



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 11:07 pm BST

PDB ID : 7Q21 / pdb_00007q21
EMDB ID : EMD-13777
Title : III2-IV2 respiratory supercomplex from Corynebacterium glutamicum
Authors : Kovalova, T.; Moe, A.; Krol, S.; Yanofsky, D.J.; Bott, M.; Sjostrand, D.;
Rubinstein, J.L.; Hogbom, M.; Brzezinski, P.
Deposited on : 2021-10-22
Resolution : 2.90 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:

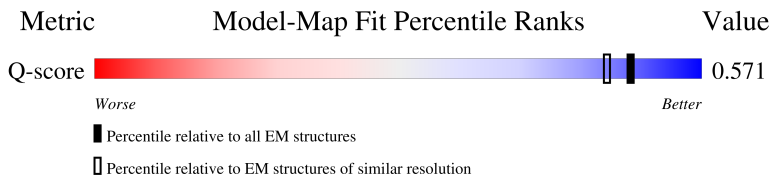
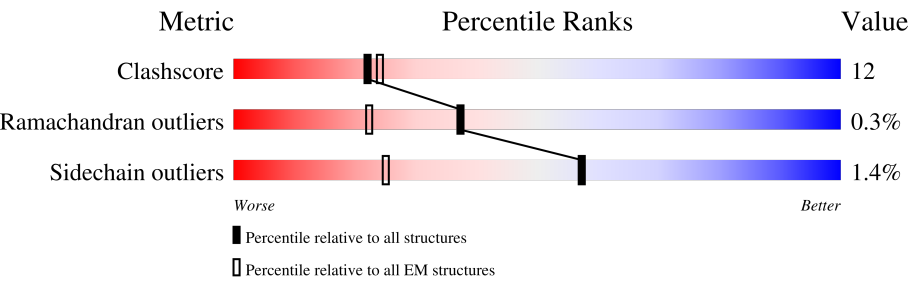
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	Y	96	98%
1	y	96	93% 5%
2	E	205	70% 21% 8%
2	e	205	76% 17% 8%

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Mol	Chain	Length	Quality of chain
3	H	147	
3	h	147	
4	F	143	
4	f	143	
5	G	359	
5	g	359	
6	D	594	
6	d	594	
7	A	408	
7	a	408	
8	L	194	
8	l	194	
9	B	539	
9	b	539	
10	C	283	
10	c	283	
11	X	21	
12	x	22	
13	V	73	
13	v	73	
14	K	65	
14	k	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	HAS	D	602	X	-	X	-
22	HAS	D	603	X	-	-	-
22	HAS	d	603	X	-	X	-
22	HAS	d	604	X	-	-	-
29	HEC	C	302	X	-	-	-
29	HEC	C	303	X	-	-	-
29	HEC	c	302	X	-	-	-
29	HEC	c	303	X	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 47749 atoms, of which 0 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 Co-purified unknown transmembrane helices built as polyALA (AscD).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Y	96	Total	C	N	O	0	0
			480	288	96	96		
1	y	91	Total	C	N	O	0	0
			455	273	91	91		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	189	Total	C	N	O	S	0	0
			1478	987	235	249	7		
2	e	189	Total	C	N	O	S	0	0
			1478	987	235	249	7		

- Molecule 3 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total	C	N	O	S	0	0
			994	643	173	177	1		
3	h	126	Total	C	N	O	S	0	0
			1003	648	174	180	1		

- Molecule 4 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	143	Total	C	N	O	S	0	0
			1094	728	167	190	9		
4	f	143	Total	C	N	O	S	0	0
			1094	728	167	190	9		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		
5	g	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		
6	d	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	-	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
d	585	ALA	-	expression tag	UNP Q79VD7
d	586	ALA	-	expression tag	UNP Q79VD7
d	587	TRP	-	expression tag	UNP Q79VD7
d	588	SER	-	expression tag	UNP Q79VD7
d	589	HIS	-	expression tag	UNP Q79VD7
d	590	PRO	-	expression tag	UNP Q79VD7
d	591	GLN	-	expression tag	UNP Q79VD7
d	592	PHE	-	expression tag	UNP Q79VD7
d	593	GLU	-	expression tag	UNP Q79VD7
d	594	LYS	-	expression tag	UNP Q79VD7

- Molecule 7 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		
8	l	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		

- Molecule 9 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		
9	b	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		
10	c	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		

- Molecule 11 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	21	Total	C	N	O	S	0	0
			106	63	21	21	1		

- Molecule 12 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	22	Total	C	N	O	S	0	0
			111	66	22	22	1		

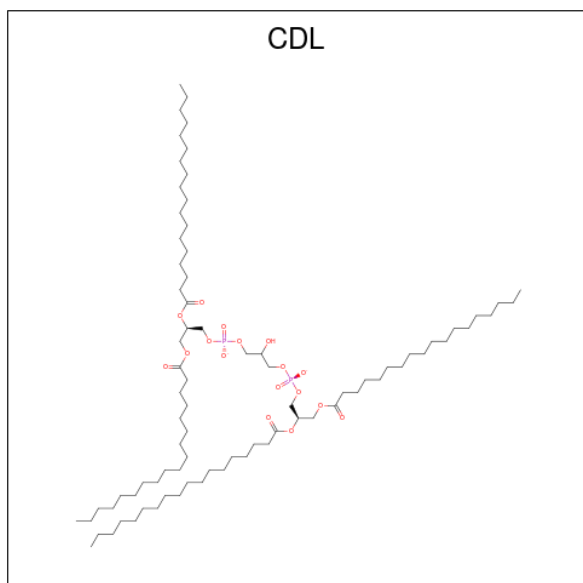
- Molecule 13 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	54	Total	C	N	O	0	0
			420	268	69	83		
13	v	54	Total	C	N	O	0	0
			420	268	69	83		

- Molecule 14 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	63	Total	C	N	O	S	0	0
			444	294	70	77	3		
14	k	63	Total	C	N	O	S	0	0
			444	294	70	77	3		

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



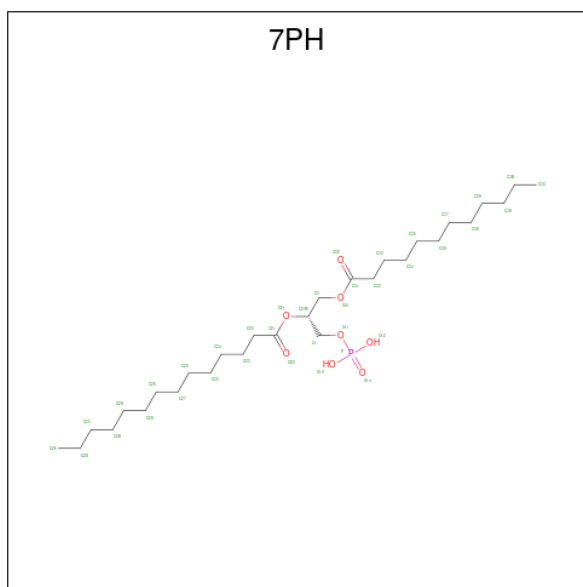
Mol	Chain	Residues	Atoms				AltConf
15	E	1	Total	C	O	P	0
			66	47	17	2	
15	F	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			74	55	17	2	
15	B	1	Total	C	O	P	0
			77	58	17	2	
15	B	1	Total	C	O	P	0
			74	55	17	2	

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Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			79	60	17	2	
15	e	1	Total	C	O	P	0
			66	47	17	2	
15	f	1	Total	C	O	P	0
			79	60	17	2	
15	d	1	Total	C	O	P	0
			79	60	17	2	
15	d	1	Total	C	O	P	0
			66	47	17	2	
15	b	1	Total	C	O	P	0
			74	55	17	2	
15	b	1	Total	C	O	P	0
			77	58	17	2	
15	c	1	Total	C	O	P	0
			79	60	17	2	

- Molecule 16 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



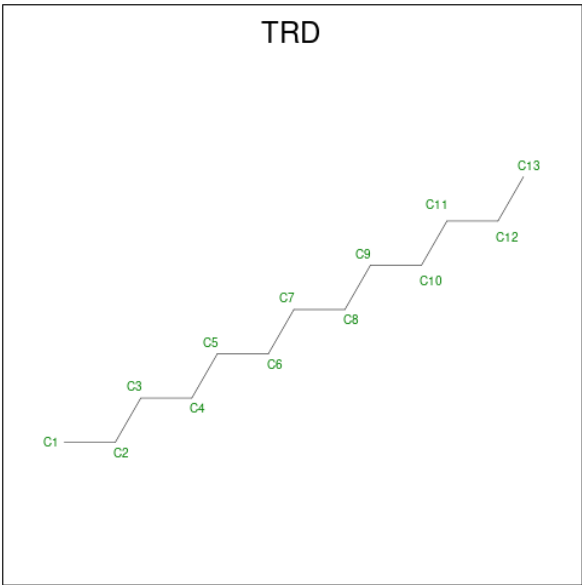
Mol	Chain	Residues	Atoms				AltConf
16	E	1	Total	C	O	P	0
			38	29	8	1	
16	H	1	Total	C	O	P	0
			38	29	8	1	
16	F	1	Total	C	O	P	0
			38	29	8	1	

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Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			38	29	8	1	
16	e	1	Total	C	O	P	0
			38	29	8	1	
16	h	1	Total	C	O	P	0
			38	29	8	1	
16	f	1	Total	C	O	P	0
			38	29	8	1	
16	g	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			38	29	8	1	
16	k	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 17 is TRIDECANE (CCD ID: TRD) (formula: C₁₃H₂₈).



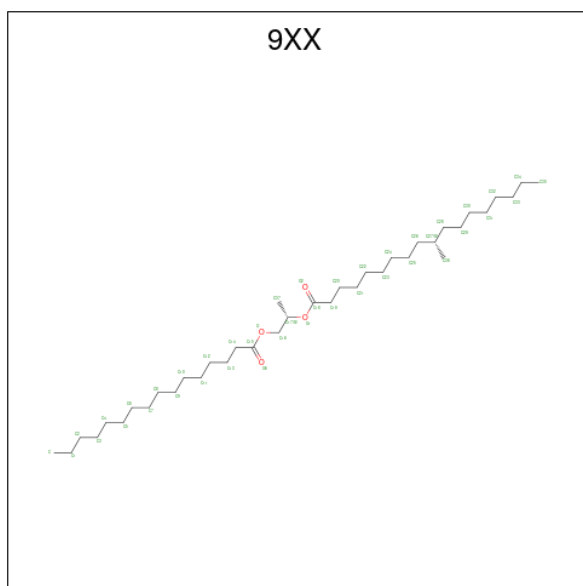
Mol	Chain	Residues	Atoms		AltConf
17	E	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	F	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	A	1	Total	C	0
			13	13	
17	B	1	Total	C	0
			13	13	
17	e	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	

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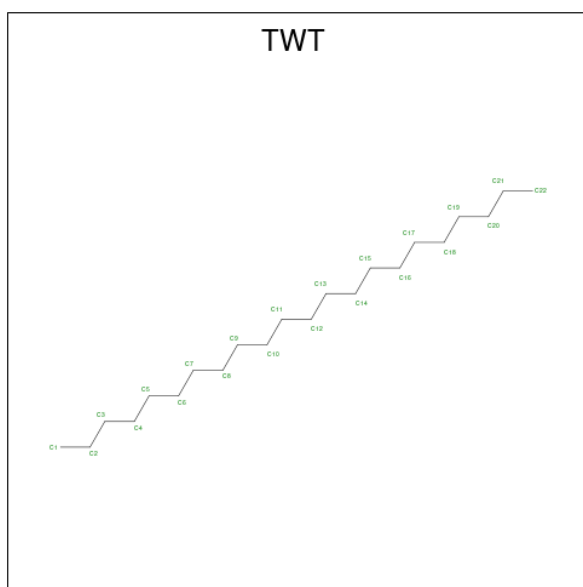
Mol	Chain	Residues	Atoms		AltConf
17	f	1	Total	C	0
			13	13	
17	f	1	Total	C	0
			13	13	
17	a	1	Total	C	0
			13	13	
17	b	1	Total	C	0
			13	13	

- Molecule 18 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
18	H	1	Total	C	O	0
			32	28	4	
18	B	1	Total	C	O	0
			32	28	4	
18	h	1	Total	C	O	0
			32	28	4	
18	h	1	Total	C	O	0
			32	28	4	

- Molecule 19 is DOCOSANE (CCD ID: TWT) (formula: $C_{22}H_{46}$).



Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C 22 22	0
19	h	1	Total C 22 22	0

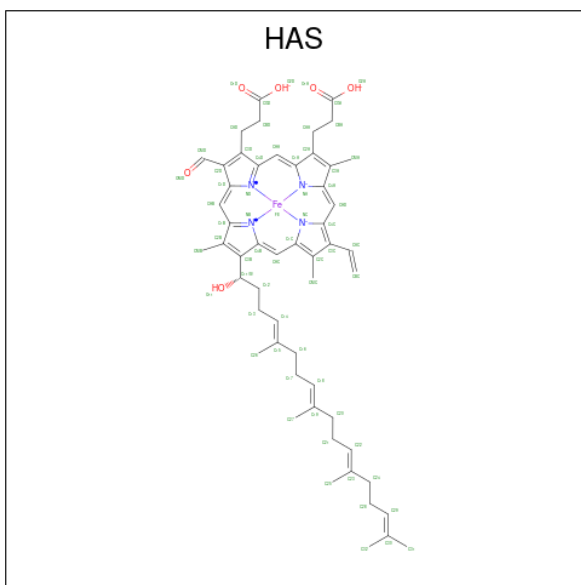
- Molecule 20 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
20	G	2	Total Cu 2 2	0
20	D	1	Total Cu 1 1	0
20	g	2	Total Cu 2 2	0
20	d	1	Total Cu 1 1	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total Mg 1 1	0
21	d	1	Total Mg 1 1	0

- Molecule 22 is HEME-AS (CCD ID: HAS) (formula: C₅₄H₆₄FeN₄O₆).

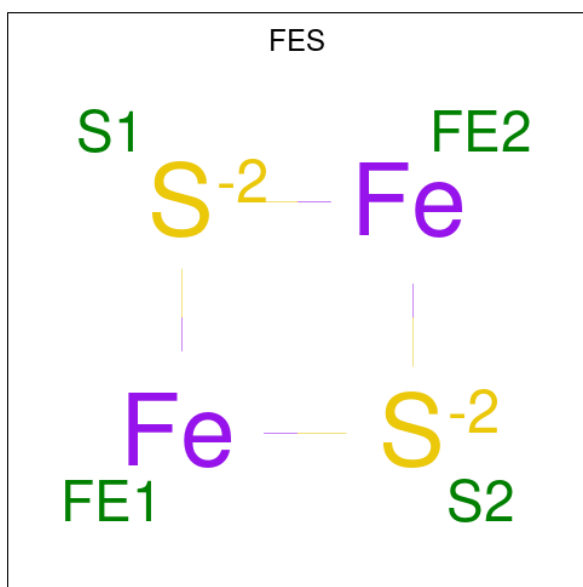


Mol	Chain	Residues	Atoms					AltConf
22	D	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	D	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	d	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
22	d	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

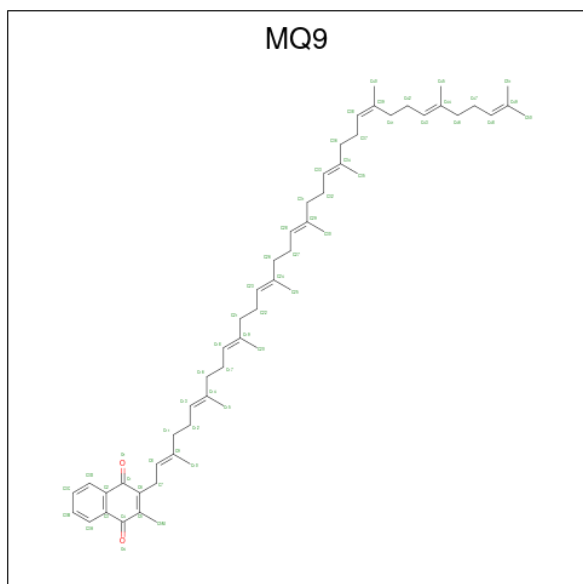
Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total	Ca	0
			1	1	
23	d	1	Total	Ca	0
			1	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	Fe	S	0
			4	2	2	
24	a	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



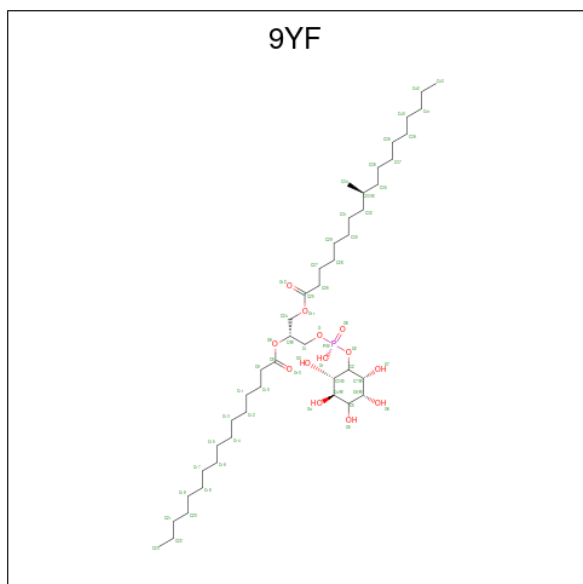
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			43	41	2	

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Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			43	41	2	
25	B	1	Total	C	O	0
			58	56	2	
25	a	1	Total	C	O	0
			43	41	2	
25	b	1	Total	C	O	0
			43	41	2	
25	b	1	Total	C	O	0
			58	56	2	

- Molecule 26 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			58	44	13	1	
26	a	1	Total	C	O	P	0
			58	44	13	1	
26	a	1	Total	C	O	P	0
			58	44	13	1	
26	l	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 27 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



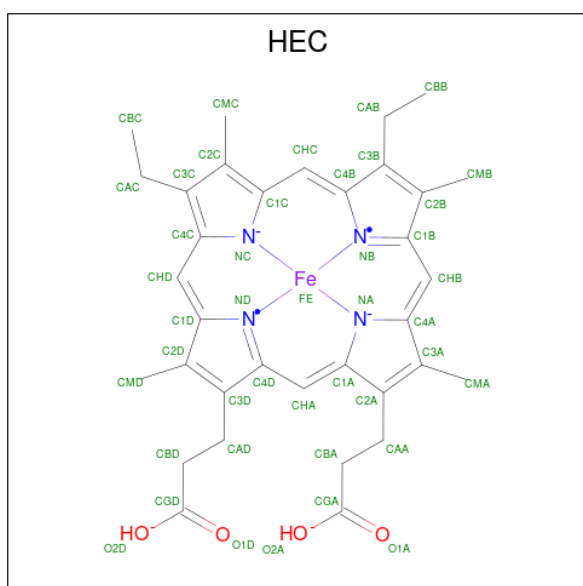
Mol	Chain	Residues	Atoms			AltConf
27	L	1	Total 11	C 10	O 1	0
27	d	1	Total 11	C 10	O 1	0
27	X	1	Total 11	C 10	O 1	0
27	x	1	Total 11	C 10	O 1	0

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	b	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	b	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 29 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).

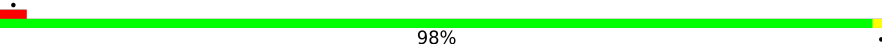


Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	c	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	c	1	Total 43	C 34	Fe 1	N 4	O 4	0

3 Residue-property plots

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

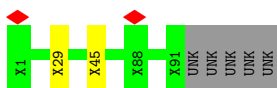
- Molecule 1: Co-purified unknown transmembrane helices built as polyALA (AscD)

Chain Y:  98%



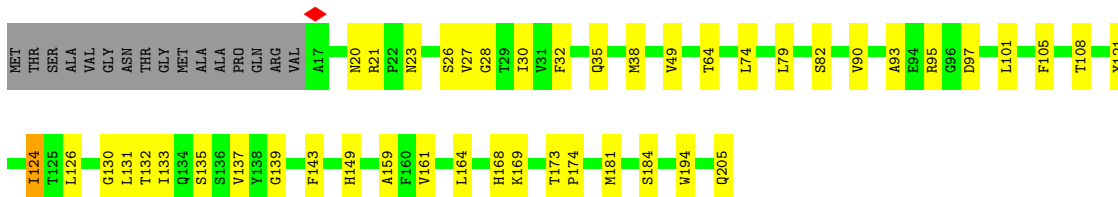
- Molecule 1: Co-purified unknown transmembrane helices built as polyALA (AscD)

Chain y:  93% 5%



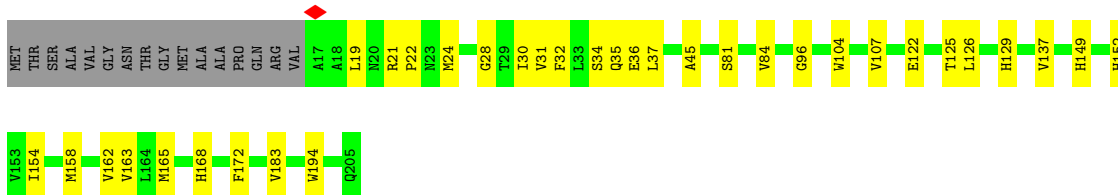
- Molecule 2: Cytochrome c oxidase subunit 3

Chain E:  70% 21% 8%



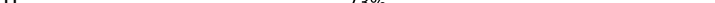
- Molecule 2: Cytochrome c oxidase subunit 3

Chain e:  76% 17% 8%



- Molecule 3: Uncharacterized membrane protein Cgl2017/cg2211

[illegible]

- Chain h:  73% 13% 14%

MET
ALA
GLY
SER
SER
HIS
THR
ILE

E9
P10
E11
I12
Y13
R14

T18

S23
A24
A25

W28

K32
R33
N34
T35

L38
A39
G40
V41
I42
S43

L75

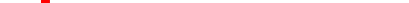
H78

E101

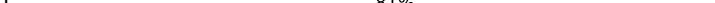
Q108

L123

A134
HIS
LEU
ARG
ALA
ALA
ALA
ASP
SER
LYS
GLU
LEU
ASP
ASN

- Chain F:  80% 20%

Category	Count
M1	1
M8	1
P11	1
M15	1
M27	1
D31	1
V38	1
V44	1
L56	1
Y59	1
V65	1
R66	1
V67	1
D68	1
V69	1
L70	1
P71	1
K82	1
F89	1
I94	1
W95	1
M99	1
L106	1
A107	1
W116	1
M117	1
L122	1
M123	1
L124	1
L126	1
I129	1
L134	1
K142	1
H143	1

- Chain f:  81% 19%

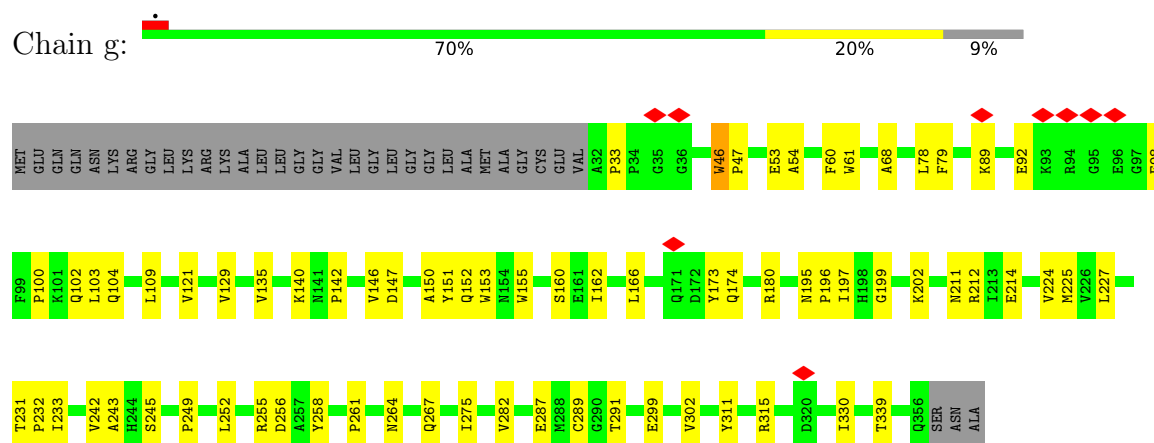
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1981	1
1984	1
1986	1
1990	1
1994	1
1998	1
2002	1
2006	1
2010	1
2014	1
2018	1
2022	1
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2105	1
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2111	1
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2153	1
2154	1
2155	1
2156	1
2157	1
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2159	1
2160	1
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2162	1
2163	1
2164	1
2165	1
2166	1
2167	1
2168	1
2169	1
2170	1
2171	1
2172	1
2173	1
2174	1
2175	1
2176	1
2177	1
2178	1
2179	1
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2182	1
2183	1
2184	1
2185	1
2186	1
2187	1
2188	1
2189	1
2190	1
2191	1
2192	1
2193	1
2194	1
2195	1
2196	1
2197	1
2198	1
2199	1
2200	1
2201	1
2202	1
2203	1
2204	1
2205	1
2206	1
2207	1
2	

- Chain G: 66% 24% 9%

R315	G199	K93	MET
I330	K202	A94	GLU
T339	V205	G95	GLN
R346	L208	F99	ASN
T355	N211	P100	LYS
Q356	R212	K101	ARG
SER	T213	Q102	LEU
ASN	E214	L103	LYS
ALA	T215	Q104	LYS
	L216	Y105	ALA
	V224	R108	LEU
	M225	Y107	LEU
	V226	P108	GLY
	L227	L109	GLY
	T231	E110	VAL
	P232	V112	LEU
	L233	I115	GLY
	V242	V121	LEU
	A243	Q132	ALA
	H244	K132	MET
	S245	V135	ALA
	F246	G135	GLY
	W247	D139	CYS
	L252	K140	GLU
	R255	N141	VAL
	D256	P142	A32
	A257	V146	P33
	Y258	D147	R43
	P261	A150	W46
	M264	W153	E53
	Q267	N154	A54
	I275	W155	F60
	V282	S160	W61
	E287	E161	W65
	M288	I162	A68
	C289	L166	I71
	G290	Y173	M75
	T291	Q174	L78
	E299	D177	A82
	V302	R180	K89
	Y311	D194	H90
		N195	A91
		P196	E92
		L197	
		H198	

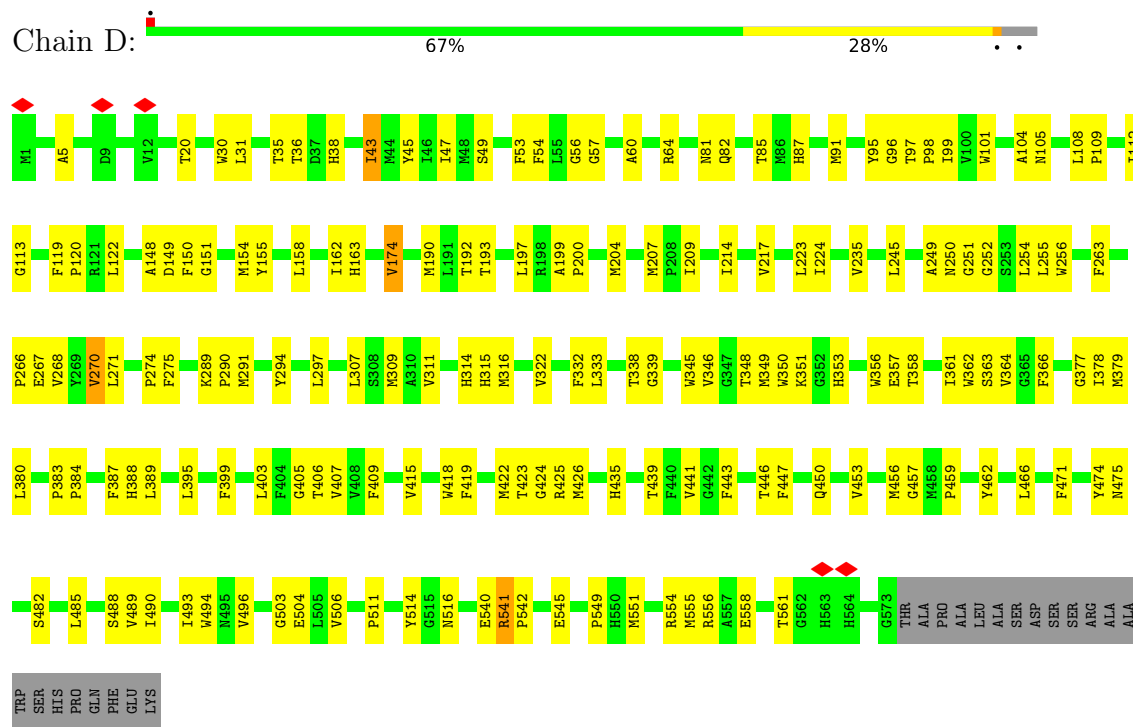
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain g:



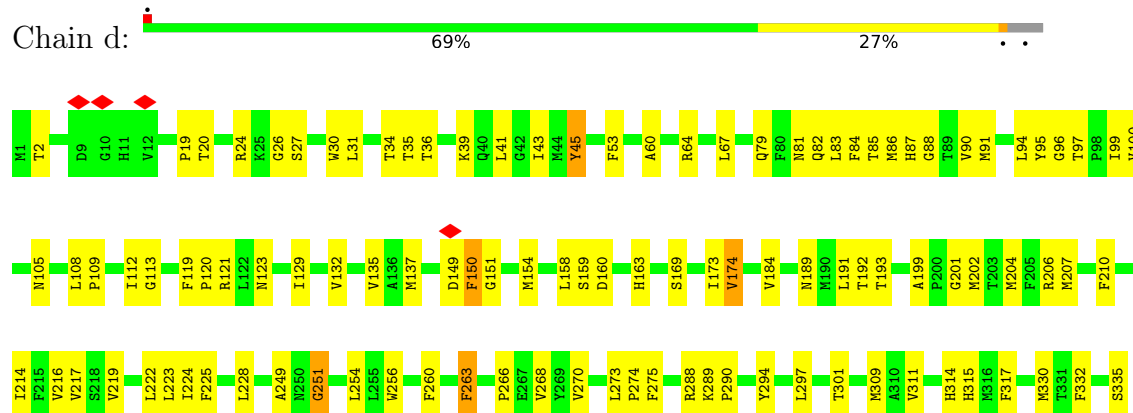
- Molecule 6: Cytochrome c oxidase subunit 1

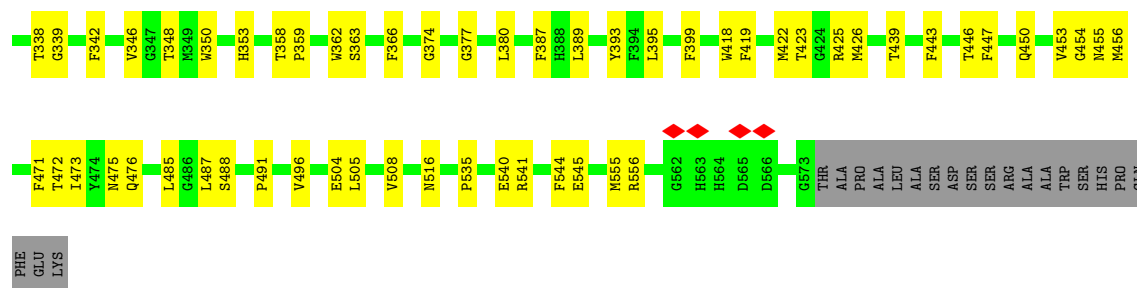
Chain D:



- Molecule 6: Cytochrome c oxidase subunit 1

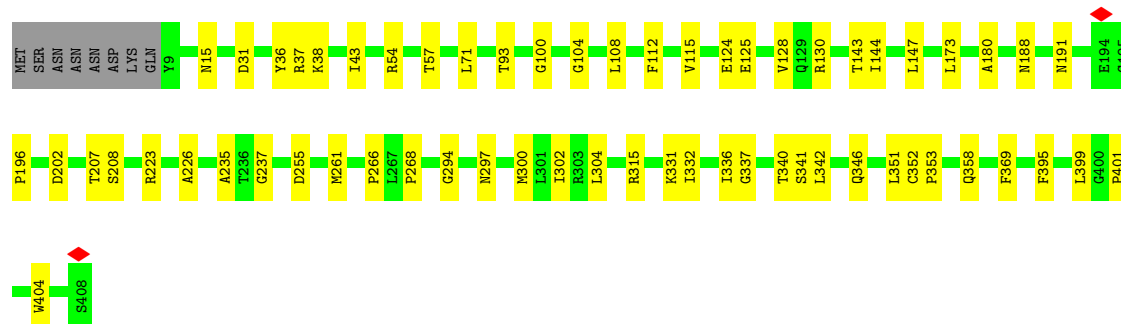
Chain d:





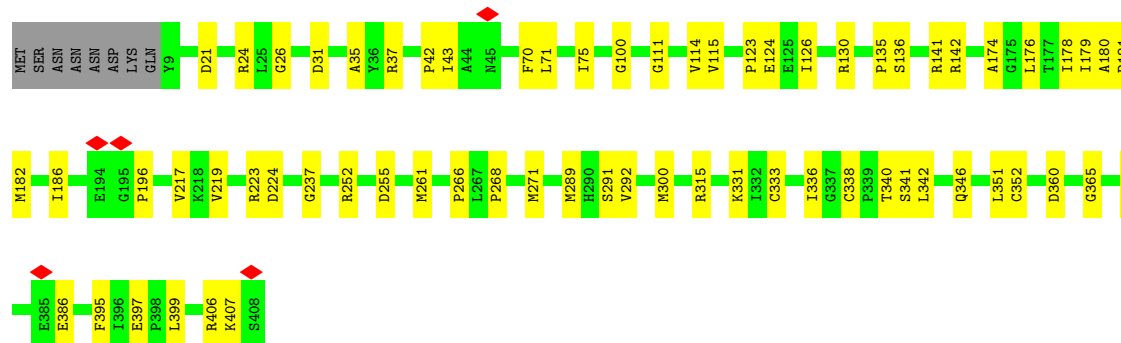
- Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A: 83% 15%



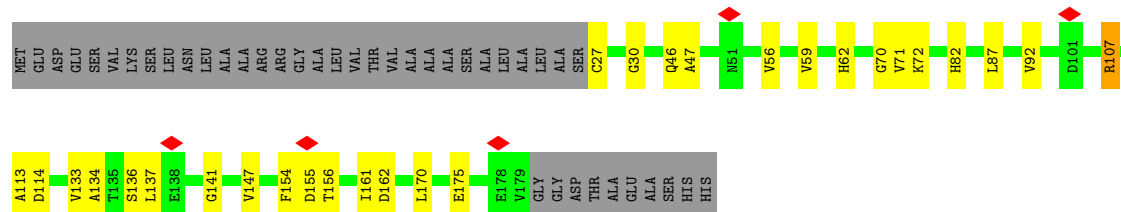
- Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain a: 82% 16%



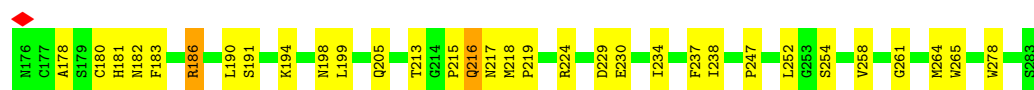
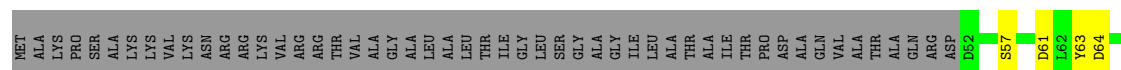
- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain L: 64% 14% 21%

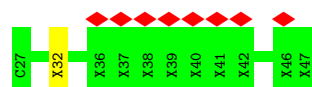


- Molecule 8: Uncharacterized protein Cgl2664/cg2949

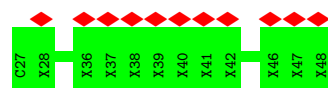
- Molecule 10: Cytochrome bc1 complex cytochrome c subunit



- Molecule 11: Co-purified unknown peptide built as polyALA (AscE)



- Molecule 12: Co-purified unknown peptide built as polyALA (AscE)

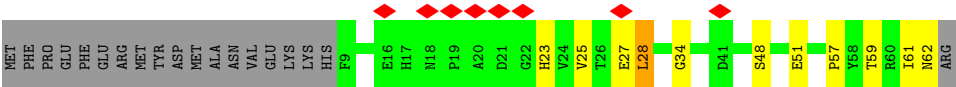


- Molecule 13: Actinobacterial supercomplex, subunit C (AscC)

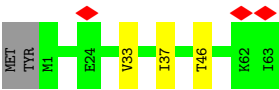
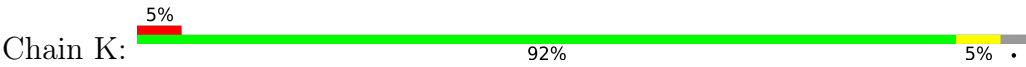


- Molecule 13: Actinobacterial supercomplex, subunit C (AscC)

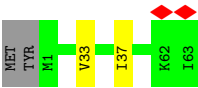
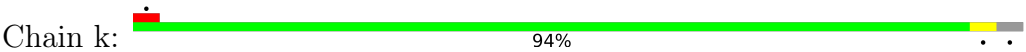




• Molecule 14: Hypothetical membrane protein



• Molecule 14: Hypothetical membrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.331	Depositor
Minimum map value	-2.395	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.541	Depositor
Map size (Å)	328.59998, 328.59998, 328.59998	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRD, FES, 9XX, CA, 7PH, TWT, PLM, HAS, CDL, MQ9, CU, HEC, HEM, 9YF, 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
2	E	0.47	0/1520	0.99	0/2071
2	e	0.47	0/1520	0.98	0/2071
3	H	0.46	0/1022	0.97	0/1397
3	h	0.47	0/1031	0.94	0/1410
4	F	0.48	0/1125	0.96	0/1529
4	f	0.47	0/1125	0.95	0/1529
5	G	0.45	0/2629	0.89	1/3586 (0.0%)
5	g	0.45	0/2629	0.88	1/3586 (0.0%)
6	D	0.49	0/4701	0.95	4/6412 (0.1%)
6	d	0.49	0/4701	0.94	1/6412 (0.0%)
7	A	0.47	0/3197	0.91	0/4352
7	a	0.47	0/3197	0.92	0/4352
8	L	0.46	0/1134	0.82	0/1553
8	l	0.47	0/1134	0.83	0/1553
9	B	0.47	0/4301	0.95	0/5861
9	b	0.48	0/4301	0.96	0/5861
10	C	0.47	0/1761	0.93	0/2383
10	c	0.48	0/1761	0.95	0/2383
11	X	0.86	0/5	0.41	0/5
12	x	0.87	0/5	0.28	0/5
13	V	0.47	0/436	0.88	0/600
13	v	0.46	0/436	0.88	0/600
14	K	0.47	0/452	1.02	0/616
14	k	0.47	0/452	1.02	0/616
All	All	0.47	0/44575	0.94	7/60743 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	267	GLU	N-CA-C	-6.23	106.31	114.04
6	D	263	PHE	CA-C-N	6.23	127.03	119.99
6	D	263	PHE	C-N-CA	6.23	127.03	119.99
5	G	33	PRO	N-CA-CB	6.00	106.34	103.22
5	g	33	PRO	N-CA-CB	5.95	106.31	103.22

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	Y	480	0	104	1	0
1	y	455	0	93	2	0
2	E	1478	0	1485	36	0
2	e	1478	0	1485	30	0
3	H	994	0	995	20	0
3	h	1003	0	1000	16	0
4	F	1094	0	1106	28	0
4	f	1094	0	1106	24	0
5	G	2556	0	2433	79	0
5	g	2556	0	2433	62	0
6	D	4532	0	4460	187	0
6	d	4532	0	4460	145	0
7	A	3117	0	3049	59	0
7	a	3117	0	3049	66	0
8	L	1120	0	1055	20	0
8	l	1120	0	1055	13	0
9	B	4186	0	4232	105	0
9	b	4186	0	4232	122	0
10	C	1729	0	1680	77	0
10	c	1729	0	1679	104	0
11	X	106	0	29	2	0
12	x	111	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	V	420	0	380	7	0
13	v	420	0	380	8	0
14	K	444	0	472	2	0
14	k	444	0	472	1	0
15	B	151	0	190	4	0
15	C	79	0	105	4	0
15	D	153	0	197	9	0
15	E	66	0	76	4	0
15	F	79	0	105	5	0
15	b	151	0	190	6	0
15	c	79	0	105	6	0
15	d	145	0	181	6	0
15	e	66	0	76	3	0
15	f	79	0	105	6	0
16	D	152	0	220	6	0
16	E	38	0	55	2	0
16	F	38	0	55	1	0
16	G	38	0	55	3	0
16	H	38	0	55	2	0
16	d	114	0	165	0	0
16	e	38	0	55	1	0
16	f	38	0	55	1	0
16	g	38	0	55	3	0
16	h	38	0	55	1	0
16	k	38	0	55	1	0
17	A	39	0	84	0	0
17	B	13	0	28	0	0
17	E	13	0	28	0	0
17	F	65	0	140	1	0
17	a	13	0	28	0	0
17	b	13	0	28	2	0
17	e	13	0	28	0	0
17	f	65	0	140	0	0
18	B	32	0	0	0	0
18	H	32	0	0	0	0
18	h	64	0	0	0	0
19	H	22	0	46	2	0
19	h	22	0	46	2	0
20	D	1	0	0	0	0
20	G	2	0	0	0	0
20	d	1	0	0	0	0
20	g	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	G	1	0	0	0	0
21	d	1	0	0	0	0
22	D	130	0	124	56	0
22	d	130	0	124	34	0
23	D	1	0	0	0	0
23	d	1	0	0	0	0
24	A	4	0	0	0	0
24	a	4	0	0	1	0
25	A	43	0	53	2	0
25	B	101	0	133	11	0
25	a	43	0	53	2	0
25	b	101	0	133	5	0
26	L	58	0	0	0	0
26	a	116	0	0	0	0
26	l	58	0	0	0	0
27	L	11	0	16	1	0
27	X	11	0	16	0	0
27	d	11	0	16	0	0
27	x	11	0	16	0	0
28	B	86	0	60	7	0
28	b	86	0	60	7	0
29	C	86	0	64	27	0
29	c	86	0	63	44	0
All	All	47749	0	46691	1088	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 12.

The worst 5 of 1088 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)
6:D:315:HIS:CE1	22:D:602:HAS:HHA	1.44	1.51
10:c:180:CYS:SG	29:c:303:HEC:HBC2	1.59	1.41
10:C:180:CYS:SG	29:C:303:HEC:CAC	2.10	1.38
10:c:67:CYS:SG	29:c:302:HEC:CAB	2.16	1.33
10:C:67:CYS:SG	29:C:302:HEC:CAB	2.15	1.33

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	
2	E	187/205 (91%)	182 (97%)	4 (2%)	1 (0%)	24	54
2	e	187/205 (91%)	182 (97%)	5 (3%)	0	100	100
3	H	123/147 (84%)	109 (89%)	13 (11%)	1 (1%)	16	44
3	h	124/147 (84%)	114 (92%)	10 (8%)	0	100	100
4	F	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
4	f	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
5	G	323/359 (90%)	295 (91%)	27 (8%)	1 (0%)	36	65
5	g	323/359 (90%)	293 (91%)	30 (9%)	0	100	100
6	D	571/594 (96%)	543 (95%)	28 (5%)	0	100	100
6	d	571/594 (96%)	540 (95%)	30 (5%)	1 (0%)	43	72
7	A	398/408 (98%)	381 (96%)	17 (4%)	0	100	100
7	a	398/408 (98%)	372 (94%)	26 (6%)	0	100	100
8	L	151/194 (78%)	131 (87%)	19 (13%)	1 (1%)	18	48
8	l	151/194 (78%)	132 (87%)	18 (12%)	1 (1%)	18	48
9	B	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	30	59
9	b	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	30	59
10	C	230/283 (81%)	203 (88%)	24 (10%)	3 (1%)	9	32
10	c	230/283 (81%)	201 (87%)	28 (12%)	1 (0%)	30	59
13	V	52/73 (71%)	45 (86%)	7 (14%)	0	100	100
13	v	52/73 (71%)	45 (86%)	7 (14%)	0	100	100
14	K	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
14	k	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
All	All	5539/6020 (92%)	5161 (93%)	364 (7%)	14 (0%)	37	65

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	141	GLY
8	l	141	GLY
2	E	130	GLY
5	G	101	LYS
3	H	111	LEU

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	
2	E	155/166 (93%)	153 (99%)	2 (1%)	61	86
2	e	155/166 (93%)	155 (100%)	0	100	100
3	H	108/125 (86%)	106 (98%)	2 (2%)	50	79
3	h	109/125 (87%)	108 (99%)	1 (1%)	70	90
4	F	114/114 (100%)	113 (99%)	1 (1%)	70	90
4	f	114/114 (100%)	113 (99%)	1 (1%)	70	90
5	G	269/292 (92%)	268 (100%)	1 (0%)	84	94
5	g	269/292 (92%)	267 (99%)	2 (1%)	76	92
6	D	472/488 (97%)	467 (99%)	5 (1%)	65	88
6	d	472/488 (97%)	466 (99%)	6 (1%)	61	86
7	A	324/332 (98%)	323 (100%)	1 (0%)	86	96
7	a	324/332 (98%)	324 (100%)	0	100	100
8	L	127/154 (82%)	126 (99%)	1 (1%)	73	90
8	l	127/154 (82%)	124 (98%)	3 (2%)	43	75
9	B	437/441 (99%)	428 (98%)	9 (2%)	47	77
9	b	437/441 (99%)	429 (98%)	8 (2%)	51	80
10	C	176/212 (83%)	169 (96%)	7 (4%)	28	62
10	c	176/212 (83%)	165 (94%)	11 (6%)	16	45
11	X	1/1 (100%)	1 (100%)	0	100	100
12	x	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	V	45/63 (71%)	44 (98%)	1 (2%)	45	77
13	v	45/63 (71%)	44 (98%)	1 (2%)	45	77
14	K	43/45 (96%)	43 (100%)	0	100	100
14	k	43/45 (96%)	43 (100%)	0	100	100
All	All	4543/4866 (93%)	4480 (99%)	63 (1%)	57	85

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	105	LEU
10	c	151	GLU
6	d	174	VAL
10	c	147	LEU
10	c	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
6	d	398	HIS
9	b	287	GLN
6	d	547	HIS
7	a	153	GLN
9	b	535	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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
17	TRD	F	203	-	12,12,12	0.39	0	11,11,11	0.62	0
15	CDL	d	607	-	65,65,99	1.01	5 (7%)	71,77,111	0.73	2 (2%)
17	TRD	f	203	-	12,12,12	0.38	0	11,11,11	0.60	0
17	TRD	f	201	-	12,12,12	0.38	0	11,11,11	0.69	0
15	CDL	f	202	-	78,78,99	0.91	4 (5%)	84,90,111	0.82	2 (2%)
17	TRD	A	503	-	12,12,12	0.39	0	11,11,11	0.62	0
25	MQ9	A	504	-	44,44,59	1.46	5 (11%)	54,57,75	1.22	7 (12%)
28	HEM	b	803	9	50,50,50	1.70	11 (22%)	66,82,82	1.97	19 (28%)
17	TRD	F	206	-	12,12,12	0.39	0	11,11,11	0.66	0
26	9YF	l	201	-	58,58,58	0.90	4 (6%)	69,71,71	1.08	3 (4%)
17	TRD	E	303	-	12,12,12	0.40	0	11,11,11	0.56	0
28	HEM	B	602	9	50,50,50	1.71	12 (24%)	66,82,82	1.98	18 (27%)
19	TWT	h	203	-	21,21,21	0.32	0	20,20,20	0.95	0
16	7PH	f	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
28	HEM	b	802	9	50,50,50	1.64	8 (16%)	66,82,82	2.20	23 (34%)
15	CDL	d	601	-	78,78,99	0.94	4 (5%)	84,90,111	0.69	0
29	HEC	c	303	10	50,50,50	2.90	26 (52%)	68,82,82	2.34	30 (44%)
26	9YF	a	601	-	58,58,58	0.92	3 (5%)	69,71,71	1.22	6 (8%)
17	TRD	f	204	-	12,12,12	0.38	0	11,11,11	0.66	0
17	TRD	f	206	-	12,12,12	0.37	0	11,11,11	0.63	0
25	MQ9	b	805	-	59,59,59	1.32	5 (8%)	72,75,75	1.22	9 (12%)
25	MQ9	b	804	-	44,44,59	1.51	6 (13%)	54,57,75	1.36	5 (9%)
22	HAS	d	604	6	71,72,72	2.10	22 (30%)	84,109,109	2.35	27 (32%)
26	9YF	a	604	-	58,58,58	0.93	4 (6%)	69,71,71	1.00	3 (4%)
25	MQ9	B	603	-	44,44,59	1.44	5 (11%)	54,57,75	1.36	9 (16%)
27	PLM	L	202	-	10,10,17	0.41	0	9,9,17	0.49	0
29	HEC	c	302	10	50,50,50	2.57	25 (50%)	68,82,82	3.13	26 (38%)
18	9XX	h	202	-	31,31,41	1.10	3 (9%)	34,34,44	1.34	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	9XX	B	608	-	31,31,41	1.12	4 (12%)	34,34,44	1.21	4 (11%)
15	CDL	b	801	-	73,73,99	0.97	5 (6%)	79,85,111	0.81	2 (2%)
15	CDL	B	605	-	76,76,99	0.95	5 (6%)	82,88,111	0.71	0
16	7PH	G	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
27	PLM	d	611	-	10,10,17	0.44	0	9,9,17	0.47	0
15	CDL	D	606	-	73,73,99	0.98	6 (8%)	79,85,111	0.76	2 (2%)
24	FES	a	603	7	0,4,4	-	-	-	-	-
15	CDL	B	607	-	73,73,99	0.88	2 (2%)	79,85,111	0.87	4 (5%)
16	7PH	H	201	-	37,37,37	0.90	2 (5%)	41,42,42	0.90	2 (4%)
25	MQ9	B	604	-	59,59,59	1.25	5 (8%)	72,75,75	1.24	10 (13%)
17	TRD	A	505	-	12,12,12	0.38	0	11,11,11	0.62	0
17	TRD	F	201	-	12,12,12	0.39	0	11,11,11	0.67	0
16	7PH	E	302	-	37,37,37	0.93	2 (5%)	41,42,42	0.92	1 (2%)
16	7PH	d	610	-	37,37,37	0.80	1 (2%)	41,42,42	0.72	0
16	7PH	e	302	-	37,37,37	0.95	3 (8%)	41,42,42	0.68	0
15	CDL	b	806	-	76,76,99	0.91	2 (2%)	82,88,111	0.80	1 (1%)
29	HEC	C	303	10	50,50,50	2.72	25 (50%)	68,82,82	2.90	34 (50%)
22	HAS	D	603	6	71,72,72	2.45	27 (38%)	84,109,109	2.21	30 (35%)
16	7PH	D	608	-	37,37,37	0.95	3 (8%)	41,42,42	0.89	1 (2%)
15	CDL	e	301	-	65,65,99	1.01	4 (6%)	71,77,111	0.80	1 (1%)
16	7PH	F	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
17	TRD	F	205	-	12,12,12	0.37	0	11,11,11	0.64	0
16	7PH	D	610	-	37,37,37	0.89	2 (5%)	41,42,42	0.72	0
16	7PH	d	608	-	37,37,37	0.91	2 (5%)	41,42,42	0.72	1 (2%)
16	7PH	d	609	-	37,37,37	0.84	0	41,42,42	0.88	1 (2%)
29	HEC	C	302	10	50,50,50	2.56	25 (50%)	68,82,82	3.06	26 (38%)
17	TRD	b	807	-	12,12,12	0.37	0	11,11,11	0.65	0
15	CDL	D	601	-	78,78,99	0.93	6 (7%)	84,90,111	0.64	0
16	7PH	k	101	-	37,37,37	0.83	1 (2%)	41,42,42	0.62	0
22	HAS	D	602	-	71,72,72	2.64	30 (42%)	84,109,109	2.39	35 (41%)
18	9XX	H	202	-	31,31,41	1.16	4 (12%)	34,34,44	1.30	3 (8%)
26	9YF	L	201	-	58,58,58	0.91	5 (8%)	69,71,71	1.07	3 (4%)
28	HEM	B	601	9	50,50,50	1.67	9 (18%)	66,82,82	2.08	19 (28%)
19	TWT	H	203	-	21,21,21	0.35	0	20,20,20	0.81	0
15	CDL	F	202	-	78,78,99	0.99	6 (7%)	84,90,111	0.81	1 (1%)
25	MQ9	a	602	-	44,44,59	1.46	5 (11%)	54,57,75	1.33	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	7PH	D	609	-	37,37,37	0.87	2 (5%)	41,42,42	0.65	0
24	FES	A	501	7	0,4,4	-	-	-		
27	PLM	x	101	-	10,10,17	0.42	0	9,9,17	0.45	0
17	TRD	a	605	-	12,12,12	0.38	0	11,11,11	0.62	0
16	7PH	h	201	-	37,37,37	0.86	2 (5%)	41,42,42	0.71	0
17	TRD	A	502	-	12,12,12	0.38	0	11,11,11	0.60	0
16	7PH	D	607	-	37,37,37	0.89	2 (5%)	41,42,42	0.77	0
17	TRD	F	204	-	12,12,12	0.37	0	11,11,11	0.68	0
17	TRD	f	205	-	12,12,12	0.37	0	11,11,11	0.71	0
17	TRD	e	303	-	12,12,12	0.39	0	11,11,11	0.58	0
22	HAS	d	603	-	71,72,72	2.63	31 (43%)	84,109,109	2.31	34 (40%)
15	CDL	c	301	-	78,78,99	0.86	3 (3%)	84,90,111	0.75	1 (1%)
15	CDL	E	301	-	65,65,99	1.01	6 (9%)	71,77,111	0.75	0
16	7PH	g	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
18	9XX	h	204	-	31,31,41	1.10	3 (9%)	34,34,44	1.24	3 (8%)
27	PLM	X	101	-	10,10,17	0.41	0	9,9,17	0.45	0
15	CDL	C	301	-	78,78,99	0.90	2 (2%)	84,90,111	0.85	2 (2%)
17	TRD	B	606	-	12,12,12	0.38	0	11,11,11	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	TRD	F	203	-	-	2/10/10/10	-
15	CDL	d	607	-	-	31/76/76/110	-
17	TRD	f	203	-	-	1/10/10/10	-
17	TRD	f	201	-	-	3/10/10/10	-
15	CDL	f	202	-	-	45/89/89/110	-
17	TRD	A	503	-	-	4/10/10/10	-
25	MQ9	A	504	-	-	12/35/55/73	0/2/2/2
28	HEM	b	803	9	-	6/14/54/54	-
17	TRD	F	206	-	-	7/10/10/10	-
26	9YF	l	201	-	-	23/54/78/78	0/1/1/1
17	TRD	E	303	-	-	8/10/10/10	-
28	HEM	B	602	9	-	5/14/54/54	-
19	TWT	h	203	-	-	5/19/19/19	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	7PH	f	207	-	-	19/39/39/39	-
28	HEM	b	802	9	-	8/14/54/54	-
15	CDL	d	601	-	-	37/89/89/110	-
29	HEC	c	303	10	1/1/3/7	11/14/54/54	-
26	9YF	a	601	-	-	35/54/78/78	0/1/1/1
17	TRD	f	204	-	-	4/10/10/10	-
17	TRD	f	206	-	-	6/10/10/10	-
25	MQ9	b	805	-	-	11/53/73/73	0/2/2/2
25	MQ9	b	804	-	-	8/35/55/73	0/2/2/2
22	HAS	d	604	6	1/1/8/18	12/42/82/82	-
26	9YF	a	604	-	-	29/54/78/78	0/1/1/1
29	HEC	c	302	10	1/1/3/7	10/14/54/54	-
25	MQ9	B	603	-	-	7/35/55/73	0/2/2/2
27	PLM	L	202	-	-	5/7/8/15	-
18	9XX	h	202	-	-	14/33/33/43	-
18	9XX	B	608	-	-	15/33/33/43	-
15	CDL	b	801	-	-	42/84/84/110	-
15	CDL	B	605	-	-	44/87/87/110	-
16	7PH	G	403	-	-	17/39/39/39	-
27	PLM	d	611	-	-	3/7/8/15	-
15	CDL	D	606	-	-	41/84/84/110	-
24	FES	a	603	7	-	-	0/1/1/1
15	CDL	B	607	-	-	42/84/84/110	-
16	7PH	H	201	-	-	19/39/39/39	-
25	MQ9	B	604	-	-	21/53/73/73	0/2/2/2
17	TRD	A	505	-	-	4/10/10/10	-
17	TRD	F	201	-	-	3/10/10/10	-
16	7PH	E	302	-	-	14/39/39/39	-
16	7PH	d	610	-	-	23/39/39/39	-
16	7PH	e	302	-	-	21/39/39/39	-
15	CDL	b	806	-	-	44/87/87/110	-
29	HEC	C	303	10	1/1/3/7	7/14/54/54	-
22	HAS	D	603	6	1/1/8/18	14/42/82/82	-
16	7PH	D	608	-	-	18/39/39/39	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	e	301	-	-	40/76/76/110	-
16	7PH	F	207	-	-	19/39/39/39	-
17	TRD	F	205	-	-	5/10/10/10	-
16	7PH	D	610	-	-	23/39/39/39	-
16	7PH	d	608	-	-	16/39/39/39	-
16	7PH	d	609	-	-	22/39/39/39	-
29	HEC	C	302	10	1/1/3/7	10/14/54/54	-
17	TRD	b	807	-	-	2/10/10/10	-
15	CDL	D	601	-	-	38/89/89/110	-
16	7PH	k	101	-	-	10/39/39/39	-
22	HAS	D	602	-	1/1/8/18	16/42/82/82	-
18	9XX	H	202	-	-	16/33/33/43	-
26	9YF	L	201	-	-	24/54/78/78	0/1/1/1
28	HEM	B	601	9	-	3/14/54/54	-
19	TWT	H	203	-	-	7/19/19/19	-
15	CDL	F	202	-	-	45/89/89/110	-
25	MQ9	a	602	-	-	12/35/55/73	0/2/2/2
16	7PH	D	609	-	-	25/39/39/39	-
24	FES	A	501	7	-	-	0/1/1/1
27	PLM	x	101	-	-	4/7/8/15	-
17	TRD	a	605	-	-	3/10/10/10	-
16	7PH	h	201	-	-	25/39/39/39	-
17	TRD	A	502	-	-	7/10/10/10	-
16	7PH	D	607	-	-	23/39/39/39	-
17	TRD	F	204	-	-	4/10/10/10	-
17	TRD	f	205	-	-	9/10/10/10	-
17	TRD	e	303	-	-	7/10/10/10	-
22	HAS	d	603	-	1/1/8/18	11/42/82/82	-
15	CDL	c	301	-	-	50/89/89/110	-
15	CDL	E	301	-	-	28/76/76/110	-
16	7PH	g	403	-	-	17/39/39/39	-
18	9XX	h	204	-	-	20/33/33/43	-
27	PLM	X	101	-	-	0/7/8/15	-
15	CDL	C	301	-	-	48/89/89/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	TRD	B	606	-	-	7/10/10/10	-

The worst 5 of 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	602	HAS	C3B-C2B	6.70	1.49	1.34
22	d	603	HAS	C3B-C2B	6.14	1.48	1.34
22	D	603	HAS	C3B-C2B	6.13	1.48	1.34
28	b	802	HEM	FE-NB	6.02	2.13	1.94
25	b	804	MQ9	C6-C5	6.01	1.46	1.35

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	302	HEC	CAC-C3C-C4C	10.76	139.85	124.92
29	C	302	HEC	CAC-C3C-C4C	10.32	139.24	124.92
29	c	302	HEC	CAC-C3C-C2C	-8.98	112.48	126.86
29	C	302	HEC	CAC-C3C-C2C	-8.54	113.19	126.86
22	d	603	HAS	C2D-C3D-C4D	-7.98	100.80	106.49

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	D	602	HAS	NA
22	D	603	HAS	NA
22	d	603	HAS	NA
22	d	604	HAS	NA
29	C	302	HEC	NA

5 of 1356 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	301	CDL	CA2-OA2-PA1-OA3
15	E	301	CDL	CB2-OB2-PB2-OB3
15	E	301	CDL	CB2-OB2-PB2-OB4
15	E	301	CDL	CB3-OB5-PB2-OB2
15	F	202	CDL	CA2-OA2-PA1-OA4

There are no ring outliers.

49 monomers are involved in 274 short contacts:

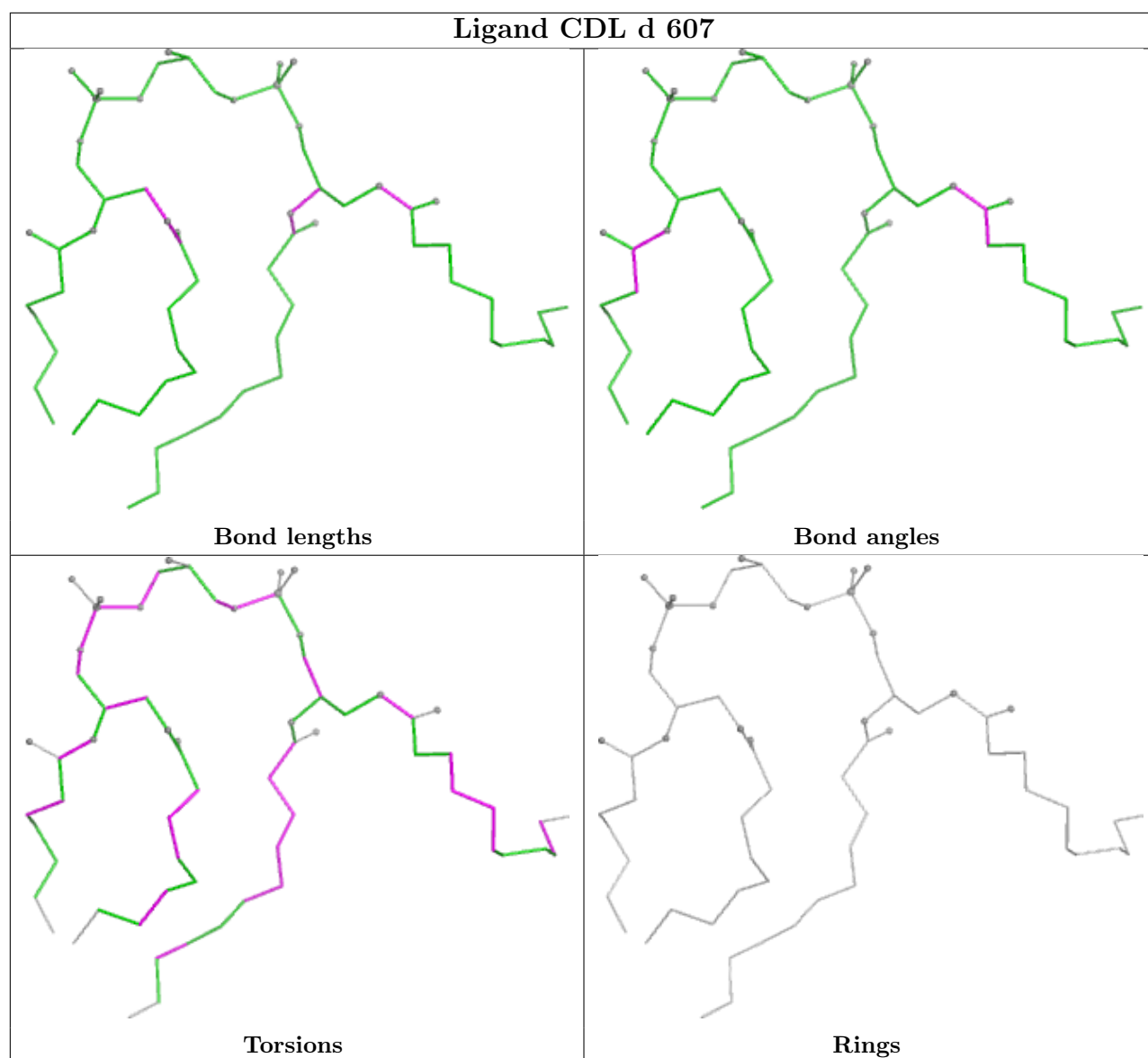
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	F	203	TRD	1	0
15	d	607	CDL	3	0
15	f	202	CDL	6	0
25	A	504	MQ9	2	0
28	b	803	HEM	4	0
28	B	602	HEM	2	0
19	h	203	TWT	2	0
16	f	207	7PH	1	0
28	b	802	HEM	3	0
15	d	601	CDL	3	0
29	c	303	HEC	32	0
25	b	805	MQ9	4	0
25	b	804	MQ9	1	0
22	d	604	HAS	4	0
25	B	603	MQ9	2	0
27	L	202	PLM	1	0
29	c	302	HEC	12	0
15	B	605	CDL	1	0
16	G	403	7PH	3	0
15	D	606	CDL	3	0
24	a	603	FES	1	0
15	B	607	CDL	3	0
16	H	201	7PH	2	0
25	B	604	MQ9	9	0
16	E	302	7PH	2	0
16	e	302	7PH	1	0
15	b	806	CDL	6	0
29	C	303	HEC	16	0
22	D	603	HAS	19	0
15	e	301	CDL	3	0
16	F	207	7PH	1	0
16	D	610	7PH	2	0
29	C	302	HEC	11	0
17	b	807	TRD	2	0
15	D	601	CDL	6	0
16	k	101	7PH	1	0
22	D	602	HAS	37	0
28	B	601	HEM	5	0
19	H	203	TWT	2	0
15	F	202	CDL	5	0
25	a	602	MQ9	2	0
16	D	609	7PH	2	0
16	h	201	7PH	1	0

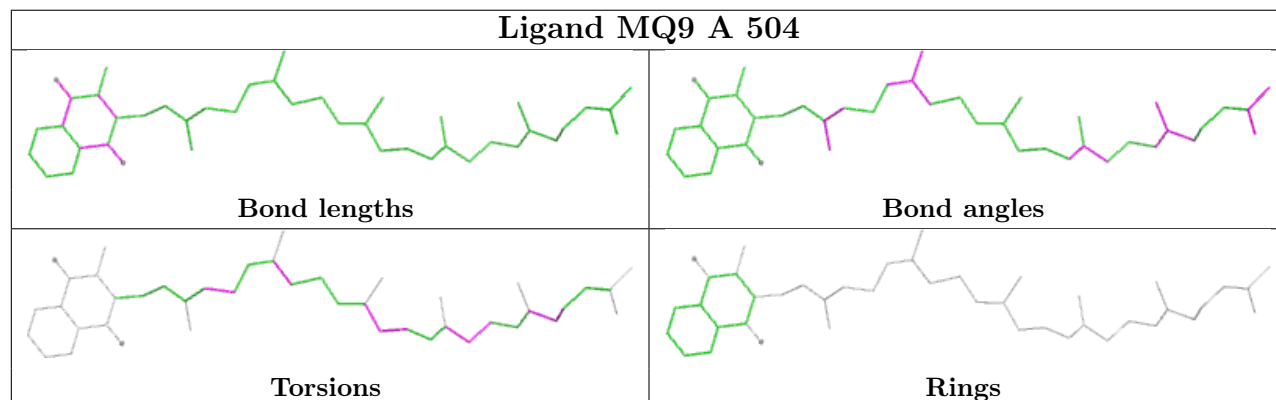
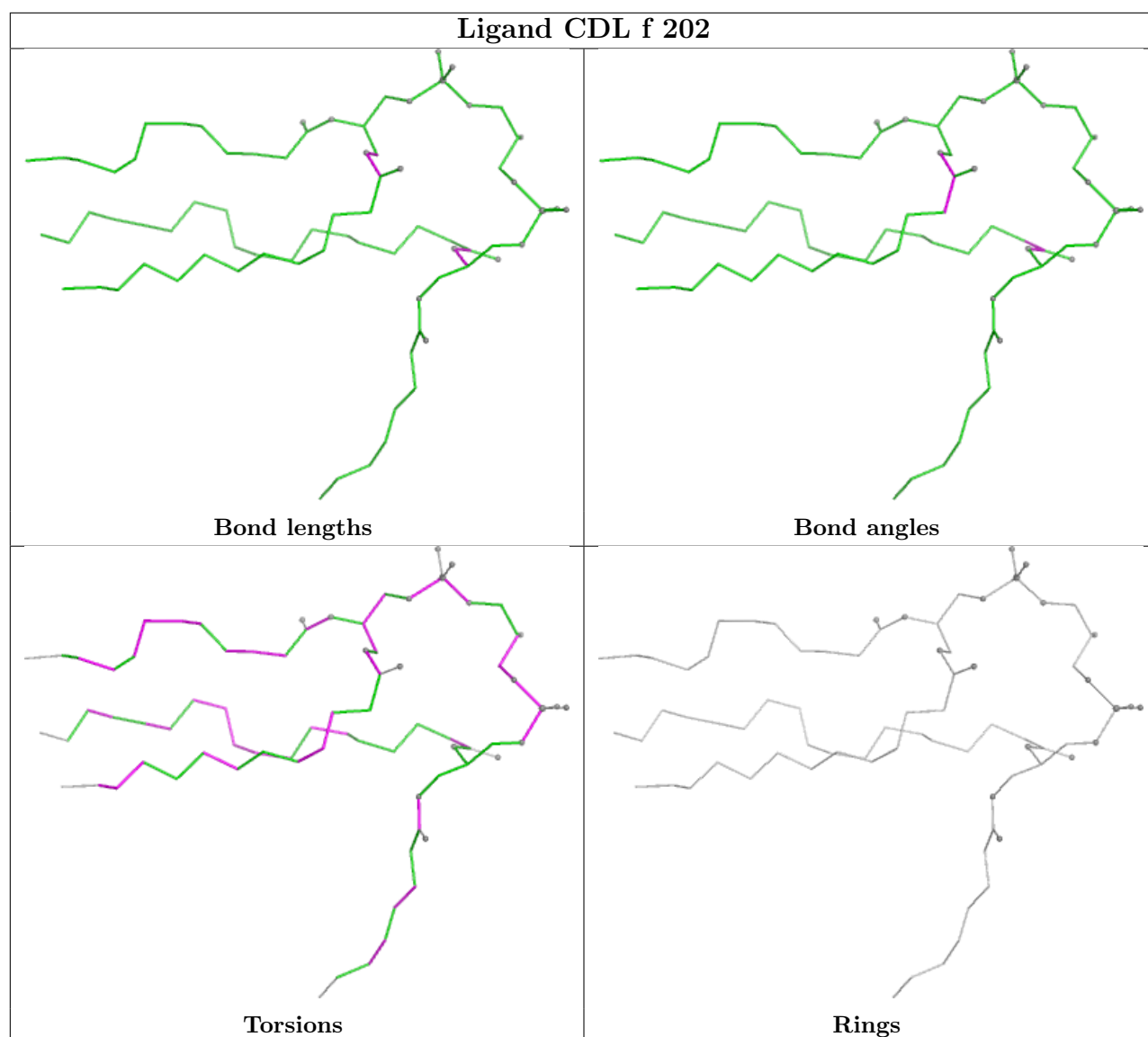
Continued on next page...

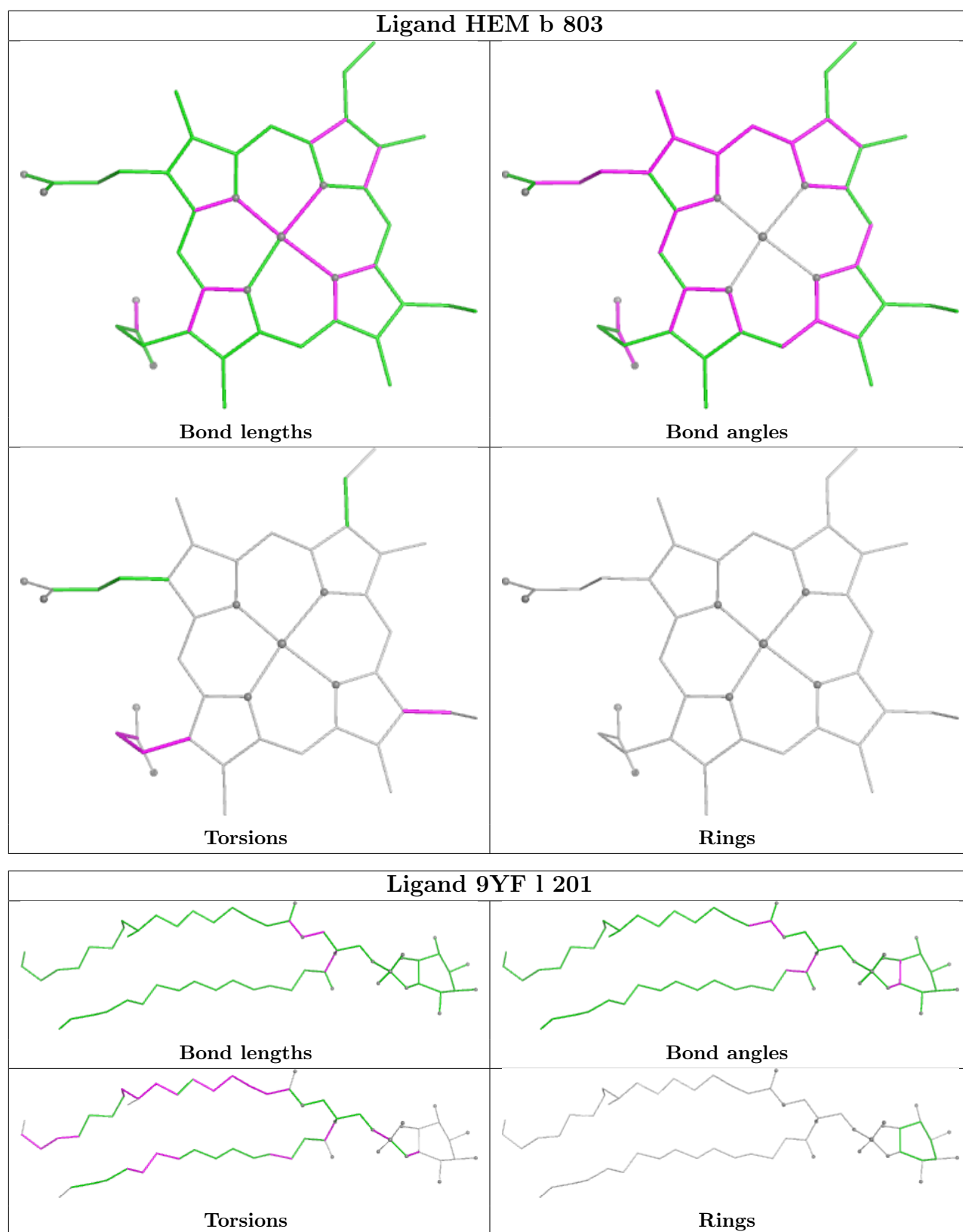
Continued from previous page...

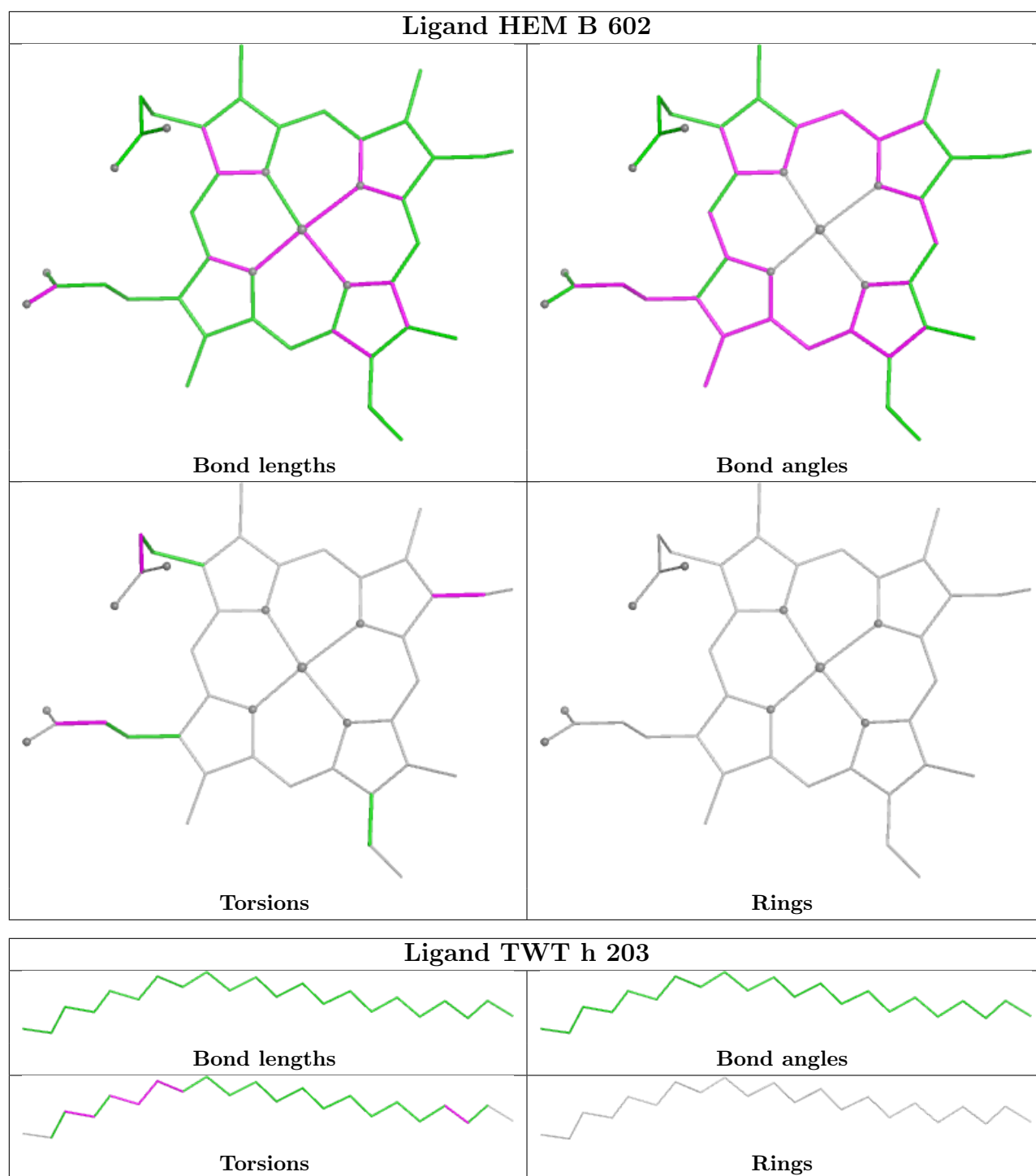
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	607	7PH	2	0
22	d	603	HAS	30	0
15	c	301	CDL	6	0
15	E	301	CDL	4	0
16	g	403	7PH	3	0
15	C	301	CDL	4	0

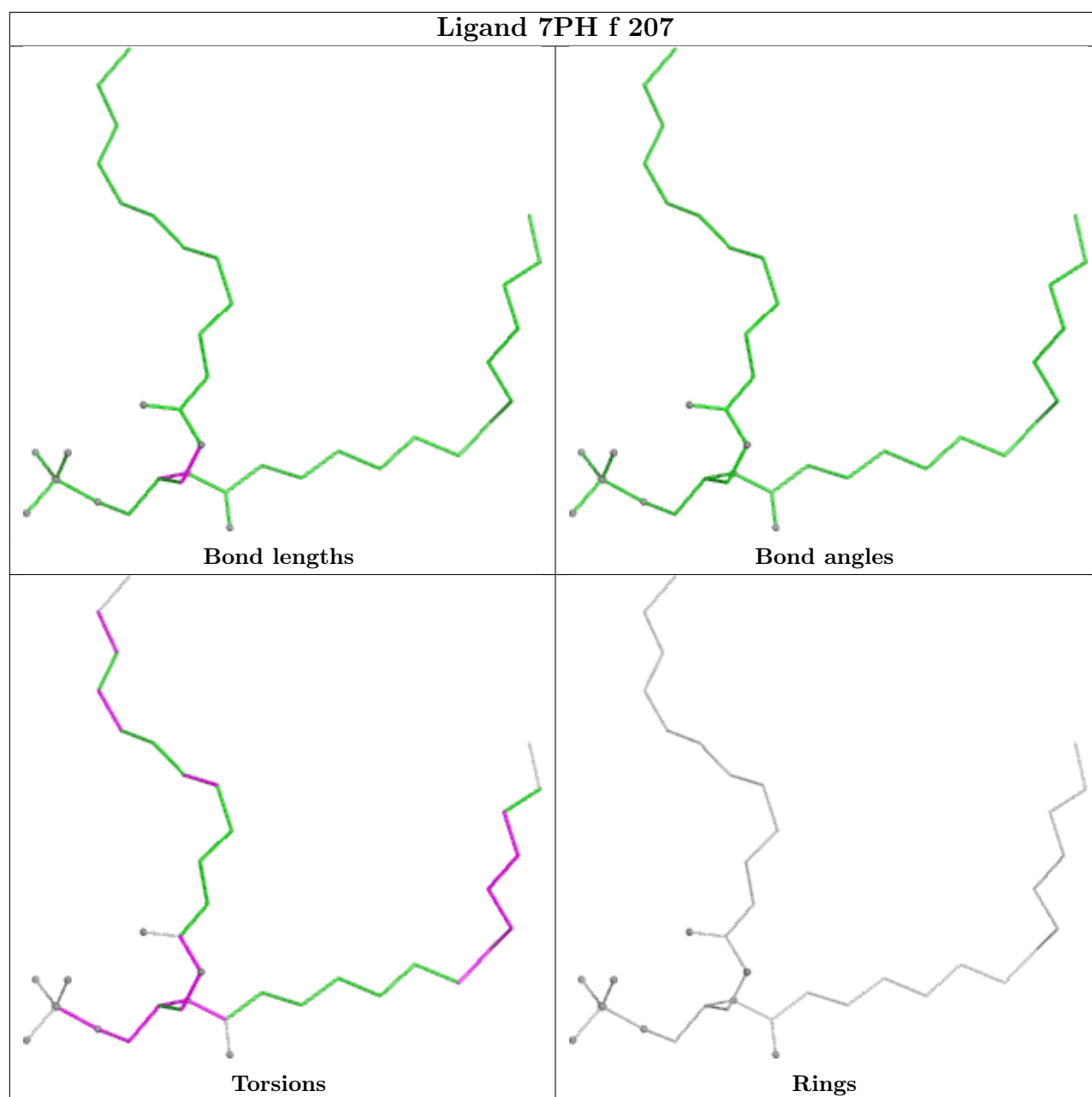
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

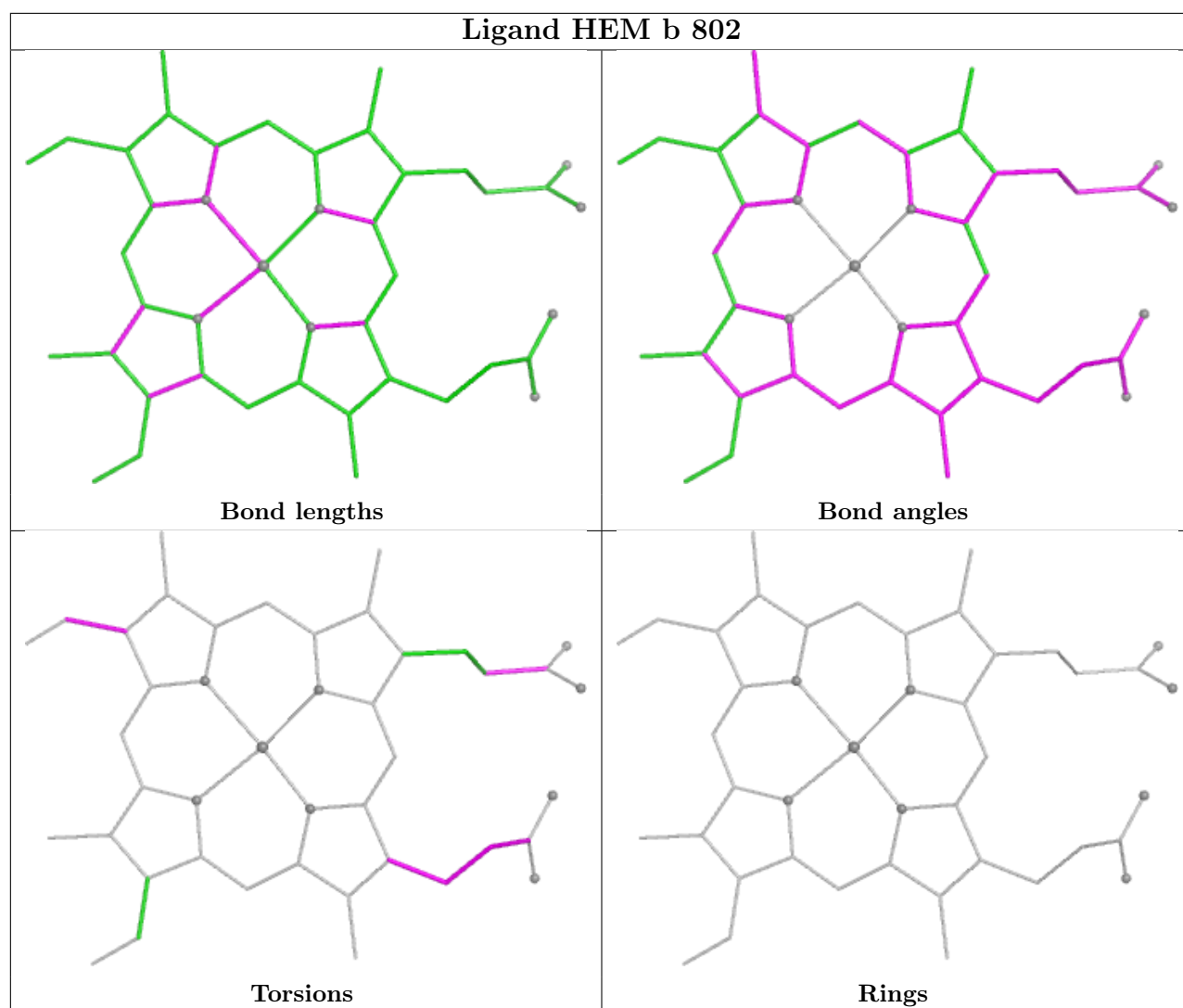


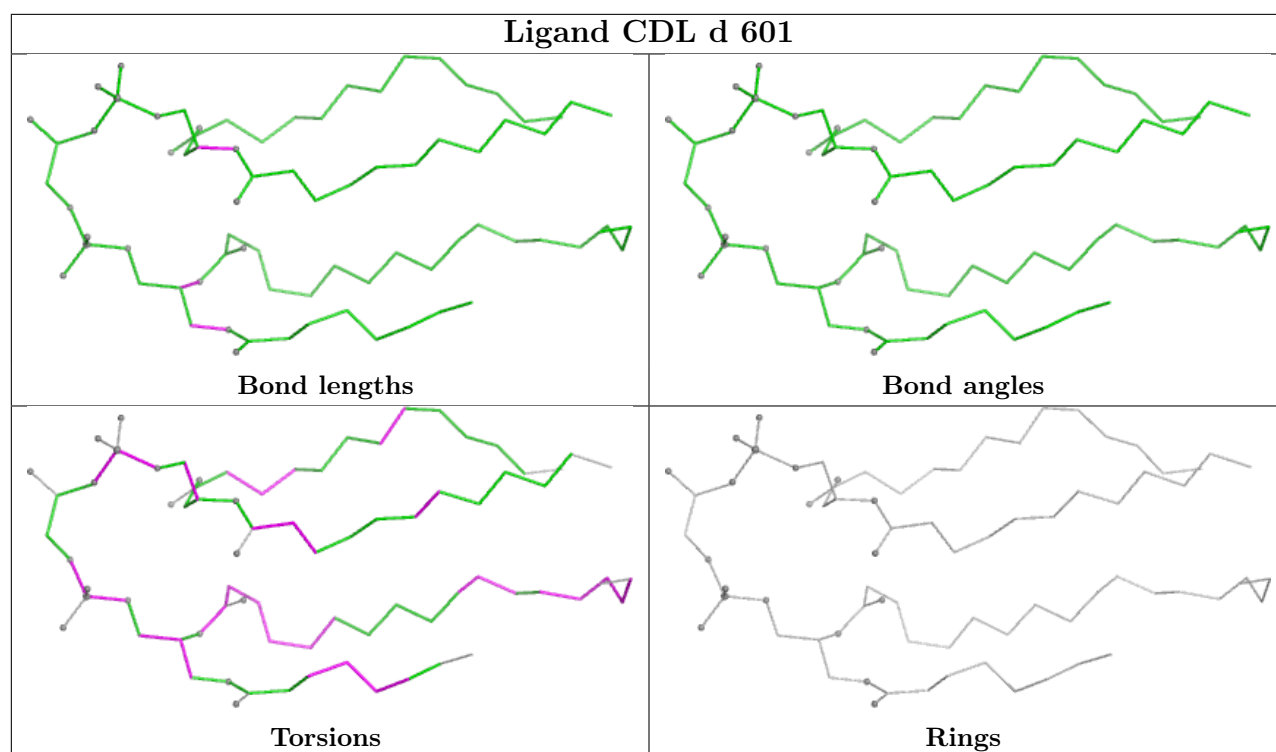


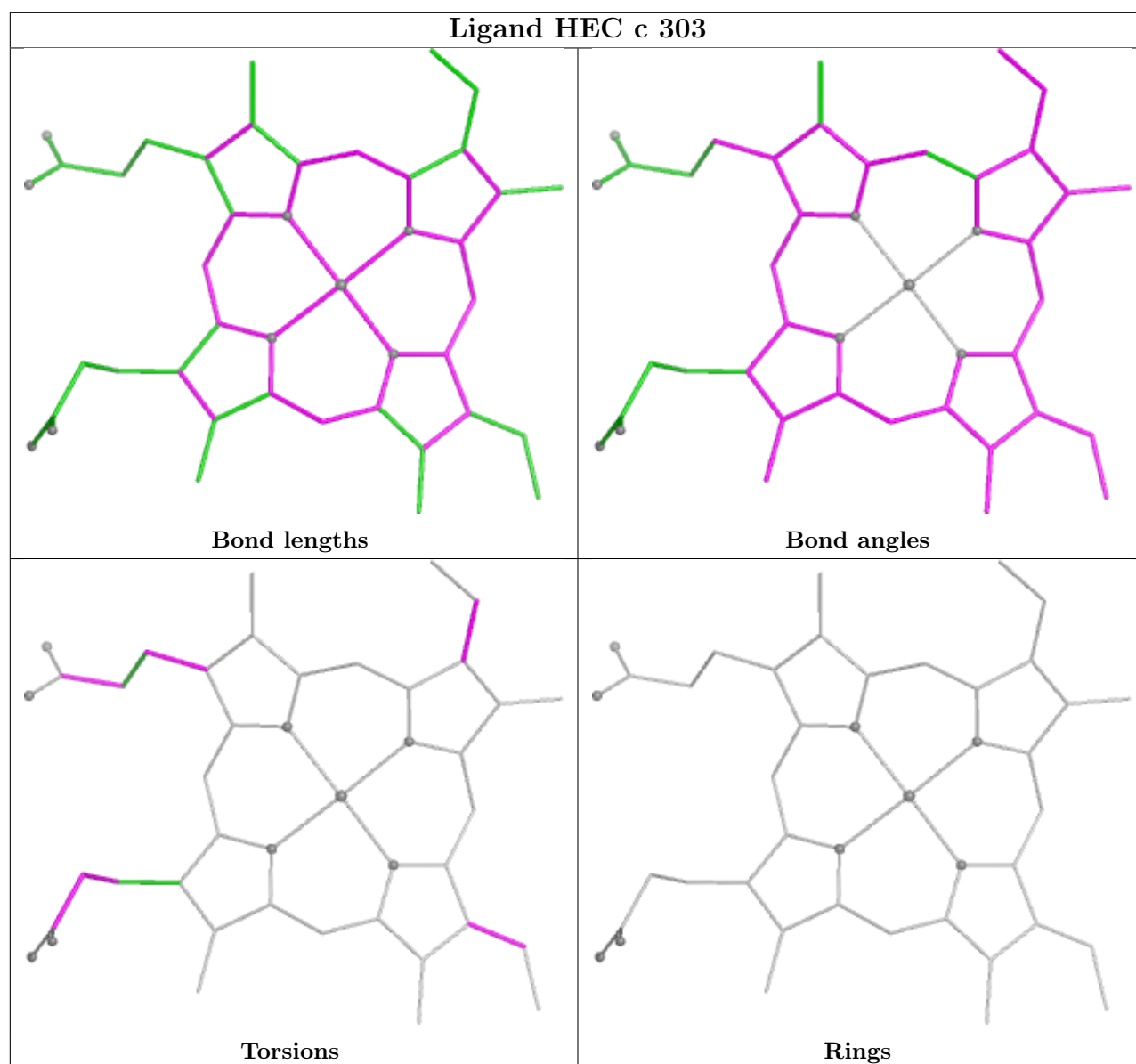


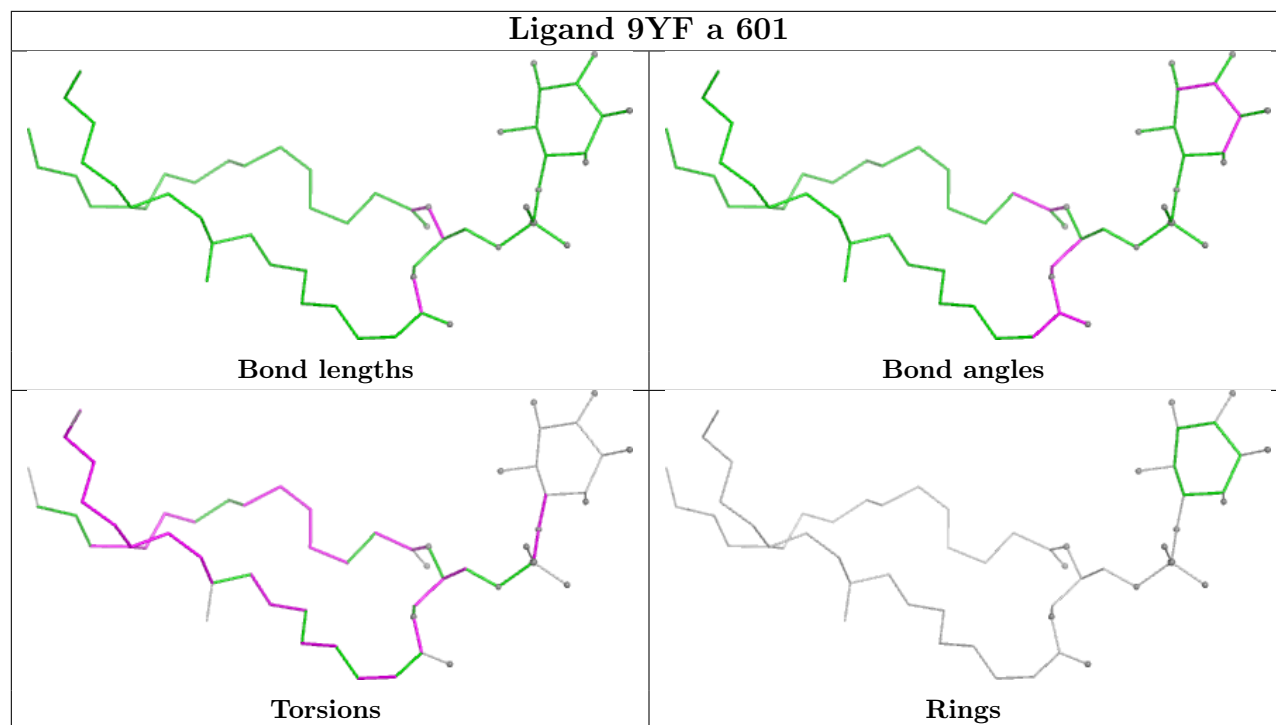


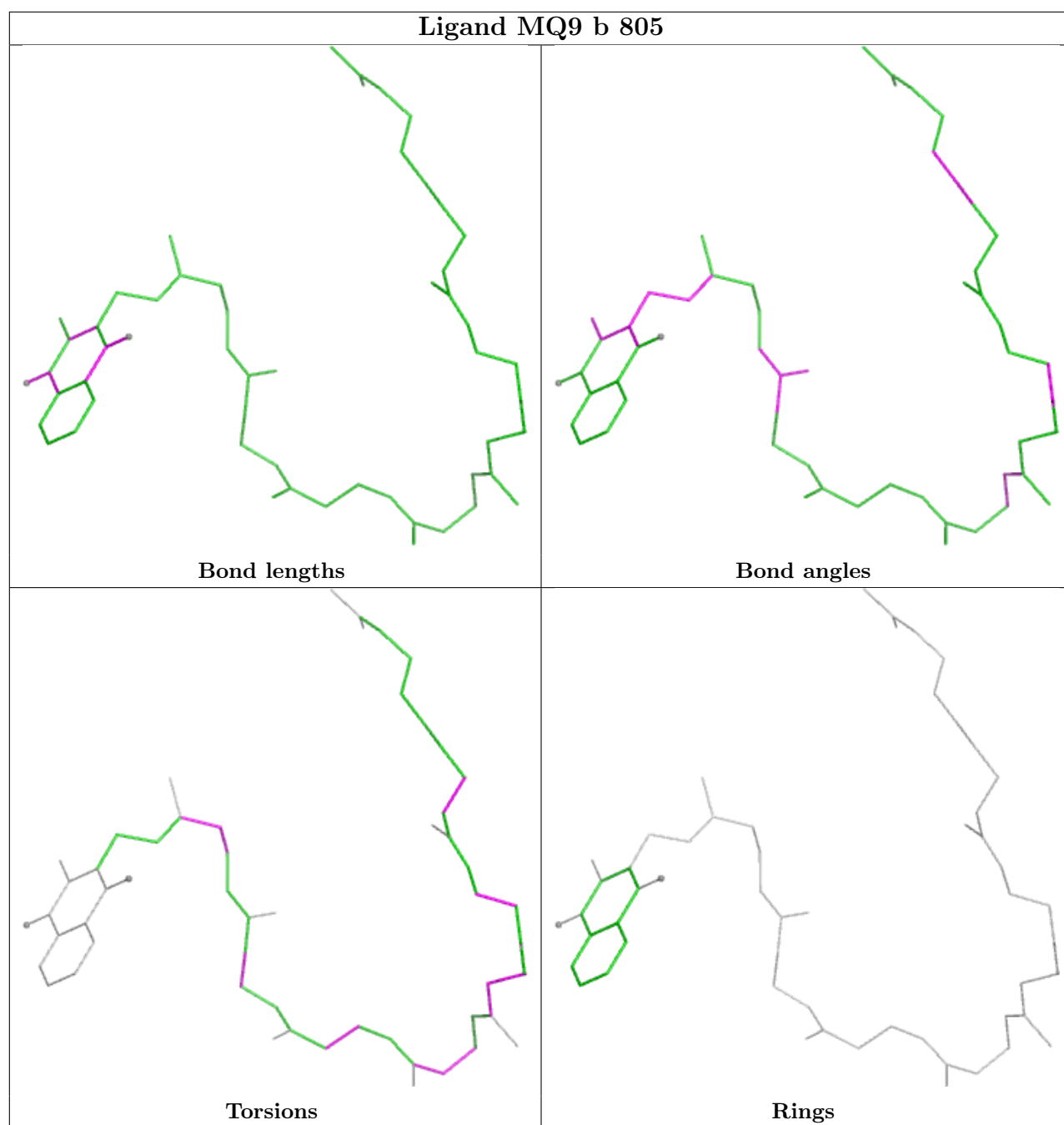


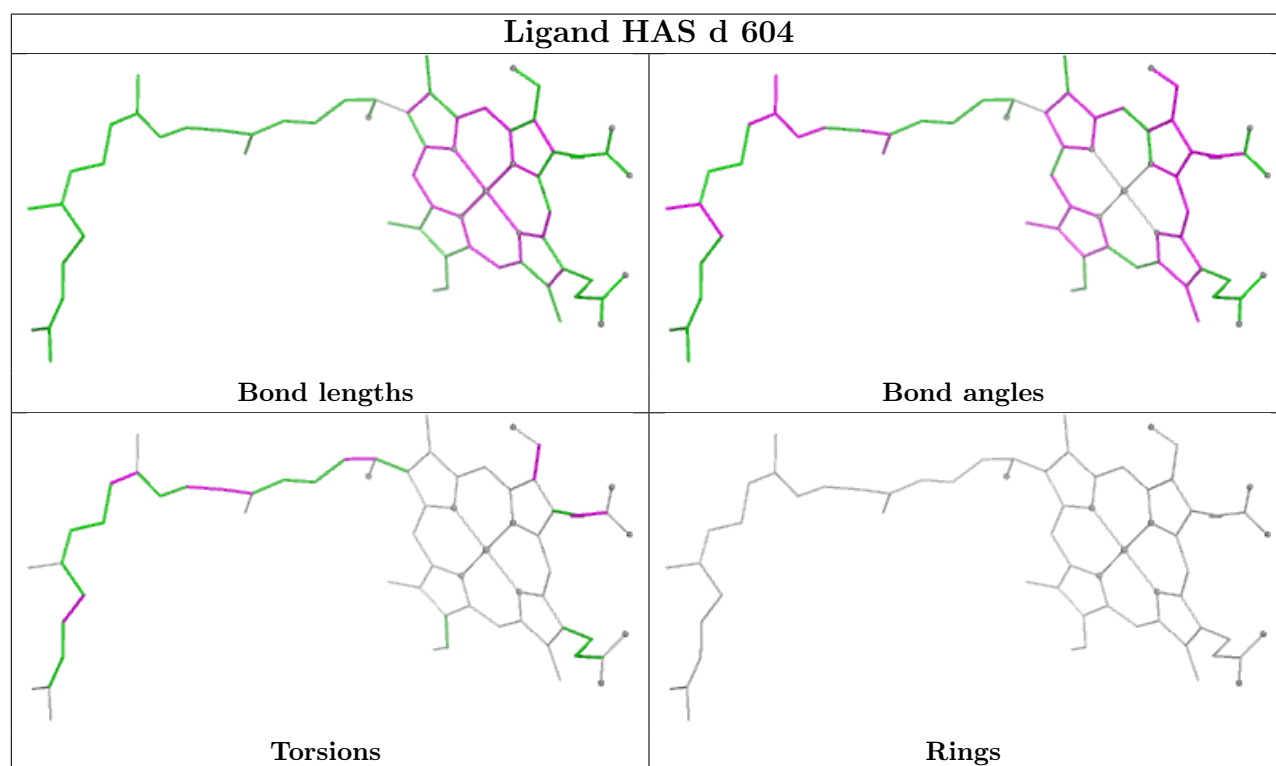
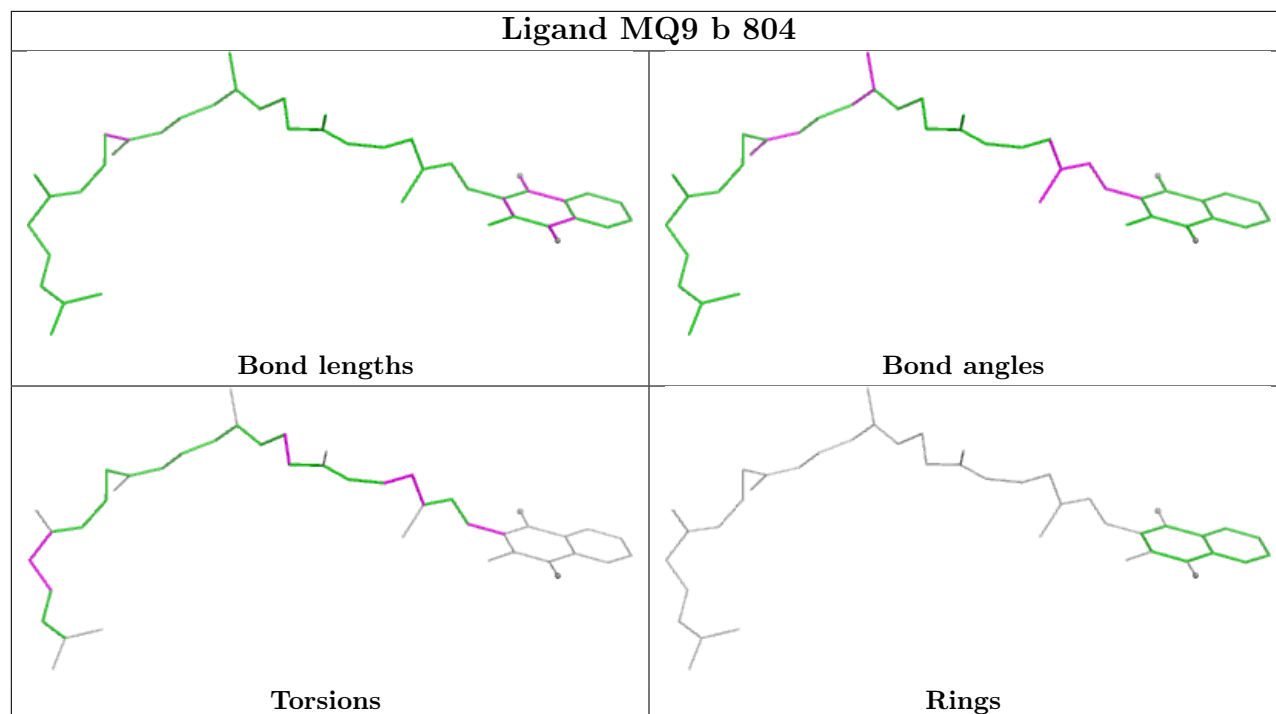


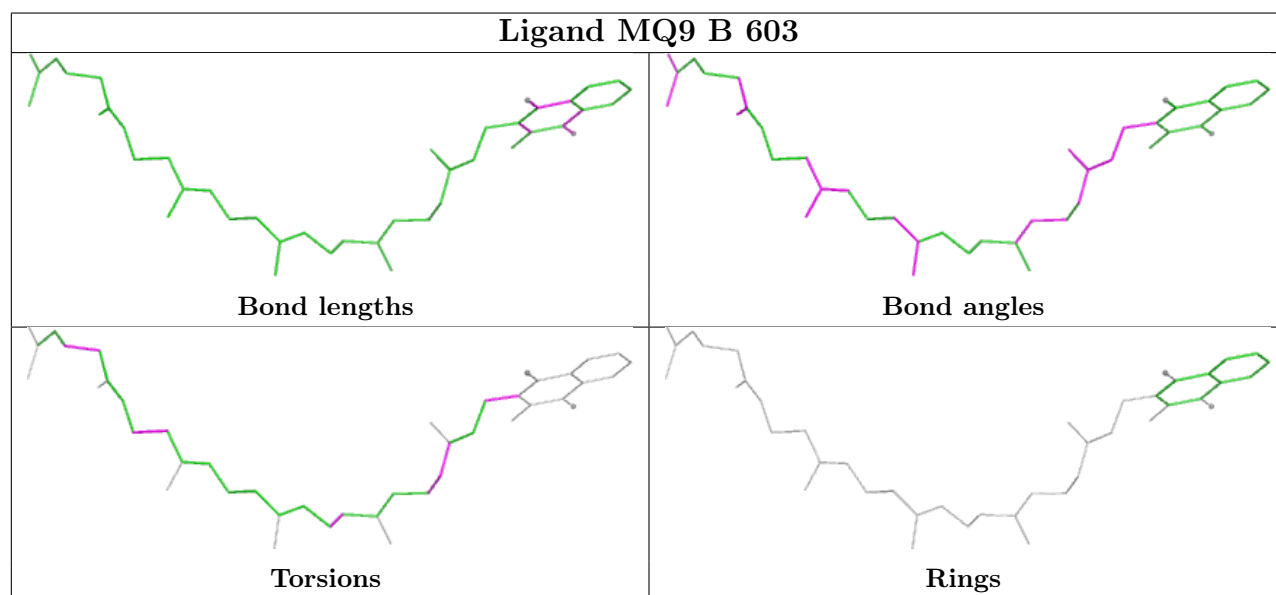
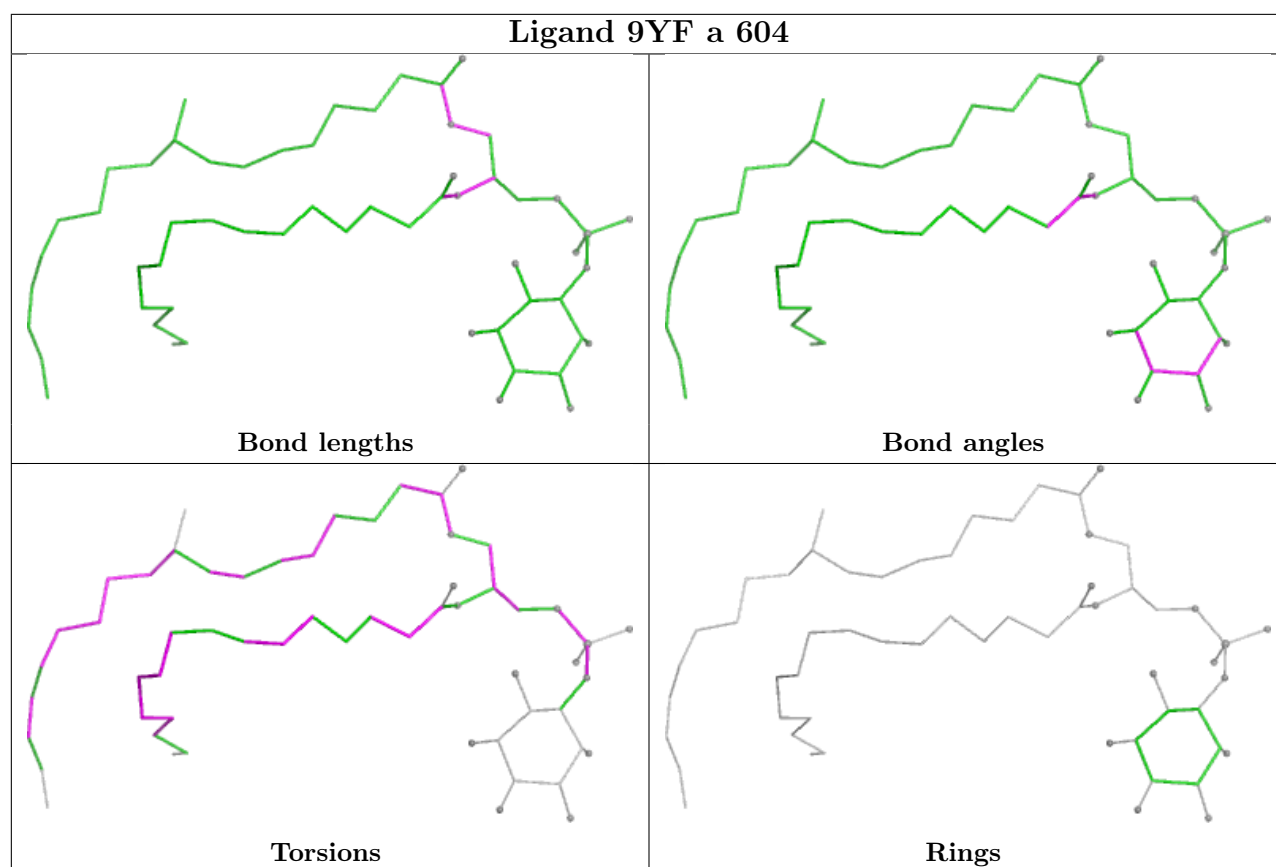


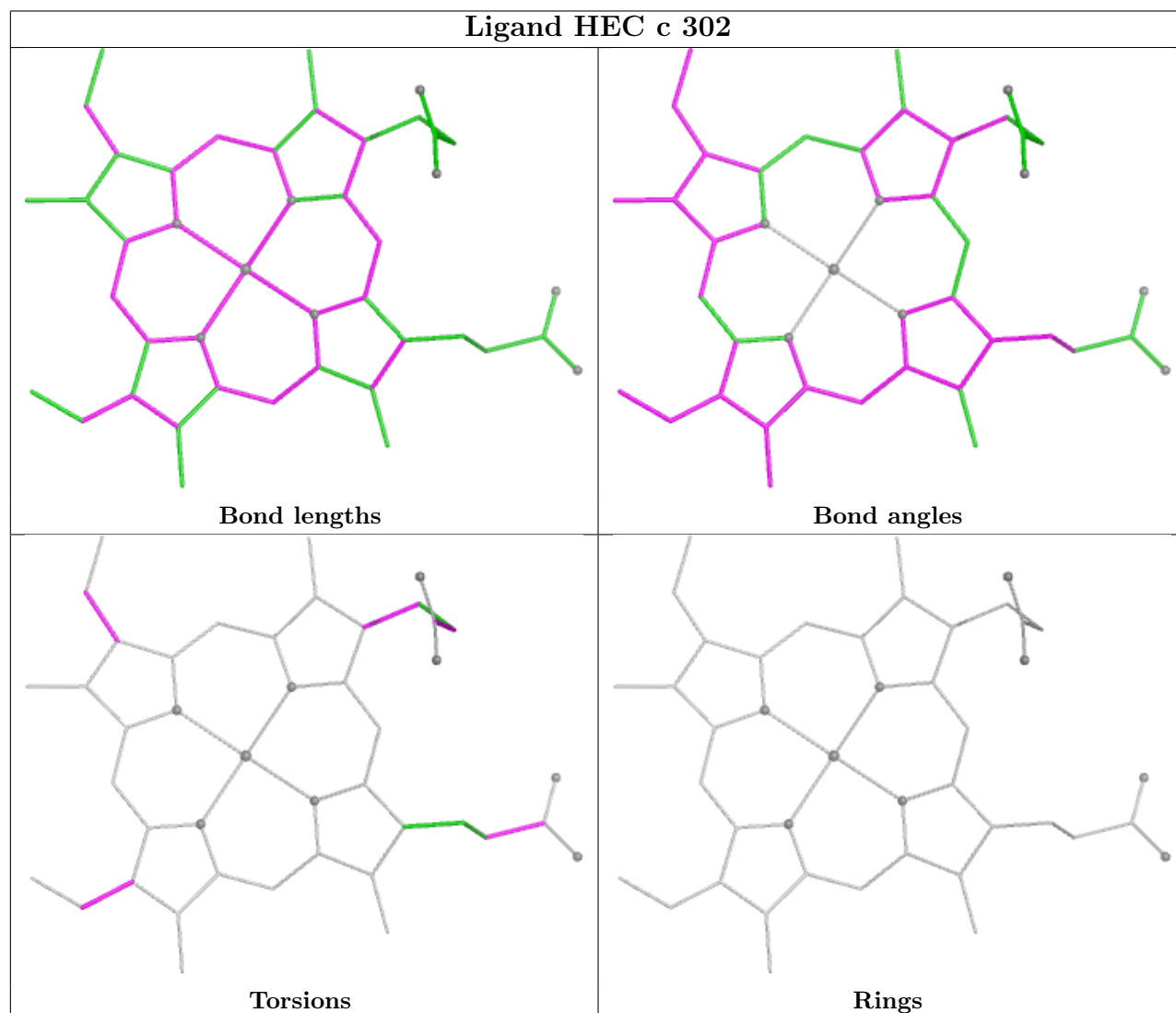
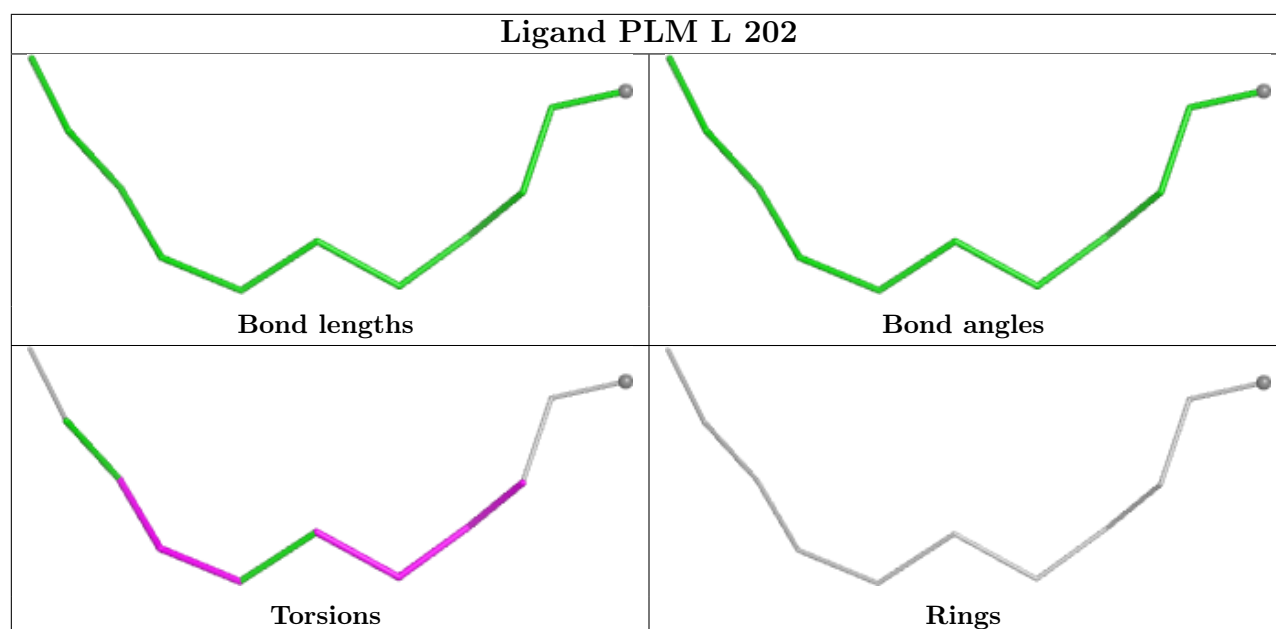


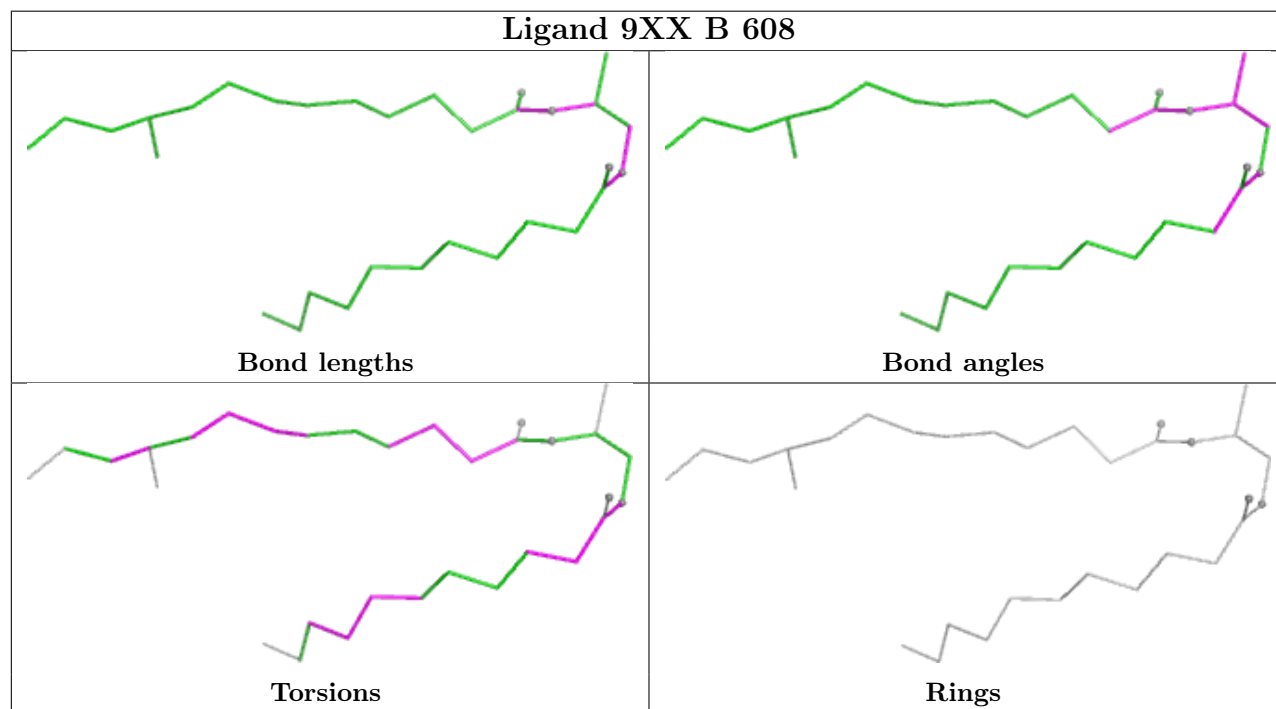
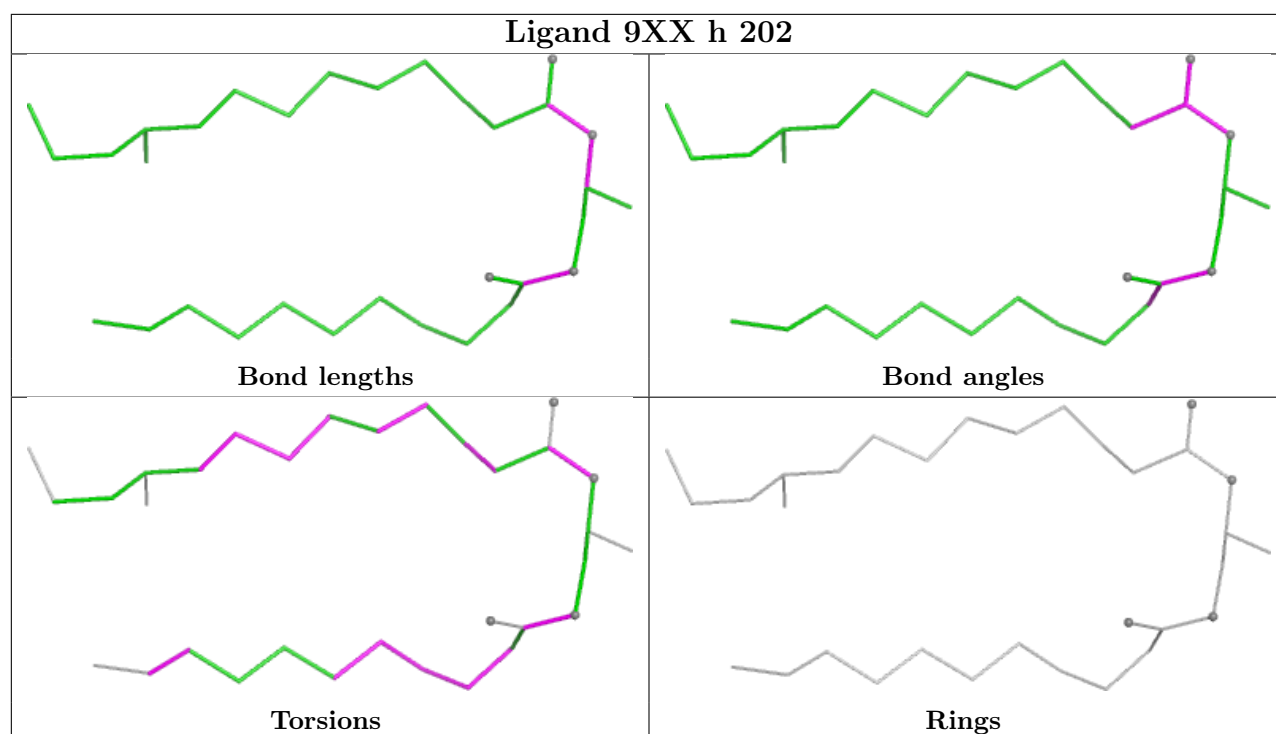


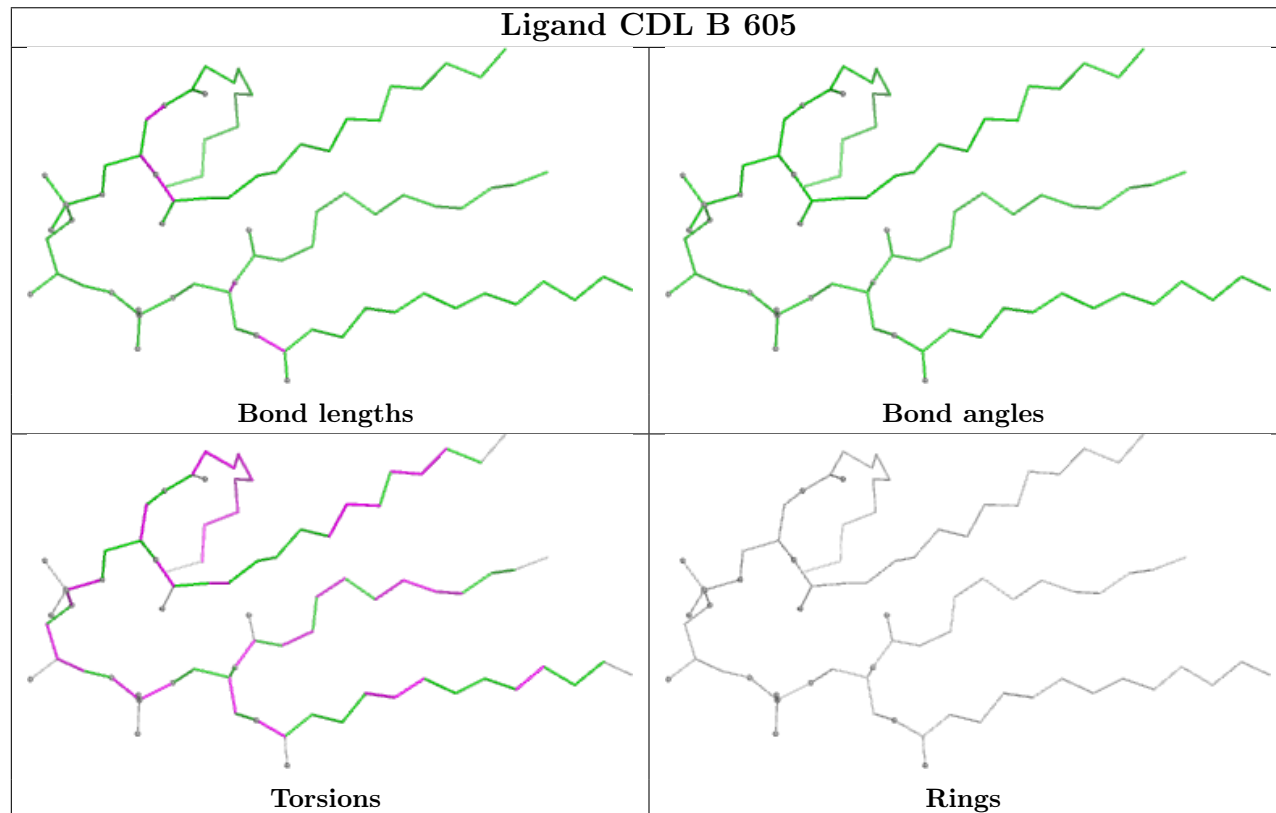
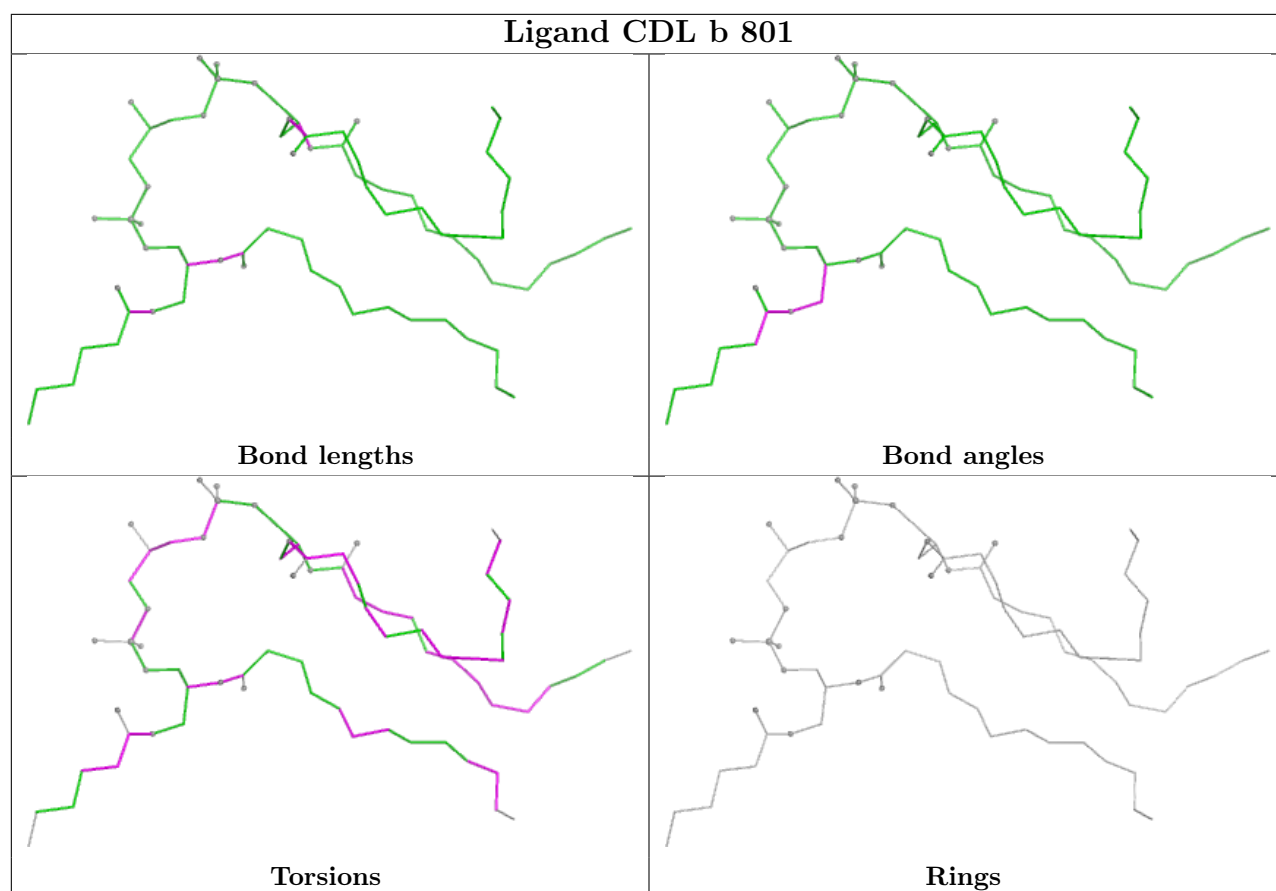


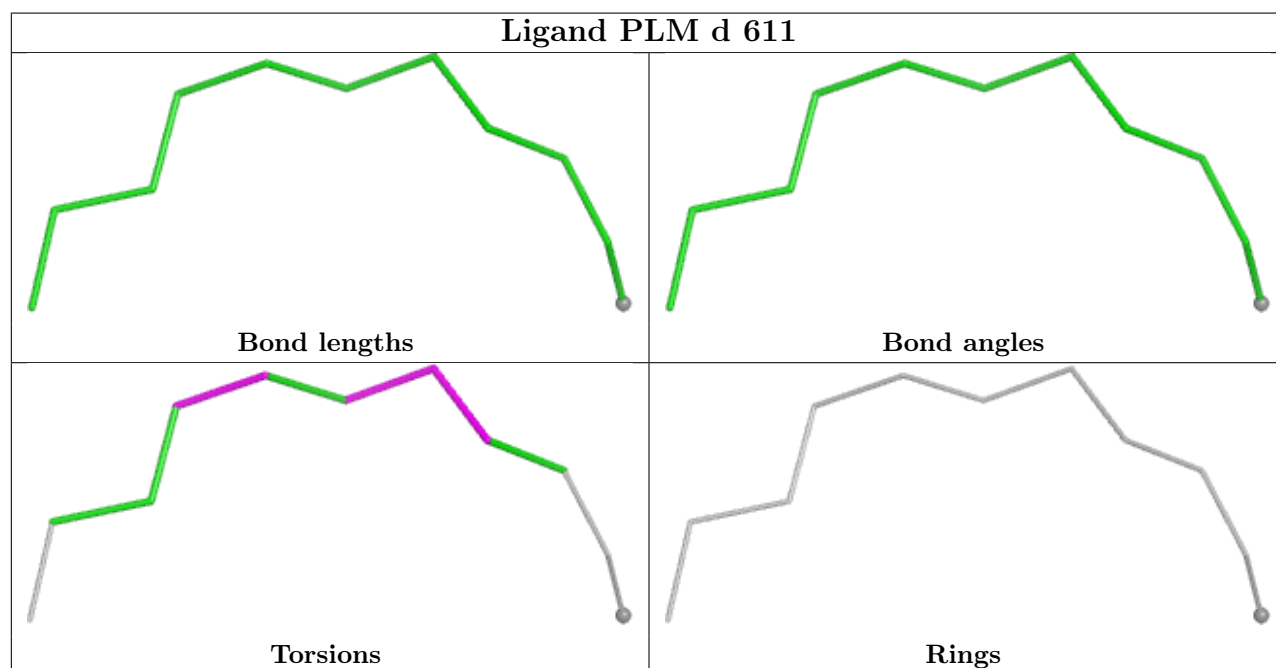
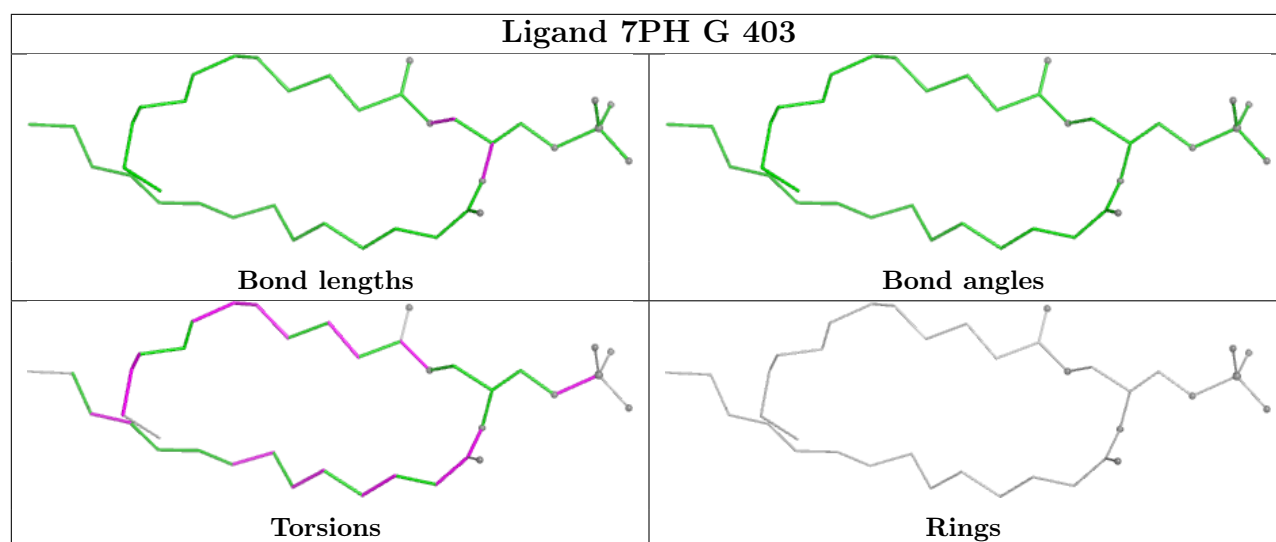


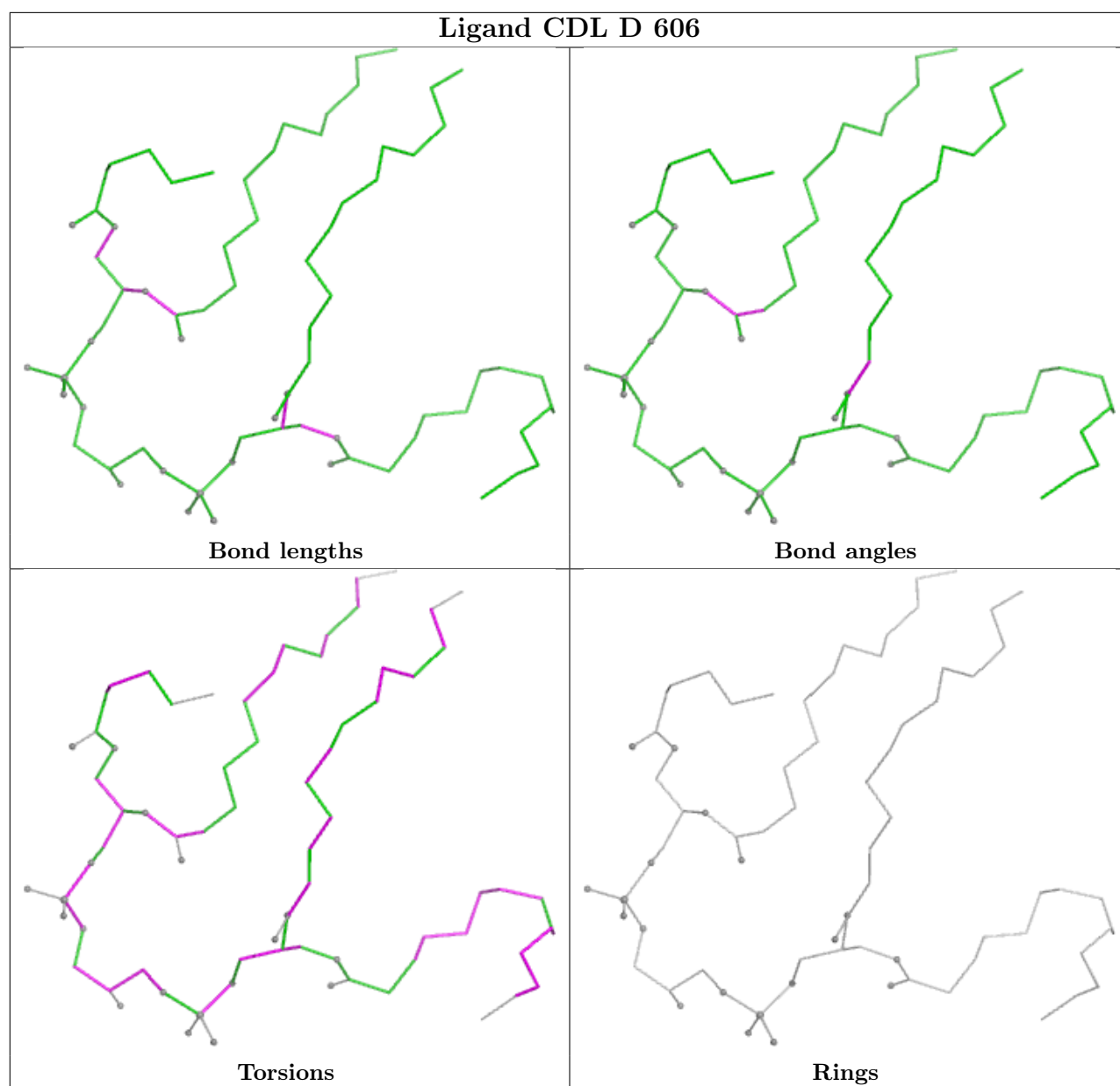


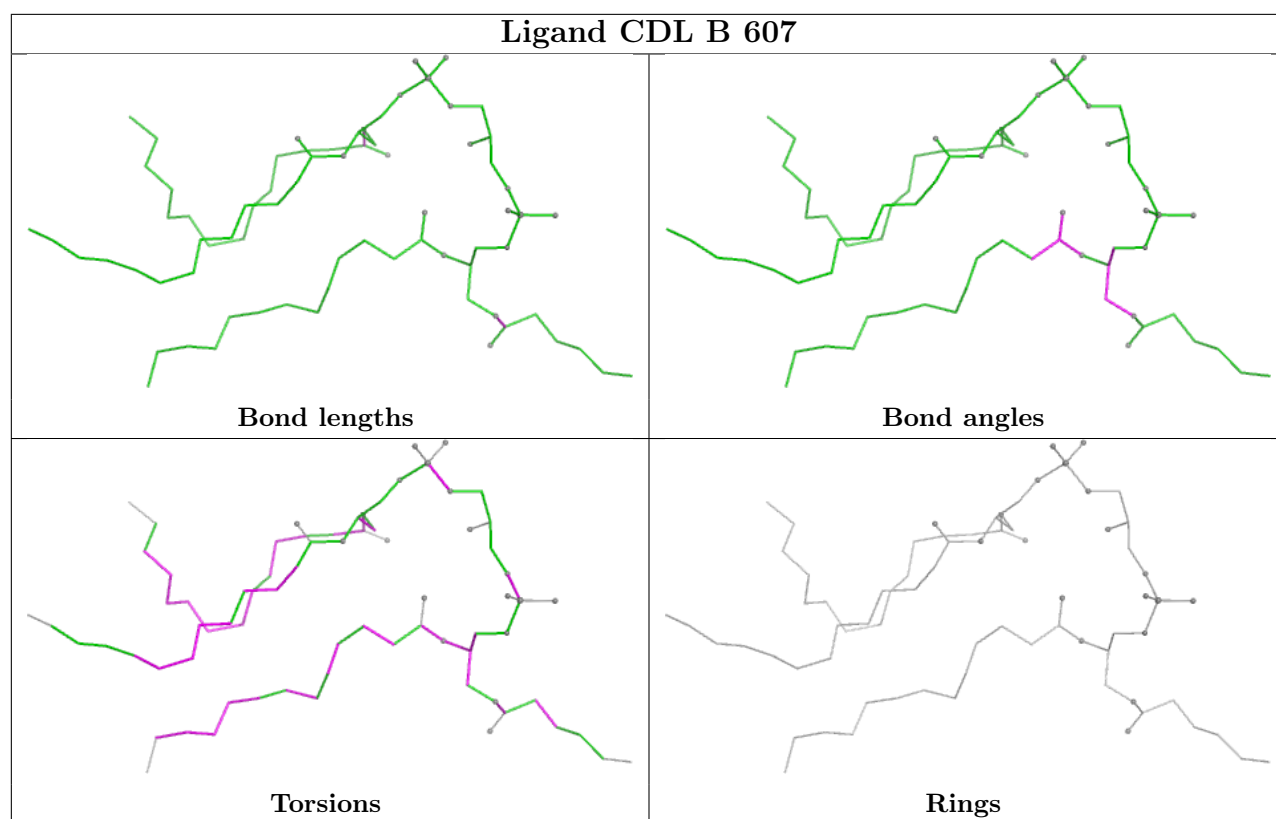


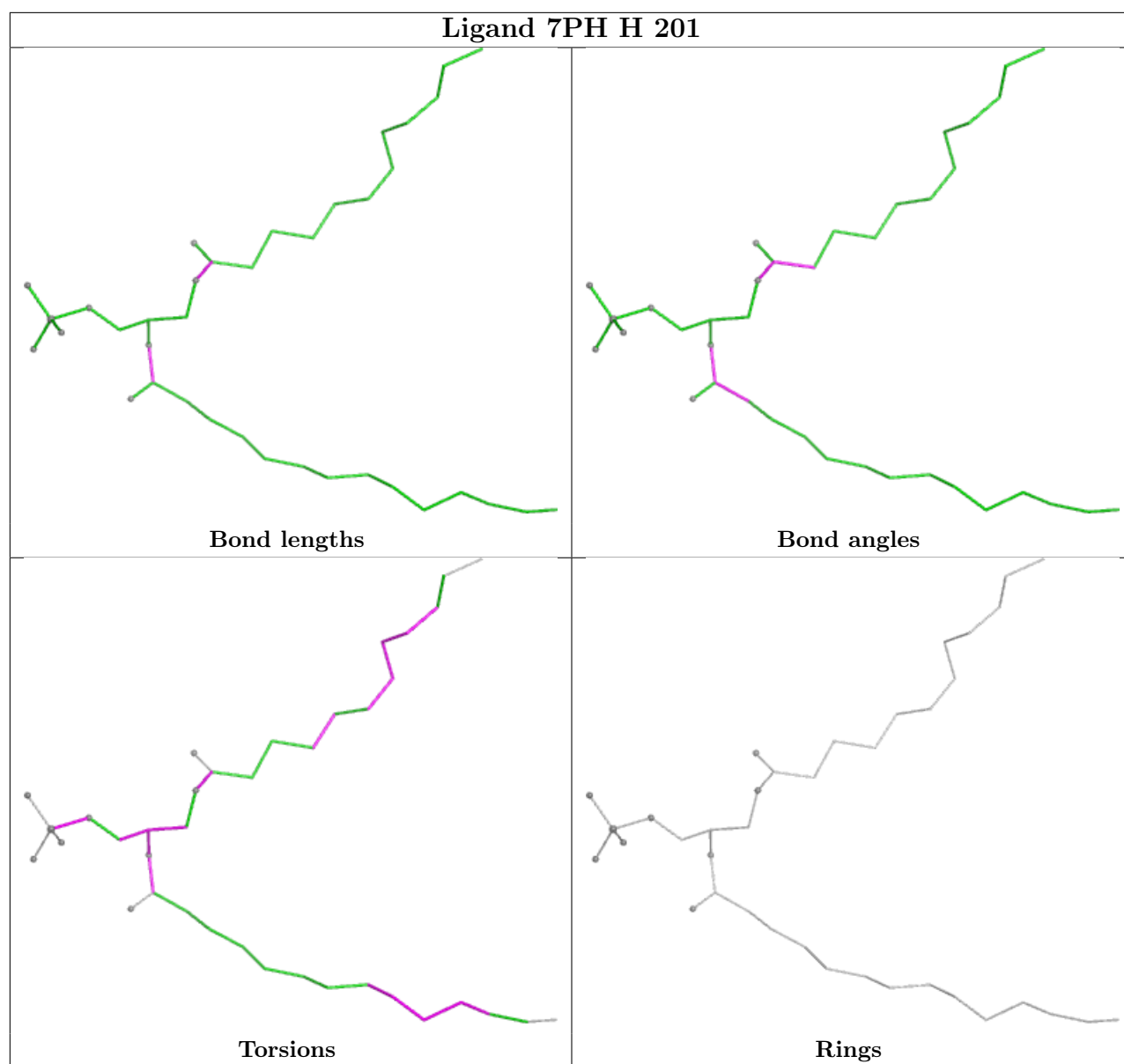


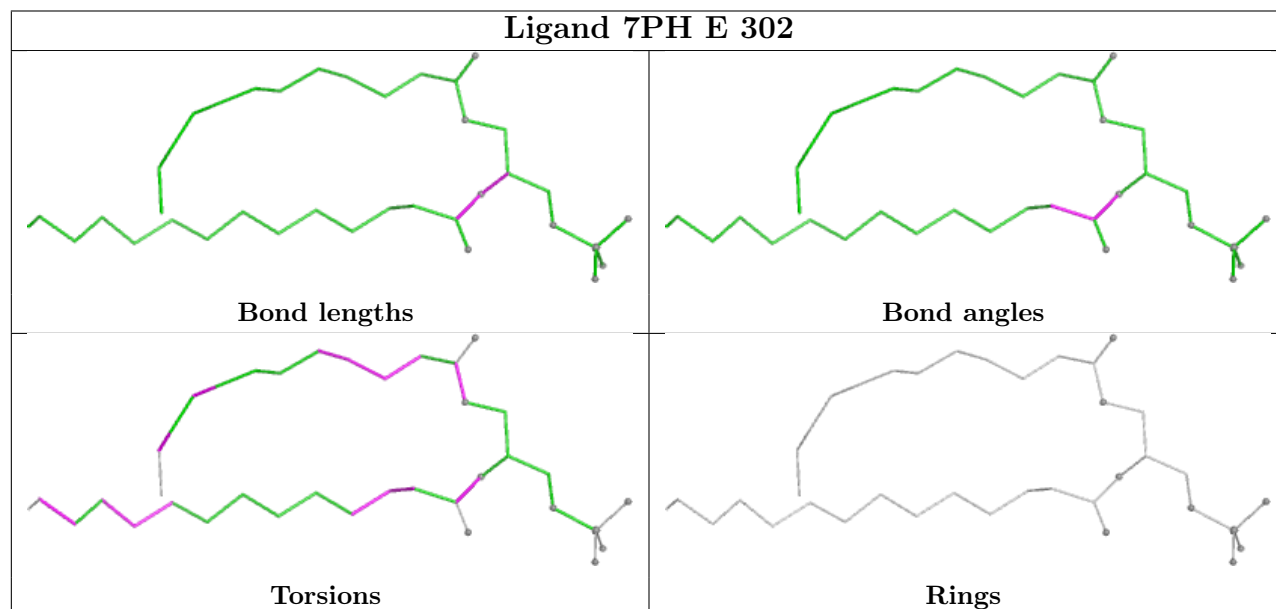
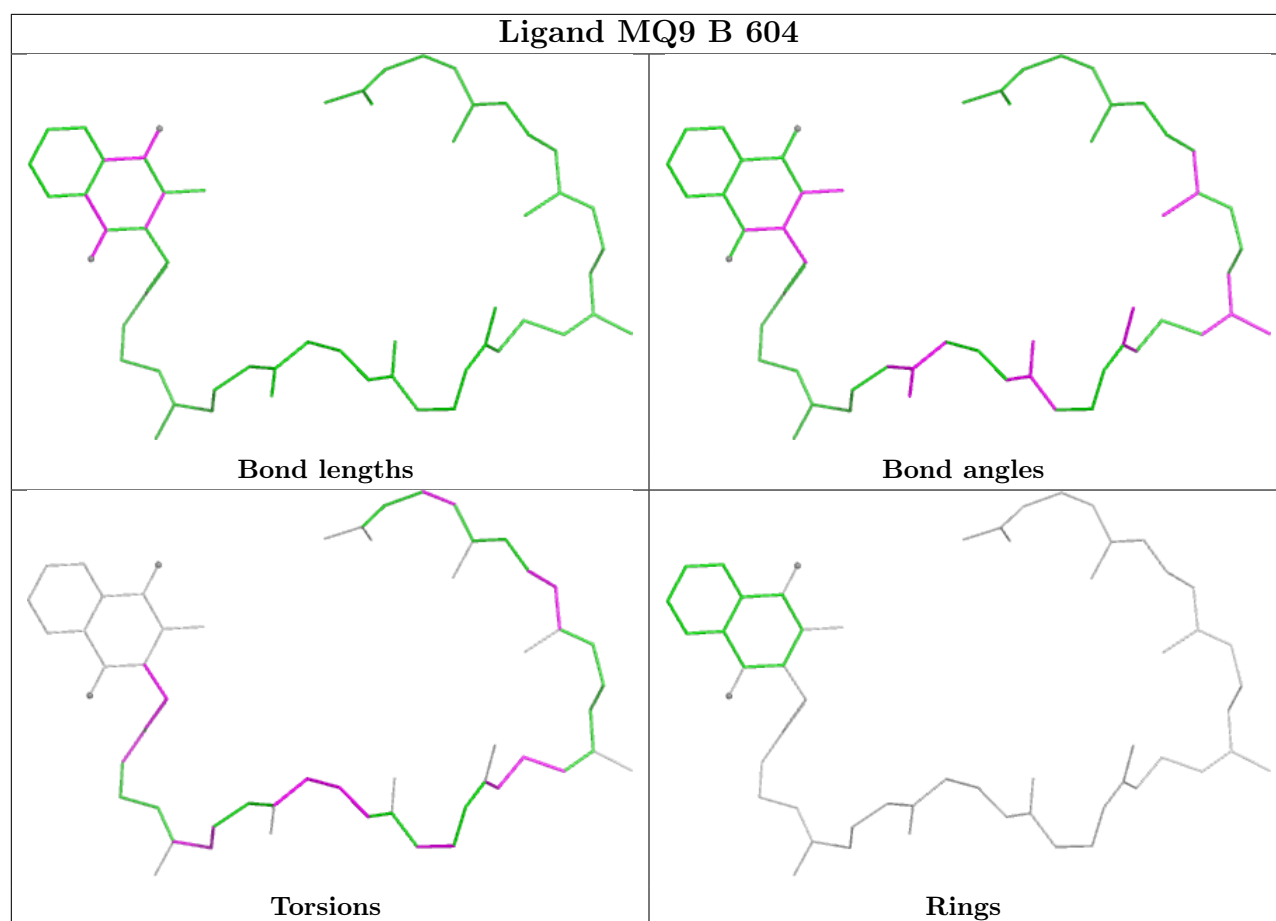


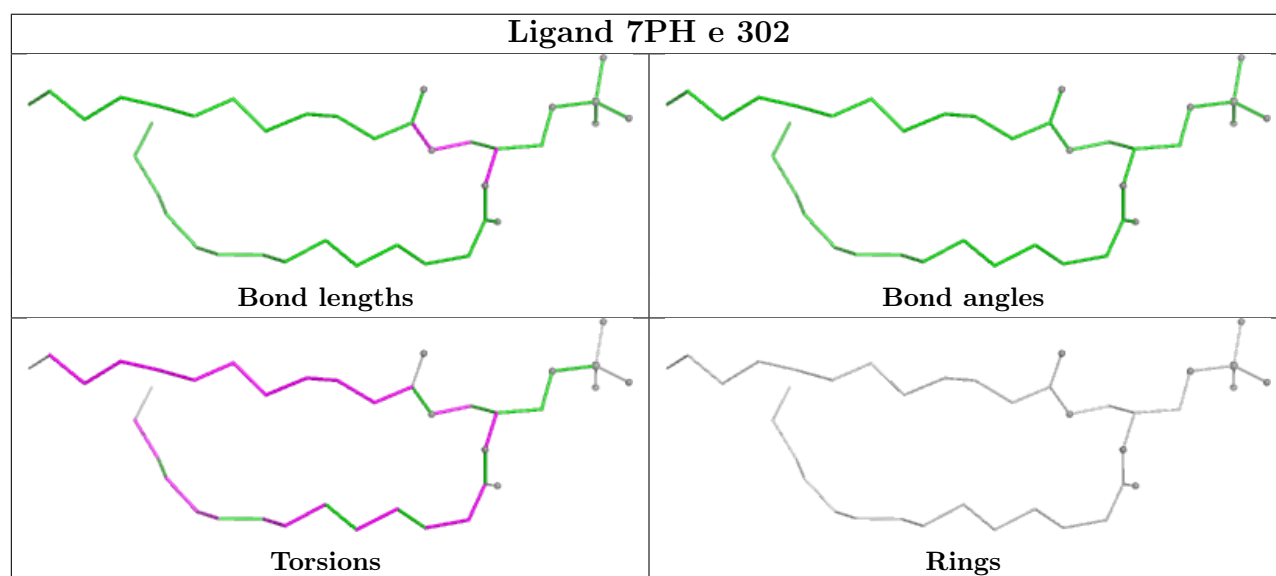
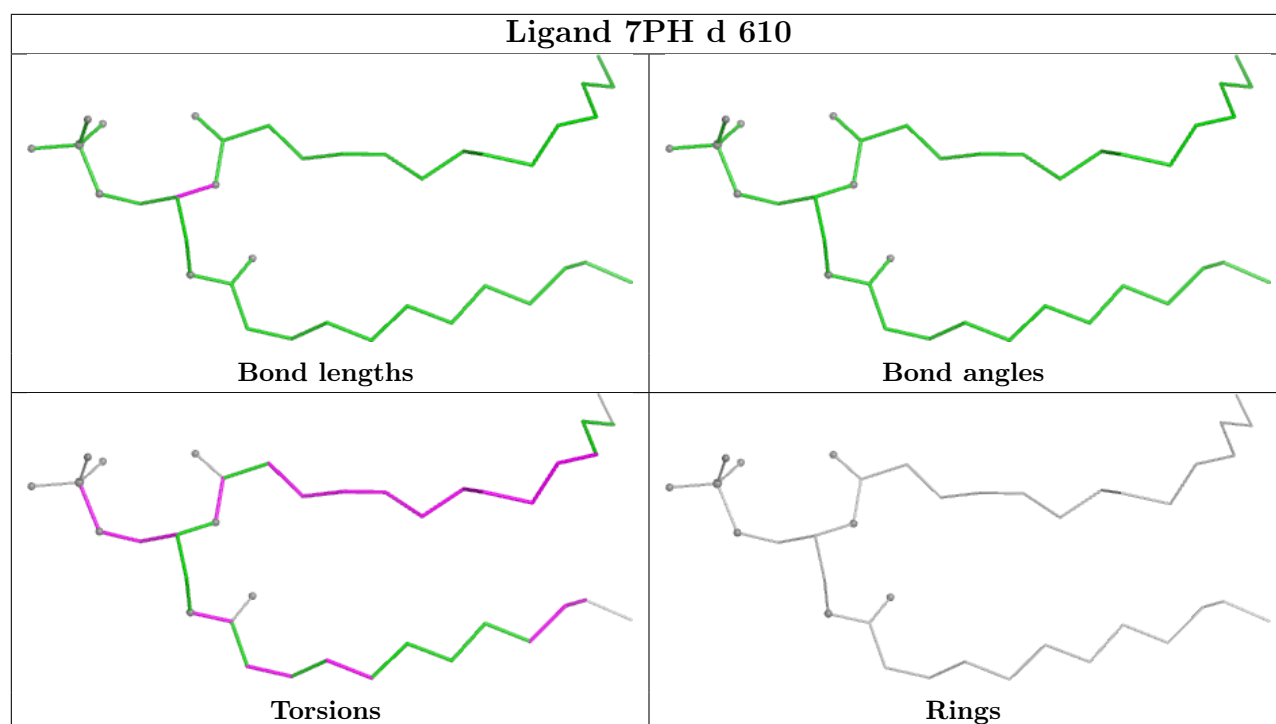


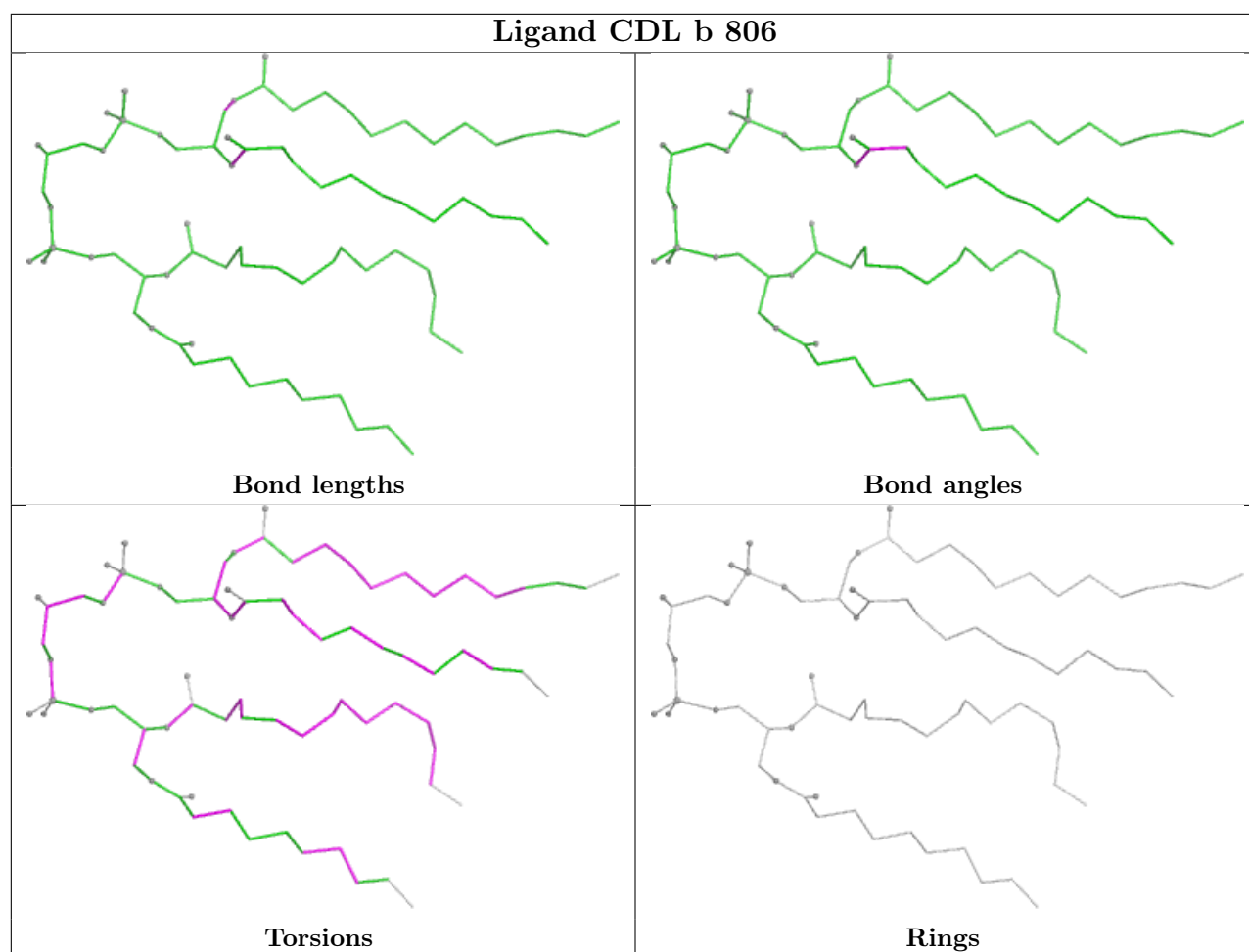


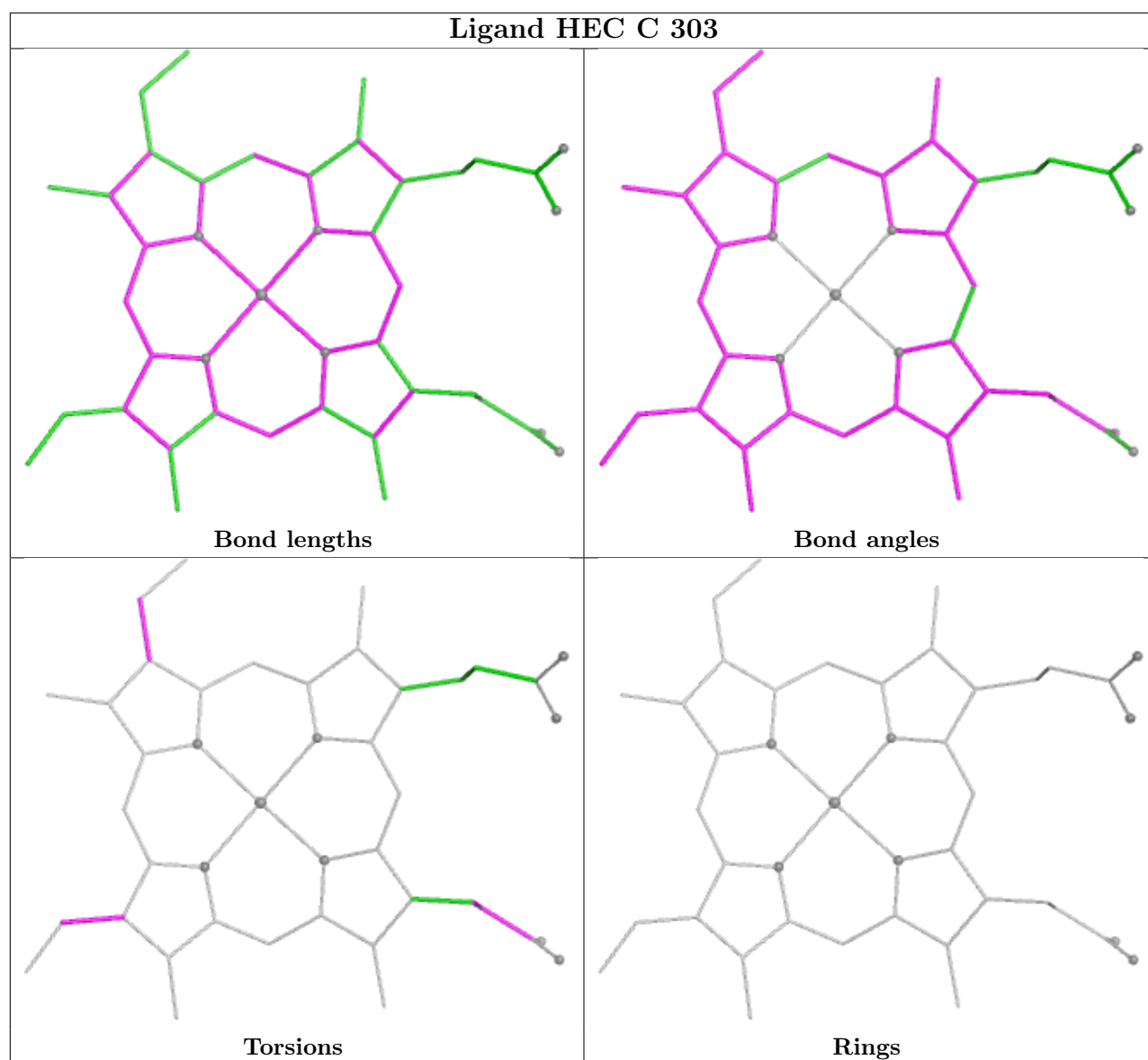


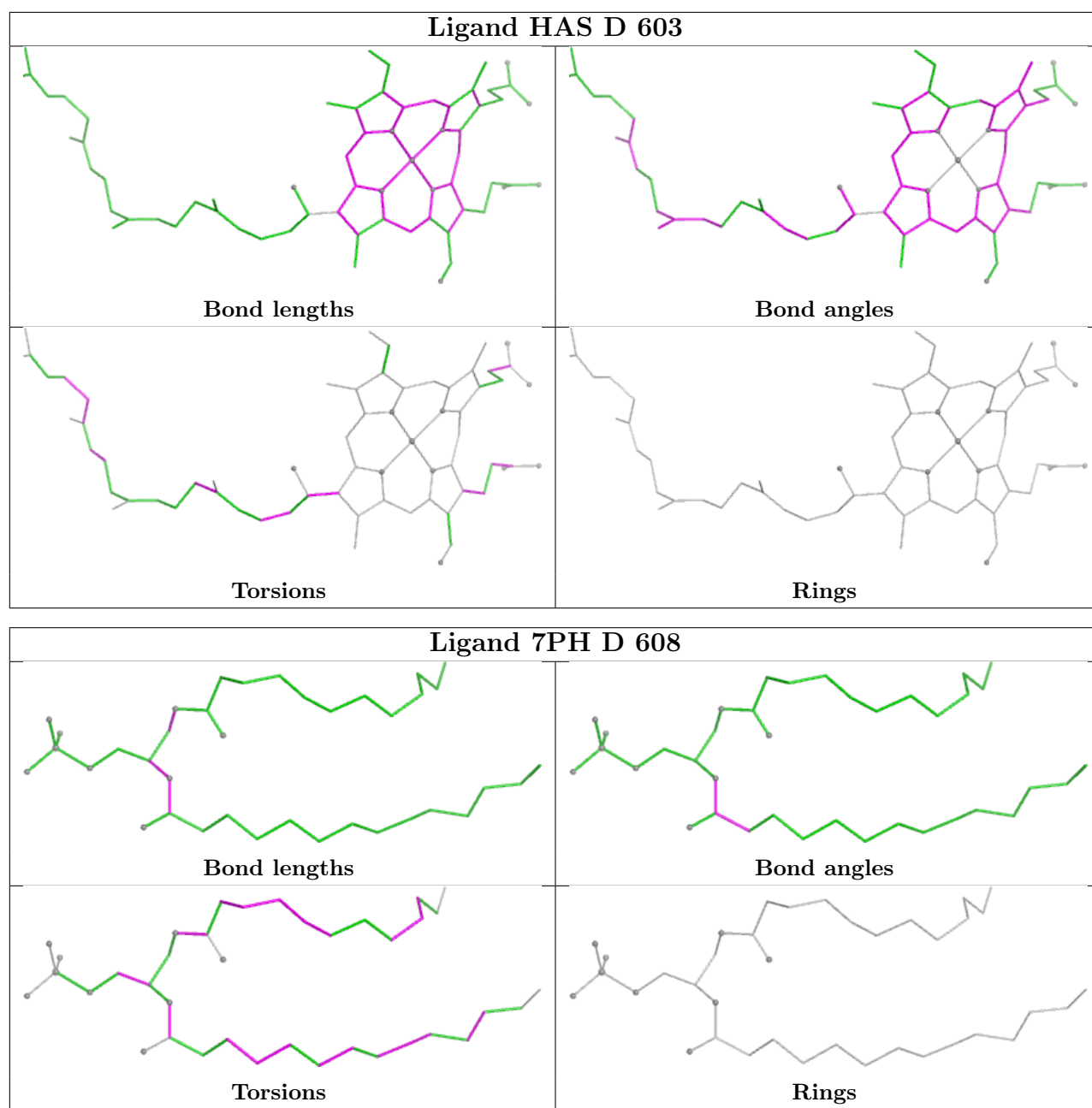


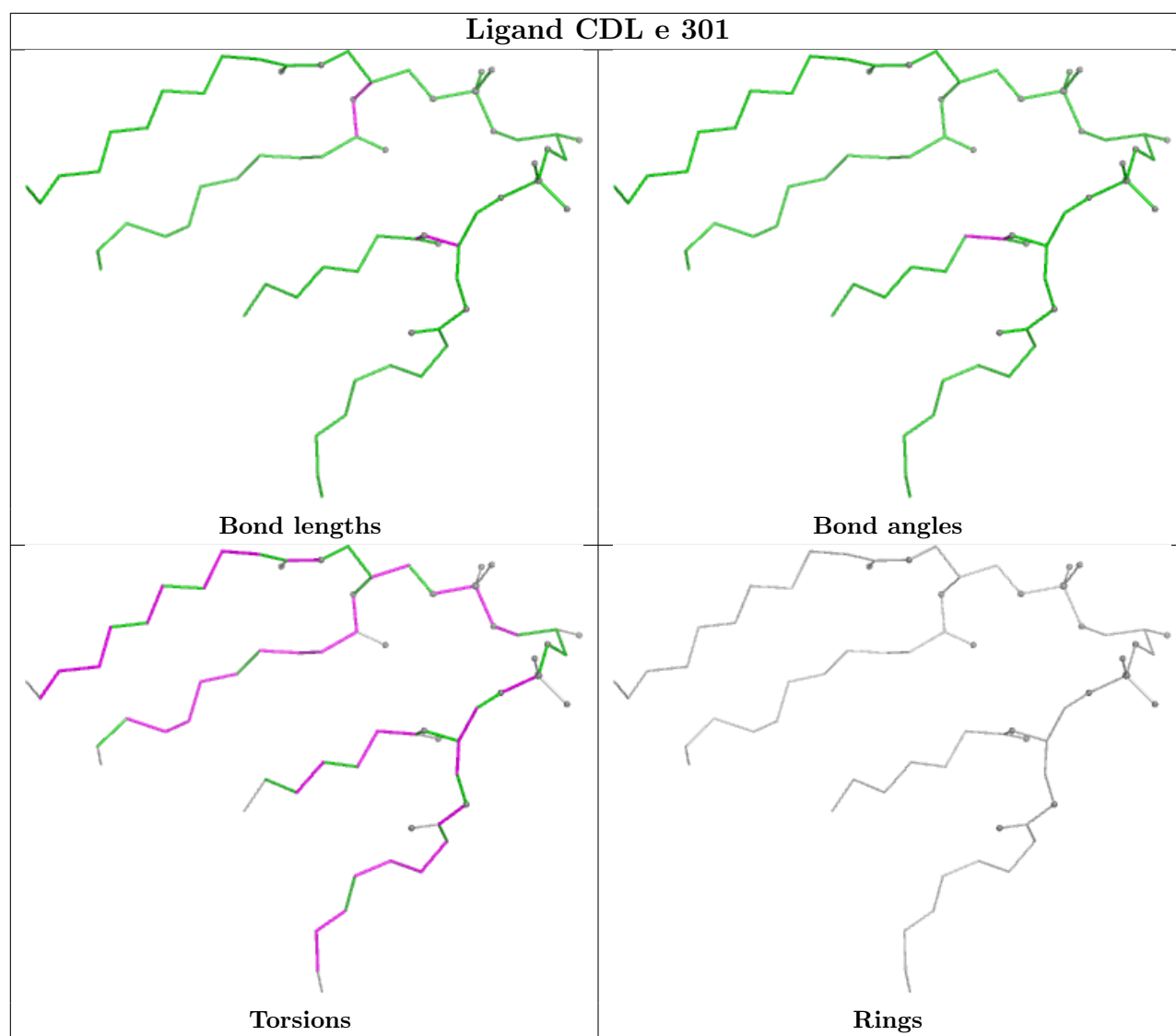


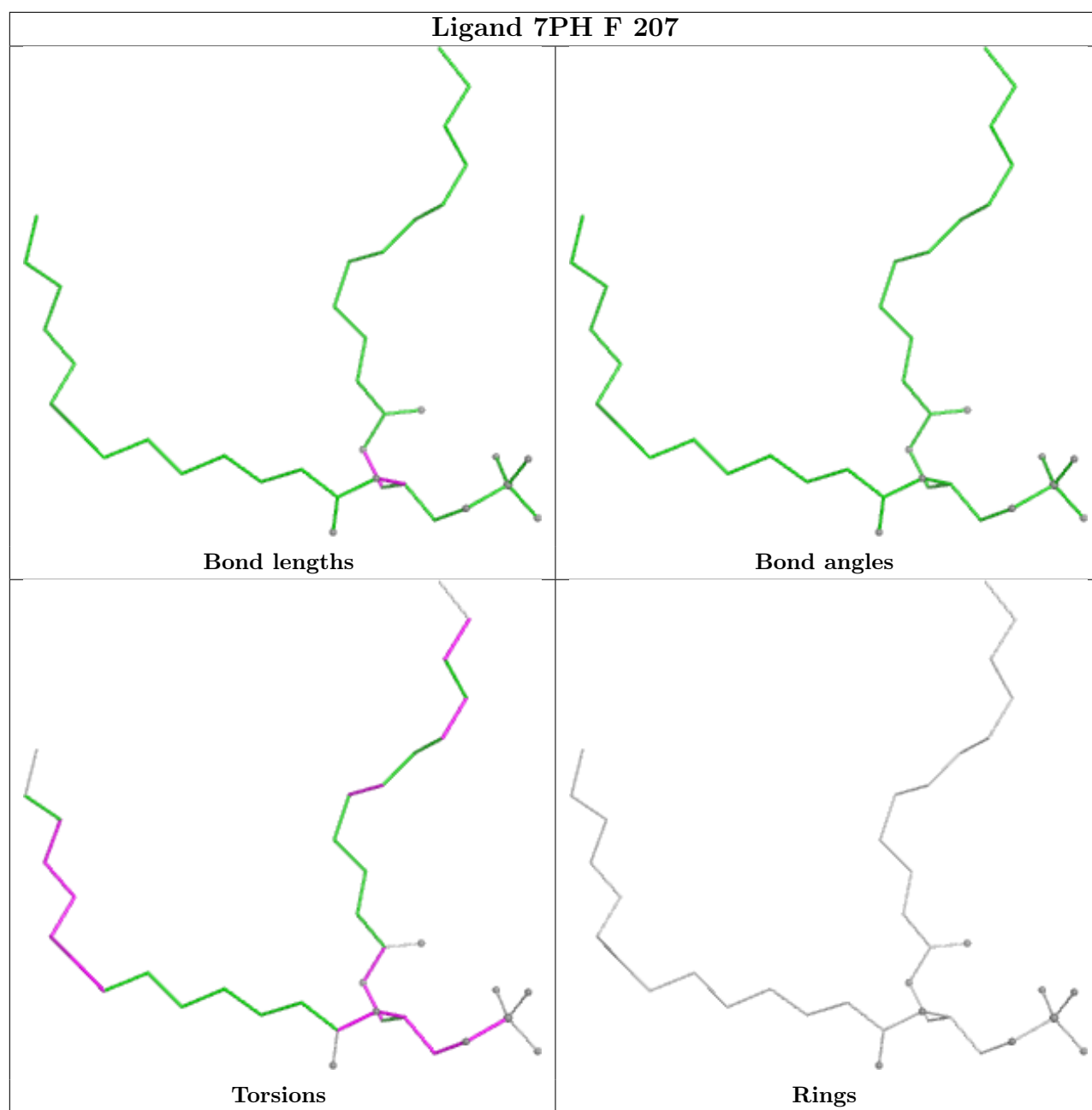


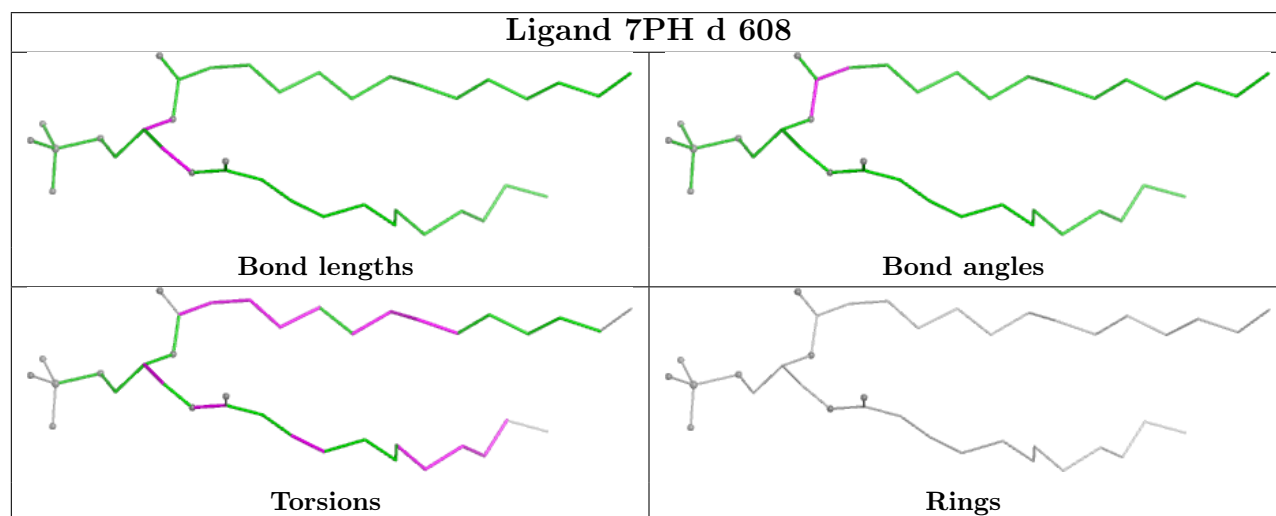
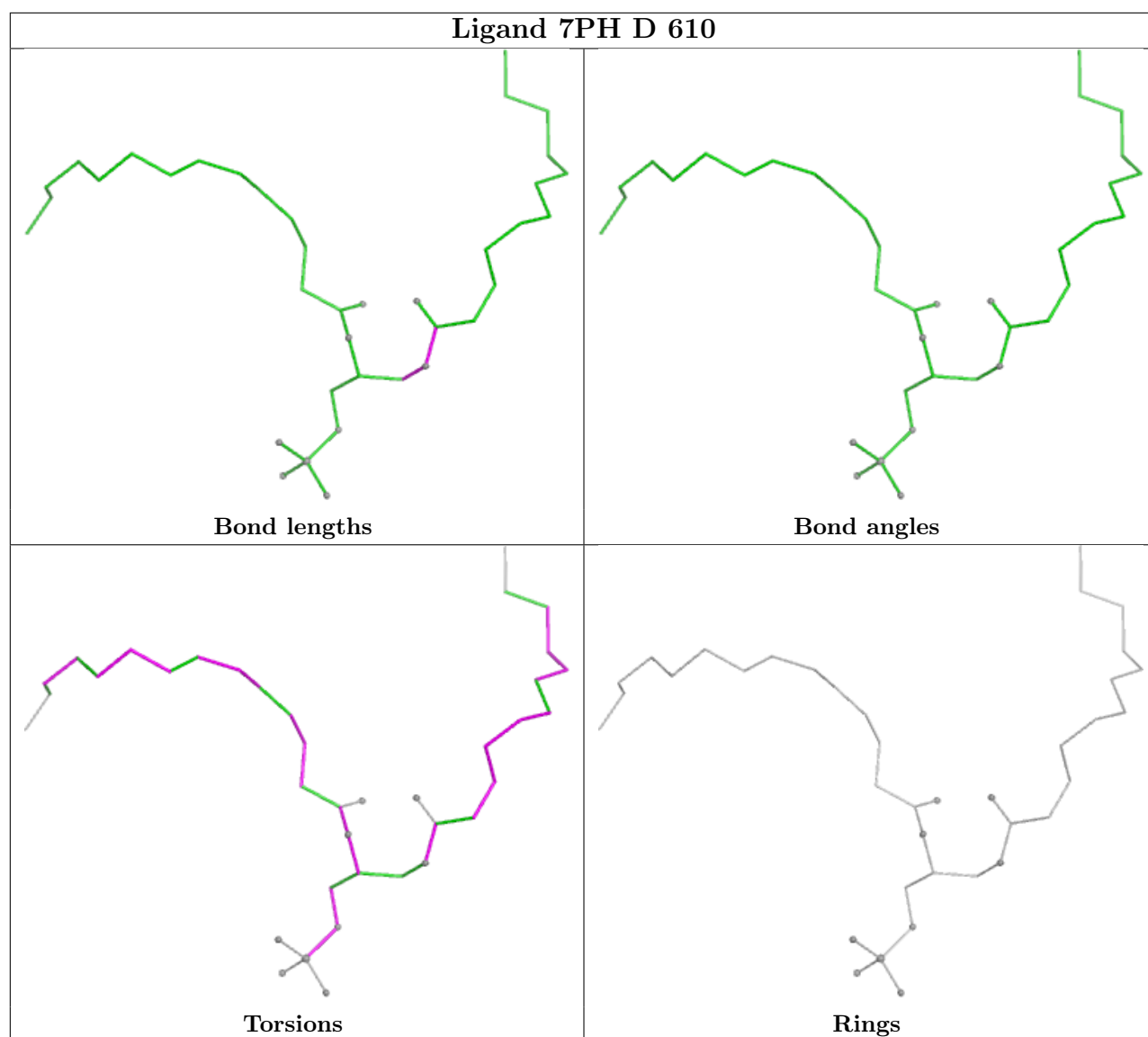


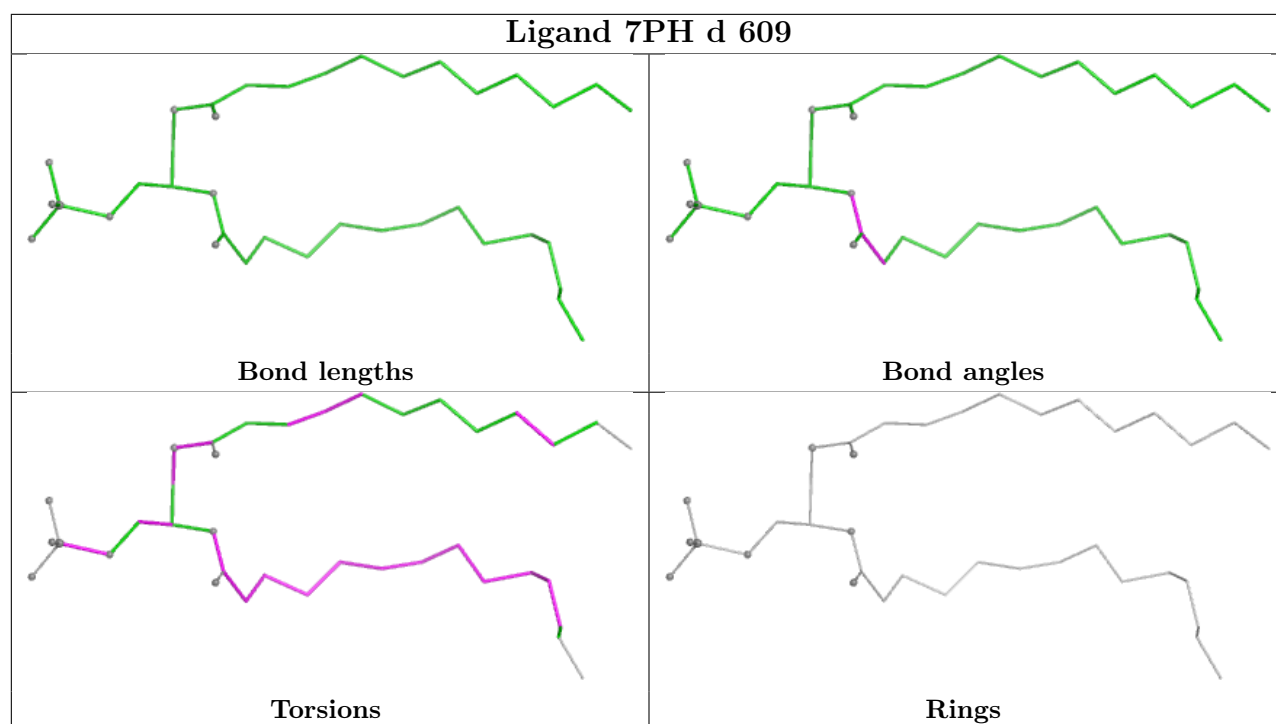


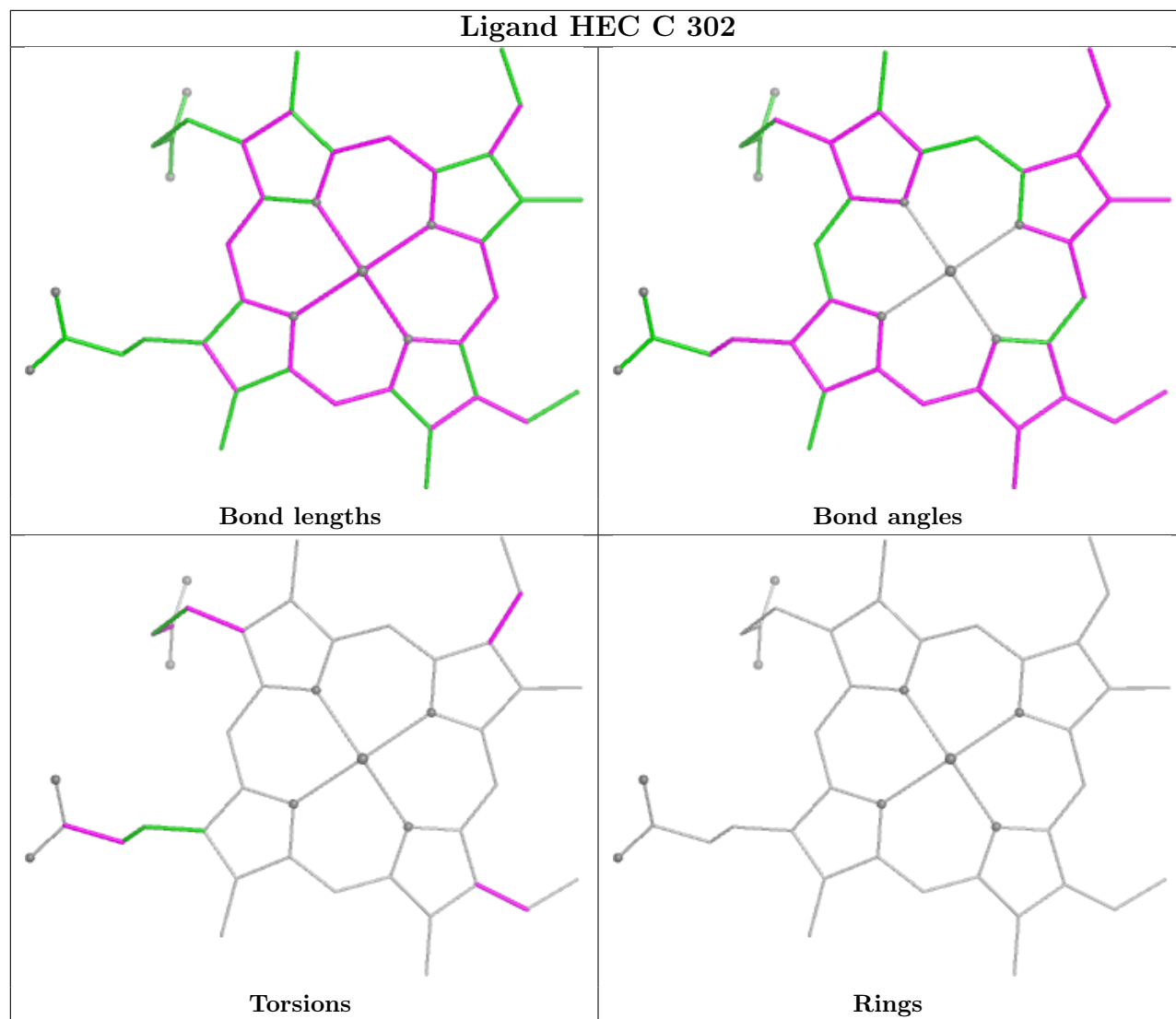


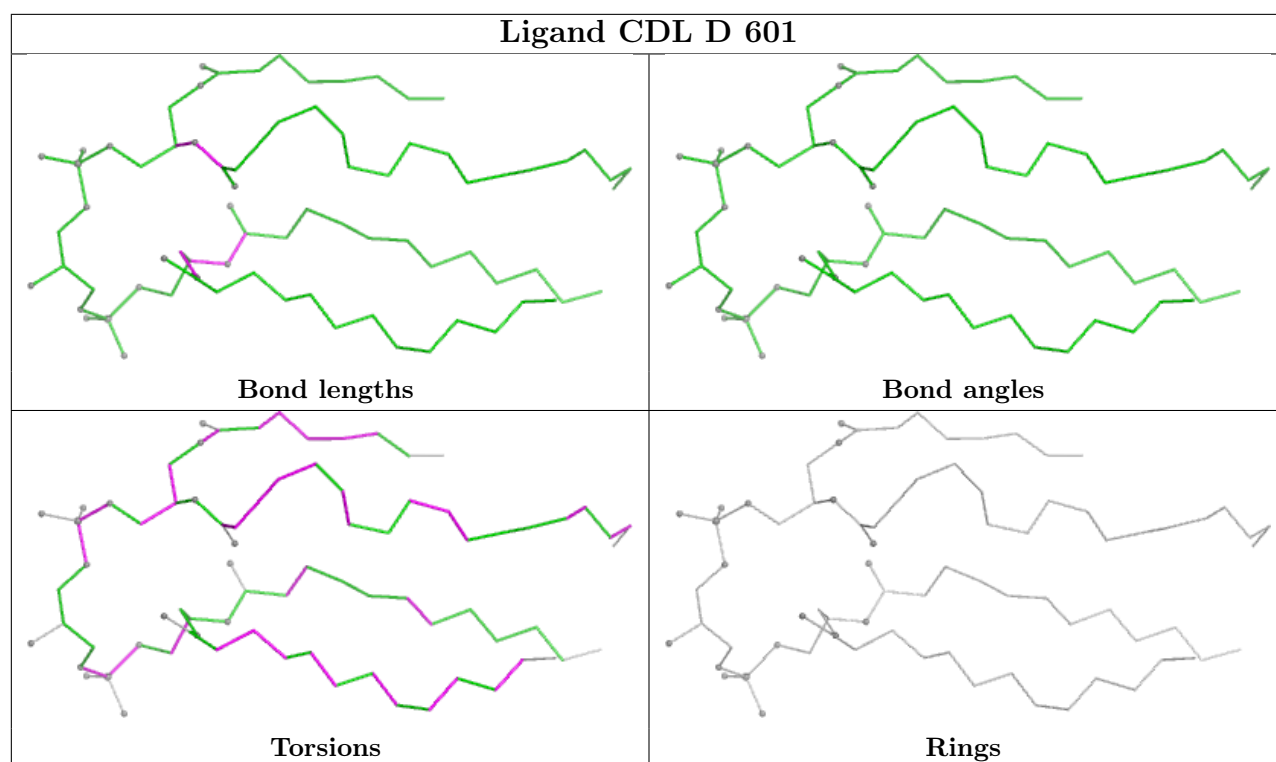


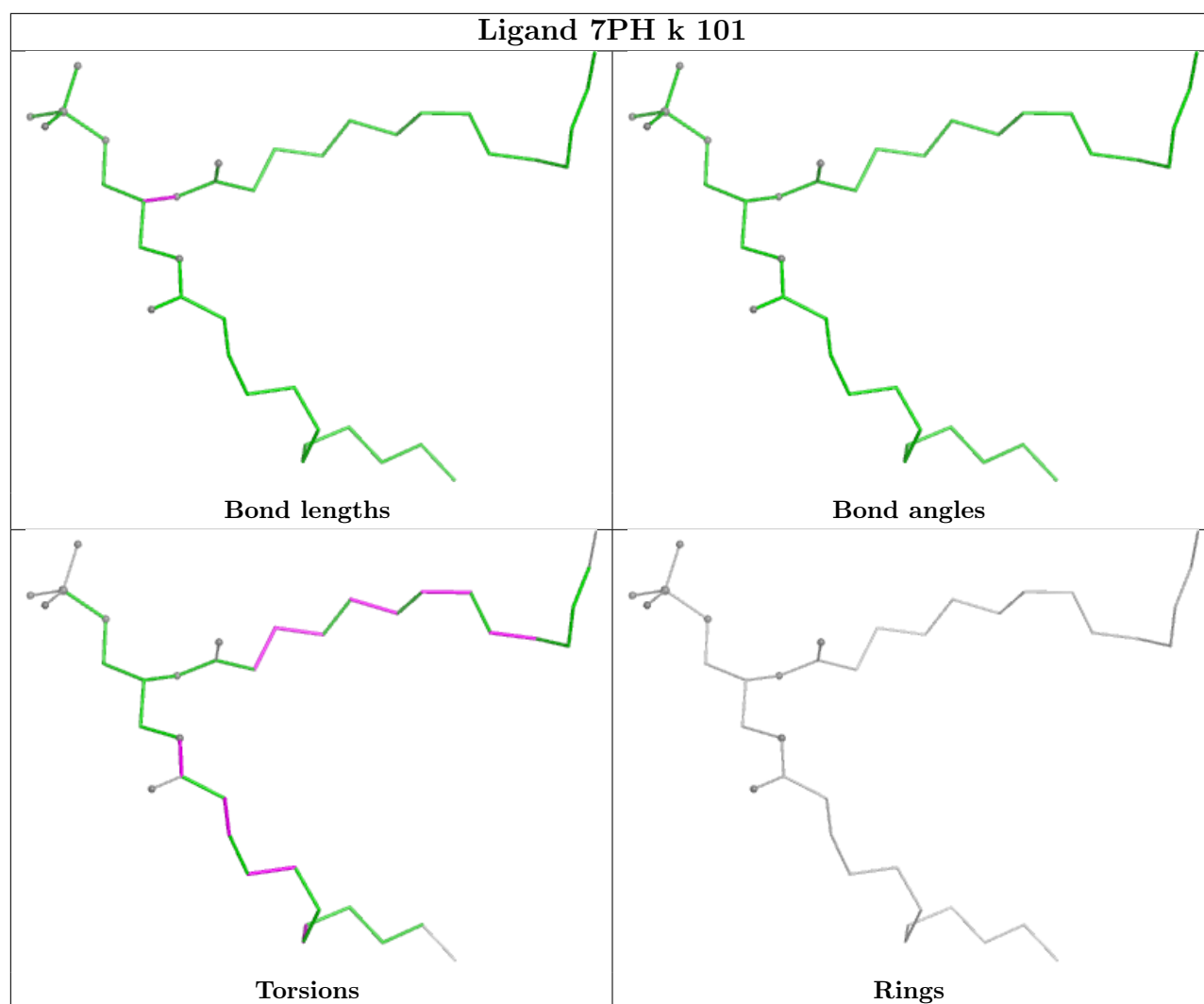


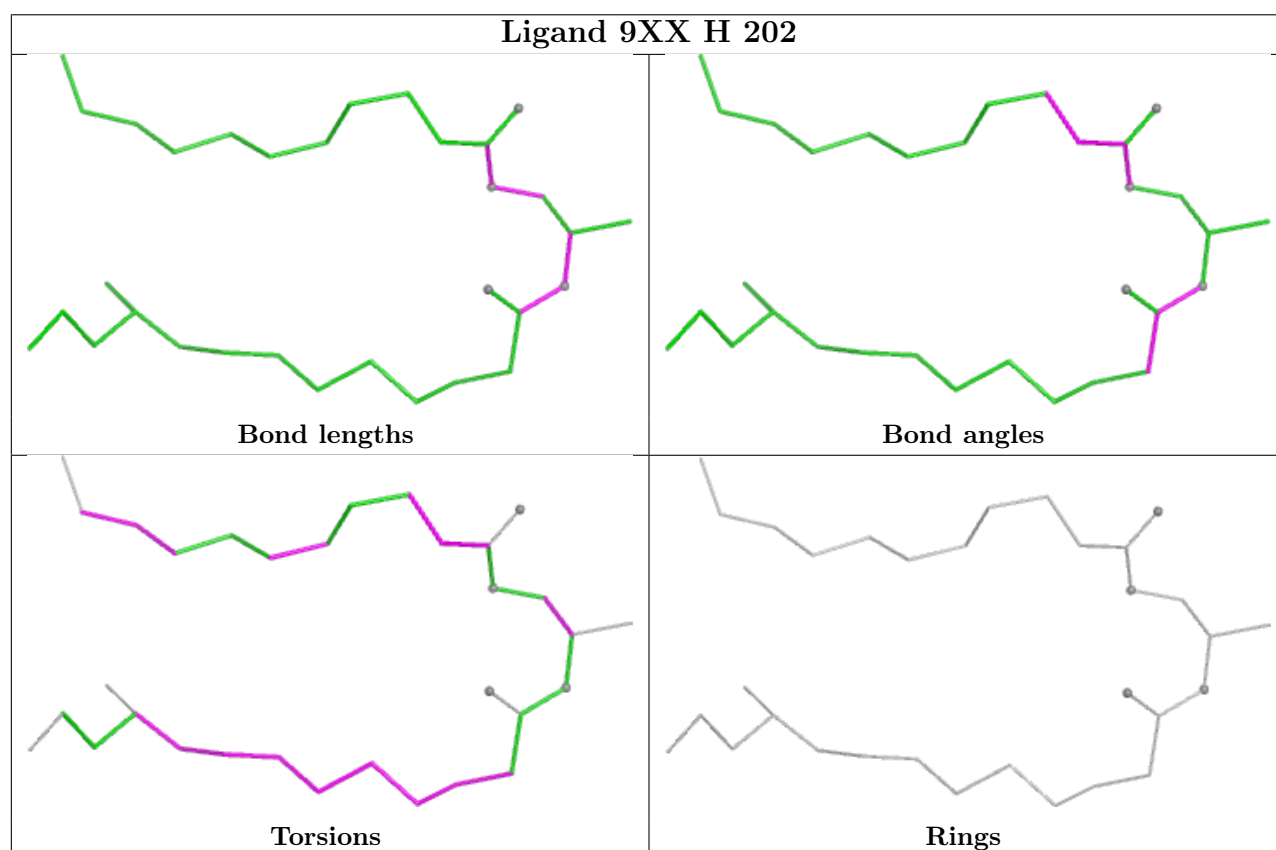
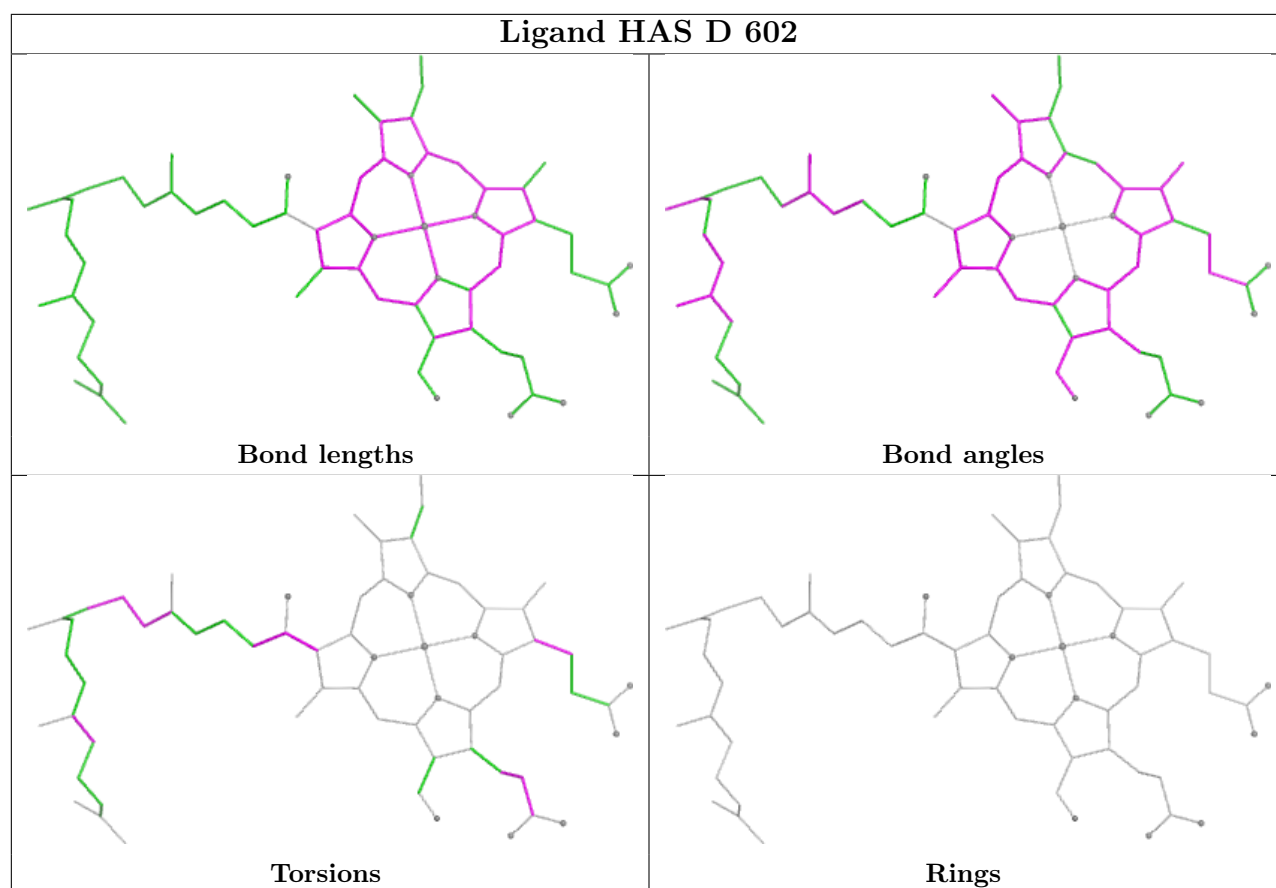


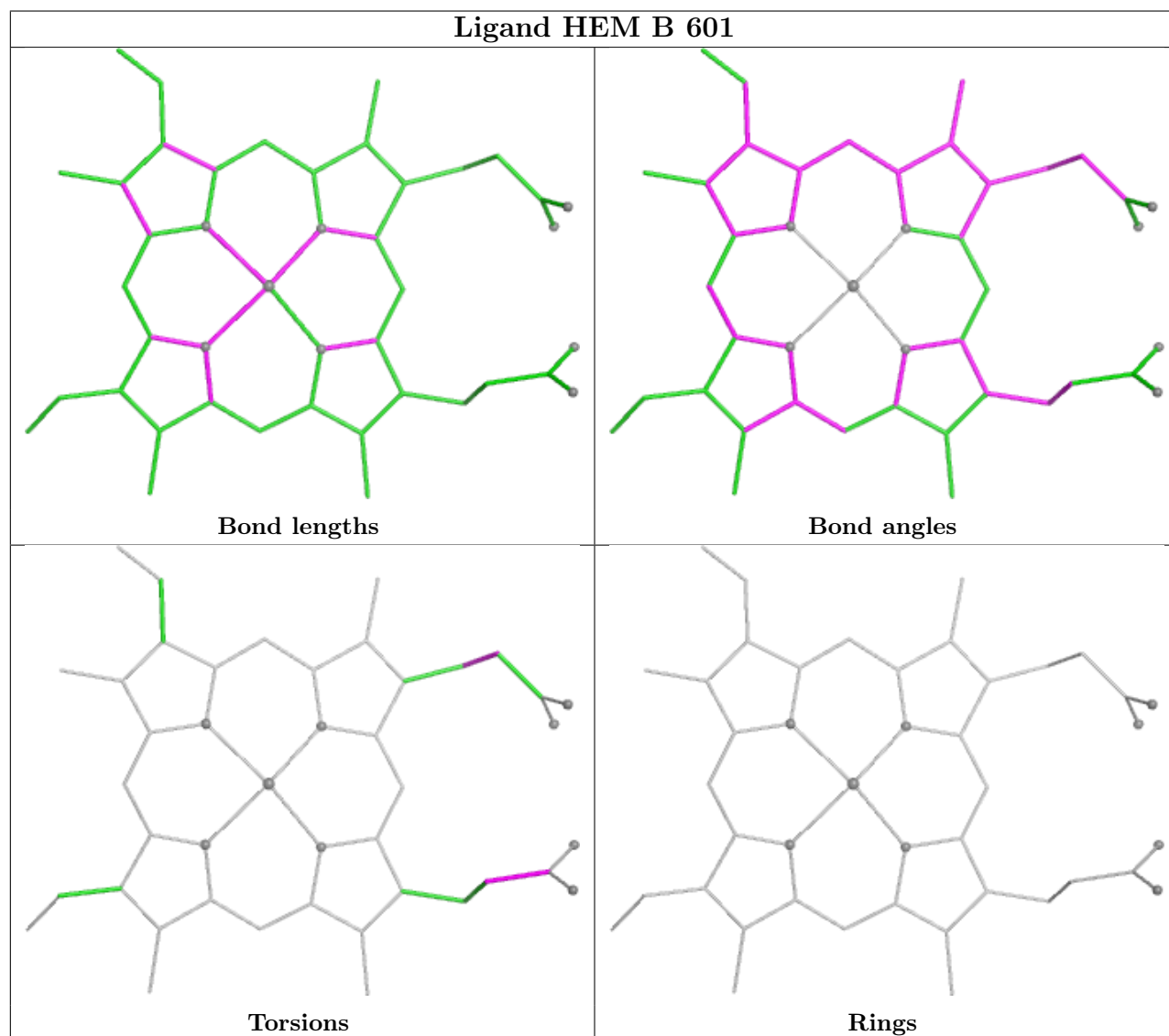
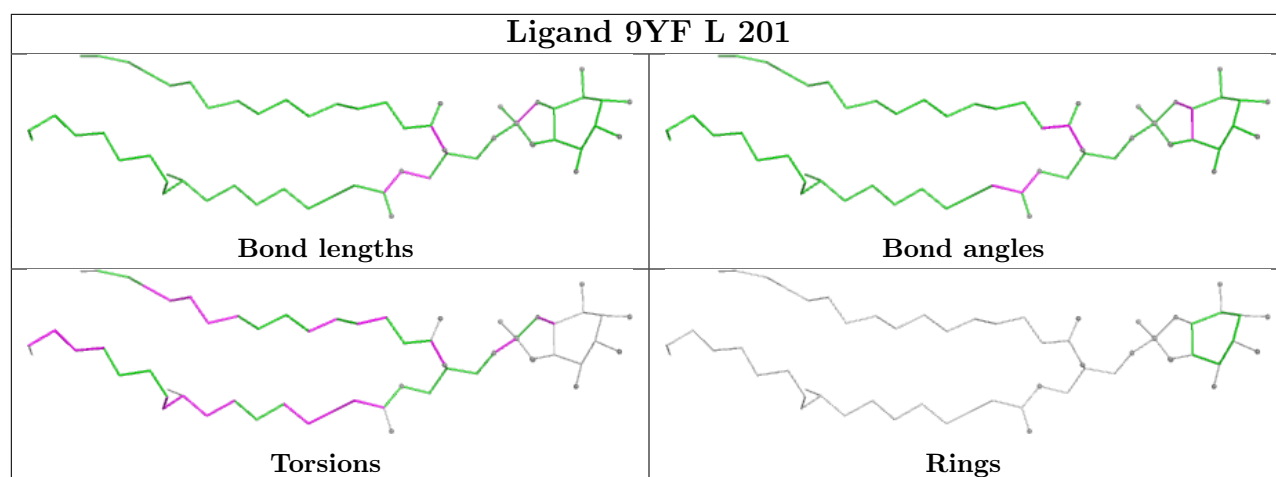


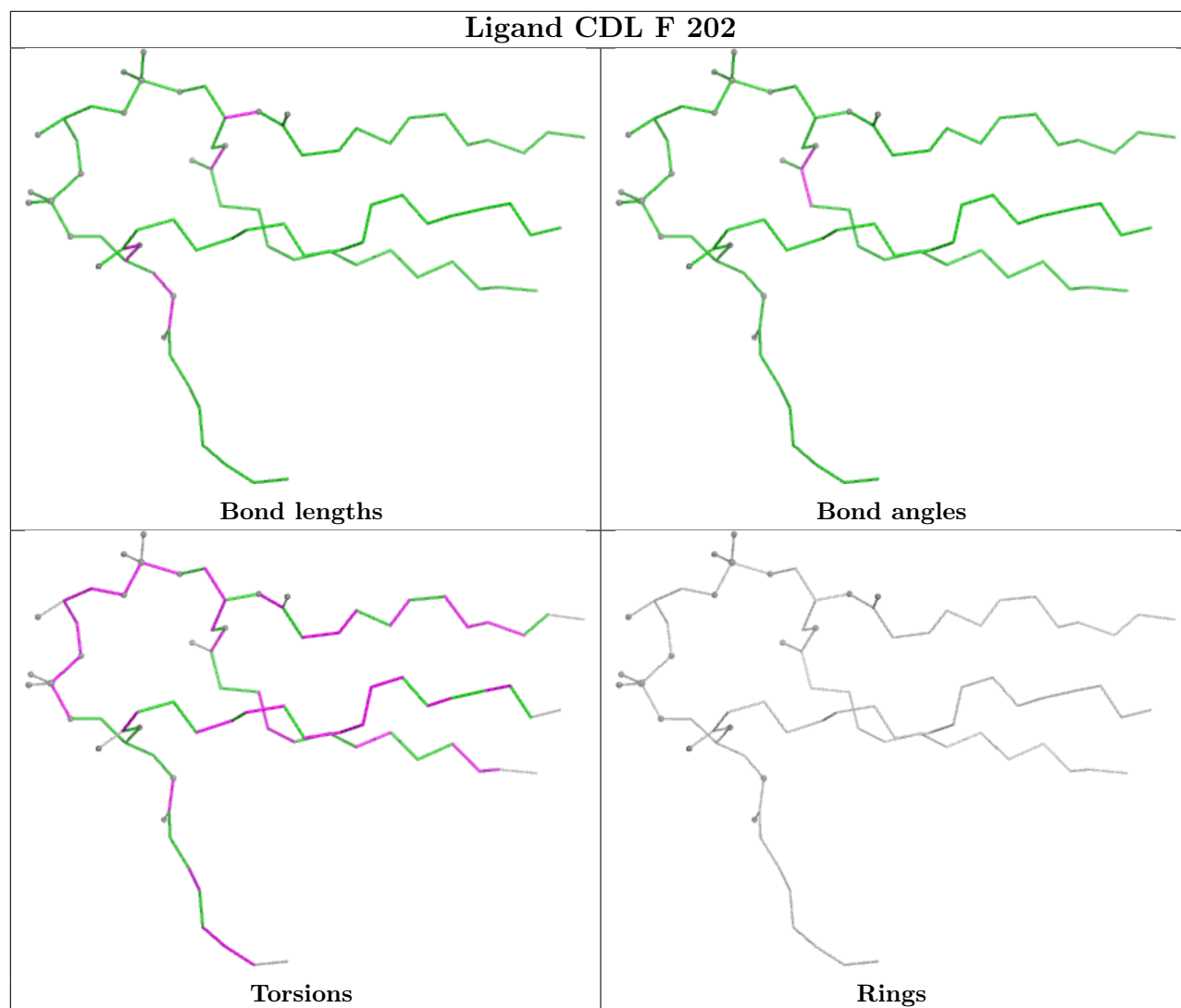
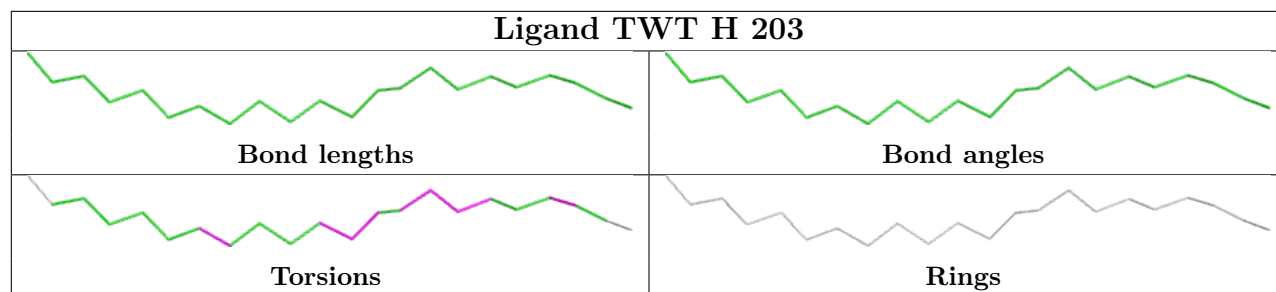


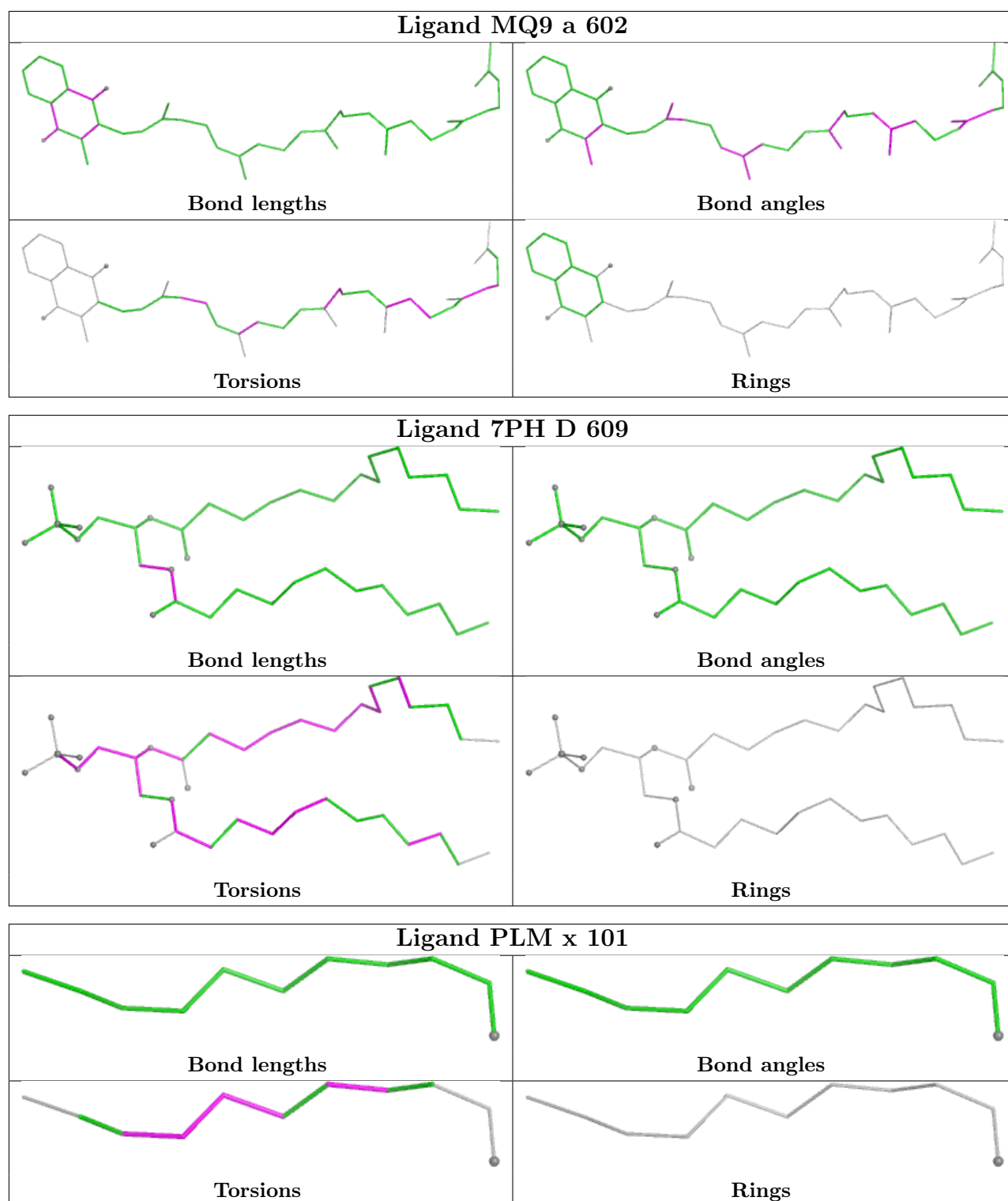


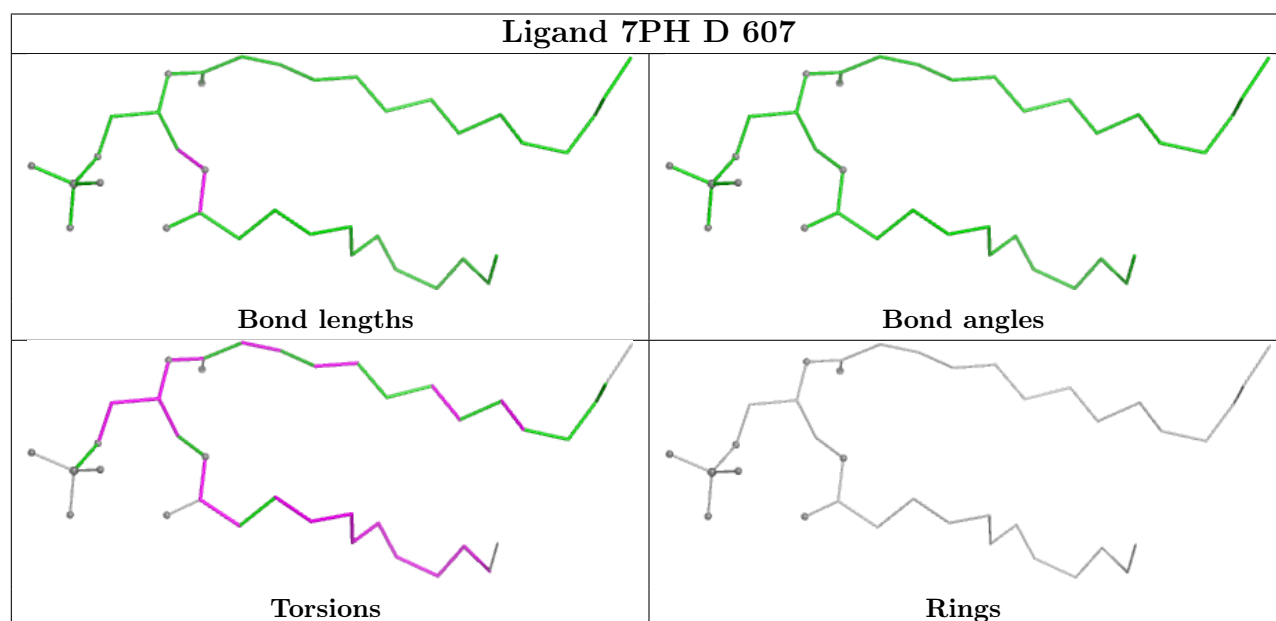
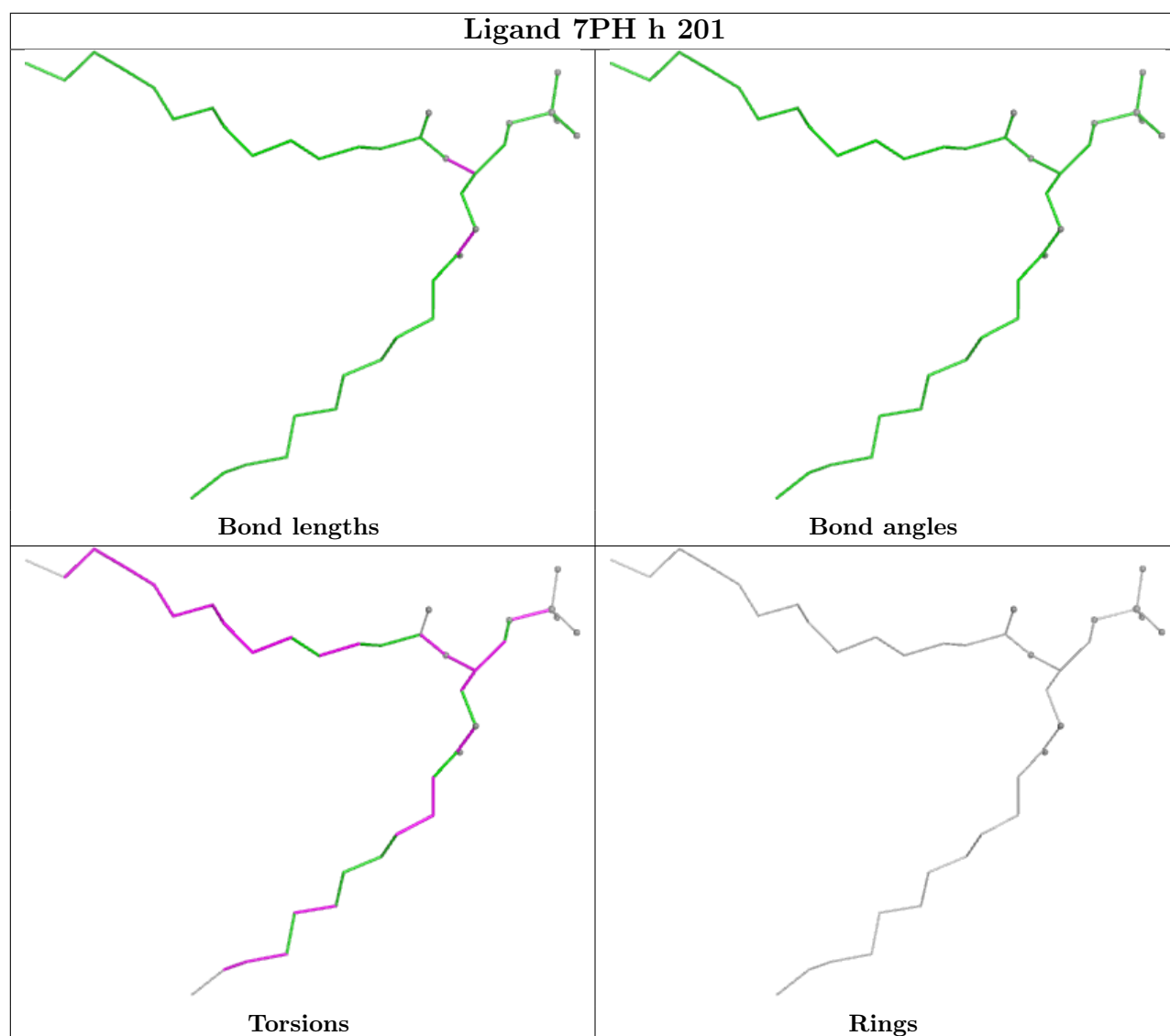


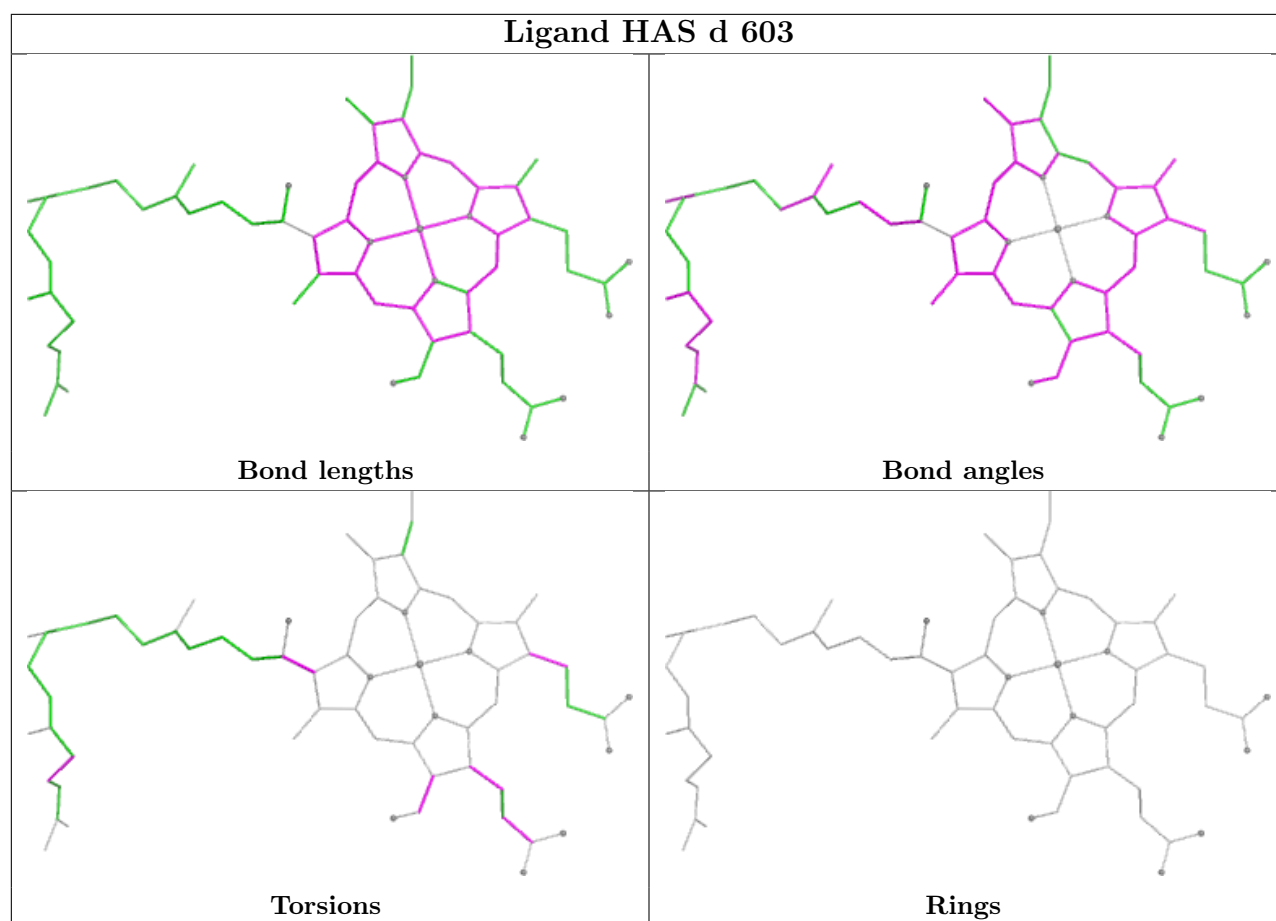


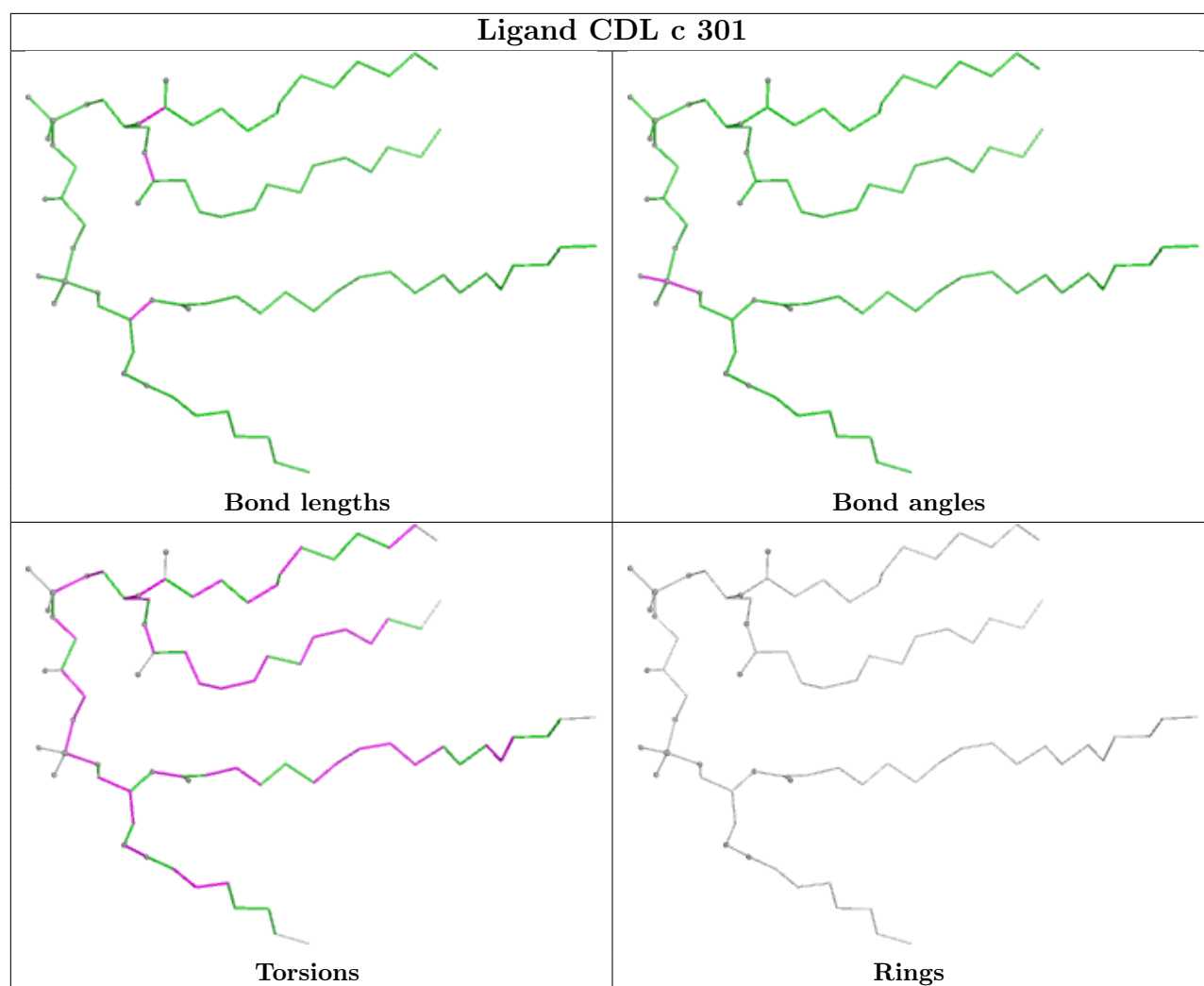


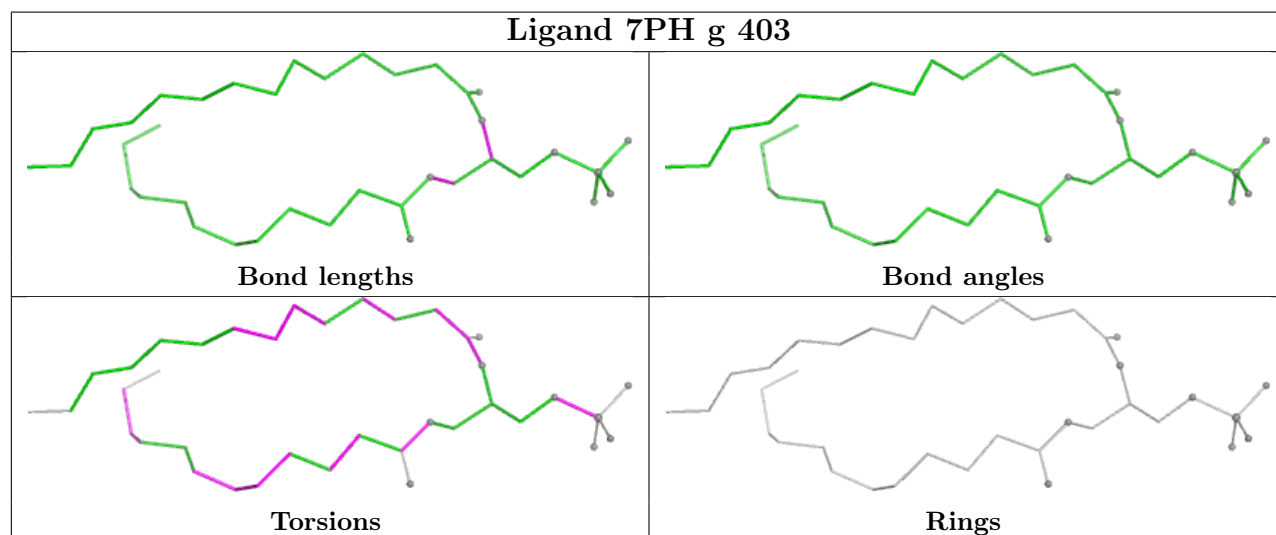
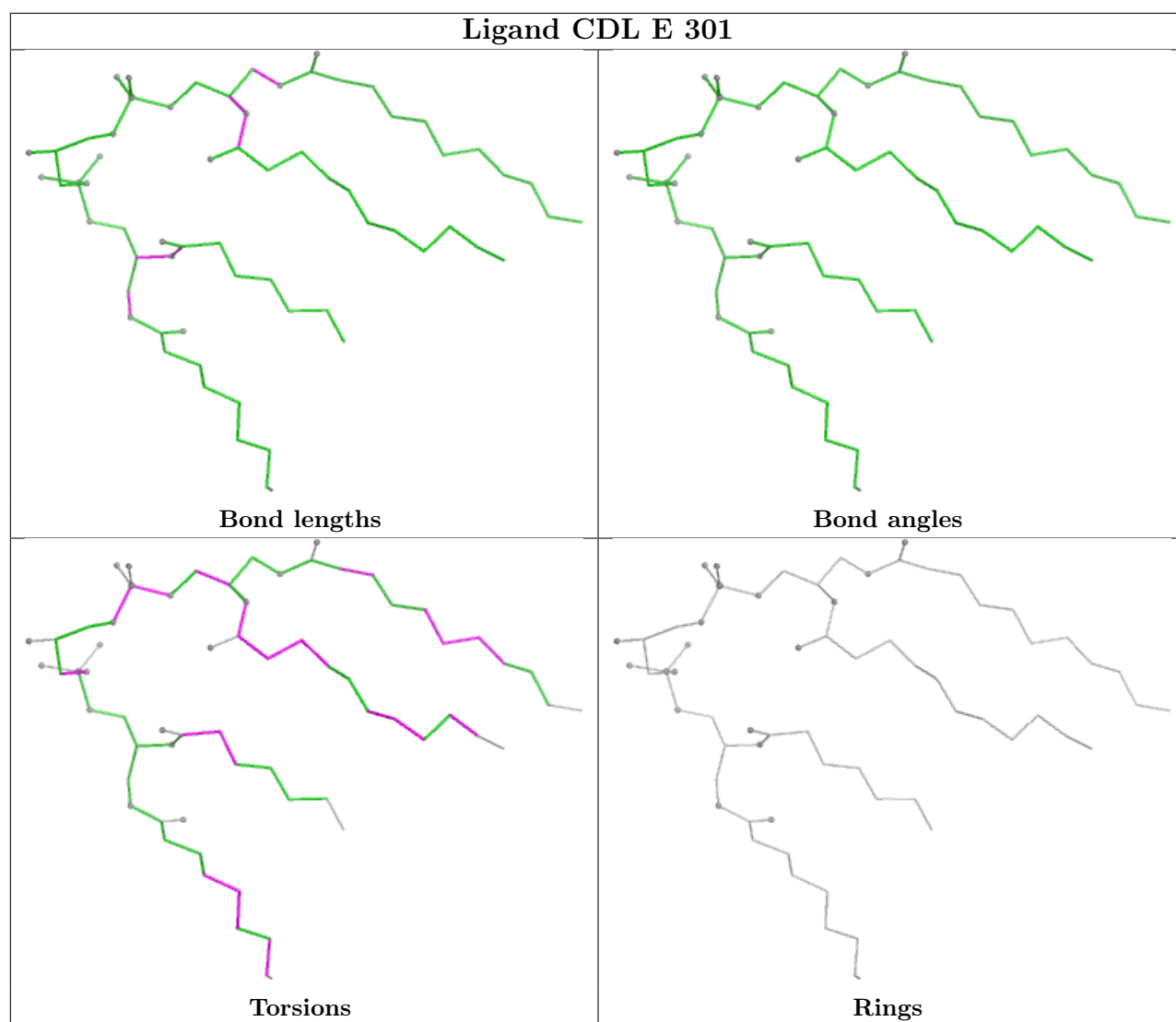


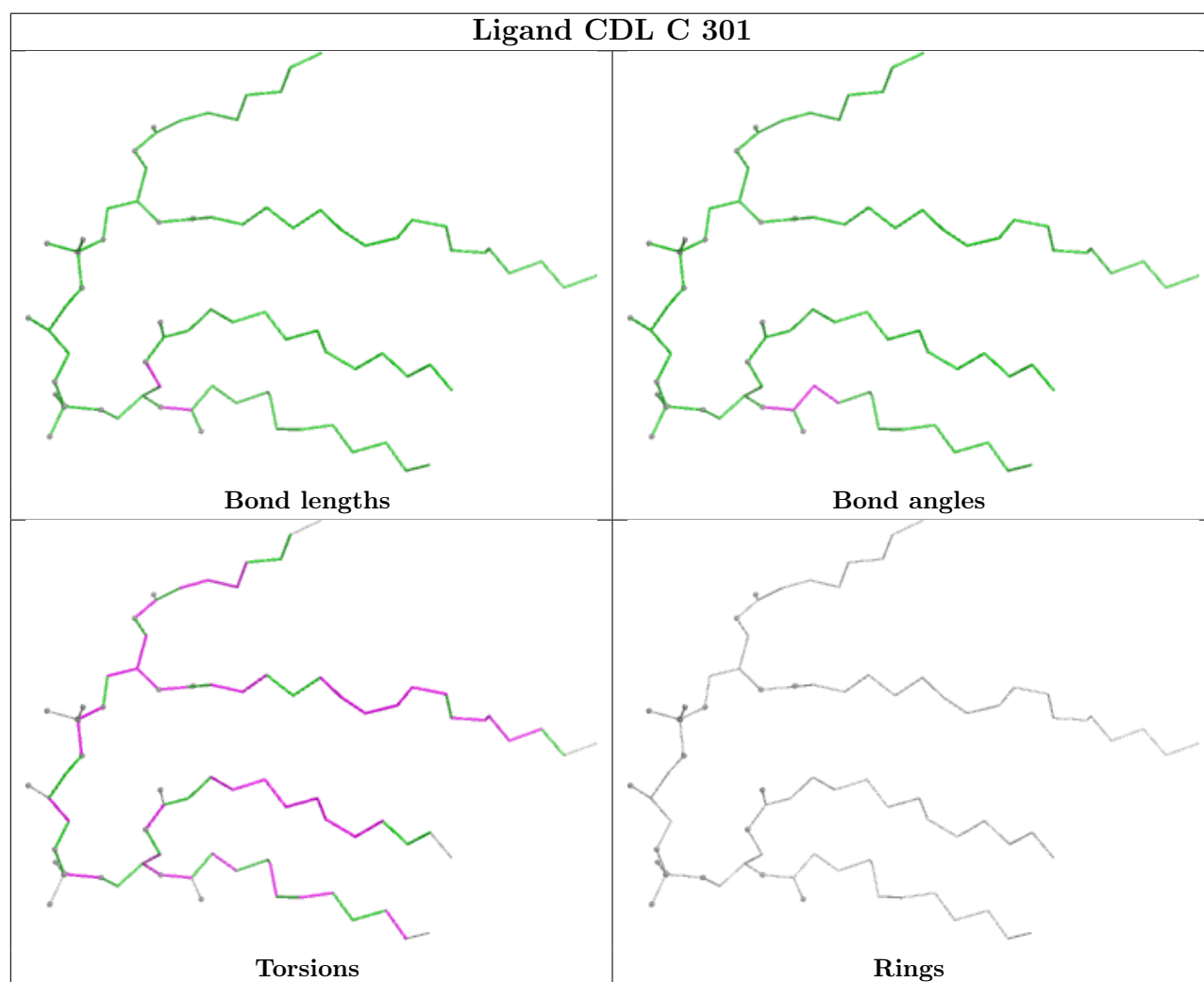
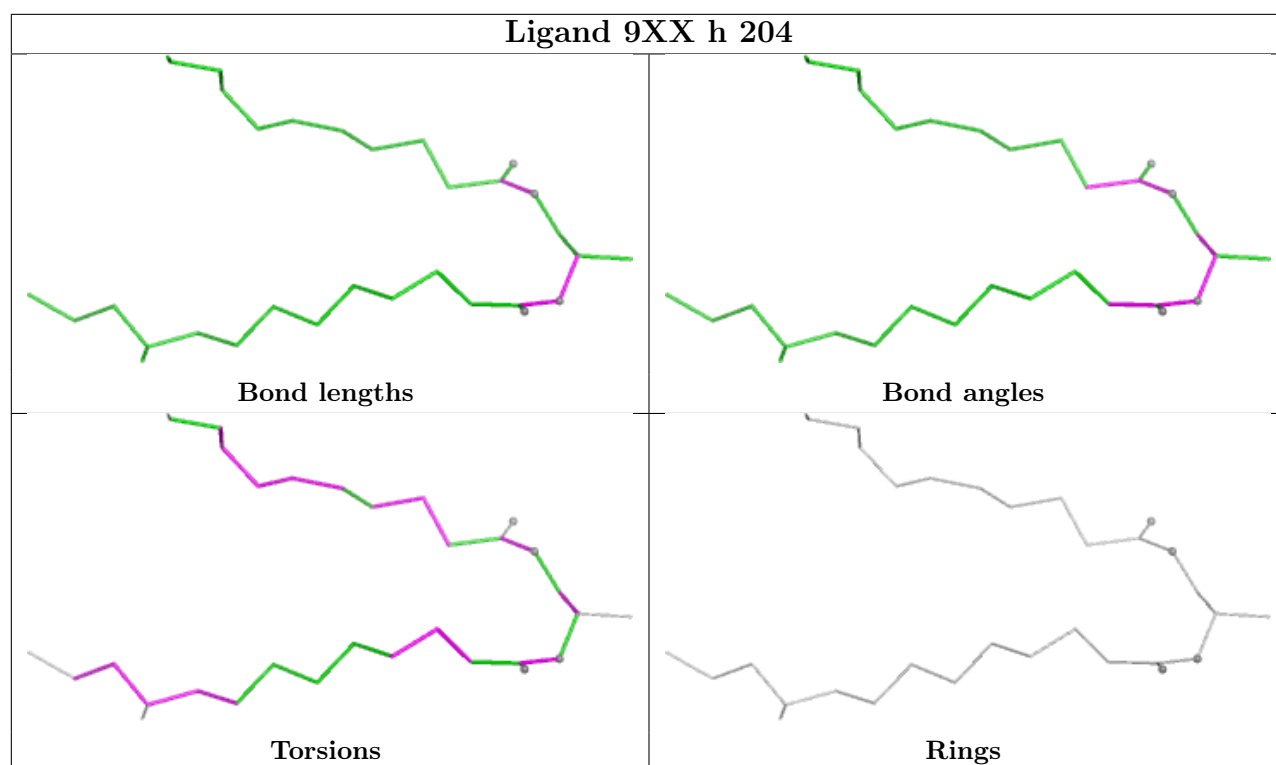












5.7 Other polymers [i](#)

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-13777. These allow visual inspection of the internal detail of the map and identification of artifacts.

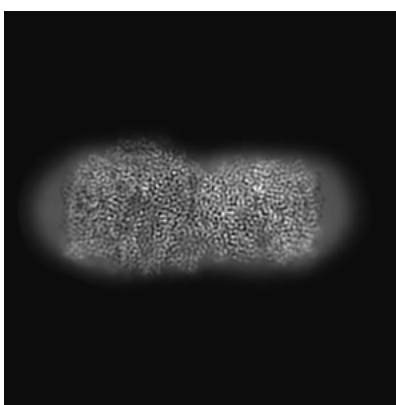
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

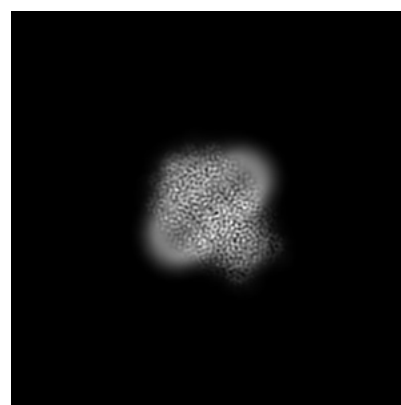
6.1.1 Primary map



X



Y

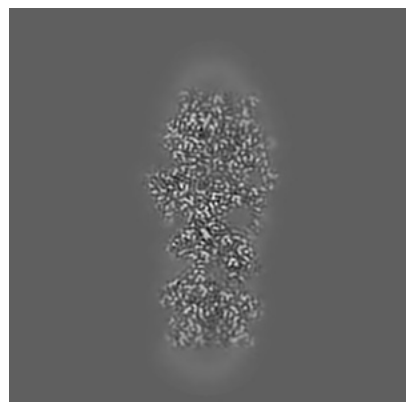


Z

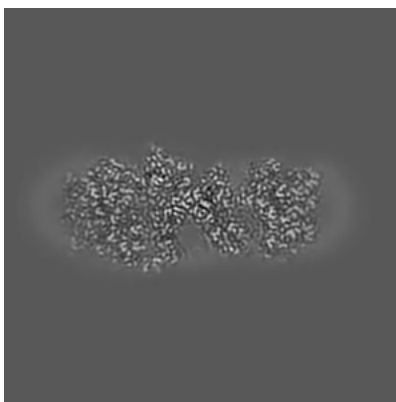
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

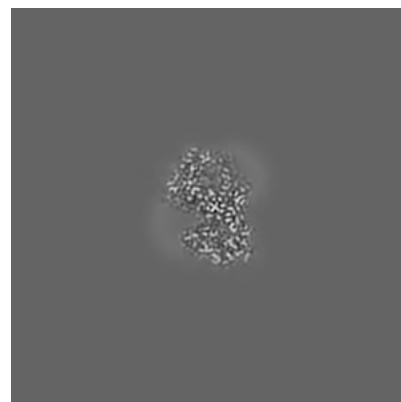
6.2.1 Primary map



X Index: 155



Y Index: 155

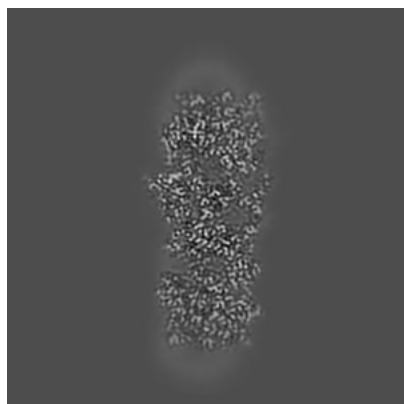


Z Index: 155

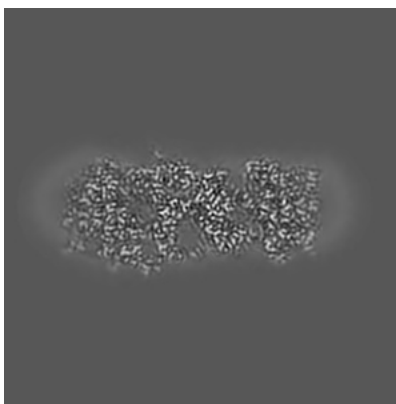
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

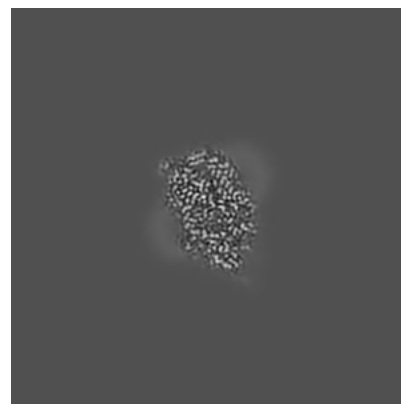
6.3.1 Primary map



X Index: 149



Y Index: 160

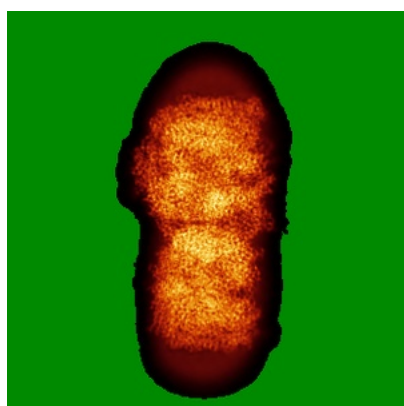


Z Index: 166

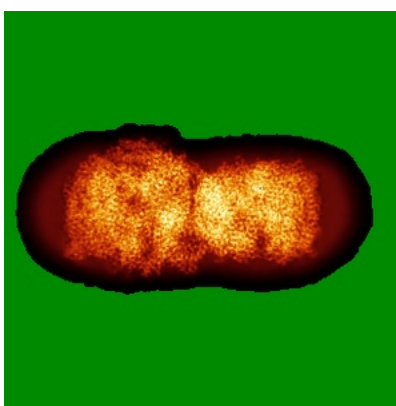
The images above show the largest variance slices of the map in three orthogonal directions.

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

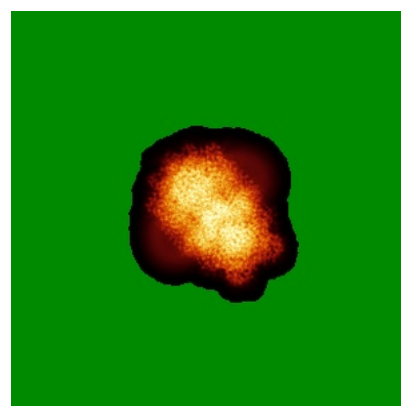
6.4.1 Primary map



X



Y



Z

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 0.541. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

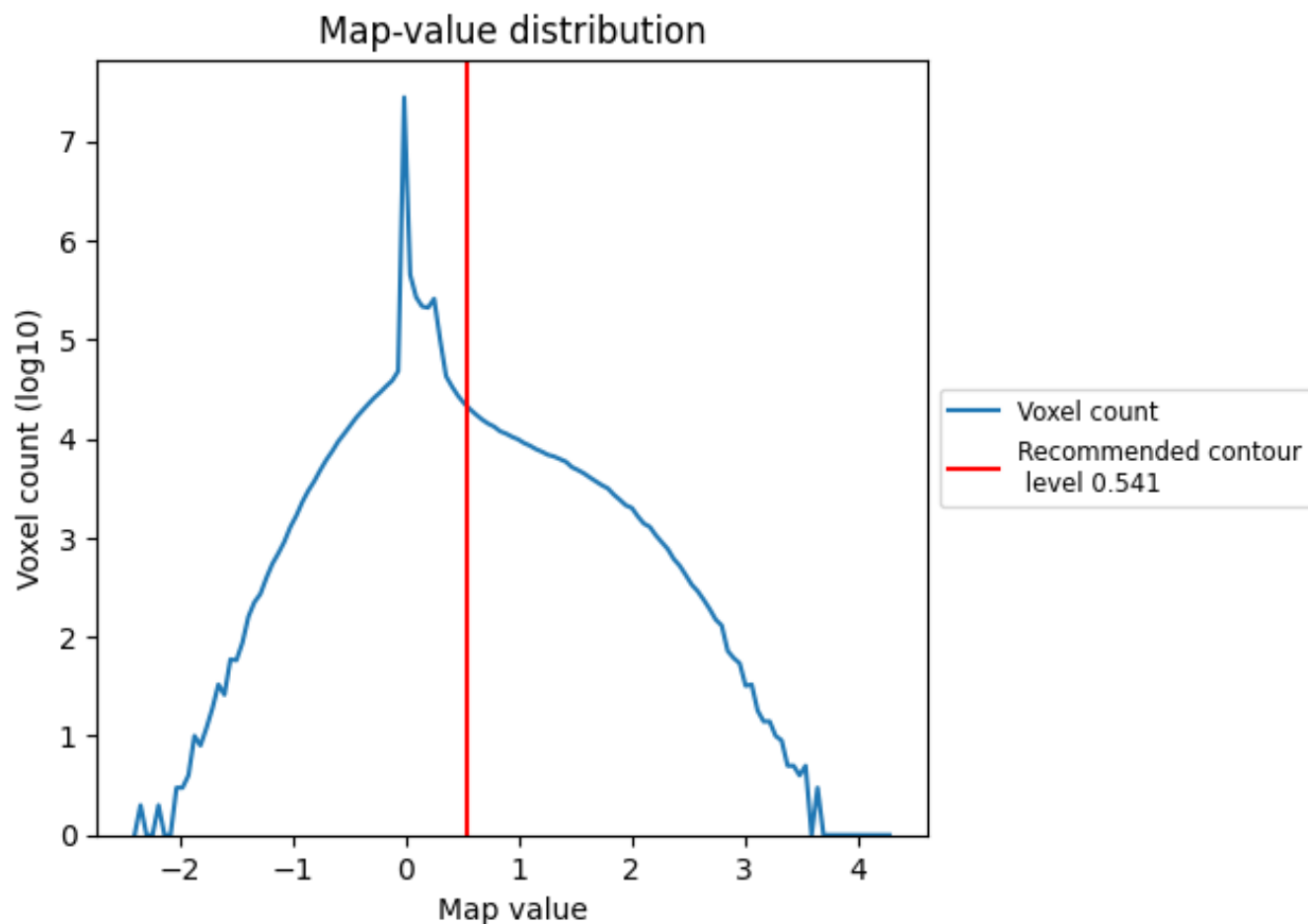
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

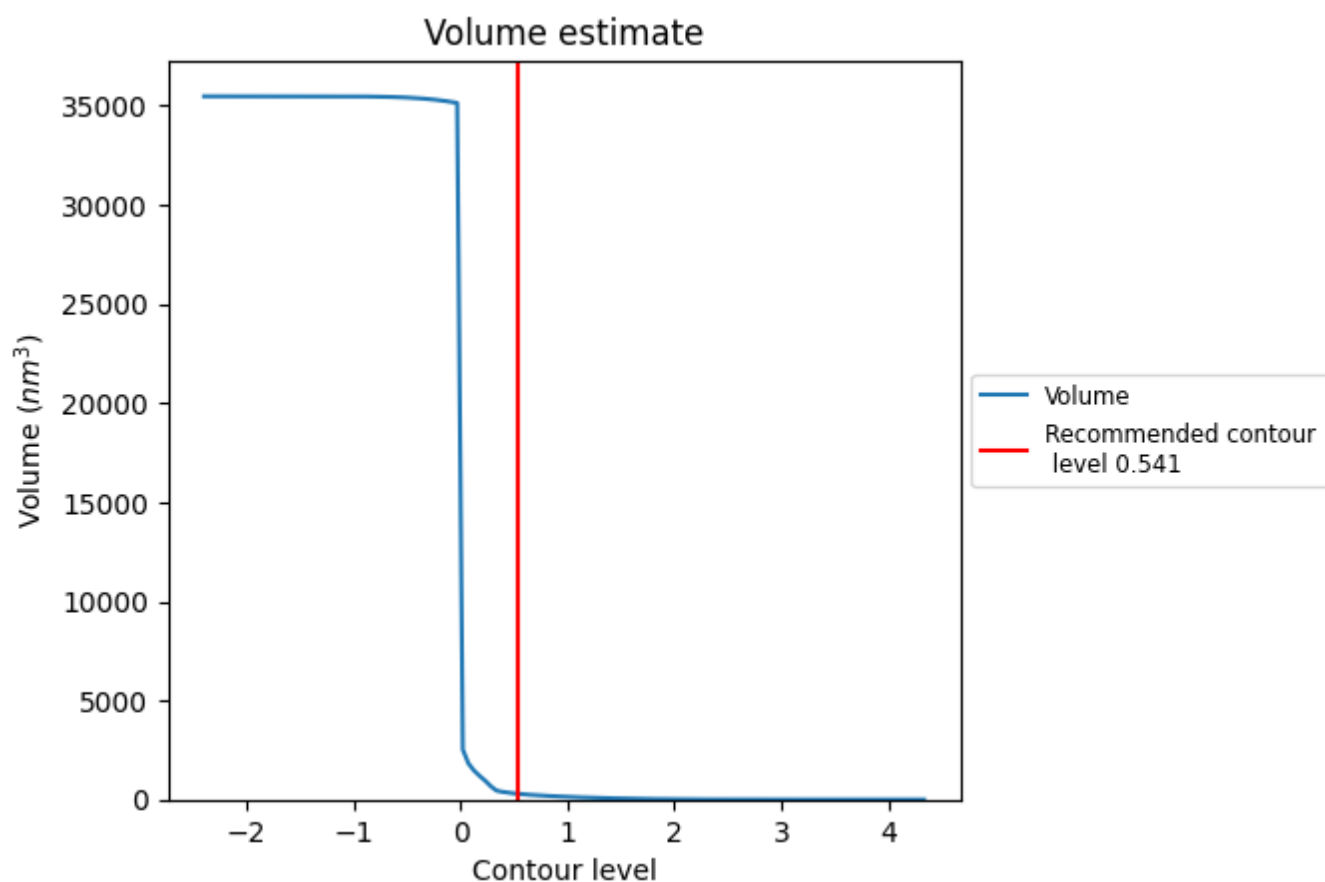
This section contains the results of statistical analysis of the map.

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.

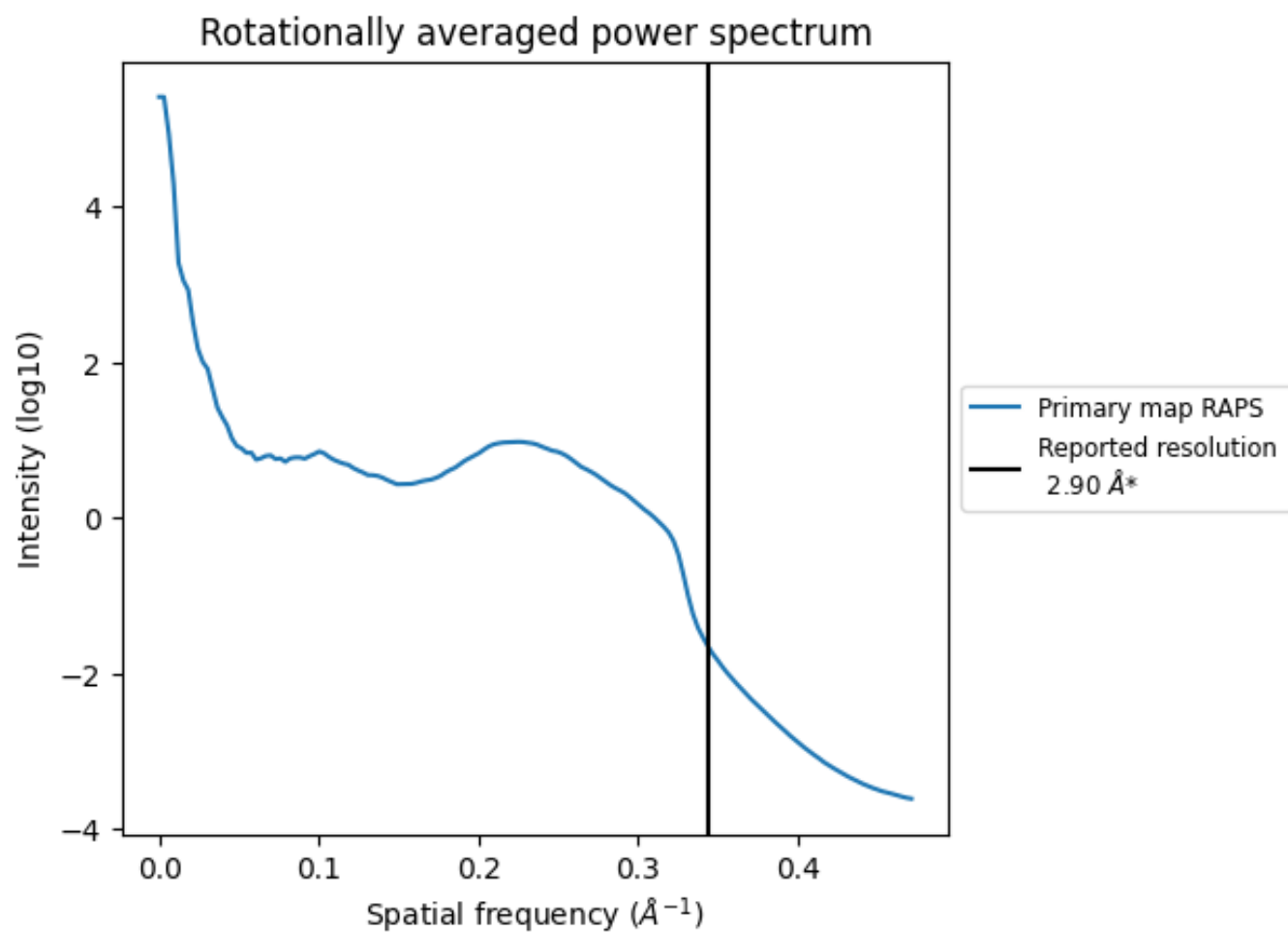
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 261 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 0.345 Å⁻¹

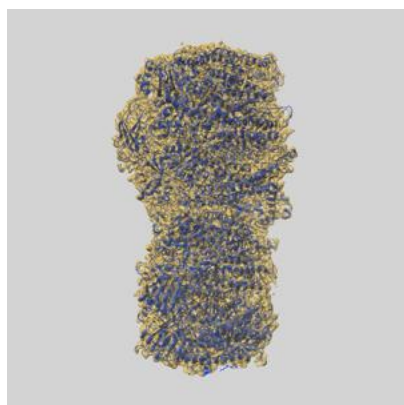
8 Fourier-Shell correlation

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

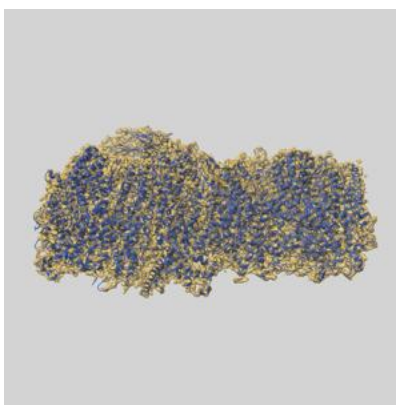
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13777 and PDB model 7Q21. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

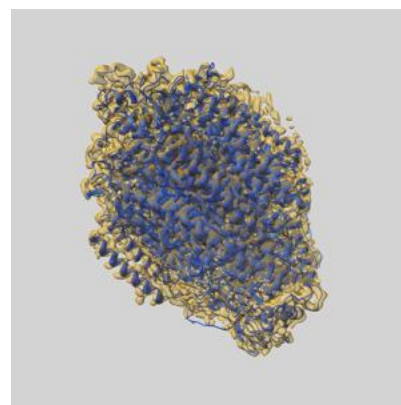
9.1 Map-model overlay [i](#)



X



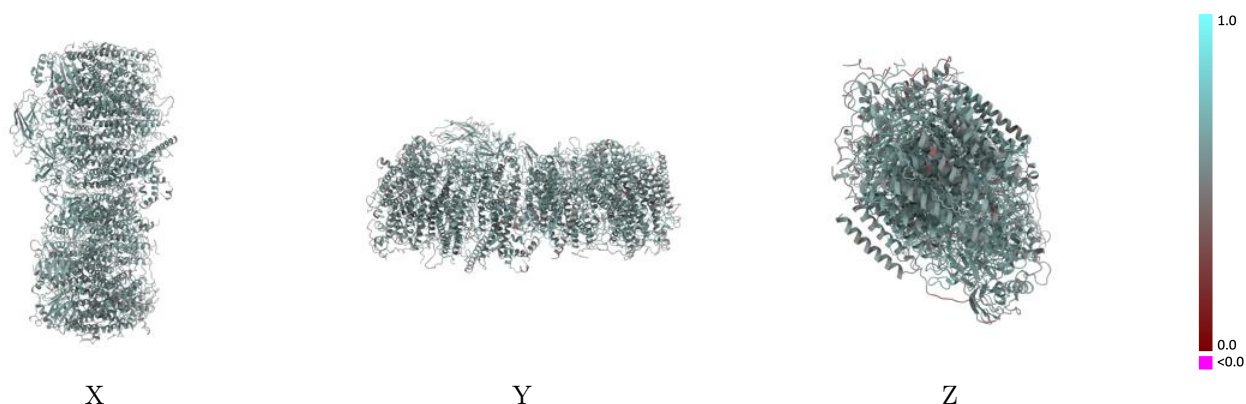
Y



Z

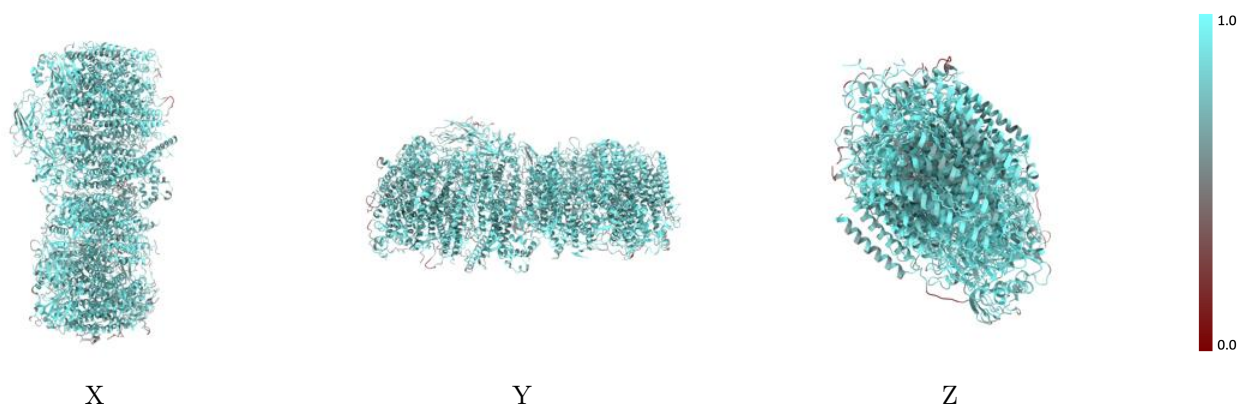
The images above show the 3D surface view of the map at the recommended contour level 0.541 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



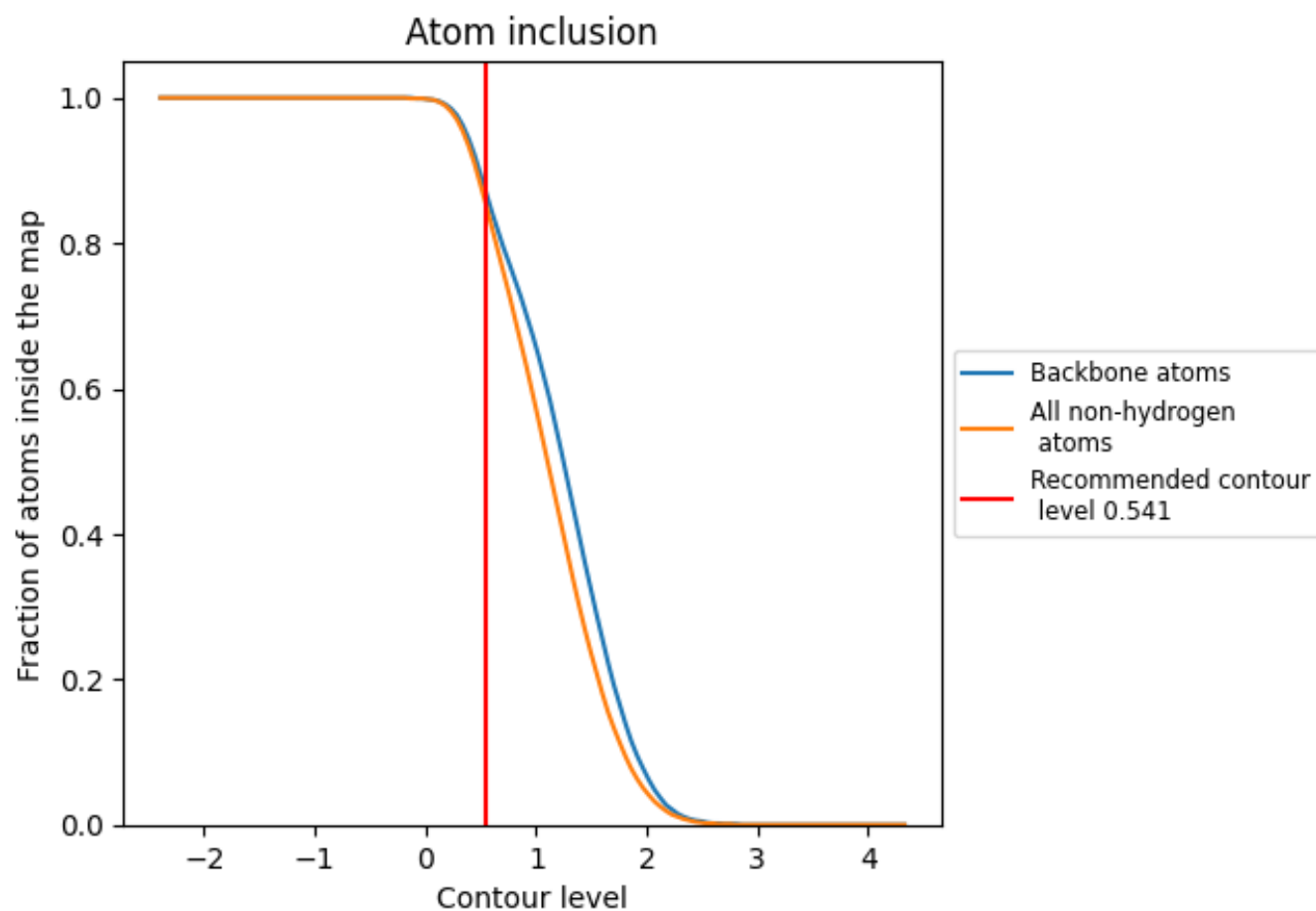
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.541).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.541) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.5710
A	 0.8860	 0.5850
B	 0.8970	 0.5910
C	 0.9010	 0.5860
D	 0.8940	 0.5860
E	 0.8820	 0.5770
F	 0.8460	 0.5750
G	 0.8390	 0.5550
H	 0.8570	 0.5590
K	 0.7210	 0.5210
L	 0.8040	 0.5490
V	 0.7660	 0.5320
X	 0.5210	 0.4590
Y	 0.8440	 0.5190
a	 0.8600	 0.5800
b	 0.8910	 0.5860
c	 0.8740	 0.5730
d	 0.8610	 0.5740
e	 0.8610	 0.5720
f	 0.8100	 0.5670
g	 0.8000	 0.5480
h	 0.8160	 0.5510
k	 0.6880	 0.5210
l	 0.7530	 0.5290
v	 0.7440	 0.5280
x	 0.4590	 0.4420
y	 0.8220	 0.5120

