



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:54 PM UTC

PDB ID : 7QHM / pdb_00007qhm
EMDB ID : EMD-13976
Title : Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from
Corynebacterium glutamicum (stigmatellin and azide bound)
Authors : Kao, W.-C.; Hunte, C.
Deposited on : 2021-12-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

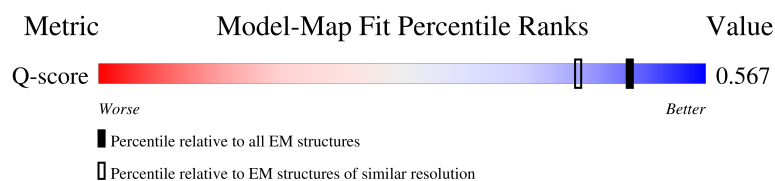
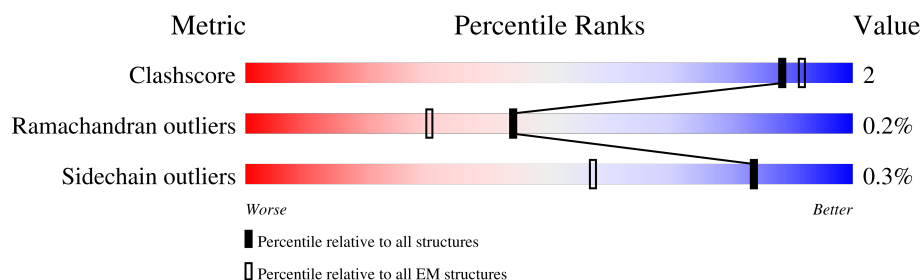
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



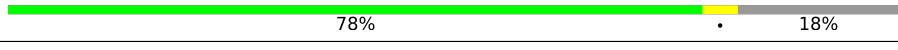
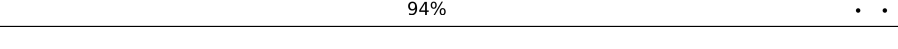
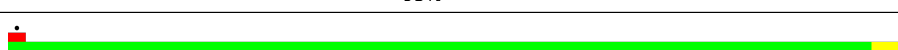
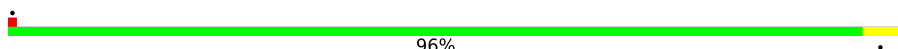
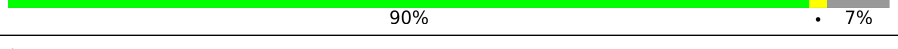
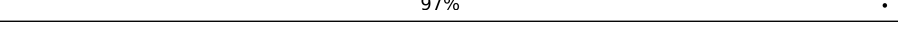
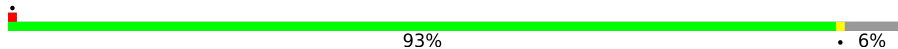
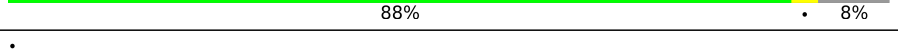
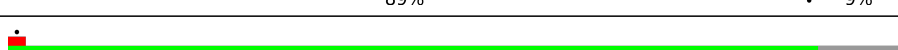
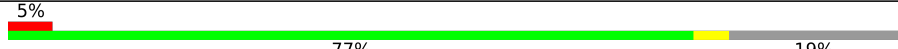
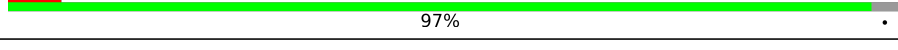
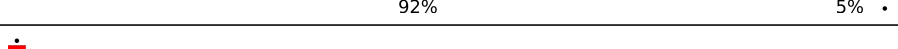
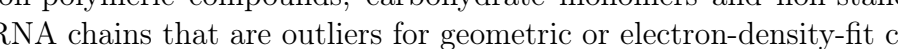
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	408	94% 5% .
1	N	408	93% 5% .
2	B	539	92% 6% .
2	O	539	94% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	283	
3	P	283	
4	D	594	
4	Q	594	
5	E	331	
5	R	331	
6	F	205	
6	S	205	
7	G	143	
7	T	143	
8	H	163	
8	U	163	
9	I	147	
9	V	147	
10	J	112	
10	W	112	
11	K	73	
11	X	73	
12	L	65	
12	Y	65	
13	M	168	
13	Z	168	

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
25	HAS	D	601	X	-	-	-
25	HAS	D	602	X	-	-	-
25	HAS	Q	601	X	-	-	-
25	HAS	Q	602	X	-	-	-
29	AZI	D	606	-	X	X	-
29	AZI	Q	605	-	X	-	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 97775 atoms, of which 48245 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 Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	402	Total	C	H	N	O	S	2	0
			6231	2004	3084	540	587	16		
1	N	401	Total	C	H	N	O	S	4	0
			6224	2004	3079	539	586	16		

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	534	Total	C	H	N	O	S	6	0
			8485	2765	4268	709	721	22		
2	O	534	Total	C	H	N	O	S	0	0
			8425	2746	4239	703	715	22		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	2	0
			3443	1089	1694	306	344	10		
3	P	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	576	Total	C	H	N	O	S	0	0
			9018	3031	4470	735	750	32		
4	Q	576	Total	C	H	N	O	S	2	0
			9034	3036	4477	736	753	32		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		
5	R	331	Total	C	H	N	O	S	2	0
			5089	1666	2482	431	499	11		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		
6	S	190	Total	C	H	N	O	S	0	0
			2980	992	1494	236	251	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	143	Total	C	H	N	O	S	2	0
			2219	734	1114	170	192	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	153	Total	C	H	N	O	S	0	0
			2174	684	1054	184	249	3		
8	U	154	Total	C	H	N	O	S	0	0
			2181	686	1057	185	250	3		

- Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	135	Total	C	H	N	O	S	0	0
			2144	691	1071	190	191	1		
9	V	135	Total	C	H	N	O	S	0	0
			2144	691	1071	190	191	1		

- Molecule 10 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	102	Total	C	H	N	O	S	0	0
			1571	506	792	134	136	3		
10	W	102	Total	C	H	N	O	S	0	0
			1571	506	792	134	136	3		

- Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	59	Total	C	H	N	O		0	0
			901	297	432	81	91			
11	X	57	Total	C	H	N	O		0	0
			864	286	413	78	87			

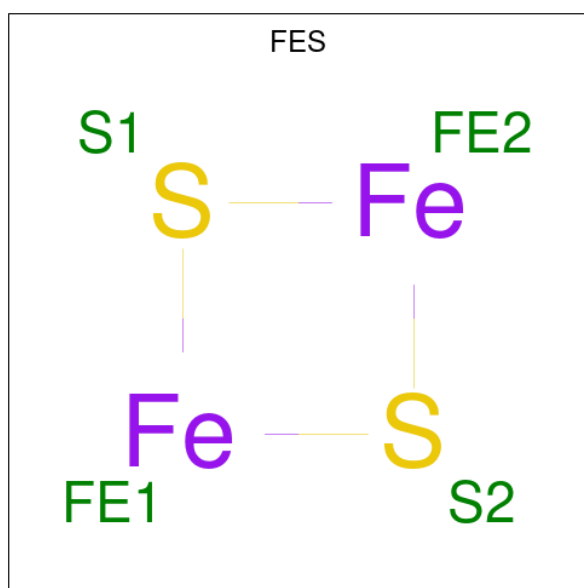
- Molecule 12 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		
12	Y	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		

- Molecule 13 is a protein called Thiamine biosynthesis protein X.

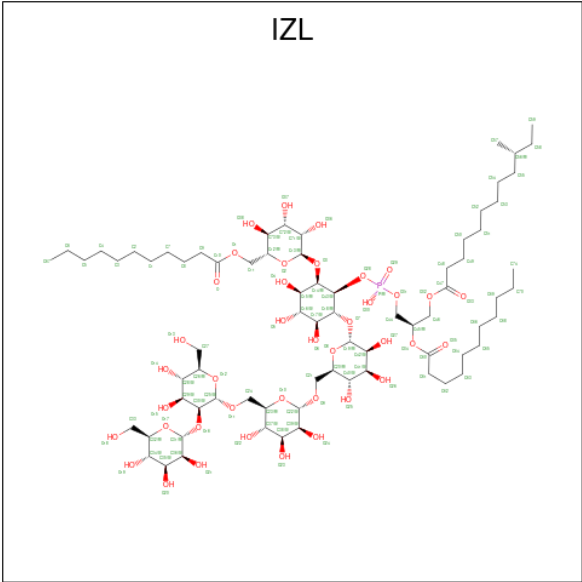
Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	22	Total	C	H	N	O	S	0	0
			330	101	159	32	37	1		
13	Z	24	Total	C	H	N	O	S	0	0
			358	110	172	35	40	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



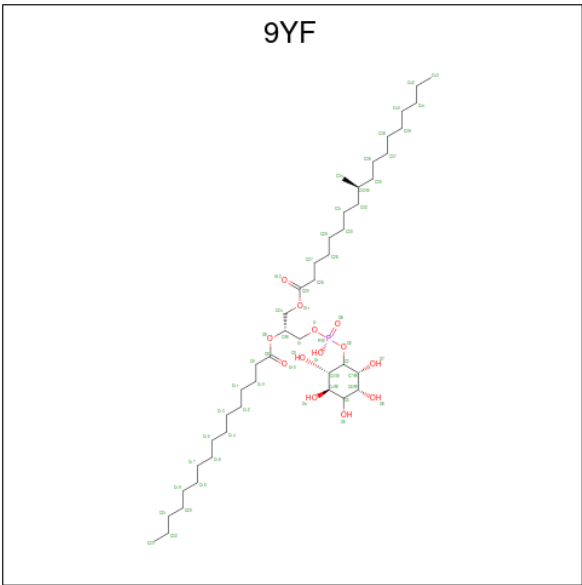
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	Fe	S	0
			4	2	2	
14	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: $\text{C}_{74}\text{H}_{133}\text{O}_{39}\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	H	O	P	0
			212	63	109	39	1	
15	N	1	Total	C	H	O	P	0
			212	63	109	39	1	

- Molecule 16 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: C₄₄H₈₅O₁₃P) (labeled as "Ligand of Interest" by depositor).



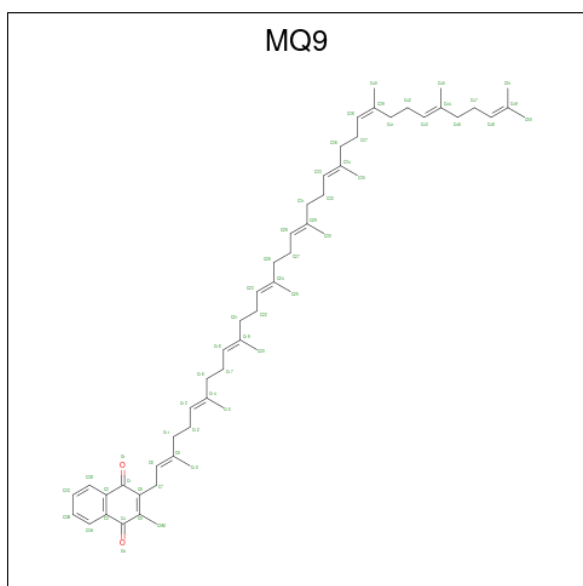
Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	H	O	P	0
			66	22	30	13	1	

Continued on next page...

Continued from previous page...

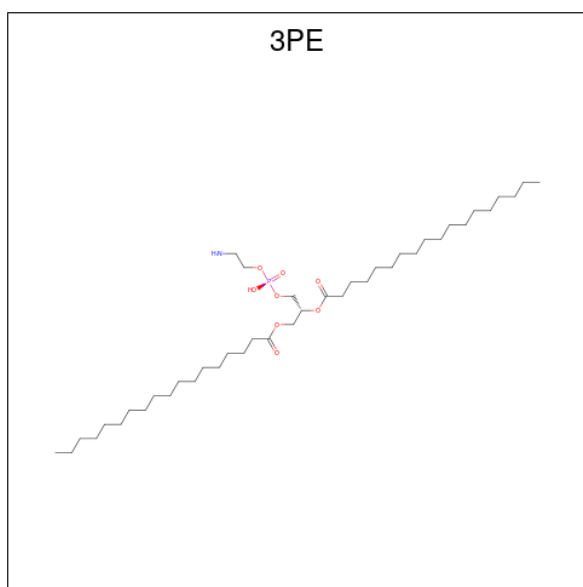
Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	H	O	P	0
			60	20	26	13	1	
16	N	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	U	1	Total	C	H	O	P	0
			75	25	36	13	1	

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	H	O	0
			138	56	80	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	N	1	Total	C	H	O	0
			78	34	42	2	
17	O	1	Total	C	H	O	0
			56	25	29	2	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



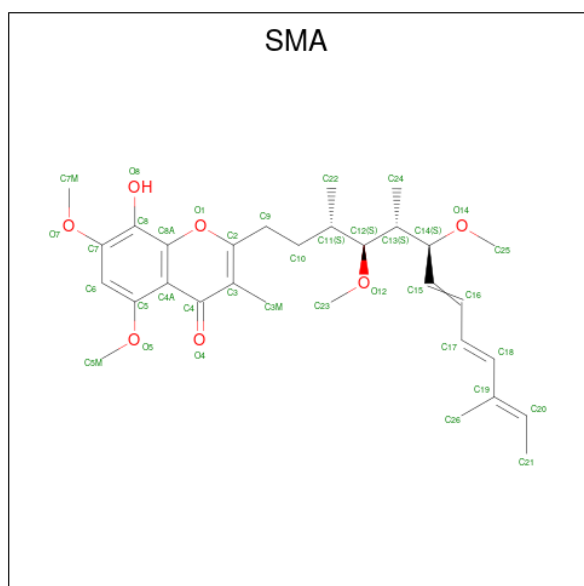
Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	H	N	O	P	0
			76	30	36	1	8	1	
18	C	1	Total	C	H	N	O	P	0
			45	15	20	1	8	1	
18	C	1	Total	C	H	N	O	P	0
			45	15	20	1	8	1	
18	D	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	F	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	
18	L	1	Total	C	H	N	O	P	0
			68	20	38	1	8	1	
18	N	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	P	1	Total	C	H	N	O	P	0
			45	17	18	1	8	1	
18	Q	1	Total	C	H	N	O	P	0
			71	29	32	1	8	1	
18	R	1	Total	C	H	N	O	P	0
			47	21	16	1	8	1	
18	S	1	Total	C	H	N	O	P	0
			95	33	52	1	8	1	
18	T	1	Total	C	H	N	O	P	0
			50	16	24	1	8	1	
18	T	1	Total	C	H	N	O	P	0
			86	32	44	1	8	1	

Continued on next page...

Continued from previous page...

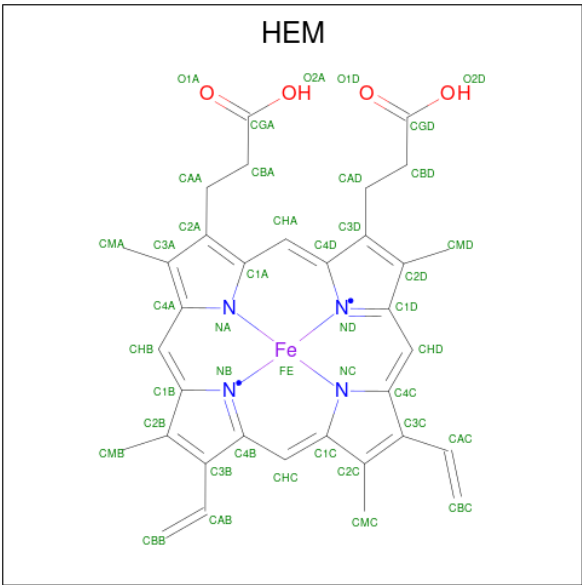
Mol	Chain	Residues	Atoms					AltConf	
18	T	1	Total	C	H	N	O	P	0
			74	28	36	1	8	1	
18	T	1	Total	C	H	N	O	P	0
			84	30	44	1	8	1	
18	W	1	Total	C	H	N	O	P	0
			115	37	68	1	8	1	

- Molecule 19 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$) (labeled as "Ligand of Interest" by depositor).



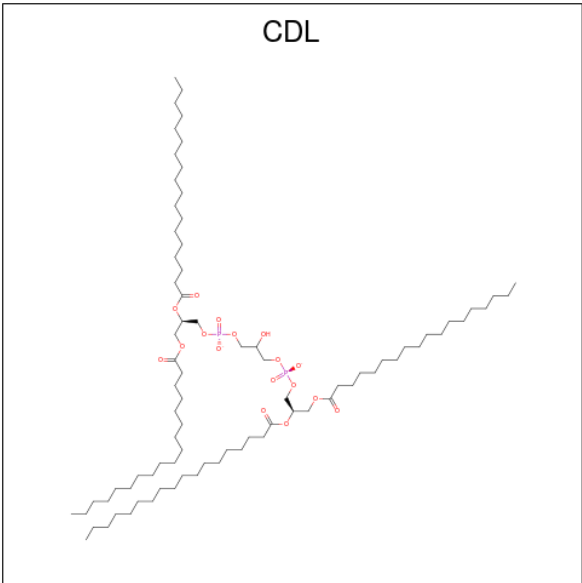
Mol	Chain	Residues	Atoms				AltConf
19	B	1	Total	C	H	O	0
			79	30	42	7	
19	O	1	Total	C	H	O	0
			79	30	42	7	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



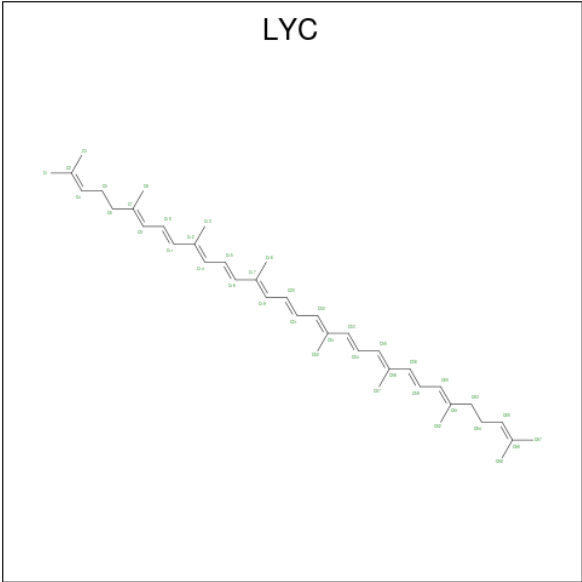
Mol	Chain	Residues	Atoms						AltConf
20	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



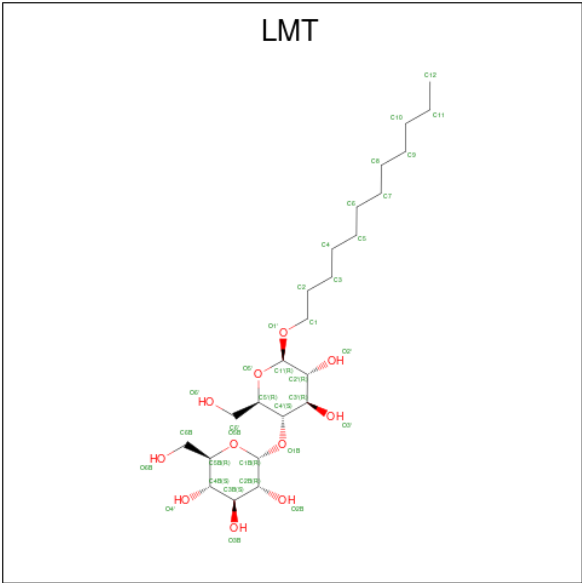
Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	H	O	P	0
			95	37	39	17	2	
21	B	1	Total	C	H	O	P	0
			72	26	27	17	2	
21	B	1	Total	C	H	O	P	0
			126	51	56	17	2	
21	D	1	Total	C	H	O	P	0
			161	58	84	17	2	
21	D	1	Total	C	H	O	P	0
			128	44	65	17	2	
21	F	1	Total	C	H	O	P	0
			94	38	37	17	2	
21	G	1	Total	C	H	O	P	0
			154	56	79	17	2	
21	G	1	Total	C	H	O	P	0
			125	50	56	17	2	
21	I	1	Total	C	H	O	P	0
			107	38	50	17	2	
21	O	1	Total	C	H	O	P	0
			145	47	79	17	2	
21	Q	1	Total	C	H	O	P	0
			183	64	100	17	2	
21	Q	1	Total	C	H	O	P	0
			145	47	79	17	2	
21	S	1	Total	C	H	O	P	0
			135	46	70	17	2	
21	T	1	Total	C	H	O	P	0
			175	61	95	17	2	
21	T	1	Total	C	H	O	P	0
			111	46	46	17	2	
21	V	1	Total	C	H	O	P	0
			159	50	90	17	2	

- Molecule 22 is LYCOPENE (CCD ID: LYC) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



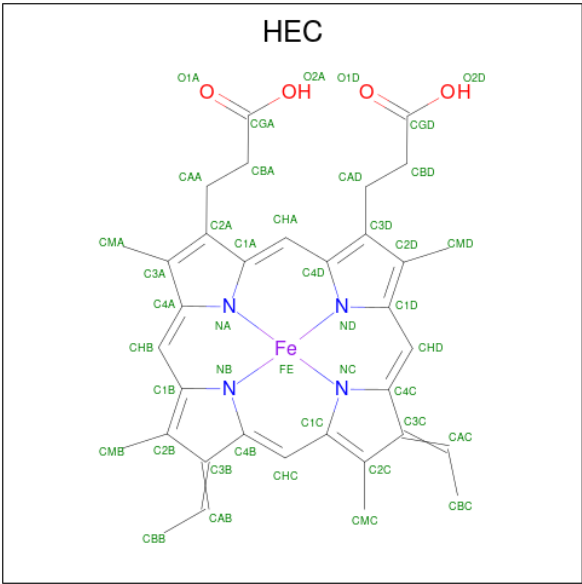
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	H	0
			96	40	56	
22	O	1	Total	C	H	0
			96	40	56	

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



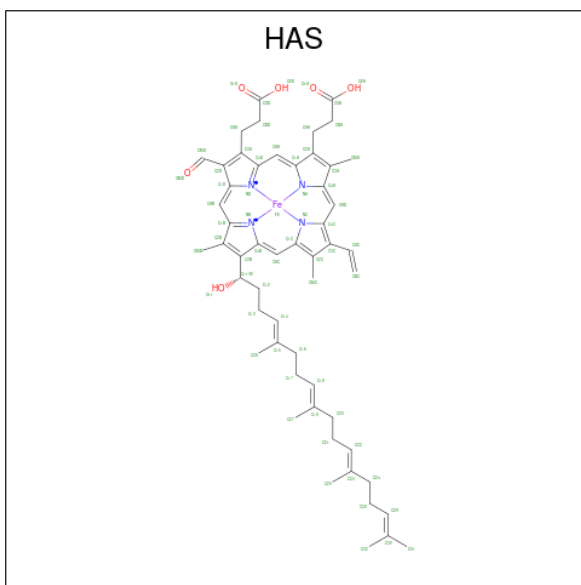
Mol	Chain	Residues	Atoms				AltConf
23	B	1	Total	C	H	O	0
			71	21	39	11	
23	O	1	Total	C	H	O	0
			71	21	39	11	

- Molecule 24 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
24	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
24	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
24	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
24	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 25 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Cu	0
			1	1	
26	Q	1	Total	Cu	0
			1	1	

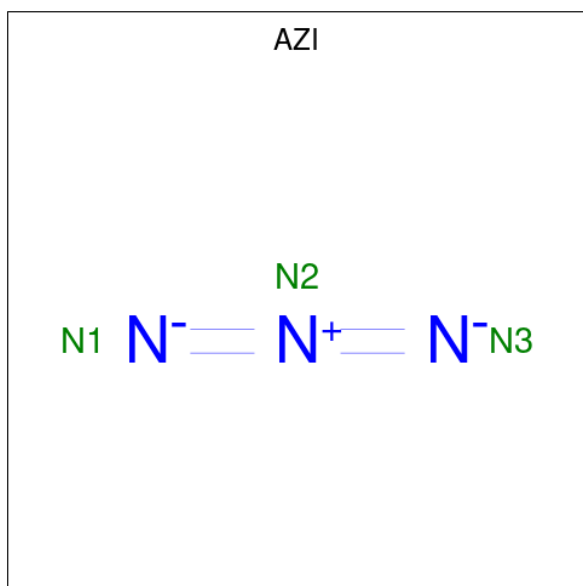
- Molecule 27 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Mn	0
			1	1	
27	R	1	Total	Mn	0
			1	1	

- Molecule 28 is CALCIUM ION (CCD ID: CA) (formula: Ca).

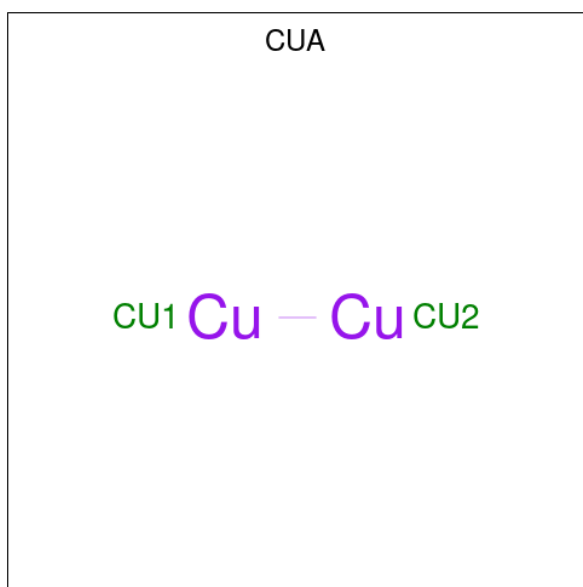
Mol	Chain	Residues	Atoms		AltConf
28	D	1	Total 1	Ca 1	0
28	Q	1	Total 1	Ca 1	0

- Molecule 29 is AZIDE ION (CCD ID: AZI) (formula: N₃) (labeled as "Ligand of Interest" by depositor).



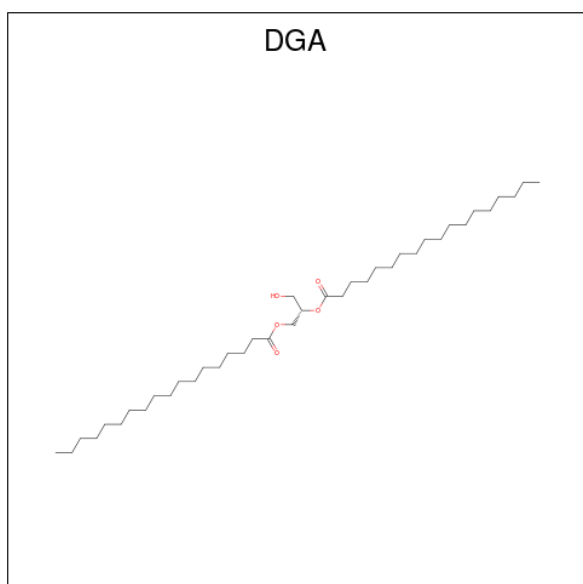
Mol	Chain	Residues	Atoms		AltConf
29	D	1	Total 3	N 3	0
29	Q	1	Total 3	N 3	0

- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



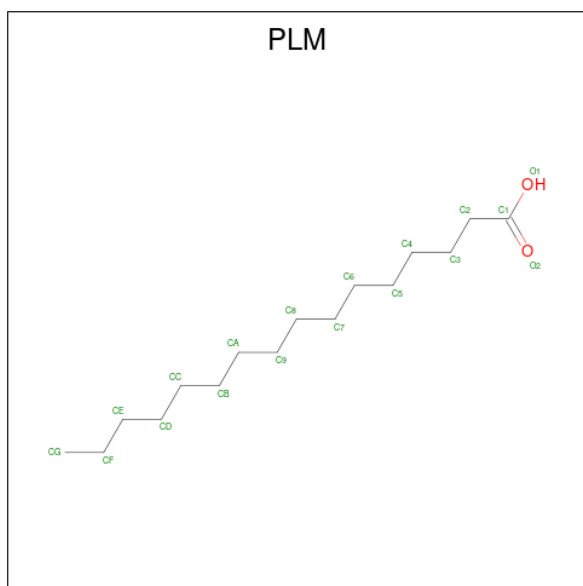
Mol	Chain	Residues	Atoms		AltConf
30	E	1	Total	Cu	0
			1	1	
30	E	1	Total	Cu	0
			1	1	
30	R	1	Total	Cu	0
			1	1	
30	R	1	Total	Cu	0
			1	1	

- Molecule 31 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total	C	O	0
			20	16	4	
31	H	1	Total	C	O	0
			17	13	4	
31	M	1	Total	C	O	0
			22	18	4	
31	R	1	Total	C	O	0
			25	21	4	
31	U	1	Total	C	O	0
			27	23	4	
31	Z	1	Total	C	O	0
			29	25	4	

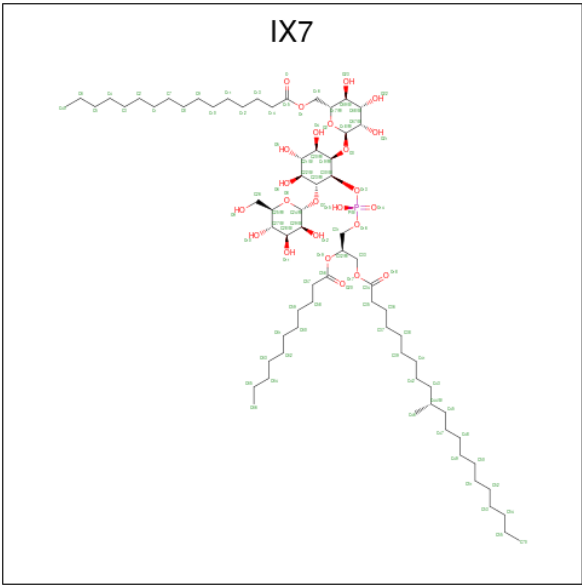
- Molecule 32 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	H	1	Total	C	H	O	0
			41	16	24	1	
32	M	1	Total	C	H	O	0
			9	4	4	1	
32	U	1	Total	C	H	O	0
			45	16	28	1	
32	Z	1	Total	C	H	O	0
			9	4	4	1	

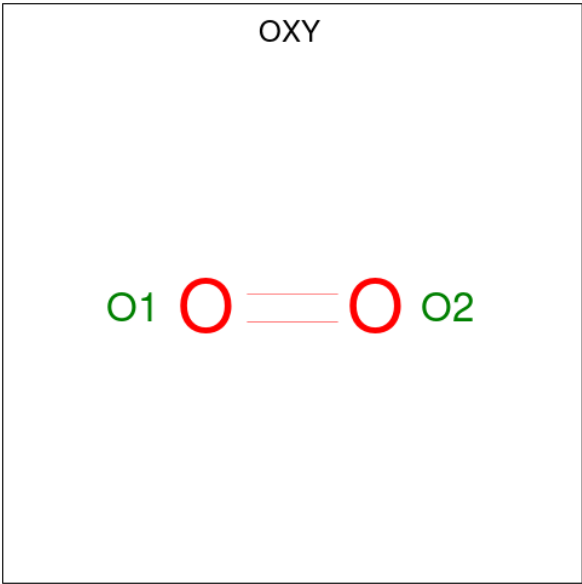
- Molecule 33 is [(2 {R})-3-[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {

S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicosanoate (CCD ID: IX7) (formula: C₇₀H₁₃₁O₂₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	H	1	Total	C	H	O	P	0
			155	47	83	24	1	
33	U	1	Total	C	H	O	P	0
			155	47	83	24	1	

- Molecule 34 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	Q	1	Total O 2 2	0

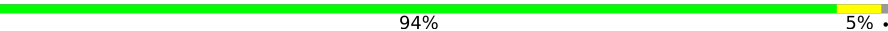
- Molecule 35 is water.

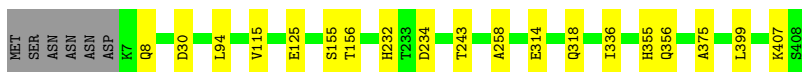
Mol	Chain	Residues	Atoms	AltConf
35	A	31	Total O 31 31	0
35	B	56	Total O 56 56	0
35	C	26	Total O 26 26	0
35	D	21	Total O 21 21	0
35	E	13	Total O 13 13	0
35	F	3	Total O 3 3	0
35	G	6	Total O 6 6	0
35	K	3	Total O 3 3	0
35	N	31	Total O 31 31	0
35	O	46	Total O 46 46	0
35	P	49	Total O 49 49	0
35	Q	53	Total O 53 53	0
35	R	44	Total O 44 44	0
35	S	5	Total O 5 5	0
35	T	13	Total O 13 13	0
35	U	12	Total O 12 12	0
35	V	2	Total O 2 2	0
35	X	2	Total O 2 2	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: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A: 



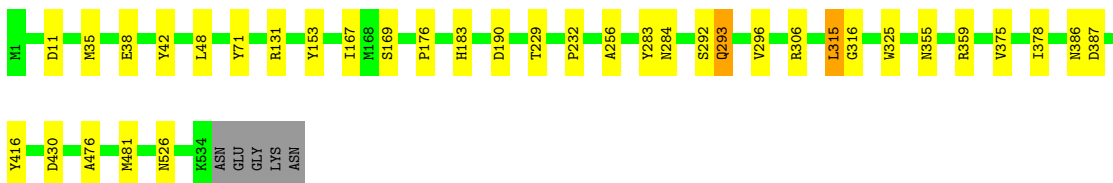
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain N: 

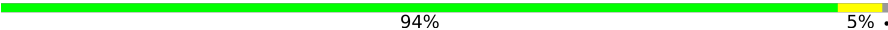


- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B: 



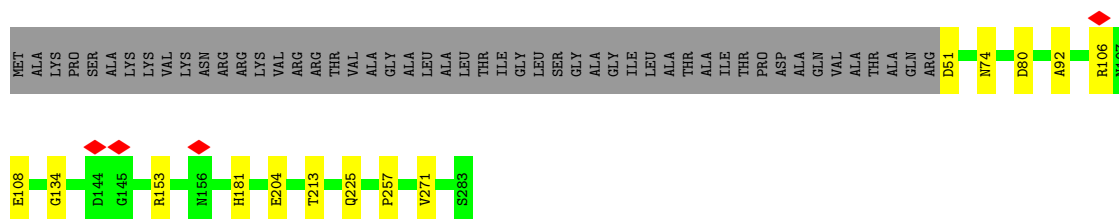
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain O: 



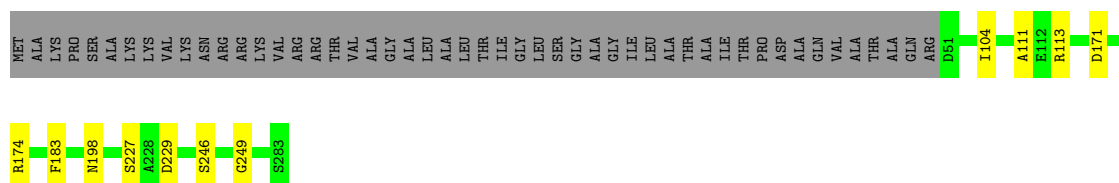
- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain C: 



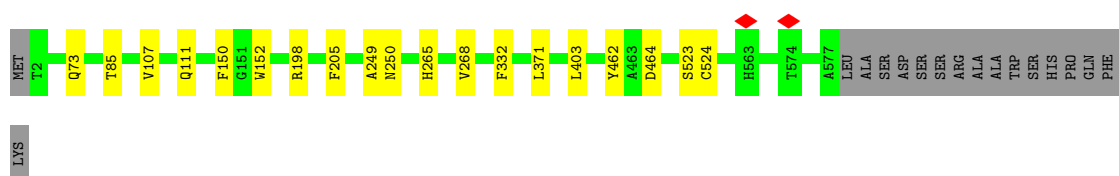
- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain P: 78% 18%



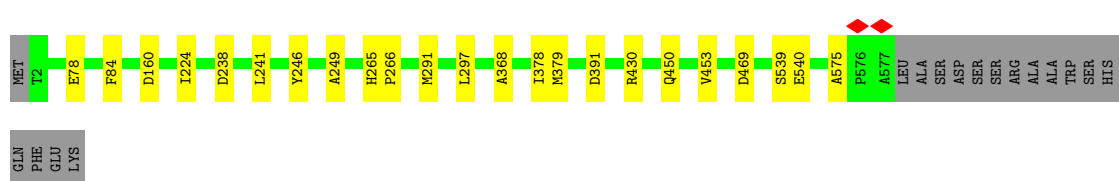
- Molecule 4: Cytochrome c oxidase subunit 1

Chain D: 94% 2%



- Molecule 4: Cytochrome c oxidase subunit 1

Chain Q: 93% 2%



- Molecule 5: Cytochrome c oxidase subunit 2

Chain E: 97% 2%



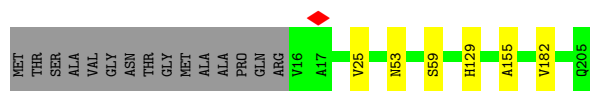
- Molecule 5: Cytochrome c oxidase subunit 2

Chain R: 96% 2%



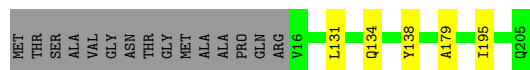
- Molecule 6: Cytochrome c oxidase subunit 3

Chain F: 90% 7%



- Molecule 6: Cytochrome c oxidase subunit 3

Chain S: 90% 7%



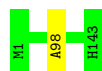
- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain G: 97%



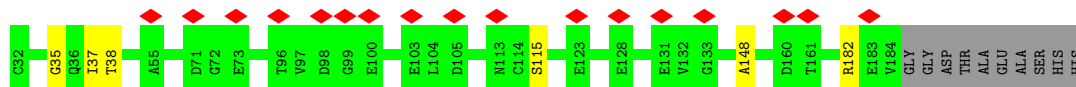
- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain T: 99%



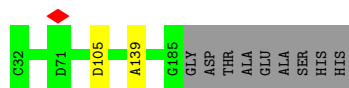
- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain H: 10% 90% 6%



- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain U: 93% 6%



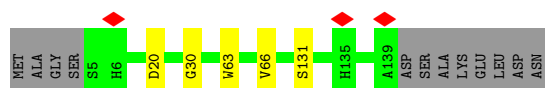
- Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain I:  88% 8%



- Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain V:  88% 8%



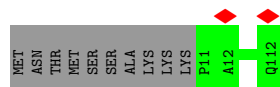
- Molecule 10: Hypothetical membrane protein

Chain J:  89% 9%



- Molecule 10: Hypothetical membrane protein

Chain W:  91% 9%



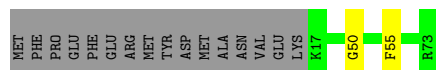
- Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

Chain K:  5% 77% 19%



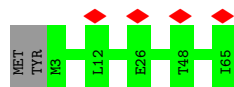
- Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

Chain X:  75% 22%

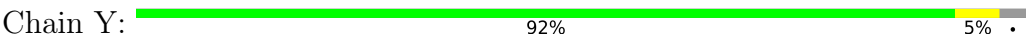


- Molecule 12: Hypothetical membrane protein

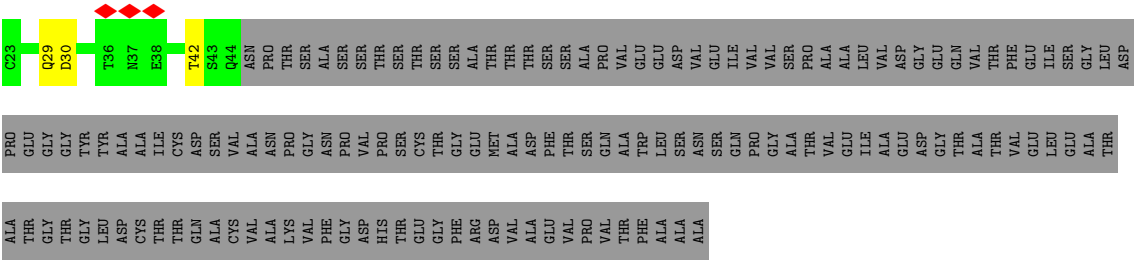
Chain L:  6% 97%



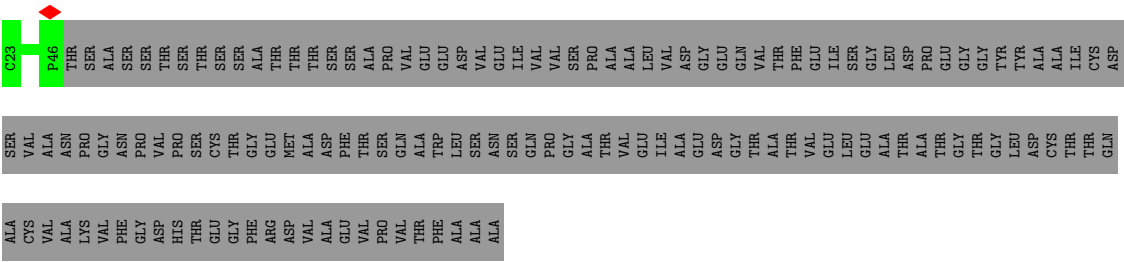
● Molecule 12: Hypothetical membrane protein



● Molecule 13: Thiamine biosynthesis protein X



● Molecule 13: Thiamine biosynthesis protein X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200424	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 ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.641	Depositor
Minimum map value	-1.574	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	281.49, 203.01399, 150.981	wwPDB
Map dimensions	177, 238, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.853, 0.853, 0.85300004	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: CDL, FES, 3PE, AZI, CA, CUA, PLM, MQ9, HEC, HAS, 9YF, IZL, DGA, HEM, IX7, CU, MN, SMA, LMT, LYC, OXY

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	0.30	0/3238	0.44	0/4403
1	N	0.32	0/3244	0.48	2/4414 (0.0%)
2	B	0.34	0/4359	0.50	4/5937 (0.1%)
2	O	0.36	0/4301	0.49	0/5860
3	C	0.26	0/1785	0.43	0/2413
3	P	0.36	0/1770	0.45	0/2394
4	D	0.31	0/4718	0.47	0/6438
4	Q	0.36	0/4734	0.50	0/6460
5	E	0.27	0/2671	0.45	0/3642
5	R	0.32	0/2686	0.45	0/3661
6	F	0.27	0/1528	0.44	0/2081
6	S	0.32	0/1528	0.48	0/2081
7	G	0.27	0/1126	0.46	0/1529
7	T	0.30	0/1144	0.42	0/1554
8	H	0.26	0/1134	0.45	0/1553
8	U	0.28	0/1138	0.44	0/1558
9	I	0.25	0/1103	0.45	0/1508
9	V	0.29	0/1103	0.47	0/1508
10	J	0.23	0/799	0.44	0/1087
10	W	0.26	0/799	0.48	0/1087
11	K	0.28	0/486	0.42	0/663
11	X	0.30	0/468	0.43	0/640
12	L	0.22	0/453	0.46	0/616
12	Y	0.26	0/453	0.53	0/616
13	M	0.21	0/174	0.41	0/238
13	Z	0.23	0/190	0.46	0/261
All	All	0.31	0/47132	0.47	6/64202 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	193	LYS	CA-C-N	5.96	132.44	121.70
1	N	193	LYS	C-N-CA	5.96	132.44	121.70
2	B	315	LEU	CA-C-N	5.38	131.39	121.70
2	B	315	LEU	C-N-CA	5.38	131.39	121.70
2	B	176	PRO	CA-C-N	5.01	130.71	121.70
2	B	176	PRO	C-N-CA	5.01	130.71	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	3084	3070	17	0
1	N	3145	3079	3063	16	0
2	B	4217	4268	4238	28	0
2	O	4186	4239	4238	21	0
3	C	1749	1694	1690	8	0
3	P	1738	1680	1680	7	0
4	D	4548	4470	4471	15	0
4	Q	4557	4477	4468	19	0
5	E	2598	2468	2468	7	0
5	R	2607	2482	2476	10	0
6	F	1486	1495	1494	5	0
6	S	1486	1494	1494	3	0
7	G	1095	1106	1106	3	0
7	T	1105	1114	1104	1	0
8	H	1120	1054	1054	5	0
8	U	1124	1057	1057	1	0
9	I	1073	1071	1071	4	0
9	V	1073	1071	1071	3	0
10	J	779	792	792	1	0
10	W	779	792	792	0	0
11	K	469	432	432	3	0
11	X	451	413	413	1	0
12	L	445	470	469	0	0
12	Y	445	470	469	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	171	159	159	2	0
13	Z	186	172	172	0	0
14	A	4	0	0	0	0
14	N	4	0	0	0	0
15	A	103	109	0	3	0
15	N	103	109	0	0	0
16	A	36	30	0	0	0
16	H	34	26	0	0	0
16	N	36	30	0	0	0
16	U	39	36	0	2	0
17	A	58	80	80	3	0
17	B	23	23	21	1	0
17	N	36	42	42	0	0
17	O	27	29	29	1	0
18	A	40	36	57	1	0
18	C	50	40	48	2	0
18	D	31	26	36	0	0
18	F	32	22	38	1	0
18	J	47	64	71	0	0
18	L	30	38	34	0	0
18	N	38	28	53	1	0
18	P	27	18	28	2	0
18	Q	39	32	55	3	0
18	R	31	16	36	3	0
18	S	43	52	60	0	0
18	T	146	148	191	1	0
18	W	47	68	68	0	0
19	B	37	42	41	1	0
19	O	37	42	41	1	0
20	B	86	60	60	3	0
20	O	86	60	60	3	0
21	B	171	122	174	2	0
21	D	140	149	171	1	0
21	F	57	37	58	1	0
21	G	144	135	179	2	0
21	I	57	50	61	0	0
21	O	66	79	79	0	0
21	Q	149	179	195	4	0
21	S	65	70	74	0	0
21	T	145	141	181	1	0
21	V	69	90	90	0	0
22	B	40	56	56	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	40	56	56	1	0
23	B	32	39	37	0	0
23	O	32	39	37	0	0
24	C	86	60	60	1	0
24	P	86	60	60	1	0
25	D	130	124	124	3	0
25	Q	130	124	124	3	0
26	D	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	R	1	0	0	0	0
28	D	1	0	0	0	0
28	Q	1	0	0	0	0
29	D	3	0	0	2	0
29	Q	3	0	0	0	0
30	E	2	0	0	0	0
30	R	2	0	0	0	0
31	E	20	0	21	0	0
31	H	17	0	15	2	0
31	M	22	0	25	1	0
31	R	25	0	31	0	0
31	U	27	0	35	3	0
31	Z	29	0	39	0	0
32	H	17	24	31	0	0
32	M	5	4	4	0	0
32	U	17	28	31	0	0
32	Z	5	4	4	0	0
33	H	72	83	0	2	0
33	U	72	83	0	2	0
34	Q	2	0	0	0	0
35	A	31	0	0	8	0
35	B	56	0	0	10	0
35	C	26	0	0	1	0
35	D	21	0	0	1	0
35	E	13	0	0	4	0
35	F	3	0	0	1	0
35	G	6	0	0	0	0
35	K	3	0	0	0	0
35	N	31	0	0	5	0
35	O	46	0	0	3	0
35	P	49	0	0	1	0
35	Q	53	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	44	0	0	2	0
35	S	5	0	0	0	0
35	T	13	0	0	0	0
35	U	12	0	0	0	0
35	V	2	0	0	0	0
35	X	2	0	0	0	0
All	All	49530	48245	48212	184	0

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

All (184) 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)
4:Q:238:ASP:OD2	35:Q:701:HOH:O	2.04	0.75
1:N:353:PRO:O	35:N:601:HOH:O	2.05	0.75
4:D:205:PHE:O	35:D:701:HOH:O	2.04	0.74
6:F:59:SER:O	35:F:401:HOH:O	2.07	0.73
3:C:257:PRO:O	35:C:401:HOH:O	2.08	0.72
2:B:190:ASP:OD1	35:B:701:HOH:O	2.07	0.72
1:A:399:LEU:O	35:A:601:HOH:O	2.08	0.72
2:B:296:VAL:O	35:B:702:HOH:O	2.08	0.71
4:Q:469:ASP:O	35:Q:702:HOH:O	2.07	0.71
5:R:292:TYR:OH	35:R:501:HOH:O	2.08	0.71
4:D:250:ASN:O	6:F:53:ASN:ND2	2.23	0.71
5:E:156:LYS:O	35:E:501:HOH:O	2.08	0.70
25:Q:602:HAS:O2A	35:Q:704:HOH:O	2.08	0.70
8:U:105:ASP:OD2	8:U:139:ALA:N	2.25	0.70
1:A:318:GLN:O	35:A:602:HOH:O	2.09	0.70
2:B:476:ALA:O	35:B:703:HOH:O	2.08	0.70
5:E:288:MET:O	35:E:502:HOH:O	2.09	0.70
1:A:258:ALA:O	35:A:603:HOH:O	2.10	0.69
1:N:225:THR:O	35:N:603:HOH:O	2.10	0.69
1:N:224:ASP:OD2	35:N:602:HOH:O	2.08	0.69
4:Q:238:ASP:OD1	35:Q:705:HOH:O	2.10	0.69
15:A:502:IZL:O6	15:A:502:IZL:O9	2.11	0.68
2:O:439:GLU:OE1	35:O:701:HOH:O	2.12	0.68
1:A:314:GLU:OE1	35:A:602:HOH:O	2.11	0.68
3:P:198:ASN:O	35:P:401:HOH:O	2.11	0.68
5:R:221:GLU:OE2	35:R:502:HOH:O	2.12	0.67
1:A:155:SER:O	1:A:156:THR:OG1	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASP:O	35:A:604:HOH:O	2.13	0.67
1:A:94:LEU:HD21	18:C:303:3PE:H222	1.76	0.67
2:B:283:TYR:O	35:B:704:HOH:O	2.12	0.67
4:Q:160:ASP:OD1	35:Q:706:HOH:O	2.13	0.66
9:I:31:LEU:HD23	9:I:36:ILE:HD11	1.77	0.66
1:A:125:GLU:O	35:A:605:HOH:O	2.14	0.65
2:B:229:THR:OG1	20:B:603:HEM:O2D	2.10	0.63
15:A:502:IZL:O6	15:A:502:IZL:O8	2.18	0.62
1:A:375:ALA:O	35:A:606:HOH:O	2.16	0.61
5:E:354:ASN:OD1	35:E:503:HOH:O	2.16	0.61
3:P:227:SER:OG	3:P:229:ASP:OD1	2.15	0.61
2:O:80:SER:OG	2:O:157:ASP:OD2	2.13	0.61
4:D:198:ARG:NH2	7:G:73:ASP:OD1	2.33	0.60
1:A:356:GLN:OE1	35:A:607:HOH:O	2.17	0.60
17:A:504:MQ9:H402	20:B:602:HEM:HBB1	1.84	0.59
19:O:602:SMA:H37	19:O:602:SMA:H33	1.85	0.59
2:O:418:ILE:CD1	21:Q:608:CDL:H712	2.33	0.59
2:B:355:ASN:ND2	35:B:709:HOH:O	2.35	0.58
4:Q:241:LEU:O	6:S:134:GLN:NE2	2.36	0.58
31:H:201:DGA:HB32	33:H:204:IX7:C7	2.34	0.58
2:O:253:LYS:NZ	35:O:708:HOH:O	2.34	0.58
25:Q:601:HAS:O2D	35:Q:707:HOH:O	2.17	0.58
16:U:203:9YF:O7	16:U:203:9YF:O8	2.22	0.58
2:B:481:MET:HE1	11:K:55:PHE:CE1	2.40	0.56
20:O:603:HEM:HBB2	20:O:603:HEM:HMB2	1.86	0.56
2:B:359:ARG:NH2	2:B:430[B]:ASP:OD2	2.39	0.56
4:Q:368:ALA:HB2	18:Q:609:3PE:H2B1	1.88	0.56
18:A:505:3PE:H282	2:O:248:PRO:HB3	1.88	0.55
2:O:418:ILE:HD12	21:Q:608:CDL:H712	1.88	0.55
2:B:232:PRO:O	35:B:705:HOH:O	2.18	0.54
4:Q:430:ARG:NE	12:Y:56:ASP:OD2	2.38	0.54
1:A:336:ILE:HD12	2:B:167:ILE:HG23	1.90	0.54
2:B:306:ARG:O	35:B:706:HOH:O	2.19	0.54
1:N:40:ARG:NH2	1:N:124:GLU:OE1	2.41	0.54
8:H:37:ILE:HG12	33:H:204:IX7:O9	2.08	0.53
2:B:42:TYR:HE1	17:B:604:MQ9:H102	1.74	0.53
4:D:464:ASP:OD2	35:E:503:HOH:O	2.18	0.53
4:Q:539:SER:OG	4:Q:540:GLU:N	2.39	0.53
4:D:85:THR:OG1	4:D:150:PHE:O	2.26	0.52
1:N:90:LEU:HD11	18:P:303:3PE:H241	1.90	0.52
2:O:337:LEU:HD22	22:O:607:LYC:H623	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:481:MET:HE2	11:X:55:PHE:CE1	2.45	0.52
4:D:371:LEU:HD21	5:E:75:MET:HB2	1.92	0.52
4:D:332:PHE:HB3	5:E:121:VAL:HG13	1.93	0.51
2:B:416:TYR:OH	9:I:31:LEU:HD22	2.09	0.51
1:N:336:ILE:HD12	2:O:167:ILE:HG23	1.93	0.51
10:J:16:MET:SD	10:J:16:MET:N	2.83	0.51
4:Q:391:ASP:OD1	35:Q:708:HOH:O	2.19	0.51
17:A:504:MQ9:H401	2:B:48:LEU:HD22	1.93	0.51
3:C:92:ALA:HA	3:C:213:THR:HG21	1.93	0.51
25:D:602:HAS:C1A	29:D:606:AZI:N3	2.65	0.51
3:C:74:ASN:OD1	8:H:115:SER:OG	2.30	0.50
1:N:157:LEU:HD22	18:N:502:3PE:H2D1	1.93	0.50
2:B:325:TRP:HB3	31:M:201:DGA:HA71	1.94	0.50
4:Q:368:ALA:CB	18:Q:609:3PE:H2B1	2.42	0.50
4:D:152:TRP:NE1	25:D:602:HAS:O1A	2.41	0.50
3:C:51:ASP:OD1	3:C:51:ASP:N	2.45	0.49
7:G:31:ASP:OD1	7:G:32:GLY:N	2.45	0.49
2:B:35:MET:HA	2:B:38:GLU:HG3	1.94	0.49
11:K:21:ASP:OD1	11:K:23:ALA:N	2.44	0.49
3:C:225:GLN:O	8:H:182:ARG:NH2	2.44	0.49
5:R:166:LEU:HD13	5:R:308:PHE:HD2	1.77	0.49
24:C:301:HEC:HBB2	24:C:301:HEC:HHC	1.94	0.49
4:Q:249:ALA:HB3	5:R:197:ILE:HG21	1.95	0.49
2:B:526:ASN:OD1	35:B:707:HOH:O	2.20	0.49
19:B:601:SMA:H36	19:B:601:SMA:H31	1.95	0.48
1:N:374:ARG:NH1	35:N:605:HOH:O	2.40	0.48
4:D:73:GLN:N	4:D:73:GLN:OE1	2.45	0.48
31:U:201:DGA:HB92	9:V:63:TRP:CZ3	2.48	0.48
1:N:81:TYR:OH	35:N:604:HOH:O	2.19	0.48
3:C:204:GLU:OE1	3:C:204:GLU:N	2.45	0.48
6:F:25:VAL:HG12	6:F:182:VAL:HG11	1.94	0.48
2:O:169:SER:OG	2:O:183:HIS:NE2	2.40	0.48
4:D:265:HIS:CE1	29:D:606:AZI:N1	2.82	0.48
1:N:406:ARG:NH1	1:N:408:SER:O	2.47	0.48
2:O:381:THR:HG22	18:T:203:3PE:H2C1	1.95	0.47
1:N:405:GLU:N	1:N:405:GLU:OE1	2.45	0.47
4:D:265:HIS:O	4:D:268:VAL:HG22	2.14	0.47
8:H:35:GLY:O	8:H:38:THR:HG23	2.14	0.47
1:A:407:LYS:HG3	15:A:502:IZL:O23	2.14	0.47
4:Q:78:GLU:OE1	4:Q:78:GLU:N	2.46	0.47
6:F:129:HIS:ND1	6:F:129:HIS:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:336:ILE:HD11	1:N:355:HIS:CE1	2.49	0.47
5:R:106:ASN:ND2	18:R:405:3PE:O22	2.47	0.47
2:B:315:LEU:N	2:B:316:GLY:HA2	2.29	0.47
1:A:336:ILE:HD11	1:A:355:HIS:CE1	2.50	0.46
1:N:94:LEU:HD11	18:P:303:3PE:H271	1.97	0.46
4:Q:378:ILE:HD12	4:Q:379:MET:N	2.30	0.46
25:Q:601:HAS:HMC1	25:Q:601:HAS:HBC1	1.98	0.46
2:O:245:ARG:NH1	35:O:707:HOH:O	2.48	0.46
8:H:148:ALA:HB2	13:M:42:THR:HB	1.98	0.46
1:N:193:LYS:N	1:N:194:GLU:HA	2.31	0.46
2:B:526:ASN:ND2	35:B:716:HOH:O	2.48	0.45
3:C:80:ASP:OD1	5:E:344:SER:OG	2.31	0.45
20:B:602:HEM:HHA	20:B:602:HEM:HBA2	1.97	0.45
5:R:103:LEU:HD23	18:R:405:3PE:H222	1.97	0.45
1:A:8:GLN:N	1:A:8:GLN:OE1	2.49	0.45
3:P:113:ARG:NH1	24:P:302:HEC:O1A	2.50	0.45
21:D:607:CDL:H781	6:F:155:ALA:HB1	1.99	0.45
1:A:94:LEU:CD2	18:C:303:3PE:H222	2.45	0.45
13:M:29:GLN:NE2	13:M:30:ASP:OD2	2.49	0.45
4:Q:246:TYR:N	35:Q:701:HOH:O	2.38	0.44
5:R:78:LEU:CD1	18:R:405:3PE:H2B2	2.48	0.44
3:P:171:ASP:OD1	3:P:174:ARG:NH1	2.48	0.44
4:Q:450:GLN:HA	4:Q:453:VAL:HG12	1.99	0.44
6:S:131:LEU:HD11	6:S:138:TYR:HD2	1.82	0.44
21:Q:607:CDL:OB7	6:S:179:ALA:HB1	2.18	0.44
17:A:504:MQ9:H302	2:O:213:LEU:HD22	2.00	0.44
31:U:201:DGA:HB82	9:V:66:VAL:HG11	1.99	0.44
16:U:203:9YF:O4	33:U:204:IX7:O21	2.36	0.44
21:G:202:CDL:HB62	21:G:202:CDL:H132	1.98	0.44
2:O:418:ILE:HD13	21:Q:608:CDL:H712	2.00	0.44
4:D:523:SER:OG	4:D:524:CYS:N	2.48	0.44
2:B:293:GLN:NE2	2:B:387:ASP:OD1	2.51	0.43
21:G:201:CDL:HB62	21:G:201:CDL:HB22	2.00	0.43
21:B:609:CDL:H711	2:O:221:ALA:HB2	1.99	0.43
2:B:375:VAL:O	2:B:378:ILE:HG22	2.19	0.43
20:O:604:HEM:HMC2	20:O:604:HEM:HBC2	2.00	0.43
12:Y:27:VAL:HG23	12:Y:28:GLY:HA2	2.00	0.43
1:N:202:ASP:OD1	1:N:207:THR:OG1	2.35	0.43
17:O:605:MQ9:H122	17:O:605:MQ9:H103	1.81	0.43
4:Q:84:PHE:HZ	5:R:288:MET:HE3	1.84	0.43
31:U:201:DGA:HB61	33:U:204:IX7:C66	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:349:THR:HG22	5:R:354:ASN:HA	2.00	0.43
1:A:232:HIS:NE2	1:A:234:ASP:OD2	2.52	0.43
18:F:301:3PE:H232	18:F:301:3PE:H321	2.01	0.42
2:B:306:ARG:NH1	2:B:386:ASN:OD1	2.52	0.42
2:O:289:SER:OG	2:O:290:ALA:N	2.51	0.42
21:F:302:CDL:OB7	21:F:302:CDL:HB31	2.19	0.42
2:O:159:LEU:HD23	3:P:183:PHE:HE1	1.85	0.42
2:B:169:SER:OG	2:B:183:HIS:NE2	2.42	0.42
3:C:106:ARG:NE	3:C:108:GLU:OE2	2.52	0.42
2:O:131:ARG:NH2	2:O:355:ASN:OD1	2.48	0.42
2:B:11:ASP:OD2	1:N:141:ARG:NH1	2.52	0.42
4:Q:224:ILE:HG21	4:Q:266:PRO:HB2	2.02	0.42
2:B:131:ARG:NH2	2:B:355:ASN:OD1	2.53	0.41
20:O:603:HEM:HHA	20:O:603:HEM:HBA2	2.01	0.41
2:B:284:ASN:ND2	35:B:718:HOH:O	2.53	0.41
21:B:605:CDL:H112	21:B:605:CDL:H512	2.02	0.41
4:D:403:LEU:HD23	25:D:602:HAS:HBC2	2.01	0.41
2:O:334:VAL:O	2:O:338:VAL:HG23	2.21	0.41
2:O:428:ARG:NH2	9:V:20:ASP:O	2.53	0.41
7:G:123:MET:N	7:G:123:MET:HE2	2.36	0.41
31:H:201:DGA:HB51	9:I:63:TRP:CZ2	2.55	0.41
3:P:104:ILE:HD11	3:P:111:ALA:HB2	2.03	0.41
5:R:136:THR:HG22	5:R:136:THR:O	2.21	0.41
7:T:98:ALA:HB1	21:T:201:CDL:H152	2.03	0.41
1:A:115:VAL:HG23	2:B:256:ALA:HB1	2.03	0.40
2:B:481:MET:HE1	11:K:55:PHE:CD1	2.57	0.40
3:P:246:SER:OG	3:P:249:GLY:O	2.35	0.40
4:Q:291:MET:HE2	4:Q:297:LEU:HD11	2.03	0.40
4:D:107:VAL:HG12	4:D:111:GLN:HG3	2.03	0.40
4:D:249:ALA:HB3	5:E:197:ILE:HG21	2.03	0.40
18:Q:609:3PE:H2B2	18:Q:609:3PE:H2E1	1.94	0.40
9:I:40:GLY:HA3	9:I:75:LEU:HD21	2.04	0.40
2:O:306:ARG:NH1	2:O:386:ASN:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/408 (98%)	382 (95%)	20 (5%)	0	100	100
1	N	403/408 (99%)	388 (96%)	14 (4%)	1 (0%)	43	72
2	B	538/539 (100%)	519 (96%)	16 (3%)	3 (1%)	21	51
2	O	532/539 (99%)	518 (97%)	14 (3%)	0	100	100
3	C	233/283 (82%)	217 (93%)	13 (6%)	3 (1%)	9	31
3	P	231/283 (82%)	214 (93%)	17 (7%)	0	100	100
4	D	574/594 (97%)	553 (96%)	21 (4%)	0	100	100
4	Q	576/594 (97%)	553 (96%)	22 (4%)	1 (0%)	43	72
5	E	329/331 (99%)	313 (95%)	14 (4%)	2 (1%)	21	51
5	R	331/331 (100%)	318 (96%)	13 (4%)	0	100	100
6	F	188/205 (92%)	185 (98%)	3 (2%)	0	100	100
6	S	188/205 (92%)	182 (97%)	6 (3%)	0	100	100
7	G	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
7	T	143/143 (100%)	137 (96%)	6 (4%)	0	100	100
8	H	151/163 (93%)	147 (97%)	4 (3%)	0	100	100
8	U	152/163 (93%)	146 (96%)	6 (4%)	0	100	100
9	I	133/147 (90%)	124 (93%)	8 (6%)	1 (1%)	16	44
9	V	133/147 (90%)	126 (95%)	6 (4%)	1 (1%)	16	44
10	J	100/112 (89%)	97 (97%)	3 (3%)	0	100	100
10	W	100/112 (89%)	95 (95%)	5 (5%)	0	100	100
11	K	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
11	X	55/73 (75%)	53 (96%)	1 (2%)	1 (2%)	6	23
12	L	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
12	Y	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
13	M	20/168 (12%)	16 (80%)	4 (20%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	22/168 (13%)	20 (91%)	2 (9%)	0	100	100
All	All	5854/6462 (91%)	5608 (96%)	233 (4%)	13 (0%)	44	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	292	SER
4	Q	575	ALA
9	V	30	GLY
2	B	71	TYR
3	C	181	HIS
5	E	194	ASP
9	I	31	LEU
2	B	293	GLN
3	C	153	ARG
1	N	272	VAL
3	C	134	GLY
11	X	50	GLY
5	E	196	PRO

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	328/332 (99%)	327 (100%)	1 (0%)	86	95
1	N	329/332 (99%)	327 (99%)	2 (1%)	78	92
2	B	443/441 (100%)	441 (100%)	2 (0%)	81	93
2	O	437/441 (99%)	434 (99%)	3 (1%)	76	91
3	C	178/212 (84%)	177 (99%)	1 (1%)	78	92
3	P	177/212 (84%)	177 (100%)	0	100	100
4	D	473/488 (97%)	472 (100%)	1 (0%)	87	96
4	Q	475/488 (97%)	475 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	274/274 (100%)	272 (99%)	2 (1%)	76	91
5	R	276/274 (101%)	274 (99%)	2 (1%)	76	91
6	F	156/166 (94%)	156 (100%)	0	100	100
6	S	156/166 (94%)	155 (99%)	1 (1%)	78	92
7	G	114/114 (100%)	114 (100%)	0	100	100
7	T	116/114 (102%)	116 (100%)	0	100	100
8	H	127/133 (96%)	127 (100%)	0	100	100
8	U	127/133 (96%)	127 (100%)	0	100	100
9	I	116/125 (93%)	116 (100%)	0	100	100
9	V	116/125 (93%)	115 (99%)	1 (1%)	70	89
10	J	81/90 (90%)	80 (99%)	1 (1%)	63	87
10	W	81/90 (90%)	81 (100%)	0	100	100
11	K	50/63 (79%)	50 (100%)	0	100	100
11	X	48/63 (76%)	48 (100%)	0	100	100
12	L	43/45 (96%)	43 (100%)	0	100	100
12	Y	43/45 (96%)	43 (100%)	0	100	100
13	M	22/135 (16%)	22 (100%)	0	100	100
13	Z	24/135 (18%)	24 (100%)	0	100	100
All	All	4810/5236 (92%)	4793 (100%)	17 (0%)	84	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	THR
2	B	153[A]	TYR
2	B	153[B]	TYR
3	C	271	VAL
4	D	462	TYR
5	E	265	LYS
5	E	302	VAL
10	J	92	VAL
1	N	120[A]	LYS
1	N	120[B]	LYS
2	O	249	LEU
2	O	295	ASP
2	O	363	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	29	CYS
5	R	160	SER
6	S	195	ILE
9	V	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	149	ASN
2	B	75	ASN
3	C	96	GLN
4	D	77	ASN
4	D	257	GLN
4	D	476	GLN
6	F	119	GLN
9	I	29	HIS
9	I	99	HIS
9	I	122	GLN
1	N	239	HIS
2	O	134	ASN
2	O	317	ASN
2	O	480	GLN
4	Q	163	HIS
4	Q	476	GLN
5	R	132	GLN
5	R	211	ASN
5	R	264	ASN
8	U	87	HIS
10	W	67	GLN
12	Y	58	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 78 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	$\# Z > 2$
21	CDL	F	302	-	56,56,99	0.39	0	62,68,111	0.60	1 (1%)
16	9YF	H	203	-	34,34,58	0.34	0	43,46,71	0.36	0
18	3PE	A	505	-	39,39,50	0.33	0	42,44,55	0.56	0
23	LMT	B	608	-	33,33,36	0.14	0	44,44,47	0.60	0
20	HEM	O	603	2	50,50,50	1.33	4 (8%)	67,82,82	1.31	7 (10%)
16	9YF	N	505	-	36,36,58	0.36	0	45,48,71	0.34	0
21	CDL	V	201	-	68,68,99	0.38	0	72,79,111	0.45	0
16	9YF	U	203	-	39,39,58	0.34	0	48,51,71	0.42	0
25	HAS	Q	602	4	72,72,72	1.21	7 (9%)	87,109,109	1.60	14 (16%)
21	CDL	B	606	-	44,44,99	0.43	0	50,56,111	0.38	0
31	DGA	H	201	-	16,16,43	0.29	0	18,18,45	0.17	0
20	HEM	B	602	2	50,50,50	1.24	3 (6%)	67,82,82	1.10	4 (5%)
20	HEM	B	603	2	50,50,50	1.26	3 (6%)	67,82,82	0.76	0
16	9YF	A	503	-	36,36,58	0.44	0	45,48,71	0.38	0
19	SMA	B	601	-	38,38,38	0.71	2 (5%)	47,52,52	0.84	2 (4%)
22	LYC	O	607	-	39,39,39	0.35	0	46,46,46	0.56	1 (2%)
18	3PE	J	201	-	46,46,50	0.33	0	49,51,55	0.65	1 (2%)
18	3PE	C	303	-	24,24,50	0.45	0	27,29,55	0.63	0
14	FES	A	501	1	0,4,4	-	-	-	-	-
29	AZI	D	606	26,25	2,2,2	2.46	2 (100%)	0,1,1	-	-
18	3PE	T	205	-	37,37,50	0.36	0	40,42,55	0.42	0
21	CDL	T	201	-	79,79,99	0.35	0	85,91,111	0.47	1 (1%)
24	HEC	C	301	3	46,50,50	1.42	2 (4%)	58,82,82	1.46	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	HEM	O	604	2	50,50,50	1.21	5 (10%)	67,82,82	0.74	1 (1%)
18	3PE	T	206	-	39,39,50	0.35	0	42,44,55	0.73	1 (2%)
17	MQ9	O	605	-	28,28,59	0.59	1 (3%)	35,37,75	1.25	3 (8%)
31	DGA	M	201	-	21,21,43	0.26	0	23,23,45	0.24	0
18	3PE	T	202	-	25,25,50	0.42	0	28,30,55	0.49	0
21	CDL	G	201	-	74,74,99	0.34	0	80,86,111	0.59	1 (1%)
32	PLM	Z	202	13	3,4,17	0.24	0	2,3,17	0.25	0
24	HEC	P	302	3	46,50,50	1.45	2 (4%)	58,82,82	1.60	3 (5%)
31	DGA	Z	201	-	28,28,43	0.23	0	30,30,45	0.35	0
24	HEC	C	302	3	46,50,50	1.45	2 (4%)	58,82,82	1.47	3 (5%)
31	DGA	U	201	-	26,26,43	0.30	0	28,28,45	0.33	0
29	AZI	Q	605	26	2,2,2	2.65	2 (100%)	0,1,1	-	-
18	3PE	S	301	-	42,42,50	0.39	0	45,47,55	0.59	1 (2%)
18	3PE	N	502	-	37,37,50	0.34	0	40,42,55	0.44	0
21	CDL	T	204	-	64,64,99	0.37	0	70,76,111	0.67	1 (1%)
21	CDL	S	302	-	64,64,99	0.38	0	70,76,111	0.58	1 (1%)
15	IZL	A	502	-	108,108,119	0.33	0	149,152,163	1.03	10 (6%)
18	3PE	C	304	-	24,24,50	0.43	0	27,29,55	0.64	1 (3%)
18	3PE	T	203	-	41,41,50	0.34	0	44,46,55	0.42	0
32	PLM	H	202	8	15,16,17	0.15	0	14,15,17	0.21	0
18	3PE	W	201	-	46,46,50	0.33	0	49,51,55	0.94	3 (6%)
15	IZL	N	504	-	108,108,119	0.43	0	149,152,163	1.09	15 (10%)
19	SMA	O	602	-	38,38,38	0.44	1 (2%)	47,52,52	0.47	0
21	CDL	Q	607	-	82,82,99	0.35	0	88,94,111	0.41	0
14	FES	N	503	1	0,4,4	-	-	-	-	-
17	MQ9	B	604	-	24,24,59	0.74	1 (4%)	31,33,75	1.43	2 (6%)
31	DGA	R	404	-	24,24,43	0.27	0	26,26,45	0.19	0
18	3PE	Q	609	-	38,38,50	0.35	0	41,43,55	0.44	0
32	PLM	U	202	8	15,16,17	0.13	0	14,15,17	0.19	0
21	CDL	D	607	-	76,76,99	0.36	0	82,88,111	0.54	1 (1%)
21	CDL	Q	608	-	65,65,99	0.37	0	71,77,111	0.43	0
25	HAS	D	602	29,4	72,72,72	1.22	7 (9%)	87,109,109	1.46	11 (12%)
18	3PE	R	405	-	30,30,50	0.37	0	33,35,55	0.48	0
22	LYC	B	607	-	39,39,39	0.22	0	46,46,46	0.39	0
18	3PE	D	609	-	30,30,50	0.39	0	33,35,55	0.38	0
21	CDL	D	608	-	62,62,99	0.39	0	68,74,111	0.56	0
17	MQ9	N	501	-	37,37,59	0.51	1 (2%)	46,48,75	0.85	2 (4%)
33	IX7	U	204	-	74,74,97	0.34	0	96,99,123	0.89	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	HAS	D	601	4	72,72,72	1.25	7 (9%)	87,109,109	1.53	11 (12%)
18	3PE	P	303	-	26,26,50	0.44	0	29,31,55	0.74	2 (6%)
21	CDL	G	202	-	68,68,99	0.36	0	74,80,111	0.64	2 (2%)
17	MQ9	A	504	-	59,59,59	0.55	2 (3%)	73,75,75	0.91	5 (6%)
21	CDL	O	606	-	65,65,99	0.39	0	71,77,111	0.59	1 (1%)
24	HEC	P	301	3	46,50,50	1.39	2 (4%)	58,82,82	1.76	2 (3%)
31	DGA	E	403	-	19,19,43	0.27	0	21,21,45	0.18	0
32	PLM	M	202	13	3,4,17	0.27	0	2,3,17	0.19	0
23	LMT	O	601	-	33,33,36	0.15	0	44,44,47	1.08	2 (4%)
18	3PE	F	301	-	31,31,50	0.39	0	34,36,55	0.86	1 (2%)
33	IX7	H	204	-	74,74,97	0.38	0	96,99,123	1.06	6 (6%)
18	3PE	L	101	-	29,29,50	0.41	0	32,34,55	0.57	0
34	OXY	Q	606	-	1,1,1	0.17	0	-		
25	HAS	Q	601	4	72,72,72	1.23	8 (11%)	87,109,109	1.31	8 (9%)
21	CDL	B	609	-	69,69,99	0.37	0	75,81,111	0.47	0
21	CDL	B	605	-	55,55,99	0.39	0	61,67,111	0.54	0
21	CDL	I	201	-	56,56,99	0.39	0	62,68,111	0.46	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
21	CDL	T	201	-	-	42/90/90/110	-
21	CDL	F	302	-	-	26/67/67/110	-
15	IZL	N	504	-	-	35/73/197/208	0/6/6/6
16	9YF	H	203	-	-	6/29/53/78	0/1/1/1
18	3PE	A	505	-	-	15/43/43/54	-
20	HEM	O	604	2	-	2/14/54/54	-
23	LMT	B	608	-	-	9/18/58/61	0/2/2/2
24	HEC	C	301	3	-	6/14/54/54	-
18	3PE	T	206	-	-	21/43/43/54	-
17	MQ9	N	501	-	-	7/27/47/73	0/2/2/2
19	SMA	O	602	-	-	11/34/34/34	0/2/2/2
21	CDL	D	608	-	-	30/73/73/110	-
20	HEM	O	603	2	-	5/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	9YF	N	505	-	-	5/31/55/78	0/1/1/1
33	IX7	U	204	-	-	25/58/122/146	0/3/3/3
21	CDL	Q	607	-	-	30/93/93/110	-
25	HAS	D	601	4	1/1/18/18	13/42/82/82	-
17	MQ9	O	605	-	-	8/16/36/73	0/2/2/2
21	CDL	V	201	-	-	37/78/78/110	-
14	FES	N	503	1	-	-	0/1/1/1
31	DGA	M	201	-	-	2/22/22/45	-
17	MQ9	B	604	-	-	3/11/31/73	0/2/2/2
16	9YF	U	203	-	-	3/34/58/78	0/1/1/1
17	MQ9	A	504	-	-	21/53/73/73	0/2/2/2
21	CDL	G	202	-	-	24/79/79/110	-
25	HAS	Q	602	4	1/1/18/18	10/42/82/82	-
18	3PE	T	202	-	-	11/29/29/54	-
21	CDL	G	201	-	-	32/85/85/110	-
32	PLM	Z	202	13	-	1/2/2/15	-
21	CDL	O	606	-	-	34/76/76/110	-
21	CDL	B	606	-	-	10/54/54/110	-
24	HEC	P	301	3	-	6/14/54/54	-
31	DGA	E	403	-	-	2/20/20/45	-
31	DGA	R	404	-	-	2/25/25/45	-
18	3PE	Q	609	-	-	14/42/42/54	-
32	PLM	M	202	13	-	0/2/2/15	-
31	DGA	H	201	-	-	0/17/17/45	-
32	PLM	U	202	8	-	2/14/14/15	-
20	HEM	B	602	2	-	2/14/54/54	-
21	CDL	D	607	-	-	38/87/87/110	-
23	LMT	O	601	-	-	11/18/58/61	0/2/2/2
18	3PE	F	301	-	-	20/35/35/54	-
24	HEC	P	302	3	-	6/14/54/54	-
24	HEC	C	302	3	-	6/14/54/54	-
20	HEM	B	603	2	-	2/14/54/54	-
31	DGA	Z	201	-	-	4/29/29/45	-
31	DGA	U	201	-	-	6/27/27/45	-
33	IX7	H	204	-	-	31/58/122/146	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	Q	608	-	-	18/76/76/110	-
16	9YF	A	503	-	-	14/31/55/78	0/1/1/1
21	CDL	I	201	-	-	25/67/67/110	-
18	3PE	L	101	-	-	12/33/33/54	-
18	3PE	S	301	-	-	21/46/46/54	-
19	SMA	B	601	-	-	10/34/34/34	0/2/2/2
22	LYC	O	607	-	-	1/43/43/43	-
32	PLM	H	202	8	-	1/14/14/15	-
18	3PE	J	201	-	-	26/50/50/54	-
18	3PE	N	502	-	-	8/41/41/54	-
18	3PE	T	205	-	-	12/41/41/54	-
21	CDL	T	204	-	-	28/75/75/110	-
25	HAS	D	602	29,4	1/1/18/18	19/42/82/82	-
18	3PE	C	303	-	-	11/28/28/54	-
14	FES	A	501	1	-	-	0/1/1/1
21	CDL	S	302	-	-	30/75/75/110	-
25	HAS	Q	601	4	1/1/18/18	10/42/82/82	-
15	IZL	A	502	-	-	31/73/197/208	0/6/6/6
18	3PE	C	304	-	-	10/28/28/54	-
18	3PE	R	405	-	-	15/34/34/54	-
22	LYC	B	607	-	-	4/43/43/43	-
21	CDL	B	609	-	-	30/80/80/110	-
18	3PE	T	203	-	-	17/45/45/54	-
18	3PE	D	609	-	-	13/34/34/54	-
21	CDL	B	605	-	-	23/66/66/110	-
18	3PE	P	303	-	-	15/30/30/54	-
18	3PE	W	201	-	-	24/50/50/54	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	302	HEC	CAC-C3C	5.87	1.54	1.35
24	P	302	HEC	CAC-C3C	5.72	1.53	1.35
24	C	301	HEC	CAC-C3C	5.59	1.53	1.35
24	C	301	HEC	CAB-C3B	5.54	1.53	1.35
24	C	302	HEC	CAB-C3B	5.51	1.52	1.35
24	P	301	HEC	CAC-C3C	5.47	1.52	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	302	HEC	CAB-C3B	5.47	1.52	1.35
25	D	601	HAS	OMD-CMD	5.33	1.33	1.22
24	P	301	HEC	CAB-C3B	5.25	1.52	1.35
25	Q	602	HAS	OMD-CMD	5.14	1.33	1.22
25	D	602	HAS	OMD-CMD	5.12	1.33	1.22
25	Q	601	HAS	OMD-CMD	4.94	1.32	1.22
20	B	603	HEM	FE-ND	4.52	2.08	1.94
20	O	603	HEM	FE-NC	4.22	2.09	1.95
20	O	603	HEM	FE-NB	4.02	2.07	1.94
20	B	602	HEM	FE-NA	3.82	2.07	1.95
20	O	604	HEM	FE-NB	3.58	2.05	1.94
19	B	601	SMA	C20-C19	3.40	1.36	1.33
17	B	604	MQ9	C6-C5	3.17	1.40	1.35
25	D	601	HAS	CMD-C2D	3.04	1.52	1.45
25	D	602	HAS	CMD-C2D	3.04	1.52	1.45
17	A	504	MQ9	C6-C1	2.94	1.54	1.47
20	B	602	HEM	FE-NC	2.94	2.04	1.95
25	Q	602	HAS	CMD-C2D	2.88	1.51	1.45
20	B	602	HEM	FE-NB	2.84	2.03	1.94
25	Q	602	HAS	FE-NB	2.82	2.03	1.94
25	Q	601	HAS	CMD-C2D	2.78	1.51	1.45
25	D	601	HAS	FE-NB	2.78	2.03	1.94
25	D	602	HAS	FE-ND	2.72	2.03	1.94
29	Q	605	AZI	N3-N2	-2.70	1.17	1.23
25	Q	601	HAS	FE-ND	2.70	2.03	1.94
17	O	605	MQ9	C6-C5	2.67	1.40	1.35
20	B	603	HEM	FE-NC	2.65	2.03	1.95
25	Q	602	HAS	FE-ND	2.63	2.03	1.94
25	D	601	HAS	FE-ND	2.62	2.03	1.94
25	D	602	HAS	FE-NB	2.61	2.02	1.94
25	Q	601	HAS	FE-NB	2.60	2.02	1.94
29	D	606	AZI	N1-N2	-2.60	1.17	1.23
29	Q	605	AZI	N1-N2	-2.59	1.17	1.23
20	O	603	HEM	FE-NA	2.56	2.03	1.95
25	Q	602	HAS	FE-NA	2.50	2.03	1.95
25	D	601	HAS	FE-NA	2.48	2.03	1.95
25	D	602	HAS	FE-NA	2.47	2.03	1.95
25	D	602	HAS	FE-NC	2.43	2.03	1.95
25	D	601	HAS	FE-NC	2.42	2.03	1.95
20	O	604	HEM	FE-NA	2.41	2.03	1.95
25	D	602	HAS	C11-C3B	-2.38	1.48	1.51
25	Q	601	HAS	FE-NA	2.37	2.03	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	602	HAS	FE-NC	2.36	2.03	1.95
25	Q	601	HAS	FE-NC	2.34	2.02	1.95
25	Q	601	HAS	CAC-C3C	2.34	1.53	1.47
20	O	604	HEM	FE-NC	2.34	2.02	1.95
29	D	606	AZI	N3-N2	-2.31	1.18	1.23
25	Q	601	HAS	C11-C3B	-2.30	1.48	1.51
17	N	501	MQ9	C6-C5	2.25	1.39	1.35
19	O	602	SMA	C13-C14	2.21	1.62	1.54
20	O	604	HEM	FE-ND	2.20	2.01	1.94
20	O	603	HEM	CAB-C3B	2.20	1.53	1.47
19	B	601	SMA	C13-C12	2.20	1.59	1.54
25	Q	602	HAS	CAC-C3C	2.16	1.53	1.47
20	B	603	HEM	CAB-C3B	2.07	1.52	1.47
25	D	601	HAS	CAC-C3C	2.02	1.52	1.47
20	O	604	HEM	CAC-C3C	2.02	1.52	1.47
17	A	504	MQ9	C6-C5	2.02	1.38	1.35

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	301	HEC	CBB-CAB-C3B	-8.44	110.56	127.43
24	P	302	HEC	CBB-CAB-C3B	-7.98	111.48	127.43
24	C	302	HEC	CBB-CAB-C3B	-7.42	112.60	127.43
24	P	301	HEC	CBC-CAC-C3C	-6.92	113.61	127.43
17	B	604	MQ9	C8-C7-C6	6.74	128.68	112.08
24	P	302	HEC	CBC-CAC-C3C	-5.96	115.52	127.43
24	C	301	HEC	CBC-CAC-C3C	-5.90	115.65	127.43
25	Q	602	HAS	C26-C15-C16	5.84	125.37	115.23
17	O	605	MQ9	C8-C7-C6	5.33	125.20	112.08
24	C	301	HEC	CBB-CAB-C3B	-5.01	117.42	127.43
25	D	601	HAS	C25-C23-C24	5.01	123.92	115.23
20	O	603	HEM	CAA-C2A-C1A	4.96	134.62	124.94
25	D	601	HAS	C27-C19-C20	4.77	123.51	115.23
25	D	602	HAS	C26-C15-C16	4.66	123.31	115.23
23	O	601	LMT	O1B-C4'-C3'	4.63	118.99	107.23
25	Q	601	HAS	C26-C15-C16	4.60	123.20	115.23
24	C	302	HEC	CBC-CAC-C3C	-4.52	118.41	127.43
25	D	602	HAS	C27-C19-C20	4.49	123.02	115.23
25	D	601	HAS	C26-C15-C14	-4.40	112.32	123.63
25	D	601	HAS	C26-C15-C16	4.36	122.80	115.23
25	Q	602	HAS	C26-C15-C14	-4.15	112.97	123.63
15	N	504	IZL	O36-C71-C13	4.04	119.70	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	602	HAS	C26-C15-C14	-3.97	113.44	123.63
15	A	502	IZL	O7-C18-C43	-3.90	97.52	107.42
25	Q	601	HAS	C26-C15-C14	-3.85	113.75	123.63
21	G	201	CDL	OB8-CB6-CB4	3.80	119.36	108.40
18	W	201	3PE	O21-C2-C3	-3.79	94.74	108.34
15	A	502	IZL	O32-C46-C45	3.79	119.32	108.40
17	N	501	MQ9	C8-C7-C6	3.79	121.41	112.08
15	N	504	IZL	O32-C46-C45	3.72	119.12	108.40
20	O	603	HEM	CAA-C2A-C3A	-3.69	118.79	127.07
20	B	602	HEM	CAA-C2A-C1A	3.64	132.05	124.94
33	H	204	IX7	O6-C22-C23	3.62	119.21	109.94
33	U	204	IX7	O7-C23-C22	-3.60	98.07	107.23
17	O	605	MQ9	C7-C6-C1	-3.53	114.86	118.58
17	B	604	MQ9	C7-C6-C1	-3.53	114.86	118.58
15	N	504	IZL	O7-C18-C17	3.49	116.11	107.23
25	Q	602	HAS	CAA-C2A-C3A	3.45	134.32	127.87
25	D	601	HAS	C25-C23-C22	-3.42	114.83	123.63
18	F	301	3PE	O21-C2-C1	3.37	120.43	108.34
17	A	504	MQ9	C7-C8-C9	3.35	132.61	126.83
25	D	602	HAS	CMC-C2C-C1C	-3.19	120.57	125.42
25	Q	602	HAS	CAA-C2A-C1A	-3.16	118.44	124.85
18	W	201	3PE	O21-C2-C1	3.15	119.65	108.34
15	A	502	IZL	C17-C18-C43	-3.03	104.91	111.72
25	Q	601	HAS	OMD-CMD-C2D	-3.00	118.85	125.62
25	Q	602	HAS	C27-C19-C18	-3.00	115.93	123.63
25	Q	602	HAS	C12-C13-C14	-2.99	104.31	112.16
25	D	602	HAS	OMD-CMD-C2D	-2.97	118.92	125.62
25	Q	602	HAS	C20-C19-C18	2.93	127.75	121.17
25	Q	601	HAS	C27-C19-C20	2.91	120.29	115.23
25	D	601	HAS	CAD-CBD-CGD	-2.87	106.05	113.67
25	Q	602	HAS	C28-C24-C23	-2.84	103.76	113.19
23	O	601	LMT	C1B-O1B-C4'	2.83	124.68	117.98
25	D	602	HAS	C27-C19-C18	-2.82	116.38	123.63
25	Q	602	HAS	OMD-CMD-C2D	-2.82	119.26	125.62
25	Q	601	HAS	C32-C30-C31	2.77	120.96	114.59
25	D	601	HAS	OMD-CMD-C2D	-2.76	119.39	125.62
20	O	603	HEM	CBA-CAA-C2A	2.75	120.13	112.53
15	A	502	IZL	C19-C42-C41	2.74	115.78	110.01
33	H	204	IX7	C24-O7-C23	2.74	124.46	117.98
33	H	204	IX7	O6-C22-C21	-2.73	103.94	110.38
20	B	602	HEM	CBA-CAA-C2A	2.73	120.08	112.53
25	D	602	HAS	C25-C23-C24	2.72	119.94	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	501	MQ9	C7-C6-C1	-2.72	115.72	118.58
33	H	204	IX7	O7-C23-C30	-2.69	100.59	107.42
24	C	301	HEC	CHD-C4C-NC	2.69	127.38	124.45
21	O	606	CDL	OB6-CB4-CB6	-2.67	98.76	108.34
18	W	201	3PE	O31-C3-C2	2.66	116.07	108.40
17	O	605	MQ9	C12-C11-C9	2.63	121.91	113.19
21	D	607	CDL	OA8-CA6-CA4	2.61	115.93	108.40
15	N	504	IZL	C49-C48-C47	2.61	123.26	113.69
17	A	504	MQ9	O1-C1-C2	-2.59	117.42	121.57
24	C	301	HEC	CHC-C4B-C3B	2.59	129.57	125.21
25	D	601	HAS	C2D-C3D-C4D	2.58	108.29	106.43
25	Q	602	HAS	CMC-C2C-C1C	-2.57	121.50	125.42
19	B	601	SMA	C22-C11-C12	2.57	115.34	111.14
18	S	301	3PE	O21-C2-C3	2.54	117.46	108.34
17	A	504	MQ9	C8-C7-C6	2.53	118.32	112.08
18	J	201	3PE	O31-C3-C2	2.52	115.67	108.40
25	Q	602	HAS	C13-C12-C11	-2.51	110.39	114.39
25	D	602	HAS	CHB-C1B-NB	2.45	127.06	124.42
33	U	204	IX7	O1-C16-C17	-2.43	103.27	108.41
15	N	504	IZL	O7-C18-C43	-2.43	101.26	107.42
21	S	302	CDL	OA6-CA4-CA6	-2.42	99.66	108.34
17	A	504	MQ9	C47-C46-C44	2.42	121.19	113.19
24	C	302	HEC	C2A-C1A-NA	-2.41	107.99	110.32
18	P	303	3PE	O31-C3-C2	2.41	115.35	108.40
33	U	204	IX7	O13-P-O14	-2.36	102.26	109.81
15	N	504	IZL	O31-P-O29	2.35	118.24	108.94
25	Q	602	HAS	C32-C30-C31	2.35	119.99	114.59
15	N	504	IZL	O15-C29-C30	2.34	115.95	109.94
20	O	603	HEM	CHA-C4D-ND	2.34	127.26	124.37
25	D	602	HAS	CMC-C2C-C3C	2.33	132.02	126.55
18	T	206	3PE	O21-C2-C3	-2.33	100.00	108.34
15	A	502	IZL	O3-C14-C43	2.32	113.32	107.42
25	D	601	HAS	C32-C30-C31	2.32	119.93	114.59
21	G	202	CDL	OA6-CA4-CA6	-2.32	100.03	108.34
25	D	602	HAS	C12-C11-C3B	-2.31	108.52	112.12
15	N	504	IZL	O14-C28-C29	-2.30	104.96	110.38
20	B	602	HEM	CHA-C4D-ND	2.29	127.20	124.37
25	Q	602	HAS	CMA-C3A-C2A	2.29	132.33	126.15
15	N	504	IZL	O12-C25-C30	-2.28	105.06	109.49
33	U	204	IX7	C18-C67-C68	2.28	114.80	110.01
22	O	607	LYC	C59-C60-C61	-2.28	124.49	127.69
25	D	601	HAS	CHB-C1B-NB	2.27	126.86	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	504	IZL	C16-C17-C18	2.24	114.77	109.68
21	T	204	CDL	OA6-CA4-CA3	2.24	116.36	108.34
25	Q	601	HAS	C20-C19-C18	-2.22	116.19	121.17
15	A	502	IZL	C22-C39-C38	2.19	114.61	110.01
20	B	602	HEM	CAA-C2A-C3A	-2.19	122.17	127.07
25	D	602	HAS	C32-C30-C29	-2.19	116.10	122.66
19	B	601	SMA	C12-C13-C14	2.18	117.94	111.99
18	P	303	3PE	O21-C2-C1	2.16	116.09	108.34
25	Q	601	HAS	C2D-C3D-C4D	2.15	107.99	106.43
21	T	201	CDL	OA6-CA4-CA6	-2.14	100.67	108.34
17	A	504	MQ9	C22-C21-C19	2.14	120.27	113.19
15	A	502	IZL	C21-O9-C22	-2.14	109.21	113.80
25	Q	602	HAS	C2D-C3D-C4D	2.14	107.97	106.43
21	G	202	CDL	OA6-CA4-CA3	2.13	116.00	108.34
15	A	502	IZL	C38-C37-C23	-2.13	106.36	110.23
15	N	504	IZL	O16-C30-C29	-2.13	101.82	107.23
15	A	502	IZL	C18-C43-C14	2.13	115.10	110.43
15	N	504	IZL	C35-C34-C32	-2.13	106.38	110.23
15	N	504	IZL	C66-C65-C64	2.12	127.66	113.36
25	D	601	HAS	C21-C20-C19	2.11	120.17	113.19
33	H	204	IX7	O19-C32-C31	2.08	115.82	108.34
20	O	603	HEM	O2A-CGA-CBA	2.08	120.58	114.00
20	O	603	HEM	CHA-C1A-C2A	2.08	129.85	125.30
24	P	302	HEC	C2A-C1A-NA	-2.06	108.33	110.32
21	F	302	CDL	OA8-CA6-CA4	-2.05	102.50	108.40
20	O	603	HEM	C4D-ND-C1D	2.02	107.61	105.21
18	C	304	3PE	O31-C3-C2	2.02	114.22	108.40
25	Q	601	HAS	CHB-C1B-NB	2.02	126.59	124.42
15	N	504	IZL	O11-C25-C30	2.01	112.12	108.31
20	O	604	HEM	CBD-CAD-C3D	-2.01	106.96	112.53
15	N	504	IZL	O32-C47-C48	-2.01	105.70	111.83
33	H	204	IX7	O17-C33-C32	2.00	114.17	108.40
15	A	502	IZL	O28-C43-C18	-2.00	104.50	108.76

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	D	601	HAS	NA
25	D	602	HAS	NA
25	Q	601	HAS	NA
25	Q	602	HAS	NA

All (1064) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	502	IZL	C44-O31-P-O28
15	A	502	IZL	C44-O31-P-O30
15	N	504	IZL	O10-C22-O9-C21
15	N	504	IZL	C61-C60-O34-C45
15	N	504	IZL	C43-O28-P-O31
16	A	503	9YF	C2-O2-P-O1
16	A	503	9YF	C1-O-P-O1
16	A	503	9YF	C1-O-P-O2
16	A	503	9YF	C1-O-P-O8
16	N	505	9YF	C2-O2-P-O1
16	N	505	9YF	C2-O2-P-O
17	A	504	MQ9	C5-C6-C7-C8
17	A	504	MQ9	C1-C6-C7-C8
17	B	604	MQ9	C5-C6-C7-C8
17	B	604	MQ9	C1-C6-C7-C8
17	O	605	MQ9	C5-C6-C7-C8
17	O	605	MQ9	C1-C6-C7-C8
18	A	505	3PE	C1-O11-P-O12
18	A	505	3PE	C11-O13-P-O14
18	A	505	3PE	O13-C11-C12-N
18	C	303	3PE	C11-O13-P-O14
18	C	303	3PE	O13-C11-C12-N
18	C	304	3PE	C1-O11-P-O12
18	C	304	3PE	C1-O11-P-O13
18	D	609	3PE	C1-O11-P-O12
18	D	609	3PE	C1-O11-P-O13
18	D	609	3PE	C11-O13-P-O14
18	D	609	3PE	C2-C1-O11-P
18	D	609	3PE	O13-C11-C12-N
18	F	301	3PE	C11-O13-P-O14
18	F	301	3PE	O13-C11-C12-N
18	J	201	3PE	C1-O11-P-O14
18	J	201	3PE	C11-O13-P-O11
18	J	201	3PE	O13-C11-C12-N
18	L	101	3PE	C11-O13-P-O11
18	L	101	3PE	C11-O13-P-O12
18	L	101	3PE	C12-C11-O13-P
18	N	502	3PE	O13-C11-C12-N
18	P	303	3PE	C1-O11-P-O12
18	P	303	3PE	C1-O11-P-O13
18	P	303	3PE	C11-O13-P-O11
18	Q	609	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	R	405	3PE	C1-O11-P-O14
18	R	405	3PE	C11-O13-P-O11
18	R	405	3PE	C11-O13-P-O12
18	R	405	3PE	C11-O13-P-O14
18	R	405	3PE	O13-C11-C12-N
18	S	301	3PE	C11-O13-P-O11
18	S	301	3PE	C11-O13-P-O12
18	S	301	3PE	C11-O13-P-O14
18	S	301	3PE	O13-C11-C12-N
18	S	301	3PE	C3-C2-O21-C21
18	S	301	3PE	C22-C21-O21-C2
18	T	202	3PE	C1-O11-P-O12
18	T	202	3PE	C11-O13-P-O14
18	T	202	3PE	O13-C11-C12-N
18	T	203	3PE	C1-O11-P-O12
18	T	203	3PE	C1-O11-P-O13
18	T	203	3PE	C1-O11-P-O14
18	T	203	3PE	O13-C11-C12-N
18	T	205	3PE	C11-O13-P-O11
18	T	205	3PE	C12-C11-O13-P
18	T	206	3PE	C11-O13-P-O14
18	T	206	3PE	O13-C11-C12-N
18	W	201	3PE	O22-C21-O21-C2
18	W	201	3PE	C22-C21-O21-C2
19	B	601	SMA	C11-C10-C9-C2
19	B	601	SMA	C10-C11-C12-C13
19	B	601	SMA	C10-C11-C12-O12
19	B	601	SMA	C22-C11-C12-C13
19	B	601	SMA	C22-C11-C12-O12
19	O	602	SMA	C12-C13-C14-C15
19	O	602	SMA	C12-C13-C14-O14
19	O	602	SMA	C24-C13-C14-C15
19	O	602	SMA	C24-C13-C14-O14
19	O	602	SMA	O14-C14-C15-C16
20	O	603	HEM	C1A-C2A-CAA-CBA
21	B	605	CDL	CA2-OA2-PA1-OA3
21	B	605	CDL	CA3-OA5-PA1-OA4
21	B	605	CDL	CB3-OB5-PB2-OB2
21	B	605	CDL	CB3-OB5-PB2-OB3
21	B	605	CDL	CB3-OB5-PB2-OB4
21	B	606	CDL	OB6-CB4-CB6-OB8
21	B	609	CDL	CB2-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	609	CDL	CA3-OA5-PA1-OA4
21	B	609	CDL	CB2-OB2-PB2-OB3
21	B	609	CDL	CB2-OB2-PB2-OB4
21	B	609	CDL	CB2-OB2-PB2-OB5
21	B	609	CDL	CB3-OB5-PB2-OB2
21	B	609	CDL	CB3-OB5-PB2-OB4
21	D	607	CDL	CA2-OA2-PA1-OA4
21	D	607	CDL	CA3-OA5-PA1-OA2
21	D	607	CDL	CA3-OA5-PA1-OA3
21	D	607	CDL	CA3-OA5-PA1-OA4
21	D	607	CDL	CB2-OB2-PB2-OB3
21	D	607	CDL	CB2-OB2-PB2-OB4
21	D	607	CDL	CB2-OB2-PB2-OB5
21	D	607	CDL	CB3-OB5-PB2-OB2
21	D	607	CDL	CB3-OB5-PB2-OB3
21	D	608	CDL	CA2-OA2-PA1-OA3
21	D	608	CDL	CA3-OA5-PA1-OA2
21	D	608	CDL	CB2-OB2-PB2-OB3
21	D	608	CDL	CB2-OB2-PB2-OB5
21	D	608	CDL	CB3-OB5-PB2-OB2
21	D	608	CDL	CB3-OB5-PB2-OB4
21	F	302	CDL	CA2-OA2-PA1-OA3
21	F	302	CDL	CA3-OA5-PA1-OA2
21	F	302	CDL	CA3-OA5-PA1-OA4
21	F	302	CDL	CB2-OB2-PB2-OB4
21	F	302	CDL	CB2-OB2-PB2-OB5
21	F	302	CDL	CB3-OB5-PB2-OB3
21	G	201	CDL	CA2-OA2-PA1-OA3
21	G	201	CDL	CA2-OA2-PA1-OA5
21	G	202	CDL	C1-CA2-OA2-PA1
21	G	202	CDL	CA2-OA2-PA1-OA3
21	G	202	CDL	CA2-OA2-PA1-OA5
21	G	202	CDL	OA7-CA5-OA6-CA4
21	G	202	CDL	C11-CA5-OA6-CA4
21	G	202	CDL	CB3-OB5-PB2-OB4
21	I	201	CDL	O1-C1-CB2-OB2
21	I	201	CDL	CA2-C1-CB2-OB2
21	I	201	CDL	CA2-OA2-PA1-OA3
21	I	201	CDL	CA2-OA2-PA1-OA5
21	I	201	CDL	CB4-CB3-OB5-PB2
21	O	606	CDL	CA2-C1-CB2-OB2
21	O	606	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	O	606	CDL	CB2-OB2-PB2-OB3
21	O	606	CDL	CB2-OB2-PB2-OB5
21	O	606	CDL	CB3-OB5-PB2-OB2
21	O	606	CDL	CB3-OB5-PB2-OB3
21	Q	607	CDL	CA3-OA5-PA1-OA4
21	Q	607	CDL	CB2-OB2-PB2-OB3
21	Q	607	CDL	CB2-OB2-PB2-OB4
21	Q	607	CDL	CB2-OB2-PB2-OB5
21	Q	608	CDL	C1-CA2-OA2-PA1
21	Q	608	CDL	CA2-OA2-PA1-OA5
21	S	302	CDL	CA3-OA5-PA1-OA2
21	S	302	CDL	CA3-OA5-PA1-OA3
21	S	302	CDL	CB2-OB2-PB2-OB3
21	S	302	CDL	CB2-OB2-PB2-OB4
21	S	302	CDL	CB2-OB2-PB2-OB5
21	T	201	CDL	CA2-OA2-PA1-OA4
21	T	201	CDL	CA2-OA2-PA1-OA5
21	T	201	CDL	CA3-OA5-PA1-OA3
21	T	201	CDL	CB2-OB2-PB2-OB3
21	T	201	CDL	CB2-OB2-PB2-OB4
21	T	201	CDL	CB3-OB5-PB2-OB2
21	T	201	CDL	CB3-OB5-PB2-OB4
21	T	204	CDL	CA3-OA5-PA1-OA2
21	T	204	CDL	CA3-OA5-PA1-OA3
21	T	204	CDL	CA3-OA5-PA1-OA4
21	T	204	CDL	CB2-OB2-PB2-OB3
21	T	204	CDL	CB3-OB5-PB2-OB3
21	V	201	CDL	O1-C1-CA2-OA2
21	V	201	CDL	CB2-C1-CA2-OA2
21	V	201	CDL	CA2-OA2-PA1-OA4
21	V	201	CDL	CA2-OA2-PA1-OA5
21	V	201	CDL	CA3-OA5-PA1-OA2
21	V	201	CDL	CA3-OA5-PA1-OA4
21	V	201	CDL	CB3-OB5-PB2-OB3
23	B	608	LMT	C2-C1-O1'-C1'
23	O	601	LMT	O5'-C1'-O1'-C1
24	C	301	HEC	C2B-C3B-CAB-CBB
24	C	301	HEC	C4B-C3B-CAB-CBB
24	C	301	HEC	C2C-C3C-CAC-CBC
24	C	301	HEC	C4C-C3C-CAC-CBC
24	C	302	HEC	C2B-C3B-CAB-CBB
24	C	302	HEC	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	302	HEC	C2C-C3C-CAC-CBC
24	C	302	HEC	C4C-C3C-CAC-CBC
24	P	301	HEC	C2B-C3B-CAB-CBB
24	P	301	HEC	C4B-C3B-CAB-CBB
24	P	301	HEC	C2C-C3C-CAC-CBC
24	P	301	HEC	C4C-C3C-CAC-CBC
24	P	302	HEC	C2B-C3B-CAB-CBB
24	P	302	HEC	C4B-C3B-CAB-CBB
24	P	302	HEC	C2C-C3C-CAC-CBC
24	P	302	HEC	C4C-C3C-CAC-CBC
25	D	601	HAS	C26-C15-C16-C17
25	Q	601	HAS	C23-C24-C28-C29
25	Q	602	HAS	C1A-C2A-CAA-CBA
31	E	403	DGA	OG1-CG1-CG2-OG2
31	E	403	DGA	OG1-CG1-CG2-CG3
31	U	201	DGA	OG1-CG1-CG2-OG2
31	U	201	DGA	OG1-CG1-CG2-CG3
32	Z	202	PLM	O2-C1-C2-C3
33	H	204	IX7	O8-C24-O7-C23
33	H	204	IX7	O20-C56-O19-C32
33	H	204	IX7	C30-O13-P-O15
33	H	204	IX7	C30-O13-P-O16
33	H	204	IX7	C31-O16-P-O13
33	H	204	IX7	C31-O16-P-O14
33	U	204	IX7	C57-C56-O19-C32
23	O	601	LMT	C3'-C4'-O1B-C1B
15	A	502	IZL	C53-C54-C55-C56
19	O	602	SMA	C15-C16-C17-C18
15	N	504	IZL	O35-C60-O34-C45
18	S	301	3PE	O22-C21-O21-C2
21	G	201	CDL	CB4-CB6-OB8-CB7
21	T	204	CDL	C11-CA5-OA6-CA4
33	H	204	IX7	C57-C56-O19-C32
17	A	504	MQ9	C25-C24-C26-C27
25	D	601	HAS	C27-C19-C20-C21
25	D	602	HAS	C26-C15-C16-C17
25	Q	601	HAS	C26-C15-C16-C17
25	D	601	HAS	C14-C15-C16-C17
25	D	602	HAS	C14-C15-C16-C17
25	Q	601	HAS	C14-C15-C16-C17
15	N	504	IZL	C48-C47-O32-C46
15	N	504	IZL	C17-C18-O7-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	609	CDL	O1-C1-CA2-OA2
21	O	606	CDL	O1-C1-CA2-OA2
18	J	201	3PE	C32-C31-O31-C3
15	A	502	IZL	C61-C60-O34-C45
18	T	206	3PE	C22-C21-O21-C2
17	O	605	MQ9	C12-C11-C9-C10
25	D	601	HAS	C25-C23-C24-C28
25	D	602	HAS	C27-C19-C20-C21
25	Q	602	HAS	C26-C15-C16-C17
17	O	605	MQ9	C12-C11-C9-C8
25	D	601	HAS	C18-C19-C20-C21
25	D	601	HAS	C22-C23-C24-C28
25	D	602	HAS	C18-C19-C20-C21
25	Q	602	HAS	C14-C15-C16-C17
17	A	504	MQ9	C19-C21-C22-C23
17	A	504	MQ9	C29-C31-C32-C33
17	A	504	MQ9	C44-C46-C47-C48
17	B	604	MQ9	C9-C11-C12-C13
17	N	501	MQ9	C9-C11-C12-C13
17	O	605	MQ9	C14-C16-C17-C18
22	O	607	LYC	C61-C63-C64-C65
25	D	601	HAS	C15-C16-C17-C18
25	D	601	HAS	C19-C20-C21-C22
25	D	602	HAS	C23-C24-C28-C29
15	N	504	IZL	C34-C32-C33-O18
18	W	201	3PE	C25-C26-C27-C28
20	B	602	HEM	C1A-C2A-CAA-CBA
25	Q	602	HAS	C3A-C2A-CAA-CBA
20	B	602	HEM	C3A-C2A-CAA-CBA
23	O	601	LMT	O5'-C5'-C6'-O6'
15	N	504	IZL	C49-C50-C51-C52
17	A	504	MQ9	C7-C8-C9-C11
18	F	301	3PE	C22-C21-O21-C2
21	S	302	CDL	C11-CA5-OA6-CA4
33	U	204	IX7	C27-C25-C26-O9
15	N	504	IZL	O33-C47-O32-C46
21	T	204	CDL	OA7-CA5-OA6-CA4
21	B	605	CDL	CB2-C1-CA2-OA2
21	F	302	CDL	CA2-C1-CB2-OB2
21	I	201	CDL	CB2-C1-CA2-OA2
21	S	302	CDL	CB2-C1-CA2-OA2
15	A	502	IZL	C48-C47-O32-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	P	303	3PE	C32-C31-O31-C3
18	W	201	3PE	C32-C31-O31-C3
18	S	301	3PE	C33-C34-C35-C36
15	N	504	IZL	O1-C11-C12-C73
23	O	601	LMT	C4'-C5'-C6'-O6'
15	N	504	IZL	O17-C31-O16-C30
15	A	502	IZL	C43-C18-O7-C19
15	N	504	IZL	O1-C11-C12-O2
21	B	605	CDL	O1-C1-CA2-OA2
21	B	605	CDL	O1-C1-CB2-OB2
21	F	302	CDL	O1-C1-CB2-OB2
21	I	201	CDL	O1-C1-CA2-OA2
21	O	606	CDL	O1-C1-CB2-OB2
21	S	302	CDL	O1-C1-CA2-OA2
21	V	201	CDL	O1-C1-CB2-OB2
18	J	201	3PE	O32-C31-O31-C3
15	N	504	IZL	O17-C32-C33-O18
23	O	601	LMT	O5B-C5B-C6B-O6B
19	B	601	SMA	C17-C18-C19-C20
15	N	504	IZL	C47-C48-C49-C50
18	J	201	3PE	C21-C22-C23-C24
21	Q	607	CDL	CB5-C51-C52-C53
15	A	502	IZL	O35-C60-O34-C45
33	U	204	IX7	O20-C56-O19-C32
16	U	203	9YF	C25-C26-C27-C28
18	W	201	3PE	C29-C2A-C2B-C2C
33	U	204	IX7	O8-C25-C26-O9
16	H	203	9YF	C25-C26-C27-C28
18	D	609	3PE	C21-C22-C23-C24
33	H	204	IX7	C56-C57-C58-C59
33	U	204	IX7	C34-C35-C36-C37
15	A	502	IZL	O1-C11-C12-O2
25	D	602	HAS	C3D-CAD-CBD-CGD
16	A	503	9YF	C25-C26-C27-C28
18	C	303	3PE	C31-C32-C33-C34
18	L	101	3PE	C21-C22-C23-C24
18	T	203	3PE	C31-C32-C33-C34
21	D	607	CDL	CB7-C71-C72-C73
21	F	302	CDL	CA7-C31-C32-C33
21	S	302	CDL	CA7-C31-C32-C33
20	O	603	HEM	C3A-C2A-CAA-CBA
21	V	201	CDL	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	608	CDL	O1-C1-CB2-OB2
15	A	502	IZL	O33-C47-O32-C46
18	P	303	3PE	O32-C31-O31-C3
21	G	202	CDL	CB7-C71-C72-C73
21	T	201	CDL	CB5-C51-C52-C53
33	H	204	IX7	C12-C13-C14-C15
18	T	206	3PE	C28-C29-C2A-C2B
18	W	201	3PE	O32-C31-O31-C3
18	W	201	3PE	C36-C37-C38-C39
18	T	206	3PE	C32-C31-O31-C3
31	U	201	DGA	CB1-CB2-CB3-CB4
15	A	502	IZL	O1-C11-C12-C73
18	F	301	3PE	O22-C21-O21-C2
18	T	206	3PE	O22-C21-O21-C2
15	A	502	IZL	C28-C26-C27-O13
21	B	605	CDL	CA2-C1-CB2-OB2
21	D	608	CDL	CA2-C1-CB2-OB2
21	G	201	CDL	CA2-C1-CB2-OB2
18	F	301	3PE	C31-C32-C33-C34
21	D	607	CDL	CA7-C31-C32-C33
33	H	204	IX7	C35-C36-C37-C38
21	S	302	CDL	OA7-CA5-OA6-CA4
23	O	601	LMT	C2'-C1'-O1'-C1
21	G	201	CDL	CA5-C11-C12-C13
25	Q	602	HAS	C23-C24-C28-C29
21	F	302	CDL	O1-C1-CA2-OA2
19	B	601	SMA	C17-C18-C19-C26
21	D	608	CDL	C1-CB2-OB2-PB2
18	W	201	3PE	C1-C2-O21-C21
21	G	202	CDL	CA3-CA4-OA6-CA5
21	T	204	CDL	CA3-CA4-OA6-CA5
21	T	204	CDL	C11-C12-C13-C14
21	I	201	CDL	C23-C24-C25-C26
33	H	204	IX7	O8-C25-C26-O9
21	B	609	CDL	OB6-CB4-CB6-OB8
21	G	201	CDL	CA7-C31-C32-C33
15	A	502	IZL	C50-C51-C52-C53
18	S	301	3PE	C36-C37-C38-C39
21	G	201	CDL	C19-C20-C21-C22
18	Q	609	3PE	C27-C28-C29-C2A
21	D	607	CDL	C15-C16-C17-C18
21	O	606	CDL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	O	606	CDL	C19-C20-C21-C22
21	T	201	CDL	C18-C19-C20-C21
21	T	204	CDL	C13-C14-C15-C16
18	S	301	3PE	C2A-C2B-C2C-C2D
18	T	205	3PE	C24-C25-C26-C27
18	T	206	3PE	C37-C38-C39-C3A
21	I	201	CDL	C11-C12-C13-C14
33	U	204	IX7	C9-C10-C11-C12
33	U	204	IX7	C62-C63-C64-C65
18	S	301	3PE	C38-C39-C3A-C3B
21	T	201	CDL	C34-C35-C36-C37
21	V	201	CDL	C38-C39-C40-C41
33	H	204	IX7	C10-C11-C12-C13
21	Q	608	CDL	C12-C13-C14-C15
15	A	502	IZL	C47-C48-C49-C50
18	T	202	3PE	C31-C32-C33-C34
21	B	609	CDL	CB5-C51-C52-C53
18	W	201	3PE	C39-C3A-C3B-C3C
21	O	606	CDL	C35-C36-C37-C38
15	N	504	IZL	C15-C14-O3-C13
15	A	502	IZL	C7-C8-C9-C10
16	H	203	9YF	C11-C10-C9-C8
18	D	609	3PE	C33-C34-C35-C36
21	B	609	CDL	C74-C75-C76-C77
21	T	201	CDL	C38-C39-C40-C41
23	B	608	LMT	C3-C4-C5-C6
21	V	201	CDL	C41-C42-C43-C44
21	V	201	CDL	C42-C43-C44-C45
31	U	201	DGA	CB6-CB7-CB8-CB9
18	T	206	3PE	C21-C22-C23-C24
21	D	608	CDL	CA7-C31-C32-C33
18	A	505	3PE	C24-C25-C26-C27
21	I	201	CDL	C22-C23-C24-C25
21	Q	607	CDL	C11-C12-C13-C14
21	S	302	CDL	C16-C17-C18-C19
21	T	201	CDL	C33-C34-C35-C36
31	U	201	DGA	CB7-CB8-CB9-CAB
21	G	202	CDL	C71-C72-C73-C74
18	A	505	3PE	C26-C27-C28-C29
23	B	608	LMT	C1-C2-C3-C4
21	I	201	CDL	C15-C16-C17-C18
21	O	606	CDL	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	S	302	CDL	C18-C19-C20-C21
15	N	504	IZL	C43-C18-O7-C19
21	Q	607	CDL	C31-C32-C33-C34
21	S	302	CDL	C13-C14-C15-C16
21	O	606	CDL	C51-CB5-OB6-CB4
21	B	609	CDL	C55-C56-C57-C58
21	D	607	CDL	C33-C34-C35-C36
21	S	302	CDL	C33-C34-C35-C36
33	U	204	IX7	C35-C36-C37-C38
18	T	206	3PE	C31-C32-C33-C34
18	S	301	3PE	C34-C35-C36-C37
21	B	609	CDL	C53-C54-C55-C56
17	A	504	MQ9	C45-C44-C46-C47
19	B	601	SMA	C16-C17-C18-C19
17	A	504	MQ9	C23-C24-C26-C27
18	L	101	3PE	C32-C33-C34-C35
18	T	206	3PE	C32-C33-C34-C35
21	D	608	CDL	C18-C19-C20-C21
21	G	202	CDL	C54-C55-C56-C57
21	V	201	CDL	C37-C38-C39-C40
33	H	204	IX7	C35-C34-O17-C33
18	Q	609	3PE	C22-C23-C24-C25
18	T	203	3PE	C22-C23-C24-C25
21	B	609	CDL	C32-C33-C34-C35
21	S	302	CDL	C36-C37-C38-C39
21	T	201	CDL	C55-C56-C57-C58
21	G	201	CDL	C14-C15-C16-C17
21	G	201	CDL	C32-C33-C34-C35
18	T	206	3PE	O32-C31-O31-C3
18	J	201	3PE	C24-C25-C26-C27
21	D	608	CDL	C21-C22-C23-C24
21	T	201	CDL	C17-C18-C19-C20
21	D	607	CDL	C58-C59-C60-C61
21	G	201	CDL	C13-C14-C15-C16
23	O	601	LMT	C1-C2-C3-C4
18	J	201	3PE	C22-C21-O21-C2
18	L	101	3PE	C22-C21-O21-C2
18	N	502	3PE	C22-C21-O21-C2
18	P	303	3PE	C22-C21-O21-C2
21	T	204	CDL	C51-CB5-OB6-CB4
21	O	606	CDL	OB7-CB5-OB6-CB4
21	B	609	CDL	C73-C74-C75-C76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	O	606	CDL	C14-C15-C16-C17
21	D	607	CDL	C38-C39-C40-C41
21	D	608	CDL	C32-C33-C34-C35
21	Q	607	CDL	C60-C61-C62-C63
21	S	302	CDL	C35-C36-C37-C38
33	U	204	IX7	C12-C13-C14-C15
15	N	504	IZL	O12-C26-C27-O13
21	D	608	CDL	C14-C15-C16-C17
25	D	602	HAS	C15-C16-C17-C18
18	L	101	3PE	C22-C23-C24-C25
18	T	203	3PE	C32-C33-C34-C35
18	W	201	3PE	C38-C39-C3A-C3B
21	G	201	CDL	C22-C23-C24-C25
21	D	607	CDL	C35-C36-C37-C38
18	C	304	3PE	O21-C2-C3-O31
18	T	202	3PE	O21-C2-C3-O31
21	D	607	CDL	OA6-CA4-CA6-OA8
21	G	201	CDL	OB6-CB4-CB6-OB8
21	O	606	CDL	OB6-CB4-CB6-OB8
18	W	201	3PE	C33-C34-C35-C36
21	D	607	CDL	C59-C60-C61-C62
21	G	201	CDL	CB5-C51-C52-C53
21	T	201	CDL	CB7-C71-C72-C73
18	T	203	3PE	C2D-C2E-C2F-C2G
33	U	204	IX7	C58-C59-C60-C61
21	B	605	CDL	C1-CA2-OA2-PA1
21	O	606	CDL	C34-C35-C36-C37
17	N	501	MQ9	C20-C19-C21-C22
18	L	101	3PE	O22-C21-O21-C2
21	F	302	CDL	CB2-C1-CA2-OA2
18	D	609	3PE	C23-C24-C25-C26
21	O	606	CDL	C31-C32-C33-C34
21	V	201	CDL	C18-C19-C20-C21
21	V	201	CDL	C32-C33-C34-C35
21	F	302	CDL	C31-CA7-OA8-CA6
18	D	609	3PE	C34-C35-C36-C37
18	J	201	3PE	C39-C3A-C3B-C3C
18	C	303	3PE	C22-C21-O21-C2
33	H	204	IX7	C7-C8-C9-C10
18	W	201	3PE	C22-C23-C24-C25
21	T	201	CDL	C16-C17-C18-C19
18	J	201	3PE	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	W	201	3PE	O11-C1-C2-C3
18	N	502	3PE	O22-C21-O21-C2
18	W	201	3PE	C32-C33-C34-C35
21	G	202	CDL	C11-C12-C13-C14
21	O	606	CDL	CA7-C31-C32-C33
21	Q	607	CDL	CA5-C11-C12-C13
17	A	504	MQ9	C18-C19-C21-C22
17	A	504	MQ9	C43-C44-C46-C47
17	N	501	MQ9	C18-C19-C21-C22
15	A	502	IZL	C17-C18-O7-C19
21	I	201	CDL	C20-C21-C22-C23
21	D	607	CDL	C31-C32-C33-C34
18	C	304	3PE	C1-C2-C3-O31
21	B	605	CDL	CA3-CA4-CA6-OA8
21	B	609	CDL	CB3-CB4-CB6-OB8
21	D	607	CDL	CA3-CA4-CA6-OA8
21	D	608	CDL	CA3-CA4-CA6-OA8
33	U	204	IX7	C61-C62-C63-C64
15	A	502	IZL	C48-C49-C50-C51
21	G	202	CDL	C59-C60-C61-C62
21	G	202	CDL	CB5-C51-C52-C53
25	D	601	HAS	C11-C12-C13-C14
18	L	101	3PE	C31-C32-C33-C34
18	Q	609	3PE	C21-C22-C23-C24
15	N	504	IZL	C43-C14-O3-C13
18	P	303	3PE	O22-C21-O21-C2
21	B	605	CDL	C52-C53-C54-C55
21	Q	607	CDL	C73-C74-C75-C76
18	S	301	3PE	C31-C32-C33-C34
21	B	609	CDL	C51-C52-C53-C54
18	W	201	3PE	C27-C28-C29-C2A
21	G	201	CDL	C53-C54-C55-C56
23	B	608	LMT	C5-C6-C7-C8
21	T	201	CDL	C13-C14-C15-C16
21	D	607	CDL	C51-C52-C53-C54
21	S	302	CDL	C51-C52-C53-C54
18	J	201	3PE	O22-C21-O21-C2
21	V	201	CDL	CA2-C1-CB2-OB2
18	S	301	3PE	C24-C25-C26-C27
33	H	204	IX7	C62-C63-C64-C65
18	R	405	3PE	C2A-C2B-C2C-C2D
21	V	201	CDL	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	T	206	3PE	C35-C36-C37-C38
21	Q	608	CDL	C32-C33-C34-C35
16	A	503	9YF	C12-C13-C14-C15
16	U	203	9YF	C28-C29-C30-C31
21	F	302	CDL	CA5-C11-C12-C13
33	U	204	IX7	C22-C23-O7-C24
16	A	503	9YF	O9-C-C24-O11
18	C	303	3PE	O21-C2-C3-O31
21	B	605	CDL	OA6-CA4-CA6-OA8
18	L	101	3PE	C24-C25-C26-C27
21	B	609	CDL	C76-C77-C78-C79
21	G	202	CDL	C33-C34-C35-C36
21	O	606	CDL	C12-C11-CA5-OA6
33	U	204	IX7	C57-C58-C59-C60
21	G	201	CDL	C24-C25-C26-C27
21	B	609	CDL	C54-C55-C56-C57
18	Q	609	3PE	C33-C34-C35-C36
18	A	505	3PE	C32-C31-O31-C3
21	D	607	CDL	CB5-C51-C52-C53
21	B	606	CDL	CB4-CB3-OB5-PB2
32	H	202	PLM	C3-C4-C5-C6
21	G	201	CDL	C71-CB7-OB8-CB6
15	N	504	IZL	C39-C22-O9-C21
18	T	203	3PE	O11-C1-C2-C3
21	Q	608	CDL	OB5-CB3-CB4-CB6
21	T	201	CDL	OB5-CB3-CB4-CB6
15	A	502	IZL	C54-C55-C56-C58
21	G	201	CDL	O1-C1-CB2-OB2
21	B	605	CDL	CA7-C31-C32-C33
21	D	608	CDL	C33-C34-C35-C36
15	A	502	IZL	C43-C14-O3-C13
21	T	201	CDL	C35-C36-C37-C38
18	S	301	3PE	C26-C27-C28-C29
15	A	502	IZL	C51-C52-C53-C54
21	Q	607	CDL	C32-C33-C34-C35
21	D	608	CDL	C16-C17-C18-C19
21	V	201	CDL	CA7-C31-C32-C33
21	T	204	CDL	OB7-CB5-OB6-CB4
23	B	608	LMT	C4B-C5B-C6B-O6B
15	A	502	IZL	O12-C26-C27-O13
16	H	203	9YF	C26-C25-O11-C24
21	I	201	CDL	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	T	202	3PE	C1-C2-C3-O31
18	W	201	3PE	C1-C2-C3-O31
21	B	606	CDL	CB3-CB4-CB6-OB8
21	G	201	CDL	CB3-CB4-CB6-OB8
21	O	606	CDL	CB3-CB4-CB6-OB8
21	T	201	CDL	CA3-CA4-CA6-OA8
21	V	201	CDL	CB3-CB4-CB6-OB8
33	H	204	IX7	C31-C32-C33-O17
17	A	504	MQ9	C20-C19-C21-C22
33	H	204	IX7	C9-C10-C11-C12
31	M	201	DGA	OG1-CG1-CG2-OG2
18	W	201	3PE	C2C-C2D-C2E-C2F
18	P	303	3PE	O11-C1-C2-O21
18	R	405	3PE	O11-C1-C2-O21
18	T	205	3PE	O11-C1-C2-O21
21	D	607	CDL	OB5-CB3-CB4-OB6
21	G	202	CDL	OB5-CB3-CB4-OB6
21	Q	607	CDL	OB5-CB3-CB4-OB6
21	T	201	CDL	OA5-CA3-CA4-OA6
21	V	201	CDL	OB5-CB3-CB4-OB6
21	I	201	CDL	C24-C25-C26-C27
18	A	505	3PE	C22-C21-O21-C2
21	O	606	CDL	C1-CB2-OB2-PB2
21	Q	608	CDL	CA4-CA3-OA5-PA1
18	A	505	3PE	O21-C2-C3-O31
18	W	201	3PE	O21-C2-C3-O31
21	Q	608	CDL	OB6-CB4-CB6-OB8
21	T	201	CDL	OA6-CA4-CA6-OA8
15	N	504	IZL	C62-C63-C64-C65
18	T	206	3PE	C36-C37-C38-C39
17	N	501	MQ9	C26-C27-C28-C29
18	T	203	3PE	C28-C29-C2A-C2B
21	F	302	CDL	OA9-CA7-OA8-CA6
18	J	201	3PE	C3B-C3C-C3D-C3E
18	N	502	3PE	C2F-C2G-C2H-C2I
18	T	203	3PE	C36-C37-C38-C39
15	N	504	IZL	C52-C53-C54-C55
17	A	504	MQ9	C34-C36-C37-C38
17	O	605	MQ9	C9-C11-C12-C13
18	N	502	3PE	C29-C2A-C2B-C2C
33	U	204	IX7	C63-C64-C65-C66
18	N	502	3PE	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	S	302	CDL	C51-CB5-OB6-CB4
18	F	301	3PE	C21-C22-C23-C24
21	V	201	CDL	C12-C13-C14-C15
21	O	606	CDL	CB2-C1-CA2-OA2
18	D	609	3PE	C24-C25-C26-C27
33	U	204	IX7	C59-C60-C61-C62
21	Q	607	CDL	C36-C37-C38-C39
18	F	301	3PE	O11-C1-C2-C3
21	B	605	CDL	OB5-CB3-CB4-CB6
21	G	202	CDL	OB5-CB3-CB4-CB6
21	I	201	CDL	OA5-CA3-CA4-CA6
21	I	201	CDL	OB5-CB3-CB4-CB6
21	Q	607	CDL	OB5-CB3-CB4-CB6
21	G	201	CDL	OB9-CB7-OB8-CB6
21	I	201	CDL	C13-C14-C15-C16
21	D	608	CDL	C13-C14-C15-C16
22	B	607	LYC	C55-C56-C58-C59
20	O	603	HEM	C2A-CAA-CBA-CGA
17	N	501	MQ9	C5-C6-C7-C8
15	A	502	IZL	C57-C56-C58-C59
18	C	303	3PE	O22-C21-O21-C2
21	T	201	CDL	C20-C21-C22-C23
23	O	601	LMT	C6-C7-C8-C9
18	T	205	3PE	C32-C33-C34-C35
21	O	606	CDL	C32-C33-C34-C35
21	D	607	CDL	C52-C53-C54-C55
18	C	303	3PE	C1-C2-O21-C21
18	F	301	3PE	C1-C2-O21-C21
21	V	201	CDL	CB5-C51-C52-C53
21	B	605	CDL	C13-C14-C15-C16
18	T	206	3PE	C27-C28-C29-C2A
21	D	607	CDL	O1-C1-CA2-OA2
15	A	502	IZL	C9-C10-O1-C11
19	O	602	SMA	O1-C2-C9-C10
18	S	301	3PE	C2D-C2E-C2F-C2G
21	T	201	CDL	C72-C73-C74-C75
16	N	505	9YF	O9-C-C1-O
18	C	304	3PE	O11-C1-C2-O21
18	J	201	3PE	O11-C1-C2-O21
18	S	301	3PE	O11-C1-C2-O21
21	B	609	CDL	OB5-CB3-CB4-OB6
21	F	302	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	I	201	CDL	OA5-CA3-CA4-OA6
21	I	201	CDL	OB5-CB3-CB4-OB6
21	O	606	CDL	OA5-CA3-CA4-OA6
21	Q	608	CDL	OB5-CB3-CB4-OB6
21	T	201	CDL	OB5-CB3-CB4-OB6
21	D	608	CDL	C11-C12-C13-C14
21	B	605	CDL	C11-C12-C13-C14
18	A	505	3PE	C1-C2-C3-O31
25	Q	602	HAS	C19-C20-C21-C22
21	G	202	CDL	C12-C13-C14-C15
17	N	501	MQ9	C1-C6-C7-C8
18	F	301	3PE	C12-C11-O13-P
18	Q	609	3PE	C12-C11-O13-P
18	R	405	3PE	C12-C11-O13-P
18	T	206	3PE	C12-C11-O13-P
18	W	201	3PE	C12-C11-O13-P
18	T	206	3PE	O21-C2-C3-O31
21	D	608	CDL	OA6-CA4-CA6-OA8
21	T	204	CDL	OA6-CA4-CA6-OA8
21	V	201	CDL	OB6-CB4-CB6-OB8
21	Q	607	CDL	C52-C53-C54-C55
31	U	201	DGA	CB5-CB6-CB7-CB8
23	O	601	LMT	C4B-C5B-C6B-O6B
21	T	204	CDL	C14-C15-C16-C17
15	N	504	IZL	C43-O28-P-O30
16	A	503	9YF	C2-O2-P-O8
16	H	203	9YF	C2-O2-P-O8
19	O	602	SMA	C13-C14-C15-C16
33	H	204	IX7	C30-O13-P-O14
18	T	202	3PE	C32-C33-C34-C35
21	B	609	CDL	C71-C72-C73-C74
17	A	504	MQ9	C15-C14-C16-C17
18	J	201	3PE	C22-C23-C24-C25
18	A	505	3PE	O32-C31-O31-C3
19	O	602	SMA	C11-C12-C13-C24
21	T	201	CDL	C12-C13-C14-C15
21	S	302	CDL	C19-C20-C21-C22
18	T	206	3PE	C26-C27-C28-C29
16	U	203	9YF	C10-C11-C12-C13
16	N	505	9YF	C10-C11-C12-C13
21	F	302	CDL	C32-C33-C34-C35
16	A	503	9YF	C24-C-C1-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	304	3PE	O11-C1-C2-C3
18	J	201	3PE	O11-C1-C2-C3
18	R	405	3PE	O11-C1-C2-C3
18	T	205	3PE	O11-C1-C2-C3
21	B	606	CDL	OB5-CB3-CB4-CB6
21	B	609	CDL	OB5-CB3-CB4-CB6
21	D	608	CDL	OB5-CB3-CB4-CB6
21	F	302	CDL	OB5-CB3-CB4-CB6
21	S	302	CDL	OA5-CA3-CA4-CA6
21	T	201	CDL	OA5-CA3-CA4-CA6
21	V	201	CDL	OB5-CB3-CB4-CB6
21	V	201	CDL	C19-C20-C21-C22
21	D	608	CDL	C51-CB5-OB6-CB4
21	T	204	CDL	C73-C74-C75-C76
18	F	301	3PE	C32-C33-C34-C35
18	T	205	3PE	C26-C27-C28-C29
21	S	302	CDL	C31-C32-C33-C34
18	T	203	3PE	C2-C1-O11-P
21	B	609	CDL	C1-CA2-OA2-PA1
21	F	302	CDL	CA4-CA3-OA5-PA1
21	T	204	CDL	C1-CA2-OA2-PA1
17	A	504	MQ9	C12-C11-C9-C10
22	B	607	LYC	C62-C61-C63-C64
21	V	201	CDL	C13-C14-C15-C16
18	P	303	3PE	C24-C25-C26-C27
21	T	204	CDL	C16-C17-C18-C19
23	B	608	LMT	C6-C7-C8-C9
16	A	503	9YF	O9-C-C1-O
18	F	301	3PE	O11-C1-C2-O21
18	T	203	3PE	O11-C1-C2-O21
18	W	201	3PE	O11-C1-C2-O21
21	B	605	CDL	OB5-CB3-CB4-OB6
21	D	608	CDL	OB5-CB3-CB4-OB6
21	S	302	CDL	OA5-CA3-CA4-OA6
33	U	204	IX7	O16-C31-C32-O19
18	T	203	3PE	C27-C28-C29-C2A
18	W	201	3PE	C2B-C2C-C2D-C2E
21	D	608	CDL	CB4-CB6-OB8-CB7
21	S	302	CDL	OA6-CA4-CA6-OA8
21	V	201	CDL	C14-C15-C16-C17
21	S	302	CDL	CB7-C71-C72-C73
16	A	503	9YF	C1-C-C24-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	303	3PE	C1-C2-C3-O31
21	Q	608	CDL	CB3-CB4-CB6-OB8
17	A	504	MQ9	C13-C14-C16-C17
33	H	204	IX7	C36-C37-C38-C39
25	D	602	HAS	O11-C11-C3B-C4B
25	Q	601	HAS	O11-C11-C3B-C4B
15	A	502	IZL	O8-C19-O7-C18
21	B	606	CDL	O1-C1-CA2-OA2
18	F	301	3PE	C32-C31-O31-C3
21	T	204	CDL	C72-C73-C74-C75
32	U	202	PLM	C5-C6-C7-C8
21	V	201	CDL	C33-C34-C35-C36
18	T	202	3PE	O31-C31-C32-C33
18	J	201	3PE	C33-C34-C35-C36
18	A	505	3PE	C1-O11-P-O13
18	C	304	3PE	C11-O13-P-O11
18	C	304	3PE	C11-O13-P-O12
18	C	304	3PE	C11-O13-P-O14
18	C	304	3PE	O13-C11-C12-N
18	D	609	3PE	C11-O13-P-O11
18	F	301	3PE	C1-O11-P-O12
18	F	301	3PE	C1-O11-P-O13
18	F	301	3PE	C1-O11-P-O14
18	F	301	3PE	C11-O13-P-O11
18	F	301	3PE	C11-O13-P-O12
18	J	201	3PE	C11-O13-P-O14
18	L	101	3PE	C1-O11-P-O12
18	P	303	3PE	C11-O13-P-O14
18	P	303	3PE	O13-C11-C12-N
18	Q	609	3PE	C11-O13-P-O11
18	Q	609	3PE	C11-O13-P-O12
18	R	405	3PE	C1-O11-P-O13
18	T	202	3PE	C1-O11-P-O13
18	T	202	3PE	C1-O11-P-O14
18	T	203	3PE	C11-O13-P-O14
18	T	205	3PE	C11-O13-P-O14
21	B	605	CDL	CA3-OA5-PA1-OA2
21	B	605	CDL	CA3-OA5-PA1-OA3
21	B	606	CDL	CA3-OA5-PA1-OA3
21	B	609	CDL	CA3-OA5-PA1-OA2
21	B	609	CDL	CA3-OA5-PA1-OA3
21	D	607	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	607	CDL	CA2-OA2-PA1-OA5
21	D	608	CDL	CA3-OA5-PA1-OA3
21	D	608	CDL	CA3-OA5-PA1-OA4
21	D	608	CDL	CB2-OB2-PB2-OB4
21	F	302	CDL	CB3-OB5-PB2-OB2
21	F	302	CDL	CB3-OB5-PB2-OB4
21	G	201	CDL	CA2-OA2-PA1-OA4
21	G	201	CDL	CA3-OA5-PA1-OA2
21	G	201	CDL	CA3-OA5-PA1-OA3
21	G	201	CDL	CA3-OA5-PA1-OA4
21	G	202	CDL	CA2-OA2-PA1-OA4
21	G	202	CDL	CB3-OB5-PB2-OB2
21	G	202	CDL	CB3-OB5-PB2-OB3
21	I	201	CDL	CA2-OA2-PA1-OA4
21	O	606	CDL	CB2-OB2-PB2-OB4
21	O	606	CDL	CB3-OB5-PB2-OB4
21	Q	607	CDL	CA2-OA2-PA1-OA3
21	Q	607	CDL	CA2-OA2-PA1-OA4
21	Q	607	CDL	CA2-OA2-PA1-OA5
21	Q	607	CDL	CA3-OA5-PA1-OA2
21	Q	607	CDL	CA3-OA5-PA1-OA3
21	Q	608	CDL	CA2-OA2-PA1-OA3
21	S	302	CDL	CA3-OA5-PA1-OA4
21	T	201	CDL	CA3-OA5-PA1-OA2
21	T	201	CDL	CA3-OA5-PA1-OA4
21	T	201	CDL	CB2-OB2-PB2-OB5
21	T	201	CDL	CB3-OB5-PB2-OB3
21	T	204	CDL	CB2-OB2-PB2-OB4
21	T	204	CDL	CB2-OB2-PB2-OB5
21	T	204	CDL	CB3-OB5-PB2-OB2
21	T	204	CDL	CB3-OB5-PB2-OB4
21	V	201	CDL	CA2-OA2-PA1-OA3
21	V	201	CDL	CA3-OA5-PA1-OA3
21	V	201	CDL	CB2-OB2-PB2-OB3
21	V	201	CDL	CB2-OB2-PB2-OB4
21	V	201	CDL	CB2-OB2-PB2-OB5
25	D	602	HAS	C11-C12-C13-C14
25	Q	601	HAS	C11-C12-C13-C14
21	Q	607	CDL	C14-C15-C16-C17
17	A	504	MQ9	C30-C29-C31-C32
23	B	608	LMT	C2-C3-C4-C5
18	Q	609	3PE	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	T	206	3PE	C2-C1-O11-P
21	Q	608	CDL	C1-CB2-OB2-PB2
21	Q	608	CDL	CB4-CB3-OB5-PB2
21	S	302	CDL	C1-CA2-OA2-PA1
22	B	607	LYC	C57-C56-C58-C59
21	D	608	CDL	OB7-CB5-OB6-CB4
21	S	302	CDL	C32-C33-C34-C35
21	G	202	CDL	C72-C71-CB7-OB8
21	T	201	CDL	C40-C41-C42-C43
15	N	504	IZL	C55-C56-C58-C59
21	V	201	CDL	C22-C23-C24-C25
18	J	201	3PE	C3-C2-O21-C21
18	P	303	3PE	C3-C2-O21-C21
21	D	608	CDL	CB6-CB4-OB6-CB5
21	F	302	CDL	CB3-CB4-OB6-CB5
15	N	504	IZL	C63-C64-C65-C66
18	P	303	3PE	O11-C1-C2-C3
21	Q	608	CDL	OA5-CA3-CA4-CA6
33	U	204	IX7	O16-C31-C32-C33
21	B	606	CDL	OB5-CB3-CB4-OB6
18	L	101	3PE	C25-C26-C27-C28
33	H	204	IX7	C32-C31-O16-P
18	S	301	3PE	O21-C2-C3-O31
33	H	204	IX7	O19-C32-C33-O17
21	G	201	CDL	CB7-C71-C72-C73
33	U	204	IX7	O8-C24-O7-C23
21	T	201	CDL	C72-C71-CB7-OB8
33	H	204	IX7	C61-C62-C63-C64
18	F	301	3PE	C23-C24-C25-C26
21	G	202	CDL	C72-C73-C74-C75
21	G	202	CDL	C52-C51-CB5-OB6
17	A	504	MQ9	C28-C29-C31-C32
18	A	505	3PE	O22-C21-O21-C2
18	R	405	3PE	O31-C31-C32-C33
21	O	606	CDL	CB4-CB3-OB5-PB2
21	F	302	CDL	C13-C14-C15-C16
15	N	504	IZL	O31-C44-C45-O34
21	G	201	CDL	OA5-CA3-CA4-OA6
21	Q	608	CDL	OA5-CA3-CA4-OA6
33	U	204	IX7	C30-C23-O7-C24
16	H	203	9YF	O12-C25-O11-C24
21	G	201	CDL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	S	301	3PE	C2C-C2D-C2E-C2F
21	T	201	CDL	C11-C12-C13-C14
18	D	609	3PE	O21-C2-C3-O31
21	O	606	CDL	OA6-CA4-CA6-OA8
21	G	201	CDL	C16-C17-C18-C19
25	Q	601	HAS	C27-C19-C20-C21
18	R	405	3PE	O32-C31-C32-C33
21	D	607	CDL	C17-C18-C19-C20
21	O	606	CDL	C12-C11-CA5-OA7
21	T	201	CDL	C1-CA2-OA2-PA1
21	D	607	CDL	C11-C12-C13-C14
33	U	204	IX7	C60-C61-C62-C63
25	D	602	HAS	C25-C23-C24-C28
22	B	607	LYC	C60-C61-C63-C64
21	G	201	CDL	C72-C73-C74-C75
21	D	607	CDL	C75-C76-C77-C78
21	I	201	CDL	C21-C22-C23-C24
33	U	204	IX7	C29-C24-O7-C23
18	Q	609	3PE	C3-C2-O21-C21
21	I	201	CDL	CB6-CB4-OB6-CB5
21	Q	608	CDL	CB6-CB4-OB6-CB5
21	V	201	CDL	CB3-CB4-OB6-CB5
18	A	505	3PE	C34-C35-C36-C37
21	G	201	CDL	C11-C12-C13-C14
25	D	602	HAS	C4D-C3D-CAD-CBD
18	A	505	3PE	C22-C23-C24-C25
21	D	607	CDL	C32-C33-C34-C35
25	D	602	HAS	CAA-CBA-CGA-O1A
15	A	502	IZL	C15-C14-O3-C13
21	S	302	CDL	O1-C1-CB2-OB2
20	B	603	HEM	CAA-CBA-CGA-O1A
15	A	502	IZL	O-C10-O1-C11
18	F	301	3PE	O32-C31-O31-C3
18	R	405	3PE	C2-C1-O11-P
15	N	504	IZL	C57-C56-C58-C59
24	C	301	HEC	CAD-CBD-CGD-O2D
25	D	601	HAS	CAA-CBA-CGA-O1A
17	N	501	MQ9	C15-C14-C16-C17
25	Q	601	HAS	C18-C19-C20-C21
18	C	303	3PE	C22-C23-C24-C25
21	I	201	CDL	C19-C20-C21-C22
33	U	204	IX7	O2-C18-O3-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	H	204	IX7	C11-C12-C13-C14
21	T	204	CDL	CB7-C71-C72-C73
20	O	604	HEM	CAA-CBA-CGA-O1A
21	Q	608	CDL	C23-C24-C25-C26
33	H	204	IX7	C60-C61-C62-C63
21	S	302	CDL	OB7-CB5-OB6-CB4
15	A	502	IZL	C55-C56-C58-C59
16	H	203	9YF	C27-C28-C29-C30
21	B	609	CDL	C52-C51-CB5-OB6
25	D	602	HAS	C22-C23-C24-C28
18	Q	609	3PE	C2E-C2F-C2G-C2H
23	O	601	LMT	O5B-C1B-O1B-C4'
21	B	605	CDL	C53-C54-C55-C56
33	H	204	IX7	C32-C33-O17-C34
31	Z	201	DGA	CA3-CA4-CA5-CA6
18	J	201	3PE	C25-C26-C27-C28
21	B	605	CDL	C34-C35-C36-C37
18	S	301	3PE	C37-C38-C39-C3A
20	O	604	HEM	CAA-CBA-CGA-O2A
24	C	301	HEC	CAD-CBD-CGD-O1D
21	B	606	CDL	CA4-CA3-OA5-PA1
21	O	606	CDL	CA4-CA3-OA5-PA1
18	J	201	3PE	C37-C38-C39-C3A
20	B	603	HEM	CAA-CBA-CGA-O2A
17	A	504	MQ9	C9-C11-C12-C13
21	T	204	CDL	CA3-CA4-CA6-OA8
21	T	204	CDL	CB3-CB4-CB6-OB8
21	O	606	CDL	C12-C13-C14-C15
21	Q	607	CDL	C37-C38-C39-C40
16	A	503	9YF	C9-C10-C11-C12
18	C	303	3PE	O11-C1-C2-O21
24	C	302	HEC	CAA-CBA-CGA-O2A
25	D	602	HAS	CAA-CBA-CGA-O2A
18	D	609	3PE	O21-C21-C22-C23
19	O	602	SMA	O12-C12-C13-C24
33	H	204	IX7	O18-C34-O17-C33
18	A	505	3PE	C21-C22-C23-C24
17	O	605	MQ9	C16-C17-C18-C19
21	Q	607	CDL	CA2-C1-CB2-OB2
25	D	601	HAS	CAA-CBA-CGA-O2A
21	Q	608	CDL	CB5-C51-C52-C53
18	J	201	3PE	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	U	204	IX7	C10-C11-C12-C13
18	C	303	3PE	O11-C1-C2-C3
18	N	502	3PE	O11-C1-C2-C3
21	D	607	CDL	OB5-CB3-CB4-CB6
21	O	606	CDL	OA5-CA3-CA4-CA6
21	G	202	CDL	C35-C36-C37-C38
18	W	201	3PE	C34-C35-C36-C37
23	O	601	LMT	C3-C4-C5-C6
21	B	609	CDL	C14-C15-C16-C17
33	H	204	IX7	C59-C60-C61-C62
18	N	502	3PE	O21-C21-C22-C23
25	D	602	HAS	C2D-C3D-CAD-CBD
21	V	201	CDL	C20-C21-C22-C23
15	N	504	IZL	C23-C24-O11-C25
24	P	302	HEC	CAA-CBA-CGA-O2A
32	U	202	PLM	C4-C5-C6-C7
18	T	206	3PE	C1-C2-O21-C21
21	D	607	CDL	CB3-CB4-OB6-CB5
18	T	203	3PE	C21-C22-C23-C24
24	C	302	HEC	CAA-CBA-CGA-O1A
21	B	609	CDL	CA4-CA3-OA5-PA1
21	F	302	CDL	OA5-CA3-CA4-OA6
17	O	605	MQ9	C11-C12-C13-C14
21	D	607	CDL	C37-C38-C39-C40
24	P	302	HEC	CAA-CBA-CGA-O1A
25	D	601	HAS	CAD-CBD-CGD-O1D
19	B	601	SMA	C15-C16-C17-C18
18	W	201	3PE	C23-C24-C25-C26
18	S	301	3PE	C27-C28-C29-C2A
21	F	302	CDL	C12-C13-C14-C15
21	Q	607	CDL	C72-C71-CB7-OB8
18	P	303	3PE	O21-C21-C22-C23
18	T	205	3PE	O21-C21-C22-C23
25	D	602	HAS	CAD-CBD-CGD-O1D
16	A	503	9YF	O9-C8-C9-C10
18	J	201	3PE	O31-C31-C32-C33
21	V	201	CDL	C44-C45-C46-C47
21	I	201	CDL	C14-C15-C16-C17
23	B	608	LMT	O5B-C5B-C6B-O6B
20	O	603	HEM	CAA-CBA-CGA-O2A
21	Q	607	CDL	C52-C51-CB5-OB6
15	A	502	IZL	C43-O28-P-O30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	N	504	IZL	C43-O28-P-O29
16	N	505	9YF	C2-O2-P-O8
19	B	601	SMA	C13-C14-C15-C16
19	O	602	SMA	C3-C2-C9-C10
25	Q	602	HAS	C3D-CAD-CBD-CGD
18	R	405	3PE	O21-C21-C22-C23
21	Q	607	CDL	C51-CB5-OB6-CB4
21	F	302	CDL	C71-C72-C73-C74
18	Q	609	3PE	C2D-C2E-C2F-C2G
18	T	205	3PE	C34-C35-C36-C37
24	P	301	HEC	CAA-CBA-CGA-O1A
21	G	201	CDL	C72-C71-CB7-OB8
21	T	201	CDL	C32-C31-CA7-OA8
31	R	404	DGA	OG1-CA1-CA2-CA3
21	G	201	CDL	C51-C52-C53-C54
25	D	602	HAS	C1A-C2A-CAA-CBA
33	H	204	IX7	O2-C18-O3-C19
25	Q	602	HAS	CAA-CBA-CGA-O1A
25	Q	602	HAS	CAA-CBA-CGA-O2A
15	A	502	IZL	C54-C55-C56-C57
18	J	201	3PE	C2A-C2B-C2C-C2D
21	Q	607	CDL	O1-C1-CB2-OB2
21	S	302	CDL	CA3-CA4-CA6-OA8
18	J	201	3PE	O21-C21-C22-C23
18	T	206	3PE	O31-C31-C32-C33
31	Z	201	DGA	OG2-CB1-CB2-CB3
21	B	606	CDL	OA6-CA4-CA6-OA8
21	Q	607	CDL	OB6-CB4-CB6-OB8
33	U	204	IX7	O19-C32-C33-O17
21	T	201	CDL	C23-C24-C25-C26
21	D	607	CDL	C12-C11-CA5-OA6
21	T	204	CDL	C12-C11-CA5-OA6
21	T	204	CDL	C52-C53-C54-C55
31	Z	201	DGA	CA7-CA8-CA9-CAA
21	T	201	CDL	C32-C33-C34-C35
21	D	608	CDL	C72-C71-CB7-OB8
15	A	502	IZL	C42-C19-O7-C18
18	W	201	3PE	C3C-C3D-C3E-C3F
21	O	606	CDL	C31-CA7-OA8-CA6
15	N	504	IZL	C61-C62-C63-C64
21	D	607	CDL	C73-C74-C75-C76
15	A	502	IZL	C44-C45-O34-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	607	CDL	CB6-CB4-OB6-CB5
21	F	302	CDL	CB6-CB4-OB6-CB5
15	N	504	IZL	C42-C19-O7-C18
21	T	201	CDL	C52-C51-CB5-OB6
21	B	609	CDL	C78-C79-C80-C81
24	P	301	HEC	CAA-CBA-CGA-O2A
17	A	504	MQ9	C21-C22-C23-C24
25	Q	601	HAS	C24-C28-C29-C30
18	T	206	3PE	O32-C31-C32-C33
15	N	504	IZL	C71-C13-O3-C14
18	F	301	3PE	C2-C1-O11-P
21	B	609	CDL	C1-CB2-OB2-PB2
25	D	602	HAS	CAD-CBD-CGD-O2D
18	P	303	3PE	O22-C21-C22-C23
18	T	202	3PE	O32-C31-C32-C33
21	T	201	CDL	C32-C31-CA7-OA9
21	I	201	CDL	C12-C11-CA5-OA6
18	R	405	3PE	O22-C21-C22-C23
31	M	201	DGA	OG2-CB1-CB2-CB3
15	N	504	IZL	O8-C19-O7-C18
18	Q	609	3PE	C24-C25-C26-C27
20	O	603	HEM	CAA-CBA-CGA-O1A
25	D	601	HAS	CAD-CBD-CGD-O2D
21	Q	608	CDL	C13-C14-C15-C16
18	T	205	3PE	C36-C37-C38-C39
33	H	204	IX7	C63-C64-C65-C66
18	J	201	3PE	C27-C28-C29-C2A
21	Q	607	CDL	C72-C71-CB7-OB9
31	Z	201	DGA	OB1-CB1-CB2-CB3
25	D	602	HAS	C3A-C2A-CAA-CBA
18	J	201	3PE	O32-C31-C32-C33
21	G	201	CDL	C72-C71-CB7-OB9
21	Q	607	CDL	C52-C51-CB5-OB7
33	H	204	IX7	C30-C19-O3-C18
31	R	404	DGA	OA1-CA1-CA2-CA3
15	N	504	IZL	C29-C30-O16-C31
16	A	503	9YF	O10-C8-C9-C10
17	A	504	MQ9	C36-C37-C38-C39
21	T	201	CDL	C51-C52-C53-C54
25	Q	602	HAS	CAD-CBD-CGD-O2D
18	T	205	3PE	O22-C21-C22-C23
23	B	608	LMT	O5B-C1B-O1B-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	606	CDL	C52-C51-CB5-OB6
33	H	204	IX7	C20-C19-O3-C18
21	T	201	CDL	C52-C51-CB5-OB7
21	T	204	CDL	C12-C11-CA5-OA7
15	N	504	IZL	O34-C60-C61-C62
33	U	204	IX7	C56-C57-C58-C59
18	T	203	3PE	C24-C25-C26-C27
25	Q	601	HAS	CAD-CBD-CGD-O1D
21	D	607	CDL	C12-C11-CA5-OA7
15	A	502	IZL	C61-C62-C63-C64
18	Q	609	3PE	C2C-C2D-C2E-C2F
25	Q	601	HAS	CAD-CBD-CGD-O2D
21	B	605	CDL	CA5-C11-C12-C13
15	N	504	IZL	O35-C60-C61-C62

There are no ring outliers.

40 monomers are involved in 59 short contacts:

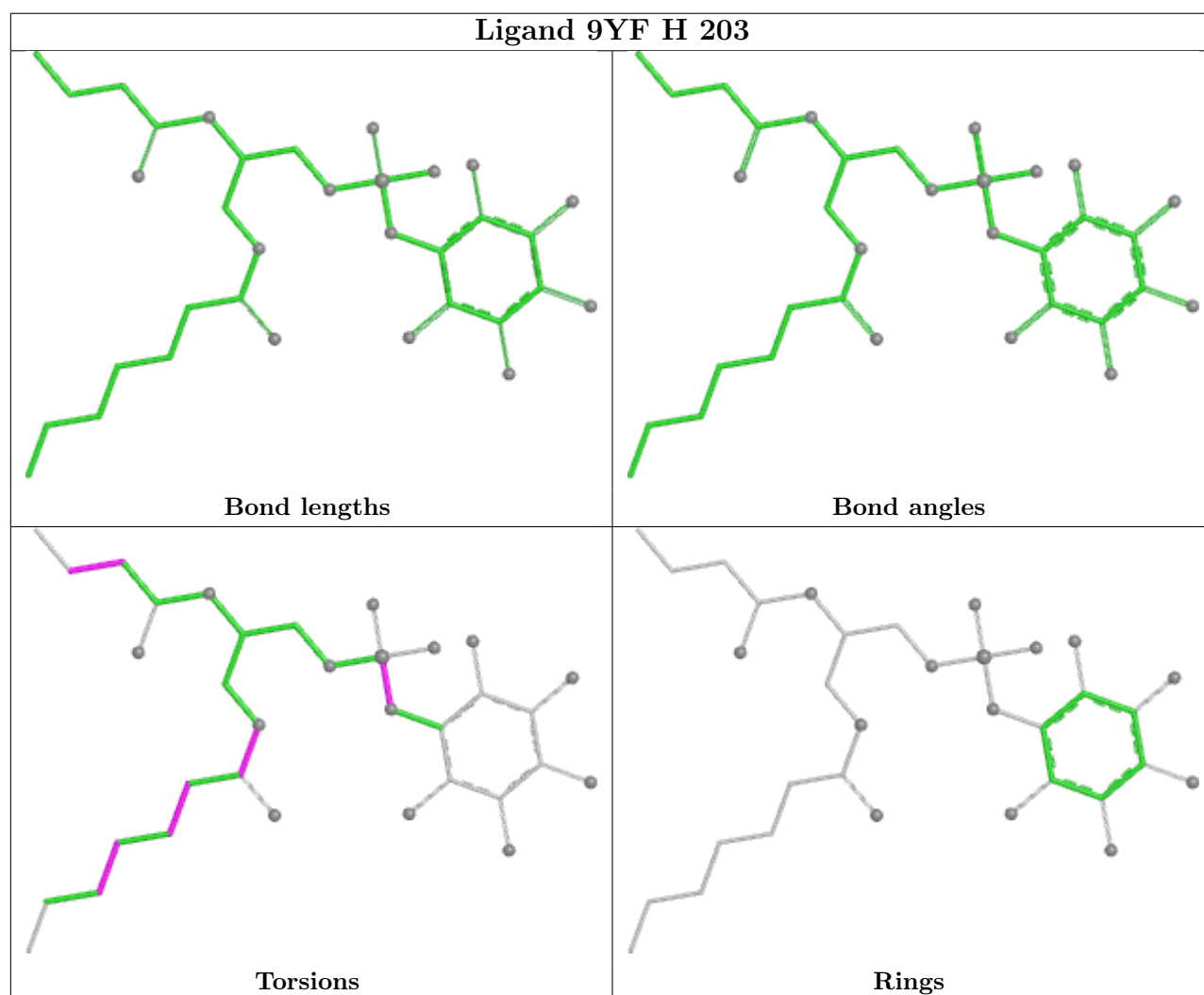
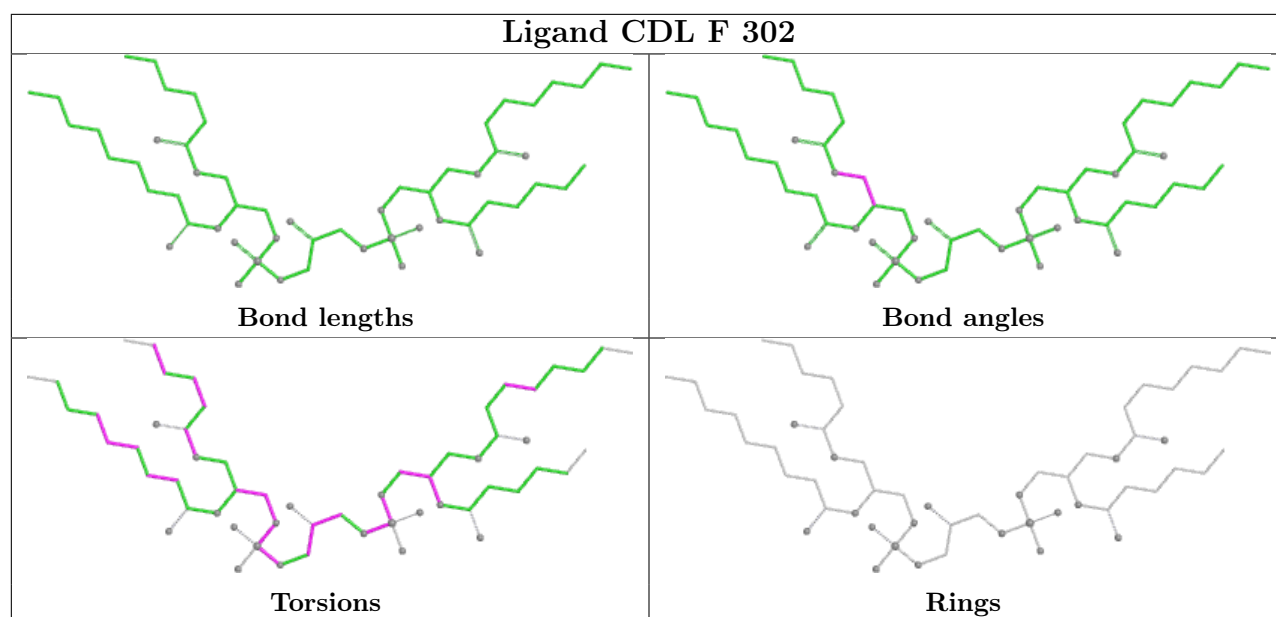
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	302	CDL	1	0
18	A	505	3PE	1	0
20	O	603	HEM	2	0
16	U	203	9YF	2	0
25	Q	602	HAS	1	0
31	H	201	DGA	2	0
20	B	602	HEM	2	0
20	B	603	HEM	1	0
19	B	601	SMA	1	0
22	O	607	LYC	1	0
18	C	303	3PE	2	0
29	D	606	AZI	2	0
21	T	201	CDL	1	0
24	C	301	HEC	1	0
20	O	604	HEM	1	0
17	O	605	MQ9	1	0
31	M	201	DGA	1	0
21	G	201	CDL	1	0
24	P	302	HEC	1	0
31	U	201	DGA	3	0
18	N	502	3PE	1	0
15	A	502	IZL	3	0
18	T	203	3PE	1	0

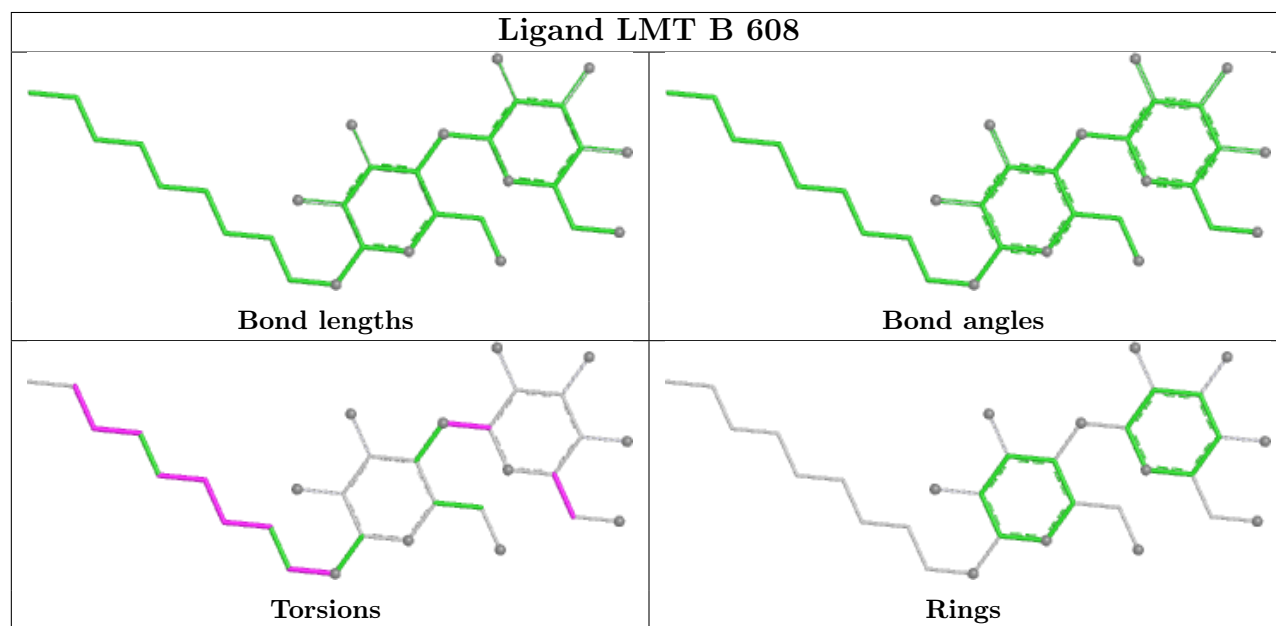
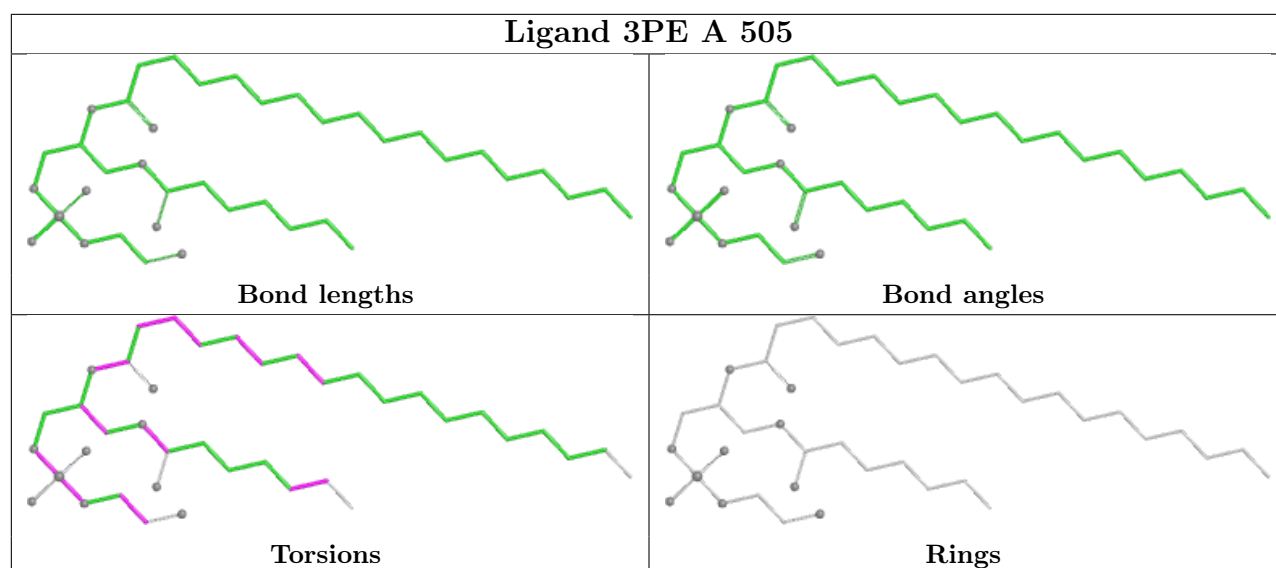
Continued on next page...

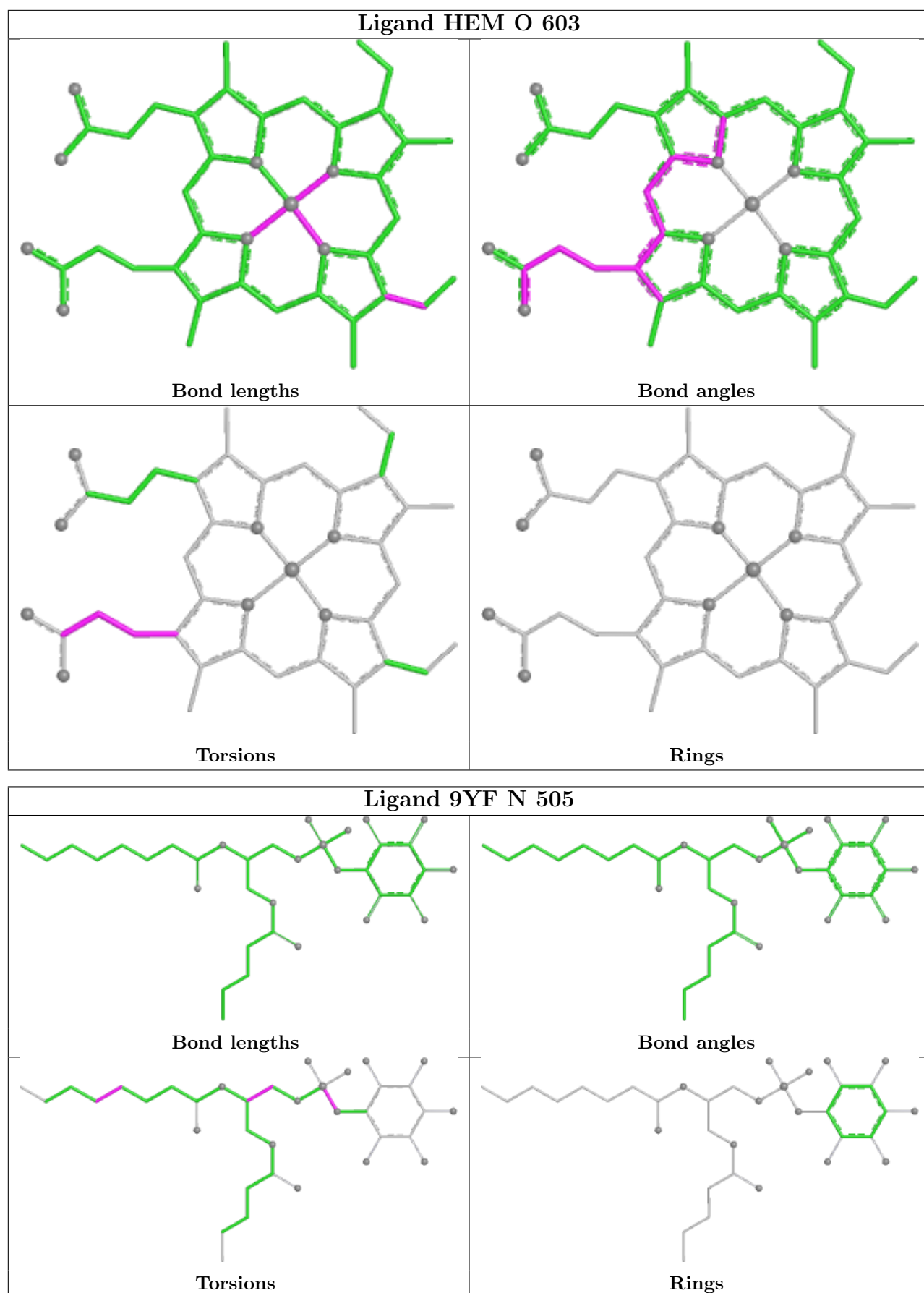
Continued from previous page...

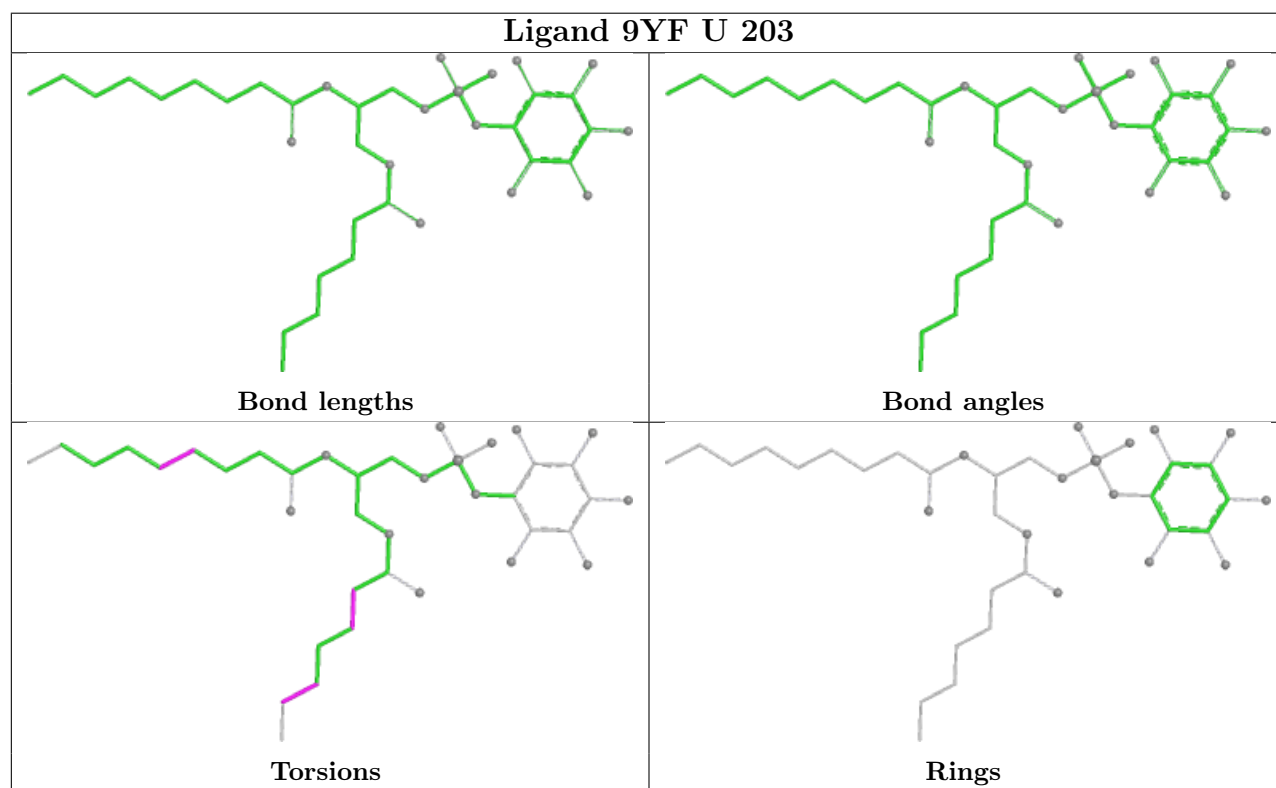
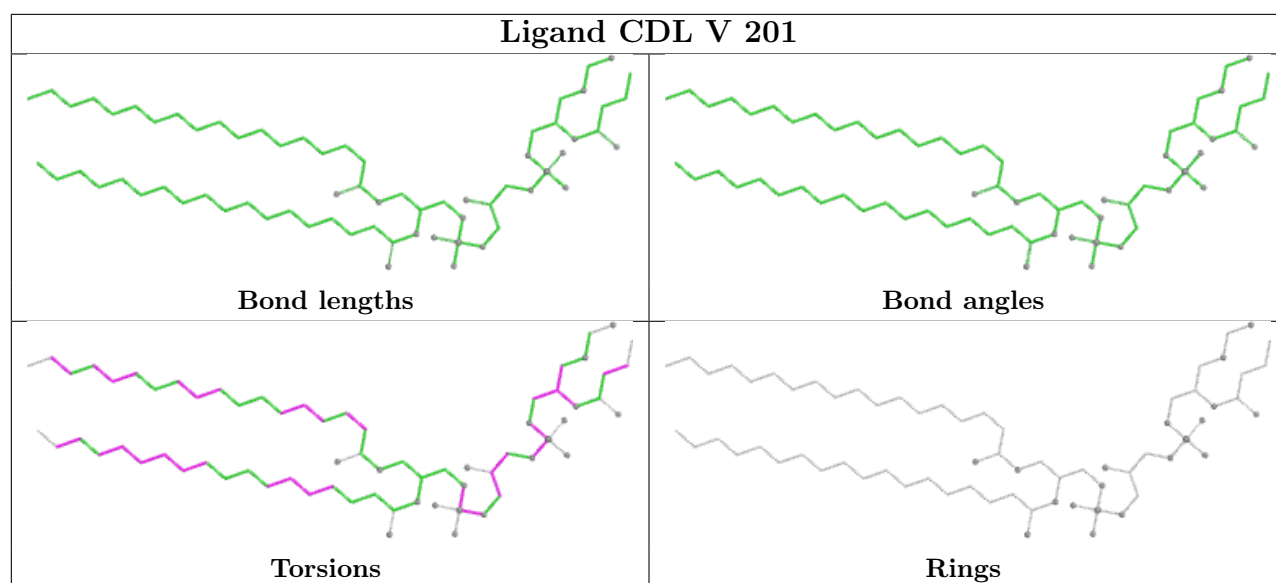
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	O	602	SMA	1	0
21	Q	607	CDL	1	0
17	B	604	MQ9	1	0
18	Q	609	3PE	3	0
21	D	607	CDL	1	0
21	Q	608	CDL	3	0
25	D	602	HAS	3	0
18	R	405	3PE	3	0
33	U	204	IX7	2	0
18	P	303	3PE	2	0
21	G	202	CDL	1	0
17	A	504	MQ9	3	0
18	F	301	3PE	1	0
33	H	204	IX7	2	0
25	Q	601	HAS	2	0
21	B	609	CDL	1	0
21	B	605	CDL	1	0

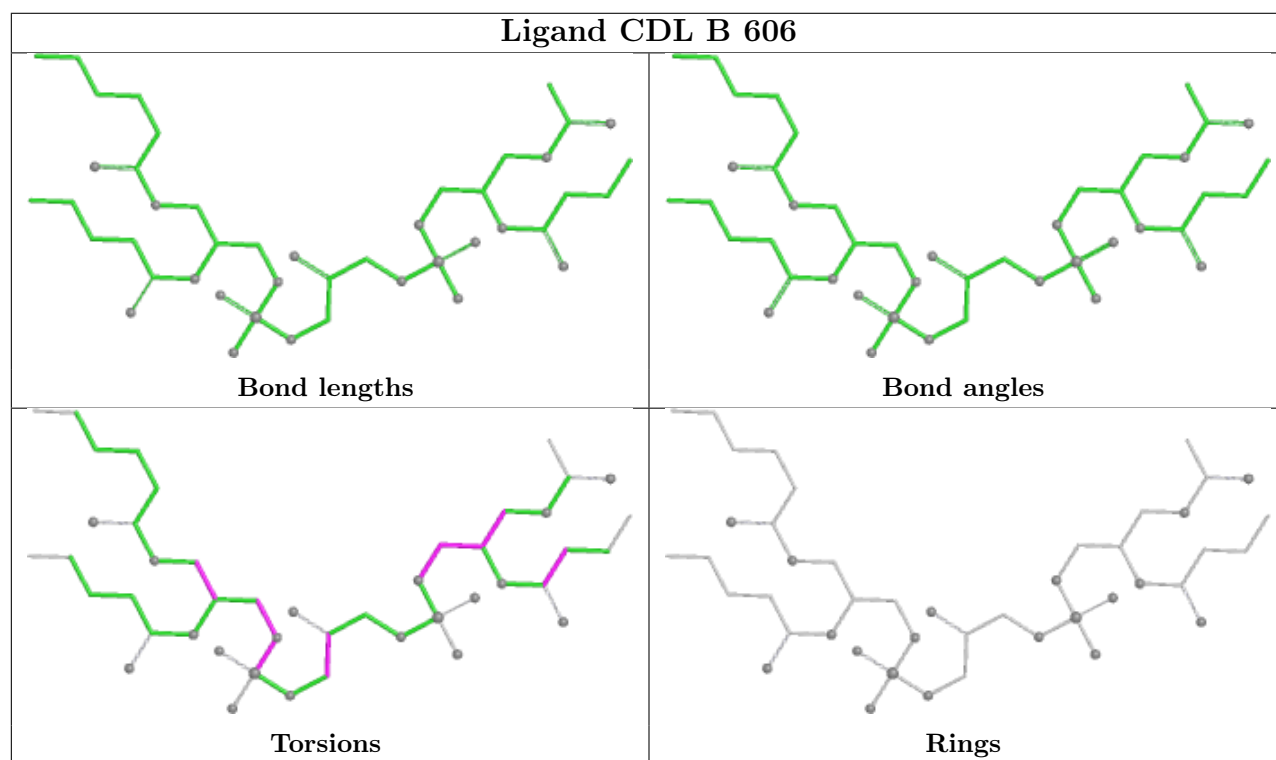
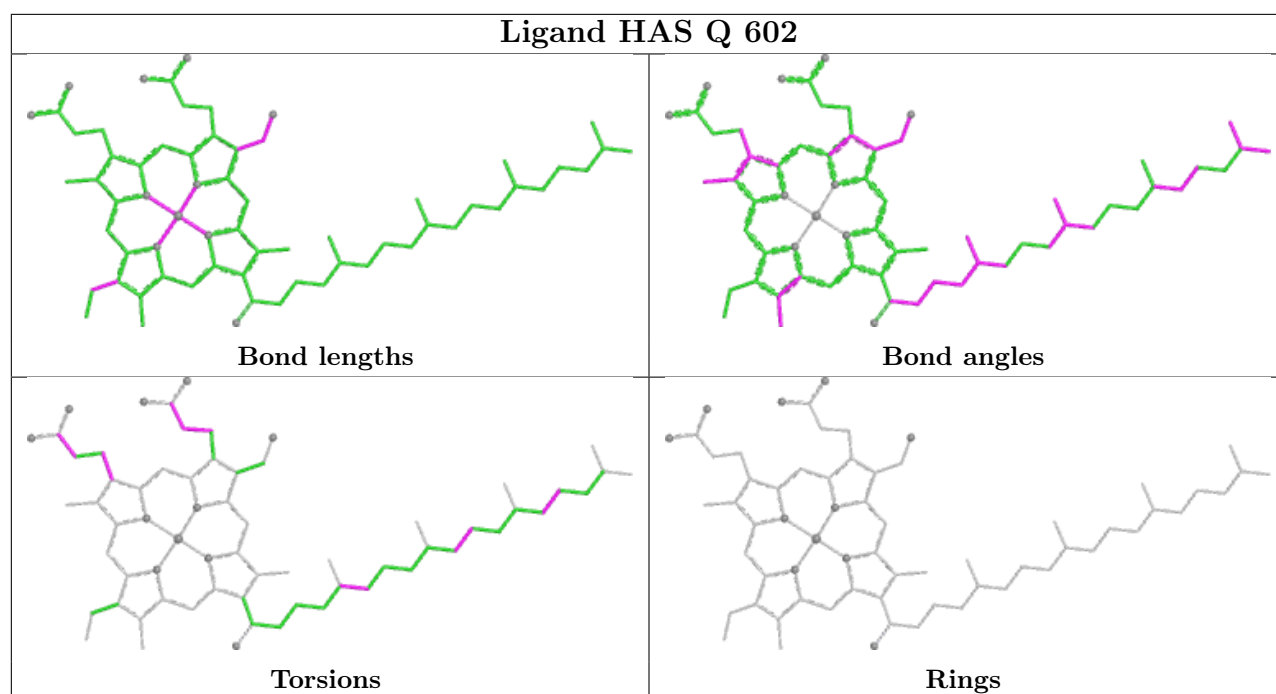
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

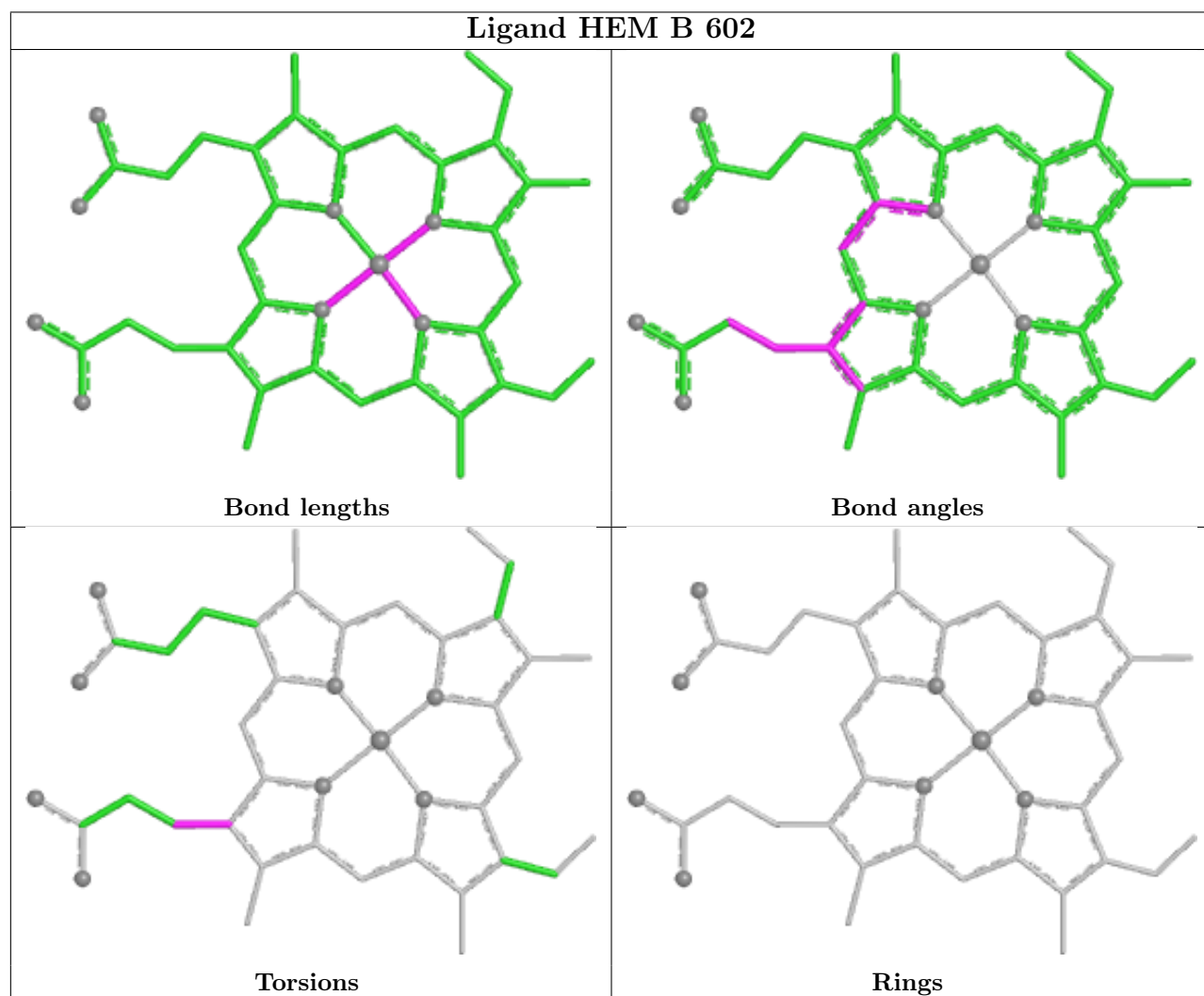
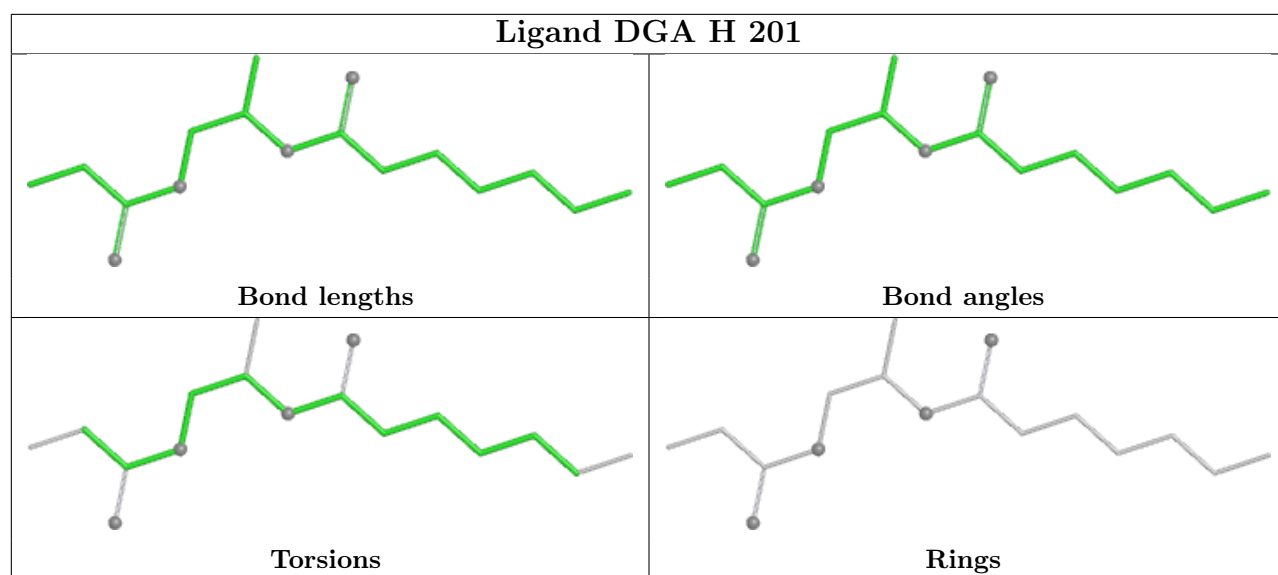


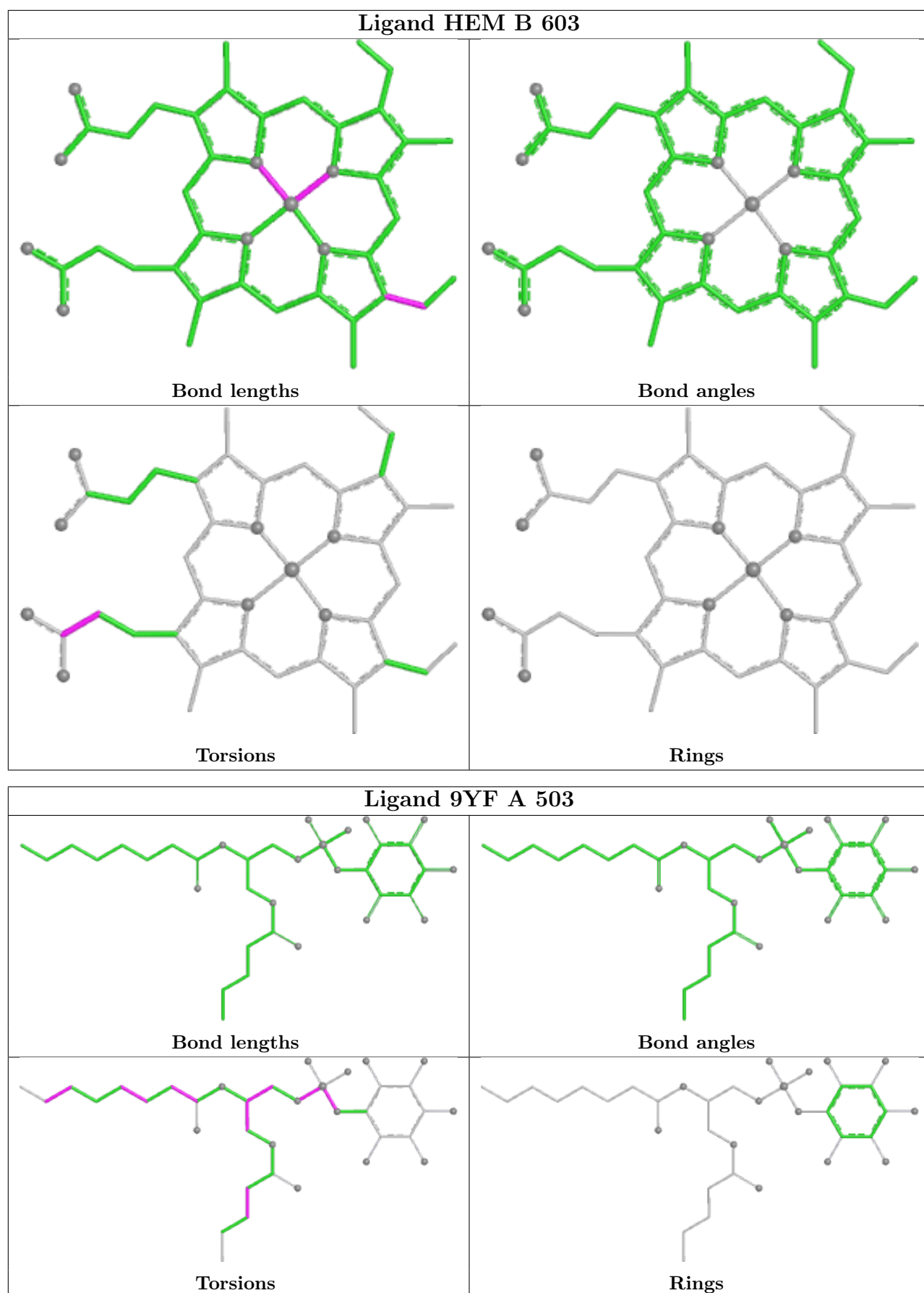


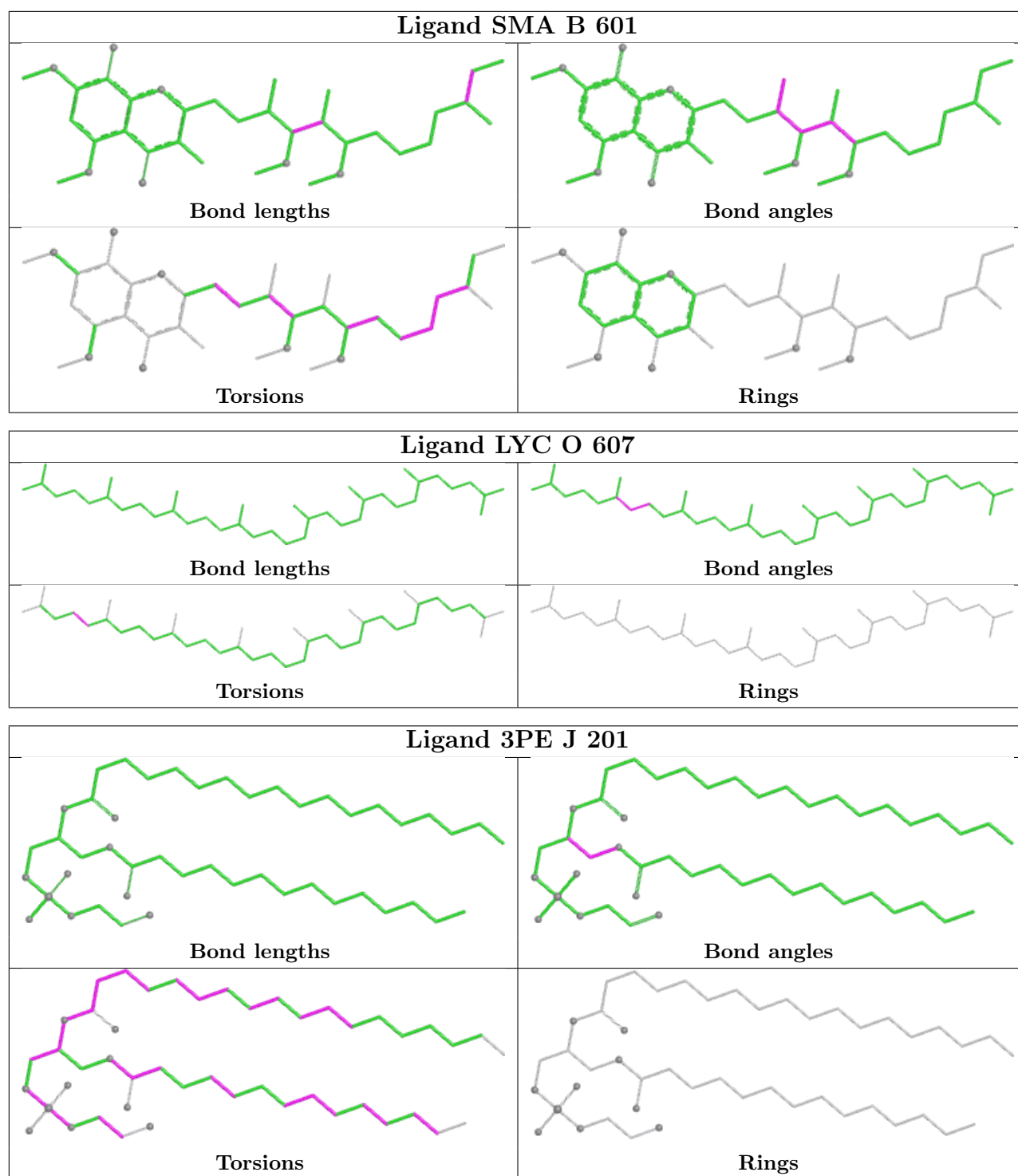


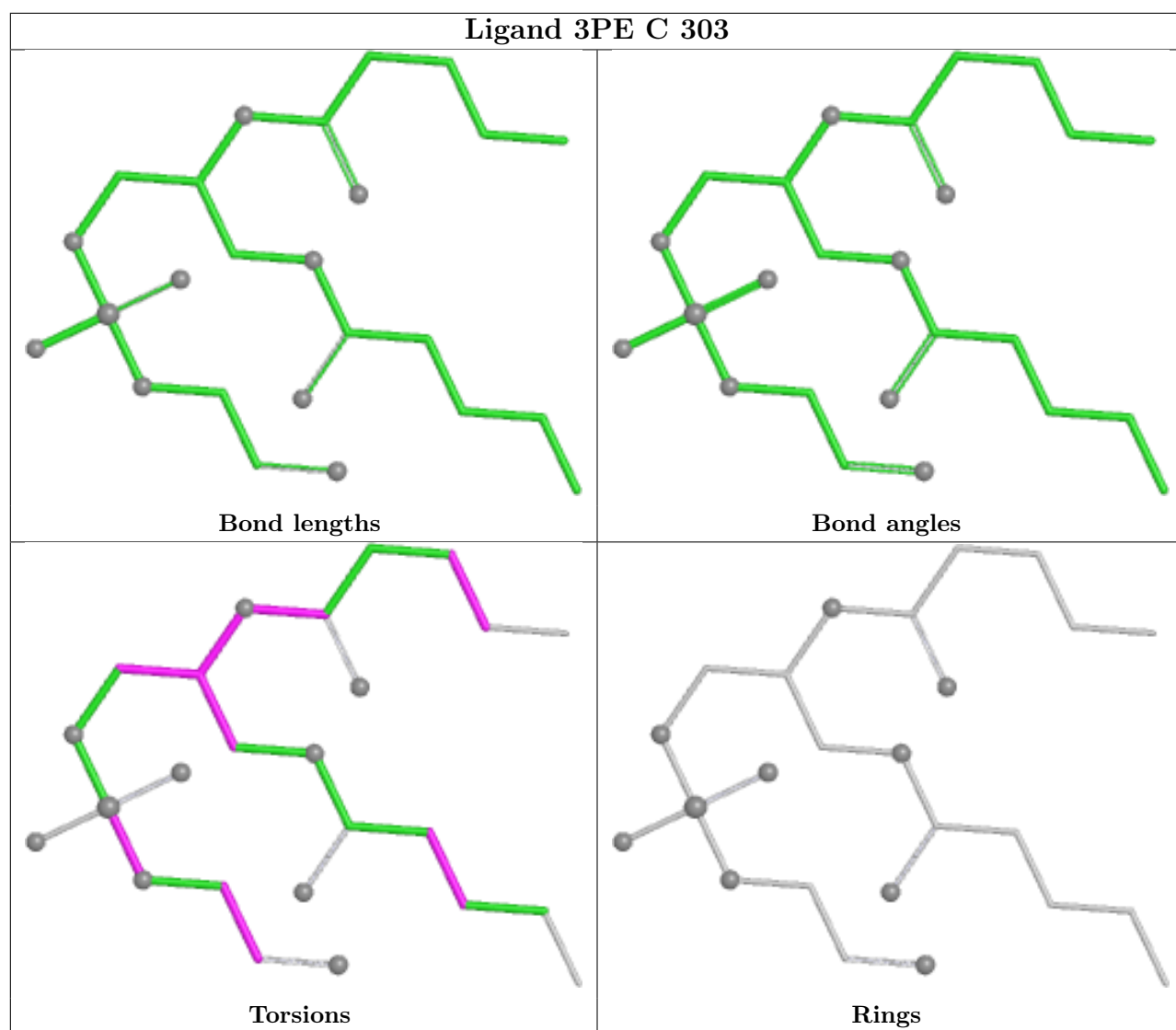


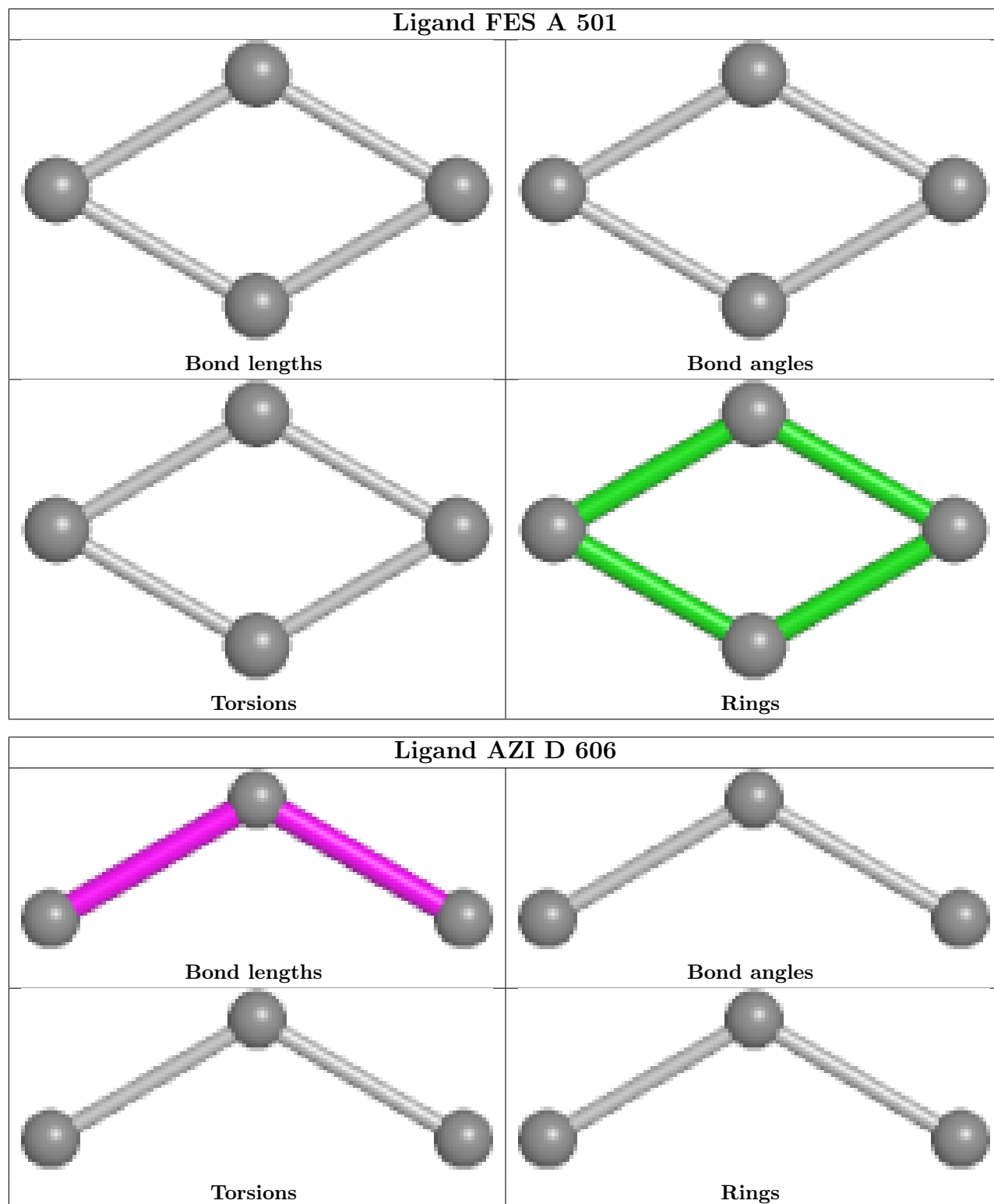


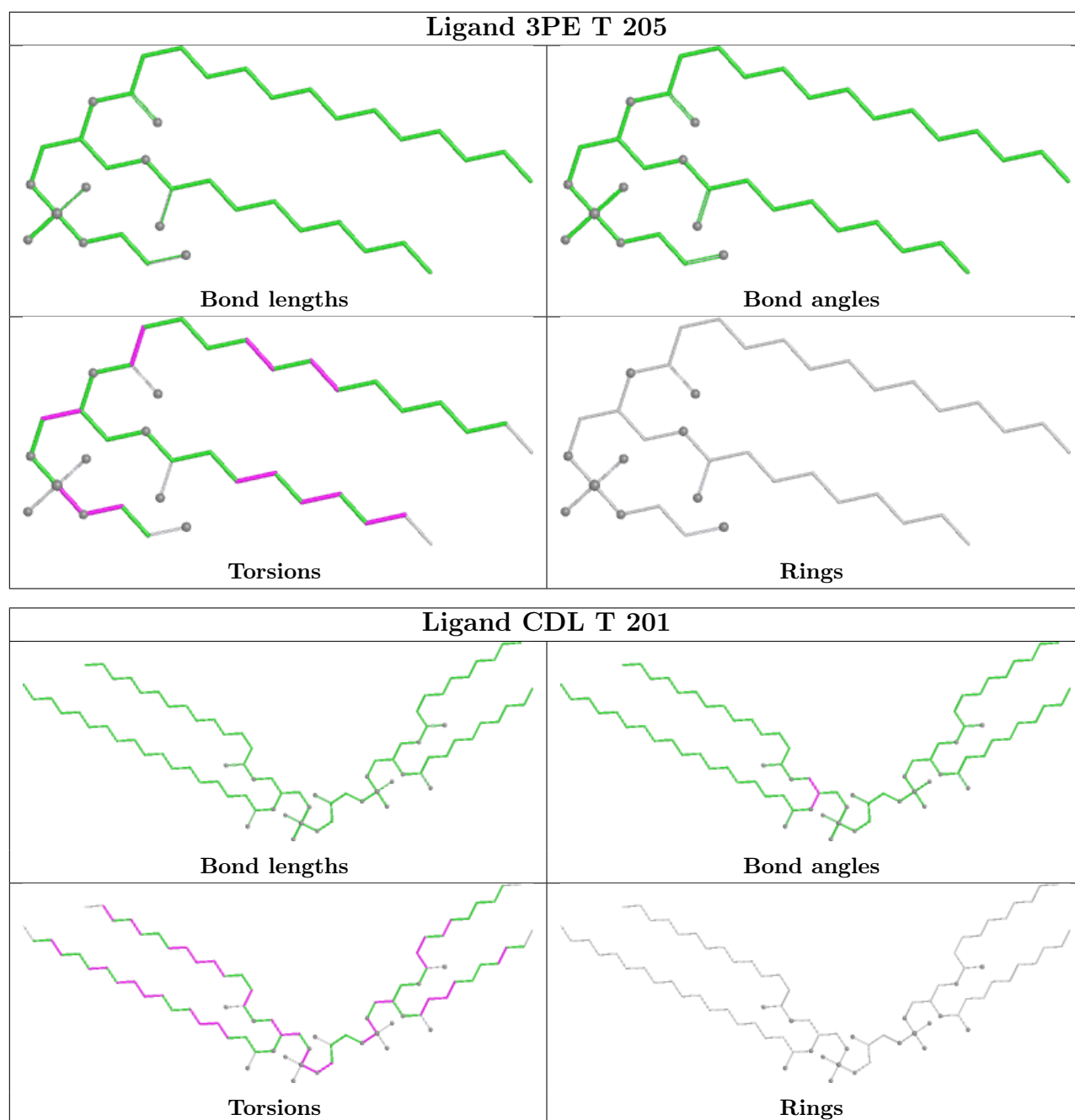




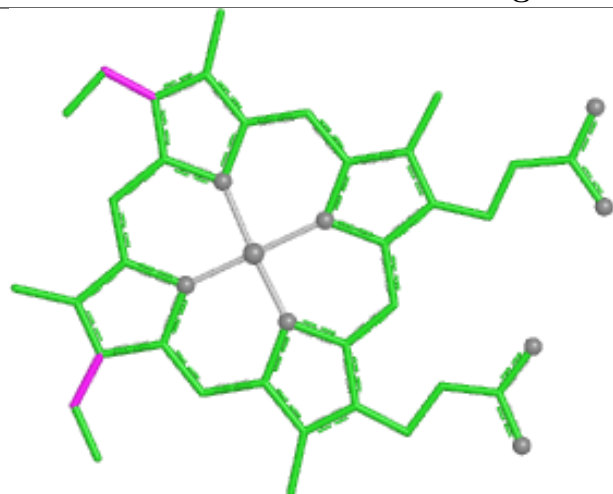




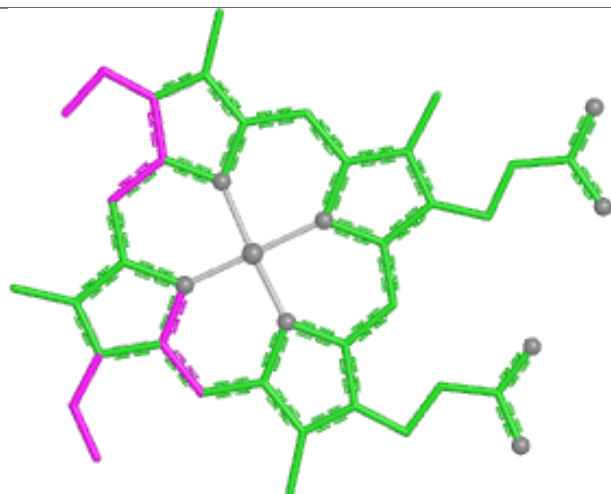




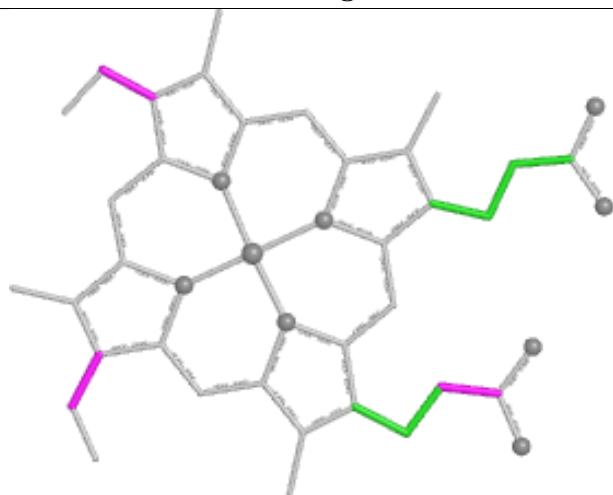
Ligand HEC C 301



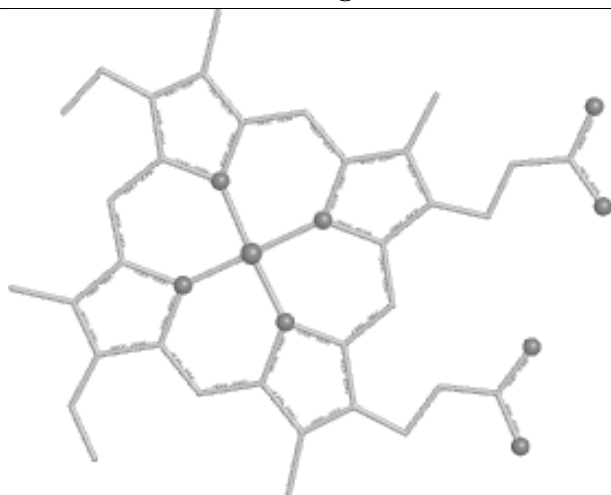
Bond lengths



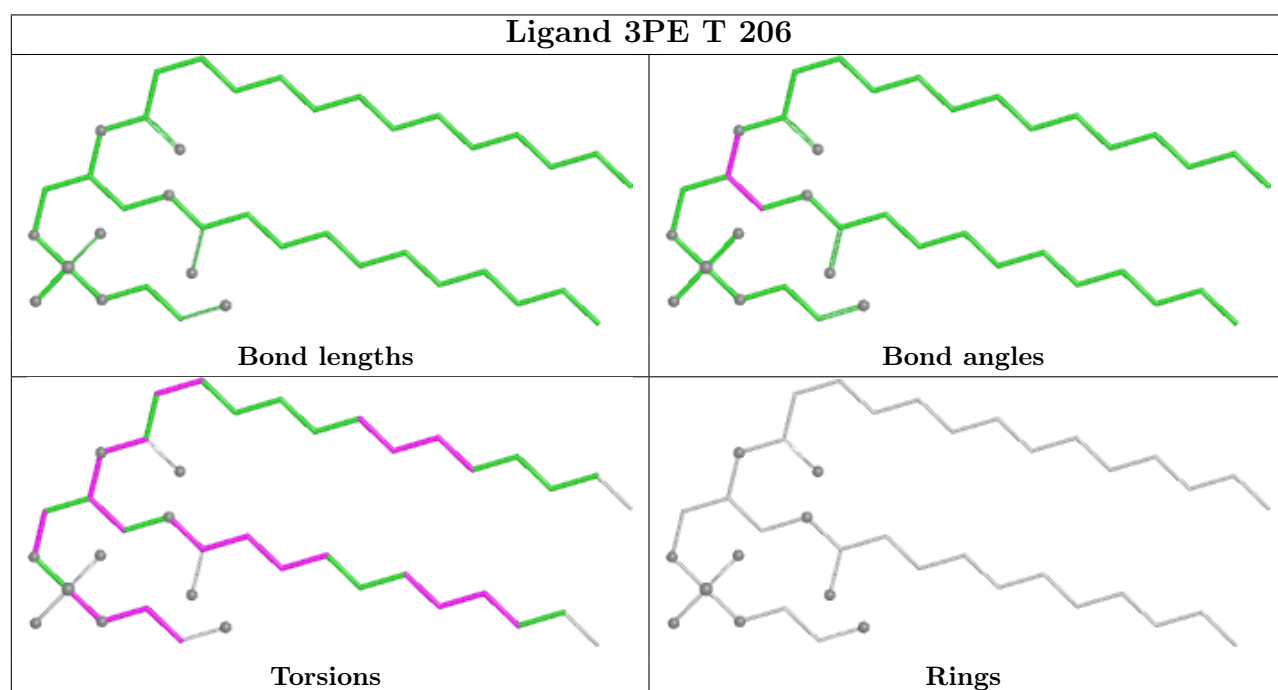
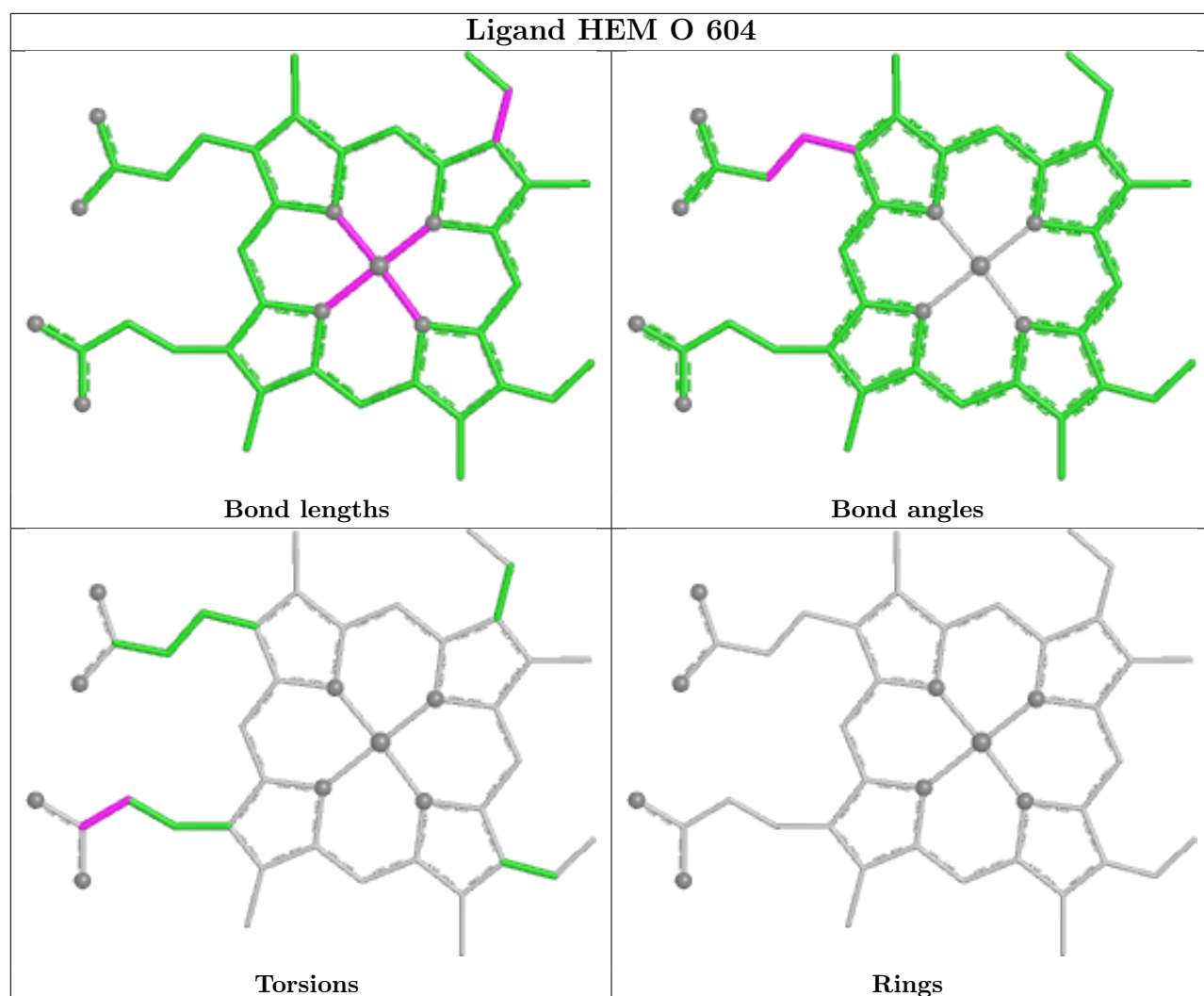
Bond angles

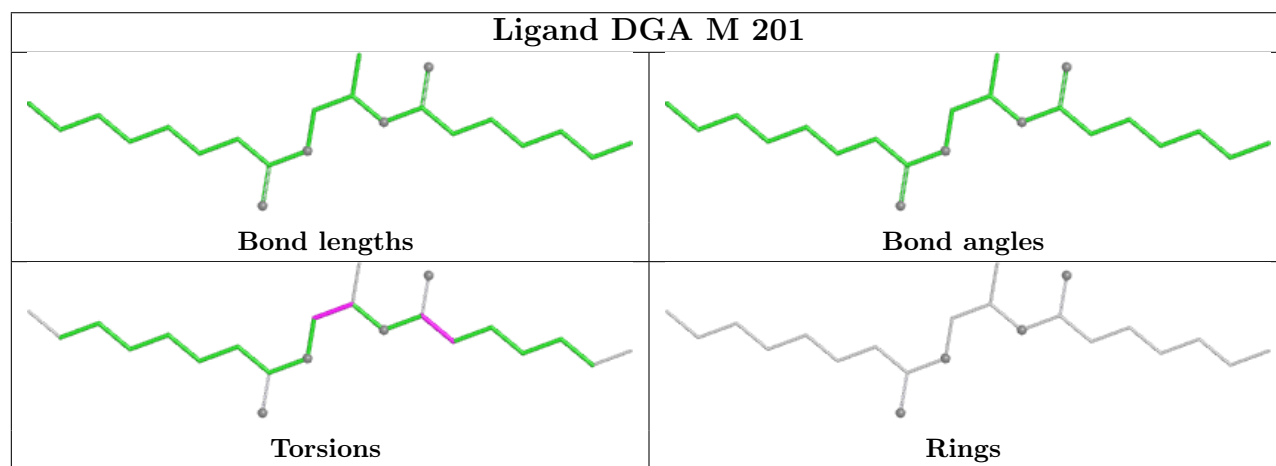
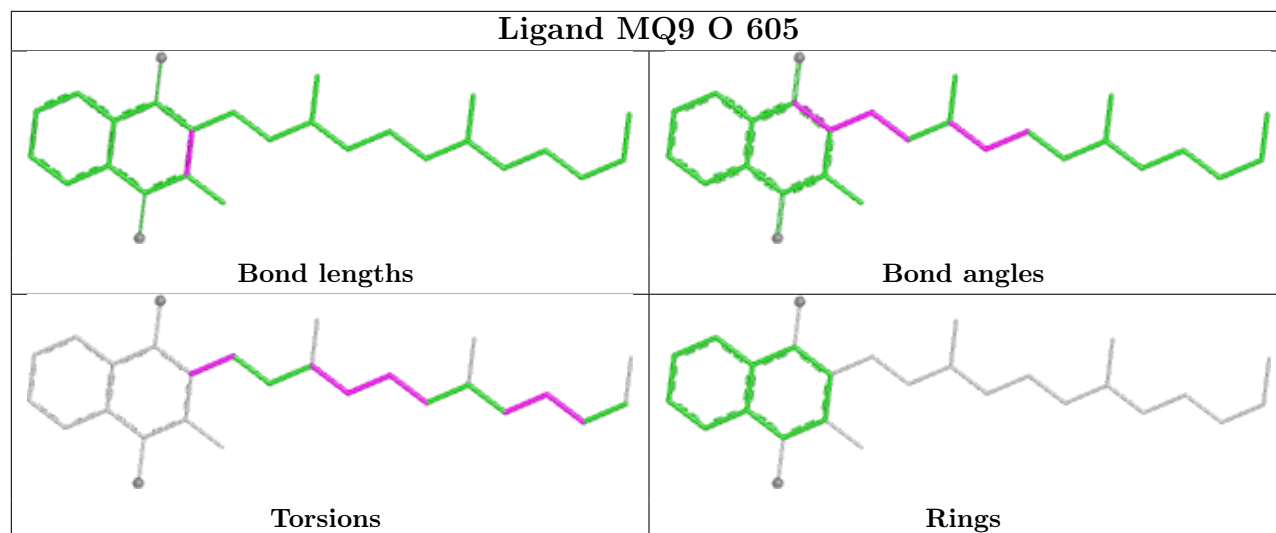


Torsions

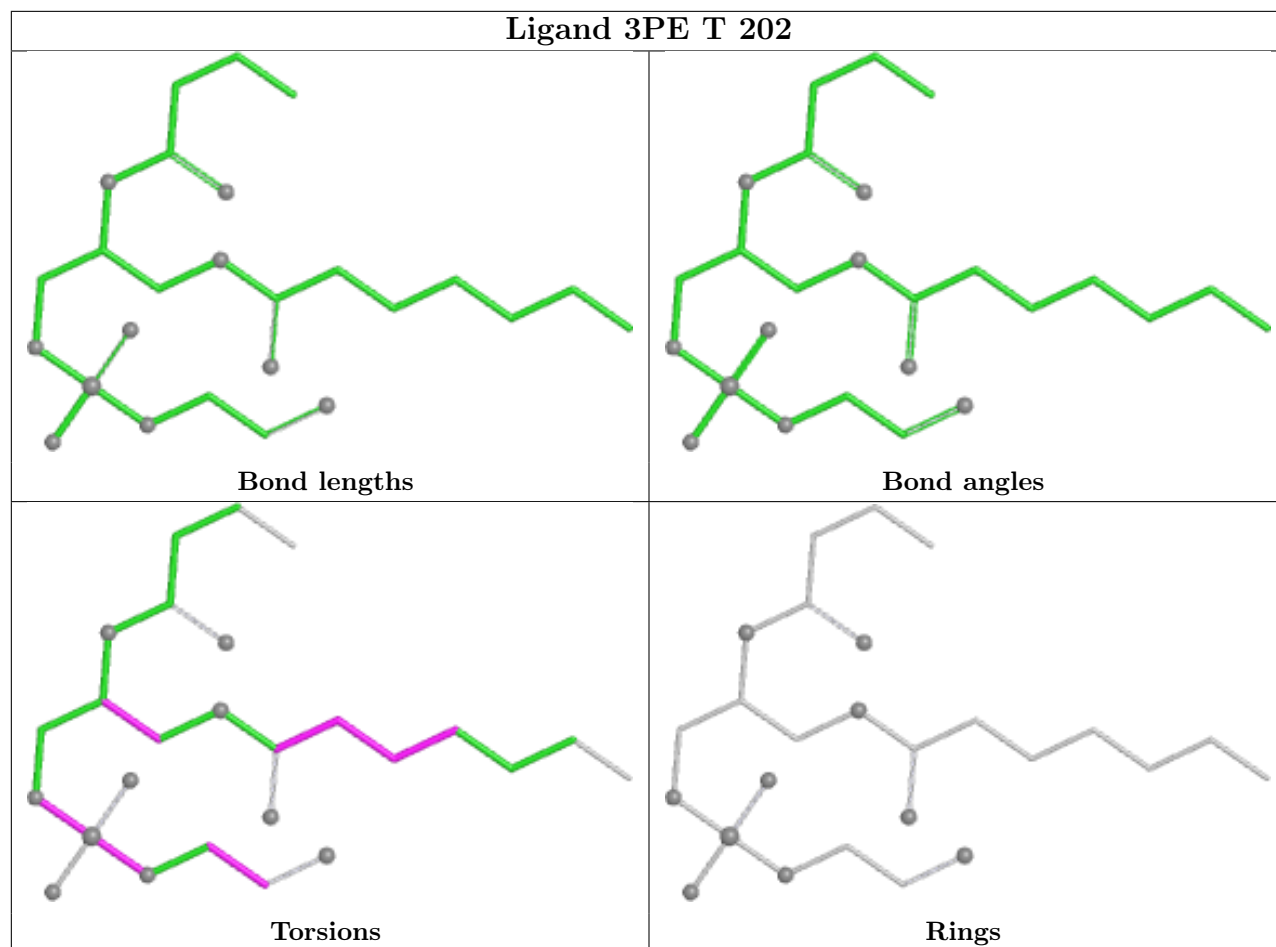


Rings

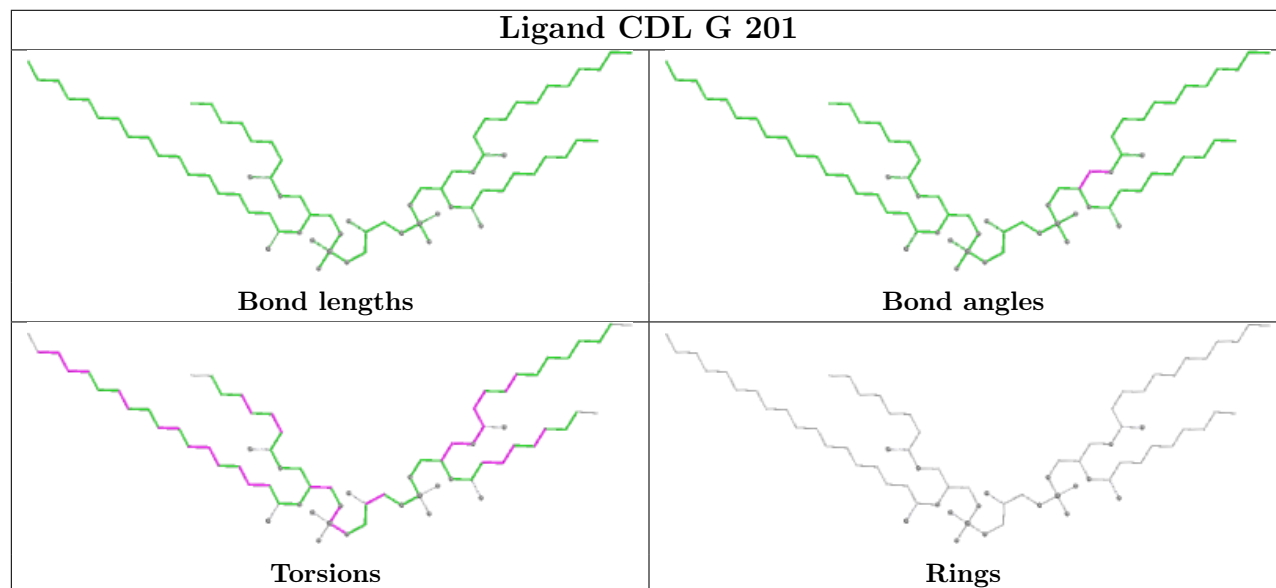


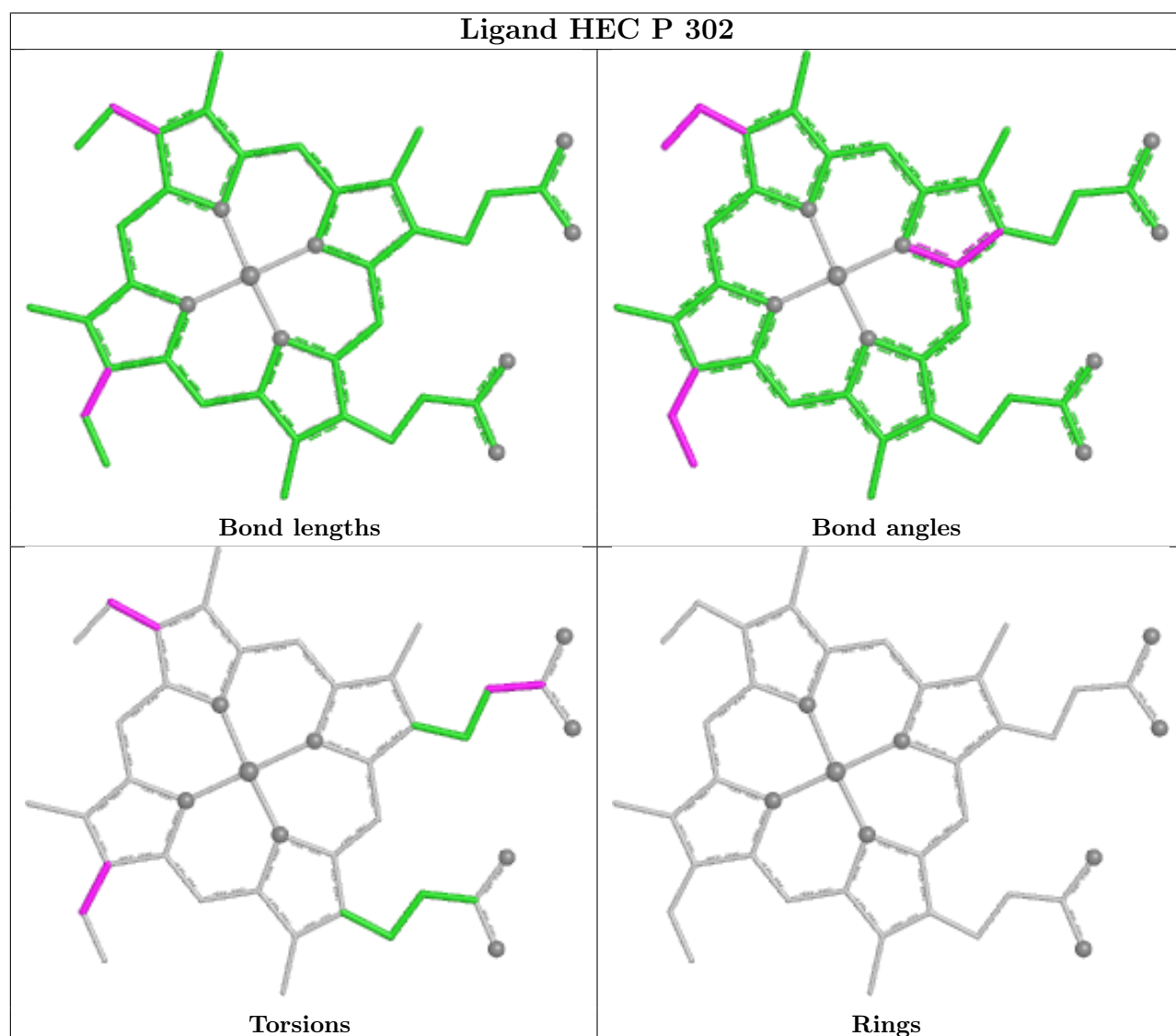
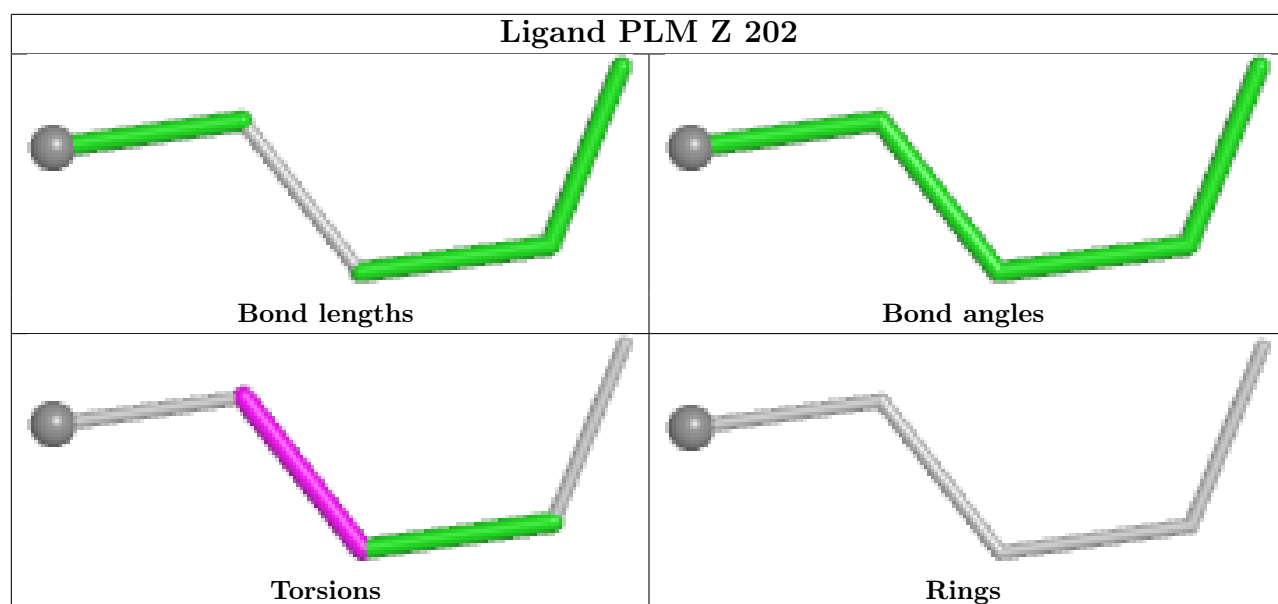


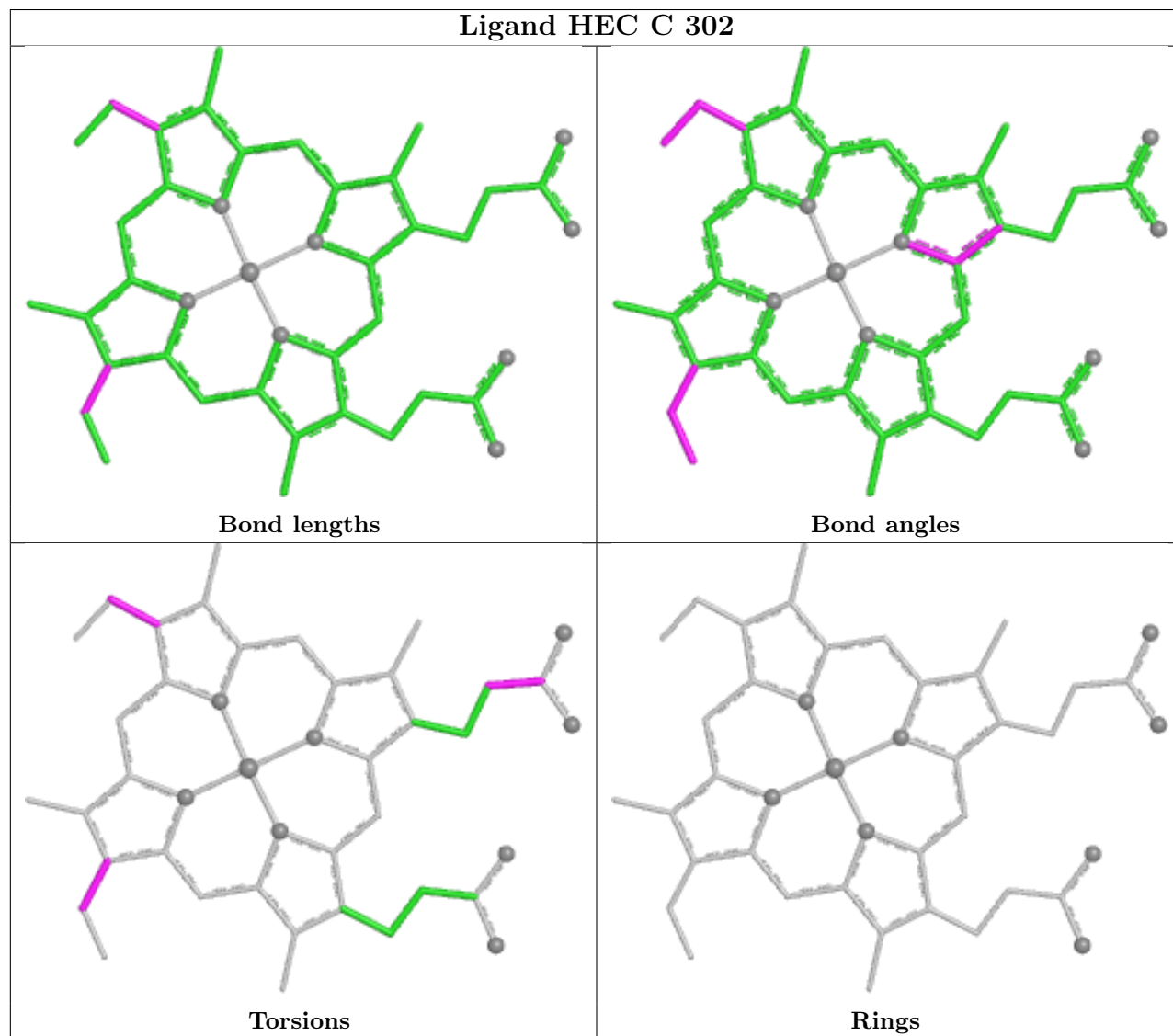
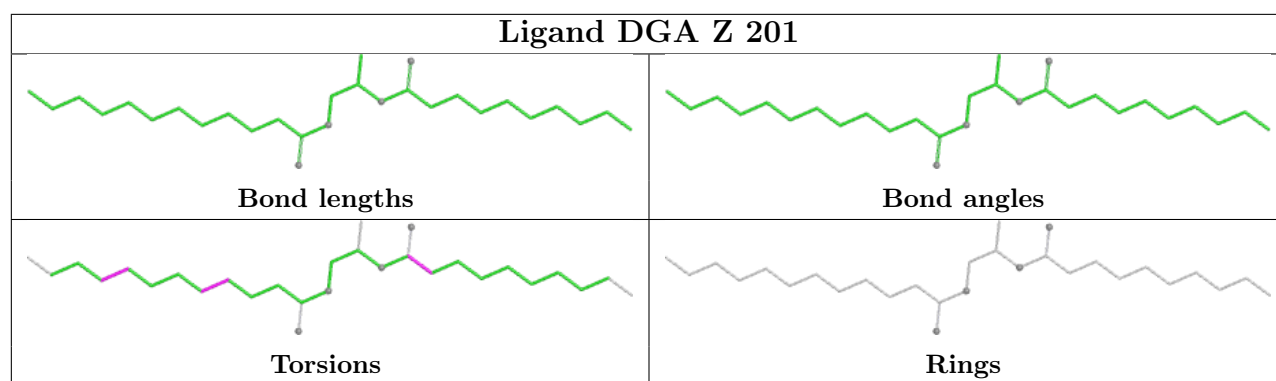
Ligand 3PE T 202

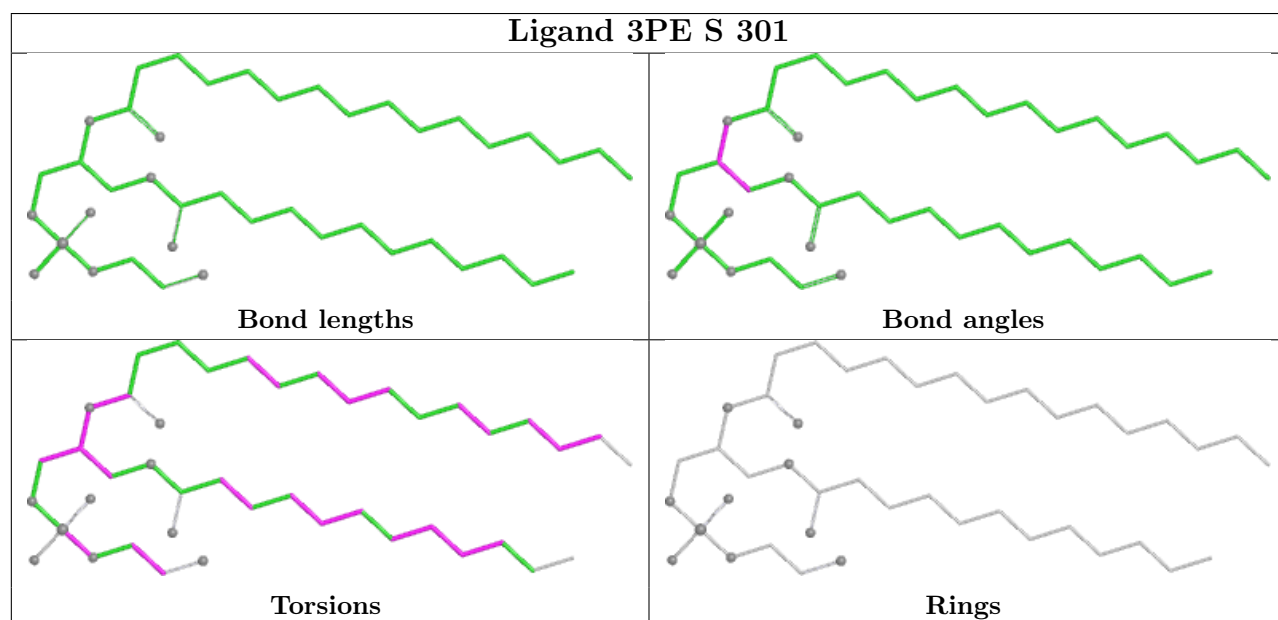
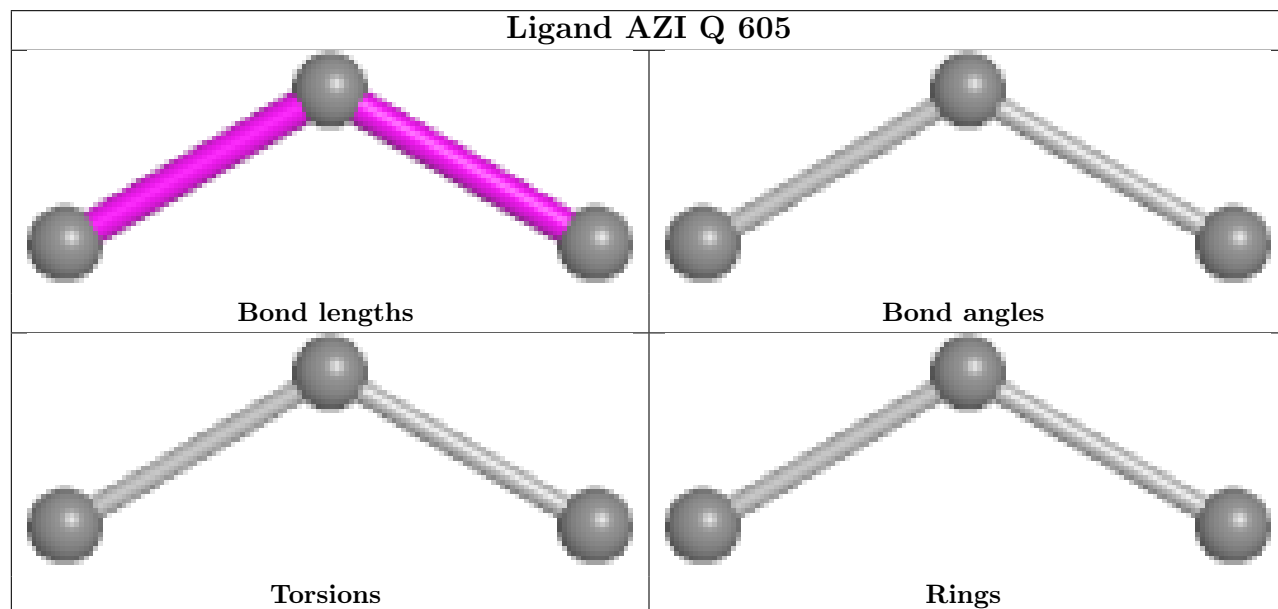
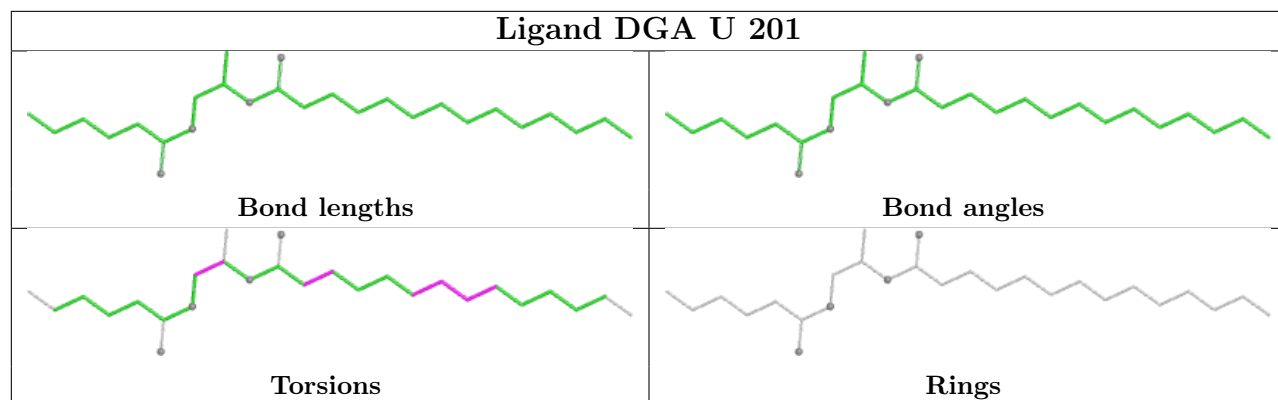


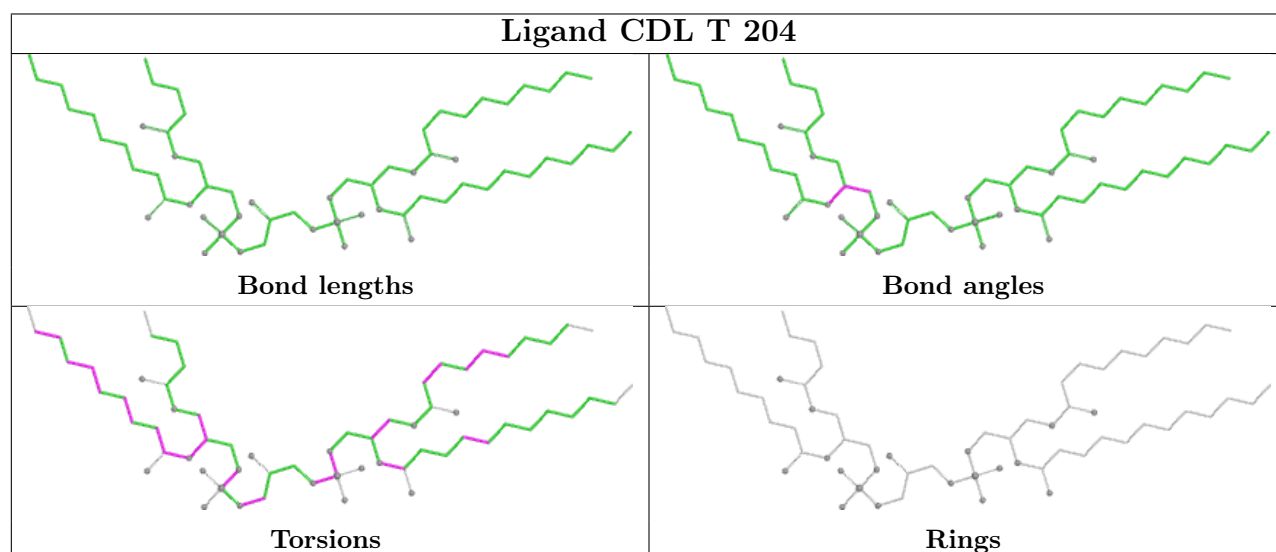
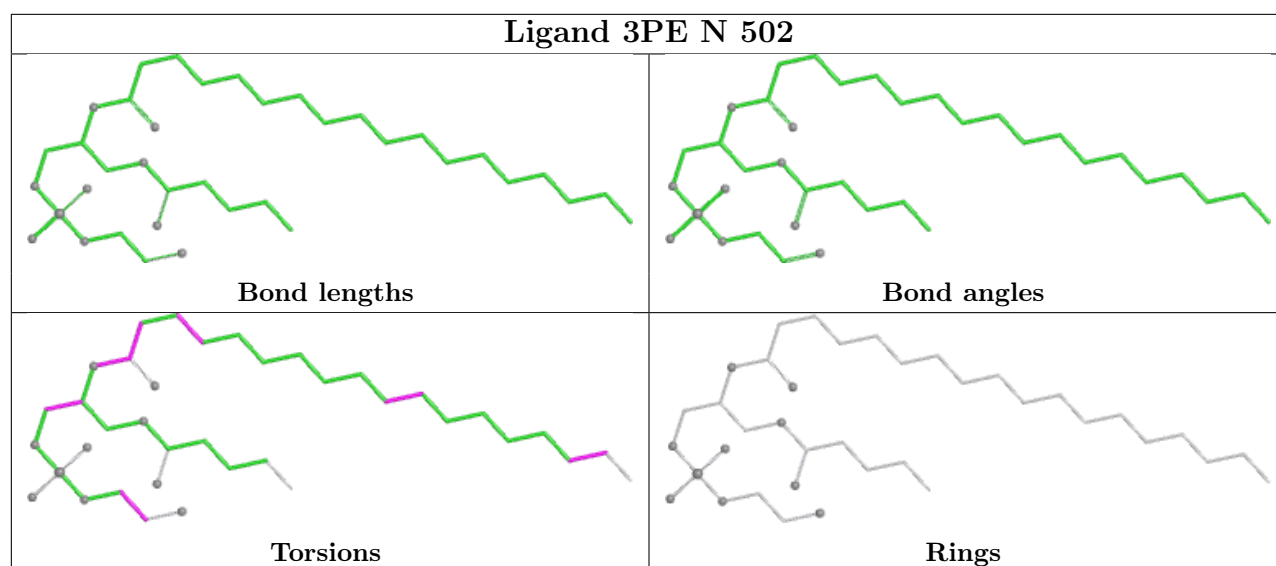
Ligand CDL G 201

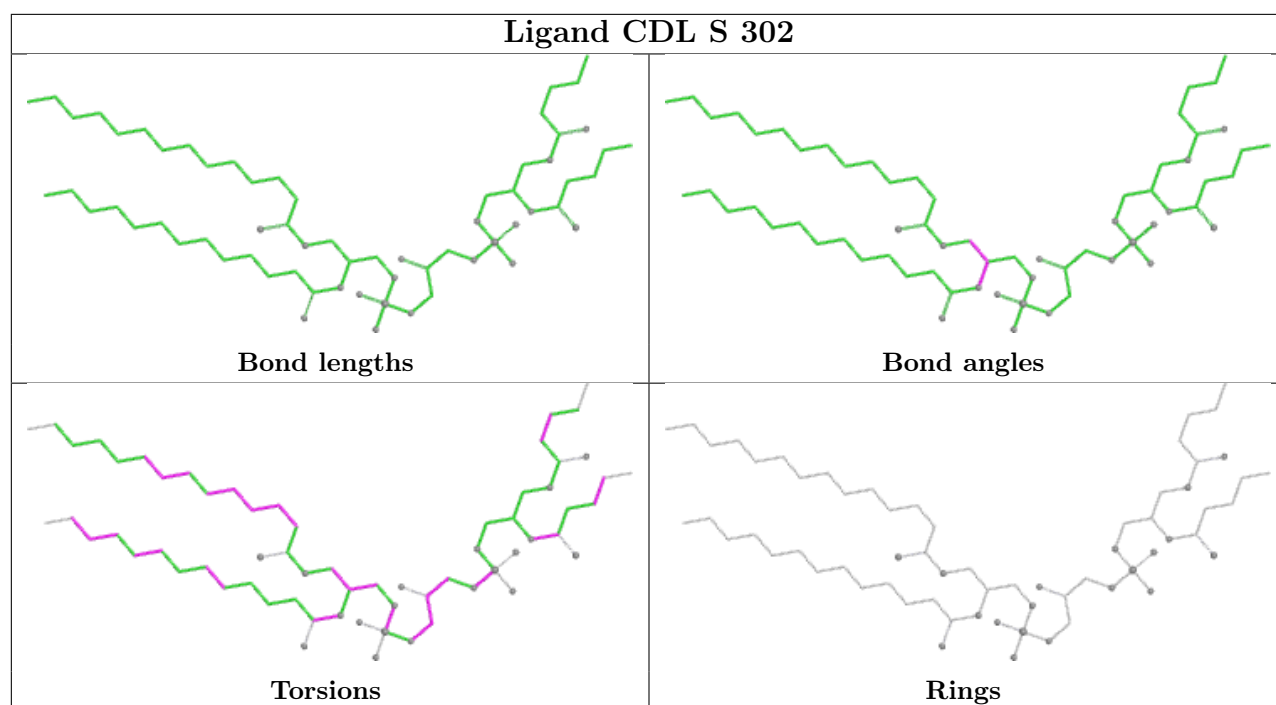


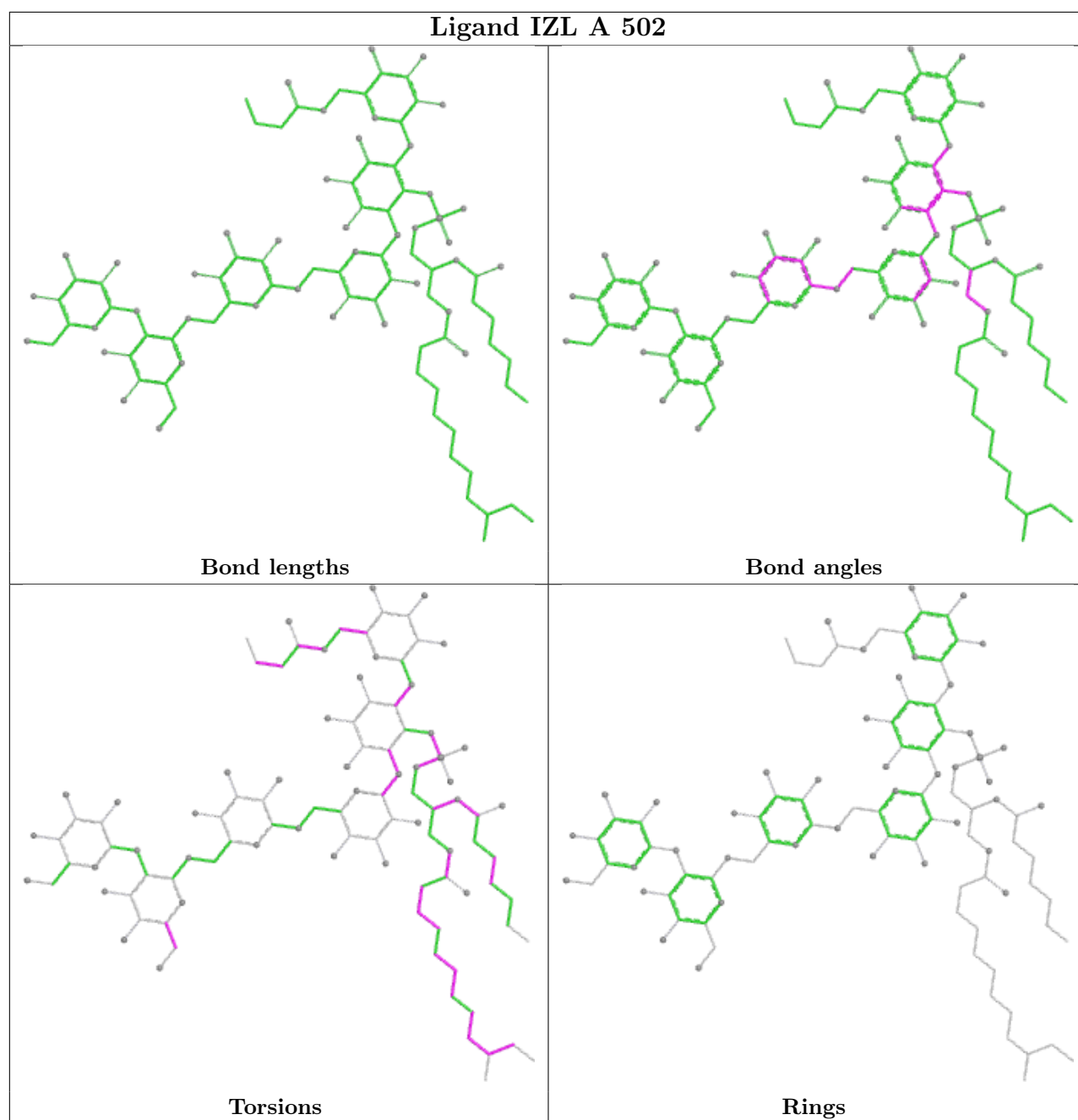


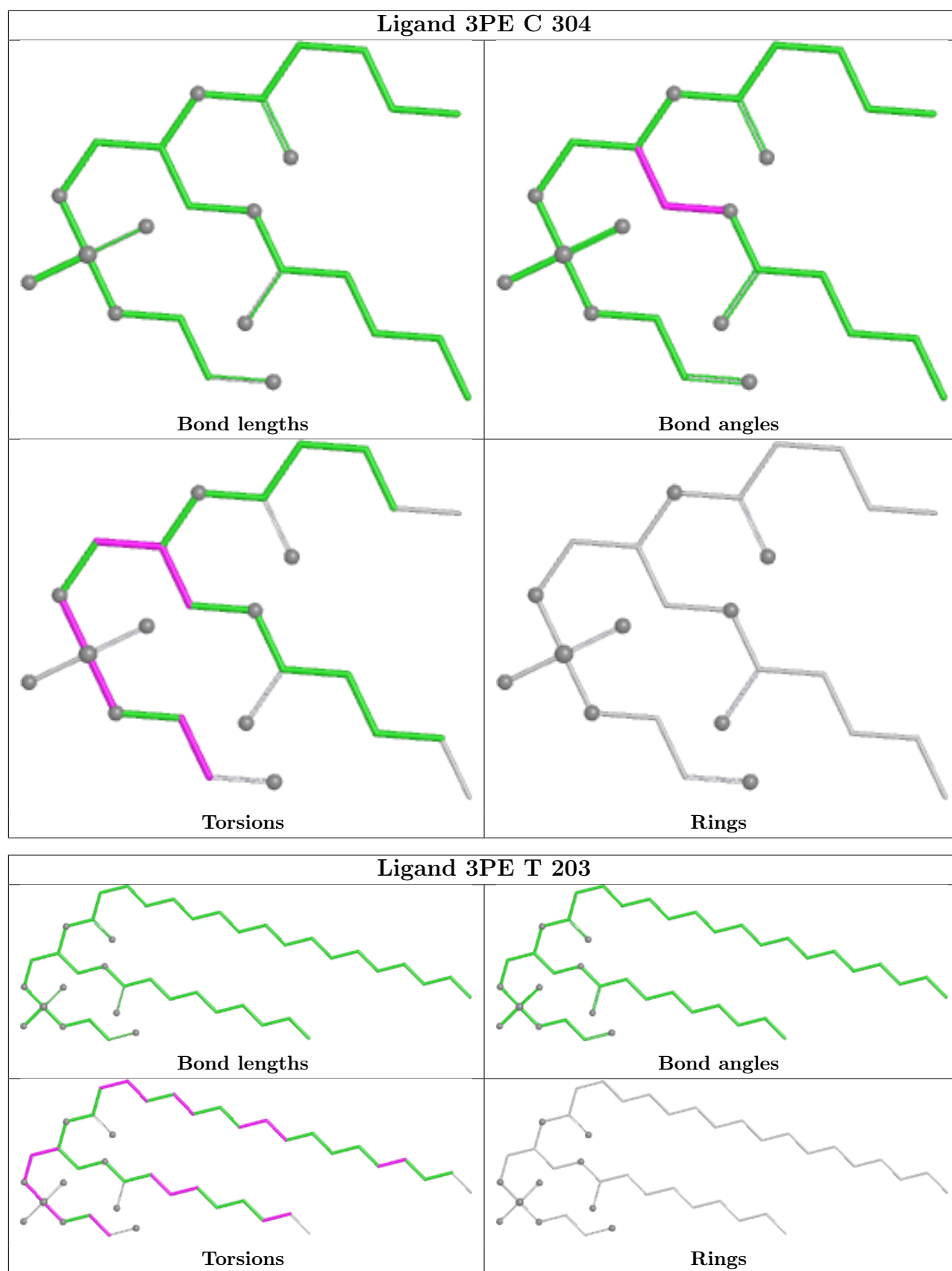


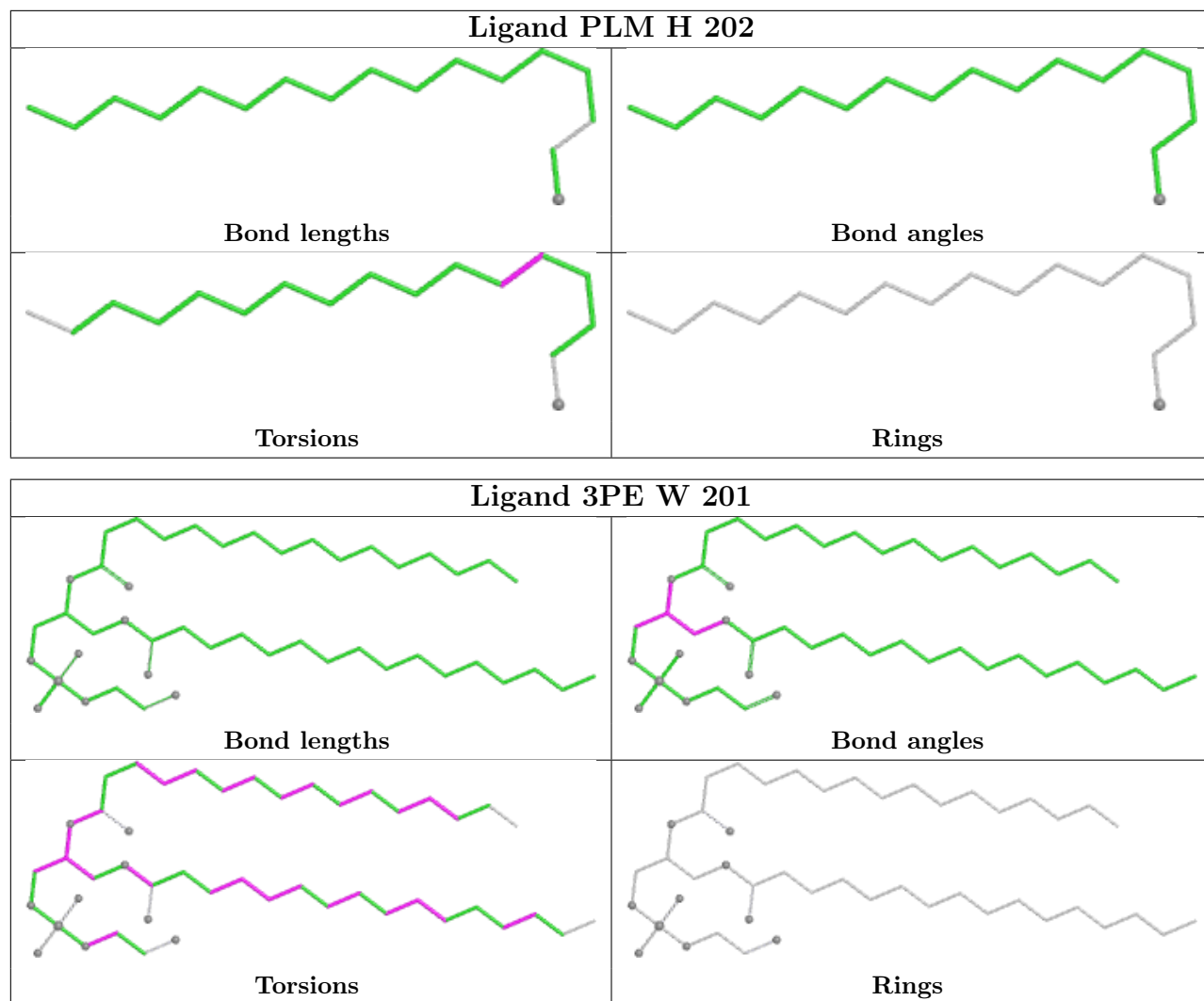


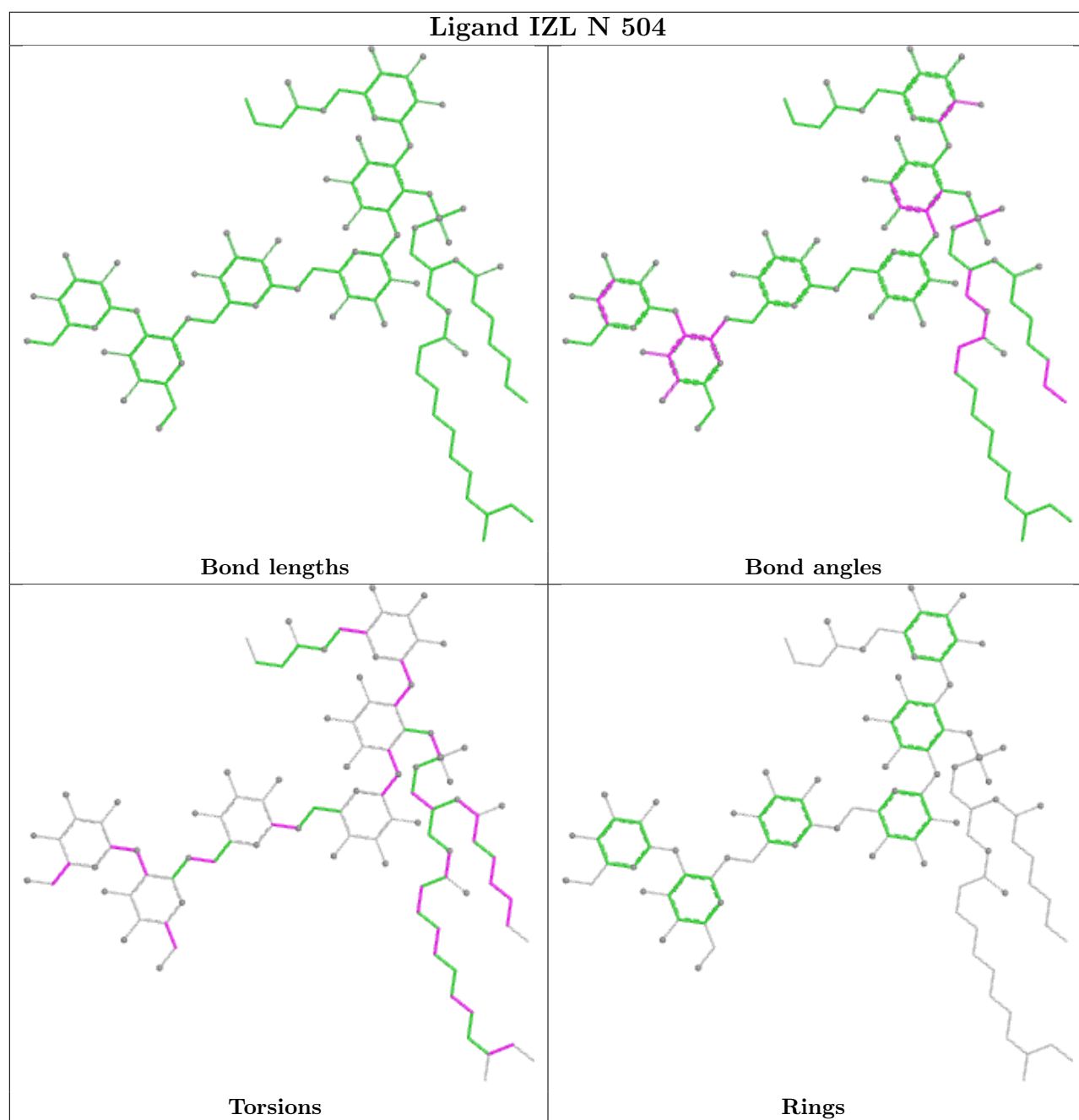


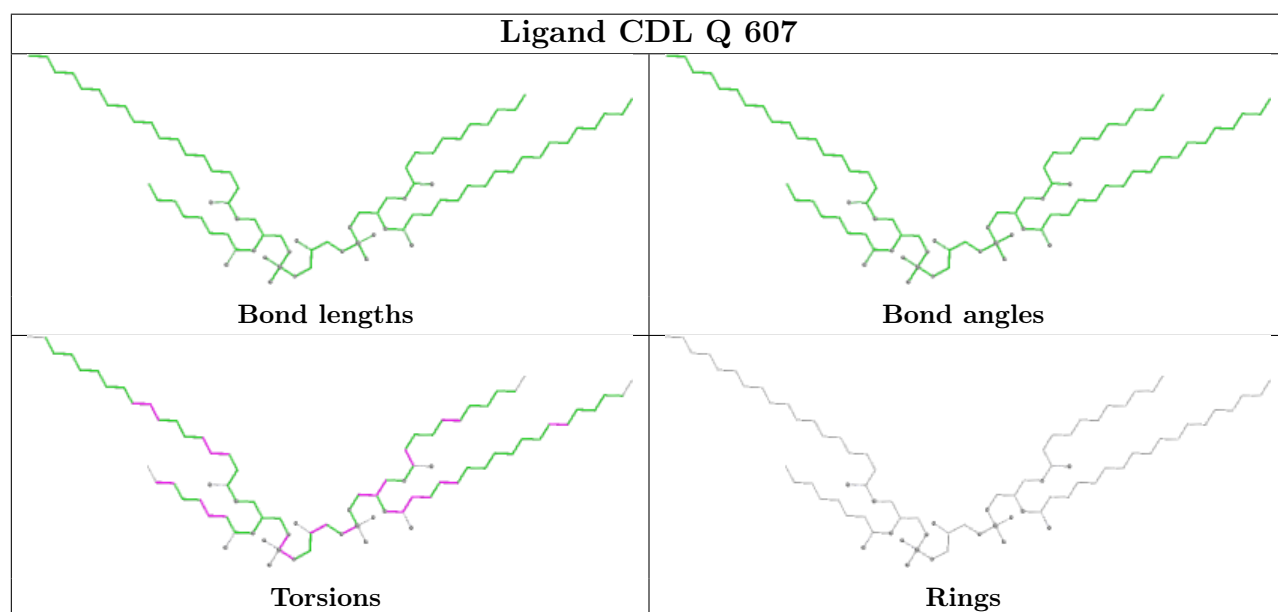
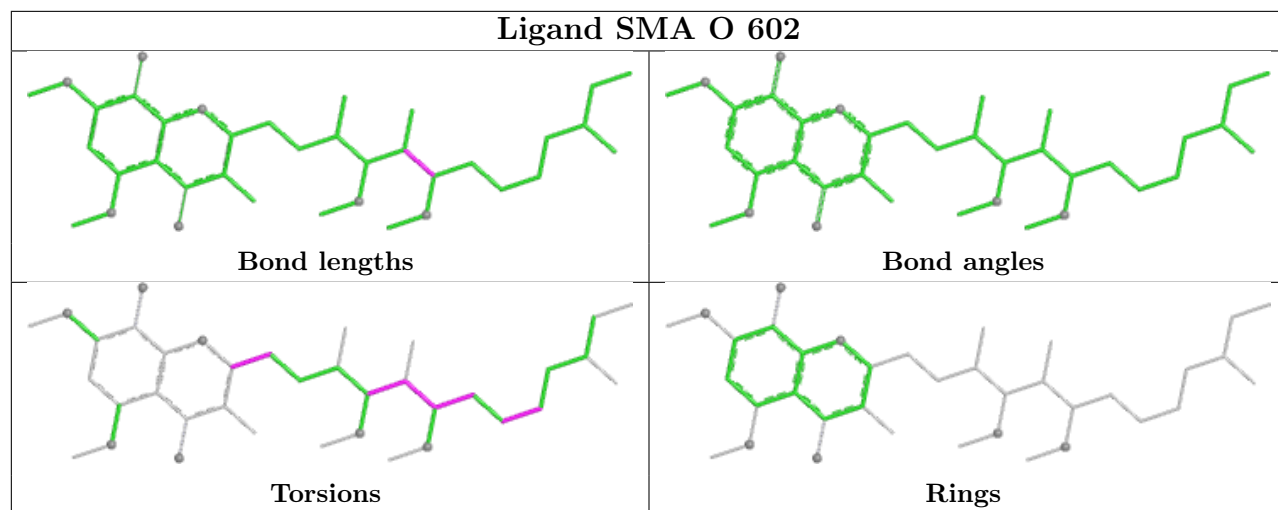


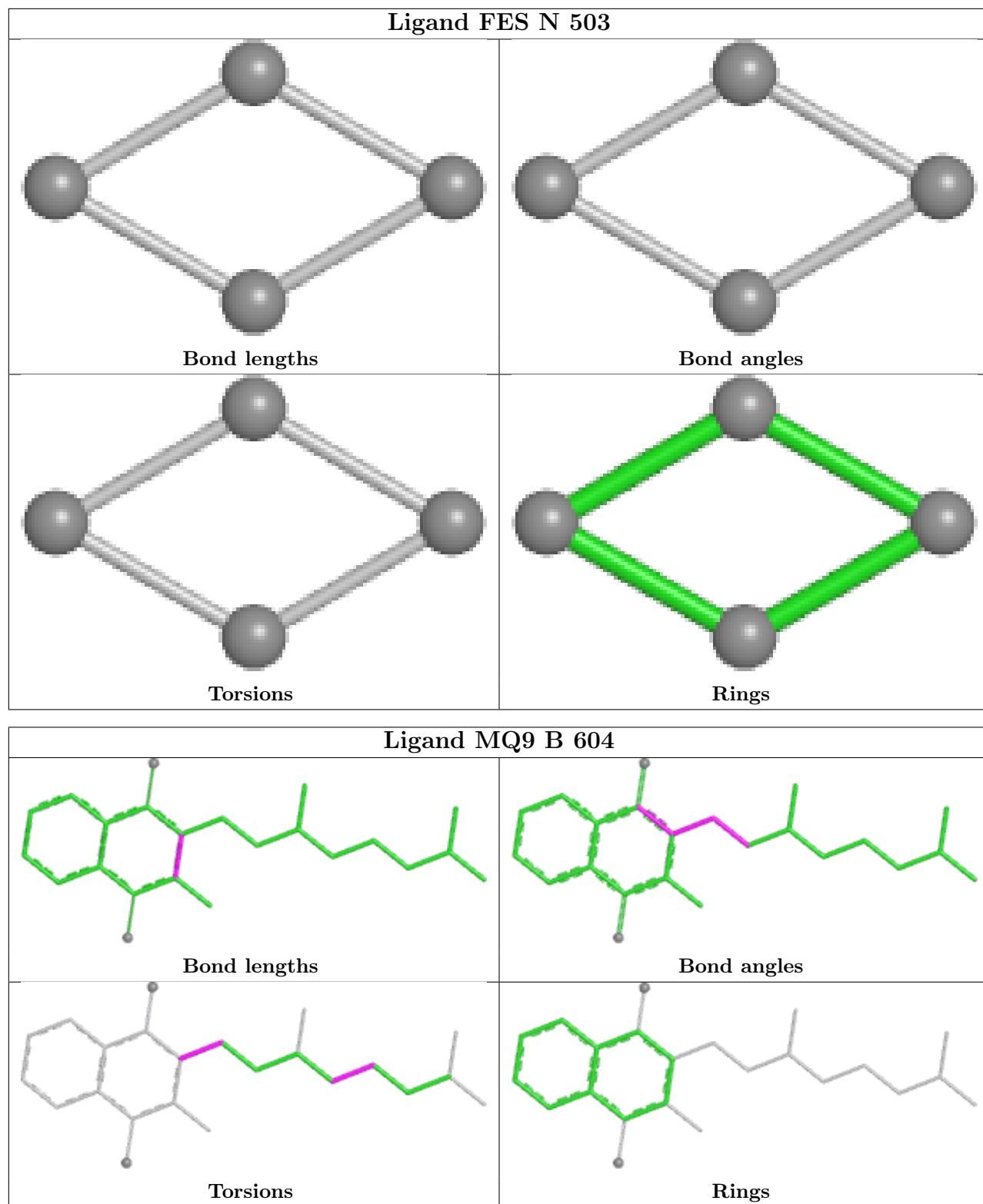


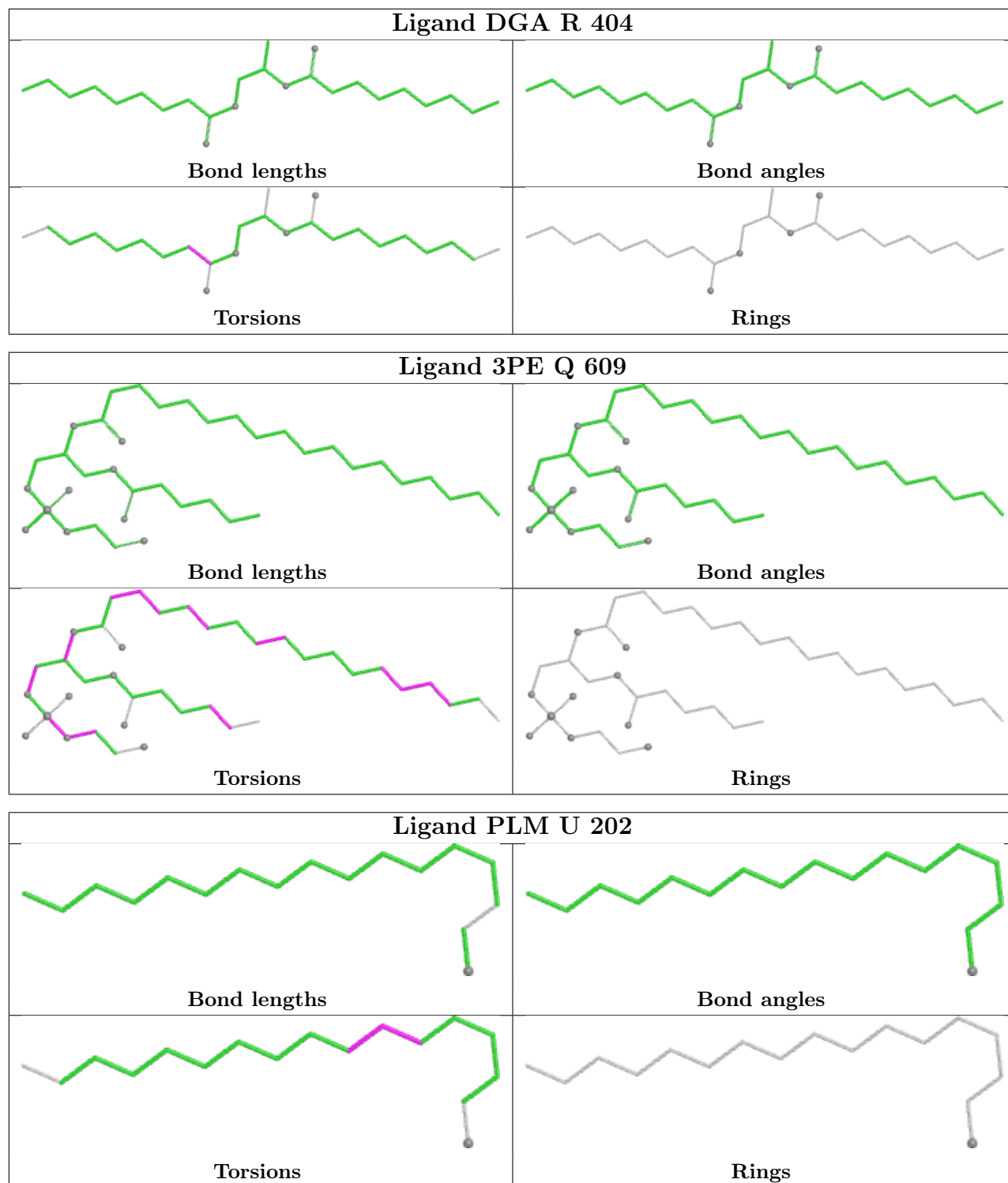


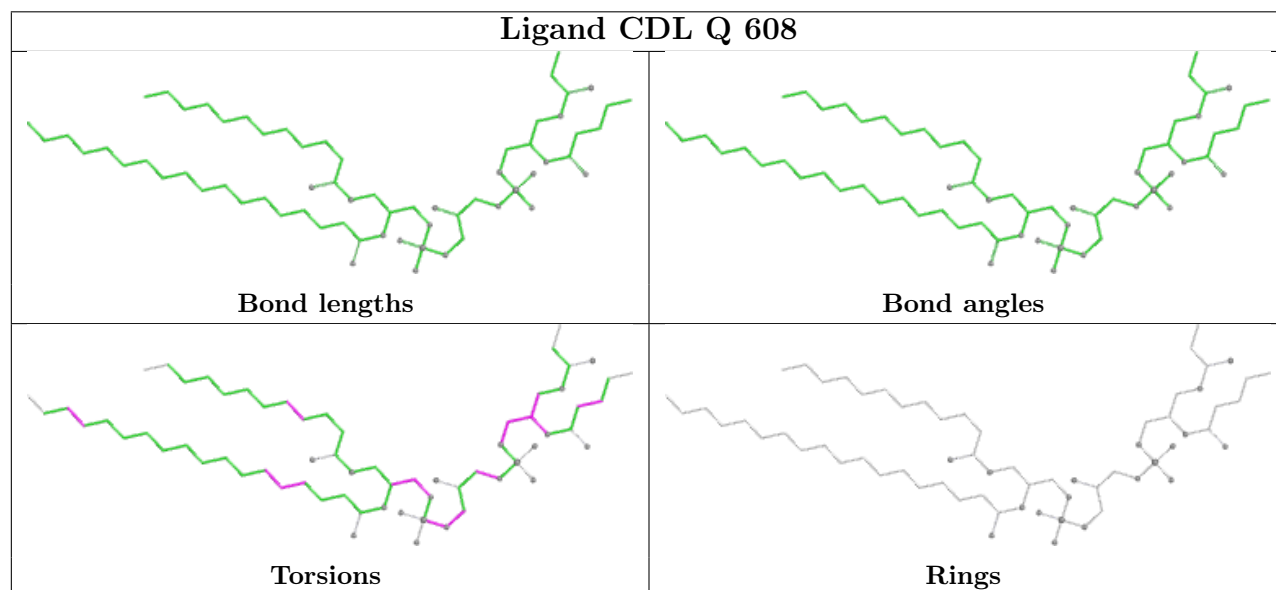
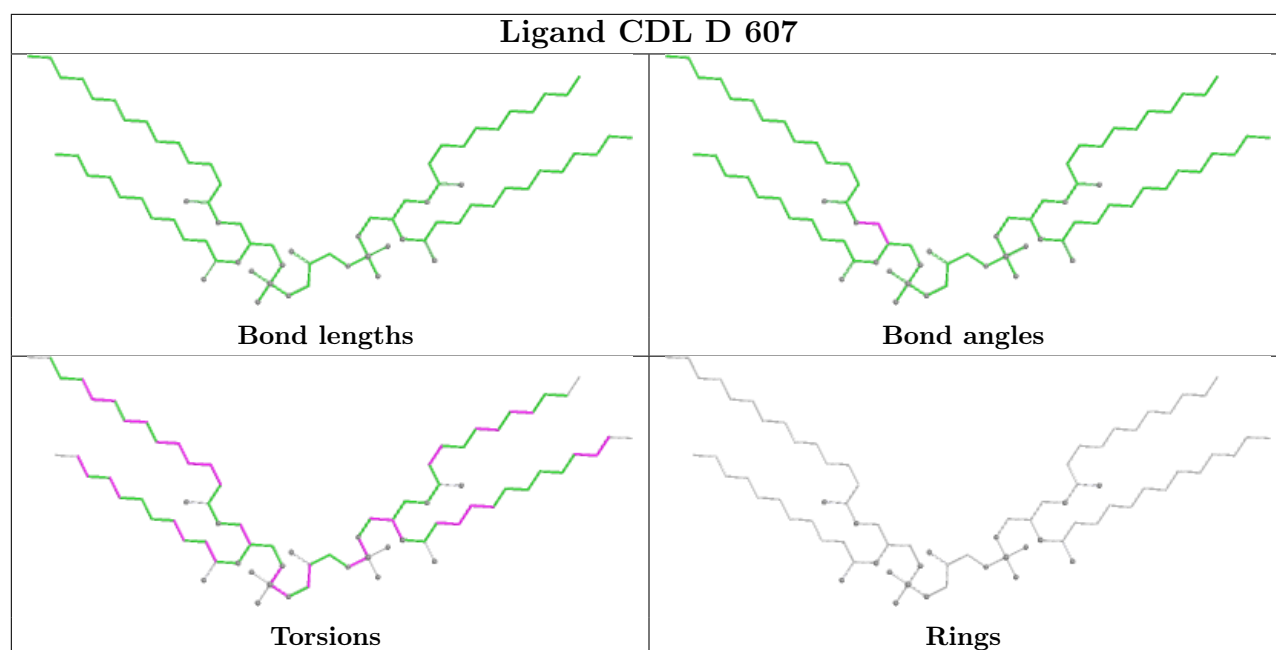


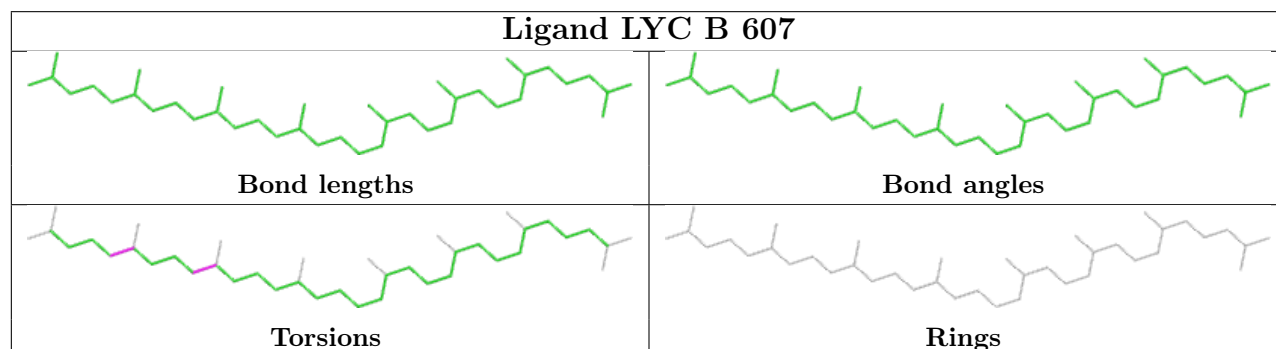
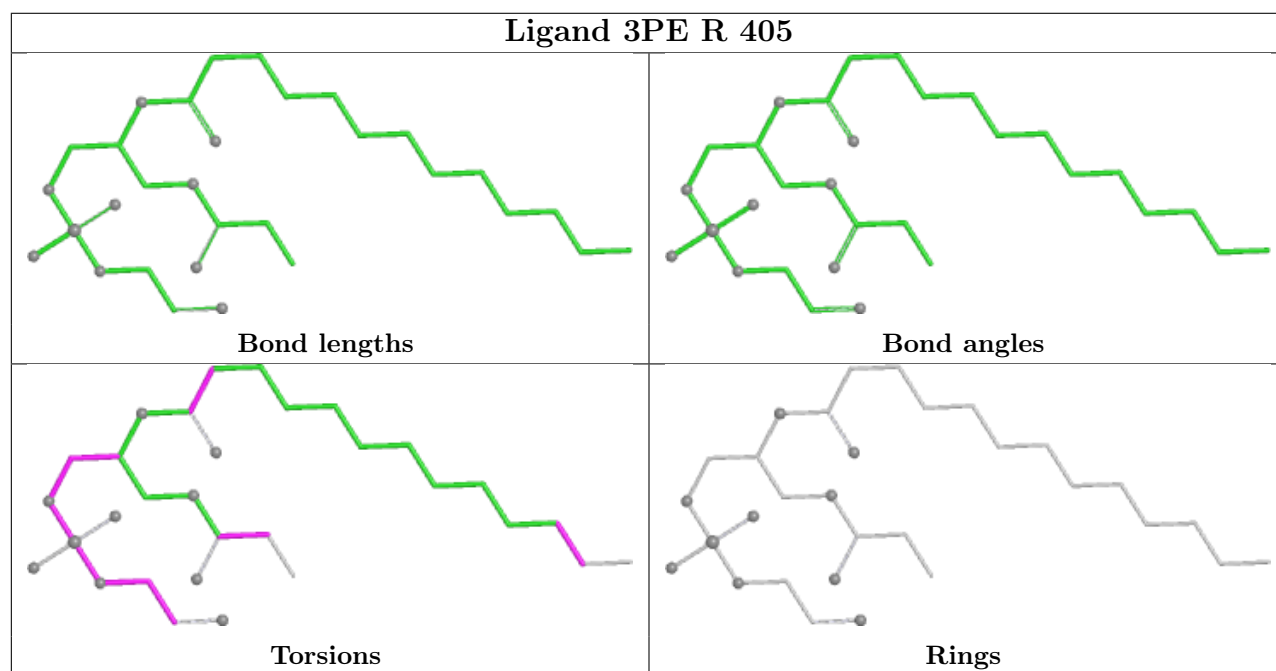
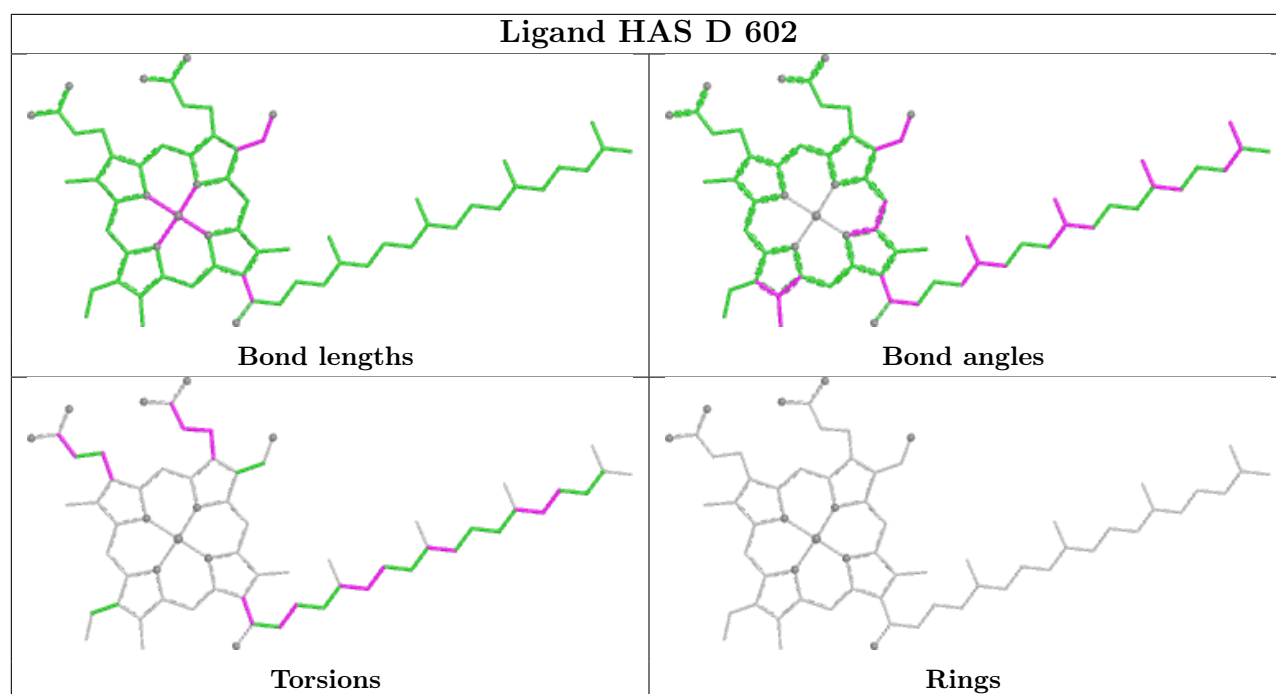


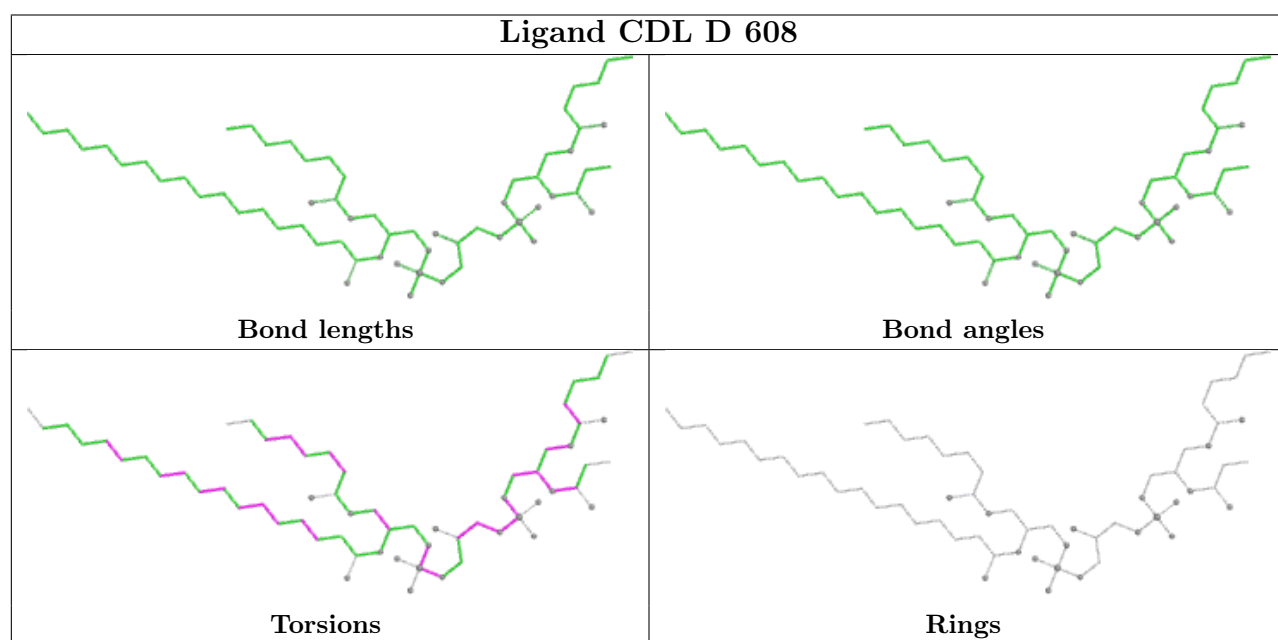
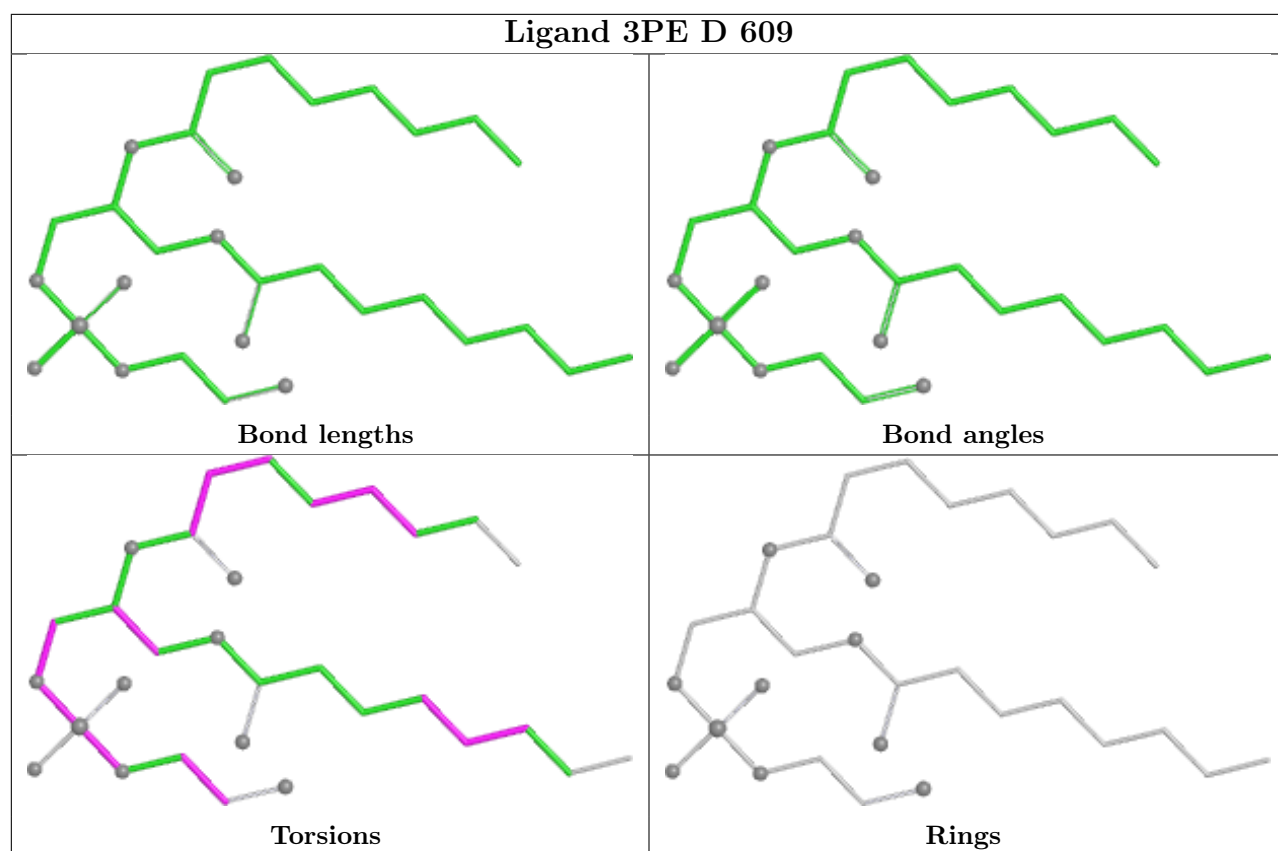


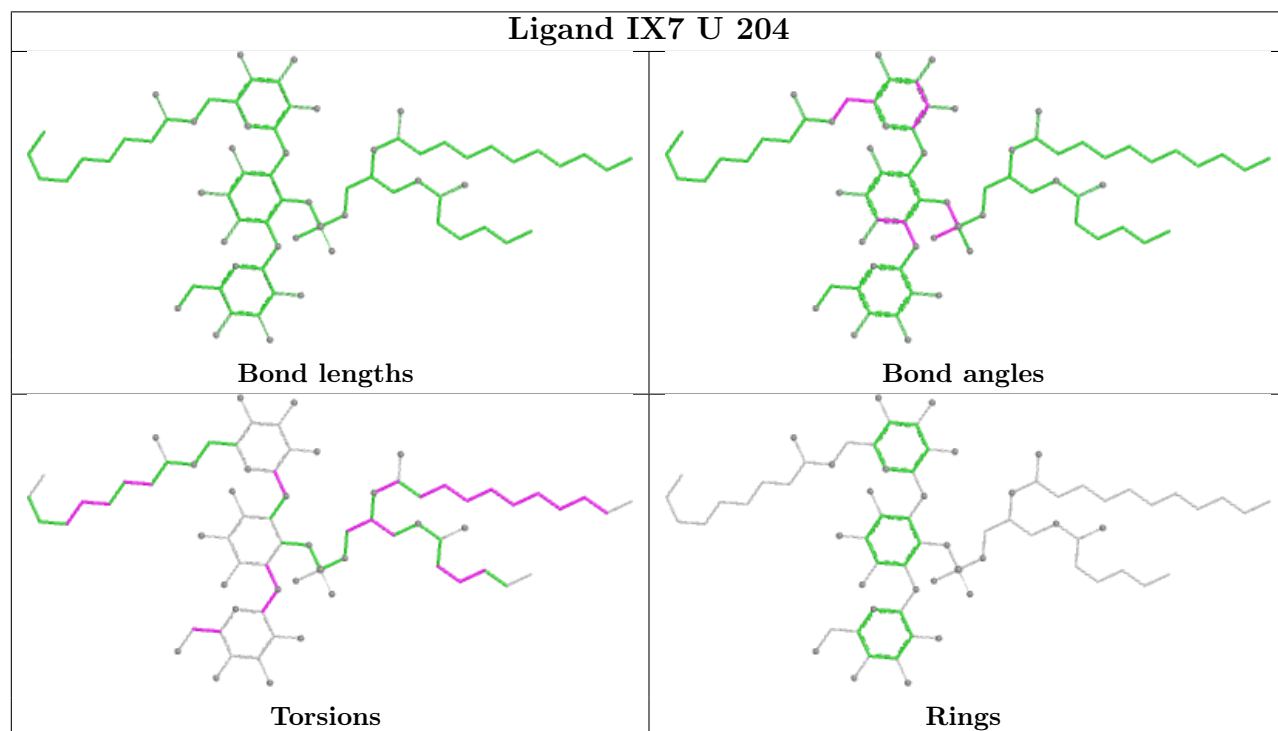
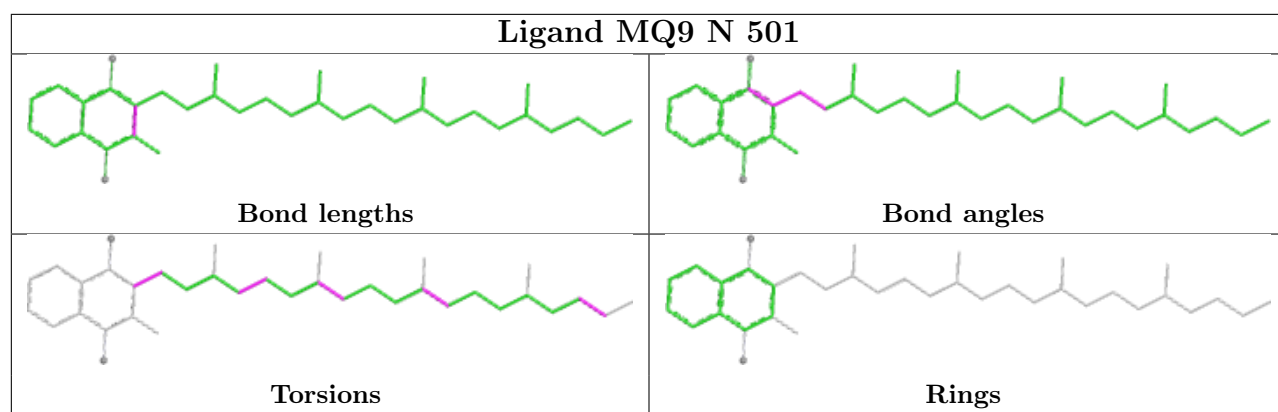




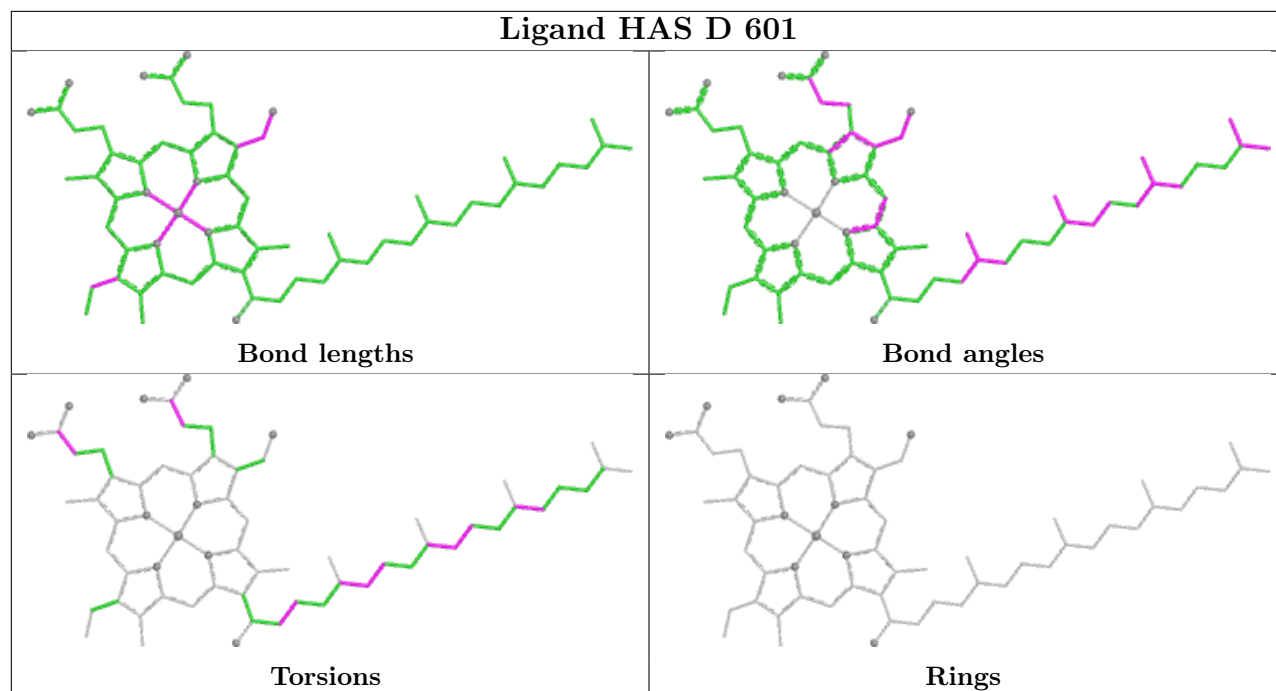




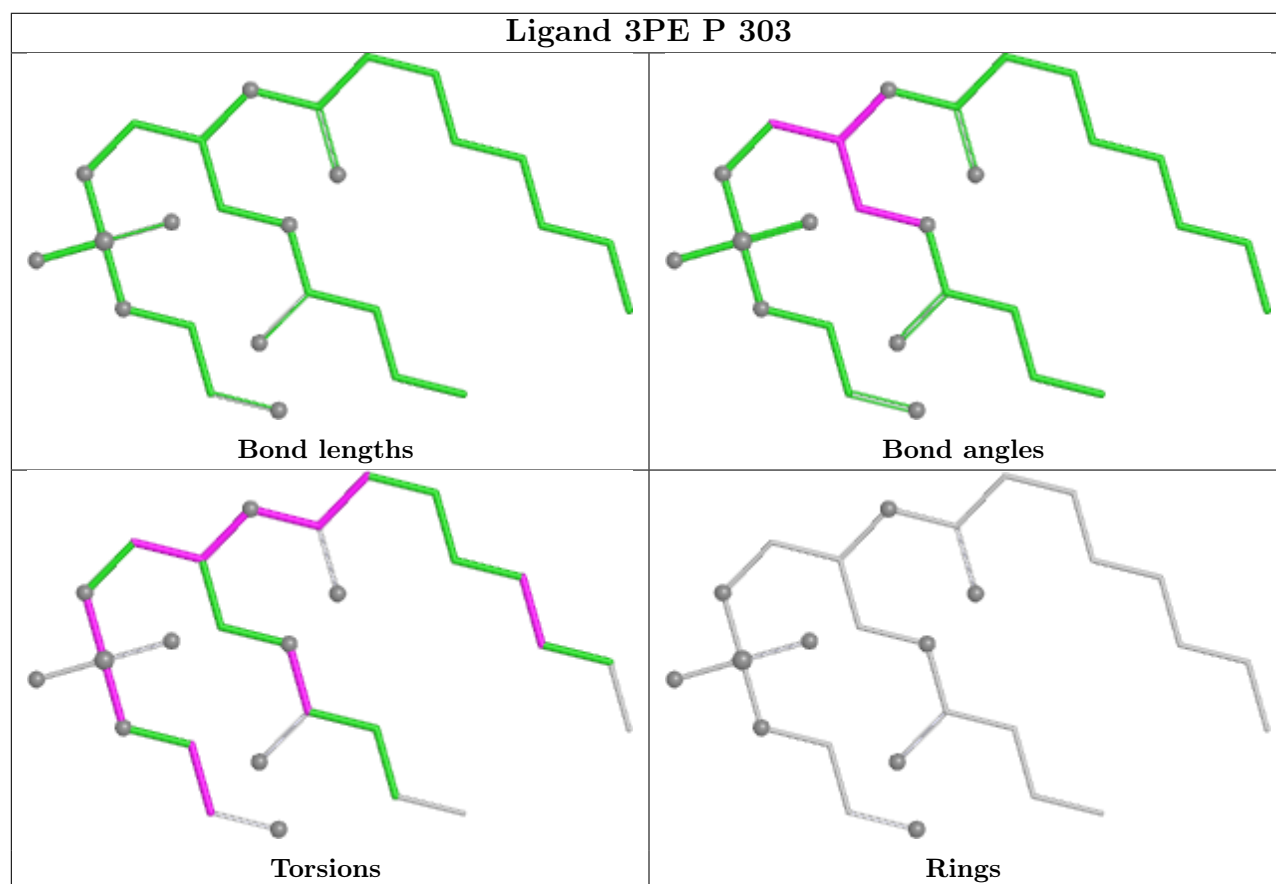


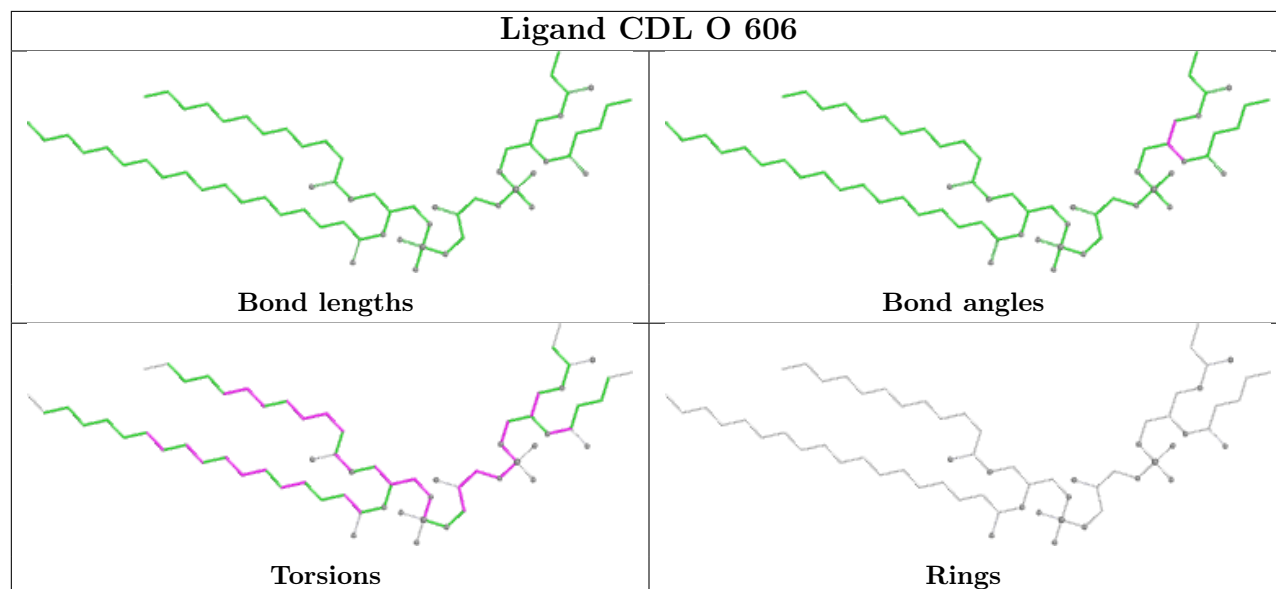
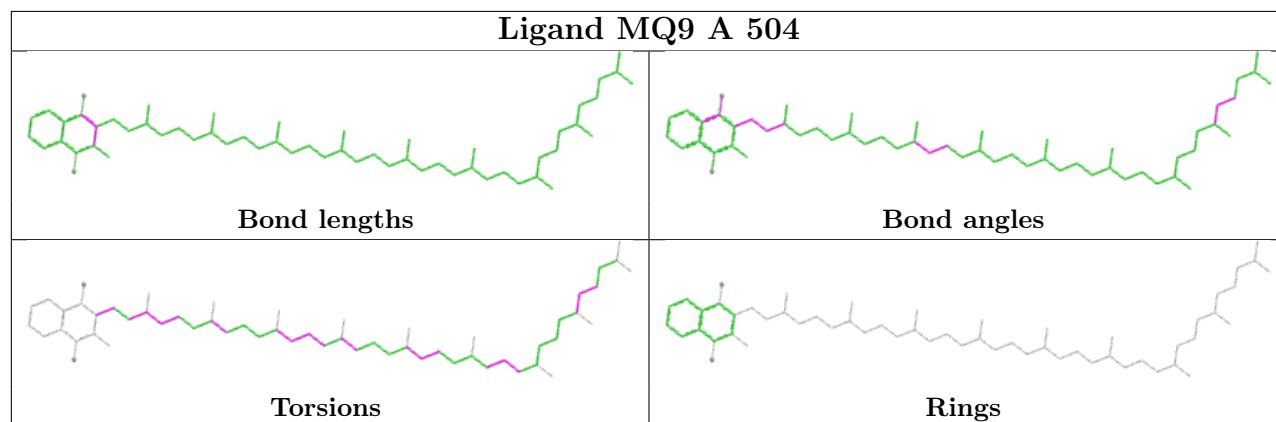
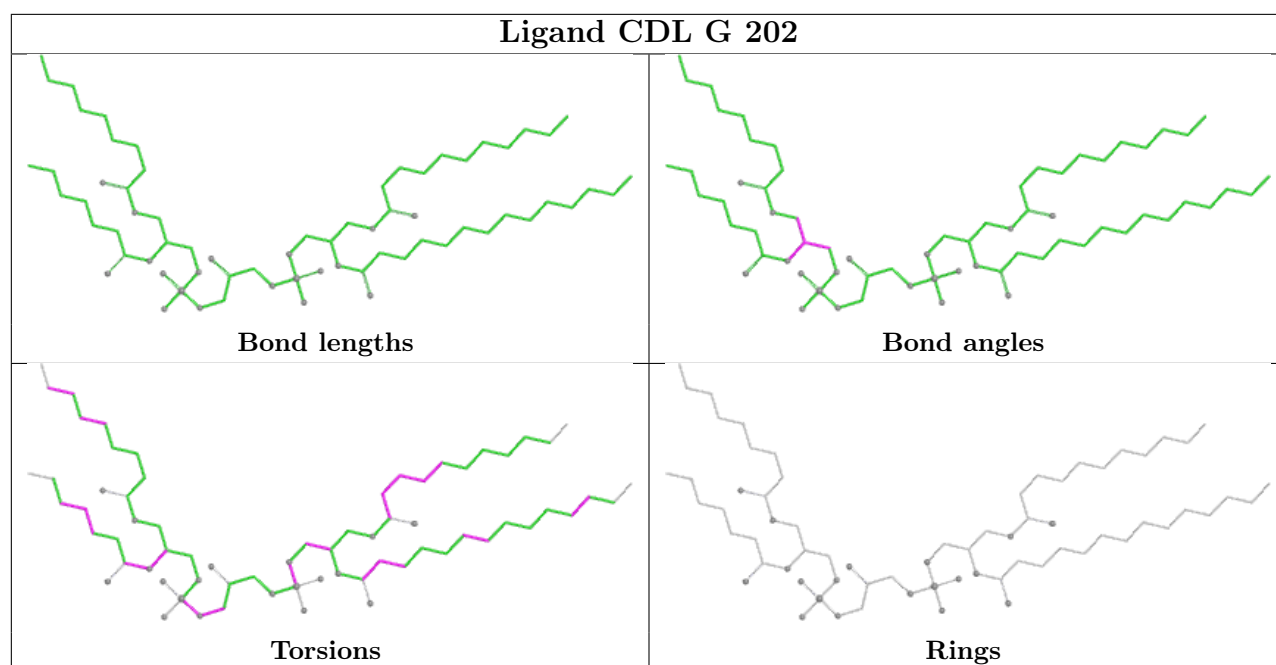


Ligand HAS D 601

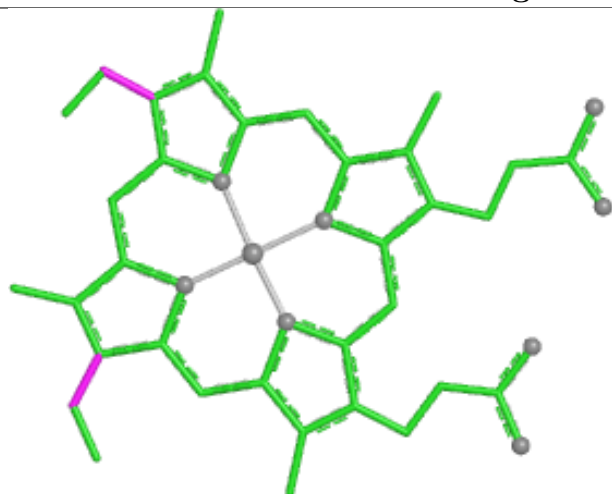


Ligand 3PE P 303

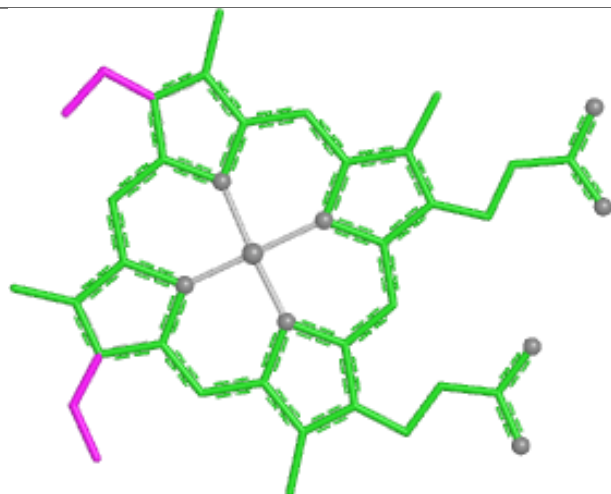




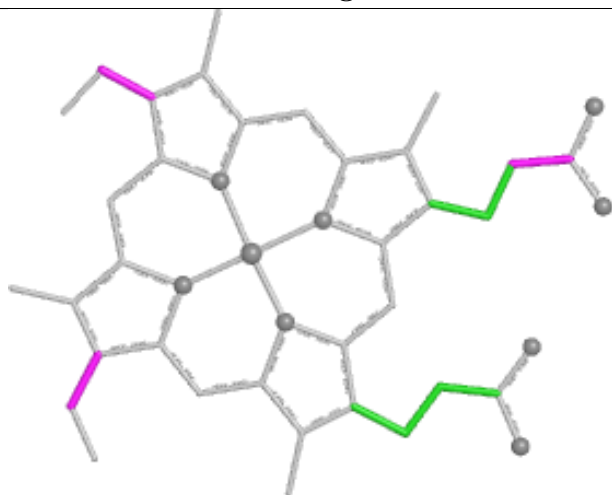
Ligand HEC P 301



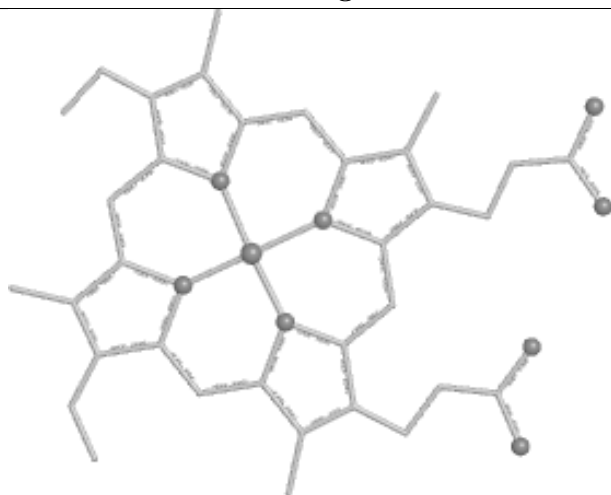
Bond lengths



Bond angles

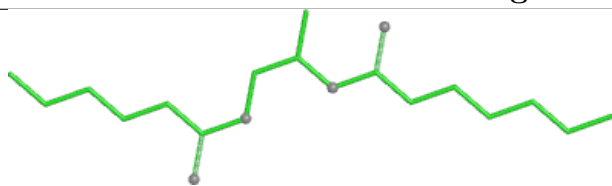


Torsions

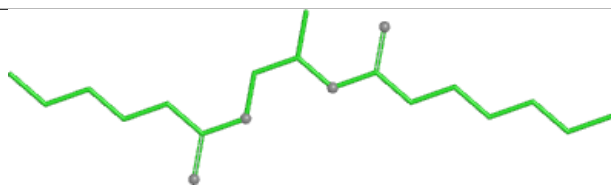


Rings

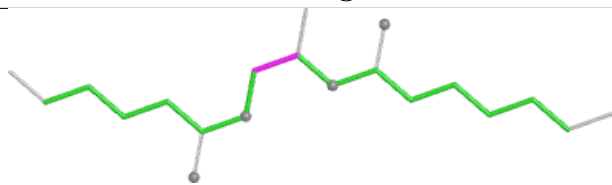
Ligand DGA E 403



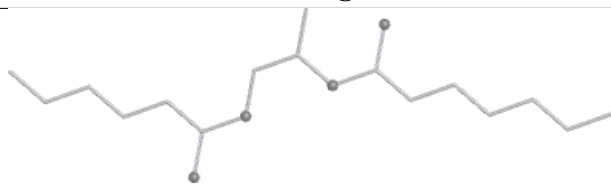
Bond lengths



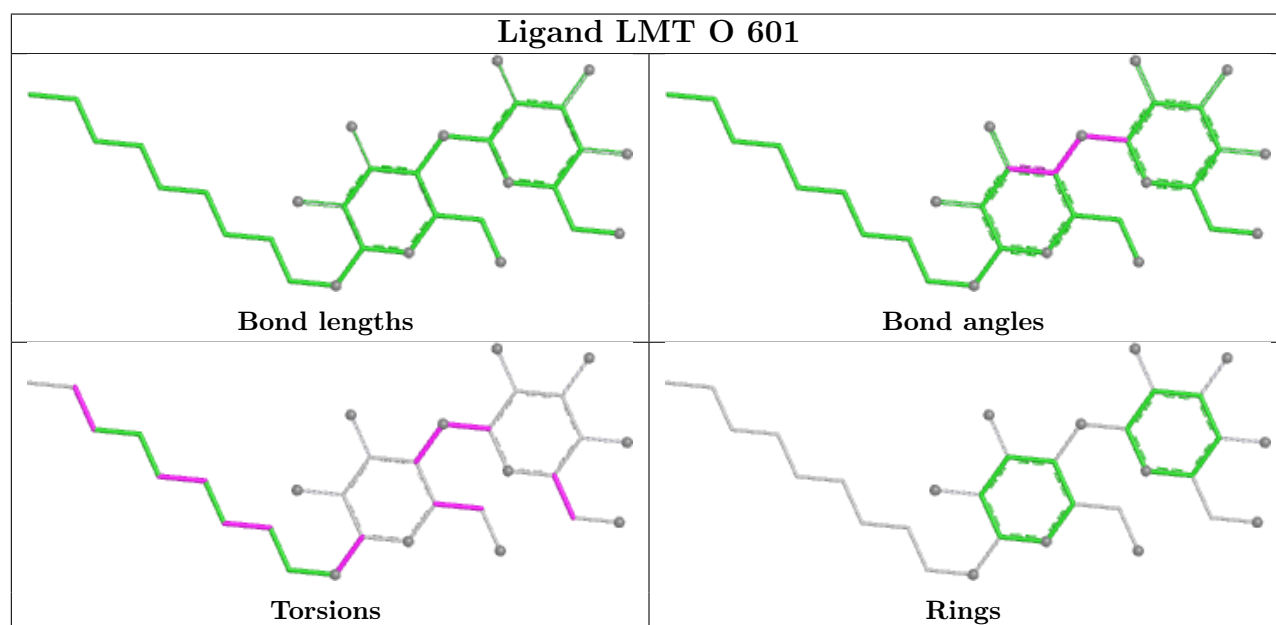
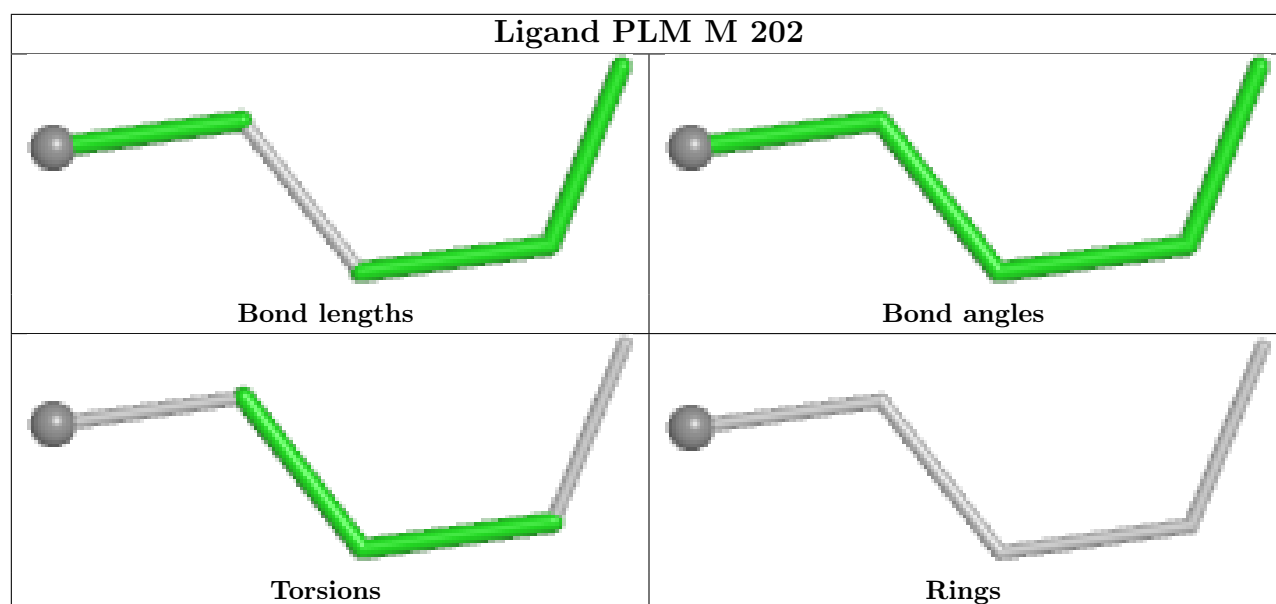
Bond angles

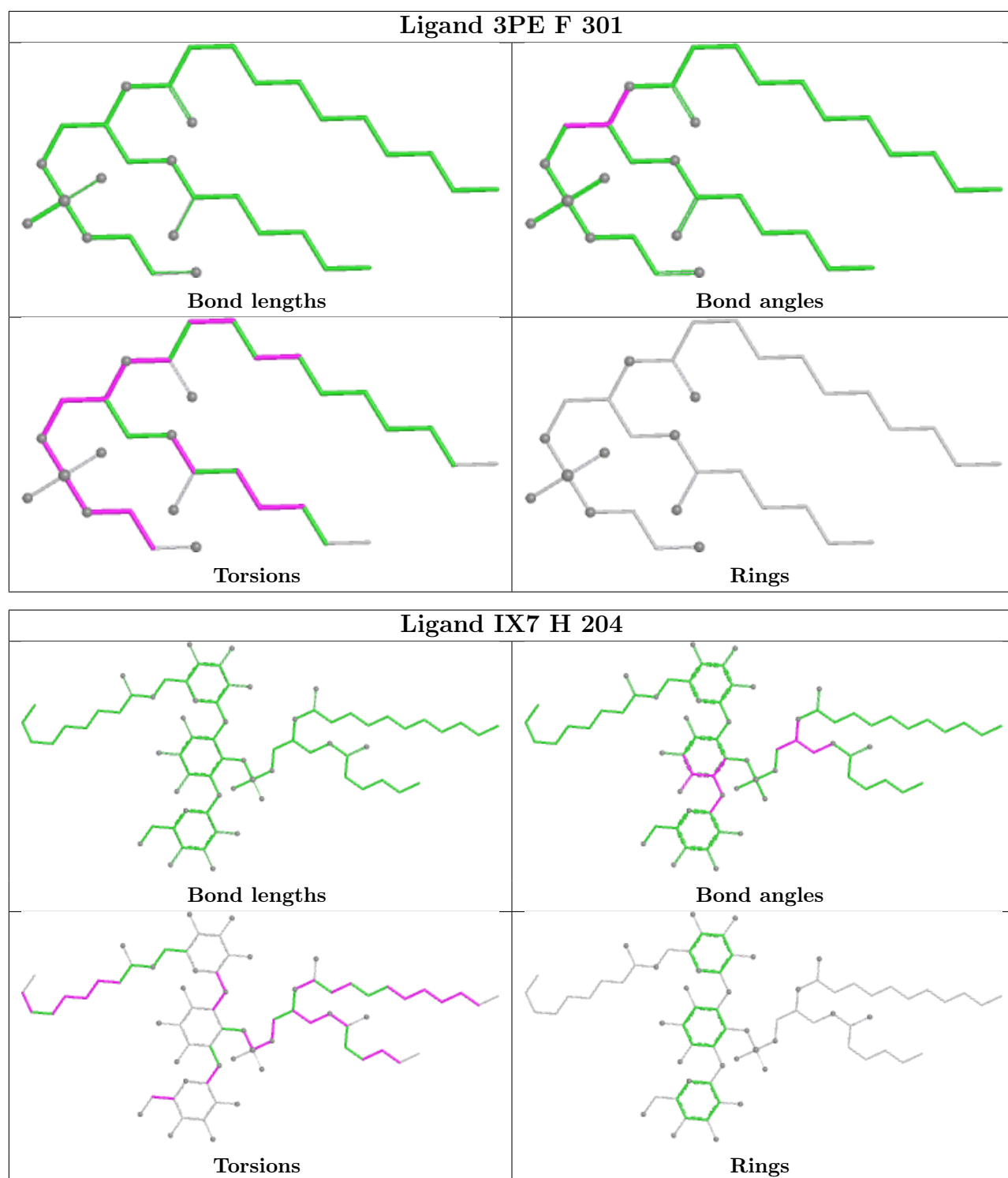


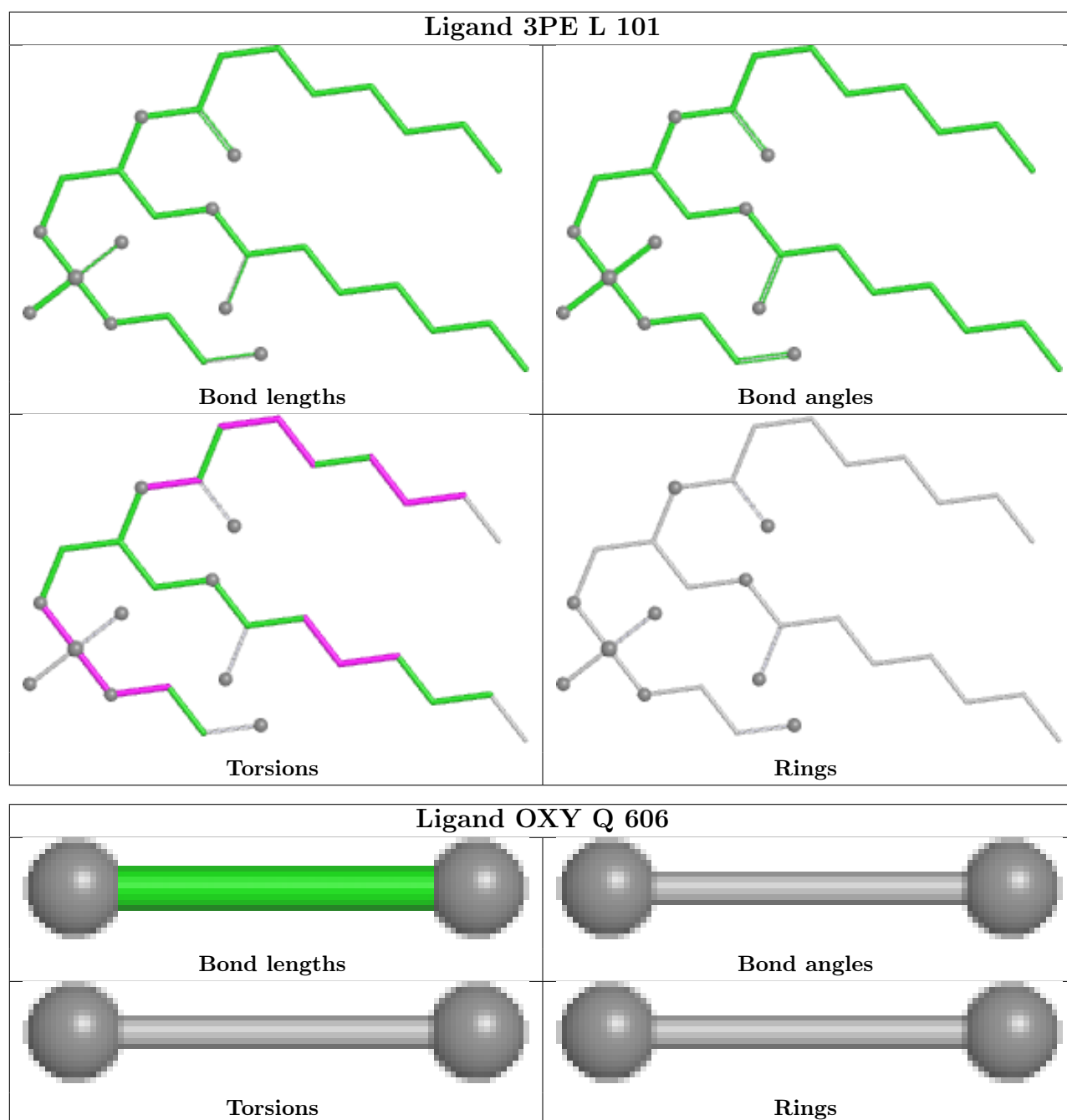
Torsions

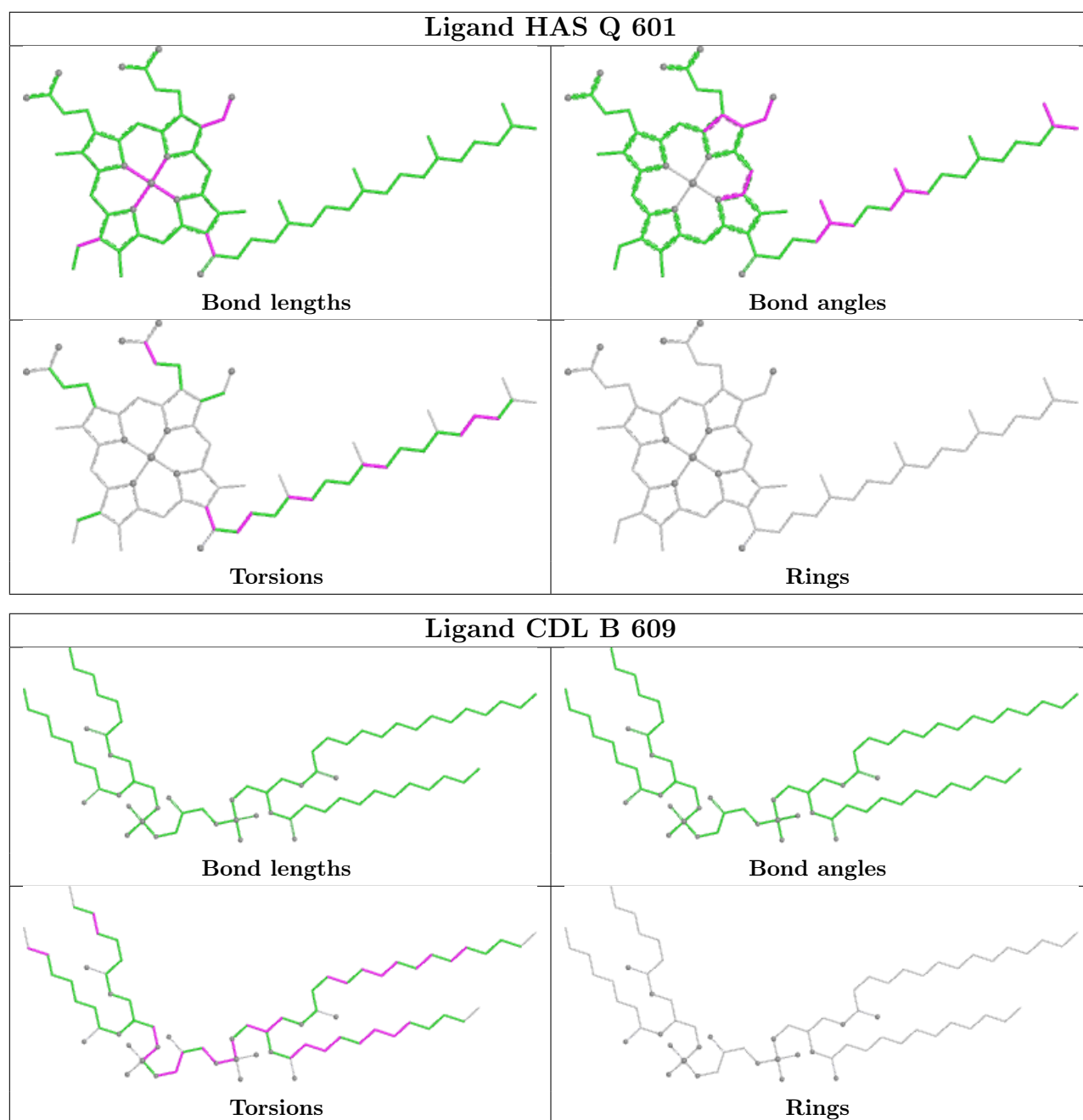


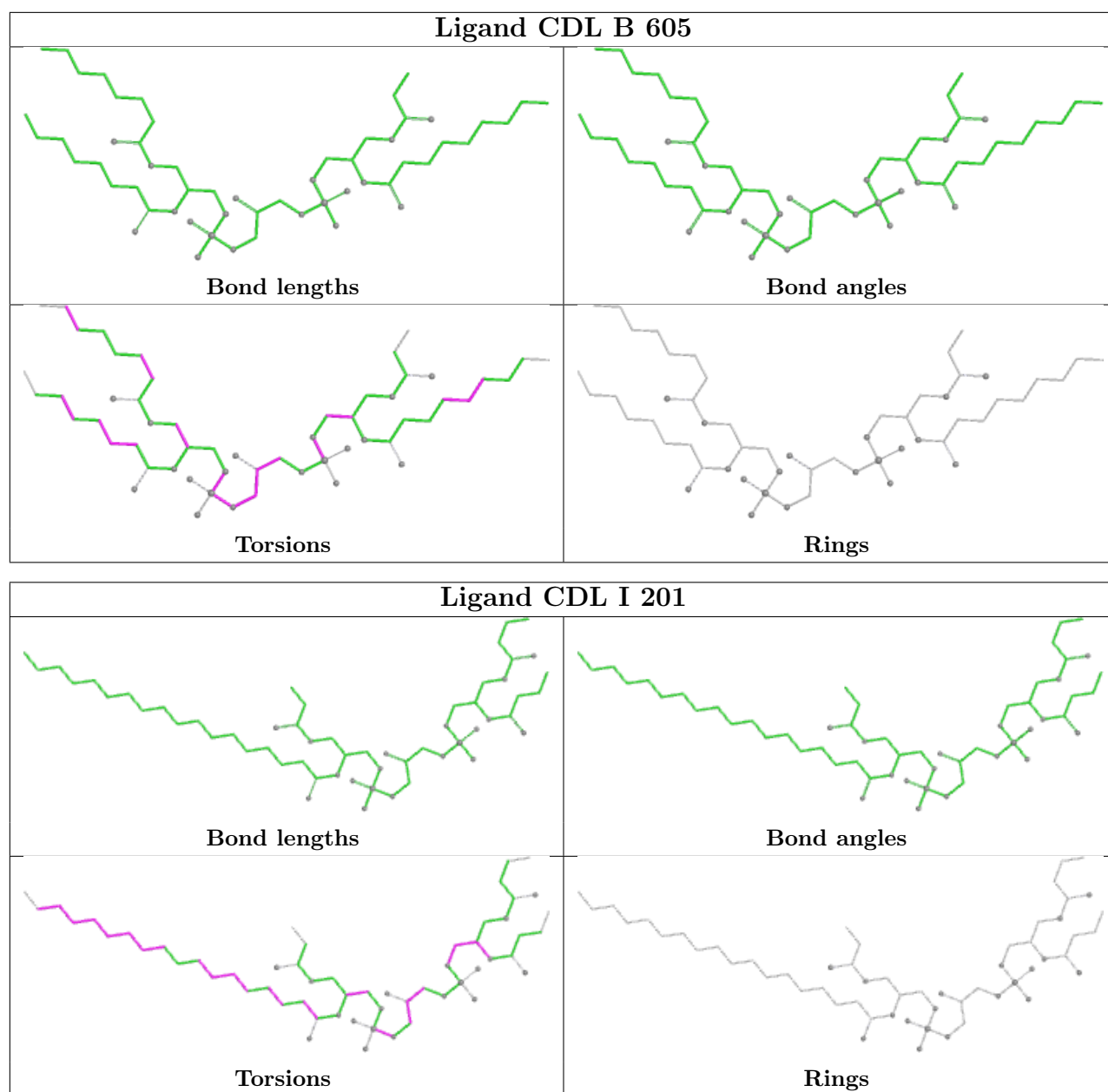
Rings











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.

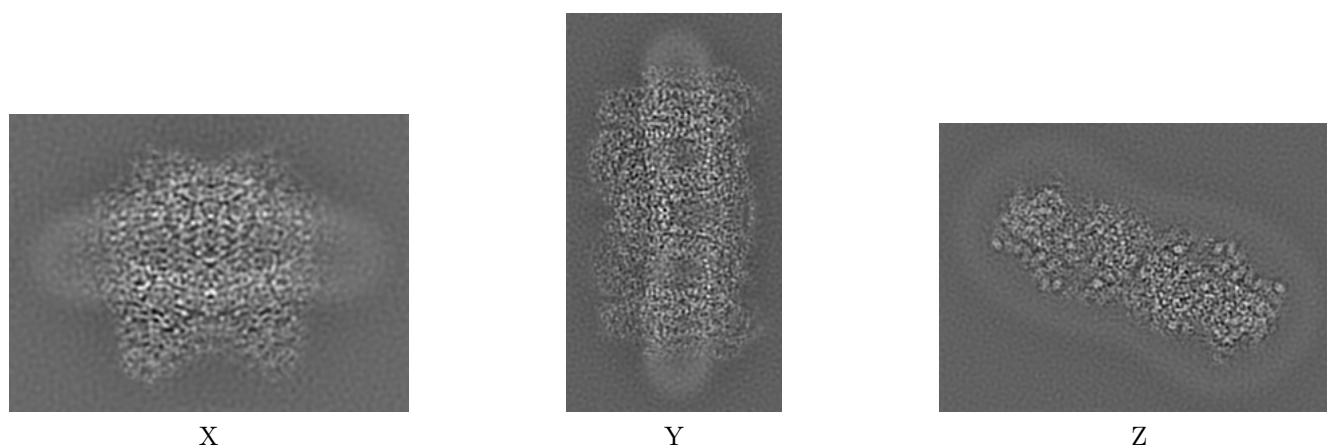
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13976. 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](#)

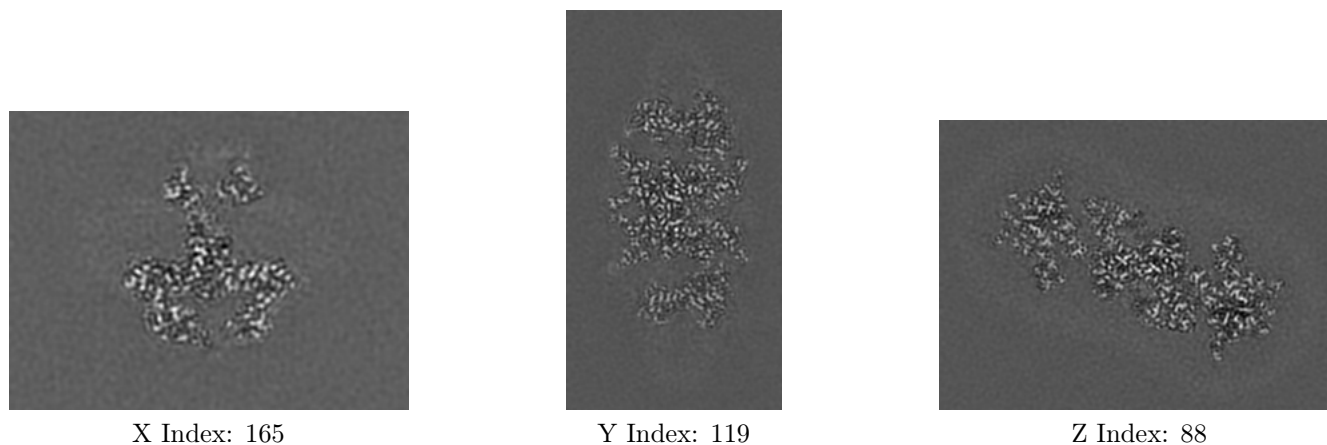
6.1.1 Primary map



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

6.2 Central slices [i](#)

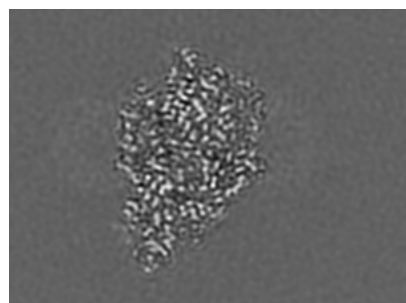
6.2.1 Primary map



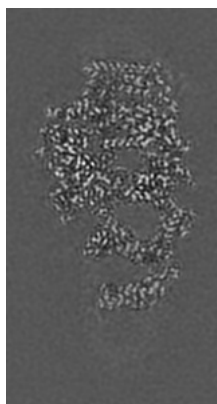
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

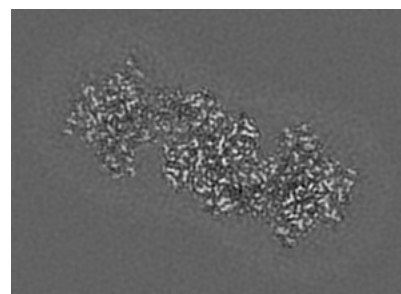
6.3.1 Primary map



X Index: 190



Y Index: 102

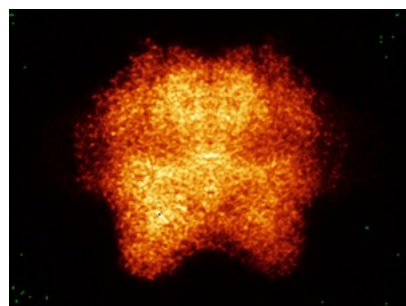


Z Index: 80

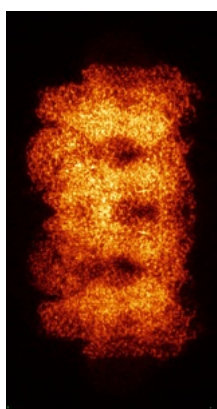
The images above show the largest variance slices of the map in three orthogonal directions.

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

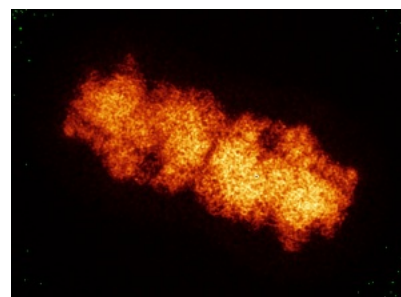
6.4.1 Primary map



X



Y

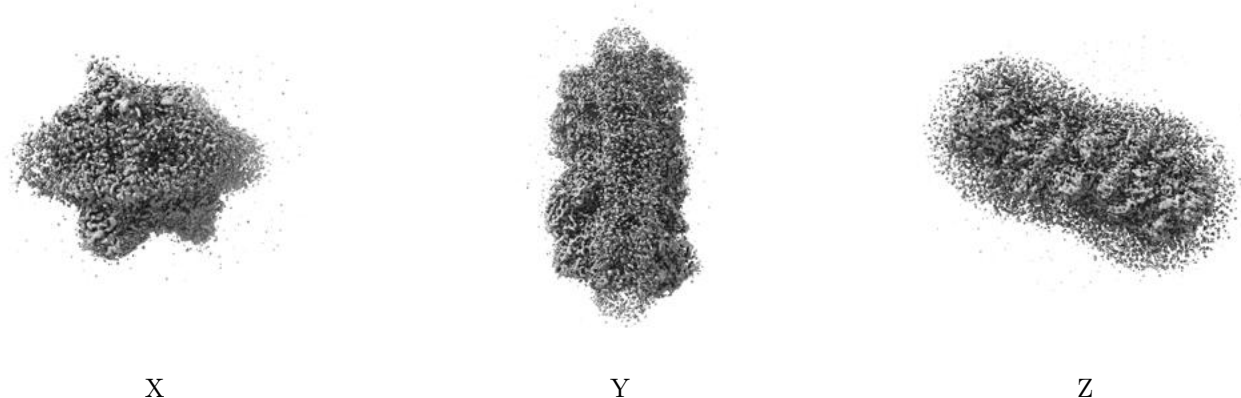


Z

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

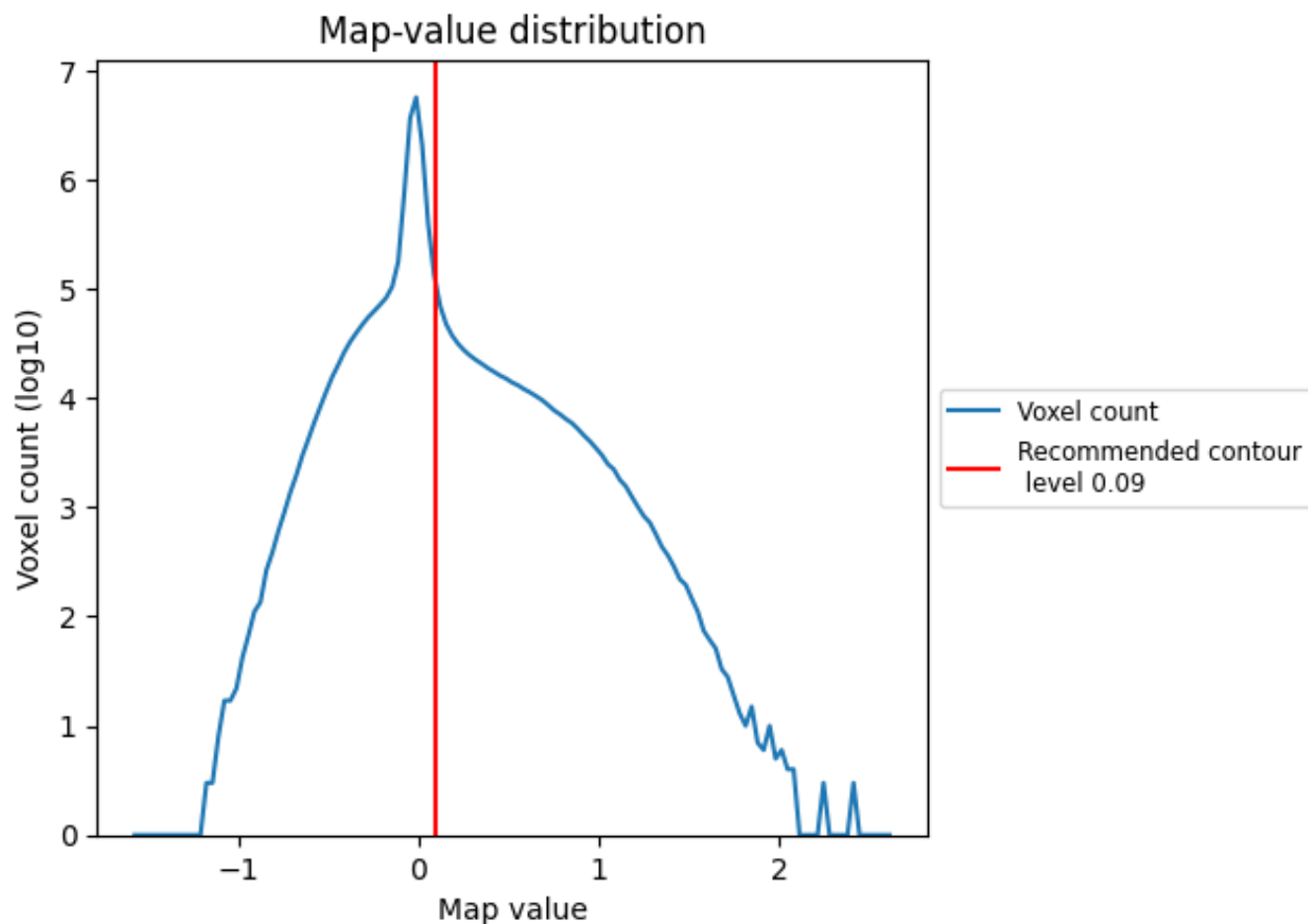
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

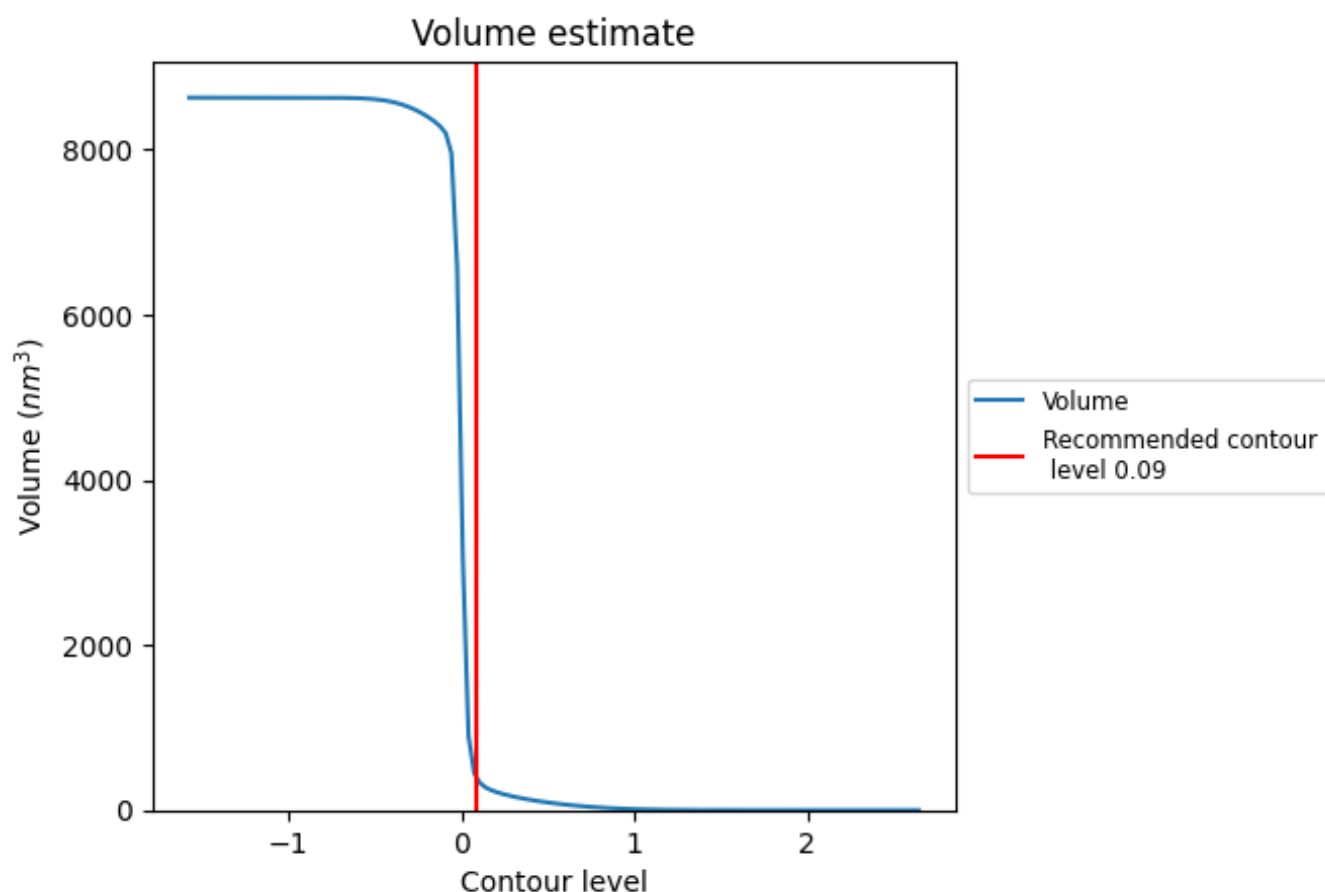
This section contains the results of statistical analysis of the map.

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 385 nm^3 ; this corresponds to an approximate mass of 348 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

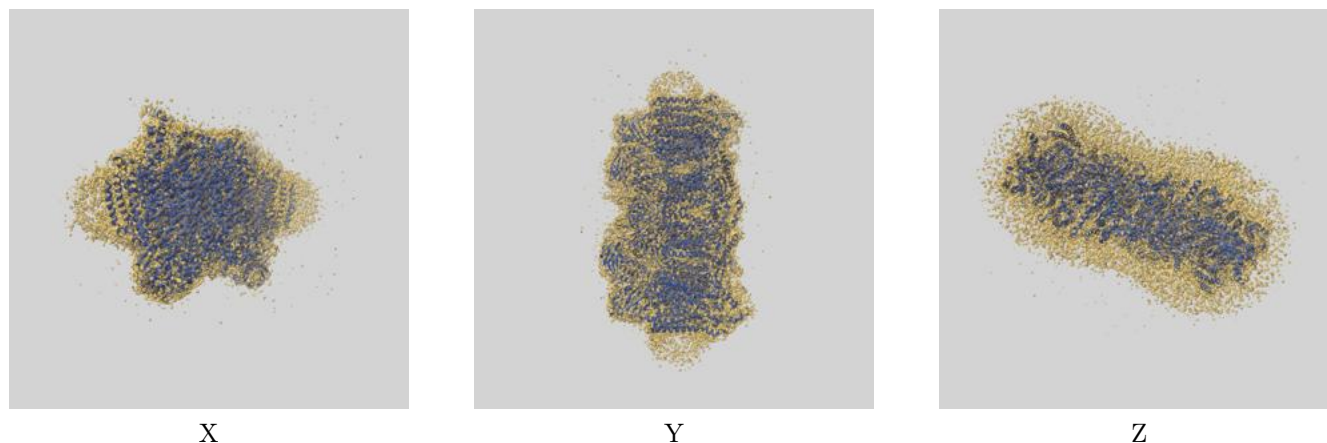
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

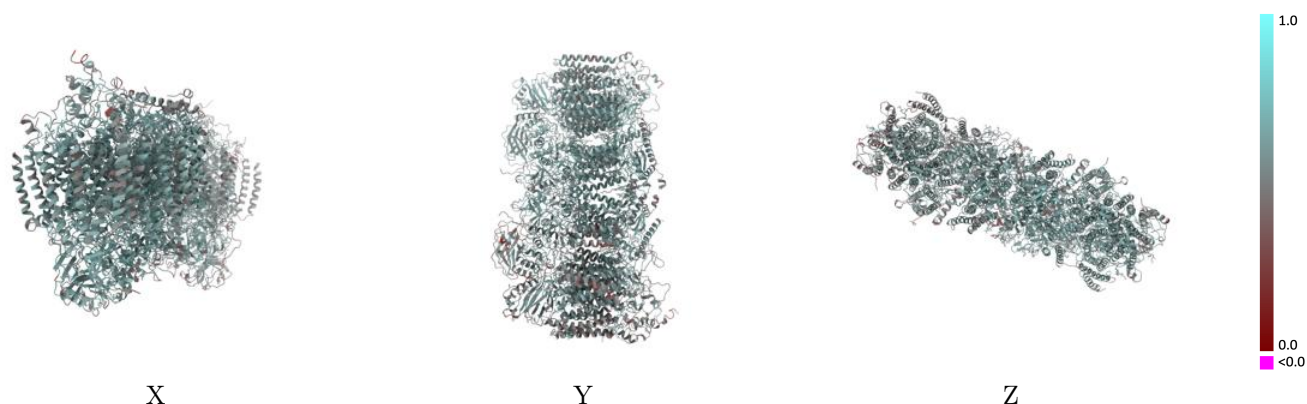
This section contains information regarding the fit between EMDB map EMD-13976 and PDB model 7QHM. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.09 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](#)

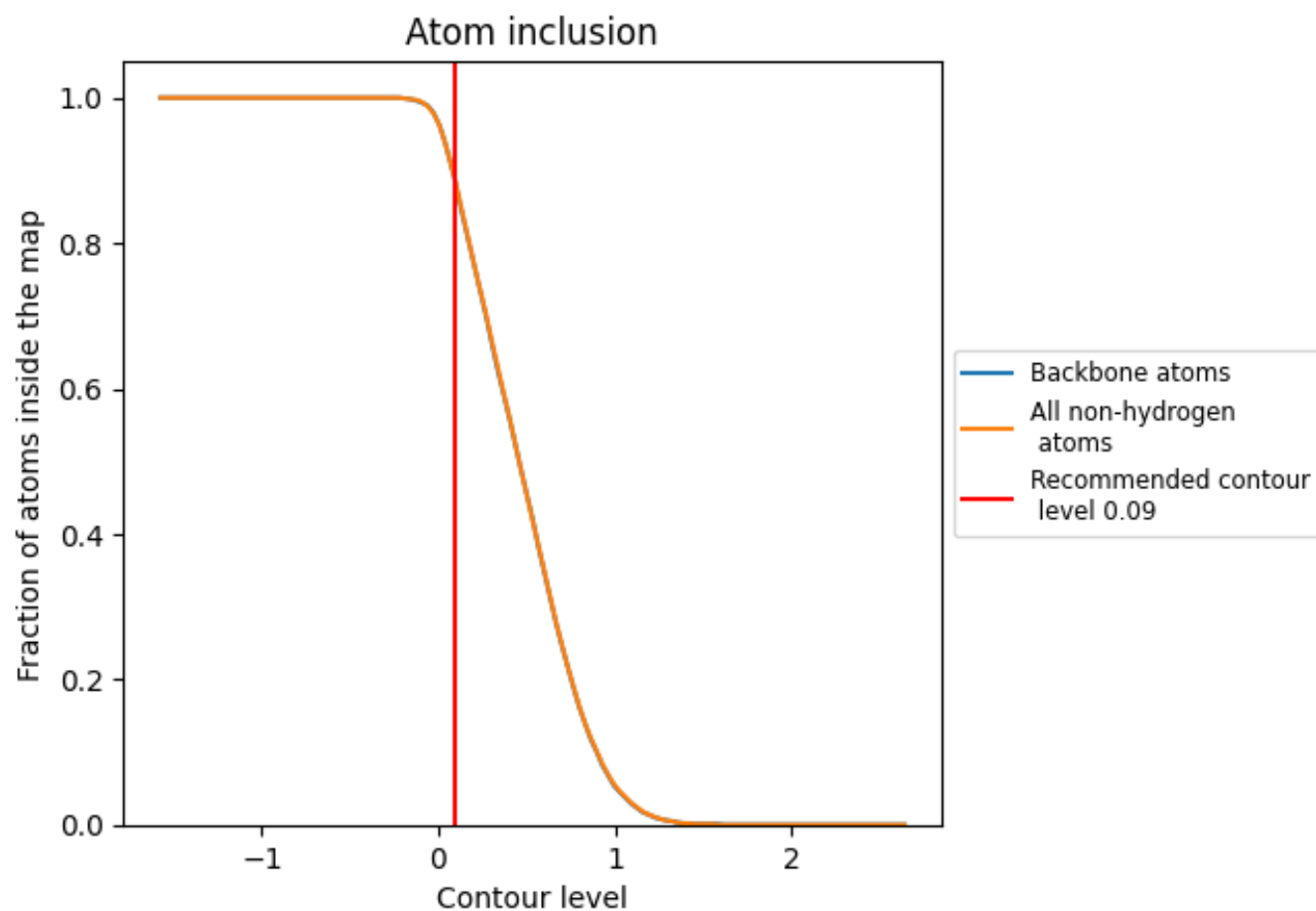


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.5670
A	 0.9130	 0.5720
B	 0.9320	 0.5910
C	 0.8600	 0.5460
D	 0.9010	 0.5660
E	 0.8130	 0.5050
F	 0.8760	 0.5400
G	 0.8600	 0.5310
H	 0.6890	 0.4700
I	 0.7980	 0.4840
J	 0.7720	 0.4750
K	 0.8110	 0.5110
L	 0.6790	 0.4380
M	 0.6380	 0.4570
N	 0.9290	 0.5880
O	 0.9530	 0.6140
P	 0.9440	 0.6130
Q	 0.9450	 0.6050
R	 0.9120	 0.5790
S	 0.9250	 0.5840
T	 0.8990	 0.5740
U	 0.9110	 0.5730
V	 0.8990	 0.5600
W	 0.8640	 0.5230
X	 0.8940	 0.5600
Y	 0.8550	 0.5380
Z	 0.7750	 0.4850

