



## Full wwPDB EM Validation Report ⓘ

Sep 23, 2024 – 01:36 pm BST

PDB ID : 9ETZ  
EMDB ID : EMD-19963  
Title : III2IV respiratory supercomplex from *Saccharomyces cerevisiae*  
Authors : Moe, A.; Brzezinski, P.  
Deposited on : 2024-03-27  
Resolution : 2.40 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](mailto: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>.

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

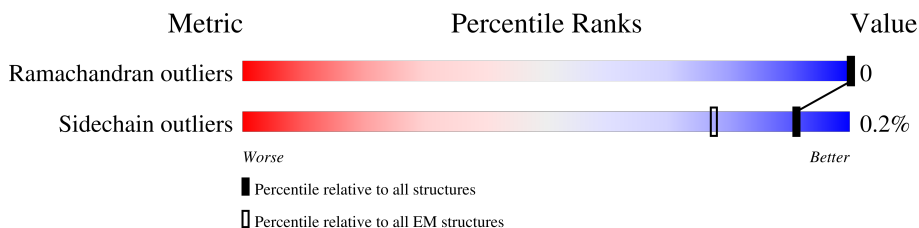
EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

# 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 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	431	100%
1	L	431	100%
2	B	352	100%
2	M	352	99%
3	C	385	100%
3	N	385	100%
4	D	247	100%
4	O	247	100%
5	E	185	64% 100%

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Mol	Chain	Length	Quality of chain
5	P	185	64% 100%
6	F	75	32% 100%
6	Q	75	36% 100%
7	G	126	• 100%
7	R	126	• 100%
8	H	93	6% 100%
8	S	93	11% 100%
9	I	57	7% 100%
9	T	57	5% 100%
10	J	76	11% 100%
10	U	76	13% 100%
11	a	534	100%
12	b	236	100%
13	c	269	100%
14	d	120	• 100%
15	f	102	• 100%
16	g	59	5% 100%
17	h	51	• 100%
18	i	55	100%
19	j	75	5% 97% •
20	k	113	100%
21	l	45	100%
22	e	133	• 100%

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 48795 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	185	1411	893	242	266	10	0	0
5	P	185	1411	893	242	266	10	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	75	633	396	109	126	2	0	0
6	Q	75	633	396	109	126	2	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	126	1019	653	173	191	2	0	0
7	R	126	1019	653	173	191	2	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	93	773	510	131	130	2	0	0
8	S	93	773	510	131	130	2	0	0

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	57	465	310	77	78	0	0
9	T	57	465	310	77	78	0	0

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	76	599	391	98	108	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	U	76	599	391	98	108	2	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a	534	4162	2778	649	713	22	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	b	236	1889	1242	286	351	10	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	c	269	2146	1430	344	357	15	0	0

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	d	120	906	571	150	180	5	0	0

- Molecule 15 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	102	851	545	137	168	1	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	g	59	484	328	83	73	0	0

- Molecule 17 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	51	Total	C	N	O	S	0	0
			409	278	66	64	1		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	75	Total	C	N	O	S	0	0
			627	403	107	112	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

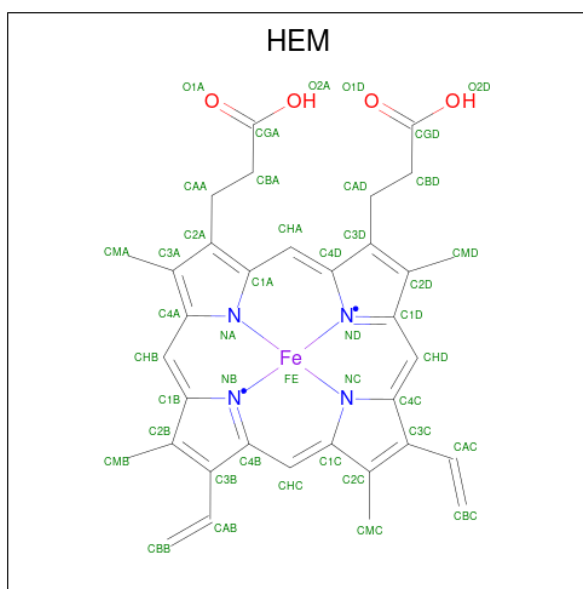
- Molecule 23 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	77	58	17	2	0
23	A	1	54	35	17	2	0
23	E	1	53	34	17	2	0
23	H	1	66	47	17	2	0
23	H	1	71	52	17	2	0
23	L	1	55	36	17	2	0
23	L	1	67	48	17	2	0
23	N	1	53	34	17	2	0
23	P	1	48	29	17	2	0
23	S	1	75	56	17	2	0
23	c	1	86	67	17	2	0

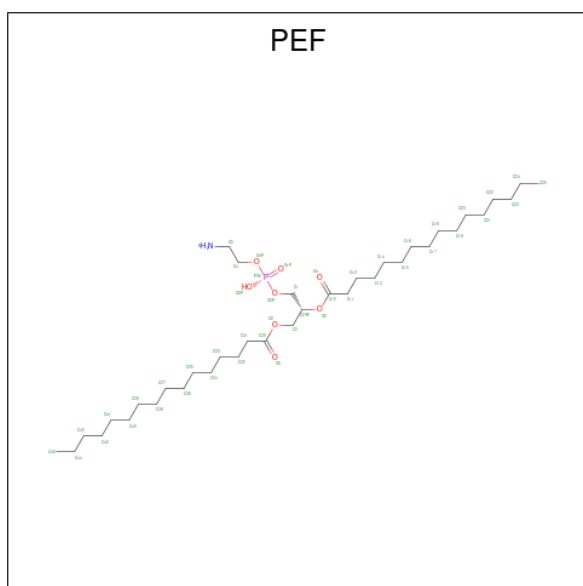
- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 25 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



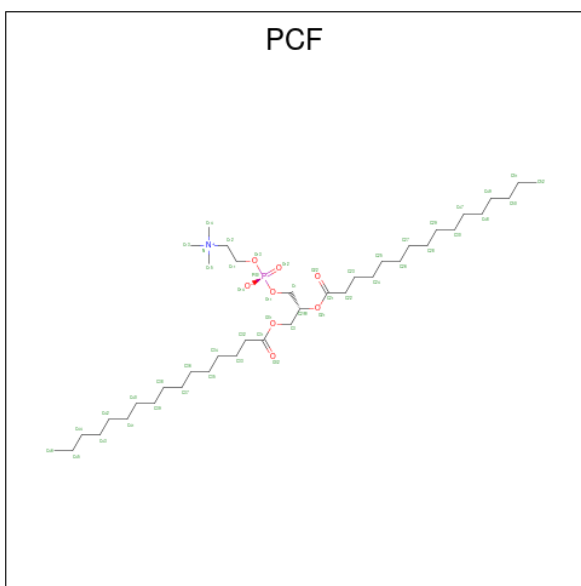
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	C	1	44	34	1	8	1	0
25	C	1	47	37	1	8	1	0
25	C	1	40	30	1	8	1	0
25	E	1	42	32	1	8	1	0
25	G	1	32	22	1	8	1	0
25	H	1	34	24	1	8	1	0
25	J	1	26	16	1	8	1	0
25	J	1	29	19	1	8	1	0
25	N	1	40	30	1	8	1	0
25	N	1	43	33	1	8	1	0
25	N	1	32	22	1	8	1	0
25	P	1	43	33	1	8	1	0
25	P	1	39	29	1	8	1	0
25	S	1	36	26	1	8	1	0
25	U	1	37	27	1	8	1	0
25	a	1	40	30	1	8	1	0
25	a	1	40	30	1	8	1	0
25	a	1	47	37	1	8	1	0
25	a	1	30	20	1	8	1	0
25	b	1	40	30	1	8	1	0
25	b	1	47	37	1	8	1	0
25	c	1	47	37	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	c	1	Total 47	C 37	N 1	O 8	P 1	0
25	h	1	Total 47	C 37	N 1	O 8	P 1	0
25	l	1	Total 47	C 37	N 1	O 8	P 1	0
25	e	1	Total 47	C 37	N 1	O 8	P 1	0

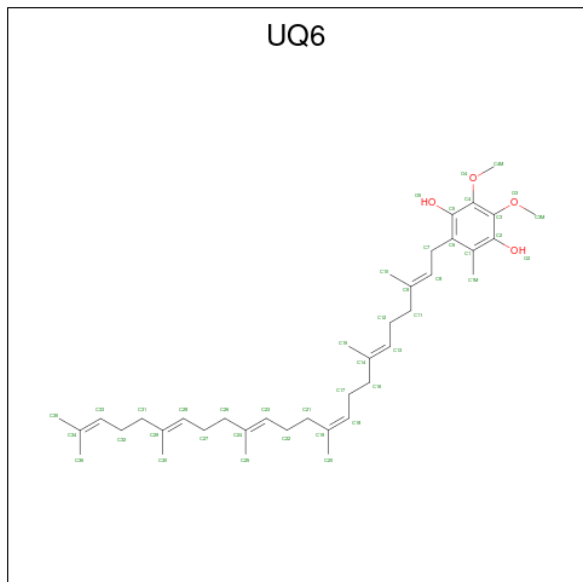
- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	C	1	Total 39	C 29	N 1	O 8	P 1	0
26	H	1	Total 32	C 22	N 1	O 8	P 1	0
26	I	1	Total 30	C 20	N 1	O 8	P 1	0
26	N	1	Total 50	C 40	N 1	O 8	P 1	0
26	T	1	Total 47	C 37	N 1	O 8	P 1	0
26	e	1	Total 50	C 40	N 1	O 8	P 1	0

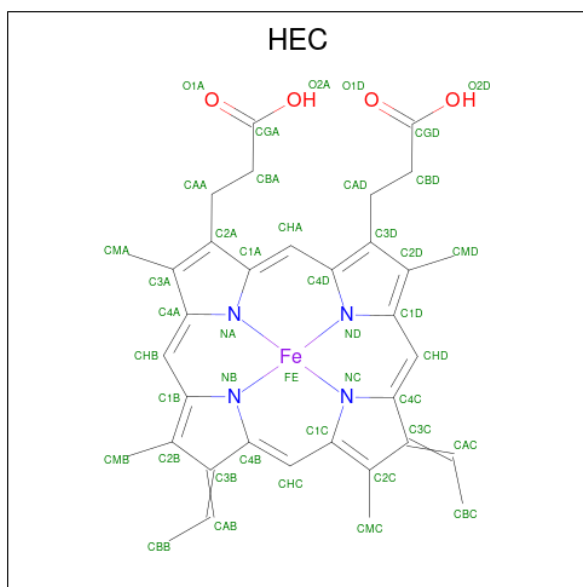
- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX

AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6)  
(formula:  $C_{39}H_{60}O_4$ ).



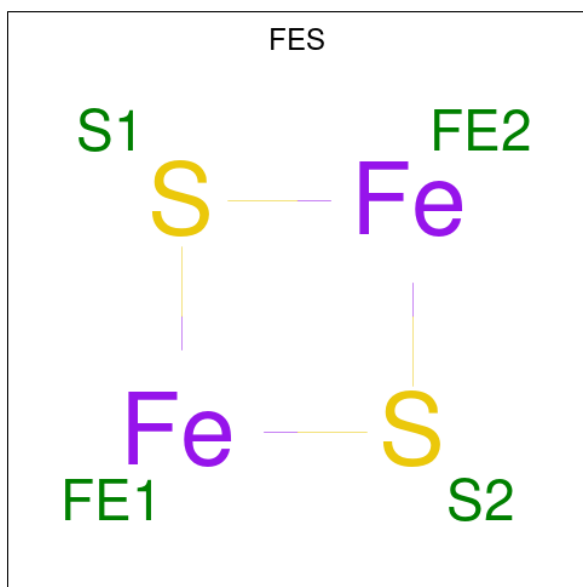
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			43	39	4	
27	N	1	Total	C	O	0
			43	39	4	

- Molecule 28 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

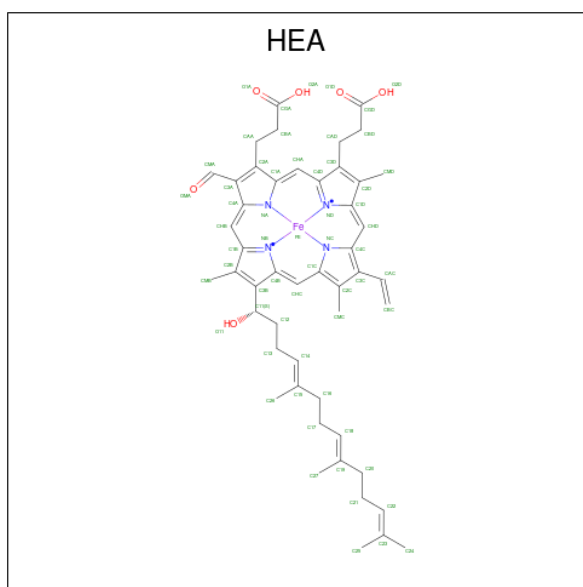


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

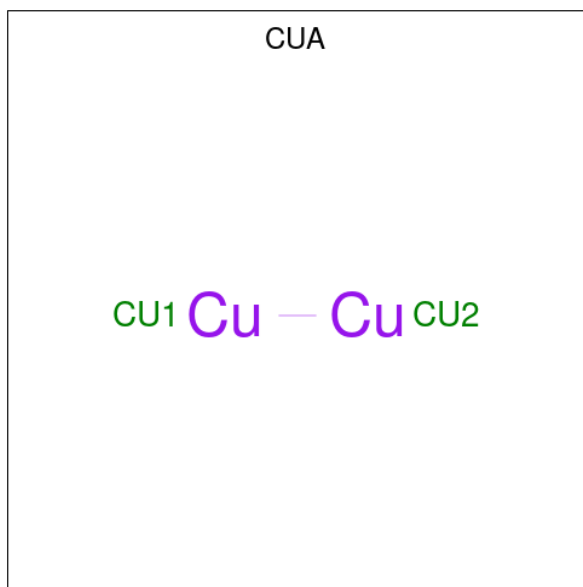
- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Ca	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total	Mg	0
			1	1	

- Molecule 34 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	AltConf
34	b	1	Total Cu 2 2	0

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
35	d	1	Total Zn 1 1	0

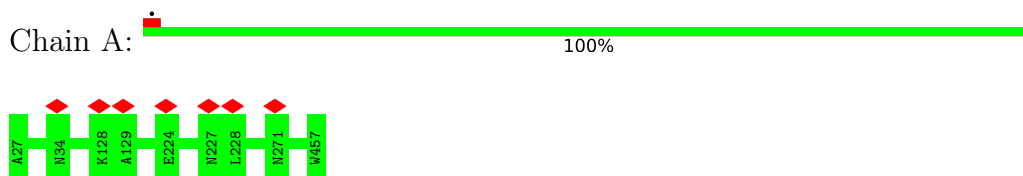
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	a	11	Total O 11 11	0

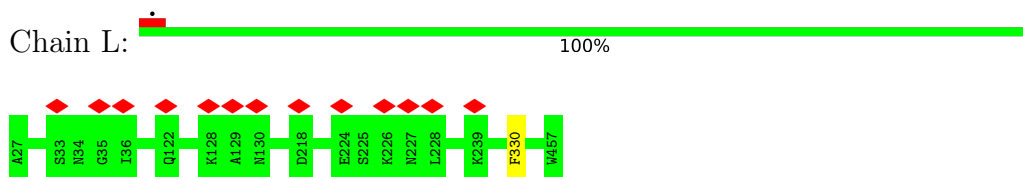
### 3 Residue-property plots [i](#)

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

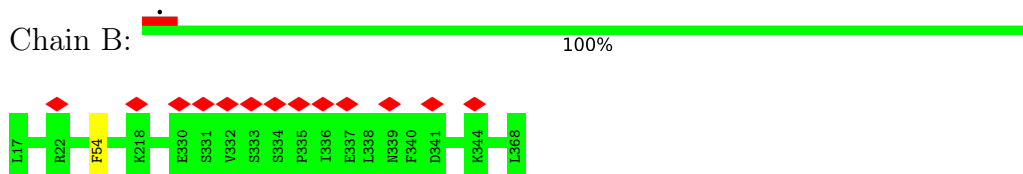
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



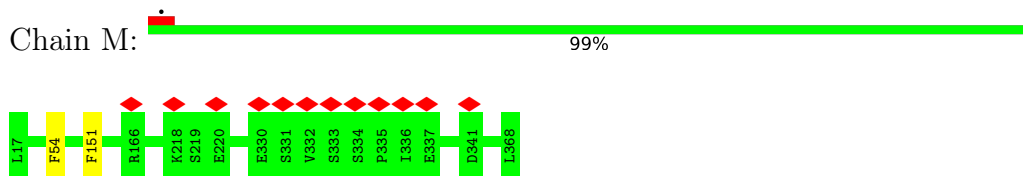
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



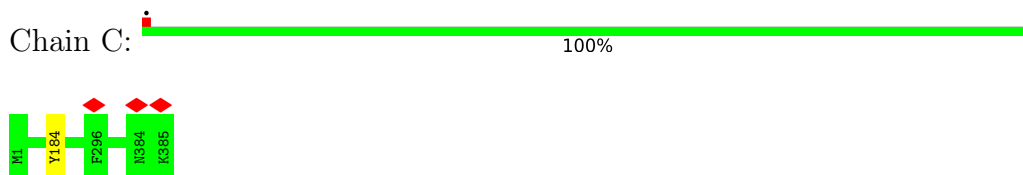
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

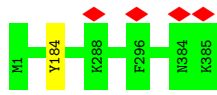


- Molecule 3: Cytochrome b

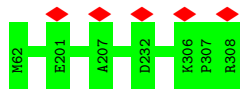




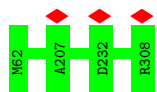
• Molecule 3: Cytochrome b



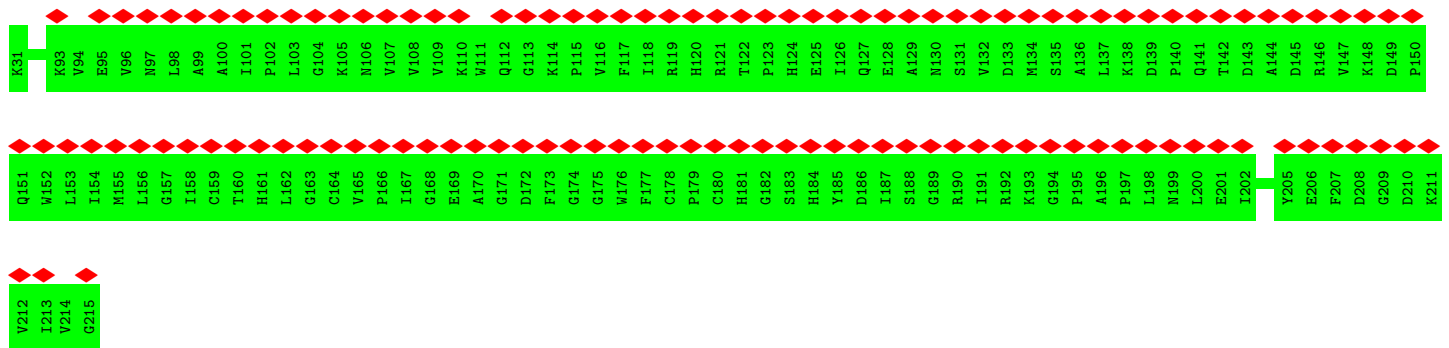
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



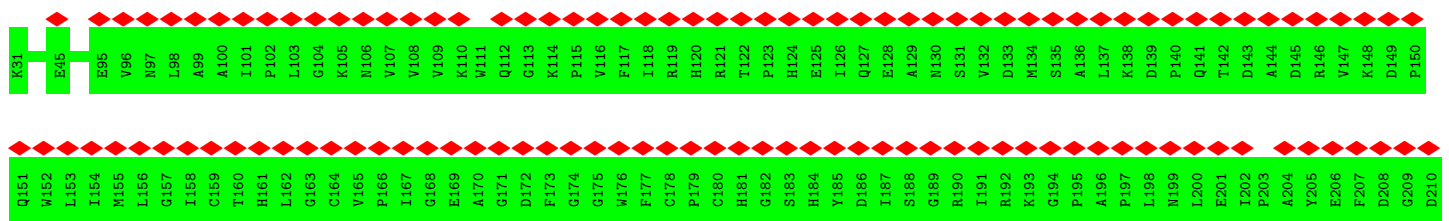
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

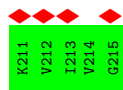


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

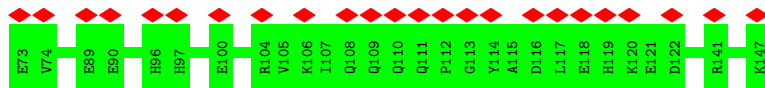


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

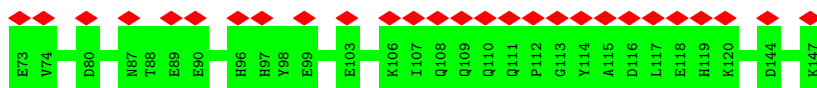




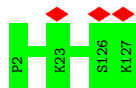
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



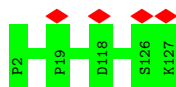
- Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



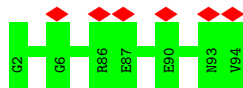
- Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



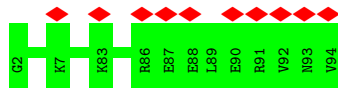
- Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial



- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial



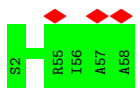
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial



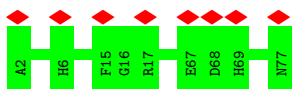
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



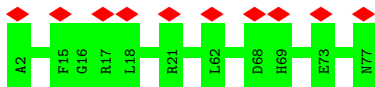
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 1



There are no outlier residues recorded for this chain.

- Molecule 12: Cytochrome c oxidase subunit 2



- Molecule 13: Cytochrome c oxidase subunit 3



- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

Chain d:  100%



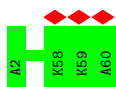
- Molecule 15: Cytochrome c oxidase subunit 6, mitochondrial

Chain f:  100%



- Molecule 16: Cytochrome c oxidase subunit 7, mitochondrial

Chain g:  5% 100%



- Molecule 17: Cytochrome c oxidase subunit 8, mitochondrial

Chain h:  100%



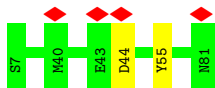
- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial

Chain j:  5% 97%




- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196457	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	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.990	Depositor
Minimum map value	-0.993	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.55	Depositor
Map size ( $\text{\AA}$ )	512.9184, 511.22562, 512.9184	wwPDB
Map dimensions	606, 604, 606	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8464, 0.8464, 0.8464	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CDL, MG, CU, PEF, HEC, HEA, CA, PCF, CUA, UQ6, ZN, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/3406	0.47	0/4615
1	L	0.26	0/3406	0.45	0/4615
2	B	0.28	0/2781	0.46	0/3764
2	M	0.28	0/2781	0.47	0/3764
3	C	0.29	0/3192	0.45	0/4354
3	N	0.29	0/3192	0.45	0/4354
4	D	0.28	0/2012	0.47	0/2740
4	O	0.28	0/2012	0.46	0/2740
5	E	0.25	0/1444	0.47	0/1957
5	P	0.25	0/1444	0.47	0/1957
6	F	0.25	0/647	0.41	0/870
6	Q	0.25	0/647	0.43	0/870
7	G	0.27	0/1040	0.48	0/1408
7	R	0.27	0/1040	0.49	0/1408
8	H	0.30	0/804	0.44	0/1088
8	S	0.29	0/804	0.42	0/1088
9	I	0.29	0/479	0.41	0/646
9	T	0.27	0/479	0.38	0/646
10	J	0.26	0/619	0.44	0/841
10	U	0.26	0/619	0.45	0/841
11	a	0.46	0/4290	0.55	0/5857
12	b	0.45	0/1941	0.54	0/2653
13	c	0.37	0/2218	0.49	0/3036
14	d	0.37	0/924	0.54	0/1258
15	f	0.41	0/868	0.51	0/1174
16	g	0.38	0/500	0.49	0/681
17	h	0.46	0/424	0.45	0/569
18	i	0.36	0/468	0.47	0/626
19	j	0.38	0/649	0.49	0/880
20	k	0.31	0/962	0.45	0/1310
21	l	0.37	0/372	0.51	0/502
22	e	0.37	0/1074	0.50	0/1451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.32	0/47538	0.48	0/64563

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
1	L	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
2	B	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
2	M	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	C	383/385 (100%)	374 (98%)	9 (2%)	0	100	100
3	N	383/385 (100%)	372 (97%)	11 (3%)	0	100	100
4	D	245/247 (99%)	241 (98%)	4 (2%)	0	100	100
4	O	245/247 (99%)	239 (98%)	6 (2%)	0	100	100
5	E	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
5	P	183/185 (99%)	164 (90%)	19 (10%)	0	100	100
6	F	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	Q	73/75 (97%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
7	R	124/126 (98%)	124 (100%)	0	0	100	100
8	H	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
8	S	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
9	I	55/57 (96%)	55 (100%)	0	0	100	100
9	T	55/57 (96%)	55 (100%)	0	0	100	100
10	J	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
10	U	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
11	a	532/534 (100%)	512 (96%)	20 (4%)	0	100	100
12	b	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
13	c	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
14	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
15	f	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
16	g	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
17	h	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
18	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	j	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
20	k	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
21	l	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
22	e	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	5782/5846 (99%)	5599 (97%)	183 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	370/370 (100%)	369 (100%)	1 (0%)	91	96
2	B	301/301 (100%)	300 (100%)	1 (0%)	91	96
2	M	301/301 (100%)	299 (99%)	2 (1%)	81	91
3	C	338/338 (100%)	337 (100%)	1 (0%)	91	96
3	N	338/338 (100%)	337 (100%)	1 (0%)	91	96
4	D	205/205 (100%)	205 (100%)	0	100	100
4	O	205/205 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	151 (100%)	0	100	100
5	P	151/151 (100%)	151 (100%)	0	100	100
6	F	68/68 (100%)	68 (100%)	0	100	100
6	Q	68/68 (100%)	68 (100%)	0	100	100
7	G	110/110 (100%)	110 (100%)	0	100	100
7	R	110/110 (100%)	110 (100%)	0	100	100
8	H	77/77 (100%)	77 (100%)	0	100	100
8	S	77/77 (100%)	77 (100%)	0	100	100
9	I	47/47 (100%)	47 (100%)	0	100	100
9	T	47/47 (100%)	47 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
10	U	65/65 (100%)	65 (100%)	0	100	100
11	a	447/447 (100%)	447 (100%)	0	100	100
12	b	209/209 (100%)	208 (100%)	1 (0%)	86	94
13	c	228/228 (100%)	227 (100%)	1 (0%)	89	95
14	d	101/101 (100%)	101 (100%)	0	100	100
15	f	91/91 (100%)	91 (100%)	0	100	100
16	g	50/50 (100%)	50 (100%)	0	100	100
17	h	41/41 (100%)	41 (100%)	0	100	100
18	i	46/46 (100%)	46 (100%)	0	100	100
19	j	67/67 (100%)	65 (97%)	2 (3%)	36	57
20	k	99/99 (100%)	99 (100%)	0	100	100
21	l	36/36 (100%)	36 (100%)	0	100	100
22	e	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4989/4989 (100%)	4979 (100%)	10 (0%)	91 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	PHE
3	C	184	TYR
1	L	330	PHE
2	M	54	PHE
2	M	151	PHE
3	N	184	TYR
12	b	85	TRP
13	c	249	TYR
19	j	44	ASP
19	j	55	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	112	GLN
9	I	29	GLN
11	a	368	HIS
15	f	117	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

Of 60 ligands modelled in this entry, 4 are monoatomic - leaving 56 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	PCF	H	104	-	31,31,49	1.32	3 (9%)	37,39,57	1.14	2 (5%)
25	PEF	N	408	-	31,31,46	1.08	4 (12%)	34,36,51	1.14	2 (5%)
25	PEF	J	102	-	28,28,46	1.13	4 (14%)	31,33,51	1.20	2 (6%)
25	PEF	a	609	-	29,29,46	1.12	4 (13%)	32,34,51	1.21	2 (6%)
23	CDL	H	101	-	65,65,99	0.42	0	71,77,111	0.26	0
23	CDL	P	304	-	47,47,99	0.44	0	53,59,111	0.30	0
23	CDL	S	101	-	74,74,99	0.37	0	80,86,111	0.21	0
25	PEF	h	101	-	46,46,46	0.89	3 (6%)	49,51,51	1.27	3 (6%)
25	PEF	e	201	-	46,46,46	0.89	4 (8%)	49,51,51	1.09	2 (4%)
27	UQ6	N	407	-	43,43,43	0.33	0	51,55,55	0.61	1 (1%)
25	PEF	P	301	-	42,42,46	0.93	4 (9%)	45,47,51	1.14	2 (4%)
26	PCF	I	101	-	29,29,49	1.38	4 (13%)	35,37,57	1.07	2 (5%)
25	PEF	J	101	-	25,25,46	1.19	4 (16%)	28,30,51	1.17	2 (7%)
25	PEF	P	303	-	38,38,46	0.96	4 (10%)	41,43,51	1.03	2 (4%)
25	PEF	a	607	-	39,39,46	0.96	3 (7%)	42,44,51	1.11	2 (4%)
23	CDL	E	303	-	52,52,99	0.44	0	58,64,111	0.29	0
25	PEF	c	301	-	46,46,46	0.91	3 (6%)	49,51,51	1.23	4 (8%)
24	HEM	C	401	3	41,50,50	1.50	5 (12%)	45,82,82	1.73	10 (22%)
25	PEF	N	405	-	42,42,46	0.92	3 (7%)	45,47,51	1.10	2 (4%)
25	PEF	N	404	-	39,39,46	0.96	4 (10%)	42,44,51	1.21	2 (4%)
26	PCF	e	202	-	49,49,49	1.10	3 (6%)	55,57,57	1.03	4 (7%)
25	PEF	a	601	-	39,39,46	0.95	4 (10%)	42,44,51	1.20	3 (7%)
26	PCF	C	405	-	38,38,49	1.21	3 (7%)	44,46,57	1.13	2 (4%)
23	CDL	c	303	-	85,85,99	0.40	0	91,97,111	0.24	0
31	HEA	a	604	11	57,67,67	2.01	16 (28%)	61,103,103	2.54	24 (39%)
23	CDL	L	502	-	66,66,99	0.39	0	72,78,111	0.23	0
23	CDL	A	502	-	53,53,99	0.44	0	59,65,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PEF	U	101	-	36,36,46	1.00	3 (8%)	39,41,51	1.15	3 (7%)
24	HEM	N	402	3	41,50,50	1.45	3 (7%)	45,82,82	1.33	6 (13%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-
25	PEF	G	201	-	31,31,46	1.07	4 (12%)	34,36,51	1.19	2 (5%)
23	CDL	A	501	-	76,76,99	0.38	0	82,88,111	0.27	0
26	PCF	T	101	-	46,46,49	1.12	3 (6%)	52,54,57	1.05	3 (5%)
25	PEF	C	404	-	46,46,46	0.89	4 (8%)	49,51,51	1.13	2 (4%)
25	PEF	c	302	-	46,46,46	0.89	3 (6%)	49,51,51	1.15	2 (4%)
25	PEF	E	302	-	41,41,46	0.94	4 (9%)	44,46,51	1.13	2 (4%)
23	CDL	N	403	-	52,52,99	0.45	0	58,64,111	0.28	0
28	HEC	O	401	4	32,50,50	2.24	3 (9%)	24,82,82	1.48	4 (16%)
25	PEF	C	403	-	43,43,46	0.91	4 (9%)	46,48,51	1.15	2 (4%)
23	CDL	H	102	-	70,70,99	0.39	0	76,82,111	0.23	0
26	PCF	N	406	-	49,49,49	1.08	3 (6%)	55,57,57	1.05	2 (3%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
25	PEF	l	101	-	46,46,46	0.89	3 (6%)	49,51,51	1.13	2 (4%)
28	HEC	D	401	4	32,50,50	2.16	3 (9%)	24,82,82	1.76	7 (29%)
25	PEF	C	407	-	39,39,46	0.96	4 (10%)	42,44,51	1.12	2 (4%)
24	HEM	C	402	3	41,50,50	1.44	3 (7%)	45,82,82	1.35	7 (15%)
27	UQ6	C	406	-	43,43,43	0.34	0	51,55,55	1.17	3 (5%)
29	FES	P	302	5	0,4,4	-	-	-	-	-
25	PEF	a	608	-	46,46,46	0.93	3 (6%)	49,51,51	1.12	2 (4%)
23	CDL	L	501	-	54,54,99	0.43	0	60,66,111	0.26	0
25	PEF	H	103	-	33,33,46	1.06	3 (9%)	36,38,51	1.05	2 (5%)
25	PEF	b	302	-	39,39,46	0.97	4 (10%)	42,44,51	1.19	2 (4%)
25	PEF	S	102	-	35,35,46	1.02	4 (11%)	38,40,51	1.11	2 (5%)
25	PEF	b	303	-	46,46,46	0.88	4 (8%)	49,51,51	1.11	2 (4%)
31	HEA	a	603	11	57,67,67	1.32	8 (14%)	61,103,103	1.67	15 (24%)
24	HEM	N	401	3	41,50,50	1.48	3 (7%)	45,82,82	1.65	9 (20%)

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
26	PCF	H	104	-	-	13/35/35/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	N	408	-	-	14/35/35/50	-
25	PEF	J	102	-	-	12/32/32/50	-
25	PEF	a	609	-	-	15/33/33/50	-
23	CDL	H	101	-	-	40/76/76/110	-
23	CDL	P	304	-	-	26/58/58/110	-
23	CDL	S	101	-	-	48/85/85/110	-
25	PEF	h	101	-	-	25/50/50/50	-
25	PEF	e	201	-	-	23/50/50/50	-
27	UQ6	N	407	-	-	11/39/39/39	0/1/1/1
25	PEF	P	301	-	-	21/46/46/50	-
26	PCF	I	101	-	-	10/33/33/53	-
25	PEF	J	101	-	-	8/29/29/50	-
25	PEF	P	303	-	-	23/42/42/50	-
25	PEF	a	607	-	-	21/43/43/50	-
23	CDL	E	303	-	-	26/63/63/110	-
25	PEF	c	301	-	-	18/50/50/50	-
24	HEM	C	401	3	-	2/12/54/54	-
25	PEF	N	405	-	-	15/46/46/50	-
25	PEF	N	404	-	-	18/43/43/50	-
26	PCF	e	202	-	-	20/53/53/53	-
25	PEF	a	601	-	-	18/43/43/50	-
26	PCF	C	405	-	-	15/42/42/53	-
23	CDL	c	303	-	-	62/96/96/110	-
31	HEA	a	604	11	-	5/32/76/76	-
23	CDL	L	502	-	-	41/77/77/110	-
23	CDL	A	502	-	-	28/64/64/110	-
25	PEF	U	101	-	-	15/40/40/50	-
24	HEM	N	402	3	-	2/12/54/54	-
25	PEF	G	201	-	-	19/35/35/50	-
23	CDL	A	501	-	-	44/87/87/110	-
26	PCF	T	101	-	-	23/50/50/53	-
25	PEF	C	404	-	-	23/50/50/50	-
25	PEF	c	302	-	-	21/50/50/50	-
25	PEF	E	302	-	-	15/45/45/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CDL	N	403	-	-	33/63/63/110	-
28	HEC	O	401	4	-	0/10/54/54	-
25	PEF	C	403	-	-	15/47/47/50	-
23	CDL	H	102	-	-	33/81/81/110	-
26	PCF	N	406	-	-	23/53/53/53	-
29	FES	E	301	5	-	-	0/1/1/1
25	PEF	l	101	-	-	19/50/50/50	-
28	HEC	D	401	4	-	2/10/54/54	-
25	PEF	C	407	-	-	23/43/43/50	-
24	HEM	C	402	3	-	4/12/54/54	-
27	UQ6	C	406	-	-	5/39/39/39	0/1/1/1
29	FES	P	302	5	-	-	0/1/1/1
25	PEF	a	608	-	-	24/50/50/50	-
23	CDL	L	501	-	-	42/64/64/110	-
25	PEF	H	103	-	-	15/37/37/50	-
25	PEF	b	302	-	-	20/43/43/50	-
25	PEF	S	102	-	-	16/39/39/50	-
25	PEF	b	303	-	-	26/50/50/50	-
31	HEA	a	603	11	-	17/32/76/76	-
24	HEM	N	401	3	-	2/12/54/54	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	O	401	HEC	C2B-C3B	-6.92	1.33	1.40
28	D	401	HEC	C3C-C2C	-6.54	1.33	1.40
28	O	401	HEC	C3C-C2C	-6.48	1.34	1.40
28	D	401	HEC	C2B-C3B	-5.94	1.34	1.40
28	D	401	HEC	C3D-C2D	5.40	1.53	1.37
28	O	401	HEC	C3D-C2D	5.37	1.53	1.37
31	a	604	HEA	C3B-C2B	4.93	1.45	1.34
31	a	604	HEA	C3A-C2A	4.68	1.46	1.40
31	a	604	HEA	CHC-C4B	4.67	1.46	1.35
31	a	604	HEA	CHD-C1D	4.67	1.46	1.35
31	a	604	HEA	C3D-C2D	4.61	1.46	1.36
31	a	604	HEA	C3C-C2C	4.11	1.46	1.40
24	N	402	HEM	C3C-C2C	-3.95	1.34	1.40
24	C	401	HEM	C3C-C2C	-3.93	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	401	HEM	C3C-C2C	-3.92	1.34	1.40
31	a	603	HEA	C3A-CMA	-3.89	1.37	1.46
24	C	402	HEM	C3C-C2C	-3.86	1.35	1.40
24	C	402	HEM	C3C-CAC	3.70	1.55	1.47
24	N	402	HEM	C3C-CAC	3.69	1.55	1.47
31	a	603	HEA	C3C-C2C	-3.67	1.35	1.40
31	a	604	HEA	FE-NB	3.65	2.14	1.96
24	N	401	HEM	C3C-CAC	3.62	1.55	1.47
24	C	401	HEM	C3C-CAC	3.58	1.55	1.47
31	a	604	HEA	C4B-C3B	3.29	1.50	1.44
26	e	202	PCF	O21-C21	3.23	1.43	1.34
26	C	405	PCF	O21-C21	3.09	1.43	1.34
26	I	101	PCF	O31-C31	3.08	1.42	1.33
26	I	101	PCF	O21-C21	3.05	1.42	1.34
31	a	603	HEA	C4B-C3B	3.04	1.49	1.44
24	C	402	HEM	CAB-C3B	3.04	1.55	1.47
24	N	402	HEM	CAB-C3B	3.04	1.55	1.47
31	a	604	HEA	C1D-ND	-3.01	1.35	1.40
26	H	104	PCF	O31-C31	2.99	1.42	1.33
26	T	101	PCF	O21-C21	2.97	1.42	1.34
25	c	302	PEF	O2-C2	-2.95	1.39	1.46
25	a	608	PEF	O2-C2	-2.95	1.39	1.46
26	H	104	PCF	O21-C21	2.94	1.42	1.34
24	N	401	HEM	CAB-C3B	2.94	1.55	1.47
25	c	301	PEF	O2-C2	-2.90	1.39	1.46
24	C	401	HEM	CAB-C3B	2.90	1.55	1.47
26	C	405	PCF	O31-C31	2.90	1.41	1.33
26	T	101	PCF	O31-C31	2.88	1.41	1.33
26	N	406	PCF	O31-C31	2.87	1.41	1.33
25	H	103	PEF	O2-C2	-2.86	1.39	1.46
26	N	406	PCF	O21-C21	2.84	1.42	1.34
31	a	604	HEA	FE-ND	2.80	2.10	1.96
26	e	202	PCF	O31-C31	2.78	1.41	1.33
25	N	405	PEF	O2-C2	-2.71	1.39	1.46
25	U	101	PEF	O2-C2	-2.71	1.39	1.46
25	a	607	PEF	O2-C2	-2.70	1.39	1.46
25	b	302	PEF	O2-C2	-2.65	1.40	1.46
25	E	302	PEF	O2-C2	-2.63	1.40	1.46
25	G	201	PEF	O2-C2	-2.62	1.40	1.46
25	l	101	PEF	O2-C2	-2.62	1.40	1.46
25	J	101	PEF	O2-C2	-2.61	1.40	1.46
31	a	604	HEA	C4B-NB	-2.60	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	102	PEF	O2-C2	-2.59	1.40	1.46
25	C	403	PEF	O2-C2	-2.57	1.40	1.46
25	l	101	PEF	O3-C3	-2.57	1.39	1.45
31	a	604	HEA	O2A-CGA	-2.56	1.22	1.30
25	a	608	PEF	O3-C3	-2.56	1.39	1.45
25	P	301	PEF	O2-C2	-2.56	1.40	1.46
25	N	408	PEF	O2-C2	-2.54	1.40	1.46
25	N	404	PEF	O2-C2	-2.53	1.40	1.46
25	h	101	PEF	O2-C2	-2.52	1.40	1.46
25	C	407	PEF	O2-C2	-2.52	1.40	1.46
25	C	404	PEF	O2-C2	-2.50	1.40	1.46
25	J	102	PEF	O2-C2	-2.48	1.40	1.46
25	C	407	PEF	O3-C30	2.48	1.40	1.33
25	N	408	PEF	O3-C30	2.45	1.40	1.33
25	H	103	PEF	O3-C30	2.45	1.40	1.33
25	a	609	PEF	O2-C2	-2.45	1.40	1.46
25	a	607	PEF	O3-C30	2.44	1.40	1.33
31	a	604	HEA	O2D-CGD	-2.44	1.22	1.30
25	e	201	PEF	O3-C3	-2.43	1.39	1.45
25	J	102	PEF	O3-C30	2.42	1.40	1.33
25	a	601	PEF	O2-C2	-2.41	1.40	1.46
25	a	609	PEF	O3-C30	2.39	1.40	1.33
25	J	101	PEF	O3-C30	2.39	1.40	1.33
31	a	604	HEA	C1C-CHC	2.39	1.47	1.41
31	a	603	HEA	C1D-C2D	2.37	1.49	1.44
25	P	303	PEF	O3-C30	2.36	1.40	1.33
25	c	302	PEF	O3-C3	-2.35	1.39	1.45
25	a	601	PEF	O3-C30	2.35	1.40	1.33
25	e	201	PEF	O2-C2	-2.35	1.40	1.46
25	e	201	PEF	O2-C10	2.33	1.40	1.34
25	U	101	PEF	O3-C3	-2.33	1.39	1.45
25	C	404	PEF	O3-C30	2.32	1.40	1.33
26	N	406	PCF	O21-C2	-2.32	1.40	1.46
24	C	401	HEM	FE-ND	2.31	2.08	1.96
25	b	302	PEF	O3-C3	-2.31	1.39	1.45
25	P	303	PEF	O2-C2	-2.31	1.40	1.46
25	P	301	PEF	O3-C30	2.29	1.40	1.33
25	b	303	PEF	O2-C2	-2.28	1.40	1.46
25	S	102	PEF	O3-C30	2.27	1.40	1.33
25	G	201	PEF	O3-C30	2.27	1.40	1.33
25	C	403	PEF	O3-C30	2.27	1.40	1.33
25	b	303	PEF	O3-C30	2.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	302	PEF	O3-C30	2.25	1.39	1.33
25	c	301	PEF	O3-C3	-2.25	1.40	1.45
25	N	404	PEF	O3-C30	2.25	1.39	1.33
25	N	405	PEF	O3-C3	-2.24	1.40	1.45
26	T	101	PCF	O21-C2	-2.24	1.41	1.46
26	e	202	PCF	O21-C2	-2.23	1.41	1.46
26	H	104	PCF	O21-C2	-2.23	1.41	1.46
25	U	101	PEF	O3-C30	2.23	1.39	1.33
25	S	102	PEF	O3-C3	-2.22	1.40	1.45
25	E	302	PEF	O3-C30	2.22	1.39	1.33
25	N	404	PEF	O3-C3	-2.21	1.40	1.45
25	N	405	PEF	O3-C30	2.21	1.39	1.33
25	P	301	PEF	O3-C3	-2.21	1.40	1.45
25	c	301	PEF	O3-C30	2.20	1.39	1.33
26	I	101	PCF	O21-C2	-2.20	1.41	1.46
25	E	302	PEF	O3-C3	-2.20	1.40	1.45
31	a	603	HEA	C3A-C2A	-2.18	1.37	1.40
25	G	201	PEF	O3-C3	-2.18	1.40	1.45
25	P	303	PEF	O2-C10	2.18	1.40	1.34
25	S	102	PEF	O2-C10	2.18	1.40	1.34
25	a	607	PEF	O3-C3	-2.17	1.40	1.45
25	H	103	PEF	O3-C3	-2.17	1.40	1.45
25	a	609	PEF	O2-C10	2.16	1.40	1.34
25	b	303	PEF	O3-C3	-2.15	1.40	1.45
25	J	102	PEF	O3-C3	-2.15	1.40	1.45
25	l	101	PEF	O2-C10	2.15	1.40	1.34
25	e	201	PEF	O3-C30	2.14	1.39	1.33
25	J	102	PEF	O2-C10	2.13	1.40	1.34
25	b	303	PEF	O2-C10	2.13	1.40	1.34
25	a	601	PEF	O3-C3	-2.13	1.40	1.45
25	C	404	PEF	O3-C3	-2.12	1.40	1.45
25	N	408	PEF	O3-C3	-2.12	1.40	1.45
25	a	608	PEF	O3-C30	2.12	1.39	1.33
25	C	403	PEF	O3-C3	-2.12	1.40	1.45
25	G	201	PEF	O2-C10	2.11	1.40	1.34
25	N	404	PEF	O2-C10	2.11	1.40	1.34
25	P	301	PEF	O2-C10	2.11	1.40	1.34
25	J	101	PEF	O3-C3	-2.10	1.40	1.45
25	P	303	PEF	O3-C3	-2.10	1.40	1.45
25	h	101	PEF	O3-C3	-2.10	1.40	1.45
31	a	604	HEA	C4C-CHD	2.10	1.46	1.41
31	a	604	HEA	C4D-ND	-2.09	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	603	HEA	CMD-C2D	2.08	1.55	1.50
25	c	302	PEF	O3-C30	2.07	1.39	1.33
25	h	101	PEF	O3-C30	2.07	1.39	1.33
25	J	101	PEF	O2-C10	2.06	1.40	1.34
25	C	407	PEF	O2-C10	2.06	1.40	1.34
25	C	404	PEF	O2-C10	2.06	1.40	1.34
31	a	603	HEA	C1C-CHC	-2.05	1.35	1.41
25	C	403	PEF	O2-C10	2.05	1.40	1.34
31	a	603	HEA	O2A-CGA	-2.05	1.23	1.30
25	N	408	PEF	O2-C10	2.04	1.40	1.34
26	C	405	PCF	O21-C2	-2.04	1.41	1.46
25	b	302	PEF	O2-C10	2.03	1.40	1.34
25	a	601	PEF	O2-C10	2.03	1.40	1.34
24	C	401	HEM	CMB-C2B	2.03	1.55	1.50
25	E	302	PEF	O2-C10	2.02	1.40	1.34
25	a	609	PEF	O3-C3	-2.02	1.40	1.45
26	I	101	PCF	C22-C21	2.01	1.56	1.50
25	C	407	PEF	O3-C3	-2.01	1.40	1.45

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	604	HEA	C2B-C1B-NB	5.82	116.85	109.88
31	a	604	HEA	C1D-C2D-C3D	-5.51	101.17	106.96
31	a	604	HEA	C3B-C4B-NB	5.26	116.08	109.84
31	a	604	HEA	C2D-C1D-ND	5.08	115.86	109.84
25	h	101	PEF	O2-C10-C11	5.00	122.29	111.50
27	C	406	UQ6	C7-C8-C9	4.90	134.85	127.24
31	a	604	HEA	CBA-CAA-C2A	-4.87	104.40	112.60
31	a	604	HEA	CMB-C2B-C1B	4.84	132.41	125.04
31	a	604	HEA	C3D-C4D-ND	4.81	115.02	110.36
25	a	609	PEF	O2-C10-C11	4.55	121.30	111.50
25	c	301	PEF	O2-C10-C11	4.52	121.25	111.50
25	C	404	PEF	O2-C10-C11	4.49	121.18	111.50
25	a	601	PEF	O2-C10-C11	4.47	121.14	111.50
25	N	404	PEF	O2-C10-C11	4.43	121.05	111.50
25	l	101	PEF	O2-C10-C11	4.40	120.98	111.50
31	a	604	HEA	C27-C19-C20	4.33	122.55	115.27
28	D	401	HEC	CMC-C2C-C1C	-4.28	121.89	128.46
25	C	403	PEF	O2-C10-C11	4.24	120.64	111.50
26	H	104	PCF	O21-C21-C22	4.16	120.47	111.50
26	C	405	PCF	O21-C21-C22	4.14	120.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	603	HEA	CMD-C2D-C1D	4.13	131.33	125.04
25	b	302	PEF	O2-C10-C11	4.10	120.34	111.50
25	b	303	PEF	O2-C10-C11	4.07	120.27	111.50
25	C	407	PEF	O2-C10-C11	4.02	120.17	111.50
25	c	302	PEF	O2-C10-C11	4.02	120.17	111.50
25	U	101	PEF	O2-C10-C11	4.01	120.15	111.50
24	C	401	HEM	CAD-C3D-C4D	4.00	131.64	124.66
25	P	301	PEF	O2-C10-C11	3.94	119.99	111.50
25	E	302	PEF	O2-C10-C11	3.93	119.96	111.50
25	G	201	PEF	O2-C10-C11	3.90	119.92	111.50
25	e	201	PEF	O2-C10-C11	3.86	119.82	111.50
25	N	405	PEF	O2-C10-C11	3.86	119.82	111.50
25	J	102	PEF	O2-C10-C11	3.84	119.78	111.50
25	J	101	PEF	O2-C10-C11	3.83	119.75	111.50
25	a	608	PEF	O2-C10-C11	3.82	119.74	111.50
25	S	102	PEF	O2-C10-C11	3.81	119.72	111.50
25	N	408	PEF	O2-C10-C11	3.76	119.60	111.50
26	I	101	PCF	O21-C21-C22	3.75	119.58	111.50
25	a	607	PEF	O2-C10-C11	3.73	119.55	111.50
24	C	401	HEM	CAD-C3D-C2D	-3.73	120.93	127.88
25	H	103	PEF	O2-C10-C11	3.72	119.52	111.50
26	N	406	PCF	O21-C21-C22	3.72	119.51	111.50
31	a	603	HEA	C4A-CHB-C1B	3.64	127.36	122.56
26	T	101	PCF	O21-C21-C22	3.61	119.29	111.50
24	N	401	HEM	CAD-C3D-C4D	3.61	130.96	124.66
31	a	604	HEA	C26-C15-C16	3.56	121.25	115.27
27	C	406	UQ6	C7-C6-C5	-3.51	116.21	120.82
24	C	401	HEM	C4C-CHD-C1D	3.49	127.16	122.56
31	a	604	HEA	C3C-C4C-NC	3.44	113.66	109.21
31	a	604	HEA	CHC-C4B-NB	-3.42	120.16	124.38
31	a	604	HEA	CMD-C2D-C1D	3.41	130.24	125.04
27	C	406	UQ6	C6-C7-C8	3.40	117.56	112.17
24	N	401	HEM	CAD-C3D-C2D	-3.39	121.56	127.88
25	P	303	PEF	O2-C10-C11	3.34	118.70	111.50
31	a	604	HEA	C1B-C2B-C3B	-3.34	102.81	106.80
25	c	301	PEF	O3-C30-C31	3.26	122.14	111.91
31	a	603	HEA	O11-C11-C12	-3.20	100.46	109.42
31	a	603	HEA	C4D-CHA-C1A	3.13	126.69	122.56
31	a	604	HEA	C4B-NB-C1B	-3.12	101.85	105.07
24	N	401	HEM	C4D-ND-C1D	3.11	108.29	105.07
28	D	401	HEC	CMB-C2B-C1B	-3.11	123.69	128.46
31	a	604	HEA	CMC-C2C-C3C	3.08	130.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	102	PEF	O3-C30-C31	3.07	121.53	111.91
24	C	401	HEM	C4D-ND-C1D	3.05	108.23	105.07
24	N	401	HEM	C4C-CHD-C1D	3.05	126.58	122.56
31	a	604	HEA	C4B-C3B-C2B	-2.93	102.41	107.41
24	C	401	HEM	C1B-NB-C4B	2.93	108.10	105.07
31	a	604	HEA	CMB-C2B-C3B	-2.92	124.77	130.34
31	a	604	HEA	CHB-C1B-NB	-2.88	121.30	124.43
25	C	407	PEF	O3-C30-C31	2.87	120.90	111.91
26	e	202	PCF	O31-C31-C32	2.86	120.89	111.91
24	C	402	HEM	C1B-NB-C4B	2.84	108.00	105.07
25	N	408	PEF	O3-C30-C31	2.82	120.77	111.91
24	C	402	HEM	C4D-ND-C1D	2.80	107.96	105.07
24	N	402	HEM	C1B-NB-C4B	2.80	107.96	105.07
25	G	201	PEF	O3-C30-C31	2.76	120.57	111.91
25	P	301	PEF	O3-C30-C31	2.75	120.54	111.91
26	C	405	PCF	O31-C31-C32	2.75	120.52	111.91
25	b	303	PEF	O3-C30-C31	2.73	120.47	111.91
31	a	603	HEA	CBA-CAA-C2A	2.71	117.17	112.60
24	N	402	HEM	C4D-ND-C1D	2.71	107.87	105.07
31	a	603	HEA	CMC-C2C-C1C	-2.70	124.31	128.46
25	a	609	PEF	O3-C30-C31	2.70	120.38	111.91
25	h	101	PEF	O3-C30-C31	2.69	120.34	111.91
24	N	401	HEM	C1B-NB-C4B	2.68	107.84	105.07
25	a	601	PEF	O3-C30-C31	2.68	120.31	111.91
25	C	404	PEF	O3-C30-C31	2.67	120.28	111.91
31	a	604	HEA	CAD-CBD-CGD	-2.65	107.91	113.60
25	b	302	PEF	O3-C30-C31	2.65	120.21	111.91
25	N	404	PEF	O3-C30-C31	2.64	120.20	111.91
26	T	101	PCF	O31-C31-C32	2.61	120.11	111.91
31	a	604	HEA	C13-C14-C15	-2.61	121.38	127.66
24	N	402	HEM	C4C-CHD-C1D	2.61	126.00	122.56
25	E	302	PEF	O3-C30-C31	2.60	120.08	111.91
25	J	101	PEF	O3-C30-C31	2.60	120.06	111.91
25	c	302	PEF	O3-C30-C31	2.60	120.06	111.91
26	N	406	PCF	O31-C31-C32	2.59	120.04	111.91
25	C	403	PEF	O3-C30-C31	2.59	120.03	111.91
26	I	101	PCF	O31-C31-C32	2.58	120.00	111.91
27	N	407	UQ6	C7-C6-C5	-2.57	117.44	120.82
25	U	101	PEF	O3-C30-C31	2.57	119.97	111.91
25	e	201	PEF	O3-C30-C31	2.56	119.93	111.91
26	e	202	PCF	C11-C12-N	-2.56	107.25	115.78
28	O	401	HEC	CAA-CBA-CGA	-2.54	106.63	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	402	HEM	C4B-CHC-C1C	2.53	125.90	122.56
24	C	401	HEM	C3D-C4D-ND	-2.50	107.38	110.17
31	a	603	HEA	CHB-C1B-C2B	-2.49	121.09	124.98
26	e	202	PCF	O21-C21-C22	2.49	116.87	111.50
25	S	102	PEF	O3-C30-C31	2.48	119.70	111.91
31	a	604	HEA	CHA-C4D-C3D	-2.48	121.19	124.84
25	a	608	PEF	O3-C30-C31	2.48	119.69	111.91
24	N	401	HEM	C4B-CHC-C1C	2.47	125.82	122.56
31	a	603	HEA	CMC-C2C-C3C	2.47	129.29	124.68
24	C	401	HEM	CHA-C4D-C3D	2.46	129.95	125.33
24	C	401	HEM	CBA-CAA-C2A	-2.46	108.42	112.62
31	a	603	HEA	C1D-C2D-C3D	-2.45	104.38	106.96
26	H	104	PCF	O31-C31-C32	2.44	119.56	111.91
24	N	401	HEM	C3D-C4D-ND	-2.43	107.47	110.17
31	a	603	HEA	C3C-C4C-NC	2.42	112.34	109.21
28	O	401	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
24	C	402	HEM	C4C-CHD-C1D	2.40	125.73	122.56
24	N	401	HEM	CBA-CAA-C2A	-2.35	108.61	112.62
25	P	303	PEF	O3-C30-C31	2.35	119.27	111.91
24	N	402	HEM	C4B-CHC-C1C	2.32	125.63	122.56
24	N	401	HEM	CMC-C2C-C3C	2.32	129.02	124.68
25	N	405	PEF	O3-C30-C31	2.30	119.13	111.91
31	a	604	HEA	C26-C15-C14	-2.30	117.79	123.68
28	D	401	HEC	CMB-C2B-C3B	2.27	128.49	125.82
28	O	401	HEC	CMB-C2B-C1B	-2.26	124.99	128.46
28	O	401	HEC	CMC-C2C-C1C	-2.25	125.01	128.46
28	D	401	HEC	CMC-C2C-C3C	-2.24	123.19	125.82
28	D	401	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
24	N	402	HEM	CMA-C3A-C4A	-2.21	125.06	128.46
31	a	603	HEA	C20-C19-C18	-2.21	116.64	121.12
25	U	101	PEF	C2-O2-C10	-2.21	112.35	117.79
25	H	103	PEF	O3-C30-C31	2.20	118.81	111.91
24	C	402	HEM	CMC-C2C-C3C	2.18	128.76	124.68
24	C	402	HEM	C3B-C2B-C1B	2.17	108.10	106.49
25	c	301	PEF	C2-O2-C10	-2.16	112.48	117.79
24	C	401	HEM	C4B-CHC-C1C	2.15	125.40	122.56
24	N	402	HEM	CMC-C2C-C3C	2.14	128.69	124.68
31	a	603	HEA	C2B-C1B-NB	2.14	112.44	109.88
26	T	101	PCF	C11-C12-N	-2.13	108.68	115.78
26	e	202	PCF	C3-C2-C1	-2.12	106.77	111.79
25	l	101	PEF	O3-C30-C31	2.12	118.56	111.91
28	D	401	HEC	CAA-CBA-CGA	-2.10	107.87	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	603	HEA	C26-C15-C14	-2.06	118.39	123.68
31	a	603	HEA	CHD-C1D-ND	-2.06	121.84	124.38
25	a	607	PEF	O3-C30-C31	2.04	118.30	111.91
25	c	301	PEF	O3-C30-O5	-2.04	118.45	123.59
25	h	101	PEF	C12-C11-C10	-2.03	106.24	113.62
28	D	401	HEC	C3C-C4C-NC	-2.03	107.11	110.94
31	a	603	HEA	O1D-CGD-CBD	-2.02	116.58	123.08
24	C	402	HEM	C3D-C4D-ND	-2.02	107.92	110.17
24	C	401	HEM	CHD-C1D-ND	2.02	126.62	124.43
25	a	601	PEF	C2-O2-C10	-2.01	112.84	117.79
31	a	604	HEA	CHB-C1B-C2B	-2.01	121.84	124.98
31	a	604	HEA	O2A-CGA-CBA	2.01	120.47	114.03

There are no chirality outliers.

All (1059) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	CDL	CA3-OA5-PA1-OA3
23	A	501	CDL	CA3-OA5-PA1-OA4
23	A	501	CDL	CA3-CA4-OA6-CA5
23	A	501	CDL	OA6-CA4-CA6-OA8
23	A	501	CDL	C11-CA5-OA6-CA4
23	A	501	CDL	CB2-OB2-PB2-OB3
23	A	501	CDL	CB2-OB2-PB2-OB4
23	A	501	CDL	CB3-OB5-PB2-OB3
23	A	502	CDL	CA2-OA2-PA1-OA3
23	A	502	CDL	CA2-OA2-PA1-OA4
23	A	502	CDL	CA2-OA2-PA1-OA5
23	A	502	CDL	C11-CA5-OA6-CA4
23	A	502	CDL	CB2-OB2-PB2-OB3
23	A	502	CDL	CB2-OB2-PB2-OB4
23	E	303	CDL	CA3-OA5-PA1-OA3
23	E	303	CDL	C11-CA5-OA6-CA4
23	E	303	CDL	CB2-OB2-PB2-OB3
23	E	303	CDL	CB2-OB2-PB2-OB4
23	E	303	CDL	CB2-OB2-PB2-OB5
23	E	303	CDL	CB3-OB5-PB2-OB4
23	H	101	CDL	CA2-OA2-PA1-OA3
23	H	101	CDL	CA2-OA2-PA1-OA4
23	H	101	CDL	CA2-OA2-PA1-OA5
23	H	101	CDL	CB2-OB2-PB2-OB3
23	H	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
23	H	101	CDL	CB2-OB2-PB2-OB5
23	H	101	CDL	CB3-OB5-PB2-OB2
23	H	101	CDL	CB3-OB5-PB2-OB4
23	H	102	CDL	CB2-OB2-PB2-OB5
23	H	102	CDL	CB3-OB5-PB2-OB3
23	H	102	CDL	CB3-OB5-PB2-OB4
23	L	501	CDL	CA2-OA2-PA1-OA3
23	L	501	CDL	CA2-OA2-PA1-OA4
23	L	501	CDL	CA2-OA2-PA1-OA5
23	L	501	CDL	CB2-OB2-PB2-OB3
23	L	501	CDL	CB2-OB2-PB2-OB4
23	L	501	CDL	CB3-OB5-PB2-OB3
23	L	501	CDL	OB5-CB3-CB4-OB6
23	L	502	CDL	CA2-C1-CB2-OB2
23	L	502	CDL	CA3-OA5-PA1-OA4
23	L	502	CDL	C11-CA5-OA6-CA4
23	L	502	CDL	OA9-CA7-OA8-CA6
23	L	502	CDL	CB2-OB2-PB2-OB3
23	L	502	CDL	CB2-OB2-PB2-OB4
23	L	502	CDL	CB3-OB5-PB2-OB3
23	L	502	CDL	CB3-OB5-PB2-OB4
23	N	403	CDL	CB2-C1-CA2-OA2
23	N	403	CDL	CA3-OA5-PA1-OA4
23	P	304	CDL	CA2-OA2-PA1-OA4
23	P	304	CDL	CA3-OA5-PA1-OA4
23	P	304	CDL	C51-CB5-OB6-CB4
23	S	101	CDL	CA2-OA2-PA1-OA3
23	S	101	CDL	CA3-OA5-PA1-OA3
23	c	303	CDL	CA2-OA2-PA1-OA3
23	c	303	CDL	CA3-OA5-PA1-OA2
23	c	303	CDL	CA3-OA5-PA1-OA3
23	c	303	CDL	CA3-OA5-PA1-OA4
23	c	303	CDL	CB2-OB2-PB2-OB3
23	c	303	CDL	CB2-OB2-PB2-OB4
24	C	401	HEM	C2D-C3D-CAD-CBD
24	C	401	HEM	C4D-C3D-CAD-CBD
24	N	401	HEM	C2D-C3D-CAD-CBD
24	N	401	HEM	C4D-C3D-CAD-CBD
25	C	403	PEF	O4P-C4-C5-N
25	C	404	PEF	O4P-C4-C5-N
25	C	407	PEF	O3P-C1-C2-O2
25	C	407	PEF	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
25	E	302	PEF	C1-O3P-P-O1P
25	G	201	PEF	O4P-C4-C5-N
25	G	201	PEF	C1-O3P-P-O1P
25	G	201	PEF	C4-O4P-P-O1P
25	G	201	PEF	C4-O4P-P-O2P
25	H	103	PEF	O4P-C4-C5-N
25	J	102	PEF	C31-C30-O3-C3
25	J	102	PEF	O5-C30-O3-C3
25	J	102	PEF	C1-O3P-P-O1P
25	N	404	PEF	O4P-C4-C5-N
25	N	404	PEF	C4-O4P-P-O1P
25	N	404	PEF	C4-O4P-P-O2P
25	N	404	PEF	C4-O4P-P-O3P
25	N	405	PEF	O4P-C4-C5-N
25	N	408	PEF	C31-C30-O3-C3
25	N	408	PEF	O5-C30-O3-C3
25	N	408	PEF	C1-O3P-P-O4P
25	P	301	PEF	O4P-C4-C5-N
25	P	301	PEF	C31-C30-O3-C3
25	P	301	PEF	O5-C30-O3-C3
25	P	301	PEF	C1-O3P-P-O1P
25	P	301	PEF	C1-O3P-P-O4P
25	P	303	PEF	O4P-C4-C5-N
25	P	303	PEF	C5-C4-O4P-P
25	P	303	PEF	C1-O3P-P-O4P
25	S	102	PEF	O4P-C4-C5-N
25	S	102	PEF	C1-O3P-P-O1P
25	S	102	PEF	C4-O4P-P-O1P
25	U	101	PEF	O4P-C4-C5-N
25	a	601	PEF	O4P-C4-C5-N
25	a	601	PEF	C4-O4P-P-O2P
25	a	607	PEF	O4P-C4-C5-N
25	a	607	PEF	C1-O3P-P-O1P
25	a	607	PEF	C4-O4P-P-O1P
25	a	608	PEF	O4P-C4-C5-N
25	a	608	PEF	C1-O3P-P-O1P
25	a	608	PEF	C1-O3P-P-O2P
25	a	608	PEF	C1-O3P-P-O4P
25	a	609	PEF	C1-O3P-P-O1P
25	a	609	PEF	C1-O3P-P-O2P
25	b	302	PEF	O3P-C1-C2-O2
25	b	302	PEF	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
25	b	303	PEF	C5-C4-O4P-P
25	b	303	PEF	C4-O4P-P-O1P
25	c	301	PEF	C4-O4P-P-O2P
25	c	302	PEF	O4P-C4-C5-N
25	h	101	PEF	O4P-C4-C5-N
25	h	101	PEF	C31-C30-O3-C3
25	h	101	PEF	O5-C30-O3-C3
25	l	101	PEF	C4-O4P-P-O1P
25	e	201	PEF	C1-O3P-P-O1P
26	C	405	PCF	C1-O11-P-O12
26	C	405	PCF	C1-O11-P-O13
26	C	405	PCF	C1-O11-P-O14
26	C	405	PCF	O13-C11-C12-N
26	H	104	PCF	O13-C11-C12-N
26	I	101	PCF	C1-O11-P-O14
26	I	101	PCF	O13-C11-C12-N
26	N	406	PCF	C1-O11-P-O12
26	N	406	PCF	C12-C11-O13-P
26	N	406	PCF	O13-C11-C12-N
26	T	101	PCF	C1-O11-P-O13
26	T	101	PCF	C1-O11-P-O14
26	T	101	PCF	C11-O13-P-O12
26	e	202	PCF	C1-O11-P-O12
26	e	202	PCF	C1-O11-P-O13
26	e	202	PCF	C1-O11-P-O14
26	e	202	PCF	O13-C11-C12-N
26	e	202	PCF	C22-C21-O21-C2
27	C	406	UQ6	C6-C7-C8-C9
27	C	406	UQ6	C29-C31-C32-C33
27	N	407	UQ6	C28-C29-C31-C32
27	N	407	UQ6	C30-C29-C31-C32
27	N	407	UQ6	C29-C31-C32-C33
31	a	603	HEA	C12-C11-C3B-C2B
31	a	603	HEA	C12-C11-C3B-C4B
31	a	603	HEA	O11-C11-C12-C13
31	a	603	HEA	C12-C13-C14-C15
31	a	603	HEA	C15-C16-C17-C18
31	a	603	HEA	C17-C18-C19-C20
23	H	102	CDL	OA9-CA7-OA8-CA6
23	S	101	CDL	OB9-CB7-OB8-CB6
23	H	102	CDL	C31-CA7-OA8-CA6
23	S	101	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
23	L	501	CDL	OB9-CB7-OB8-CB6
23	P	304	CDL	OB9-CB7-OB8-CB6
23	c	303	CDL	OA9-CA7-OA8-CA6
25	C	407	PEF	O5-C30-O3-C3
25	U	101	PEF	O5-C30-O3-C3
26	T	101	PCF	O32-C31-O31-C3
23	A	501	CDL	OA7-CA5-OA6-CA4
23	A	502	CDL	OA7-CA5-OA6-CA4
23	E	303	CDL	OA7-CA5-OA6-CA4
23	L	502	CDL	OA7-CA5-OA6-CA4
23	P	304	CDL	OB7-CB5-OB6-CB4
26	e	202	PCF	O22-C21-O21-C2
23	L	502	CDL	C31-CA7-OA8-CA6
23	c	303	CDL	C31-CA7-OA8-CA6
25	C	404	PEF	C31-C30-O3-C3
25	C	407	PEF	C31-C30-O3-C3
26	T	101	PCF	C32-C31-O31-C3
23	H	101	CDL	C71-CB7-OB8-CB6
23	L	501	CDL	C71-CB7-OB8-CB6
23	P	304	CDL	C71-CB7-OB8-CB6
25	U	101	PEF	C31-C30-O3-C3
31	a	603	HEA	C13-C14-C15-C26
23	c	303	CDL	OB7-CB5-OB6-CB4
31	a	603	HEA	C13-C14-C15-C16
23	N	403	CDL	OB9-CB7-OB8-CB6
25	C	404	PEF	O5-C30-O3-C3
25	c	302	PEF	O5-C30-O3-C3
23	L	501	CDL	OA9-CA7-OA8-CA6
23	A	501	CDL	O1-C1-CB2-OB2
23	A	502	CDL	O1-C1-CB2-OB2
23	E	303	CDL	O1-C1-CA2-OA2
23	H	101	CDL	O1-C1-CB2-OB2
23	L	501	CDL	O1-C1-CB2-OB2
23	N	403	CDL	O1-C1-CA2-OA2
23	N	403	CDL	O1-C1-CB2-OB2
23	P	304	CDL	O1-C1-CB2-OB2
23	S	101	CDL	O1-C1-CB2-OB2
23	c	303	CDL	O1-C1-CB2-OB2
23	N	403	CDL	C31-CA7-OA8-CA6
23	N	403	CDL	C71-CB7-OB8-CB6
23	H	101	CDL	C11-CA5-OA6-CA4
23	c	303	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
25	P	303	PEF	C11-C10-O2-C2
23	H	101	CDL	CB7-C71-C72-C73
23	S	101	CDL	C75-C76-C77-C78
23	L	501	CDL	C31-CA7-OA8-CA6
23	A	501	CDL	C71-C72-C73-C74
23	A	501	CDL	C32-C33-C34-C35
25	a	609	PEF	C31-C30-O3-C3
25	c	302	PEF	C31-C30-O3-C3
23	H	101	CDL	OA7-CA5-OA6-CA4
23	H	101	CDL	OB9-CB7-OB8-CB6
23	A	501	CDL	C34-C35-C36-C37
31	a	603	HEA	C21-C22-C23-C25
23	N	403	CDL	OA9-CA7-OA8-CA6
25	a	609	PEF	O5-C30-O3-C3
27	N	407	UQ6	C19-C21-C22-C23
27	N	407	UQ6	C24-C26-C27-C28
23	S	101	CDL	C11-CA5-OA6-CA4
31	a	603	HEA	C17-C18-C19-C27
23	H	101	CDL	C72-C73-C74-C75
23	H	101	CDL	CA2-C1-CB2-OB2
23	H	102	CDL	CA2-C1-CB2-OB2
23	N	403	CDL	CA2-C1-CB2-OB2
23	S	101	CDL	CA2-C1-CB2-OB2
23	c	303	CDL	CB2-C1-CA2-OA2
25	b	303	PEF	C31-C30-O3-C3
25	a	601	PEF	C30-C31-C32-C33
25	P	301	PEF	C34-C35-C36-C37
23	c	303	CDL	C39-C40-C41-C42
23	c	303	CDL	C74-C75-C76-C77
23	c	303	CDL	OA5-CA3-CA4-OA6
25	c	302	PEF	O3P-C1-C2-O2
23	L	502	CDL	O1-C1-CB2-OB2
23	c	303	CDL	O1-C1-CA2-OA2
25	P	301	PEF	C10-C11-C12-C13
25	b	302	PEF	C30-C31-C32-C33
23	H	102	CDL	OB6-CB4-CB6-OB8
23	L	501	CDL	C54-C55-C56-C57
25	c	302	PEF	C38-C39-C40-C41
23	H	101	CDL	C51-CB5-OB6-CB4
23	H	102	CDL	C11-CA5-OA6-CA4
23	S	101	CDL	C11-C12-C13-C14
23	A	501	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	E	302	PEF	C30-C31-C32-C33
25	N	404	PEF	C10-C11-C12-C13
25	b	303	PEF	O5-C30-O3-C3
25	U	101	PEF	C31-C32-C33-C34
26	e	202	PCF	C47-C48-C49-C50
23	H	101	CDL	CA7-C31-C32-C33
23	N	403	CDL	CB7-C71-C72-C73
23	P	304	CDL	CA7-C31-C32-C33
25	E	302	PEF	C10-C11-C12-C13
25	a	607	PEF	C10-C11-C12-C13
26	N	406	PCF	C31-C32-C33-C34
23	A	501	CDL	C18-C19-C20-C21
23	S	101	CDL	OA7-CA5-OA6-CA4
25	P	303	PEF	O4-C10-O2-C2
23	A	502	CDL	CA7-C31-C32-C33
23	A	502	CDL	C52-C53-C54-C55
23	N	403	CDL	C34-C35-C36-C37
27	C	406	UQ6	C9-C11-C12-C13
27	C	406	UQ6	C14-C16-C17-C18
27	N	407	UQ6	C14-C16-C17-C18
23	L	501	CDL	CB7-C71-C72-C73
25	b	303	PEF	C10-C11-C12-C13
25	c	301	PEF	C30-C31-C32-C33
23	H	102	CDL	O1-C1-CB2-OB2
23	H	102	CDL	OA7-CA5-OA6-CA4
23	P	304	CDL	CB7-C71-C72-C73
23	L	501	CDL	C51-CB5-OB6-CB4
23	L	502	CDL	C32-C33-C34-C35
23	A	501	CDL	CA3-OA5-PA1-OA2
23	A	501	CDL	CB2-OB2-PB2-OB5
23	A	502	CDL	CB2-OB2-PB2-OB5
23	A	502	CDL	CB3-OB5-PB2-OB2
23	E	303	CDL	CB3-OB5-PB2-OB2
23	H	101	CDL	CA3-OA5-PA1-OA2
23	H	102	CDL	CB3-OB5-PB2-OB2
23	L	501	CDL	CA3-OA5-PA1-OA2
23	L	501	CDL	CB2-OB2-PB2-OB5
23	L	501	CDL	CB3-OB5-PB2-OB2
23	L	502	CDL	CA3-OA5-PA1-OA2
23	L	502	CDL	CB2-OB2-PB2-OB5
23	L	502	CDL	CB3-OB5-PB2-OB2
23	N	403	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
23	N	403	CDL	CA3-OA5-PA1-OA2
23	P	304	CDL	CA2-OA2-PA1-OA5
23	P	304	CDL	CA3-OA5-PA1-OA2
23	S	101	CDL	CA2-OA2-PA1-OA5
23	S	101	CDL	CB2-OB2-PB2-OB5
23	S	101	CDL	CB3-OB5-PB2-OB2
23	c	303	CDL	CA2-OA2-PA1-OA5
23	c	303	CDL	CB2-OB2-PB2-OB5
23	c	303	CDL	CB3-OB5-PB2-OB2
25	G	201	PEF	C4-O4P-P-O3P
25	N	404	PEF	C1-O3P-P-O4P
25	P	301	PEF	C4-O4P-P-O3P
25	S	102	PEF	C4-O4P-P-O3P
25	a	607	PEF	C4-O4P-P-O3P
25	a	609	PEF	C1-O3P-P-O4P
25	c	301	PEF	C4-O4P-P-O3P
25	l	101	PEF	C4-O4P-P-O3P
25	e	201	PEF	C1-O3P-P-O4P
26	I	101	PCF	C1-O11-P-O13
26	N	406	PCF	C11-O13-P-O11
23	S	101	CDL	CB7-C71-C72-C73
25	P	303	PEF	C30-C31-C32-C33
26	C	405	PCF	C32-C31-O31-C3
23	A	502	CDL	CA2-C1-CB2-OB2
23	H	101	CDL	OB7-CB5-OB6-CB4
23	L	501	CDL	OB7-CB5-OB6-CB4
23	A	501	CDL	C59-C60-C61-C62
23	H	101	CDL	C71-C72-C73-C74
26	e	202	PCF	C24-C25-C26-C27
23	c	303	CDL	C11-CA5-OA6-CA4
23	A	501	CDL	C57-C58-C59-C60
23	E	303	CDL	C52-C53-C54-C55
23	H	101	CDL	C31-C32-C33-C34
23	H	102	CDL	C11-C12-C13-C14
25	E	302	PEF	C32-C33-C34-C35
25	P	303	PEF	C13-C14-C15-C16
25	S	102	PEF	C32-C33-C34-C35
25	a	608	PEF	C15-C16-C17-C18
25	c	302	PEF	C20-C21-C22-C23
25	h	101	PEF	C13-C14-C15-C16
25	h	101	PEF	C40-C41-C42-C43
25	l	101	PEF	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
25	e	201	PEF	C17-C18-C19-C20
25	e	201	PEF	C31-C32-C33-C34
23	L	502	CDL	C73-C74-C75-C76
23	N	403	CDL	C33-C34-C35-C36
25	C	403	PEF	C36-C37-C38-C39
25	C	407	PEF	C12-C13-C14-C15
25	N	408	PEF	C11-C12-C13-C14
25	N	408	PEF	C34-C35-C36-C37
25	P	301	PEF	C33-C34-C35-C36
25	a	601	PEF	C13-C14-C15-C16
25	b	303	PEF	C13-C14-C15-C16
25	c	302	PEF	C11-C12-C13-C14
25	c	302	PEF	C16-C17-C18-C19
25	l	101	PEF	C37-C38-C39-C40
26	T	101	PCF	C41-C42-C43-C44
26	e	202	PCF	C41-C42-C43-C44
23	c	303	CDL	OA7-CA5-OA6-CA4
25	e	201	PEF	C10-C11-C12-C13
23	A	501	CDL	C55-C56-C57-C58
23	H	102	CDL	C61-C62-C63-C64
23	L	502	CDL	C18-C19-C20-C21
23	S	101	CDL	C73-C74-C75-C76
25	G	201	PEF	C34-C35-C36-C37
25	a	609	PEF	C11-C12-C13-C14
23	A	501	CDL	C31-C32-C33-C34
23	H	102	CDL	C35-C36-C37-C38
23	S	101	CDL	C57-C58-C59-C60
23	c	303	CDL	C63-C64-C65-C66
25	C	403	PEF	C32-C33-C34-C35
25	N	405	PEF	C17-C18-C19-C20
23	H	101	CDL	C37-C38-C39-C40
23	H	101	CDL	C38-C39-C40-C41
23	H	102	CDL	C14-C15-C16-C17
23	S	101	CDL	C56-C57-C58-C59
25	S	102	PEF	C31-C32-C33-C34
25	b	303	PEF	C20-C21-C22-C23
25	l	101	PEF	C12-C13-C14-C15
25	l	101	PEF	C38-C39-C40-C41
26	C	405	PCF	C21-C22-C23-C24
23	A	502	CDL	C12-C13-C14-C15
23	E	303	CDL	C71-C72-C73-C74
23	L	502	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	C	404	PEF	C32-C33-C34-C35
25	C	407	PEF	C33-C34-C35-C36
25	P	301	PEF	C35-C36-C37-C38
25	b	303	PEF	C32-C33-C34-C35
27	N	407	UQ6	C15-C14-C16-C17
23	H	101	CDL	C11-C12-C13-C14
23	c	303	CDL	C37-C38-C39-C40
25	C	403	PEF	C34-C35-C36-C37
23	A	501	CDL	C75-C76-C77-C78
23	H	102	CDL	C15-C16-C17-C18
23	H	102	CDL	C37-C38-C39-C40
23	L	502	CDL	C20-C21-C22-C23
23	N	403	CDL	C32-C33-C34-C35
23	S	101	CDL	C63-C64-C65-C66
23	c	303	CDL	C11-C12-C13-C14
25	C	404	PEF	C37-C38-C39-C40
25	P	303	PEF	C16-C17-C18-C19
25	a	601	PEF	C34-C35-C36-C37
25	h	101	PEF	C34-C35-C36-C37
25	l	101	PEF	C34-C35-C36-C37
26	e	202	PCF	C25-C26-C27-C28
25	N	405	PEF	C12-C13-C14-C15
25	P	303	PEF	C32-C33-C34-C35
25	c	301	PEF	C40-C41-C42-C43
23	A	501	CDL	C37-C38-C39-C40
23	c	303	CDL	C15-C16-C17-C18
25	N	404	PEF	C31-C32-C33-C34
26	e	202	PCF	C29-C30-C47-C48
23	L	502	CDL	CB7-C71-C72-C73
23	c	303	CDL	CB7-C71-C72-C73
23	A	501	CDL	C11-C12-C13-C14
23	A	501	CDL	C17-C18-C19-C20
23	S	101	CDL	C59-C60-C61-C62
23	S	101	CDL	C77-C78-C79-C80
23	c	303	CDL	C34-C35-C36-C37
25	C	403	PEF	C31-C32-C33-C34
25	C	407	PEF	C34-C35-C36-C37
25	a	607	PEF	C12-C13-C14-C15
25	a	608	PEF	C16-C17-C18-C19
25	a	608	PEF	C40-C41-C42-C43
25	c	302	PEF	C36-C37-C38-C39
25	h	101	PEF	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	l	101	PEF	C40-C41-C42-C43
27	N	407	UQ6	C9-C11-C12-C13
23	H	101	CDL	C36-C37-C38-C39
23	L	502	CDL	C72-C73-C74-C75
23	c	303	CDL	C55-C56-C57-C58
25	C	403	PEF	C38-C39-C40-C41
25	C	404	PEF	C13-C14-C15-C16
25	N	404	PEF	C13-C14-C15-C16
25	N	408	PEF	C31-C32-C33-C34
25	P	301	PEF	C31-C32-C33-C34
25	a	607	PEF	C34-C35-C36-C37
25	c	301	PEF	C36-C37-C38-C39
25	h	101	PEF	C35-C36-C37-C38
25	C	407	PEF	O4P-C4-C5-N
25	l	101	PEF	O4P-C4-C5-N
25	b	303	PEF	C11-C12-C13-C14
25	N	405	PEF	C10-C11-C12-C13
23	L	502	CDL	C23-C24-C25-C26
23	c	303	CDL	C59-C60-C61-C62
25	C	404	PEF	C36-C37-C38-C39
25	G	201	PEF	C11-C12-C13-C14
25	N	408	PEF	C32-C33-C34-C35
25	P	303	PEF	C34-C35-C36-C37
25	b	303	PEF	C16-C17-C18-C19
26	e	202	PCF	C27-C28-C29-C30
23	c	303	CDL	C77-C78-C79-C80
31	a	603	HEA	C21-C22-C23-C24
23	L	502	CDL	C19-C20-C21-C22
25	U	101	PEF	C13-C14-C15-C16
25	b	302	PEF	C12-C13-C14-C15
26	e	202	PCF	C48-C49-C50-C51
25	C	407	PEF	C10-C11-C12-C13
26	C	405	PCF	O32-C31-O31-C3
23	H	102	CDL	C63-C64-C65-C66
23	S	101	CDL	C60-C61-C62-C63
25	C	404	PEF	C18-C19-C20-C21
25	E	302	PEF	C36-C37-C38-C39
23	S	101	CDL	C61-C62-C63-C64
25	b	303	PEF	C12-C13-C14-C15
26	H	104	PCF	C32-C31-O31-C3
27	N	407	UQ6	C13-C14-C16-C17
23	E	303	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
23	S	101	CDL	C72-C73-C74-C75
23	c	303	CDL	C42-C43-C44-C45
23	c	303	CDL	C56-C57-C58-C59
25	C	403	PEF	C13-C14-C15-C16
25	C	404	PEF	C31-C32-C33-C34
25	E	302	PEF	C35-C36-C37-C38
25	b	302	PEF	C34-C35-C36-C37
25	b	302	PEF	C36-C37-C38-C39
25	c	302	PEF	C31-C32-C33-C34
23	H	102	CDL	C51-C52-C53-C54
25	E	302	PEF	C12-C13-C14-C15
25	N	404	PEF	C33-C34-C35-C36
25	a	607	PEF	C35-C36-C37-C38
23	c	303	CDL	C51-C52-C53-C54
25	U	101	PEF	C12-C13-C14-C15
23	E	303	CDL	CB2-C1-CA2-OA2
23	H	102	CDL	C34-C35-C36-C37
23	L	501	CDL	C13-C14-C15-C16
25	b	302	PEF	C11-C12-C13-C14
25	a	607	PEF	C36-C37-C38-C39
25	h	101	PEF	C39-C40-C41-C42
25	l	101	PEF	C13-C14-C15-C16
23	E	303	CDL	CB7-C71-C72-C73
25	C	403	PEF	C10-C11-C12-C13
25	e	201	PEF	C19-C20-C21-C22
25	e	201	PEF	C36-C37-C38-C39
26	H	104	PCF	C22-C23-C24-C25
23	P	304	CDL	C11-CA5-OA6-CA4
25	P	301	PEF	C11-C10-O2-C2
25	U	101	PEF	C11-C10-O2-C2
25	c	301	PEF	C11-C10-O2-C2
26	H	104	PCF	C22-C21-O21-C2
23	c	303	CDL	C43-C44-C45-C46
25	a	608	PEF	C34-C35-C36-C37
26	N	406	PCF	C40-C41-C42-C43
23	H	101	CDL	CA5-C11-C12-C13
23	E	303	CDL	C31-C32-C33-C34
23	L	502	CDL	C74-C75-C76-C77
23	S	101	CDL	C32-C33-C34-C35
26	H	104	PCF	O32-C31-O31-C3
25	b	303	PEF	C31-C32-C33-C34
26	N	406	PCF	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
25	E	302	PEF	O4-C10-O2-C2
26	H	104	PCF	O22-C21-O21-C2
23	A	502	CDL	C16-C17-C18-C19
23	L	502	CDL	C51-C52-C53-C54
23	H	101	CDL	C16-C17-C18-C19
23	H	102	CDL	C57-C58-C59-C60
26	H	104	PCF	C23-C24-C25-C26
26	e	202	PCF	C35-C36-C37-C38
25	b	303	PEF	C41-C42-C43-C44
25	e	201	PEF	C37-C38-C39-C40
23	A	502	CDL	CB5-C51-C52-C53
23	H	102	CDL	C13-C14-C15-C16
23	H	102	CDL	C31-C32-C33-C34
23	L	502	CDL	C17-C18-C19-C20
23	c	303	CDL	C36-C37-C38-C39
25	c	301	PEF	C31-C32-C33-C34
25	C	403	PEF	C40-C41-C42-C43
26	e	202	PCF	C36-C37-C38-C39
23	S	101	CDL	C52-C53-C54-C55
23	c	303	CDL	C75-C76-C77-C78
25	N	404	PEF	C36-C37-C38-C39
25	C	403	PEF	C11-C10-O2-C2
25	E	302	PEF	C11-C10-O2-C2
26	N	406	PCF	C22-C21-O21-C2
23	L	502	CDL	C71-C72-C73-C74
25	U	101	PEF	C17-C18-C19-C20
25	a	609	PEF	C13-C14-C15-C16
23	P	304	CDL	OA7-CA5-OA6-CA4
25	c	301	PEF	O4-C10-O2-C2
25	h	101	PEF	C10-C11-C12-C13
23	c	303	CDL	C76-C77-C78-C79
25	C	404	PEF	C34-C35-C36-C37
26	I	101	PCF	O21-C2-C3-O31
25	C	407	PEF	C13-C14-C15-C16
23	A	501	CDL	C51-C52-C53-C54
23	H	101	CDL	C13-C14-C15-C16
25	C	404	PEF	C14-C15-C16-C17
25	a	601	PEF	C21-C22-C23-C24
25	a	608	PEF	C37-C38-C39-C40
26	e	202	PCF	C42-C43-C44-C45
23	c	303	CDL	C61-C62-C63-C64
25	P	301	PEF	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	b	302	PEF	C31-C32-C33-C34
23	c	303	CDL	C62-C63-C64-C65
25	P	301	PEF	C37-C38-C39-C40
25	h	101	PEF	C38-C39-C40-C41
25	C	403	PEF	O4-C10-O2-C2
25	P	301	PEF	O4-C10-O2-C2
25	U	101	PEF	O4-C10-O2-C2
25	G	201	PEF	C11-C10-O2-C2
23	H	102	CDL	C54-C55-C56-C57
23	A	501	CDL	CB3-OB5-PB2-OB2
25	J	101	PEF	C4-O4P-P-O3P
25	J	102	PEF	C1-O3P-P-O4P
25	a	601	PEF	C4-O4P-P-O3P
25	b	303	PEF	C1-O3P-P-O4P
25	b	303	PEF	C4-O4P-P-O3P
26	N	406	PCF	C1-O11-P-O13
26	T	101	PCF	C11-O13-P-O11
25	h	101	PEF	C17-C18-C19-C20
25	e	201	PEF	C18-C19-C20-C21
23	H	102	CDL	C59-C60-C61-C62
25	l	101	PEF	C15-C16-C17-C18
25	e	201	PEF	C13-C14-C15-C16
23	L	501	CDL	OB5-CB3-CB4-CB6
25	C	403	PEF	O3P-C1-C2-C3
25	C	407	PEF	O3P-C1-C2-C3
25	N	405	PEF	C11-C12-C13-C14
25	N	405	PEF	C34-C35-C36-C37
23	c	303	CDL	C72-C73-C74-C75
25	N	405	PEF	C31-C32-C33-C34
25	P	303	PEF	C10-C11-C12-C13
25	b	302	PEF	C13-C14-C15-C16
23	H	101	CDL	C52-C53-C54-C55
25	P	303	PEF	C15-C16-C17-C18
25	h	101	PEF	C12-C13-C14-C15
23	E	303	CDL	CA7-C31-C32-C33
23	S	101	CDL	C34-C35-C36-C37
25	N	405	PEF	C35-C36-C37-C38
23	A	501	CDL	CA3-CA4-CA6-OA8
23	A	502	CDL	CA3-CA4-CA6-OA8
23	P	304	CDL	CA3-CA4-CA6-OA8
23	S	101	CDL	CA3-CA4-CA6-OA8
23	S	101	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
23	c	303	CDL	CB3-CB4-CB6-OB8
25	J	101	PEF	C31-C32-C33-C34
25	J	102	PEF	C1-C2-C3-O3
25	P	301	PEF	C1-C2-C3-O3
25	S	102	PEF	C1-C2-C3-O3
25	a	609	PEF	C1-C2-C3-O3
25	e	201	PEF	C14-C15-C16-C17
25	h	101	PEF	C32-C33-C34-C35
25	l	101	PEF	C11-C12-C13-C14
26	e	202	PCF	C31-C32-C33-C34
23	A	501	CDL	C19-C20-C21-C22
25	N	405	PEF	C16-C17-C18-C19
23	N	403	CDL	C37-C38-C39-C40
25	G	201	PEF	C12-C13-C14-C15
25	c	302	PEF	C42-C43-C44-C45
23	L	501	CDL	C72-C73-C74-C75
23	c	303	CDL	C44-C45-C46-C47
25	c	301	PEF	C12-C13-C14-C15
25	c	301	PEF	C37-C38-C39-C40
25	e	201	PEF	C16-C17-C18-C19
23	A	501	CDL	CA7-C31-C32-C33
23	A	501	CDL	C77-C78-C79-C80
25	b	303	PEF	C21-C22-C23-C24
25	a	601	PEF	C31-C32-C33-C34
25	H	103	PEF	C10-C11-C12-C13
23	H	102	CDL	C32-C33-C34-C35
23	H	102	CDL	C38-C39-C40-C41
25	C	404	PEF	C42-C43-C44-C45
26	N	406	PCF	O22-C21-O21-C2
25	a	608	PEF	C32-C33-C34-C35
23	L	501	CDL	C12-C13-C14-C15
25	C	404	PEF	C17-C18-C19-C20
25	h	101	PEF	C36-C37-C38-C39
25	e	201	PEF	C34-C35-C36-C37
23	c	303	CDL	C60-C61-C62-C63
25	C	407	PEF	C11-C12-C13-C14
25	N	404	PEF	C34-C35-C36-C37
26	N	406	PCF	C26-C27-C28-C29
25	E	302	PEF	O3P-C1-C2-O2
25	H	103	PEF	O3P-C1-C2-O2
25	J	101	PEF	O3P-C1-C2-O2
25	c	301	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	T	101	PCF	O11-C1-C2-O21
25	J	102	PEF	C10-C11-C12-C13
23	L	502	CDL	C52-C53-C54-C55
25	H	103	PEF	C36-C37-C38-C39
26	C	405	PCF	C27-C28-C29-C30
26	H	104	PCF	C21-C22-C23-C24
23	E	303	CDL	C54-C55-C56-C57
23	A	502	CDL	OA6-CA4-CA6-OA8
25	e	201	PEF	O2-C2-C3-O3
23	c	303	CDL	C38-C39-C40-C41
25	l	101	PEF	C33-C34-C35-C36
23	H	101	CDL	C73-C74-C75-C76
25	N	404	PEF	C18-C19-C20-C21
23	A	502	CDL	C14-C15-C16-C17
25	J	101	PEF	C12-C13-C14-C15
25	C	403	PEF	C35-C36-C37-C38
25	a	607	PEF	C18-C19-C20-C21
25	a	608	PEF	C11-C12-C13-C14
25	a	608	PEF	C31-C32-C33-C34
23	A	501	CDL	CA2-C1-CB2-OB2
25	C	407	PEF	C11-C10-O2-C2
25	U	101	PEF	C16-C17-C18-C19
25	C	404	PEF	C35-C36-C37-C38
23	A	501	CDL	OB5-CB3-CB4-CB6
23	A	502	CDL	OB5-CB3-CB4-CB6
23	N	403	CDL	OA5-CA3-CA4-CA6
23	c	303	CDL	OA5-CA3-CA4-CA6
25	a	601	PEF	O3P-C1-C2-C3
25	b	302	PEF	O3P-C1-C2-C3
25	c	302	PEF	O3P-C1-C2-C3
26	C	405	PCF	O11-C1-C2-C3
26	T	101	PCF	O11-C1-C2-C3
23	L	501	CDL	C11-C12-C13-C14
25	a	601	PEF	C20-C21-C22-C23
25	C	404	PEF	C33-C34-C35-C36
25	G	201	PEF	O4-C10-O2-C2
25	a	601	PEF	C19-C20-C21-C22
25	c	302	PEF	C13-C14-C15-C16
26	N	406	PCF	C41-C42-C43-C44
25	a	608	PEF	C42-C43-C44-C45
23	L	502	CDL	C1-CB2-OB2-PB2
25	G	201	PEF	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	N	403	CDL	C51-C52-C53-C54
25	a	601	PEF	C22-C23-C24-C25
25	c	301	PEF	C17-C18-C19-C20
25	c	302	PEF	C32-C33-C34-C35
26	H	104	PCF	C25-C26-C27-C28
25	b	302	PEF	C32-C33-C34-C35
25	h	101	PEF	C31-C32-C33-C34
23	E	303	CDL	CB3-CB4-CB6-OB8
23	H	102	CDL	CA3-CA4-CA6-OA8
23	H	102	CDL	CB3-CB4-CB6-OB8
25	C	404	PEF	C1-C2-C3-O3
25	G	201	PEF	C1-C2-C3-O3
25	N	404	PEF	C1-C2-C3-O3
25	a	608	PEF	C1-C2-C3-O3
25	h	101	PEF	C1-C2-C3-O3
26	C	405	PCF	C1-C2-C3-O31
26	H	104	PCF	C1-C2-C3-O31
26	N	406	PCF	C1-C2-C3-O31
23	A	502	CDL	CA5-C11-C12-C13
23	c	303	CDL	C54-C55-C56-C57
26	N	406	PCF	C35-C36-C37-C38
23	S	101	CDL	C13-C14-C15-C16
25	E	302	PEF	C37-C38-C39-C40
25	a	607	PEF	C16-C17-C18-C19
25	N	408	PEF	C35-C36-C37-C38
25	l	101	PEF	C32-C33-C34-C35
25	e	201	PEF	C42-C43-C44-C45
23	L	501	CDL	C71-C72-C73-C74
25	U	101	PEF	C32-C33-C34-C35
23	A	502	CDL	OB5-CB3-CB4-OB6
23	N	403	CDL	OA5-CA3-CA4-OA6
25	e	201	PEF	O3P-C1-C2-O2
26	I	101	PCF	O11-C1-C2-O21
23	A	501	CDL	C72-C73-C74-C75
25	C	404	PEF	C39-C40-C41-C42
25	H	103	PEF	C31-C32-C33-C34
23	L	501	CDL	OB6-CB4-CB6-OB8
23	S	101	CDL	OB6-CB4-CB6-OB8
25	C	404	PEF	O2-C2-C3-O3
25	N	404	PEF	O2-C2-C3-O3
25	S	102	PEF	O2-C2-C3-O3
25	b	303	PEF	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
26	C	405	PCF	O21-C2-C3-O31
26	H	104	PCF	O21-C2-C3-O31
26	N	406	PCF	O21-C2-C3-O31
26	T	101	PCF	O21-C2-C3-O31
25	b	302	PEF	C11-C10-O2-C2
23	L	501	CDL	CB5-C51-C52-C53
23	P	304	CDL	CA2-C1-CB2-OB2
25	C	407	PEF	O4-C10-O2-C2
25	S	102	PEF	C33-C34-C35-C36
25	a	608	PEF	C17-C18-C19-C20
23	E	303	CDL	C1-CA2-OA2-PA1
23	c	303	CDL	C73-C74-C75-C76
25	C	407	PEF	C14-C15-C16-C17
25	h	101	PEF	C11-C12-C13-C14
26	C	405	PCF	C30-C47-C48-C49
23	N	403	CDL	C35-C36-C37-C38
25	l	101	PEF	C10-C11-C12-C13
25	l	101	PEF	C11-C10-O2-C2
25	a	609	PEF	C32-C33-C34-C35
25	b	303	PEF	C14-C15-C16-C17
23	P	304	CDL	C71-C72-C73-C74
25	a	608	PEF	C33-C34-C35-C36
25	E	302	PEF	O3P-C1-C2-C3
25	P	303	PEF	O3P-C1-C2-C3
25	a	609	PEF	O3P-C1-C2-C3
25	b	303	PEF	O3P-C1-C2-C3
26	I	101	PCF	O11-C1-C2-C3
26	N	406	PCF	O11-C1-C2-C3
25	e	201	PEF	C11-C12-C13-C14
23	S	101	CDL	C54-C55-C56-C57
23	S	101	CDL	C36-C37-C38-C39
23	c	303	CDL	C78-C79-C80-C81
25	P	301	PEF	C15-C16-C17-C18
23	c	303	CDL	C41-C42-C43-C44
25	c	301	PEF	C10-C11-C12-C13
25	a	609	PEF	C12-C13-C14-C15
25	a	607	PEF	C30-C31-C32-C33
23	L	501	CDL	CB3-CB4-CB6-OB8
25	a	601	PEF	C1-C2-C3-O3
25	c	302	PEF	C2-C1-O3P-P
26	I	101	PCF	C1-C2-C3-O31
23	L	502	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
25	C	403	PEF	O3P-C1-C2-O2
25	G	201	PEF	O3P-C1-C2-O2
25	N	408	PEF	O3P-C1-C2-O2
25	P	303	PEF	O3P-C1-C2-O2
25	a	601	PEF	O3P-C1-C2-O2
25	b	303	PEF	O3P-C1-C2-O2
23	A	501	CDL	C74-C75-C76-C77
25	a	608	PEF	C12-C13-C14-C15
23	L	502	CDL	C13-C14-C15-C16
23	L	501	CDL	CA2-C1-CB2-OB2
25	b	302	PEF	O4-C10-O2-C2
25	l	101	PEF	O4-C10-O2-C2
23	E	303	CDL	C73-C74-C75-C76
23	H	102	CDL	OA6-CA4-CA6-OA8
23	N	403	CDL	OB6-CB4-CB6-OB8
23	S	101	CDL	OA6-CA4-CA6-OA8
25	G	201	PEF	O2-C2-C3-O3
25	c	302	PEF	O2-C2-C3-O3
25	h	101	PEF	C33-C34-C35-C36
25	a	601	PEF	C18-C19-C20-C21
25	h	101	PEF	O4-C10-O2-C2
26	T	101	PCF	C40-C41-C42-C43
23	A	501	CDL	C15-C16-C17-C18
25	N	408	PEF	C36-C37-C38-C39
25	b	303	PEF	C40-C41-C42-C43
26	e	202	PCF	C32-C33-C34-C35
23	E	303	CDL	CA2-OA2-PA1-OA5
23	E	303	CDL	CA3-OA5-PA1-OA2
25	E	302	PEF	C1-O3P-P-O4P
25	b	302	PEF	C1-O3P-P-O4P
26	I	101	PCF	C11-O13-P-O11
26	e	202	PCF	C11-O13-P-O11
23	A	501	CDL	CA4-CA3-OA5-PA1
23	N	403	CDL	CB4-CB3-OB5-PB2
23	S	101	CDL	CA4-CA3-OA5-PA1
25	H	103	PEF	C2-C1-O3P-P
25	h	101	PEF	C2-C1-O3P-P
25	C	407	PEF	C32-C33-C34-C35
23	A	501	CDL	CB3-OB5-PB2-OB4
23	A	502	CDL	CB3-OB5-PB2-OB3
23	A	502	CDL	CB3-OB5-PB2-OB4
23	E	303	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
23	H	101	CDL	CA3-OA5-PA1-OA3
23	H	101	CDL	CB3-OB5-PB2-OB3
23	L	501	CDL	CA3-OA5-PA1-OA3
23	L	501	CDL	CA3-OA5-PA1-OA4
23	L	501	CDL	CB3-OB5-PB2-OB4
23	N	403	CDL	CA2-OA2-PA1-OA3
23	N	403	CDL	CA2-OA2-PA1-OA4
23	P	304	CDL	CA2-OA2-PA1-OA3
23	S	101	CDL	CA2-OA2-PA1-OA4
23	S	101	CDL	CA3-OA5-PA1-OA4
23	S	101	CDL	CB2-OB2-PB2-OB3
23	S	101	CDL	CB2-OB2-PB2-OB4
23	S	101	CDL	CB3-OB5-PB2-OB3
23	c	303	CDL	CA2-OA2-PA1-OA4
23	c	303	CDL	CB3-OB5-PB2-OB3
25	J	101	PEF	C4-O4P-P-O2P
25	N	404	PEF	C1-O3P-P-O2P
25	P	301	PEF	C4-O4P-P-O1P
25	P	301	PEF	C4-O4P-P-O2P
25	P	303	PEF	C4-O4P-P-O2P
25	S	102	PEF	C4-O4P-P-O2P
25	U	101	PEF	C4-O4P-P-O2P
25	a	601	PEF	C4-O4P-P-O1P
25	a	608	PEF	C4-O4P-P-O2P
25	c	301	PEF	C4-O4P-P-O1P
26	I	101	PCF	C1-O11-P-O12
26	N	406	PCF	C11-O13-P-O12
26	T	101	PCF	C1-O11-P-O12
23	S	101	CDL	OB5-CB3-CB4-CB6
25	G	201	PEF	O3P-C1-C2-C3
25	H	103	PEF	O3P-C1-C2-C3
25	J	101	PEF	O3P-C1-C2-C3
25	N	408	PEF	O3P-C1-C2-C3
25	U	101	PEF	O3P-C1-C2-C3
25	a	607	PEF	O3P-C1-C2-C3
25	c	301	PEF	O3P-C1-C2-C3
25	e	201	PEF	O3P-C1-C2-C3
23	S	101	CDL	C31-C32-C33-C34
23	N	403	CDL	CA7-C31-C32-C33
25	N	405	PEF	C32-C33-C34-C35
23	c	303	CDL	C33-C34-C35-C36
25	G	201	PEF	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
25	e	201	PEF	C15-C16-C17-C18
25	H	103	PEF	C5-C4-O4P-P
25	b	302	PEF	C5-C4-O4P-P
31	a	603	HEA	C3B-C11-C12-C13
25	S	102	PEF	C30-C31-C32-C33
25	C	407	PEF	C2-C3-O3-C30
25	H	103	PEF	C12-C13-C14-C15
23	c	303	CDL	CA2-C1-CB2-OB2
23	c	303	CDL	C40-C41-C42-C43
23	A	501	CDL	OB5-CB3-CB4-OB6
23	S	101	CDL	OB5-CB3-CB4-OB6
25	a	609	PEF	O3P-C1-C2-O2
26	C	405	PCF	O11-C1-C2-O21
26	N	406	PCF	O11-C1-C2-O21
31	a	603	HEA	O11-C11-C3B-C2B
23	c	303	CDL	C58-C59-C60-C61
23	c	303	CDL	C64-C65-C66-C67
23	A	501	CDL	C38-C39-C40-C41
25	h	101	PEF	C11-C10-O2-C2
23	N	403	CDL	CA3-CA4-CA6-OA8
23	N	403	CDL	CB3-CB4-CB6-OB8
25	E	302	PEF	C34-C35-C36-C37
26	T	101	PCF	O13-C11-C12-N
23	E	303	CDL	OB6-CB4-CB6-OB8
23	N	403	CDL	OA6-CA4-CA6-OA8
23	P	304	CDL	OA6-CA4-CA6-OA8
23	c	303	CDL	OB6-CB4-CB6-OB8
25	J	102	PEF	O2-C2-C3-O3
25	P	301	PEF	O2-C2-C3-O3
25	a	608	PEF	O2-C2-C3-O3
25	h	101	PEF	O2-C2-C3-O3
25	N	404	PEF	C35-C36-C37-C38
23	A	501	CDL	C53-C54-C55-C56
23	H	101	CDL	C51-C52-C53-C54
25	P	303	PEF	C35-C36-C37-C38
25	S	102	PEF	C34-C35-C36-C37
25	a	608	PEF	C30-C31-C32-C33
25	l	101	PEF	C16-C17-C18-C19
23	L	501	CDL	OA7-CA5-OA6-CA4
25	P	303	PEF	C38-C39-C40-C41
23	L	502	CDL	C11-C12-C13-C14
23	H	101	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	H	101	CDL	C74-C75-C76-C77
23	S	101	CDL	CA6-CA4-OA6-CA5
25	P	303	PEF	C3-C2-O2-C10
25	c	302	PEF	C37-C38-C39-C40
25	a	609	PEF	C2-C1-O3P-P
23	L	502	CDL	C21-C22-C23-C24
25	C	404	PEF	C11-C12-C13-C14
23	c	303	CDL	C52-C53-C54-C55
23	L	501	CDL	C56-C57-C58-C59
23	L	501	CDL	C11-CA5-OA6-CA4
26	N	406	PCF	C22-C23-C24-C25
25	a	609	PEF	O2-C2-C3-O3
23	A	502	CDL	CA3-OA5-PA1-OA2
23	N	403	CDL	CB3-OB5-PB2-OB2
25	C	407	PEF	C4-O4P-P-O3P
25	H	103	PEF	C1-O3P-P-O4P
25	J	101	PEF	C1-O3P-P-O4P
25	a	607	PEF	C1-O3P-P-O4P
26	C	405	PCF	C11-O13-P-O11
25	G	201	PEF	C37-C38-C39-C40
25	b	303	PEF	C34-C35-C36-C37
25	H	103	PEF	C1-C2-C3-O3
25	e	201	PEF	C1-C2-C3-O3
23	S	101	CDL	C78-C79-C80-C81
25	J	102	PEF	C12-C13-C14-C15
25	N	408	PEF	C11-C10-O2-C2
25	h	101	PEF	C18-C19-C20-C21
25	C	407	PEF	C36-C37-C38-C39
26	H	104	PCF	C31-C32-C33-C34
25	N	404	PEF	C2-C1-O3P-P
23	A	502	CDL	C51-C52-C53-C54
25	H	103	PEF	C30-C31-C32-C33
25	N	408	PEF	O4-C10-O2-C2
23	P	304	CDL	C51-C52-C53-C54
25	a	608	PEF	C36-C37-C38-C39
25	E	302	PEF	O4P-C4-C5-N
25	P	303	PEF	C36-C37-C38-C39
23	L	501	CDL	C55-C56-C57-C58
23	L	501	CDL	C15-C16-C17-C18
23	A	501	CDL	C73-C74-C75-C76
25	S	102	PEF	C37-C38-C39-C40
25	J	102	PEF	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	E	303	CDL	CB4-CB3-OB5-PB2
23	H	102	CDL	CA4-CA3-OA5-PA1
23	L	502	CDL	C1-CA2-OA2-PA1
25	e	201	PEF	C2-C1-O3P-P
25	N	405	PEF	C21-C22-C23-C24
25	e	201	PEF	C35-C36-C37-C38
25	a	608	PEF	C38-C39-C40-C41
26	N	406	PCF	C47-C48-C49-C50
25	b	302	PEF	C33-C34-C35-C36
26	N	406	PCF	C42-C43-C44-C45
23	P	304	CDL	C52-C53-C54-C55
25	e	201	PEF	C20-C21-C22-C23
26	N	406	PCF	C38-C39-C40-C41
25	J	101	PEF	C1-C2-C3-O3
25	N	405	PEF	C1-C2-C3-O3
25	c	302	PEF	C1-C2-C3-O3
26	T	101	PCF	C28-C29-C30-C47
23	L	502	CDL	C33-C34-C35-C36
27	N	407	UQ6	C20-C19-C21-C22
25	a	607	PEF	C32-C33-C34-C35
25	N	404	PEF	C12-C13-C14-C15
23	P	304	CDL	CB3-OB5-PB2-OB2
26	T	101	PCF	C37-C38-C39-C40
23	L	501	CDL	OA5-CA3-CA4-OA6
25	N	405	PEF	O3P-C1-C2-C3
25	a	609	PEF	C10-C11-C12-C13
31	a	603	HEA	CAA-CBA-CGA-O2A
25	C	404	PEF	C10-C11-C12-C13
25	H	103	PEF	O2-C2-C3-O3
31	a	604	HEA	CAD-CBD-CGD-O1D
25	C	404	PEF	C40-C41-C42-C43
23	L	502	CDL	C24-C25-C26-C27
23	L	501	CDL	C52-C53-C54-C55
23	L	502	CDL	C22-C23-C24-C25
23	S	101	CDL	C53-C54-C55-C56
31	a	604	HEA	CAD-CBD-CGD-O2D
23	N	403	CDL	C71-C72-C73-C74
23	L	501	CDL	C52-C51-CB5-OB6
26	T	101	PCF	C39-C40-C41-C42
23	L	501	CDL	C53-C54-C55-C56
24	C	402	HEM	CAA-CBA-CGA-O2A
25	a	601	PEF	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	a	603	HEA	C27-C19-C20-C21
23	A	501	CDL	C76-C77-C78-C79
23	N	403	CDL	OB5-CB3-CB4-OB6
25	U	101	PEF	O3P-C1-C2-O2
23	L	502	CDL	CA5-C11-C12-C13
25	a	608	PEF	C21-C22-C23-C24
24	C	402	HEM	CAD-CBD-CGD-O1D
25	b	302	PEF	C39-C40-C41-C42
25	b	303	PEF	O3-C30-C31-C32
23	N	403	CDL	C1-CB2-OB2-PB2
23	P	304	CDL	CB4-CB3-OB5-PB2
25	S	102	PEF	C11-C12-C13-C14
25	J	102	PEF	C31-C32-C33-C34
23	A	501	CDL	C36-C37-C38-C39
25	C	407	PEF	C1-O3P-P-O4P
23	c	303	CDL	C16-C17-C18-C19
23	P	304	CDL	C52-C51-CB5-OB6
26	T	101	PCF	C23-C24-C25-C26
25	b	302	PEF	O3-C30-C31-C32
25	c	302	PEF	O3-C30-C31-C32
23	S	101	CDL	CA3-CA4-OA6-CA5
25	c	302	PEF	C12-C13-C14-C15
25	C	407	PEF	O3-C30-C31-C32
27	C	406	UQ6	C12-C11-C9-C10
23	H	101	CDL	C33-C34-C35-C36
26	T	101	PCF	C1-C2-C3-O31
23	E	303	CDL	C51-C52-C53-C54
23	H	101	CDL	OB5-CB3-CB4-OB6
25	P	303	PEF	C31-C32-C33-C34
23	c	303	CDL	CB5-C51-C52-C53
31	a	603	HEA	CAD-CBD-CGD-O2D
25	N	405	PEF	C37-C38-C39-C40
25	h	101	PEF	C42-C43-C44-C45
23	L	501	CDL	CA5-C11-C12-C13
24	C	402	HEM	CAA-CBA-CGA-O1A
23	L	502	CDL	OB5-CB3-CB4-CB6
25	P	303	PEF	C11-C12-C13-C14
23	H	101	CDL	C72-C71-CB7-OB8
23	S	101	CDL	CA7-C31-C32-C33
25	H	103	PEF	C32-C33-C34-C35
31	a	604	HEA	CAA-CBA-CGA-O1A
25	C	404	PEF	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
26	T	101	PCF	C33-C34-C35-C36
24	N	402	HEM	CAD-CBD-CGD-O1D
26	T	101	PCF	O31-C31-C32-C33
23	H	102	CDL	C72-C71-CB7-OB8
23	A	502	CDL	C72-C71-CB7-OB8
26	T	101	PCF	C24-C25-C26-C27
31	a	604	HEA	C2A-CAA-CBA-CGA
24	C	402	HEM	CAD-CBD-CGD-O2D
25	a	608	PEF	C39-C40-C41-C42
25	c	301	PEF	O3-C30-C31-C32
25	C	404	PEF	C20-C21-C22-C23
26	T	101	PCF	O32-C31-C32-C33
25	N	408	PEF	C33-C34-C35-C36
23	c	303	CDL	C32-C33-C34-C35
25	P	303	PEF	C17-C18-C19-C20
25	b	303	PEF	C39-C40-C41-C42
25	a	607	PEF	C31-C30-O3-C3
25	b	302	PEF	C38-C39-C40-C41
25	b	303	PEF	C1-C2-C3-O3
25	a	607	PEF	O3-C30-C31-C32
23	H	101	CDL	C72-C71-CB7-OB9
25	b	302	PEF	O5-C30-C31-C32
26	e	202	PCF	C26-C27-C28-C29
25	a	607	PEF	O5-C30-O3-C3
25	S	102	PEF	C36-C37-C38-C39
25	P	301	PEF	C2-C1-O3P-P
23	P	304	CDL	C52-C51-CB5-OB7
23	P	304	CDL	CB3-OB5-PB2-OB3
25	C	407	PEF	C4-O4P-P-O1P
25	N	405	PEF	C4-O4P-P-O1P
25	P	303	PEF	C1-O3P-P-O2P
25	U	101	PEF	C1-O3P-P-O1P
25	c	301	PEF	C1-O3P-P-O1P
26	C	405	PCF	C11-O13-P-O12
26	H	104	PCF	C1-O11-P-O12
25	C	407	PEF	O5-C30-C31-C32
25	b	303	PEF	O5-C30-C31-C32
25	J	102	PEF	O4P-C4-C5-N
25	G	201	PEF	C35-C36-C37-C38
26	N	406	PCF	C23-C24-C25-C26
25	l	101	PEF	C17-C18-C19-C20
28	D	401	HEC	CAD-CBD-CGD-O2D

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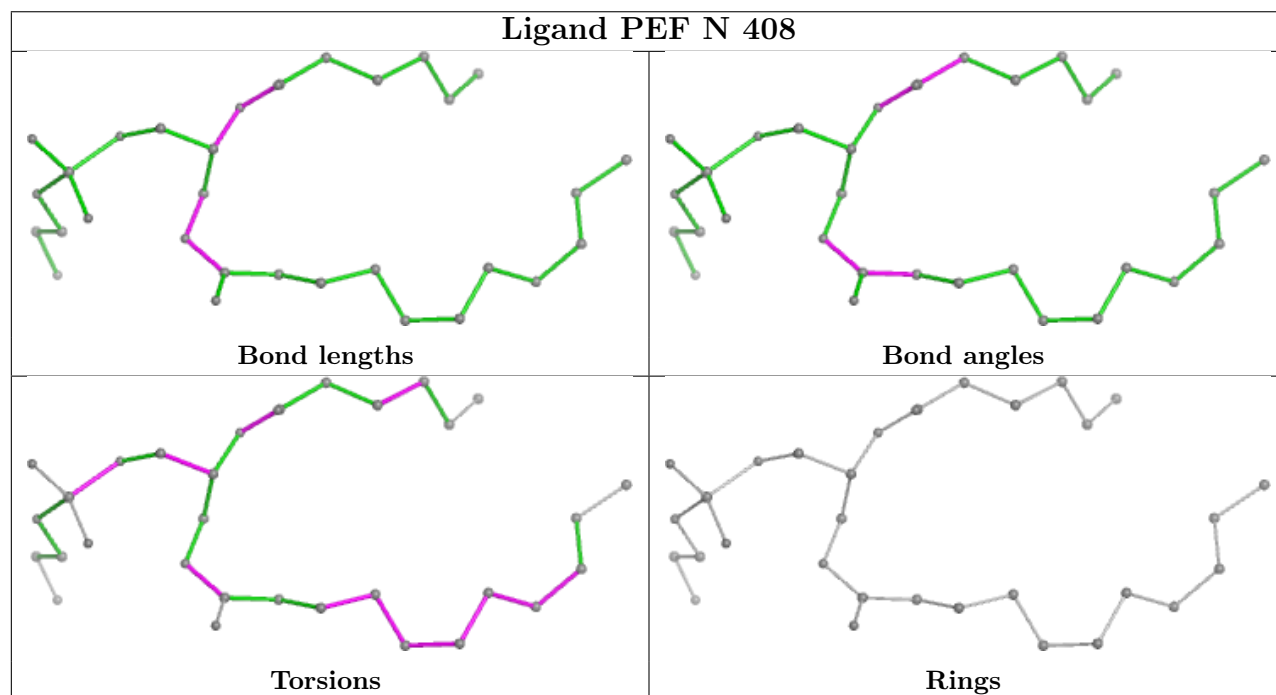
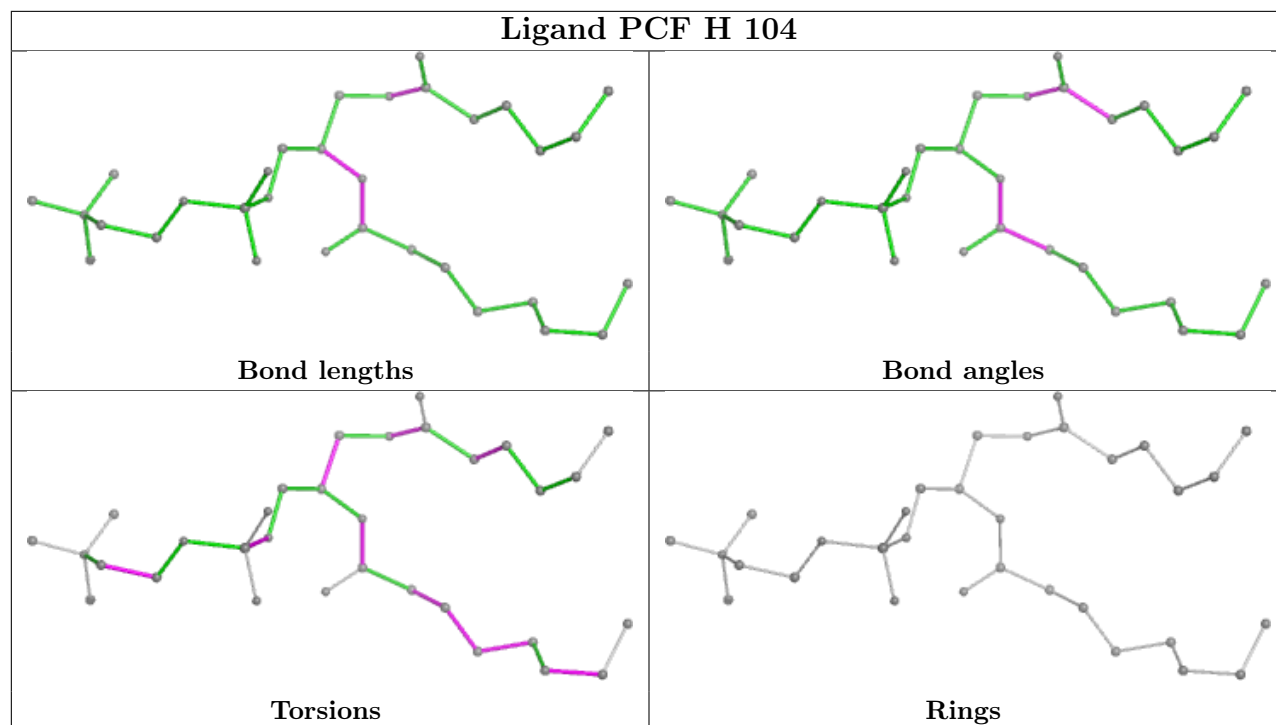
Mol	Chain	Res	Type	Atoms
23	H	102	CDL	CA6-CA4-OA6-CA5
25	G	201	PEF	C5-C4-O4P-P
25	S	102	PEF	C5-C4-O4P-P
26	I	101	PCF	C12-C11-O13-P
23	A	502	CDL	C72-C71-CB7-OB9
25	c	302	PEF	O5-C30-C31-C32
31	a	603	HEA	CAA-CBA-CGA-O1A
26	T	101	PCF	C21-C22-C23-C24
25	J	102	PEF	O2-C10-C11-C12
25	C	403	PEF	C42-C43-C44-C45
23	L	502	CDL	C52-C51-CB5-OB6
23	N	403	CDL	C52-C51-CB5-OB6
25	a	607	PEF	O2-C10-C11-C12
23	S	101	CDL	CB2-C1-CA2-OA2
24	N	402	HEM	CAD-CBD-CGD-O2D
25	H	103	PEF	C14-C15-C16-C17
23	c	303	CDL	C57-C58-C59-C60
27	N	407	UQ6	C18-C19-C21-C22
28	D	401	HEC	CAD-CBD-CGD-O1D
25	c	301	PEF	O5-C30-C31-C32
25	a	601	PEF	C14-C15-C16-C17
23	P	304	CDL	C12-C11-CA5-OA6
25	a	607	PEF	O5-C30-C31-C32
23	L	502	CDL	C52-C51-CB5-OB7
25	a	607	PEF	O4-C10-C11-C12
31	a	604	HEA	CAA-CBA-CGA-O2A

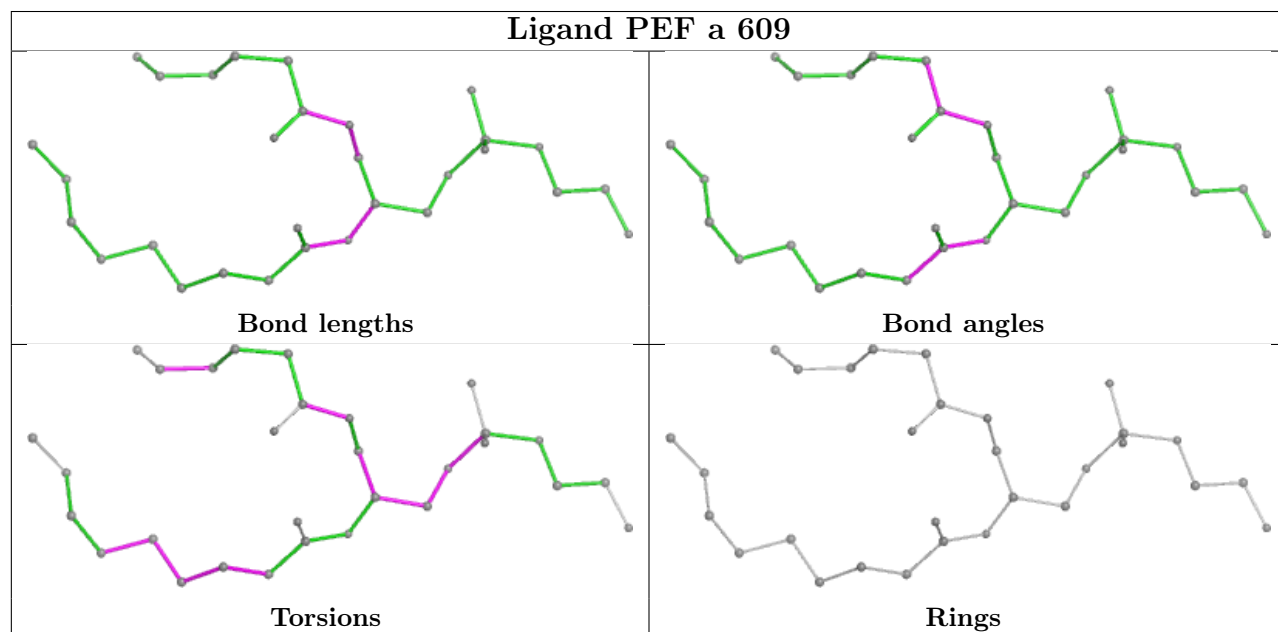
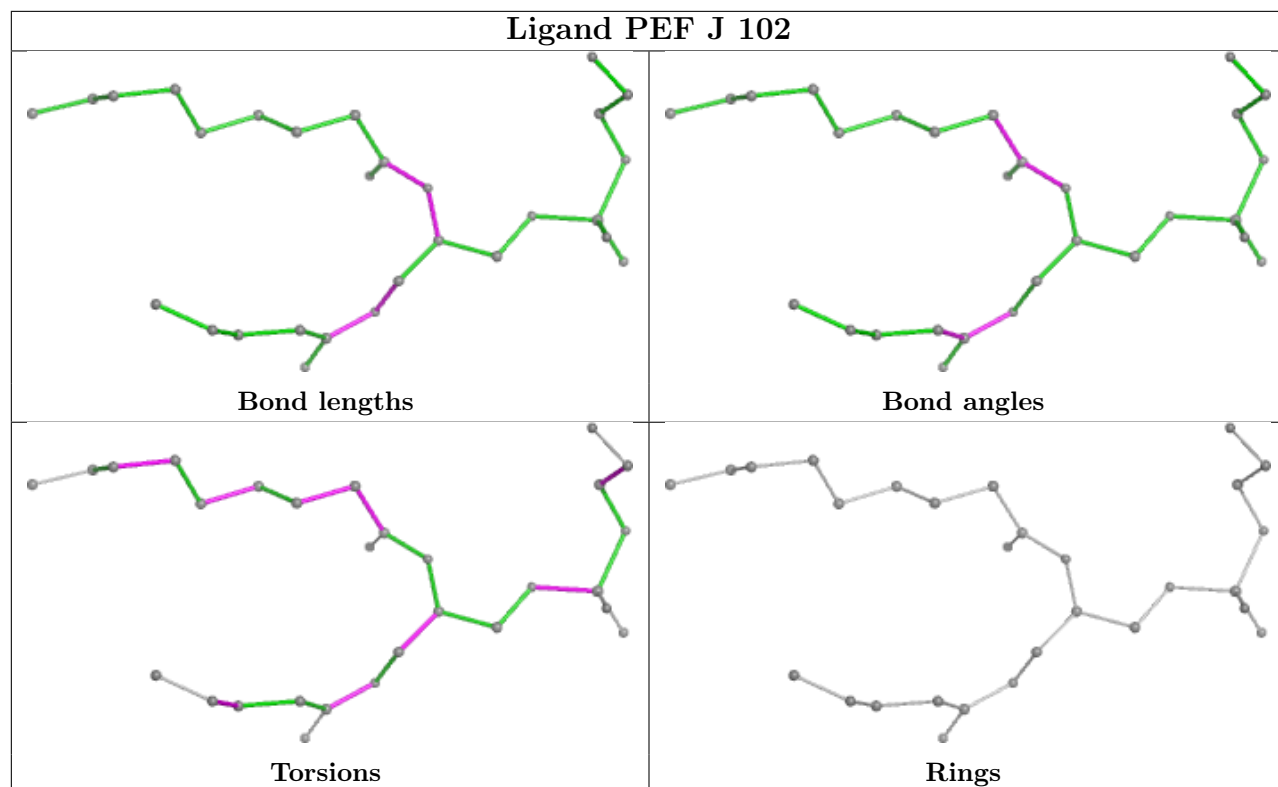
There are no ring outliers.

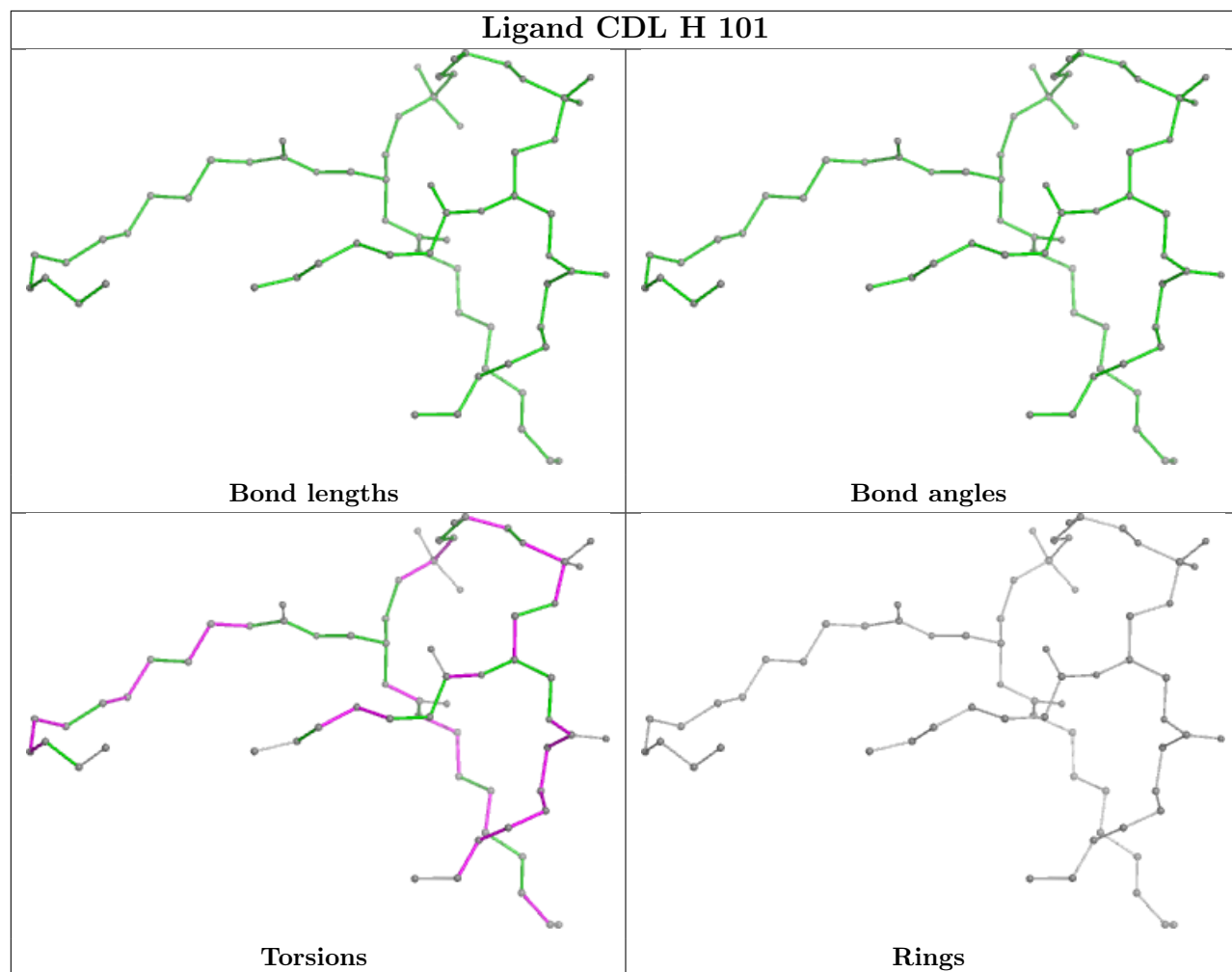
No monomer is involved in short contacts.

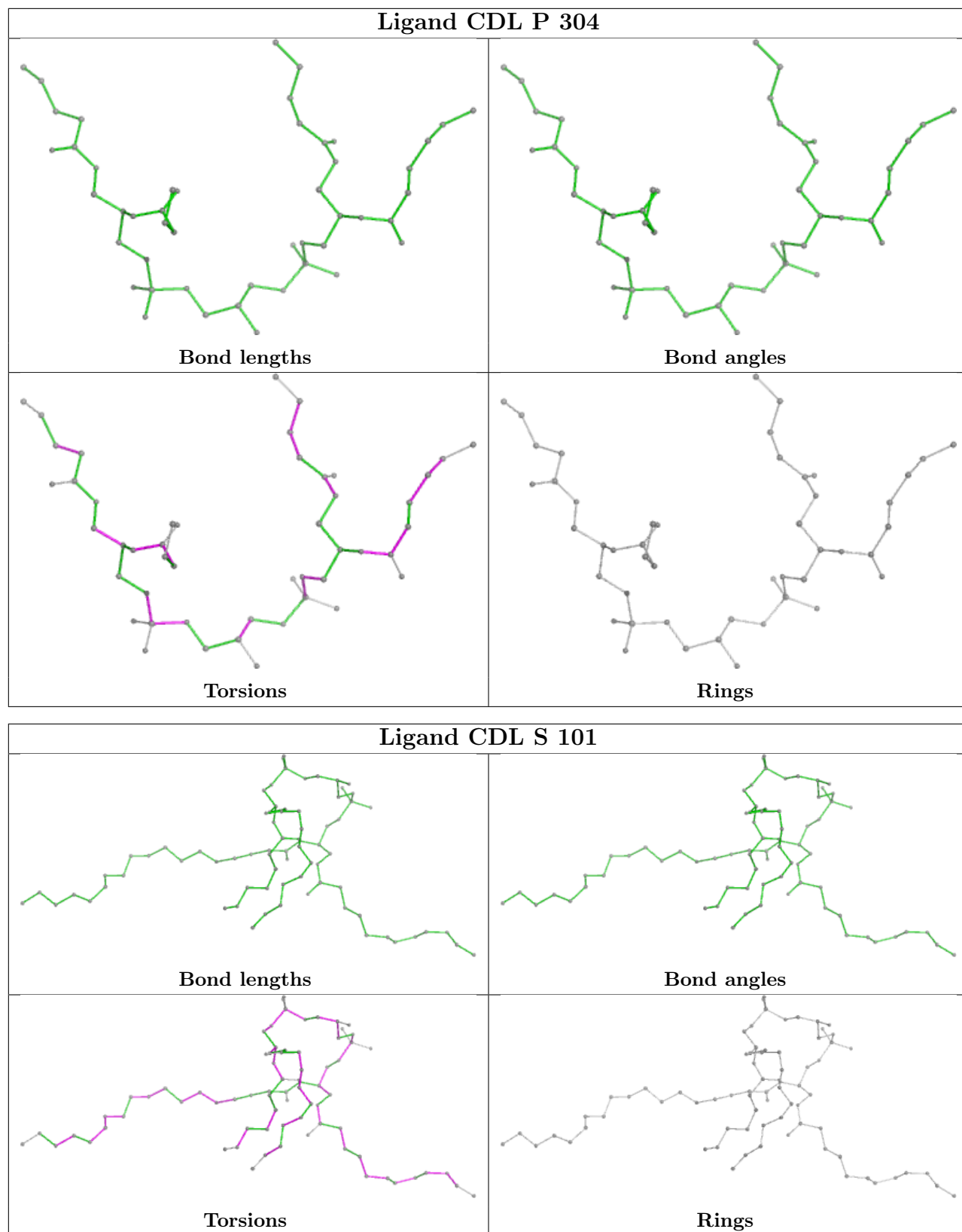
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

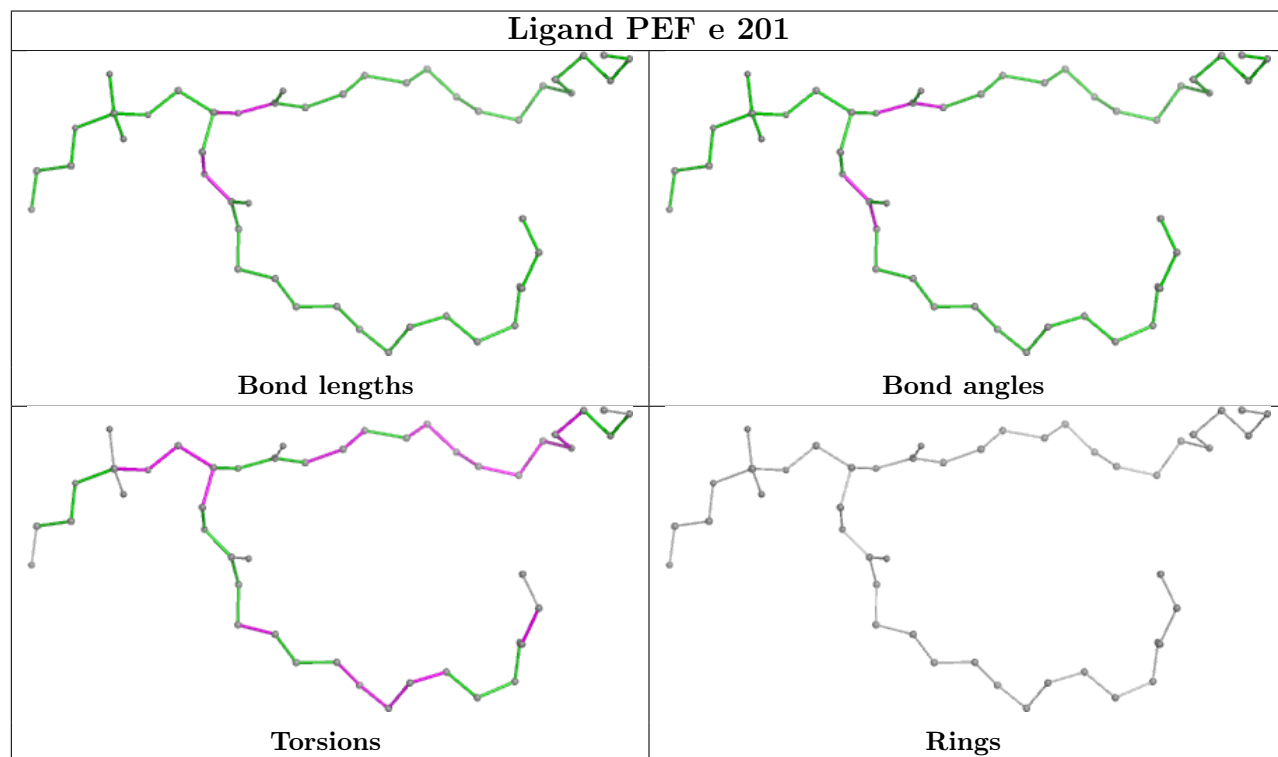
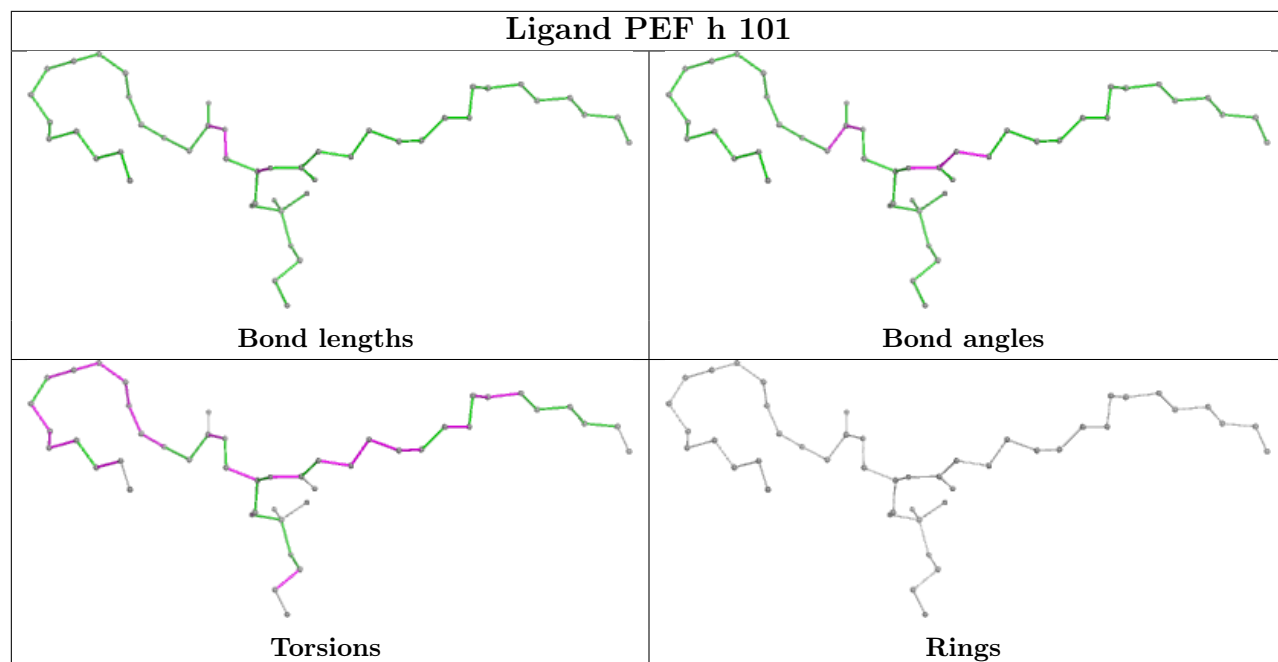


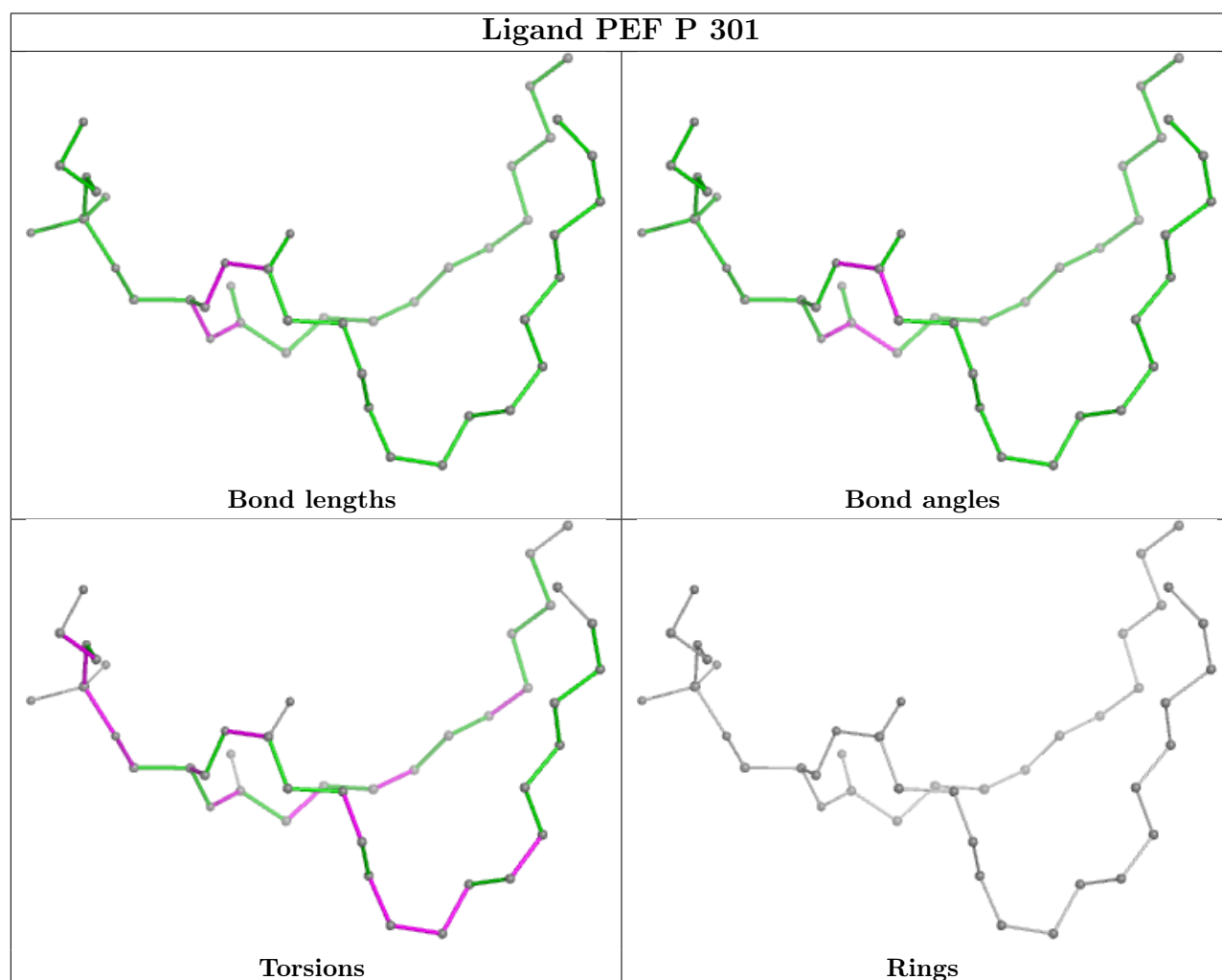
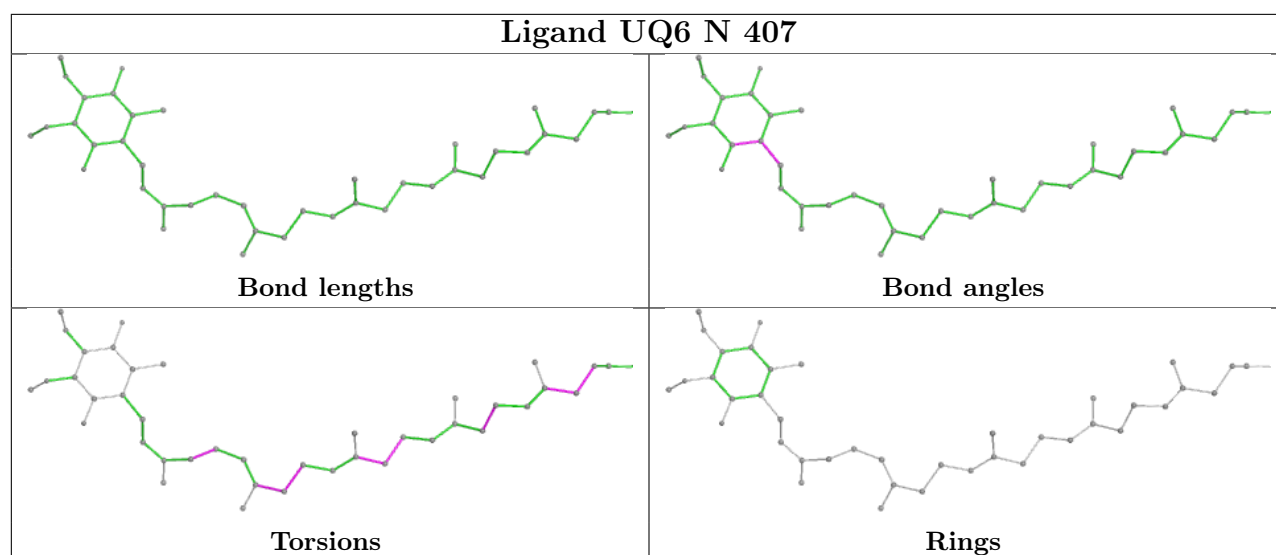


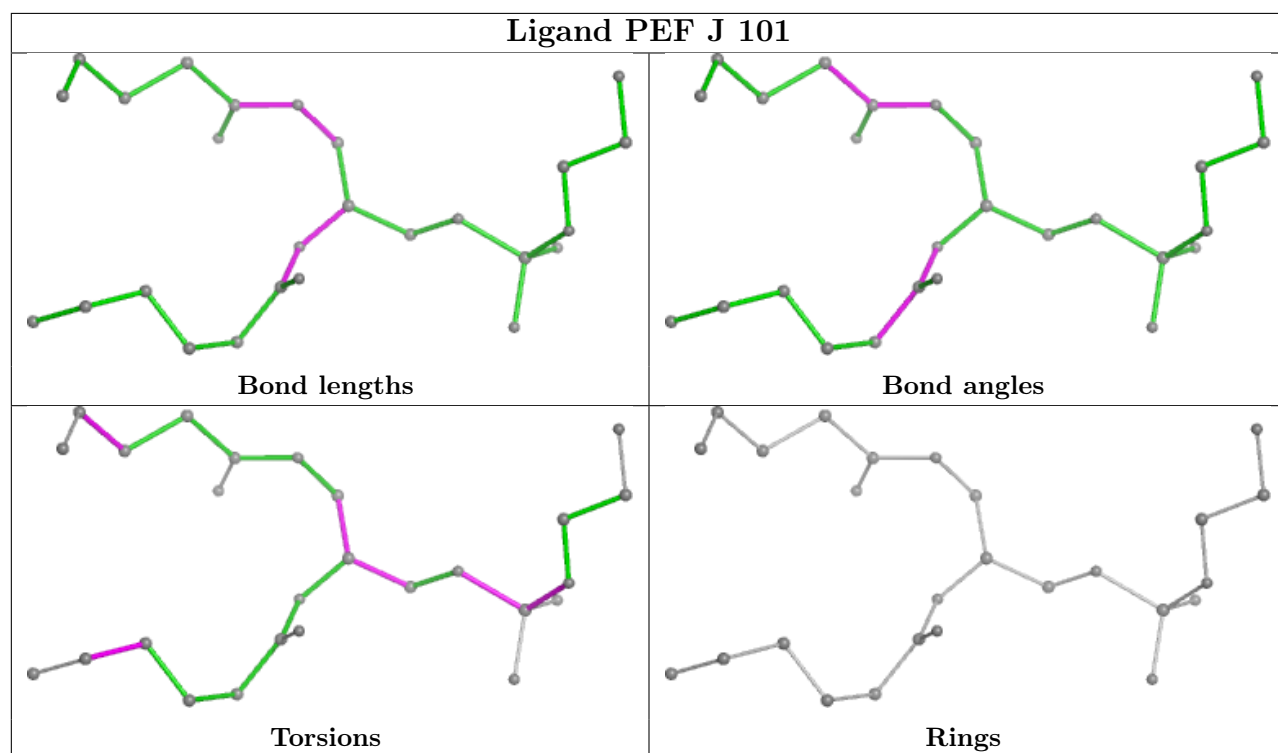
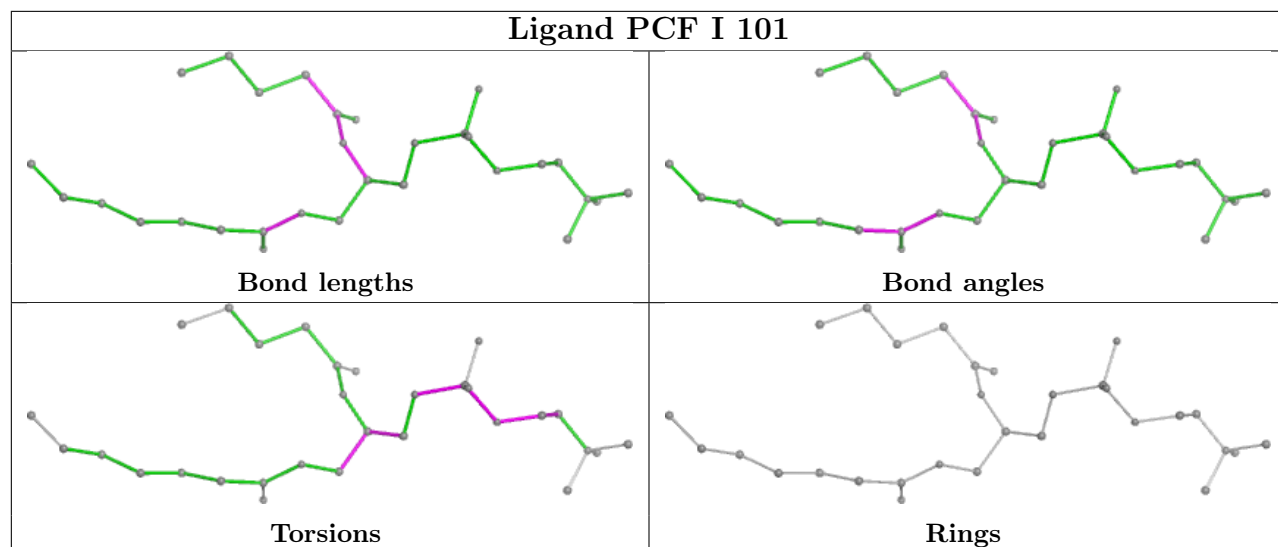


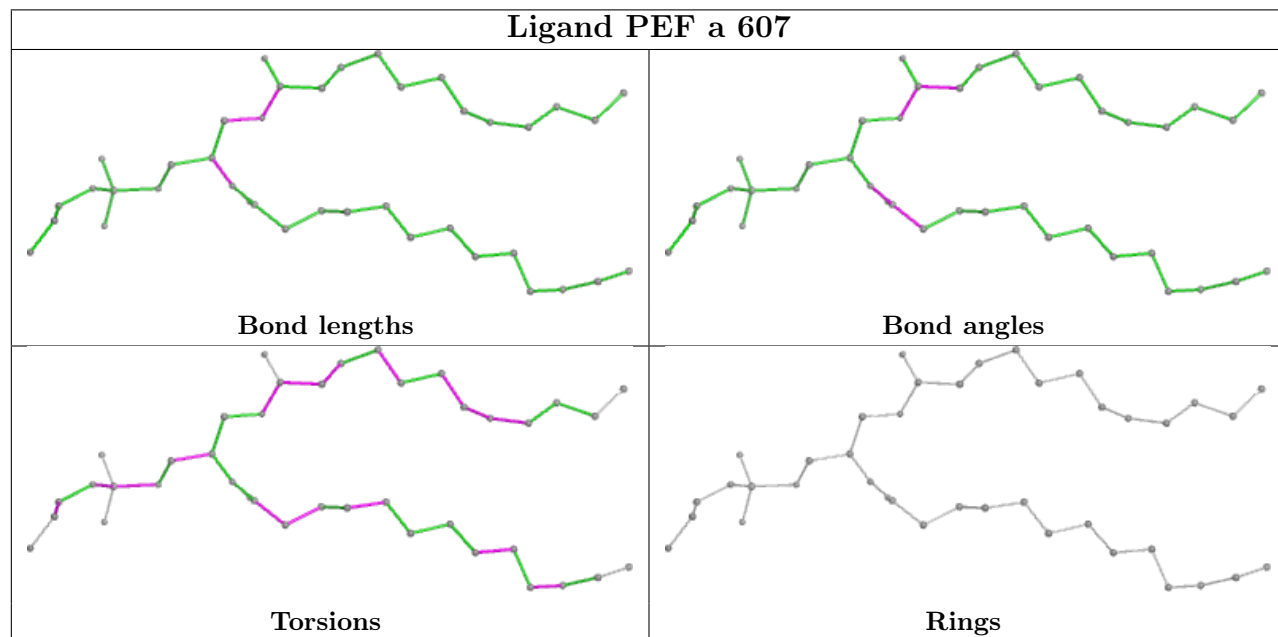
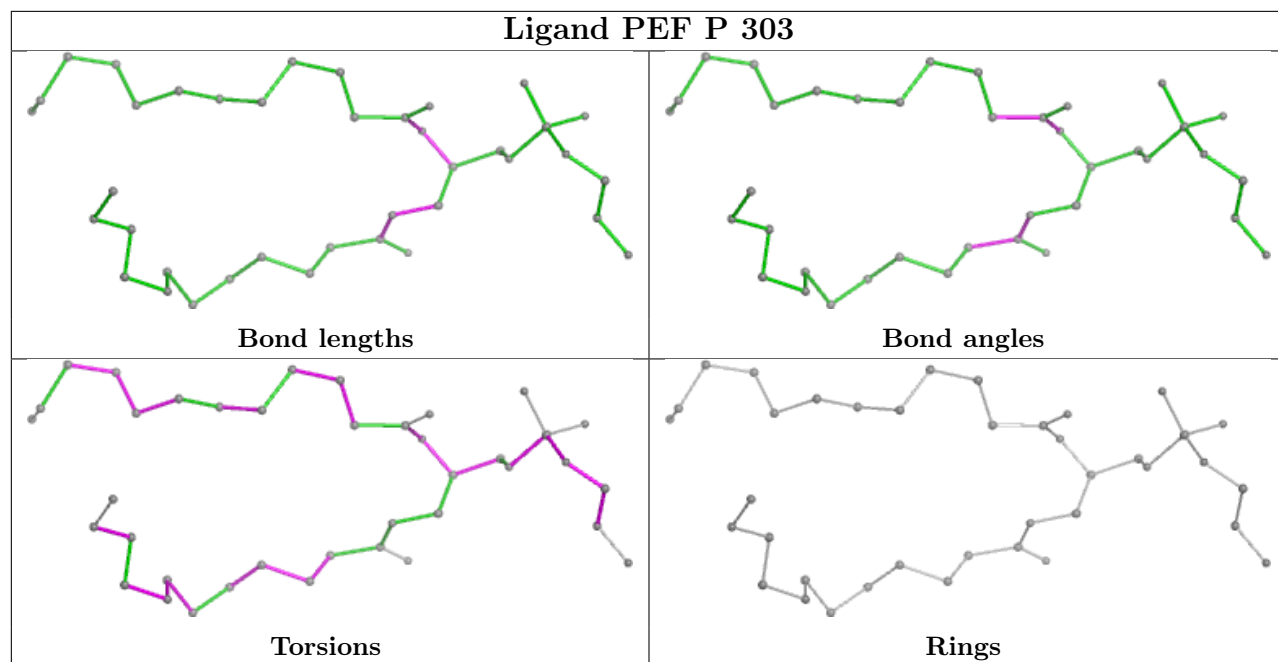




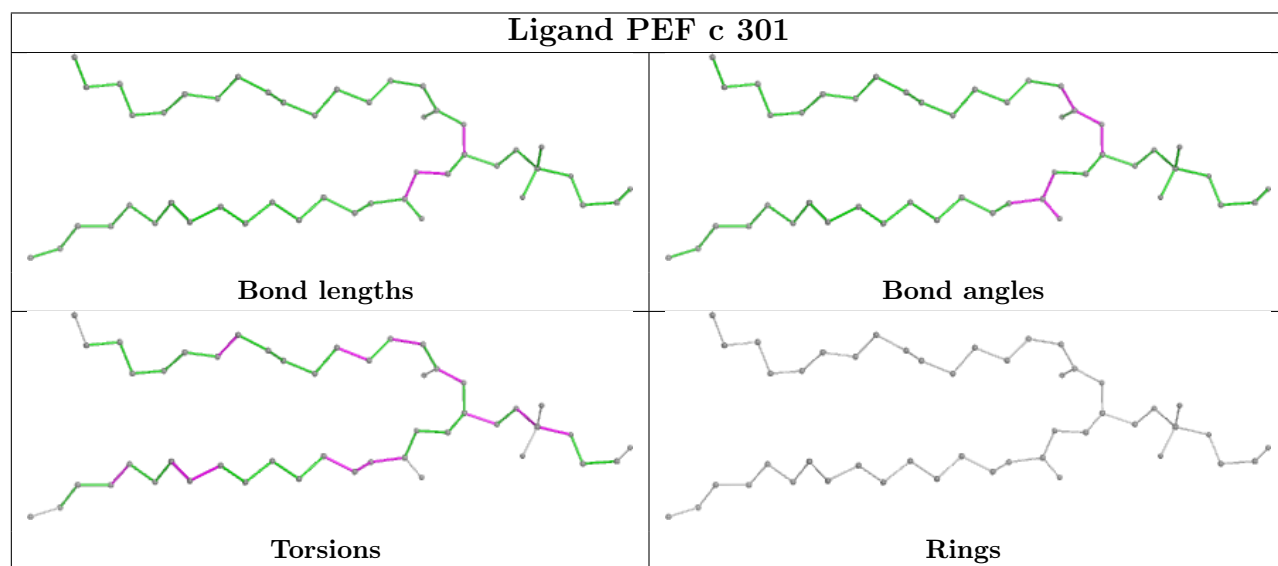
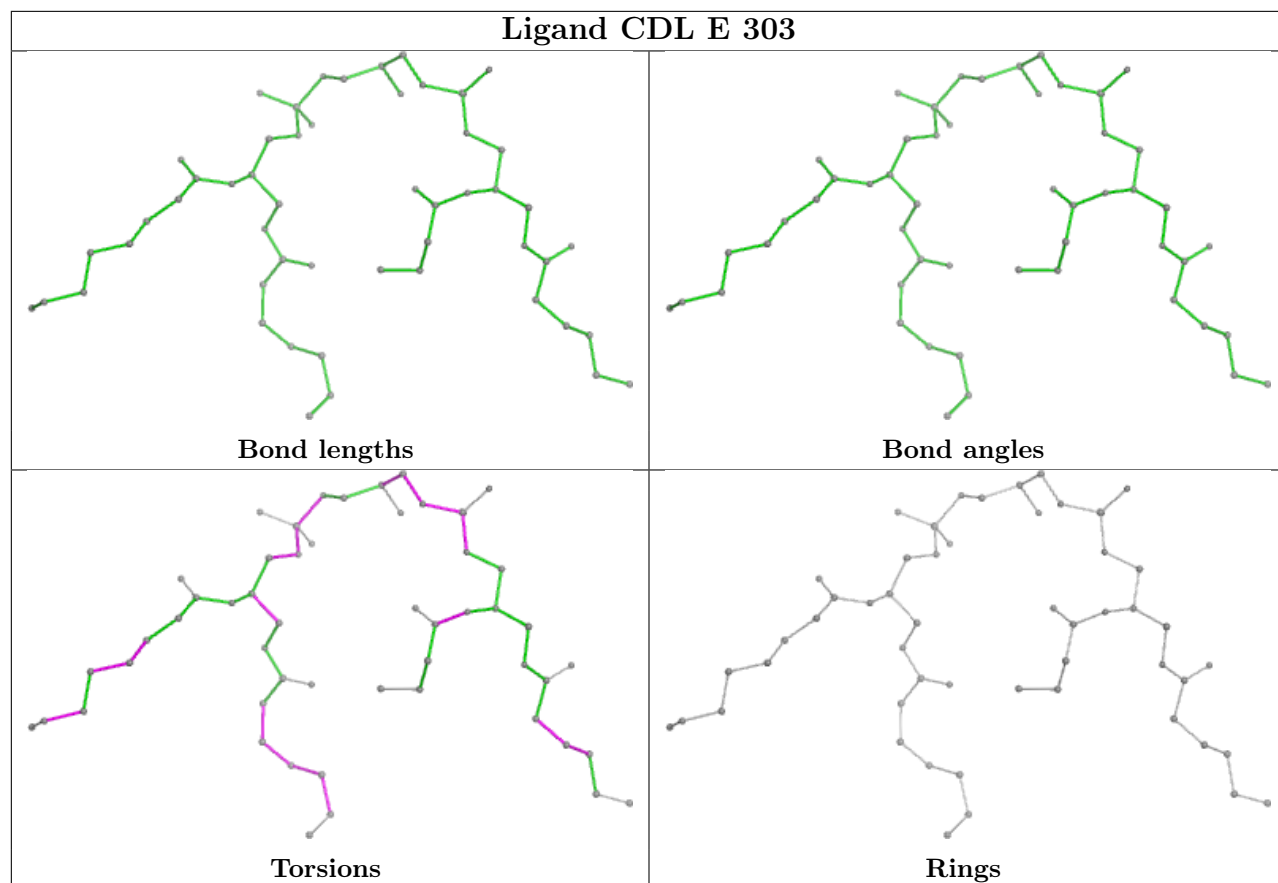


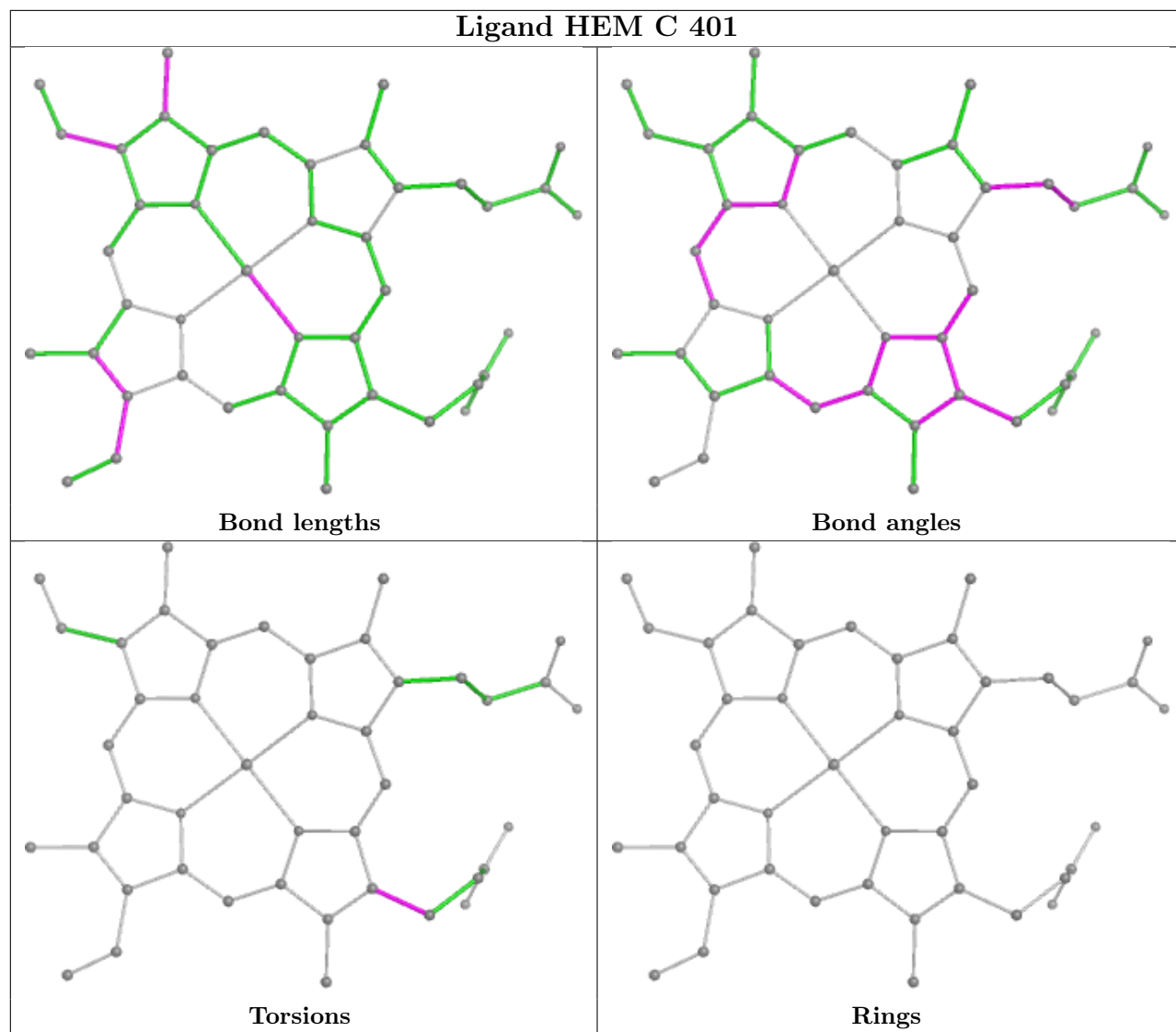


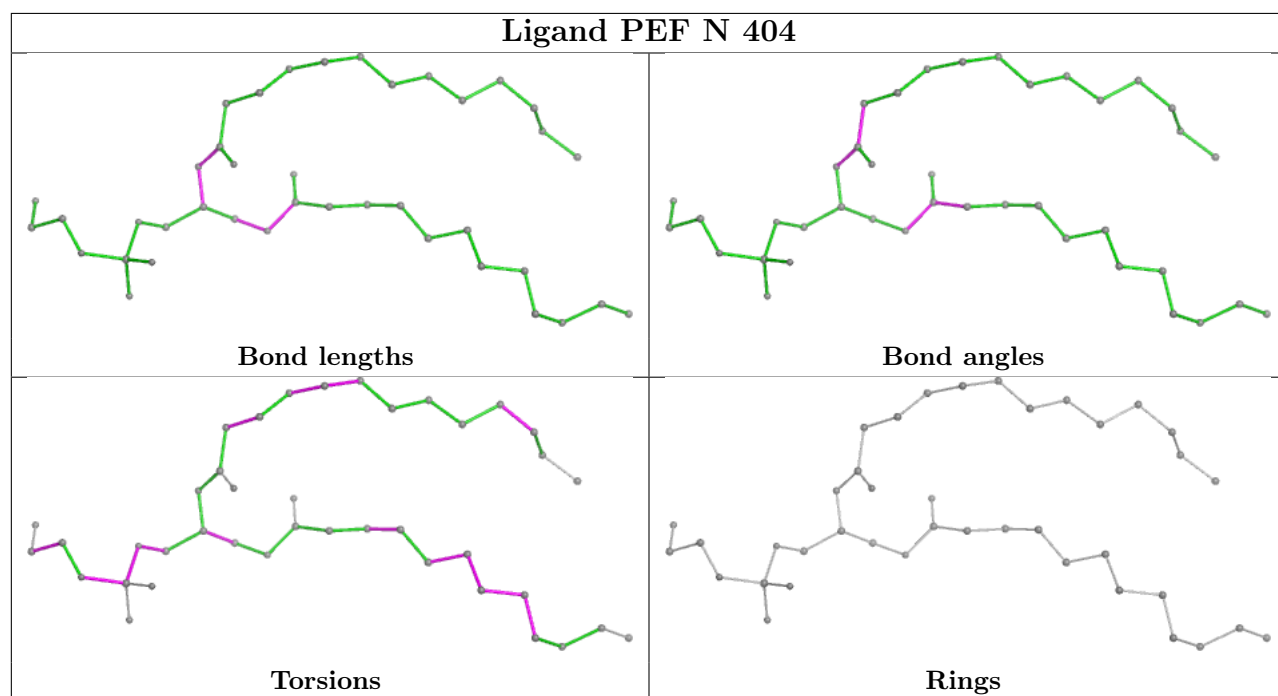
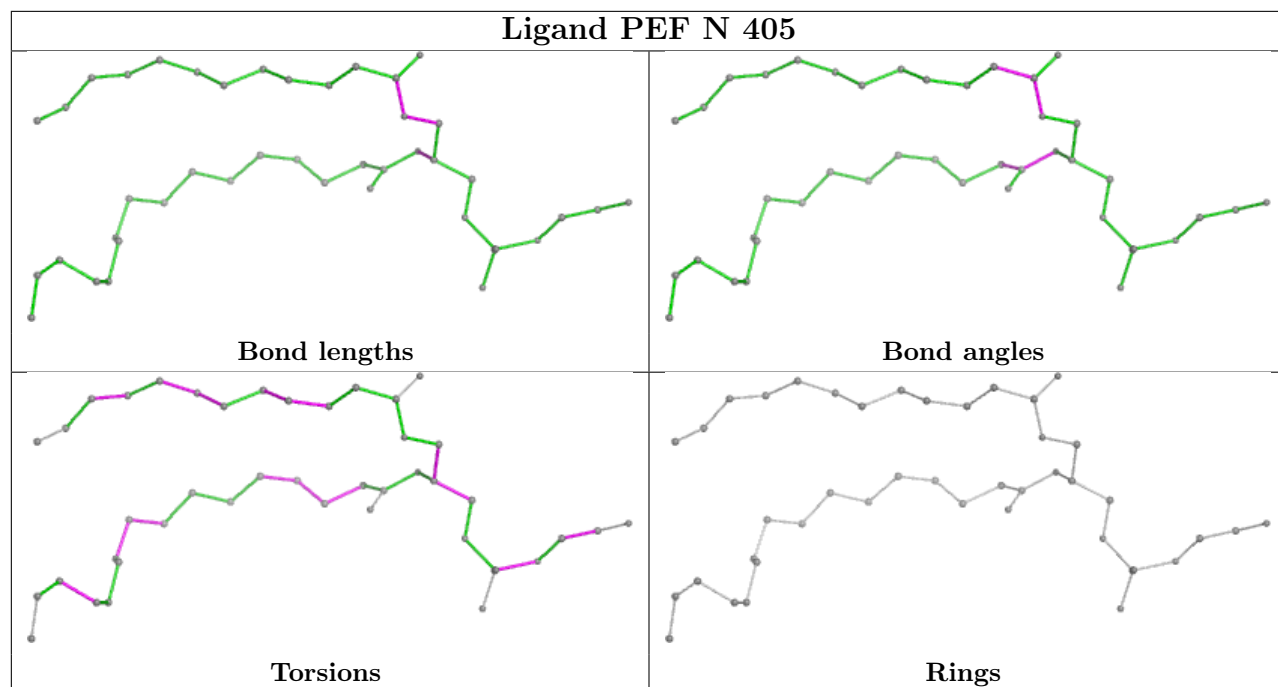


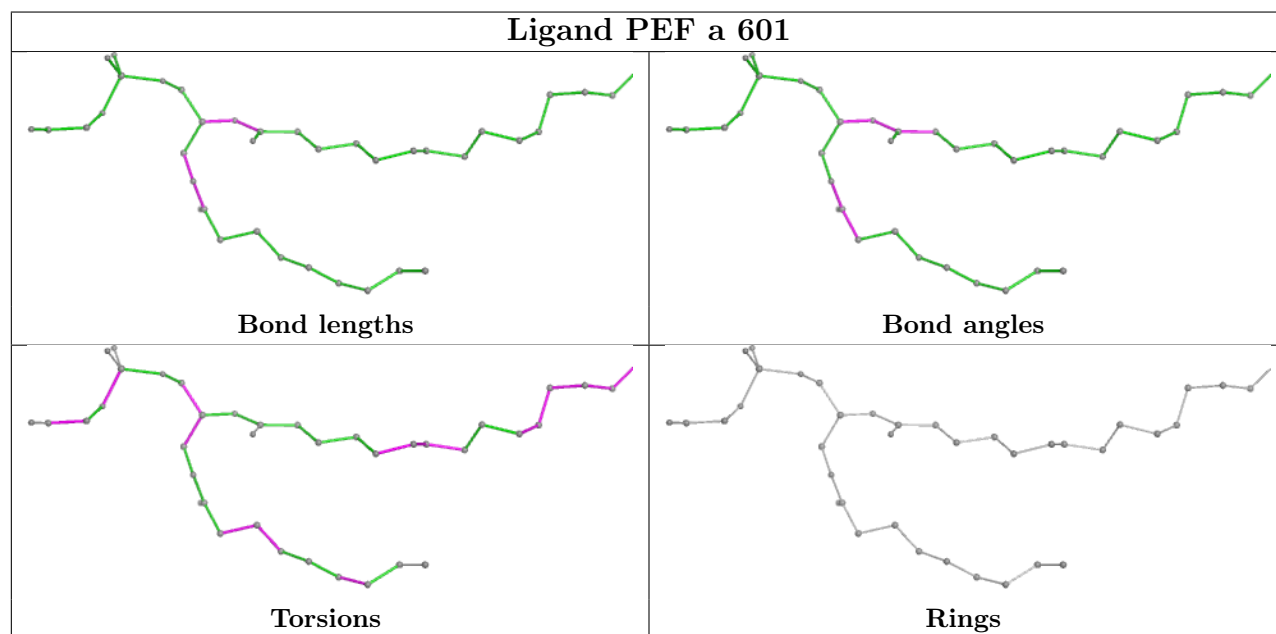
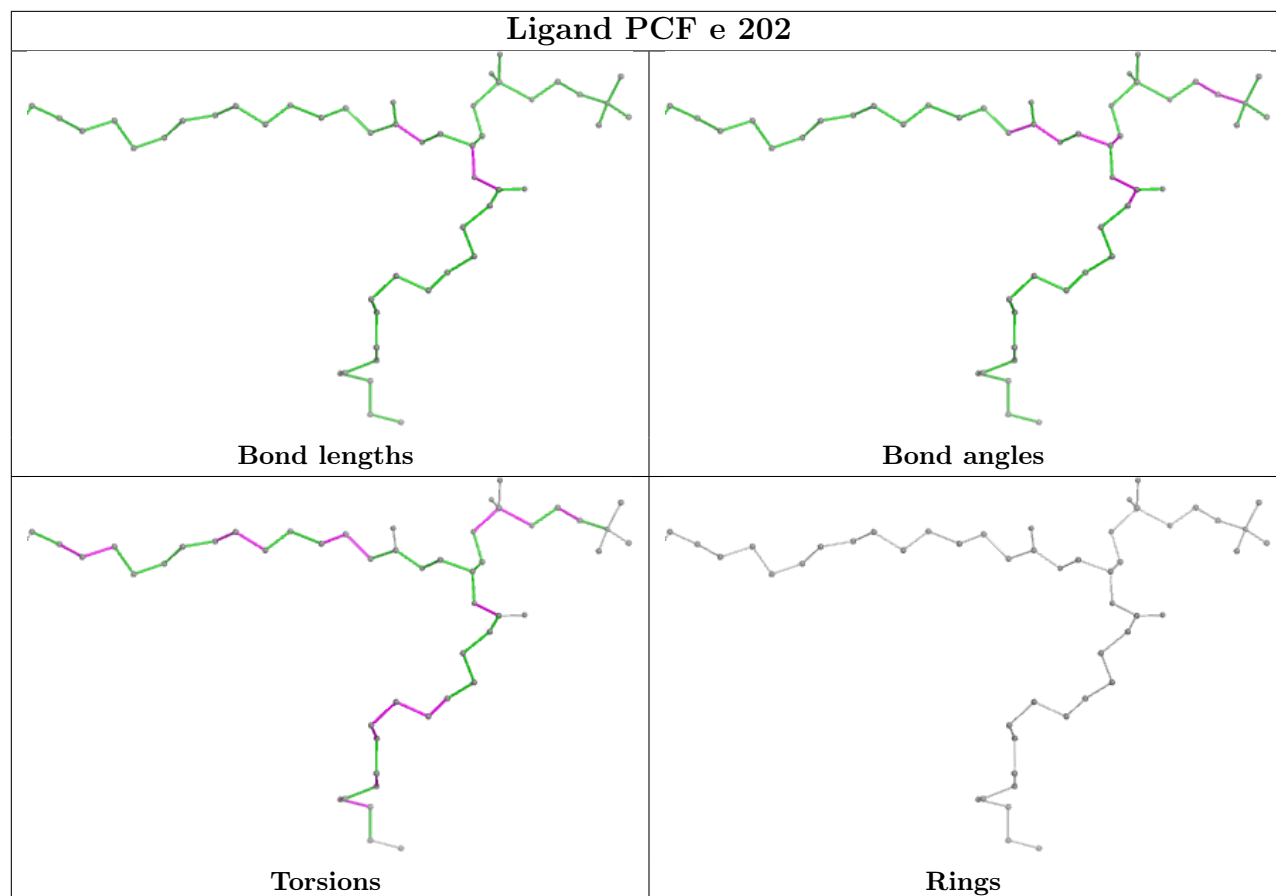


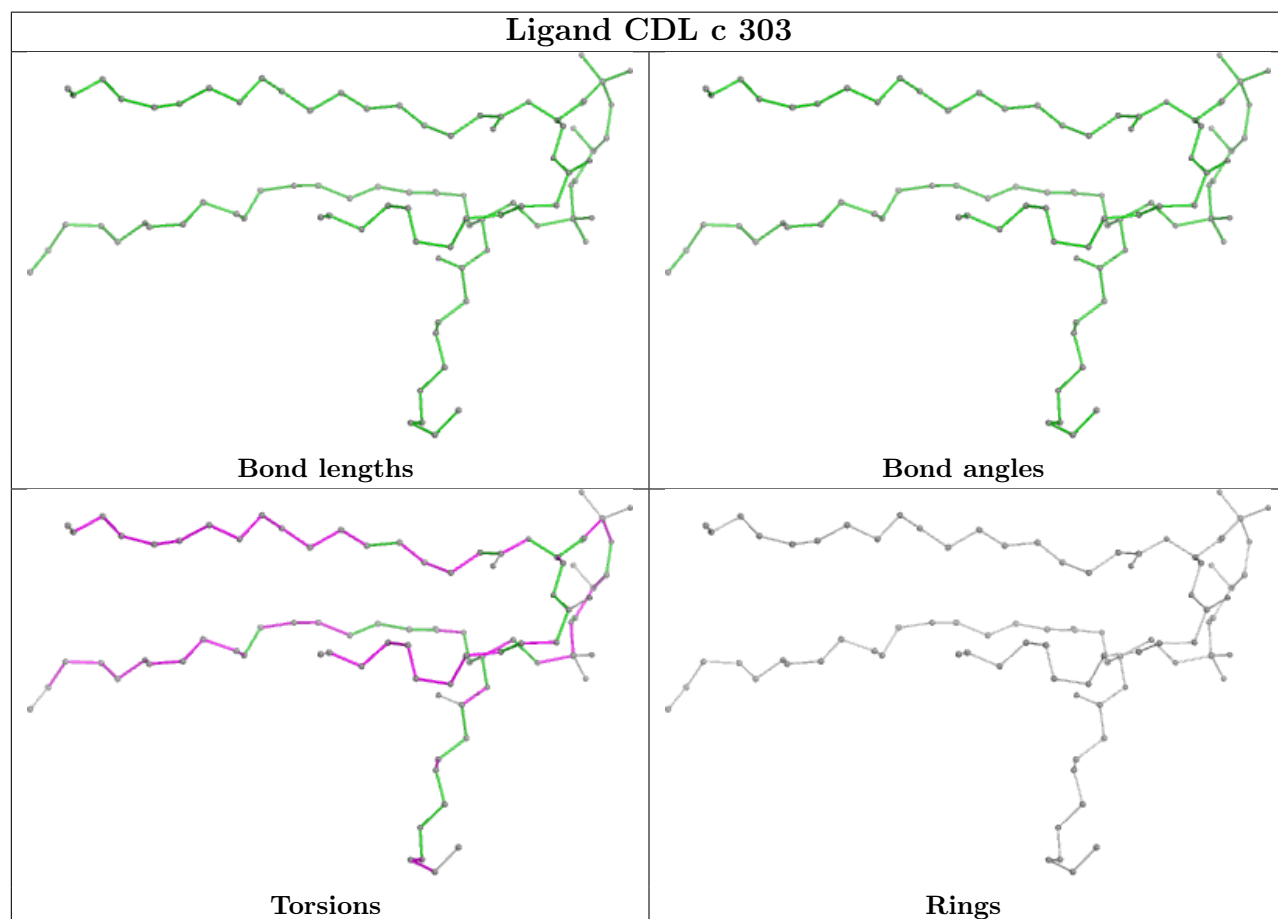
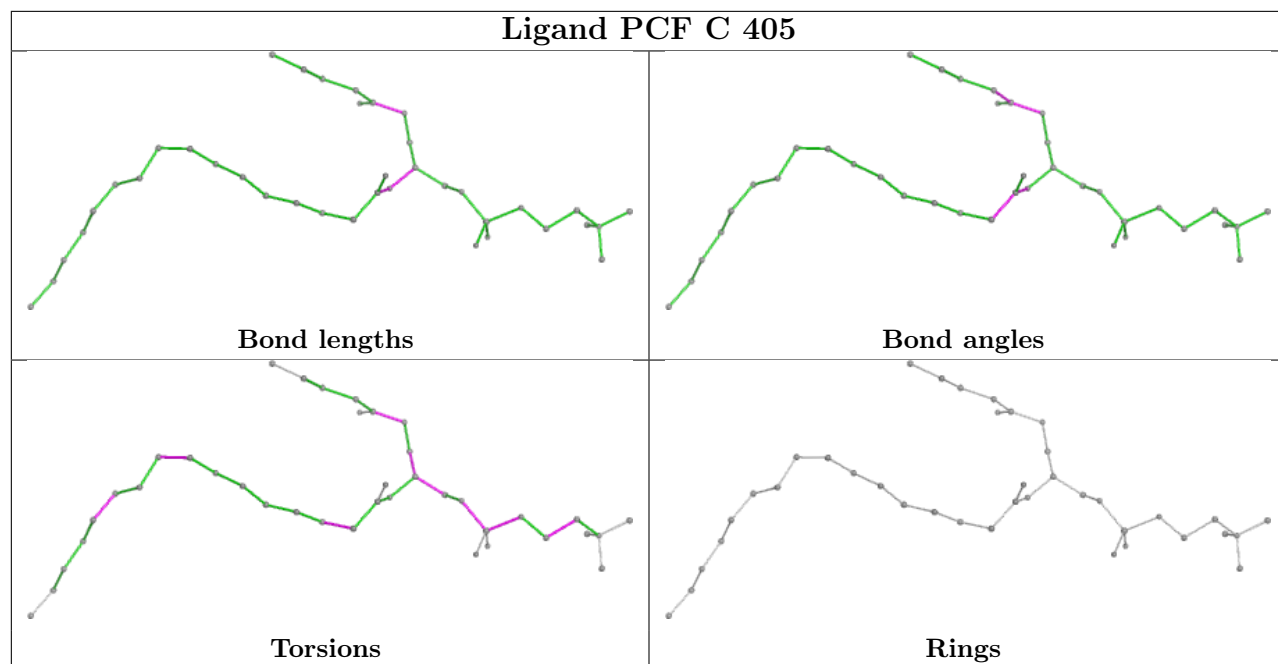


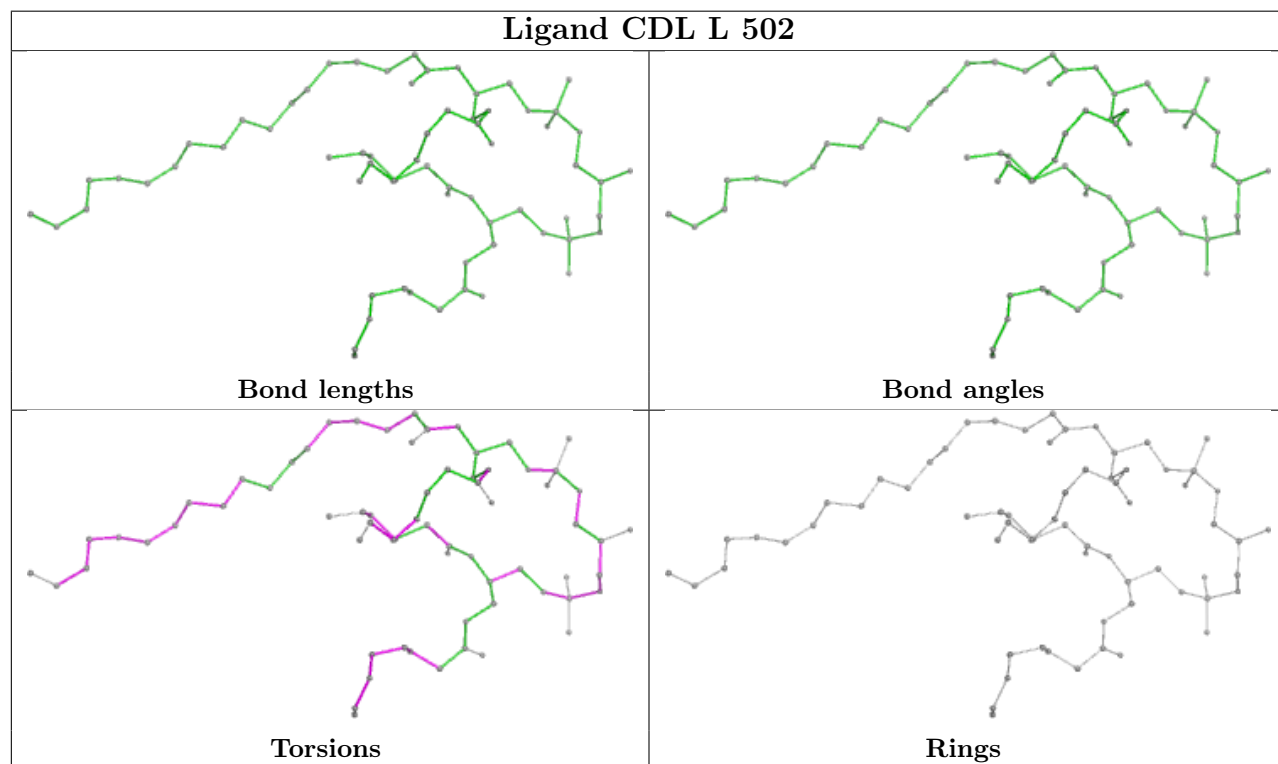
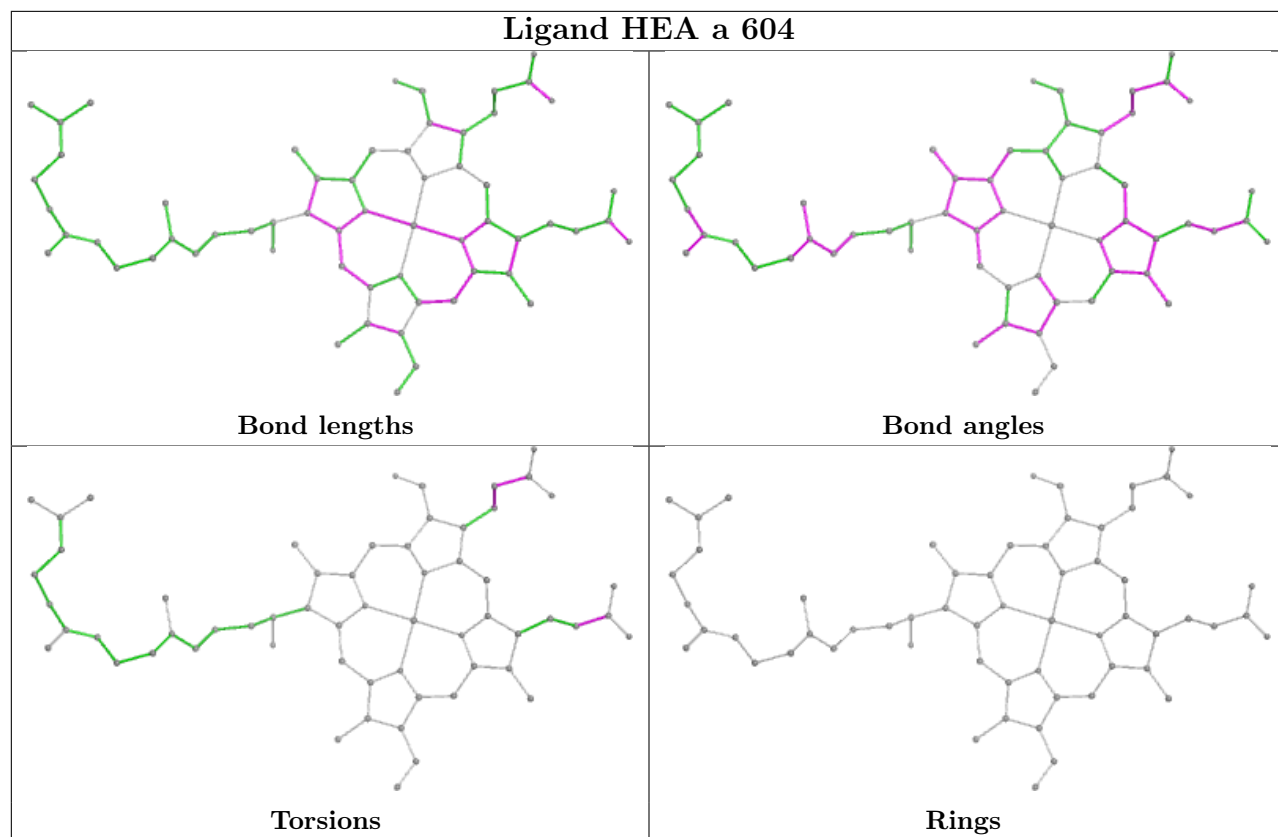


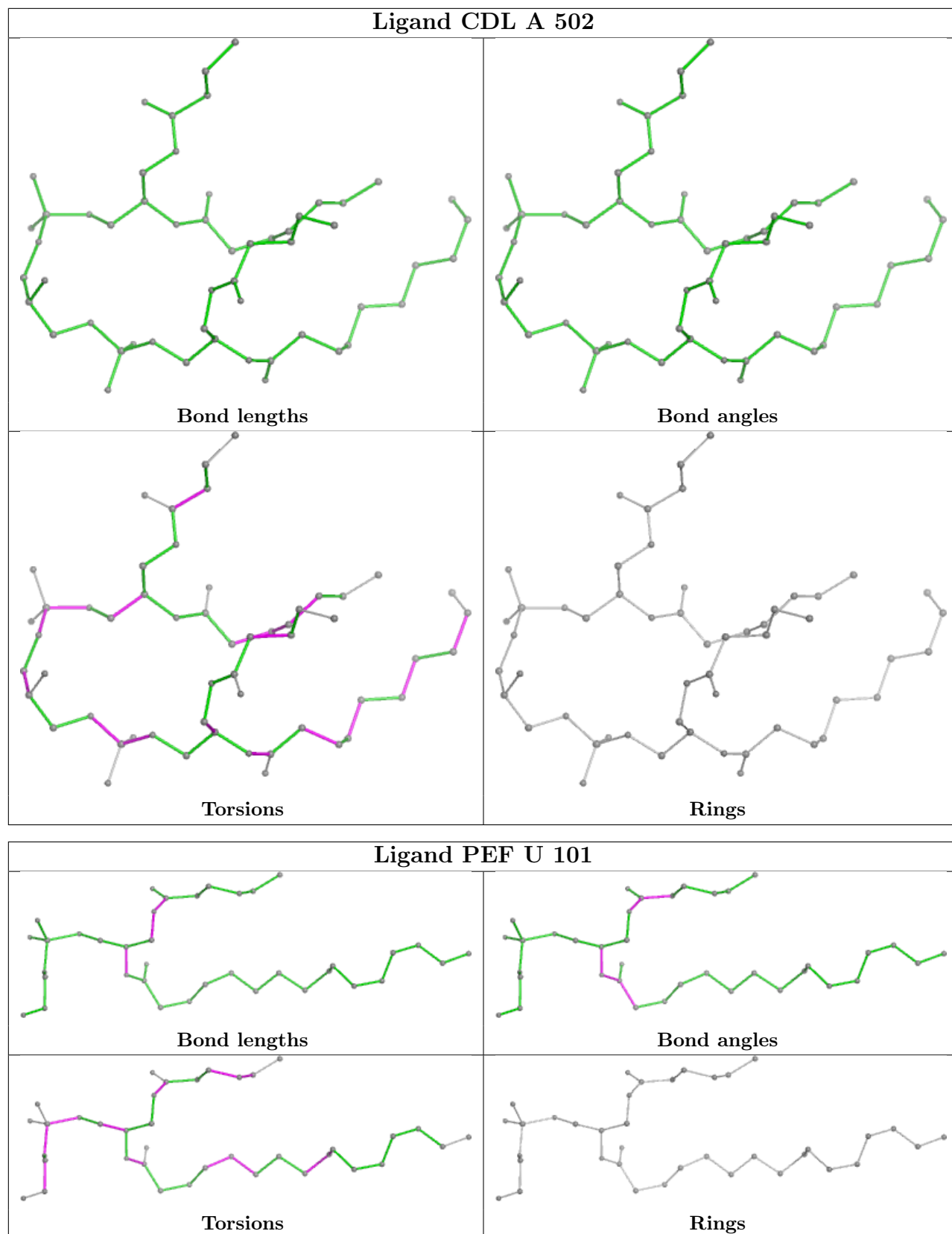


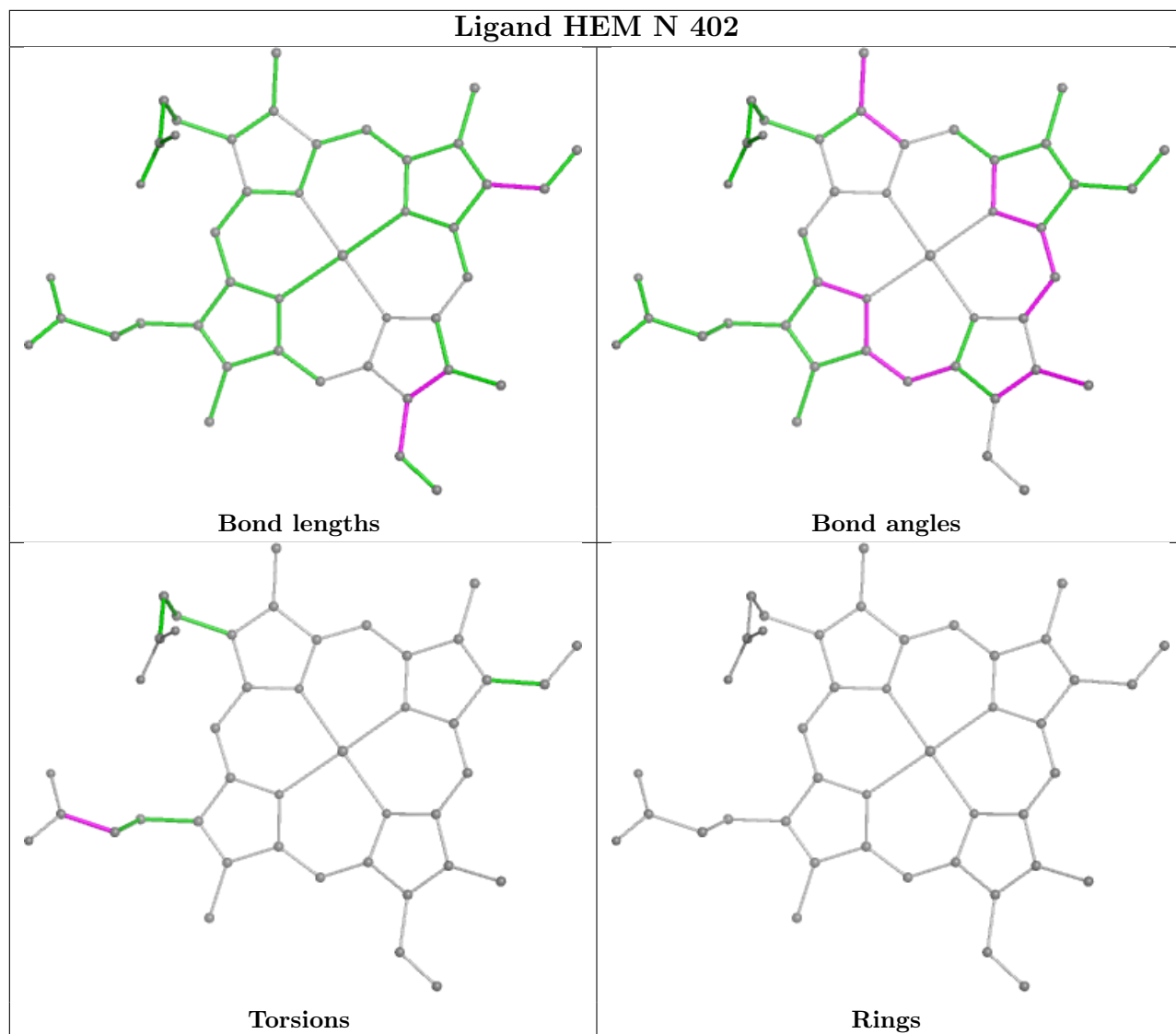




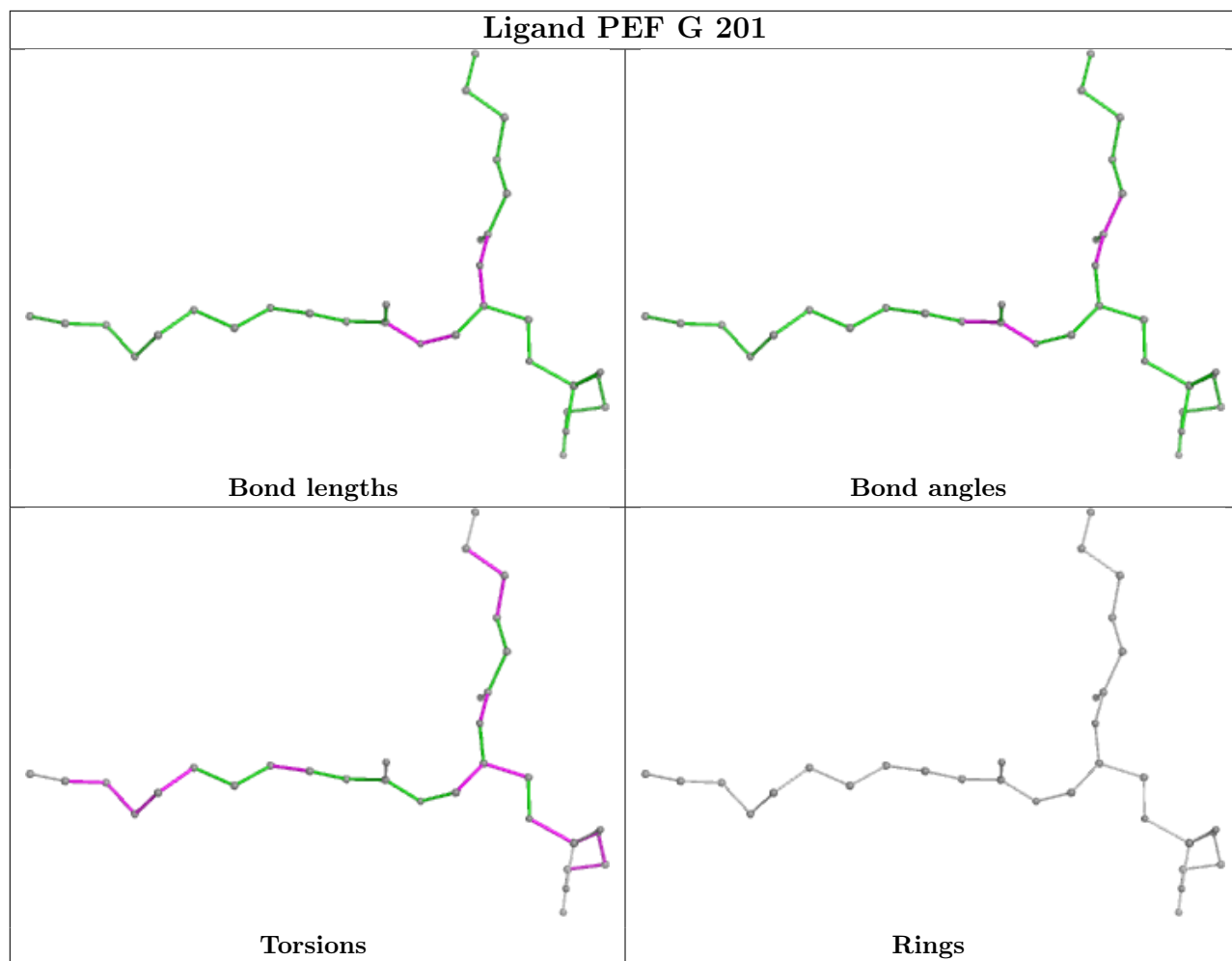


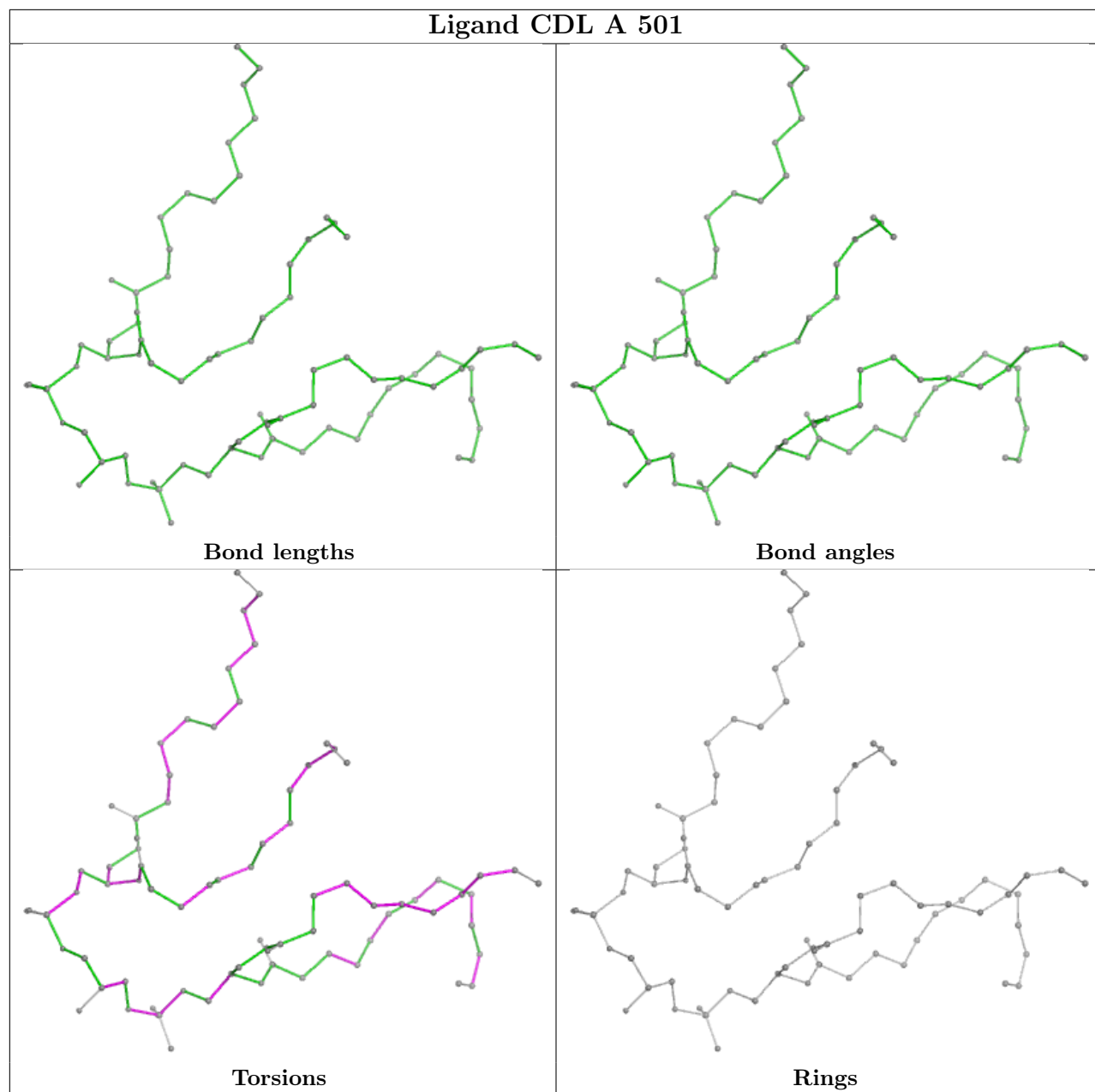


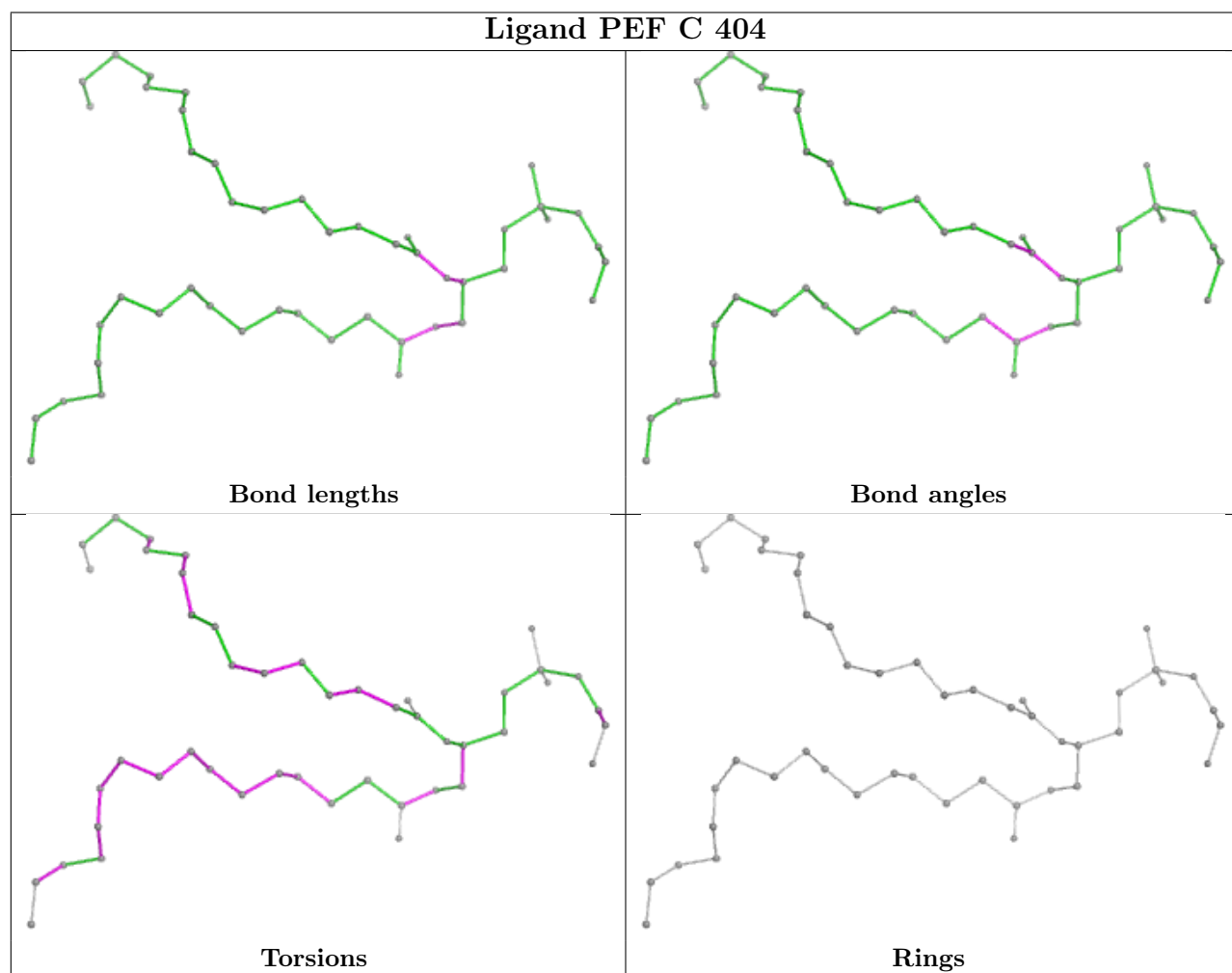
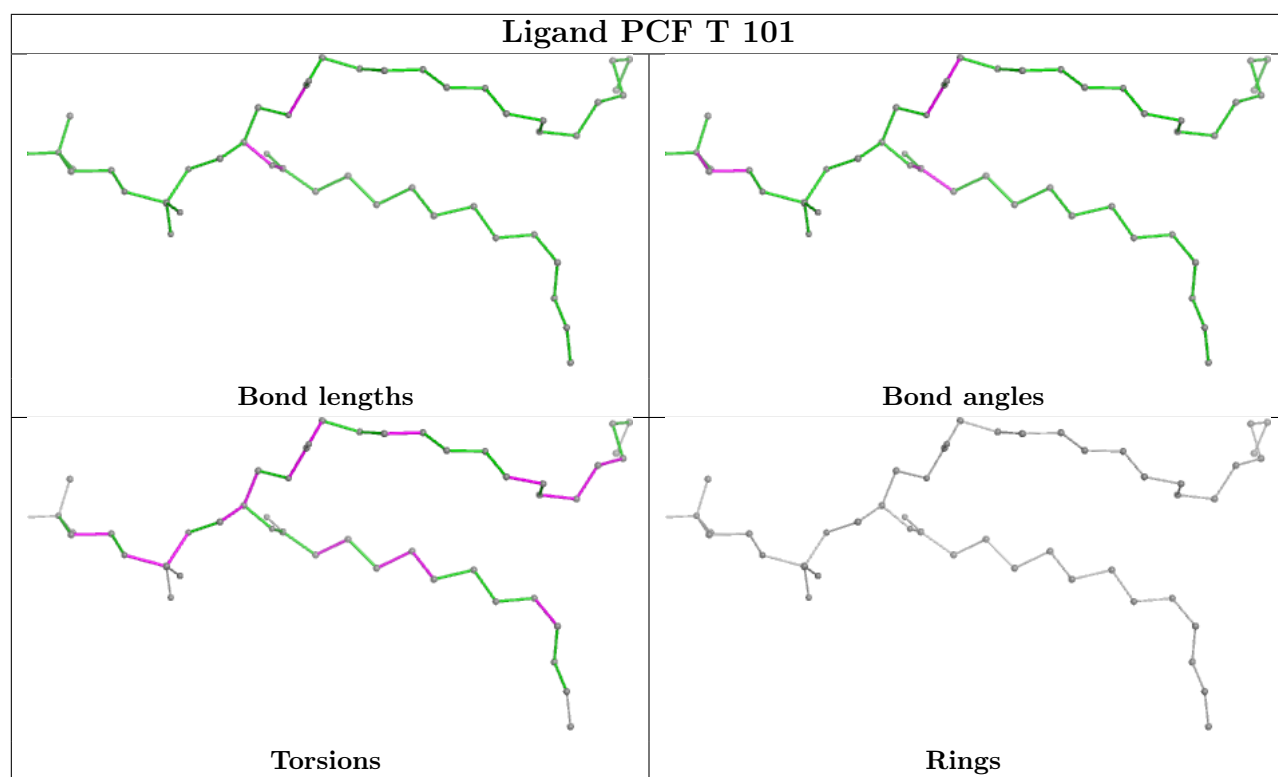


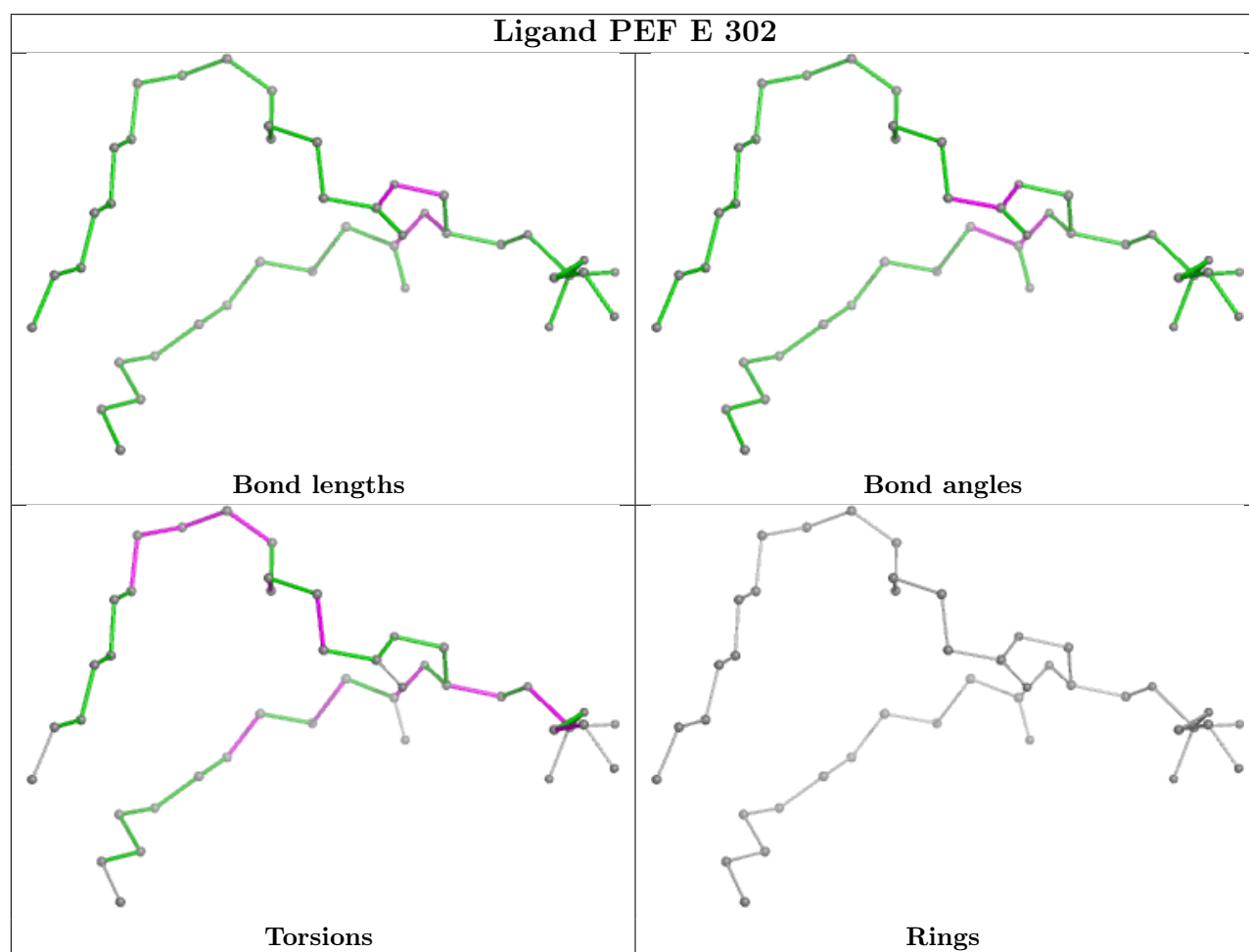
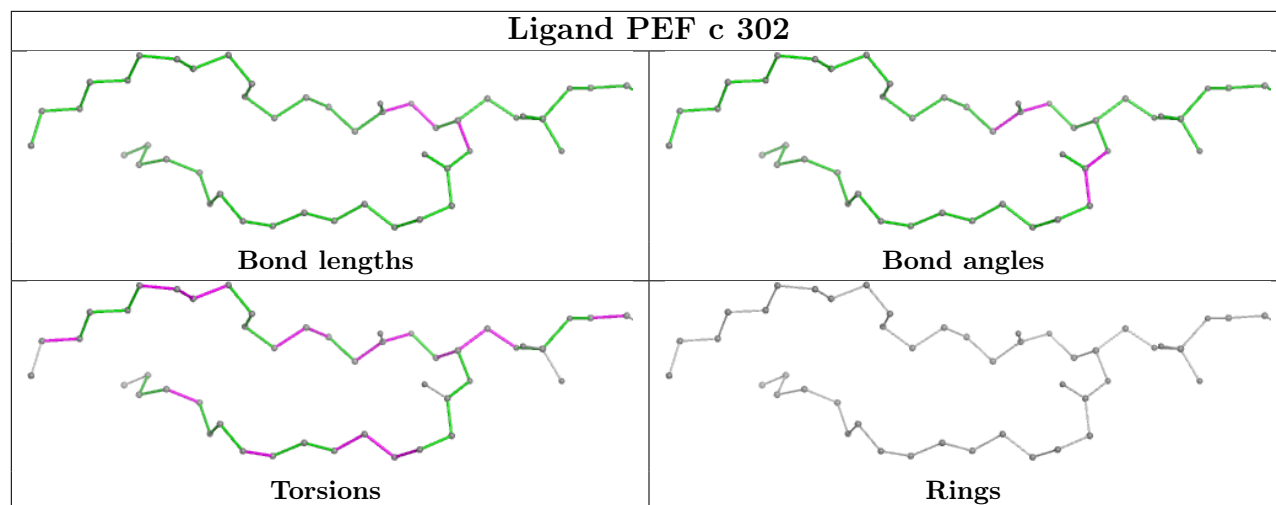


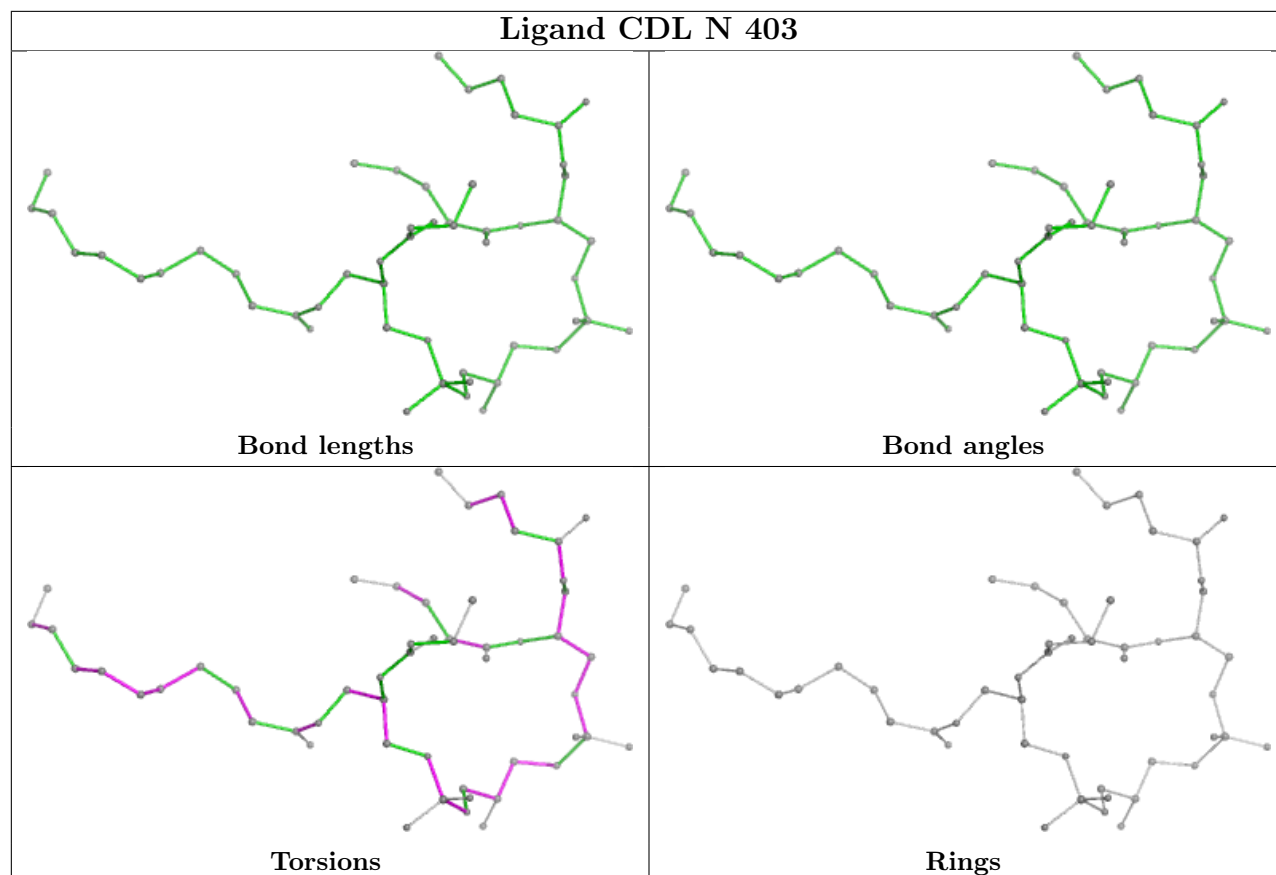


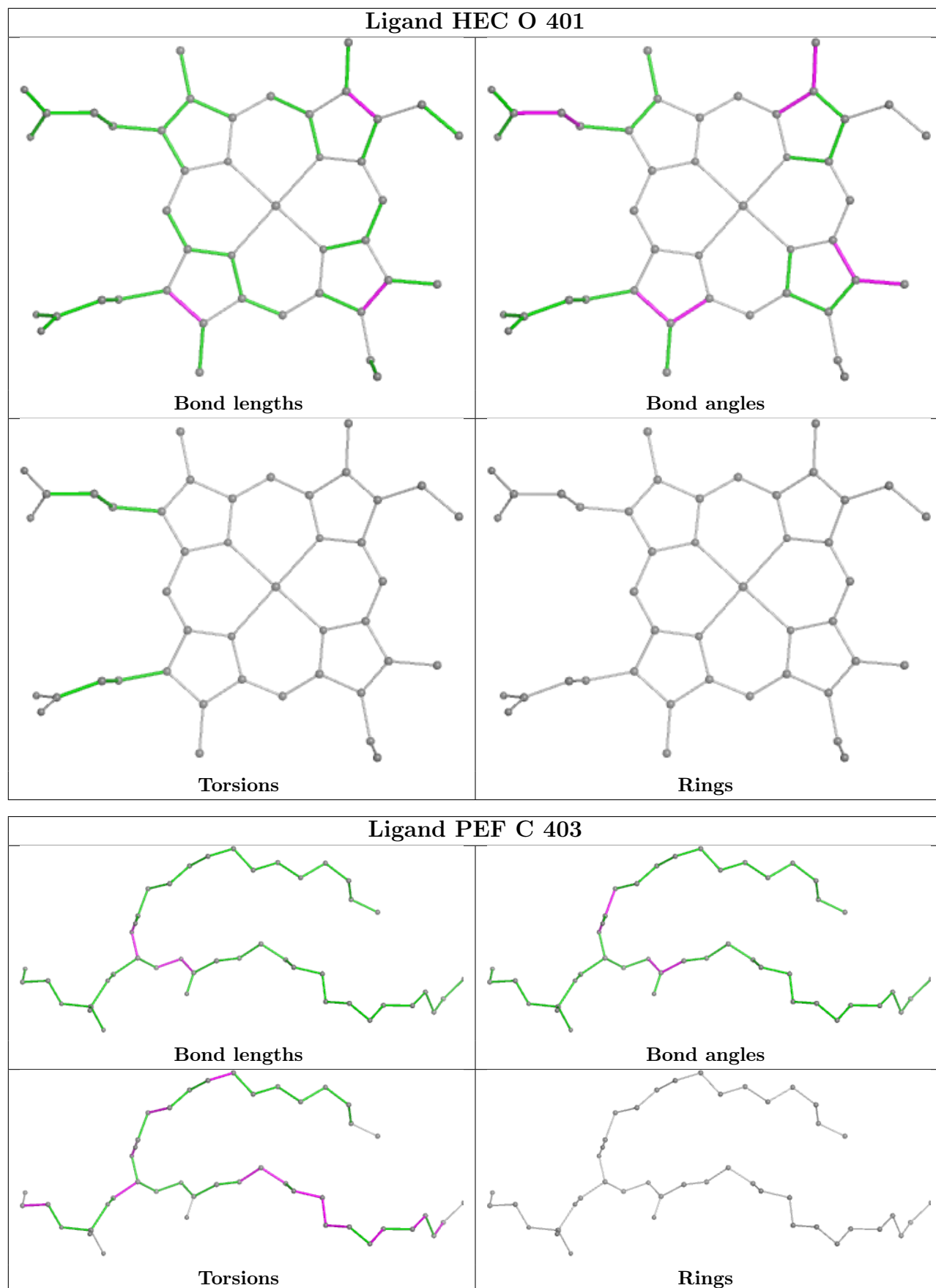


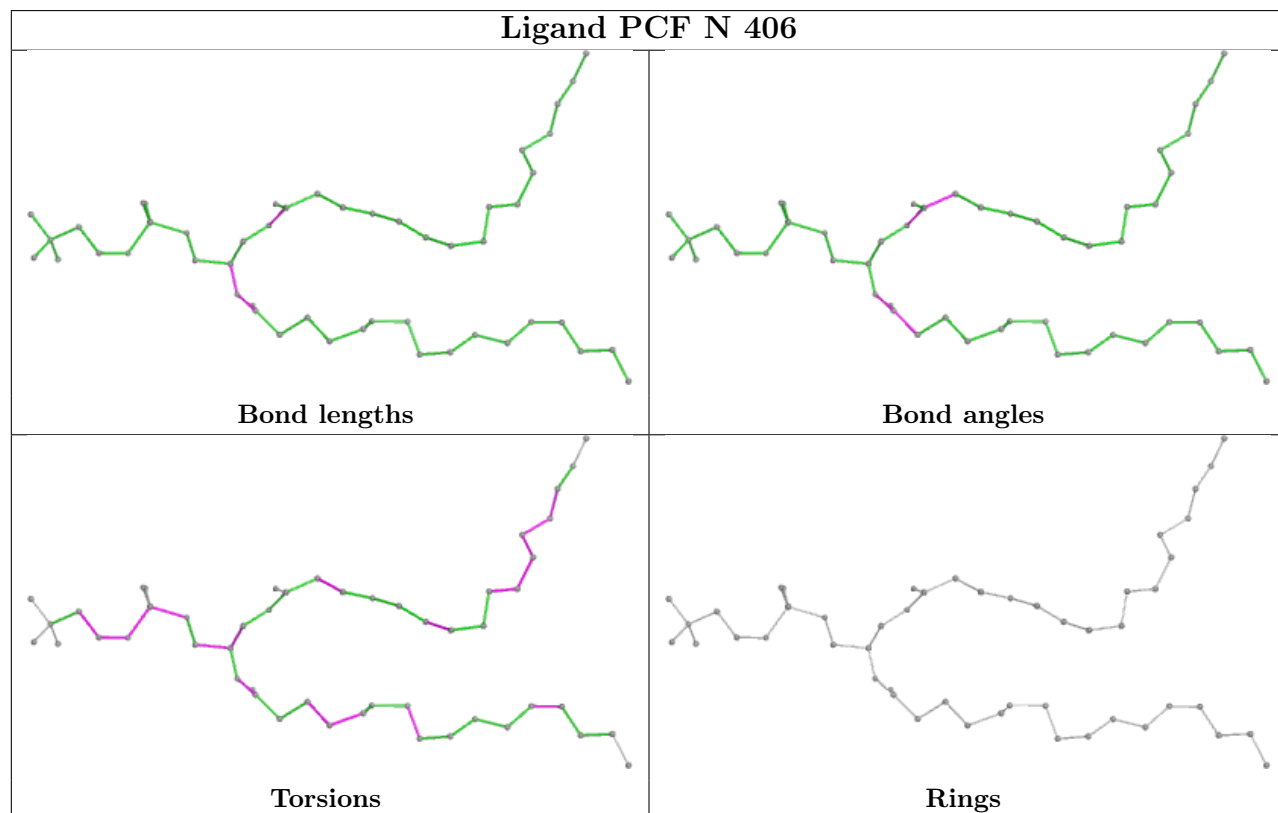
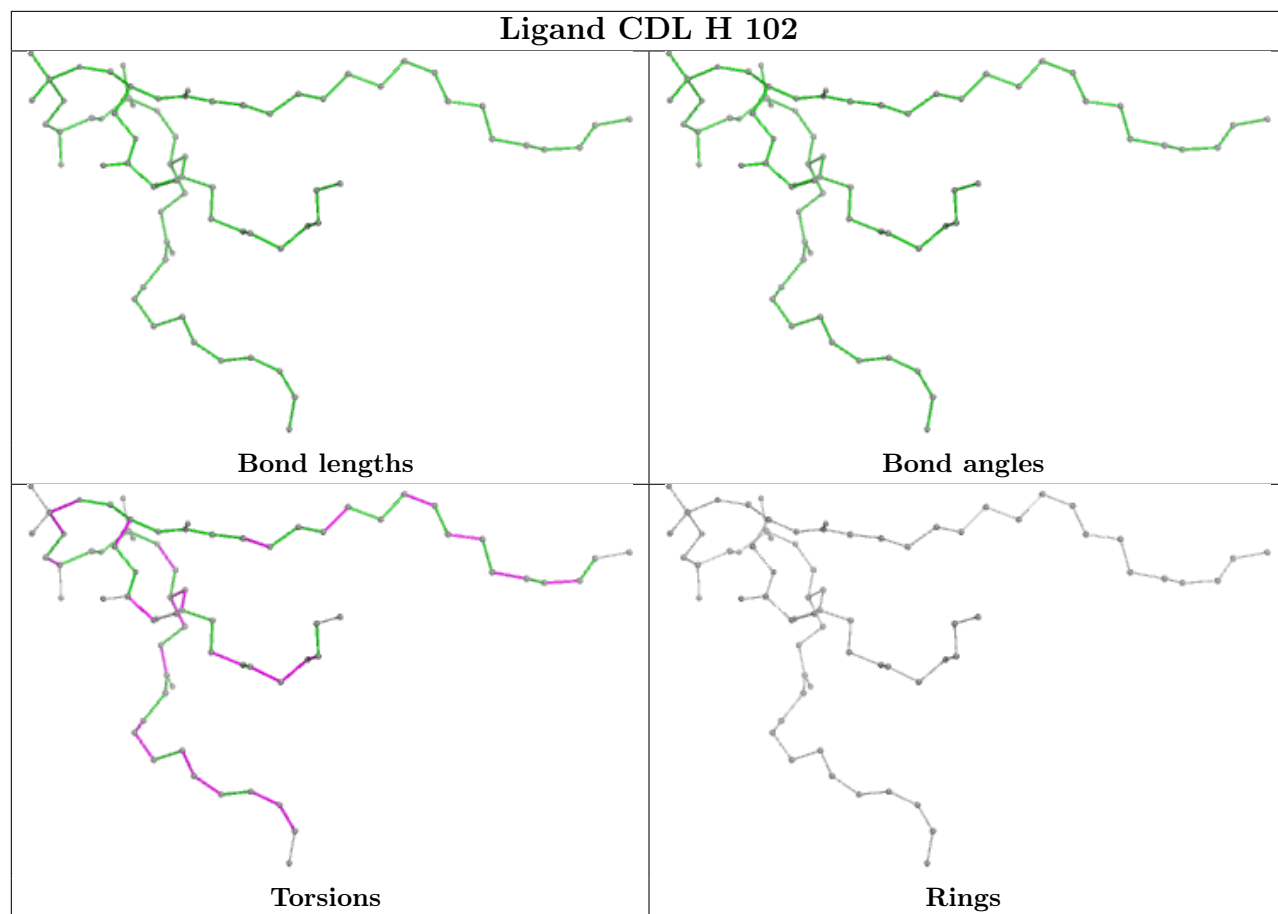


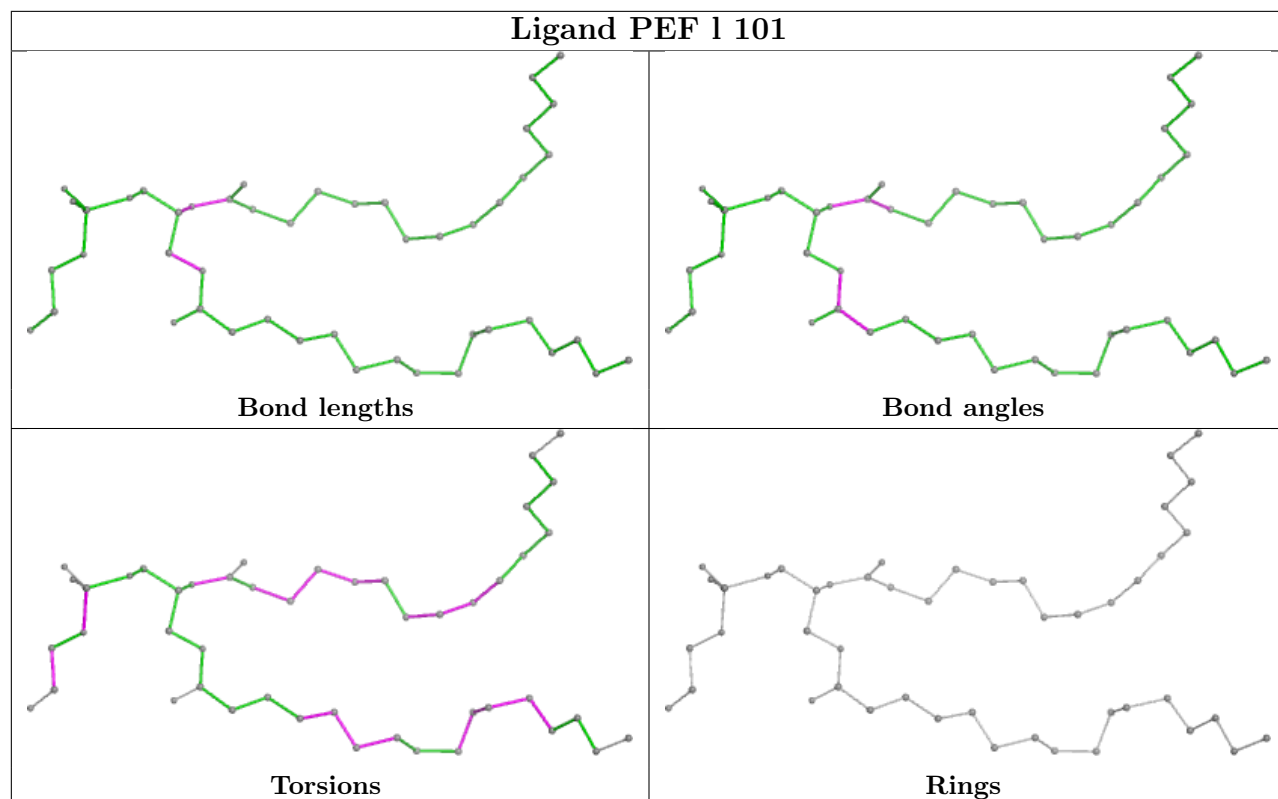




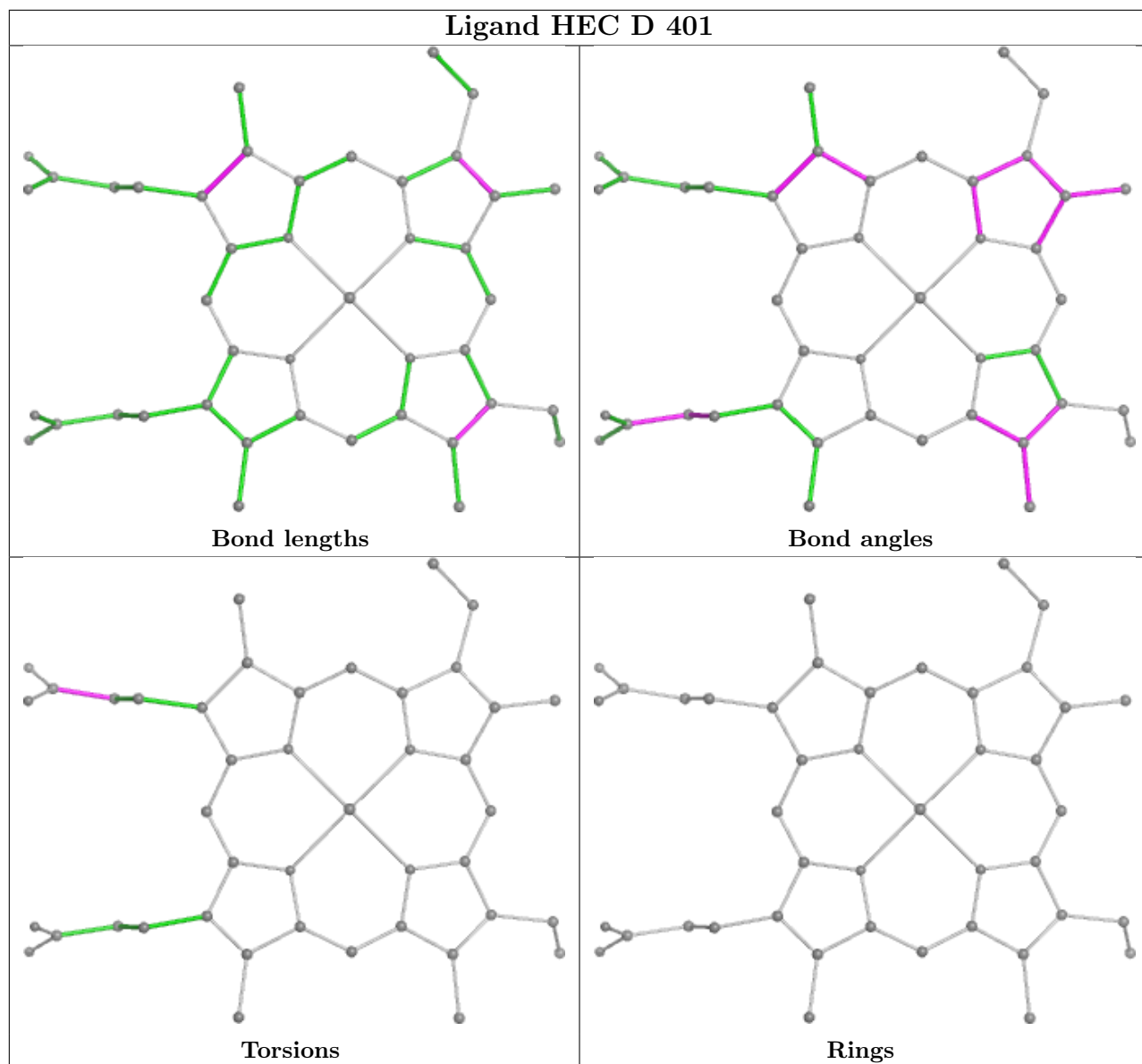


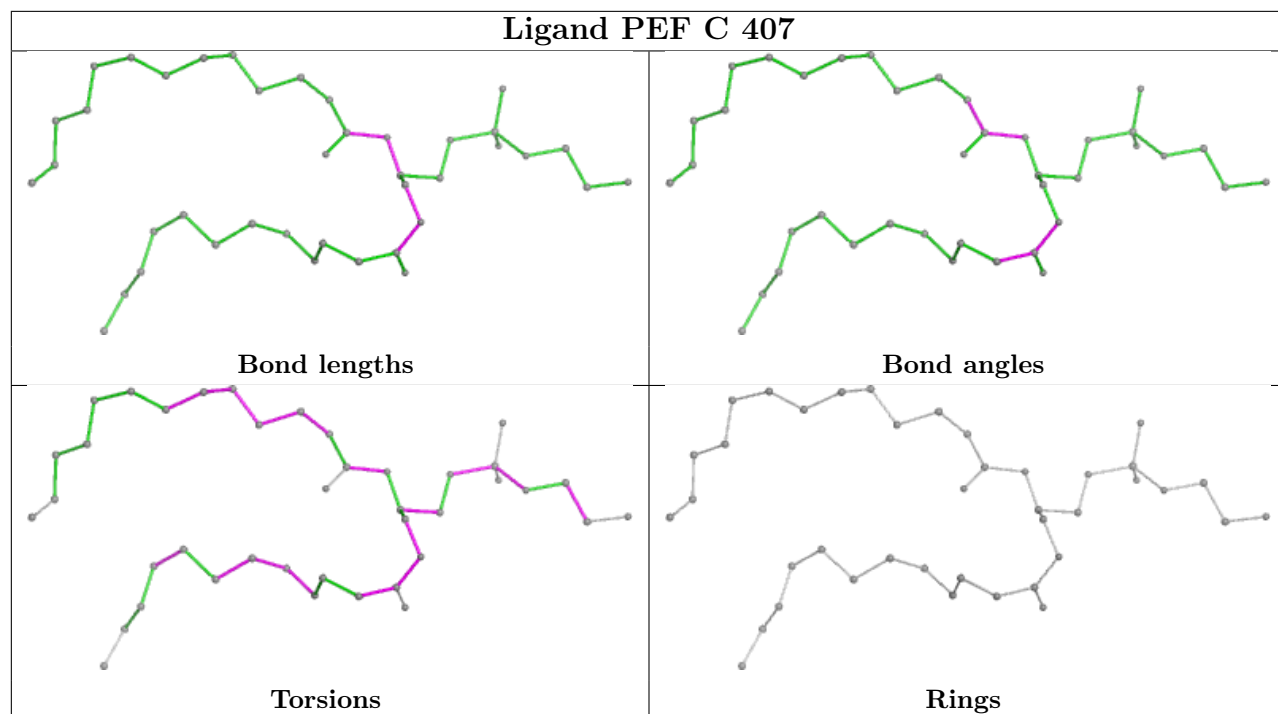


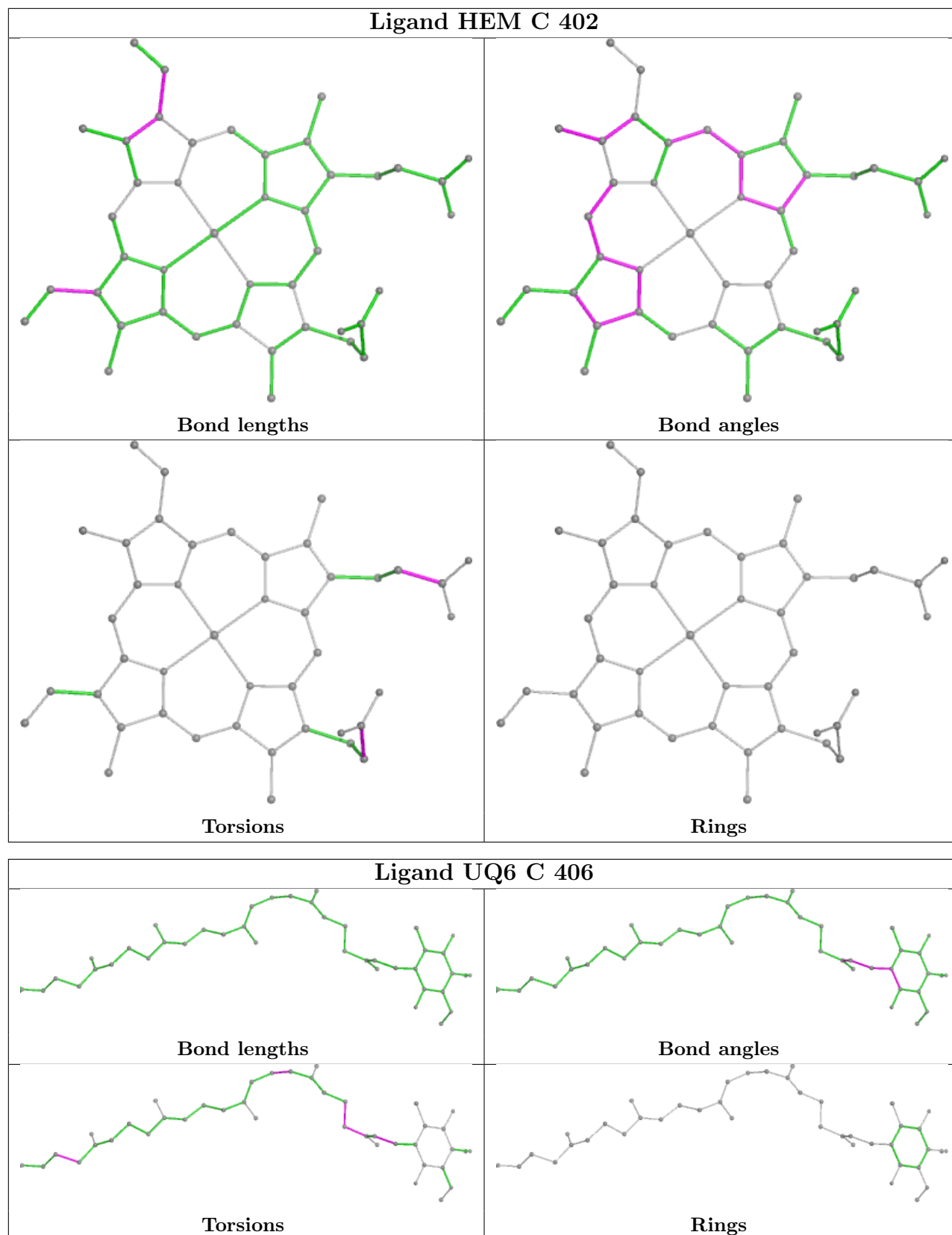


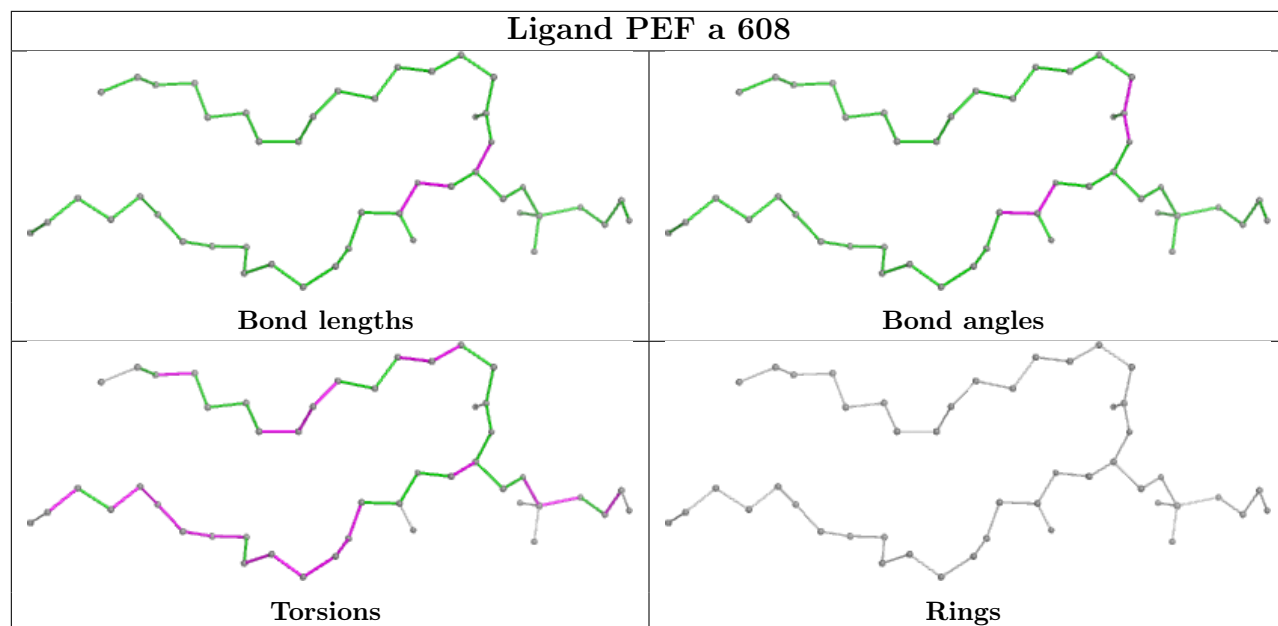


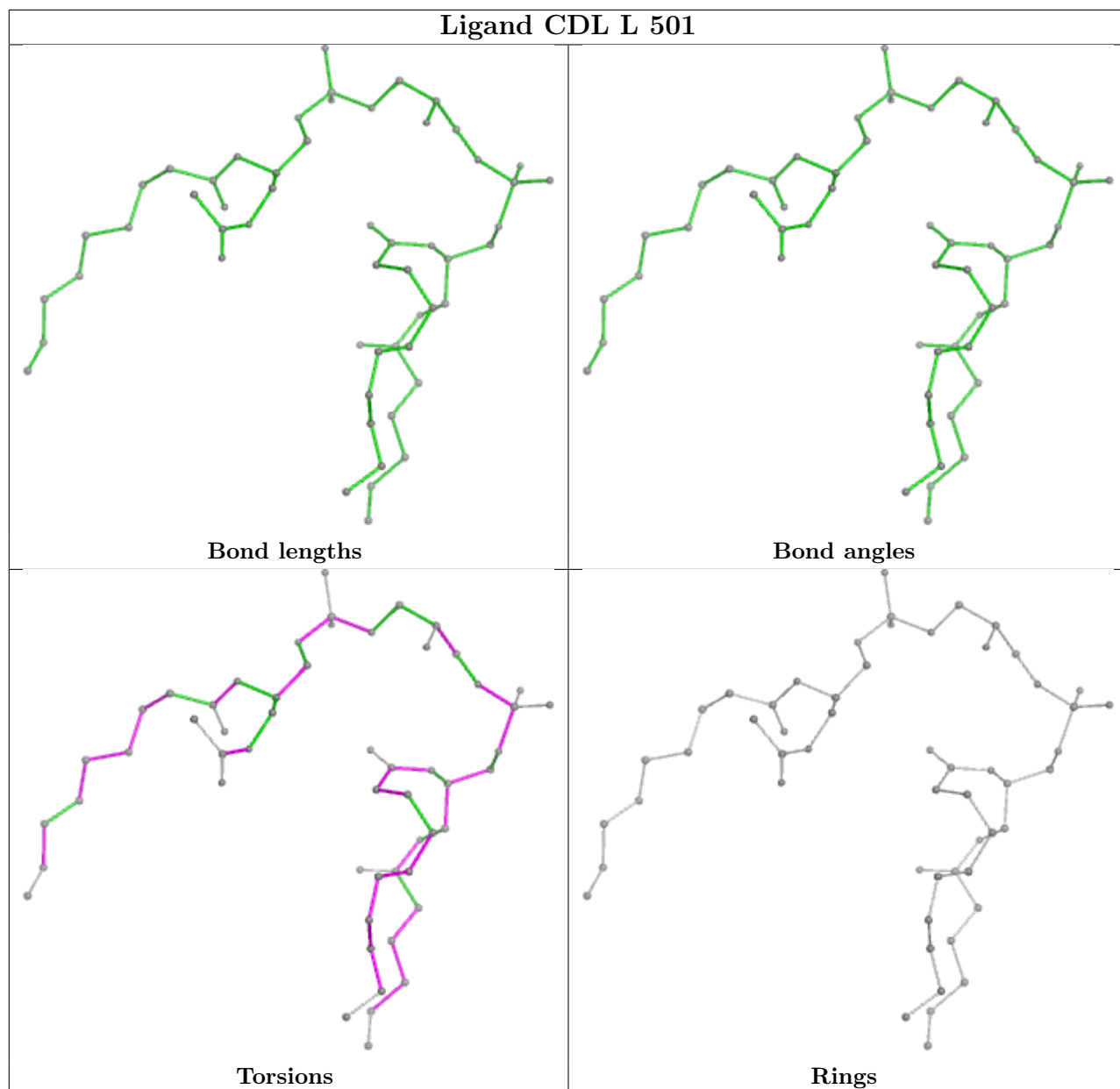


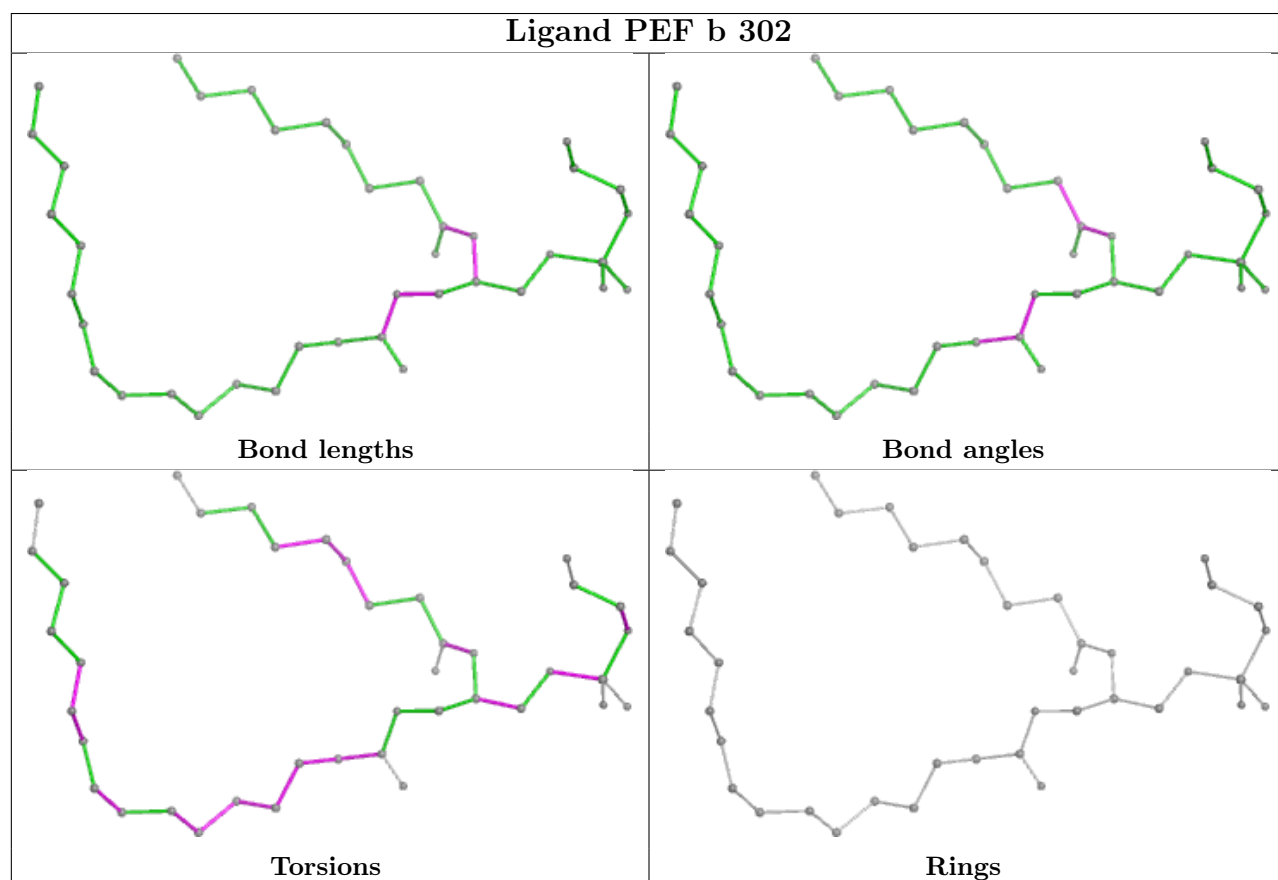
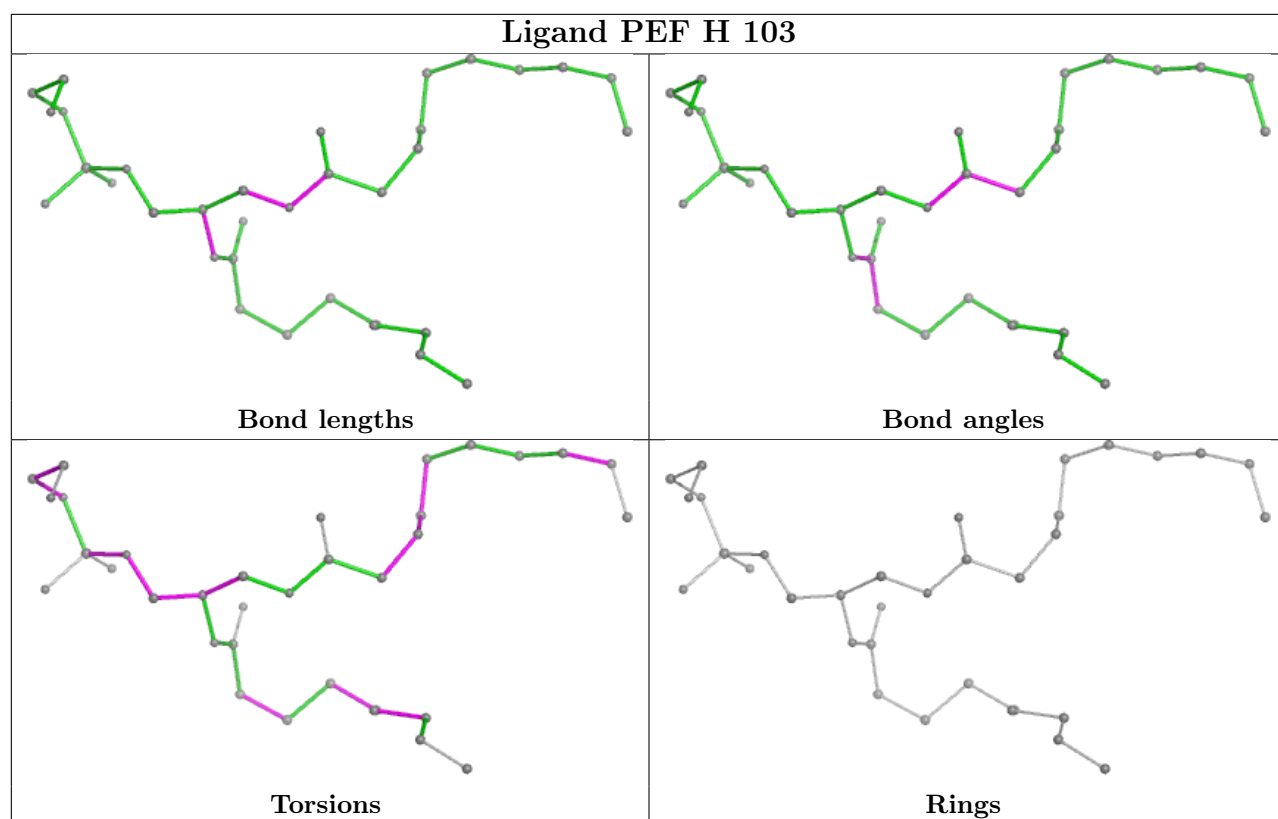


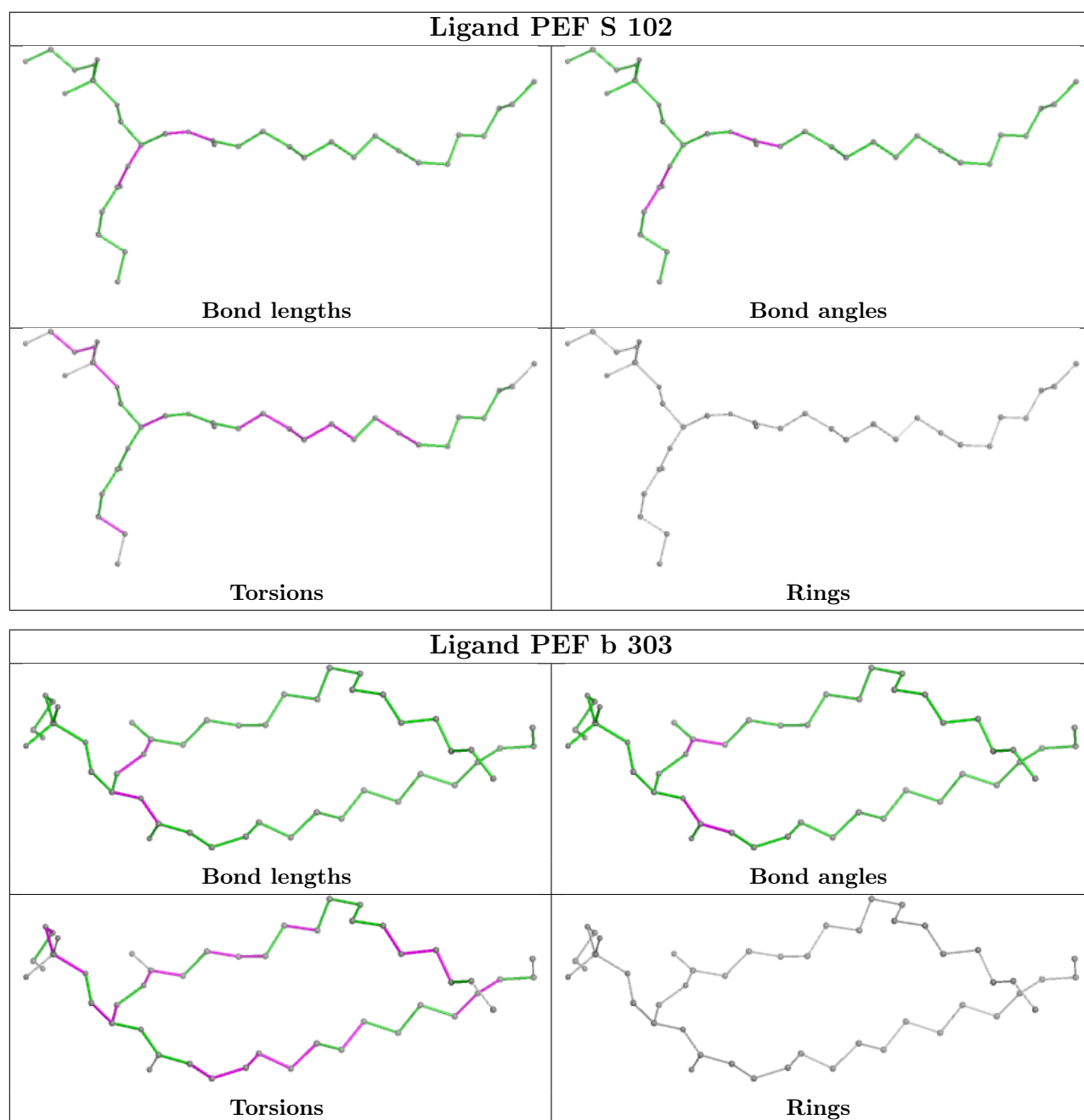


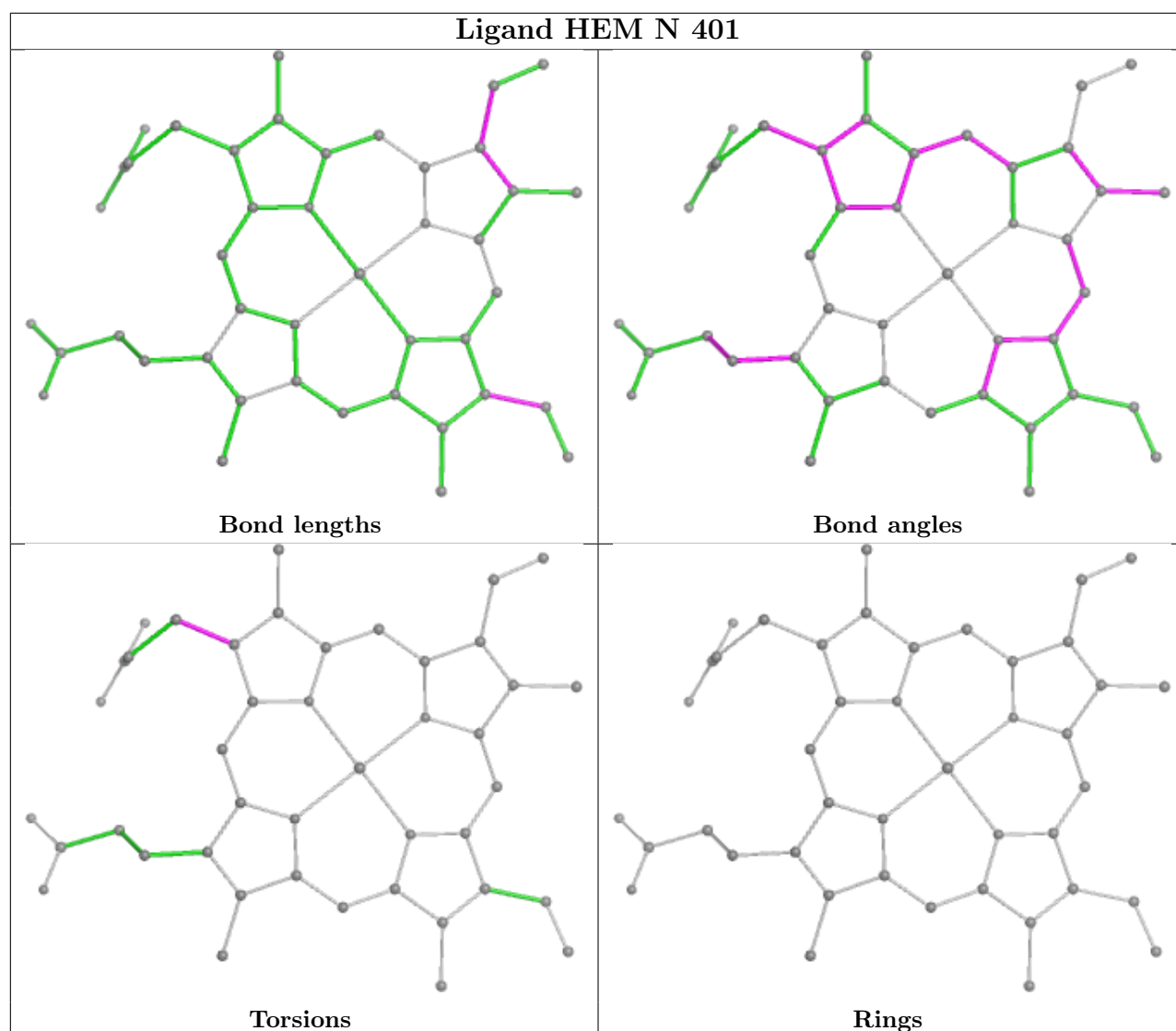
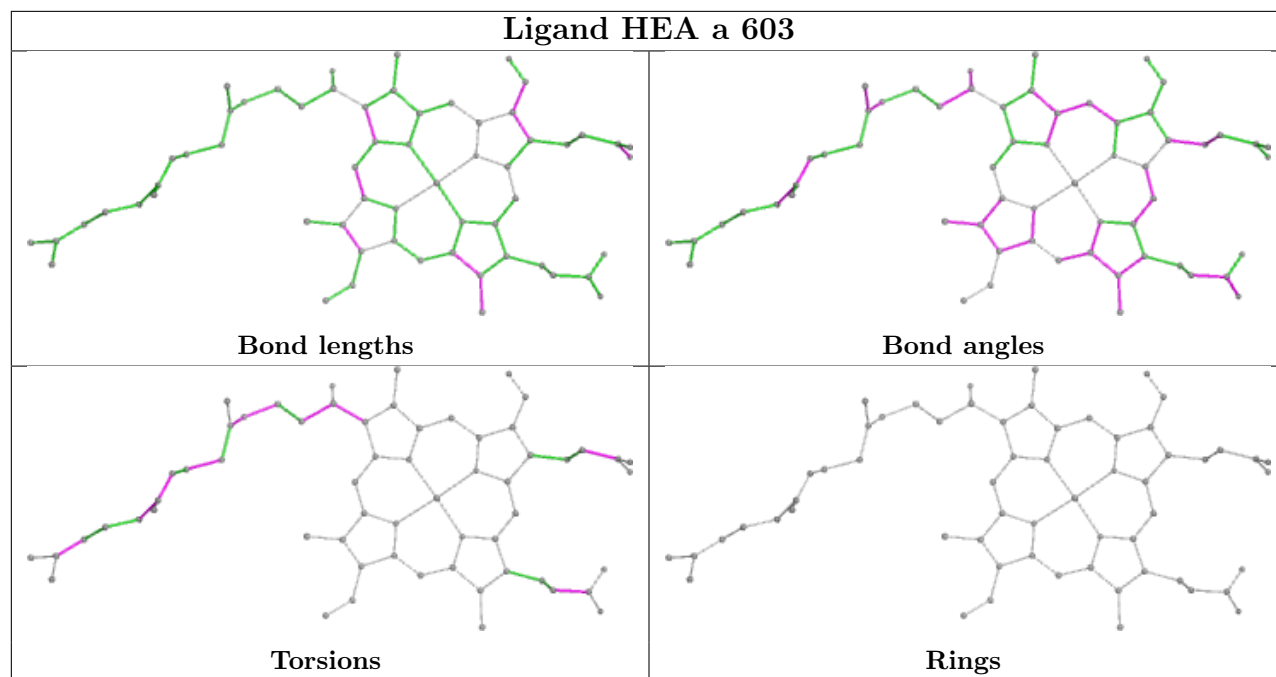














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

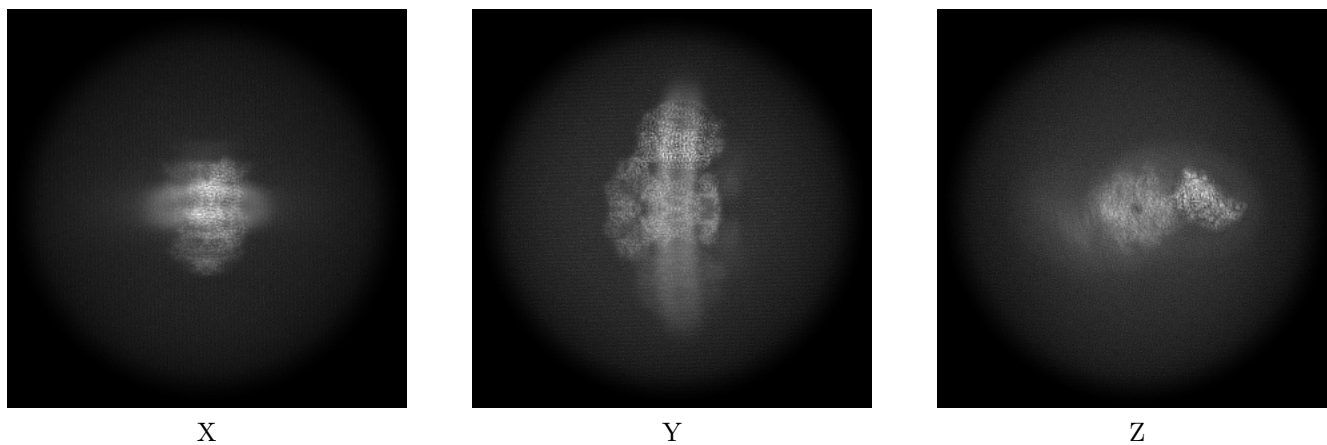
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19963. 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](#)

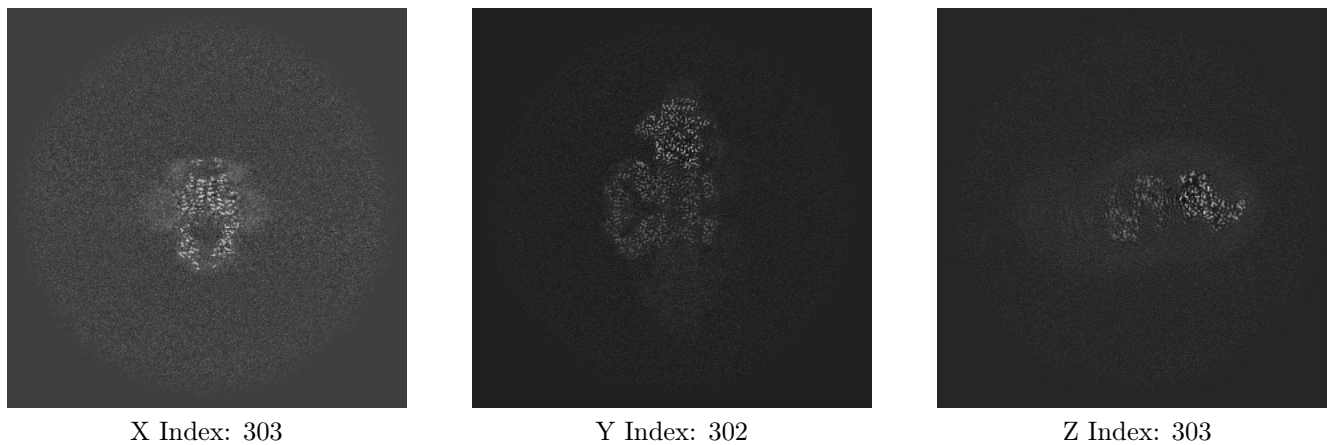
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

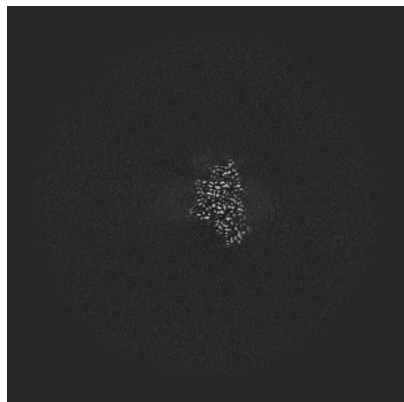
#### 6.2.1 Primary map



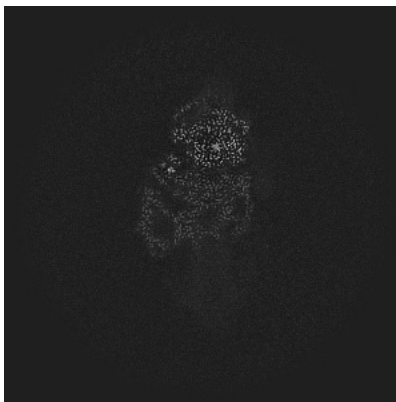
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

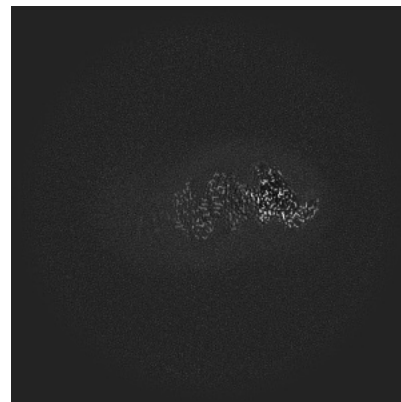
### 6.3.1 Primary map



X Index: 387



Y Index: 313

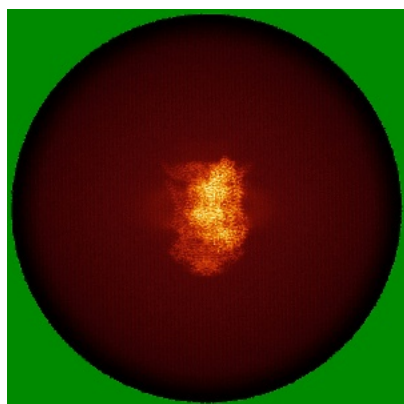


Z Index: 294

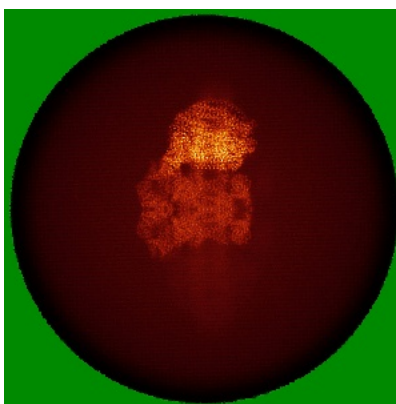
The images above show the largest variance slices of the map in three orthogonal directions.

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

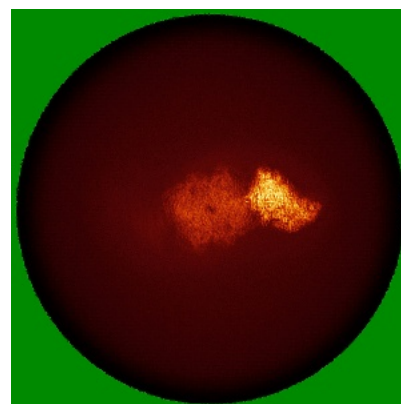
### 6.4.1 Primary map



X



Y

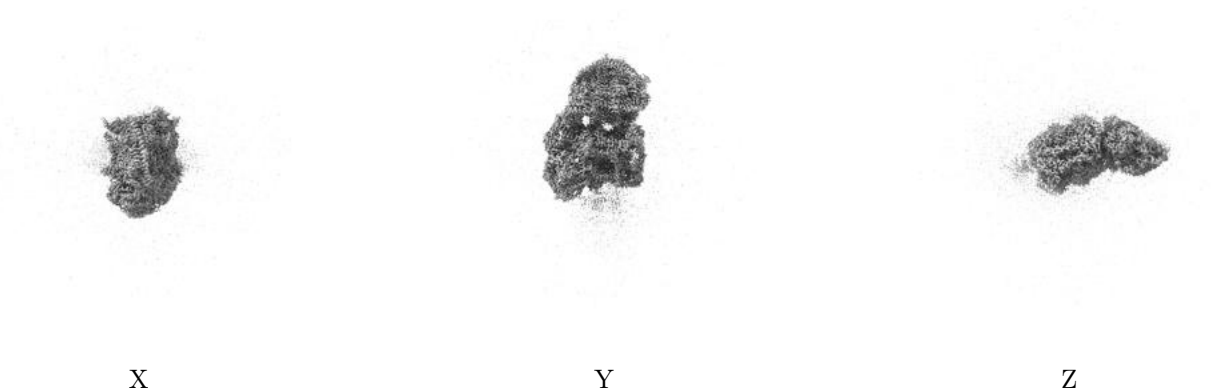


Z

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

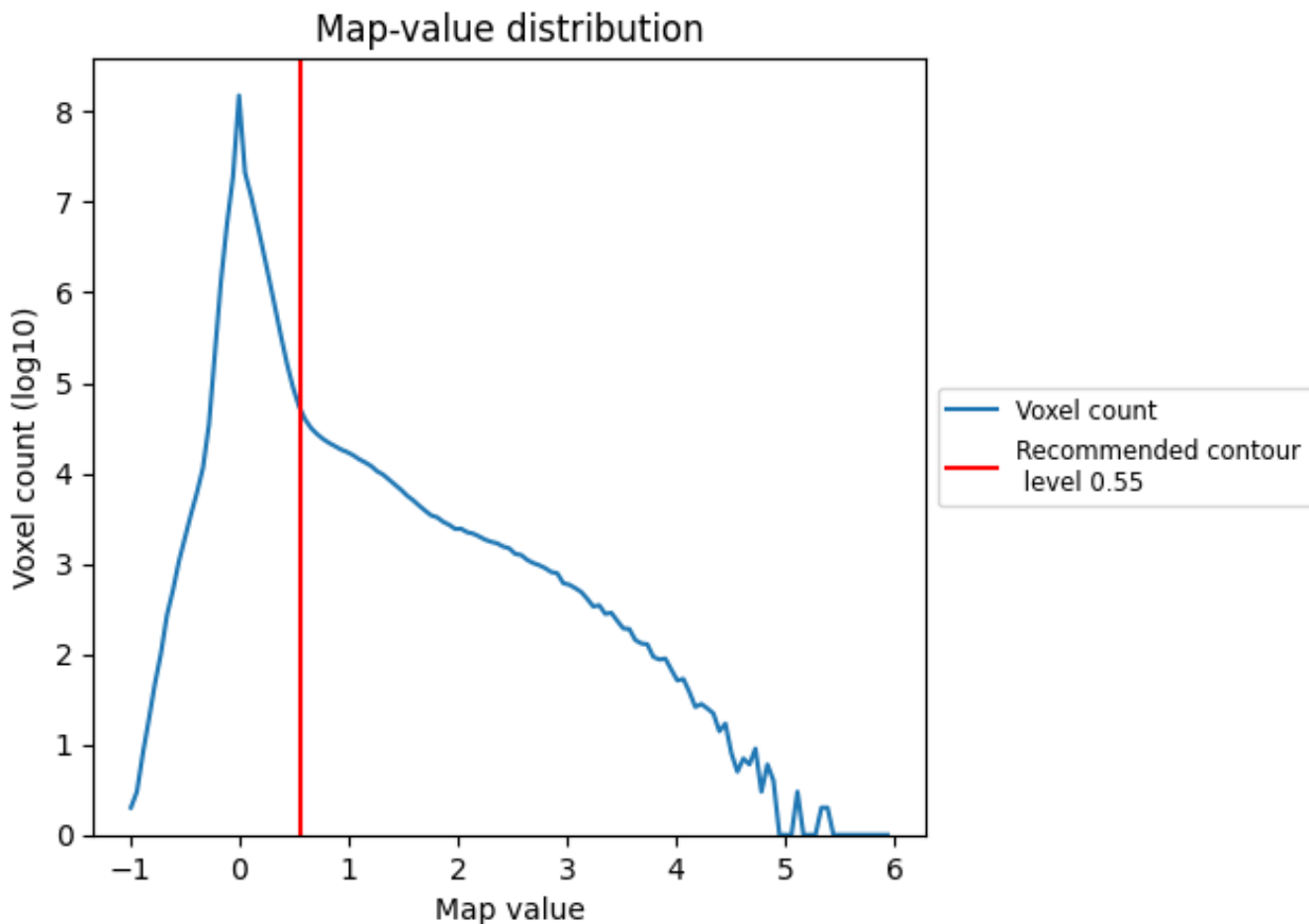
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

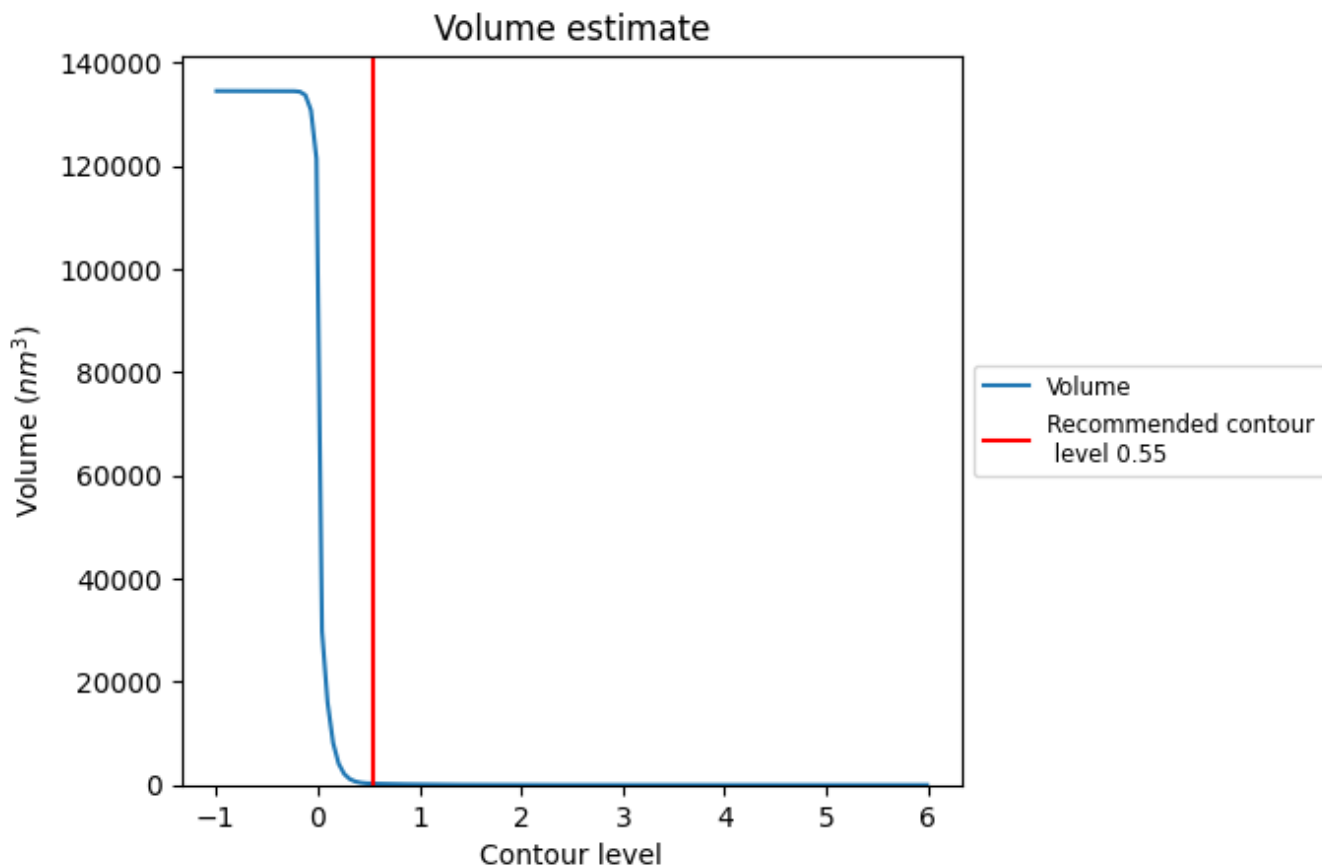
This section contains the results of statistical analysis of the map.

### 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 251 nm<sup>3</sup>; this corresponds to an approximate mass of 227 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.

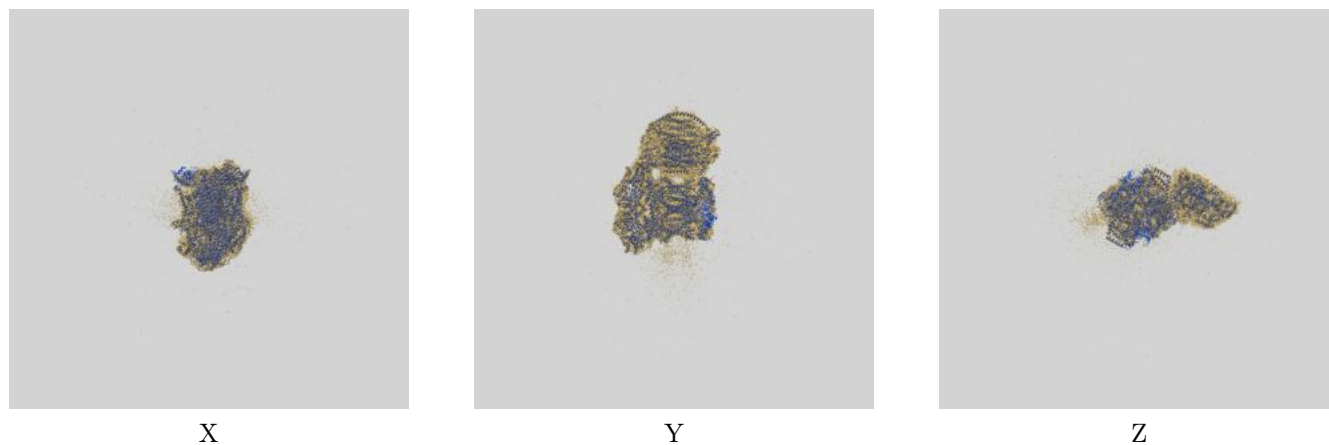
## 8 Fourier-Shell correlation

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-19963 and PDB model 9ETZ. Per-residue inclusion information can be found in section 3 on page 16.

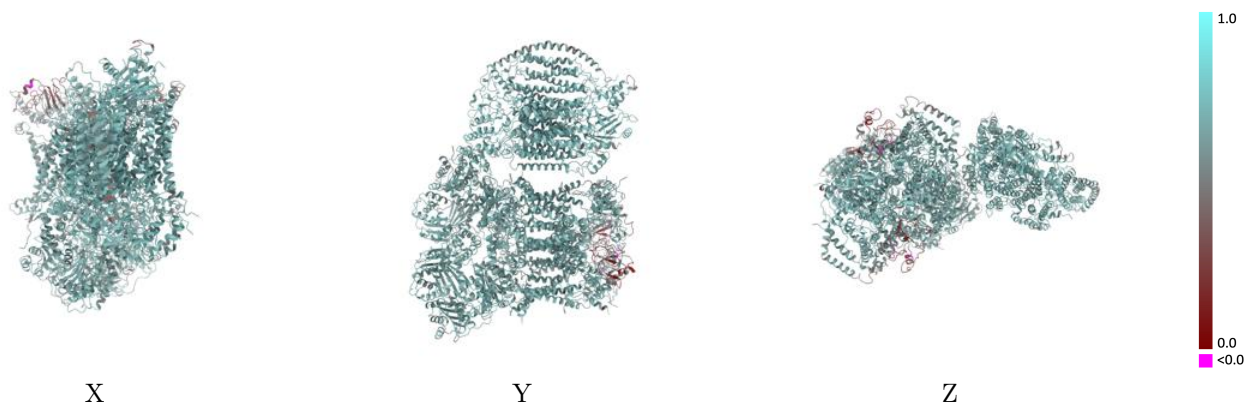
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

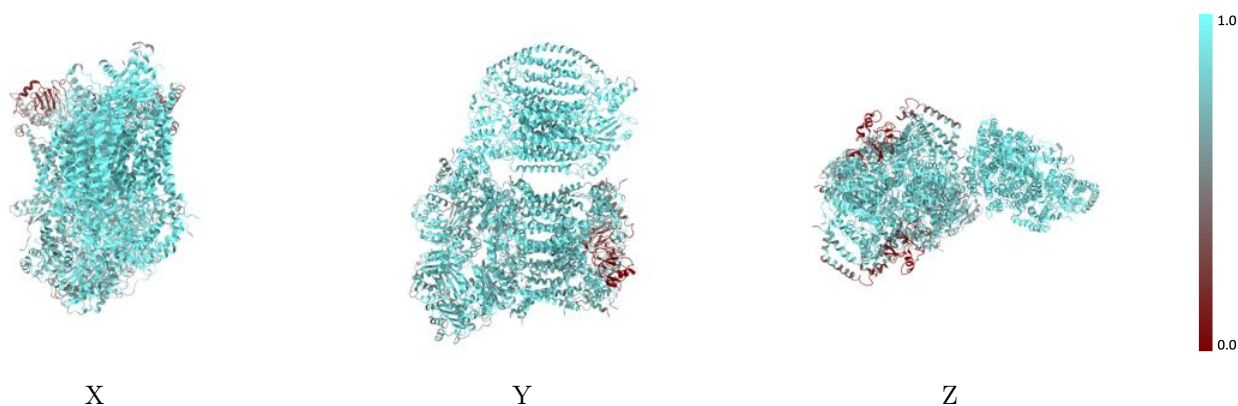


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



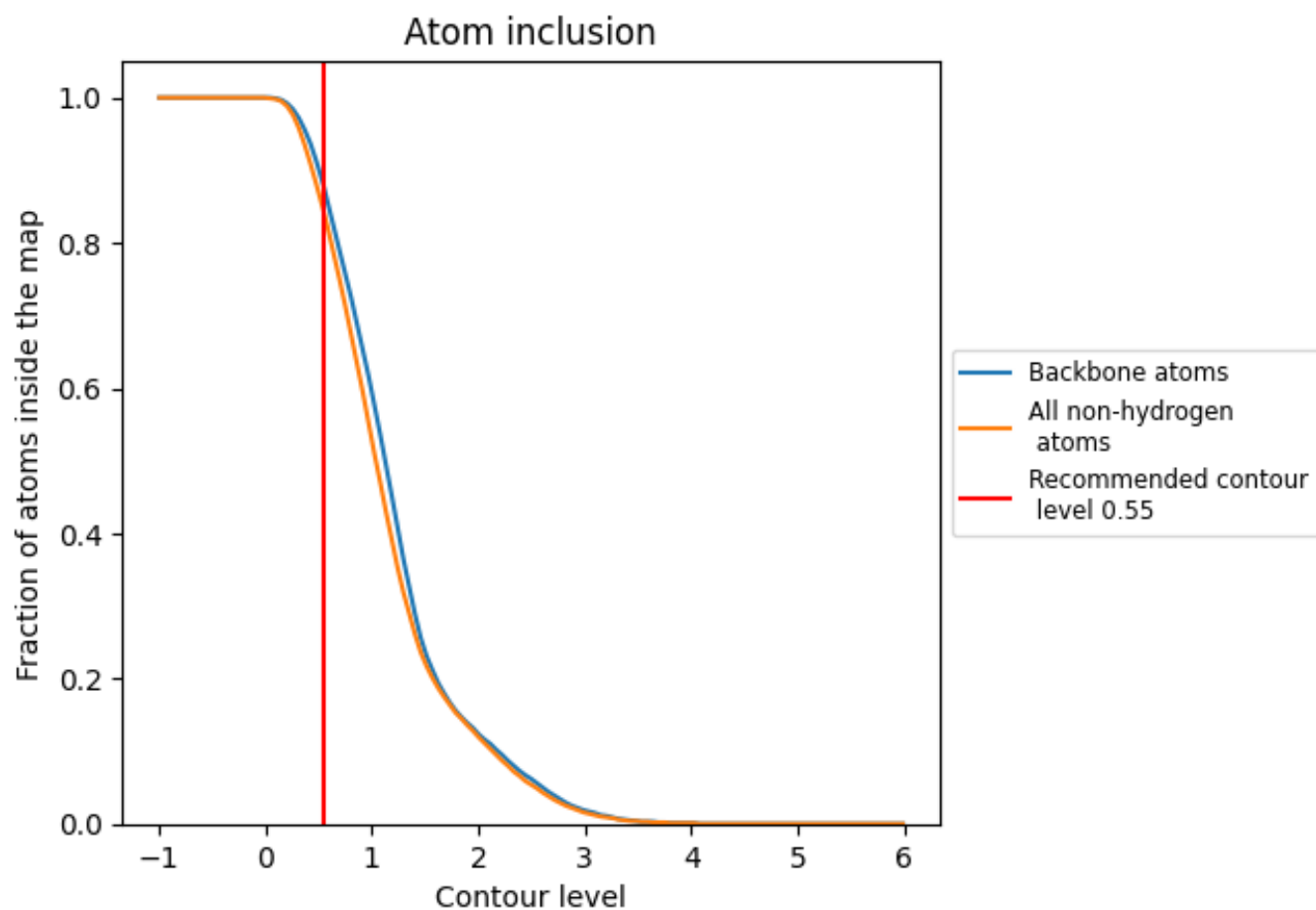
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.6390
A	 0.8520	 0.6480
B	 0.8340	 0.6430
C	 0.8950	 0.6620
D	 0.8780	 0.6470
E	 0.3550	 0.4380
F	 0.5750	 0.5590
G	 0.8510	 0.6460
H	 0.8130	 0.6340
I	 0.8380	 0.6410
J	 0.7160	 0.6240
L	 0.8330	 0.6470
M	 0.8340	 0.6430
N	 0.8920	 0.6650
O	 0.8790	 0.6590
P	 0.3340	 0.4320
Q	 0.5480	 0.5710
R	 0.8440	 0.6510
S	 0.7820	 0.6320
T	 0.8020	 0.6320
U	 0.6920	 0.6200
a	 0.9890	 0.6920
b	 0.9690	 0.6790
c	 0.9720	 0.6730
d	 0.9410	 0.6670
e	 0.9370	 0.6540
f	 0.9570	 0.6650
g	 0.9430	 0.6510
h	 0.9560	 0.6710
i	 0.9250	 0.6330
j	 0.8830	 0.6330
k	 0.8420	 0.6090
l	 0.9700	 0.6620

