



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 06:22 pm GMT

PDB ID : 6T0B
EMDB ID : EMD-10340
Title : The III2-IV(5B)2 respiratory supercomplex from *S. cerevisiae*
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.
Deposited on : 2019-10-02
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

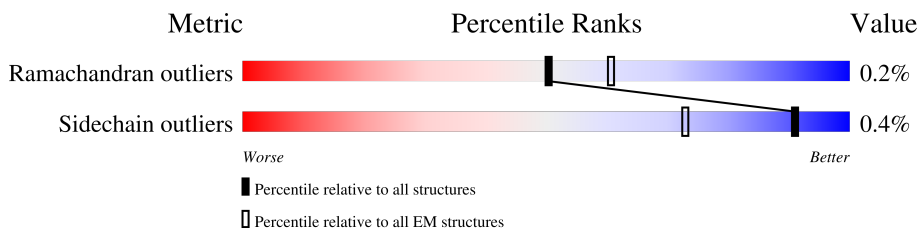
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	431	100%
1	L	431	100%
2	B	352	99% .
2	M	352	99% .
3	C	385	99% .
3	N	385	100%
4	D	248	100%
4	O	248	100%
5	E	185	94% 6%

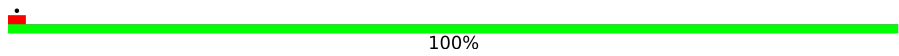
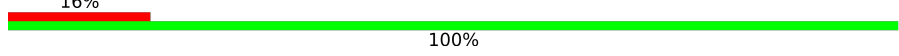
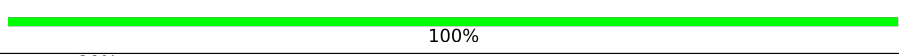
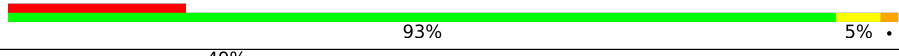
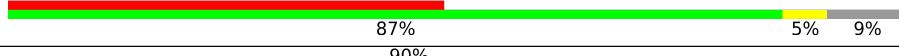



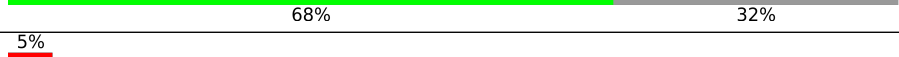
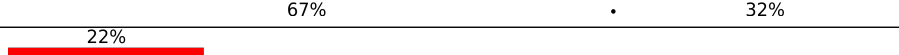
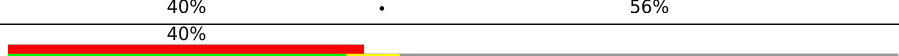
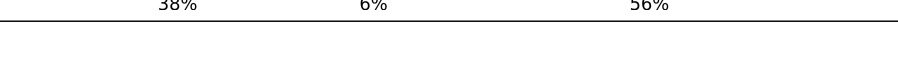
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Mol	Chain	Length	Quality of chain
5	P	185	5% 89% 9%
6	F	147	51% 49%
6	Q	147	50% 49%
7	G	127	98% ..
7	R	127	99% .
8	H	94	99% .
8	S	94	99% .
9	I	66	86% 14%
9	T	66	86% 14%
10	J	77	5% 96% ..
10	U	77	5% 97% ..
11	a	534	99% .
11	n	534	9% 99% .
12	b	236	100%
12	o	236	14% 97% .
13	c	269	100%
13	p	269	39% 99% .
14	d	130	92% 8% .
14	q	130	28% 88% 5% 7%
15	e	134	99% .
15	r	134	98% ..
16	f	108	94% 6%
16	s	108	91% 6% .
17	g	59	10% 100%
17	t	59	42% 100%

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Mol	Chain	Length	Quality of chain
18	h	51	 100%
18	u	51	 100%
19	i	55	 100%
19	v	55	 93%
20	j	82	 87%
20	w	82	 90%
21	k	131	 85%
21	x	131	 80%
22	l	66	 68%
22	y	66	 67%
23	m	224	 40%
23	z	224	 38%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	HEA	a	602	X	-	-	-
31	HEA	a	603	X	-	-	-
31	HEA	n	602	X	-	-	-
31	HEA	n	603	X	-	-	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 64478 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.

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.

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.

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.

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.

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
11	n	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
12	o	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
13	p	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
14	q	121	913	576	151	181	5	0	0

- Molecule 15 is a protein called Cytochrome c oxidase polypeptide 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	e	133	1075	689	187	197	2	0	0
15	r	133	1075	689	187	197	2	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7.

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

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

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

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799
x	130	GLY	-	expression tag	UNP P32799
x	131	ALA	-	expression tag	UNP P32799
x	132	ARG	-	expression tag	UNP P32799
x	133	GLY	-	expression tag	UNP P32799
x	134	SER	-	expression tag	UNP P32799
x	135	HIS	-	expression tag	UNP P32799
x	136	HIS	-	expression tag	UNP P32799
x	137	HIS	-	expression tag	UNP P32799
x	138	HIS	-	expression tag	UNP P32799
x	139	HIS	-	expression tag	UNP P32799
x	140	HIS	-	expression tag	UNP P32799

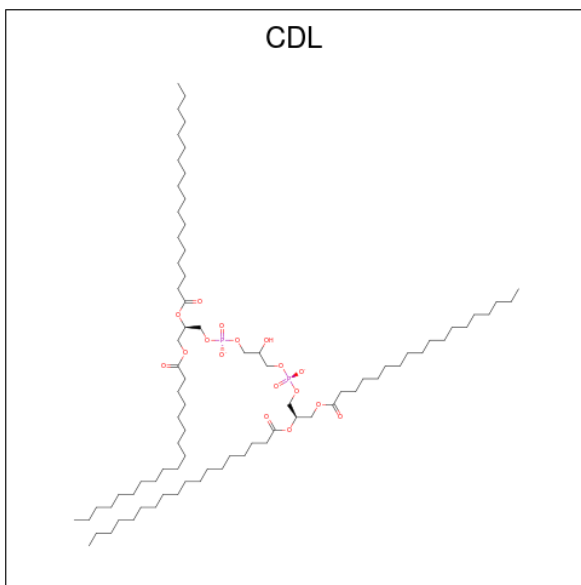
- Molecule 22 is a protein called Cox26.

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

- Molecule 23 is a protein called Respiratory supercomplex factor 2, mitochondrial.

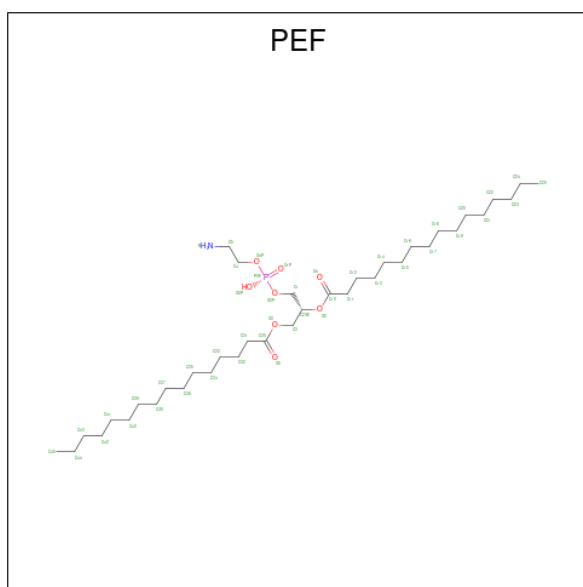
Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	99	Total	C	N	O	S	0	0
			799	511	140	144	4		
23	z	99	Total	C	N	O	S	0	0
			799	511	140	144	4		

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			58	39	17	2	
24	C	1	Total	C	O	P	0
			66	47	17	2	
24	D	1	Total	C	O	P	0
			71	52	17	2	
24	H	1	Total	C	O	P	0
			53	34	17	2	
24	L	1	Total	C	O	P	0
			55	36	17	2	
24	N	1	Total	C	O	P	0
			128	90	34	4	
24	N	1	Total	C	O	P	0
			128	90	34	4	
24	S	1	Total	C	O	P	0
			48	29	17	2	

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



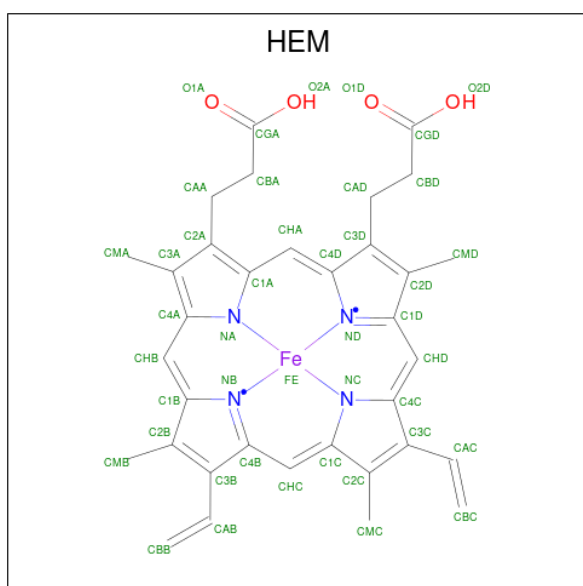
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	A	1	Total 36	C 26	N 1	O 8	P 1	0
25	C	1	Total 83	C 63	N 2	O 16	P 2	0
25	C	1	Total 83	C 63	N 2	O 16	P 2	0
25	E	1	Total 116	C 86	N 3	O 24	P 3	0
25	E	1	Total 116	C 86	N 3	O 24	P 3	0
25	E	1	Total 116	C 86	N 3	O 24	P 3	0
25	H	1	Total 32	C 22	N 1	O 8	P 1	0
25	J	1	Total 29	C 19	N 1	O 8	P 1	0
25	L	1	Total 31	C 21	N 1	O 8	P 1	0
25	N	1	Total 83	C 63	N 2	O 16	P 2	0
25	N	1	Total 83	C 63	N 2	O 16	P 2	0
25	O	1	Total 43	C 33	N 1	O 8	P 1	0
25	S	1	Total 36	C 26	N 1	O 8	P 1	0
25	a	1	Total 33	C 23	N 1	O 8	P 1	0

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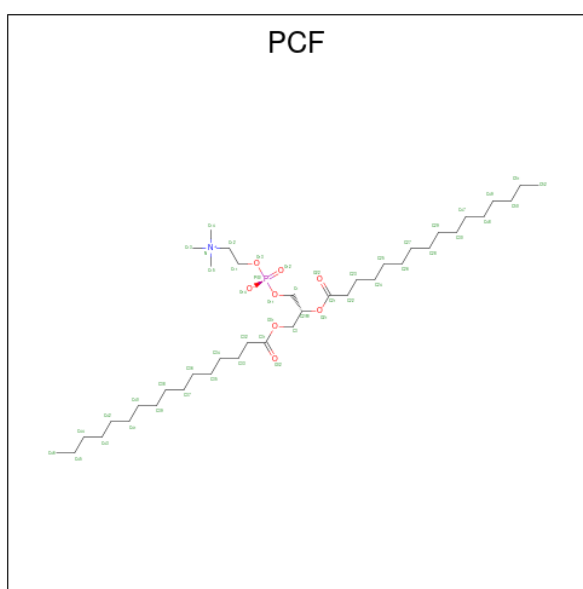
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	b	1	Total	C	N	O	P	0
			80	60	2	16	2	
25	b	1	Total	C	N	O	P	0
			80	60	2	16	2	
25	c	1	Total	C	N	O	P	0
			70	50	2	16	2	
25	c	1	Total	C	N	O	P	0
			70	50	2	16	2	
25	e	1	Total	C	N	O	P	0
			41	31	1	8	1	
25	l	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	n	1	Total	C	N	O	P	0
			113	83	3	24	3	
25	n	1	Total	C	N	O	P	0
			113	83	3	24	3	
25	n	1	Total	C	N	O	P	0
			113	83	3	24	3	
25	o	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	p	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	r	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



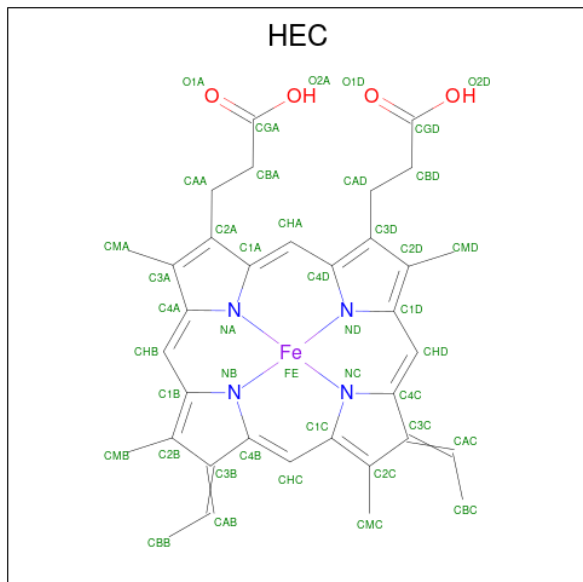
Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
26	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
26	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
26	N	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



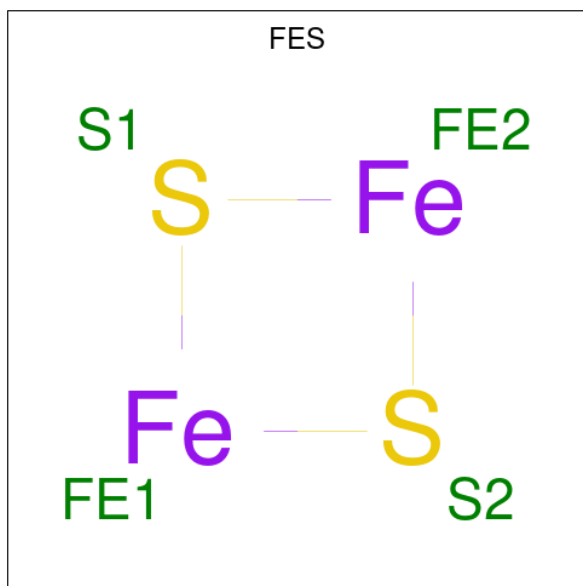
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	I	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	T	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	r	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

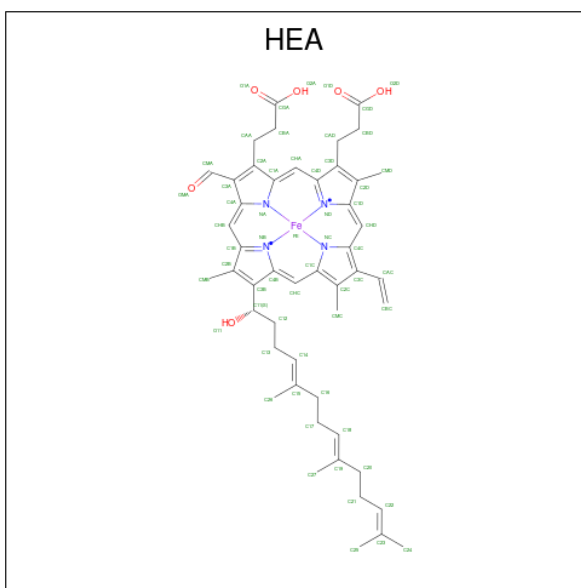


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
31	a	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
31	n	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
31	n	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

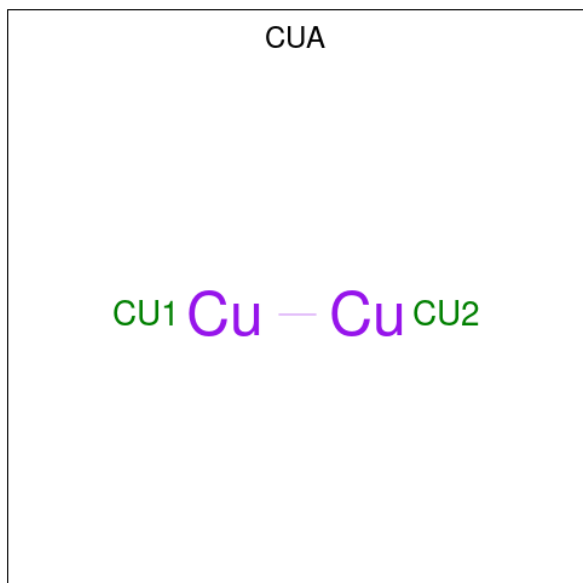
- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 34 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

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

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

Chain A:  100%



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

Chain L:  100%



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

Chain B:  99%



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

Chain M:  99%



- Molecule 3: Cytochrome b

Chain C:  99%



- Molecule 3: Cytochrome b

Chain N: 100%



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 100%



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O: 100%



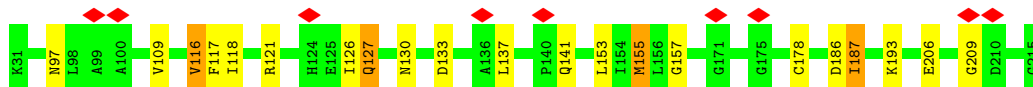
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 94% 6%



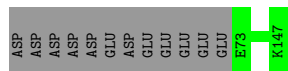
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P: 89% 9% 5%



- Molecule 6: Cytochrome b-c1 complex subunit 6

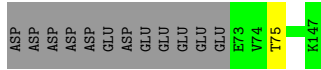
Chain F: 51% 49%



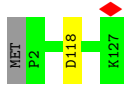
- Molecule 6: Cytochrome b-c1 complex subunit 6

Chain Q: 50% 49%





• Molecule 7: Cytochrome b-c1 complex subunit 7



• Molecule 7: Cytochrome b-c1 complex subunit 7



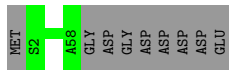
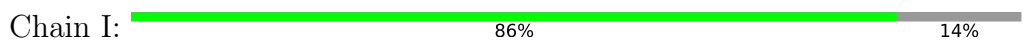
• Molecule 8: Cytochrome b-c1 complex subunit 8



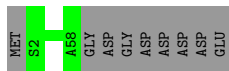
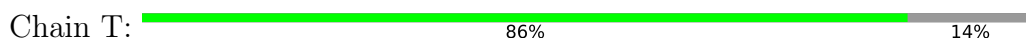
• Molecule 8: Cytochrome b-c1 complex subunit 8



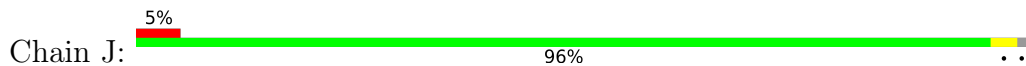
• Molecule 9: Cytochrome b-c1 complex subunit 9

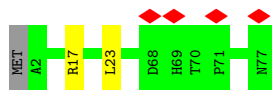


• Molecule 9: Cytochrome b-c1 complex subunit 9

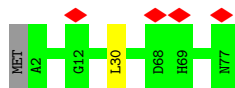


• Molecule 10: Cytochrome b-c1 complex subunit 10





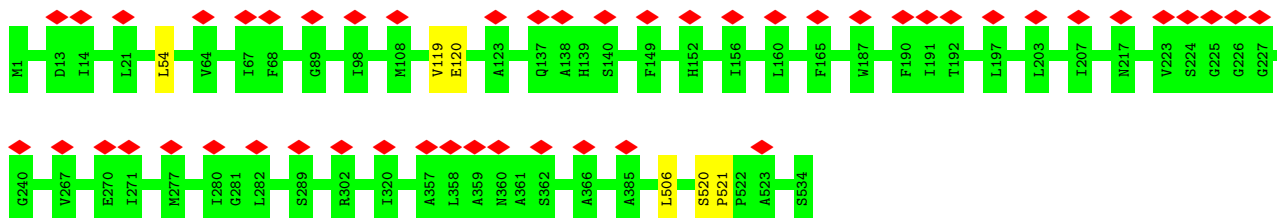
- Molecule 10: Cytochrome b-c1 complex subunit 10



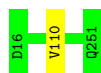
- Molecule 11: Cytochrome c oxidase subunit 1



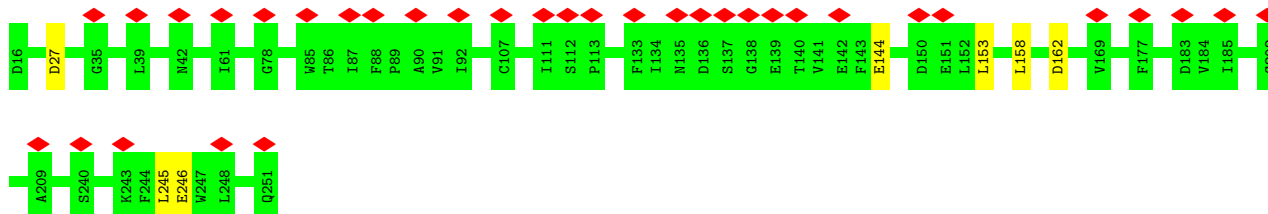
- Molecule 11: Cytochrome c oxidase subunit 1



- Molecule 12: Cytochrome c oxidase subunit 2

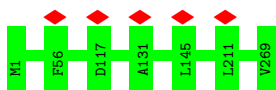


- Molecule 12: Cytochrome c oxidase subunit 2

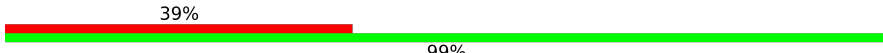


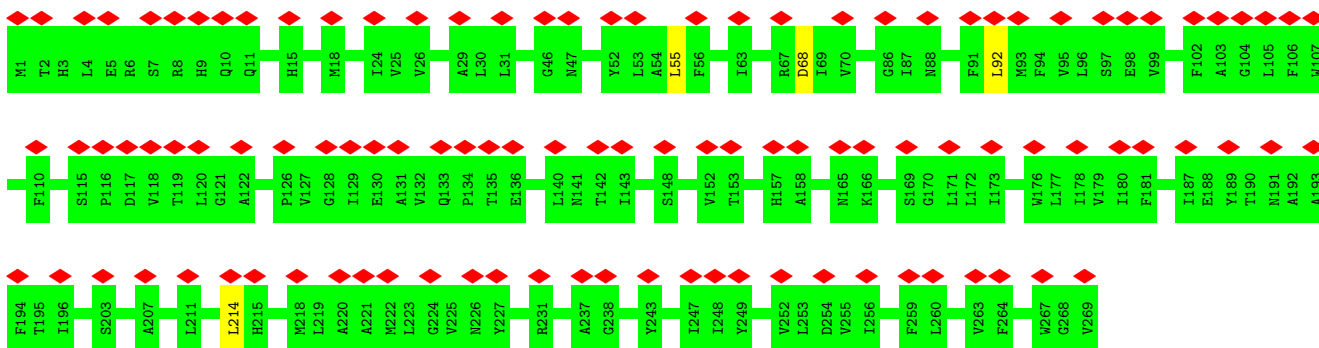
- Molecule 13: Cytochrome c oxidase subunit 3

Chain c:  100%



- Molecule 13: Cytochrome c oxidase subunit 3

Chain p:  99%




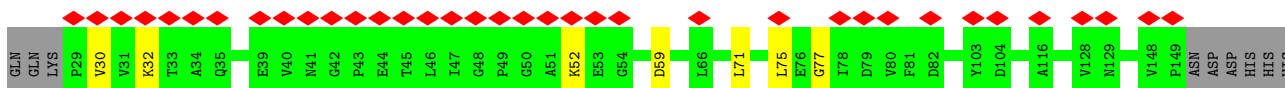
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

Chain d:  92% 8%



- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

Chain q:  88% 28% 5% 7%



- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain e:  99%



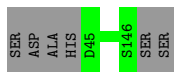
- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain r:  98%



- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain f:  94% 6%



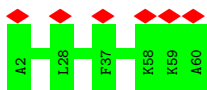
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain s:  91% 6%




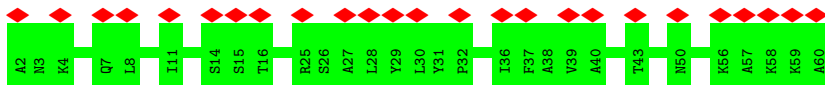
- Molecule 17: Cytochrome c oxidase subunit 7

Chain g:  10% 100%



- Molecule 17: Cytochrome c oxidase subunit 7

Chain t:  42% 100%



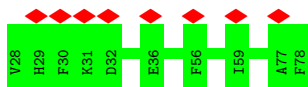
- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:  100%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain u:  16% 100%

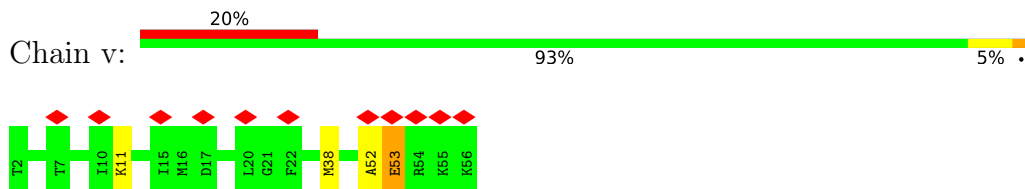


- Molecule 19: Cytochrome c oxidase subunit 7A

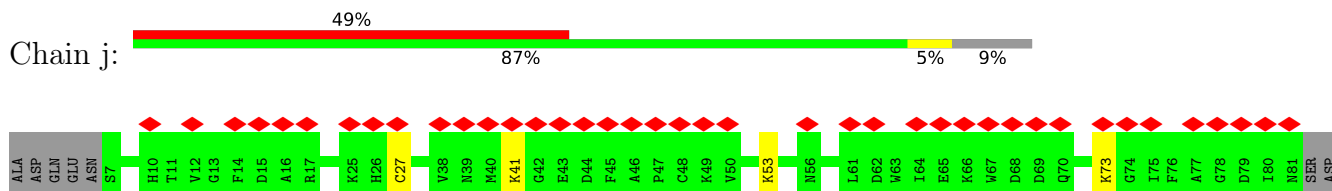
Chain i:  100%

There are no outlier residues recorded for this chain.

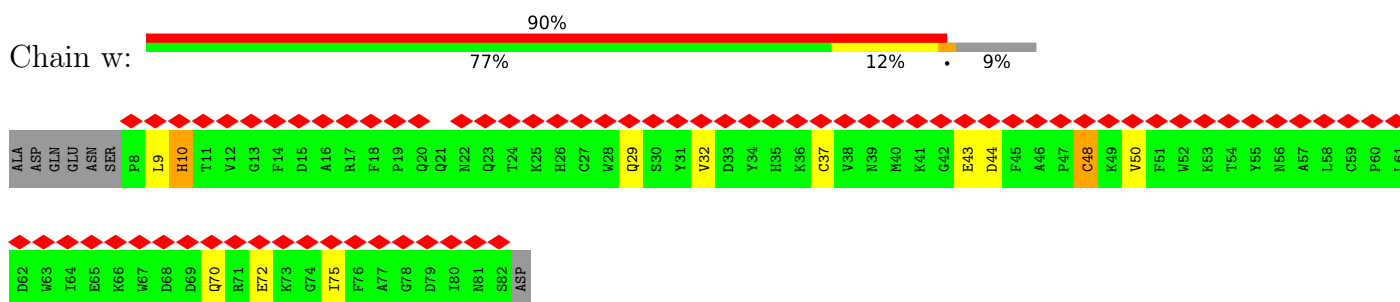
• Molecule 19: Cytochrome c oxidase subunit 7A



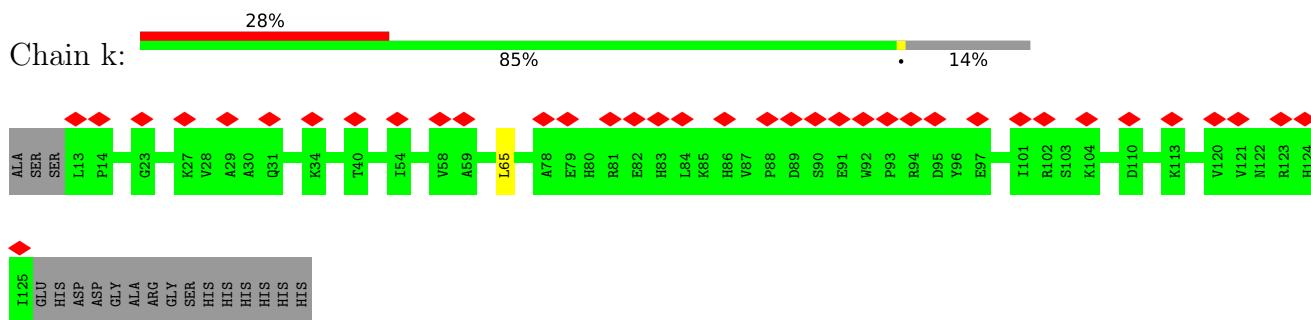
• Molecule 20: Cytochrome c oxidase subunit 6B



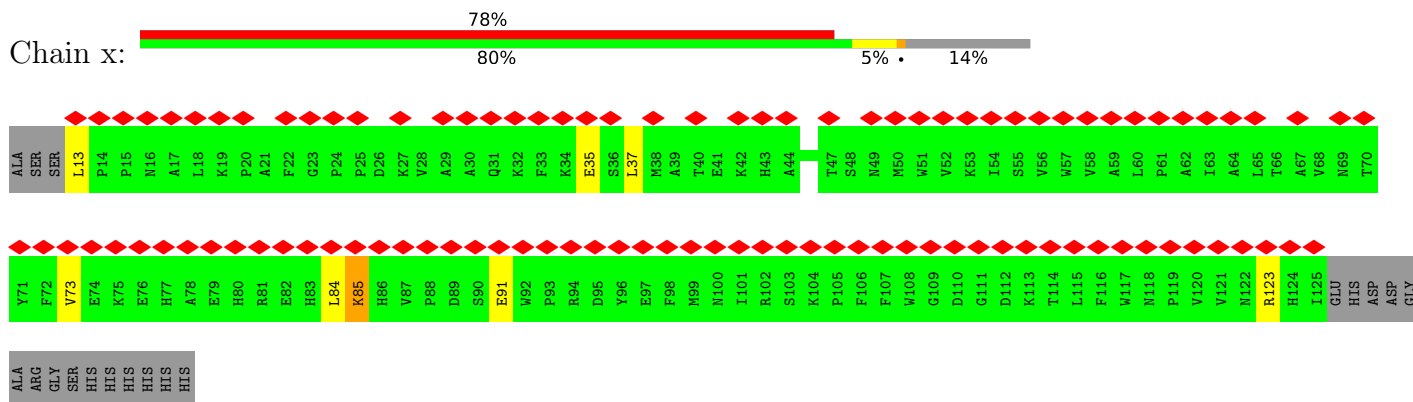
• Molecule 20: Cytochrome c oxidase subunit 6B



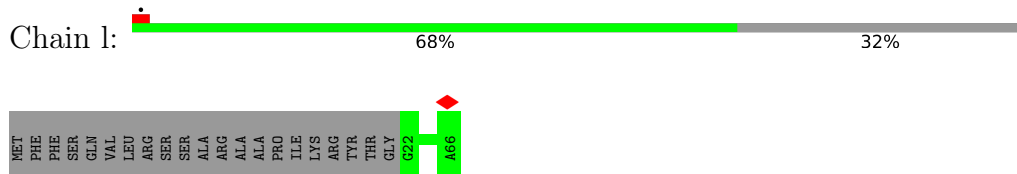
• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



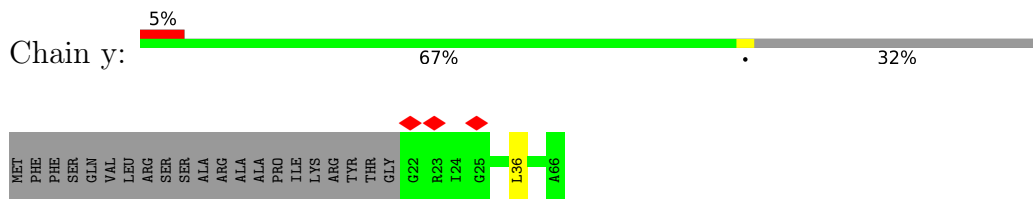
• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



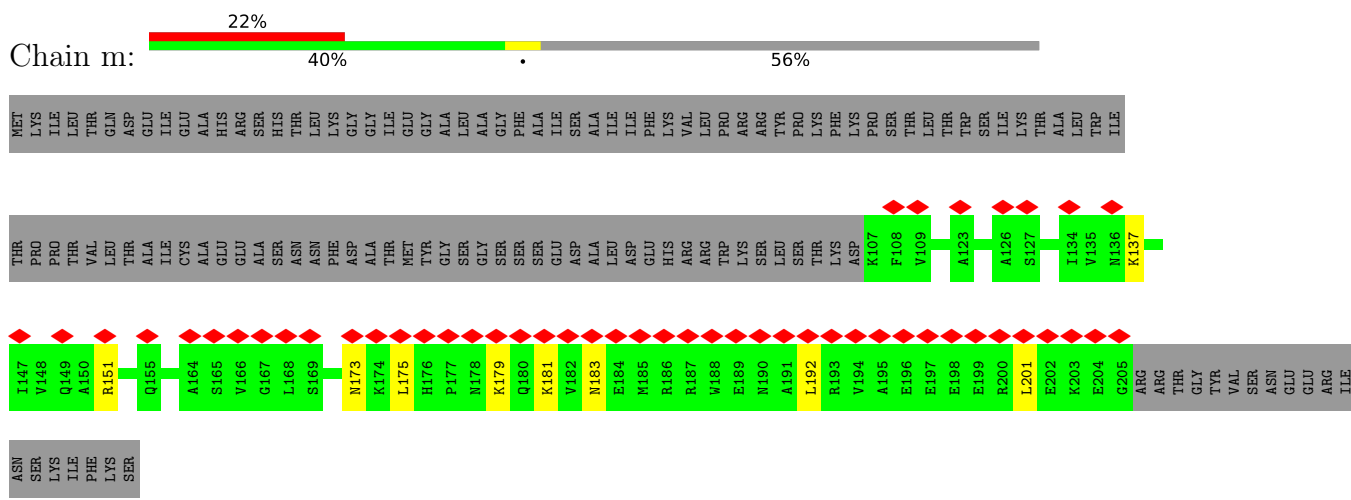
• Molecule 22: Cox26



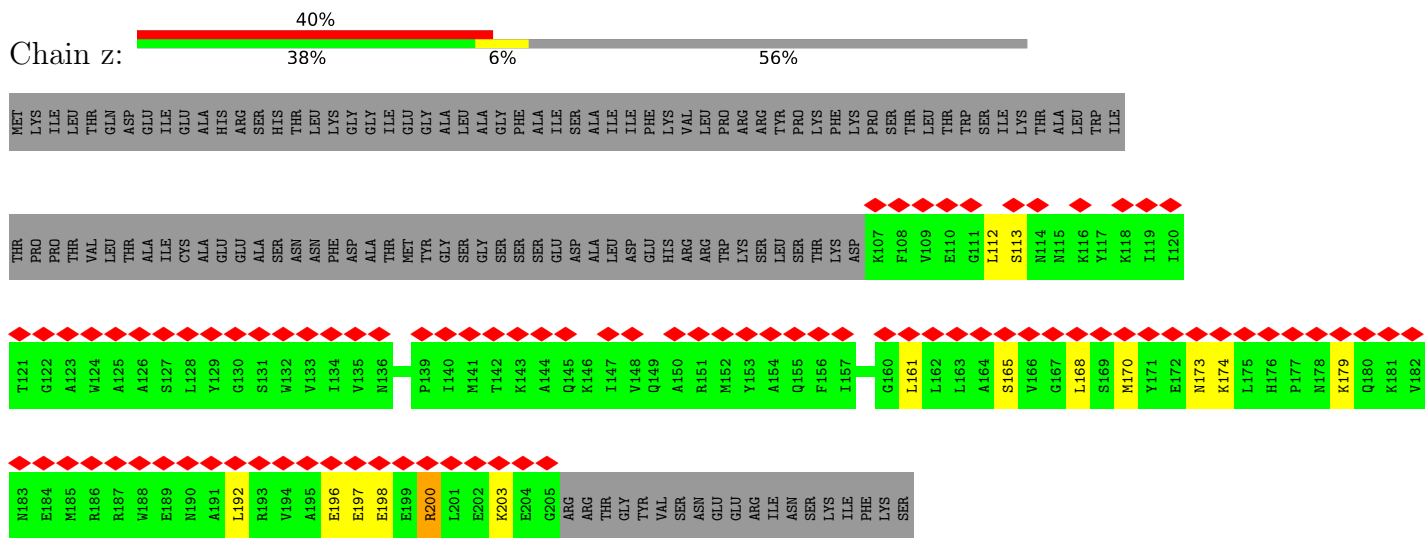
• Molecule 22: Cox26



• Molecule 23: Respiratory supercomplex factor 2, mitochondrial



• Molecule 23: Respiratory supercomplex factor 2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65999	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 ($e^-/\text{\AA}^2$)	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.028	Depositor
Minimum map value	-1.743	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	486.08002, 486.08002, 486.08002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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, PEF, HEC, PCF, CA, FES, MG, CUA, ZN, HEA, CU, CDL

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	0.60	0/3406	0.61	0/4615
1	L	0.56	0/3406	0.60	0/4615
2	B	0.59	0/2781	0.60	1/3764 (0.0%)
2	M	0.58	0/2781	0.60	1/3764 (0.0%)
3	C	0.70	1/3192 (0.0%)	0.63	1/4354 (0.0%)
3	N	0.66	0/3192	0.62	0/4354
4	D	0.64	0/2012	0.55	0/2740
4	O	0.62	0/2012	0.54	0/2740
5	E	0.53	0/1444	0.84	5/1957 (0.3%)
5	P	0.65	2/1444 (0.1%)	0.98	7/1957 (0.4%)
6	F	0.44	0/647	0.51	0/870
6	Q	0.45	0/647	0.57	0/870
7	G	0.54	0/1040	0.58	1/1408 (0.1%)
7	R	0.54	0/1040	0.55	0/1408
8	H	0.60	0/804	0.52	0/1088
8	S	0.60	0/804	0.52	0/1088
9	I	0.56	0/479	0.51	0/646
9	T	0.57	0/479	0.48	0/646
10	J	0.40	0/619	0.59	1/841 (0.1%)
10	U	0.37	0/619	0.58	1/841 (0.1%)
11	a	0.65	0/4290	0.63	1/5857 (0.0%)
11	n	0.53	0/4290	0.67	2/5857 (0.0%)
12	b	0.61	0/1941	0.63	1/2653 (0.0%)
12	o	0.59	1/1941 (0.1%)	0.80	4/2653 (0.2%)
13	c	0.53	0/2218	0.57	0/3036
13	p	0.42	0/2218	0.70	4/3036 (0.1%)
14	d	0.61	0/924	0.65	0/1258
14	q	0.49	0/932	0.76	1/1269 (0.1%)
15	e	0.54	0/1103	0.56	0/1493
15	r	0.46	0/1103	0.63	1/1493 (0.1%)
16	f	0.63	0/868	0.61	0/1174
16	s	0.54	1/868 (0.1%)	0.71	2/1174 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.60	0/500	0.59	0/681
17	t	0.41	0/500	0.64	0/681
18	h	0.63	0/424	0.60	0/569
18	u	0.43	0/424	0.58	0/569
19	i	0.49	0/468	0.56	0/626
19	v	0.67	2/468 (0.4%)	0.76	1/626 (0.2%)
20	j	0.53	1/649 (0.2%)	0.79	2/880 (0.2%)
20	w	0.54	0/649	0.96	1/879 (0.1%)
21	k	0.35	0/962	0.54	1/1310 (0.1%)
21	x	0.47	0/962	0.93	4/1310 (0.3%)
22	l	0.50	0/372	0.59	0/502
22	y	0.46	0/372	0.79	1/502 (0.2%)
23	m	0.53	0/813	0.92	3/1093 (0.3%)
23	z	0.53	0/813	1.03	7/1093 (0.6%)
All	All	0.57	8/63920 (0.0%)	0.66	54/86840 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	M	0	1
3	C	0	1
5	E	0	4
5	P	0	12
11	a	0	2
11	n	0	2
12	o	0	3
14	d	0	1
14	q	0	2
16	s	0	1
19	v	0	3
20	w	0	8
21	x	0	3
23	m	0	2
23	z	0	5
All	All	0	51

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	127	GLN	CB-CG	9.28	1.77	1.52
19	v	53	GLU	CG-CD	-8.61	1.39	1.51
20	j	41	LYS	CD-CE	-6.26	1.35	1.51
12	o	144	GLU	CB-CG	-5.78	1.41	1.52
16	s	108	PHE	CD1-CE1	-5.64	1.27	1.39
3	C	21	PRO	C-N	-5.28	1.22	1.34
5	P	130	ASN	CG-OD1	5.12	1.35	1.24
19	v	53	GLU	CD-OE1	-5.06	1.20	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	m	192	LEU	CA-CB-CG	10.16	138.67	115.30
5	P	153	LEU	CA-CB-CG	10.07	138.46	115.30
15	r	131	ASP	CB-CG-OD1	8.78	126.20	118.30
5	E	145	ASP	CB-CG-OD1	8.54	125.98	118.30
5	P	118	ILE	CG1-CB-CG2	-7.77	94.31	111.40
11	a	517	LEU	CB-CG-CD1	-7.48	98.28	111.00
21	x	13	LEU	CA-CB-CG	7.11	131.64	115.30
7	G	118	ASP	CB-CG-OD1	6.97	124.57	118.30
13	p	55	LEU	CA-CB-CG	6.96	131.31	115.30
5	P	121	ARG	C-N-CA	6.87	138.87	121.70
16	s	111	LEU	CB-CG-CD1	-6.73	99.55	111.00
23	z	168	LEU	CA-CB-CG	6.64	130.58	115.30
20	j	41	LYS	CD-CE-NZ	-6.59	96.54	111.70
5	P	133	ASP	CB-CG-OD2	6.54	124.19	118.30
12	o	158	LEU	CA-CB-CG	6.36	129.93	115.30
23	z	112	LEU	CA-CB-CG	6.33	129.85	115.30
12	o	153	LEU	CA-CB-CG	6.23	129.62	115.30
12	o	162	ASP	CB-CG-OD2	-6.22	112.70	118.30
2	B	203	GLU	CA-CB-CG	6.21	127.05	113.40
23	z	161	LEU	CA-CB-CG	6.19	129.54	115.30
22	y	36	LEU	CA-CB-CG	6.12	129.38	115.30
23	z	200	ARG	CA-CB-CG	6.10	126.83	113.40
19	v	53	GLU	CA-CB-CG	5.95	126.48	113.40
23	m	201	LEU	CA-CB-CG	5.84	128.73	115.30
10	U	30	LEU	CA-CB-CG	5.83	128.71	115.30
13	p	68	ASP	CB-CG-OD1	5.69	123.42	118.30
23	m	175	LEU	CA-CB-CG	5.68	128.36	115.30
23	z	196	GLU	CA-CB-CG	5.65	125.84	113.40
5	E	164	CYS	CA-CB-SG	5.65	124.17	114.00
21	x	37	LEU	CA-CB-CG	5.64	128.26	115.30
21	x	84	LEU	CA-CB-CG	5.62	128.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	k	65	LEU	CA-CB-CG	5.61	128.20	115.30
5	E	98	LEU	CA-CB-CG	5.57	128.11	115.30
23	z	192	LEU	CB-CG-CD2	5.56	120.45	111.00
5	E	137	LEU	CB-CG-CD1	-5.50	101.65	111.00
21	x	85	LYS	CA-CB-CG	5.48	125.45	113.40
5	P	116	VAL	CG1-CB-CG2	-5.43	102.21	110.90
5	P	178	CYS	CA-CB-SG	5.43	123.77	114.00
20	j	73	LYS	CA-CB-CG	5.42	125.33	113.40
2	M	291	ASP	CB-CG-OD1	5.42	123.17	118.30
14	q	71	LEU	CB-CG-CD1	-5.41	101.81	111.00
5	E	178	CYS	CA-CB-SG	5.38	123.69	114.00
13	p	92	LEU	CA-CB-CG	5.38	127.66	115.30
16	s	143	LEU	CA-CB-CG	5.35	127.61	115.30
10	J	23	LEU	CA-CB-CG	5.34	127.59	115.30
11	n	54	LEU	CB-CG-CD1	-5.27	102.04	111.00
13	p	214	LEU	CA-CB-CG	5.21	127.28	115.30
12	o	153	LEU	CB-CG-CD1	-5.20	102.16	111.00
23	z	168	LEU	CB-CG-CD1	5.15	119.75	111.00
3	C	101	LEU	CA-CB-CG	5.12	127.07	115.30
5	P	126	ILE	CA-CB-CG1	5.09	120.67	111.00
20	w	75	ILE	CG1-CB-CG2	-5.05	100.29	111.40
11	n	506	LEU	CA-CB-CG	5.02	126.84	115.30
12	b	110	VAL	CG1-CB-CG2	-5.01	102.88	110.90

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	VAL	Peptide
3	C	107	ARG	Peptide
5	E	127	GLN	Peptide
5	E	135	SER	Peptide
5	E	173	PHE	Peptide
5	E	97	ASN	Peptide
2	M	94	LEU	Peptide
5	P	117	PHE	Peptide
5	P	127	GLN	Sidechain
5	P	137	LEU	Peptide
5	P	141	GLN	Peptide
5	P	155	MET	Peptide
5	P	157	GLY	Peptide
5	P	186	ASP	Peptide

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Mol	Chain	Res	Type	Group
5	P	187	ILE	Peptide
5	P	193	LYS	Peptide
5	P	206	GLU	Peptide
5	P	209	GLY	Peptide
5	P	97	ASN	Peptide
11	a	119	VAL	Peptide
11	a	520	SER	Peptide
14	d	32	LYS	Peptide
23	m	173	ASN	Peptide
23	m	183	ASN	Peptide
11	n	119	VAL	Peptide
11	n	520	SER	Peptide
12	o	245	LEU	Peptide
12	o	246	GLU	Peptide
12	o	27	ASP	Peptide
14	q	59	ASP	Peptide
14	q	75	LEU	Peptide
16	s	46	GLU	Peptide
19	v	38	MET	Peptide
19	v	52	ALA	Peptide
19	v	53	GLU	Peptide
20	w	10	HIS	Peptide
20	w	29	GLN	Peptide
20	w	43	GLU	Peptide
20	w	48	CYS	Peptide
20	w	50	VAL	Peptide
20	w	70	GLN	Peptide
20	w	72	GLU	Peptide
20	w	9	LEU	Peptide
21	x	35	GLU	Peptide
21	x	85	LYS	Peptide
21	x	91	GLU	Peptide
23	z	165	SER	Peptide
23	z	170	MET	Peptide
23	z	174	LYS	Peptide
23	z	197	GLU	Peptide
23	z	198	GLU	Peptide

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	401 (94%)	28 (6%)	0	100	100
1	L	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
2	B	350/352 (99%)	329 (94%)	21 (6%)	0	100	100
2	M	350/352 (99%)	328 (94%)	22 (6%)	0	100	100
3	C	383/385 (100%)	370 (97%)	13 (3%)	0	100	100
3	N	383/385 (100%)	373 (97%)	10 (3%)	0	100	100
4	D	245/248 (99%)	238 (97%)	7 (3%)	0	100	100
4	O	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	157 (86%)	26 (14%)	0	100	100
5	P	183/185 (99%)	149 (81%)	33 (18%)	1 (0%)	29	61
6	F	73/147 (50%)	67 (92%)	6 (8%)	0	100	100
6	Q	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
7	G	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
7	R	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
8	H	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
8	S	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
9	I	55/66 (83%)	55 (100%)	0	0	100	100
9	T	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	504 (95%)	27 (5%)	1 (0%)	47	78
11	n	532/534 (100%)	502 (94%)	28 (5%)	2 (0%)	34	66
12	b	234/236 (99%)	215 (92%)	19 (8%)	0	100	100
12	o	234/236 (99%)	206 (88%)	28 (12%)	0	100	100
13	c	267/269 (99%)	260 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	p	267/269 (99%)	263 (98%)	4 (2%)	0	100	100
14	d	118/130 (91%)	98 (83%)	20 (17%)	0	100	100
14	q	119/130 (92%)	101 (85%)	16 (13%)	2 (2%)	9	29
15	e	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
15	r	131/134 (98%)	115 (88%)	15 (12%)	1 (1%)	19	49
16	f	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
16	s	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
17	t	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
18	h	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
18	u	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	v	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
20	j	73/82 (89%)	68 (93%)	5 (7%)	0	100	100
20	w	73/82 (89%)	62 (85%)	9 (12%)	2 (3%)	5	17
21	k	111/131 (85%)	104 (94%)	7 (6%)	0	100	100
21	x	111/131 (85%)	95 (86%)	16 (14%)	0	100	100
22	l	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
22	y	43/66 (65%)	38 (88%)	5 (12%)	0	100	100
23	m	97/224 (43%)	90 (93%)	7 (7%)	0	100	100
23	z	97/224 (43%)	87 (90%)	7 (7%)	3 (3%)	4	14
All	All	7745/8382 (92%)	7252 (94%)	481 (6%)	12 (0%)	50	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	187	ILE
11	n	120	GLU
11	n	521	PRO
20	w	10	HIS
23	z	173	ASN
11	a	521	PRO
20	w	44	ASP
23	z	179	LYS
14	q	30	VAL

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Mol	Chain	Res	Type
23	z	200	ARG
15	r	39	PRO
14	q	77	GLY

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%)	369 (100%)	1 (0%)	92	98
1	L	370/370 (100%)	369 (100%)	1 (0%)	92	98
2	B	301/301 (100%)	301 (100%)	0	100	100
2	M	301/301 (100%)	301 (100%)	0	100	100
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	338 (100%)	0	100	100
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	149 (99%)	2 (1%)	69	91
5	P	151/151 (100%)	148 (98%)	3 (2%)	55	84
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	65	89
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	S	77/78 (99%)	77 (100%)	0	100	100
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	64 (98%)	1 (2%)	65	89
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	447 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	n	447/447 (100%)	447 (100%)	0	100	100
12	b	209/209 (100%)	209 (100%)	0	100	100
12	o	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	228 (100%)	0	100	100
13	p	228/228 (100%)	228 (100%)	0	100	100
14	d	101/111 (91%)	100 (99%)	1 (1%)	76	93
14	q	102/111 (92%)	100 (98%)	2 (2%)	55	84
15	e	114/115 (99%)	114 (100%)	0	100	100
15	r	114/115 (99%)	114 (100%)	0	100	100
16	f	91/96 (95%)	91 (100%)	0	100	100
16	s	91/96 (95%)	91 (100%)	0	100	100
17	g	50/50 (100%)	50 (100%)	0	100	100
17	t	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
18	u	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
19	v	46/46 (100%)	45 (98%)	1 (2%)	52	83
20	j	67/73 (92%)	65 (97%)	2 (3%)	41	75
20	w	67/73 (92%)	64 (96%)	3 (4%)	27	60
21	k	99/113 (88%)	99 (100%)	0	100	100
21	x	99/113 (88%)	97 (98%)	2 (2%)	55	84
22	l	36/53 (68%)	36 (100%)	0	100	100
22	y	36/53 (68%)	36 (100%)	0	100	100
23	m	84/191 (44%)	80 (95%)	4 (5%)	25	58
23	z	84/191 (44%)	82 (98%)	2 (2%)	49	81
All	All	6691/7158 (94%)	6665 (100%)	26 (0%)	91	97

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ARG
5	E	110	LYS
5	E	180	CYS

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Mol	Chain	Res	Type
10	J	17	ARG
1	L	449	ARG
5	P	109	VAL
5	P	116	VAL
5	P	155	MET
6	Q	75	THR
14	d	32	LYS
20	j	27	CYS
20	j	53	LYS
23	m	137	LYS
23	m	151	ARG
23	m	179	LYS
23	m	181	LYS
14	q	32	LYS
14	q	52	LYS
19	v	11	LYS
20	w	32	VAL
20	w	37	CYS
20	w	48	CYS
21	x	73	VAL
21	x	123	ARG
23	z	113	SER
23	z	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	42	HIS
1	A	67	ASN
1	A	171	ASN
1	A	187	ASN
1	A	274	ASN
1	A	283	GLN
1	A	298	GLN
1	A	317	HIS
1	A	352	ASN
1	A	388	ASN
2	B	49	HIS
2	B	103	ASN
2	B	157	ASN
2	B	352	ASN

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Mol	Chain	Res	Type
2	B	361	ASN
3	C	22	GLN
3	C	138	GLN
3	C	177	GLN
3	C	253	HIS
3	C	256	ASN
3	C	343	HIS
4	D	70	HIS
4	D	79	ASN
4	D	127	ASN
4	D	185	HIS
4	D	256	ASN
5	E	97	ASN
5	E	112	GLN
5	E	141	GLN
5	E	199	ASN
6	F	87	ASN
6	F	110	GLN
7	G	30	ASN
9	I	42	ASN
9	I	44	ASN
10	J	29	ASN
1	L	187	ASN
1	L	199	ASN
1	L	274	ASN
1	L	283	GLN
1	L	298	GLN
1	L	305	ASN
1	L	317	HIS
1	L	350	GLN
1	L	388	ASN
2	M	103	ASN
2	M	191	ASN
2	M	352	ASN
2	M	361	ASN
3	N	177	GLN
3	N	222	HIS
3	N	253	HIS
3	N	256	ASN
3	N	384	ASN
4	O	78	HIS
4	O	79	ASN

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Mol	Chain	Res	Type
4	O	127	ASN
4	O	169	ASN
5	P	47	ASN
5	P	106	ASN
5	P	112	GLN
5	P	130	ASN
5	P	199	ASN
6	Q	87	ASN
9	T	44	ASN
11	a	478	ASN
11	a	482	ASN
12	b	33	GLN
12	b	135	ASN
12	b	157	GLN
13	c	11	GLN
13	c	141	ASN
13	c	165	ASN
13	c	185	GLN
14	d	41	ASN
14	d	62	GLN
14	d	119	HIS
15	e	84	HIS
18	h	29	HIS
18	h	53	HIS
19	i	42	ASN
21	k	43	HIS
22	l	42	GLN
11	n	51	ASN
11	n	164	ASN
11	n	399	GLN
11	n	482	ASN
12	o	40	HIS
12	o	251	GLN
13	p	141	ASN
13	p	226	ASN
13	p	234	HIS
14	q	129	ASN
15	r	127	GLN
16	s	133	GLN
17	t	13	GLN
21	x	16	ASN
21	x	49	ASN

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Mol	Chain	Res	Type
22	y	42	GLN
23	z	136	ASN
23	z	155	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 8 are monoatomic - leaving 55 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	$\# Z > 2$
25	PEF	r	201	-	40,40,46	0.99	2 (5%)	43,45,51	1.13	3 (6%)
25	PEF	l	101	-	32,32,46	1.10	2 (6%)	35,37,51	1.28	4 (11%)
25	PEF	E	303	-	39,39,46	1.00	2 (5%)	42,44,51	1.24	3 (7%)
25	PEF	N	605	-	39,39,46	1.00	2 (5%)	42,44,51	1.16	3 (7%)
24	CDL	N	604	-	74,74,99	1.04	5 (6%)	80,86,111	1.19	6 (7%)
29	FES	P	301	5	0,4,4	-	-	-	-	-
25	PEF	c	301	-	35,35,46	1.05	2 (5%)	38,40,51	1.13	3 (7%)
25	PEF	N	606	-	42,42,46	0.93	2 (4%)	45,47,51	1.19	4 (8%)
31	HEA	n	603	11	57,67,67	1.98	15 (26%)	61,103,103	2.53	26 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEF	a	606	-	32,32,46	1.14	2 (6%)	35,37,51	1.07	3 (8%)
25	PEF	C	604	-	43,43,46	0.97	2 (4%)	46,48,51	1.10	3 (6%)
25	PEF	n	608	-	32,32,46	1.13	2 (6%)	35,37,51	1.12	2 (5%)
25	PEF	o	302	-	39,39,46	1.04	2 (5%)	42,44,51	1.08	4 (9%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-
24	CDL	H	101	-	52,52,99	1.22	4 (7%)	58,64,111	1.32	8 (13%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
28	HEC	O	401	4	32,50,50	2.12	10 (31%)	24,82,82	2.30	9 (37%)
31	HEA	n	602	11	57,67,67	1.93	15 (26%)	61,103,103	2.60	31 (50%)
24	CDL	D	402	-	70,70,99	1.03	4 (5%)	76,82,111	1.27	7 (9%)
25	PEF	S	102	-	35,35,46	1.06	2 (5%)	38,40,51	1.22	3 (7%)
25	PEF	c	302	-	33,33,46	1.11	2 (6%)	36,38,51	1.06	2 (5%)
25	PEF	H	102	-	31,31,46	1.11	2 (6%)	34,36,51	1.33	4 (11%)
24	CDL	L	501	-	54,54,99	1.12	4 (7%)	60,66,111	1.27	5 (8%)
25	PEF	C	605	-	38,38,46	1.01	2 (5%)	41,43,51	1.10	2 (4%)
26	HEM	C	602	3	41,50,50	1.55	7 (17%)	45,82,82	1.94	12 (26%)
28	HEC	D	401	4	32,50,50	2.13	9 (28%)	24,82,82	2.35	9 (37%)
34	CUA	o	301	12	0,1,1	-	-	-	-	-
24	CDL	S	101	-	47,47,99	1.31	4 (8%)	53,59,111	1.41	9 (16%)
27	PCF	N	607	-	49,49,49	0.91	3 (6%)	55,57,57	1.16	4 (7%)
25	PEF	n	607	-	32,32,46	1.13	2 (6%)	35,37,51	1.20	3 (8%)
24	CDL	A	501	-	57,57,99	1.18	4 (7%)	63,69,111	1.40	8 (12%)
25	PEF	L	502	-	30,30,46	1.15	2 (6%)	33,35,51	1.20	4 (12%)
26	HEM	N	602	3	41,50,50	1.52	7 (17%)	45,82,82	1.96	11 (24%)
27	PCF	H	103	-	31,31,49	1.17	2 (6%)	37,39,57	1.18	4 (10%)
25	PEF	J	101	-	28,28,46	1.23	2 (7%)	31,33,51	1.26	3 (9%)
25	PEF	p	301	-	35,35,46	1.09	3 (8%)	38,40,51	1.12	3 (7%)
25	PEF	A	502	-	35,35,46	1.06	2 (5%)	38,40,51	1.14	3 (7%)
27	PCF	e	202	-	35,35,49	1.15	2 (5%)	41,43,57	1.16	3 (7%)
25	PEF	b	302	-	39,39,46	1.01	2 (5%)	42,44,51	1.12	3 (7%)
25	PEF	E	304	-	33,33,46	1.08	2 (6%)	36,38,51	1.26	5 (13%)
27	PCF	C	606	-	38,38,49	1.06	2 (5%)	44,46,57	1.31	6 (13%)
26	HEM	C	601	3	41,50,50	1.53	6 (14%)	45,82,82	2.10	12 (26%)
24	CDL	N	603	-	52,52,99	1.22	4 (7%)	58,64,111	1.43	7 (12%)
27	PCF	T	101	-	46,46,49	0.99	2 (4%)	52,54,57	1.14	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	HEA	a	602	11	57,67,67	1.91	15 (26%)	61,103,103	2.84	30 (49%)
27	PCF	I	101	-	29,29,49	1.27	2 (6%)	35,37,57	1.30	4 (11%)
24	CDL	C	603	-	65,65,99	1.12	4 (6%)	71,77,111	1.38	7 (9%)
25	PEF	b	303	-	39,39,46	1.04	2 (5%)	42,44,51	1.09	3 (7%)
25	PEF	n	606	-	46,46,46	0.95	2 (4%)	49,51,51	1.15	4 (8%)
26	HEM	N	601	3	41,50,50	1.47	7 (17%)	45,82,82	2.20	10 (22%)
25	PEF	E	302	-	41,41,46	1.00	2 (4%)	44,46,51	1.08	3 (6%)
25	PEF	e	201	-	40,40,46	0.96	2 (5%)	43,45,51	1.35	5 (11%)
31	HEA	a	603	11	57,67,67	1.92	14 (24%)	61,103,103	2.51	27 (44%)
27	PCF	r	202	-	35,35,49	1.14	2 (5%)	41,43,57	1.03	2 (4%)
25	PEF	O	402	-	42,42,46	0.99	2 (4%)	45,47,51	1.09	3 (6%)

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
25	PEF	r	201	-	-	15/44/44/50	-
25	PEF	l	101	-	-	7/36/36/50	-
25	PEF	E	303	-	-	19/43/43/50	-
25	PEF	N	605	-	-	19/43/43/50	-
24	CDL	N	604	-	-	34/85/85/110	-
29	FES	P	301	5	-	-	0/1/1/1
25	PEF	c	301	-	-	11/39/39/50	-
25	PEF	N	606	-	-	11/46/46/50	-
31	HEA	n	603	11	2/2/7/16	4/32/76/76	-
25	PEF	a	606	-	-	13/36/36/50	-
25	PEF	C	604	-	-	15/47/47/50	-
25	PEF	n	608	-	-	8/36/36/50	-
25	PEF	o	302	-	-	14/43/43/50	-
24	CDL	H	101	-	-	29/63/63/110	-
29	FES	E	301	5	-	-	0/1/1/1
28	HEC	O	401	4	-	3/10/54/54	-
31	HEA	n	602	11	2/2/7/16	7/32/76/76	-
24	CDL	D	402	-	-	24/81/81/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	S	102	-	-	12/39/39/50	-
25	PEF	c	302	-	-	14/37/37/50	-
25	PEF	H	102	-	-	8/35/35/50	-
24	CDL	L	501	-	-	30/64/64/110	-
25	PEF	C	605	-	-	9/42/42/50	-
26	HEM	C	602	3	-	4/12/54/54	-
28	HEC	D	401	4	-	1/10/54/54	-
24	CDL	S	101	-	-	16/58/58/110	-
27	PCF	N	607	-	-	21/53/53/53	-
25	PEF	n	607	-	-	16/36/36/50	-
24	CDL	A	501	-	-	25/68/68/110	-
25	PEF	L	502	-	-	17/34/34/50	-
26	HEM	N	602	3	-	4/12/54/54	-
27	PCF	H	103	-	-	17/35/35/53	-
25	PEF	J	101	-	-	12/32/32/50	-
25	PEF	p	301	-	-	12/39/39/50	-
25	PEF	A	502	-	-	11/39/39/50	-
27	PCF	e	202	-	-	11/39/39/53	-
25	PEF	b	302	-	-	15/43/43/50	-
25	PEF	E	304	-	-	16/37/37/50	-
27	PCF	C	606	-	-	20/42/42/53	-
26	HEM	C	601	3	-	8/12/54/54	-
24	CDL	N	603	-	-	23/63/63/110	-
27	PCF	T	101	-	-	4/50/50/53	-
31	HEA	a	602	11	2/2/7/16	9/32/76/76	-
27	PCF	I	101	-	-	5/33/33/53	-
24	CDL	C	603	-	-	28/76/76/110	-
25	PEF	b	303	-	-	17/43/43/50	-
25	PEF	n	606	-	-	19/50/50/50	-
26	HEM	N	601	3	-	8/12/54/54	-
25	PEF	E	302	-	-	19/45/45/50	-
31	HEA	a	603	11	2/2/7/16	6/32/76/76	-
25	PEF	e	201	-	-	17/44/44/50	-
27	PCF	r	202	-	-	10/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	O	402	-	-	21/46/46/50	-

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	401	HEC	C3C-C2C	5.73	1.46	1.40
28	O	401	HEC	C3C-C2C	5.62	1.46	1.40
31	a	603	HEA	C3B-C2B	5.00	1.46	1.34
31	n	603	HEA	C3B-C2B	4.96	1.45	1.34
31	n	602	HEA	C3B-C2B	4.83	1.45	1.34
31	n	603	HEA	C3A-C2A	4.76	1.47	1.40
28	O	401	HEC	C2B-C3B	4.74	1.45	1.40
31	n	603	HEA	C3D-C2D	4.72	1.46	1.36
31	a	603	HEA	C3D-C2D	4.70	1.46	1.36
31	n	602	HEA	CHC-C4B	4.68	1.47	1.35
31	n	603	HEA	C3C-C2C	4.61	1.46	1.40
31	a	603	HEA	CHD-C1D	4.60	1.46	1.35
31	n	603	HEA	CHD-C1D	4.60	1.46	1.35
28	D	401	HEC	C2B-C3B	4.56	1.45	1.40
31	a	602	HEA	CHC-C4B	4.52	1.46	1.35
31	n	602	HEA	CHD-C1D	4.46	1.46	1.35
31	n	602	HEA	C3D-C2D	4.44	1.46	1.36
31	a	603	HEA	CHC-C4B	4.42	1.46	1.35
31	a	602	HEA	C3B-C2B	4.41	1.44	1.34
31	a	602	HEA	CHD-C1D	4.41	1.46	1.35
31	a	602	HEA	C3D-C2D	4.36	1.46	1.36
31	a	602	HEA	C3A-C2A	4.34	1.46	1.40
25	b	303	PEF	O2-C10	4.34	1.46	1.34
31	n	602	HEA	C3C-C2C	4.33	1.46	1.40
25	J	101	PEF	O3-C30	4.31	1.45	1.33
31	n	603	HEA	CHC-C4B	4.31	1.46	1.35
26	C	602	HEM	C1B-NB	-4.30	1.32	1.40
25	E	303	PEF	O3-C30	4.30	1.45	1.33
26	N	602	HEM	C1B-NB	-4.29	1.32	1.40
24	S	101	CDL	OA6-CA5	4.27	1.46	1.34
27	r	202	PCF	O31-C31	4.26	1.45	1.33
25	E	302	PEF	O2-C10	4.25	1.46	1.34
24	N	604	CDL	OB8-CB7	4.25	1.45	1.33
26	C	602	HEM	C4D-ND	-4.23	1.33	1.40
25	C	605	PEF	O2-C10	4.22	1.46	1.34
31	n	602	HEA	C3A-C2A	4.22	1.46	1.40
24	S	101	CDL	OB8-CB7	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	603	HEA	C3A-C2A	4.22	1.46	1.40
24	H	101	CDL	OB8-CB7	4.21	1.45	1.33
24	A	501	CDL	OA8-CA7	4.20	1.45	1.33
25	n	607	PEF	O3-C30	4.18	1.45	1.33
27	e	202	PCF	O31-C31	4.18	1.45	1.33
25	p	301	PEF	O3-C30	4.17	1.45	1.33
25	o	302	PEF	O3-C30	4.17	1.45	1.33
27	H	103	PCF	O31-C31	4.15	1.45	1.33
25	a	606	PEF	O3-C30	4.15	1.45	1.33
25	o	302	PEF	O2-C10	4.15	1.46	1.34
25	L	502	PEF	O3-C30	4.14	1.45	1.33
25	O	402	PEF	O2-C10	4.14	1.46	1.34
25	c	302	PEF	O2-C10	4.14	1.46	1.34
25	b	302	PEF	O3-C30	4.14	1.45	1.33
27	I	101	PCF	O31-C31	4.13	1.45	1.33
25	n	607	PEF	O2-C10	4.13	1.45	1.34
24	C	603	CDL	OA6-CA5	4.13	1.45	1.34
25	S	102	PEF	O2-C10	4.12	1.45	1.34
24	C	603	CDL	OB6-CB5	4.12	1.45	1.34
25	n	606	PEF	O2-C10	4.11	1.45	1.34
25	c	302	PEF	O3-C30	4.11	1.45	1.33
25	r	201	PEF	O3-C30	4.11	1.45	1.33
25	E	304	PEF	O2-C10	4.10	1.45	1.34
25	n	606	PEF	O3-C30	4.09	1.45	1.33
25	N	605	PEF	O2-C10	4.08	1.45	1.34
24	C	603	CDL	OA8-CA7	4.08	1.45	1.33
24	A	501	CDL	OA6-CA5	4.07	1.45	1.34
24	S	101	CDL	OB6-CB5	4.07	1.45	1.34
25	n	608	PEF	O3-C30	4.05	1.45	1.33
25	b	303	PEF	O3-C30	4.05	1.45	1.33
25	J	101	PEF	O2-C10	4.04	1.45	1.34
25	O	402	PEF	O3-C30	4.04	1.45	1.33
25	C	604	PEF	O2-C10	4.04	1.45	1.34
24	L	501	CDL	OA6-CA5	4.04	1.45	1.34
25	n	608	PEF	O2-C10	4.04	1.45	1.34
25	A	502	PEF	O3-C30	4.02	1.45	1.33
25	C	604	PEF	O3-C30	4.02	1.45	1.33
25	E	302	PEF	O3-C30	4.01	1.45	1.33
31	a	602	HEA	C3C-C2C	4.00	1.45	1.40
26	C	601	HEM	C1B-NB	-4.00	1.33	1.40
24	A	501	CDL	OB8-CB7	4.00	1.45	1.33
27	I	101	PCF	O21-C21	4.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	502	PEF	O2-C10	3.99	1.45	1.34
25	b	302	PEF	O2-C10	3.98	1.45	1.34
26	N	602	HEM	C4D-ND	-3.98	1.33	1.40
24	N	603	CDL	OB6-CB5	3.98	1.45	1.34
27	e	202	PCF	O21-C21	3.98	1.45	1.34
24	L	501	CDL	OB8-CB7	3.96	1.44	1.33
27	H	103	PCF	O21-C21	3.96	1.45	1.34
25	H	102	PEF	O2-C10	3.96	1.45	1.34
24	H	101	CDL	OA6-CA5	3.94	1.45	1.34
27	r	202	PCF	O21-C21	3.94	1.45	1.34
27	C	606	PCF	O21-C21	3.94	1.45	1.34
25	a	606	PEF	O2-C10	3.94	1.45	1.34
25	c	301	PEF	O3-C30	3.92	1.44	1.33
25	l	101	PEF	O2-C10	3.92	1.45	1.34
24	N	603	CDL	OA8-CA7	3.92	1.44	1.33
25	L	502	PEF	O2-C10	3.91	1.45	1.34
25	c	301	PEF	O2-C10	3.89	1.45	1.34
27	T	101	PCF	O21-C21	3.89	1.45	1.34
24	L	501	CDL	OB6-CB5	3.88	1.45	1.34
27	T	101	PCF	O31-C31	3.88	1.44	1.33
24	H	101	CDL	OB6-CB5	3.87	1.45	1.34
25	H	102	PEF	O3-C30	3.87	1.44	1.33
25	N	605	PEF	O3-C30	3.87	1.44	1.33
24	D	402	CDL	OB8-CB7	3.87	1.44	1.33
24	N	604	CDL	OA6-CA5	3.86	1.45	1.34
24	N	604	CDL	OB6-CB5	3.86	1.45	1.34
25	S	102	PEF	O3-C30	3.85	1.44	1.33
25	C	605	PEF	O3-C30	3.85	1.44	1.33
25	p	301	PEF	O2-C10	3.85	1.45	1.34
24	S	101	CDL	OA8-CA7	3.85	1.44	1.33
25	l	101	PEF	O3-C30	3.84	1.44	1.33
25	r	201	PEF	O2-C10	3.83	1.45	1.34
25	N	606	PEF	O2-C10	3.83	1.45	1.34
25	E	304	PEF	O3-C30	3.81	1.44	1.33
24	D	402	CDL	OB6-CB5	3.80	1.45	1.34
25	e	201	PEF	O3-C30	3.80	1.44	1.33
24	A	501	CDL	OB6-CB5	3.78	1.45	1.34
27	C	606	PCF	O31-C31	3.77	1.44	1.33
24	N	603	CDL	OA6-CA5	3.77	1.44	1.34
24	N	604	CDL	OA8-CA7	3.74	1.44	1.33
26	N	601	HEM	C1B-NB	-3.74	1.33	1.40
24	D	402	CDL	OA6-CA5	3.73	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	603	CDL	OB8-CB7	3.72	1.44	1.33
24	H	101	CDL	OA8-CA7	3.72	1.44	1.33
25	N	606	PEF	O3-C30	3.71	1.44	1.33
28	D	401	HEC	C3C-C4C	3.70	1.49	1.43
28	O	401	HEC	C3C-C4C	3.70	1.49	1.43
25	e	201	PEF	O2-C10	3.69	1.44	1.34
31	a	603	HEA	C3C-C2C	3.68	1.45	1.40
25	E	303	PEF	O2-C10	3.67	1.44	1.34
24	D	402	CDL	OA8-CA7	3.66	1.44	1.33
28	D	401	HEC	C4B-C3B	3.65	1.49	1.43
27	N	607	PCF	O31-C31	3.64	1.44	1.33
28	O	401	HEC	C4B-C3B	3.63	1.49	1.43
24	C	603	CDL	OB8-CB7	3.55	1.43	1.33
26	C	601	HEM	C4D-ND	-3.54	1.34	1.40
31	a	602	HEA	C1D-ND	-3.48	1.34	1.40
31	a	603	HEA	C1D-ND	-3.48	1.34	1.40
27	N	607	PCF	O21-C21	3.43	1.44	1.34
31	n	602	HEA	C1D-ND	-3.41	1.34	1.40
31	a	603	HEA	C4B-NB	-3.39	1.34	1.40
31	n	603	HEA	C4B-NB	-3.34	1.34	1.40
31	a	602	HEA	C4B-NB	-3.30	1.34	1.40
26	N	601	HEM	C4D-ND	-3.29	1.34	1.40
31	n	603	HEA	C1D-ND	-3.19	1.34	1.40
31	n	602	HEA	C4B-NB	-3.05	1.35	1.40
28	D	401	HEC	C3D-C2D	2.98	1.46	1.37
28	O	401	HEC	C3D-C2D	2.92	1.46	1.37
28	D	401	HEC	C2A-C3A	2.89	1.46	1.37
28	O	401	HEC	C2A-C3A	2.80	1.46	1.37
31	n	603	HEA	FE-NB	2.77	2.10	1.96
31	n	602	HEA	FE-NB	2.76	2.10	1.96
31	n	603	HEA	FE-ND	2.75	2.10	1.96
31	a	603	HEA	FE-ND	2.73	2.10	1.96
31	a	603	HEA	FE-NB	2.71	2.10	1.96
31	a	602	HEA	FE-NB	2.71	2.10	1.96
26	C	601	HEM	C1D-ND	-2.70	1.33	1.38
31	a	602	HEA	FE-ND	2.69	2.10	1.96
26	N	601	HEM	C1D-ND	-2.69	1.33	1.38
26	N	601	HEM	FE-NB	2.69	2.10	1.96
31	n	602	HEA	FE-ND	2.68	2.10	1.96
26	C	601	HEM	FE-NB	2.67	2.10	1.96
26	C	602	HEM	C4B-NB	-2.63	1.33	1.38
26	C	602	HEM	C1D-ND	-2.57	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	602	HEM	C1D-ND	-2.56	1.33	1.38
26	N	602	HEM	FE-NB	2.55	2.09	1.96
31	n	602	HEA	C4B-C3B	2.55	1.48	1.44
26	N	602	HEM	C4B-NB	-2.53	1.33	1.38
24	L	501	CDL	OA8-CA7	2.50	1.45	1.33
28	D	401	HEC	C2A-C1A	2.50	1.48	1.42
26	C	602	HEM	FE-NB	2.50	2.09	1.96
31	a	603	HEA	C1B-NB	-2.46	1.33	1.38
31	a	602	HEA	C4B-C3B	2.43	1.48	1.44
31	a	602	HEA	C1B-NB	-2.43	1.33	1.38
26	C	601	HEM	C4B-NB	-2.43	1.33	1.38
28	D	401	HEC	C1C-CHC	2.42	1.47	1.41
26	C	602	HEM	FE-ND	-2.42	1.84	1.96
27	N	607	PCF	O21-C2	-2.40	1.40	1.46
26	N	602	HEM	FE-ND	-2.39	1.85	1.96
28	O	401	HEC	C2A-C1A	2.37	1.47	1.42
31	n	603	HEA	C2A-C1A	2.36	1.47	1.42
31	n	603	HEA	C4D-ND	-2.33	1.34	1.38
31	n	602	HEA	C2A-C1A	2.31	1.47	1.42
28	O	401	HEC	C1C-CHC	2.29	1.47	1.41
26	N	601	HEM	C4B-NB	-2.29	1.34	1.38
31	a	603	HEA	C4D-ND	-2.29	1.34	1.38
31	n	603	HEA	C4B-C3B	2.28	1.48	1.44
31	a	602	HEA	C2A-C1A	2.27	1.47	1.42
26	C	602	HEM	C1B-C2B	-2.24	1.40	1.44
26	N	602	HEM	C1B-C2B	-2.23	1.40	1.44
31	n	602	HEA	C4D-ND	-2.21	1.34	1.38
28	O	401	HEC	C4D-CHA	2.20	1.47	1.41
31	n	603	HEA	C1B-NB	-2.20	1.34	1.38
28	D	401	HEC	C4D-CHA	2.20	1.47	1.41
28	O	401	HEC	C1D-CHD	2.19	1.47	1.41
31	n	602	HEA	C1C-CHC	2.18	1.47	1.41
31	n	602	HEA	C1B-NB	-2.16	1.34	1.38
31	a	603	HEA	C4B-C3B	2.15	1.48	1.44
26	C	601	HEM	FE-ND	-2.10	1.86	1.96
31	n	603	HEA	C4C-CHD	2.08	1.46	1.41
31	a	602	HEA	C4D-ND	-2.08	1.34	1.38
26	N	601	HEM	FE-ND	-2.06	1.86	1.96
26	N	601	HEM	C4D-C3D	2.04	1.48	1.45
31	a	602	HEA	C1C-CHC	2.04	1.46	1.41
31	a	603	HEA	C4C-CHD	2.04	1.46	1.41
25	p	301	PEF	O2-C2	-2.04	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	604	CDL	OA6-CA4	-2.02	1.41	1.46

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C13-C12-C11	-7.92	102.46	114.35
31	a	603	HEA	C3D-C4D-ND	7.39	117.51	110.36
31	n	603	HEA	C3D-C4D-ND	6.78	116.92	110.36
31	a	602	HEA	C2B-C1B-NB	6.55	117.72	109.88
28	D	401	HEC	C1D-C2D-C3D	-6.51	102.47	107.00
31	n	602	HEA	C3D-C4D-ND	6.32	116.47	110.36
28	O	401	HEC	C1D-C2D-C3D	-6.26	102.64	107.00
26	N	601	HEM	CAD-C3D-C4D	6.26	135.59	124.66
31	a	602	HEA	C3D-C4D-ND	6.12	116.28	110.36
26	C	601	HEM	CAD-C3D-C4D	6.07	135.27	124.66
31	a	603	HEA	C2B-C1B-NB	5.98	117.04	109.88
31	n	603	HEA	C2B-C1B-NB	5.77	116.79	109.88
31	n	602	HEA	C2B-C1B-NB	5.69	116.70	109.88
31	n	603	HEA	C2D-C1D-ND	5.66	116.54	109.84
31	n	603	HEA	C3B-C4B-NB	5.61	116.48	109.84
31	a	602	HEA	C26-C15-C16	5.52	124.56	115.27
26	N	601	HEM	CHD-C1D-ND	5.49	130.40	124.43
26	N	601	HEM	CHC-C4B-NB	5.46	130.36	124.43
31	a	602	HEA	CBA-CAA-C2A	-5.43	103.45	112.60
31	n	602	HEA	C2D-C1D-ND	5.41	116.25	109.84
31	a	603	HEA	C2D-C1D-ND	5.38	116.22	109.84
27	C	606	PCF	O21-C21-C22	5.30	122.93	111.50
26	C	602	HEM	CHC-C4B-NB	5.26	130.15	124.43
31	n	602	HEA	C13-C12-C11	-5.26	106.45	114.35
31	a	602	HEA	C2D-C1D-ND	5.22	116.03	109.84
26	N	602	HEM	CHC-C4B-NB	5.19	130.07	124.43
31	a	603	HEA	C3B-C4B-NB	5.16	115.96	109.84
26	C	601	HEM	CHC-C4B-NB	4.88	129.74	124.43
24	D	402	CDL	OB6-CB5-C51	4.79	121.83	111.50
24	A	501	CDL	OA6-CA5-C11	4.73	121.70	111.50
31	n	602	HEA	C3B-C4B-NB	4.73	115.44	109.84
26	N	602	HEM	CHD-C1D-ND	4.71	129.54	124.43
31	n	603	HEA	C1D-C2D-C3D	-4.68	102.04	106.96
31	n	603	HEA	CMC-C2C-C3C	4.63	133.34	124.68
26	C	601	HEM	CHD-C1D-ND	4.63	129.46	124.43
25	E	304	PEF	O2-C10-C11	4.60	121.41	111.50
26	N	601	HEM	CAD-C3D-C2D	-4.54	119.42	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	607	PEF	O2-C10-C11	4.52	121.23	111.50
31	n	602	HEA	C3C-C4C-NC	4.50	115.03	109.21
25	n	606	PEF	O2-C10-C11	4.44	121.07	111.50
31	n	603	HEA	C13-C12-C11	-4.43	107.69	114.35
28	D	401	HEC	CMB-C2B-C3B	4.40	131.00	125.82
24	L	501	CDL	OA6-CA5-C11	4.40	120.98	111.50
25	L	502	PEF	O2-C10-C11	4.39	120.96	111.50
25	e	201	PEF	C2-O2-C10	-4.39	106.99	117.79
27	I	101	PCF	O21-C21-C22	4.37	120.91	111.50
31	n	602	HEA	CMC-C2C-C3C	4.37	132.85	124.68
26	C	602	HEM	CHD-C1D-ND	4.36	129.17	124.43
24	C	603	CDL	OB6-CB5-C51	4.34	120.85	111.50
31	n	602	HEA	C1D-C2D-C3D	-4.33	102.40	106.96
31	a	603	HEA	C1D-C2D-C3D	-4.31	102.42	106.96
24	N	603	CDL	OA6-CA5-C11	4.31	120.79	111.50
24	S	101	CDL	OB6-CB5-C51	4.30	120.77	111.50
24	N	604	CDL	OB6-CB5-C51	4.27	120.71	111.50
25	N	606	PEF	O2-C10-C11	4.26	120.69	111.50
26	C	601	HEM	CAD-C3D-C2D	-4.26	119.94	127.88
28	O	401	HEC	CMB-C2B-C3B	4.25	130.81	125.82
31	n	602	HEA	C26-C15-C16	4.23	122.39	115.27
24	C	603	CDL	OA6-CA5-C11	4.18	120.51	111.50
27	e	202	PCF	O21-C21-C22	4.18	120.50	111.50
25	H	102	PEF	O2-C10-C11	4.15	120.45	111.50
31	a	602	HEA	C1B-C2B-C3B	-4.15	101.84	106.80
31	a	602	HEA	C3B-C4B-NB	4.14	114.74	109.84
31	a	602	HEA	C3C-C4C-NC	4.13	114.55	109.21
24	A	501	CDL	OB6-CB5-C51	4.13	120.39	111.50
24	H	101	CDL	OA6-CA5-C11	4.12	120.39	111.50
24	N	603	CDL	OB6-CB5-C51	4.12	120.38	111.50
31	a	603	HEA	C13-C12-C11	-4.08	108.22	114.35
25	S	102	PEF	O2-C10-C11	4.06	120.26	111.50
26	C	602	HEM	C1B-NB-C4B	4.06	109.26	105.07
25	l	101	PEF	O2-C10-C11	4.04	120.20	111.50
31	n	603	HEA	C3C-C4C-NC	4.02	114.41	109.21
25	c	301	PEF	O2-C10-C11	3.98	120.07	111.50
25	C	605	PEF	O2-C10-C11	3.97	120.05	111.50
25	O	402	PEF	O2-C10-C11	3.97	120.05	111.50
26	C	602	HEM	CHA-C4D-ND	3.96	129.27	124.38
25	A	502	PEF	O2-C10-C11	3.96	120.03	111.50
24	S	101	CDL	OA6-CA5-C11	3.95	120.02	111.50
25	b	302	PEF	O2-C10-C11	3.93	119.97	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	303	PEF	O2-C10-C11	3.92	119.96	111.50
25	o	302	PEF	O2-C10-C11	3.92	119.94	111.50
25	E	303	PEF	C2-O2-C10	-3.91	108.17	117.79
27	r	202	PCF	O21-C21-C22	3.90	119.90	111.50
31	n	602	HEA	CAD-CBD-CGD	-3.89	105.23	113.60
24	N	604	CDL	OA6-CA5-C11	3.89	119.87	111.50
25	J	101	PEF	O2-C10-C11	3.86	119.83	111.50
31	a	602	HEA	C1D-C2D-C3D	-3.85	102.90	106.96
25	n	608	PEF	O2-C10-C11	3.85	119.81	111.50
31	a	603	HEA	C1B-C2B-C3B	-3.85	102.19	106.80
25	E	303	PEF	O2-C10-C11	3.85	119.80	111.50
24	D	402	CDL	OB8-CB7-C71	3.85	121.47	111.38
26	N	602	HEM	CHA-C4D-ND	3.84	129.13	124.38
25	E	302	PEF	O2-C10-C11	3.80	119.69	111.50
26	N	602	HEM	C1B-NB-C4B	3.79	108.98	105.07
25	c	302	PEF	O2-C10-C11	3.78	119.66	111.50
25	e	201	PEF	O2-C10-C11	3.77	119.63	111.50
26	C	602	HEM	CHB-C1B-NB	3.75	129.02	124.38
25	N	605	PEF	O2-C10-C11	3.74	119.55	111.50
24	L	501	CDL	OB6-CB5-C51	3.72	119.53	111.50
27	N	607	PCF	O21-C21-C22	3.71	119.50	111.50
26	N	601	HEM	C1B-NB-C4B	3.69	108.89	105.07
24	H	101	CDL	OB6-CB5-C51	3.68	119.43	111.50
27	T	101	PCF	O21-C21-C22	3.67	119.42	111.50
26	N	601	HEM	CHD-C1D-C2D	-3.67	119.25	124.98
31	n	603	HEA	C1B-C2B-C3B	-3.67	102.41	106.80
24	N	603	CDL	CA4-OA6-CA5	-3.66	108.77	117.79
25	C	604	PEF	O2-C10-C11	3.66	119.39	111.50
25	r	201	PEF	O2-C10-C11	3.60	119.26	111.50
31	a	602	HEA	CHB-C1B-C2B	-3.58	119.38	124.98
28	O	401	HEC	CMC-C2C-C3C	3.57	130.02	125.82
31	a	602	HEA	CAD-C3D-C4D	3.55	130.87	124.66
31	n	602	HEA	C1B-C2B-C3B	-3.55	102.55	106.80
25	p	301	PEF	O2-C10-C11	3.53	119.10	111.50
31	a	603	HEA	CAD-CBD-CGD	-3.52	106.04	113.60
31	a	603	HEA	C4D-C3D-C2D	-3.51	101.78	106.90
31	a	603	HEA	CMC-C2C-C3C	3.51	131.24	124.68
26	C	601	HEM	CBD-CAD-C3D	3.51	122.37	112.63
31	a	602	HEA	CAD-CBD-CGD	-3.51	106.06	113.60
24	A	501	CDL	OB8-CB7-C71	3.47	122.81	111.91
31	a	603	HEA	C3C-C4C-NC	3.47	113.70	109.21
26	C	601	HEM	CHB-C1B-NB	3.47	128.66	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	603	HEA	CAD-CBD-CGD	-3.46	106.16	113.60
26	N	601	HEM	CBD-CAD-C3D	3.45	122.22	112.63
26	N	602	HEM	CHB-C1B-NB	3.43	128.61	124.38
26	C	601	HEM	C1B-NB-C4B	3.41	108.60	105.07
27	N	607	PCF	O31-C31-C32	3.40	122.58	111.91
28	O	401	HEC	CAA-CBA-CGA	-3.38	104.28	113.76
25	l	101	PEF	C2-O2-C10	-3.34	109.57	117.79
31	a	602	HEA	CMC-C2C-C3C	3.32	130.90	124.68
31	a	602	HEA	C4D-C3D-C2D	-3.31	102.07	106.90
25	H	102	PEF	O3-C30-C31	3.29	122.22	111.91
25	E	302	PEF	O3-C30-C31	3.28	122.20	111.91
31	a	602	HEA	CHA-C4D-ND	-3.27	120.88	124.43
27	T	101	PCF	C3-C2-C1	-3.24	104.12	111.79
28	D	401	HEC	CAA-CBA-CGA	-3.23	104.70	113.76
28	D	401	HEC	CMA-C3A-C2A	3.21	130.99	124.94
25	J	101	PEF	O3-C30-C31	3.21	121.98	111.91
24	D	402	CDL	OA6-CA5-C11	3.20	118.40	111.50
26	C	601	HEM	CHD-C1D-C2D	-3.20	119.99	124.98
25	n	606	PEF	O3-C30-C31	3.19	121.91	111.91
27	N	607	PCF	C2-O21-C21	-3.18	109.96	117.79
31	a	602	HEA	C16-C15-C14	-3.18	114.69	121.12
31	n	603	HEA	C4D-C3D-C2D	-3.17	102.28	106.90
25	a	606	PEF	O2-C10-C11	3.12	118.22	111.50
31	n	602	HEA	C4D-C3D-C2D	-3.10	102.38	106.90
27	C	606	PCF	O31-C31-C32	3.10	121.64	111.91
31	n	602	HEA	OMA-CMA-C3A	-3.09	118.18	124.91
24	C	603	CDL	CB4-OB6-CB5	-3.08	110.20	117.79
24	A	501	CDL	CB4-OB6-CB5	-3.07	110.23	117.79
25	r	201	PEF	C2-O2-C10	-3.06	110.27	117.79
24	H	101	CDL	OB8-CB7-C71	3.05	121.49	111.91
31	n	603	HEA	C4B-C3B-C2B	-3.05	102.20	107.41
24	C	603	CDL	OA8-CA7-C31	3.05	121.48	111.91
26	N	601	HEM	CHB-C1B-NB	3.04	128.13	124.38
31	a	602	HEA	C27-C19-C20	3.02	120.35	115.27
27	T	101	PCF	O31-C31-C32	3.00	121.32	111.91
31	n	603	HEA	CHA-C4D-ND	-2.98	121.19	124.43
26	N	602	HEM	CHD-C1D-C2D	-2.95	120.38	124.98
31	a	603	HEA	C4B-C3B-C2B	-2.92	102.42	107.41
31	a	603	HEA	C27-C19-C20	2.92	120.18	115.27
31	a	603	HEA	C1D-ND-C4D	-2.90	102.07	105.07
25	C	604	PEF	C2-O2-C10	-2.89	110.68	117.79
26	C	601	HEM	CBA-CAA-C2A	-2.88	107.70	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	603	HEA	C4B-NB-C1B	-2.87	102.11	105.07
27	H	103	PCF	O31-C31-C32	2.84	120.82	111.91
25	N	605	PEF	O3-C30-C31	2.83	120.78	111.91
26	N	602	HEM	CAD-CBD-CGD	-2.83	107.52	113.60
25	b	303	PEF	O3-C30-C31	2.82	120.75	111.91
24	S	101	CDL	OA8-CA7-C31	2.81	120.73	111.91
24	H	101	CDL	OA8-CA7-C31	2.81	120.73	111.91
25	n	607	PEF	O3-C30-C31	2.79	120.68	111.91
24	N	604	CDL	OB8-CB7-C71	2.79	120.66	111.91
25	A	502	PEF	O3-C30-C31	2.78	120.63	111.91
25	O	402	PEF	O3-C30-C31	2.78	120.62	111.91
26	N	602	HEM	C4D-ND-C1D	2.78	107.94	105.07
25	E	303	PEF	O3-C30-C31	2.78	120.62	111.91
31	n	602	HEA	C4B-C3B-C2B	-2.77	102.67	107.41
31	n	603	HEA	C1D-ND-C4D	-2.77	102.21	105.07
28	D	401	HEC	CMC-C2C-C3C	2.77	129.07	125.82
27	N	607	PCF	O31-C31-O32	-2.76	116.64	123.59
25	a	606	PEF	O3-C30-C31	2.75	120.53	111.91
24	C	603	CDL	OB8-CB6-CB4	-2.75	100.44	108.43
27	e	202	PCF	O31-C31-C32	2.75	120.52	111.91
24	D	402	CDL	OA8-CA7-C31	2.74	120.51	111.91
25	E	304	PEF	O3-C30-C31	2.73	120.48	111.91
31	n	602	HEA	C17-C18-C19	-2.73	121.10	127.66
24	S	101	CDL	OB8-CB7-C71	2.72	120.44	111.91
25	o	302	PEF	O3-C30-C31	2.71	120.42	111.91
31	n	602	HEA	CBA-CAA-C2A	-2.71	108.04	112.60
25	l	101	PEF	O3-C30-C31	2.71	120.41	111.91
25	b	302	PEF	O3-C30-C31	2.70	120.39	111.91
31	a	603	HEA	CBA-CAA-C2A	-2.70	108.06	112.60
31	a	602	HEA	C4B-NB-C1B	-2.70	102.29	105.07
26	C	602	HEM	CHD-C1D-C2D	-2.70	120.77	124.98
25	S	102	PEF	C2-O2-C10	-2.68	111.18	117.79
25	C	604	PEF	O3-C30-C31	2.68	120.31	111.91
27	I	101	PCF	C3-C2-C1	-2.67	105.47	111.79
24	N	603	CDL	CB4-OB6-CB5	-2.67	111.22	117.79
31	a	603	HEA	CHA-C4D-ND	-2.67	121.53	124.43
31	n	603	HEA	CMB-C2B-C1B	2.66	129.10	125.04
31	a	602	HEA	C12-C13-C14	-2.66	105.20	112.23
25	p	301	PEF	O3-C30-C31	2.66	120.25	111.91
31	a	603	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
24	A	501	CDL	OA8-CA7-C31	2.64	120.20	111.91
28	O	401	HEC	CMA-C3A-C2A	2.63	129.91	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	p	301	PEF	C2-O2-C10	-2.63	111.32	117.79
31	a	603	HEA	C4B-NB-C1B	-2.63	102.36	105.07
25	N	606	PEF	C2-O2-C10	-2.62	111.33	117.79
26	C	602	HEM	C4D-ND-C1D	2.62	107.78	105.07
25	N	605	PEF	C2-O2-C10	-2.61	111.36	117.79
31	a	603	HEA	CHB-C1B-C2B	-2.61	120.90	124.98
28	D	401	HEC	C4C-C3C-C2C	-2.61	103.53	106.35
24	N	603	CDL	OB8-CB7-C71	2.61	120.10	111.91
26	N	602	HEM	CMC-C2C-C3C	2.60	129.54	124.68
25	N	606	PEF	O3-C30-C31	2.57	119.96	111.91
31	a	602	HEA	C13-C14-C15	-2.56	121.48	127.66
31	n	603	HEA	CHB-C1B-NB	-2.56	121.65	124.43
28	D	401	HEC	CMD-C2D-C3D	2.54	129.74	124.94
31	a	603	HEA	C13-C14-C15	-2.53	121.56	127.66
24	L	501	CDL	OB8-CB7-C71	2.53	119.86	111.91
31	a	603	HEA	CAD-C3D-C2D	2.53	132.59	127.88
31	a	602	HEA	C17-C18-C19	-2.53	121.58	127.66
25	H	102	PEF	C2-O2-C10	-2.52	111.58	117.79
28	O	401	HEC	CAD-CBD-CGD	-2.52	106.71	113.76
27	H	103	PCF	C3-C2-C1	-2.51	105.85	111.79
24	C	603	CDL	CA4-OA6-CA5	-2.51	111.61	117.79
24	L	501	CDL	CB4-OB6-CB5	-2.51	111.61	117.79
31	a	602	HEA	CMD-C2D-C1D	2.51	128.85	125.04
31	n	602	HEA	C27-C19-C20	2.51	119.48	115.27
31	n	603	HEA	C13-C14-C15	-2.50	121.64	127.66
31	n	602	HEA	C1D-ND-C4D	-2.50	102.49	105.07
27	H	103	PCF	O21-C21-C22	2.50	116.89	111.50
25	c	301	PEF	O3-C30-C31	2.50	119.75	111.91
27	I	101	PCF	O31-C31-C32	2.49	119.73	111.91
26	C	602	HEM	CAD-CBD-CGD	-2.49	108.25	113.60
28	D	401	HEC	CAD-CBD-CGD	-2.47	106.83	113.76
25	L	502	PEF	O3-C30-C31	2.46	119.63	111.91
31	a	602	HEA	CMB-C2B-C1B	2.45	128.78	125.04
25	r	201	PEF	O3-C30-C31	2.45	119.59	111.91
24	S	101	CDL	CB4-OB6-CB5	-2.43	111.80	117.79
25	n	606	PEF	C32-C31-C30	-2.43	104.79	113.62
24	N	603	CDL	OA8-CA7-C31	2.42	119.52	111.91
24	D	402	CDL	OB8-CB7-OB9	-2.42	117.48	123.59
24	L	501	CDL	CA4-OA6-CA5	-2.42	111.83	117.79
31	n	602	HEA	CHA-C4D-ND	-2.42	121.81	124.43
24	H	101	CDL	CA4-OA6-CA5	-2.41	111.85	117.79
27	T	101	PCF	O31-C31-O32	-2.41	117.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	e	202	PCF	C2-O21-C21	-2.40	111.88	117.79
25	H	102	PEF	O3-C30-O5	-2.40	117.53	123.59
28	D	401	HEC	CBD-CAD-C3D	-2.40	108.53	112.62
24	N	604	CDL	OA8-CA7-C31	2.39	119.39	111.91
24	A	501	CDL	OB8-CB7-OB9	-2.38	117.58	123.59
31	n	602	HEA	CHB-C1B-NB	-2.37	121.85	124.43
25	A	502	PEF	O3-C30-O5	-2.37	117.61	123.59
26	C	602	HEM	CHB-C1B-C2B	-2.37	120.16	126.72
24	N	604	CDL	CB2-C1-CA2	-2.37	105.81	112.79
31	a	602	HEA	C27-C19-C18	-2.37	117.60	123.68
31	a	602	HEA	C4B-C3B-C2B	-2.37	103.37	107.41
26	N	602	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
31	n	602	HEA	CMB-C2B-C1B	2.36	128.64	125.04
31	n	602	HEA	C4B-NB-C1B	-2.36	102.64	105.07
31	n	603	HEA	C27-C19-C20	2.36	119.23	115.27
31	n	602	HEA	CAD-C3D-C4D	2.35	128.77	124.66
25	E	304	PEF	C2-O2-C10	-2.33	112.05	117.79
24	S	101	CDL	OA8-CA7-OA9	-2.32	117.74	123.59
31	n	603	HEA	CHD-C1D-C2D	-2.32	120.31	126.72
25	e	201	PEF	O3-C30-C31	2.31	119.16	111.91
26	N	602	HEM	CHB-C1B-C2B	-2.29	120.38	126.72
27	C	606	PCF	O31-C31-O32	-2.29	117.81	123.59
25	n	608	PEF	O3-C30-C31	2.29	119.10	111.91
31	n	603	HEA	CBA-CAA-C2A	-2.29	108.74	112.60
25	L	502	PEF	C2-O2-C10	-2.29	112.16	117.79
31	a	602	HEA	C1D-ND-C4D	-2.29	102.71	105.07
24	H	101	CDL	OA8-CA7-OA9	-2.28	117.83	123.59
24	D	402	CDL	CB4-OB6-CB5	-2.28	112.18	117.79
31	n	602	HEA	C25-C23-C24	2.28	119.64	114.60
31	n	602	HEA	CHD-C1D-C2D	-2.27	120.45	126.72
31	n	602	HEA	CHB-C1B-C2B	-2.26	121.44	124.98
31	a	603	HEA	CHB-C1B-NB	-2.26	121.97	124.43
28	O	401	HEC	CBD-CAD-C3D	-2.25	108.78	112.62
24	H	101	CDL	CB4-OB6-CB5	-2.25	112.25	117.79
25	S	102	PEF	O3-C30-C31	2.25	118.96	111.91
25	E	302	PEF	O3-C30-O5	-2.24	117.93	123.59
24	S	101	CDL	OA6-CA4-CA6	2.24	116.51	108.40
27	H	103	PCF	O21-C2-C1	2.23	116.46	108.40
28	O	401	HEC	CMD-C2D-C3D	2.22	129.13	124.94
31	a	603	HEA	C25-C23-C24	2.22	119.50	114.60
25	o	302	PEF	C2-O2-C10	-2.22	112.33	117.79
31	a	602	HEA	C21-C22-C23	-2.21	120.18	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	603	HEA	CHB-C1B-C2B	-2.21	121.53	124.98
27	C	606	PCF	C2-O21-C21	-2.20	112.37	117.79
31	a	603	HEA	CAA-CBA-CGA	-2.20	107.59	113.76
31	n	603	HEA	C25-C23-C24	2.20	119.46	114.60
25	b	302	PEF	C2-O2-C10	-2.20	112.39	117.79
25	C	605	PEF	O3-C30-C31	2.19	118.79	111.91
31	a	602	HEA	CHD-C1D-C2D	-2.19	120.67	126.72
25	l	101	PEF	O3-C30-O5	-2.18	118.08	123.59
26	C	601	HEM	CHB-C1B-C2B	-2.17	120.73	126.72
25	N	606	PEF	O3-C30-O5	-2.16	118.13	123.59
26	N	601	HEM	CBA-CAA-C2A	-2.15	108.94	112.62
24	S	101	CDL	CA6-CA4-CA3	-2.15	106.69	111.79
27	C	606	PCF	O21-C21-O22	-2.15	118.51	123.70
25	J	101	PEF	O3-C30-O5	-2.15	118.17	123.59
31	a	602	HEA	C21-C20-C19	-2.15	105.92	112.98
28	O	401	HEC	C4C-C3C-C2C	-2.14	104.04	106.35
25	a	606	PEF	C3-C2-C1	-2.14	106.73	111.79
26	C	602	HEM	O2A-CGA-CBA	2.14	120.89	114.03
24	S	101	CDL	OB4-PB2-OB3	2.13	122.78	112.24
24	N	603	CDL	OB4-PB2-OB3	2.13	122.77	112.24
26	C	602	HEM	CMB-C2B-C1B	-2.13	121.80	125.04
26	C	602	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
31	n	602	HEA	CHA-C4D-C3D	-2.12	121.72	124.84
31	a	603	HEA	CMB-C2B-C1B	2.12	128.26	125.04
31	a	603	HEA	CHD-C1D-C2D	-2.11	120.88	126.72
25	c	302	PEF	O3-C30-C31	2.11	118.51	111.91
31	n	602	HEA	CAA-CBA-CGA	-2.10	107.86	113.76
27	C	606	PCF	O14-P-O12	2.10	122.60	112.24
24	C	603	CDL	OB8-CB7-C71	2.10	118.48	111.91
24	H	101	CDL	OB4-PB2-OB3	2.09	122.57	112.24
25	n	606	PEF	C2-O2-C10	-2.09	112.65	117.79
24	N	604	CDL	CB4-OB6-CB5	-2.08	112.67	117.79
25	O	402	PEF	C2-O2-C10	-2.08	112.67	117.79
31	n	602	HEA	C12-C13-C14	-2.07	106.76	112.23
26	N	601	HEM	C4D-ND-C1D	2.07	107.21	105.07
27	I	101	PCF	O21-C21-O22	-2.07	118.71	123.70
25	n	607	PEF	O2-C10-O4	-2.06	118.72	123.70
27	r	202	PCF	O31-C31-C32	2.06	118.38	111.91
25	o	302	PEF	O3-C30-O5	-2.06	118.40	123.59
24	D	402	CDL	OB6-CB5-OB7	-2.05	118.75	123.70
24	A	501	CDL	OA6-CA5-OA7	-2.04	118.77	123.70
25	e	201	PEF	C12-C11-C10	-2.04	106.20	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	602	HEA	CMD-C2D-C1D	2.03	128.14	125.04
31	n	603	HEA	CAA-CBA-CGA	-2.03	108.06	113.76
26	C	601	HEM	O2D-CGD-CBD	2.03	120.55	114.03
31	n	602	HEA	C13-C14-C15	-2.03	122.78	127.66
25	b	303	PEF	O3-C30-O5	-2.03	118.48	123.59
31	a	603	HEA	CHC-C4B-NB	-2.01	121.89	124.38
26	C	601	HEM	CAD-CBD-CGD	-2.01	109.27	113.60
25	c	301	PEF	C2-O2-C10	-2.01	112.84	117.79
31	n	603	HEA	CHA-C4D-C3D	-2.01	121.88	124.84
25	L	502	PEF	O2-C10-O4	-2.01	118.84	123.70
25	E	304	PEF	O3-C30-O5	-2.01	118.52	123.59
24	A	501	CDL	OB6-CB5-OB7	-2.00	118.86	123.70
25	E	304	PEF	O2-C10-O4	-2.00	118.86	123.70
31	n	603	HEA	CMD-C2D-C1D	2.00	128.09	125.04
25	e	201	PEF	O3-C3-C2	-2.00	102.61	108.43

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	a	602	HEA	ND
31	a	602	HEA	NB
31	a	603	HEA	ND
31	a	603	HEA	NB
31	n	602	HEA	ND
31	n	602	HEA	NB
31	n	603	HEA	ND
31	n	603	HEA	NB

All (718) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	501	CDL	CA2-OA2-PA1-OA3
24	A	501	CDL	CA3-OA5-PA1-OA3
24	C	603	CDL	CA3-OA5-PA1-OA3
24	C	603	CDL	CB2-OB2-PB2-OB4
24	D	402	CDL	CA2-OA2-PA1-OA3
24	D	402	CDL	CA3-OA5-PA1-OA2
24	D	402	CDL	CA3-OA5-PA1-OA3
24	D	402	CDL	CA3-OA5-PA1-OA4
24	D	402	CDL	CB3-OB5-PB2-OB2
24	D	402	CDL	CB3-OB5-PB2-OB3
24	D	402	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
24	H	101	CDL	CA2-OA2-PA1-OA3
24	H	101	CDL	CA2-OA2-PA1-OA4
24	H	101	CDL	CB2-OB2-PB2-OB3
24	H	101	CDL	CB2-OB2-PB2-OB4
24	L	501	CDL	CA2-OA2-PA1-OA3
24	L	501	CDL	CA2-OA2-PA1-OA4
24	L	501	CDL	CA3-OA5-PA1-OA3
24	L	501	CDL	CB2-OB2-PB2-OB3
24	L	501	CDL	CB3-OB5-PB2-OB2
24	L	501	CDL	CB3-OB5-PB2-OB3
24	L	501	CDL	CB3-OB5-PB2-OB4
24	N	603	CDL	CA2-OA2-PA1-OA3
24	N	603	CDL	CA2-OA2-PA1-OA4
24	N	603	CDL	CA2-OA2-PA1-OA5
24	N	603	CDL	CA3-OA5-PA1-OA2
24	N	603	CDL	CA3-OA5-PA1-OA4
24	N	603	CDL	CB2-OB2-PB2-OB3
24	N	603	CDL	CB2-OB2-PB2-OB4
24	N	604	CDL	O1-C1-CB2-OB2
24	N	604	CDL	CA3-OA5-PA1-OA3
24	N	604	CDL	CB3-OB5-PB2-OB2
24	N	604	CDL	CB3-OB5-PB2-OB3
24	N	604	CDL	CB3-OB5-PB2-OB4
24	S	101	CDL	CA3-OA5-PA1-OA2
24	S	101	CDL	C11-CA5-OA6-CA4
25	C	604	PEF	O4P-C4-C5-N
25	C	604	PEF	C1-O3P-P-O2P
25	E	302	PEF	C1-O3P-P-O1P
25	E	302	PEF	C1-O3P-P-O4P
25	E	302	PEF	C4-O4P-P-O1P
25	E	302	PEF	C4-O4P-P-O2P
25	E	303	PEF	C1-O3P-P-O1P
25	E	303	PEF	C1-O3P-P-O2P
25	E	303	PEF	C1-O3P-P-O4P
25	E	303	PEF	C4-O4P-P-O1P
25	E	303	PEF	C4-O4P-P-O2P
25	E	304	PEF	C1-O3P-P-O1P
25	E	304	PEF	C1-O3P-P-O4P
25	J	101	PEF	C1-O3P-P-O2P
25	J	101	PEF	C4-O4P-P-O1P
25	L	502	PEF	C1-O3P-P-O1P
25	L	502	PEF	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
25	L	502	PEF	C4-O4P-P-O1P
25	L	502	PEF	C4-O4P-P-O2P
25	N	605	PEF	C1-O3P-P-O1P
25	N	605	PEF	C1-O3P-P-O2P
25	N	605	PEF	C1-O3P-P-O4P
25	N	605	PEF	C4-O4P-P-O1P
25	N	606	PEF	C4-O4P-P-O2P
25	O	402	PEF	C31-C30-O3-C3
25	O	402	PEF	O5-C30-O3-C3
25	S	102	PEF	C4-O4P-P-O1P
25	S	102	PEF	C4-O4P-P-O2P
25	S	102	PEF	C4-O4P-P-O3P
25	a	606	PEF	O4P-C4-C5-N
25	a	606	PEF	C1-O3P-P-O1P
25	a	606	PEF	C4-O4P-P-O1P
25	a	606	PEF	C4-O4P-P-O2P
25	b	302	PEF	O2-C2-C3-O3
25	b	302	PEF	O4P-C4-C5-N
25	b	302	PEF	C4-O4P-P-O1P
25	b	302	PEF	C4-O4P-P-O2P
25	b	302	PEF	C4-O4P-P-O3P
25	b	303	PEF	C11-C10-O2-C2
25	b	303	PEF	O4-C10-O2-C2
25	b	303	PEF	C1-O3P-P-O2P
25	c	301	PEF	C1-O3P-P-O4P
25	c	302	PEF	O4P-C4-C5-N
25	c	302	PEF	C1-O3P-P-O1P
25	e	201	PEF	C11-C10-O2-C2
25	l	101	PEF	C4-O4P-P-O1P
25	n	606	PEF	C4-O4P-P-O1P
25	n	606	PEF	C4-O4P-P-O2P
25	n	607	PEF	C11-C10-O2-C2
25	n	607	PEF	O4-C10-O2-C2
25	n	607	PEF	C1-O3P-P-O1P
25	n	607	PEF	C1-O3P-P-O4P
25	n	607	PEF	C4-O4P-P-O1P
25	n	607	PEF	C4-O4P-P-O3P
25	n	608	PEF	C4-O4P-P-O1P
25	o	302	PEF	C4-O4P-P-O2P
25	p	301	PEF	C1-O3P-P-O1P
25	p	301	PEF	C1-O3P-P-O2P
25	p	301	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
25	r	201	PEF	C1-O3P-P-O2P
26	C	601	HEM	C2B-C3B-CAB-CBB
26	C	601	HEM	C4B-C3B-CAB-CBB
26	C	601	HEM	C2D-C3D-CAD-CBD
26	C	601	HEM	C4D-C3D-CAD-CBD
26	N	601	HEM	C2B-C3B-CAB-CBB
26	N	601	HEM	C4B-C3B-CAB-CBB
26	N	601	HEM	C2D-C3D-CAD-CBD
26	N	601	HEM	C4D-C3D-CAD-CBD
27	C	606	PCF	C1-O11-P-O12
27	H	103	PCF	C1-O11-P-O14
27	H	103	PCF	C11-O13-P-O12
27	r	202	PCF	C22-C21-O21-C2
31	a	602	HEA	C11-C12-C13-C14
31	n	602	HEA	C2A-CAA-CBA-CGA
31	n	602	HEA	C11-C12-C13-C14
31	n	602	HEA	C26-C15-C16-C17
24	N	604	CDL	OB9-CB7-OB8-CB6
24	S	101	CDL	OA7-CA5-OA6-CA4
25	E	302	PEF	O4-C10-O2-C2
25	e	201	PEF	O4-C10-O2-C2
27	r	202	PCF	O22-C21-O21-C2
24	L	501	CDL	OA9-CA7-OA8-CA6
24	L	501	CDL	C71-CB7-OB8-CB6
24	N	604	CDL	C71-CB7-OB8-CB6
24	L	501	CDL	C31-CA7-OA8-CA6
24	C	603	CDL	O1-C1-CB2-OB2
24	D	402	CDL	O1-C1-CB2-OB2
25	C	604	PEF	C11-C10-O2-C2
25	E	302	PEF	C11-C10-O2-C2
24	L	501	CDL	OB9-CB7-OB8-CB6
31	a	602	HEA	C26-C15-C16-C17
31	a	602	HEA	C14-C15-C16-C17
31	n	602	HEA	C14-C15-C16-C17
24	S	101	CDL	C51-CB5-OB6-CB4
24	N	604	CDL	CA2-C1-CB2-OB2
25	C	604	PEF	O4-C10-O2-C2
24	S	101	CDL	C71-CB7-OB8-CB6
25	a	606	PEF	C30-C31-C32-C33
25	A	502	PEF	O3P-C1-C2-O2
24	H	101	CDL	O1-C1-CA2-OA2
24	H	101	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
24	L	501	CDL	CB5-C51-C52-C53
24	S	101	CDL	CB5-C51-C52-C53
27	N	607	PCF	C21-C22-C23-C24
31	a	602	HEA	C2A-CAA-CBA-CGA
31	n	603	HEA	C2A-CAA-CBA-CGA
25	E	303	PEF	C30-C31-C32-C33
25	J	101	PEF	C10-C11-C12-C13
25	n	606	PEF	C30-C31-C32-C33
25	p	301	PEF	C10-C11-C12-C13
27	C	606	PCF	C31-C32-C33-C34
27	C	606	PCF	C21-C22-C23-C24
24	S	101	CDL	OB9-CB7-OB8-CB6
25	C	605	PEF	C30-C31-C32-C33
25	E	302	PEF	C10-C11-C12-C13
25	S	102	PEF	C30-C31-C32-C33
27	I	101	PCF	C11-C12-N-C14
24	H	101	CDL	CA7-C31-C32-C33
27	H	103	PCF	C21-C22-C23-C24
27	N	607	PCF	C31-C32-C33-C34
25	O	402	PEF	C11-C10-O2-C2
24	A	501	CDL	O1-C1-CB2-OB2
25	c	302	PEF	C11-C10-O2-C2
24	A	501	CDL	CA2-OA2-PA1-OA5
24	A	501	CDL	CA3-OA5-PA1-OA2
24	A	501	CDL	CB2-OB2-PB2-OB5
24	A	501	CDL	CB3-OB5-PB2-OB2
24	C	603	CDL	CA3-OA5-PA1-OA2
24	C	603	CDL	CB2-OB2-PB2-OB5
24	D	402	CDL	CB2-OB2-PB2-OB5
24	H	101	CDL	CA2-OA2-PA1-OA5
24	H	101	CDL	CB2-OB2-PB2-OB5
24	H	101	CDL	CB3-OB5-PB2-OB2
24	L	501	CDL	CA2-OA2-PA1-OA5
24	L	501	CDL	CA3-OA5-PA1-OA2
24	L	501	CDL	CB2-OB2-PB2-OB5
24	N	603	CDL	CB2-OB2-PB2-OB5
24	S	101	CDL	CA2-OA2-PA1-OA5
25	A	502	PEF	C4-O4P-P-O3P
25	C	604	PEF	C1-O3P-P-O4P
25	C	604	PEF	C4-O4P-P-O3P
25	E	302	PEF	C4-O4P-P-O3P
25	E	303	PEF	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
25	E	304	PEF	C4-O4P-P-O3P
25	H	102	PEF	C1-O3P-P-O4P
25	H	102	PEF	C4-O4P-P-O3P
25	J	101	PEF	C1-O3P-P-O4P
25	J	101	PEF	C4-O4P-P-O3P
25	L	502	PEF	C1-O3P-P-O4P
25	L	502	PEF	C4-O4P-P-O3P
25	O	402	PEF	C1-O3P-P-O4P
25	O	402	PEF	C4-O4P-P-O3P
25	a	606	PEF	C4-O4P-P-O3P
25	b	303	PEF	C1-O3P-P-O4P
25	b	303	PEF	C4-O4P-P-O3P
25	c	302	PEF	C1-O3P-P-O4P
25	c	302	PEF	C4-O4P-P-O3P
25	e	201	PEF	C1-O3P-P-O4P
25	e	201	PEF	C4-O4P-P-O3P
25	n	606	PEF	C4-O4P-P-O3P
25	o	302	PEF	C4-O4P-P-O3P
25	r	201	PEF	C4-O4P-P-O3P
27	C	606	PCF	C11-O13-P-O11
24	A	501	CDL	CA2-C1-CB2-OB2
24	H	101	CDL	OA7-CA5-OA6-CA4
24	S	101	CDL	OB7-CB5-OB6-CB4
25	O	402	PEF	O4-C10-O2-C2
25	c	302	PEF	O4-C10-O2-C2
27	I	101	PCF	C11-C12-N-C15
24	S	101	CDL	CA7-C31-C32-C33
24	N	604	CDL	C11-CA5-OA6-CA4
25	E	303	PEF	C11-C10-O2-C2
27	H	103	PCF	C22-C21-O21-C2
25	N	606	PEF	C13-C14-C15-C16
25	O	402	PEF	C41-C42-C43-C44
25	b	302	PEF	C39-C40-C41-C42
25	b	303	PEF	C34-C35-C36-C37
25	o	302	PEF	C12-C13-C14-C15
25	N	606	PEF	C31-C32-C33-C34
24	S	101	CDL	CA6-CA4-OA6-CA5
24	N	604	CDL	OA7-CA5-OA6-CA4
25	E	303	PEF	O4-C10-O2-C2
27	H	103	PCF	O22-C21-O21-C2
24	C	603	CDL	CB5-C51-C52-C53
25	E	304	PEF	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	e	201	PEF	C15-C16-C17-C18
25	o	302	PEF	C34-C35-C36-C37
27	T	101	PCF	C39-C40-C41-C42
25	E	304	PEF	C32-C33-C34-C35
24	L	501	CDL	O1-C1-CB2-OB2
25	o	302	PEF	C16-C17-C18-C19
24	N	604	CDL	C57-C58-C59-C60
24	D	402	CDL	C51-C52-C53-C54
25	C	604	PEF	C34-C35-C36-C37
25	n	606	PEF	C37-C38-C39-C40
25	n	606	PEF	C13-C14-C15-C16
25	J	101	PEF	O4-C10-O2-C2
24	C	603	CDL	C11-CA5-OA6-CA4
24	N	603	CDL	C11-CA5-OA6-CA4
25	J	101	PEF	C11-C10-O2-C2
25	O	402	PEF	C40-C41-C42-C43
24	C	603	CDL	C36-C37-C38-C39
25	E	303	PEF	C11-C12-C13-C14
25	O	402	PEF	C33-C34-C35-C36
25	n	606	PEF	C35-C36-C37-C38
25	E	303	PEF	C21-C22-C23-C24
25	E	303	PEF	O4P-C4-C5-N
25	E	303	PEF	C13-C14-C15-C16
25	o	302	PEF	C10-C11-C12-C13
24	N	604	CDL	C56-C57-C58-C59
25	r	201	PEF	C12-C13-C14-C15
25	N	606	PEF	C11-C12-C13-C14
24	N	604	CDL	C32-C33-C34-C35
25	E	302	PEF	C15-C16-C17-C18
25	o	302	PEF	C15-C16-C17-C18
25	n	606	PEF	C40-C41-C42-C43
25	O	402	PEF	C34-C35-C36-C37
24	N	604	CDL	C51-CB5-OB6-CB4
25	C	605	PEF	C11-C10-O2-C2
25	r	201	PEF	C11-C10-O2-C2
27	N	607	PCF	C30-C47-C48-C49
24	C	603	CDL	C71-C72-C73-C74
24	N	604	CDL	C31-C32-C33-C34
25	C	605	PEF	C11-C12-C13-C14
25	n	606	PEF	C31-C32-C33-C34
24	N	603	CDL	CA5-C11-C12-C13
24	D	402	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
24	N	603	CDL	C34-C35-C36-C37
24	D	402	CDL	CA2-C1-CB2-OB2
25	N	605	PEF	C34-C35-C36-C37
24	N	603	CDL	OA7-CA5-OA6-CA4
24	N	604	CDL	OB7-CB5-OB6-CB4
25	r	201	PEF	O4-C10-O2-C2
25	N	605	PEF	C11-C12-C13-C14
25	O	402	PEF	C14-C15-C16-C17
25	e	201	PEF	C19-C20-C21-C22
27	I	101	PCF	C11-C12-N-C13
25	N	606	PEF	C35-C36-C37-C38
24	A	501	CDL	C51-CB5-OB6-CB4
25	L	502	PEF	C11-C10-O2-C2
25	N	605	PEF	C11-C10-O2-C2
25	n	606	PEF	C41-C42-C43-C44
27	e	202	PCF	C21-C22-C23-C24
25	C	604	PEF	C37-C38-C39-C40
25	E	304	PEF	C34-C35-C36-C37
24	A	501	CDL	OB7-CB5-OB6-CB4
24	C	603	CDL	OA7-CA5-OA6-CA4
25	C	605	PEF	O4-C10-O2-C2
27	N	607	PCF	O22-C21-O21-C2
27	C	606	PCF	C32-C31-O31-C3
25	b	303	PEF	C16-C17-C18-C19
24	C	603	CDL	C73-C74-C75-C76
25	n	606	PEF	C39-C40-C41-C42
27	H	103	PCF	C23-C24-C25-C26
27	N	607	PCF	C22-C21-O21-C2
24	L	501	CDL	OB5-CB3-CB4-OB6
25	L	502	PEF	O3P-C1-C2-O2
25	r	201	PEF	C34-C35-C36-C37
25	L	502	PEF	O4-C10-O2-C2
24	A	501	CDL	CA5-C11-C12-C13
24	A	501	CDL	OB6-CB4-CB6-OB8
27	I	101	PCF	O21-C2-C3-O31
25	E	302	PEF	C38-C39-C40-C41
25	n	606	PEF	C11-C12-C13-C14
27	e	202	PCF	C11-C12-N-C13
25	b	302	PEF	C30-C31-C32-C33
25	r	201	PEF	C30-C31-C32-C33
24	N	604	CDL	C71-C72-C73-C74
25	N	605	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
25	a	606	PEF	C11-C10-O2-C2
25	n	606	PEF	C20-C21-C22-C23
24	D	402	CDL	CA2-OA2-PA1-OA5
25	N	606	PEF	C4-O4P-P-O3P
25	b	302	PEF	C1-O3P-P-O4P
24	H	101	CDL	CB5-C51-C52-C53
25	L	502	PEF	C30-C31-C32-C33
27	N	607	PCF	C38-C39-C40-C41
24	N	603	CDL	OA5-CA3-CA4-CA6
25	o	302	PEF	O3P-C1-C2-C3
24	A	501	CDL	C52-C53-C54-C55
24	L	501	CDL	C51-C52-C53-C54
25	e	201	PEF	C18-C19-C20-C21
27	N	607	PCF	C35-C36-C37-C38
25	N	605	PEF	C33-C34-C35-C36
25	o	302	PEF	C14-C15-C16-C17
24	D	402	CDL	C11-CA5-OA6-CA4
25	C	605	PEF	C15-C16-C17-C18
27	C	606	PCF	C27-C28-C29-C30
24	H	101	CDL	CA3-CA4-CA6-OA8
24	H	101	CDL	CB3-CB4-CB6-OB8
24	L	501	CDL	CB3-CB4-CB6-OB8
24	N	604	CDL	CB3-CB4-CB6-OB8
25	A	502	PEF	C1-C2-C3-O3
25	C	604	PEF	C1-C2-C3-O3
25	N	605	PEF	C1-C2-C3-O3
25	O	402	PEF	C1-C2-C3-O3
25	S	102	PEF	C1-C2-C3-O3
25	b	302	PEF	C1-C2-C3-O3
25	n	607	PEF	C1-C2-C3-O3
27	e	202	PCF	C32-C33-C34-C35
25	N	606	PEF	C20-C21-C22-C23
27	C	606	PCF	O32-C31-O31-C3
24	N	604	CDL	C73-C74-C75-C76
25	o	302	PEF	C33-C34-C35-C36
25	E	304	PEF	C11-C10-O2-C2
25	n	606	PEF	C42-C43-C44-C45
25	n	607	PEF	C32-C33-C34-C35
27	H	103	PCF	C1-C2-O21-C21
25	a	606	PEF	O4-C10-O2-C2
24	C	603	CDL	C53-C54-C55-C56
25	N	605	PEF	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
24	S	101	CDL	C71-C72-C73-C74
25	E	302	PEF	C37-C38-C39-C40
25	N	605	PEF	C15-C16-C17-C18
25	b	302	PEF	C33-C34-C35-C36
24	D	402	CDL	C31-CA7-OA8-CA6
25	S	102	PEF	C10-C11-C12-C13
24	D	402	CDL	CA7-C31-C32-C33
25	O	402	PEF	C10-C11-C12-C13
24	N	604	CDL	OB6-CB4-CB6-OB8
25	a	606	PEF	O2-C2-C3-O3
25	p	301	PEF	O2-C2-C3-O3
25	c	302	PEF	C36-C37-C38-C39
27	N	607	PCF	C22-C23-C24-C25
25	O	402	PEF	C32-C33-C34-C35
25	N	605	PEF	C19-C20-C21-C22
24	D	402	CDL	C11-C12-C13-C14
25	C	604	PEF	C35-C36-C37-C38
25	J	101	PEF	C31-C32-C33-C34
25	e	201	PEF	C31-C30-O3-C3
24	C	603	CDL	C74-C75-C76-C77
25	n	608	PEF	C31-C30-O3-C3
31	a	603	HEA	C4D-C3D-CAD-CBD
25	O	402	PEF	C31-C32-C33-C34
27	e	202	PCF	C11-C12-N-C15
24	A	501	CDL	OA5-CA3-CA4-CA6
25	A	502	PEF	O3P-C1-C2-C3
25	L	502	PEF	O3P-C1-C2-C3
25	n	608	PEF	O3P-C1-C2-C3
25	p	301	PEF	O3P-C1-C2-C3
25	r	201	PEF	O3P-C1-C2-C3
27	C	606	PCF	O11-C1-C2-C3
31	n	602	HEA	C15-C16-C17-C18
25	N	605	PEF	O4P-C4-C5-N
25	S	102	PEF	O4P-C4-C5-N
25	c	302	PEF	C32-C33-C34-C35
27	C	606	PCF	C29-C30-C47-C48
25	E	303	PEF	C22-C23-C24-C25
25	l	101	PEF	C31-C30-O3-C3
24	A	501	CDL	C11-C12-C13-C14
24	D	402	CDL	OA9-CA7-OA8-CA6
25	b	303	PEF	C19-C20-C21-C22
24	A	501	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
24	N	603	CDL	CB3-CB4-CB6-OB8
24	N	604	CDL	CA3-CA4-CA6-OA8
25	r	201	PEF	C1-C2-C3-O3
24	C	603	CDL	C51-C52-C53-C54
25	C	605	PEF	C12-C13-C14-C15
27	e	202	PCF	C11-C12-N-C14
27	e	202	PCF	C35-C36-C37-C38
25	n	608	PEF	C4-O4P-P-O3P
25	r	201	PEF	C1-O3P-P-O4P
27	r	202	PCF	C21-C22-C23-C24
25	e	201	PEF	O5-C30-O3-C3
27	N	607	PCF	C36-C37-C38-C39
24	H	101	CDL	OB5-CB3-CB4-OB6
24	N	604	CDL	OB5-CB3-CB4-OB6
25	n	607	PEF	O3P-C1-C2-O2
27	e	202	PCF	O11-C1-C2-O21
25	E	304	PEF	O4-C10-O2-C2
24	C	603	CDL	CA5-C11-C12-C13
25	S	102	PEF	C40-C41-C42-C43
24	C	603	CDL	OB6-CB4-CB6-OB8
24	L	501	CDL	OB6-CB4-CB6-OB8
25	C	604	PEF	O2-C2-C3-O3
25	n	608	PEF	O2-C2-C3-O3
27	H	103	PCF	O21-C2-C3-O31
27	N	607	PCF	O21-C2-C3-O31
24	L	501	CDL	C13-C14-C15-C16
24	L	501	CDL	C52-C53-C54-C55
24	H	101	CDL	CB2-C1-CA2-OA2
27	C	606	PCF	C25-C26-C27-C28
24	D	402	CDL	OA7-CA5-OA6-CA4
25	c	302	PEF	C33-C34-C35-C36
24	N	604	CDL	C55-C56-C57-C58
25	o	302	PEF	C17-C18-C19-C20
25	b	303	PEF	C31-C32-C33-C34
25	N	606	PEF	C12-C13-C14-C15
25	E	302	PEF	C41-C42-C43-C44
24	A	501	CDL	OB5-CB3-CB4-CB6
24	C	603	CDL	OB5-CB3-CB4-CB6
24	H	101	CDL	OB5-CB3-CB4-CB6
25	S	102	PEF	O3P-C1-C2-C3
27	e	202	PCF	O11-C1-C2-C3
27	r	202	PCF	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	c	302	PEF	C31-C32-C33-C34
25	E	302	PEF	C36-C37-C38-C39
24	H	101	CDL	C71-CB7-OB8-CB6
31	a	603	HEA	C2D-C3D-CAD-CBD
24	N	603	CDL	C35-C36-C37-C38
25	n	607	PEF	C3-C2-O2-C10
24	C	603	CDL	C31-C32-C33-C34
24	C	603	CDL	CB3-CB4-CB6-OB8
24	N	604	CDL	CA4-CA3-OA5-PA1
27	C	606	PCF	C1-C2-C3-O31
27	I	101	PCF	C1-C2-C3-O31
27	N	607	PCF	C1-C2-C3-O31
27	e	202	PCF	C22-C21-O21-C2
25	S	102	PEF	O3P-C1-C2-O2
25	r	201	PEF	O3P-C1-C2-O2
27	C	606	PCF	C28-C29-C30-C47
27	H	103	PCF	C32-C33-C34-C35
27	N	607	PCF	C27-C28-C29-C30
25	n	608	PEF	O5-C30-O3-C3
24	H	101	CDL	OA6-CA4-CA6-OA8
24	N	604	CDL	OA6-CA4-CA6-OA8
25	A	502	PEF	O2-C2-C3-O3
25	J	101	PEF	O2-C2-C3-O3
25	N	605	PEF	O2-C2-C3-O3
25	S	102	PEF	O2-C2-C3-O3
25	n	606	PEF	O2-C2-C3-O3
25	n	607	PEF	O2-C2-C3-O3
27	r	202	PCF	C32-C31-O31-C3
25	E	303	PEF	C14-C15-C16-C17
25	l	101	PEF	O5-C30-O3-C3
25	H	102	PEF	C34-C35-C36-C37
24	S	101	CDL	CA5-C11-C12-C13
25	E	302	PEF	C35-C36-C37-C38
27	N	607	PCF	C48-C49-C50-C51
27	H	103	PCF	C32-C31-O31-C3
24	C	603	CDL	C52-C53-C54-C55
25	b	303	PEF	C13-C14-C15-C16
27	N	607	PCF	C39-C40-C41-C42
25	p	301	PEF	O4-C10-O2-C2
24	L	501	CDL	C12-C13-C14-C15
24	N	604	CDL	C58-C59-C60-C61
25	b	303	PEF	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	r	202	PCF	O32-C31-O31-C3
27	e	202	PCF	O22-C21-O21-C2
24	N	604	CDL	CA2-OA2-PA1-OA5
25	N	605	PEF	C4-O4P-P-O3P
25	a	606	PEF	C1-O3P-P-O4P
27	H	103	PCF	C1-O11-P-O13
24	H	101	CDL	C1-CA2-OA2-PA1
24	A	501	CDL	CA2-OA2-PA1-OA4
24	A	501	CDL	CA3-OA5-PA1-OA4
24	A	501	CDL	CB2-OB2-PB2-OB3
24	A	501	CDL	CB3-OB5-PB2-OB3
24	D	402	CDL	CB2-OB2-PB2-OB3
24	H	101	CDL	CB3-OB5-PB2-OB3
24	L	501	CDL	CA3-OA5-PA1-OA4
24	L	501	CDL	CB2-OB2-PB2-OB4
24	N	603	CDL	CA3-OA5-PA1-OA3
24	S	101	CDL	CA2-OA2-PA1-OA3
24	S	101	CDL	CA3-OA5-PA1-OA4
25	A	502	PEF	C4-O4P-P-O1P
25	C	604	PEF	C4-O4P-P-O1P
25	E	304	PEF	C4-O4P-P-O1P
25	H	102	PEF	C1-O3P-P-O1P
25	H	102	PEF	C4-O4P-P-O1P
25	J	101	PEF	C1-O3P-P-O1P
25	J	101	PEF	C4-O4P-P-O2P
25	N	605	PEF	C4-O4P-P-O2P
25	N	606	PEF	C4-O4P-P-O1P
25	O	402	PEF	C1-O3P-P-O1P
25	O	402	PEF	C4-O4P-P-O1P
25	O	402	PEF	C4-O4P-P-O2P
25	b	302	PEF	C1-O3P-P-O1P
25	b	302	PEF	C1-O3P-P-O2P
25	b	303	PEF	C4-O4P-P-O1P
25	c	301	PEF	C1-O3P-P-O2P
25	c	302	PEF	C4-O4P-P-O2P
25	e	201	PEF	C1-O3P-P-O1P
25	e	201	PEF	C4-O4P-P-O1P
25	o	302	PEF	C4-O4P-P-O1P
25	r	201	PEF	C1-O3P-P-O1P
25	r	201	PEF	C4-O4P-P-O1P
27	C	606	PCF	C11-O13-P-O12
24	L	501	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
24	L	501	CDL	OB5-CB3-CB4-CB6
24	N	604	CDL	OB5-CB3-CB4-CB6
25	N	606	PEF	O3P-C1-C2-C3
25	e	201	PEF	C22-C23-C24-C25
24	N	604	CDL	C75-C76-C77-C78
24	N	603	CDL	C71-C72-C73-C74
25	E	302	PEF	C30-C31-C32-C33
25	E	303	PEF	C10-C11-C12-C13
25	e	201	PEF	C34-C35-C36-C37
25	c	301	PEF	C35-C36-C37-C38
27	C	606	PCF	C23-C24-C25-C26
24	L	501	CDL	CA2-C1-CB2-OB2
24	A	501	CDL	OA5-CA3-CA4-OA6
24	A	501	CDL	OB5-CB3-CB4-OB6
24	C	603	CDL	OB5-CB3-CB4-OB6
24	D	402	CDL	OB5-CB3-CB4-OB6
24	L	501	CDL	OA5-CA3-CA4-OA6
24	N	603	CDL	OA5-CA3-CA4-OA6
25	b	302	PEF	O3P-C1-C2-O2
25	n	608	PEF	O3P-C1-C2-O2
25	o	302	PEF	O3P-C1-C2-O2
25	p	301	PEF	O3P-C1-C2-O2
27	C	606	PCF	O11-C1-C2-O21
27	H	103	PCF	O32-C31-O31-C3
25	l	101	PEF	C11-C10-O2-C2
27	e	202	PCF	C23-C24-C25-C26
27	N	607	PCF	C11-C12-N-C14
27	H	103	PCF	C33-C34-C35-C36
25	c	301	PEF	C30-C31-C32-C33
27	T	101	PCF	O13-C11-C12-N
24	H	101	CDL	OB6-CB4-CB6-OB8
25	E	304	PEF	O2-C10-C11-C12
25	L	502	PEF	C13-C14-C15-C16
25	p	301	PEF	C11-C10-O2-C2
31	a	602	HEA	C15-C16-C17-C18
24	H	101	CDL	OB9-CB7-OB8-CB6
25	b	303	PEF	C20-C21-C22-C23
24	N	603	CDL	C31-C32-C33-C34
25	C	605	PEF	C13-C14-C15-C16
25	C	605	PEF	C3-C2-O2-C10
24	D	402	CDL	OB5-CB3-CB4-CB6
25	c	301	PEF	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	n	607	PEF	O3P-C1-C2-C3
25	l	101	PEF	O4-C10-O2-C2
25	c	302	PEF	C31-C30-O3-C3
25	E	304	PEF	C35-C36-C37-C38
25	S	102	PEF	C37-C38-C39-C40
27	N	607	PCF	C34-C35-C36-C37
25	E	302	PEF	O3-C30-C31-C32
25	c	302	PEF	O5-C30-O3-C3
25	c	301	PEF	O3P-C1-C2-O2
27	r	202	PCF	O11-C1-C2-O21
27	N	607	PCF	C11-C12-N-C15
27	r	202	PCF	C34-C35-C36-C37
25	O	402	PEF	O2-C2-C3-O3
25	r	201	PEF	O2-C2-C3-O3
24	C	603	CDL	CA2-OA2-PA1-OA5
24	H	101	CDL	CA3-OA5-PA1-OA2
24	N	603	CDL	CB3-OB5-PB2-OB2
25	c	301	PEF	C4-O4P-P-O3P
25	l	101	PEF	C1-O3P-P-O4P
25	n	606	PEF	C1-O3P-P-O4P
25	p	301	PEF	C4-O4P-P-O3P
25	e	201	PEF	C1-C2-C3-O3
25	n	606	PEF	C1-C2-C3-O3
25	p	301	PEF	C1-C2-C3-O3
25	L	502	PEF	C11-C12-C13-C14
25	E	304	PEF	C36-C37-C38-C39
24	S	101	CDL	CB4-CB3-OB5-PB2
24	C	603	CDL	CA2-C1-CB2-OB2
25	H	102	PEF	C31-C30-O3-C3
25	E	304	PEF	C10-C11-C12-C13
25	b	303	PEF	C11-C12-C13-C14
26	C	602	HEM	CAD-CBD-CGD-O2D
26	N	602	HEM	CAD-CBD-CGD-O2D
25	E	304	PEF	C15-C16-C17-C18
25	H	102	PEF	O5-C30-O3-C3
25	b	303	PEF	O3P-C1-C2-O2
25	E	303	PEF	C19-C20-C21-C22
25	C	604	PEF	C11-C12-C13-C14
25	e	201	PEF	C12-C13-C14-C15
24	N	604	CDL	C61-C62-C63-C64
26	C	602	HEM	CAD-CBD-CGD-O1D
26	N	602	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	a	602	HEA	CAD-CBD-CGD-O1D
25	b	302	PEF	C32-C33-C34-C35
25	J	101	PEF	C1-C2-C3-O3
25	c	302	PEF	C1-C2-C3-O3
25	E	302	PEF	O5-C30-O3-C3
25	N	605	PEF	C35-C36-C37-C38
24	N	604	CDL	CA6-CA4-OA6-CA5
25	c	301	PEF	C32-C33-C34-C35
27	N	607	PCF	C11-C12-N-C13
24	C	603	CDL	CA7-C31-C32-C33
24	N	603	CDL	CB4-CB3-OB5-PB2
24	A	501	CDL	C51-C52-C53-C54
25	E	303	PEF	O3P-C1-C2-O2
25	E	302	PEF	C31-C30-O3-C3
25	b	302	PEF	O3P-C1-C2-C3
24	N	604	CDL	C63-C64-C65-C66
31	a	602	HEA	CAD-CBD-CGD-O2D
25	L	502	PEF	C31-C32-C33-C34
25	A	502	PEF	O4-C10-O2-C2
24	A	501	CDL	C15-C16-C17-C18
27	N	607	PCF	C33-C34-C35-C36
31	n	603	HEA	CAD-CBD-CGD-O2D
31	a	603	HEA	CAD-CBD-CGD-O2D
26	N	602	HEM	CAA-CBA-CGA-O2A
26	N	601	HEM	CAD-CBD-CGD-O2D
25	E	304	PEF	C33-C34-C35-C36
24	N	604	CDL	C35-C36-C37-C38
31	a	603	HEA	CAD-CBD-CGD-O1D
26	C	601	HEM	CAA-CBA-CGA-O2A
25	b	303	PEF	O4P-C4-C5-N
25	C	605	PEF	O3-C30-C31-C32
24	H	101	CDL	CA5-C11-C12-C13
27	N	607	PCF	C40-C41-C42-C43
24	N	603	CDL	OB6-CB4-CB6-OB8
25	n	606	PEF	C19-C20-C21-C22
27	H	103	PCF	C11-O13-P-O11
25	b	303	PEF	O2-C10-C11-C12
27	T	101	PCF	C37-C38-C39-C40
26	C	601	HEM	CAA-CBA-CGA-O1A
26	N	601	HEM	CAA-CBA-CGA-O2A
31	n	603	HEA	CAD-CBD-CGD-O1D
25	a	606	PEF	C3-C2-O2-C10

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Mol	Chain	Res	Type	Atoms
26	C	602	HEM	CAA-CBA-CGA-O2A
25	L	502	PEF	C10-C11-C12-C13
26	C	601	HEM	CAD-CBD-CGD-O2D
31	n	602	HEA	CAD-CBD-CGD-O1D
25	L	502	PEF	O2-C10-C11-C12
25	E	304	PEF	C2-C1-O3P-P
27	H	103	PCF	C1-C2-C3-O31
26	N	602	HEM	CAA-CBA-CGA-O1A
25	e	201	PEF	O3P-C1-C2-O2
28	O	401	HEC	CAD-CBD-CGD-O2D
25	O	402	PEF	C17-C18-C19-C20
25	A	502	PEF	O3-C30-C31-C32
25	n	606	PEF	C12-C13-C14-C15
27	C	606	PCF	C30-C47-C48-C49
26	C	602	HEM	CAA-CBA-CGA-O1A
26	N	601	HEM	CAA-CBA-CGA-O1A
26	N	601	HEM	CAD-CBD-CGD-O1D
28	O	401	HEC	CAD-CBD-CGD-O1D
24	C	603	CDL	C13-C14-C15-C16
25	e	201	PEF	O3P-C1-C2-C3
27	N	607	PCF	O11-C1-C2-C3
26	C	601	HEM	CAD-CBD-CGD-O1D
24	C	603	CDL	C72-C71-CB7-OB8
24	H	101	CDL	C12-C11-CA5-OA6
25	a	606	PEF	C13-C14-C15-C16
25	o	302	PEF	C11-C12-C13-C14
31	n	602	HEA	CAD-CBD-CGD-O2D
25	C	604	PEF	C32-C33-C34-C35
24	H	101	CDL	C54-C55-C56-C57
27	r	202	PCF	C23-C24-C25-C26
25	l	101	PEF	C33-C34-C35-C36
27	C	606	PCF	C22-C21-O21-C2
25	n	607	PEF	O3-C30-C31-C32
24	D	402	CDL	C72-C71-CB7-OB9
25	A	502	PEF	O5-C30-C31-C32
25	a	606	PEF	C1-C2-C3-O3
25	n	608	PEF	C1-C2-C3-O3
27	C	606	PCF	C1-O11-P-O13
25	n	607	PEF	C11-C12-C13-C14
25	L	502	PEF	O4-C10-C11-C12
27	C	606	PCF	O22-C21-O21-C2
24	C	603	CDL	CA2-OA2-PA1-OA3

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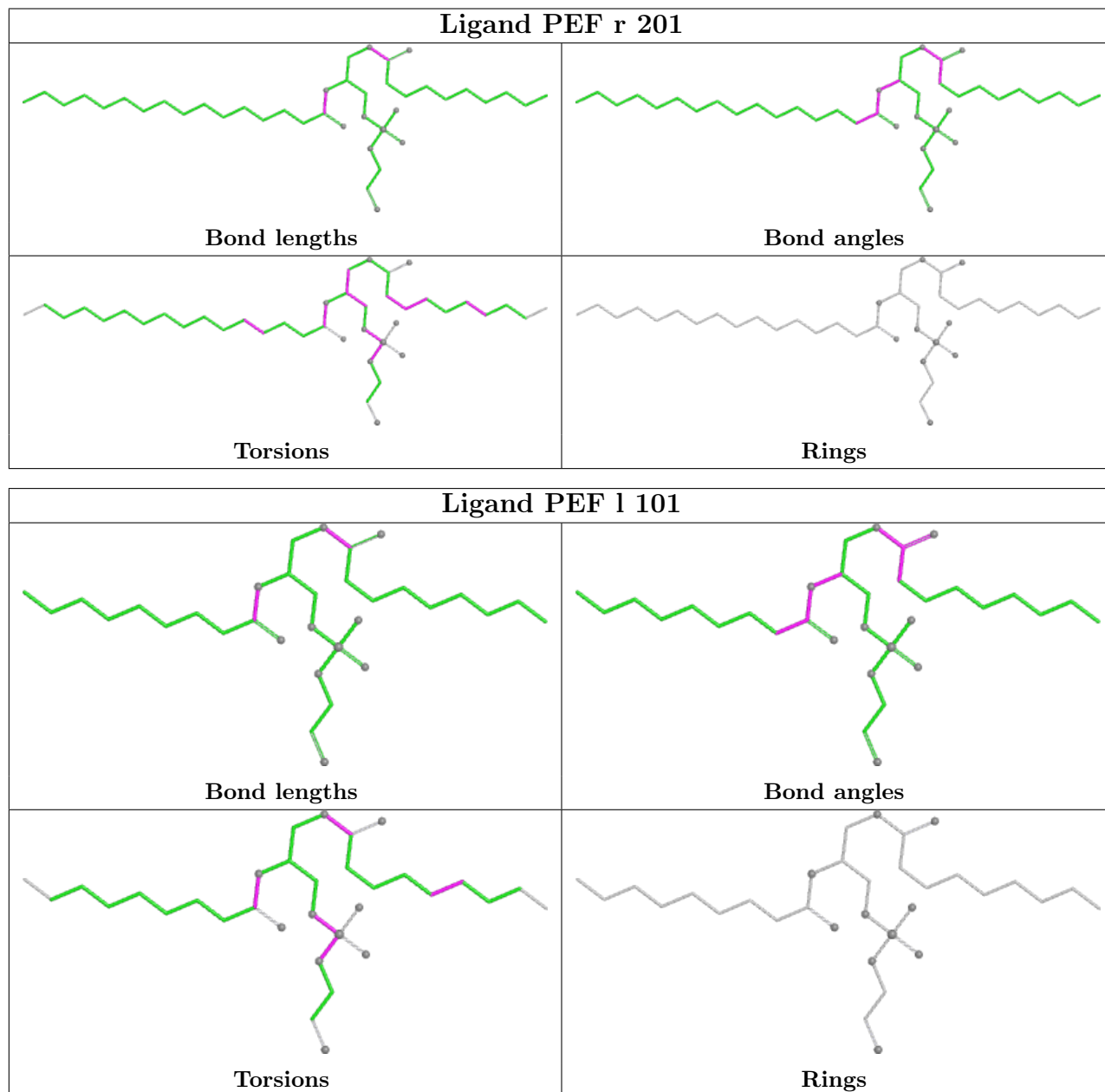
Mol	Chain	Res	Type	Atoms
24	H	101	CDL	CA3-OA5-PA1-OA3
24	N	603	CDL	CB3-OB5-PB2-OB3
27	H	103	PCF	C1-O11-P-O12
27	H	103	PCF	C11-O13-P-O14
25	E	302	PEF	O4P-C4-C5-N
25	O	402	PEF	O4P-C4-C5-N
24	N	604	CDL	C33-C34-C35-C36
25	E	303	PEF	C33-C34-C35-C36
24	L	501	CDL	OB7-CB5-OB6-CB4
28	O	401	HEC	CAA-CBA-CGA-O2A
31	a	603	HEA	C26-C15-C16-C17
31	n	603	HEA	C26-C15-C16-C17
25	c	301	PEF	O5-C30-O3-C3
25	A	502	PEF	O2-C10-C11-C12
25	c	301	PEF	C11-C12-C13-C14
25	n	607	PEF	C30-C31-C32-C33
27	T	101	PCF	C36-C37-C38-C39
25	c	301	PEF	C10-C11-C12-C13
25	N	605	PEF	C13-C14-C15-C16
25	N	606	PEF	O3-C30-C31-C32
31	a	602	HEA	CAA-CBA-CGA-O2A
24	C	603	CDL	C72-C71-CB7-OB9
24	H	101	CDL	C12-C11-CA5-OA7
25	r	201	PEF	C31-C32-C33-C34
25	A	502	PEF	O4-C10-C11-C12
24	D	402	CDL	C72-C71-CB7-OB8
25	n	607	PEF	O5-C30-C31-C32
31	a	603	HEA	CAA-CBA-CGA-O1A
25	H	102	PEF	O2-C10-C11-C12
27	C	606	PCF	O21-C21-C22-C23
25	C	604	PEF	C38-C39-C40-C41
28	D	401	HEC	CAA-CBA-CGA-O2A
25	p	301	PEF	O2-C10-C11-C12
27	r	202	PCF	O31-C31-C32-C33
31	a	602	HEA	CAA-CBA-CGA-O1A

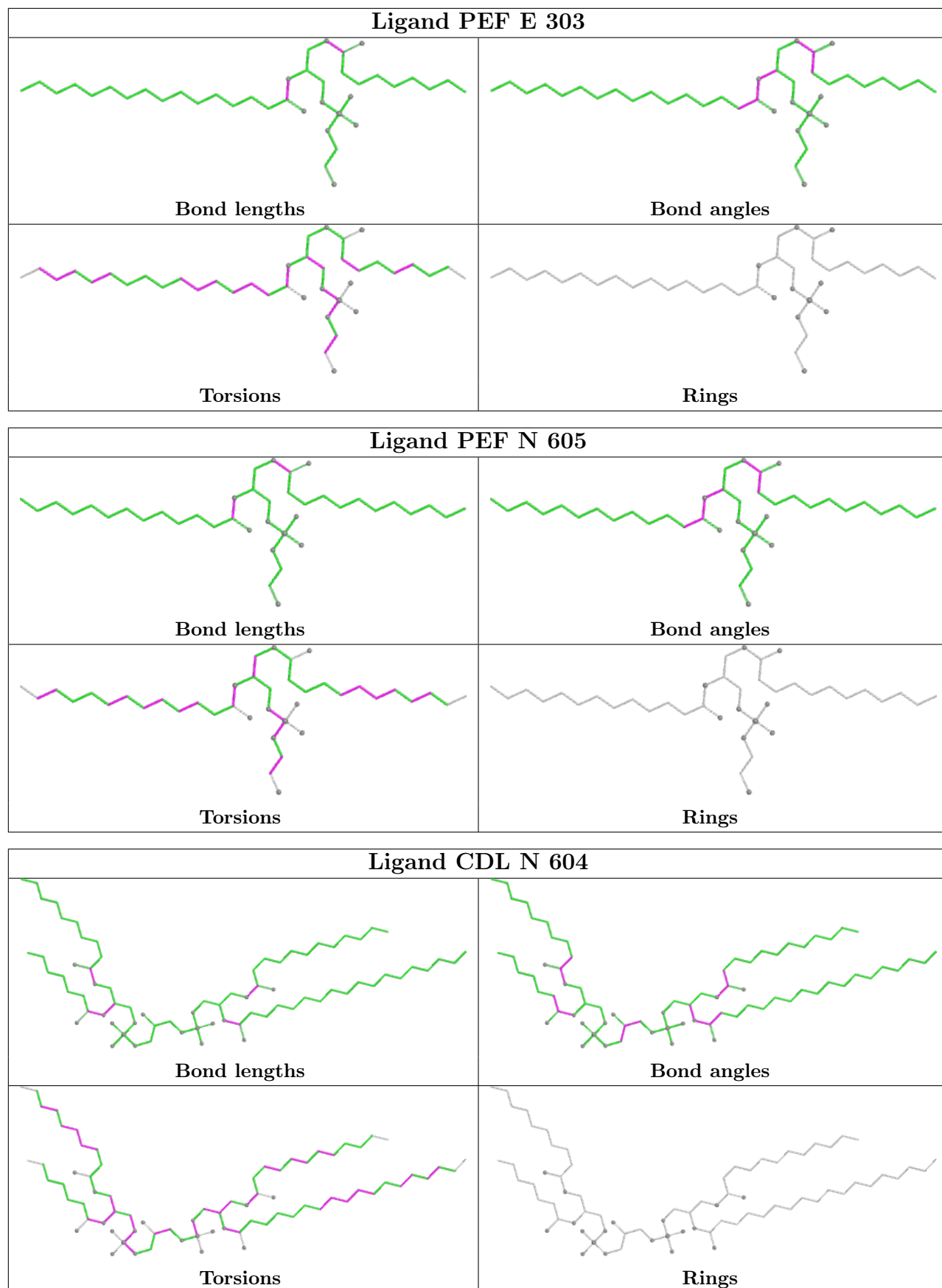
There are no ring outliers.

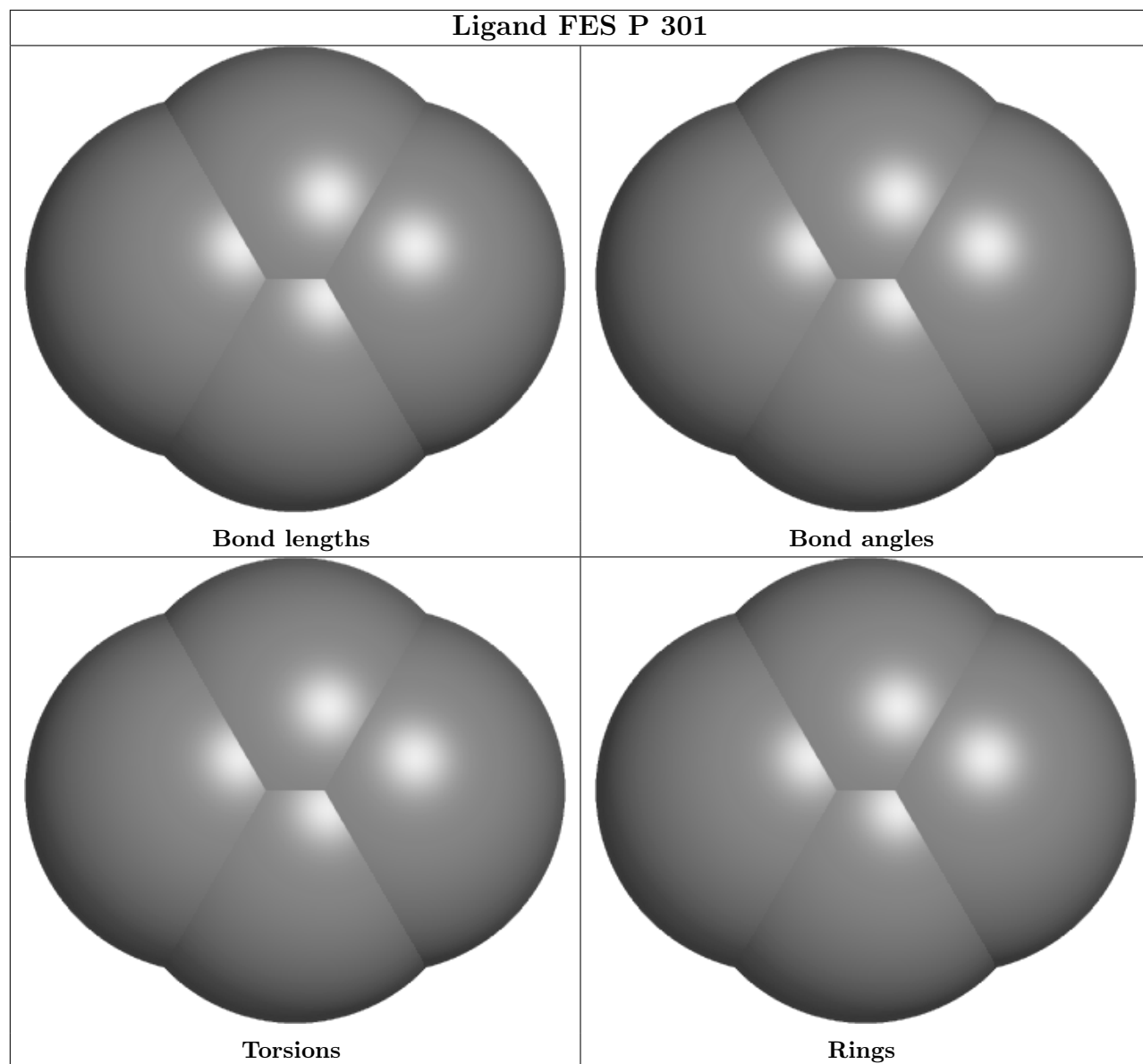
No monomer is involved in short contacts.

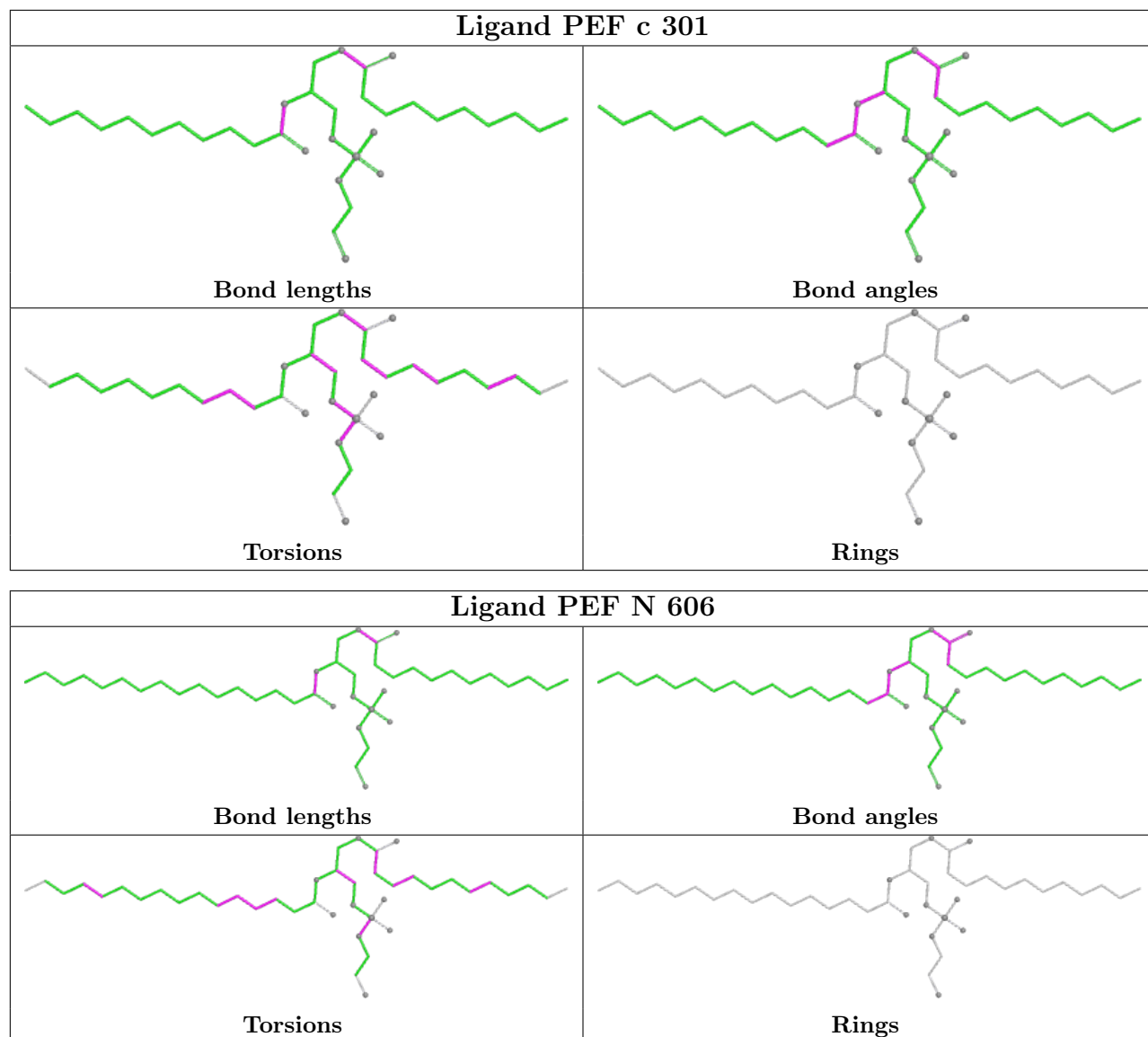
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

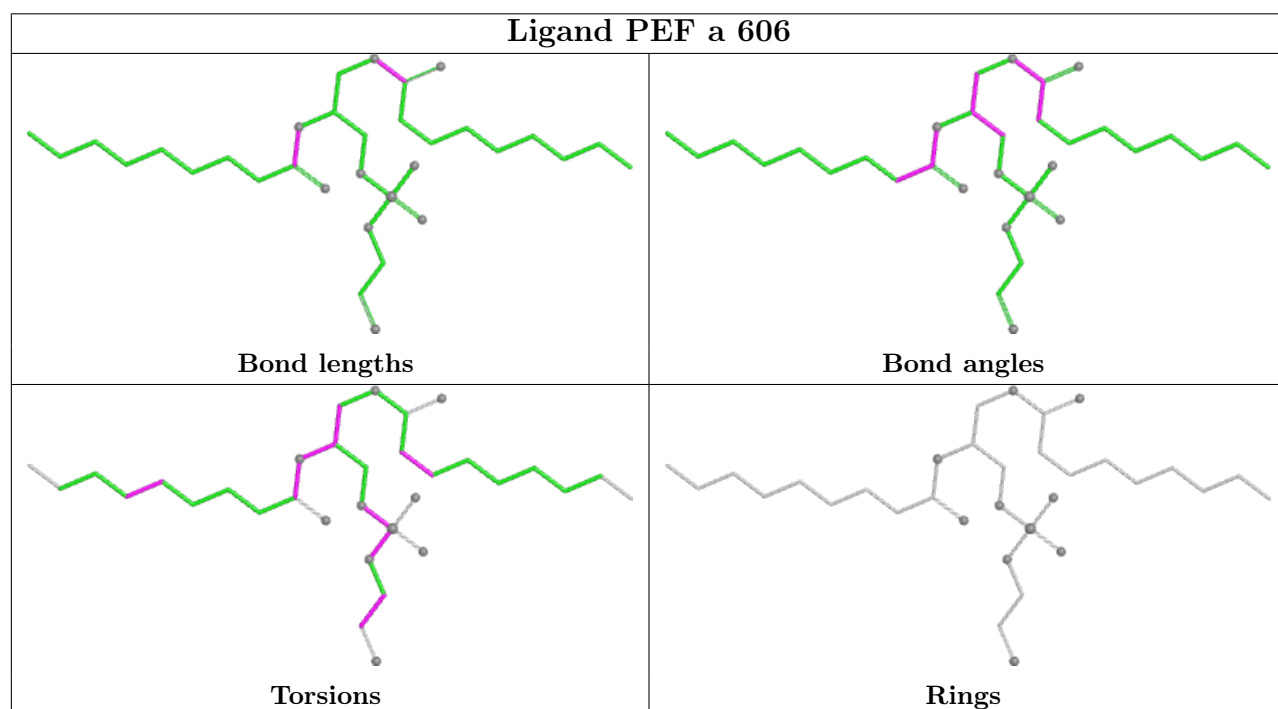
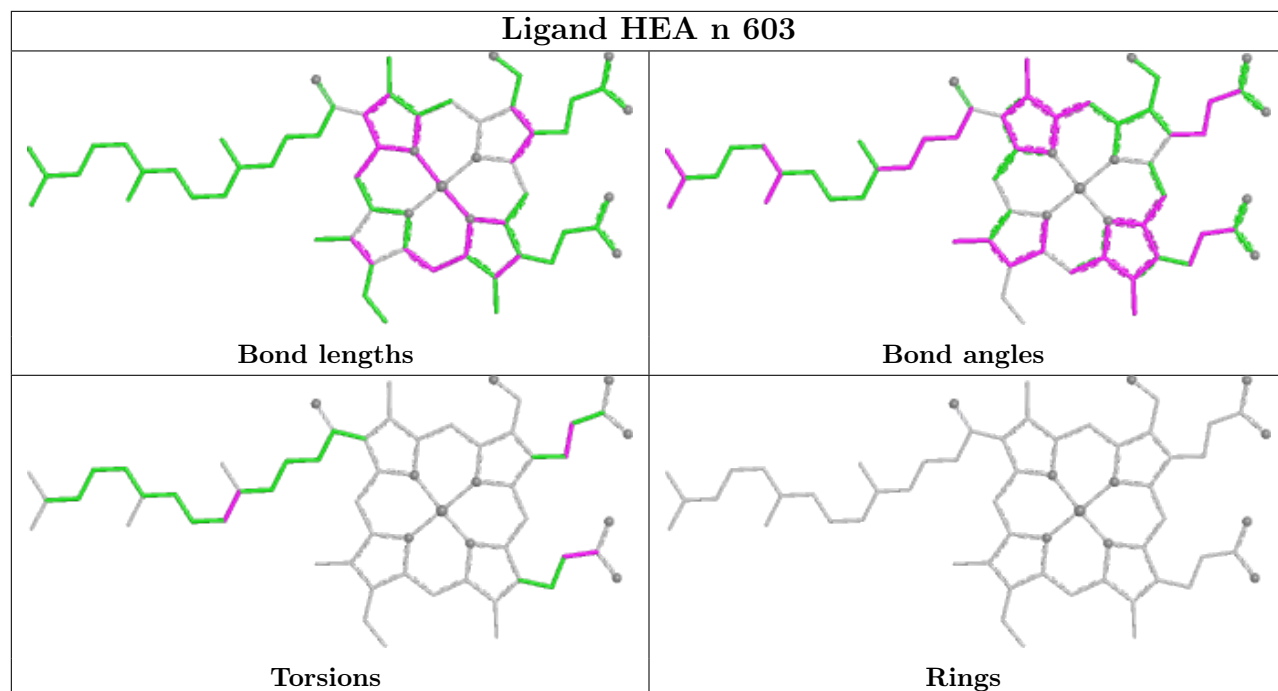
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

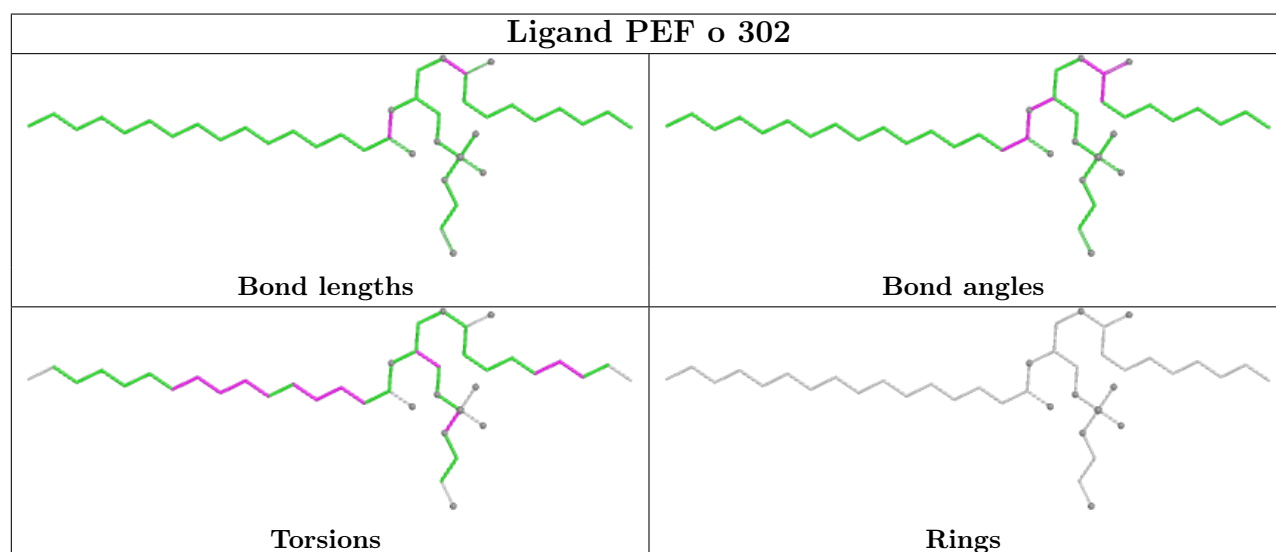
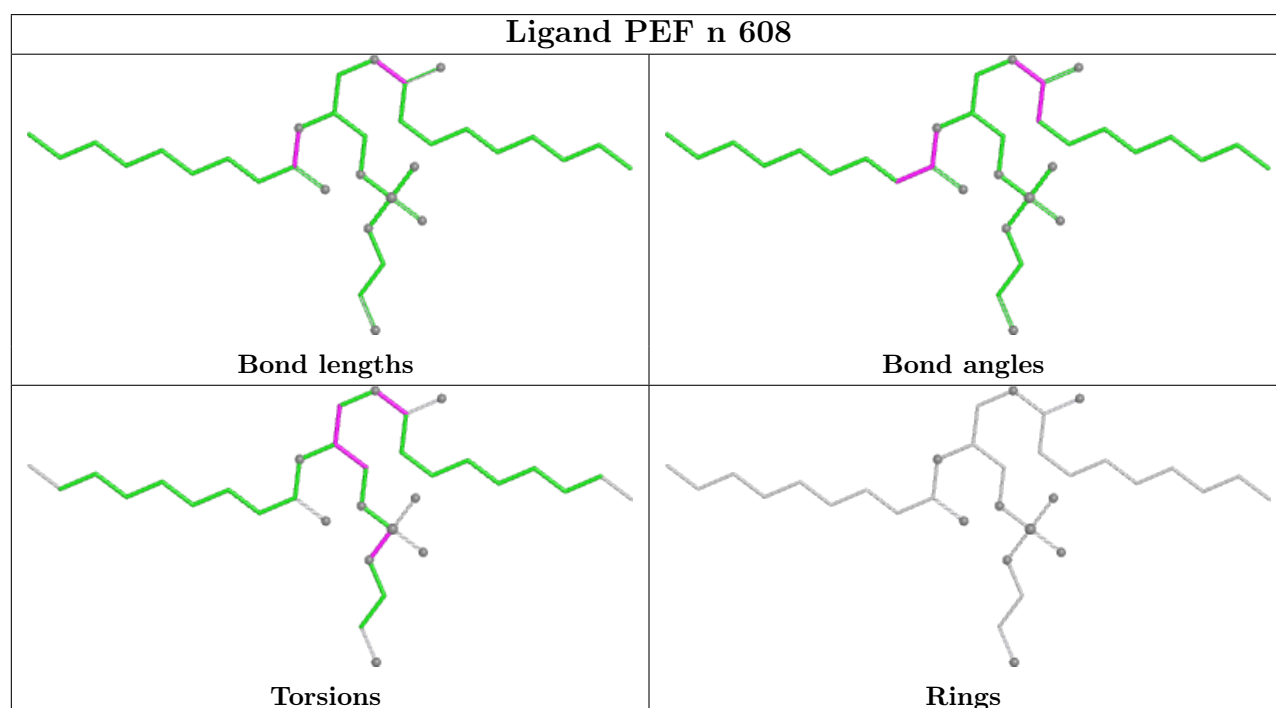
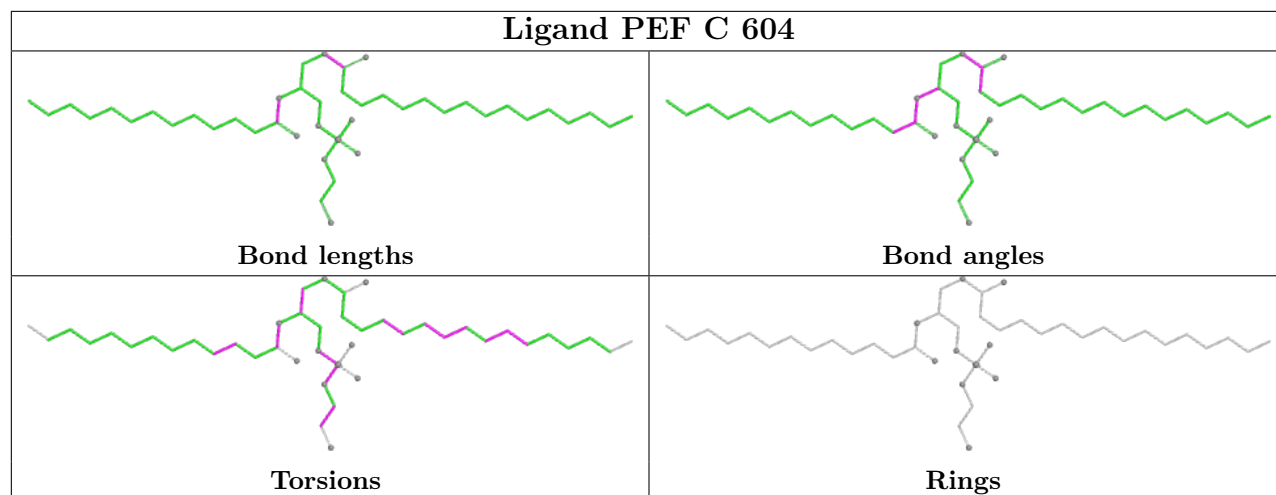


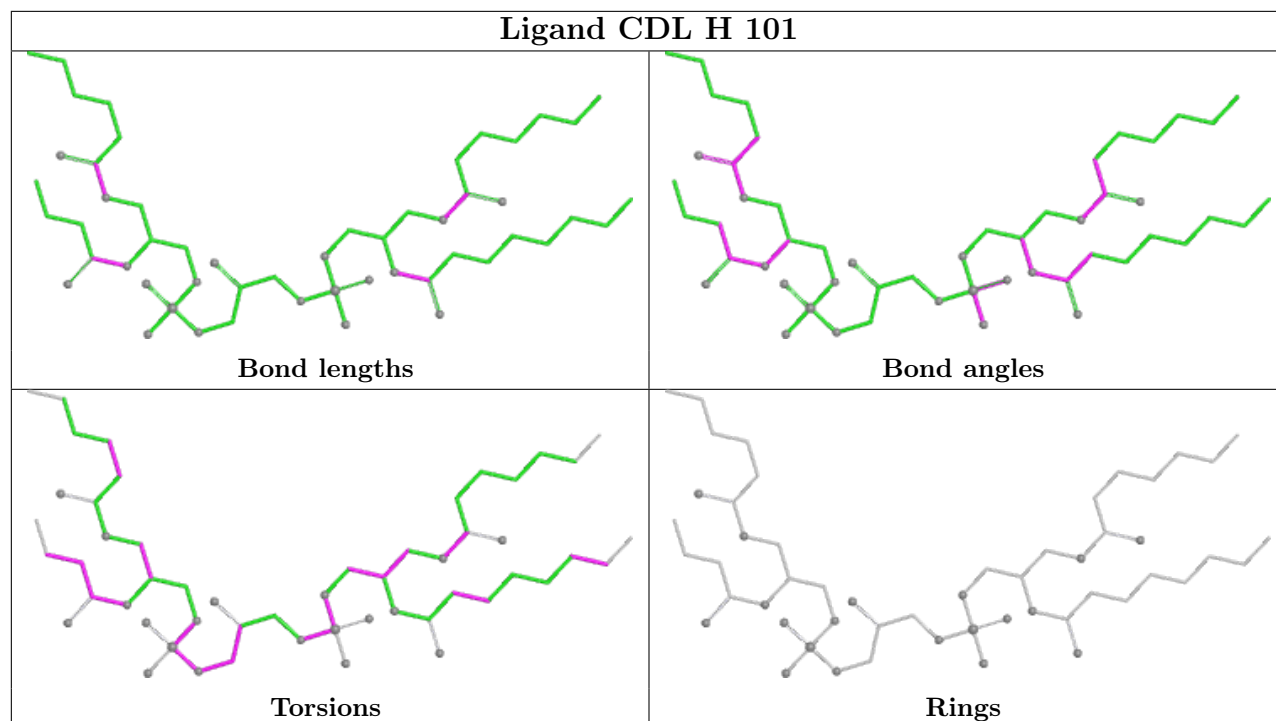


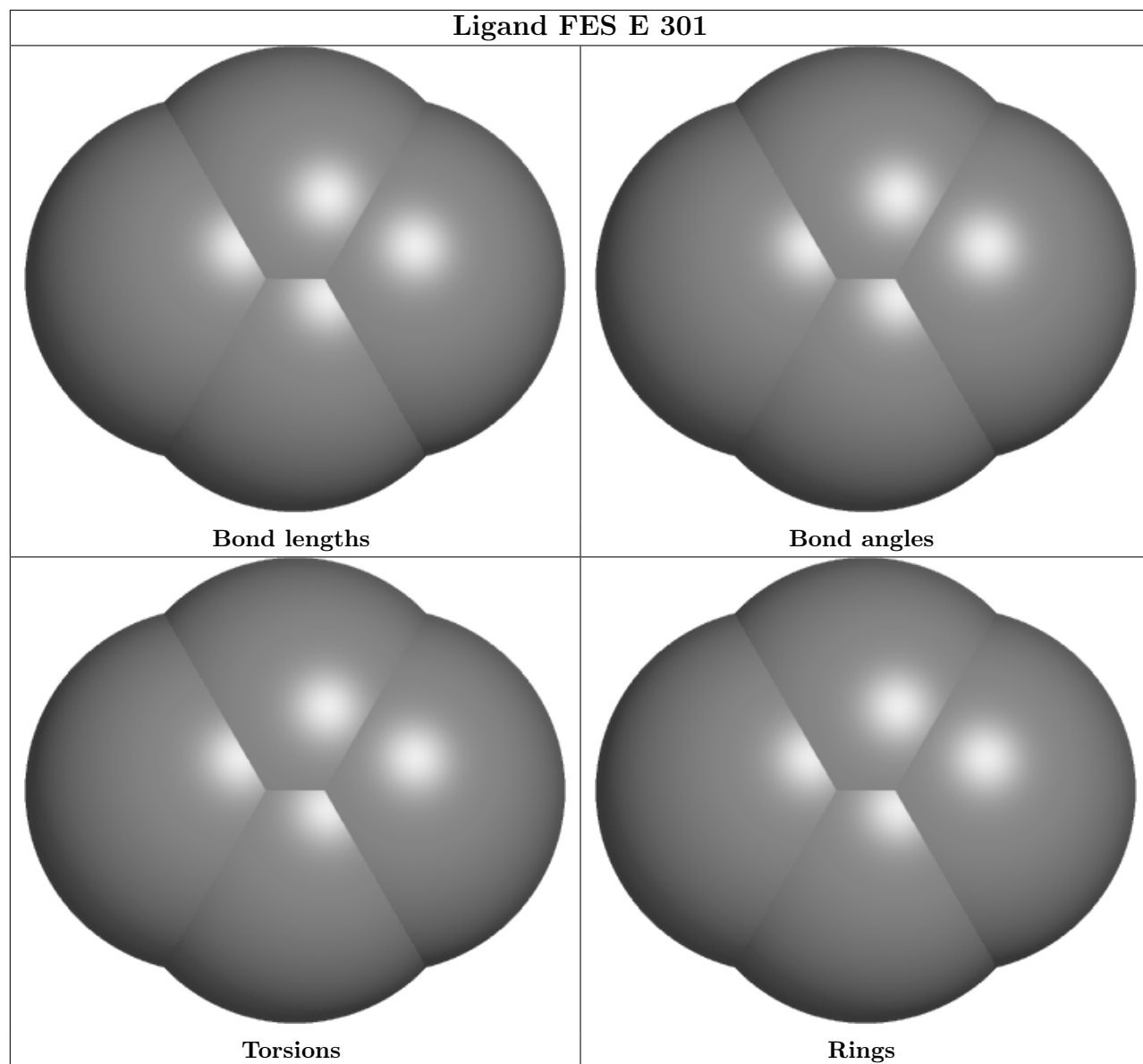


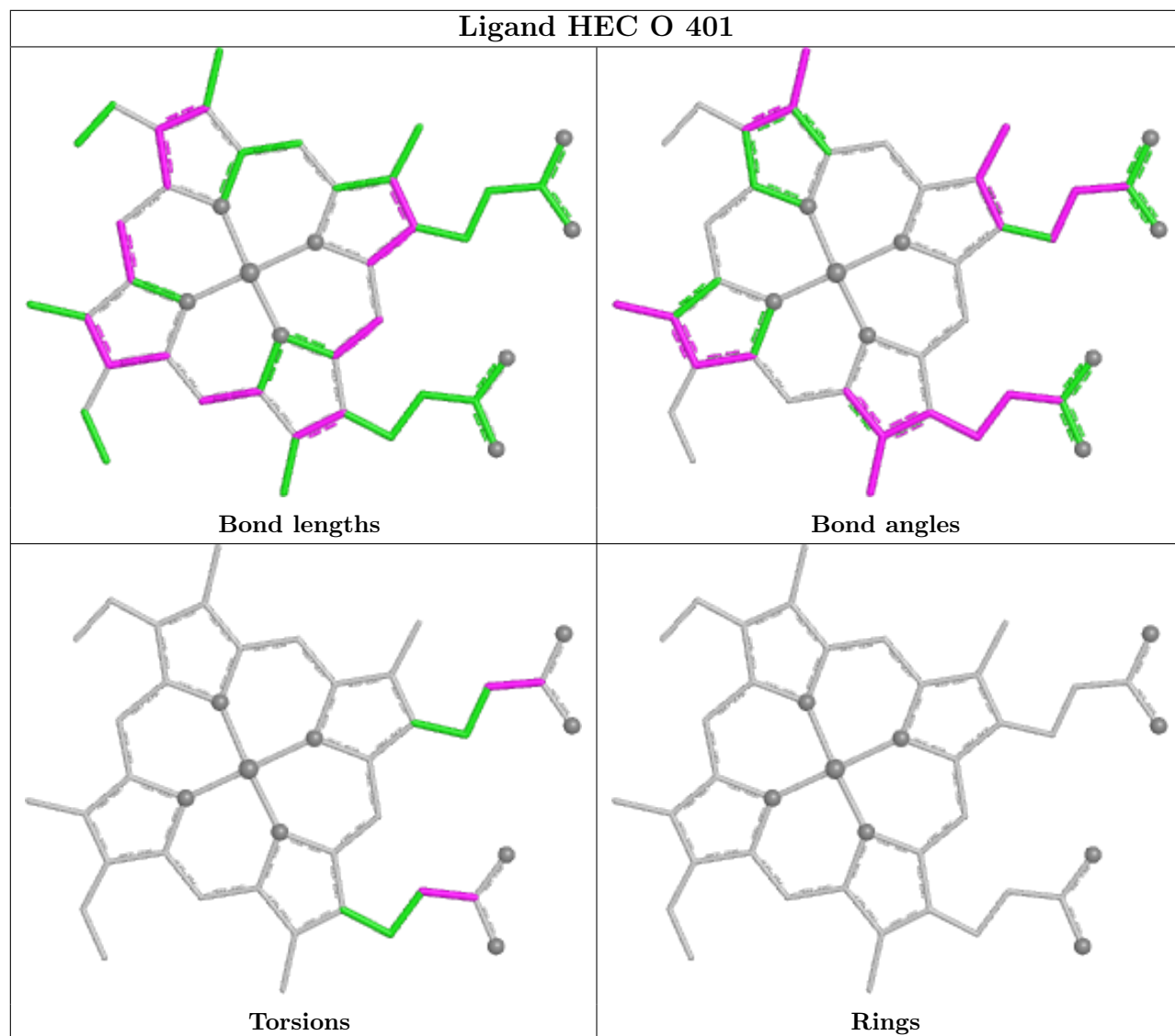


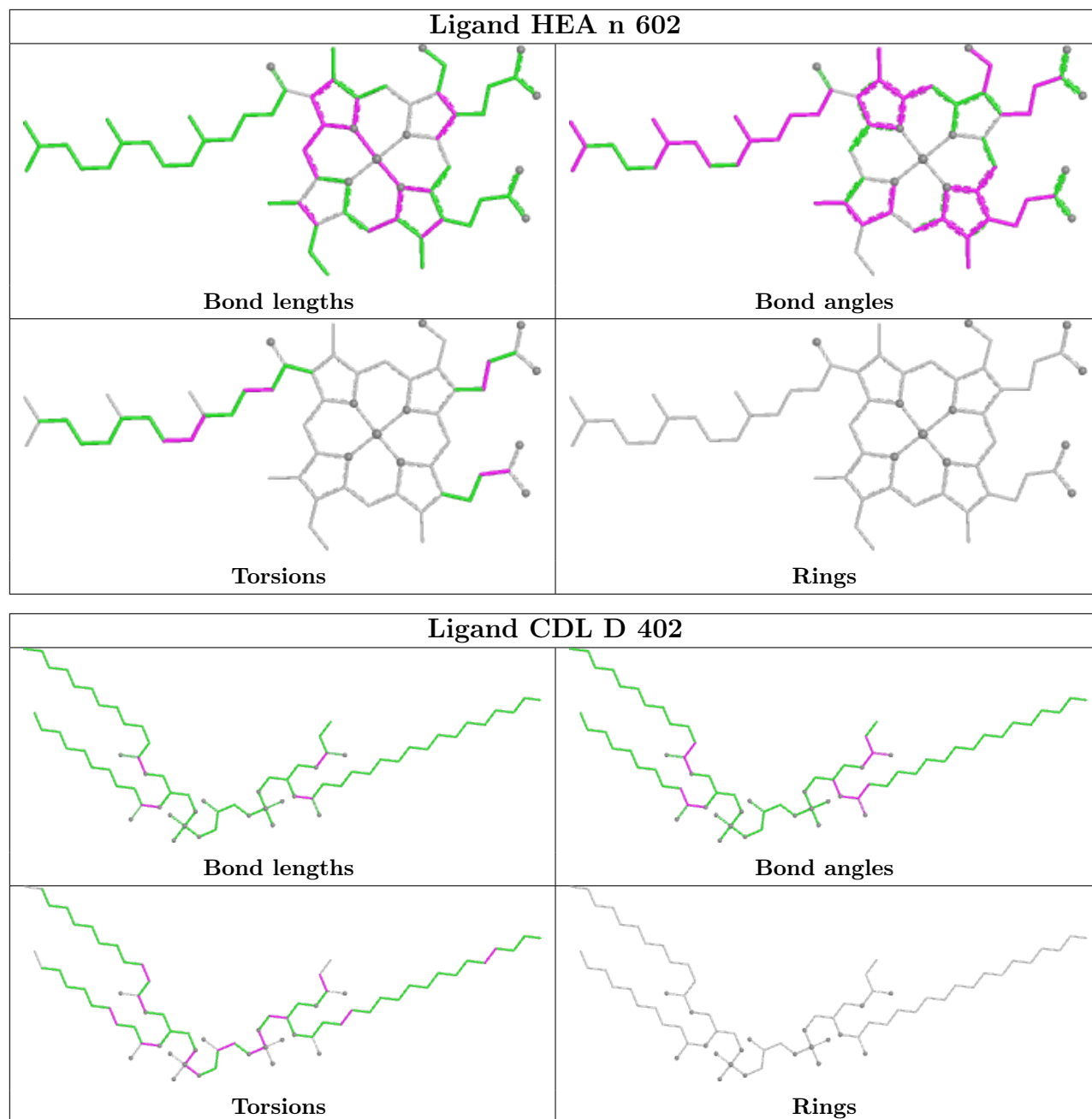


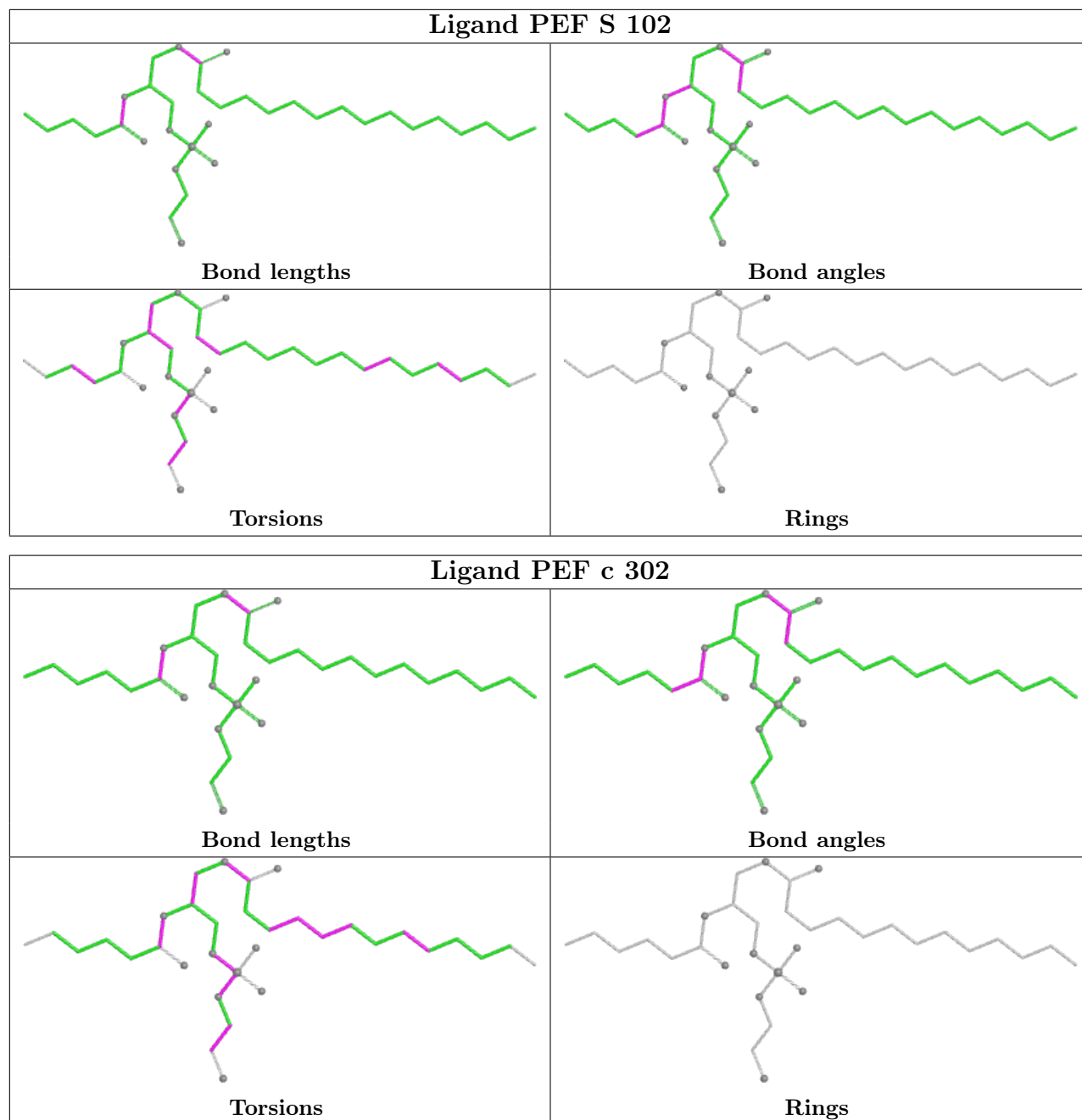


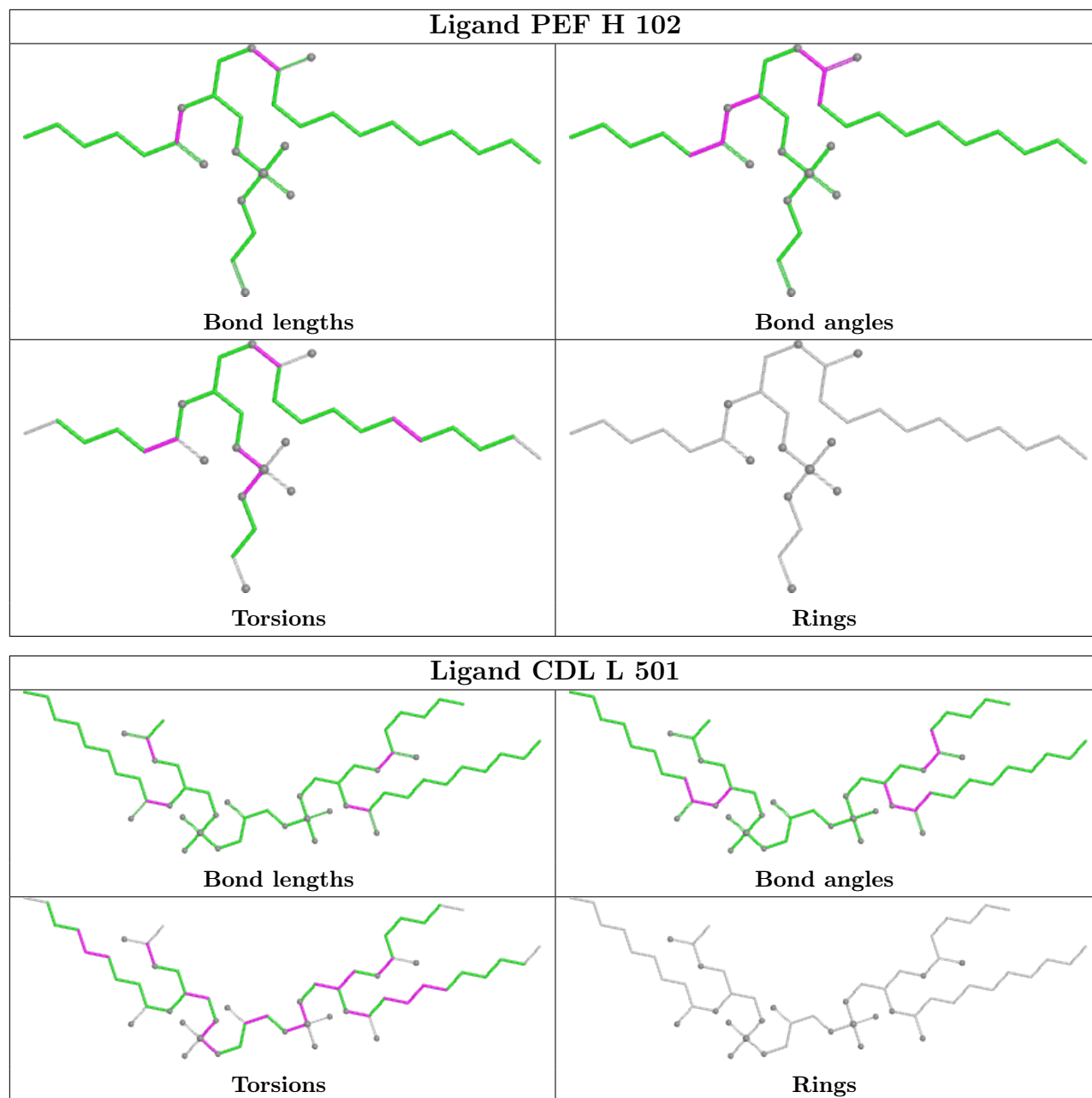


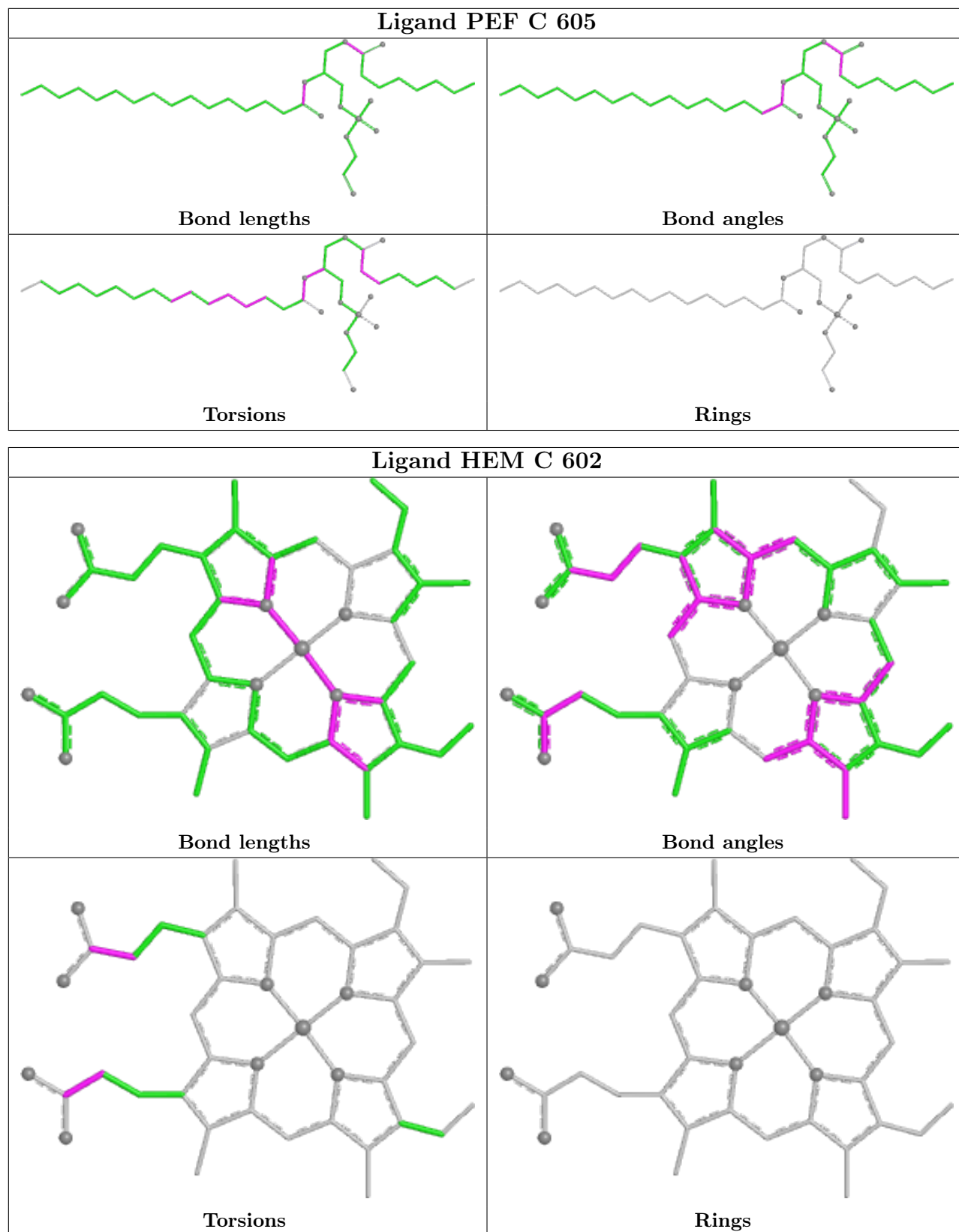


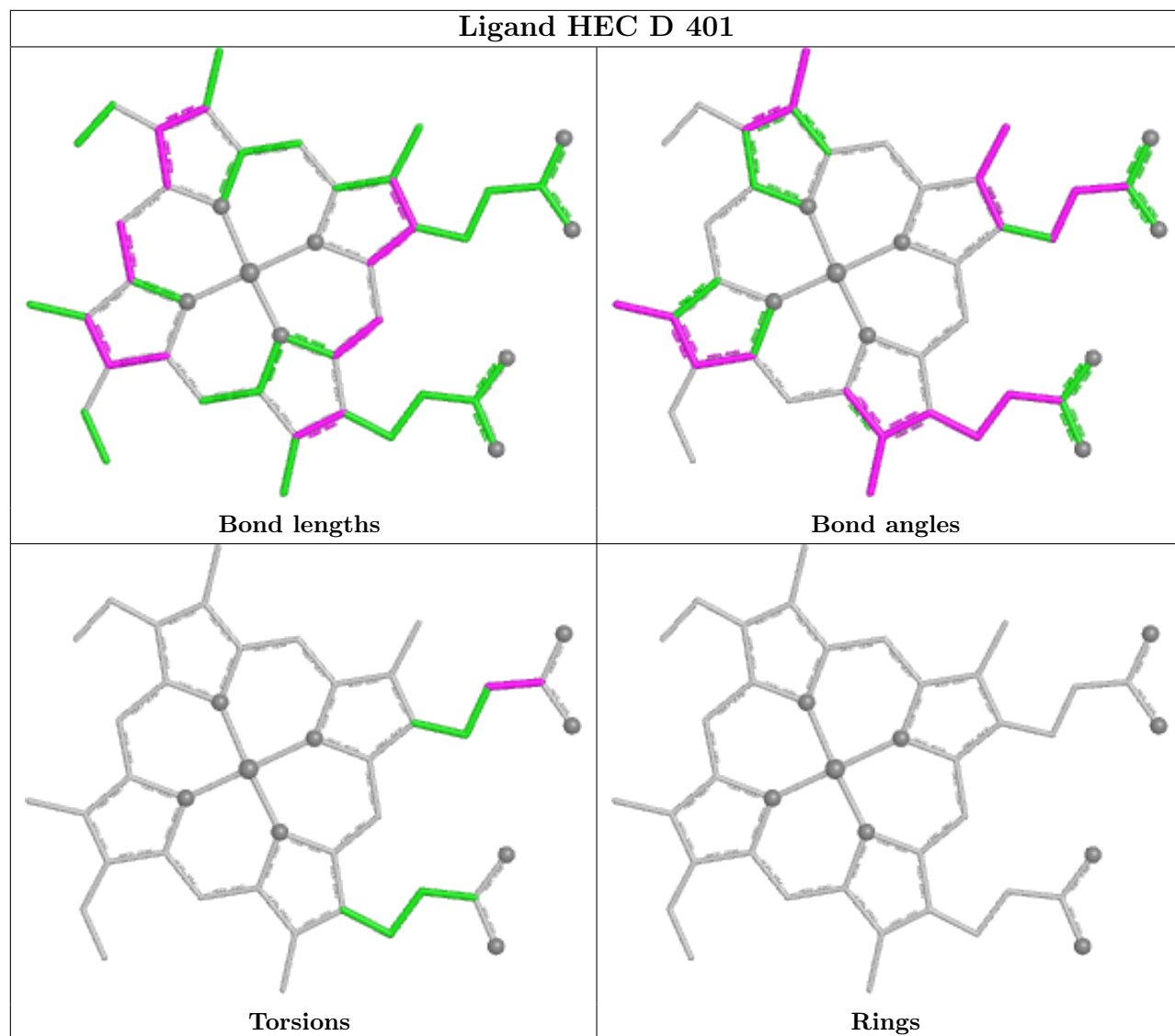


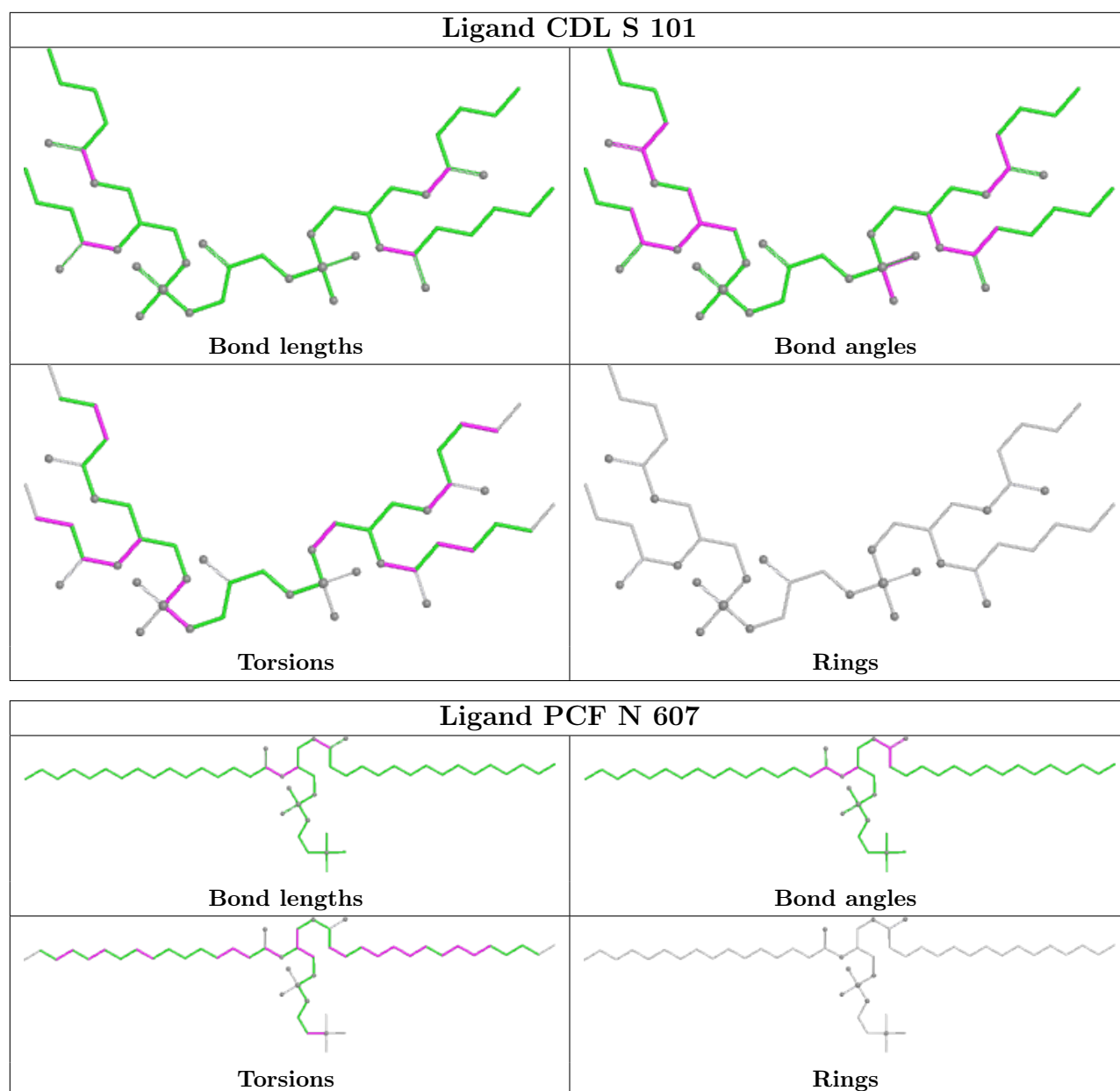


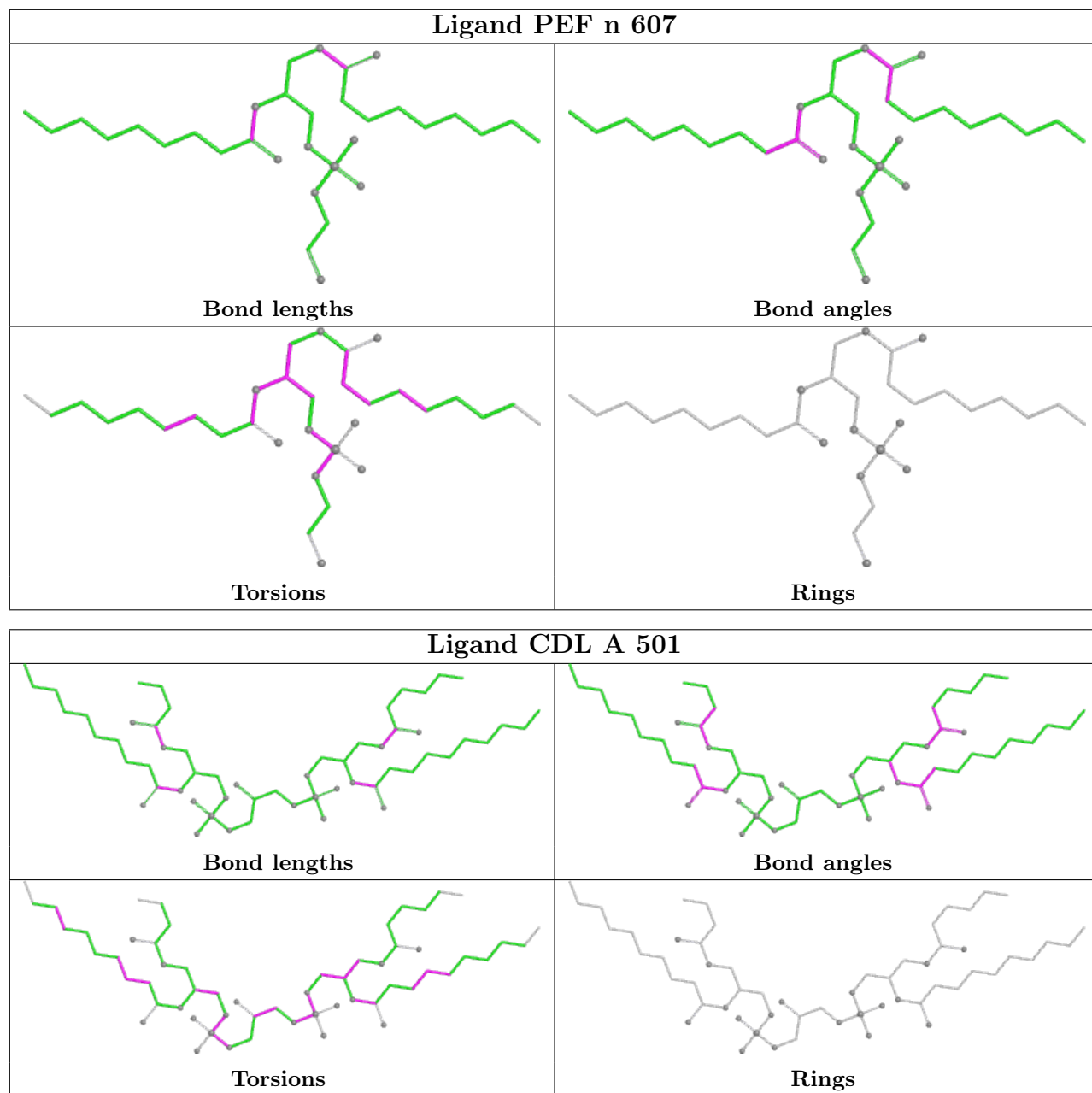


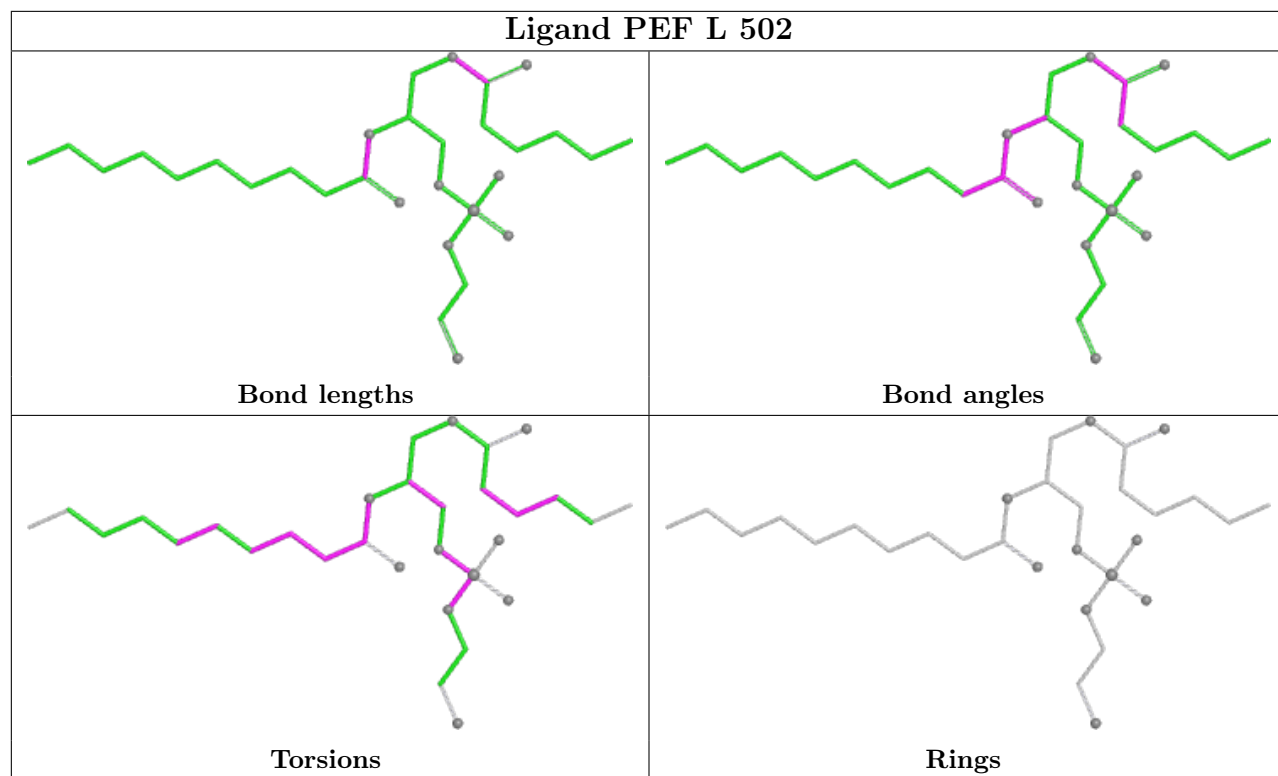


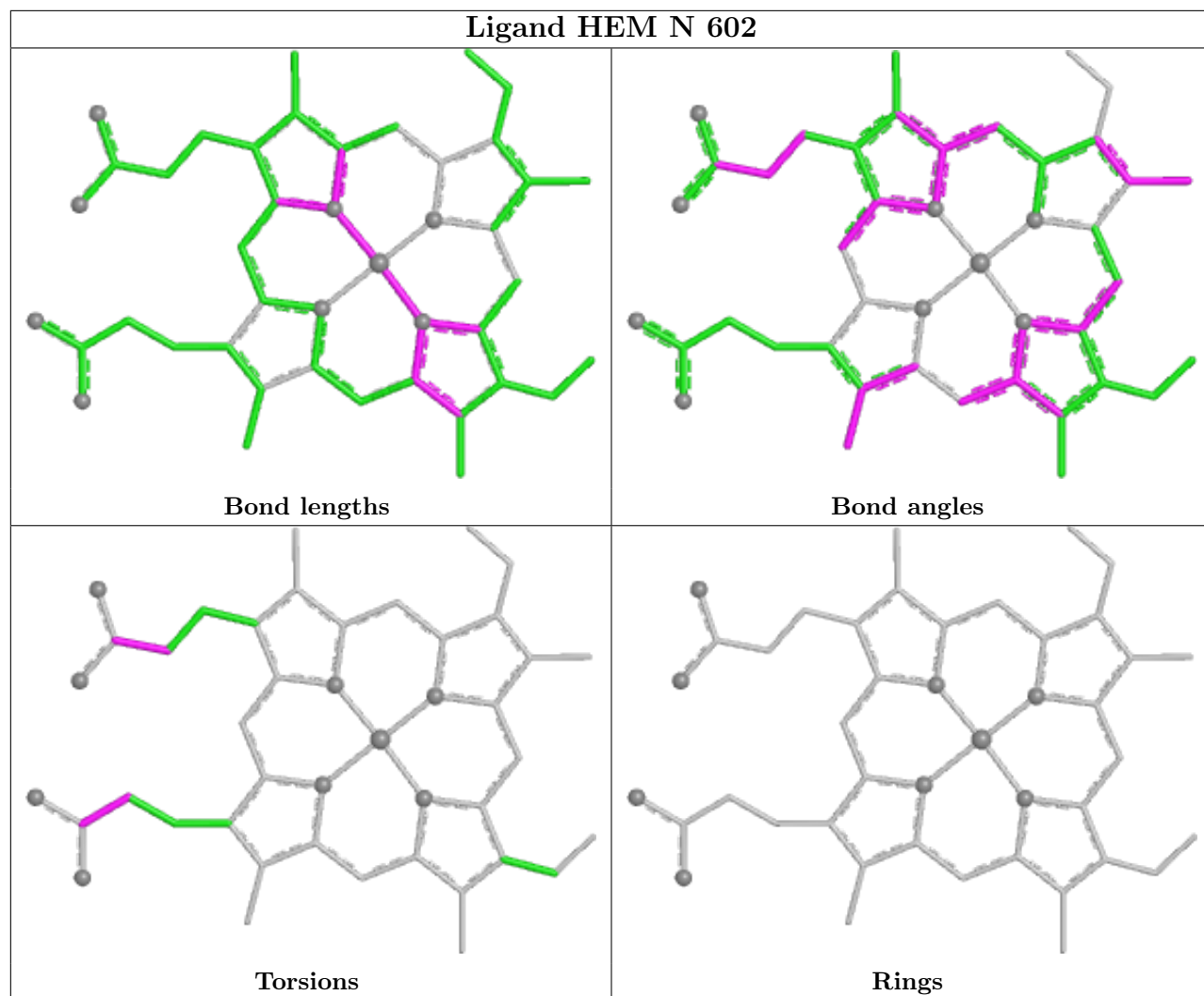


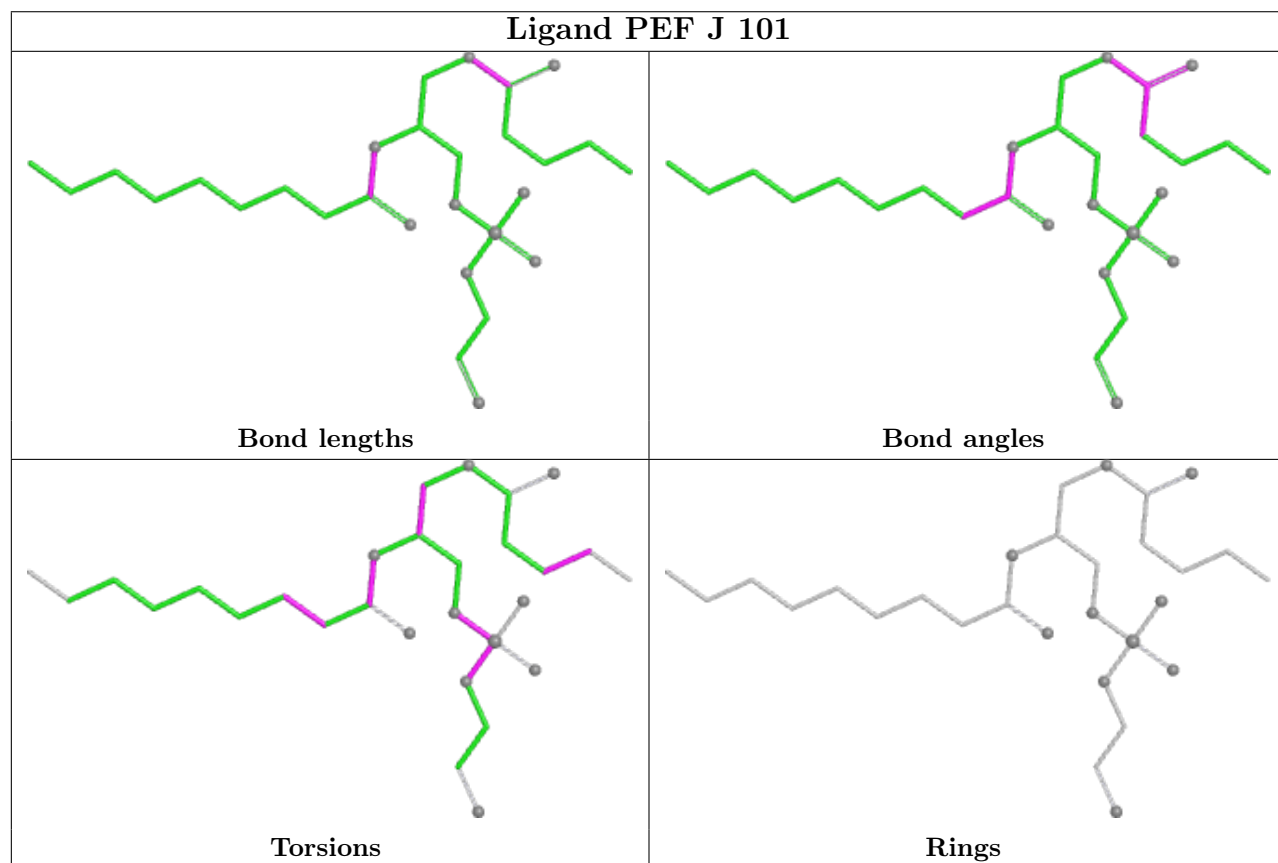
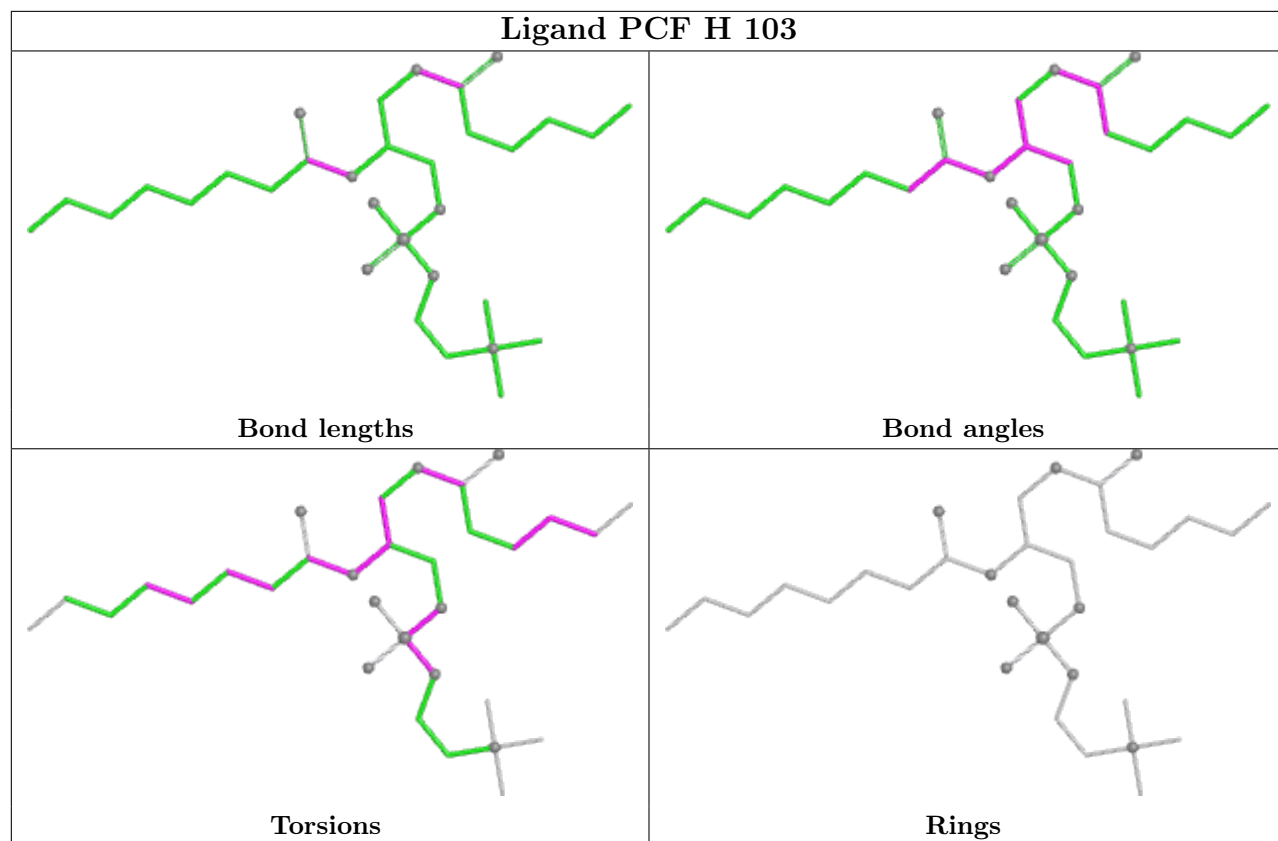


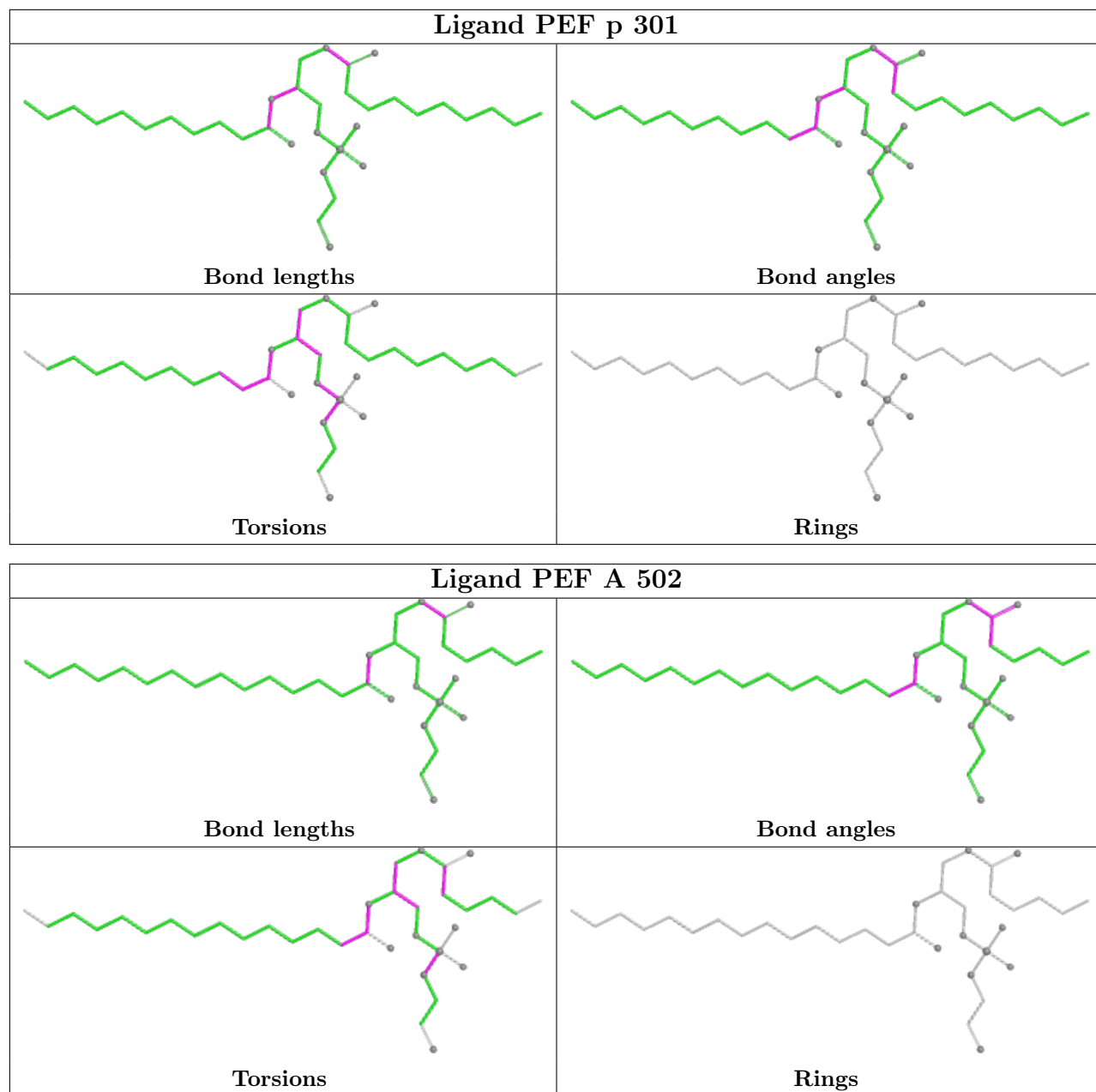


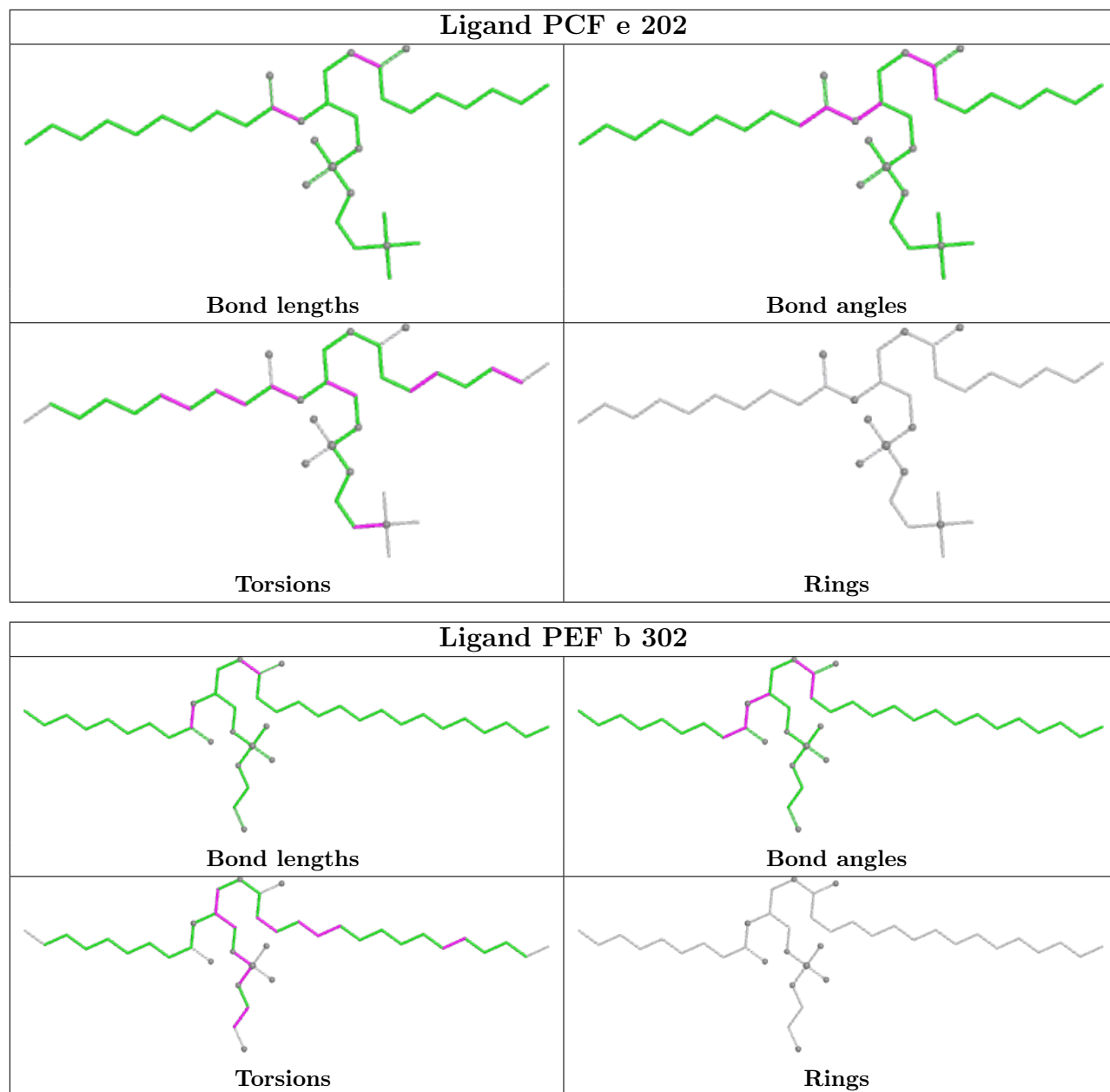


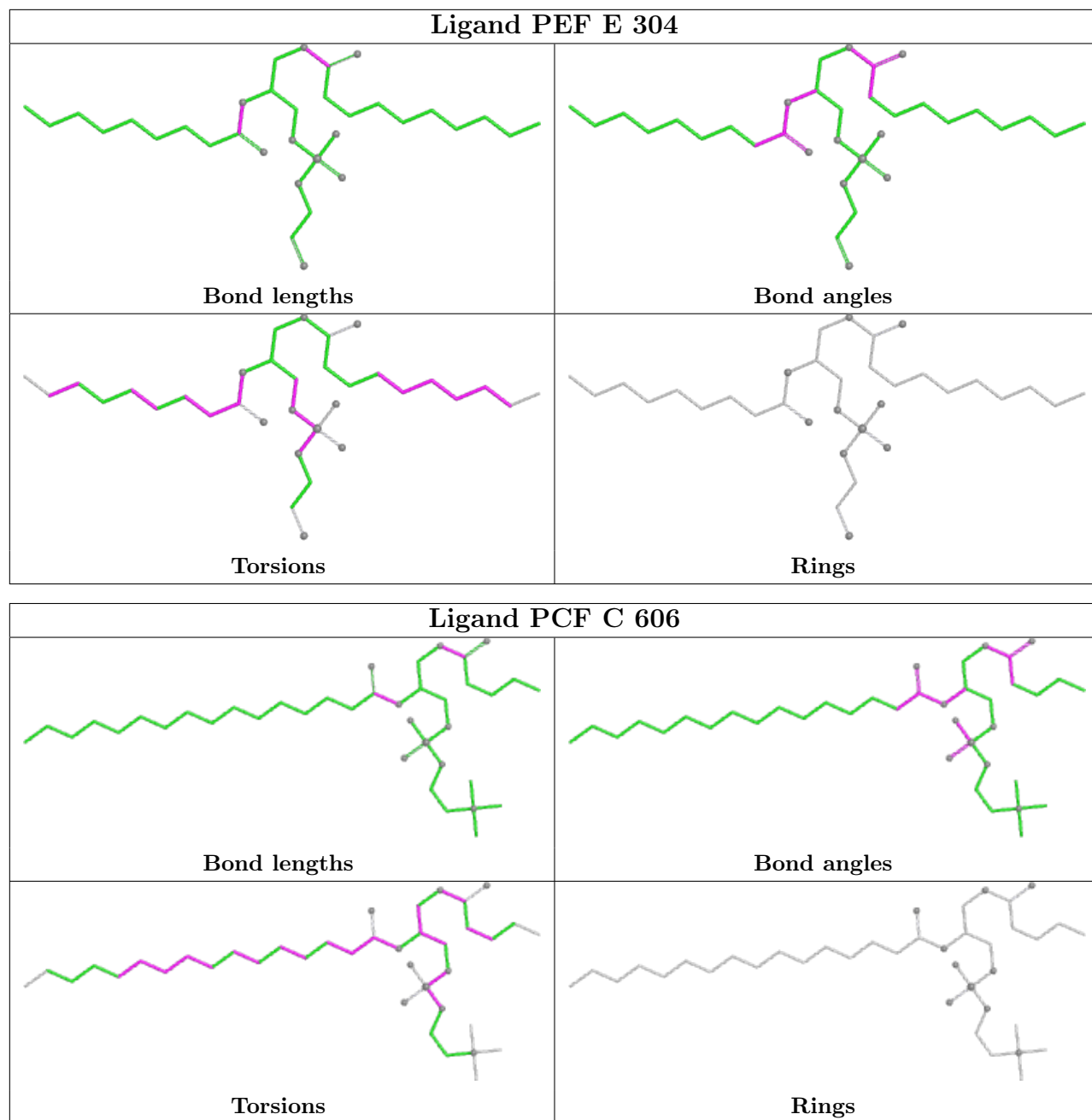


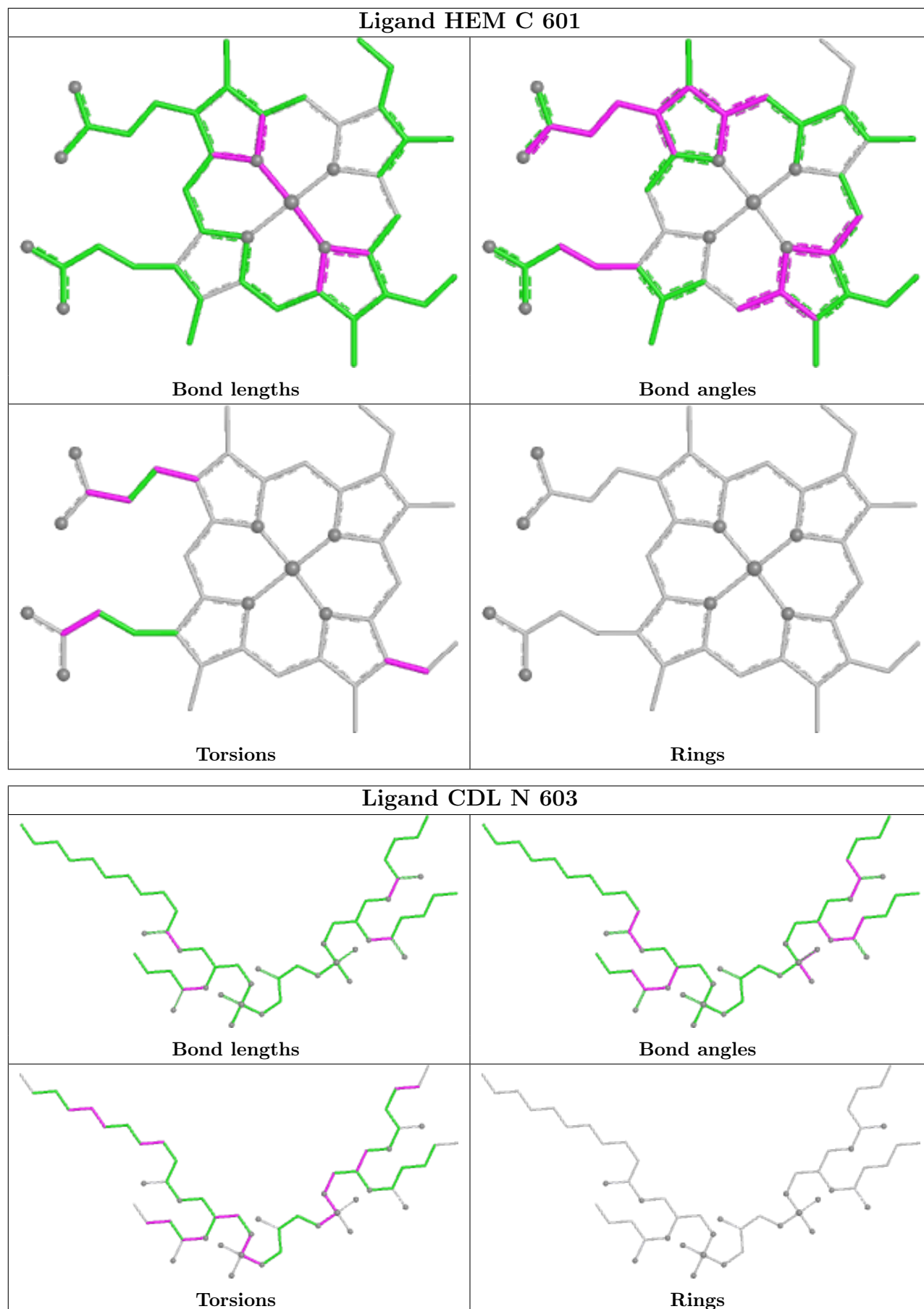


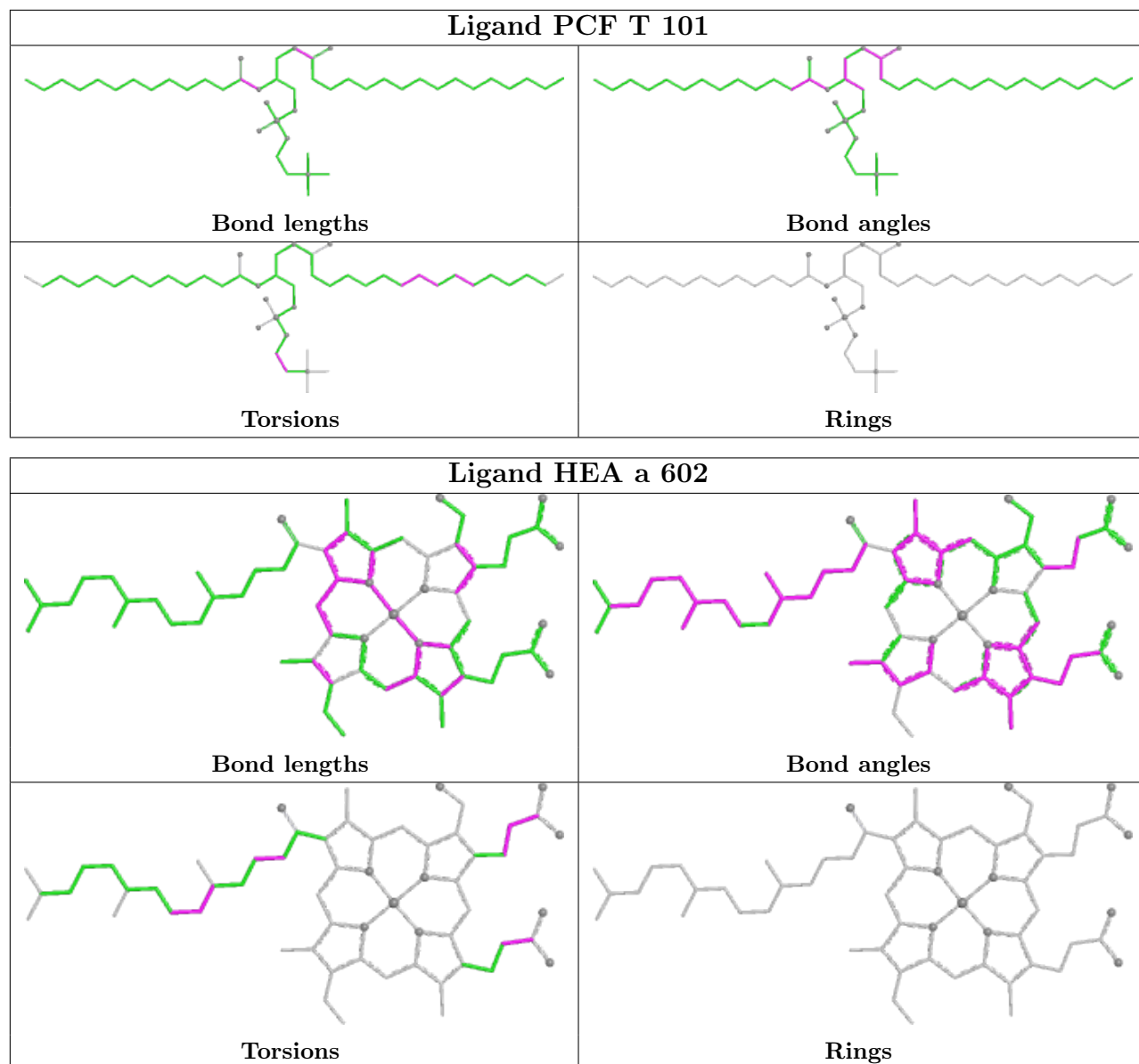


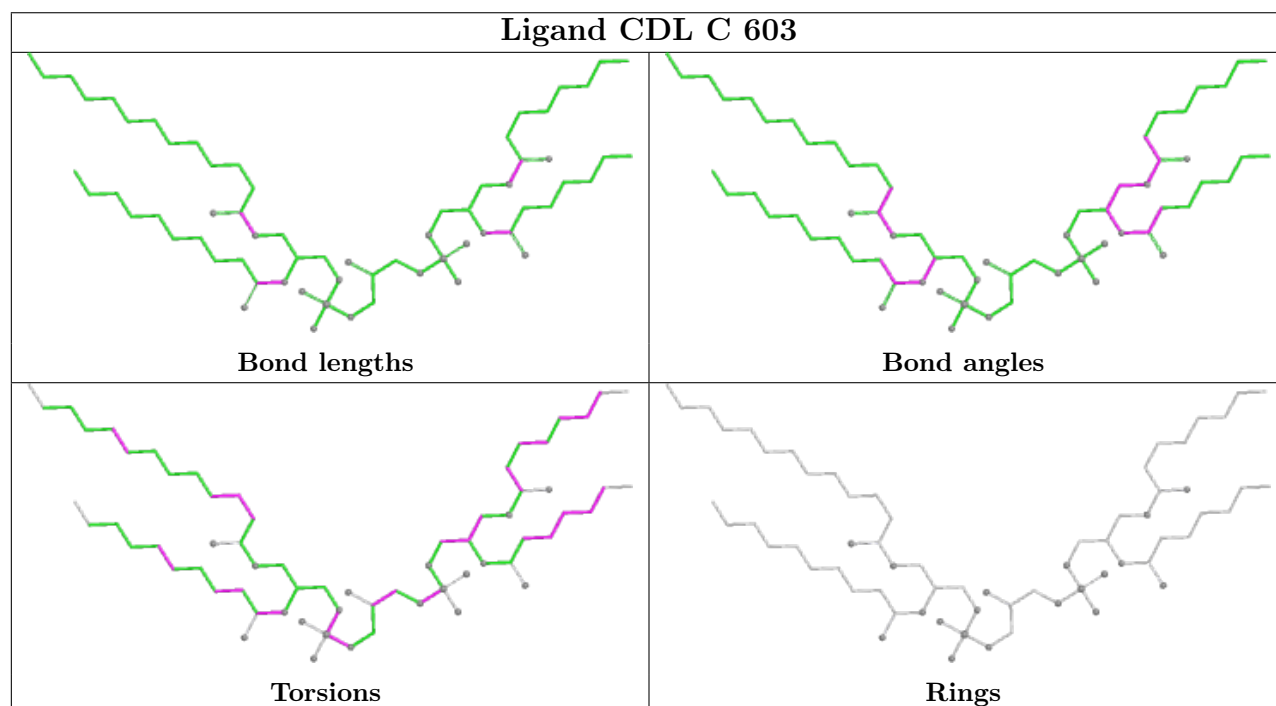
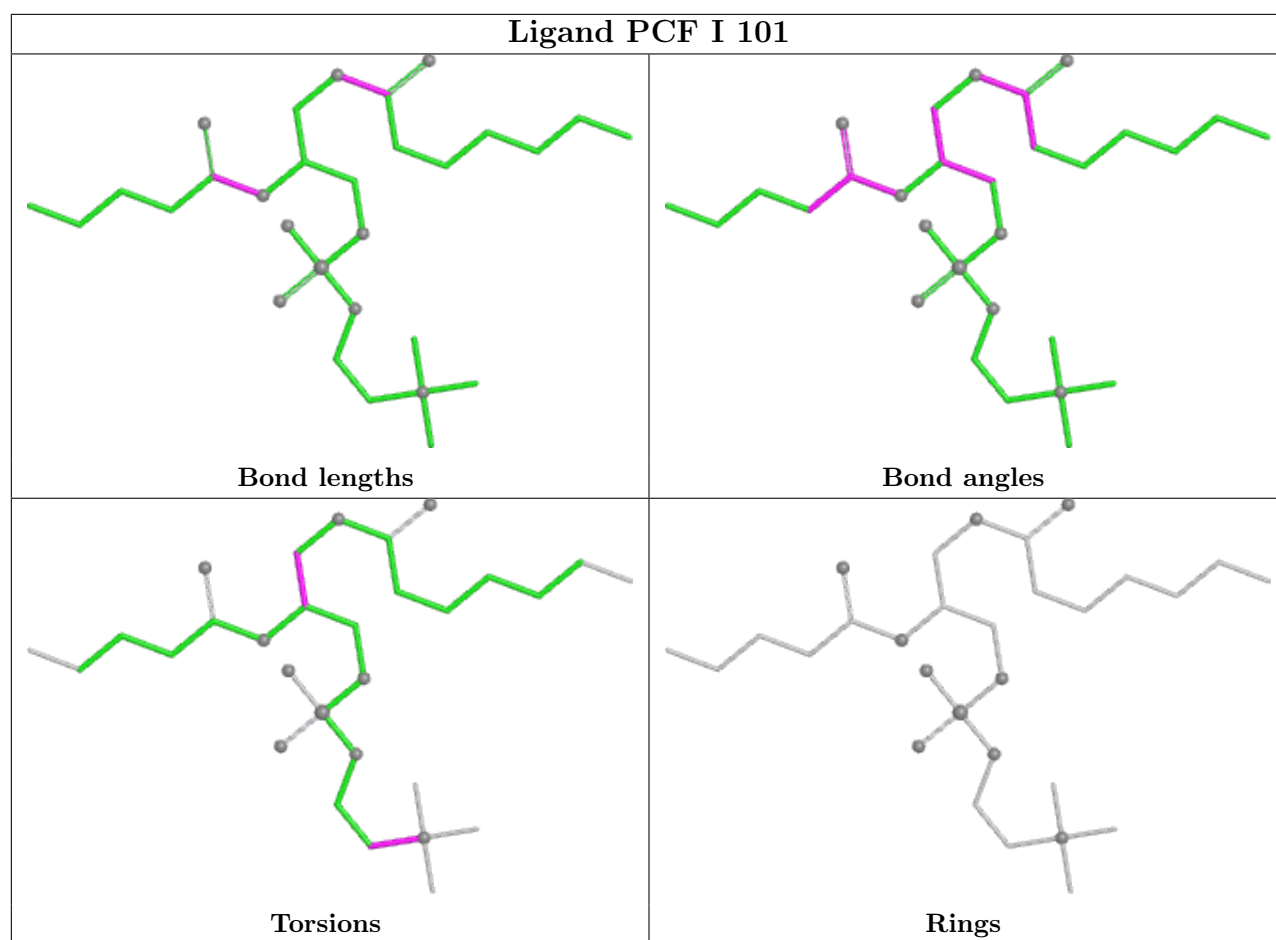


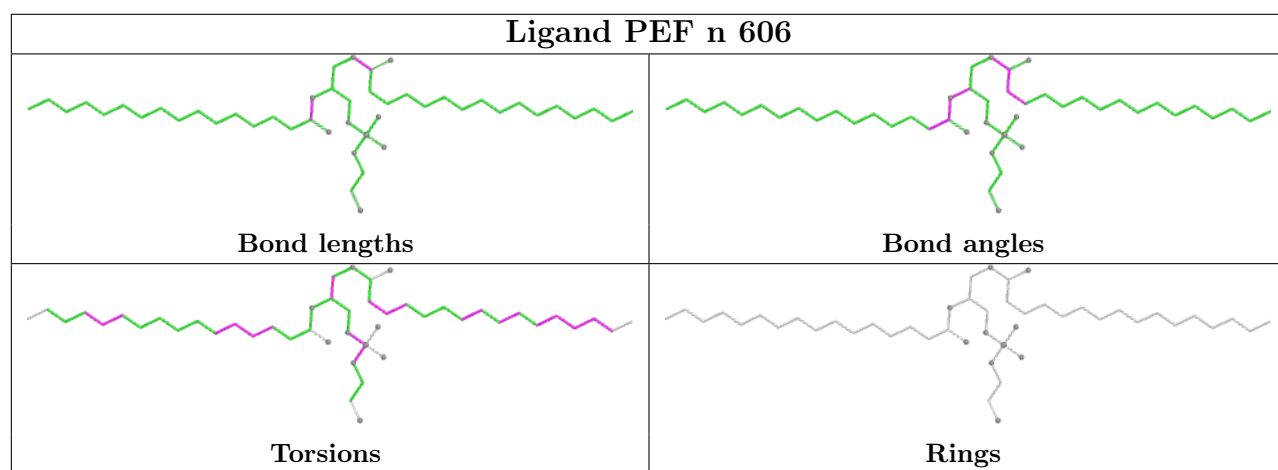
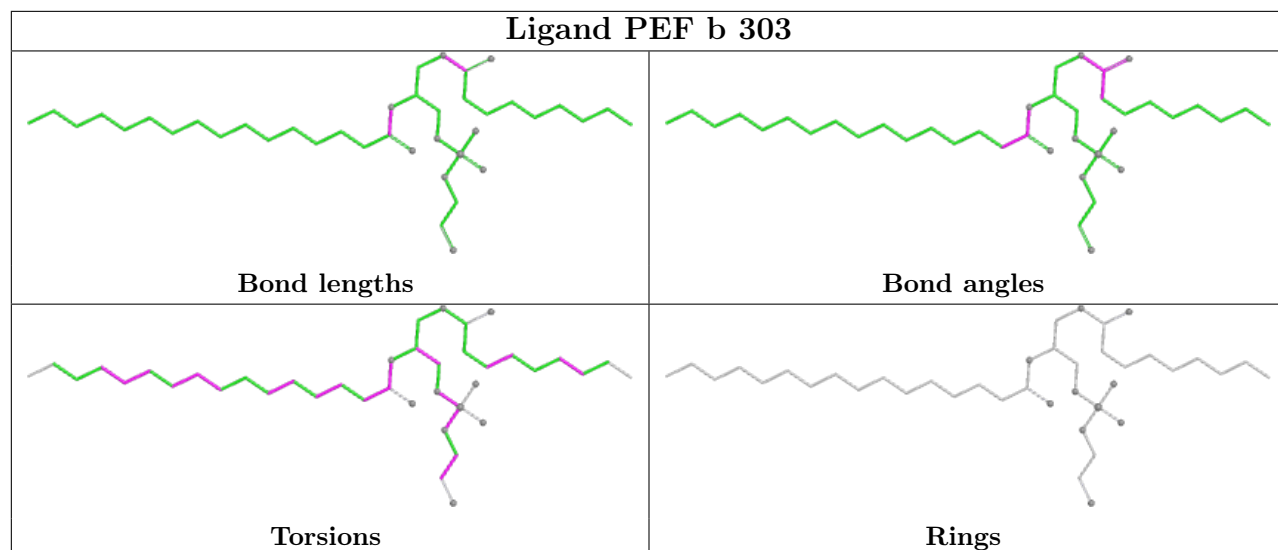


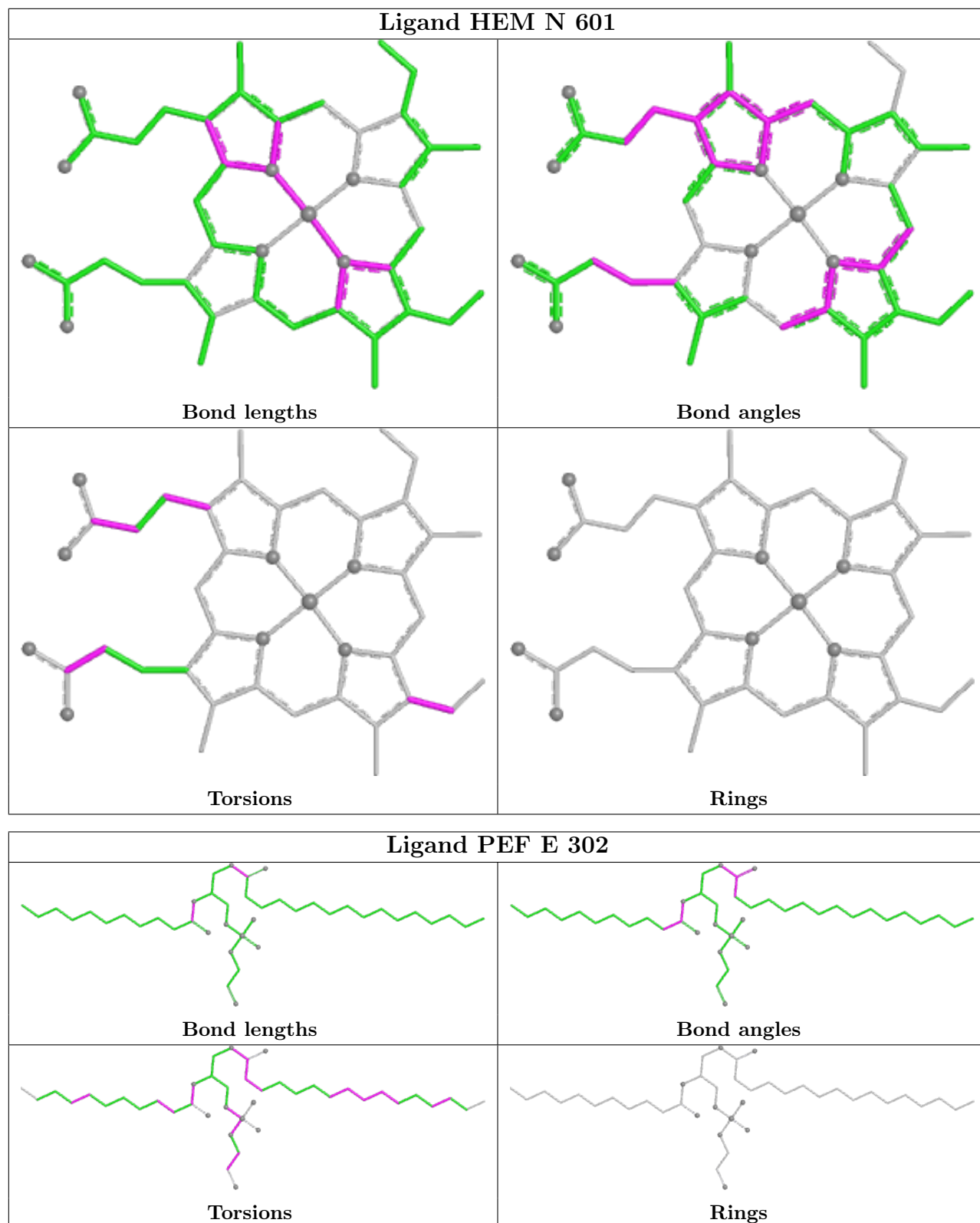


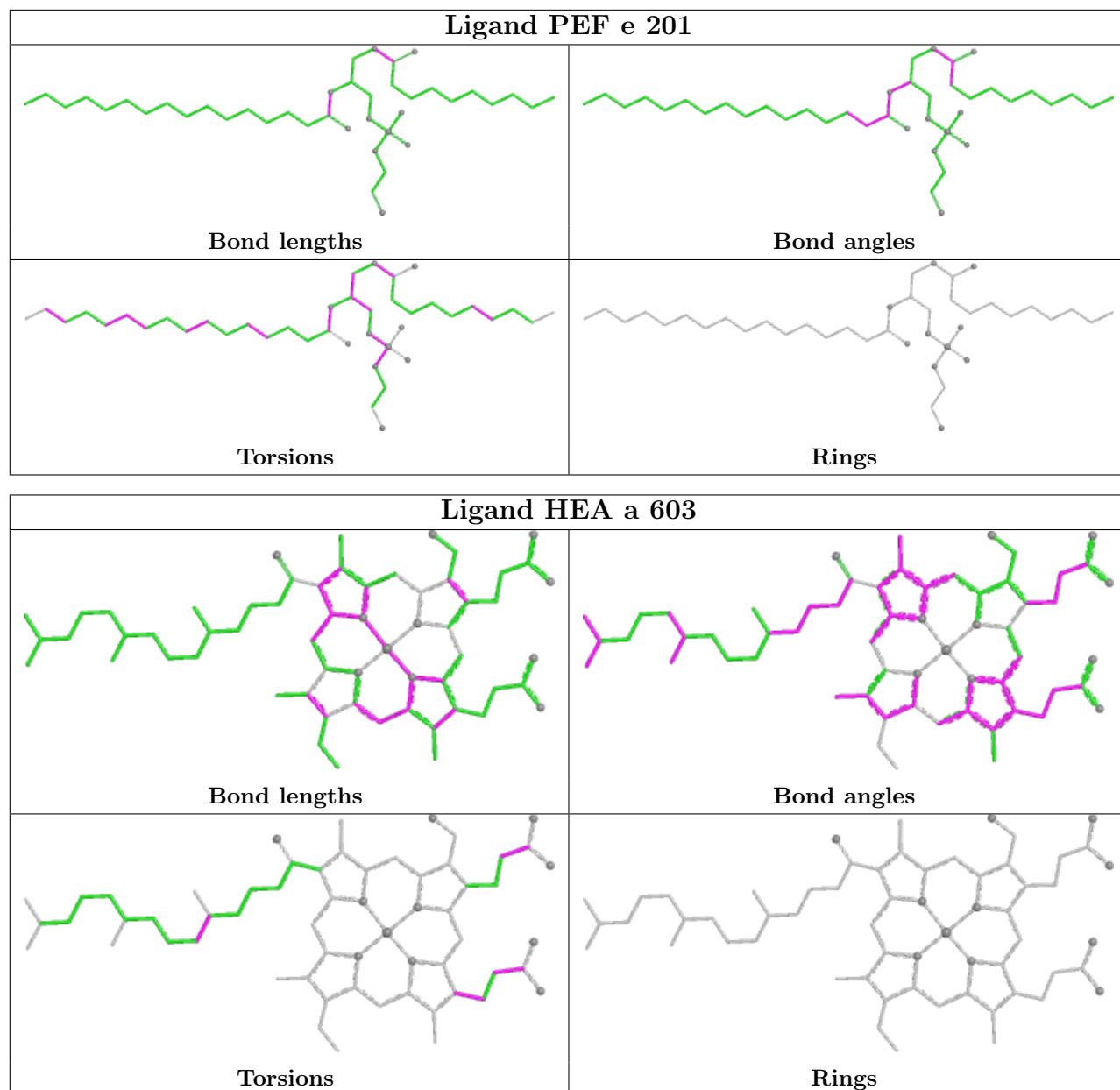


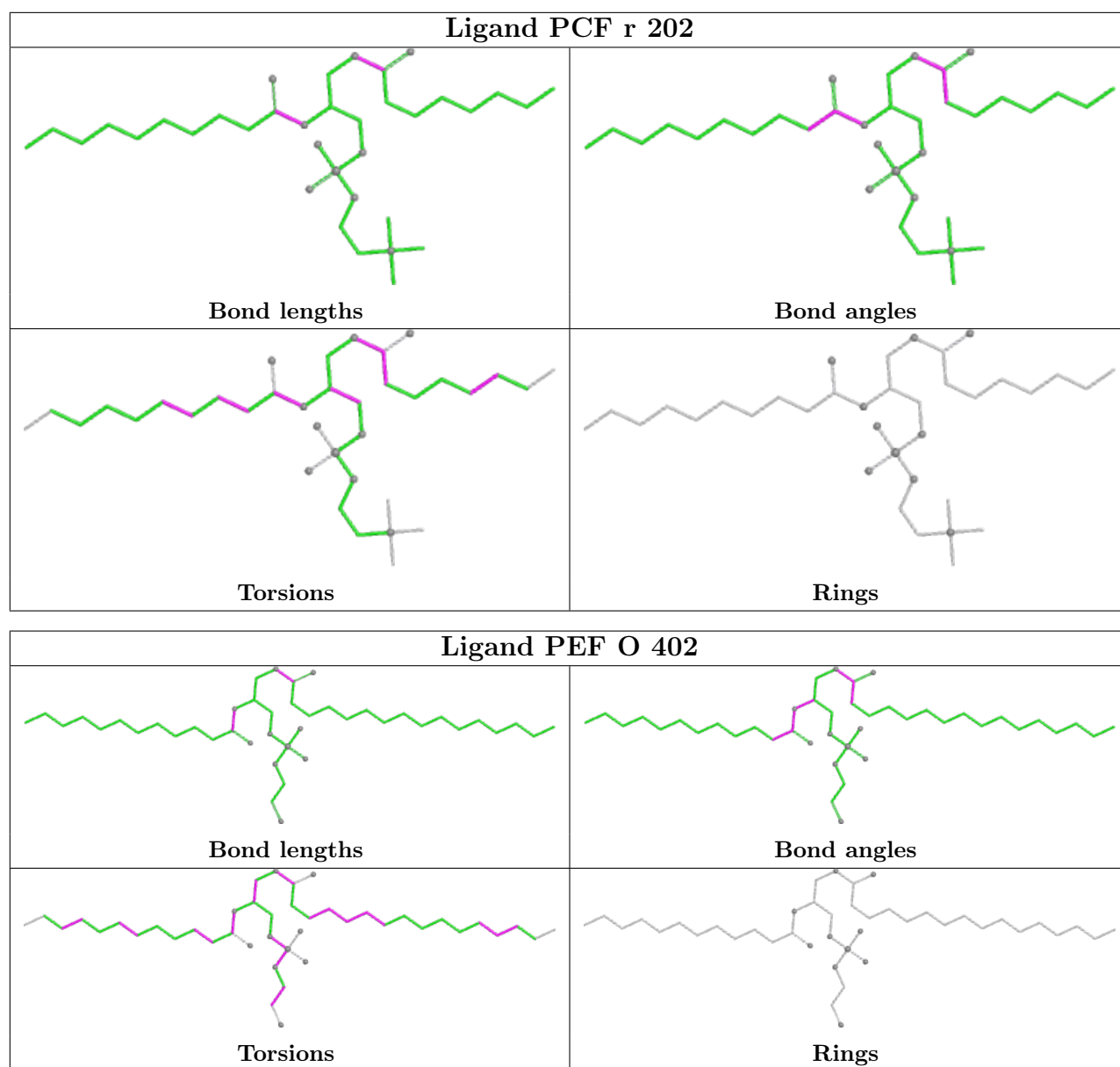












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

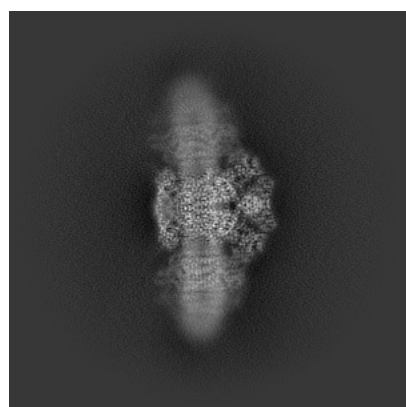
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10340. These allow visual inspection of the internal detail of the map and identification of artifacts.

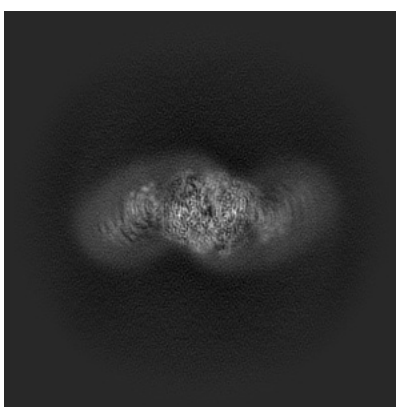
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

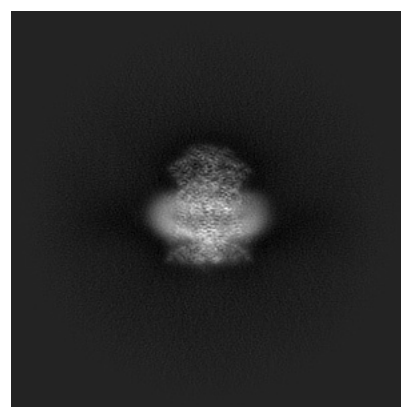
6.1.1 Primary map



X



Y

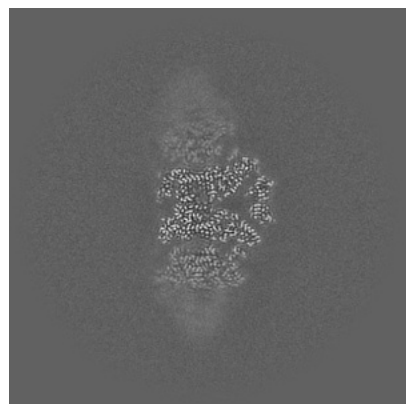


Z

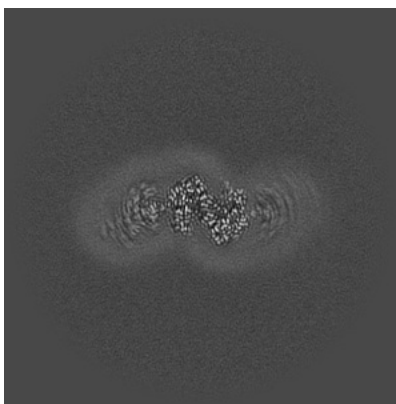
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

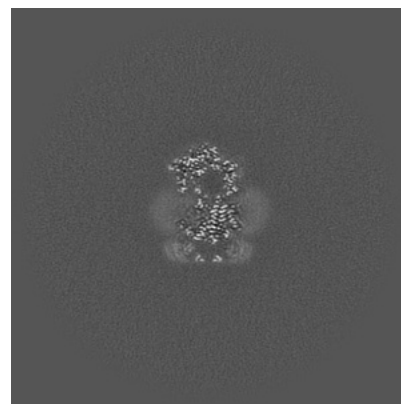
6.2.1 Primary map



X Index: 224



Y Index: 224

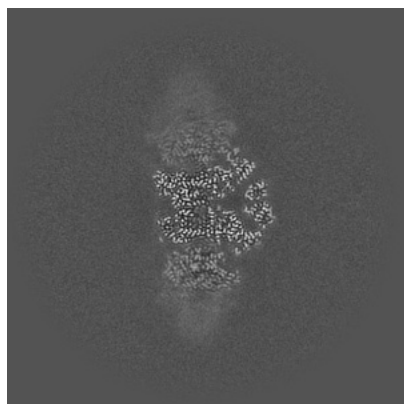


Z Index: 224

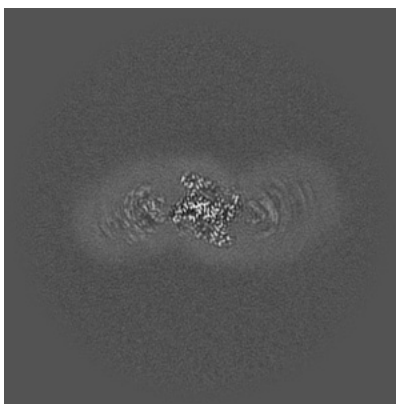
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

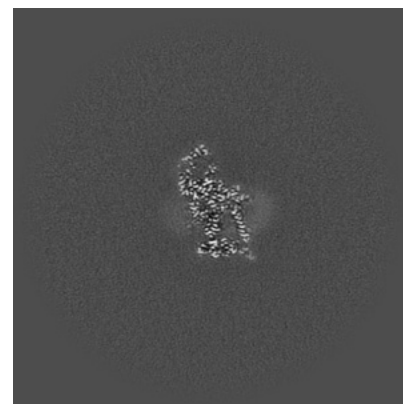
6.3.1 Primary map



X Index: 218



Y Index: 202



Z Index: 200

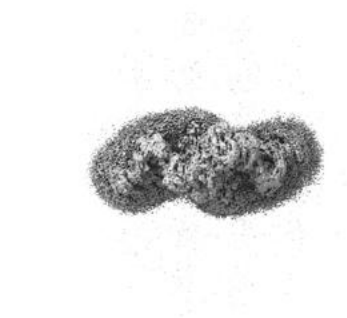
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

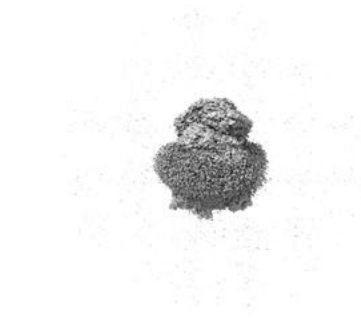
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

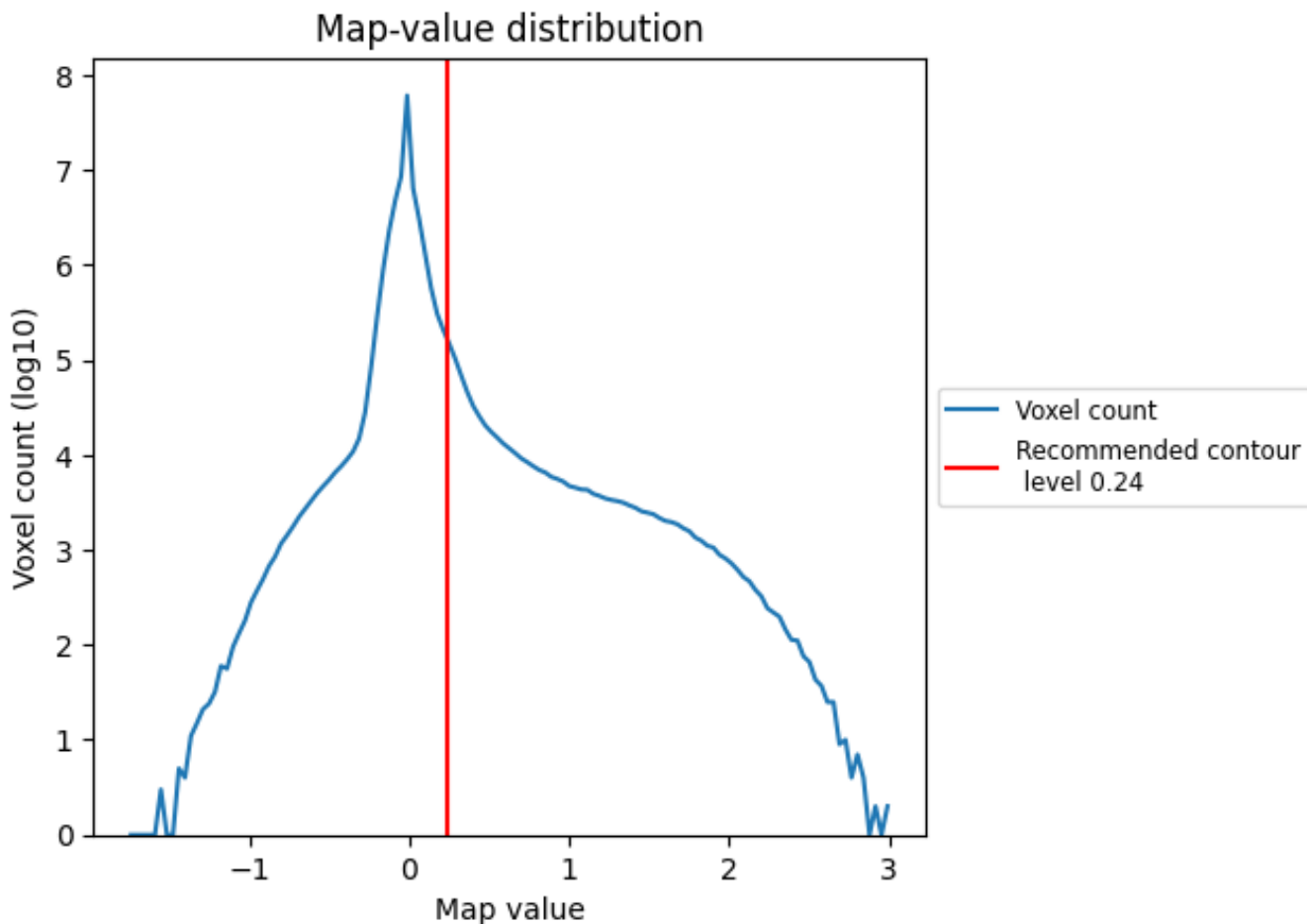
6.5 Mask visualisation

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

7 Map analysis [i](#)

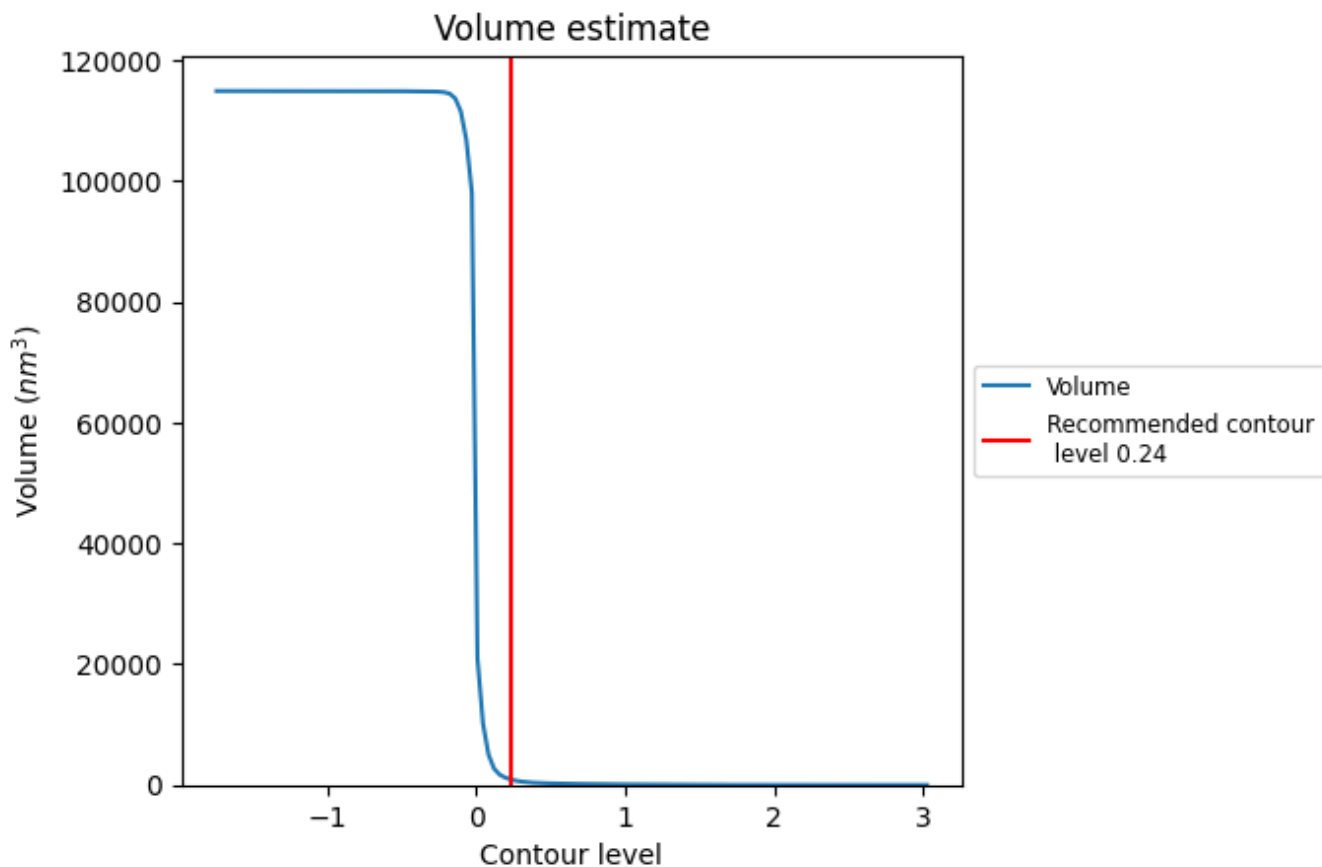
This section contains the results of statistical analysis of the map.

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.

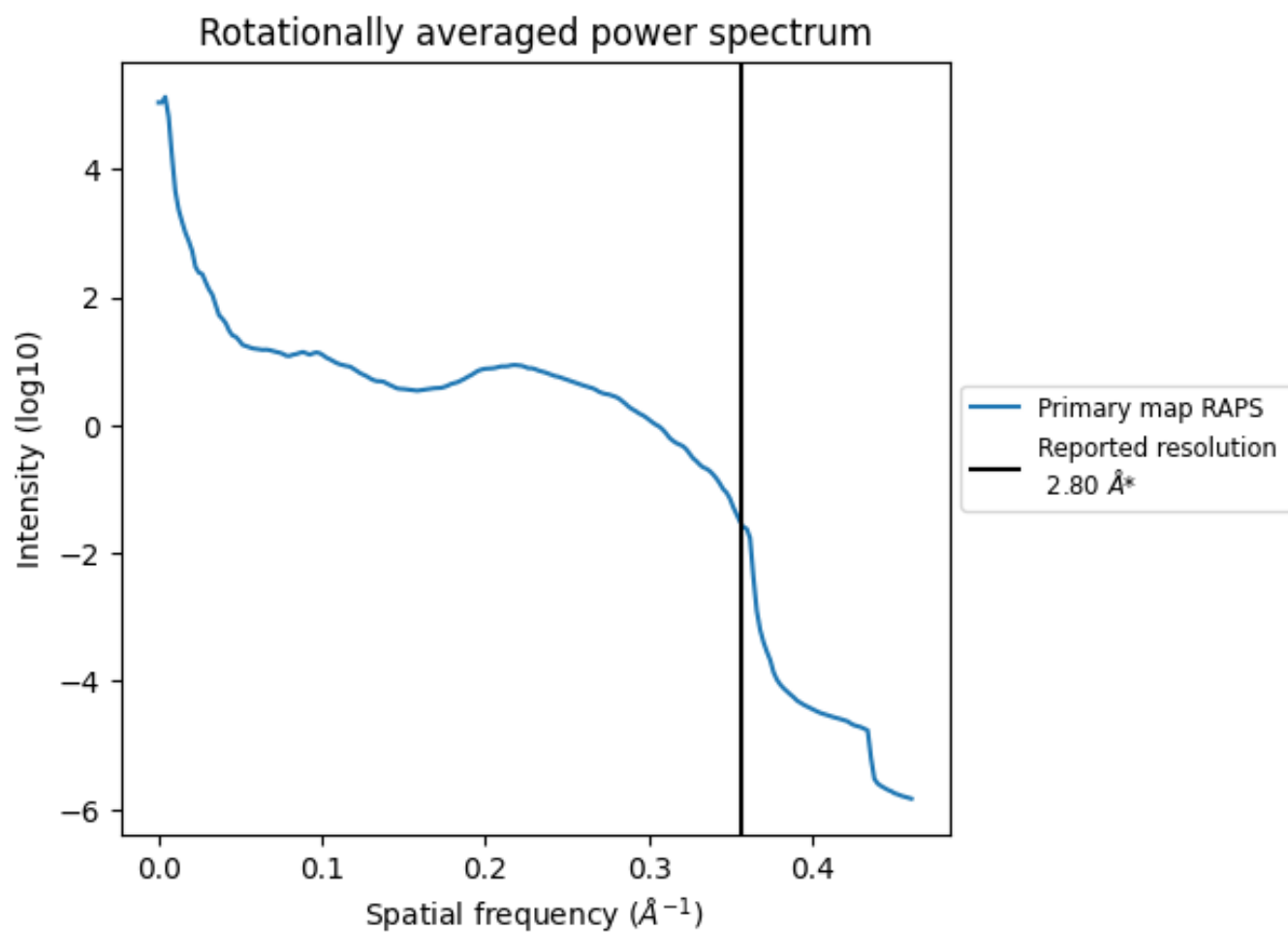
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 878 nm³; this corresponds to an approximate mass of 793 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](#)

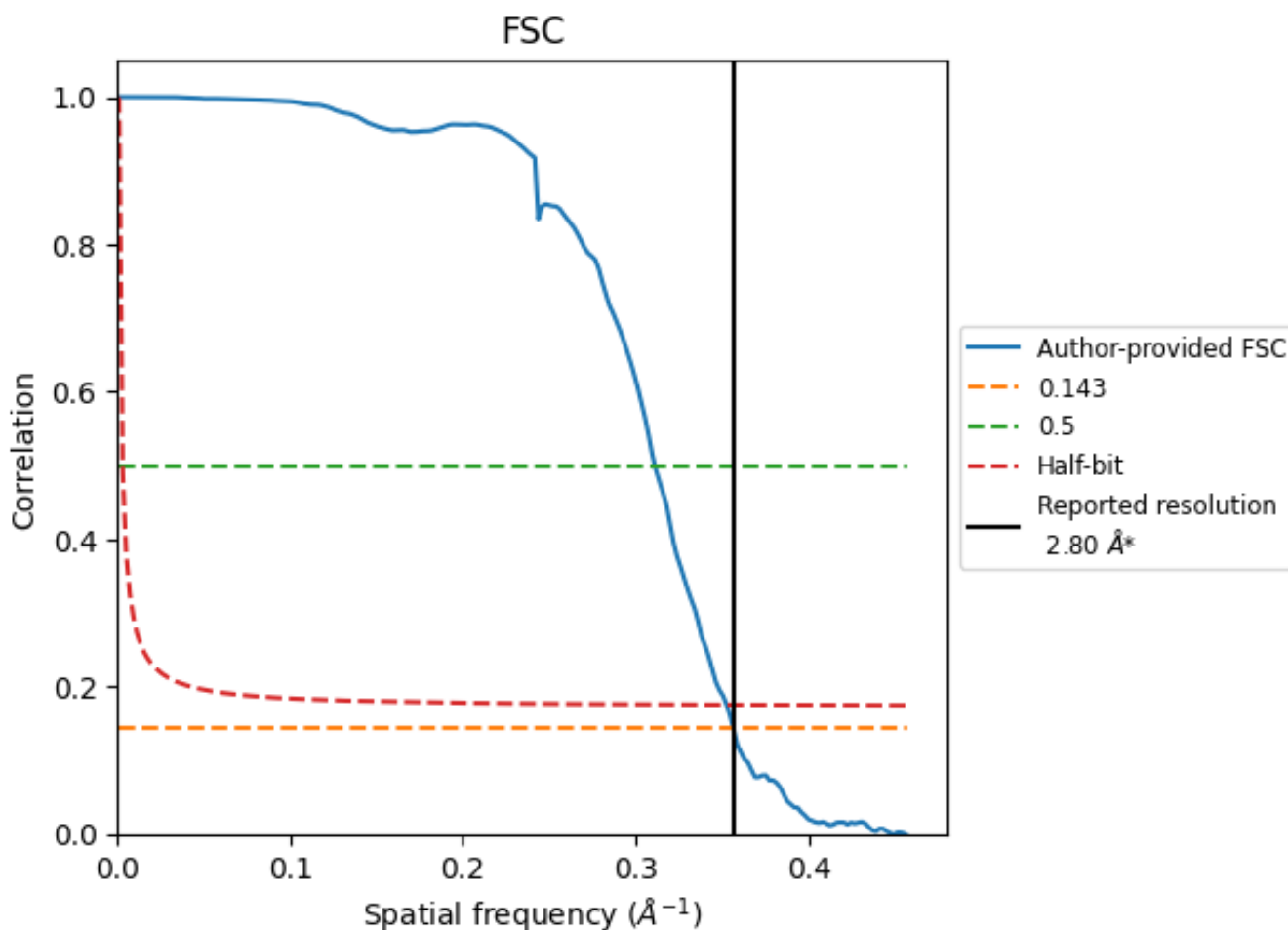


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



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

8.2 Resolution estimates [i](#)

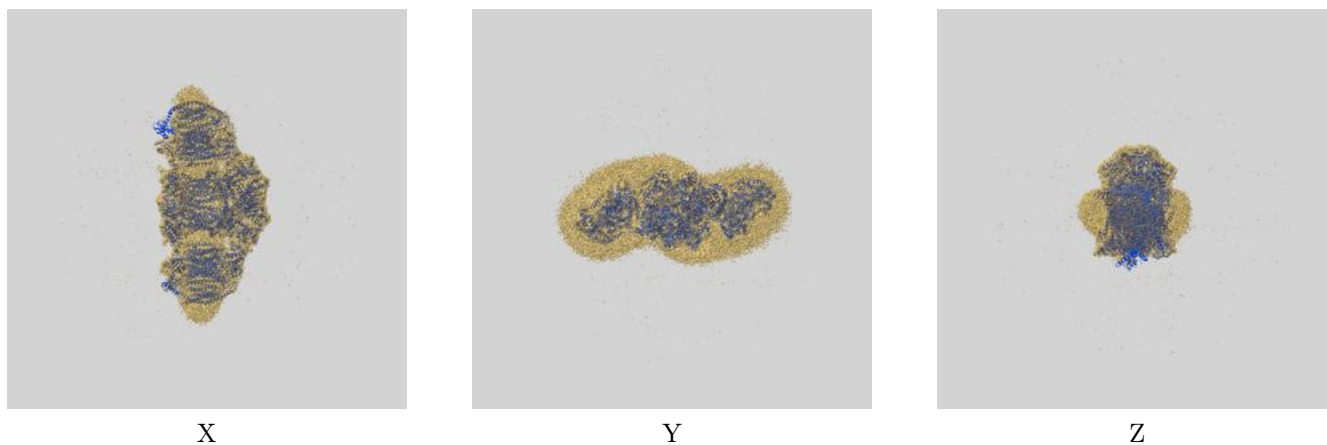
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.21	2.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

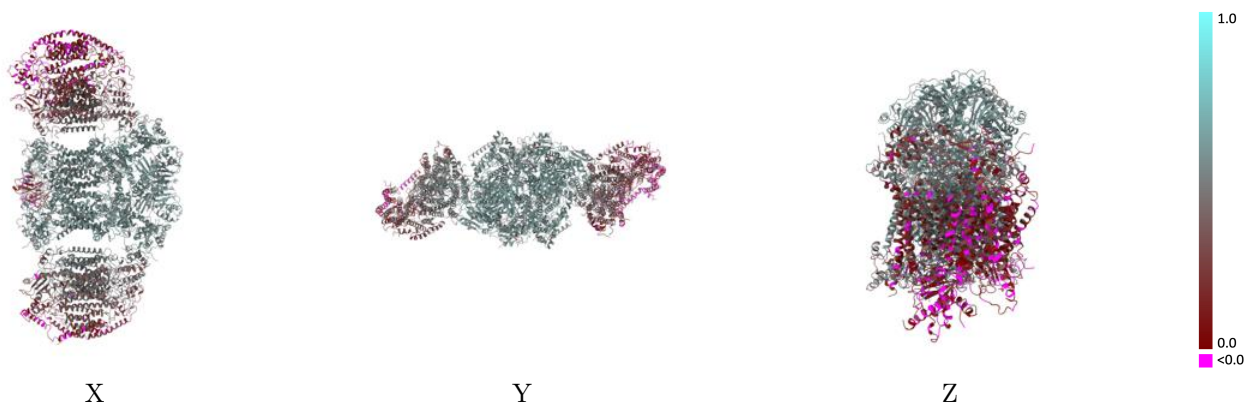
This section contains information regarding the fit between EMDB map EMD-10340 and PDB model 6T0B. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



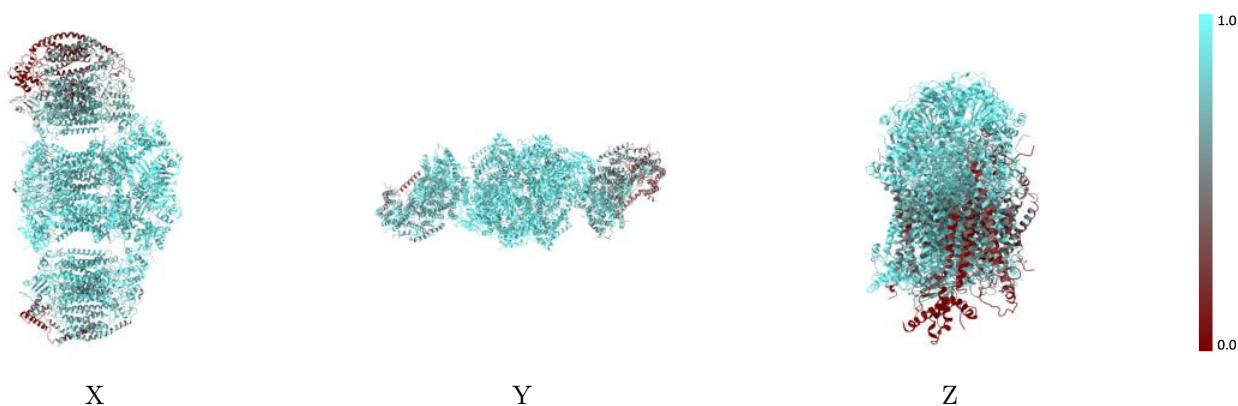
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



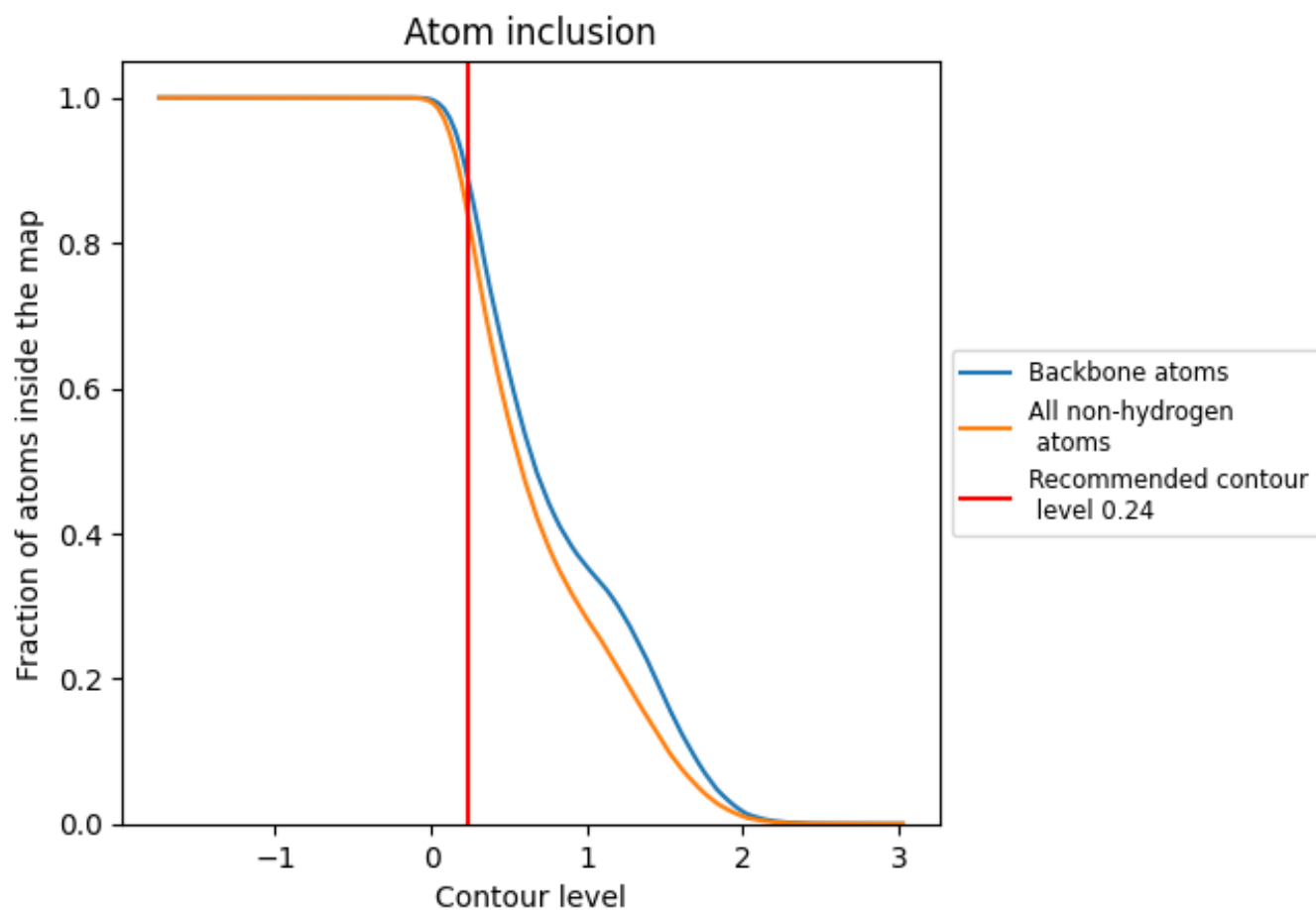
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8346	 0.4360
A	 0.9735	 0.5720
B	 0.9829	 0.5720
C	 0.9749	 0.5820
D	 0.9797	 0.5780
E	 0.8542	 0.3440
F	 0.9423	 0.5070
G	 0.9689	 0.5670
H	 0.9712	 0.5690
I	 0.9774	 0.5700
J	 0.8417	 0.4960
L	 0.9779	 0.5700
M	 0.9781	 0.5630
N	 0.9796	 0.5850
O	 0.9789	 0.5750
P	 0.8658	 0.3400
Q	 0.9535	 0.5130
R	 0.9659	 0.5680
S	 0.9725	 0.5690
T	 0.9563	 0.5650
U	 0.8288	 0.4880
a	 0.9051	 0.4820
b	 0.8750	 0.4200
c	 0.8113	 0.3190
d	 0.8779	 0.3740
e	 0.9168	 0.5060
f	 0.9182	 0.4260
g	 0.7797	 0.2750
h	 0.8911	 0.4360
i	 0.8781	 0.3990
j	 0.4269	 0.2400
k	 0.5257	 0.1690
l	 0.8822	 0.4460
m	 0.3862	 0.0990
n	 0.7248	 0.3360



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Chain	Atom inclusion	Q-score
o	 0.6555	 0.2310
p	 0.4865	 0.1790
q	 0.5756	 0.2320
r	 0.8549	 0.4200
s	 0.8255	 0.3080
t	 0.4873	 0.1540
u	 0.6782	 0.2870
v	 0.6050	 0.2010
w	 0.0341	 0.0850
x	 0.1435	 0.0690
y	 0.7536	 0.3060
z	 0.1419	 0.0450