



Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 04:06 PM EST

PDB ID : 8E7S
EMDB ID : EMD-27940
Title : III2IV2 respiratory supercomplex from *Saccharomyces cerevisiae* with 4 bound UQ6
Authors : Hryc, C.F.; Mileykovskaya, E.; Baker, M.; Dowhan, W.
Deposited on : 2022-08-24
Resolution : 3.20 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:

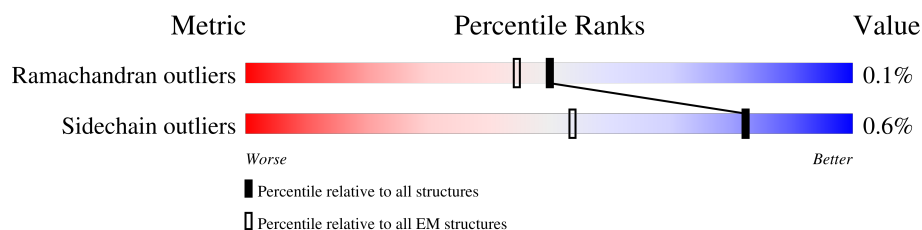
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.20 Å.

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




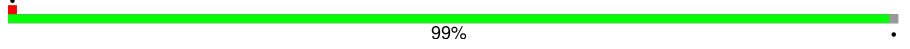
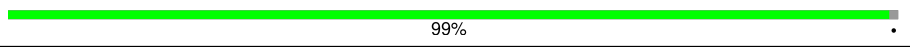
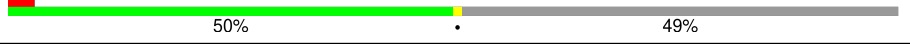
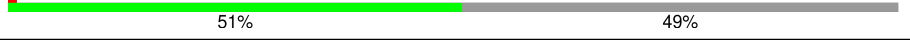
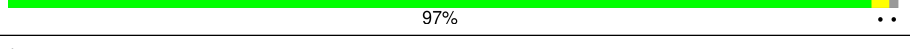
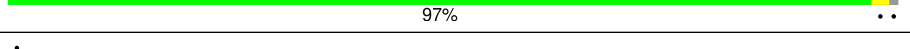
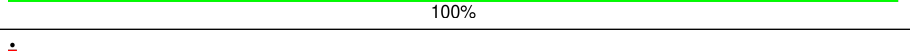
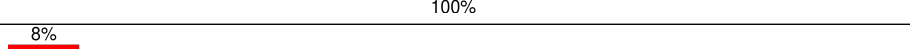
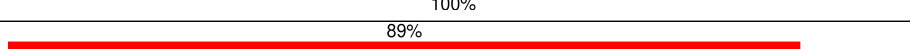
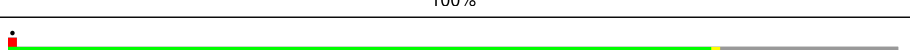

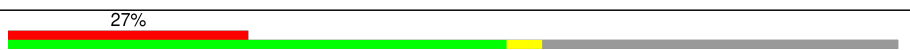

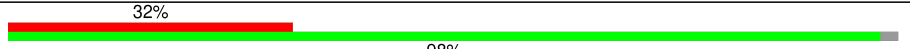
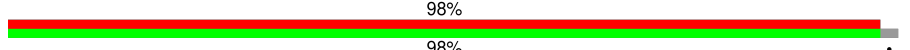


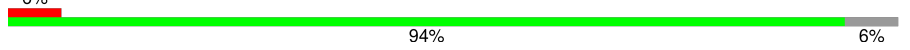
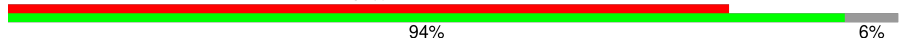
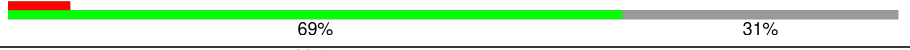

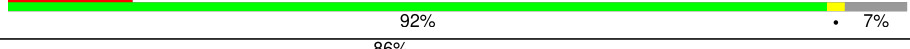
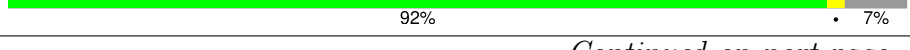

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	457	 94% • 6%
1	a	457	 94% • 6%
2	B	368	 95% •
2	b	368	 96% •
3	C	215	 10% 86% 14%
3	c	215	 16% 86% 14%
4	D	77	 8% 86% 14%
4	d	77	 25% 86% 14%
5	E	66	 86% 14%

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Mol	Chain	Length	Quality of chain
5	e	66	
6	F	127	
6	f	127	
7	G	147	
7	g	147	
8	H	94	
8	h	94	
9	J	385	
9	j	385	
10	K	534	
10	k	534	
11	L	309	
11	l	309	
12	M	78	
12	m	78	
13	N	60	
13	n	60	
14	O	269	
14	o	269	
15	P	251	
15	p	251	
16	Q	148	
16	q	148	
17	R	59	
17	r	59	

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Mol	Chain	Length	Quality of chain
18	S	129	
18	s	129	
19	T	155	
19	t	155	
20	U	83	
20	u	83	
21	V	66	
21	v	66	
22	W	153	
22	w	153	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CDL	C	302	X	-	-	-
25	CDL	H	601	X	-	-	-
25	CDL	J	403	X	-	-	-
25	CDL	K	603	X	-	-	-
25	CDL	L	402	X	-	-	-
25	CDL	c	302	X	-	-	-
25	CDL	h	601	X	-	-	-
25	CDL	h	602	X	-	-	-
25	CDL	j	402	X	-	-	-
25	CDL	k	602	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 62847 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
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	a	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
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	b	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
3	c	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			521	344	84	91	2		
4	d	66	Total	C	N	O	S	0	0
			521	344	84	91	2		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	57	Total	C	N	O	0	0
			465	310	77	78		
5	e	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
6	f	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
7	g	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

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

- Molecule 9 is a protein called Cytochrome b.

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

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

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

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

- Molecule 11 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
11	l	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	47	Total	C	N	O	S	0	0
			382	261	62	58	1		
12	m	47	Total	C	N	O	S	0	0
			382	261	62	58	1		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		
15	p	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

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

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	55	Total	C	N	O	S	0	0
			455	300	79	73	3		
17	r	55	Total	C	N	O	S	0	0
			455	300	79	73	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	121	Total	C	N	O	S	0	0
			913	576	151	181	5		
19	t	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	77	Total	C	N	O	S	0	0
			642	410	109	118	5		
20	u	77	Total	C	N	O	S	0	0
			642	410	109	118	5		

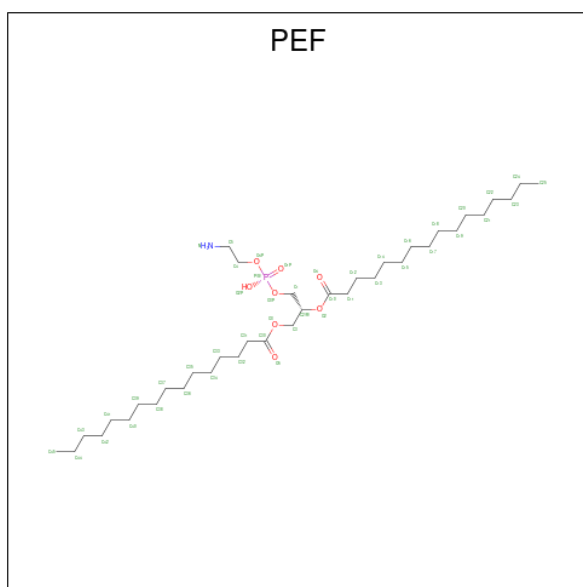
- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

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

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

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

- Molecule 23 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$) (labeled as "Ligand of Interest" by depositor).



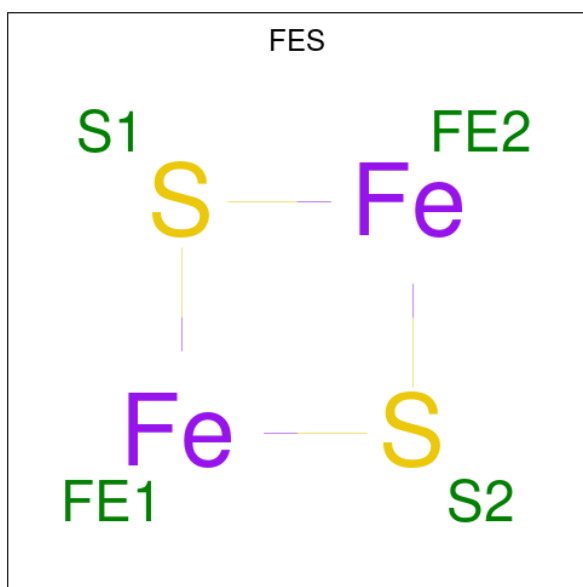
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	C	1	Total	C	N	O	P	0
			32	22	1	8	1	

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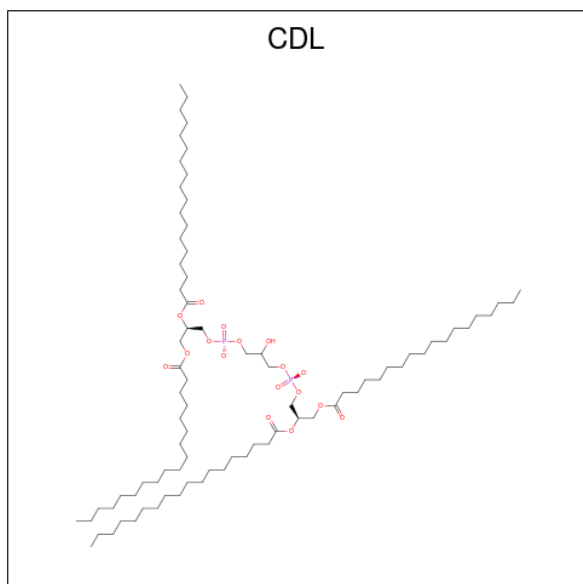
Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	V	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	a	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	c	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	c	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	e	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	j	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	j	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	j	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	v	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	w	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	w	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			4	2	2	
24	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



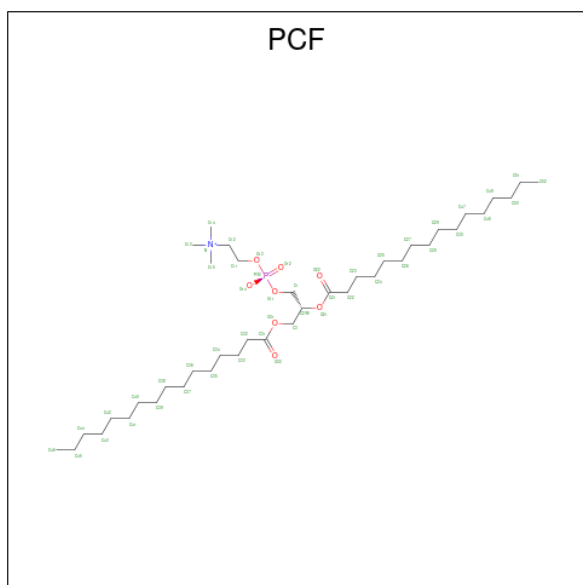
Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O	P	0
			53	34	17	2	

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Mol	Chain	Residues	Atoms				AltConf
25	H	1	Total	C	O	P	0
			53	34	17	2	
25	J	1	Total	C	O	P	0
			56	37	17	2	
25	K	1	Total	C	O	P	0
			67	48	17	2	
25	L	1	Total	C	O	P	0
			67	48	17	2	
25	c	1	Total	C	O	P	0
			48	29	17	2	
25	h	1	Total	C	O	P	0
			53	34	17	2	
25	h	1	Total	C	O	P	0
			67	48	17	2	
25	j	1	Total	C	O	P	0
			56	37	17	2	
25	k	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



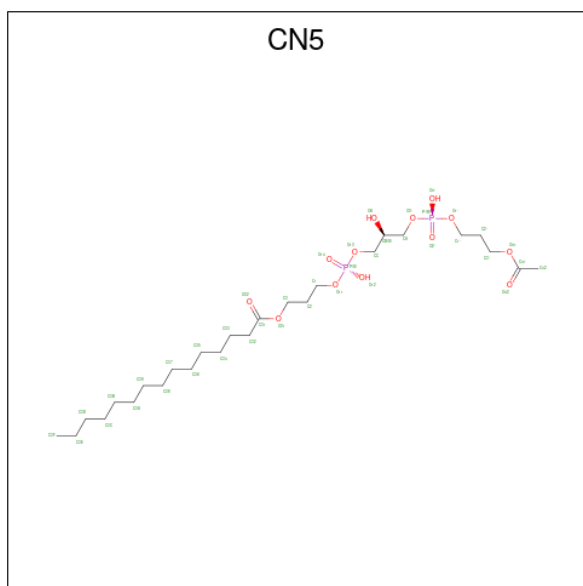
Mol	Chain	Residues	Atoms					AltConf
26	E	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	H	1	Total	C	N	O	P	0
			50	40	1	8	1	

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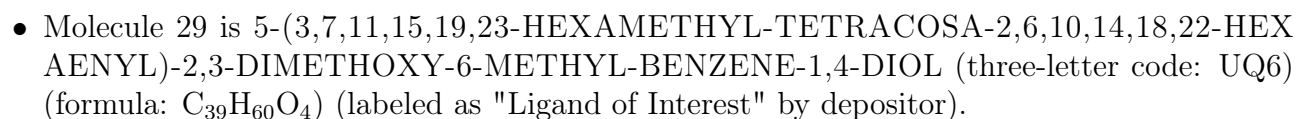
Mol	Chain	Residues	Atoms					AltConf
26	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	k	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	w	1	Total	C	N	O	P	0
			50	40	1	8	1	

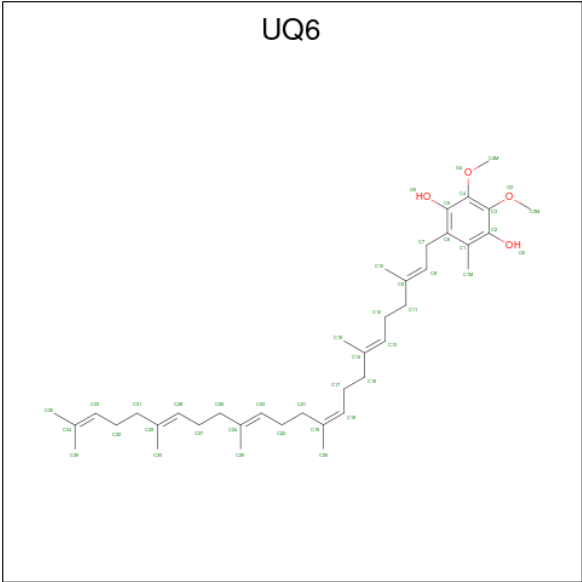
- Molecule 27 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (three-letter code: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



Mol	Chain	Residues	Atoms				AltConf
27	J	1	Total	C	O	P	0
			41	26	13	2	

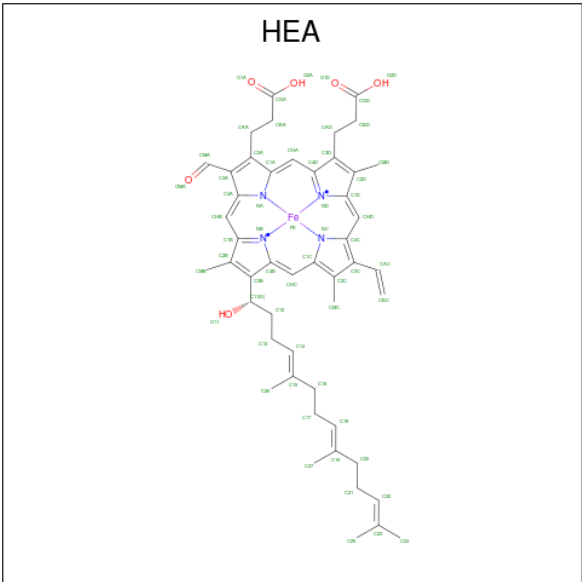
- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			43	39	4	
29	J	1	Total	C	O	0
			20	16	4	
29	j	1	Total	C	O	0
			43	39	4	
29	j	1	Total	C	O	0
			43	39	4	

- Molecule 30 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

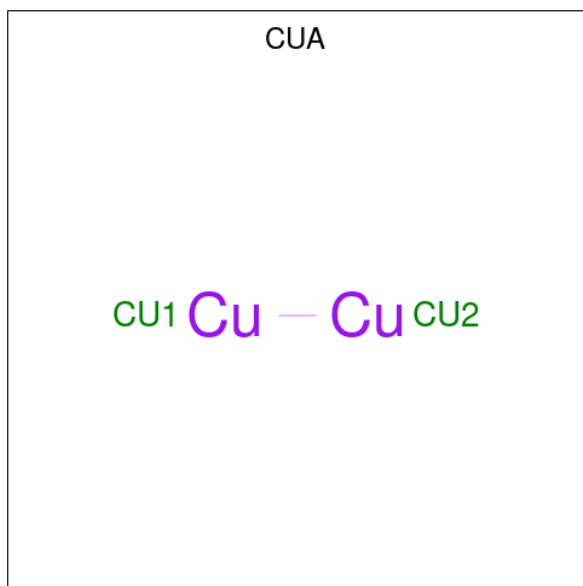


Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 31 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
31	K	1	Total	Cu	0
			1	1	
31	k	1	Total	Cu	0
			1	1	

- Molecule 32 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



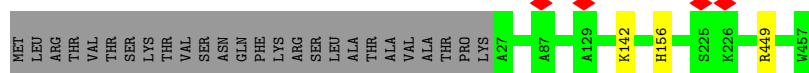
Mol	Chain	Residues	Atoms		AltConf
32	P	1	Total	Cu	0
			1	1	
32	P	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	

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.

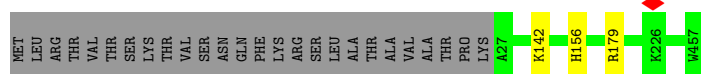
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:  94% 6%



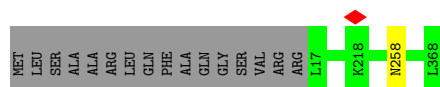
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain a:  94% 6%



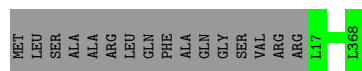
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  95%




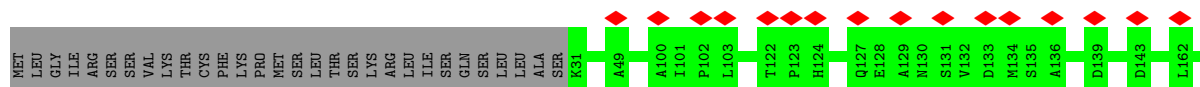
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

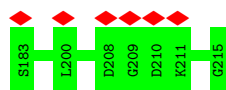
Chain b:  96%



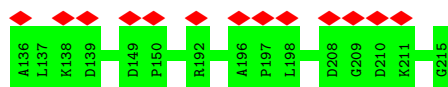
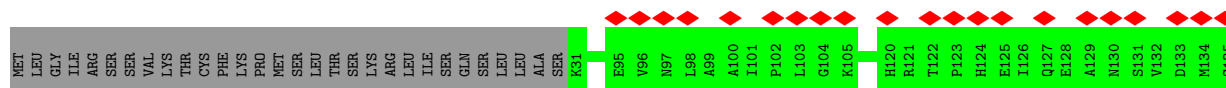
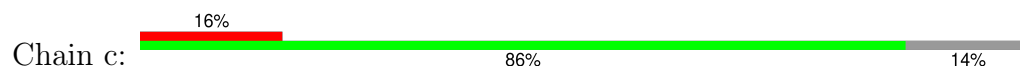
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C:  10% 86% 14%

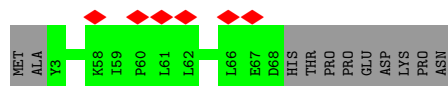
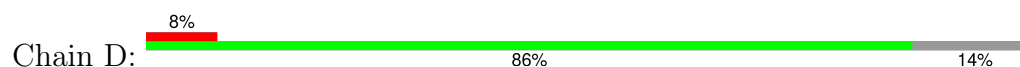




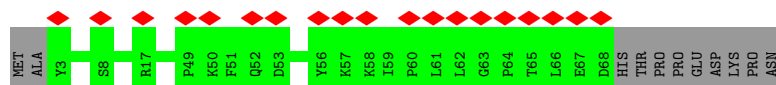
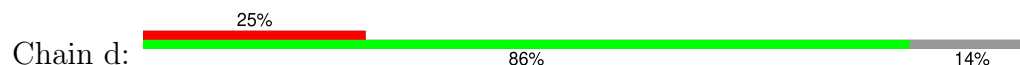
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



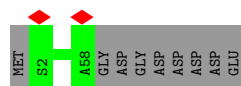
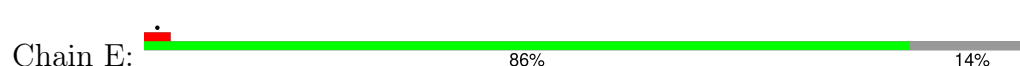
- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



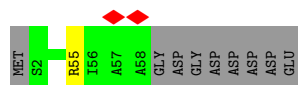
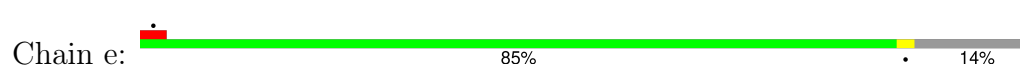
- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial

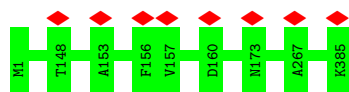


- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7, mitochondrial





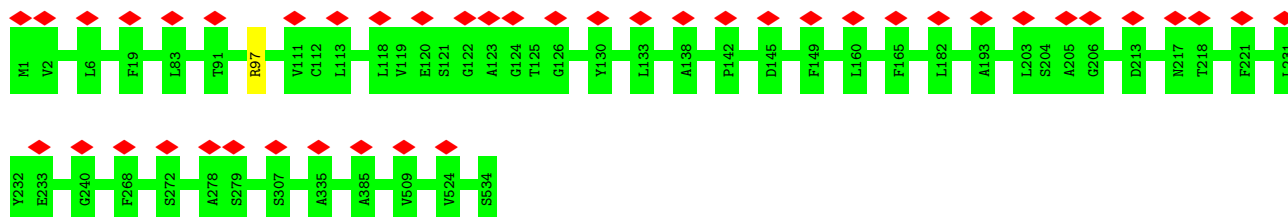
- Molecule 9: Cytochrome b

Chain j: 100%



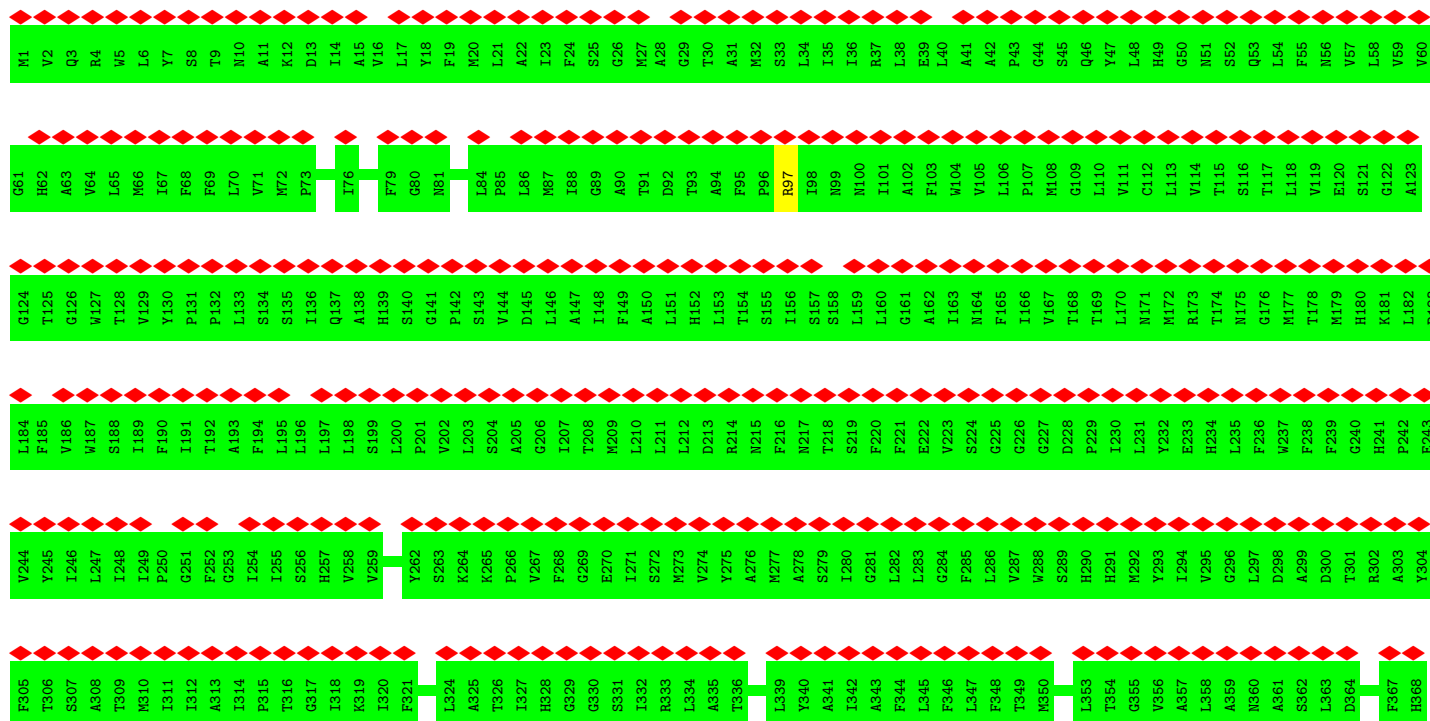
- Molecule 10: Cytochrome c oxidase subunit 1

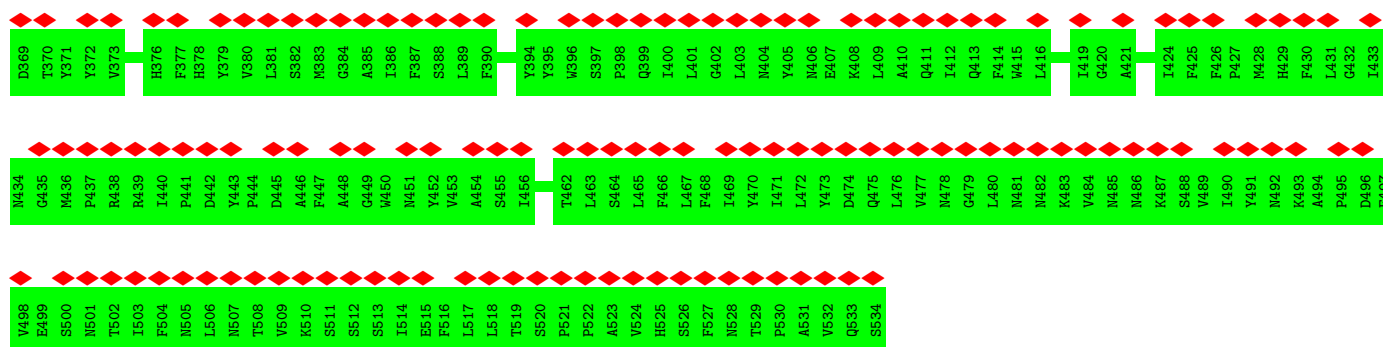
Chain K: 8% 100%



- Molecule 10: Cytochrome c oxidase subunit 1

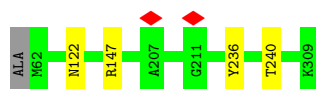
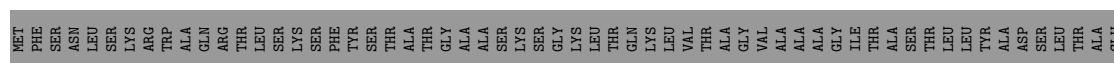
Chain k: 89% 100%





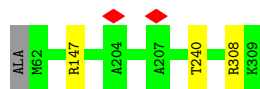
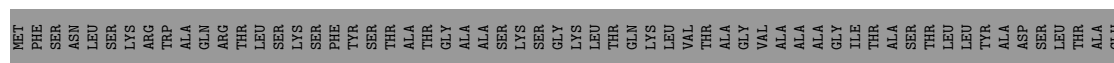
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain L: 79% 20%



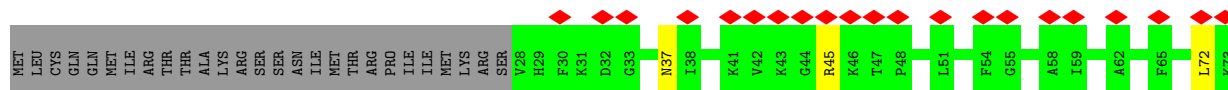
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain l: 79% 20%



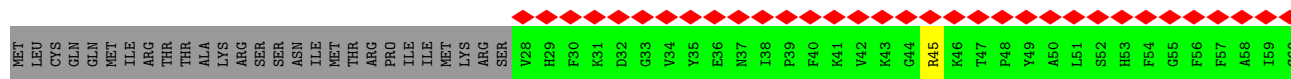
- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial

Chain M: 27% 56% 40%



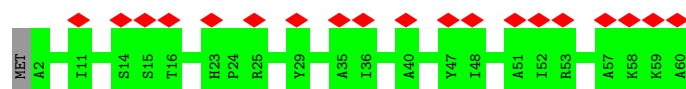
- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial

Chain m: 60% 58% 40%





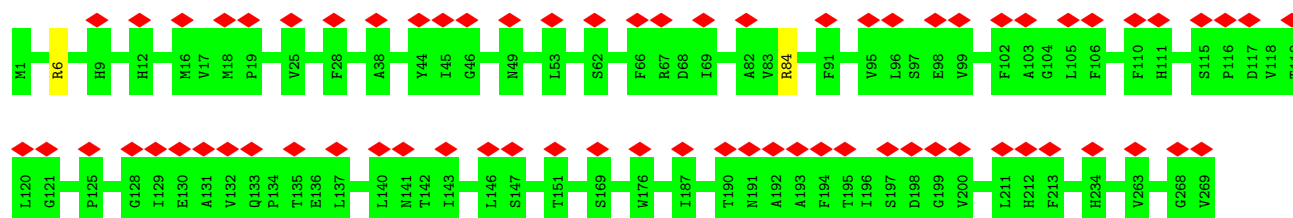
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial



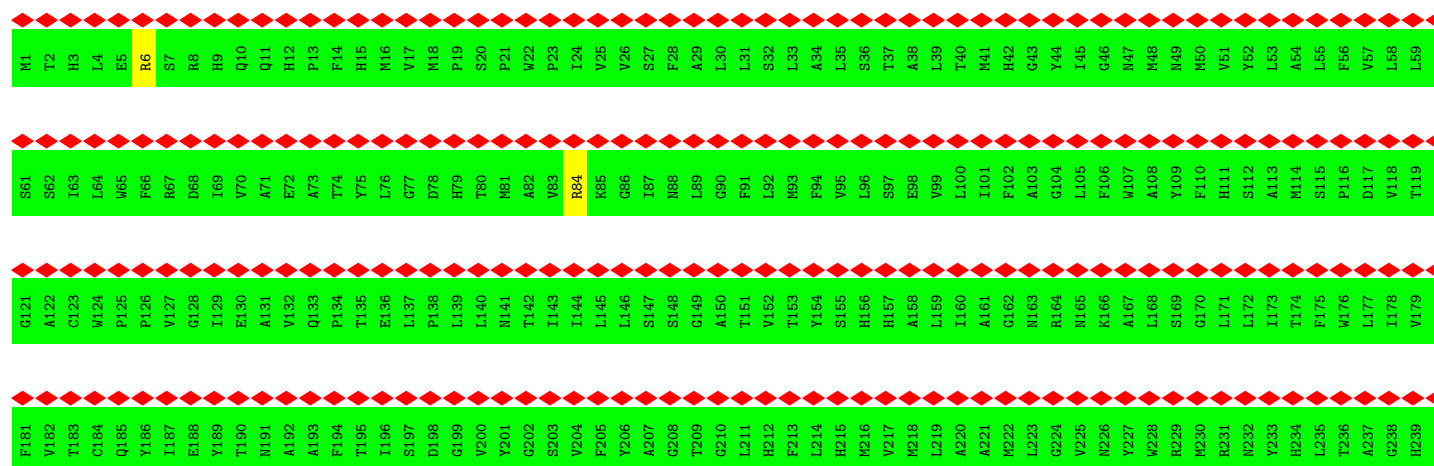
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial



- Molecule 14: Cytochrome c oxidase subunit 3

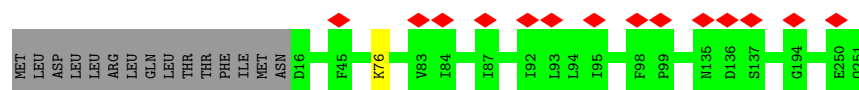


- Molecule 14: Cytochrome c oxidase subunit 3

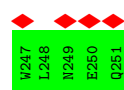
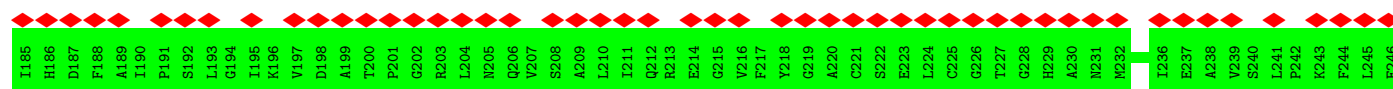
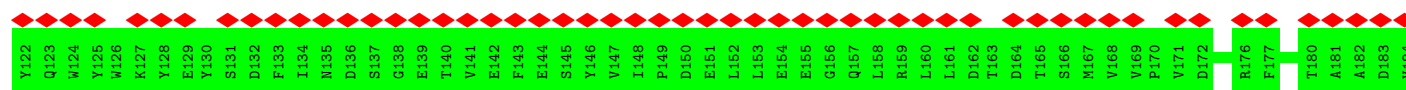
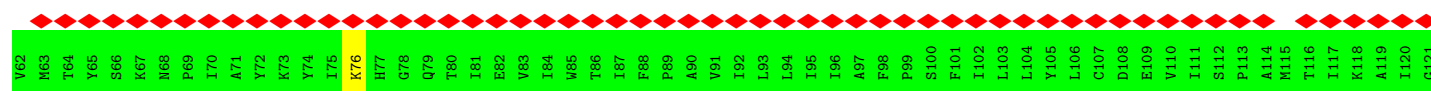
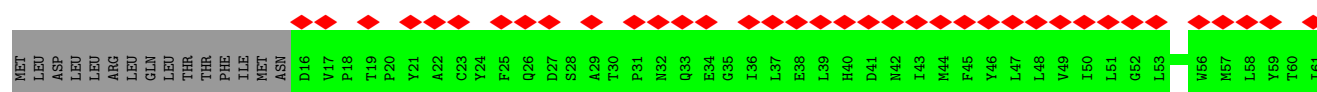
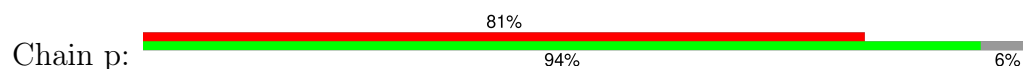




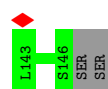
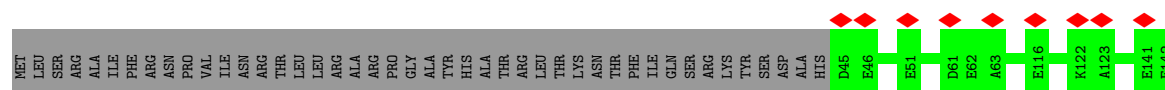
• Molecule 15: Cytochrome c oxidase subunit 2



• Molecule 15: Cytochrome c oxidase subunit 2

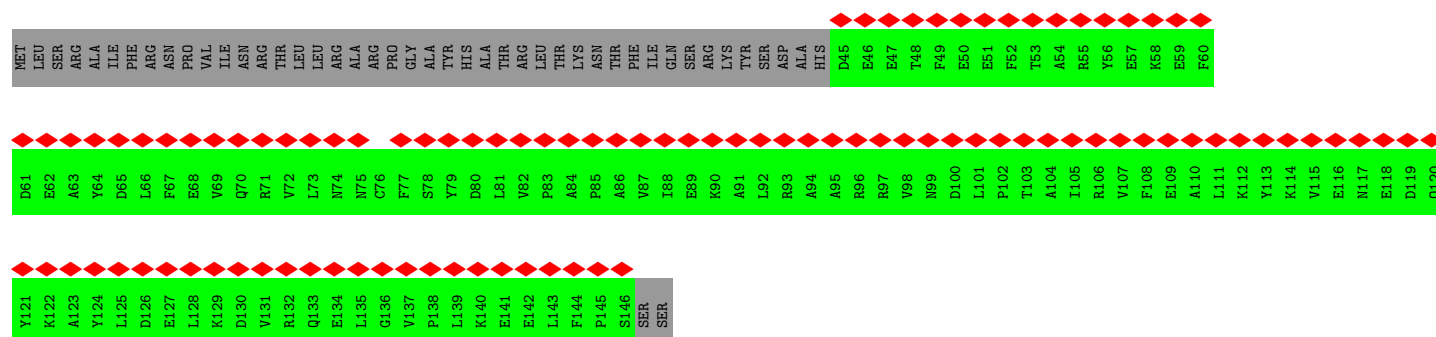


• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

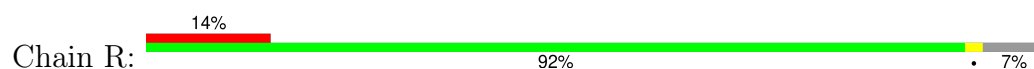


• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

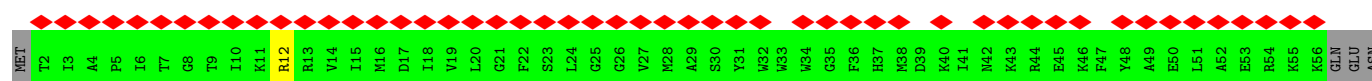
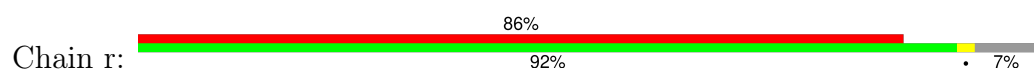




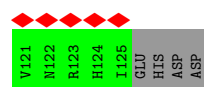
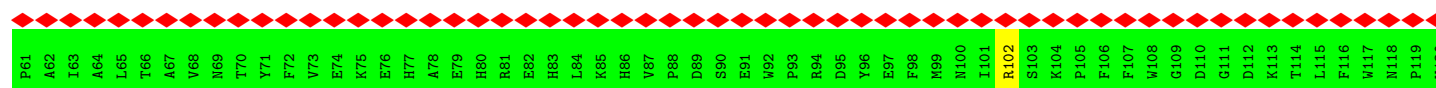
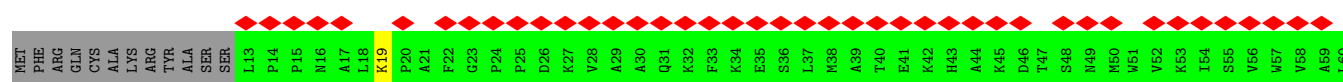
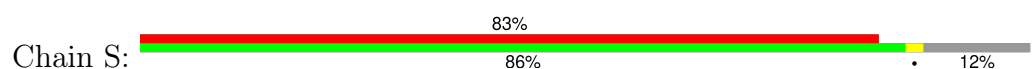
- Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial



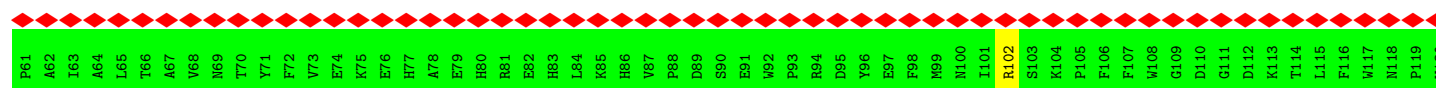
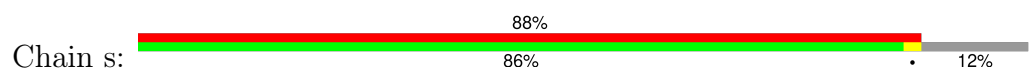
- Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial

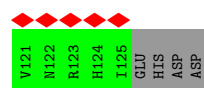


- Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial

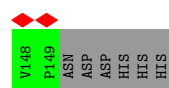
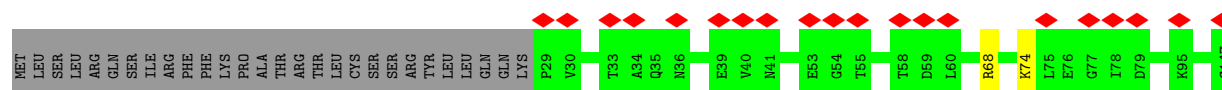
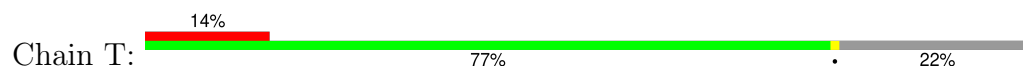


- Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial

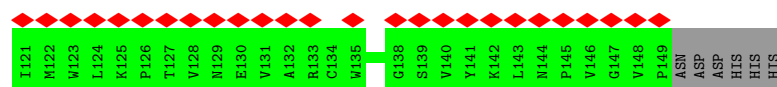
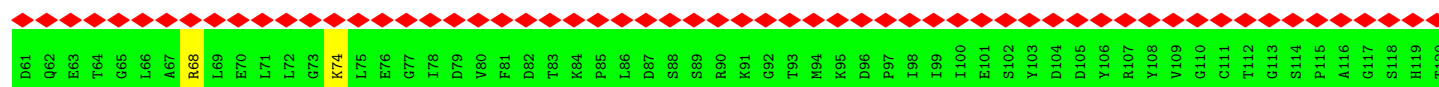
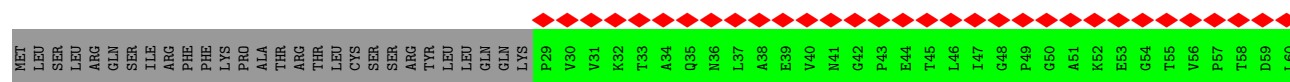
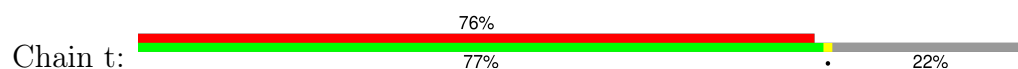




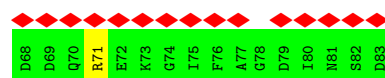
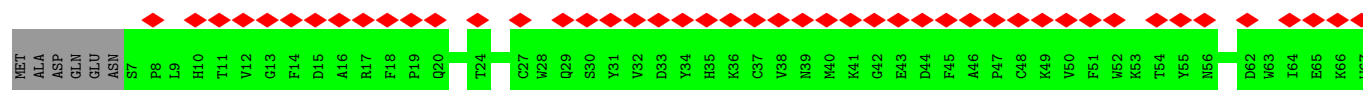
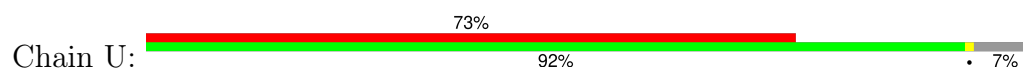
- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial



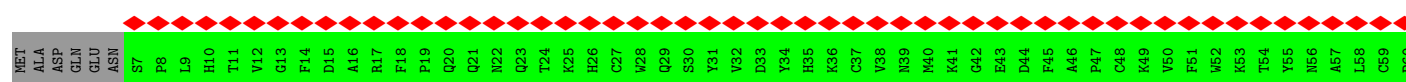
- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial



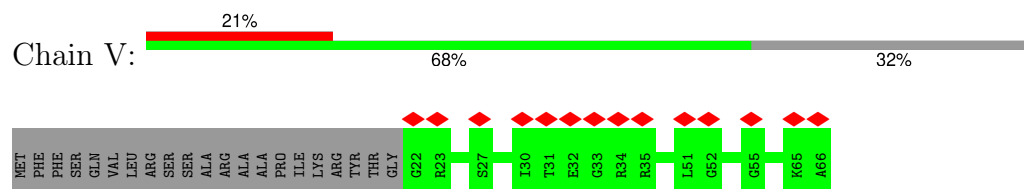
- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



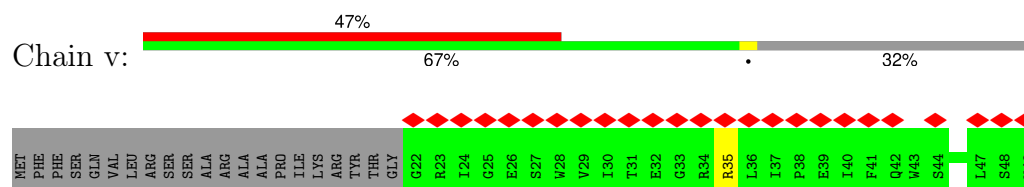
- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



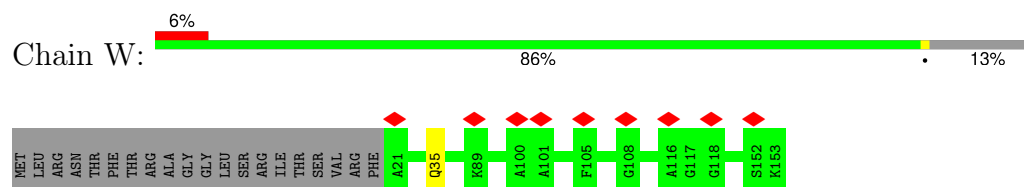
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



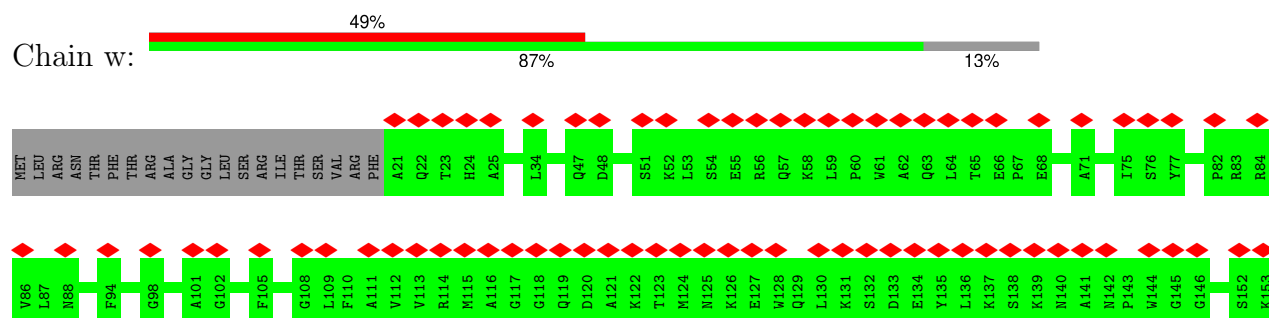
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	493055	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.844	Depositor
Minimum map value	-0.873	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.245	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEA, CN5, PCF, CDL, CUA, PEF, HEM, UQ6, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/3406	0.52	0/4615
1	a	0.33	0/3406	0.53	0/4615
2	B	0.36	0/2781	0.53	0/3764
2	b	0.35	0/2781	0.52	0/3764
3	C	0.27	0/1444	0.50	0/1957
3	c	0.28	0/1444	0.50	0/1957
4	D	0.27	0/537	0.54	0/728
4	d	0.26	0/537	0.54	0/728
5	E	0.31	0/479	0.44	0/646
5	e	0.32	0/479	0.51	0/646
6	F	0.31	0/1040	0.53	0/1408
6	f	0.31	0/1040	0.52	0/1408
7	G	0.28	0/647	0.49	0/870
7	g	0.29	0/647	0.50	0/870
8	H	0.33	0/804	0.46	0/1088
8	h	0.36	0/804	0.49	0/1088
9	J	0.37	0/3192	0.52	0/4354
9	j	0.36	0/3192	0.51	0/4354
10	K	0.28	0/4290	0.47	0/5857
10	k	0.26	0/4290	0.47	0/5857
11	L	0.34	0/2022	0.51	0/2751
11	l	0.35	0/2022	0.54	0/2751
12	M	0.29	0/396	0.53	1/533 (0.2%)
12	m	0.27	0/396	0.54	1/533 (0.2%)
13	N	0.25	0/500	0.47	0/681
13	n	0.24	0/500	0.46	0/681
14	O	0.24	0/2218	0.47	0/3036
14	o	0.24	0/2218	0.48	0/3036
15	P	0.26	0/1941	0.47	0/2653
15	p	0.25	0/1941	0.47	0/2653
16	Q	0.28	0/868	0.52	0/1174
16	q	0.26	0/868	0.51	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.24	0/467	0.51	0/626
17	r	0.24	0/467	0.52	0/626
18	S	0.24	0/962	0.44	0/1310
18	s	0.24	0/962	0.43	0/1310
19	T	0.25	0/932	0.50	0/1269
19	t	0.24	0/932	0.49	0/1269
20	U	0.24	0/664	0.41	0/899
20	u	0.24	0/664	0.44	0/899
21	V	0.27	0/372	0.53	0/502
21	v	0.26	0/372	0.54	0/502
22	W	0.26	0/1074	0.51	0/1451
22	w	0.26	0/1074	0.48	0/1451
All	All	0.30	0/62072	0.50	2/84344 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	72	LEU	CA-CB-CG	5.32	127.54	115.30
12	m	72	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/457 (94%)	368 (86%)	60 (14%)	1 (0%)	44	75
1	a	429/457 (94%)	366 (85%)	62 (14%)	1 (0%)	44	75
2	B	350/368 (95%)	324 (93%)	26 (7%)	0	100	100
2	b	350/368 (95%)	319 (91%)	31 (9%)	0	100	100
3	C	183/215 (85%)	166 (91%)	17 (9%)	0	100	100
3	c	183/215 (85%)	167 (91%)	16 (9%)	0	100	100
4	D	64/77 (83%)	59 (92%)	5 (8%)	0	100	100
4	d	64/77 (83%)	61 (95%)	3 (5%)	0	100	100
5	E	55/66 (83%)	55 (100%)	0	0	100	100
5	e	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
6	F	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
6	f	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
7	G	73/147 (50%)	72 (99%)	1 (1%)	0	100	100
7	g	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
8	H	91/94 (97%)	84 (92%)	5 (6%)	2 (2%)	5	30
8	h	91/94 (97%)	82 (90%)	8 (9%)	1 (1%)	12	44
9	J	383/385 (100%)	352 (92%)	31 (8%)	0	100	100
9	j	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
10	K	532/534 (100%)	493 (93%)	39 (7%)	0	100	100
10	k	532/534 (100%)	506 (95%)	26 (5%)	0	100	100
11	L	246/309 (80%)	210 (85%)	33 (13%)	3 (1%)	11	43
11	l	246/309 (80%)	211 (86%)	34 (14%)	1 (0%)	30	64
12	M	45/78 (58%)	43 (96%)	2 (4%)	0	100	100
12	m	45/78 (58%)	40 (89%)	5 (11%)	0	100	100
13	N	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
13	n	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
14	O	267/269 (99%)	245 (92%)	22 (8%)	0	100	100
14	o	267/269 (99%)	246 (92%)	21 (8%)	0	100	100
15	P	234/251 (93%)	218 (93%)	16 (7%)	0	100	100
15	p	234/251 (93%)	222 (95%)	12 (5%)	0	100	100
16	Q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100
16	q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
17	r	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
18	S	111/129 (86%)	103 (93%)	8 (7%)	0	100	100
18	s	111/129 (86%)	102 (92%)	9 (8%)	0	100	100
19	T	119/155 (77%)	109 (92%)	10 (8%)	0	100	100
19	t	119/155 (77%)	110 (92%)	9 (8%)	0	100	100
20	U	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
20	u	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
21	V	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
21	v	43/66 (65%)	39 (91%)	4 (9%)	0	100	100
22	W	131/153 (86%)	115 (88%)	16 (12%)	0	100	100
22	w	131/153 (86%)	119 (91%)	12 (9%)	0	100	100
All	All	7530/8460 (89%)	6898 (92%)	623 (8%)	9 (0%)	50	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	40	ILE
11	L	240	THR
11	l	240	THR
11	L	122	ASN
1	A	156	HIS
1	a	156	HIS
11	L	236	TYR
8	H	30	SER
8	h	30	SER

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/393 (94%)	368 (100%)	2 (0%)	86	93
1	a	370/393 (94%)	368 (100%)	2 (0%)	86	93
2	B	301/313 (96%)	300 (100%)	1 (0%)	91	96
2	b	301/313 (96%)	301 (100%)	0	100	100
3	C	151/179 (84%)	151 (100%)	0	100	100
3	c	151/179 (84%)	151 (100%)	0	100	100
4	D	56/66 (85%)	56 (100%)	0	100	100
4	d	56/66 (85%)	56 (100%)	0	100	100
5	E	47/54 (87%)	47 (100%)	0	100	100
5	e	47/54 (87%)	46 (98%)	1 (2%)	48	74
6	F	110/111 (99%)	110 (100%)	0	100	100
6	f	110/111 (99%)	110 (100%)	0	100	100
7	G	68/131 (52%)	67 (98%)	1 (2%)	60	81
7	g	68/131 (52%)	68 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	h	77/78 (99%)	76 (99%)	1 (1%)	65	83
9	J	338/338 (100%)	338 (100%)	0	100	100
9	j	338/338 (100%)	337 (100%)	1 (0%)	91	96
10	K	447/447 (100%)	446 (100%)	1 (0%)	92	97
10	k	447/447 (100%)	446 (100%)	1 (0%)	92	97
11	L	206/251 (82%)	205 (100%)	1 (0%)	86	93
11	l	206/251 (82%)	204 (99%)	2 (1%)	73	87
12	M	39/67 (58%)	37 (95%)	2 (5%)	20	53
12	m	39/67 (58%)	38 (97%)	1 (3%)	41	70
13	N	50/51 (98%)	50 (100%)	0	100	100
13	n	50/51 (98%)	50 (100%)	0	100	100
14	O	228/228 (100%)	226 (99%)	2 (1%)	75	89
14	o	228/228 (100%)	226 (99%)	2 (1%)	75	89
15	P	209/224 (93%)	208 (100%)	1 (0%)	86	93
15	p	209/224 (93%)	208 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	91/131 (70%)	91 (100%)	0	100	100
16	q	91/131 (70%)	91 (100%)	0	100	100
17	R	46/50 (92%)	45 (98%)	1 (2%)	47	73
17	r	46/50 (92%)	45 (98%)	1 (2%)	47	73
18	S	99/113 (88%)	97 (98%)	2 (2%)	50	75
18	s	99/113 (88%)	97 (98%)	2 (2%)	50	75
19	T	102/135 (76%)	100 (98%)	2 (2%)	50	75
19	t	102/135 (76%)	100 (98%)	2 (2%)	50	75
20	U	69/74 (93%)	68 (99%)	1 (1%)	62	82
20	u	69/74 (93%)	68 (99%)	1 (1%)	62	82
21	V	36/53 (68%)	36 (100%)	0	100	100
21	v	36/53 (68%)	35 (97%)	1 (3%)	38	68
22	W	110/127 (87%)	109 (99%)	1 (1%)	75	89
22	w	110/127 (87%)	110 (100%)	0	100	100
All	All	6500/7228 (90%)	6463 (99%)	37 (1%)	82	92

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LYS
1	A	449	ARG
2	B	258	ASN
7	G	108	GLN
10	K	97	ARG
11	L	147	ARG
12	M	37	ASN
12	M	45	ARG
14	O	6	ARG
14	O	84	ARG
15	P	76	LYS
17	R	12	ARG
18	S	19	LYS
18	S	102	ARG
19	T	68	ARG
19	T	74	LYS
20	U	71	ARG
22	W	35	GLN

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Mol	Chain	Res	Type
1	a	142	LYS
1	a	179	ARG
5	e	55	ARG
8	h	38	GLN
9	j	79	ARG
10	k	97	ARG
11	l	147	ARG
11	l	308	ARG
12	m	45	ARG
14	o	6	ARG
14	o	84	ARG
15	p	76	LYS
17	r	12	ARG
18	s	19	LYS
18	s	102	ARG
19	t	68	ARG
19	t	74	LYS
20	u	71	ARG
21	v	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	157	ASN
2	B	184	ASN
3	C	161	HIS
9	J	138	GLN
9	J	332	ASN
9	J	338	GLN
10	K	485	ASN
11	L	169	ASN
1	a	67	ASN
2	b	145	GLN
3	c	181	HIS
8	h	38	GLN
9	j	82	HIS
9	j	222	HIS
9	j	332	ASN
10	k	100	ASN
11	l	169	ASN
15	p	229	HIS
16	q	70	GLN

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Mol	Chain	Res	Type
16	q	117	ASN
22	w	22	GLN
22	w	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - leaving 57 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	$\# Z > 2$
23	PEF	J	401	-	44,44,46	0.45	0	47,49,51	1.21	4 (8%)
29	UQ6	J	406	-	43,43,43	0.50	0	54,55,55	1.70	13 (24%)
23	PEF	a	501	-	39,39,46	0.46	0	42,44,51	1.36	5 (11%)
25	CDL	H	601	-	52,52,99	1.22	6 (11%)	58,64,111	0.96	4 (6%)
23	PEF	c	303	-	28,28,46	0.49	0	31,33,51	1.33	4 (12%)
26	PCF	W	203	-	35,35,49	0.71	0	41,43,57	0.55	0
28	HEM	J	404	9	42,50,50	1.52	7 (16%)	46,82,82	2.06	13 (28%)
25	CDL	j	402	-	55,55,99	1.20	6 (10%)	61,67,111	0.93	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	HEM	L	401	11	42,50,50	1.46	6 (14%)	46,82,82	1.99	12 (26%)
23	PEF	a	504	-	39,39,46	0.45	0	42,44,51	1.24	4 (9%)
26	PCF	a	502	-	46,46,49	0.63	0	52,54,57	0.58	0
23	PEF	C	304	-	31,31,46	0.48	0	34,36,51	1.32	4 (11%)
25	CDL	c	302	-	47,47,99	1.28	6 (12%)	53,59,111	1.02	5 (9%)
29	UQ6	j	407	-	43,43,43	0.47	0	54,55,55	1.57	13 (24%)
23	PEF	A	503	-	39,39,46	0.44	0	42,44,51	1.28	4 (9%)
25	CDL	C	302	-	52,52,99	1.22	6 (11%)	58,64,111	0.94	3 (5%)
28	HEM	j	403	9	42,50,50	1.51	6 (14%)	46,82,82	2.07	13 (28%)
23	PEF	A	502	-	30,30,46	0.48	0	33,35,51	1.38	4 (12%)
23	PEF	e	101	-	31,31,46	0.51	0	34,36,51	1.33	5 (14%)
30	HEA	K	604	10	58,67,67	2.02	14 (24%)	63,103,103	2.57	31 (49%)
26	PCF	H	602	-	49,49,49	0.62	0	55,57,57	0.50	0
23	PEF	w	202	-	40,40,46	0.46	0	43,45,51	1.24	4 (9%)
23	PEF	J	407	-	42,42,46	0.46	0	45,47,51	1.30	5 (11%)
25	CDL	K	603	-	66,66,99	1.08	6 (9%)	72,78,111	0.89	2 (2%)
27	CN5	J	402	-	40,40,40	0.50	0	44,48,48	0.92	1 (2%)
24	FES	c	301	3	0,4,4	-	-	-	-	-
23	PEF	a	503	-	30,30,46	0.49	0	33,35,51	1.32	4 (12%)
23	PEF	w	201	-	35,35,46	0.48	0	38,40,51	1.32	4 (10%)
23	PEF	W	201	-	35,35,46	0.46	0	38,40,51	1.32	4 (10%)
25	CDL	L	402	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
25	CDL	h	601	-	52,52,99	1.23	6 (11%)	58,64,111	0.97	4 (6%)
26	PCF	E	101	-	46,46,49	0.63	0	52,54,57	0.62	1 (1%)
26	PCF	k	605	-	35,35,49	0.71	0	41,43,57	0.54	0
25	CDL	J	403	-	55,55,99	1.19	6 (10%)	61,67,111	0.97	4 (6%)
23	PEF	c	304	-	31,31,46	0.47	0	34,36,51	1.34	4 (11%)
29	UQ6	j	405	-	43,43,43	0.46	0	54,55,55	1.60	14 (25%)
23	PEF	j	406	-	42,42,46	0.44	0	45,47,51	1.29	4 (8%)
23	PEF	W	202	-	40,40,46	0.45	0	43,45,51	1.27	4 (9%)
23	PEF	E	102	-	31,31,46	0.49	0	34,36,51	1.34	5 (14%)
23	PEF	J	409	-	28,28,46	0.50	0	31,33,51	1.39	4 (12%)
23	PEF	j	401	-	44,44,46	0.44	0	47,49,51	1.20	4 (8%)
30	HEA	k	604	10	58,67,67	2.03	17 (29%)	63,103,103	2.59	32 (50%)
28	HEM	j	404	9	42,50,50	1.51	6 (14%)	46,82,82	2.12	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PEF	v	101	-	32,32,46	0.48	0	35,37,51	1.31	5 (14%)
26	PCF	w	203	-	49,49,49	0.63	0	55,57,57	0.53	0
23	PEF	V	101	-	32,32,46	0.49	0	35,37,51	1.34	5 (14%)
30	HEA	K	601	10	58,67,67	2.03	16 (27%)	63,103,103	2.60	33 (52%)
25	CDL	h	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
30	HEA	k	603	10	58,67,67	2.06	18 (31%)	63,103,103	2.50	32 (50%)
28	HEM	l	401	11	42,50,50	1.48	7 (16%)	46,82,82	1.91	12 (26%)
29	UQ6	J	408	-	20,20,43	0.59	0	25,27,55	1.67	5 (20%)
23	PEF	A	501	-	39,39,46	0.45	0	42,44,51	1.27	4 (9%)
24	FES	C	301	3	0,4,4	-	-	-	-	-
25	CDL	k	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.87	2 (2%)
23	PEF	j	408	-	28,28,46	0.51	0	31,33,51	1.32	4 (12%)
28	HEM	J	405	9	42,50,50	1.51	6 (14%)	46,82,82	2.14	12 (26%)
23	PEF	C	303	-	28,28,46	0.52	0	31,33,51	1.38	5 (16%)

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
23	PEF	J	401	-	-	16/48/48/50	-
29	UQ6	J	406	-	-	11/39/39/39	0/1/1/1
25	CDL	H	601	-	1/1/9/9	28/63/63/110	-
23	PEF	a	501	-	-	9/43/43/50	-
23	PEF	c	303	-	-	8/32/32/50	-
26	PCF	W	203	-	-	10/39/39/53	-
28	HEM	J	404	9	-	5/12/54/54	-
25	CDL	j	402	-	1/1/9/9	23/66/66/110	-
28	HEM	L	401	11	-	6/12/54/54	-
23	PEF	a	504	-	-	7/43/43/50	-
26	PCF	a	502	-	-	13/50/50/53	-
23	PEF	C	304	-	-	8/35/35/50	-
25	CDL	c	302	-	1/1/9/9	22/58/58/110	-
29	UQ6	j	407	-	-	9/39/39/39	0/1/1/1
23	PEF	A	503	-	-	11/43/43/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	C	302	-	1/1/9/9	27/63/63/110	-
28	HEM	j	403	9	-	10/12/54/54	-
23	PEF	A	502	-	-	1/34/34/50	-
23	PEF	e	101	-	-	6/35/35/50	-
30	HEA	K	604	10	-	16/32/76/76	-
26	PCF	H	602	-	-	16/53/53/53	-
23	PEF	w	202	-	-	6/44/44/50	-
23	PEF	J	407	-	-	10/46/46/50	-
25	CDL	K	603	-	1/1/9/9	34/77/77/110	-
27	CN5	J	402	-	-	8/44/44/44	-
24	FES	c	301	3	-	-	0/1/1/1
23	PEF	a	503	-	-	6/34/34/50	-
25	CDL	L	402	-	1/1/9/9	33/77/77/110	-
25	CDL	h	601	-	1/1/9/9	26/63/63/110	-
23	PEF	W	201	-	-	7/39/39/50	-
23	PEF	w	201	-	-	10/39/39/50	-
26	PCF	E	101	-	-	12/50/50/53	-
26	PCF	k	605	-	-	7/39/39/53	-
25	CDL	J	403	-	1/1/9/9	27/66/66/110	-
23	PEF	c	304	-	-	10/35/35/50	-
29	UQ6	j	405	-	-	7/39/39/39	0/1/1/1
23	PEF	j	406	-	-	14/46/46/50	-
23	PEF	W	202	-	-	8/44/44/50	-
23	PEF	E	102	-	-	8/35/35/50	-
23	PEF	J	409	-	-	11/32/32/50	-
23	PEF	j	401	-	-	11/48/48/50	-
30	HEA	k	604	10	-	14/32/76/76	-
28	HEM	j	404	9	-	6/12/54/54	-
23	PEF	v	101	-	-	7/36/36/50	-
26	PCF	w	203	-	-	15/53/53/53	-
23	PEF	V	101	-	-	9/36/36/50	-
30	HEA	K	601	10	-	14/32/76/76	-
25	CDL	h	602	-	1/1/9/9	26/77/77/110	-
30	HEA	k	603	10	-	15/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	HEM	l	401	11	-	4/12/54/54	-
29	UQ6	J	408	-	-	2/12/12/39	0/1/1/1
23	PEF	A	501	-	-	8/43/43/50	-
24	FES	C	301	3	-	-	0/1/1/1
25	CDL	k	602	-	1/1/9/9	33/77/77/110	-
23	PEF	j	408	-	-	5/32/32/50	-
28	HEM	J	405	9	-	7/12/54/54	-
23	PEF	C	303	-	-	9/32/32/50	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	k	603	HEA	C3A-C2A	5.19	1.47	1.40
30	k	604	HEA	C3A-C2A	5.18	1.47	1.40
30	K	604	HEA	C3A-C2A	5.02	1.47	1.40
30	K	601	HEA	C3A-C2A	5.02	1.47	1.40
30	k	603	HEA	CHC-C4B	4.97	1.46	1.34
30	K	601	HEA	CHD-C1D	4.87	1.46	1.34
30	k	603	HEA	CHD-C1D	4.82	1.46	1.34
30	k	604	HEA	CHD-C1D	4.81	1.46	1.34
30	K	604	HEA	CHC-C4B	4.81	1.46	1.34
30	k	604	HEA	CHC-C4B	4.80	1.46	1.34
30	K	601	HEA	CHC-C4B	4.70	1.46	1.34
30	k	603	HEA	C3A-C4A	4.69	1.48	1.41
30	K	604	HEA	CHD-C1D	4.67	1.46	1.34
30	k	604	HEA	C3A-C4A	4.52	1.48	1.41
30	K	601	HEA	C3D-C2D	4.46	1.46	1.36
30	k	603	HEA	C3D-C2D	4.45	1.46	1.36
30	K	601	HEA	C3A-C4A	4.44	1.47	1.41
30	K	604	HEA	C3D-C2D	4.38	1.46	1.36
30	k	604	HEA	C3D-C2D	4.37	1.46	1.36
30	k	603	HEA	C3B-C2B	4.32	1.44	1.34
30	K	604	HEA	C3A-C4A	4.30	1.47	1.41
30	k	604	HEA	C3B-C2B	4.27	1.44	1.34
30	K	601	HEA	C3B-C2B	4.18	1.44	1.34
30	K	604	HEA	C3B-C2B	4.15	1.44	1.34
30	k	603	HEA	C3C-C2C	4.09	1.45	1.40
28	j	404	HEM	C1B-NB	-3.97	1.33	1.40
28	J	404	HEM	C1B-NB	-3.89	1.33	1.40
28	J	405	HEM	C1B-NB	-3.86	1.33	1.40
30	k	604	HEA	C3C-C2C	3.83	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	604	HEA	C3C-C2C	3.82	1.45	1.40
28	j	403	HEM	C1B-NB	-3.82	1.33	1.40
28	l	401	HEM	C1B-NB	-3.72	1.33	1.40
30	K	604	HEA	C11-C3B	-3.67	1.46	1.51
30	K	601	HEA	C11-C3B	-3.64	1.46	1.51
30	K	601	HEA	C3C-C2C	3.59	1.45	1.40
28	L	401	HEM	C1B-NB	-3.58	1.34	1.40
30	K	604	HEA	C1D-ND	-3.55	1.34	1.40
30	K	601	HEA	C4B-NB	-3.36	1.34	1.40
30	k	603	HEA	C1D-ND	-3.35	1.34	1.40
28	J	405	HEM	C4D-ND	-3.33	1.34	1.40
28	J	404	HEM	C4D-ND	-3.32	1.34	1.40
30	K	601	HEA	C1D-ND	-3.32	1.34	1.40
25	h	601	CDL	PA1-OA4	-3.30	1.40	1.55
28	l	401	HEM	C4D-ND	-3.30	1.34	1.40
28	j	403	HEM	C4D-ND	-3.28	1.34	1.40
25	L	402	CDL	PA1-OA4	-3.28	1.40	1.55
28	j	404	HEM	C4D-ND	-3.27	1.34	1.40
25	h	602	CDL	PA1-OA4	-3.27	1.40	1.55
30	k	604	HEA	C1D-ND	-3.25	1.34	1.40
25	J	403	CDL	PA1-OA4	-3.25	1.40	1.55
30	K	604	HEA	C4B-NB	-3.24	1.34	1.40
25	j	402	CDL	PA1-OA4	-3.24	1.40	1.55
25	H	601	CDL	PA1-OA4	-3.23	1.40	1.55
25	K	603	CDL	PA1-OA4	-3.21	1.40	1.55
25	C	302	CDL	PA1-OA4	-3.20	1.40	1.55
25	k	602	CDL	PA1-OA4	-3.19	1.40	1.55
25	c	302	CDL	PA1-OA4	-3.18	1.40	1.55
28	j	404	HEM	C1D-ND	-3.11	1.32	1.38
28	L	401	HEM	C4D-ND	-3.11	1.34	1.40
28	J	405	HEM	C1D-ND	-3.05	1.32	1.38
30	k	604	HEA	C11-C3B	-3.04	1.47	1.51
25	h	602	CDL	PB2-OB4	-3.04	1.41	1.55
28	J	404	HEM	C1D-ND	-3.04	1.32	1.38
25	J	403	CDL	PB2-OB4	-3.03	1.41	1.55
25	h	601	CDL	PB2-OB4	-3.03	1.41	1.55
25	L	402	CDL	PA1-OA3	-3.02	1.40	1.50
25	H	601	CDL	PB2-OB4	-3.01	1.41	1.55
25	c	302	CDL	PB2-OB4	-3.00	1.41	1.55
30	k	603	HEA	C4B-NB	-3.00	1.35	1.40
25	j	402	CDL	PB2-OB4	-2.99	1.41	1.55
25	C	302	CDL	PB2-OB4	-2.99	1.41	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	602	CDL	PA1-OA3	-2.97	1.40	1.50
25	j	402	CDL	PB2-OB3	-2.96	1.40	1.50
25	L	402	CDL	PB2-OB3	-2.96	1.40	1.50
25	L	402	CDL	PB2-OB4	-2.96	1.41	1.55
25	h	601	CDL	PA1-OA3	-2.96	1.40	1.50
25	h	602	CDL	PB2-OB3	-2.96	1.40	1.50
25	h	601	CDL	PB2-OB3	-2.95	1.40	1.50
25	H	601	CDL	PA1-OA3	-2.95	1.40	1.50
25	K	603	CDL	PB2-OB4	-2.95	1.41	1.55
30	k	604	HEA	C4B-NB	-2.95	1.35	1.40
25	k	602	CDL	PB2-OB4	-2.94	1.41	1.55
25	C	302	CDL	PB2-OB3	-2.94	1.40	1.50
30	k	603	HEA	C11-C3B	-2.93	1.47	1.51
25	J	403	CDL	PA1-OA3	-2.93	1.40	1.50
28	j	403	HEM	C1D-ND	-2.93	1.33	1.38
25	c	302	CDL	PA1-OA3	-2.92	1.40	1.50
28	l	401	HEM	C1D-ND	-2.92	1.33	1.38
25	j	402	CDL	PA1-OA3	-2.91	1.40	1.50
25	c	302	CDL	PB2-OB3	-2.91	1.40	1.50
28	J	405	HEM	C4B-NB	-2.91	1.33	1.38
25	H	601	CDL	PB2-OB3	-2.90	1.40	1.50
25	J	403	CDL	PB2-OB3	-2.90	1.40	1.50
25	K	603	CDL	PB2-OB3	-2.90	1.40	1.50
25	k	602	CDL	PB2-OB3	-2.89	1.40	1.50
28	J	404	HEM	C4B-NB	-2.88	1.33	1.38
25	C	302	CDL	PA1-OA3	-2.88	1.40	1.50
25	k	602	CDL	PA1-OA3	-2.86	1.40	1.50
25	K	603	CDL	PA1-OA3	-2.86	1.40	1.50
28	j	404	HEM	C4B-NB	-2.85	1.33	1.38
28	j	403	HEM	C4B-NB	-2.84	1.33	1.38
28	L	401	HEM	C1D-ND	-2.79	1.33	1.38
28	l	401	HEM	C4B-NB	-2.69	1.33	1.38
30	K	604	HEA	C1B-NB	-2.55	1.33	1.38
25	k	602	CDL	PB2-OB5	2.54	1.69	1.59
25	j	402	CDL	PB2-OB5	2.53	1.69	1.59
25	K	603	CDL	PB2-OB5	2.52	1.69	1.59
25	L	402	CDL	PB2-OB5	2.52	1.69	1.59
25	c	302	CDL	PB2-OB5	2.50	1.69	1.59
25	c	302	CDL	PA1-OA5	2.49	1.69	1.59
25	K	603	CDL	PA1-OA5	2.49	1.69	1.59
30	K	601	HEA	C1B-NB	-2.49	1.34	1.38
25	k	602	CDL	PA1-OA5	2.46	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	601	CDL	PB2-OB5	2.45	1.69	1.59
25	C	302	CDL	PA1-OA5	2.44	1.69	1.59
25	J	403	CDL	PB2-OB5	2.43	1.68	1.59
25	C	302	CDL	PB2-OB5	2.43	1.68	1.59
25	h	601	CDL	PB2-OB5	2.43	1.68	1.59
25	J	403	CDL	PA1-OA5	2.41	1.68	1.59
25	h	602	CDL	PB2-OB5	2.40	1.68	1.59
30	k	603	HEA	C1B-NB	-2.38	1.34	1.38
28	L	401	HEM	C4B-NB	-2.38	1.34	1.38
25	h	602	CDL	PA1-OA5	2.37	1.68	1.59
30	K	604	HEA	C4D-ND	-2.36	1.34	1.38
25	j	402	CDL	PA1-OA5	2.36	1.68	1.59
30	k	604	HEA	C1B-NB	-2.36	1.34	1.38
25	L	402	CDL	PA1-OA5	2.31	1.68	1.59
30	k	604	HEA	C2A-C1A	2.31	1.47	1.42
30	k	604	HEA	C4B-C3B	2.26	1.48	1.44
25	h	601	CDL	PA1-OA5	2.26	1.68	1.59
30	k	603	HEA	C4B-C3B	2.25	1.48	1.44
30	K	604	HEA	C2A-C1A	2.24	1.47	1.42
25	H	601	CDL	PA1-OA5	2.22	1.68	1.59
28	l	401	HEM	CHB-C1B	2.20	1.40	1.34
30	k	604	HEA	FE-ND	2.18	2.10	1.98
28	L	401	HEM	FE-NB	2.18	2.10	1.98
28	l	401	HEM	FE-ND	-2.18	1.85	1.98
28	j	403	HEM	FE-ND	-2.18	1.85	1.98
30	k	603	HEA	C1C-CHC	2.18	1.47	1.41
30	k	604	HEA	FE-NB	2.17	2.10	1.98
30	k	603	HEA	C2A-C1A	2.16	1.47	1.42
30	K	601	HEA	C2A-C1A	2.15	1.47	1.42
28	J	405	HEM	FE-NB	2.14	2.10	1.98
28	J	404	HEM	FE-ND	-2.13	1.86	1.98
30	k	603	HEA	C4D-ND	-2.13	1.34	1.38
28	j	404	HEM	FE-ND	-2.13	1.86	1.98
28	j	404	HEM	FE-NB	2.13	2.09	1.98
28	J	405	HEM	FE-ND	-2.12	1.86	1.98
30	K	601	HEA	FE-ND	2.11	2.09	1.98
30	k	603	HEA	FE-NB	2.11	2.09	1.98
28	J	404	HEM	FE-NB	2.11	2.09	1.98
30	k	603	HEA	FE-ND	2.10	2.09	1.98
30	K	601	HEA	C4D-ND	-2.08	1.34	1.38
30	K	601	HEA	FE-NB	2.08	2.09	1.98
30	k	604	HEA	C1C-CHC	2.08	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	403	HEM	FE-NB	2.05	2.09	1.98
28	L	401	HEM	FE-ND	-2.05	1.86	1.98
30	k	603	HEA	C4C-CHD	2.03	1.46	1.41
30	K	604	HEA	C1C-CHC	2.03	1.46	1.41
30	k	604	HEA	C4C-CHD	2.02	1.46	1.41
28	J	404	HEM	C1A-CHA	-2.01	1.35	1.41
30	K	601	HEA	C4C-CHD	2.00	1.46	1.41
28	l	401	HEM	FE-NB	2.00	2.09	1.98

All (388) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	601	HEA	C3D-C4D-ND	6.70	116.82	110.35
30	k	603	HEA	C3D-C4D-ND	6.60	116.73	110.35
30	k	604	HEA	C3D-C4D-ND	6.50	116.63	110.35
28	j	404	HEM	CAD-C3D-C4D	6.45	135.95	124.70
30	K	604	HEA	C3D-C4D-ND	6.42	116.56	110.35
29	J	408	UQ6	C7-C8-C9	-6.14	118.62	127.42
28	J	405	HEM	CAD-C3D-C4D	6.01	135.18	124.70
29	J	406	UQ6	C7-C8-C9	-5.79	119.13	127.42
30	K	604	HEA	C13-C12-C11	-5.71	105.28	114.39
30	k	604	HEA	C2B-C1B-NB	5.64	116.42	109.90
30	K	601	HEA	C2B-C1B-NB	5.55	116.32	109.90
30	k	604	HEA	C13-C12-C11	-5.40	105.77	114.39
30	K	604	HEA	C2B-C1B-NB	5.39	116.14	109.90
28	J	404	HEM	CAD-C3D-C4D	5.36	134.04	124.70
30	K	601	HEA	C3B-C4B-NB	5.27	115.89	109.84
30	k	604	HEA	C3B-C4B-NB	5.16	115.77	109.84
30	K	601	HEA	C13-C12-C11	-5.15	106.17	114.39
28	j	403	HEM	CAD-C3D-C4D	5.12	133.62	124.70
30	k	603	HEA	C13-C12-C11	-5.07	106.29	114.39
28	j	403	HEM	CHC-C4B-NB	5.06	129.88	124.44
30	k	603	HEA	C2B-C1B-NB	5.01	115.70	109.90
30	k	604	HEA	C2D-C1D-ND	5.01	115.60	109.84
28	J	405	HEM	CHC-C4B-NB	4.90	129.71	124.44
30	K	604	HEA	C2D-C1D-ND	4.89	115.47	109.84
28	J	404	HEM	CHC-C4B-NB	4.89	129.69	124.44
30	k	603	HEA	C2D-C1D-ND	4.83	115.39	109.84
28	j	404	HEM	CHC-C4B-NB	4.80	129.60	124.44
28	L	401	HEM	CAD-C3D-C4D	4.78	133.04	124.70
30	K	601	HEA	C2D-C1D-ND	4.77	115.32	109.84
30	k	603	HEA	C3B-C4B-NB	4.76	115.31	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	604	HEA	C3B-C4B-NB	4.73	115.28	109.84
30	K	601	HEA	CBA-CAA-C2A	-4.70	104.81	112.55
29	j	407	UQ6	C7-C8-C9	-4.64	120.77	127.42
29	j	405	UQ6	C7-C8-C9	-4.52	120.94	127.42
28	j	404	HEM	CAD-C3D-C2D	-4.50	119.43	127.87
28	l	401	HEM	CAD-C3D-C4D	4.45	132.45	124.70
28	l	401	HEM	CHC-C4B-NB	4.37	129.14	124.44
28	j	403	HEM	CHD-C1D-ND	4.26	129.01	124.44
30	K	601	HEA	CAD-C3D-C4D	4.24	132.09	124.70
28	j	403	HEM	CHB-C1B-NB	4.21	129.59	124.37
30	k	603	HEA	C26-C15-C16	4.20	122.52	115.23
28	j	404	HEM	CBD-CAD-C3D	4.19	124.11	112.53
28	J	405	HEM	CAD-C3D-C2D	-4.18	120.04	127.87
28	J	405	HEM	CHD-C1D-ND	4.17	128.92	124.44
23	w	201	PEF	O2-C10-C11	4.16	120.49	111.48
23	a	504	PEF	O2-C10-C11	4.15	120.45	111.48
30	k	604	HEA	C26-C15-C16	4.14	122.42	115.23
30	k	604	HEA	CAD-C3D-C4D	4.12	131.88	124.70
28	J	404	HEM	CHD-C1D-ND	4.08	128.82	124.44
28	l	401	HEM	C1B-NB-C4B	4.07	110.03	105.21
23	W	202	PEF	O2-C10-C11	4.05	120.24	111.48
28	J	405	HEM	CBD-CAD-C3D	4.04	123.70	112.53
28	J	404	HEM	CHB-C1B-NB	4.02	129.35	124.37
28	L	401	HEM	CHD-C1D-ND	4.01	128.75	124.44
23	W	201	PEF	O2-C10-C11	3.99	120.11	111.48
23	A	503	PEF	O2-C10-C11	3.98	120.09	111.48
30	K	601	HEA	C4D-C3D-C2D	-3.95	101.14	106.89
28	L	401	HEM	CHC-C4B-NB	3.94	128.68	124.44
28	j	404	HEM	CHD-C1D-ND	3.94	128.68	124.44
23	A	502	PEF	O2-C10-C11	3.94	120.00	111.48
30	k	603	HEA	CAD-C3D-C4D	3.90	131.50	124.70
23	j	406	PEF	O2-C10-C11	3.89	119.90	111.48
30	K	601	HEA	C26-C15-C16	3.87	121.94	115.23
23	C	304	PEF	O2-C10-C11	3.87	119.85	111.48
23	A	501	PEF	O2-C10-C11	3.86	119.84	111.48
23	w	202	PEF	O2-C10-C11	3.85	119.81	111.48
28	L	401	HEM	CHB-C1B-NB	3.84	129.14	124.37
23	J	409	PEF	O2-C10-C11	3.84	119.79	111.48
30	k	603	HEA	C4D-C3D-C2D	-3.84	101.31	106.89
28	L	401	HEM	C3B-C4B-NB	-3.81	106.73	109.47
23	c	304	PEF	O2-C10-C11	3.78	119.66	111.48
30	k	604	HEA	CBA-CAA-C2A	-3.76	106.35	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	408	PEF	O2-C10-C11	3.75	119.60	111.48
23	j	401	PEF	O2-C10-C11	3.73	119.56	111.48
30	K	604	HEA	C3C-C4C-NC	3.71	114.01	109.21
30	K	604	HEA	C4D-C3D-C2D	-3.70	101.50	106.89
23	a	503	PEF	O2-C10-C11	3.70	119.49	111.48
30	k	604	HEA	C4D-C3D-C2D	-3.69	101.53	106.89
30	k	603	HEA	C3C-C4C-NC	3.68	113.97	109.21
23	C	303	PEF	O2-C10-C11	3.68	119.43	111.48
23	J	401	PEF	O2-C10-C11	3.68	119.43	111.48
30	K	601	HEA	CHB-C1B-C2B	-3.62	119.31	125.03
23	v	101	PEF	O2-C10-C11	3.62	119.31	111.48
30	k	604	HEA	C3C-C4C-NC	3.61	113.88	109.21
28	L	401	HEM	C1B-NB-C4B	3.61	109.49	105.21
30	k	604	HEA	CHB-C1B-C2B	-3.61	119.33	125.03
23	V	101	PEF	O2-C10-C11	3.59	119.24	111.48
28	J	404	HEM	CAD-C3D-C2D	-3.58	121.17	127.87
28	l	401	HEM	C3B-C4B-NB	-3.56	106.91	109.47
30	K	604	HEA	CHB-C1B-C2B	-3.54	119.43	125.03
28	l	401	HEM	CHD-C1D-ND	3.54	128.24	124.44
23	E	102	PEF	O2-C10-C11	3.54	119.14	111.48
28	J	405	HEM	CBA-CAA-C2A	-3.51	106.64	112.54
29	j	405	UQ6	C12-C13-C14	-3.50	119.61	127.62
28	j	403	HEM	CAD-C3D-C2D	-3.50	121.31	127.87
30	K	601	HEA	C3C-C4C-NC	3.48	113.71	109.21
28	J	405	HEM	CHB-C1B-NB	3.47	128.67	124.37
23	J	407	PEF	C2-O2-C10	3.46	126.08	117.80
23	a	501	PEF	C2-O2-C10	3.45	126.06	117.80
30	K	604	HEA	CAD-C3D-C4D	3.44	130.69	124.70
30	K	604	HEA	C26-C15-C16	3.44	121.19	115.23
23	c	303	PEF	O2-C10-C11	3.43	118.90	111.48
28	j	404	HEM	CHB-C1B-NB	3.43	128.62	124.37
30	K	604	HEA	C17-C18-C19	-3.42	119.80	127.62
30	K	604	HEA	CMC-C2C-C3C	3.40	131.47	124.68
23	a	501	PEF	P-O4P-C4	-3.38	105.17	121.26
28	l	401	HEM	CHB-C1B-NB	3.34	128.51	124.37
23	J	407	PEF	O2-C10-C11	3.33	118.68	111.48
30	K	604	HEA	C1D-C2D-C3D	-3.33	103.48	106.98
28	j	404	HEM	C1B-NB-C4B	3.32	109.13	105.21
28	j	403	HEM	C1B-NB-C4B	3.30	109.12	105.21
30	K	604	HEA	CBA-CAA-C2A	-3.30	107.11	112.55
23	e	101	PEF	O2-C10-C11	3.30	118.61	111.48
25	H	601	CDL	OA4-PA1-OA3	3.29	127.74	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	405	UQ6	C22-C23-C24	-3.29	120.10	127.62
23	j	406	PEF	P-O4P-C4	-3.26	105.73	121.26
28	J	404	HEM	CBA-CAA-C2A	-3.25	107.08	112.54
30	k	604	HEA	C1D-C2D-C3D	-3.24	103.57	106.98
23	A	502	PEF	P-O4P-C4	-3.24	105.84	121.26
30	k	603	HEA	CBA-CAA-C2A	-3.24	107.22	112.55
25	j	402	CDL	OA4-PA1-OA3	3.23	127.48	112.44
29	j	405	UQ6	C27-C28-C29	-3.22	120.24	127.62
29	J	406	UQ6	C22-C23-C24	-3.22	120.25	127.62
25	h	601	CDL	OA4-PA1-OA3	3.21	127.40	112.44
25	L	402	CDL	OA4-PA1-OA3	3.19	127.28	112.44
29	J	406	UQ6	C27-C28-C29	-3.19	120.33	127.62
23	J	401	PEF	P-O4P-C4	-3.17	106.15	121.26
30	k	604	HEA	C4B-C3B-C2B	-3.17	102.11	107.44
25	K	603	CDL	OA4-PA1-OA3	3.17	127.17	112.44
23	J	407	PEF	P-O4P-C4	-3.17	106.19	121.26
23	W	201	PEF	P-O4P-C4	-3.16	106.20	121.26
25	k	602	CDL	OA4-PA1-OA3	3.16	127.14	112.44
29	j	407	UQ6	C27-C28-C29	-3.16	120.39	127.62
28	J	404	HEM	C1B-NB-C4B	3.16	108.95	105.21
30	k	603	HEA	CHB-C1B-C2B	-3.14	120.07	125.03
28	J	404	HEM	CBD-CAD-C3D	3.14	121.22	112.53
25	J	403	CDL	OA4-PA1-OA3	3.14	127.05	112.44
23	j	401	PEF	P-O4P-C4	-3.14	106.31	121.26
25	C	302	CDL	OA4-PA1-OA3	3.14	127.04	112.44
30	k	604	HEA	CMC-C2C-C3C	3.14	130.95	124.68
28	j	403	HEM	CBA-CAA-C2A	-3.14	107.26	112.54
30	k	603	HEA	CMC-C2C-C3C	3.14	130.95	124.68
30	K	601	HEA	C1B-C2B-C3B	-3.13	103.17	106.80
30	k	603	HEA	C1D-C2D-C3D	-3.12	103.69	106.98
29	j	407	UQ6	C10-C9-C11	3.12	120.65	115.23
30	k	603	HEA	C4B-C3B-C2B	-3.12	102.19	107.44
23	A	503	PEF	P-O4P-C4	-3.12	106.42	121.26
30	K	604	HEA	C1B-C2B-C3B	-3.12	103.19	106.80
23	a	501	PEF	O2-C10-C11	3.11	118.22	111.48
23	c	304	PEF	P-O4P-C4	-3.11	106.45	121.26
25	h	602	CDL	OA4-PA1-OA3	3.10	126.86	112.44
25	c	302	CDL	OA4-PA1-OA3	3.08	126.76	112.44
23	W	202	PEF	P-O4P-C4	-3.07	106.63	121.26
30	K	601	HEA	C4B-C3B-C2B	-3.06	102.29	107.44
28	L	401	HEM	CAD-C3D-C2D	-3.06	122.13	127.87
30	K	604	HEA	CAD-CBD-CGD	-3.06	105.54	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	503	PEF	P-O4P-C4	-3.06	106.70	121.26
30	K	604	HEA	C27-C19-C20	3.05	120.52	115.23
25	C	302	CDL	OB4-PB2-OB3	3.04	126.58	112.44
28	L	401	HEM	CBD-CAD-C3D	3.04	120.93	112.53
23	V	101	PEF	P-O4P-C4	-3.03	106.83	121.26
23	j	408	PEF	P-O4P-C4	-3.03	106.85	121.26
23	w	202	PEF	P-O4P-C4	-3.03	106.86	121.26
23	C	304	PEF	P-O4P-C4	-3.02	106.89	121.26
28	J	405	HEM	C1B-NB-C4B	3.01	108.78	105.21
23	c	303	PEF	P-O4P-C4	-3.01	106.91	121.26
25	c	302	CDL	OB4-PB2-OB3	3.01	126.44	112.44
23	v	101	PEF	P-O4P-C4	-3.01	106.95	121.26
29	J	406	UQ6	C3M-O3-C3	-3.00	106.59	114.74
23	A	501	PEF	P-O4P-C4	-3.00	106.99	121.26
23	J	409	PEF	O3-C30-C31	2.99	120.94	111.83
30	k	604	HEA	C27-C19-C20	2.98	120.41	115.23
30	K	601	HEA	C1D-C2D-C3D	-2.97	103.85	106.98
30	k	603	HEA	C17-C18-C19	-2.97	120.82	127.62
23	E	102	PEF	P-O4P-C4	-2.97	107.12	121.26
30	K	601	HEA	CMC-C2C-C3C	2.97	130.62	124.68
29	J	406	UQ6	C12-C13-C14	-2.97	120.83	127.62
23	J	409	PEF	P-O4P-C4	-2.96	107.16	121.26
28	j	403	HEM	CBD-CAD-C3D	2.95	120.69	112.53
30	k	604	HEA	CHA-C4D-C3D	-2.94	120.49	124.77
30	K	604	HEA	CHA-C4D-C3D	-2.93	120.49	124.77
23	e	101	PEF	P-O4P-C4	-2.93	107.33	121.26
29	j	407	UQ6	C17-C18-C19	-2.92	120.93	127.62
30	K	604	HEA	C13-C14-C15	-2.92	120.94	127.62
30	k	604	HEA	C17-C18-C19	-2.92	120.95	127.62
23	w	201	PEF	P-O4P-C4	-2.92	107.38	121.26
28	l	401	HEM	CBD-CAD-C3D	2.90	120.55	112.53
30	k	604	HEA	C1B-C2B-C3B	-2.90	103.44	106.80
30	K	601	HEA	C27-C19-C20	2.90	120.26	115.23
30	K	604	HEA	C16-C15-C14	-2.90	114.66	121.17
29	J	406	UQ6	C25-C24-C26	2.89	120.24	115.23
25	j	402	CDL	OB4-PB2-OB3	2.89	125.88	112.44
23	C	303	PEF	P-O4P-C4	-2.88	107.53	121.26
29	j	405	UQ6	C17-C18-C19	-2.88	121.03	127.62
30	K	604	HEA	C4B-C3B-C2B	-2.88	102.60	107.44
25	h	601	CDL	OB4-PB2-OB3	2.87	125.80	112.44
23	C	303	PEF	O3-C30-C31	2.86	120.56	111.83
30	K	601	HEA	CBD-CAD-C3D	2.85	120.43	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	k	604	HEA	CAD-CBD-CGD	-2.85	106.09	113.67
28	J	405	HEM	CMC-C2C-C3C	2.85	130.38	124.68
28	l	401	HEM	CAD-C3D-C2D	-2.84	122.55	127.87
25	J	403	CDL	OB4-PB2-OB3	2.83	125.59	112.44
30	k	603	HEA	CAD-CBD-CGD	-2.82	106.18	113.67
25	h	602	CDL	OB4-PB2-OB3	2.82	125.54	112.44
23	j	406	PEF	O3-C30-C31	2.81	120.42	111.83
25	k	602	CDL	OB4-PB2-OB3	2.81	125.52	112.44
23	A	503	PEF	P-O3P-C1	-2.81	105.24	121.35
25	H	601	CDL	OB4-PB2-OB3	2.80	125.46	112.44
25	L	402	CDL	OB4-PB2-OB3	2.80	125.45	112.44
23	a	501	PEF	P-O3P-C1	-2.79	105.37	121.35
29	j	405	UQ6	C4M-O4-C4	-2.78	107.19	114.74
25	K	603	CDL	OB4-PB2-OB3	2.78	125.39	112.44
30	k	603	HEA	C27-C19-C20	2.78	120.05	115.23
29	J	406	UQ6	C15-C14-C16	2.78	120.05	115.23
23	a	503	PEF	O3-C30-C31	2.77	120.29	111.83
23	V	101	PEF	C2-O2-C10	2.77	124.43	117.80
23	c	303	PEF	O3-C30-C31	2.76	120.25	111.83
29	j	407	UQ6	C15-C14-C16	2.76	120.02	115.23
23	j	401	PEF	P-O3P-C1	-2.75	105.61	121.35
29	j	405	UQ6	C3M-O3-C3	-2.75	107.29	114.74
23	c	304	PEF	O3-C30-C31	2.75	120.21	111.83
30	K	604	HEA	C12-C13-C14	-2.74	104.95	112.16
29	J	408	UQ6	C4M-O4-C4	-2.73	107.34	114.74
30	K	601	HEA	CHA-C4D-C3D	-2.72	120.81	124.77
23	e	101	PEF	C2-O2-C10	2.72	124.31	117.80
23	J	401	PEF	O3-C30-C31	2.72	120.11	111.83
30	K	604	HEA	C21-C20-C19	-2.71	104.19	113.19
23	E	102	PEF	O3-C30-C31	2.71	120.10	111.83
23	j	406	PEF	P-O3P-C1	-2.70	105.86	121.35
30	K	601	HEA	CAD-CBD-CGD	-2.70	106.50	113.67
23	c	304	PEF	P-O3P-C1	-2.70	105.87	121.35
23	A	501	PEF	O3-C30-C31	2.70	120.07	111.83
23	e	101	PEF	O3-C30-C31	2.70	120.07	111.83
23	J	401	PEF	P-O3P-C1	-2.70	105.89	121.35
30	K	601	HEA	C17-C18-C19	-2.70	121.45	127.62
23	a	504	PEF	P-O4P-C4	-2.68	108.50	121.26
23	A	502	PEF	O3-C30-C31	2.68	120.00	111.83
23	j	401	PEF	O3-C30-C31	2.67	119.98	111.83
29	j	407	UQ6	C4M-O4-C4	-2.67	107.49	114.74
23	c	303	PEF	P-O3P-C1	-2.65	106.14	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	k	603	HEA	C1B-C2B-C3B	-2.65	103.73	106.80
28	J	405	HEM	CHD-C1D-C2D	-2.65	120.84	125.03
23	a	501	PEF	O3-C30-C31	2.65	119.91	111.83
23	A	502	PEF	P-O3P-C1	-2.64	106.21	121.35
28	L	401	HEM	CHD-C1D-C2D	-2.64	120.86	125.03
27	J	402	CN5	O31-C31-C32	2.63	119.85	111.83
29	J	406	UQ6	C30-C29-C31	2.62	119.78	115.23
23	w	202	PEF	O3-C30-C31	2.62	119.83	111.83
30	k	604	HEA	C4A-CHB-C1B	2.61	126.01	122.56
23	a	504	PEF	O3-C30-C31	2.61	119.79	111.83
25	c	302	CDL	CA4-OA6-CA5	2.61	124.03	117.80
23	V	101	PEF	P-O3P-C1	-2.60	106.43	121.35
23	j	408	PEF	O3-C30-C31	2.60	119.76	111.83
30	k	604	HEA	C21-C20-C19	-2.60	104.58	113.19
30	k	603	HEA	CHA-C4D-C3D	-2.60	120.99	124.77
23	w	202	PEF	P-O3P-C1	-2.58	106.55	121.35
23	w	201	PEF	O3-C30-C31	2.58	119.71	111.83
23	v	101	PEF	O3-C30-C31	2.58	119.70	111.83
23	V	101	PEF	O3-C30-C31	2.58	119.69	111.83
23	W	202	PEF	P-O3P-C1	-2.57	106.62	121.35
23	C	304	PEF	O3-C30-C31	2.56	119.65	111.83
23	E	102	PEF	P-O3P-C1	-2.56	106.67	121.35
23	W	201	PEF	P-O3P-C1	-2.56	106.68	121.35
23	e	101	PEF	P-O3P-C1	-2.55	106.73	121.35
23	j	408	PEF	P-O3P-C1	-2.55	106.75	121.35
23	J	409	PEF	P-O3P-C1	-2.55	106.76	121.35
23	a	503	PEF	P-O3P-C1	-2.55	106.76	121.35
28	j	403	HEM	CHA-C4D-ND	2.54	127.53	124.37
23	J	407	PEF	P-O3P-C1	-2.54	106.79	121.35
30	k	603	HEA	C12-C13-C14	-2.54	105.49	112.16
29	J	406	UQ6	C17-C18-C19	-2.54	121.82	127.62
23	v	101	PEF	P-O3P-C1	-2.54	106.81	121.35
23	W	202	PEF	O3-C30-C31	2.53	119.56	111.83
30	k	603	HEA	C21-C20-C19	-2.53	104.80	113.19
23	C	304	PEF	P-O3P-C1	-2.53	106.86	121.35
29	j	405	UQ6	C20-C19-C21	2.53	119.62	115.23
29	J	406	UQ6	C10-C9-C11	2.52	119.60	115.23
28	j	403	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
28	J	404	HEM	CHD-C1D-C2D	-2.50	121.08	125.03
30	k	603	HEA	C13-C14-C15	-2.49	121.92	127.62
30	k	604	HEA	C4B-NB-C1B	-2.49	102.26	105.21
30	k	604	HEA	C12-C13-C14	-2.49	105.62	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	503	PEF	O3-C30-C31	2.49	119.42	111.83
30	K	601	HEA	C21-C20-C19	-2.49	104.94	113.19
23	J	407	PEF	O3-C30-C31	2.48	119.39	111.83
29	j	407	UQ6	C20-C19-C21	2.48	119.53	115.23
30	k	603	HEA	C4A-CHB-C1B	2.47	125.82	122.56
28	L	401	HEM	CHA-C4D-ND	2.46	127.42	124.37
29	j	407	UQ6	C12-C13-C14	-2.46	122.00	127.62
25	h	602	CDL	OB6-CB5-OB7	-2.45	117.97	123.70
26	E	101	PCF	C11-C12-N	-2.45	107.96	115.82
30	k	604	HEA	C4D-CHA-C1A	2.44	125.78	122.56
23	a	504	PEF	P-O3P-C1	-2.43	107.41	121.35
30	K	601	HEA	C4B-NB-C1B	-2.43	102.33	105.21
29	j	407	UQ6	C30-C29-C31	2.42	119.43	115.23
28	j	404	HEM	C3B-C4B-NB	-2.42	107.73	109.47
23	W	201	PEF	O3-C30-C31	2.42	119.20	111.83
28	j	403	HEM	C3B-C4B-NB	-2.42	107.73	109.47
29	J	408	UQ6	C10-C9-C11	2.42	119.42	115.23
29	j	405	UQ6	C10-C9-C11	2.41	119.41	115.23
28	j	404	HEM	CHD-C1D-C2D	-2.41	121.22	125.03
23	E	102	PEF	C2-O2-C10	2.40	123.55	117.80
30	K	601	HEA	C4A-CHB-C1B	2.40	125.73	122.56
23	C	303	PEF	P-O3P-C1	-2.40	107.61	121.35
29	j	407	UQ6	C25-C24-C26	2.39	119.38	115.23
29	J	406	UQ6	C4M-O4-C4	-2.38	108.27	114.74
28	l	401	HEM	CAA-CBA-CGA	-2.38	107.43	113.83
30	K	601	HEA	C16-C15-C14	-2.37	115.86	121.17
23	C	303	PEF	C2-O2-C10	2.37	123.46	117.80
29	J	406	UQ6	C20-C19-C21	2.36	119.33	115.23
28	J	404	HEM	CHA-C4D-ND	2.36	127.30	124.37
25	J	403	CDL	OA6-CA5-OA7	-2.36	118.19	123.70
23	A	501	PEF	P-O3P-C1	-2.36	107.83	121.35
29	j	407	UQ6	C36-C34-C35	2.36	120.02	114.59
29	j	405	UQ6	C25-C24-C26	2.35	119.31	115.23
30	K	601	HEA	C12-C13-C14	-2.35	105.98	112.16
30	k	603	HEA	CMB-C2B-C1B	2.34	128.69	125.03
29	j	405	UQ6	C36-C34-C35	2.33	119.96	114.59
30	K	601	HEA	C4D-CHA-C1A	2.33	125.63	122.56
29	j	407	UQ6	C3M-O3-C3	-2.33	108.42	114.74
30	K	604	HEA	C4A-CHB-C1B	2.32	125.62	122.56
30	K	604	HEA	C21-C22-C23	-2.32	119.91	127.64
23	v	101	PEF	C2-O2-C10	2.31	123.33	117.80
30	k	604	HEA	CMD-C2D-C1D	2.30	128.62	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	408	UQ6	C3M-O3-C3	-2.29	108.52	114.74
29	j	407	UQ6	C22-C23-C24	-2.28	122.40	127.62
30	k	604	HEA	C13-C14-C15	-2.27	122.43	127.62
28	L	401	HEM	CBA-CAA-C2A	-2.26	108.74	112.54
28	J	404	HEM	CHB-C1B-C2B	-2.26	120.55	126.94
30	K	604	HEA	C4D-CHA-C1A	2.25	125.53	122.56
28	j	403	HEM	CHB-C1B-C2B	-2.25	120.56	126.94
30	K	601	HEA	CMB-C2B-C1B	2.25	128.54	125.03
30	K	601	HEA	C13-C14-C15	-2.23	122.51	127.62
30	K	604	HEA	CHD-C1D-C2D	-2.23	120.62	126.94
25	c	302	CDL	OB6-CB5-OB7	-2.23	118.49	123.70
28	j	404	HEM	CBA-CAA-C2A	-2.23	108.79	112.54
29	J	406	UQ6	C36-C34-C35	2.23	119.71	114.59
29	j	405	UQ6	C15-C14-C16	2.22	119.08	115.23
25	j	402	CDL	OB6-CB5-OB7	-2.22	118.53	123.70
28	L	401	HEM	CHB-C1B-C2B	-2.21	120.68	126.94
23	w	201	PEF	P-O3P-C1	-2.20	108.75	121.35
25	L	402	CDL	OB6-CB5-OB7	-2.19	118.58	123.70
30	K	604	HEA	CMB-C2B-C1B	2.19	128.46	125.03
29	j	405	UQ6	C32-C33-C34	-2.19	120.33	127.64
25	h	601	CDL	OB6-CB5-OB7	-2.19	118.58	123.70
25	J	403	CDL	OB6-CB5-OB7	-2.19	118.59	123.70
28	j	404	HEM	CMC-C2C-C3C	2.19	129.05	124.68
28	l	401	HEM	CHA-C4D-ND	2.17	127.06	124.37
30	k	603	HEA	C27-C19-C18	-2.16	118.07	123.63
30	k	603	HEA	CHC-C4B-NB	-2.16	121.70	124.37
29	j	405	UQ6	C30-C29-C31	2.16	118.97	115.23
30	k	604	HEA	C1D-ND-C4D	-2.15	102.67	105.21
25	H	601	CDL	OA6-CA5-OA7	-2.14	118.70	123.70
30	k	604	HEA	CBD-CAD-C3D	2.14	118.44	112.53
28	J	404	HEM	CMC-C2C-C3C	2.14	128.95	124.68
28	j	403	HEM	CAA-CBA-CGA	-2.12	108.12	113.83
30	k	603	HEA	CMD-C2D-C1D	2.12	128.35	125.03
30	k	604	HEA	CHD-C1D-C2D	-2.12	120.94	126.94
30	k	604	HEA	CMB-C2B-C1B	2.12	128.34	125.03
25	h	601	CDL	OA6-CA5-OA7	-2.12	118.75	123.70
25	C	302	CDL	OB6-CB5-OB7	-2.11	118.76	123.70
30	K	604	HEA	C25-C23-C24	2.11	119.45	114.59
30	K	601	HEA	CMD-C2D-C1D	2.11	128.33	125.03
25	h	602	CDL	OA6-CA5-OA7	-2.11	118.78	123.70
30	K	601	HEA	CHD-C1D-C2D	-2.11	120.97	126.94
25	L	402	CDL	OA6-CA5-OA7	-2.10	118.79	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	k	603	HEA	C16-C15-C14	-2.10	116.46	121.17
28	l	401	HEM	CHD-C1D-C2D	-2.10	121.72	125.03
28	J	404	HEM	C3B-C4B-NB	-2.08	107.97	109.47
30	k	603	HEA	CBD-CAD-C3D	2.08	118.29	112.53
30	K	604	HEA	C26-C15-C14	-2.07	118.30	123.63
28	j	404	HEM	CHB-C1B-C2B	-2.07	121.07	126.94
25	H	601	CDL	OB6-CB5-OB7	-2.07	118.86	123.70
30	K	601	HEA	C27-C19-C18	-2.06	118.32	123.63
28	J	405	HEM	CHB-C1B-C2B	-2.06	121.10	126.94
30	k	604	HEA	C16-C15-C14	-2.06	116.55	121.17
30	k	603	HEA	CHD-C1D-C2D	-2.05	121.12	126.94
29	J	408	UQ6	C6-C7-C8	2.05	115.57	112.06
28	l	401	HEM	O2A-CGA-O1A	-2.05	118.05	123.33
25	c	302	CDL	OA6-CA5-OA7	-2.04	118.94	123.70
28	J	405	HEM	CHA-C4D-ND	2.03	126.89	124.37
30	K	604	HEA	C4B-NB-C1B	-2.03	102.80	105.21
30	K	601	HEA	C25-C23-C24	2.02	119.25	114.59
25	j	402	CDL	OA6-CA5-OA7	-2.02	118.98	123.70
30	k	603	HEA	C4D-CHA-C1A	2.01	125.21	122.56
30	K	601	HEA	O11-C11-C3B	-2.01	107.58	111.26
30	k	604	HEA	C27-C19-C18	-2.01	118.48	123.63
30	k	603	HEA	CHA-C4D-ND	-2.00	122.28	124.44

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	302	CDL	CA4
25	H	601	CDL	CA4
25	J	403	CDL	CA4
25	K	603	CDL	CA4
25	L	402	CDL	CA4
25	c	302	CDL	CA4
25	h	601	CDL	CA4
25	h	602	CDL	CA4
25	j	402	CDL	CA4
25	k	602	CDL	CA4

All (691) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	PEF	O2-C2-C3-O3
23	A	503	PEF	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
23	A	503	PEF	C4-O4P-P-O3P
23	C	303	PEF	C11-C10-O2-C2
23	E	102	PEF	C1-O3P-P-O1P
23	J	401	PEF	C4-O4P-P-O1P
23	J	401	PEF	C4-O4P-P-O3P
23	J	409	PEF	C11-C10-O2-C2
23	J	409	PEF	C31-C30-O3-C3
23	J	409	PEF	O5-C30-O3-C3
23	W	201	PEF	O2-C2-C3-O3
23	a	501	PEF	O2-C2-C3-O3
23	a	501	PEF	O4P-C4-C5-N
23	a	504	PEF	C4-O4P-P-O1P
23	a	504	PEF	C4-O4P-P-O3P
23	j	401	PEF	C11-C10-O2-C2
25	C	302	CDL	CA2-OA2-PA1-OA3
25	C	302	CDL	CA2-OA2-PA1-OA5
25	C	302	CDL	CA3-OA5-PA1-OA2
25	C	302	CDL	CA3-OA5-PA1-OA3
25	C	302	CDL	OA6-CA4-CA6-OA8
25	C	302	CDL	CB3-OB5-PB2-OB2
25	C	302	CDL	CB3-OB5-PB2-OB3
25	C	302	CDL	CB3-OB5-PB2-OB4
25	C	302	CDL	C51-CB5-OB6-CB4
25	H	601	CDL	O1-C1-CB2-OB2
25	H	601	CDL	CA2-C1-CB2-OB2
25	H	601	CDL	CA2-OA2-PA1-OA4
25	H	601	CDL	CA2-OA2-PA1-OA5
25	H	601	CDL	CA3-OA5-PA1-OA3
25	H	601	CDL	OA7-CA5-OA6-CA4
25	H	601	CDL	C11-CA5-OA6-CA4
25	H	601	CDL	OB6-CB4-CB6-OB8
25	J	403	CDL	CA3-OA5-PA1-OA3
25	J	403	CDL	OA7-CA5-OA6-CA4
25	J	403	CDL	CB2-OB2-PB2-OB4
25	J	403	CDL	CB2-OB2-PB2-OB5
25	J	403	CDL	CB3-OB5-PB2-OB2
25	J	403	CDL	CB3-OB5-PB2-OB3
25	J	403	CDL	CB3-OB5-PB2-OB4
25	K	603	CDL	CA2-OA2-PA1-OA3
25	K	603	CDL	CA2-OA2-PA1-OA5
25	K	603	CDL	CA3-OA5-PA1-OA2
25	K	603	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
25	K	603	CDL	OA7-CA5-OA6-CA4
25	K	603	CDL	C11-CA5-OA6-CA4
25	K	603	CDL	CB2-OB2-PB2-OB3
25	K	603	CDL	CB2-OB2-PB2-OB5
25	K	603	CDL	CB3-OB5-PB2-OB3
25	L	402	CDL	CA2-OA2-PA1-OA3
25	L	402	CDL	CA2-OA2-PA1-OA5
25	L	402	CDL	CA3-OA5-PA1-OA2
25	L	402	CDL	CA3-OA5-PA1-OA3
25	L	402	CDL	CA3-OA5-PA1-OA4
25	L	402	CDL	CB2-OB2-PB2-OB5
25	L	402	CDL	CB3-OB5-PB2-OB3
25	L	402	CDL	CB3-OB5-PB2-OB4
25	c	302	CDL	O1-C1-CA2-OA2
25	c	302	CDL	CA3-OA5-PA1-OA2
25	c	302	CDL	CA3-OA5-PA1-OA3
25	c	302	CDL	CA3-OA5-PA1-OA4
25	c	302	CDL	C11-CA5-OA6-CA4
25	c	302	CDL	CB3-OB5-PB2-OB4
25	c	302	CDL	CB4-CB3-OB5-PB2
25	h	601	CDL	OA7-CA5-OA6-CA4
25	h	601	CDL	C11-CA5-OA6-CA4
25	h	601	CDL	CB2-OB2-PB2-OB3
25	h	601	CDL	CB2-OB2-PB2-OB4
25	h	601	CDL	CB3-OB5-PB2-OB2
25	h	601	CDL	CB3-OB5-PB2-OB3
25	h	601	CDL	CB3-OB5-PB2-OB4
25	h	601	CDL	C51-CB5-OB6-CB4
25	h	602	CDL	CA3-OA5-PA1-OA2
25	h	602	CDL	OA7-CA5-OA6-CA4
25	h	602	CDL	C11-CA5-OA6-CA4
25	h	602	CDL	CB2-OB2-PB2-OB3
25	h	602	CDL	CB2-OB2-PB2-OB4
25	h	602	CDL	CB2-OB2-PB2-OB5
25	j	402	CDL	CA2-OA2-PA1-OA3
25	j	402	CDL	CA2-OA2-PA1-OA4
25	j	402	CDL	CA3-OA5-PA1-OA2
25	j	402	CDL	CA4-CA3-OA5-PA1
25	j	402	CDL	CB2-OB2-PB2-OB3
25	j	402	CDL	CB2-OB2-PB2-OB5
25	k	602	CDL	CA2-OA2-PA1-OA3
25	k	602	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
25	k	602	CDL	CA2-OA2-PA1-OA5
25	k	602	CDL	CA3-OA5-PA1-OA2
25	k	602	CDL	CA3-OA5-PA1-OA4
25	k	602	CDL	CB2-OB2-PB2-OB3
25	k	602	CDL	CB3-OB5-PB2-OB2
25	k	602	CDL	CB3-OB5-PB2-OB3
26	E	101	PCF	C1-O11-P-O12
26	E	101	PCF	C11-O13-P-O12
26	E	101	PCF	O21-C2-C3-O31
26	H	602	PCF	C1-O11-P-O12
26	a	502	PCF	C1-O11-P-O12
26	a	502	PCF	O13-C11-C12-N
26	w	203	PCF	C1-O11-P-O12
27	J	402	CN5	CC-O13-P-O11
27	J	402	CN5	CC-O13-P-O12
27	J	402	CN5	CC-O13-P-O14
27	J	402	CN5	C1'-O1'-P'-O2'
28	J	404	HEM	C2D-C3D-CAD-CBD
28	J	404	HEM	C4D-C3D-CAD-CBD
28	J	405	HEM	C2D-C3D-CAD-CBD
28	J	405	HEM	C4D-C3D-CAD-CBD
28	j	403	HEM	C2D-C3D-CAD-CBD
28	j	403	HEM	C4D-C3D-CAD-CBD
28	j	404	HEM	C2A-CAA-CBA-CGA
28	j	404	HEM	C2D-C3D-CAD-CBD
28	j	404	HEM	C4D-C3D-CAD-CBD
28	l	401	HEM	C2B-C3B-CAB-CBB
28	l	401	HEM	C4B-C3B-CAB-CBB
29	J	408	UQ6	C12-C11-C9-C8
29	J	408	UQ6	C12-C11-C9-C10
29	j	405	UQ6	C9-C11-C12-C13
29	j	407	UQ6	C20-C19-C21-C22
30	K	601	HEA	C2A-CAA-CBA-CGA
30	K	601	HEA	C13-C14-C15-C26
30	K	601	HEA	C20-C21-C22-C23
30	K	601	HEA	C21-C22-C23-C24
30	K	604	HEA	C1A-C2A-CAA-CBA
30	K	604	HEA	C3A-C2A-CAA-CBA
30	k	603	HEA	C1A-C2A-CAA-CBA
30	k	604	HEA	C2A-CAA-CBA-CGA
30	k	604	HEA	C21-C22-C23-C24
25	K	603	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
25	h	602	CDL	OB9-CB7-OB8-CB6
25	j	402	CDL	OB9-CB7-OB8-CB6
25	k	602	CDL	OB9-CB7-OB8-CB6
30	K	601	HEA	C21-C22-C23-C25
30	k	604	HEA	C21-C22-C23-C25
25	K	603	CDL	C71-CB7-OB8-CB6
25	h	602	CDL	C31-CA7-OA8-CA6
25	k	602	CDL	C71-CB7-OB8-CB6
25	J	403	CDL	OA9-CA7-OA8-CA6
25	L	402	CDL	OA9-CA7-OA8-CA6
25	h	602	CDL	OA9-CA7-OA8-CA6
26	W	203	PCF	O32-C31-O31-C3
26	k	605	PCF	O32-C31-O31-C3
23	j	401	PEF	O4-C10-O2-C2
25	K	603	CDL	OB7-CB5-OB6-CB4
25	h	601	CDL	OB7-CB5-OB6-CB4
25	L	402	CDL	C31-CA7-OA8-CA6
25	h	602	CDL	C71-CB7-OB8-CB6
25	j	402	CDL	C71-CB7-OB8-CB6
26	W	203	PCF	C32-C31-O31-C3
26	k	605	PCF	C32-C31-O31-C3
25	J	403	CDL	C11-CA5-OA6-CA4
25	K	603	CDL	C51-CB5-OB6-CB4
29	J	406	UQ6	C25-C24-C26-C27
29	j	407	UQ6	C25-C24-C26-C27
30	k	603	HEA	C27-C19-C20-C21
29	j	407	UQ6	C18-C19-C21-C22
29	j	407	UQ6	C23-C24-C26-C27
30	k	603	HEA	C18-C19-C20-C21
28	L	401	HEM	C2D-C3D-CAD-CBD
30	k	603	HEA	C2D-C3D-CAD-CBD
25	J	403	CDL	C31-CA7-OA8-CA6
30	K	601	HEA	C17-C18-C19-C27
30	k	604	HEA	C17-C18-C19-C27
30	K	601	HEA	C17-C18-C19-C20
30	k	604	HEA	C17-C18-C19-C20
25	H	601	CDL	OB9-CB7-OB8-CB6
28	L	401	HEM	C4D-C3D-CAD-CBD
30	K	604	HEA	C4D-C3D-CAD-CBD
30	k	603	HEA	C4D-C3D-CAD-CBD
23	C	303	PEF	O4-C10-O2-C2
23	J	409	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
25	C	302	CDL	OB7-CB5-OB6-CB4
25	c	302	CDL	OA7-CA5-OA6-CA4
25	C	302	CDL	O1-C1-CA2-OA2
25	c	302	CDL	O1-C1-CB2-OB2
25	h	601	CDL	O1-C1-CB2-OB2
25	k	602	CDL	C11-CA5-OA6-CA4
25	k	602	CDL	C51-CB5-OB6-CB4
25	H	601	CDL	C71-CB7-OB8-CB6
25	c	302	CDL	C31-CA7-OA8-CA6
29	j	405	UQ6	C30-C29-C31-C32
30	K	604	HEA	C27-C19-C20-C21
29	J	406	UQ6	C23-C24-C26-C27
29	J	406	UQ6	C24-C26-C27-C28
29	j	407	UQ6	C9-C11-C12-C13
29	j	407	UQ6	C24-C26-C27-C28
30	K	601	HEA	C19-C20-C21-C22
30	K	604	HEA	C15-C16-C17-C18
30	K	604	HEA	C19-C20-C21-C22
30	k	603	HEA	C15-C16-C17-C18
30	k	604	HEA	C19-C20-C21-C22
30	k	603	HEA	C3D-CAD-CBD-CGD
25	c	302	CDL	OA9-CA7-OA8-CA6
25	k	602	CDL	OA7-CA5-OA6-CA4
25	k	602	CDL	OB7-CB5-OB6-CB4
25	C	302	CDL	CB2-C1-CA2-OA2
25	J	403	CDL	CA2-C1-CB2-OB2
25	L	402	CDL	C71-CB7-OB8-CB6
29	j	405	UQ6	C28-C29-C31-C32
30	K	604	HEA	C18-C19-C20-C21
25	J	403	CDL	O1-C1-CB2-OB2
25	L	402	CDL	O1-C1-CB2-OB2
25	L	402	CDL	OB9-CB7-OB8-CB6
23	J	407	PEF	O2-C2-C3-O3
23	j	406	PEF	O2-C2-C3-O3
25	L	402	CDL	OB6-CB4-CB6-OB8
29	J	406	UQ6	C9-C11-C12-C13
29	J	406	UQ6	C19-C21-C22-C23
29	j	405	UQ6	C19-C21-C22-C23
30	k	603	HEA	C19-C20-C21-C22
23	c	304	PEF	C10-C11-C12-C13
25	c	302	CDL	C51-CB5-OB6-CB4
26	w	203	PCF	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
23	J	409	PEF	C30-C31-C32-C33
25	J	403	CDL	CB7-C71-C72-C73
25	h	601	CDL	CB5-C51-C52-C53
25	h	602	CDL	O1-C1-CA2-OA2
25	j	402	CDL	O1-C1-CB2-OB2
25	H	601	CDL	C51-CB5-OB6-CB4
23	A	501	PEF	C30-C31-C32-C33
25	H	601	CDL	OB7-CB5-OB6-CB4
25	c	302	CDL	OB7-CB5-OB6-CB4
25	L	402	CDL	CA2-C1-CB2-OB2
25	c	302	CDL	CA2-C1-CB2-OB2
25	h	602	CDL	CB2-C1-CA2-OA2
26	H	602	PCF	C11-C12-N-C14
26	H	602	PCF	C11-C12-N-C15
26	W	203	PCF	C11-C12-N-C13
26	W	203	PCF	C11-C12-N-C14
26	W	203	PCF	C11-C12-N-C15
26	k	605	PCF	C11-C12-N-C15
26	w	203	PCF	C11-C12-N-C13
26	w	203	PCF	C11-C12-N-C14
26	w	203	PCF	C11-C12-N-C15
25	j	402	CDL	C51-CB5-OB6-CB4
25	j	402	CDL	OB7-CB5-OB6-CB4
23	e	101	PEF	C10-C11-C12-C13
30	k	604	HEA	C15-C16-C17-C18
25	H	601	CDL	O1-C1-CA2-OA2
27	J	402	CN5	O1'-C1'-C2'-C3'
26	H	602	PCF	C2-C1-O11-P
30	K	604	HEA	C2D-C3D-CAD-CBD
28	J	404	HEM	C3D-CAD-CBD-CGD
26	H	602	PCF	C11-C12-N-C13
26	k	605	PCF	C11-C12-N-C13
26	k	605	PCF	C11-C12-N-C14
23	j	406	PEF	C31-C32-C33-C34
23	j	408	PEF	C11-C12-C13-C14
26	E	101	PCF	C33-C34-C35-C36
28	J	405	HEM	C2A-CAA-CBA-CGA
23	C	304	PEF	C10-C11-C12-C13
23	J	409	PEF	C11-C12-C13-C14
23	W	202	PEF	C19-C20-C21-C22
23	j	401	PEF	C13-C14-C15-C16
28	L	401	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
23	w	202	PEF	C19-C20-C21-C22
25	K	603	CDL	C33-C34-C35-C36
25	k	602	CDL	C33-C34-C35-C36
26	H	602	PCF	C34-C35-C36-C37
30	K	601	HEA	C14-C15-C16-C17
25	k	602	CDL	CA5-C11-C12-C13
26	H	602	PCF	C31-C32-C33-C34
26	w	203	PCF	C22-C23-C24-C25
23	c	303	PEF	C12-C13-C14-C15
23	j	406	PEF	C11-C12-C13-C14
25	j	402	CDL	C52-C53-C54-C55
23	J	401	PEF	C11-C10-O2-C2
23	c	304	PEF	C11-C10-O2-C2
23	v	101	PEF	C11-C10-O2-C2
25	C	302	CDL	C11-CA5-OA6-CA4
25	L	402	CDL	C51-CB5-OB6-CB4
25	C	302	CDL	CB7-C71-C72-C73
30	k	603	HEA	C3A-C2A-CAA-CBA
28	L	401	HEM	C2B-C3B-CAB-CBB
23	J	401	PEF	C16-C17-C18-C19
26	w	203	PCF	C25-C26-C27-C28
25	C	302	CDL	OA5-CA3-CA4-OA6
25	h	602	CDL	C11-C12-C13-C14
26	H	602	PCF	C27-C28-C29-C30
26	H	602	PCF	C25-C26-C27-C28
25	K	603	CDL	CB5-C51-C52-C53
23	J	401	PEF	O2-C2-C3-O3
23	w	201	PEF	O2-C2-C3-O3
25	J	403	CDL	OB6-CB4-CB6-OB8
25	h	601	CDL	OA6-CA4-CA6-OA8
23	j	406	PEF	C18-C19-C20-C21
26	E	101	PCF	C2-C1-O11-P
23	a	503	PEF	C11-C12-C13-C14
23	c	304	PEF	O4-C10-O2-C2
23	v	101	PEF	O4-C10-O2-C2
25	K	603	CDL	CA2-C1-CB2-OB2
25	c	302	CDL	CB2-C1-CA2-OA2
28	J	404	HEM	C2A-CAA-CBA-CGA
23	E	102	PEF	C11-C10-O2-C2
23	C	303	PEF	O3P-C1-C2-C3
23	W	201	PEF	O3P-C1-C2-C3
23	j	406	PEF	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	C	302	CDL	OA5-CA3-CA4-CA6
26	a	502	PCF	O11-C1-C2-C3
26	w	203	PCF	O11-C1-C2-C3
23	J	407	PEF	C35-C36-C37-C38
25	L	402	CDL	C53-C54-C55-C56
23	A	501	PEF	C12-C13-C14-C15
23	j	401	PEF	C12-C13-C14-C15
23	j	408	PEF	C10-C11-C12-C13
23	W	201	PEF	C1-C2-C3-O3
23	a	501	PEF	C1-C2-C3-O3
23	a	504	PEF	C1-C2-C3-O3
23	j	406	PEF	C1-C2-C3-O3
25	h	601	CDL	CA3-CA4-CA6-OA8
25	j	402	CDL	CB3-CB4-CB6-OB8
26	E	101	PCF	C1-C2-C3-O31
26	W	203	PCF	C23-C24-C25-C26
25	C	302	CDL	O1-C1-CB2-OB2
25	K	603	CDL	CA7-C31-C32-C33
23	J	401	PEF	C30-C31-C32-C33
26	w	203	PCF	C31-C32-C33-C34
29	J	406	UQ6	C30-C29-C31-C32
25	L	402	CDL	OB7-CB5-OB6-CB4
23	E	102	PEF	C3-C2-O2-C10
25	k	602	CDL	CA6-CA4-OA6-CA5
23	j	406	PEF	C32-C33-C34-C35
26	w	203	PCF	C34-C35-C36-C37
25	h	602	CDL	C52-C53-C54-C55
25	j	402	CDL	CA2-C1-CB2-OB2
23	E	102	PEF	O3P-C1-C2-O2
25	J	403	CDL	OA5-CA3-CA4-OA6
26	a	502	PCF	O11-C1-C2-O21
23	a	503	PEF	C30-C31-C32-C33
26	w	203	PCF	C27-C28-C29-C30
23	j	401	PEF	C40-C41-C42-C43
30	k	604	HEA	C20-C21-C22-C23
26	H	602	PCF	C24-C25-C26-C27
25	K	603	CDL	C12-C13-C14-C15
25	K	603	CDL	C52-C53-C54-C55
30	K	604	HEA	C3B-C11-C12-C13
23	V	101	PEF	C31-C32-C33-C34
23	a	503	PEF	C32-C33-C34-C35
23	J	401	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
25	C	302	CDL	OA7-CA5-OA6-CA4
25	H	601	CDL	CA4-CA3-OA5-PA1
25	h	602	CDL	C1-CB2-OB2-PB2
25	k	602	CDL	C52-C53-C54-C55
23	E	102	PEF	O3P-C1-C2-C3
23	J	407	PEF	O3P-C1-C2-C3
23	V	101	PEF	O3P-C1-C2-C3
23	c	303	PEF	O3P-C1-C2-C3
23	j	408	PEF	O3P-C1-C2-C3
23	v	101	PEF	O3P-C1-C2-C3
25	L	402	CDL	OB5-CB3-CB4-CB6
25	c	302	CDL	OB5-CB3-CB4-CB6
25	j	402	CDL	OB5-CB3-CB4-CB6
23	J	409	PEF	C10-C11-C12-C13
25	K	603	CDL	CB7-C71-C72-C73
23	w	201	PEF	C37-C38-C39-C40
25	k	602	CDL	C31-C32-C33-C34
26	a	502	PCF	C21-C22-C23-C24
23	J	401	PEF	C41-C42-C43-C44
25	H	601	CDL	CB2-C1-CA2-OA2
25	k	602	CDL	CA2-C1-CB2-OB2
25	C	302	CDL	C31-CA7-OA8-CA6
23	J	409	PEF	C12-C13-C14-C15
23	J	401	PEF	C1-C2-C3-O3
23	J	407	PEF	C1-C2-C3-O3
23	J	409	PEF	C1-C2-C3-O3
23	w	201	PEF	C1-C2-C3-O3
25	L	402	CDL	CB3-CB4-CB6-OB8
25	h	601	CDL	CB3-CB4-CB6-OB8
23	e	101	PEF	C14-C15-C16-C17
23	c	303	PEF	C30-C31-C32-C33
25	k	602	CDL	C54-C55-C56-C57
29	J	406	UQ6	C20-C19-C21-C22
26	w	203	PCF	C26-C27-C28-C29
23	C	303	PEF	O3P-C1-C2-O2
23	C	304	PEF	O3P-C1-C2-O2
23	W	201	PEF	O3P-C1-C2-O2
23	W	202	PEF	O3P-C1-C2-O2
23	c	303	PEF	O3P-C1-C2-O2
23	j	401	PEF	O3P-C1-C2-O2
23	j	406	PEF	O3P-C1-C2-O2
23	j	408	PEF	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
23	v	101	PEF	O3P-C1-C2-O2
23	w	202	PEF	O3P-C1-C2-O2
25	L	402	CDL	OA5-CA3-CA4-OA6
25	c	302	CDL	OB5-CB3-CB4-OB6
25	h	602	CDL	OB5-CB3-CB4-OB6
25	j	402	CDL	OB5-CB3-CB4-OB6
23	a	504	PEF	C34-C35-C36-C37
23	j	406	PEF	C10-C11-C12-C13
28	j	403	HEM	C3D-CAD-CBD-CGD
23	J	409	PEF	O2-C2-C3-O3
25	h	602	CDL	OA6-CA4-CA6-OA8
25	j	402	CDL	OB6-CB4-CB6-OB8
23	E	102	PEF	O4-C10-O2-C2
26	E	101	PCF	C21-C22-C23-C24
23	A	503	PEF	C33-C34-C35-C36
23	A	503	PEF	C36-C37-C38-C39
29	j	405	UQ6	C25-C24-C26-C27
25	C	302	CDL	OB5-CB3-CB4-CB6
25	H	601	CDL	OA5-CA3-CA4-CA6
25	h	602	CDL	OB5-CB3-CB4-CB6
25	J	403	CDL	C1-CA2-OA2-PA1
25	k	602	CDL	CB7-C71-C72-C73
23	W	201	PEF	C35-C36-C37-C38
28	j	403	HEM	C2B-C3B-CAB-CBB
23	a	501	PEF	C1-C2-O2-C10
23	e	101	PEF	C3-C2-O2-C10
25	H	601	CDL	CA3-CA4-OA6-CA5
25	K	603	CDL	CA6-CA4-OA6-CA5
25	K	603	CDL	CB6-CB4-OB6-CB5
25	c	302	CDL	CA3-CA4-OA6-CA5
25	h	601	CDL	CA3-CA4-OA6-CA5
26	a	502	PCF	C26-C27-C28-C29
23	V	101	PEF	O3P-C1-C2-O2
23	e	101	PEF	O3P-C1-C2-O2
23	w	201	PEF	O3P-C1-C2-O2
25	C	302	CDL	OB5-CB3-CB4-OB6
25	L	402	CDL	OB5-CB3-CB4-OB6
25	C	302	CDL	OA9-CA7-OA8-CA6
23	A	501	PEF	C1-C2-C3-O3
23	A	503	PEF	C1-C2-C3-O3
23	v	101	PEF	C1-C2-C3-O3
25	C	302	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
25	H	601	CDL	CB3-CB4-CB6-OB8
25	h	602	CDL	CA3-CA4-CA6-OA8
25	k	602	CDL	CA3-CA4-CA6-OA8
30	K	601	HEA	C15-C16-C17-C18
25	h	601	CDL	CB7-C71-C72-C73
28	j	403	HEM	C4B-C3B-CAB-CBB
30	K	601	HEA	O11-C11-C12-C13
30	K	604	HEA	O11-C11-C12-C13
30	k	604	HEA	O11-C11-C12-C13
29	j	405	UQ6	C23-C24-C26-C27
26	k	605	PCF	C23-C24-C25-C26
23	a	504	PEF	O2-C2-C3-O3
25	h	601	CDL	OB6-CB4-CB6-OB8
25	k	602	CDL	OA6-CA4-CA6-OA8
23	J	407	PEF	C16-C17-C18-C19
25	H	601	CDL	CB5-C51-C52-C53
23	j	408	PEF	C13-C14-C15-C16
23	E	102	PEF	C2-C1-O3P-P
23	E	102	PEF	C16-C17-C18-C19
26	E	101	PCF	O13-C11-C12-N
26	H	602	PCF	O13-C11-C12-N
26	W	203	PCF	O13-C11-C12-N
26	k	605	PCF	O13-C11-C12-N
26	w	203	PCF	O13-C11-C12-N
25	h	601	CDL	CA2-C1-CB2-OB2
23	A	501	PEF	C15-C16-C17-C18
27	J	402	CN5	C32-C31-O31-C3
23	w	201	PEF	C31-C32-C33-C34
23	C	304	PEF	C31-C30-O3-C3
29	j	407	UQ6	C12-C11-C9-C10
23	C	304	PEF	O3P-C1-C2-C3
23	J	401	PEF	O3P-C1-C2-C3
23	W	202	PEF	O3P-C1-C2-C3
23	a	501	PEF	O3P-C1-C2-C3
23	c	304	PEF	O3P-C1-C2-C3
23	e	101	PEF	O3P-C1-C2-C3
23	w	201	PEF	O3P-C1-C2-C3
23	w	202	PEF	O3P-C1-C2-C3
25	J	403	CDL	OA5-CA3-CA4-CA6
25	L	402	CDL	OA5-CA3-CA4-CA6
25	h	601	CDL	OA5-CA3-CA4-CA6
25	j	402	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
25	K	603	CDL	C32-C33-C34-C35
25	k	602	CDL	C12-C13-C14-C15
23	J	401	PEF	O3P-C1-C2-O2
23	c	304	PEF	O3P-C1-C2-O2
25	H	601	CDL	OA5-CA3-CA4-OA6
25	h	601	CDL	OA5-CA3-CA4-OA6
25	j	402	CDL	OA5-CA3-CA4-OA6
26	w	203	PCF	O11-C1-C2-O21
30	K	604	HEA	C3D-CAD-CBD-CGD
23	w	201	PEF	C32-C33-C34-C35
26	a	502	PCF	C11-C12-N-C15
23	A	502	PEF	C11-C12-C13-C14
26	E	101	PCF	C23-C24-C25-C26
27	J	402	CN5	O32-C31-O31-C3
23	w	202	PEF	C1-C2-C3-O3
25	J	403	CDL	CB3-CB4-CB6-OB8
25	K	603	CDL	CA3-CA4-CA6-OA8
25	h	602	CDL	O1-C1-CB2-OB2
23	C	304	PEF	O5-C30-O3-C3
23	A	503	PEF	C32-C33-C34-C35
23	J	401	PEF	C14-C15-C16-C17
23	A	503	PEF	C4-O4P-P-O2P
23	V	101	PEF	C4-O4P-P-O1P
23	W	201	PEF	C1-O3P-P-O1P
23	W	202	PEF	C1-O3P-P-O1P
23	W	202	PEF	C4-O4P-P-O1P
23	a	504	PEF	C4-O4P-P-O2P
23	c	304	PEF	C4-O4P-P-O1P
23	j	401	PEF	C4-O4P-P-O1P
23	j	406	PEF	C1-O3P-P-O1P
23	j	406	PEF	C1-O3P-P-O4P
23	w	201	PEF	C1-O3P-P-O1P
23	w	202	PEF	C1-O3P-P-O1P
25	H	601	CDL	CA2-OA2-PA1-OA3
25	H	601	CDL	CA3-OA5-PA1-OA2
25	H	601	CDL	CA3-OA5-PA1-OA4
25	K	603	CDL	CA2-OA2-PA1-OA4
25	K	603	CDL	CB2-OB2-PB2-OB4
25	L	402	CDL	CA2-OA2-PA1-OA4
25	L	402	CDL	CB2-OB2-PB2-OB3
25	L	402	CDL	CB3-OB5-PB2-OB2
25	h	601	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
25	h	602	CDL	CA3-OA5-PA1-OA3
25	j	402	CDL	CA2-OA2-PA1-OA5
25	j	402	CDL	CA3-OA5-PA1-OA3
25	j	402	CDL	CB2-OB2-PB2-OB4
26	E	101	PCF	C11-O13-P-O11
30	K	604	HEA	C11-C12-C13-C14
30	k	603	HEA	C11-C12-C13-C14
23	j	401	PEF	C35-C36-C37-C38
29	J	406	UQ6	C28-C29-C31-C32
25	C	302	CDL	C1-CA2-OA2-PA1
25	J	403	CDL	CA4-CA3-OA5-PA1
25	c	302	CDL	C1-CA2-OA2-PA1
25	c	302	CDL	C1-CB2-OB2-PB2
25	h	601	CDL	CA4-CA3-OA5-PA1
25	h	602	CDL	CB4-CB3-OB5-PB2
23	j	401	PEF	C30-C31-C32-C33
25	k	602	CDL	CB5-C51-C52-C53
25	L	402	CDL	CB5-C51-C52-C53
23	a	501	PEF	C13-C14-C15-C16
23	J	407	PEF	C3-C2-O2-C10
23	V	101	PEF	C3-C2-O2-C10
23	v	101	PEF	C3-C2-O2-C10
25	J	403	CDL	CA3-CA4-OA6-CA5
25	k	602	CDL	CB6-CB4-OB6-CB5
23	j	406	PEF	C35-C36-C37-C38
29	j	405	UQ6	C14-C16-C17-C18
26	a	502	PCF	C11-C12-N-C13
23	j	401	PEF	O3P-C1-C2-C3
26	H	602	PCF	O11-C1-C2-C3
25	K	603	CDL	C34-C35-C36-C37
23	a	501	PEF	O3P-C1-C2-O2
23	c	303	PEF	C10-C11-C12-C13
23	J	407	PEF	C18-C19-C20-C21
23	J	401	PEF	C11-C12-C13-C14
23	A	503	PEF	O2-C2-C3-O3
25	J	403	CDL	OA6-CA4-CA6-OA8
25	K	603	CDL	OA6-CA4-CA6-OA8
23	c	304	PEF	C31-C30-O3-C3
23	A	501	PEF	C31-C32-C33-C34
26	H	602	PCF	C26-C27-C28-C29
25	C	302	CDL	C72-C73-C74-C75
25	H	601	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	C	304	PEF	C2-C1-O3P-P
25	k	602	CDL	CA4-CA3-OA5-PA1
23	J	407	PEF	C13-C14-C15-C16
23	c	304	PEF	O5-C30-O3-C3
25	L	402	CDL	CB7-C71-C72-C73
28	L	401	HEM	C4B-C3B-CAB-CBB
25	H	601	CDL	C36-C37-C38-C39
25	K	603	CDL	O1-C1-CB2-OB2
25	L	402	CDL	O1-C1-CA2-OA2
26	a	502	PCF	C22-C23-C24-C25
29	J	406	UQ6	C15-C14-C16-C17
23	J	407	PEF	C12-C13-C14-C15
25	h	602	CDL	C1-CA2-OA2-PA1
26	W	203	PCF	C24-C25-C26-C27
30	k	604	HEA	CAA-CBA-CGA-O1A
26	a	502	PCF	C24-C25-C26-C27
25	C	302	CDL	CA2-C1-CB2-OB2
26	a	502	PCF	C34-C35-C36-C37
23	W	202	PEF	C1-C2-C3-O3
29	j	407	UQ6	C29-C31-C32-C33
23	c	304	PEF	C11-C12-C13-C14
25	k	602	CDL	C52-C51-CB5-OB6
23	C	303	PEF	C1-C2-O2-C10
23	j	406	PEF	C30-C31-C32-C33
30	K	604	HEA	C14-C15-C16-C17
23	a	503	PEF	C12-C13-C14-C15
26	a	502	PCF	C11-C12-N-C14
26	W	203	PCF	C21-C22-C23-C24
23	C	304	PEF	C30-C31-C32-C33
28	l	401	HEM	CAA-CBA-CGA-O2A
23	e	101	PEF	C2-C1-O3P-P
25	c	302	CDL	CA4-CA3-OA5-PA1
27	J	402	CN5	CB-CC-O13-P
23	a	501	PEF	C30-C31-C32-C33
28	J	405	HEM	CAA-CBA-CGA-O1A
23	A	503	PEF	O3P-C1-C2-C3
30	K	601	HEA	CAA-CBA-CGA-O2A
30	k	603	HEA	CAA-CBA-CGA-O1A
23	J	401	PEF	C32-C33-C34-C35
23	A	501	PEF	C34-C35-C36-C37
23	W	202	PEF	C20-C21-C22-C23
28	j	404	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	J	406	UQ6	C18-C19-C21-C22
30	k	603	HEA	C14-C15-C16-C17
30	K	604	HEA	CAA-CBA-CGA-O1A
25	h	601	CDL	CA5-C11-C12-C13
28	j	403	HEM	CAD-CBD-CGD-O1D
28	j	404	HEM	CAA-CBA-CGA-O1A
30	K	601	HEA	CAA-CBA-CGA-O1A
30	k	603	HEA	C26-C15-C16-C17
30	k	604	HEA	CAD-CBD-CGD-O2D
23	a	504	PEF	C2-C1-O3P-P
23	c	304	PEF	C2-C1-O3P-P
25	C	302	CDL	CB4-CB3-OB5-PB2
29	j	407	UQ6	C12-C11-C9-C8
23	j	406	PEF	C12-C13-C14-C15
26	w	203	PCF	C30-C47-C48-C49
28	J	405	HEM	CAA-CBA-CGA-O2A
23	V	101	PEF	C1-C2-C3-O3
25	J	403	CDL	CA3-CA4-CA6-OA8
25	j	402	CDL	O1-C1-CA2-OA2
23	V	101	PEF	O4-C10-O2-C2
26	H	602	PCF	O11-C1-C2-O21
25	c	302	CDL	C52-C51-CB5-OB6
25	L	402	CDL	C31-C32-C33-C34
26	W	203	PCF	C22-C23-C24-C25
25	h	602	CDL	C74-C75-C76-C77
30	k	603	HEA	CAA-CBA-CGA-O2A
28	j	404	HEM	CAD-CBD-CGD-O2D
25	J	403	CDL	C52-C53-C54-C55
25	H	601	CDL	OB5-CB3-CB4-CB6
26	E	101	PCF	O11-C1-C2-C3
23	c	303	PEF	O2-C2-C3-O3
23	J	401	PEF	C40-C41-C42-C43
25	J	403	CDL	C53-C54-C55-C56
23	j	401	PEF	C33-C34-C35-C36
23	C	304	PEF	C15-C16-C17-C18
30	k	604	HEA	C27-C19-C20-C21
28	j	403	HEM	CAA-CBA-CGA-O2A
28	l	401	HEM	CAD-CBD-CGD-O2D
25	k	602	CDL	C34-C35-C36-C37
23	a	503	PEF	C1-C2-C3-O3
30	k	604	HEA	CAA-CBA-CGA-O2A
23	W	201	PEF	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	a	502	PCF	C38-C39-C40-C41
28	L	401	HEM	CAD-CBD-CGD-O1D
25	h	601	CDL	C72-C71-CB7-OB8
25	K	603	CDL	C55-C56-C57-C58
30	K	604	HEA	CAA-CBA-CGA-O2A
25	J	403	CDL	C32-C31-CA7-OA8
23	V	101	PEF	C11-C10-O2-C2
30	K	601	HEA	C3B-C11-C12-C13
23	J	401	PEF	C35-C36-C37-C38
25	k	602	CDL	O1-C1-CB2-OB2
28	j	403	HEM	CAD-CBD-CGD-O2D
23	c	303	PEF	O4-C10-O2-C2
23	A	501	PEF	O3P-C1-C2-O2
29	J	406	UQ6	C13-C14-C16-C17
30	k	604	HEA	CAD-CBD-CGD-O1D
23	C	303	PEF	O2-C10-C11-C12
25	K	603	CDL	C61-C62-C63-C64
23	C	303	PEF	O2-C2-C3-O3
30	K	604	HEA	CAD-CBD-CGD-O2D
25	h	602	CDL	C52-C51-CB5-OB6
25	H	601	CDL	CB7-C71-C72-C73
23	A	503	PEF	C15-C16-C17-C18
23	W	202	PEF	C35-C36-C37-C38
23	J	409	PEF	C1-C2-O2-C10
25	J	403	CDL	CA6-CA4-OA6-CA5
26	H	602	PCF	C48-C49-C50-C51
26	E	101	PCF	C40-C41-C42-C43
23	J	407	PEF	C2-C1-O3P-P
23	a	503	PEF	C2-C1-O3P-P
25	L	402	CDL	C52-C53-C54-C55
25	K	603	CDL	C62-C63-C64-C65
25	h	602	CDL	C52-C51-CB5-OB7
23	C	303	PEF	C12-C13-C14-C15
23	C	303	PEF	O4-C10-C11-C12
25	h	601	CDL	C72-C71-CB7-OB9
23	v	101	PEF	C31-C32-C33-C34
28	j	403	HEM	C3A-C2A-CAA-CBA
23	w	201	PEF	O4-C10-O2-C2
23	w	202	PEF	O2-C2-C3-O3
25	L	402	CDL	OA6-CA4-CA6-OA8
23	A	503	PEF	C34-C35-C36-C37
23	V	101	PEF	C33-C34-C35-C36

Continued on next page...

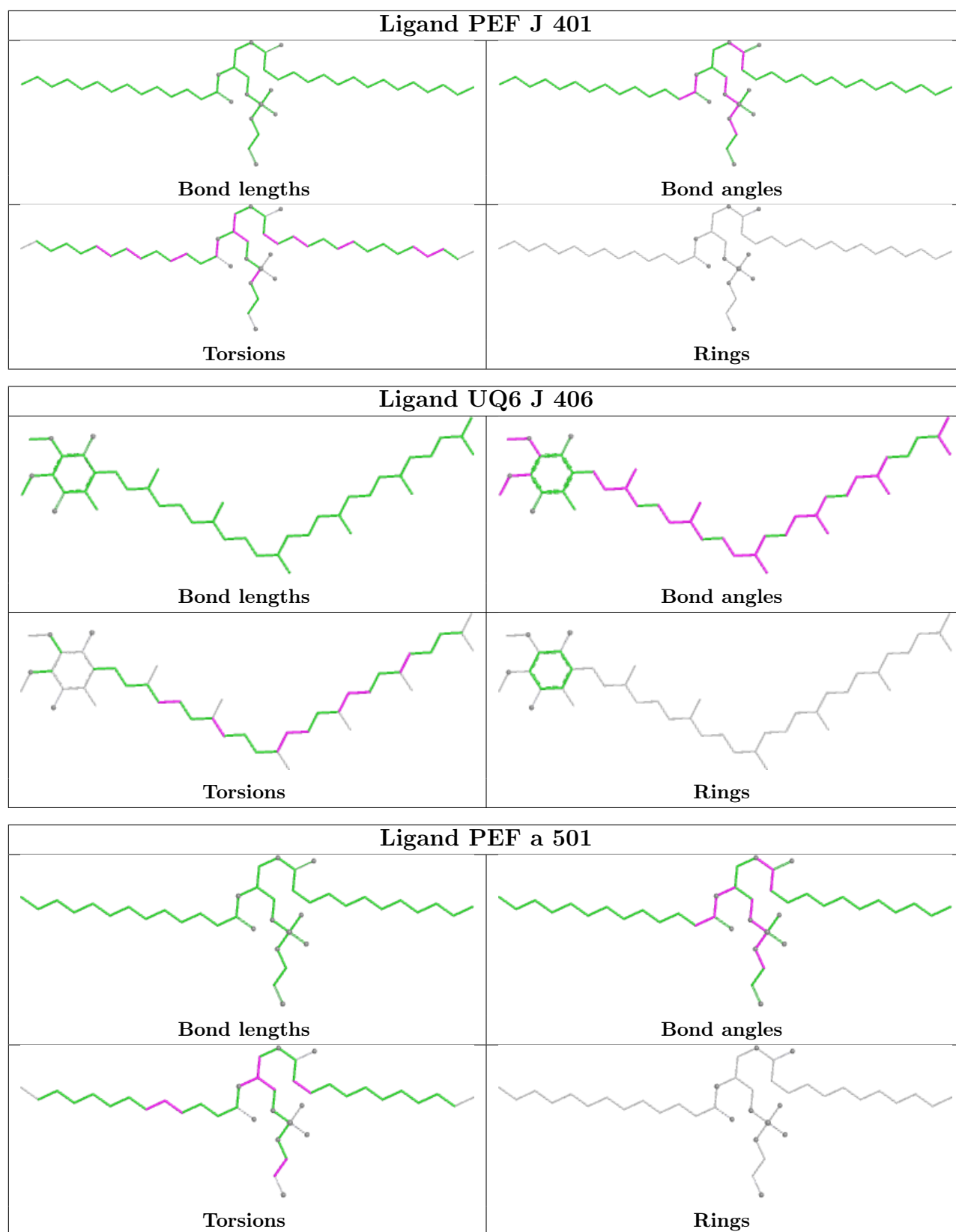
Continued from previous page...

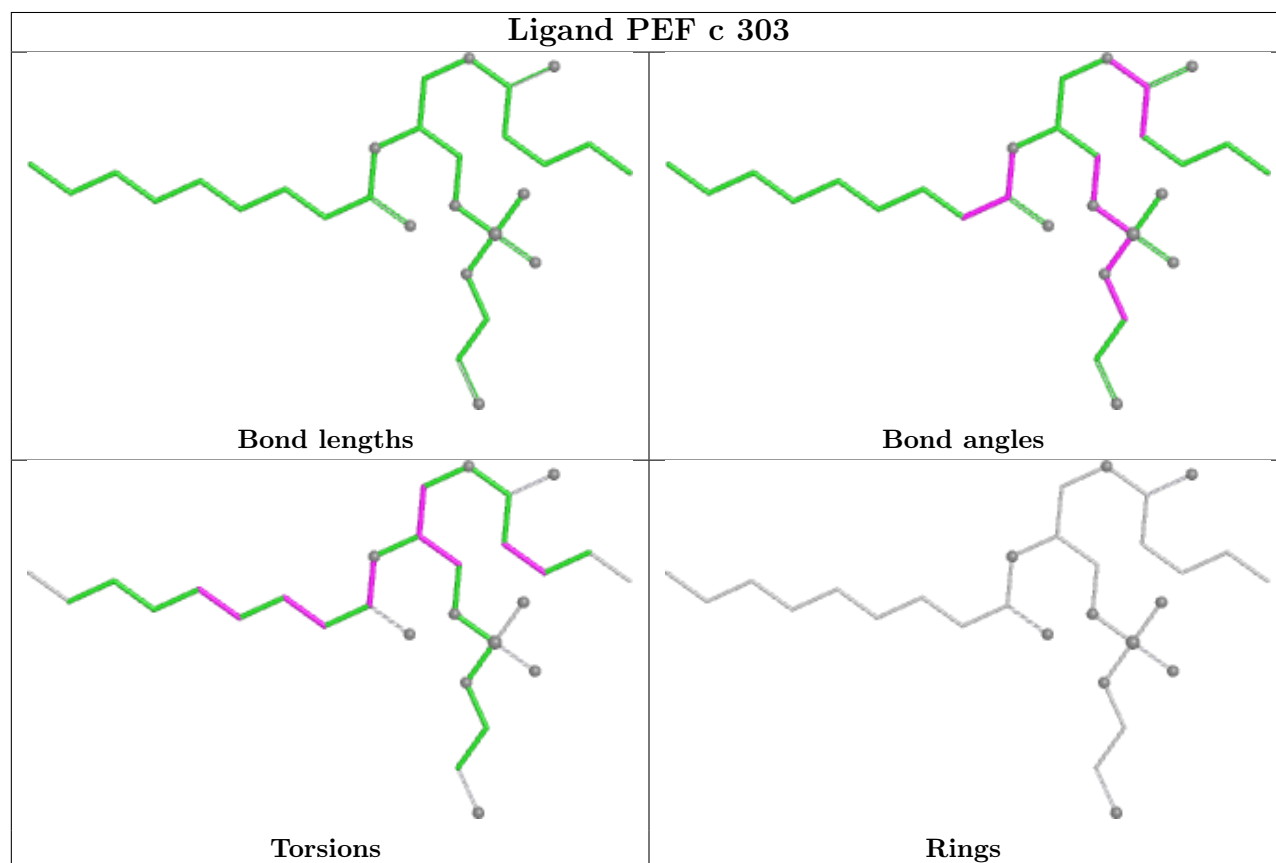
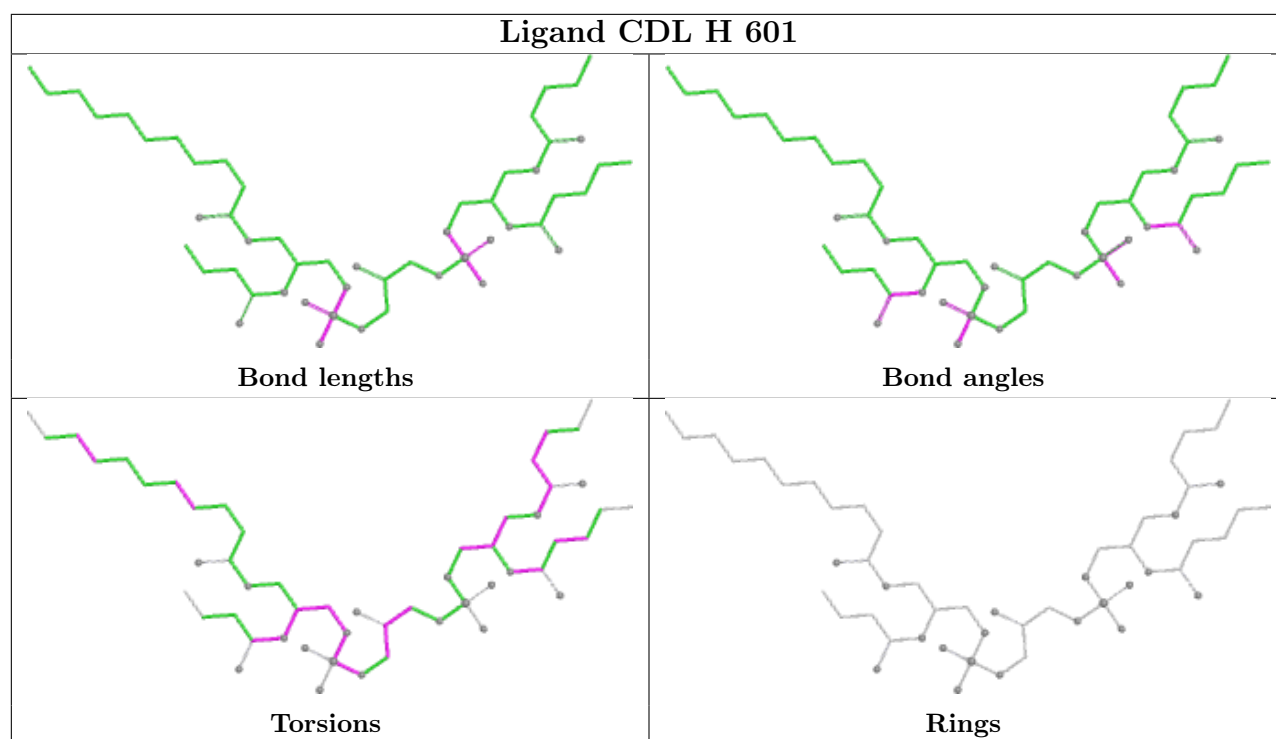
Mol	Chain	Res	Type	Atoms
25	J	403	CDL	C11-C12-C13-C14
25	H	601	CDL	C72-C71-CB7-OB8
25	K	603	CDL	C52-C51-CB5-OB6
23	a	501	PEF	C12-C13-C14-C15
26	H	602	PCF	C1-C2-C3-O31
28	J	405	HEM	CAD-CBD-CGD-O2D
25	L	402	CDL	C72-C71-CB7-OB8
28	J	405	HEM	CAD-CBD-CGD-O1D
25	h	601	CDL	CA7-C31-C32-C33
25	k	602	CDL	C12-C11-CA5-OA6
25	k	602	CDL	C72-C71-CB7-OB8
28	j	403	HEM	C1A-C2A-CAA-CBA
23	c	303	PEF	C11-C10-O2-C2
23	w	201	PEF	C11-C10-O2-C2
25	K	603	CDL	C72-C71-CB7-OB8
28	J	404	HEM	CAD-CBD-CGD-O1D
30	k	603	HEA	CAD-CBD-CGD-O1D

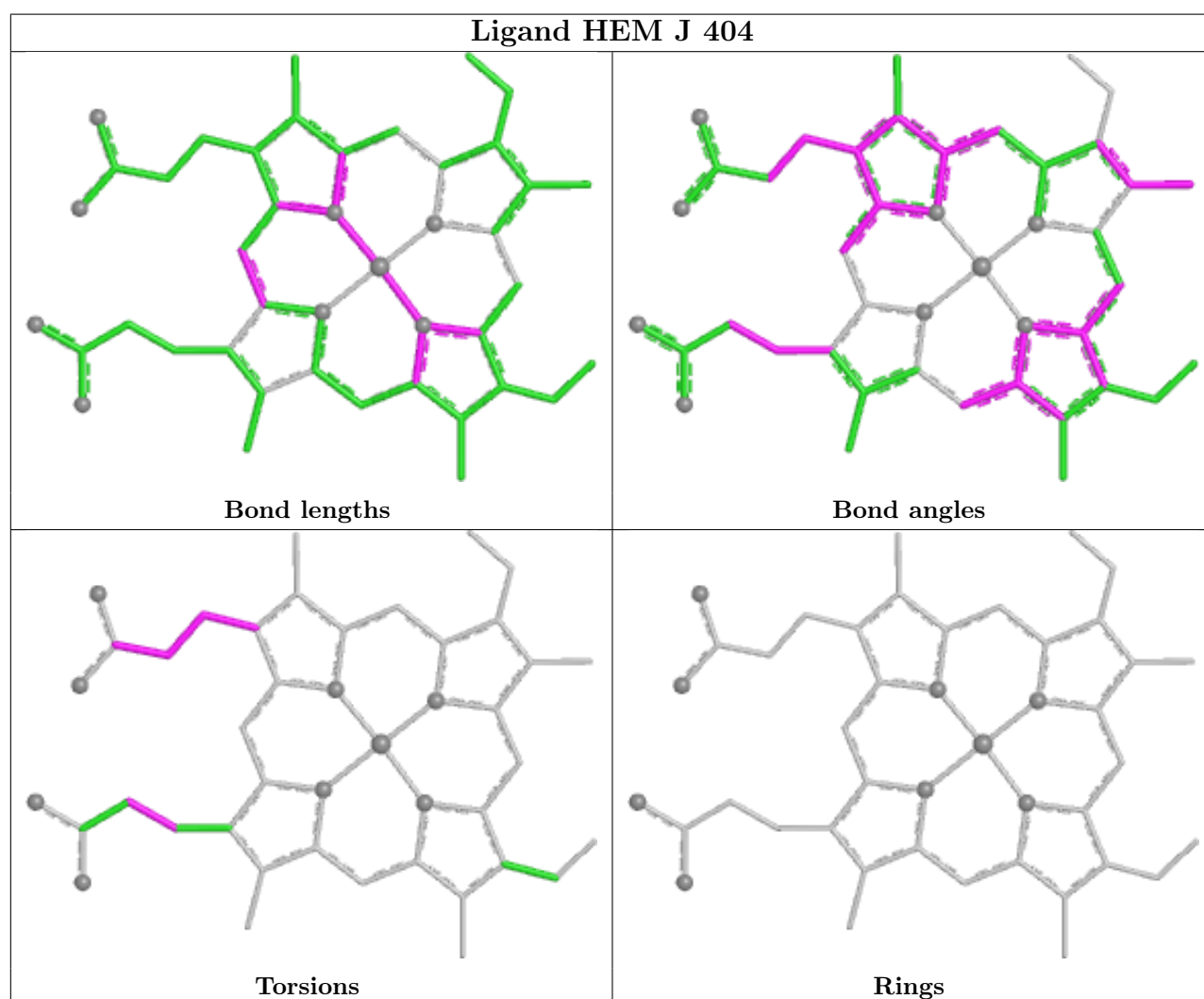
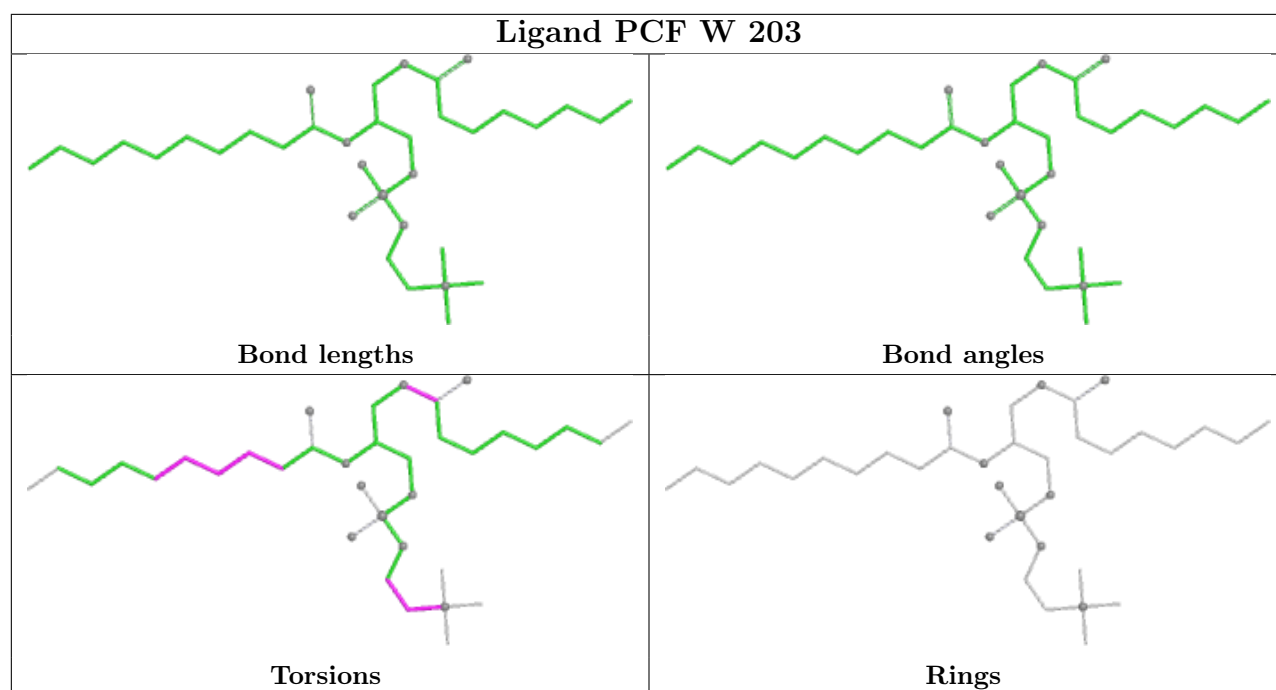
There are no ring outliers.

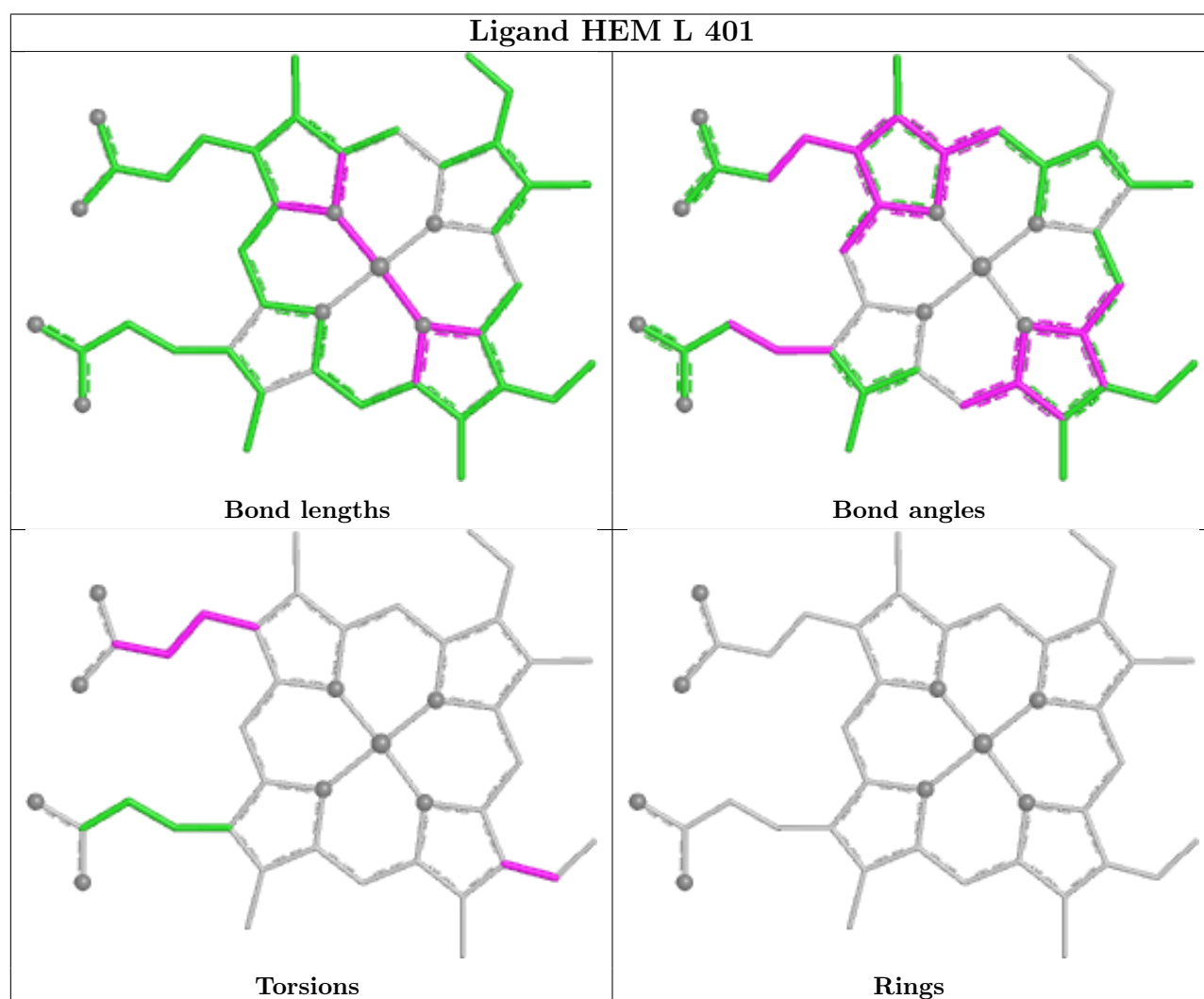
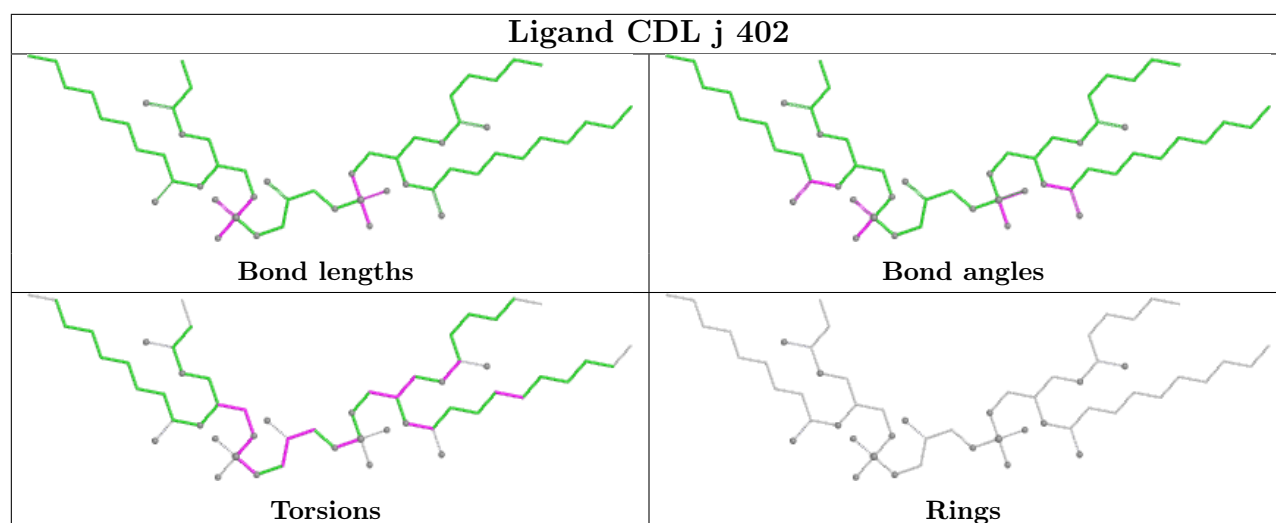
No monomer is involved in short contacts.

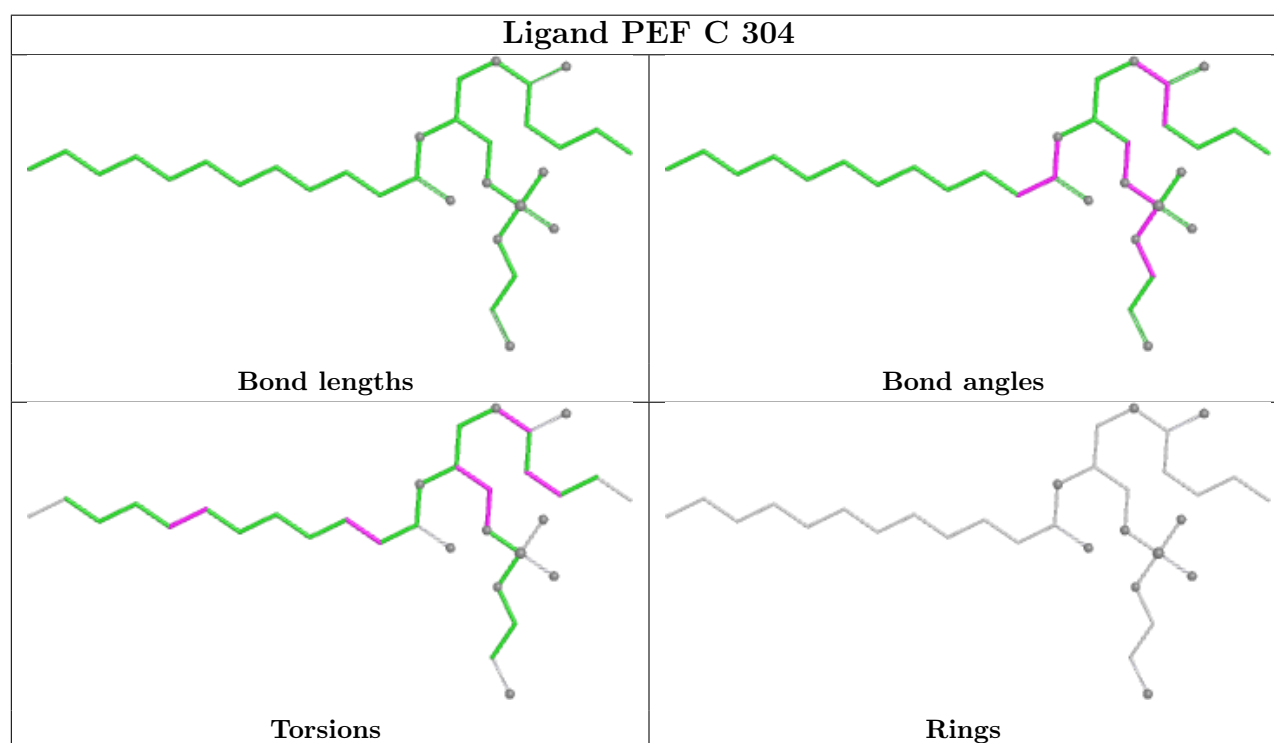
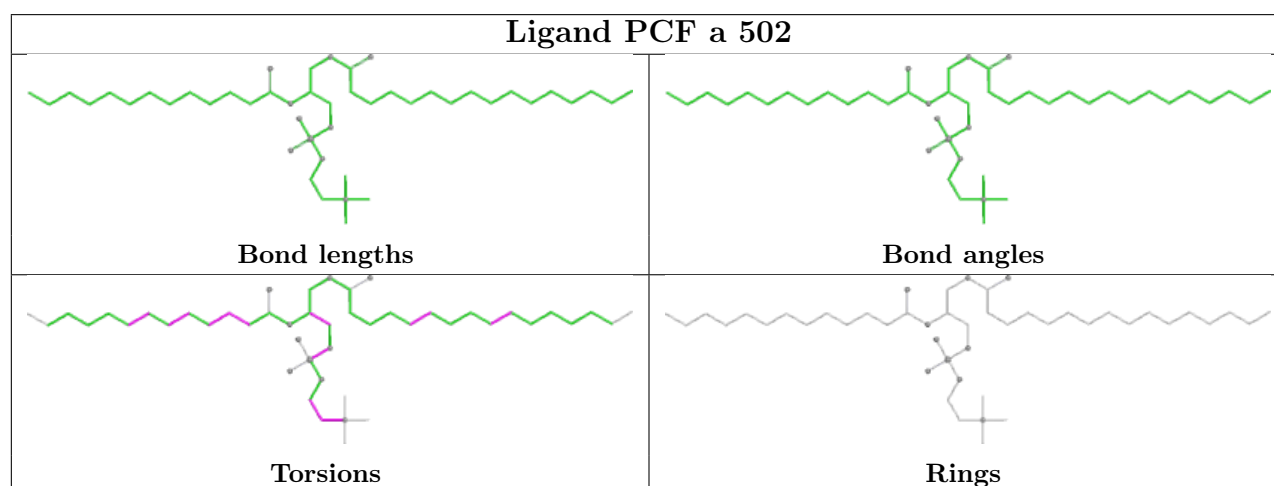
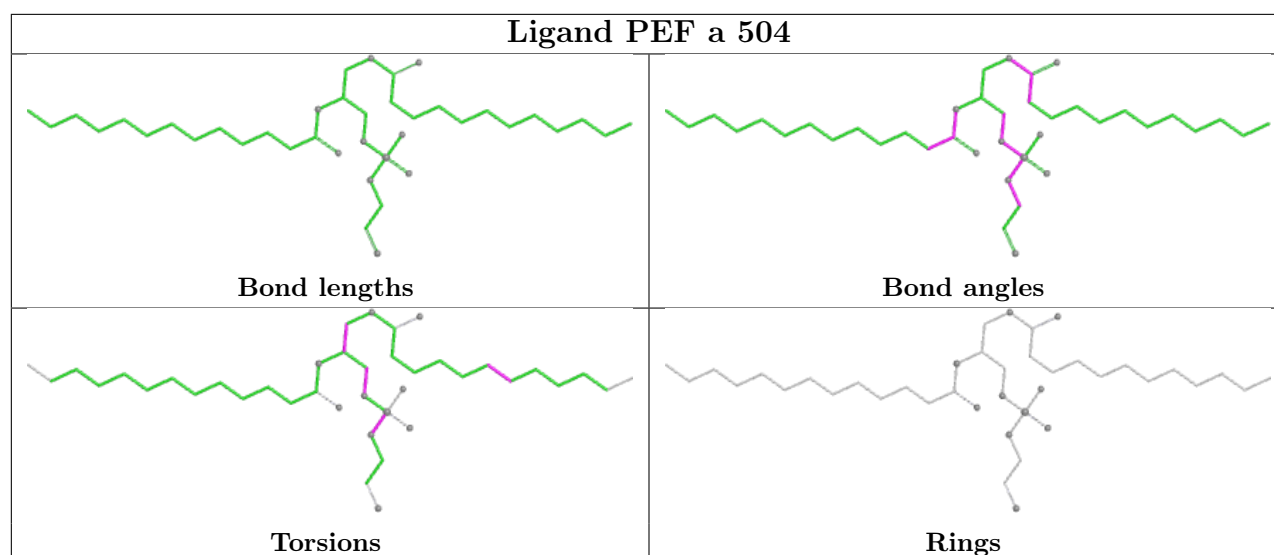
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

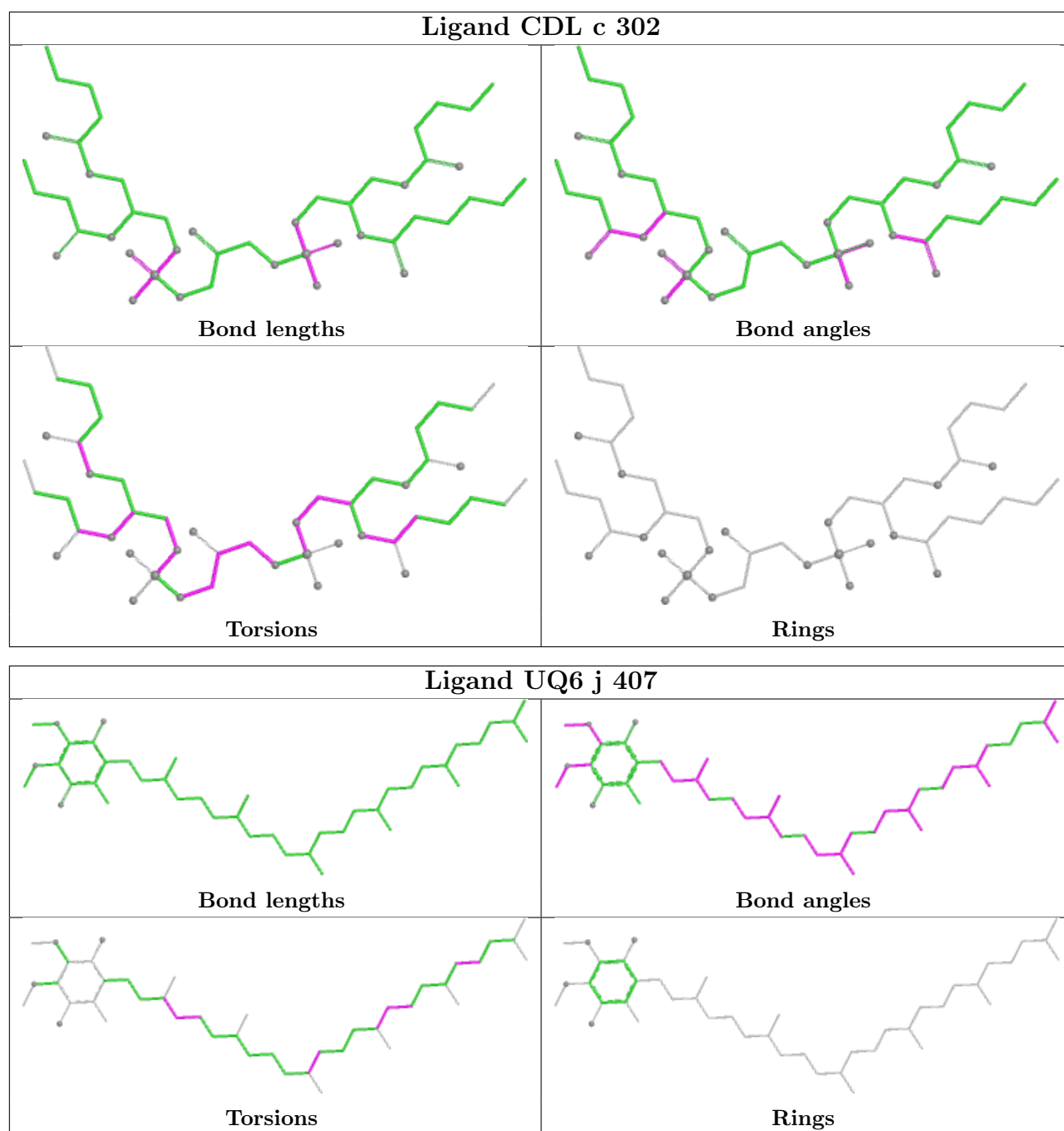


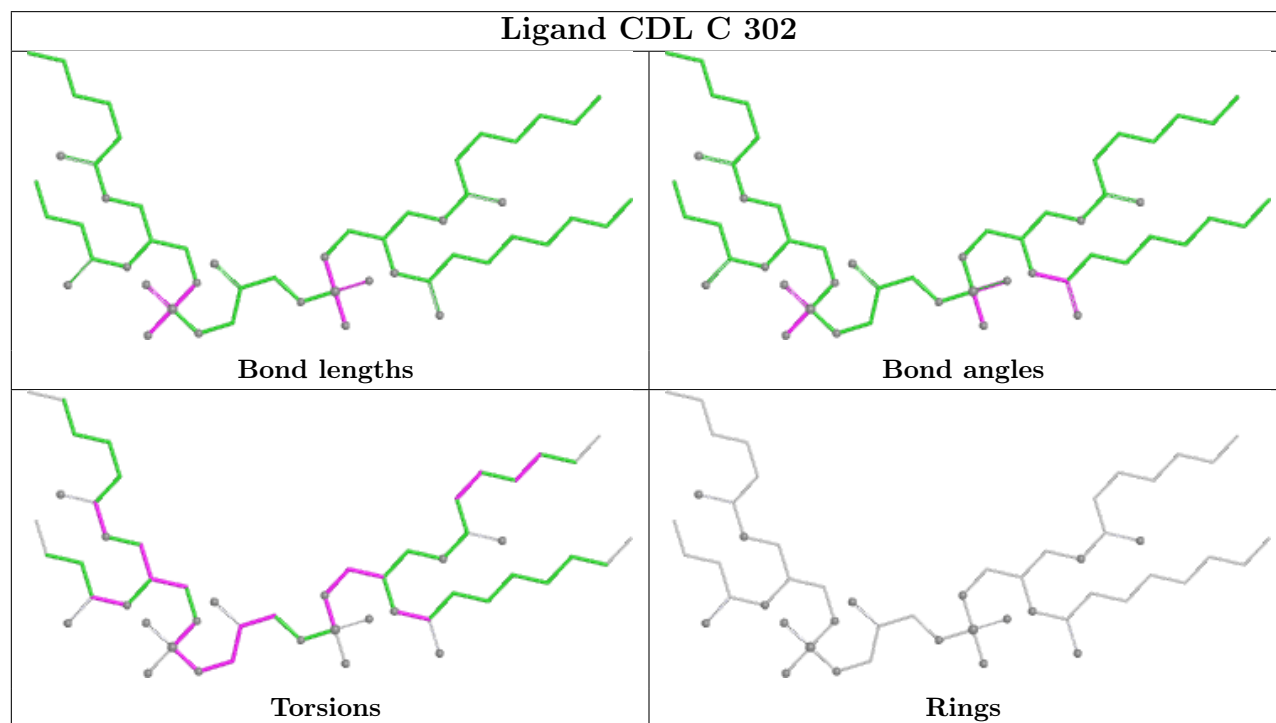
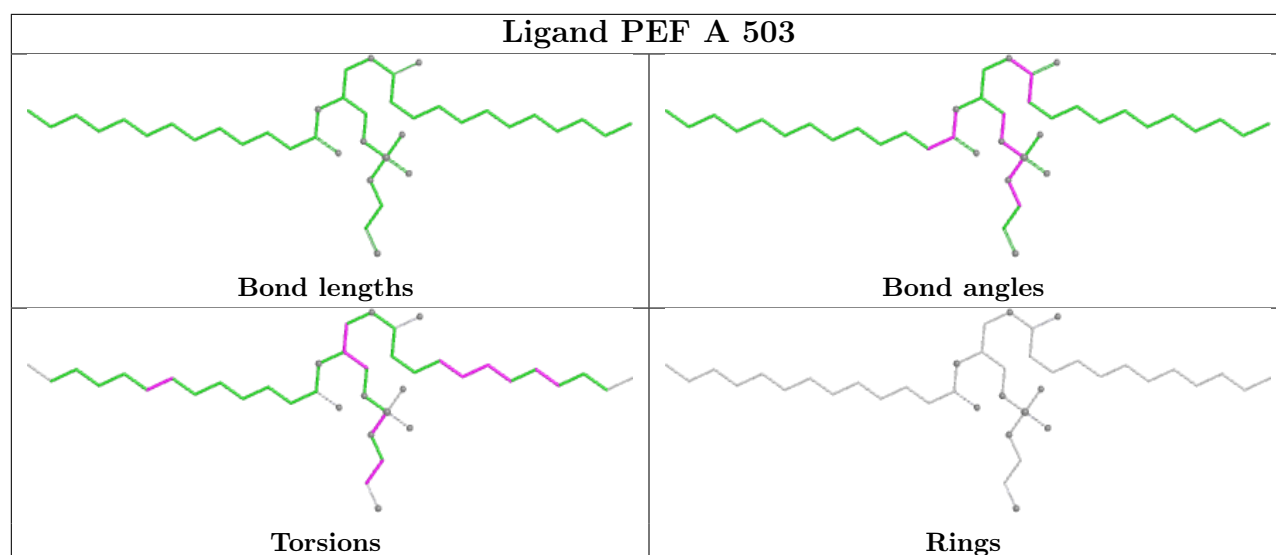


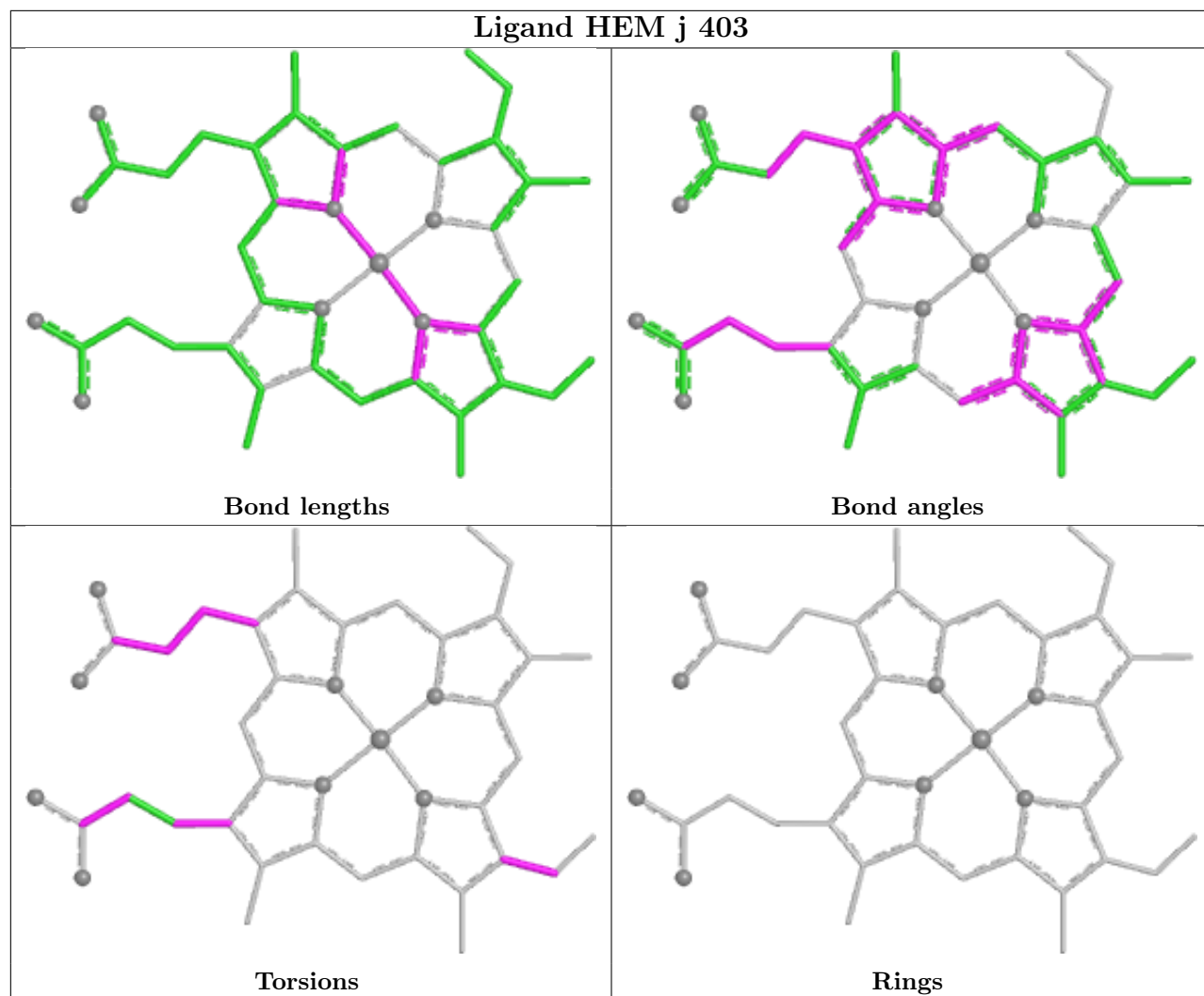


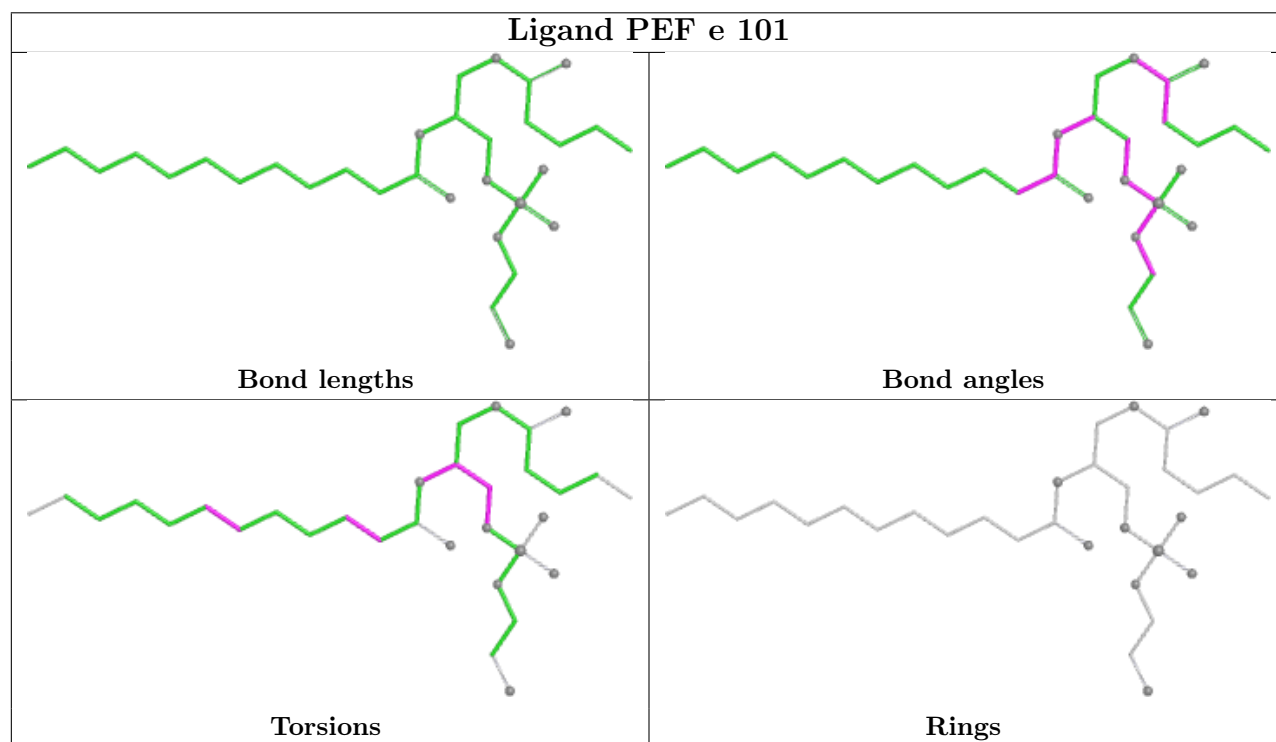
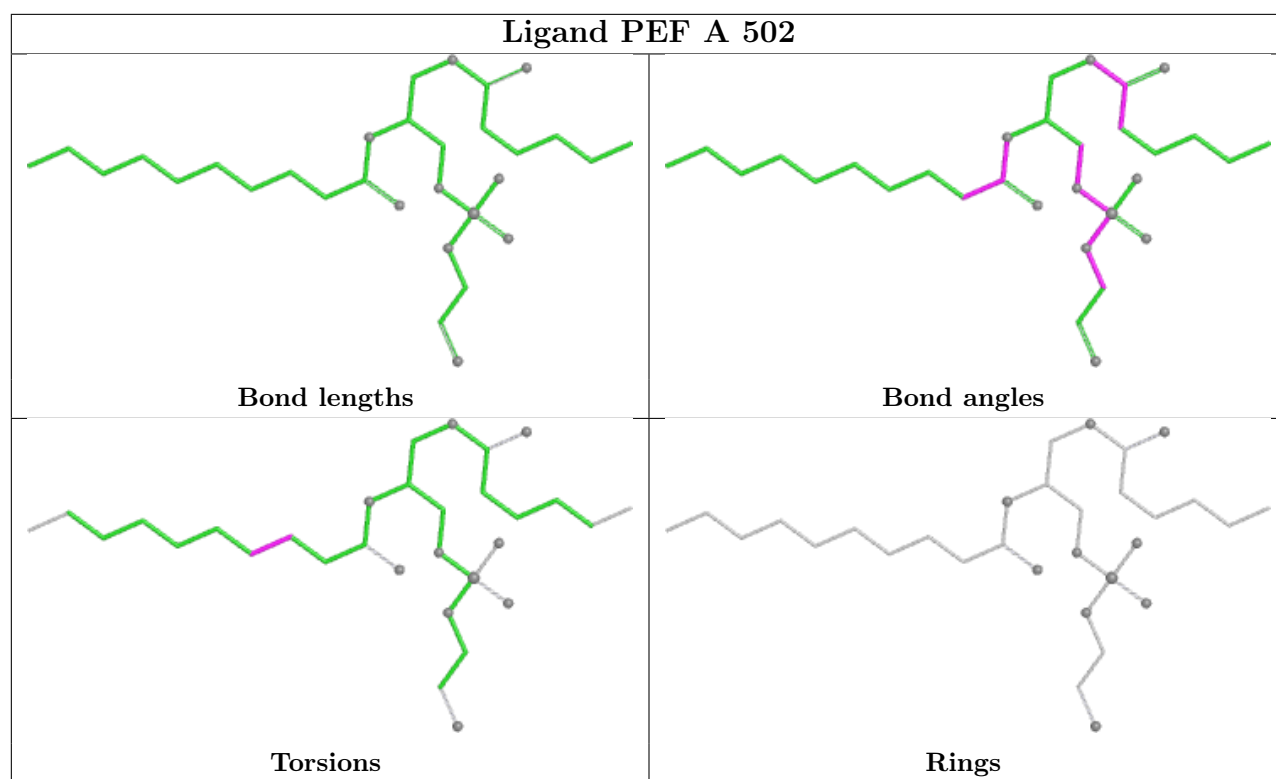


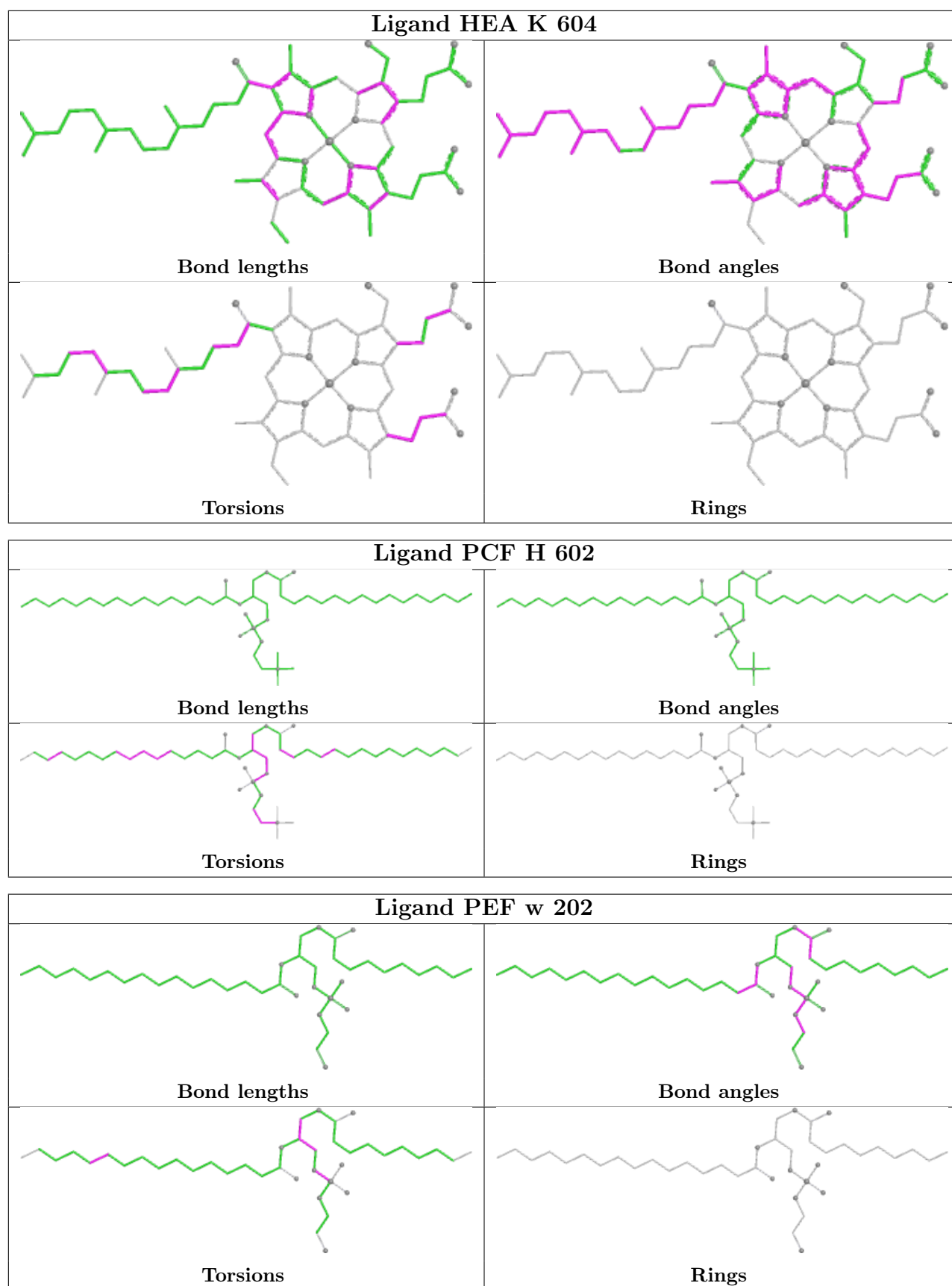


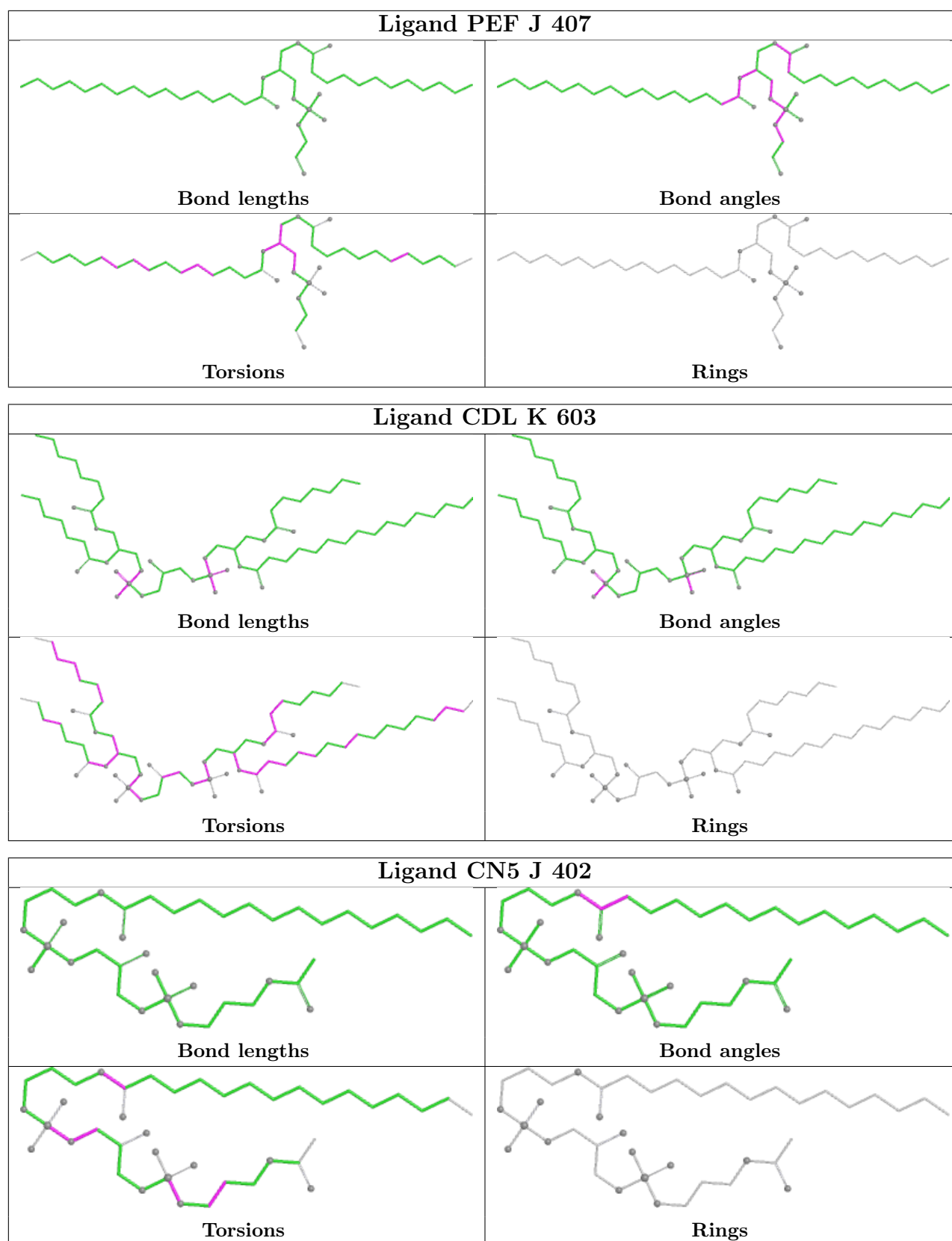


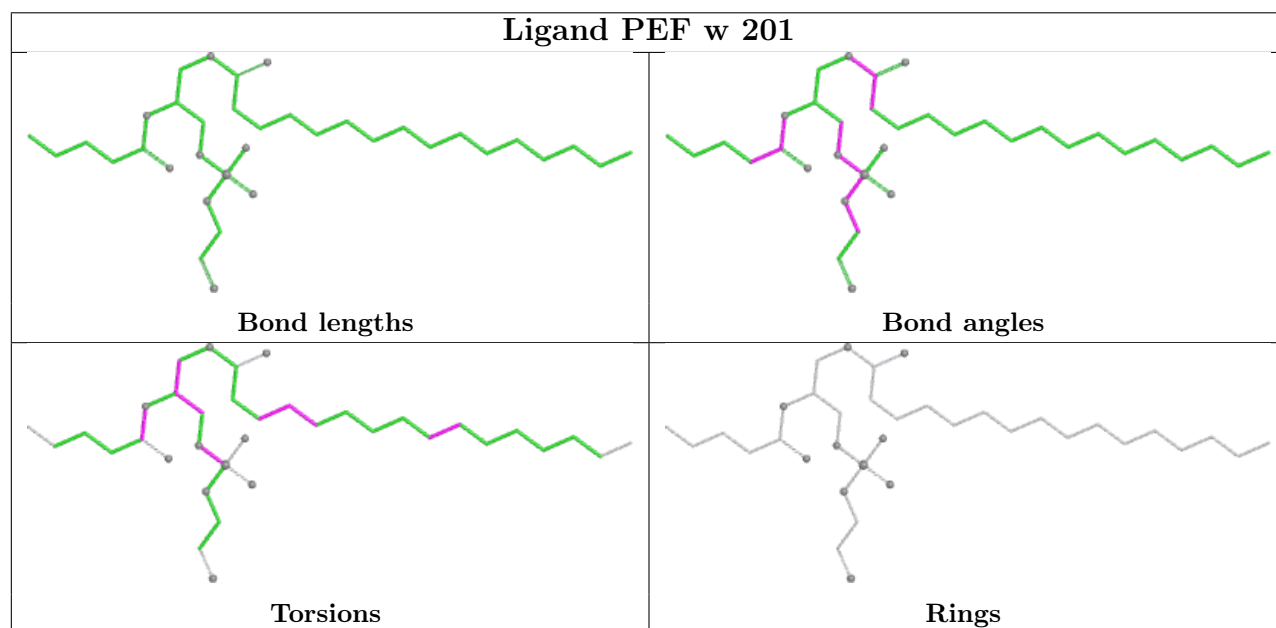
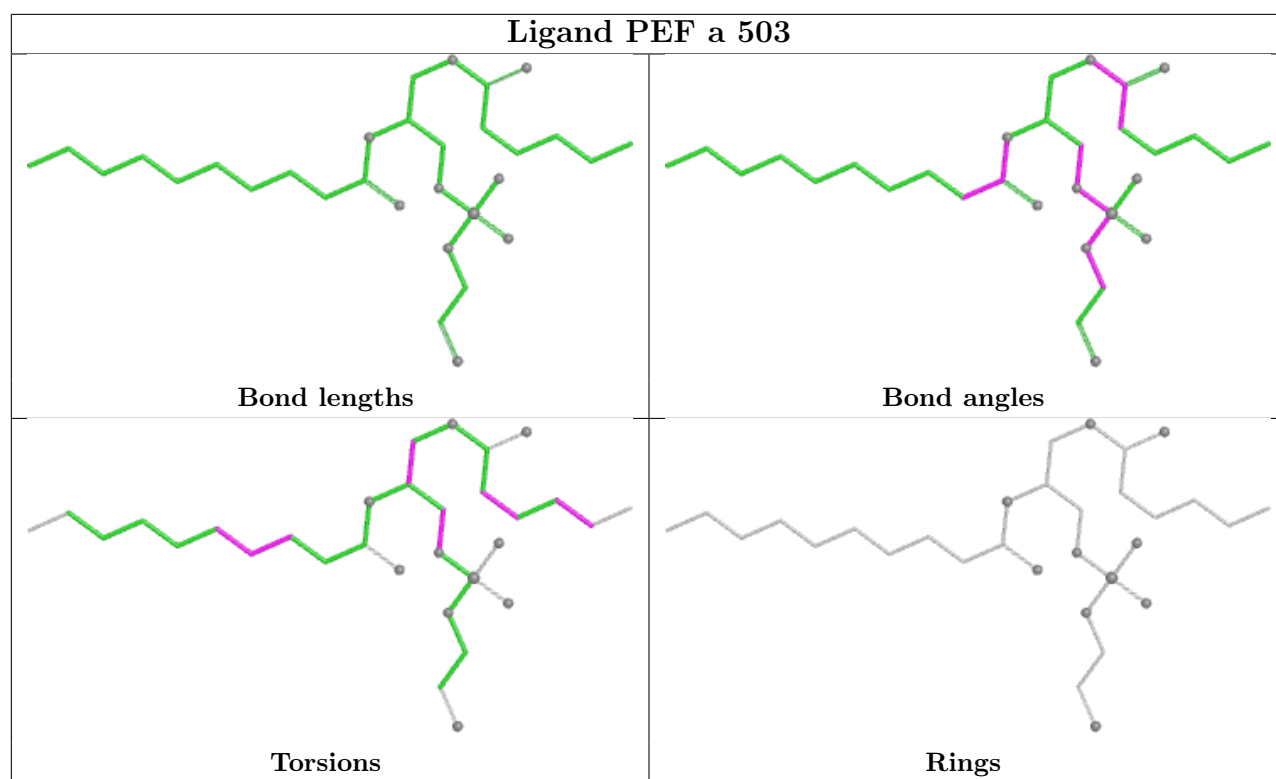


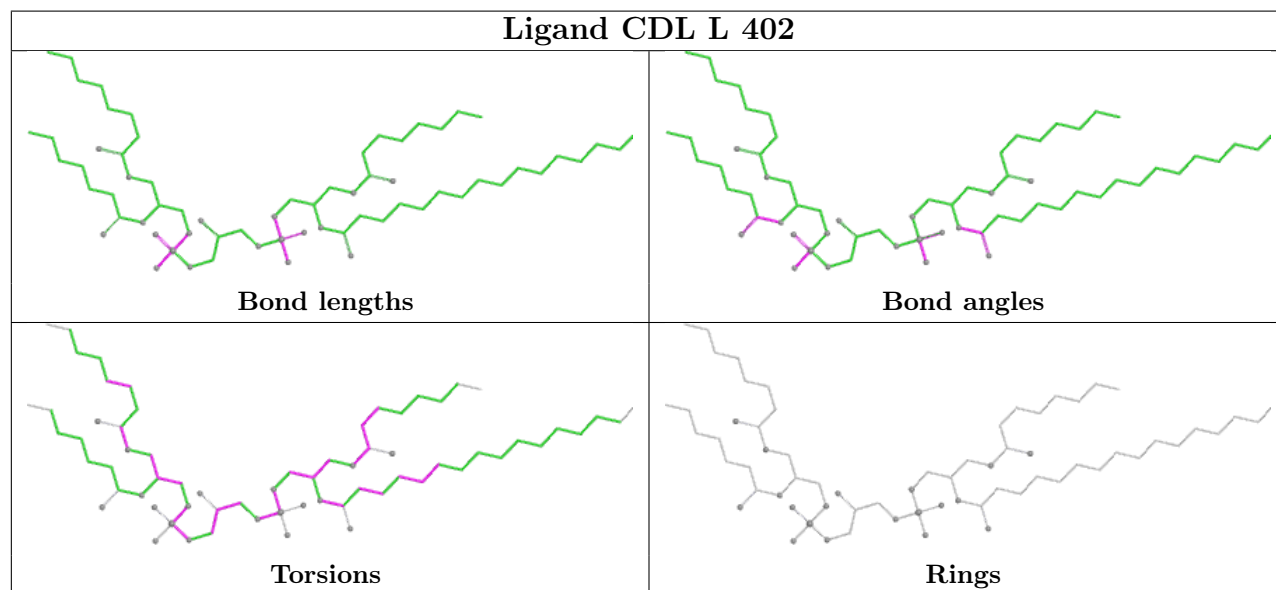
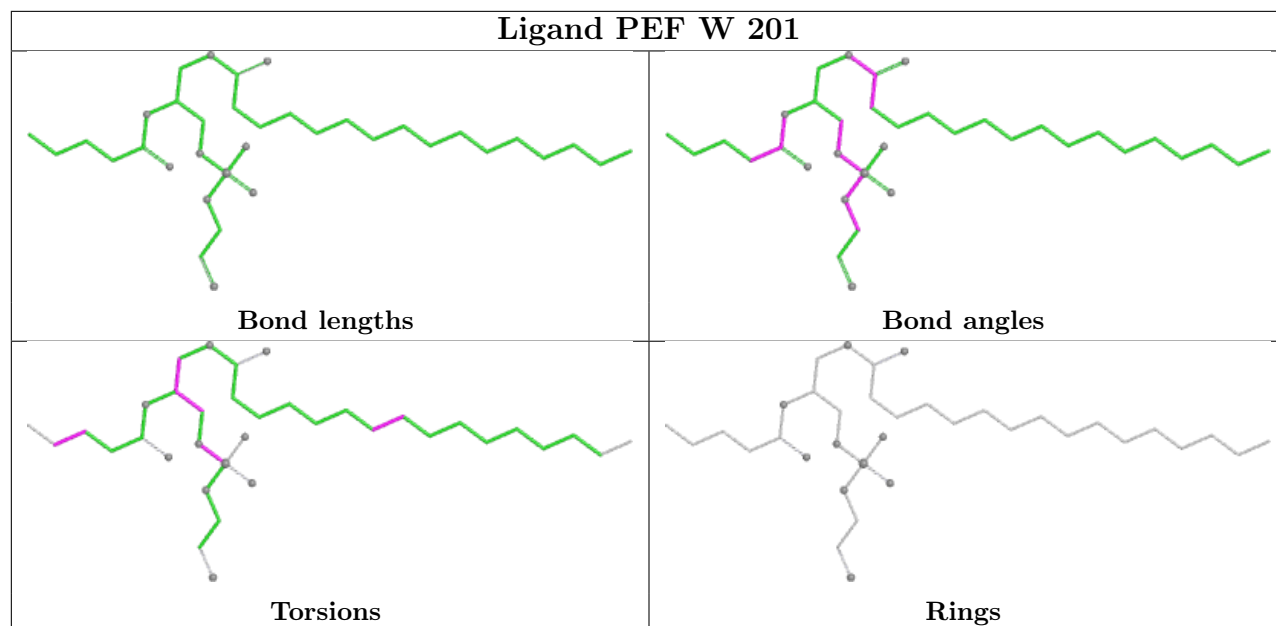


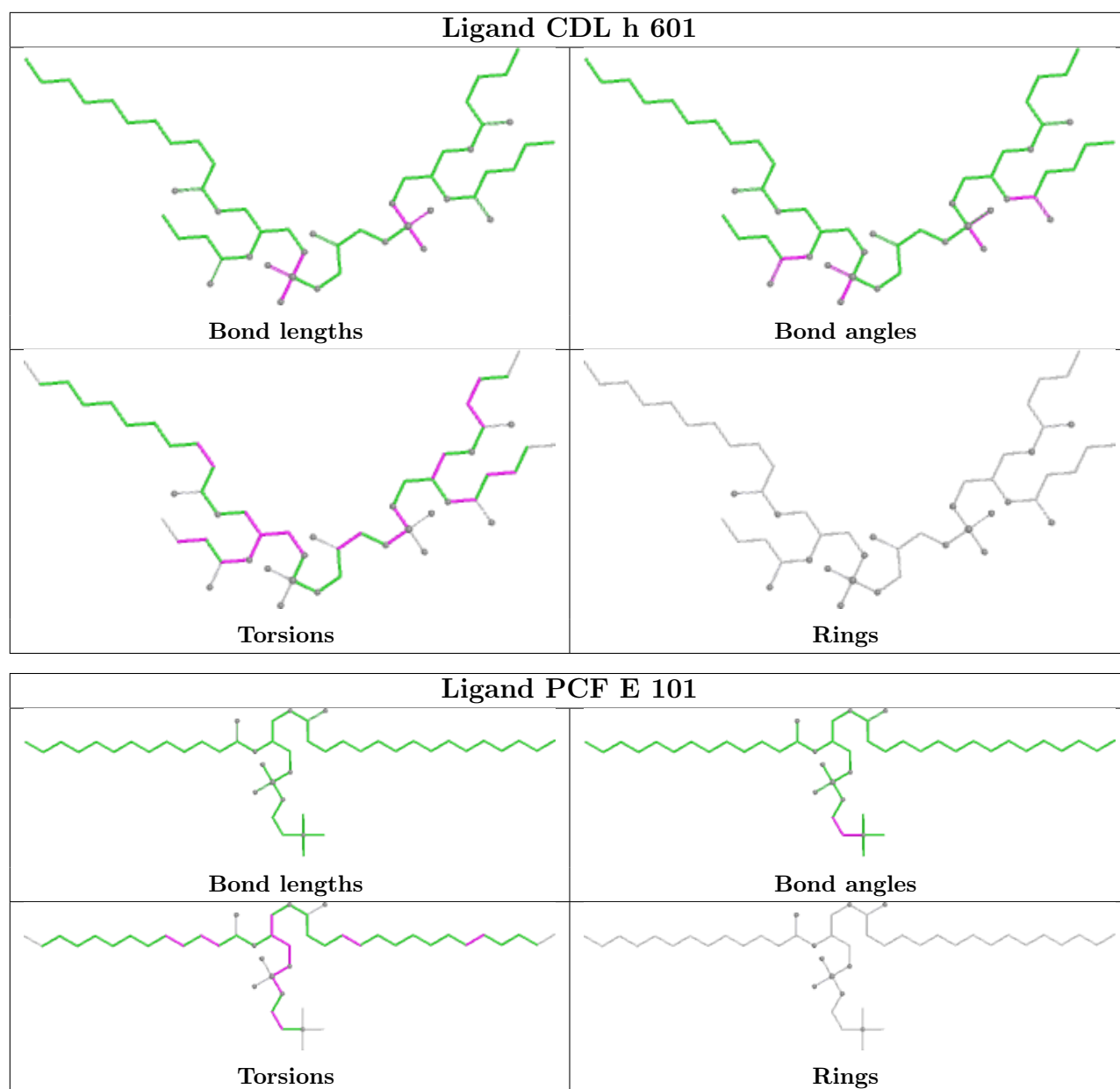


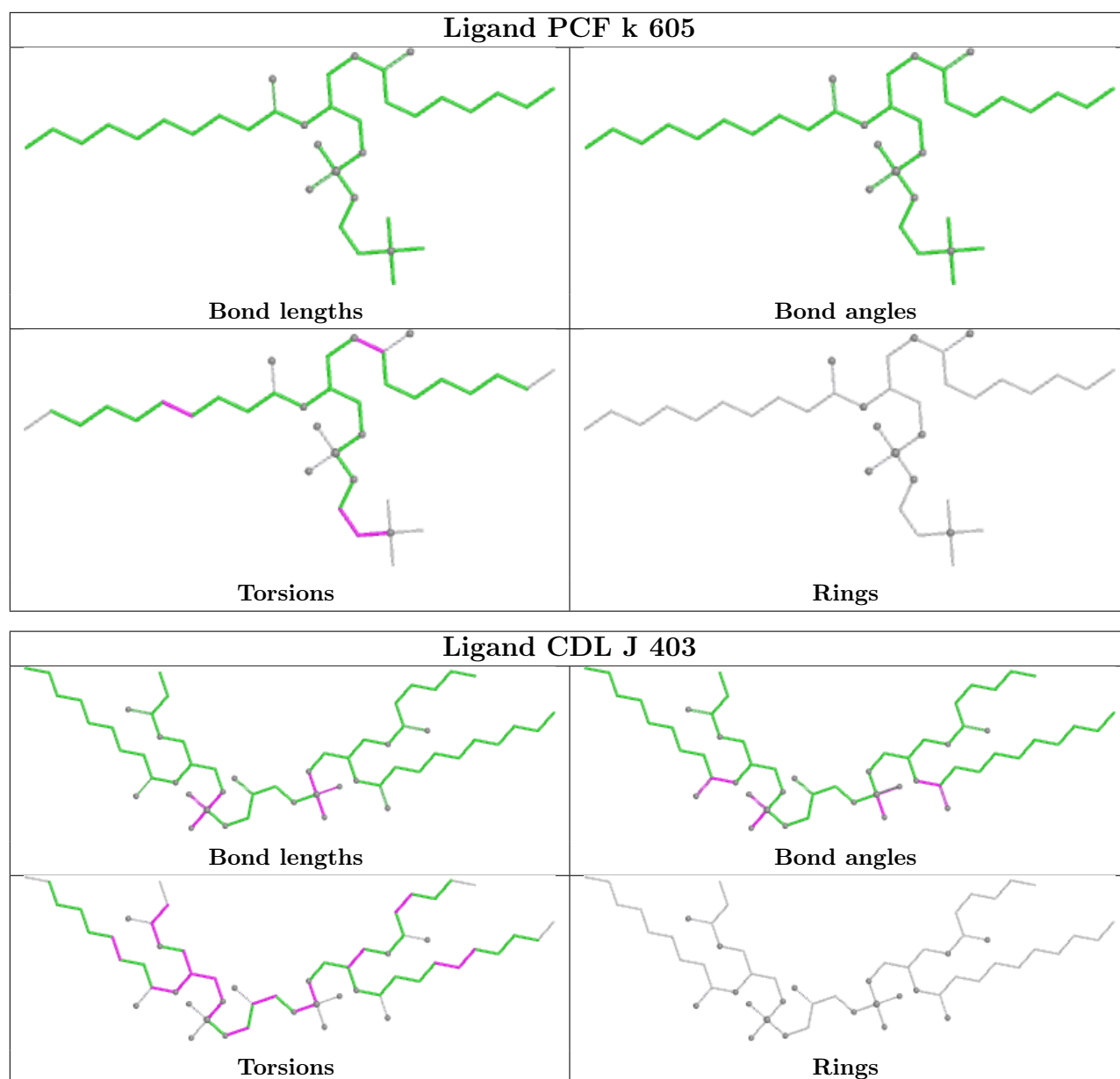


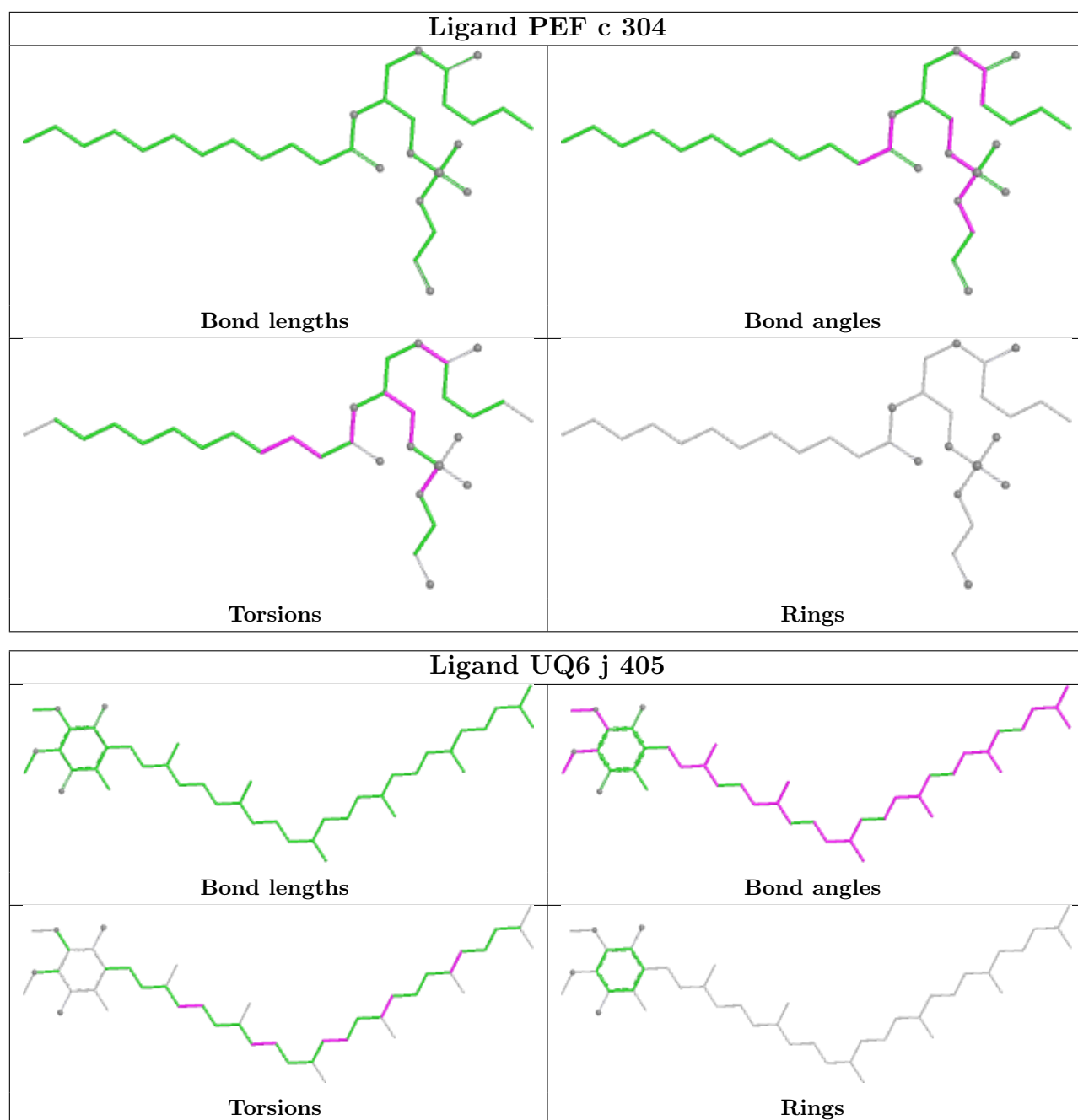


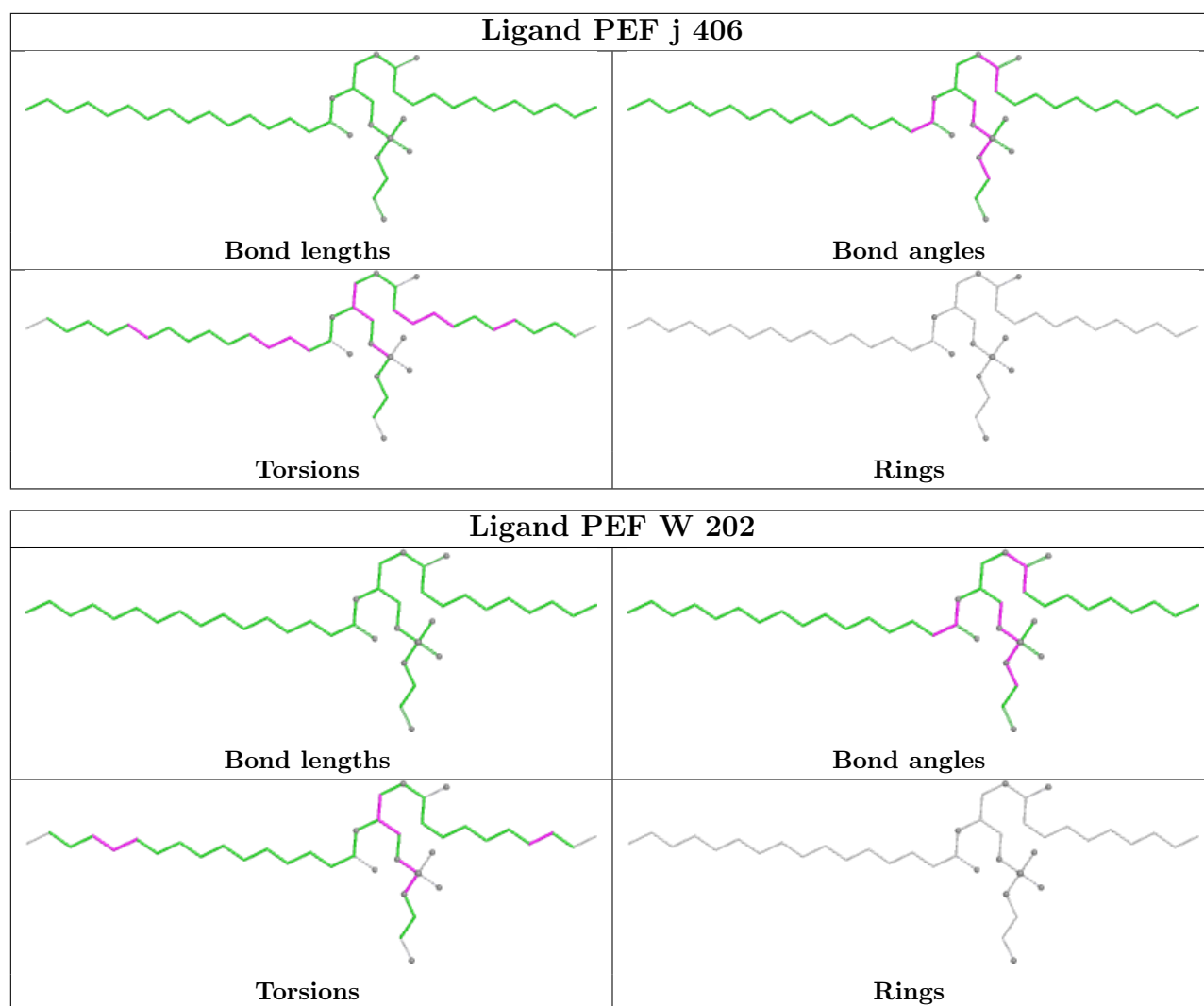


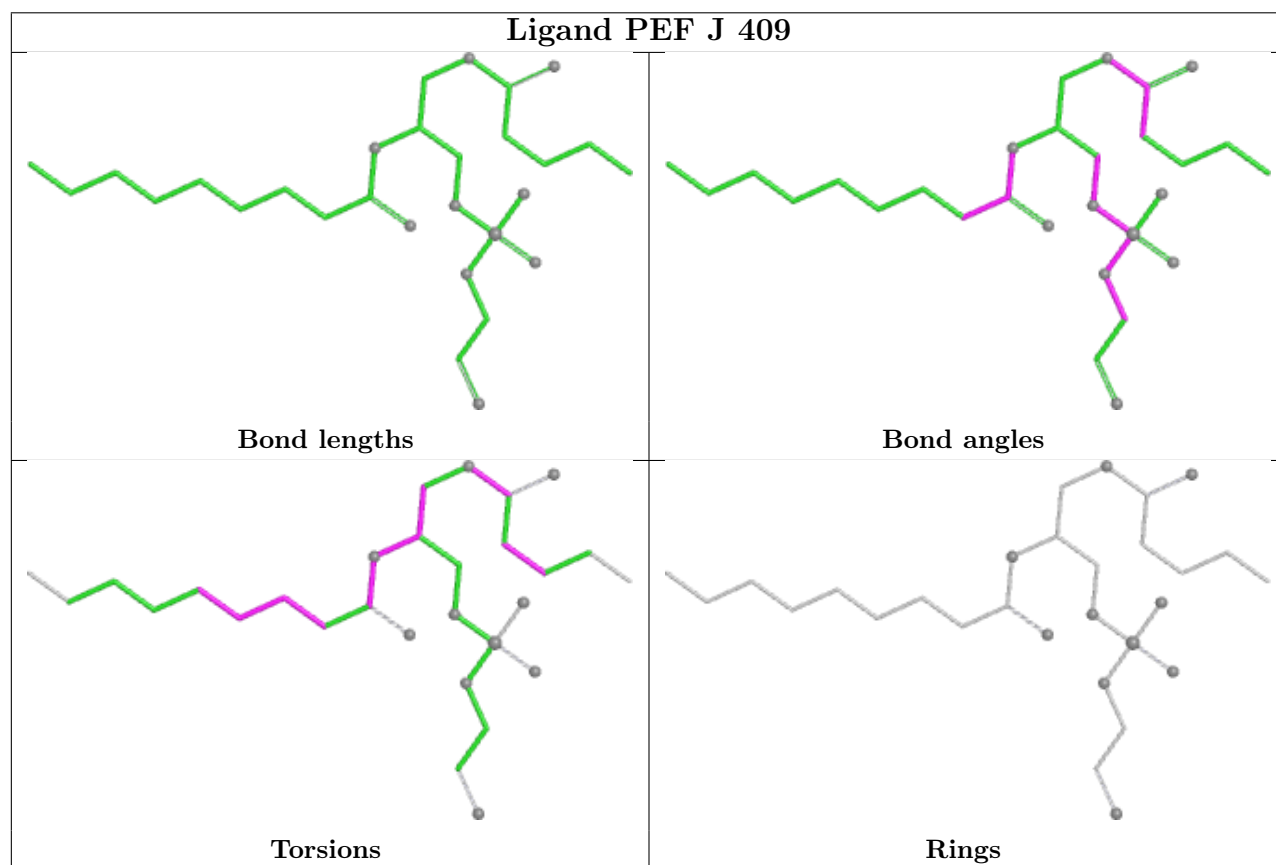
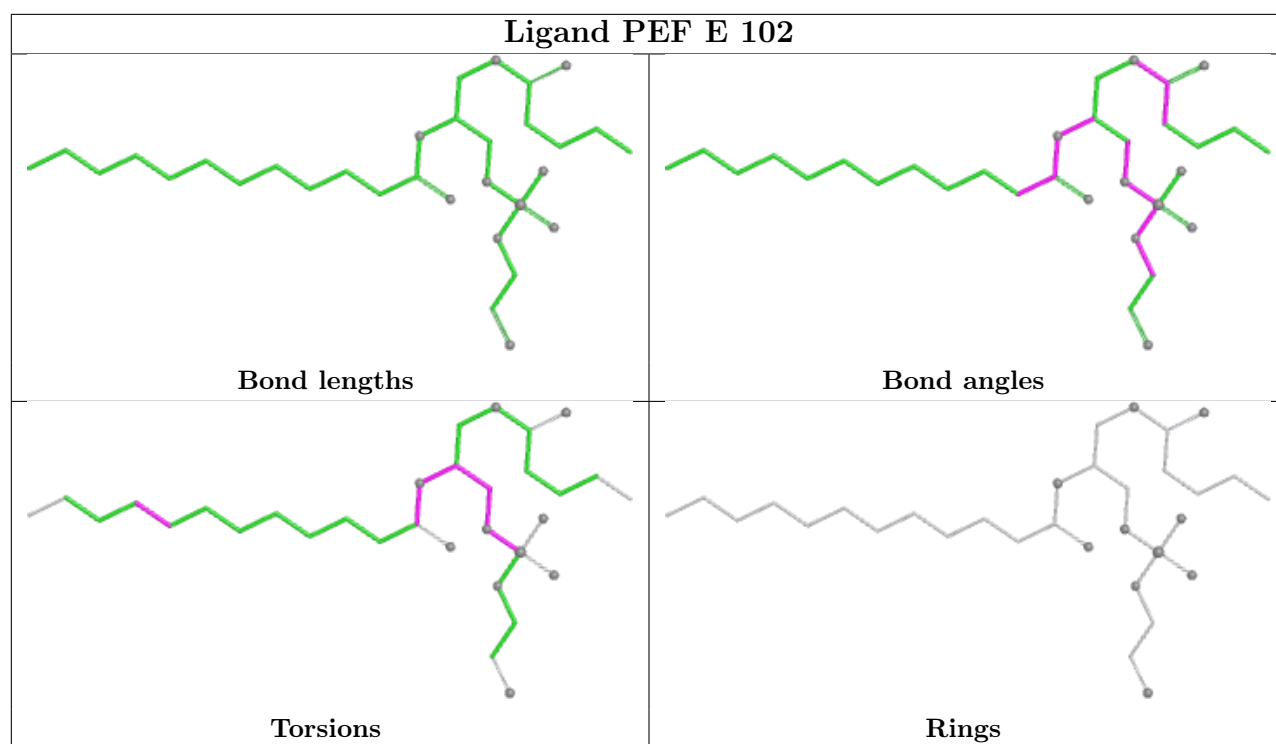


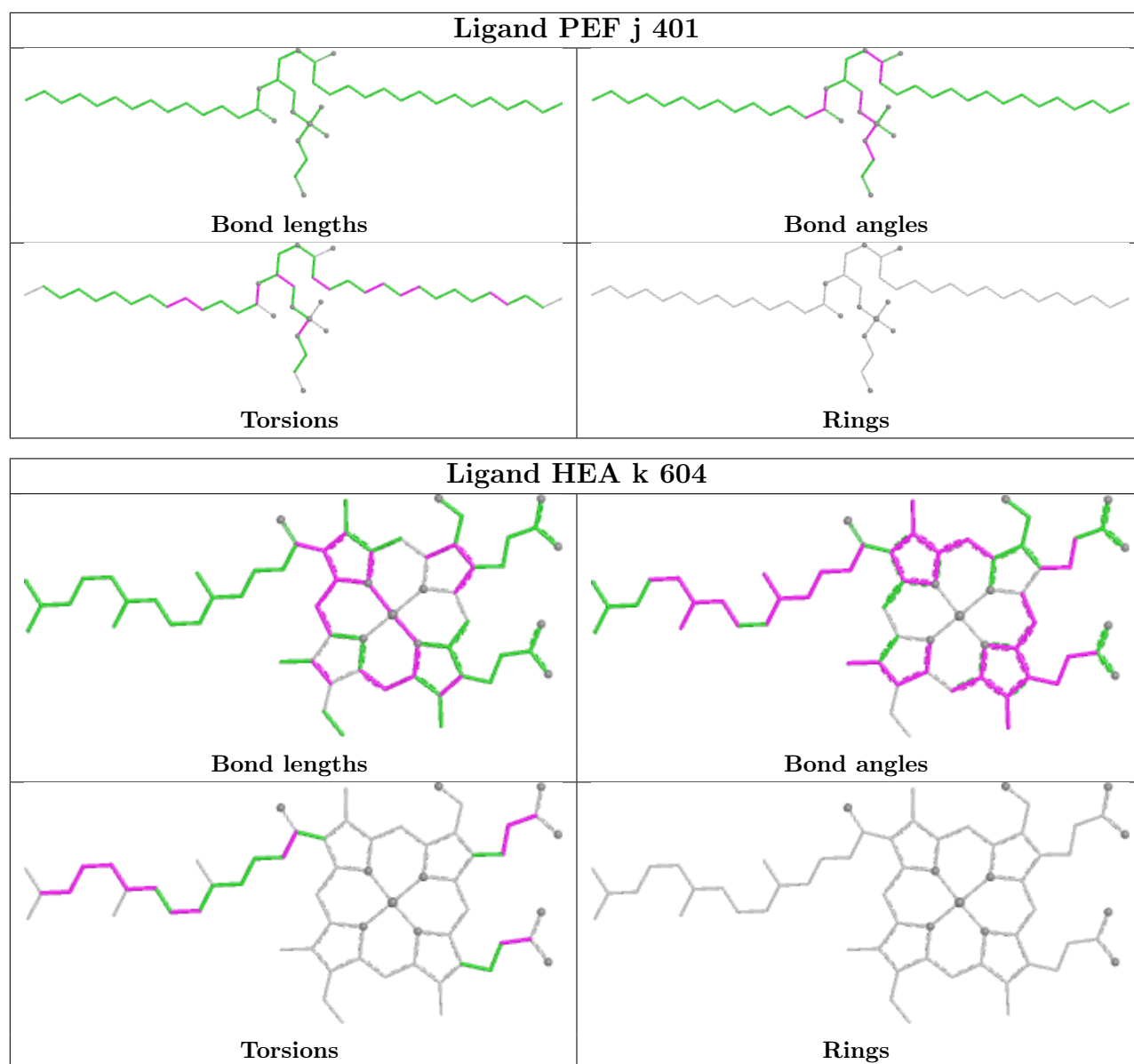




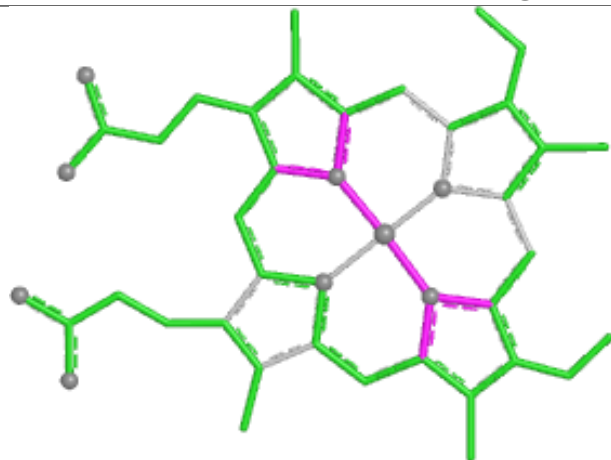




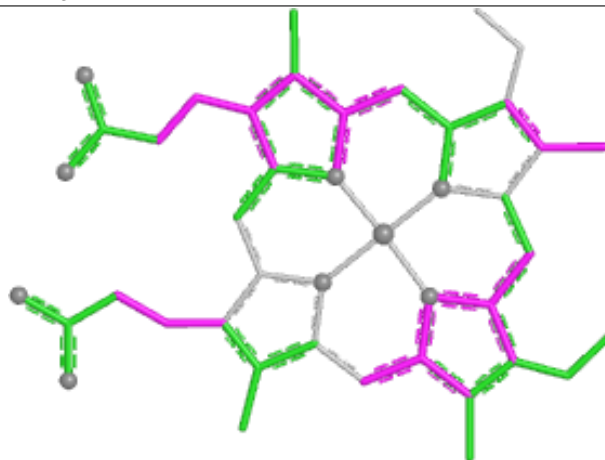




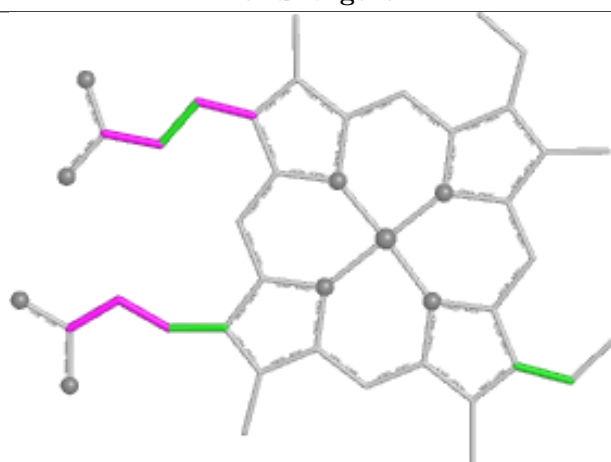
Ligand HEM j 404



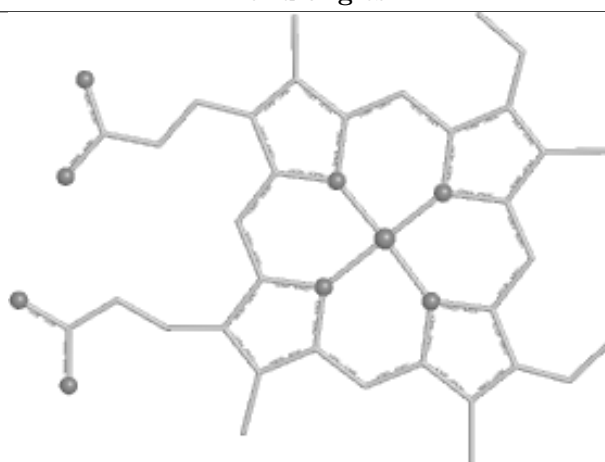
Bond lengths



Bond angles

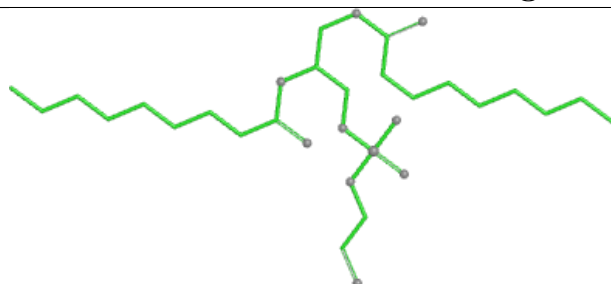


Torsions

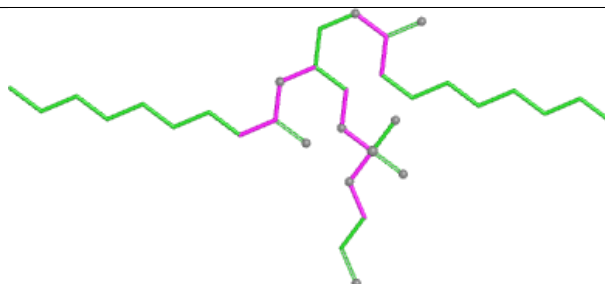


Rings

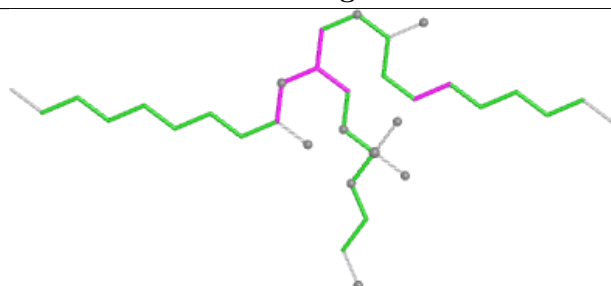
Ligand PEF v 101



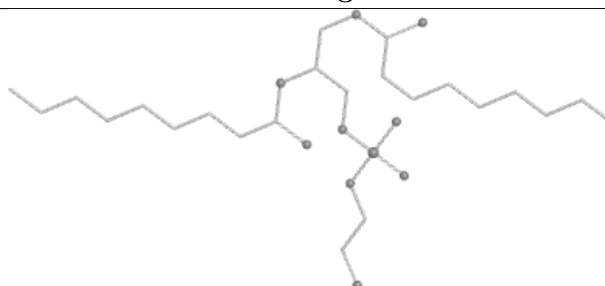
Bond lengths



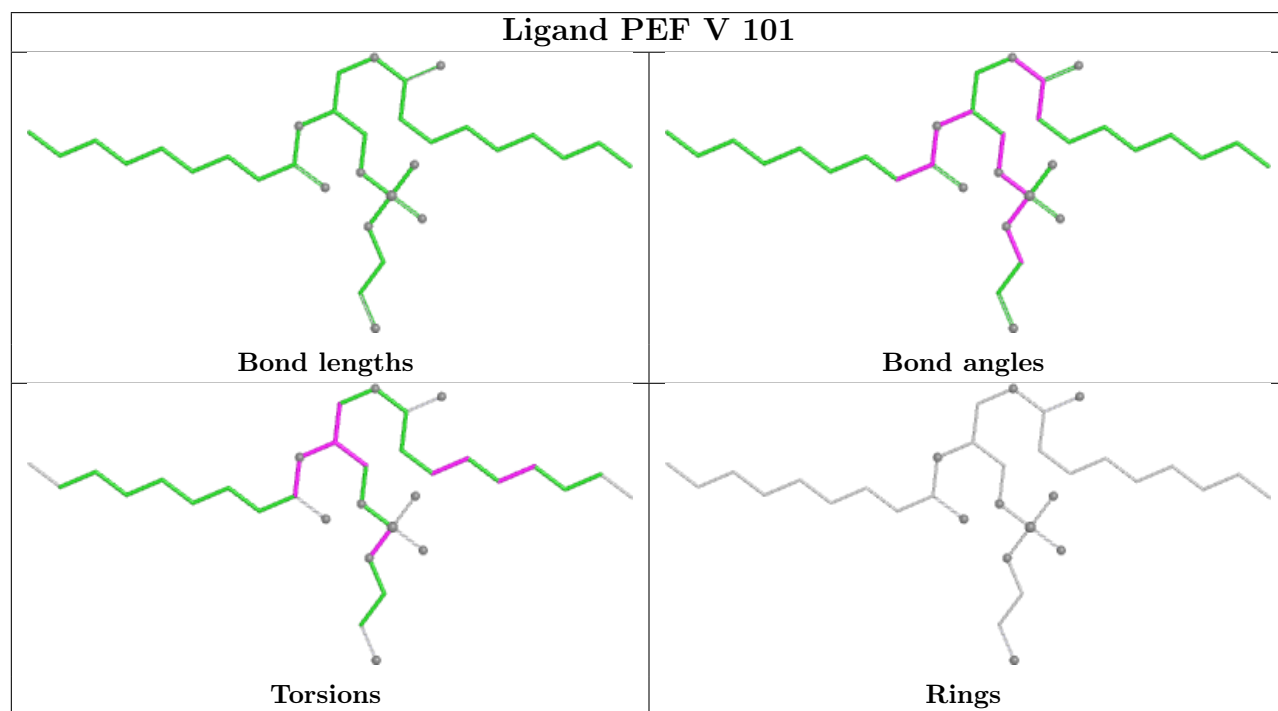
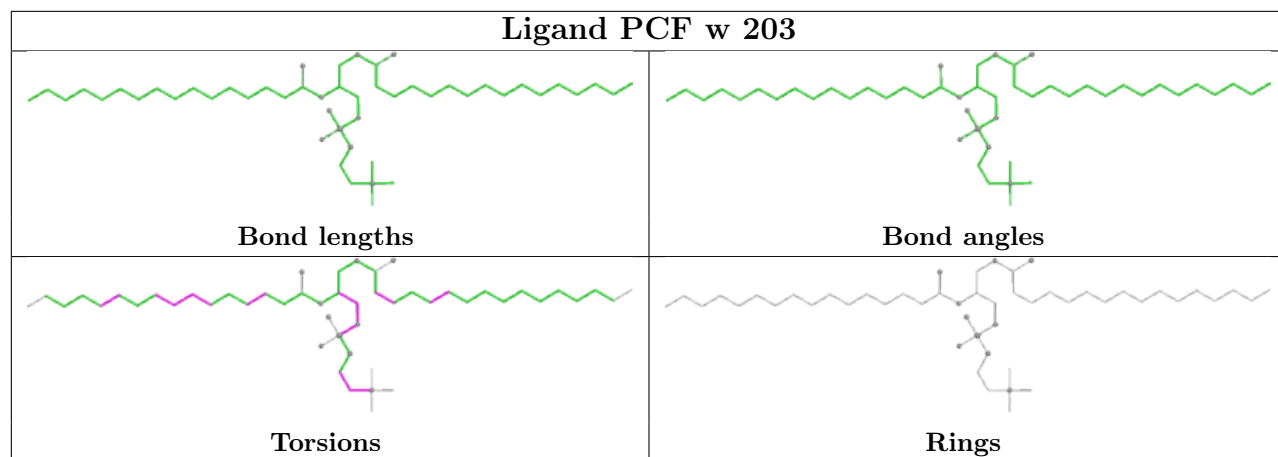
Bond angles

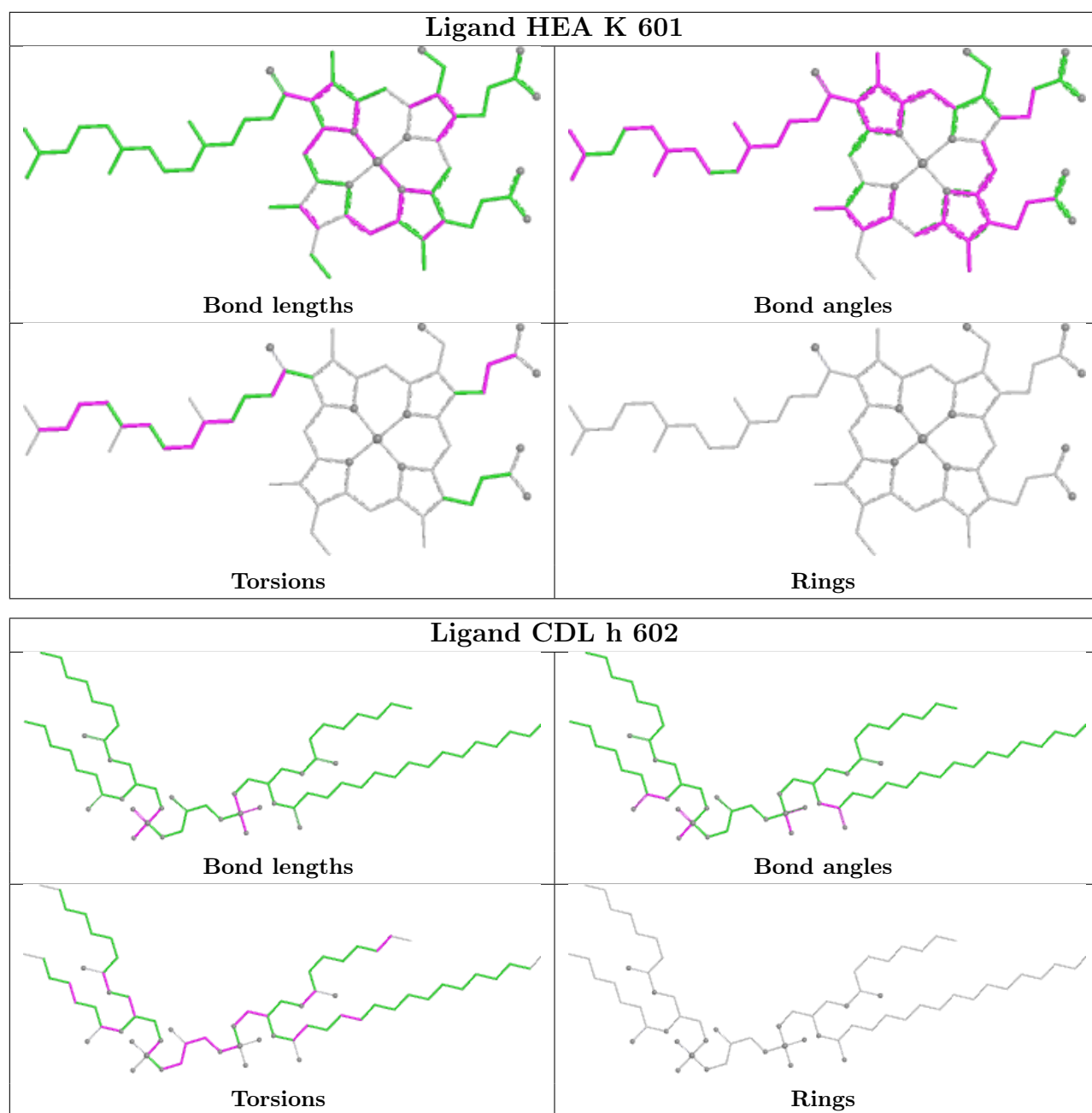


Torsions

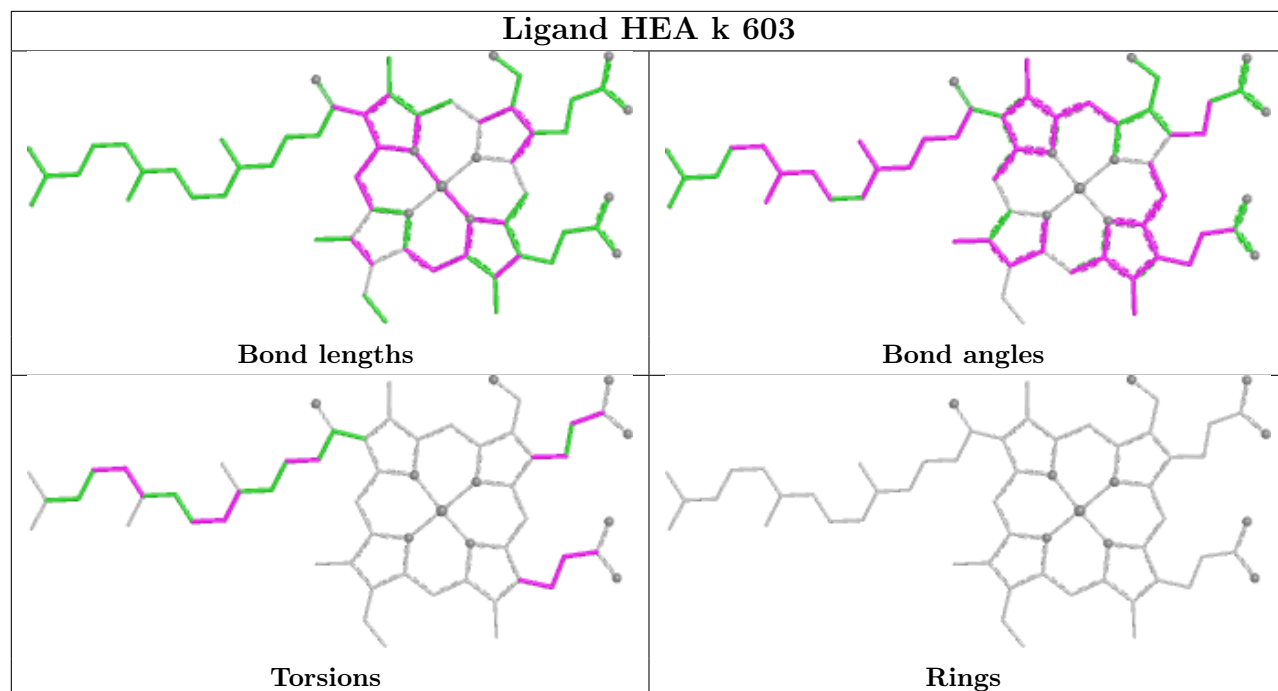


Rings

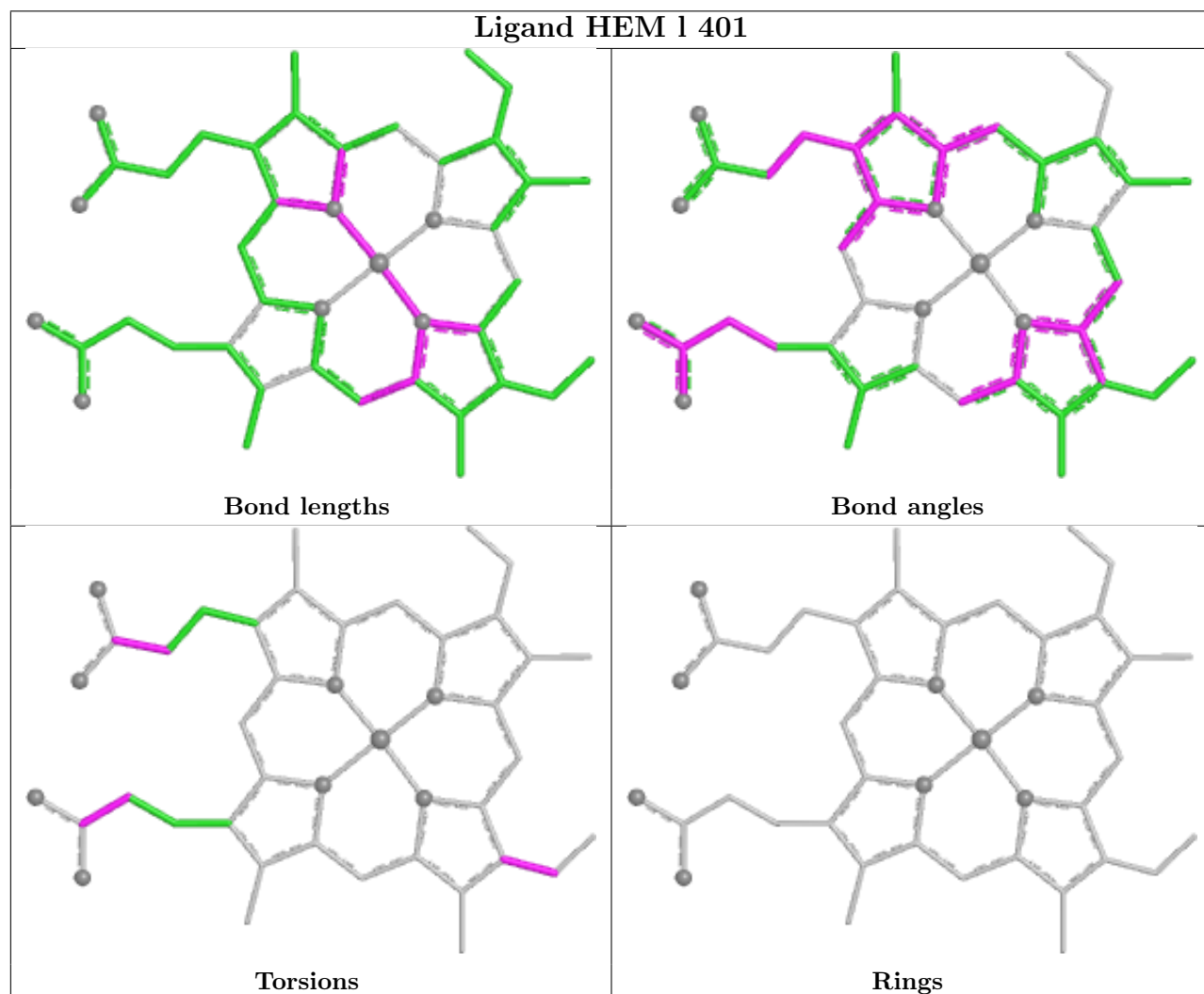


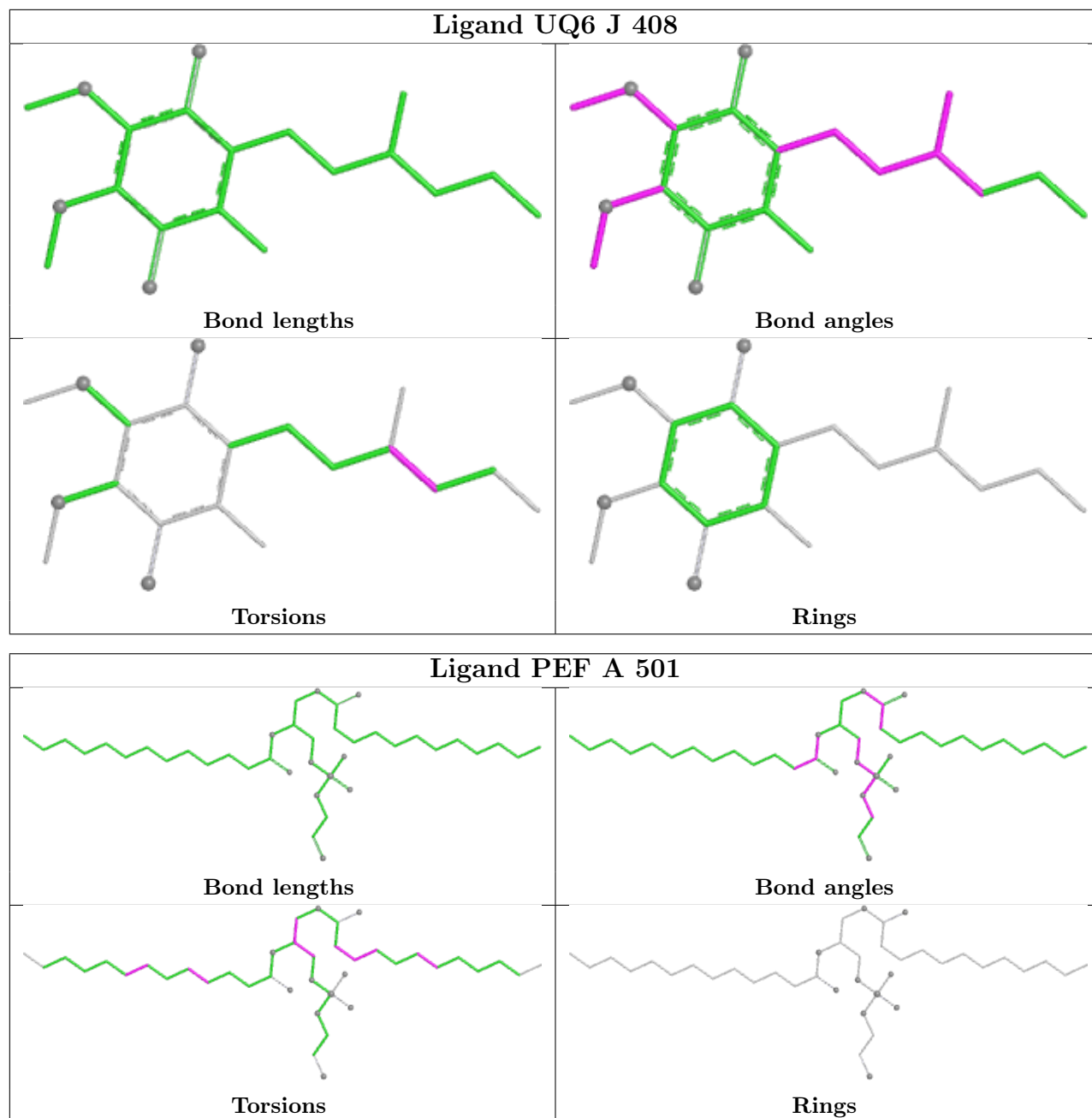


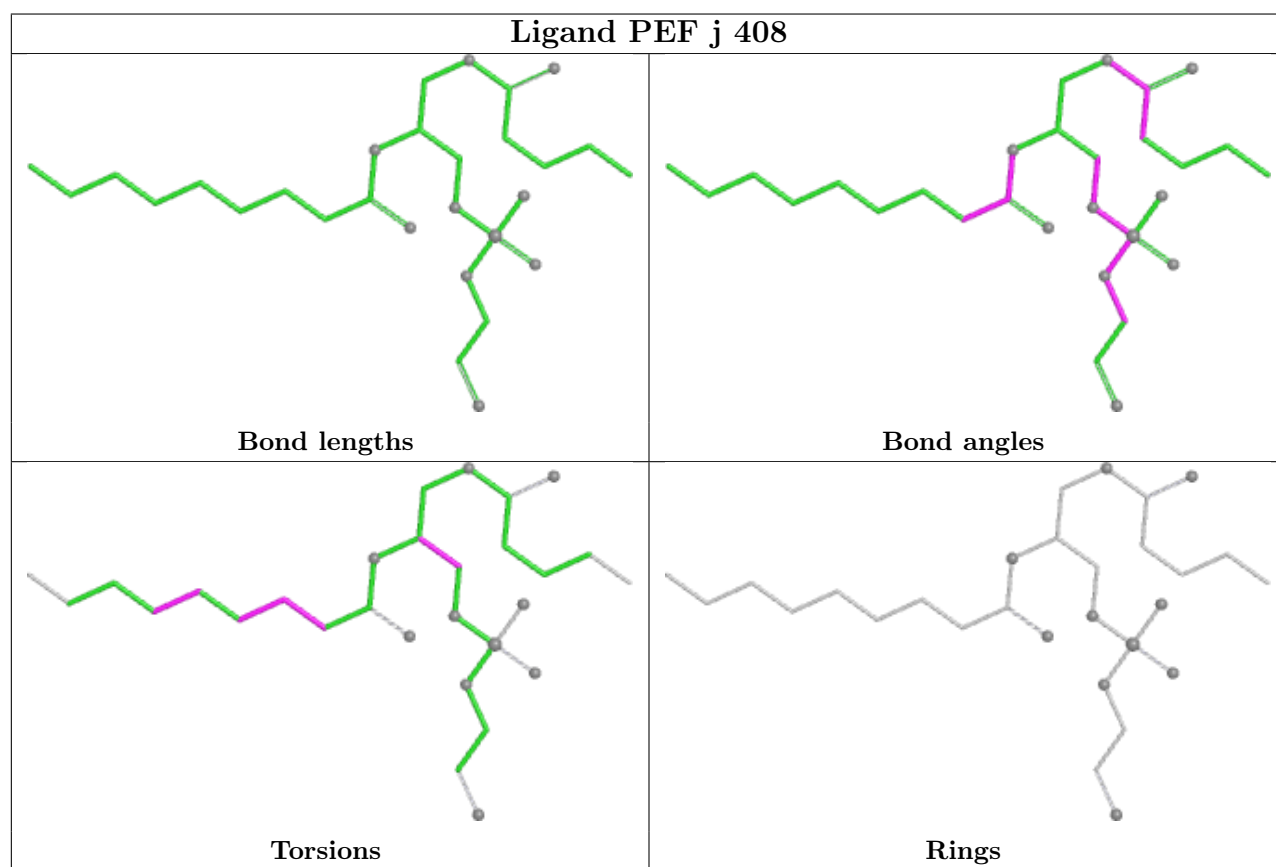
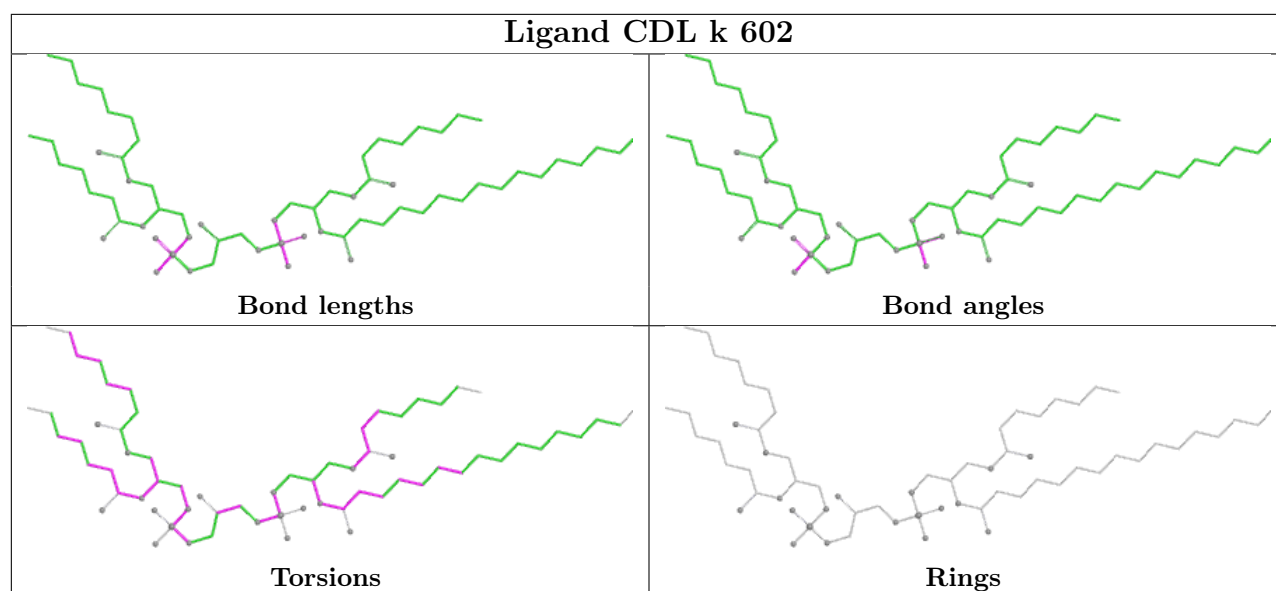
Ligand HEA k 603

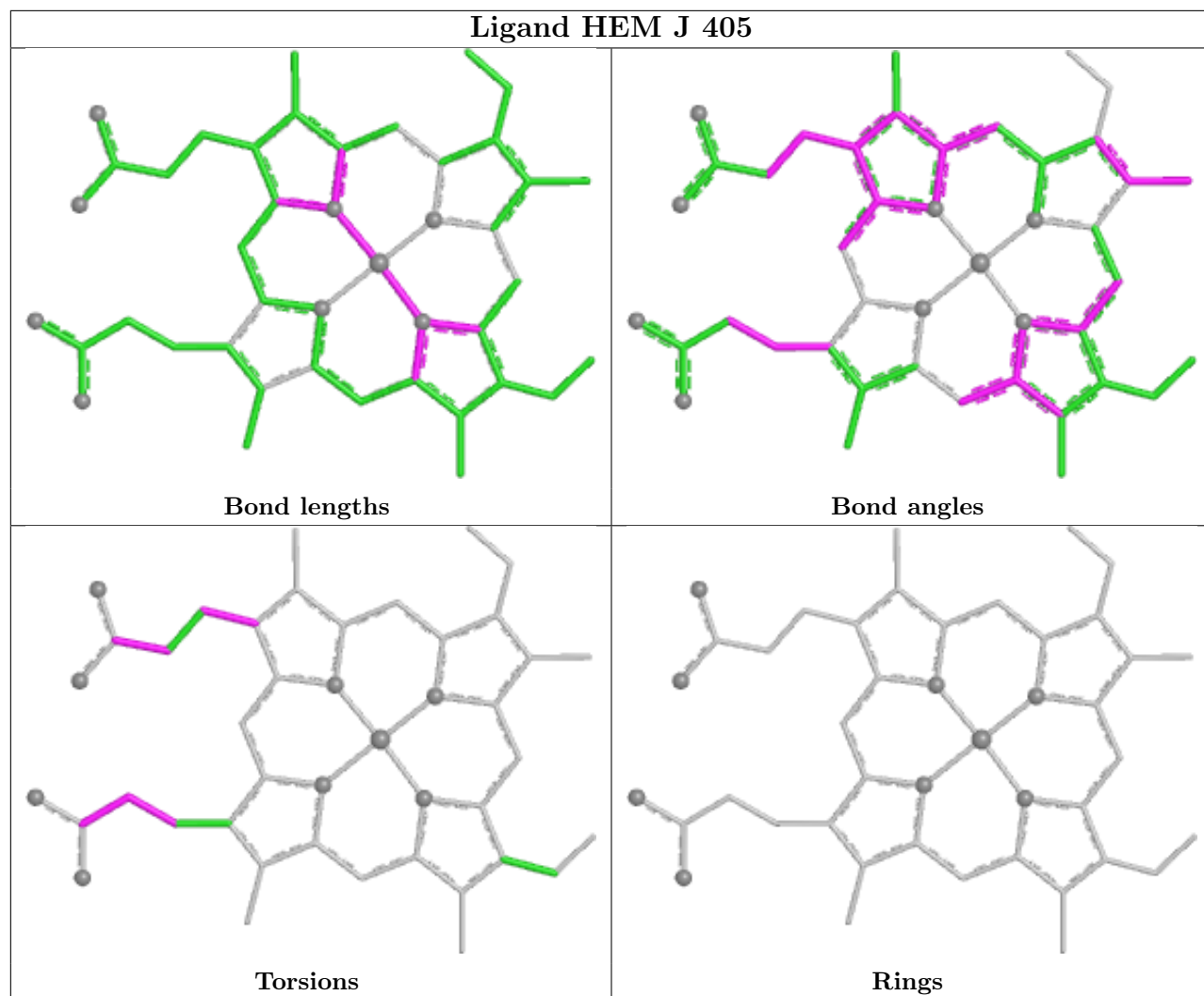


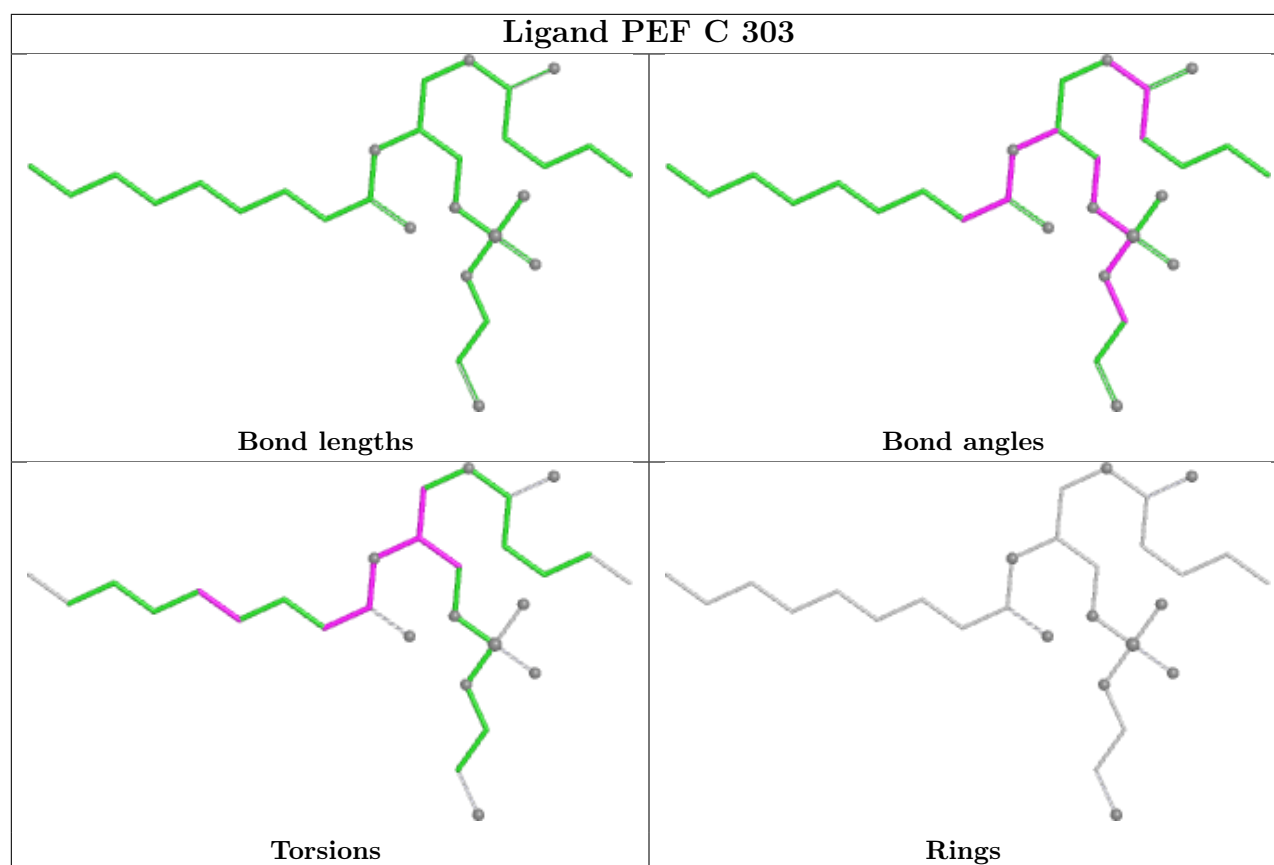
Ligand HEM l 401











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.

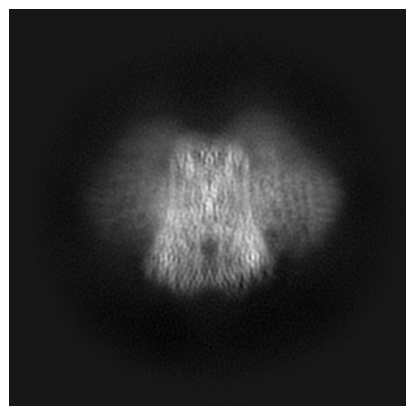
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27940. These allow visual inspection of the internal detail of the map and identification of artifacts.

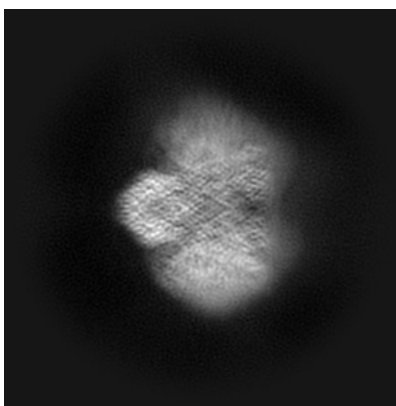
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

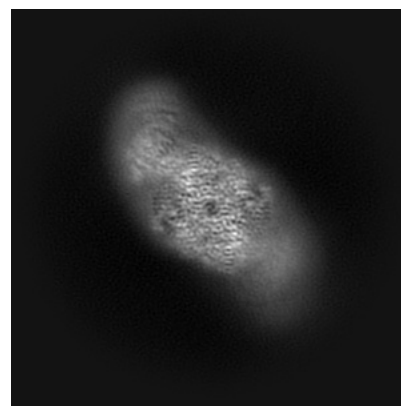
6.1.1 Primary map



X

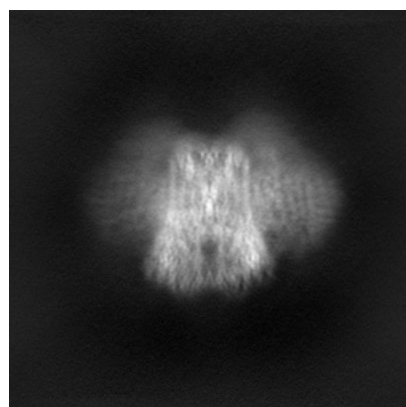


Y

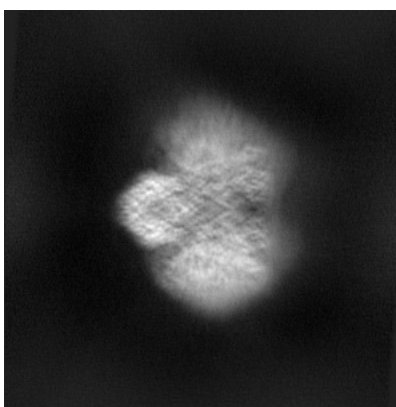


Z

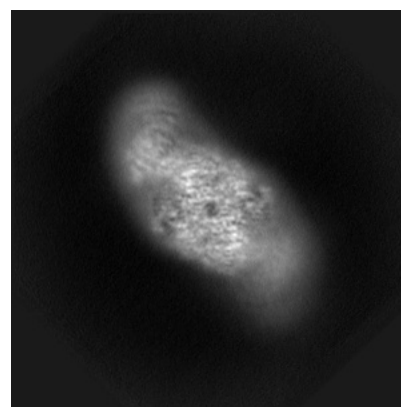
6.1.2 Raw map



X



Y

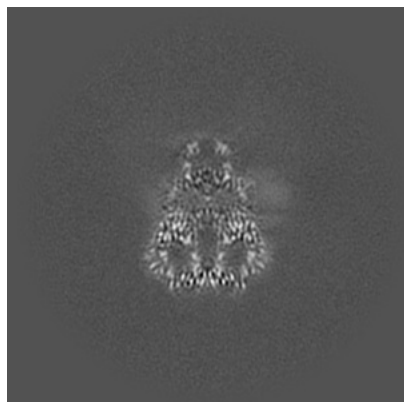


Z

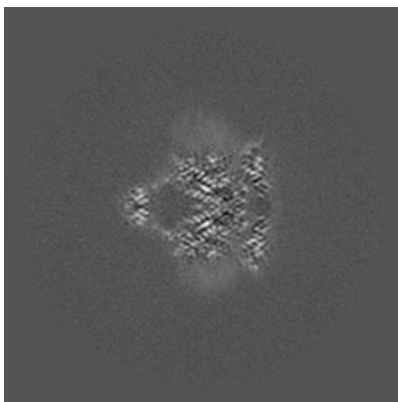
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

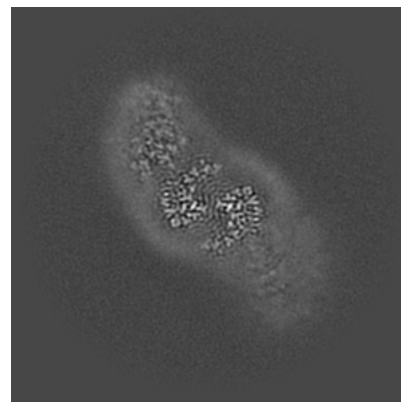
6.2.1 Primary map



X Index: 180

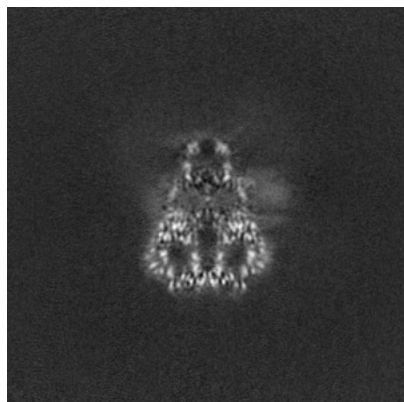


Y Index: 180

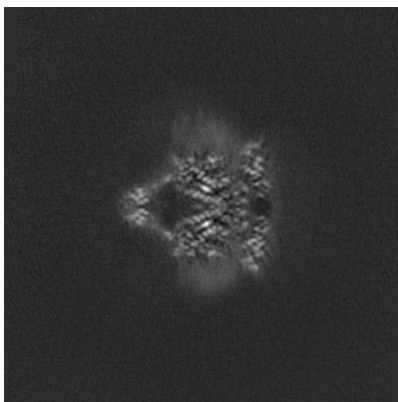


Z Index: 180

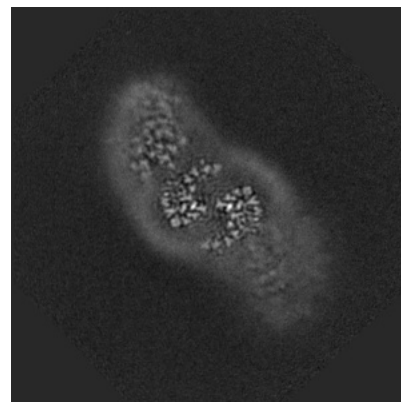
6.2.2 Raw map



X Index: 180



Y Index: 180

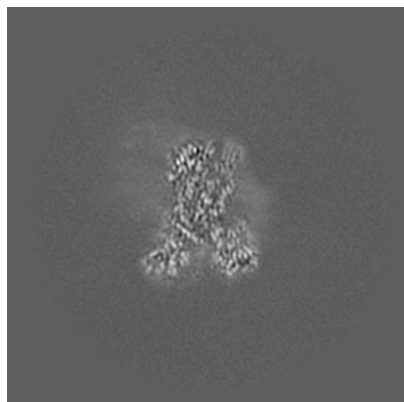


Z Index: 180

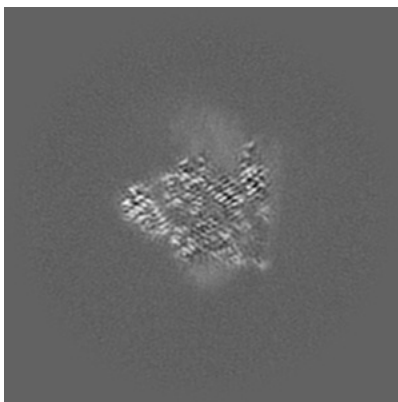
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

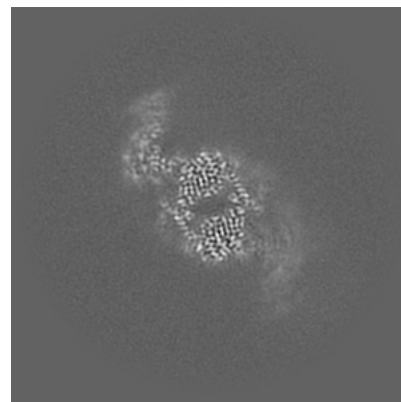
6.3.1 Primary map



X Index: 202

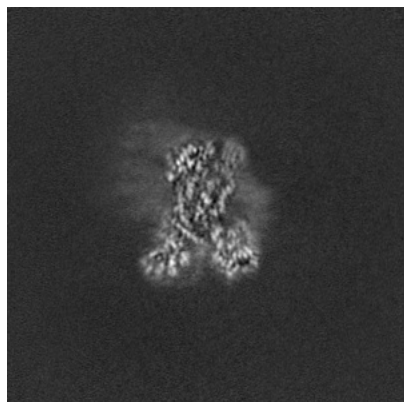


Y Index: 170

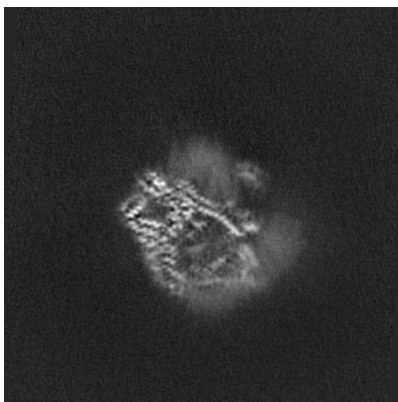


Z Index: 153

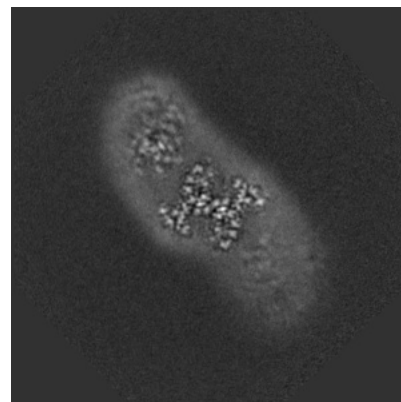
6.3.2 Raw map



X Index: 202



Y Index: 214

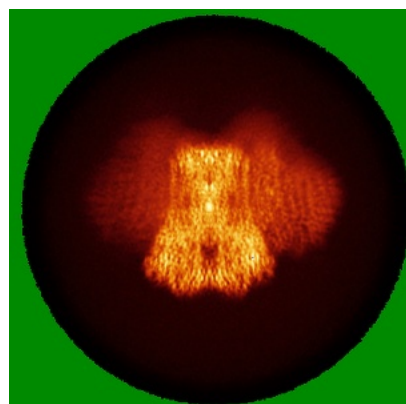


Z Index: 197

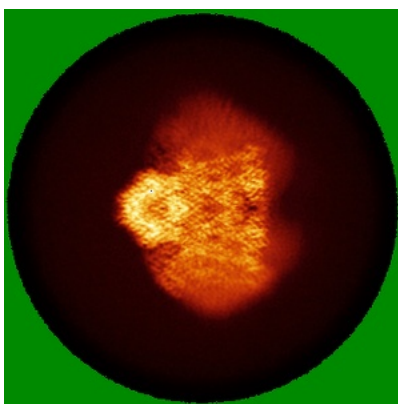
The images above show the largest variance slices of the map in three orthogonal directions.

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

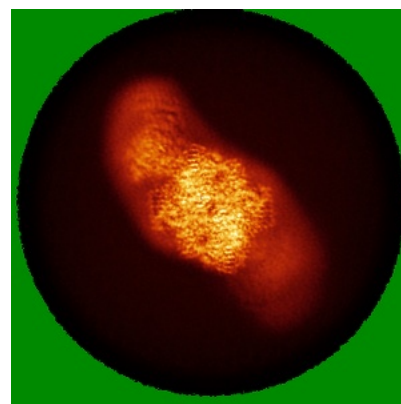
6.4.1 Primary map



X

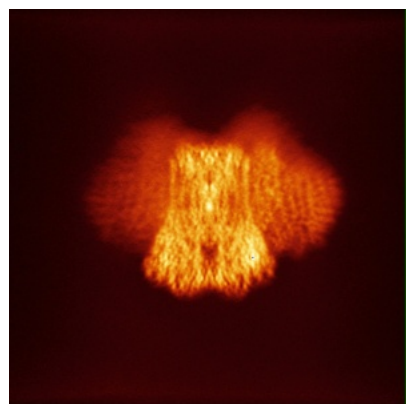


Y

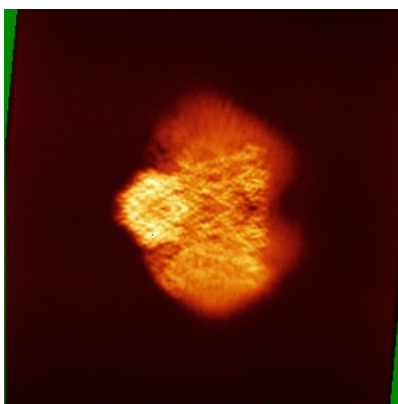


Z

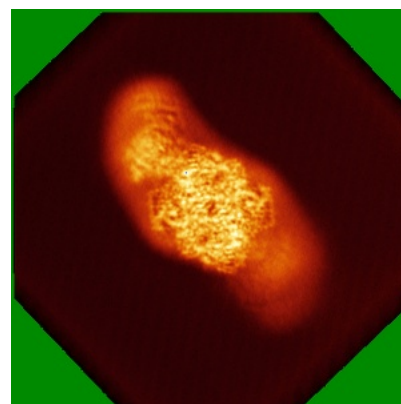
6.4.2 Raw map



X



Y

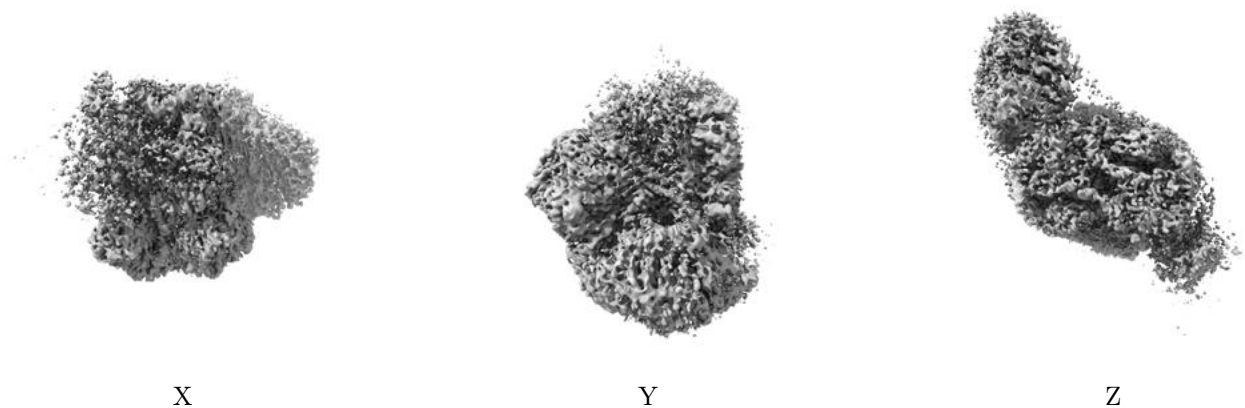


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

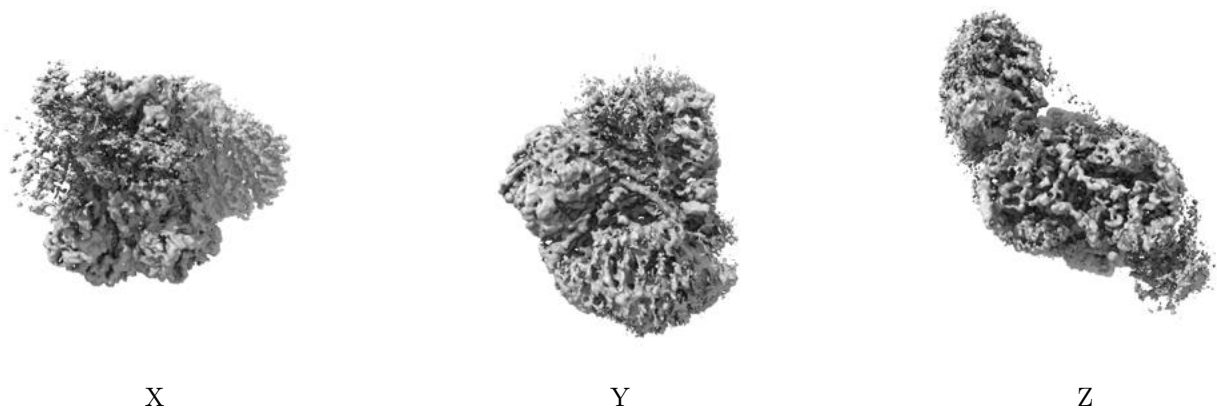
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

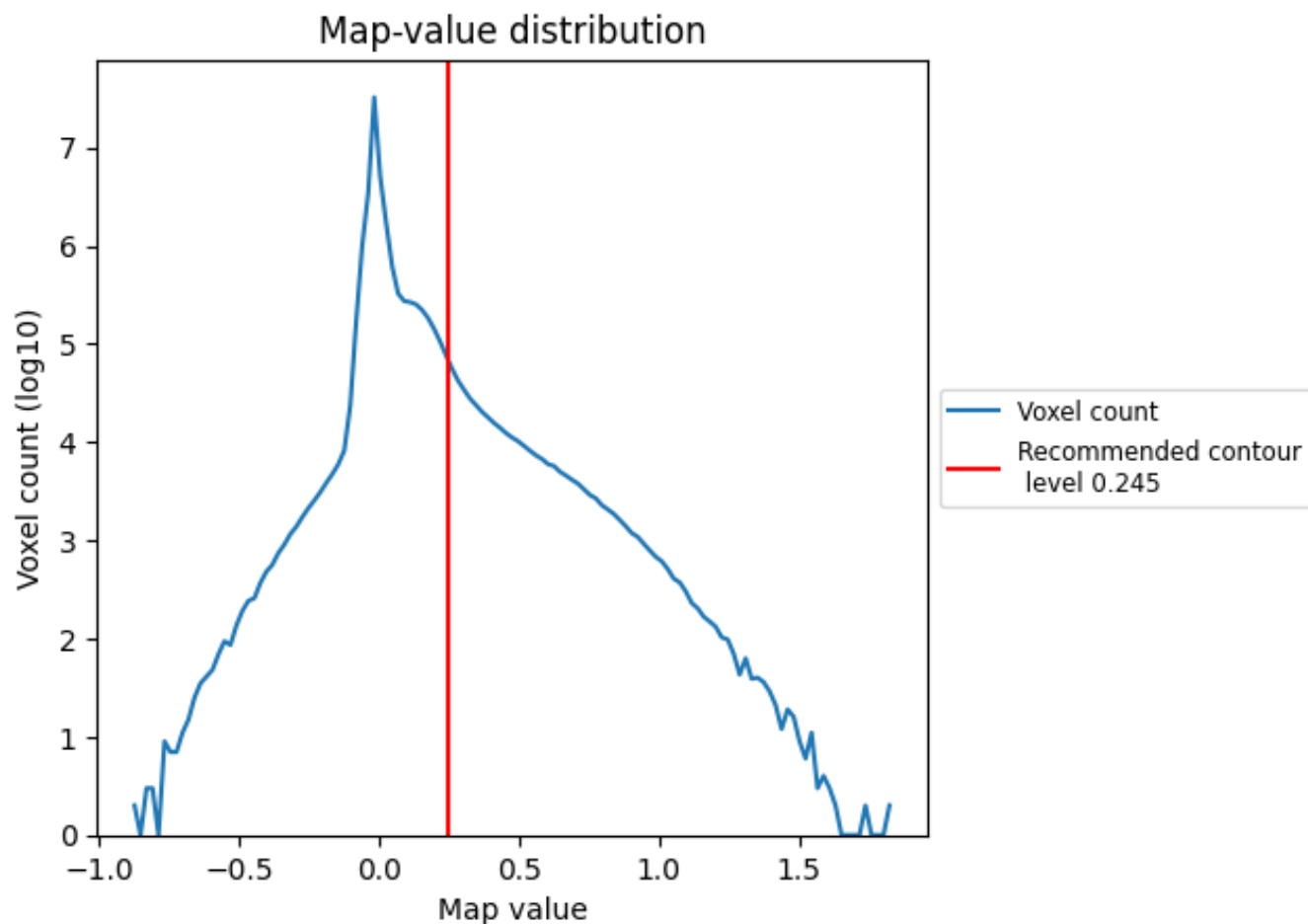
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

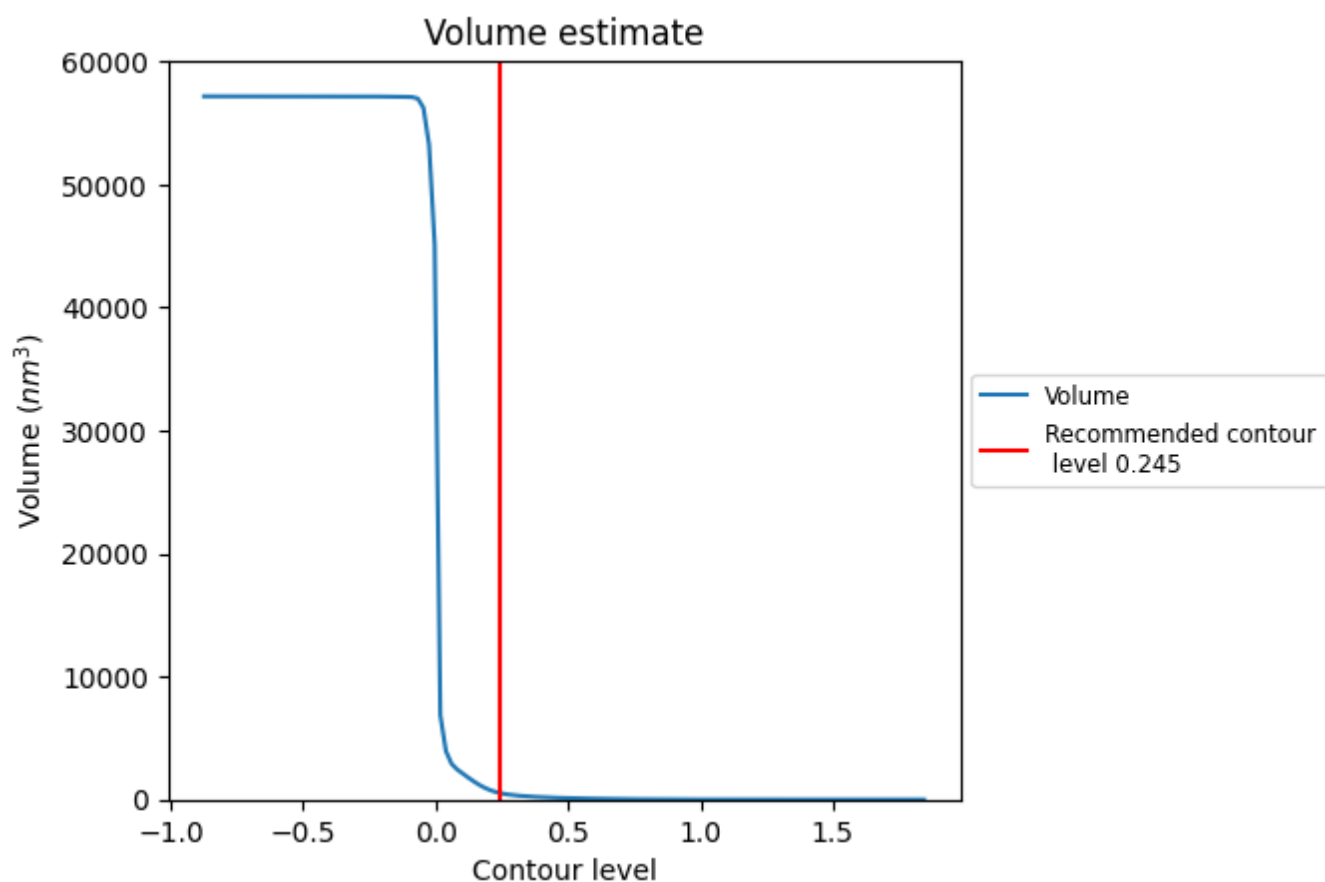
This section contains the results of statistical analysis of the map.

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.

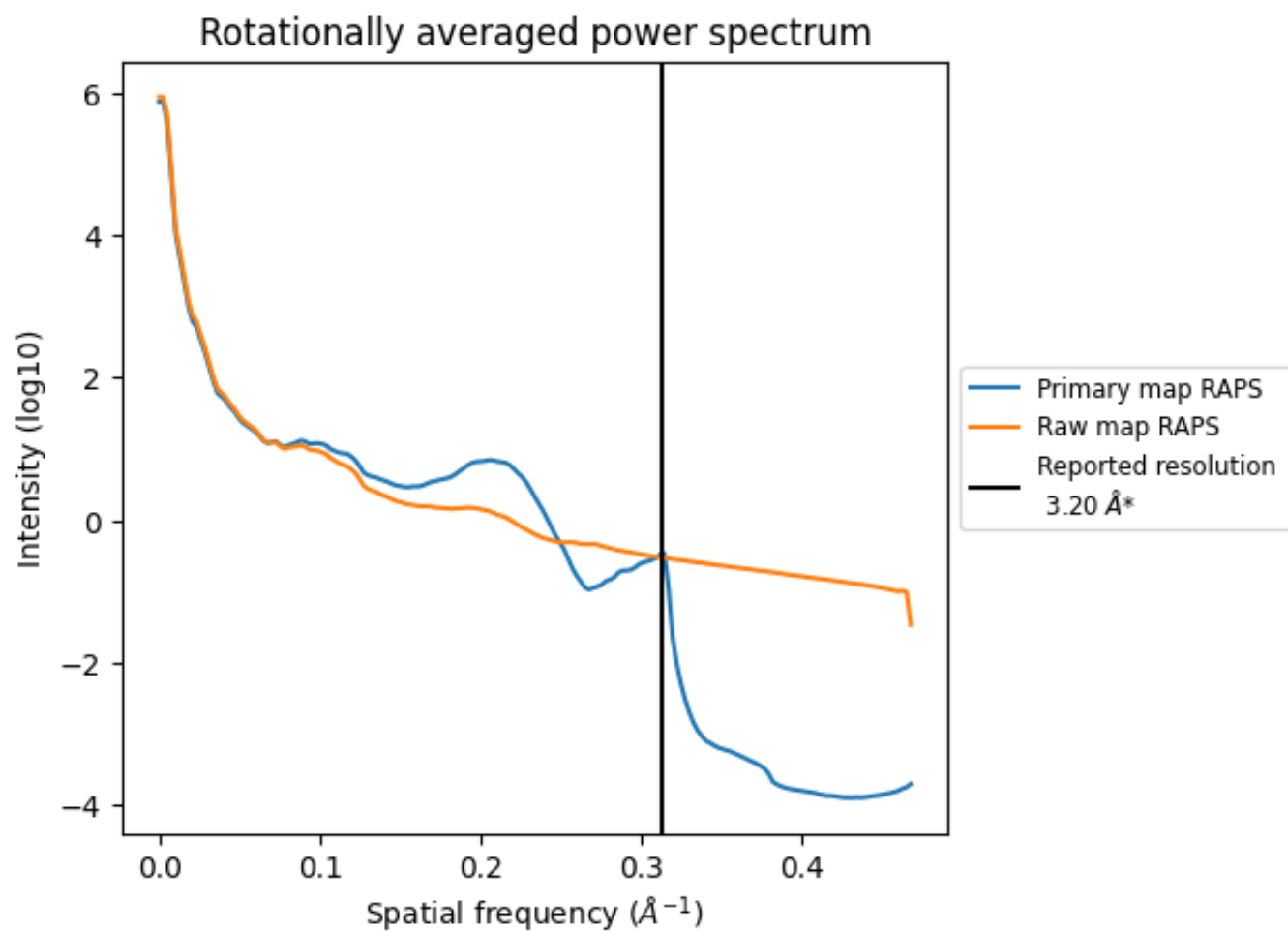
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 525 nm³; this corresponds to an approximate mass of 474 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

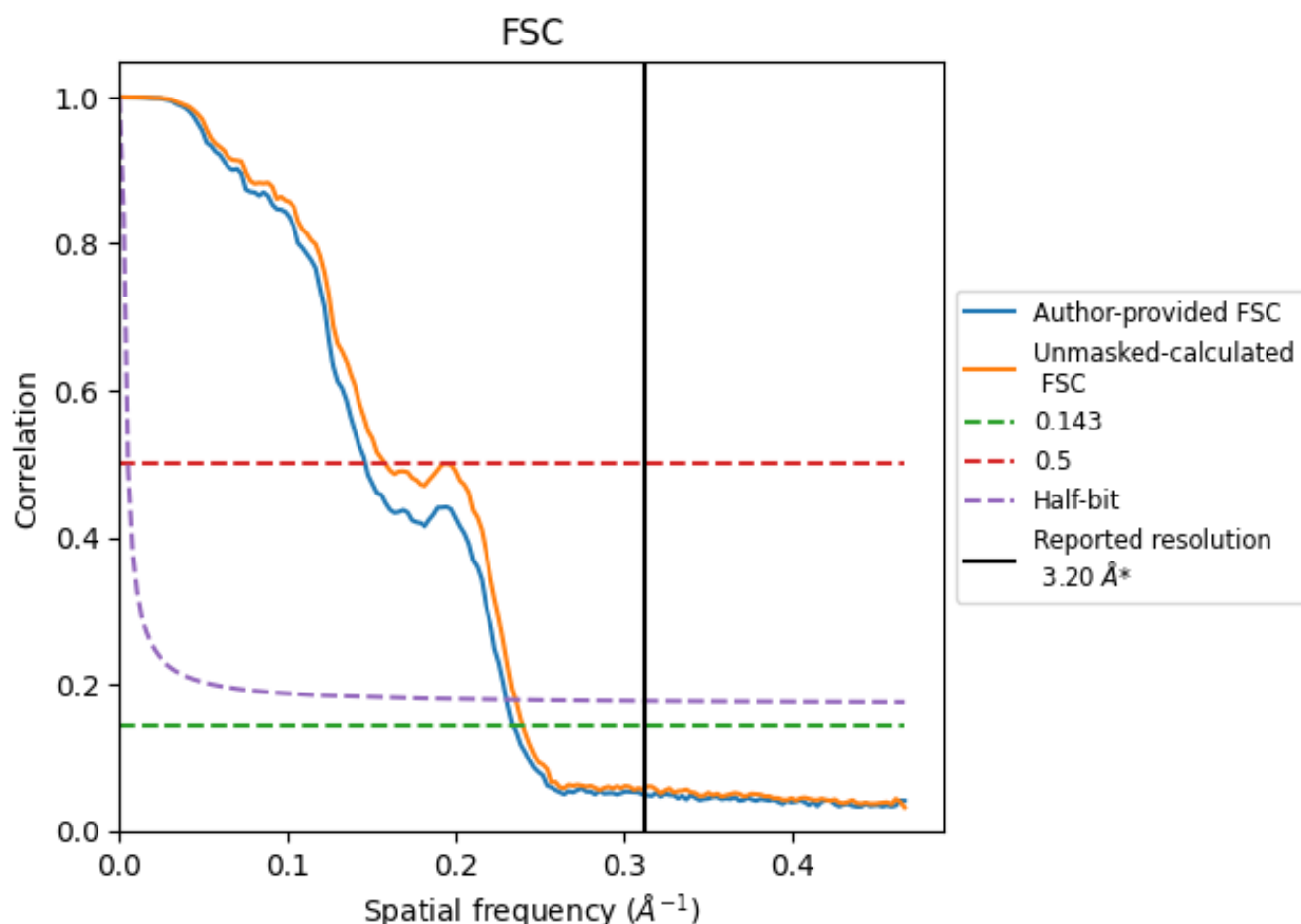


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.27	6.84	4.34
Unmasked-calculated*	4.17	6.32	4.24

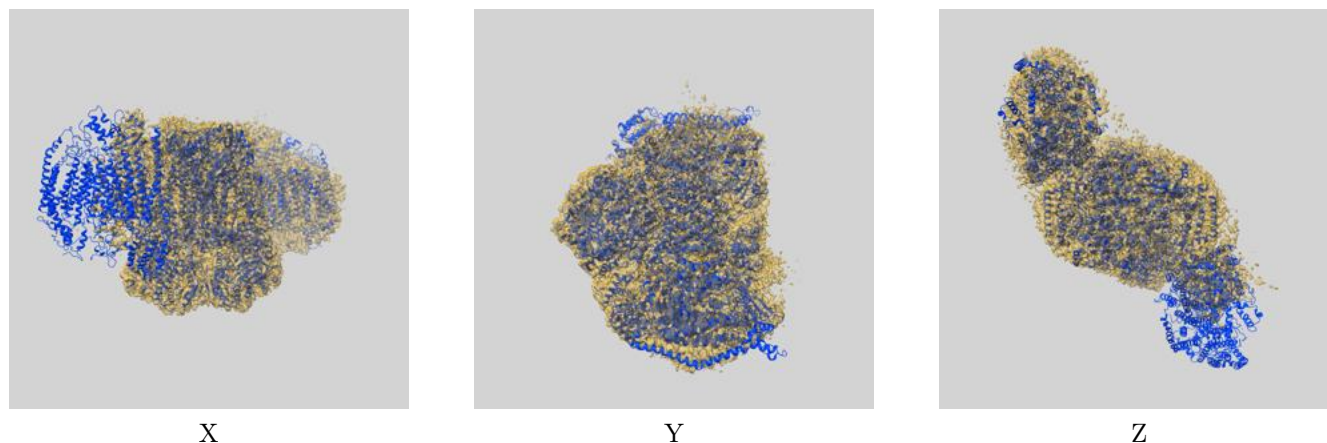
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

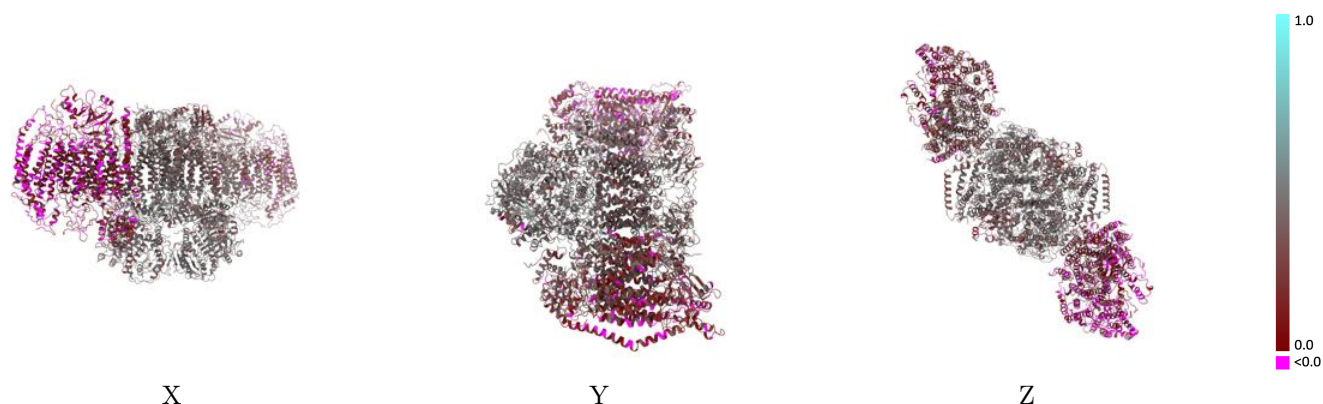
This section contains information regarding the fit between EMDB map EMD-27940 and PDB model 8E7S. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



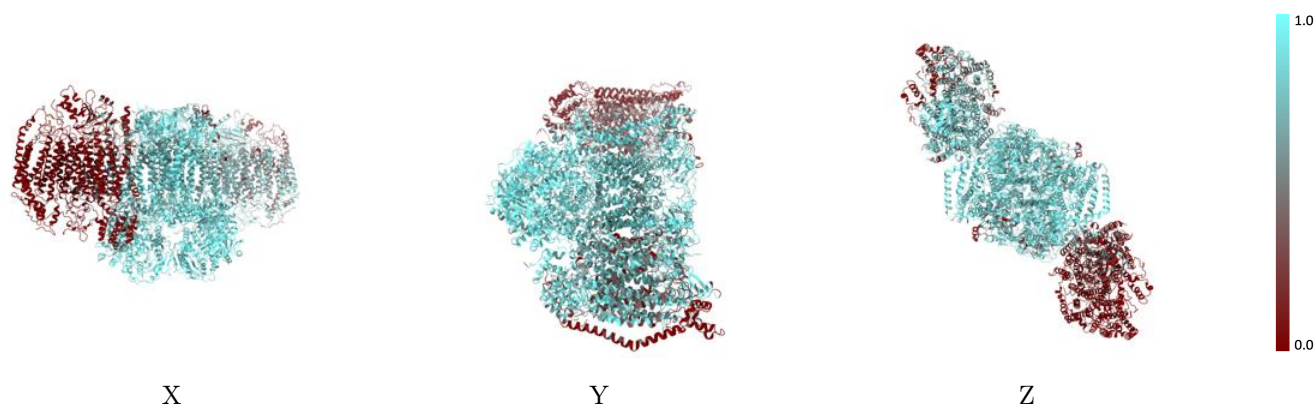
The images above show the 3D surface view of the map at the recommended contour level 0.245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



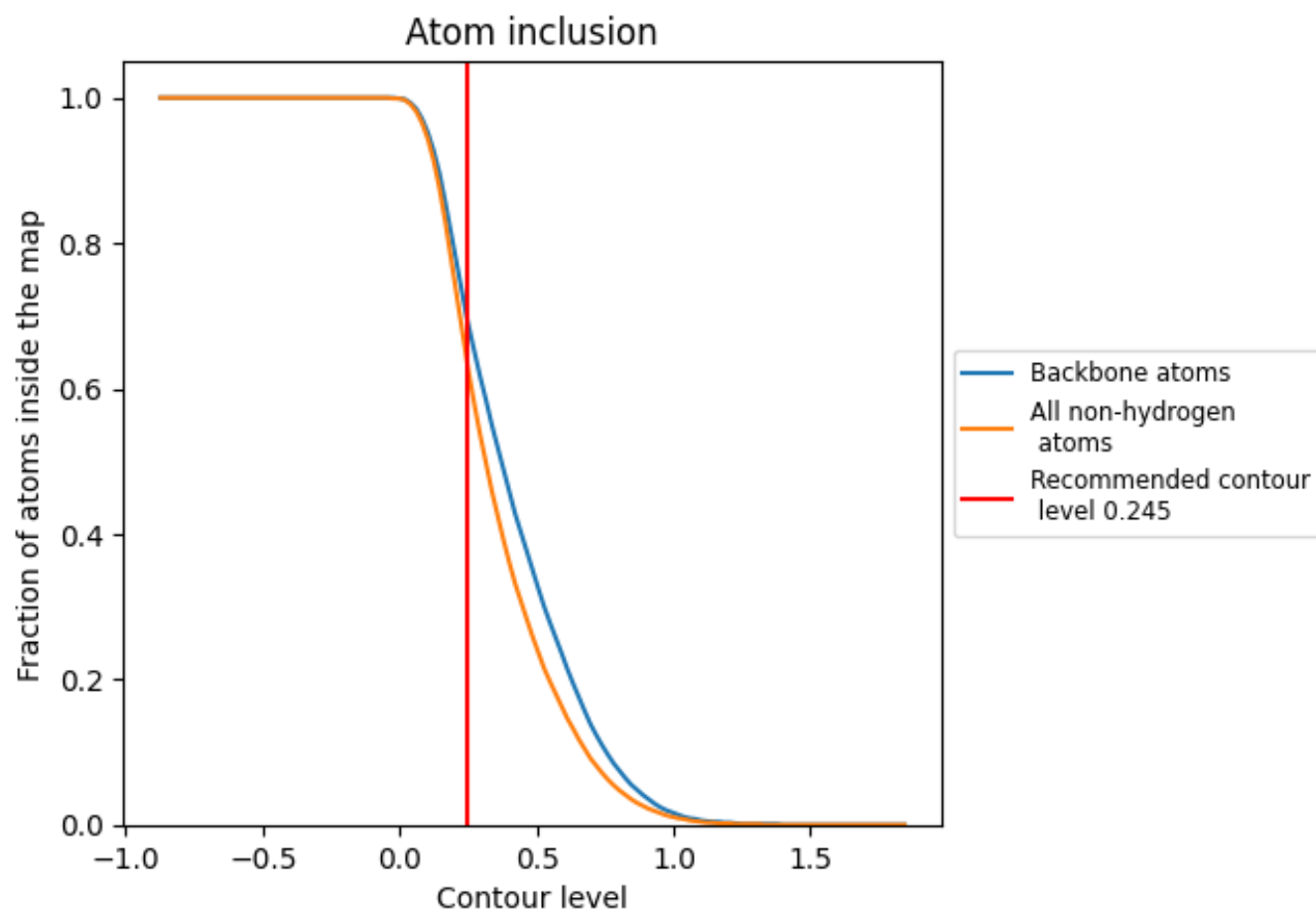
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.245).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.3120
A	 0.9260	 0.4260
B	 0.9380	 0.4330
C	 0.7330	 0.3570
D	 0.7440	 0.3710
E	 0.7950	 0.4000
F	 0.9010	 0.4340
G	 0.8490	 0.3690
H	 0.8320	 0.4310
J	 0.8400	 0.4220
K	 0.7100	 0.3240
L	 0.9050	 0.4290
M	 0.4320	 0.2750
N	 0.5230	 0.2610
O	 0.6000	 0.1920
P	 0.8130	 0.2850
Q	 0.7890	 0.2870
R	 0.7200	 0.2440
S	 0.0580	 0.1440
T	 0.7080	 0.2960
U	 0.1840	 0.1570
V	 0.5940	 0.2850
W	 0.7810	 0.3480
a	 0.9270	 0.4310
b	 0.9430	 0.4290
c	 0.6810	 0.3420
d	 0.5920	 0.3560
e	 0.7970	 0.3840
f	 0.9050	 0.4280
g	 0.8450	 0.3860
h	 0.8990	 0.4320
j	 0.8680	 0.4220
k	 0.1350	 0.1560
l	 0.9090	 0.4210
m	 0.0000	 0.1350



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Chain	Atom inclusion	Q-score
n	 0.0000	 0.0710
o	 0.0010	 0.0460
p	 0.1510	 0.1210
q	 0.0530	 0.1440
r	 0.1020	 0.0670
s	 0.0000	 0.0210
t	 0.0280	 0.0850
u	 0.0000	 0.0380
v	 0.2750	 0.1630
w	 0.3370	 0.2200