



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 07:09 PM UTC

PDB ID : 9G9Z / pdb_00009g9z
EMDB ID : EMD-51162
Title : Respiratory supercomplex CI1-CIII2-CIV1 (respirasome) from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-25
Resolution : 4.03 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

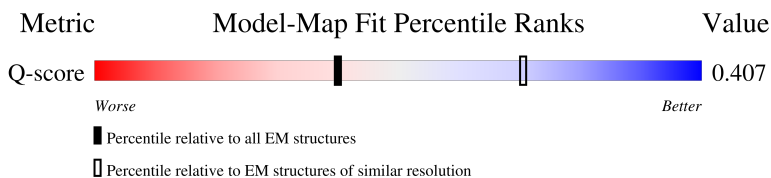
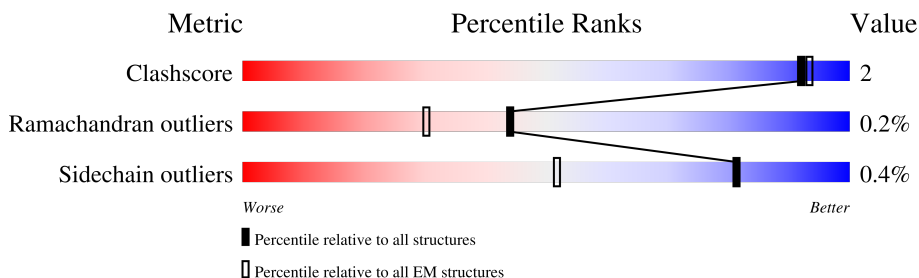
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.03 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6618 (3.54 - 4.53)

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	121	<div> <div>23%</div> <div>93%</div> <div>7%</div> </div>
2	B	175	<div> <div>13%</div> <div>86%</div> <div>6%</div> <div>7%</div> </div>
3	C	208	<div> <div>11%</div> <div>90%</div> <div>7%</div> </div>
4	D	412	<div> <div>13%</div> <div>94%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	239	
6	F	431	
7	G	674	
8	H	345	
9	I	163	
10	J	199	
11	K	101	
12	L	703	
13	M	513	
14	N	499	
15	P	330	
16	Q	103	
17	R	62	
18	Z	217	
19	a	440	
19	d	440	
20	b	450	
20	e	450	
21	c	195	
21	f	195	
22	g	558	
23	h	298	
24	i	274	
25	j	66	
26	o	176	

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Mol	Chain	Length	Quality of chain
26	p	176	
27	q	124	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 68831 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 NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

- Molecule 12 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

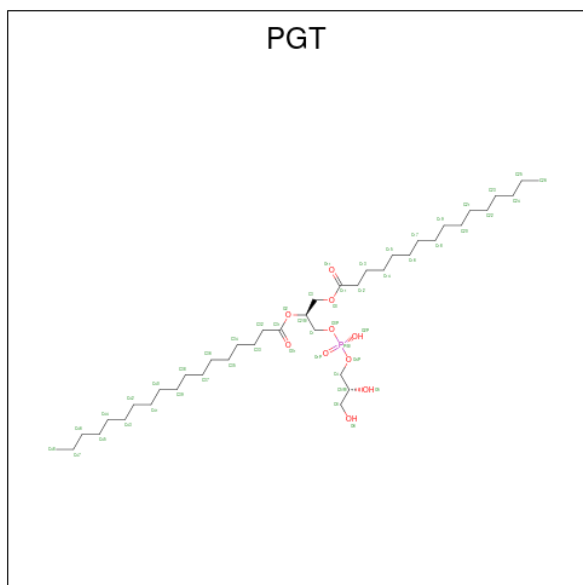
- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		
26	p	45	Total	C	N	O	S	0	0
			330	218	50	60	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYL)OXY]METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



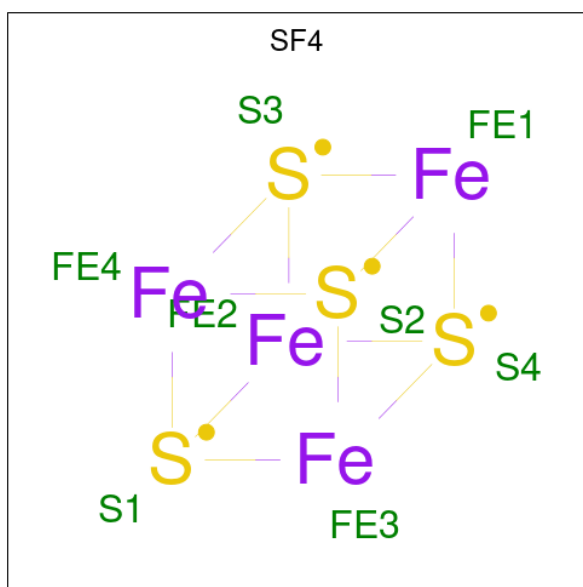
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			51	40	10	1	
28	A	1	Total	C	O	P	0
			51	40	10	1	
28	J	1	Total	C	O	P	0
			51	40	10	1	
28	L	1	Total	C	O	P	0
			51	40	10	1	
28	P	1	Total	C	O	P	0
			51	40	10	1	
28	q	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 29 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



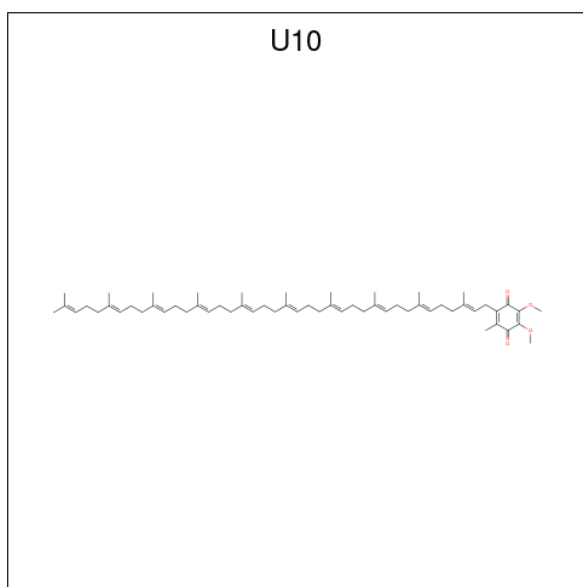
Mol	Chain	Residues	Atoms			AltCon
29	A	1	Total 37	C 32	O 5	0
29	H	1	Total 37	C 32	O 5	0
29	J	1	Total 37	C 32	O 5	0
29	J	1	Total 37	C 32	O 5	0
29	M	1	Total 37	C 32	O 5	0
29	M	1	Total 37	C 32	O 5	0
29	c	1	Total 37	C 32	O 5	0
29	c	1	Total 37	C 32	O 5	0
29	i	1	Total 37	C 32	O 5	0

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	Fe	S	0
			8	4	4	
30	F	1	Total	Fe	S	0
			8	4	4	
30	G	1	Total	Fe	S	0
			8	4	4	
30	G	1	Total	Fe	S	0
			8	4	4	
30	I	1	Total	Fe	S	0
			8	4	4	
30	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 31 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

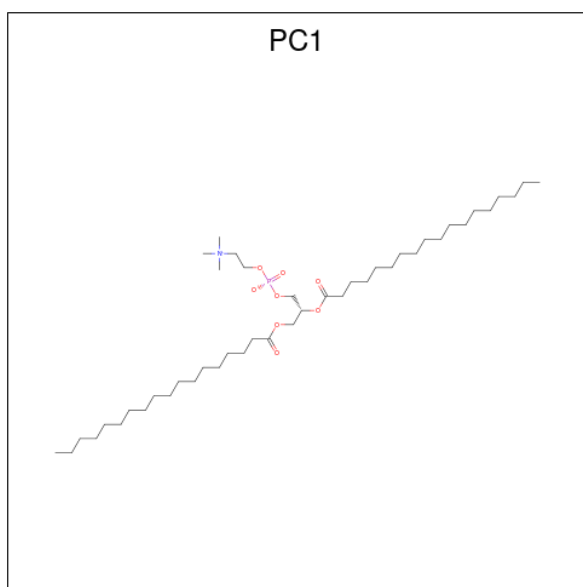


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			63	59	4	
31	a	1	Total	C	O	0
			63	59	4	
31	a	1	Total	C	O	0
			63	59	4	
31	d	1	Total	C	O	0
			63	59	4	
31	d	1	Total	C	O	0
			63	59	4	

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
32	D	1	Total	Ca	0
			1	1	
32	b	1	Total	Ca	0
			1	1	
32	e	1	Total	Ca	0
			1	1	
32	g	1	Total	Ca	0
			1	1	

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



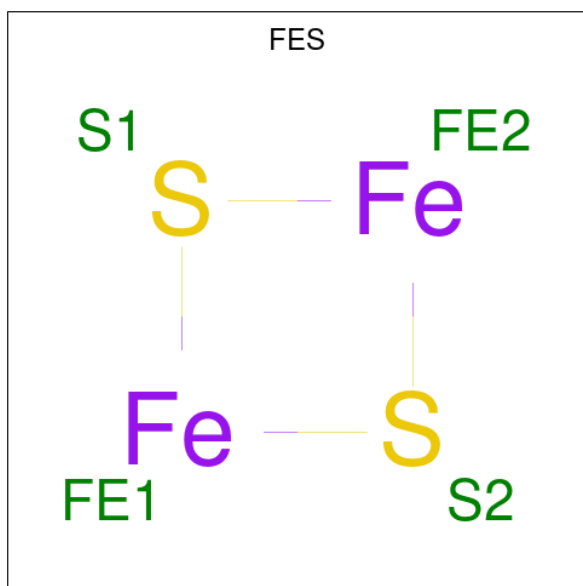
Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	d	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	

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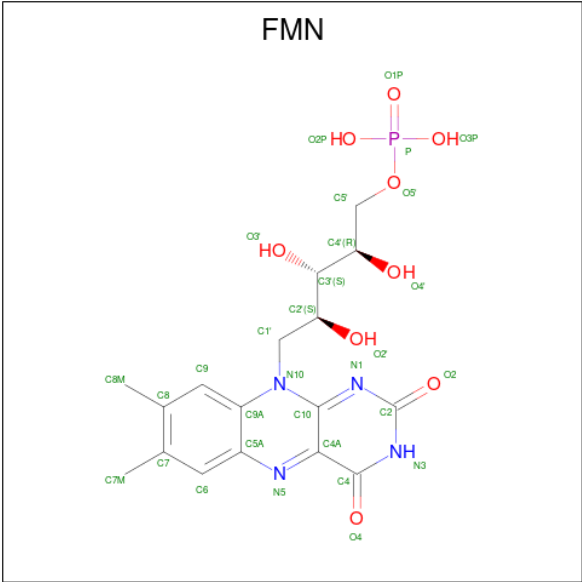
Mol	Chain	Residues	Atoms					AltConf
33	j	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



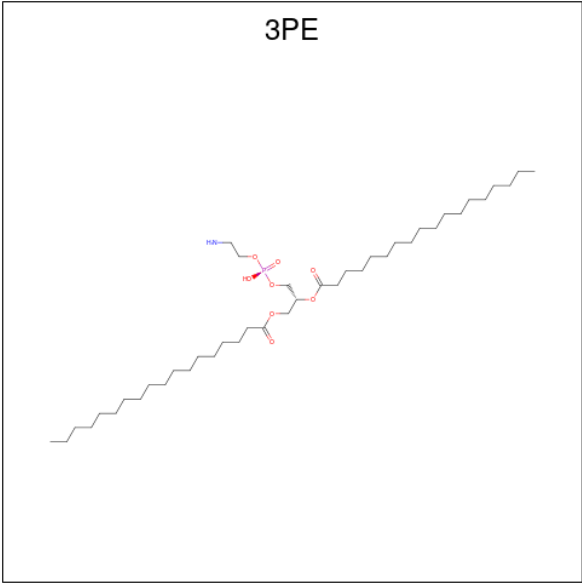
Mol	Chain	Residues	Atoms			AltConf
34	E	1	Total	Fe	S	0
			4	2	2	
34	G	1	Total	Fe	S	0
			4	2	2	
34	c	1	Total	Fe	S	0
			4	2	2	
34	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 35 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 36 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



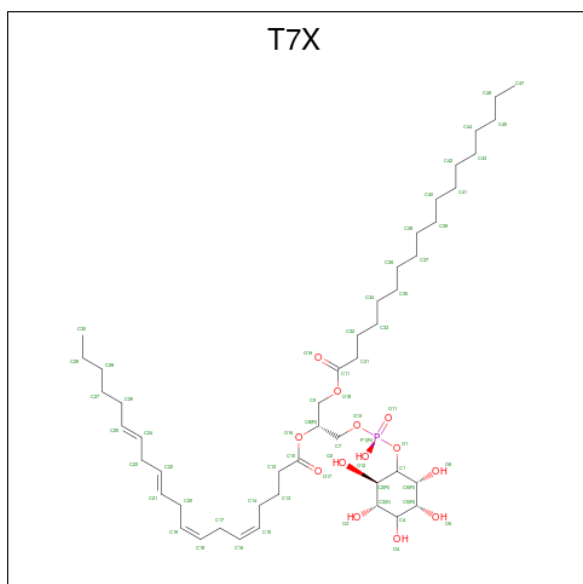
Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

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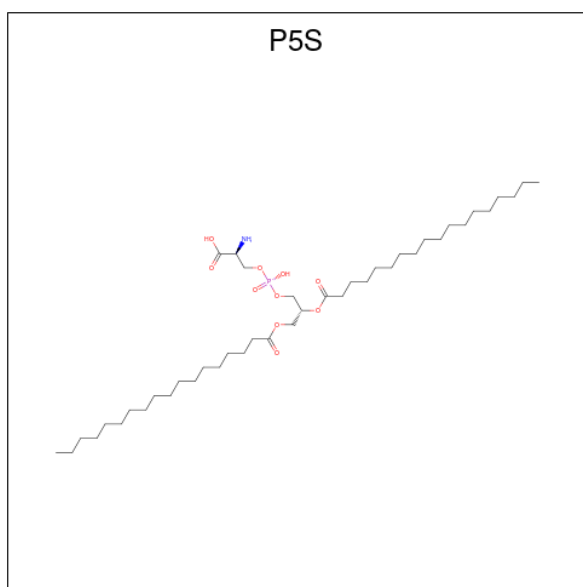
Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	c	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 37 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



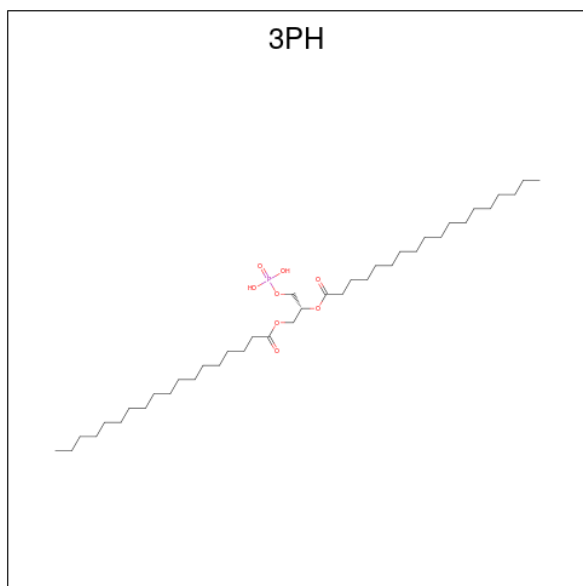
Mol	Chain	Residues	Atoms				AltConf
37	J	1	Total	C	O	P	0
			61	47	13	1	

- Molecule 38 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
38	L	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
39	L	1	Total	C	O	P	0
			48	39	8	1	
39	L	1	Total	C	O	P	0
			48	39	8	1	

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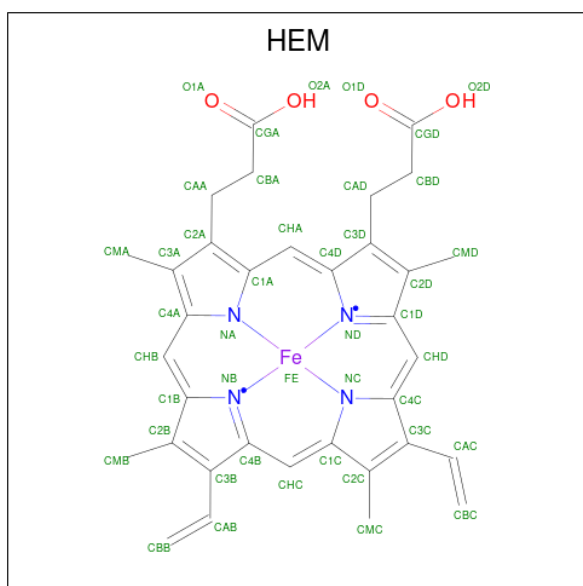
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Mol	Chain	Residues	Atoms				AltConf
39	M	1	Total	C	O	P	0
			48	39	8	1	
39	a	1	Total	C	O	P	0
			48	39	8	1	
39	c	1	Total	C	O	P	0
			48	39	8	1	
39	f	1	Total	C	O	P	0
			48	39	8	1	
39	i	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	R	1	Total	Zn	0
			1	1	
40	i	1	Total	Zn	0
			1	1	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



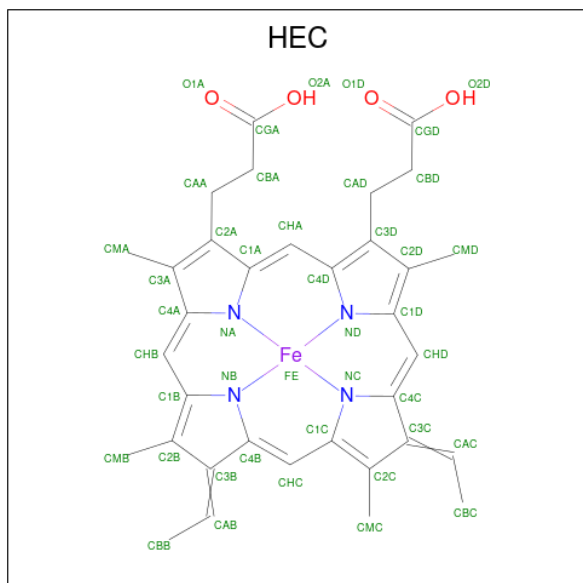
Mol	Chain	Residues	Atoms					AltConf
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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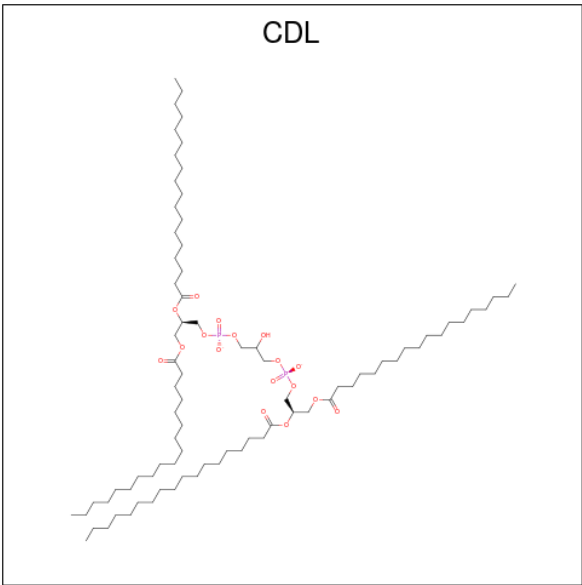
Mol	Chain	Residues	Atoms					AltConf
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



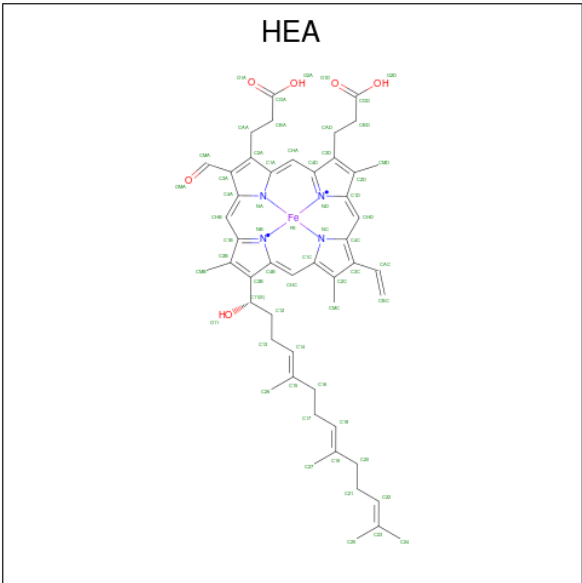
Mol	Chain	Residues	Atoms					AltConf
42	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 43 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
43	d	1	100	81	17	2	0

- Molecule 44 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

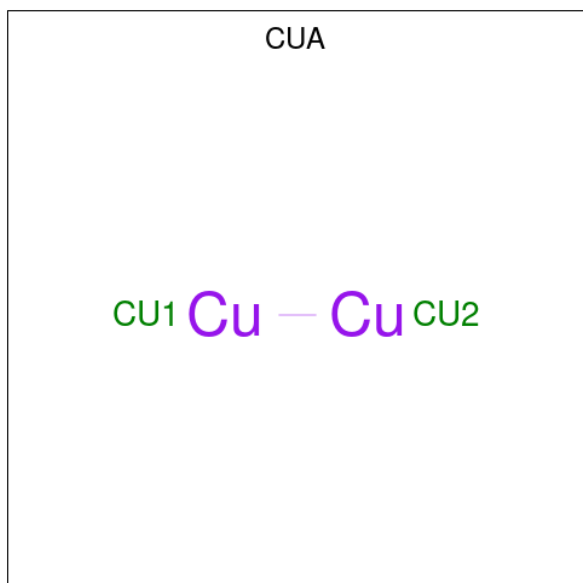
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
45	g	1	Total	Cu	0
			1	1	

- Molecule 46 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
46	g	1	Total	Mn	0
			1	1	

- Molecule 47 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

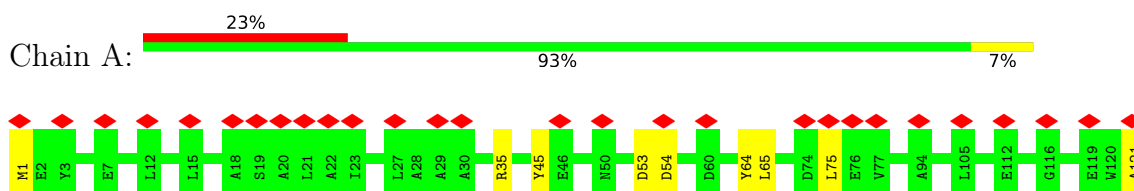


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total	Cu	0
			2	2	

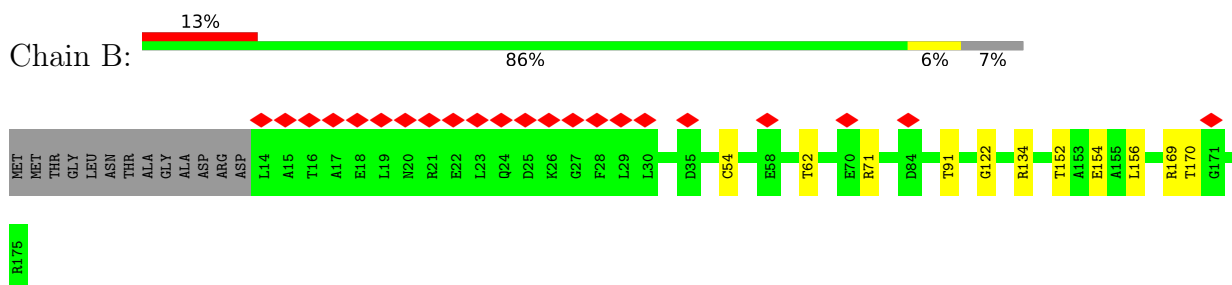
3 Residue-property plots [i](#)

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

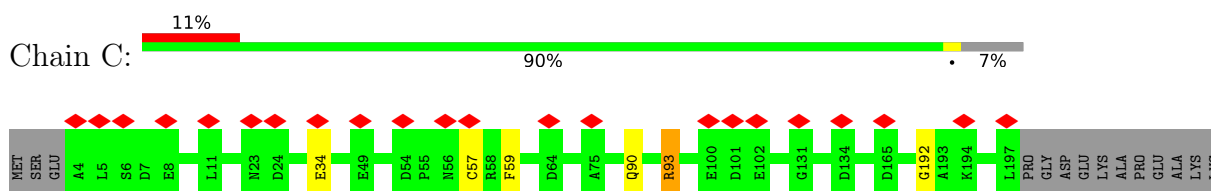
- Molecule 1: NADH-quinone oxidoreductase subunit A



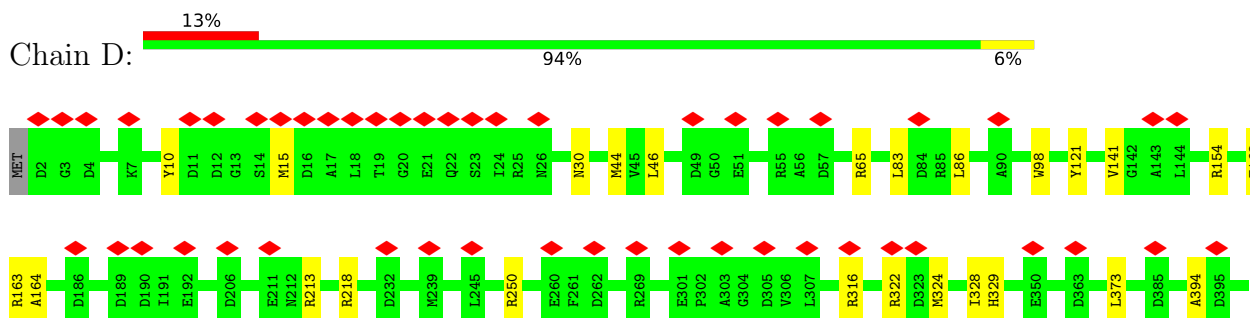
- Molecule 2: NADH-quinone oxidoreductase subunit B

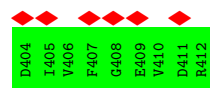


- Molecule 3: NADH-quinone oxidoreductase subunit C

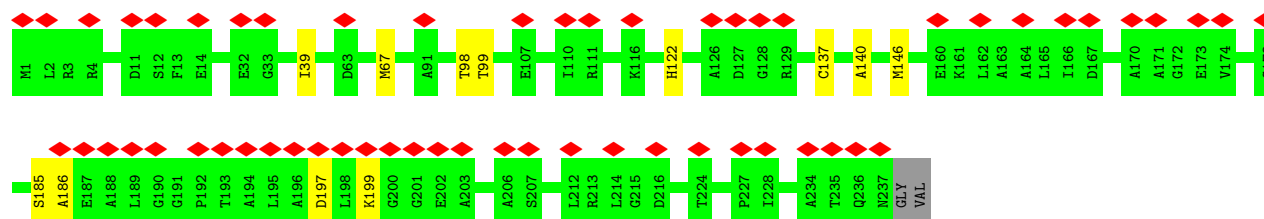
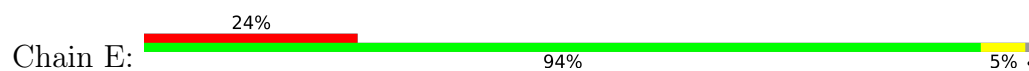


- Molecule 4: NADH-quinone oxidoreductase subunit D

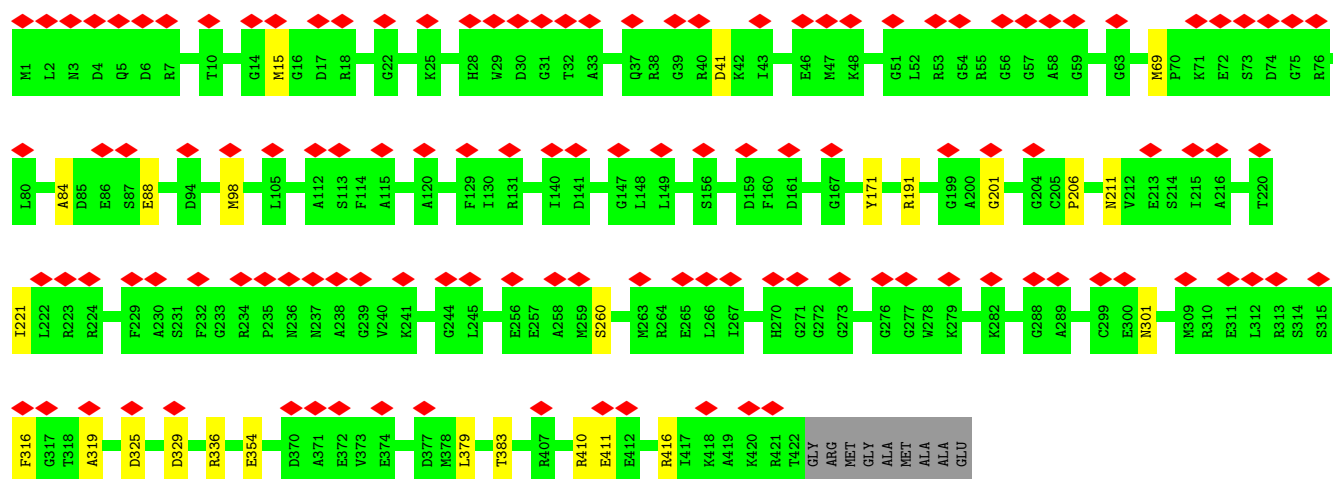
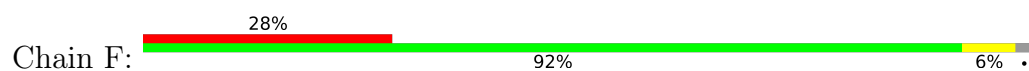




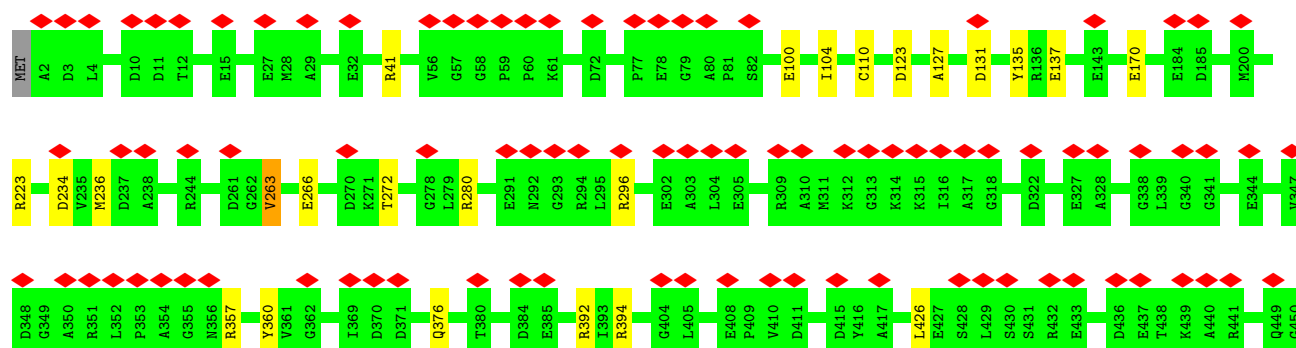
• Molecule 5: NADH dehydrogenase subunit E

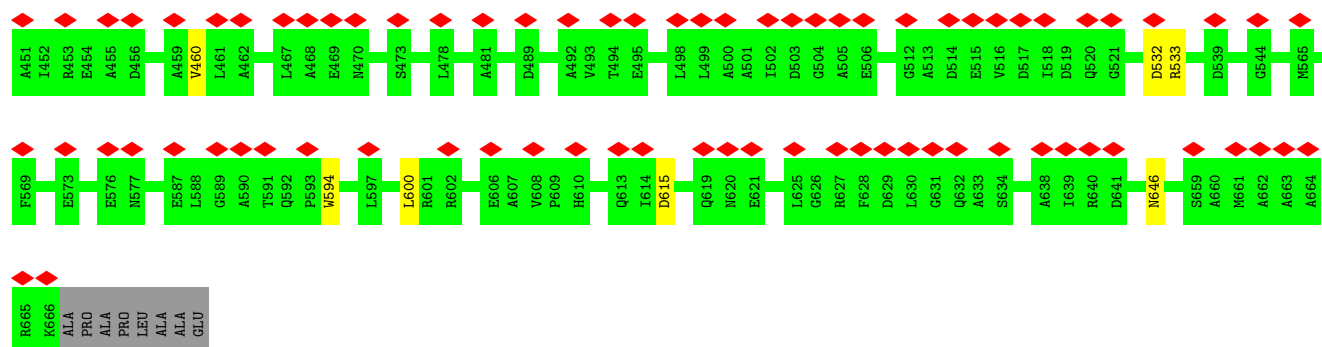


• Molecule 6: NADH-quinone oxidoreductase subunit F



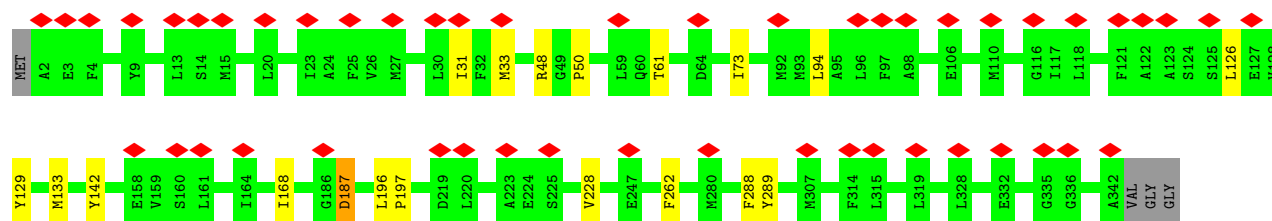
• Molecule 7: NADH-quinone oxidoreductase





- Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H: 14% 93% 5% .



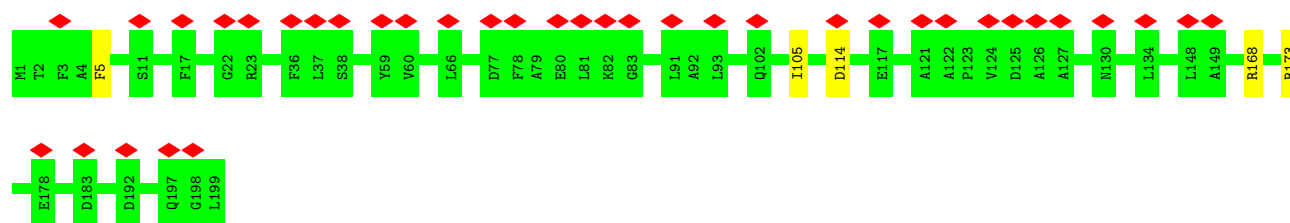
- Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I: 7% 96% . .



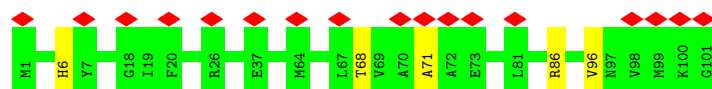
- Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J: 19% 97% .

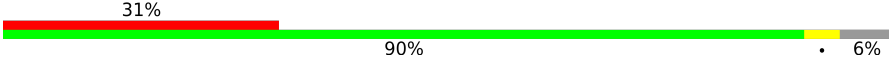


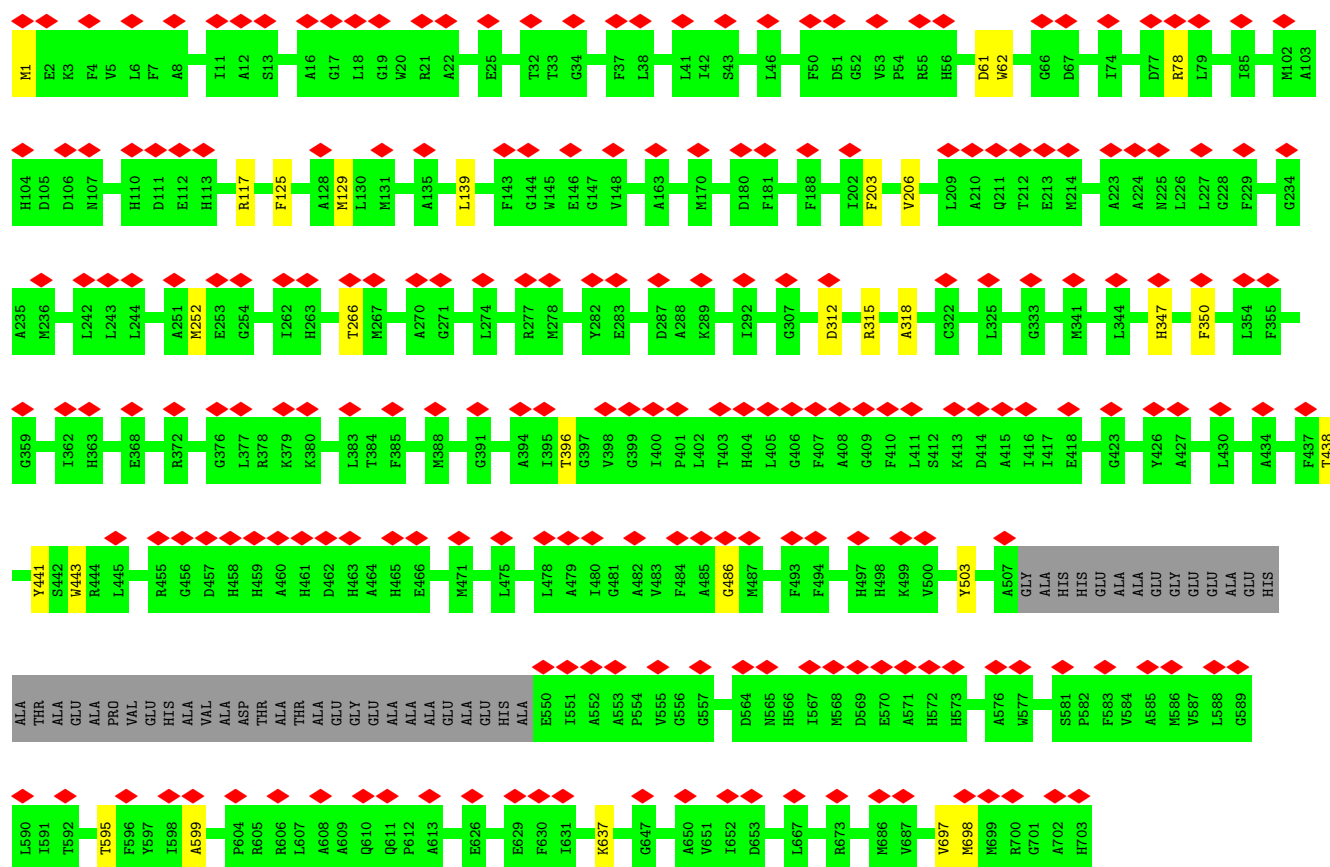
- Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K: 17% 95% 5%

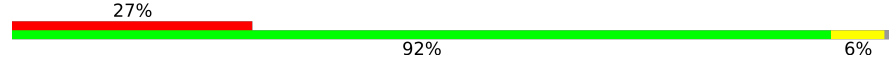


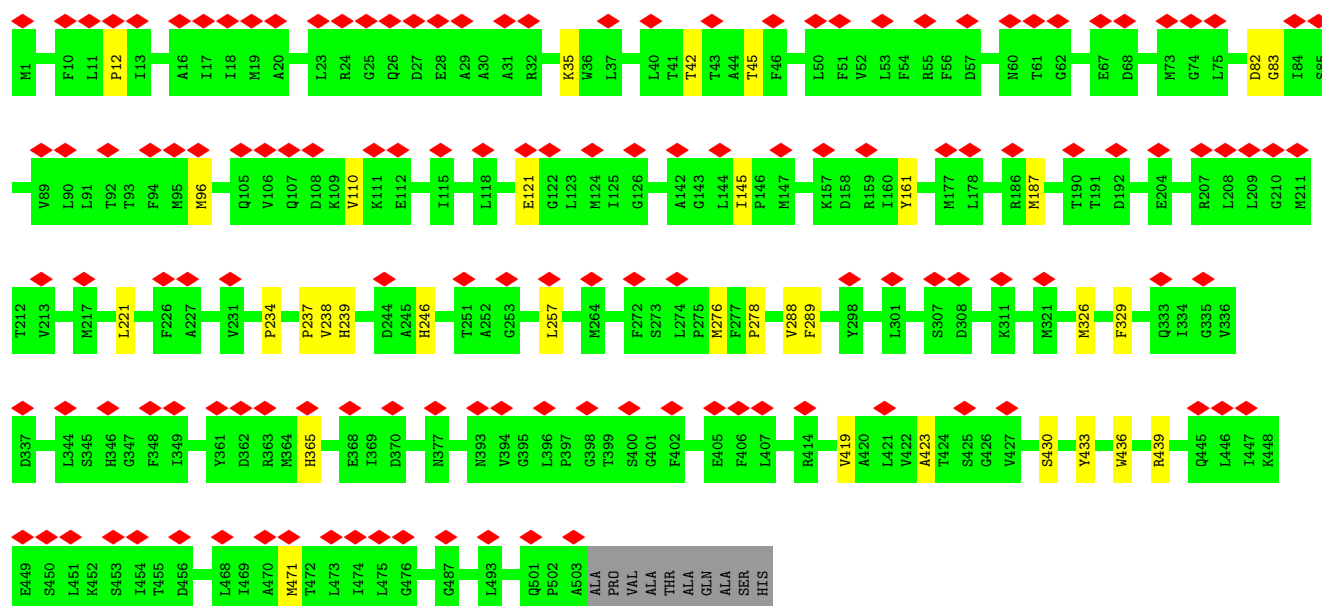
- Molecule 12: NADH dehydrogenase subunit L

Chain L:  31% 90% 6%

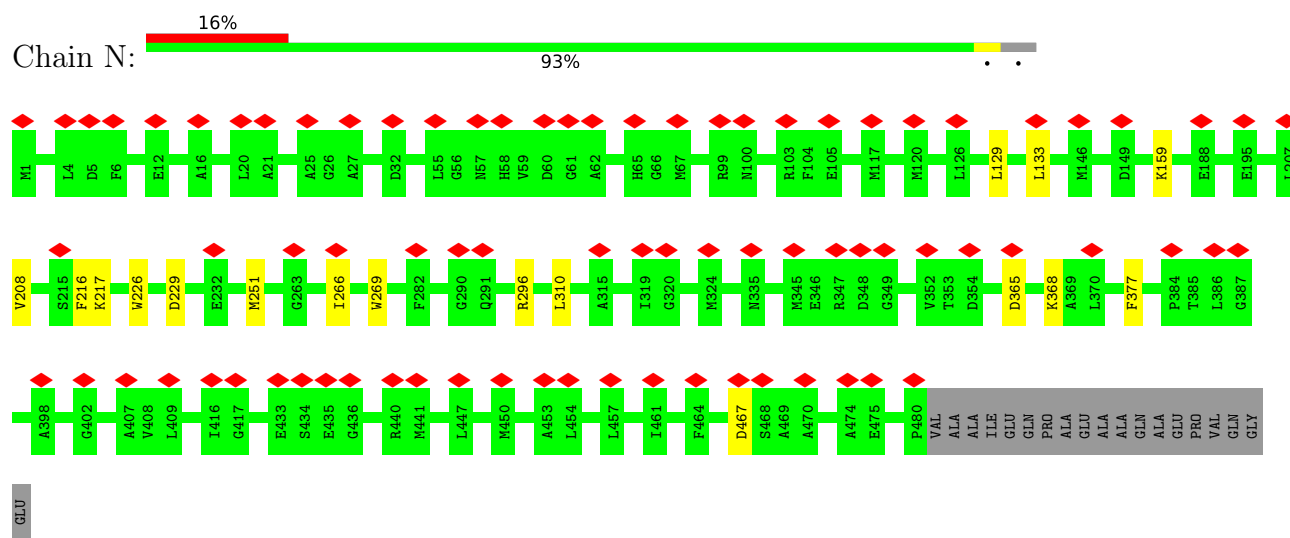


• Molecule 13: NADH dehydrogenase subunit M

Chain M:  27% 92% 6%



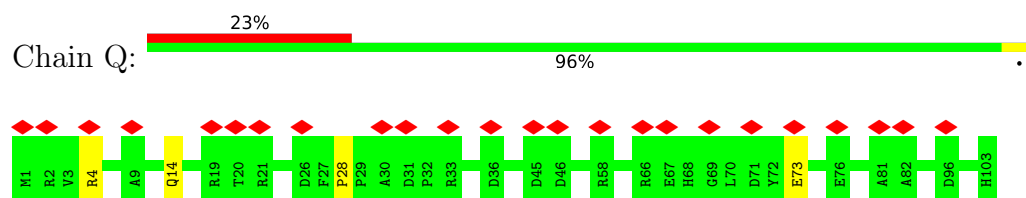
- Molecule 14: NADH-quinone oxidoreductase subunit N



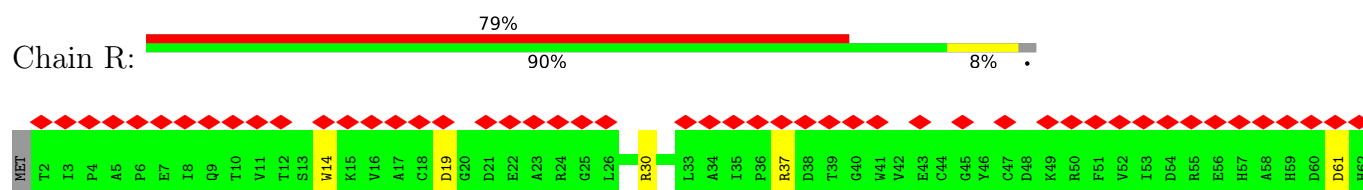
- Molecule 15: NAD-dependent epimerase/dehydratase



- Molecule 16: ETC complex I subunit conserved region

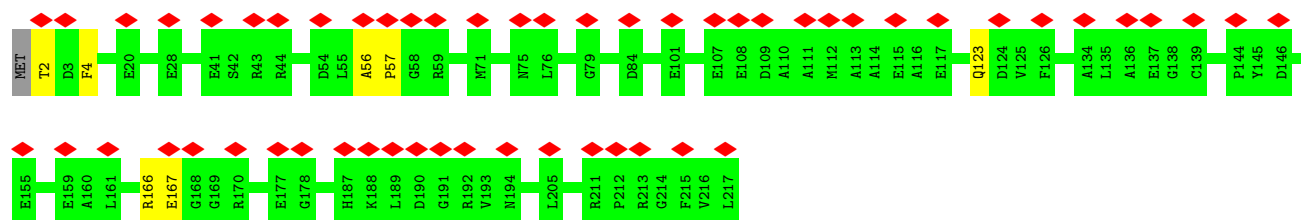


- Molecule 17: Zinc finger CHCC-type domain-containing protein



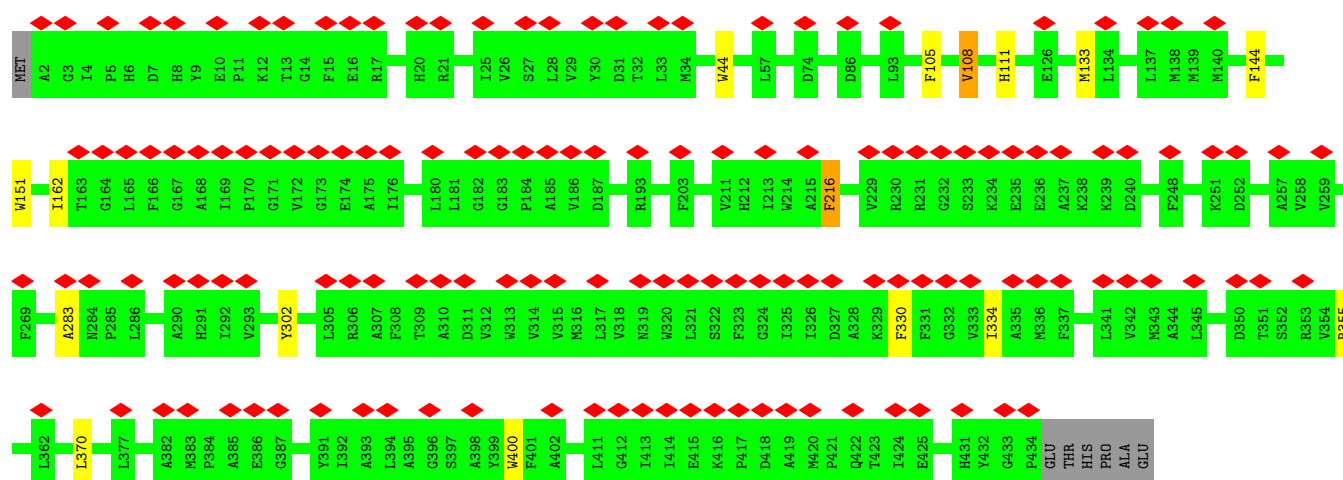
- Molecule 18: Protein-L-isoaspartate O-methyltransferase

Chain Z:  25% 96%

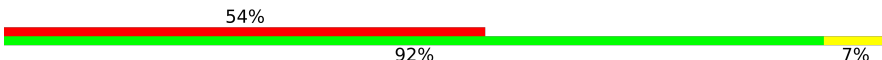


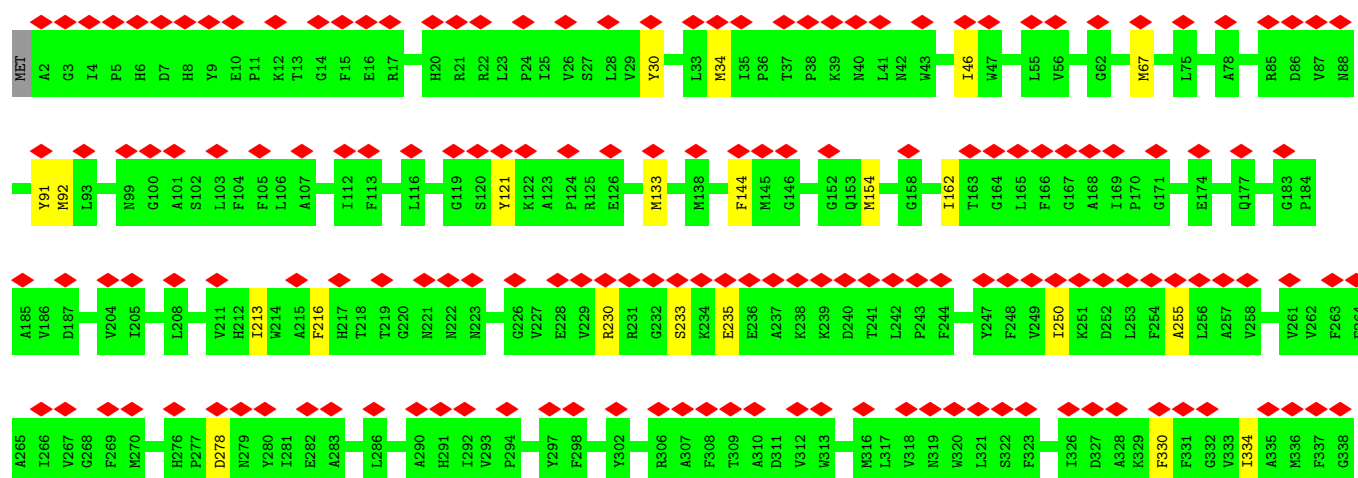
- Molecule 19: Cytochrome b

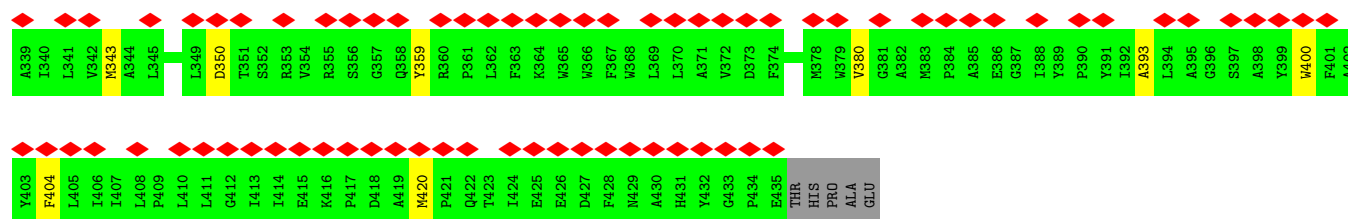
Chain a:  32% 95%



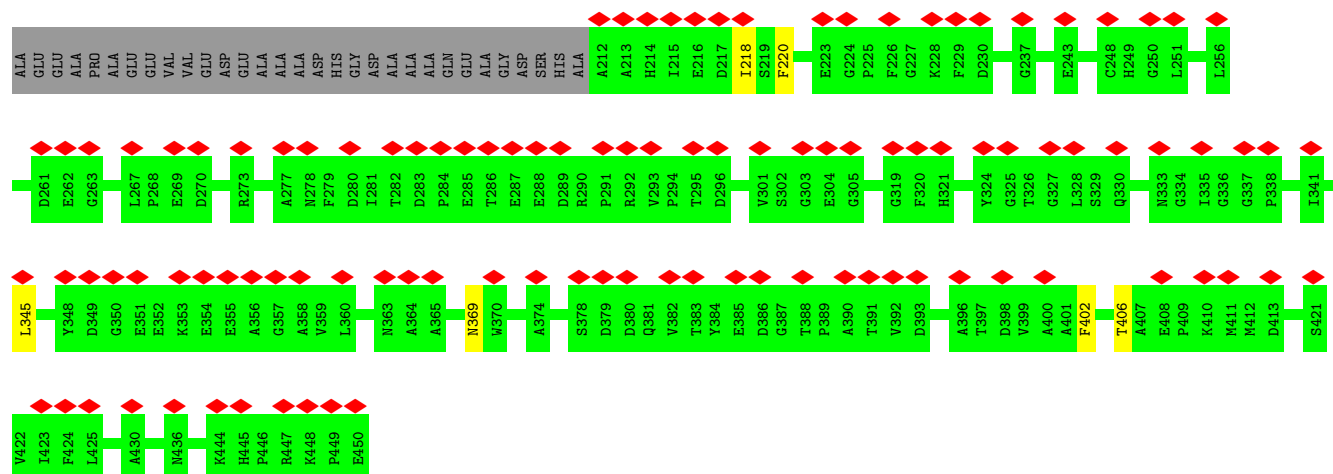
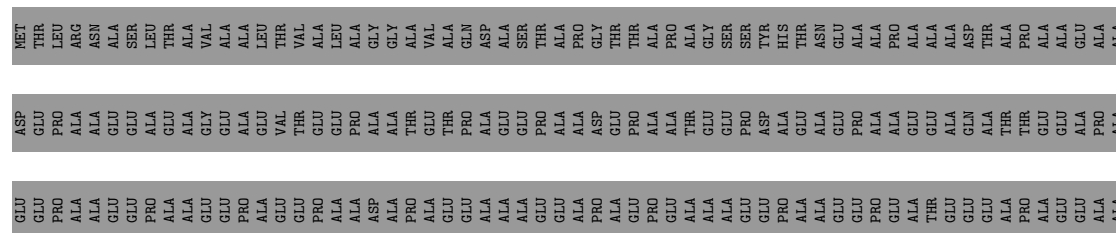
- Molecule 19: Cytochrome b

Chain d:  54% 92% 7%

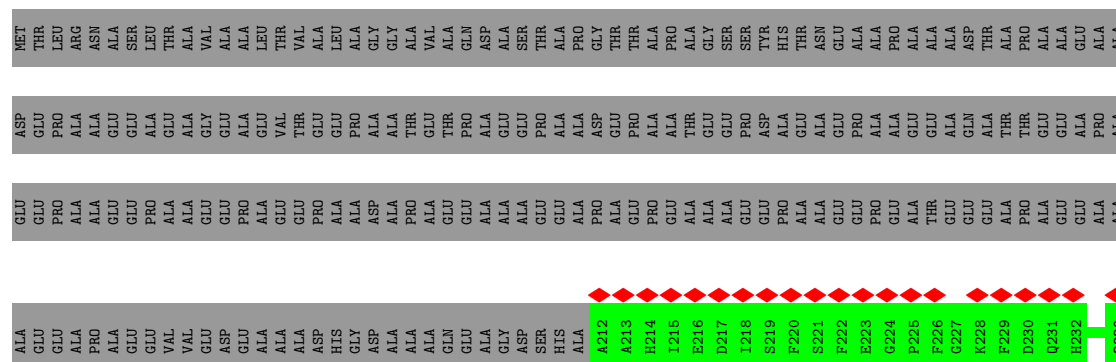


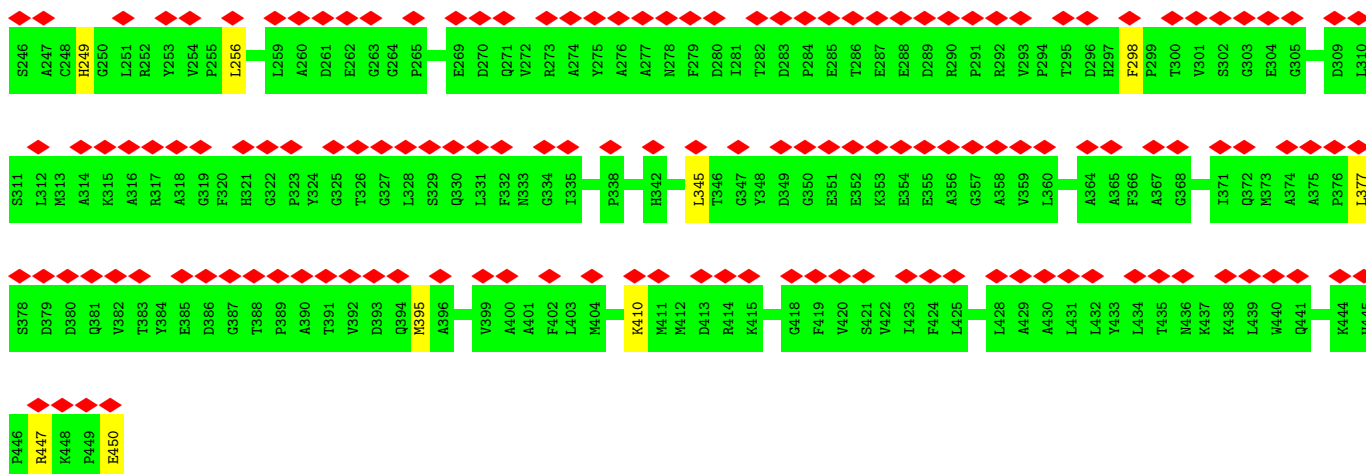


• Molecule 20: Cytochrome c1

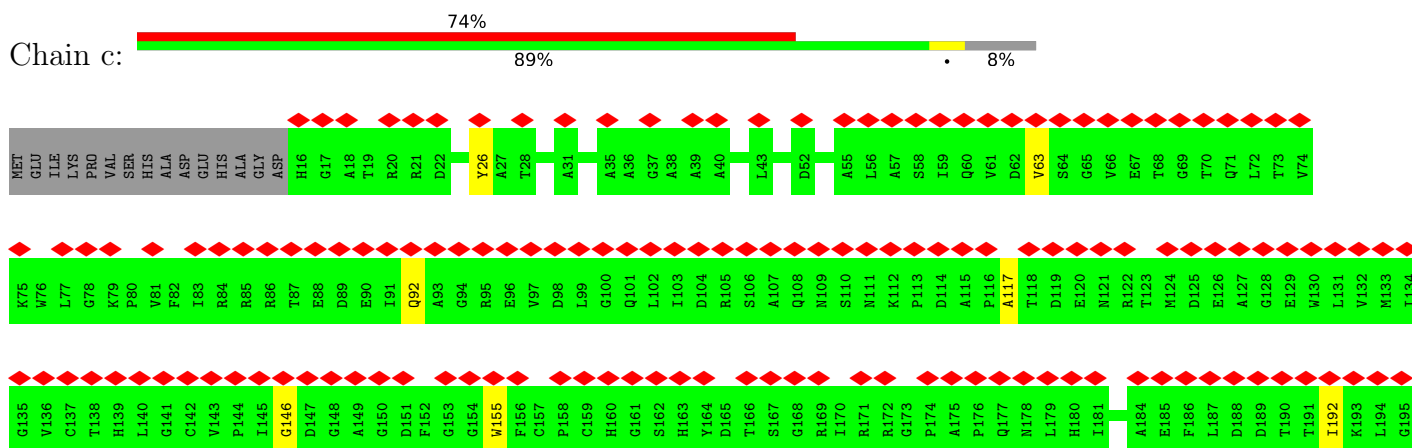


• Molecule 20: Cytochrome c1

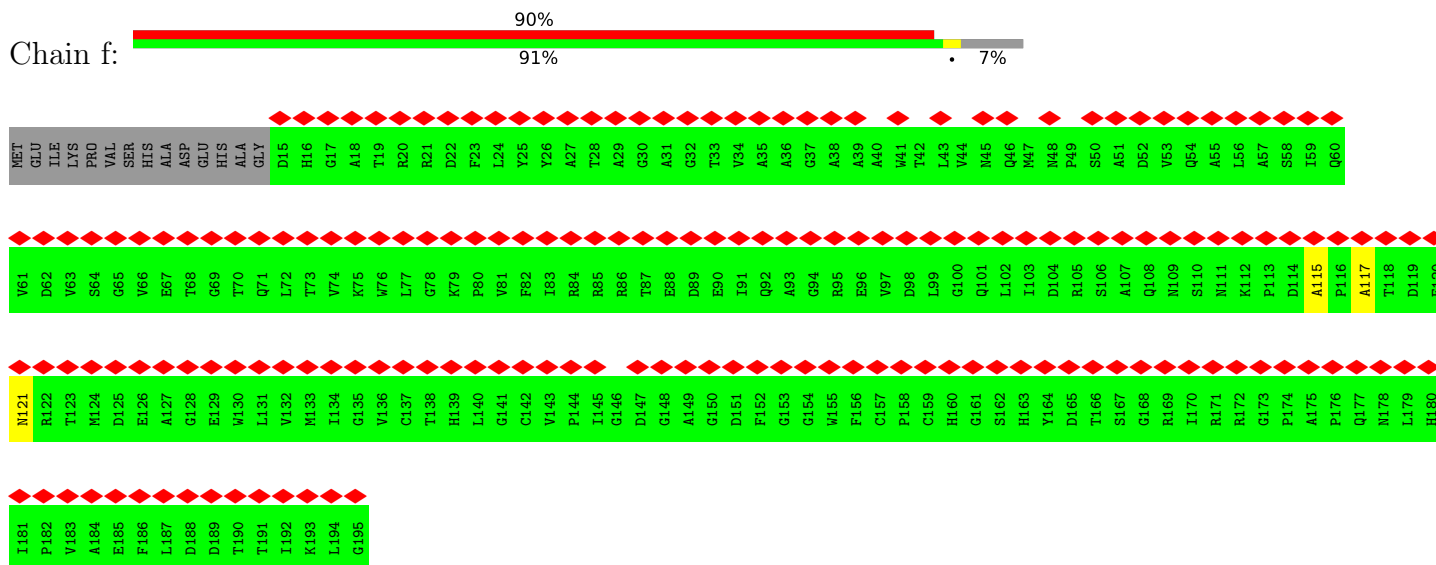




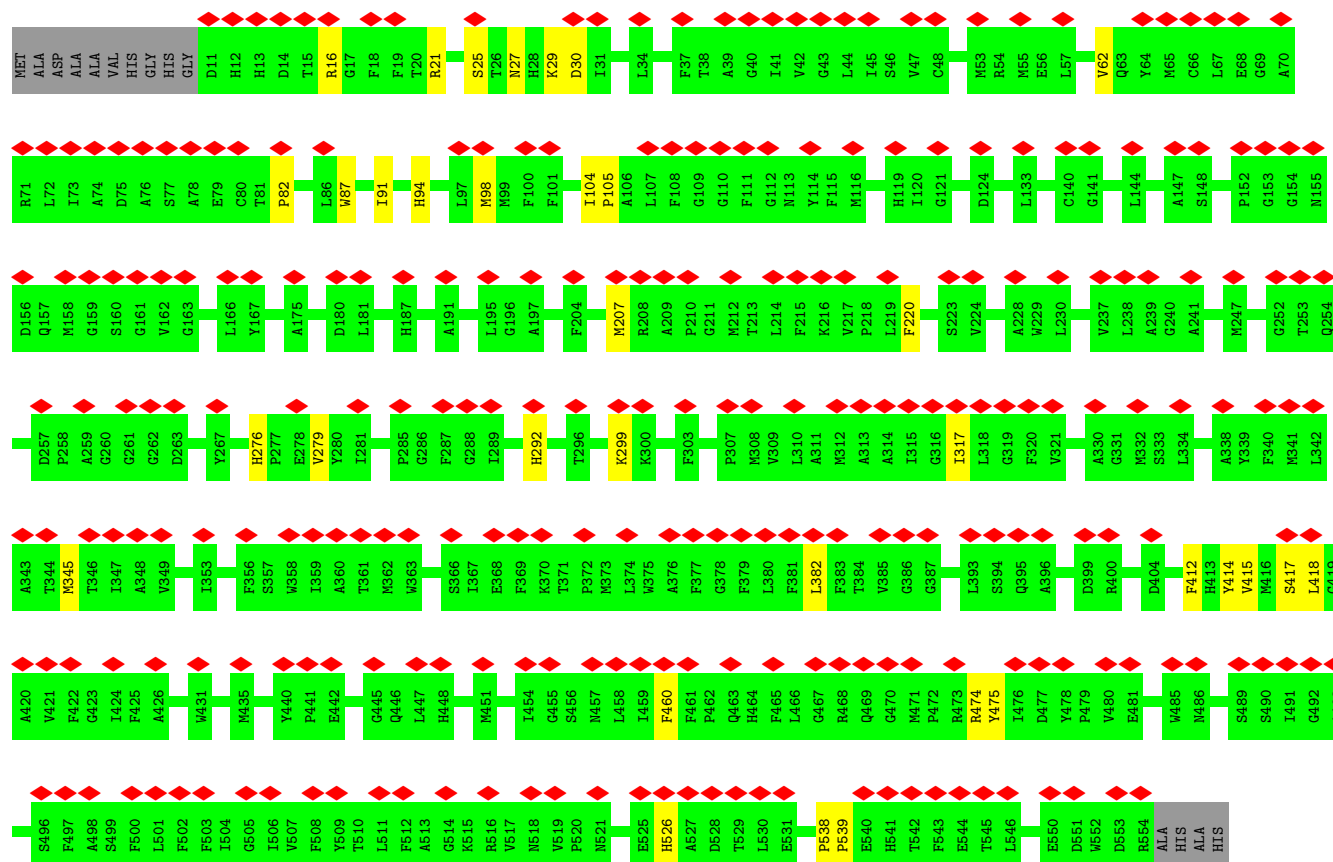
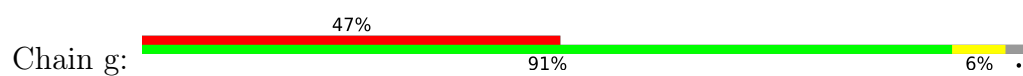
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

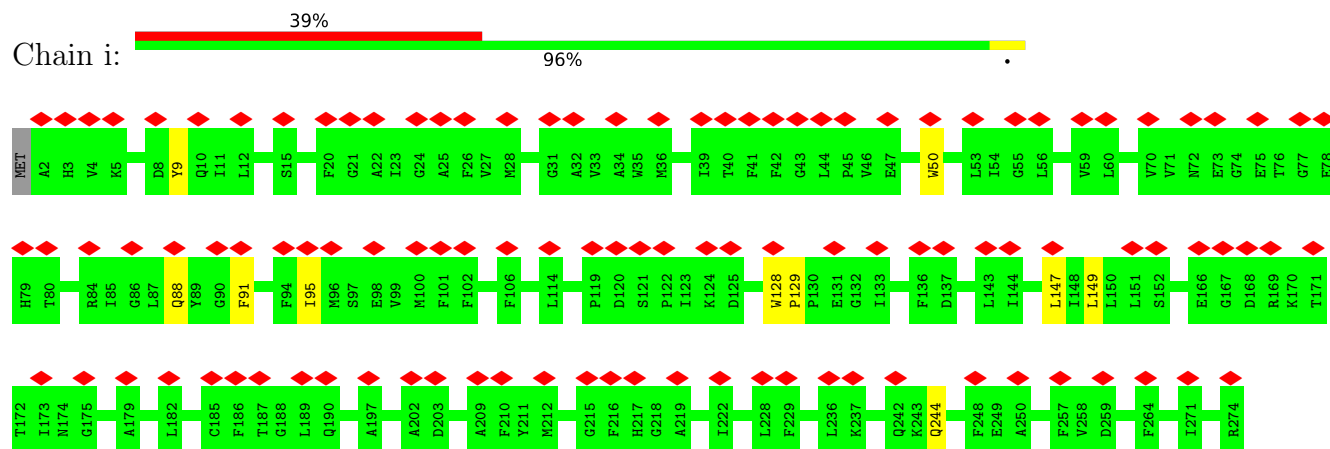


- Molecule 22: Cytochrome c oxidase subunit 1



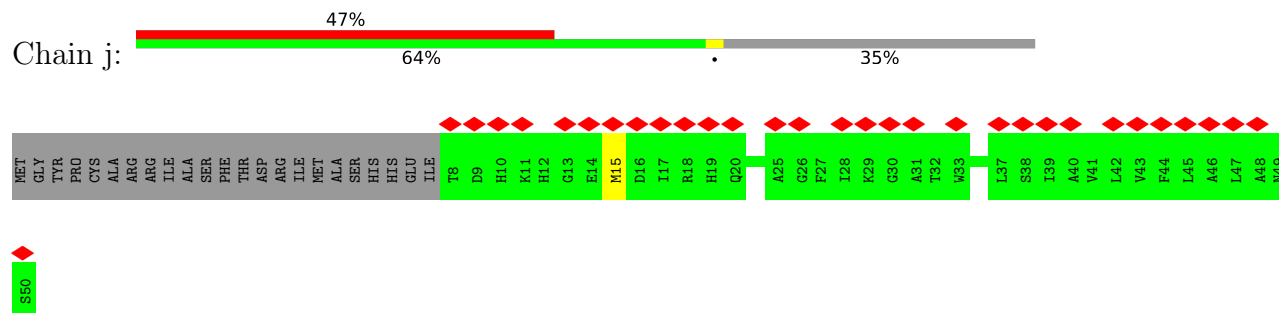
- Molecule 24: cytochrome-c oxidase

Chain i:



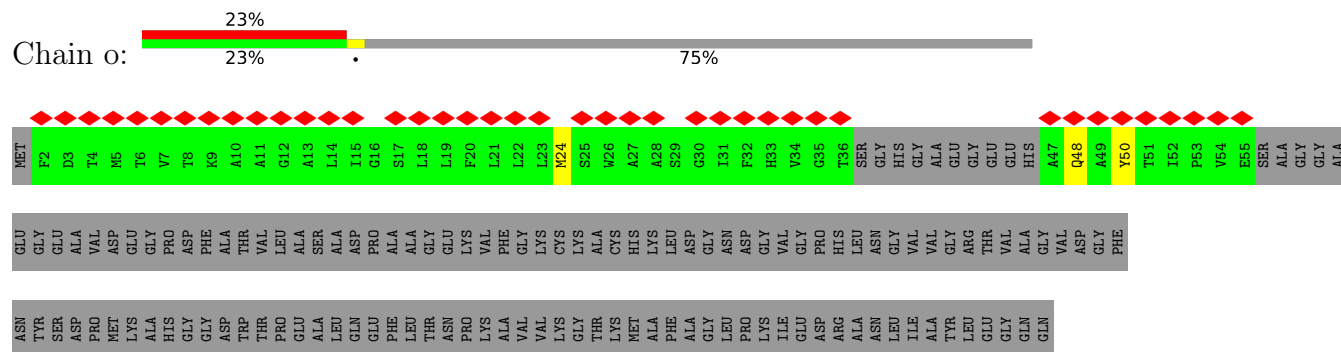
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV

Chain j:



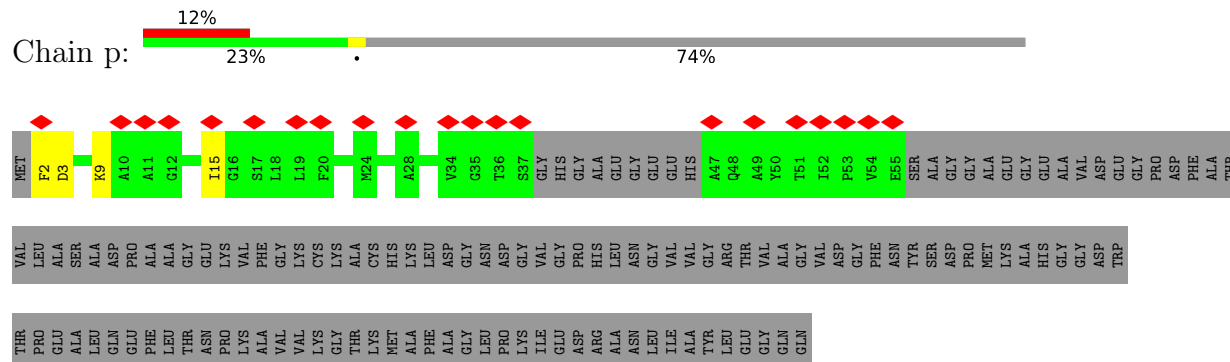
- Molecule 26: Cytochrome c, class I

Chain o:

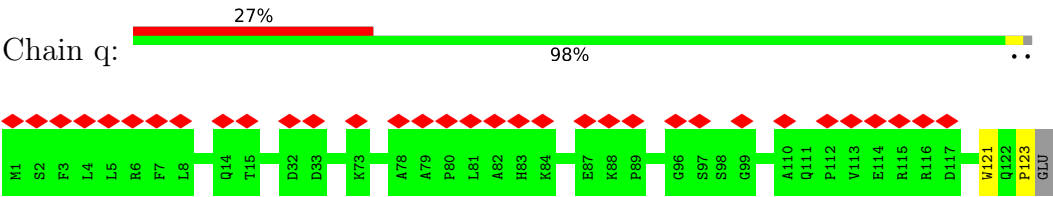


- Molecule 26: Cytochrome c, class I

Chain p:



● Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16429	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.040	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, HEM, FMN, T7X, CA, P5S, SF4, FES, CUA, PGT, DU0, 3PH, U10, FME, PC1, MN, HEA, CU, 2MR, 3PE, HEC, ZN

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	0.37	0/988	0.53	0/1345
2	B	0.46	0/1297	0.62	0/1758
3	C	0.40	0/1624	0.58	0/2208
4	D	0.43	0/3339	0.60	0/4520
5	E	0.30	0/1865	0.58	0/2537
6	F	0.30	0/3308	0.57	0/4456
7	G	0.35	0/5156	0.59	0/6982
8	H	0.38	0/2815	0.58	0/3837
9	I	0.47	0/1354	0.62	0/1828
10	J	0.35	0/1548	0.60	0/2104
11	K	0.39	0/775	0.56	0/1050
12	L	0.30	0/5379	0.53	0/7323
13	M	0.34	0/4010	0.57	0/5460
14	N	0.35	0/3634	0.54	0/4935
15	P	0.29	0/2511	0.59	0/3409
16	Q	0.34	0/872	0.57	0/1181
17	R	0.27	0/503	0.59	0/685
18	Z	0.32	0/1669	0.60	0/2266
19	a	0.35	0/3641	0.55	0/4993
19	d	0.29	0/3650	0.55	0/5005
20	b	0.29	0/1906	0.53	0/2592
20	e	0.24	0/1906	0.60	0/2592
21	c	0.25	0/1382	0.55	0/1880
21	f	0.25	0/1390	0.59	0/1891
22	g	0.29	0/4483	0.57	0/6118
23	h	0.24	0/2033	0.56	0/2787
24	i	0.30	0/2270	0.53	0/3107
25	j	0.25	0/339	0.47	0/457
26	o	0.22	0/330	0.53	0/448
26	p	0.30	0/336	0.54	0/456
27	q	0.34	0/1049	0.59	0/1434

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.33	0/67362	0.57	0/91644

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
4	D	0	3
6	F	0	2
7	G	0	3
9	I	0	2
13	M	0	1
14	N	0	1
19	a	0	1
19	d	0	1
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
3	C	93	ARG	Sidechain
4	D	154	ARG	Sidechain
4	D	250	ARG	Sidechain
4	D	316	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	970	9	0
2	B	1270	0	1268	4	0
3	C	1586	0	1562	5	0
4	D	3277	0	3217	16	0
5	E	1822	0	1796	6	0
6	F	3241	0	3188	14	0
7	G	5068	0	5037	15	0
8	H	2722	0	2744	12	0
9	I	1319	0	1259	3	0
10	J	1528	0	1612	5	0
11	K	764	0	817	5	0
12	L	5215	0	5174	16	0
13	M	3915	0	4024	17	0
14	N	3556	0	3656	9	0
15	P	2468	0	2498	3	0
16	Q	849	0	812	2	0
17	R	488	0	450	3	0
18	Z	1642	0	1643	3	0
19	a	3504	0	3483	10	0
19	d	3513	0	3489	16	0
20	b	1855	0	1773	4	0
20	e	1855	0	1773	7	0
21	c	1353	0	1297	3	0
21	f	1361	0	1301	1	0
22	g	4322	0	4225	22	0
23	h	1976	0	1960	9	0
24	i	2183	0	2144	9	0
25	j	332	0	331	1	0
26	o	324	0	330	1	0
26	p	330	0	335	3	0
27	q	1018	0	942	1	0
28	A	102	0	156	0	0
28	J	51	0	78	0	0
28	L	51	0	78	0	0
28	P	51	0	78	0	0
28	q	51	0	78	0	0
29	A	37	0	0	0	0
29	H	37	0	0	0	0
29	J	74	0	0	0	0
29	M	74	0	0	0	0
29	c	74	0	0	0	0
29	i	37	0	0	0	0
30	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	8	0	0	0	0
30	G	16	0	0	0	0
30	I	16	0	0	0	0
31	B	63	0	90	0	0
31	a	126	0	180	3	0
31	d	126	0	180	7	0
32	D	1	0	0	0	0
32	b	1	0	0	0	0
32	e	1	0	0	0	0
32	g	1	0	0	0	0
33	D	54	0	88	1	0
33	H	54	0	88	1	0
33	L	54	0	88	1	0
33	M	108	0	176	0	0
33	a	216	0	352	0	0
33	d	54	0	88	0	0
33	i	216	0	352	3	0
33	j	54	0	88	2	0
34	E	4	0	0	0	0
34	G	4	0	0	0	0
34	c	4	0	0	0	0
34	f	4	0	0	0	0
35	F	31	0	19	3	0
36	H	51	0	82	0	0
36	I	51	0	82	0	0
36	L	51	0	82	1	0
36	b	51	0	82	0	0
36	c	51	0	82	0	0
36	d	51	0	82	0	0
36	i	102	0	164	0	0
37	J	61	0	0	0	0
38	L	54	0	80	0	0
39	L	96	0	150	1	0
39	M	48	0	75	0	0
39	a	48	0	75	1	0
39	c	48	0	75	0	0
39	f	48	0	75	0	0
39	i	48	0	75	0	0
40	R	1	0	0	0	0
40	i	1	0	0	0	0
41	a	86	0	60	1	0
41	d	86	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	b	43	0	30	3	0
42	e	43	0	30	4	0
43	d	100	0	156	0	0
44	g	120	0	108	5	0
45	g	1	0	0	0	0
46	g	1	0	0	0	0
47	h	2	0	0	0	0
All	All	68831	0	69072	213	0

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

The worst 5 of 213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD11	11:K:71:ALA:HB3	1.58	0.84
1:A:64:TYR:OH	11:K:86:ARG:NH2	2.19	0.76
31:d:506:U10:H1M1	31:d:506:U10:H1O2	1.71	0.71
13:M:96:MET:HE3	13:M:121:GLU:HB2	1.75	0.68
12:L:438:THR:HA	12:L:441:TYR:CE2	2.31	0.66

There are no symmetry-related clashes.

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	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
2	B	160/175 (91%)	152 (95%)	7 (4%)	1 (1%)	21	57
3	C	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
4	D	408/412 (99%)	395 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	235/239 (98%)	224 (95%)	9 (4%)	2 (1%)	14	48
6	F	420/431 (97%)	396 (94%)	23 (6%)	1 (0%)	43	75
7	G	663/674 (98%)	635 (96%)	26 (4%)	2 (0%)	36	69
8	H	339/345 (98%)	324 (96%)	15 (4%)	0	100	100
9	I	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
10	J	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
11	K	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	45
12	L	657/703 (94%)	628 (96%)	28 (4%)	1 (0%)	43	75
13	M	501/513 (98%)	493 (98%)	7 (1%)	1 (0%)	43	75
14	N	478/499 (96%)	468 (98%)	10 (2%)	0	100	100
15	P	326/330 (99%)	314 (96%)	11 (3%)	1 (0%)	36	69
16	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
17	R	59/62 (95%)	56 (95%)	2 (3%)	1 (2%)	7	35
18	Z	214/217 (99%)	206 (96%)	8 (4%)	0	100	100
19	a	431/440 (98%)	423 (98%)	8 (2%)	0	100	100
19	d	432/440 (98%)	421 (98%)	11 (2%)	0	100	100
20	b	237/450 (53%)	235 (99%)	1 (0%)	1 (0%)	30	64
20	e	237/450 (53%)	229 (97%)	7 (3%)	1 (0%)	30	64
21	c	178/195 (91%)	168 (94%)	9 (5%)	1 (1%)	21	57
21	f	179/195 (92%)	170 (95%)	8 (4%)	1 (1%)	21	57
22	g	542/558 (97%)	524 (97%)	18 (3%)	0	100	100
23	h	250/298 (84%)	238 (95%)	11 (4%)	1 (0%)	30	64
24	i	271/274 (99%)	266 (98%)	5 (2%)	0	100	100
25	j	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
26	o	40/176 (23%)	40 (100%)	0	0	100	100
26	p	41/176 (23%)	41 (100%)	0	0	100	100
27	q	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
All	All	8328/9337 (89%)	8039 (96%)	273 (3%)	16 (0%)	44	75

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS

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Mol	Chain	Res	Type
13	M	238	VAL
15	P	87	GLY
20	b	369	ASN
6	F	201	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	134 (98%)	2 (2%)	57	70
3	C	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	326 (98%)	5 (2%)	57	70
7	G	530/535 (99%)	527 (99%)	3 (1%)	78	80
8	H	277/279 (99%)	275 (99%)	2 (1%)	76	79
9	I	136/137 (99%)	135 (99%)	1 (1%)	76	79
10	J	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	81 (100%)	0	100	100
12	L	520/543 (96%)	519 (100%)	1 (0%)	87	87
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	82
14	N	357/369 (97%)	356 (100%)	1 (0%)	86	85
15	P	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	86 (99%)	1 (1%)	65	74
17	R	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	166 (99%)	1 (1%)	78	80
19	a	360/366 (98%)	357 (99%)	3 (1%)	73	77
19	d	361/366 (99%)	359 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100
21	c	139/151 (92%)	138 (99%)	1 (1%)	76	79
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	445 (100%)	2 (0%)	84	83
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	82
24	i	220/221 (100%)	220 (100%)	0	100	100
25	j	34/53 (64%)	34 (100%)	0	100	100
26	o	33/126 (26%)	32 (97%)	1 (3%)	36	57
26	p	34/126 (27%)	34 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
All	All	6754/7366 (92%)	6725 (100%)	29 (0%)	81	83

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	365	HIS
23	h	30	GLN
16	Q	73	GLU
19	d	250	ILE
14	N	129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
16	Q	78	HIS
21	c	45	ASN
25	j	49	ASN
18	Z	78	ASN
20	b	436	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
13	FME	M	1	13	8,9,10	1.00	0	8,9,11	0.91	0
10	FME	J	1	10	8,9,10	1.00	0	8,9,11	0.98	0
4	2MR	D	65	4	10,12,13	2.12	3 (30%)	5,13,15	0.95	0
27	FME	q	1	27	8,9,10	1.01	0	8,9,11	0.90	0
12	FME	L	1	12	8,9,10	1.03	1 (12%)	8,9,11	0.82	0
1	FME	A	1	1	8,9,10	0.94	0	8,9,11	1.10	1 (12%)

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
13	FME	M	1	13	-	1/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
4	2MR	D	65	4	-	0/10/13/15	-
27	FME	q	1	27	-	0/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	2MR	CZ-NH2	4.24	1.42	1.33
4	D	65	2MR	CZ-NE	3.94	1.42	1.34
4	D	65	2MR	CQ1-NH1	-2.27	1.41	1.46
12	L	1	FME	CA-N	-2.08	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CB-CA-N	2.06	114.26	110.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 8 are monoatomic - leaving 73 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	$\# Z > 2$
44	HEA	g	604	22	67,67,67	1.36	6 (8%)	81,103,103	2.32	29 (35%)
33	PC1	L	802	-	53,53,53	0.96	3 (5%)	59,61,61	1.00	2 (3%)
29	DU0	M	2004	-	42,42,42	0.79	0	64,66,66	0.97	4 (6%)
33	PC1	j	1001	-	53,53,53	0.97	4 (7%)	59,61,61	0.89	4 (6%)
33	PC1	M	2005	-	53,53,53	0.97	3 (5%)	59,61,61	0.88	2 (3%)
36	3PE	i	1004	-	50,50,50	0.98	4 (8%)	53,55,55	1.12	5 (9%)
33	PC1	H	403	-	53,53,53	0.97	4 (7%)	59,61,61	0.84	2 (3%)
28	PGT	q	1000	-	50,50,50	0.93	4 (8%)	53,56,56	0.84	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SF4	G	702	7	0,12,12	-	-	-		
39	3PH	a	503	-	47,47,47	1.38	5 (10%)	50,52,52	1.05	2 (4%)
33	PC1	M	2003	-	53,53,53	0.99	3 (5%)	59,61,61	0.84	1 (1%)
39	3PH	L	806	-	47,47,47	1.34	6 (12%)	50,52,52	1.16	5 (10%)
43	CDL	d	501	-	99,99,99	0.93	7 (7%)	105,111,111	0.92	6 (5%)
36	3PE	d	505	-	50,50,50	0.96	4 (8%)	53,55,55	0.96	3 (5%)
30	SF4	G	703	7	0,12,12	-	-	-		
29	DU0	c	204	-	42,42,42	0.71	0	64,66,66	1.20	7 (10%)
41	HEM	d	503	19	50,50,50	1.28	5 (10%)	67,82,82	1.01	2 (2%)
29	DU0	A	1002	-	42,42,42	0.67	0	64,66,66	1.07	4 (6%)
39	3PH	f	202	-	47,47,47	1.40	6 (12%)	50,52,52	0.96	5 (10%)
41	HEM	a	505	19	50,50,50	1.28	6 (12%)	67,82,82	1.07	2 (2%)
28	PGT	J	203	-	50,50,50	0.93	4 (8%)	53,56,56	0.83	4 (7%)
41	HEM	a	507	19	50,50,50	1.32	7 (14%)	67,82,82	1.01	2 (2%)
28	PGT	A	1003	-	50,50,50	0.93	4 (8%)	53,56,56	0.88	4 (7%)
36	3PE	I	203	-	50,50,50	0.97	4 (8%)	53,55,55	0.94	1 (1%)
36	3PE	c	201	-	50,50,50	0.96	4 (8%)	53,55,55	0.94	2 (3%)
36	3PE	b	501	-	50,50,50	0.95	4 (8%)	53,55,55	1.14	6 (11%)
37	T7X	J	201	-	61,61,61	0.95	4 (6%)	70,73,73	0.98	4 (5%)
38	P5S	L	803	-	52,53,53	0.94	3 (5%)	54,60,60	0.79	3 (5%)
42	HEC	e	502	20	46,50,50	1.88	5 (10%)	58,82,82	1.52	7 (12%)
33	PC1	D	502	-	53,53,53	0.95	3 (5%)	59,61,61	0.95	2 (3%)
30	SF4	B	1001	2	0,12,12	-	-	-		
29	DU0	H	401	-	42,42,42	0.68	0	64,66,66	0.89	1 (1%)
28	PGT	L	804	-	50,50,50	0.95	4 (8%)	53,56,56	1.23	7 (13%)
34	FES	f	201	21	0,4,4	-	-	-		
42	HEC	b	502	20	46,50,50	1.89	5 (10%)	58,82,82	1.60	8 (13%)
29	DU0	J	204	-	42,42,42	0.65	0	64,66,66	0.95	4 (6%)
31	U10	B	1002	-	63,63,63	0.71	0	78,79,79	1.24	5 (6%)
33	PC1	a	504	-	53,53,53	0.94	3 (5%)	59,61,61	0.86	2 (3%)
31	U10	d	504	-	63,63,63	0.68	0	78,79,79	1.06	2 (2%)
35	FMN	F	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.25	8 (16%)
30	SF4	I	201	9	0,12,12	-	-	-		
33	PC1	d	507	-	53,53,53	0.96	3 (5%)	59,61,61	0.87	3 (5%)
29	DU0	J	202	-	42,42,42	0.73	0	64,66,66	0.94	1 (1%)
41	HEM	d	502	19	50,50,50	1.23	4 (8%)	67,82,82	1.02	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PC1	a	502	-	53,53,53	0.96	3 (5%)	59,61,61	0.84	1 (1%)
34	FES	c	203	21	0,4,4	-	-	-		
31	U10	d	506	-	63,63,63	0.71	0	78,79,79	1.22	6 (7%)
28	PGT	A	1001	-	50,50,50	0.94	4 (8%)	53,56,56	0.90	3 (5%)
39	3PH	M	2001	-	47,47,47	1.38	5 (10%)	50,52,52	1.10	4 (8%)
34	FES	G	701	7	0,4,4	-	-	-		
29	DU0	i	1008	-	42,42,42	0.66	0	64,66,66	1.18	4 (6%)
29	DU0	c	202	-	42,42,42	0.71	0	64,66,66	1.10	5 (7%)
33	PC1	a	509	-	53,53,53	0.95	3 (5%)	59,61,61	0.90	1 (1%)
33	PC1	i	1005	-	53,53,53	0.96	3 (5%)	59,61,61	0.95	3 (5%)
33	PC1	i	1006	-	53,53,53	0.95	3 (5%)	59,61,61	0.91	3 (5%)
34	FES	E	401	5	0,4,4	-	-	-		
33	PC1	i	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.84	1 (1%)
30	SF4	F	501	6	0,12,12	-	-	-		
30	SF4	I	202	9	0,12,12	-	-	-		
33	PC1	a	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.91	2 (3%)
36	3PE	L	801	-	50,50,50	0.95	4 (8%)	53,55,55	1.05	4 (7%)
36	3PE	i	1007	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	3 (5%)
39	3PH	c	205	-	47,47,47	1.36	5 (10%)	50,52,52	1.08	6 (12%)
39	3PH	i	1009	-	47,47,47	1.36	5 (10%)	50,52,52	1.05	5 (10%)
29	DU0	M	2002	-	42,42,42	0.75	0	64,66,66	0.99	7 (10%)
33	PC1	i	1003	-	53,53,53	0.98	3 (5%)	59,61,61	0.90	2 (3%)
36	3PE	H	402	-	50,50,50	0.96	4 (8%)	53,55,55	1.13	5 (9%)
28	PGT	P	401	-	50,50,50	0.93	4 (8%)	53,56,56	0.87	3 (5%)
31	U10	a	508	-	63,63,63	0.71	0	78,79,79	0.96	4 (5%)
31	U10	a	506	-	63,63,63	0.66	0	78,79,79	0.80	3 (3%)
39	3PH	L	805	-	47,47,47	1.37	5 (10%)	50,52,52	1.04	5 (10%)
44	HEA	g	601	22	67,67,67	1.37	8 (11%)	81,103,103	2.32	30 (37%)
47	CUA	h	301	23	0,1,1	-	-	-		

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
44	HEA	g	604	22	-	4/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PC1	L	802	-	-	9/57/57/57	-
29	DU0	M	2004	-	-	0/10/98/98	0/6/6/6
33	PC1	j	1001	-	-	18/57/57/57	-
33	PC1	M	2005	-	-	9/57/57/57	-
36	3PE	i	1004	-	-	5/54/54/54	-
33	PC1	H	403	-	-	12/57/57/57	-
28	PGT	q	1000	-	-	13/55/55/55	-
39	3PH	a	503	-	-	8/49/49/49	-
43	CDL	d	501	-	-	23/110/110/110	-
33	PC1	M	2003	-	-	8/57/57/57	-
39	3PH	L	806	-	-	11/49/49/49	-
30	SF4	G	702	7	-	-	0/6/5/5
36	3PE	d	505	-	-	10/54/54/54	-
30	SF4	G	703	7	-	-	0/6/5/5
29	DU0	c	204	-	-	3/10/98/98	0/6/6/6
34	FES	E	401	5	-	-	0/1/1/1
41	HEM	d	503	19	-	6/14/54/54	-
29	DU0	A	1002	-	-	0/10/98/98	0/6/6/6
39	3PH	f	202	-	-	5/49/49/49	-
28	PGT	J	203	-	-	15/55/55/55	-
41	HEM	a	507	19	-	8/14/54/54	-
28	PGT	A	1003	-	-	5/55/55/55	-
36	3PE	I	203	-	-	9/54/54/54	-
36	3PE	c	201	-	-	9/54/54/54	-
36	3PE	b	501	-	-	12/54/54/54	-
37	T7X	J	201	-	-	12/56/80/80	0/1/1/1
38	P5S	L	803	-	-	7/59/59/59	-
42	HEC	e	502	20	-	4/14/54/54	-
33	PC1	D	502	-	-	17/57/57/57	-
30	SF4	B	1001	2	-	-	0/6/5/5
29	DU0	H	401	-	-	0/10/98/98	0/6/6/6
28	PGT	L	804	-	-	8/55/55/55	-
34	FES	f	201	21	-	-	0/1/1/1
42	HEC	b	502	20	-	7/14/54/54	-
29	DU0	J	204	-	-	2/10/98/98	0/6/6/6
31	U10	B	1002	-	-	22/63/87/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PC1	a	504	-	-	20/57/57/57	-
31	U10	d	504	-	-	3/63/87/87	0/1/1/1
35	FMN	F	502	-	-	1/18/18/18	0/3/3/3
30	SF4	I	201	9	-	-	0/6/5/5
33	PC1	d	507	-	-	17/57/57/57	-
29	DU0	J	202	-	-	0/10/98/98	0/6/6/6
41	HEM	d	502	19	-	7/14/54/54	-
33	PC1	a	502	-	-	9/57/57/57	-
34	FES	c	203	21	-	-	0/1/1/1
31	U10	d	506	-	-	11/63/87/87	0/1/1/1
28	PGT	A	1001	-	-	12/55/55/55	-
39	3PH	M	2001	-	-	8/49/49/49	-
41	HEM	a	505	19	-	7/14/54/54	-
29	DU0	i	1008	-	-	0/10/98/98	0/6/6/6
29	DU0	c	202	-	-	0/10/98/98	0/6/6/6
33	PC1	a	509	-	-	10/57/57/57	-
33	PC1	i	1005	-	-	13/57/57/57	-
33	PC1	i	1006	-	-	13/57/57/57	-
36	3PE	L	801	-	-	11/54/54/54	-
33	PC1	i	1001	-	-	12/57/57/57	-
33	PC1	a	501	-	-	10/57/57/57	-
30	SF4	F	501	6	-	-	0/6/5/5
30	SF4	I	202	9	-	-	0/6/5/5
36	3PE	i	1007	-	-	10/54/54/54	-
39	3PH	c	205	-	-	7/49/49/49	-
39	3PH	i	1009	-	-	6/49/49/49	-
29	DU0	M	2002	-	-	0/10/98/98	0/6/6/6
33	PC1	i	1003	-	-	9/57/57/57	-
36	3PE	H	402	-	-	13/54/54/54	-
28	PGT	P	401	-	-	11/55/55/55	-
31	U10	a	508	-	-	7/63/87/87	0/1/1/1
31	U10	a	506	-	-	9/63/87/87	0/1/1/1
39	3PH	L	805	-	-	8/49/49/49	-
44	HEA	g	601	22	-	6/36/76/76	-
34	FES	G	701	7	-	-	0/1/1/1

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	f	202	3PH	P-O11	7.50	1.84	1.60
39	a	503	3PH	P-O11	7.42	1.83	1.60
39	M	2001	3PH	P-O11	7.31	1.83	1.60
39	L	805	3PH	P-O11	7.21	1.83	1.60
39	i	1009	3PH	P-O11	7.15	1.82	1.60

The worst 5 of 275 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	506	U10	C6-C1-C2	6.74	124.48	119.17
44	g	604	HEA	C3A-C2A-C1A	-6.72	100.69	107.05
44	g	601	HEA	C3A-C2A-C1A	-6.05	101.33	107.05
42	b	502	HEC	CBB-CAB-C3B	-5.71	116.03	127.43
42	e	502	HEC	CBB-CAB-C3B	-5.31	116.83	127.43

There are no chirality outliers.

5 of 531 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	1001	PGT	C1-O3P-P-O2P
28	A	1001	PGT	O4P-C4-C5-C6
28	J	203	PGT	C5-C4-O4P-P
28	L	804	PGT	C5-C4-O4P-P
28	P	401	PGT	C1-O3P-P-O1P

There are no ring outliers.

17 monomers are involved in 35 short contacts:

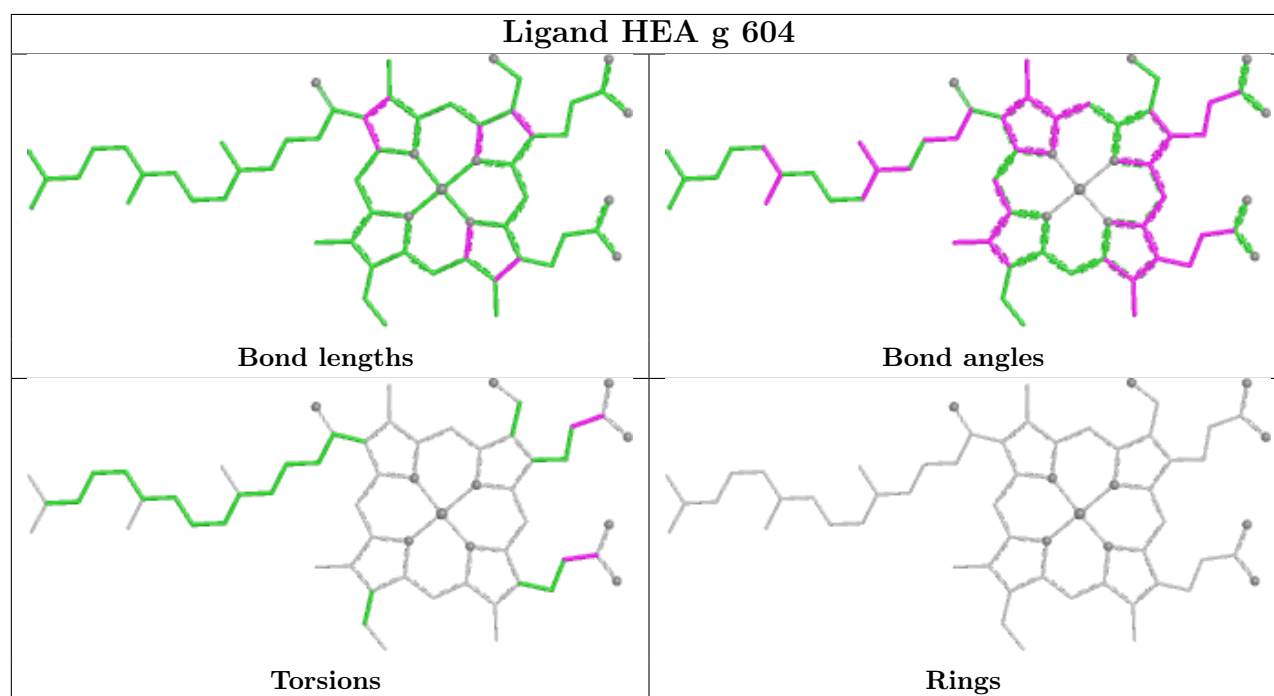
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	L	802	PC1	1	0
33	j	1001	PC1	2	0
33	H	403	PC1	1	0
39	a	503	3PH	1	0
39	L	806	3PH	1	0
41	a	507	HEM	1	0
42	e	502	HEC	4	0
33	D	502	PC1	1	0
42	b	502	HEC	3	0
31	d	504	U10	2	0
35	F	502	FMN	3	0
31	d	506	U10	5	0
33	i	1005	PC1	1	0

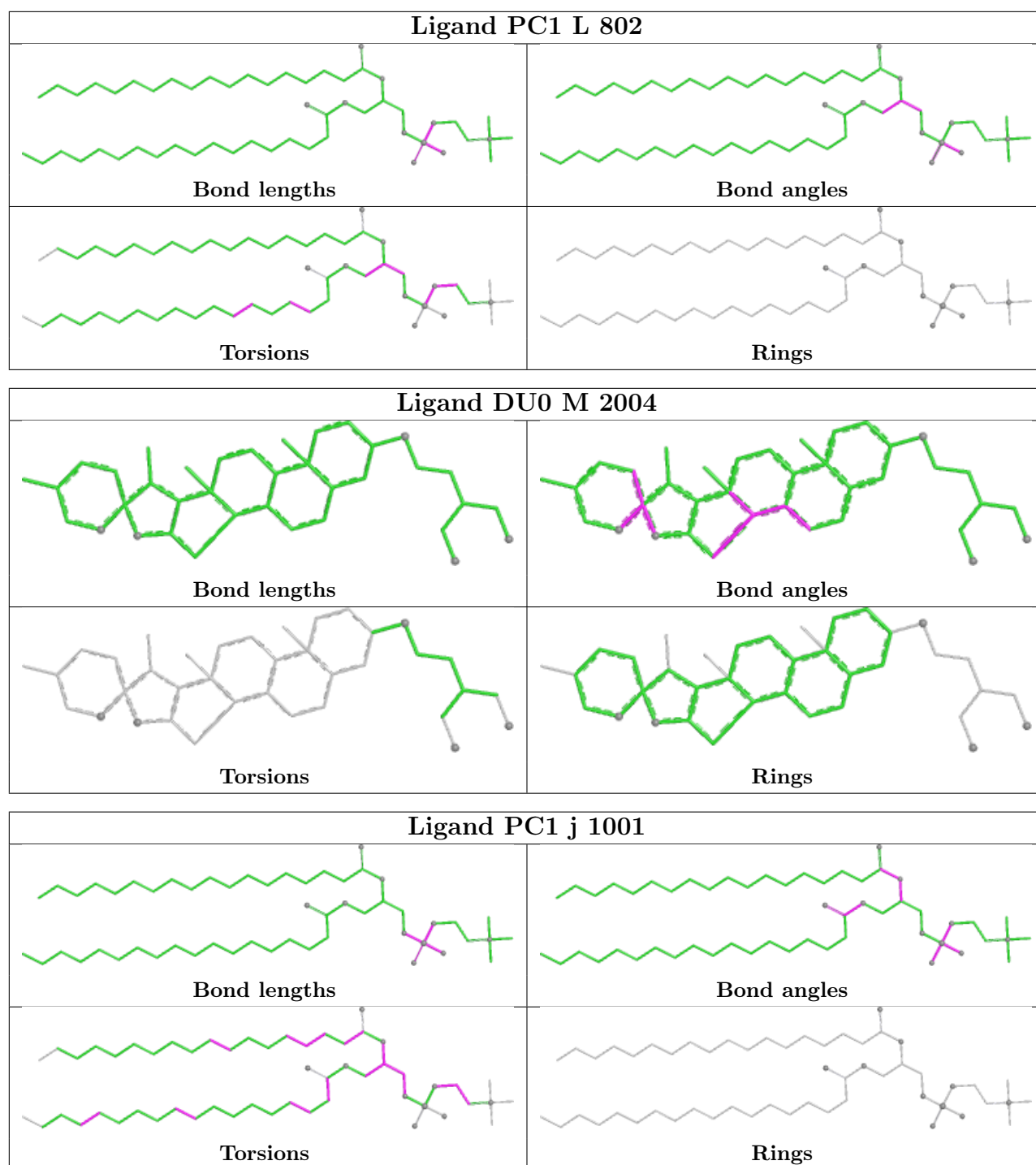
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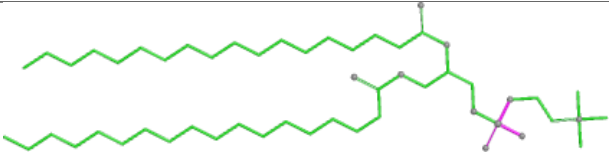
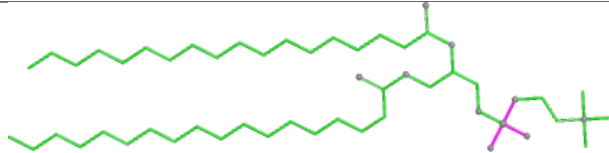
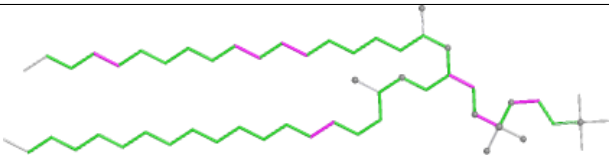
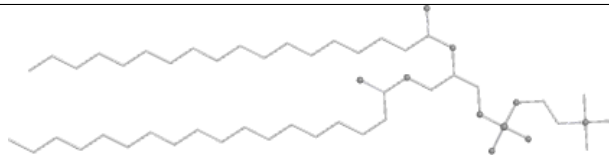
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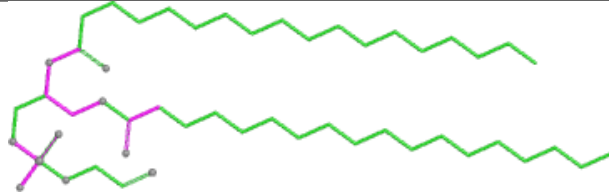
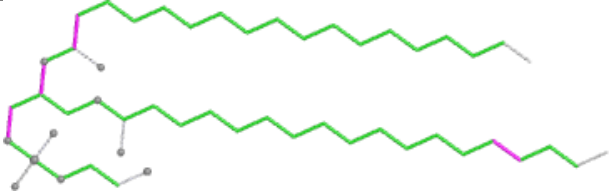
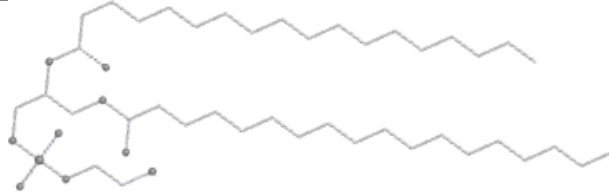
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	i	1006	PC1	2	0
36	L	801	3PE	1	0
31	a	508	U10	3	0
44	g	601	HEA	5	0

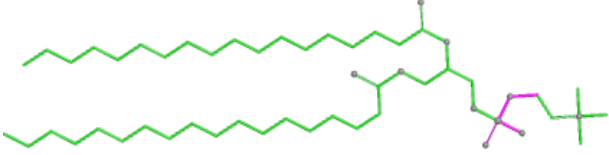
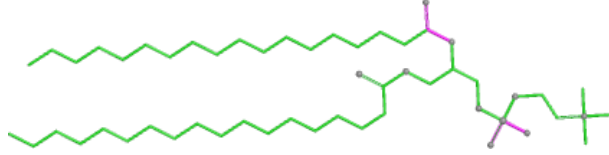
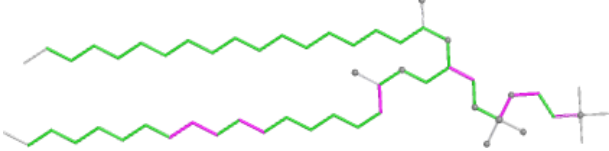
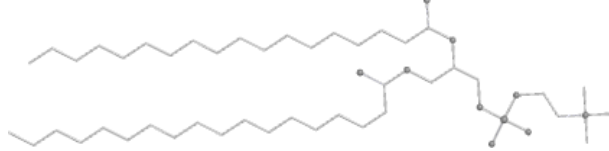
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

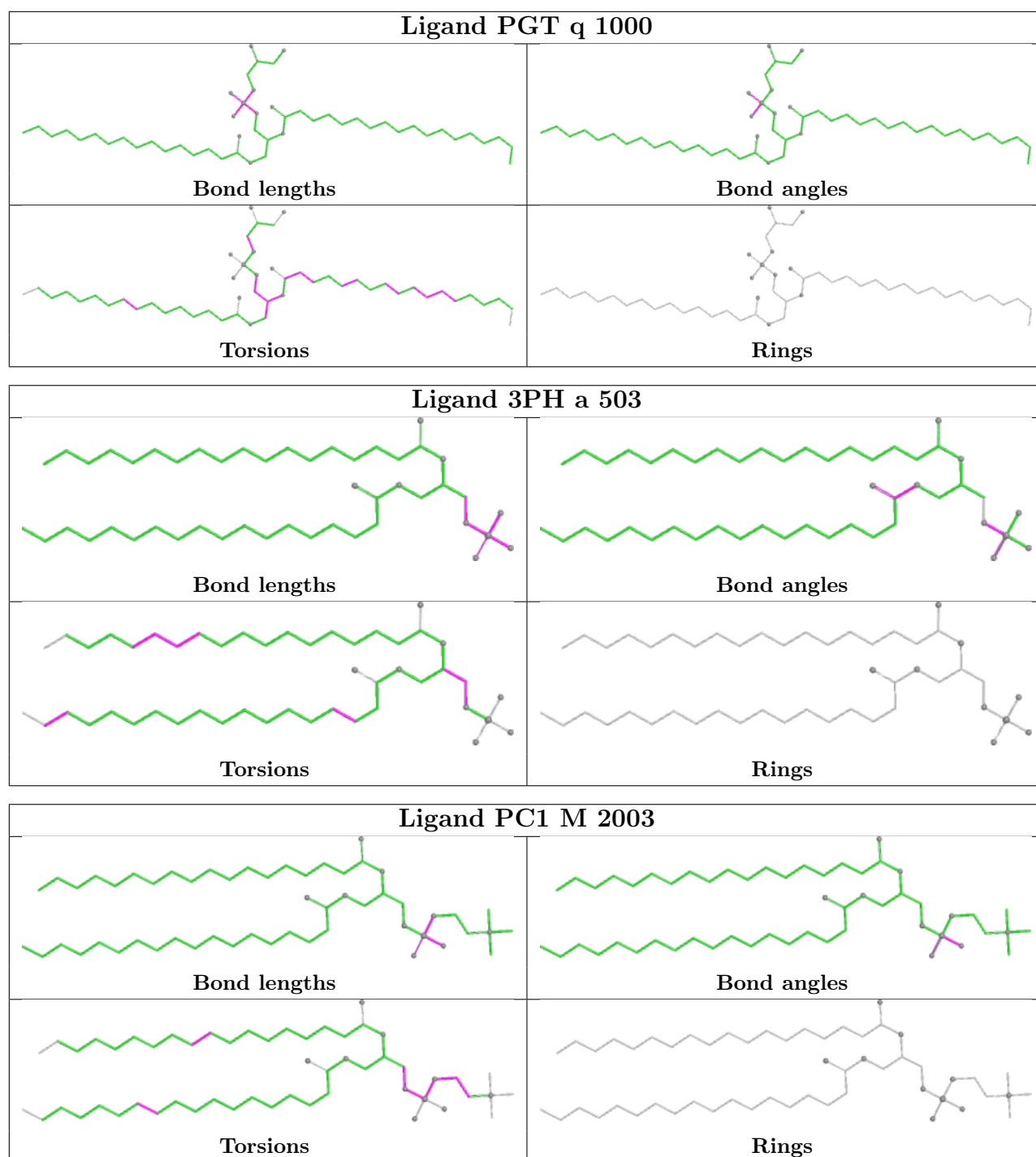


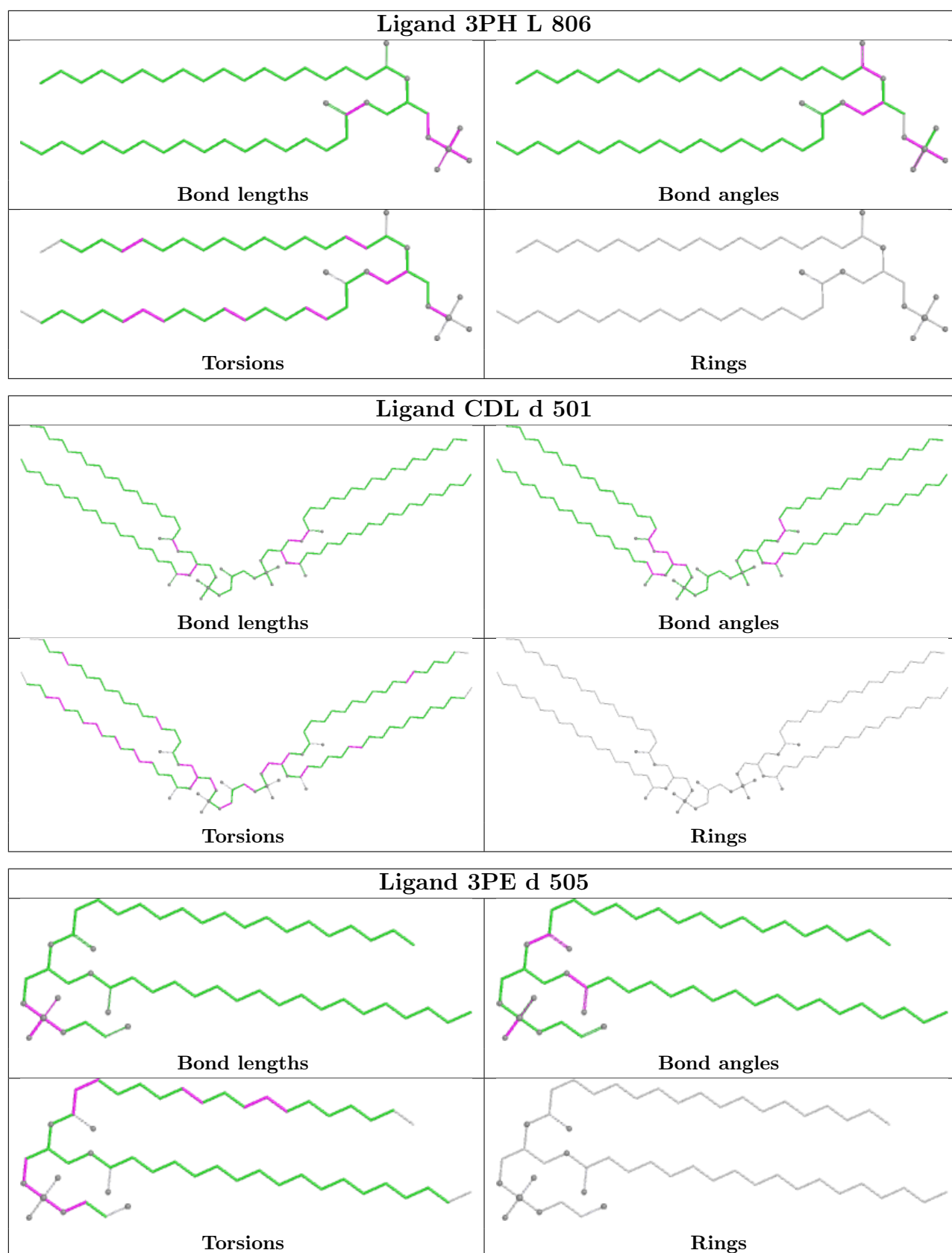


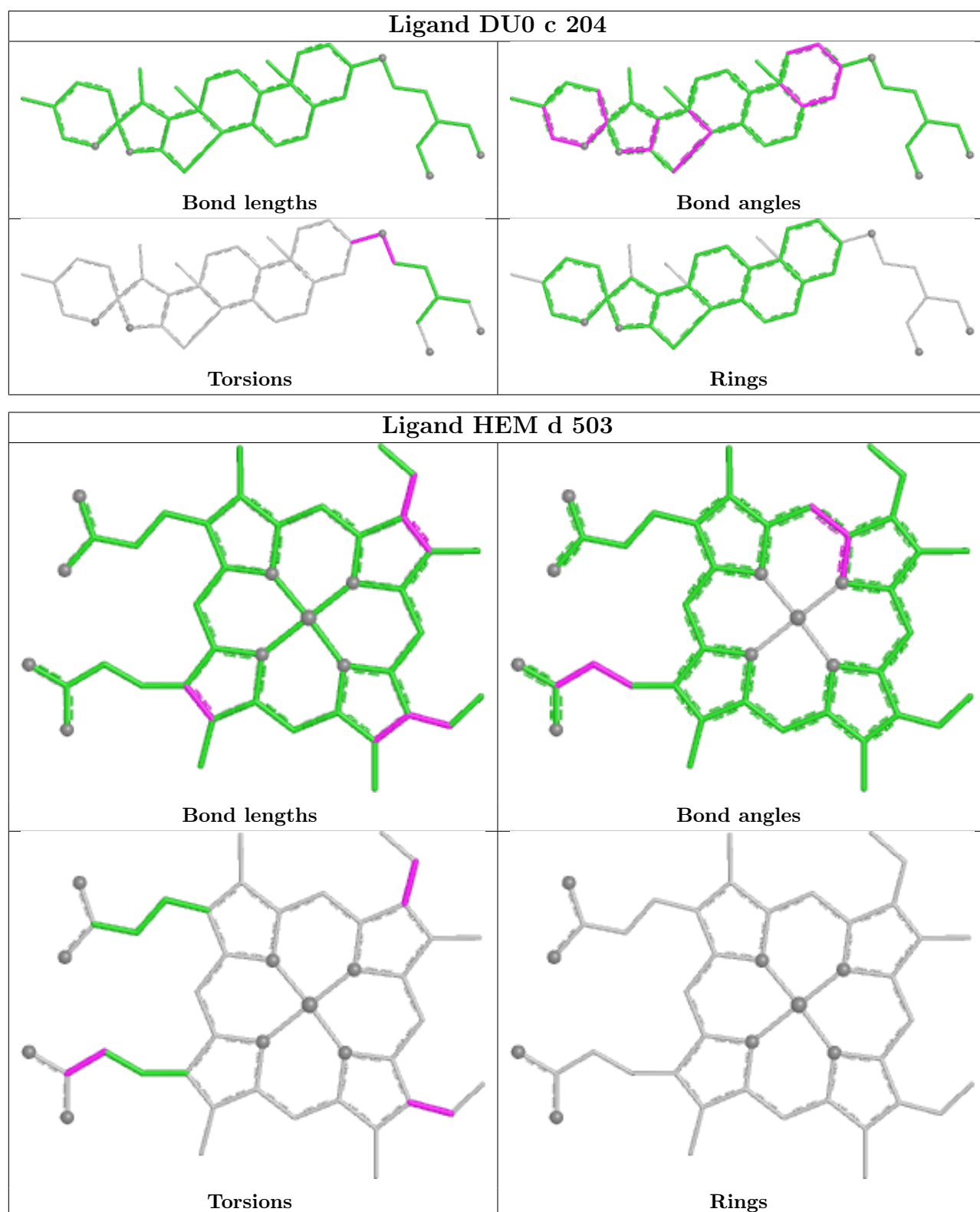
Ligand PC1 M 2005	
	
Bond lengths	Bond angles
	
Torsions	Rings

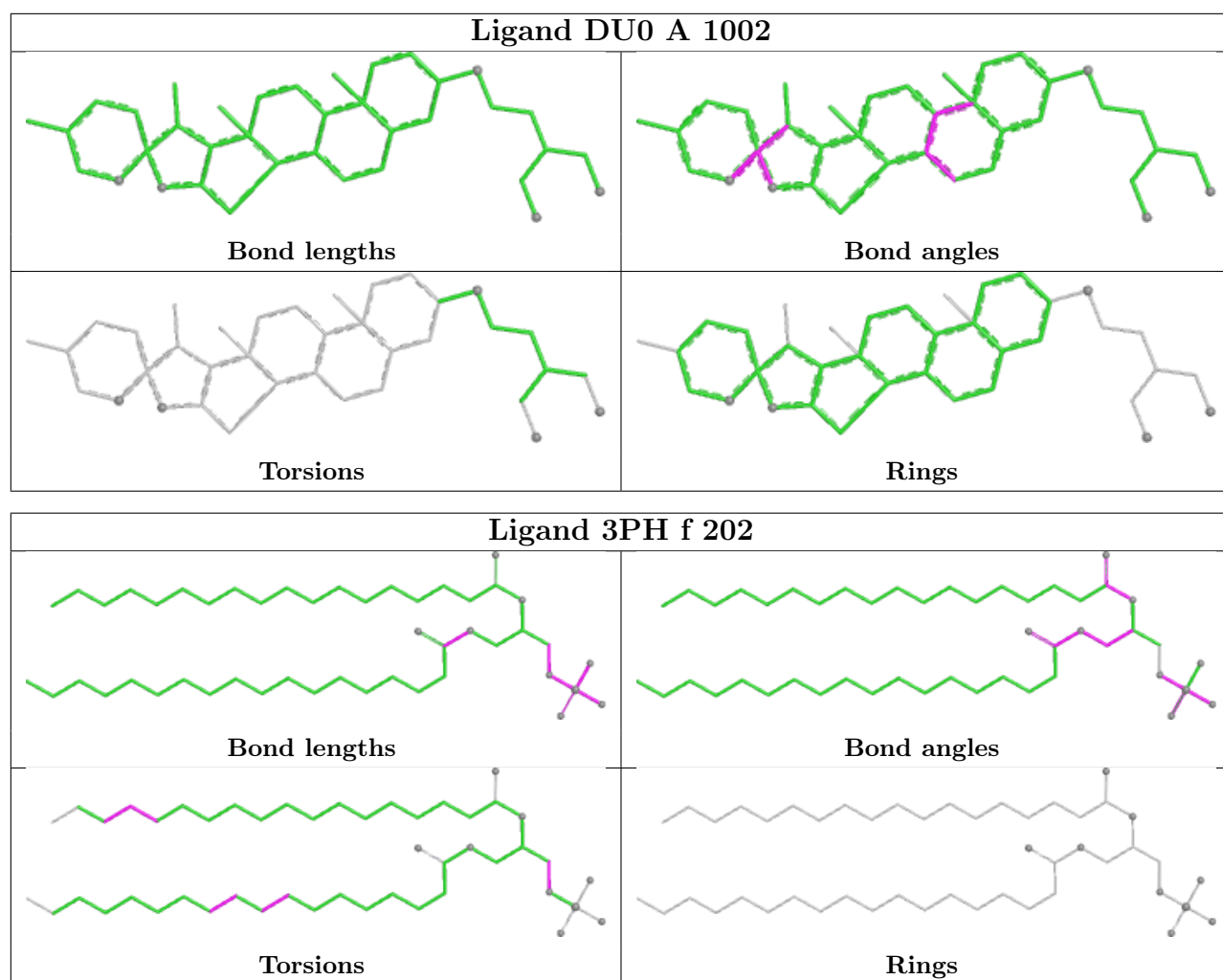
Ligand 3PE i 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

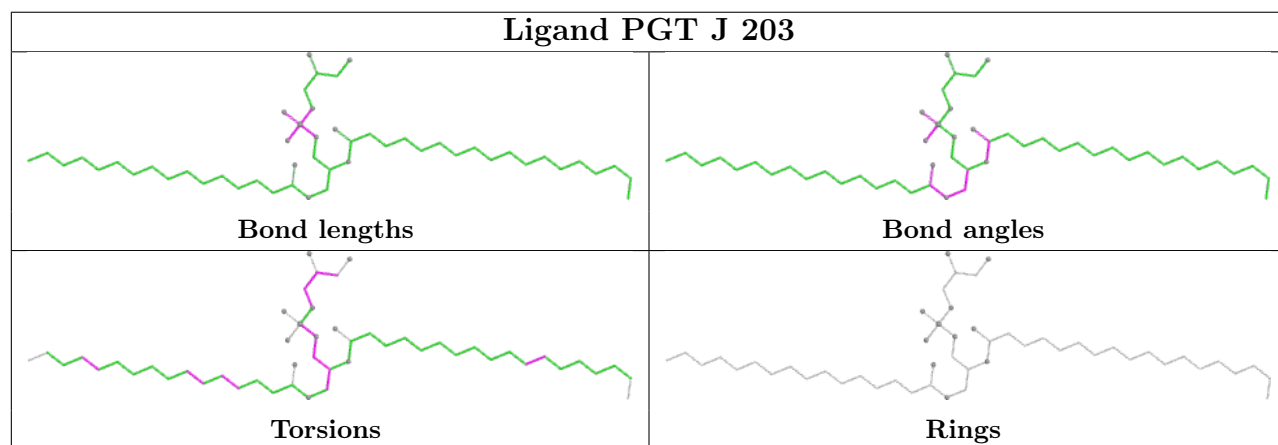
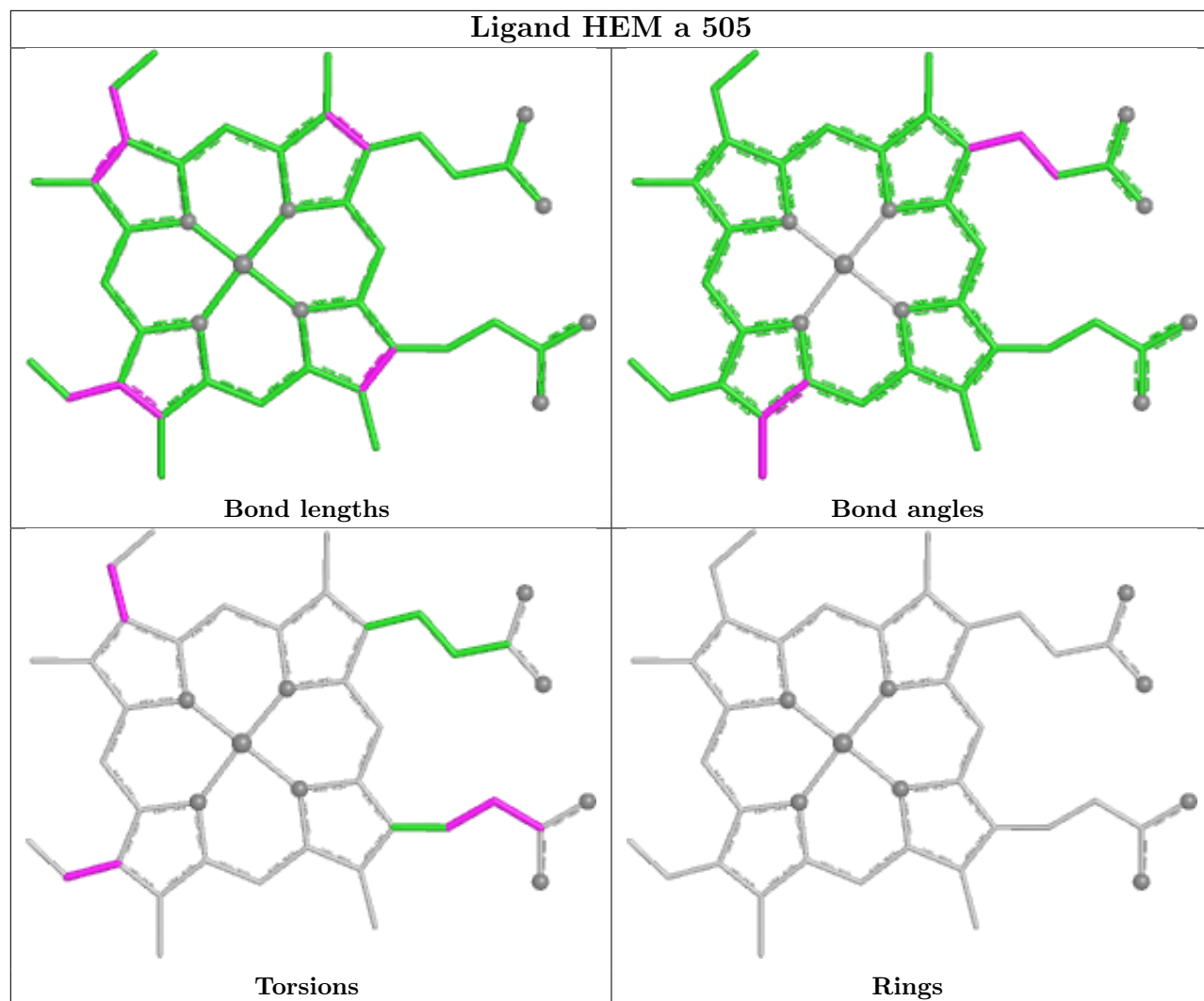
Ligand PC1 H 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

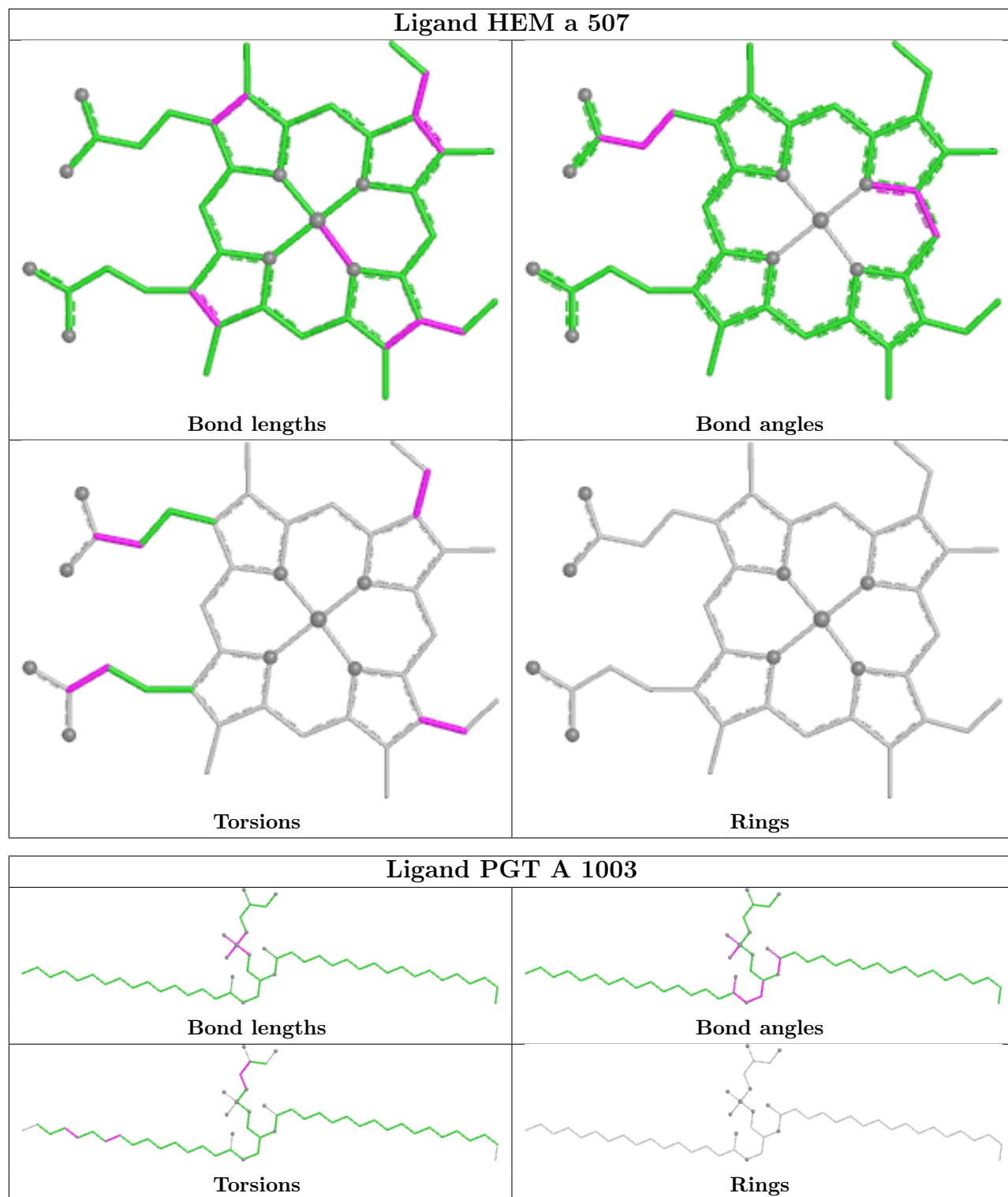


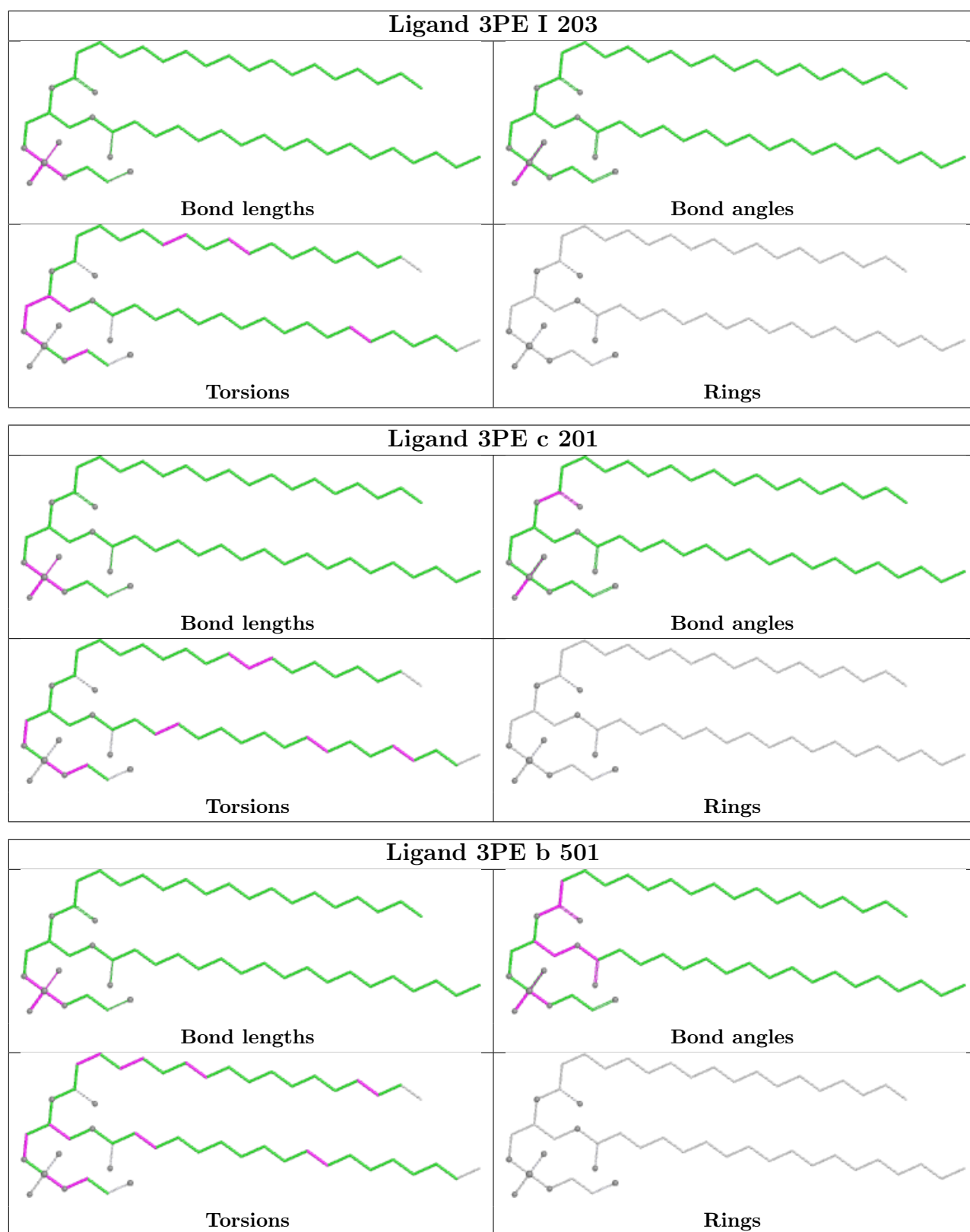


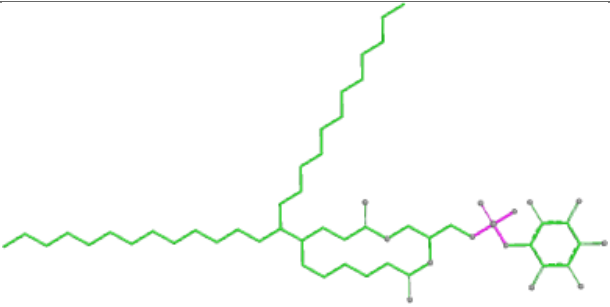
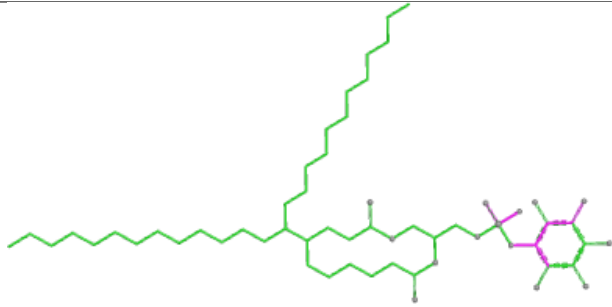
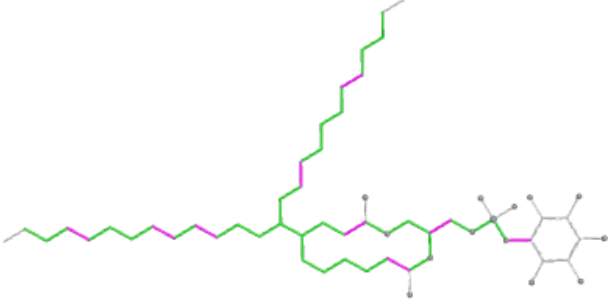
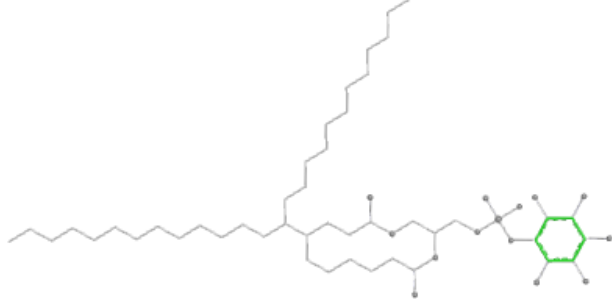





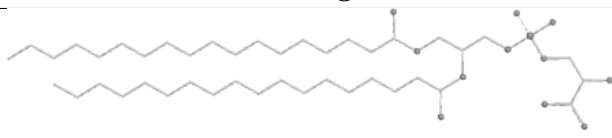




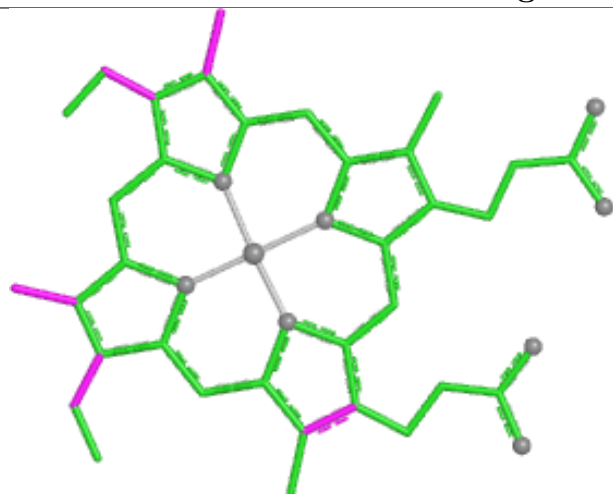




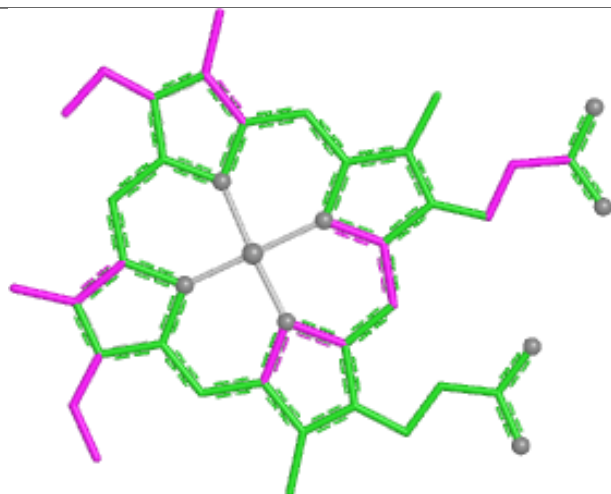
Ligand T7X J 201			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand P5S L 803			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

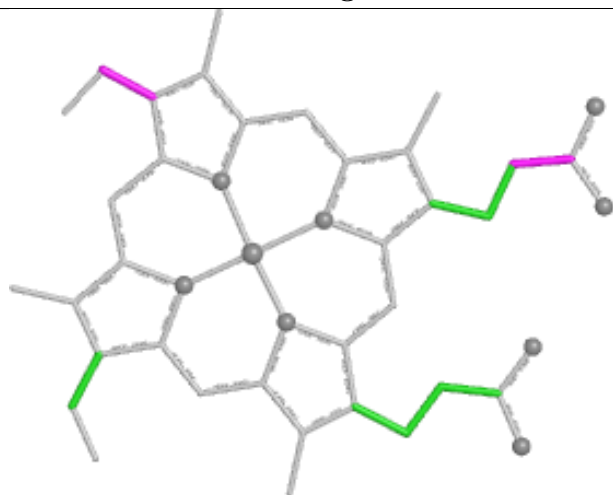
Ligand HEC e 502



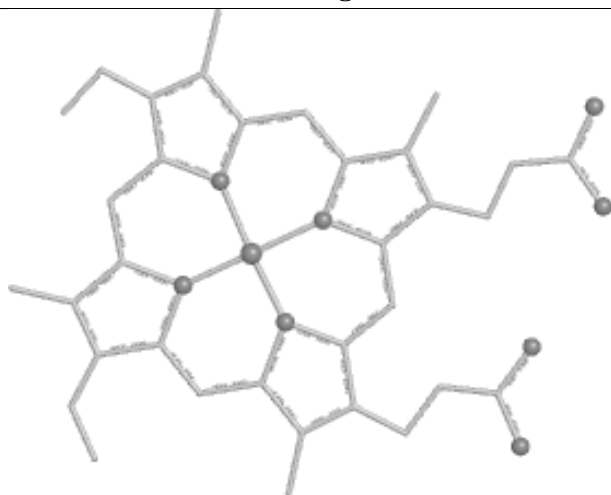
Bond lengths



Bond angles

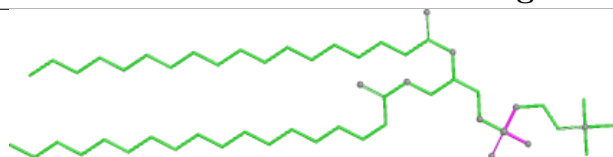


Torsions



Rings

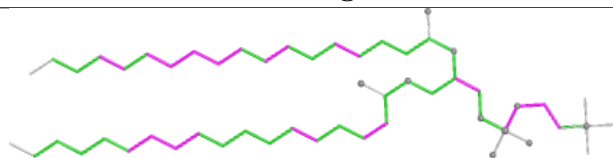
Ligand PC1 D 502



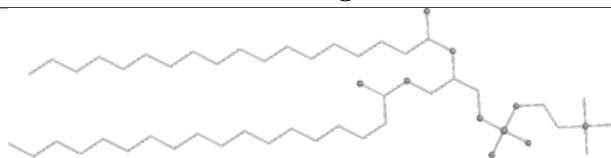
Bond lengths



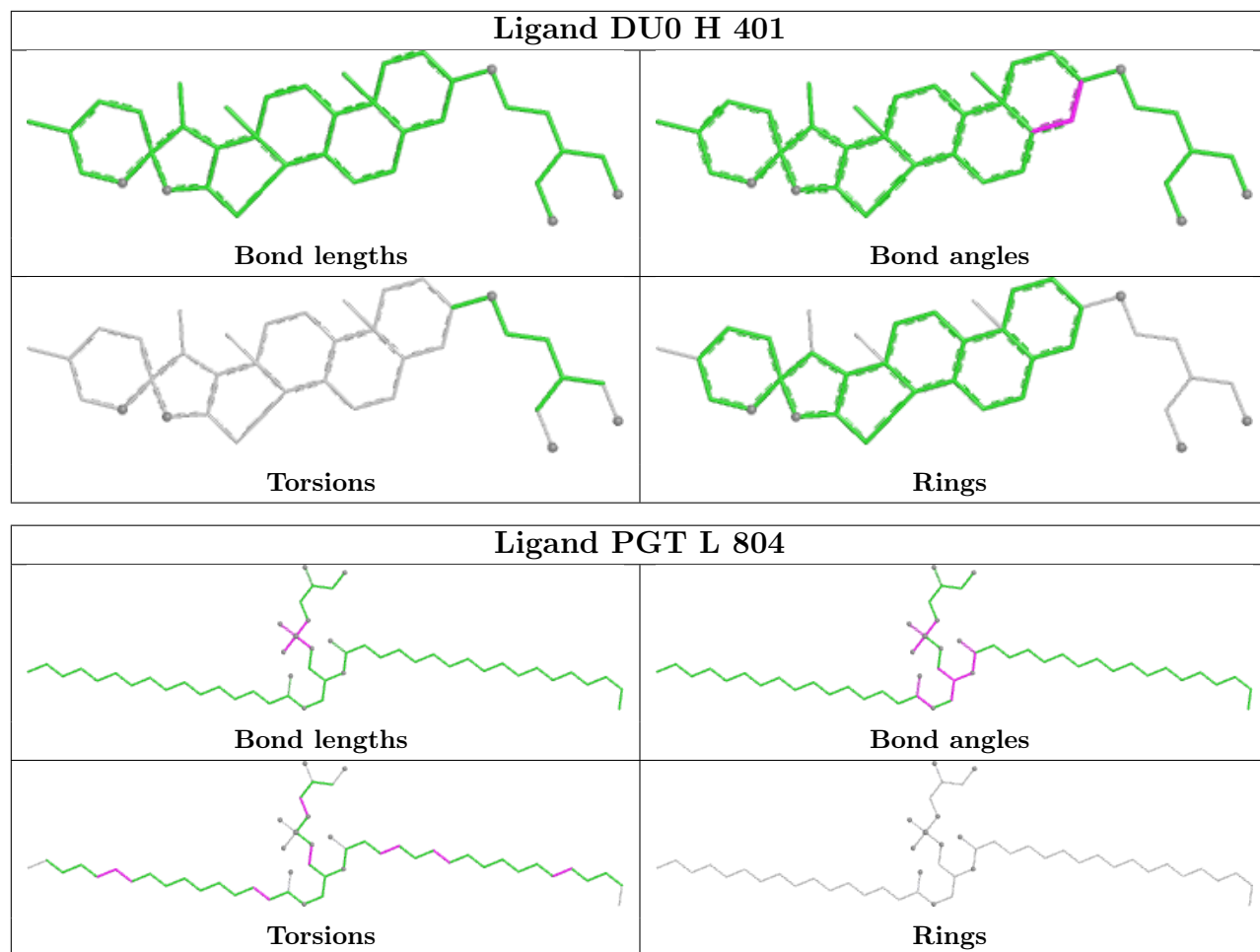
Bond angles



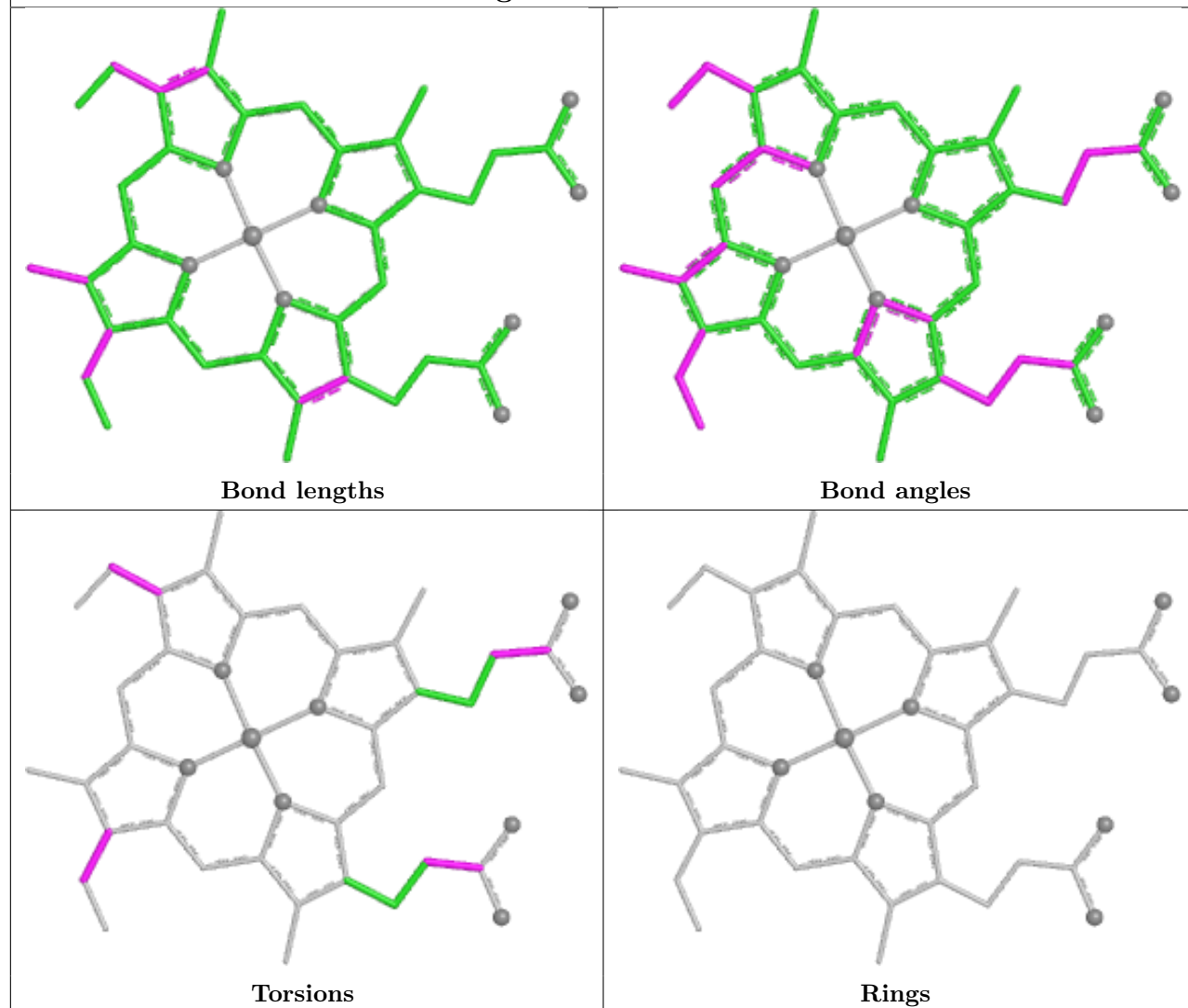
Torsions



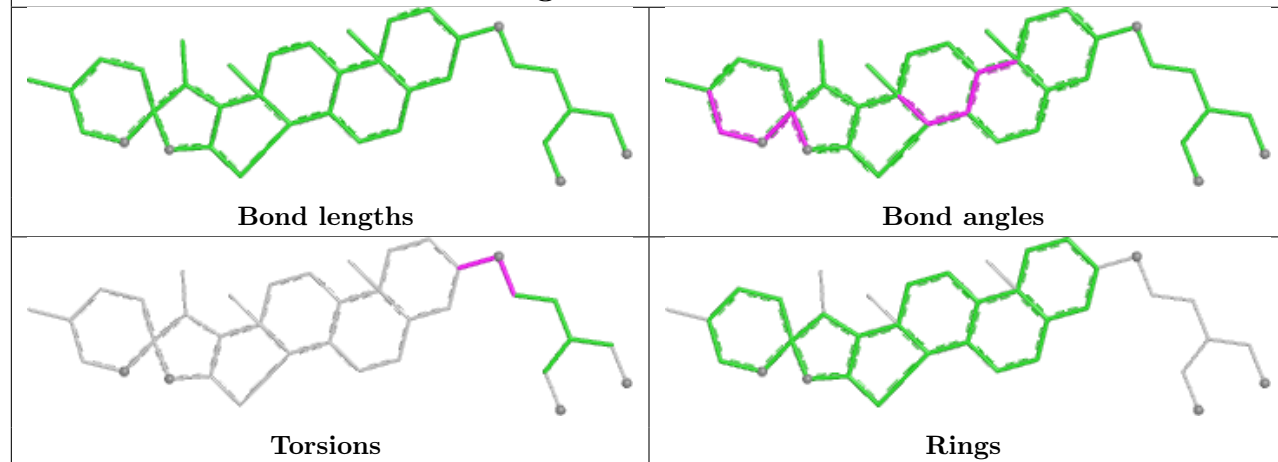
Rings

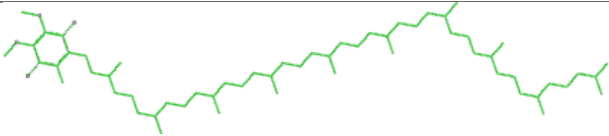

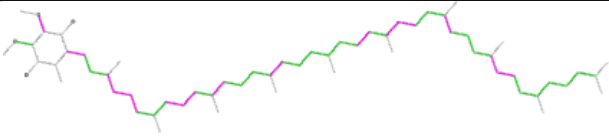



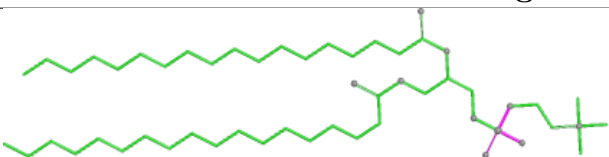
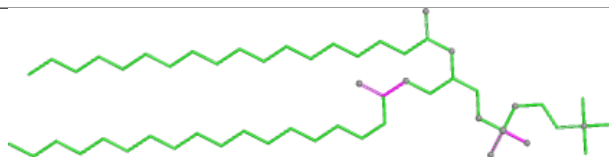
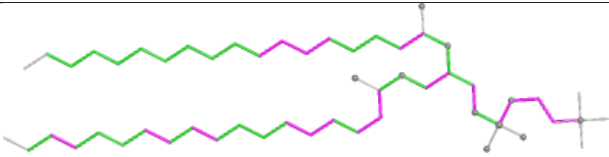
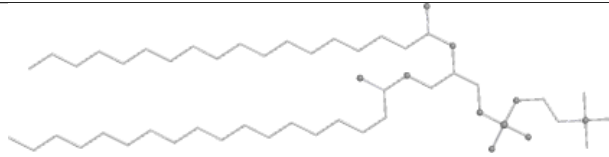
Ligand HEC b 502

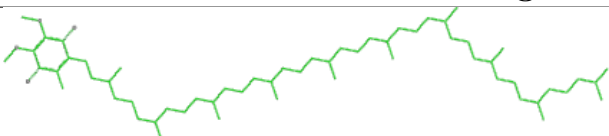
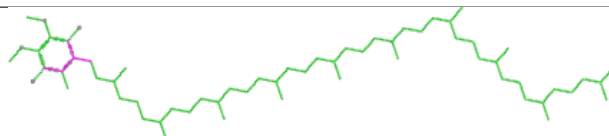
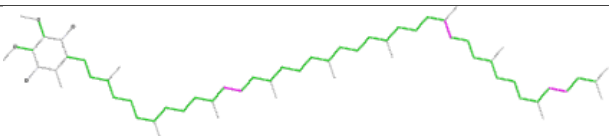
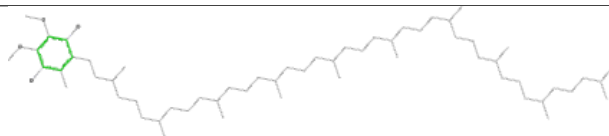


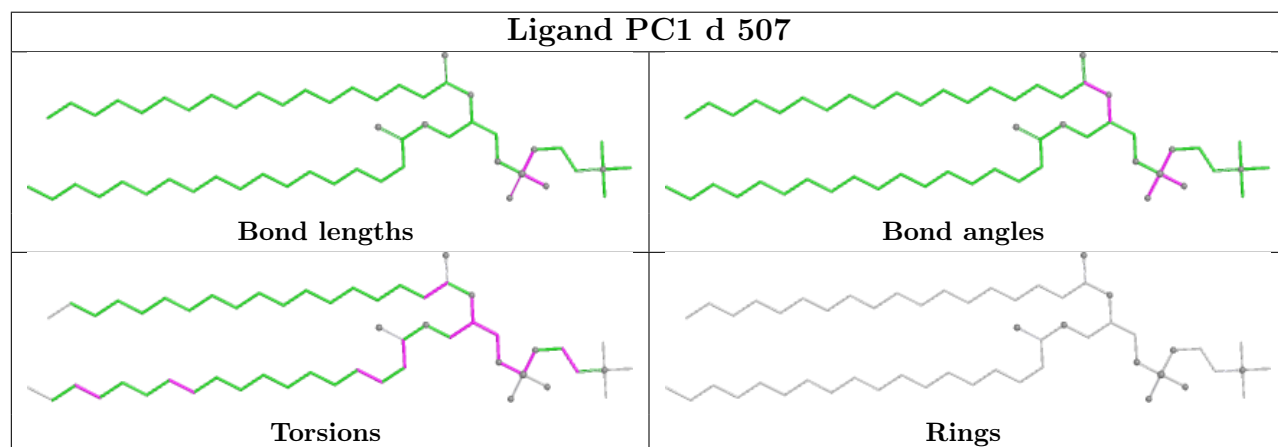
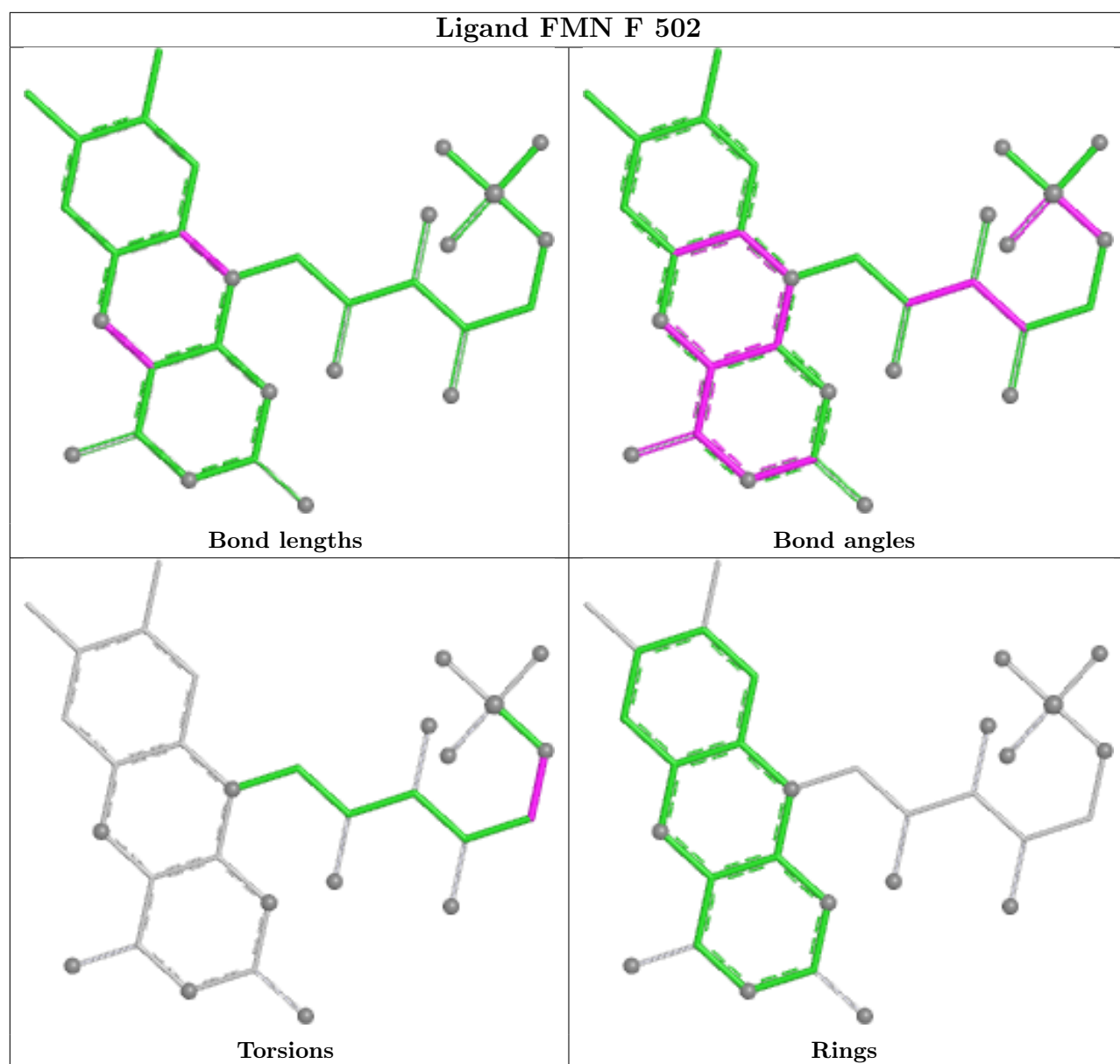
Ligand DU0 J 204



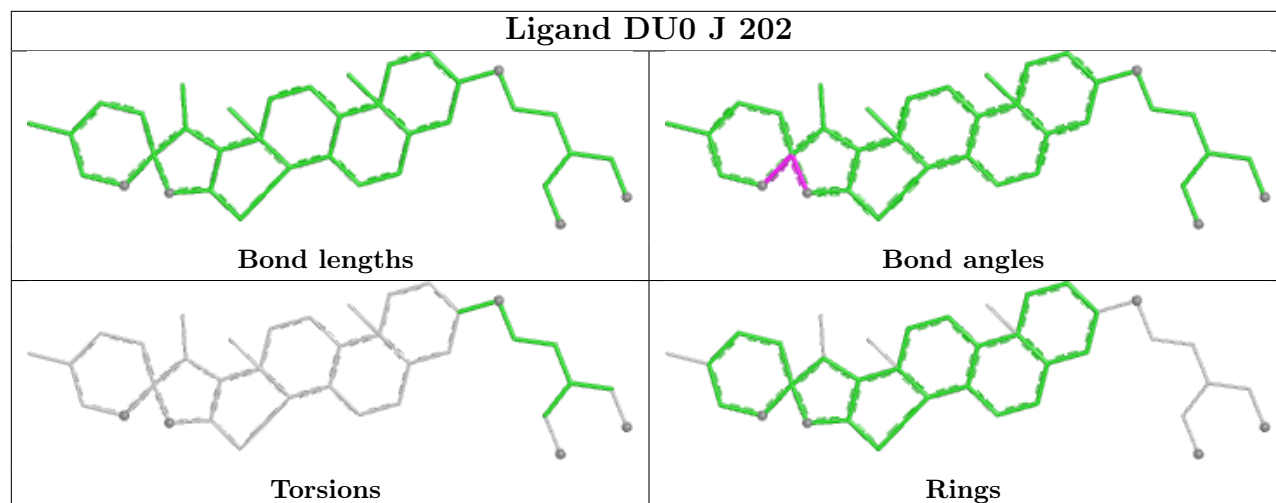
Ligand U10 B 1002	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand PC1 a 504	
	Bond lengths
	Bond angles
	Torsions
	Rings

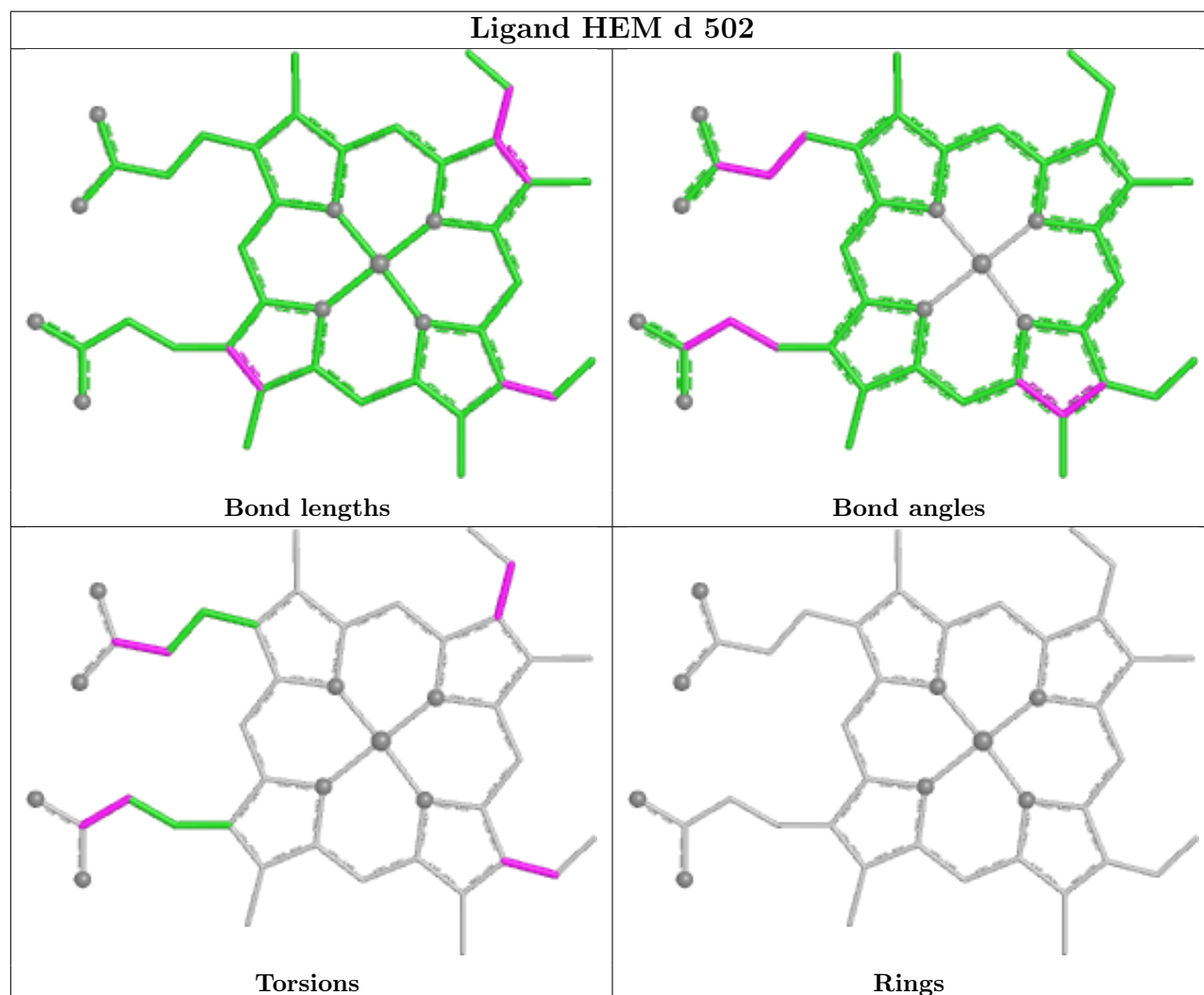
Ligand U10 d 504	
	Bond lengths
	Bond angles
	Torsions
	Rings

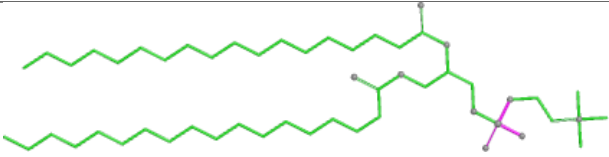
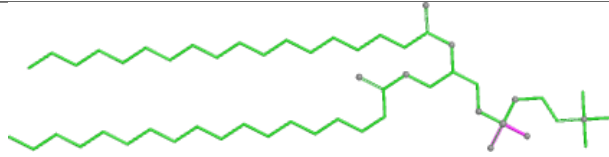
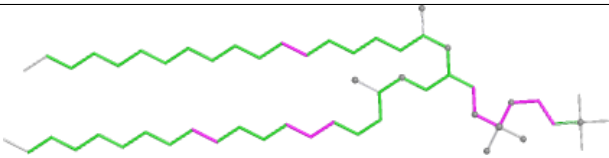
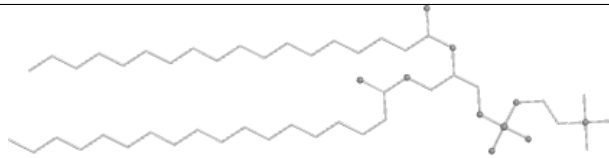
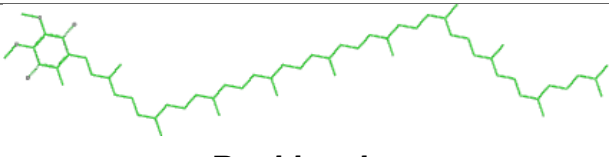
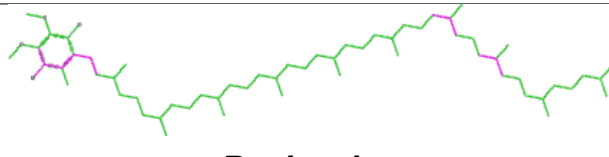
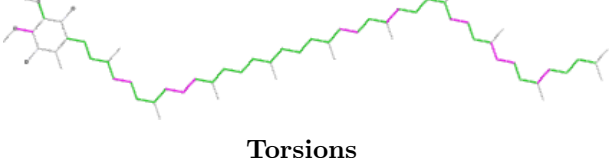

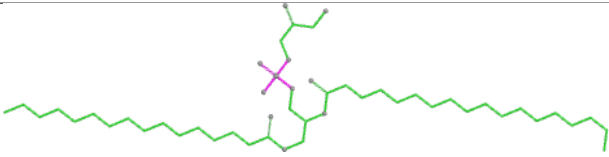
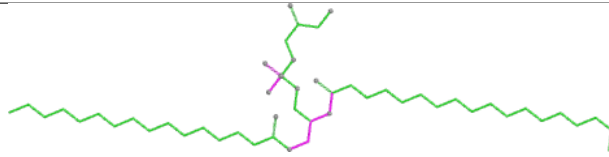
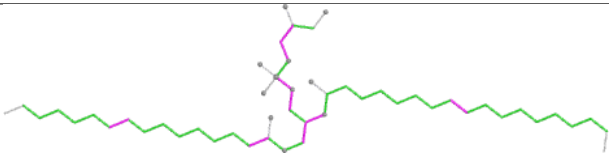
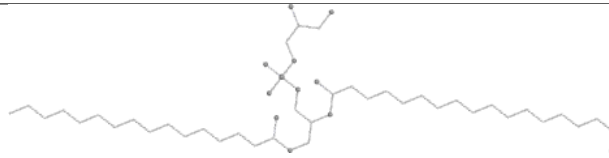


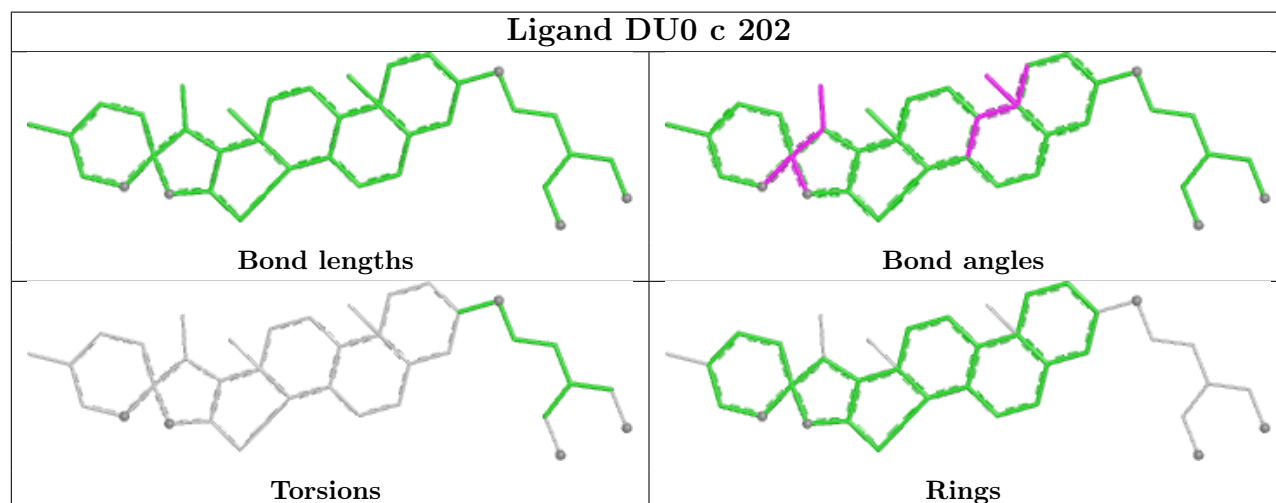
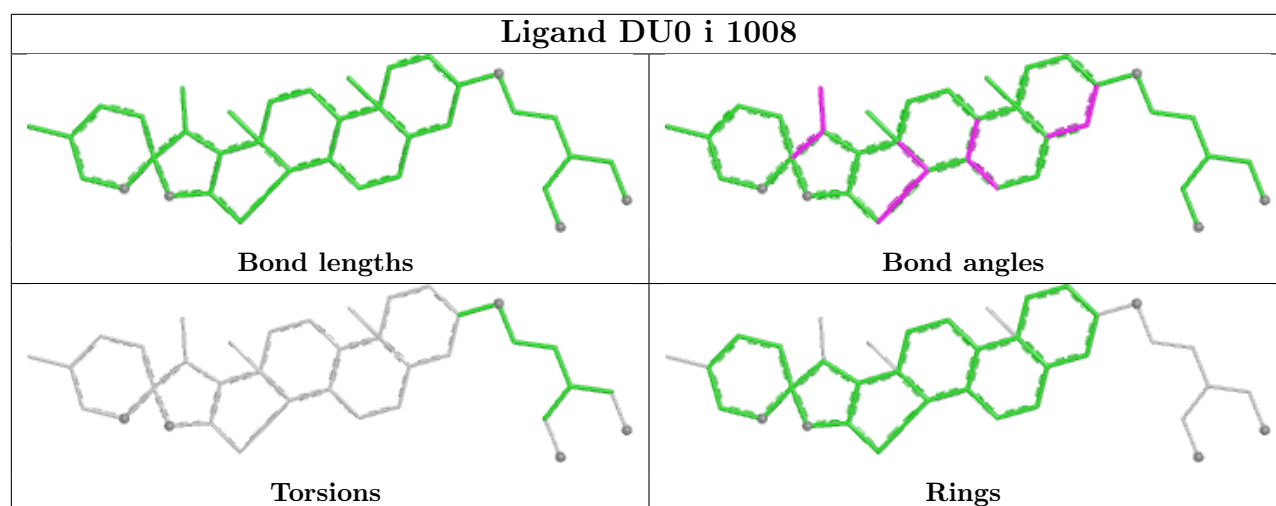
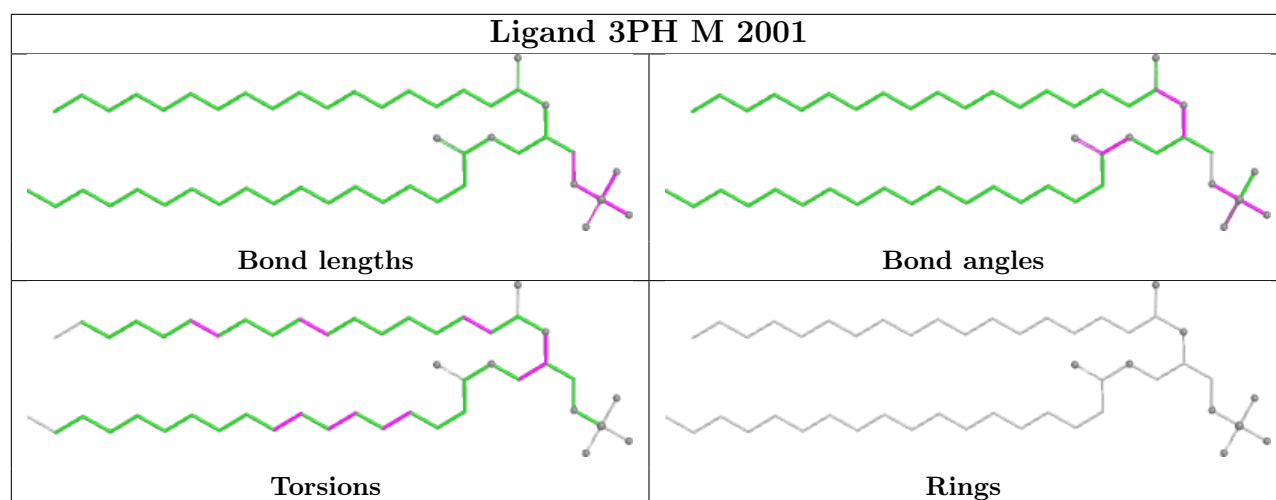
Ligand DU0 J 202

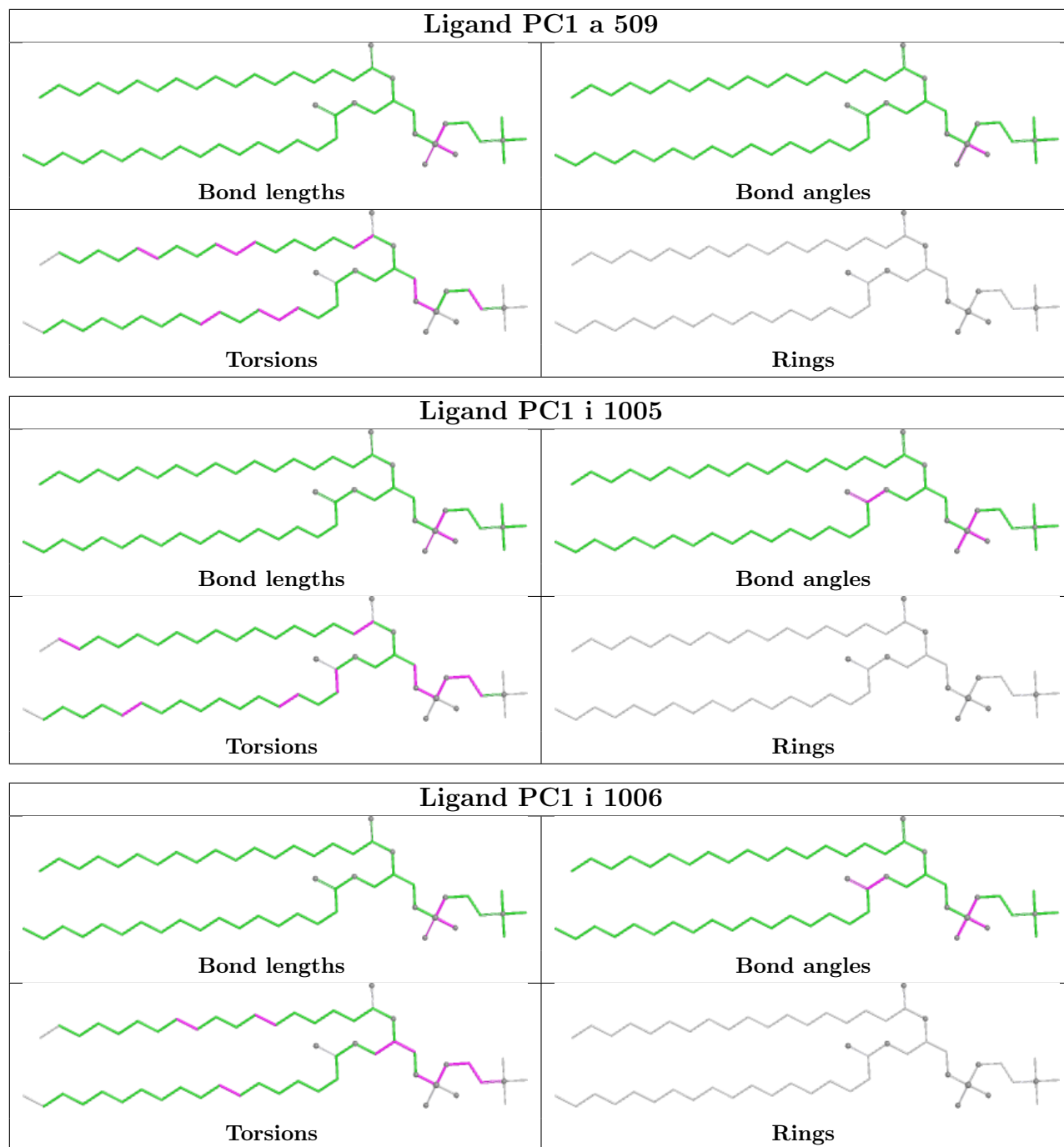


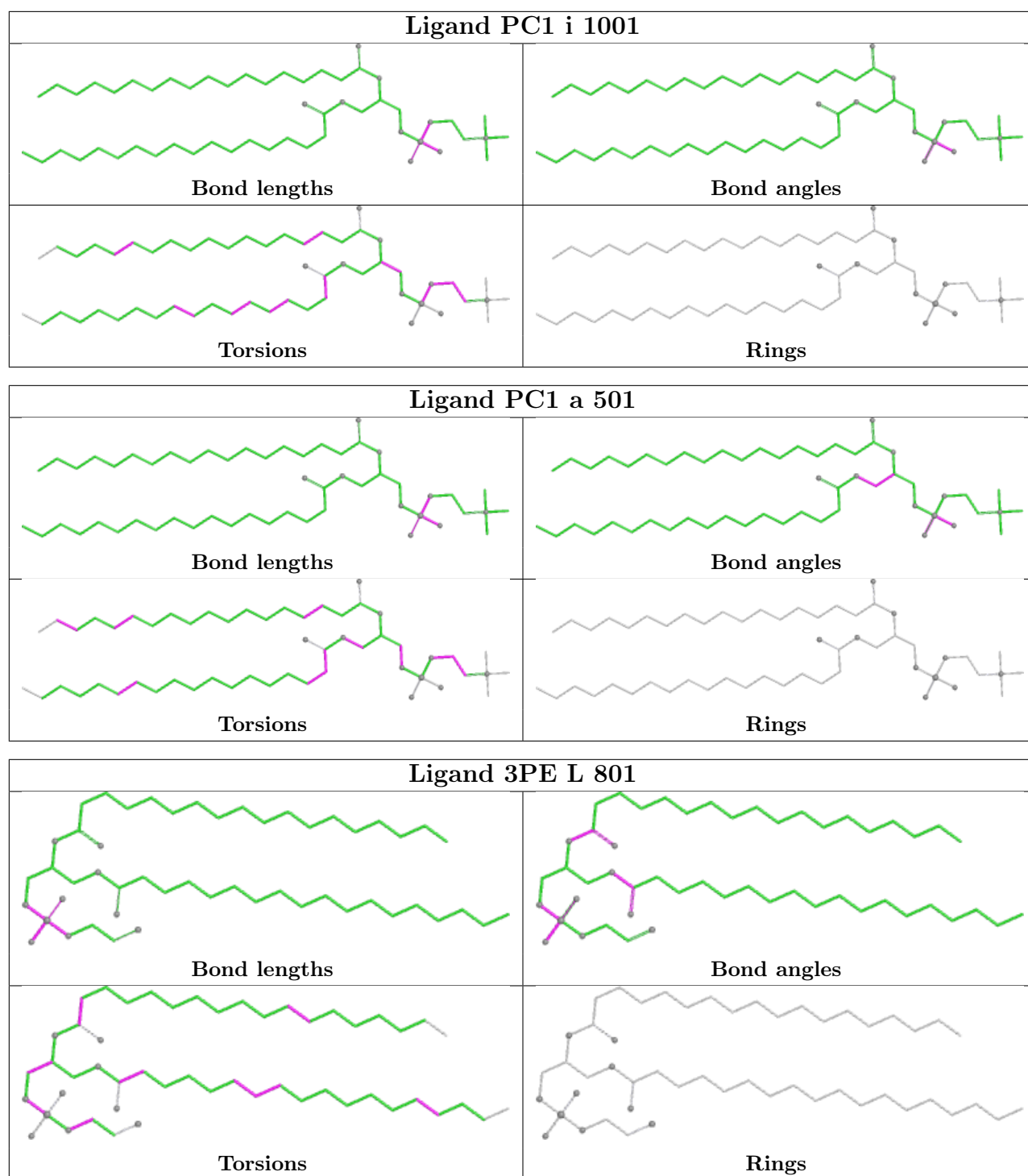
Ligand HEM d 502

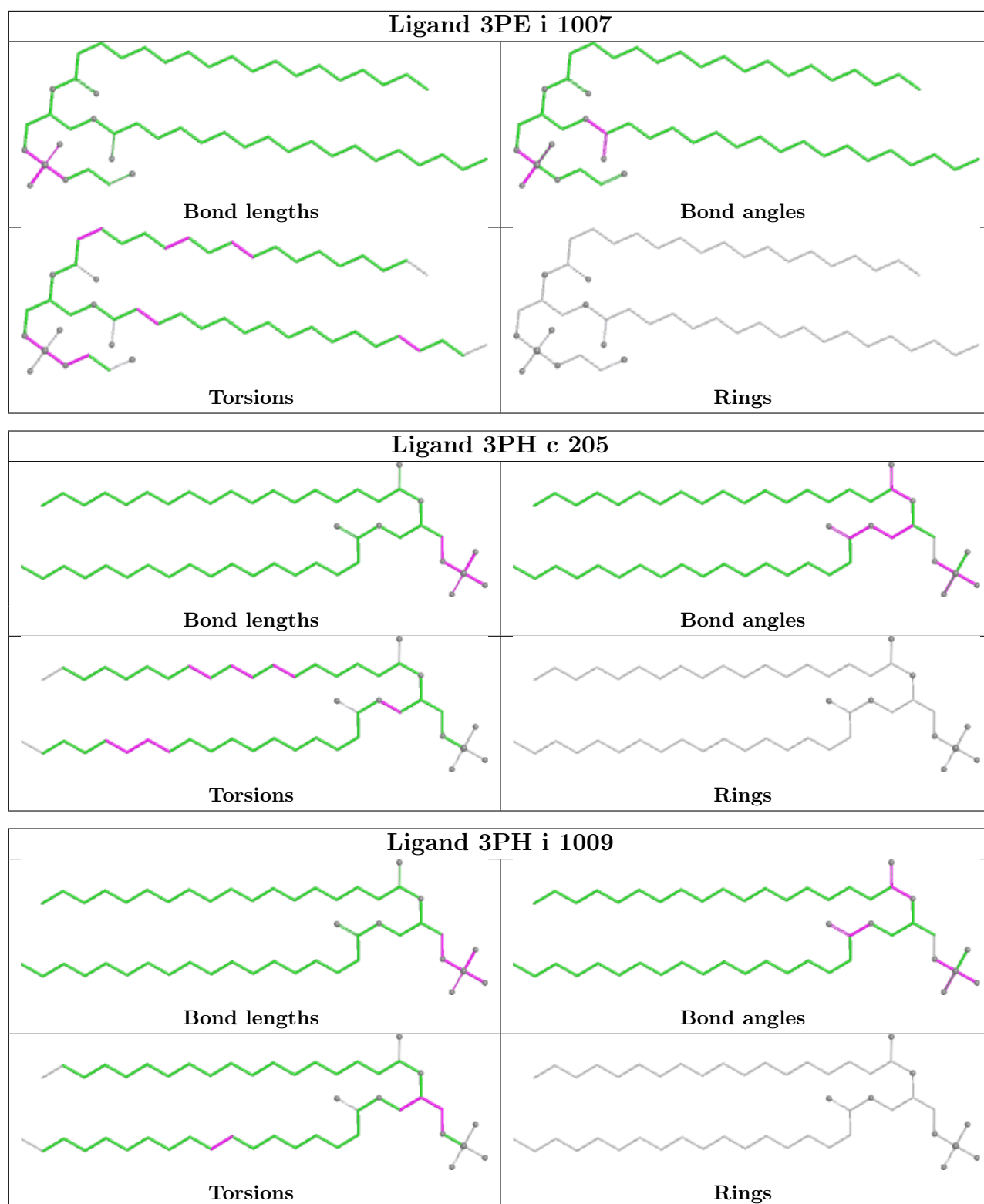


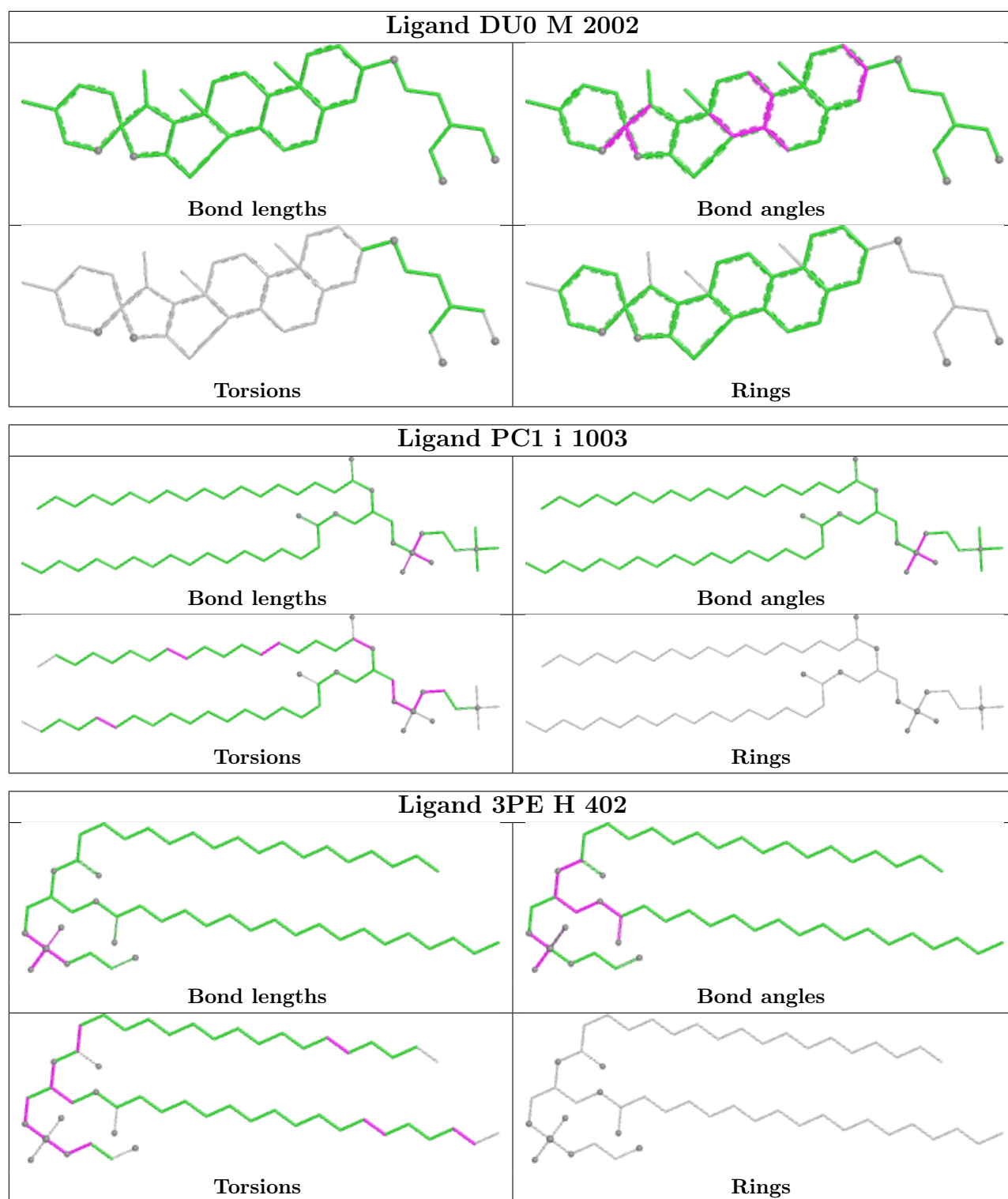
Ligand PC1 a 502	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 d 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PGT A 1001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

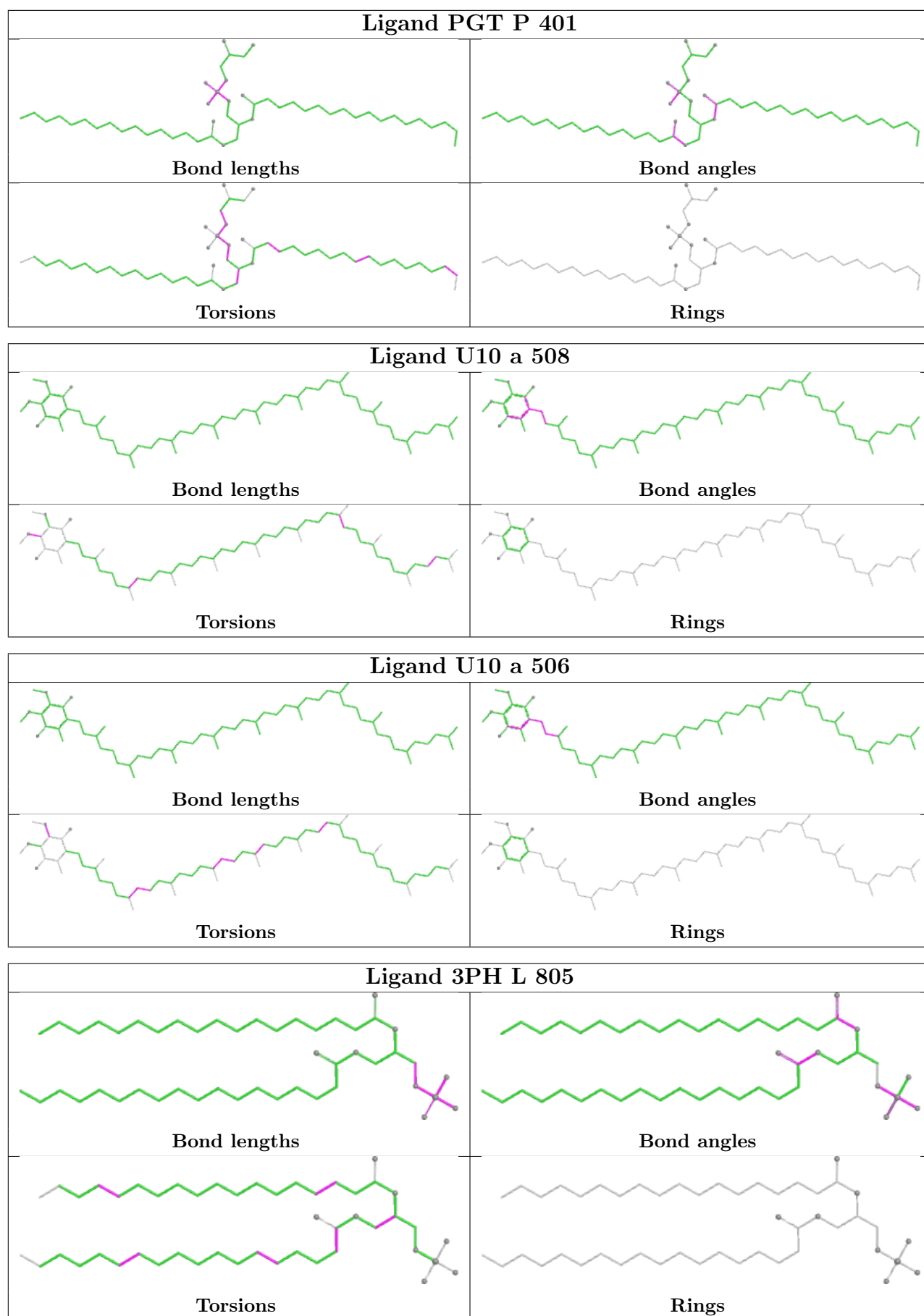


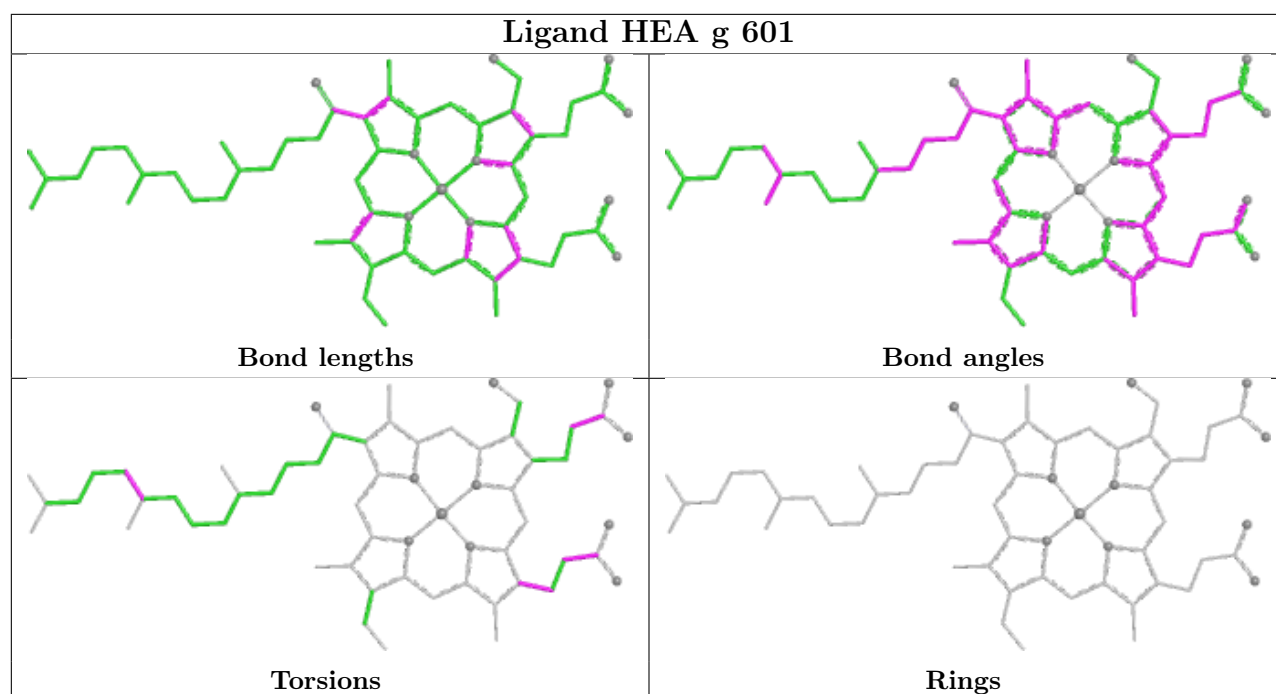












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

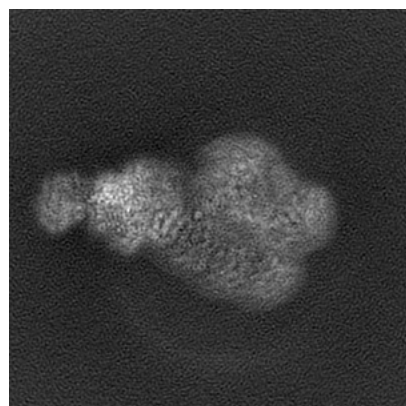
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51162. These allow visual inspection of the internal detail of the map and identification of artifacts.

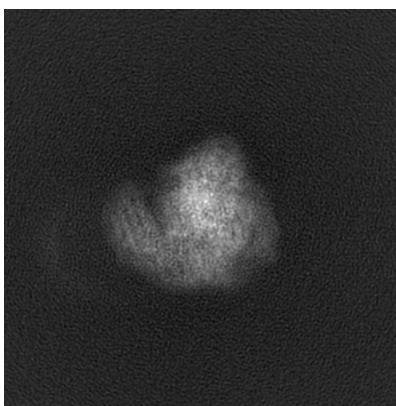
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

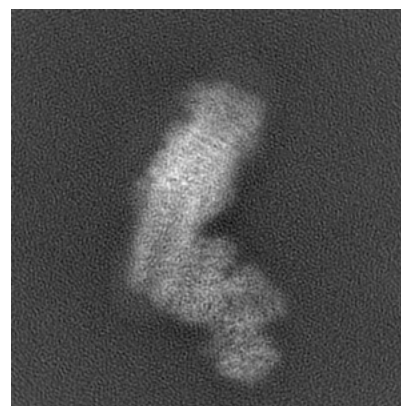
6.1.1 Primary map



X

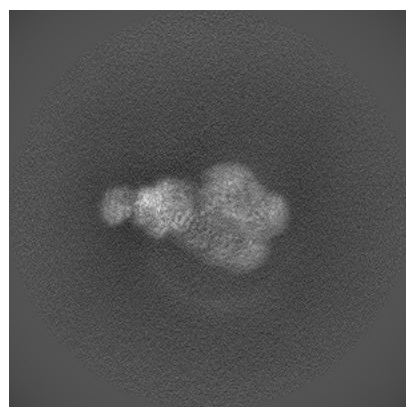


Y

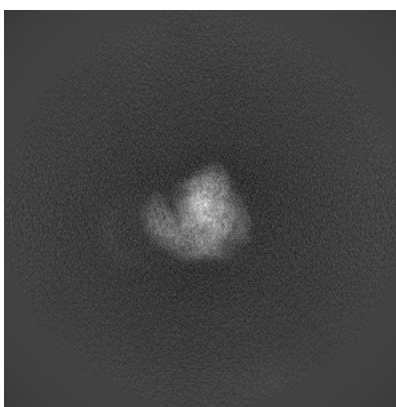


Z

6.1.2 Raw map



X



Y

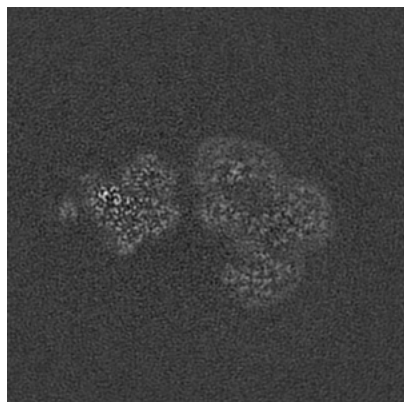


Z

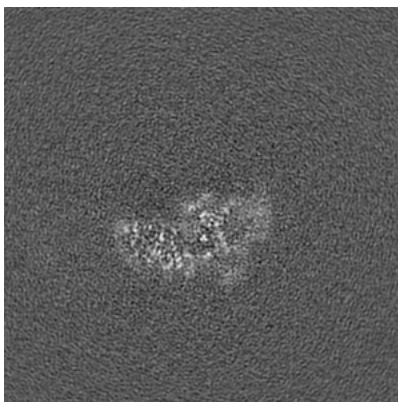
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

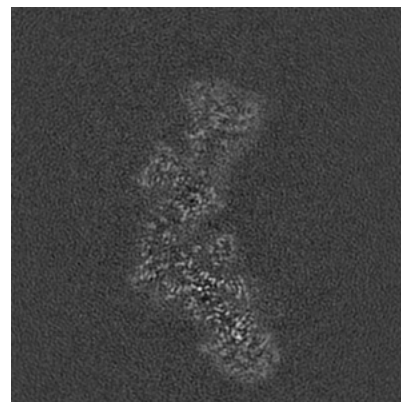
6.2.1 Primary map



X Index: 187

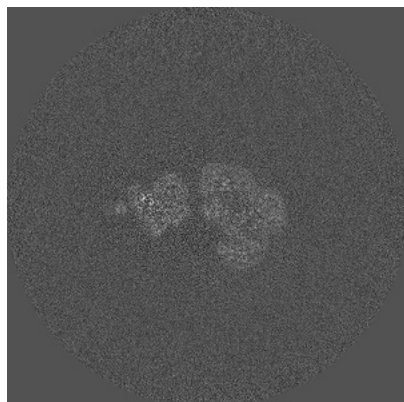


Y Index: 187

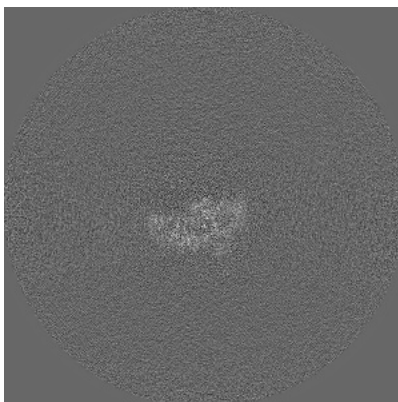


Z Index: 187

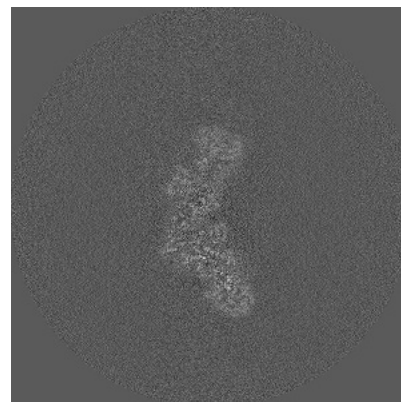
6.2.2 Raw map



X Index: 300



Y Index: 300

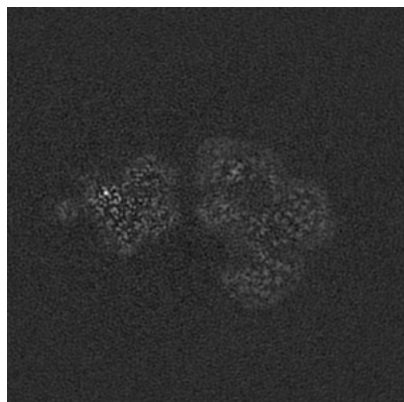


Z Index: 300

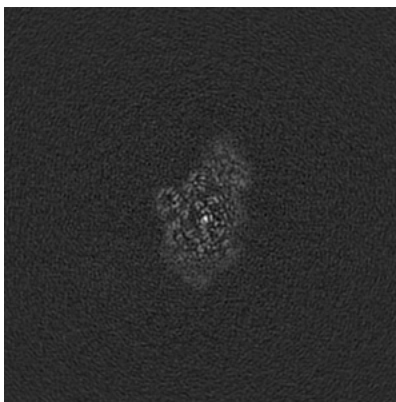
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

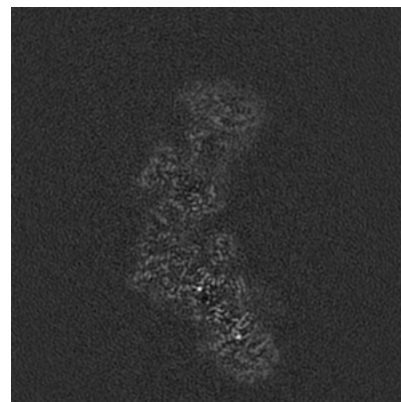
6.3.1 Primary map



X Index: 188

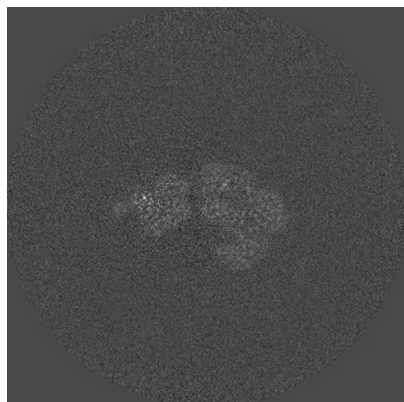


Y Index: 111

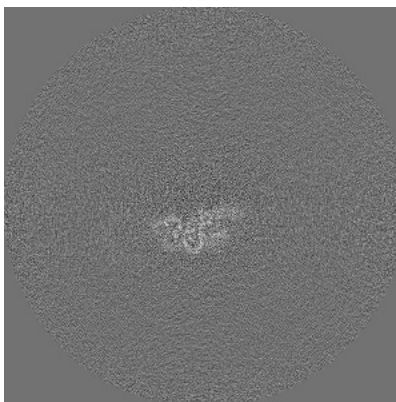


Z Index: 188

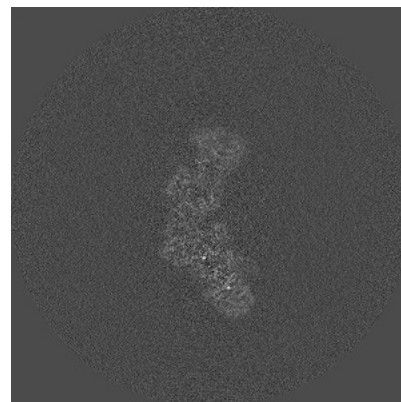
6.3.2 Raw map



X Index: 301



Y Index: 289

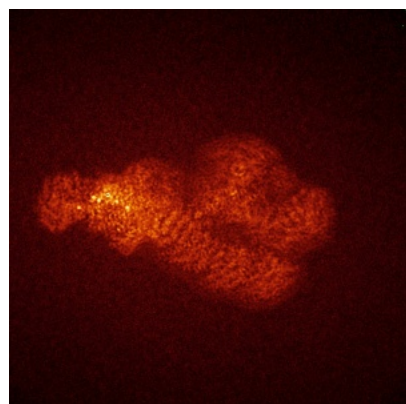


Z Index: 301

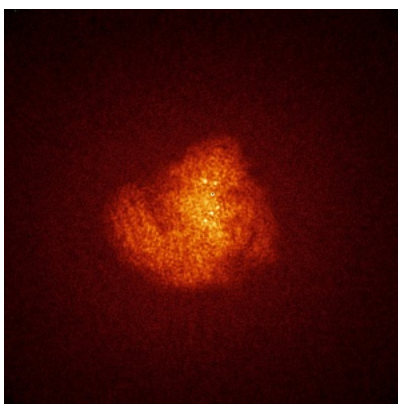
The images above show the largest variance slices of the map in three orthogonal directions.

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

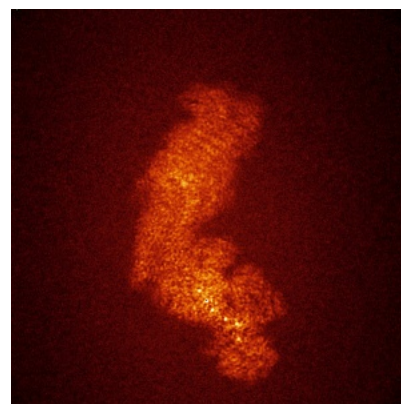
6.4.1 Primary map



X

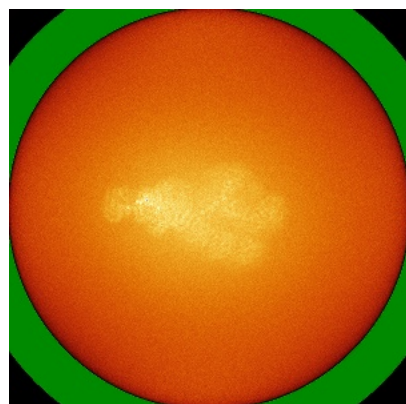


Y

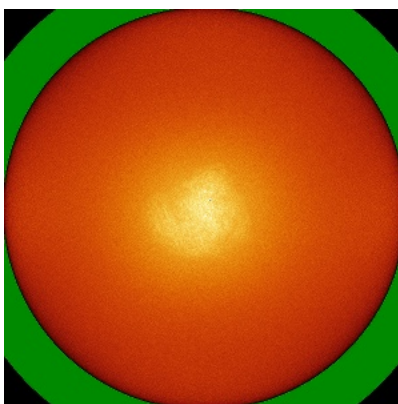


Z

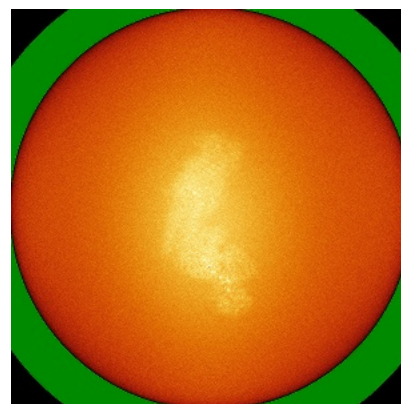
6.4.2 Raw map



X



Y

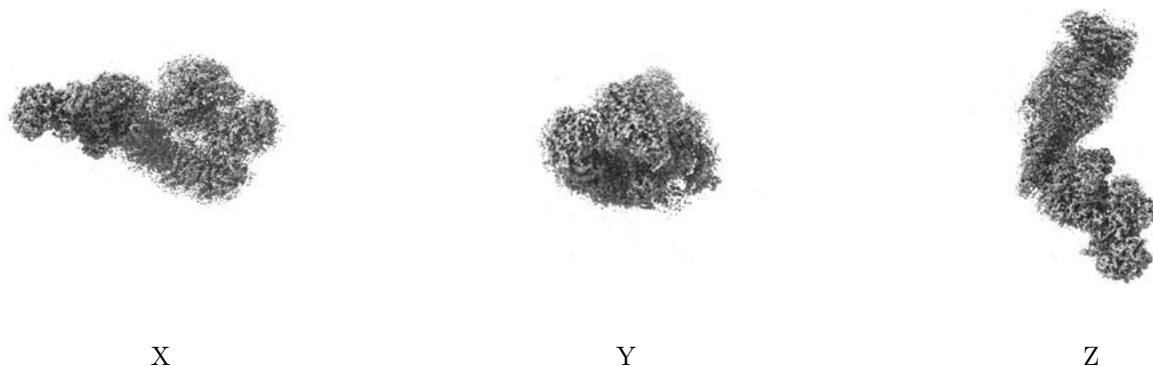


Z

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.

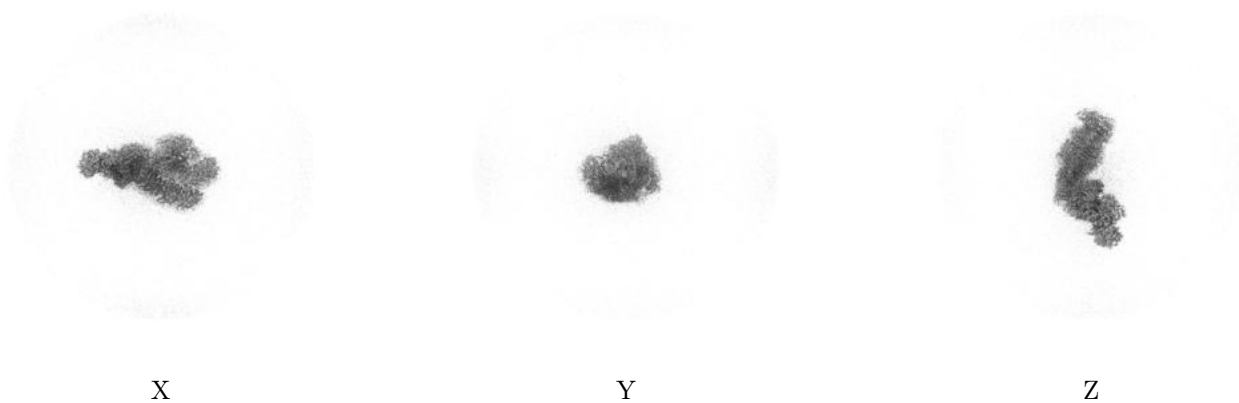
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

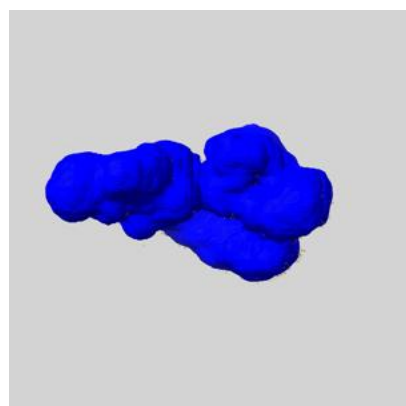
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

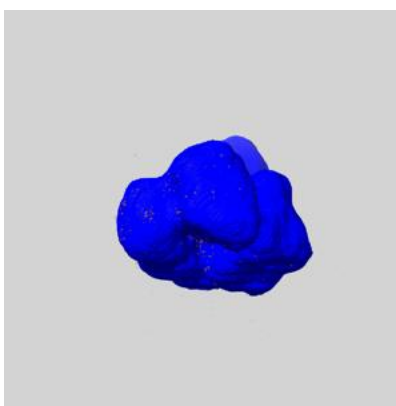
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

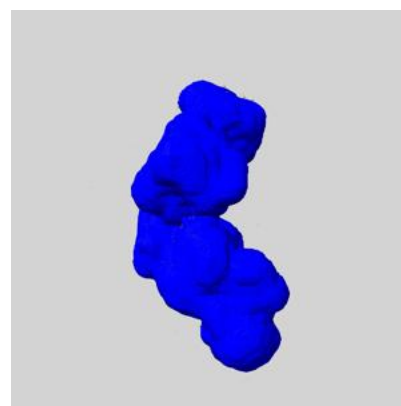
6.6.1 emd_51162_msk_1.map [i](#)



X

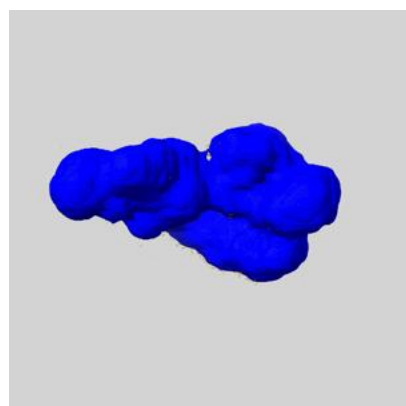


Y

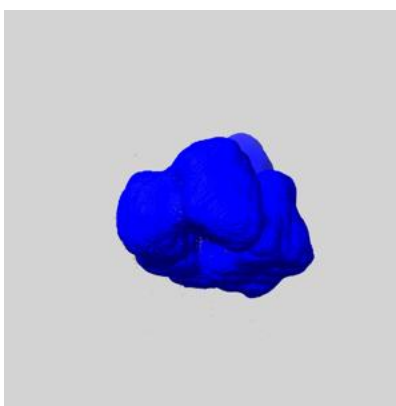


Z

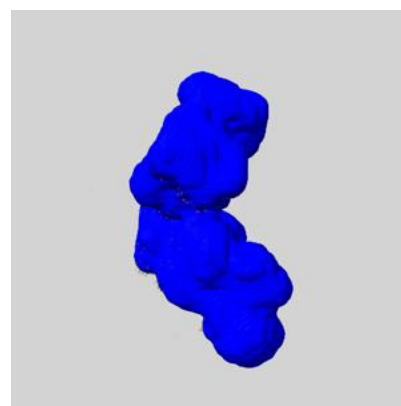
6.6.2 emd_51162_msk_2.map [i](#)



X



Y

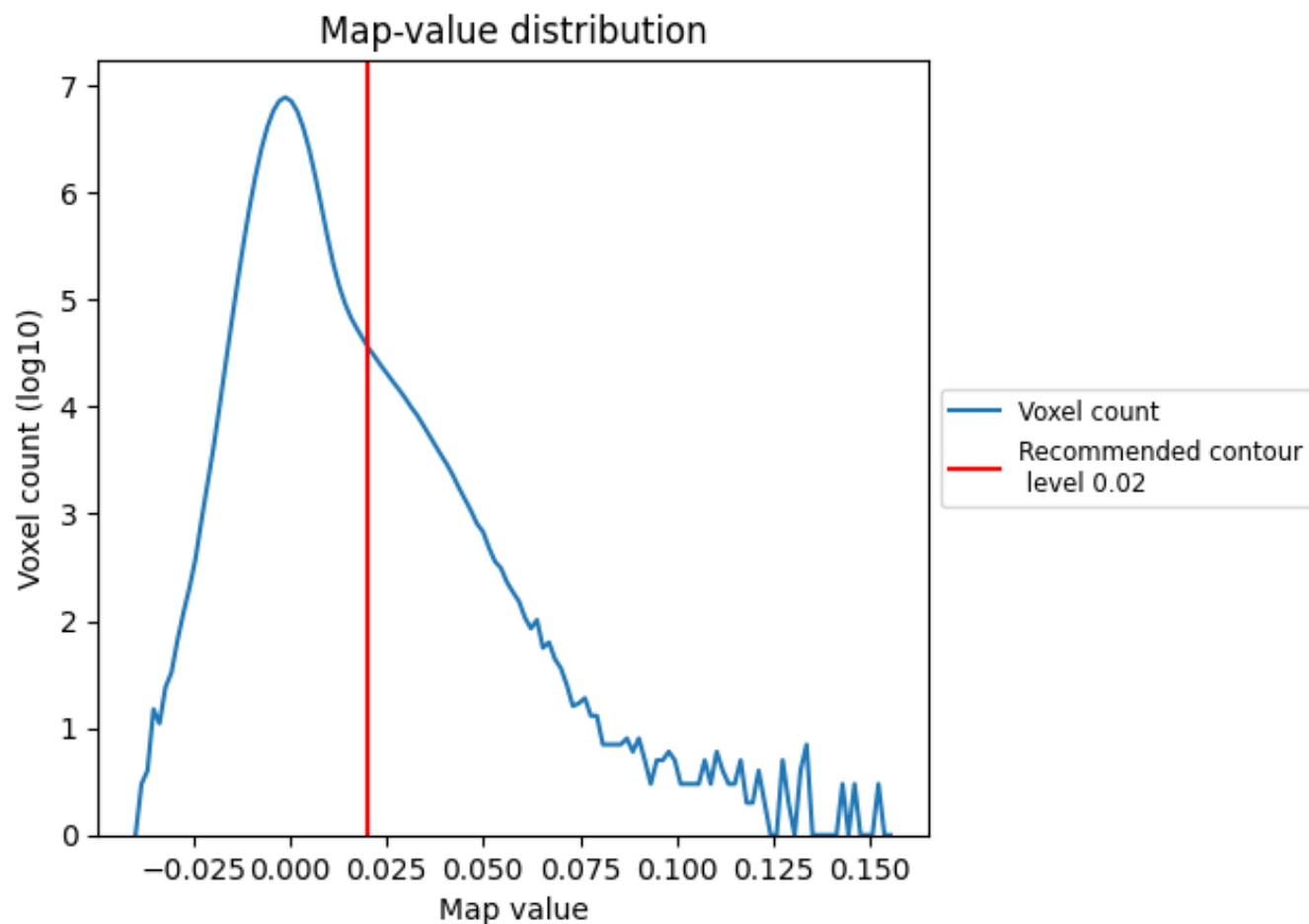


Z

7 Map analysis [i](#)

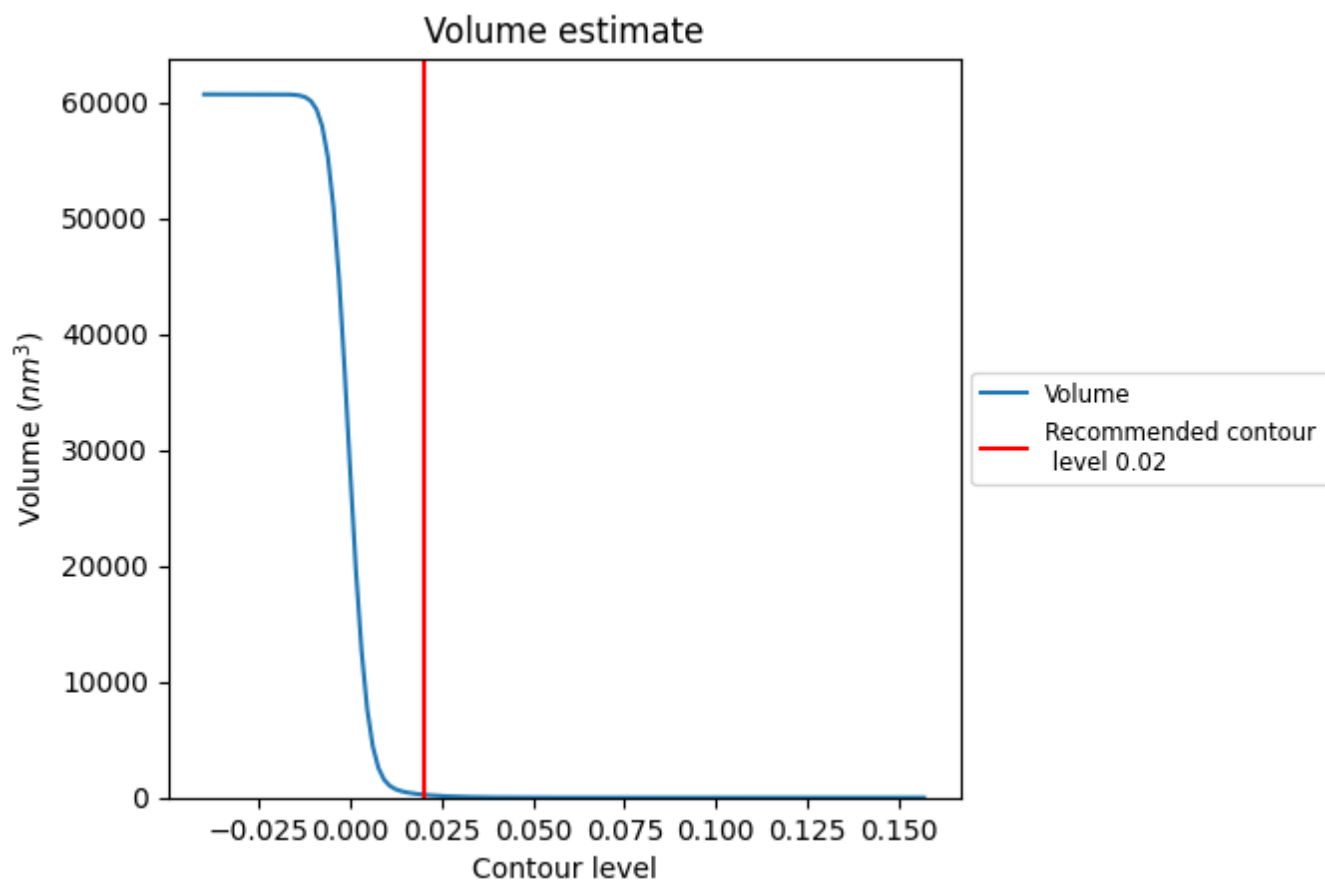
This section contains the results of statistical analysis of the map.

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.

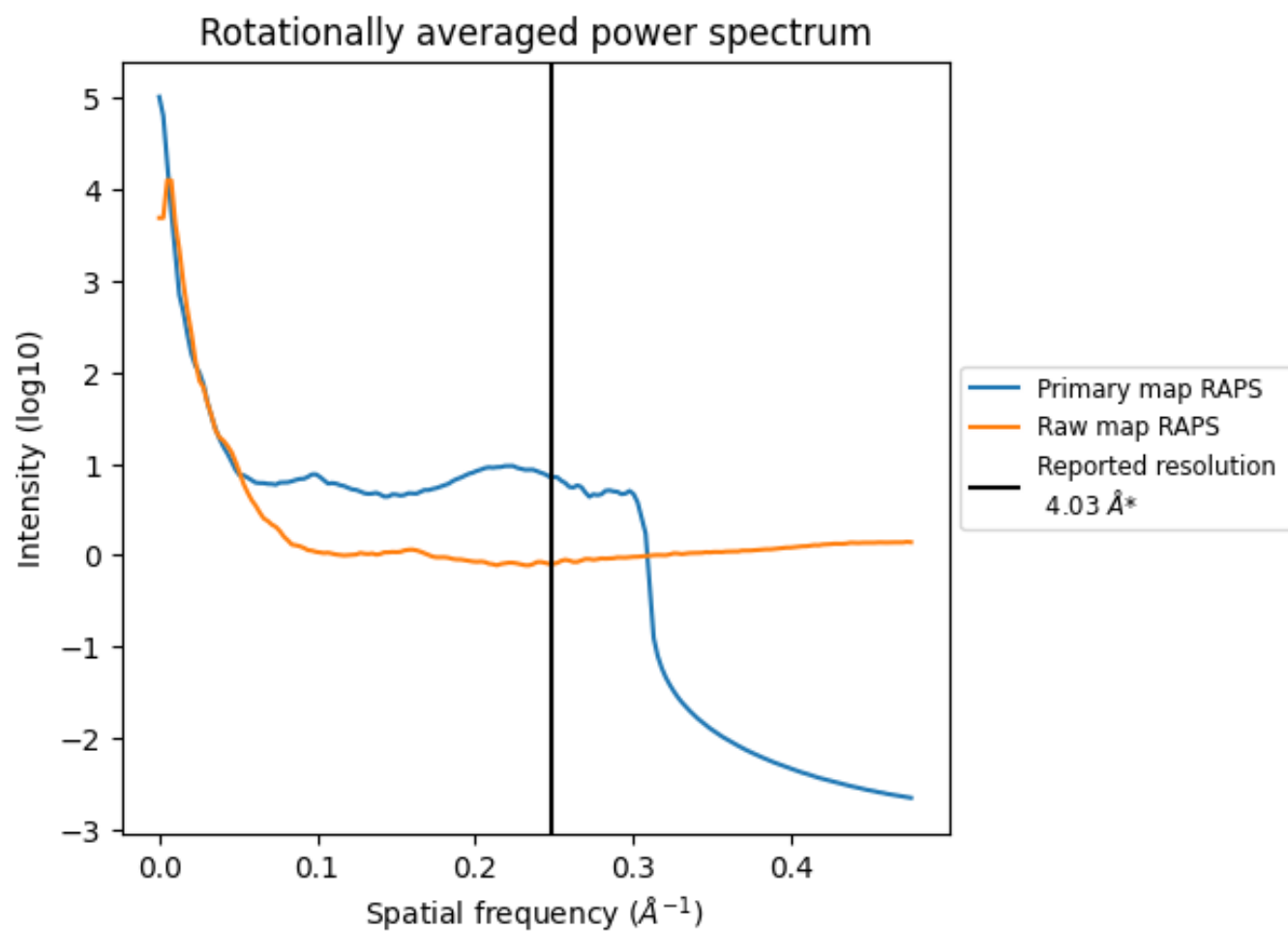
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm^3 ; this corresponds to an approximate mass of 226 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 ⓘ

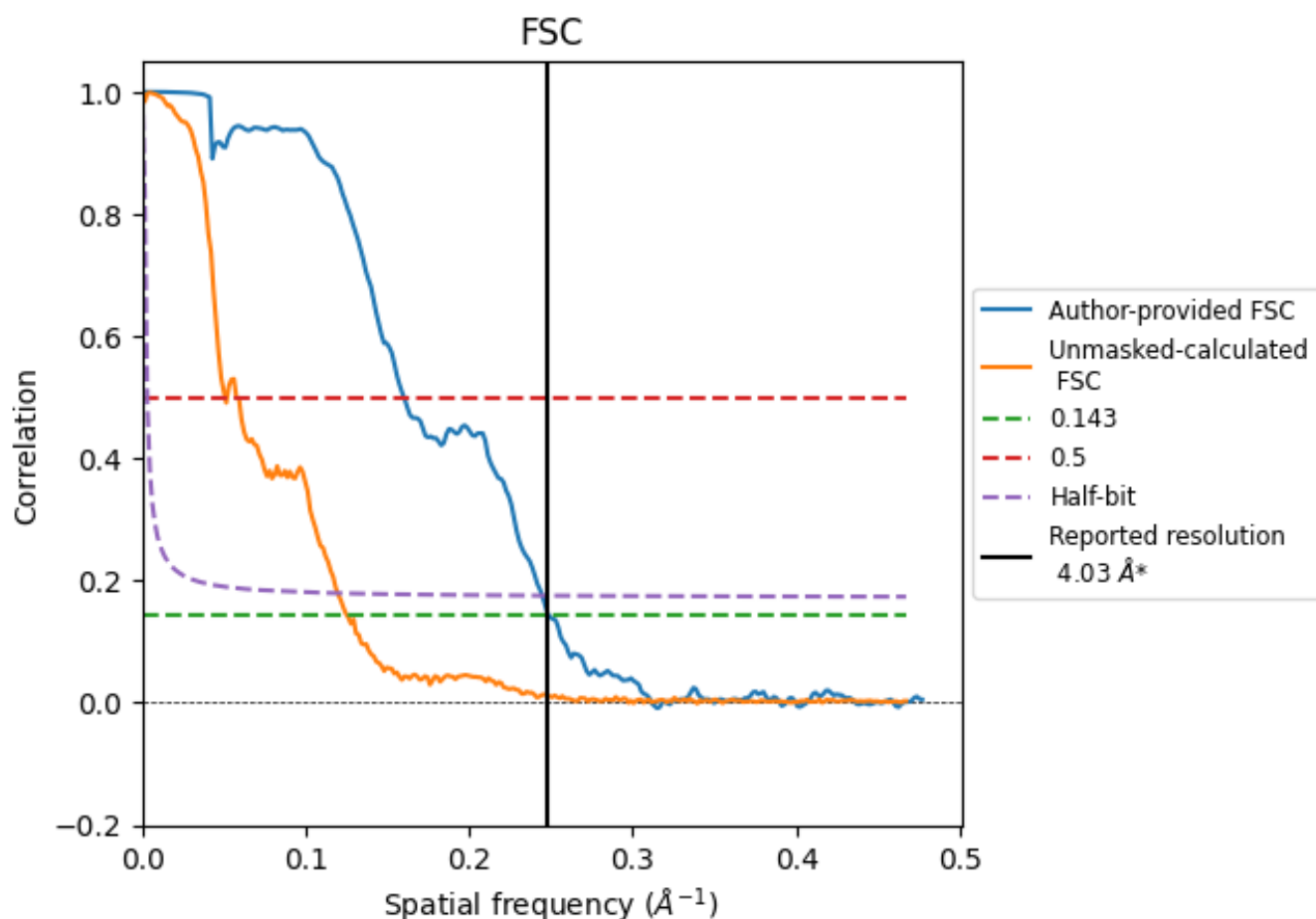


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.248 \AA^{-1}

8.2 Resolution estimates [i](#)

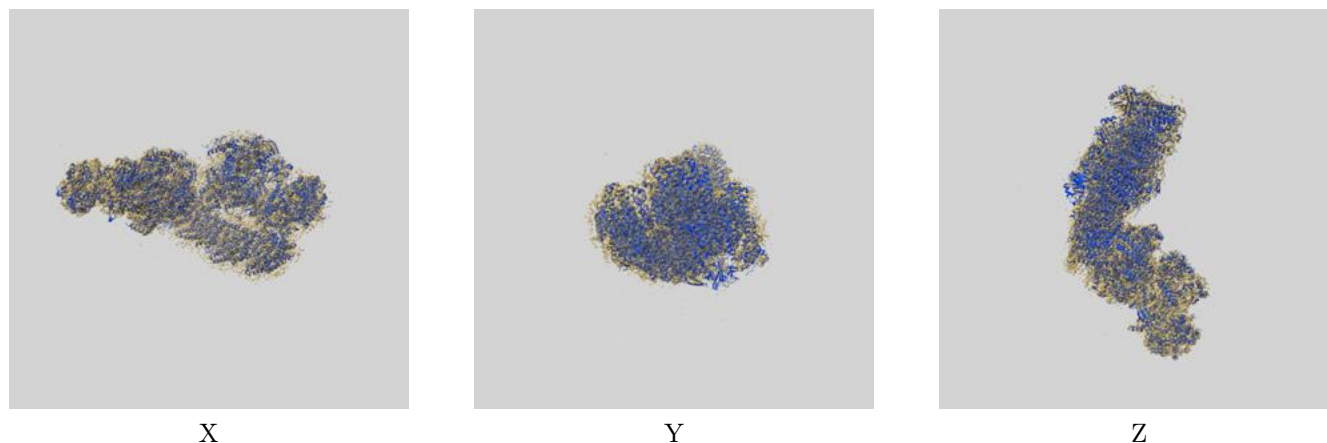
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.02	6.25	4.09
Unmasked-calculated*	7.99	19.72	8.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 4.03 by more than 10 %

9 Map-model fit [i](#)

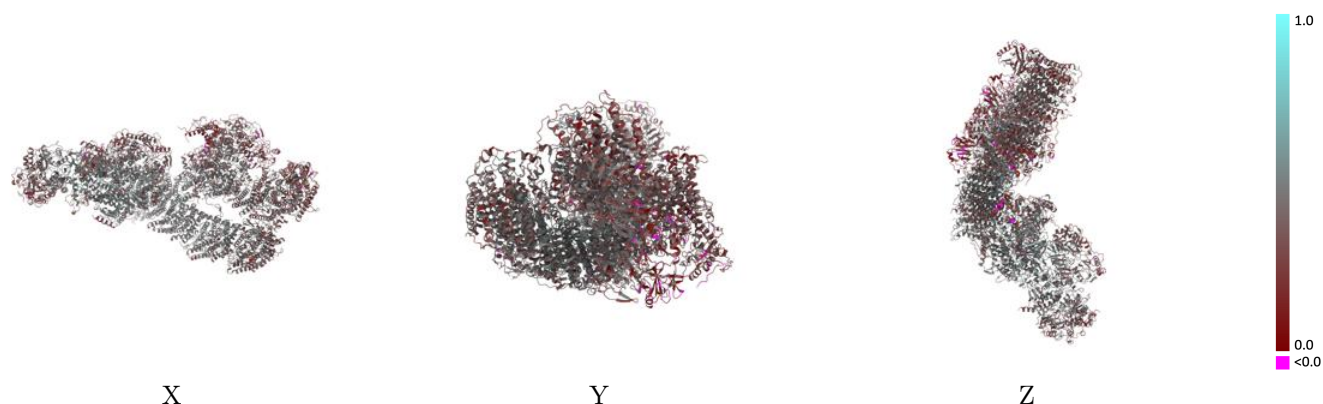
This section contains information regarding the fit between EMDB map EMD-51162 and PDB model 9G9Z. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



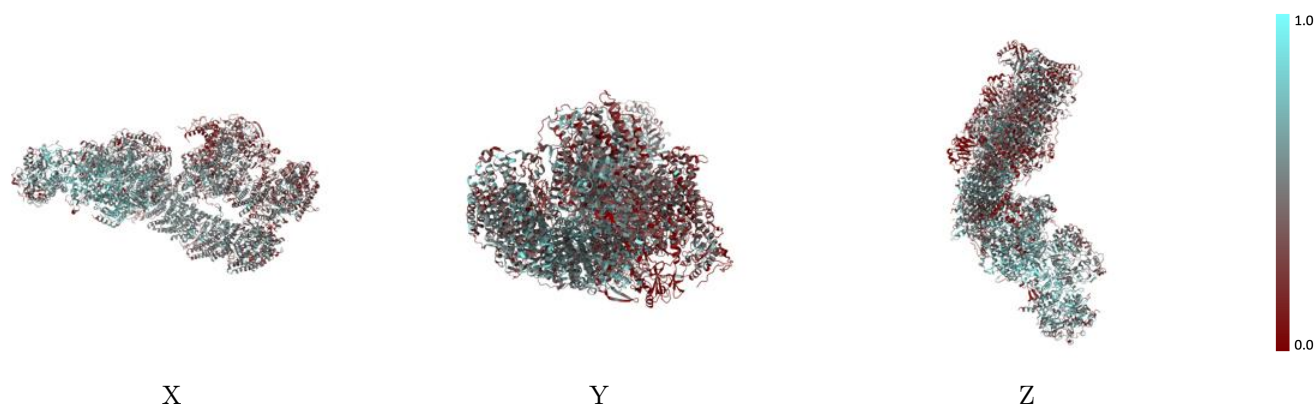
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



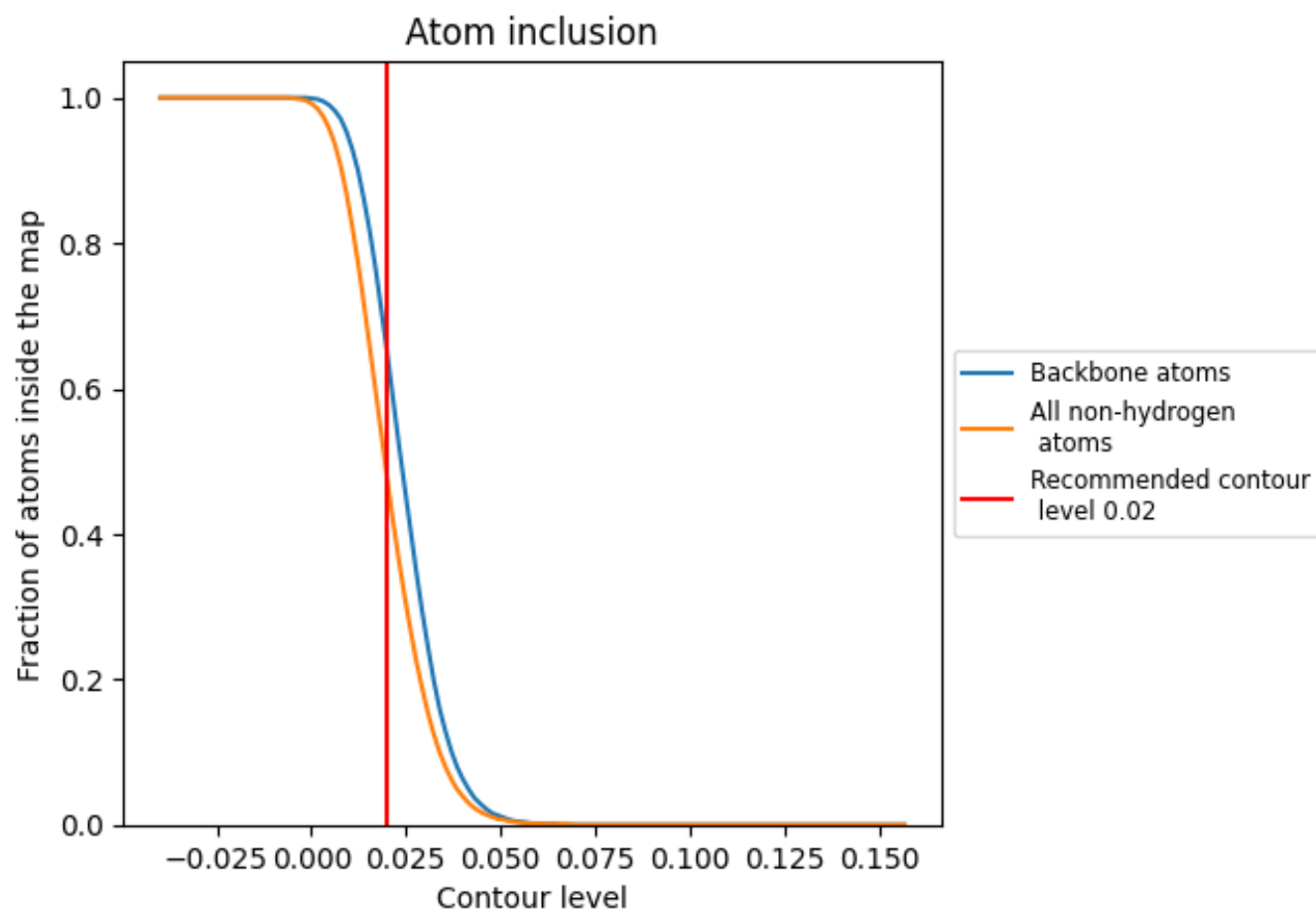
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

































































9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 48% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4790	 0.4070
A	 0.5140	 0.4470
B	 0.6030	 0.4740
C	 0.6630	 0.4790
D	 0.6410	 0.4830
E	 0.5590	 0.4070
F	 0.5320	 0.3890
G	 0.5660	 0.4250
H	 0.5770	 0.4620
I	 0.6990	 0.5010
J	 0.5200	 0.4530
K	 0.5510	 0.4670
L	 0.4730	 0.4060
M	 0.5090	 0.4390
N	 0.5620	 0.4530
P	 0.4070	 0.3740
Q	 0.5990	 0.4550
R	 0.2320	 0.4130
Z	 0.5410	 0.4340
a	 0.4820	 0.4300
b	 0.4300	 0.3720
c	 0.2150	 0.2920
d	 0.3570	 0.3540
e	 0.2870	 0.3130
f	 0.0810	 0.2240
g	 0.4210	 0.3760
h	 0.3150	 0.3070
i	 0.4160	 0.4000
j	 0.2470	 0.3250
o	 0.0930	 0.2540
p	 0.3990	 0.3930
q	 0.5560	 0.4320

