



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:11 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

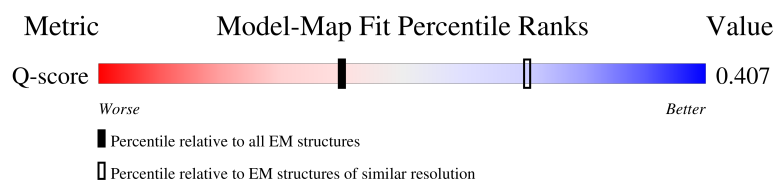
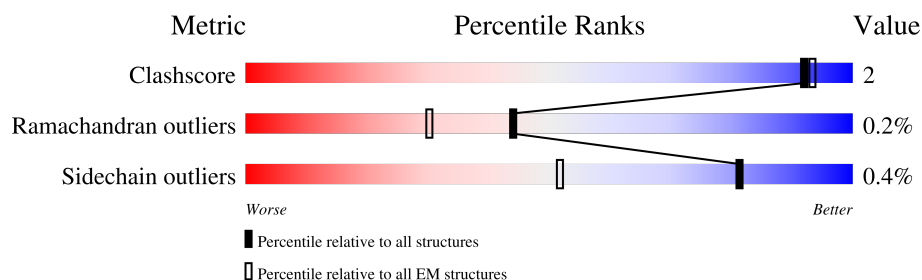
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	<div><div><div></div><div></div><div></div></div><div>12%23%74%</div></div>
27	q	124	<div><div><div></div><div></div><div></div></div><div>27%98%</div></div>

## 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		

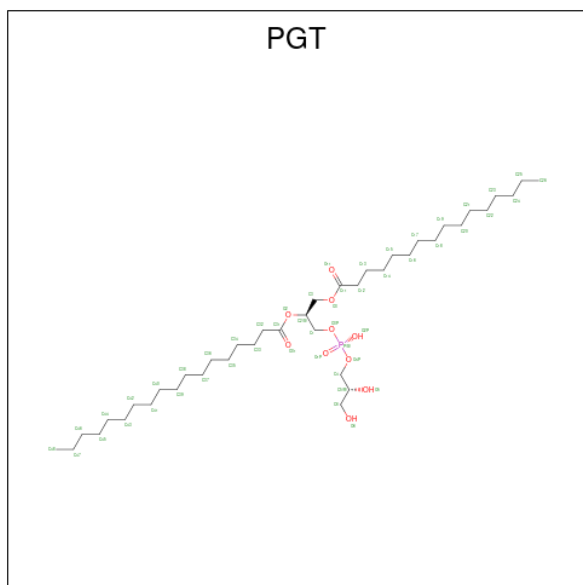
- Molecule 26 is a protein called Cytochrome c, class I.

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.

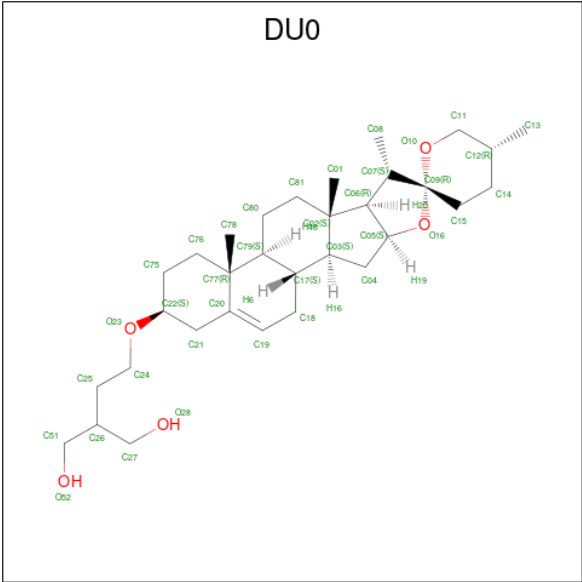
Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



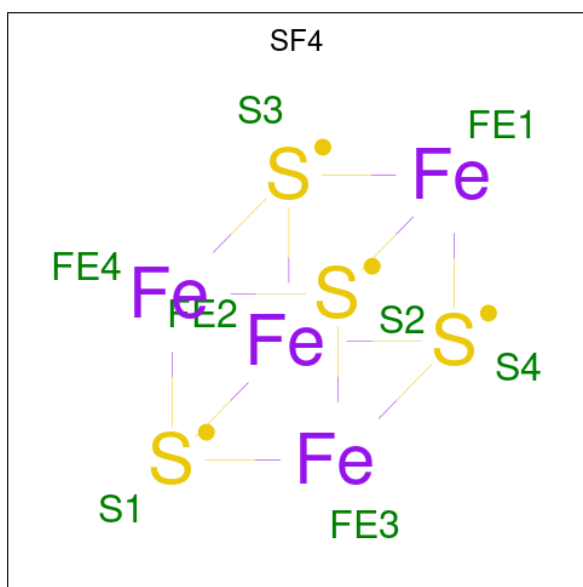
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			51	40	10	1	
28	A	1	Total	C	O	P	0
			51	40	10	1	
28	J	1	Total	C	O	P	0
			51	40	10	1	
28	L	1	Total	C	O	P	0
			51	40	10	1	
28	P	1	Total	C	O	P	0
			51	40	10	1	
28	q	1	Total	C	O	P	0
			51	40	10	1	

- 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<sup>2,9</sup>.0<sup>4,8</sup>.0<sup>13,18</sup>]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C<sub>32</sub>H<sub>52</sub>O<sub>5</sub>).



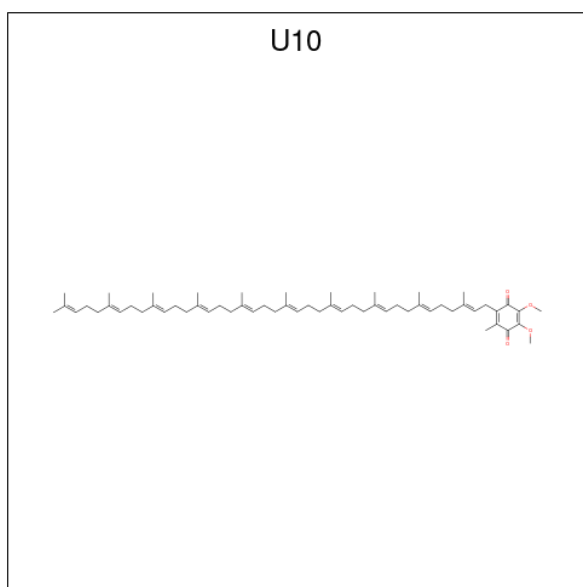
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			37	32	5	
29	H	1	Total	C	O	0
			37	32	5	
29	J	1	Total	C	O	0
			37	32	5	
29	J	1	Total	C	O	0
			37	32	5	
29	M	1	Total	C	O	0
			37	32	5	
29	M	1	Total	C	O	0
			37	32	5	
29	c	1	Total	C	O	0
			37	32	5	
29	c	1	Total	C	O	0
			37	32	5	
29	i	1	Total	C	O	0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

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).

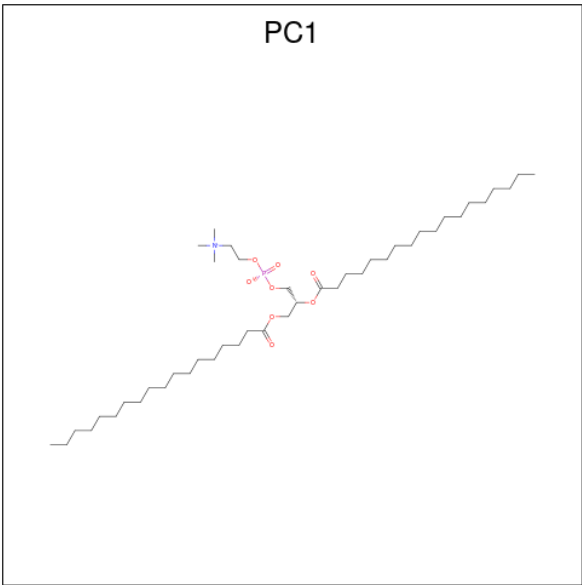


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			63	59	4	
31	a	1	Total	C	O	0
			63	59	4	
31	a	1	Total	C	O	0
			63	59	4	
31	d	1	Total	C	O	0
			63	59	4	
31	d	1	Total	C	O	0
			63	59	4	

- 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: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



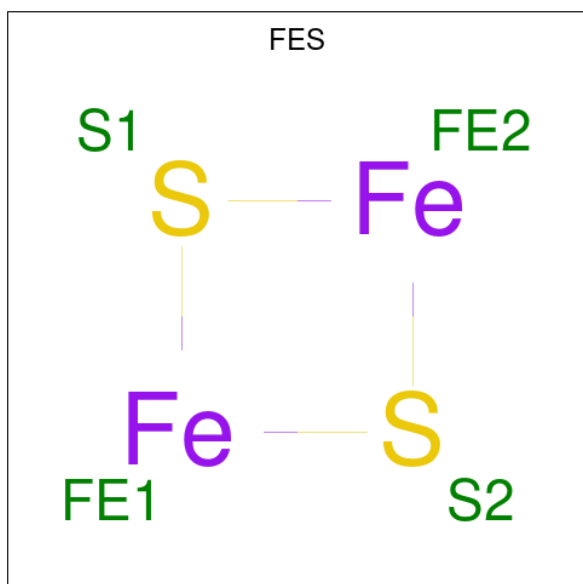
Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44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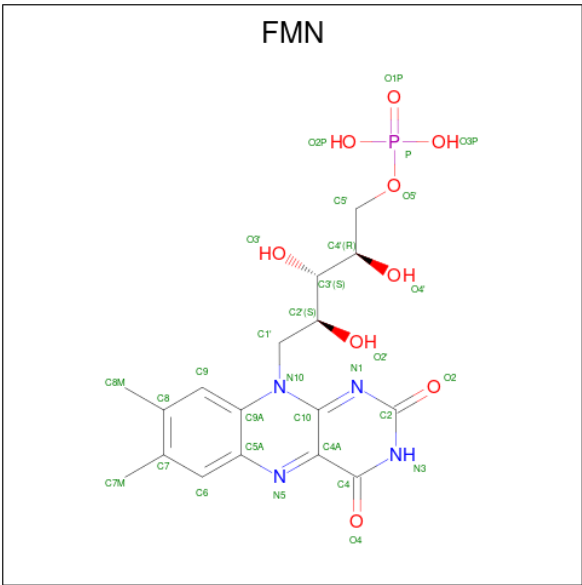
Mol	Chain	Residues	Atoms					AltConf
33	j	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



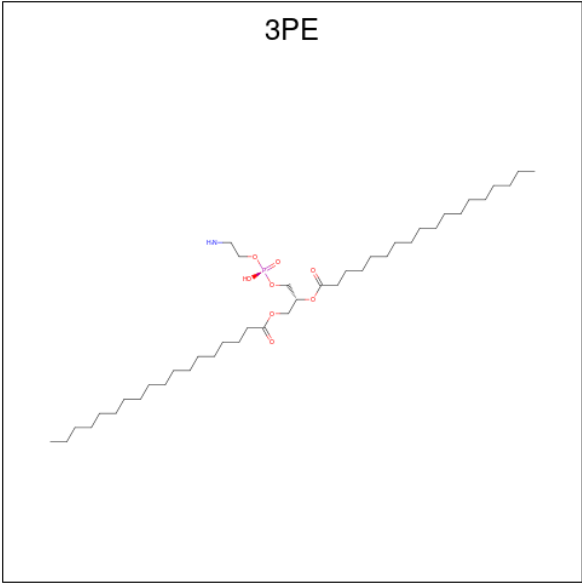
Mol	Chain	Residues	Atoms			AltConf
34	E	1	Total	Fe	S	0
			4	2	2	
34	G	1	Total	Fe	S	0
			4	2	2	
34	c	1	Total	Fe	S	0
			4	2	2	
34	f	1	Total	Fe	S	0
			4	2	2	

- 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:  $C_{41}H_{82}NO_8P$ ).



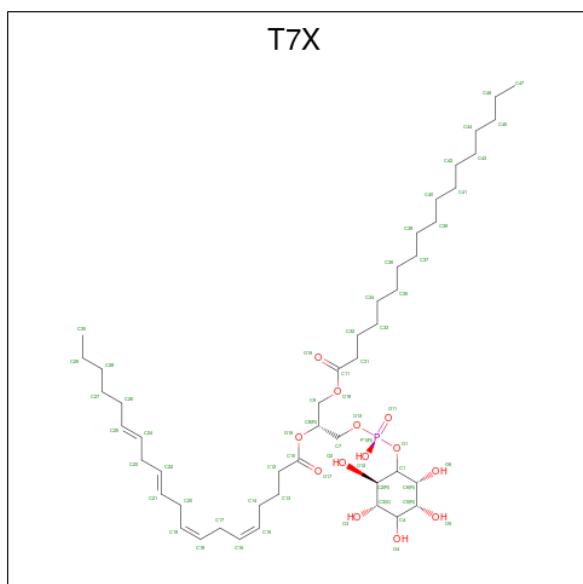
Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

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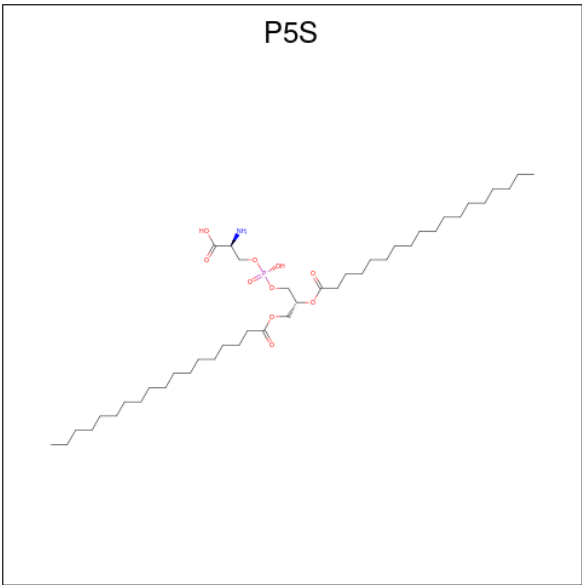
Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	c	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
36	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



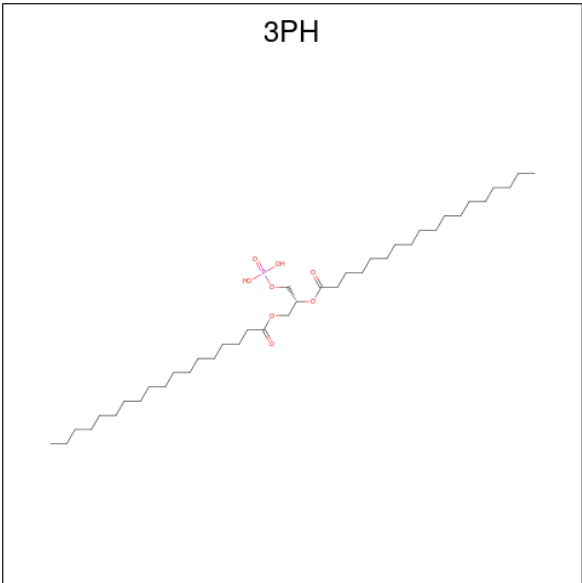
Mol	Chain	Residues	Atoms				AltConf
37	J	1	Total	C	O	P	0
			61	47	13	1	

- 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
			Total	C	N	O	P	
38	L	1	54	42	1	10	1	0

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



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

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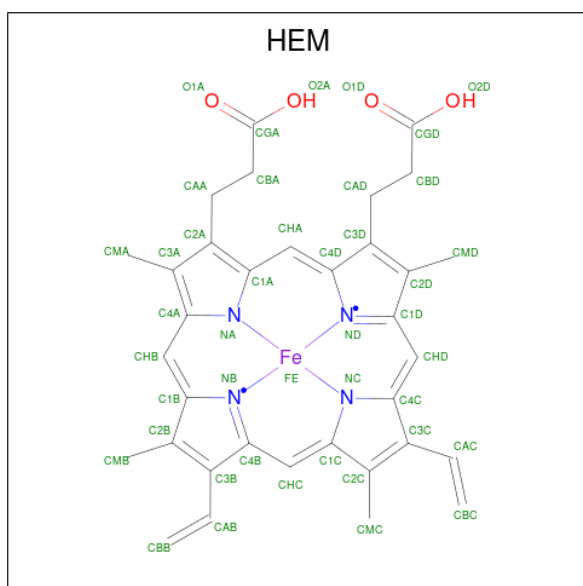
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Mol	Chain	Residues	Atoms				AltConf
39	M	1	Total	C	O	P	0
			48	39	8	1	
39	a	1	Total	C	O	P	0
			48	39	8	1	
39	c	1	Total	C	O	P	0
			48	39	8	1	
39	f	1	Total	C	O	P	0
			48	39	8	1	
39	i	1	Total	C	O	P	0
			48	39	8	1	

- 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: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



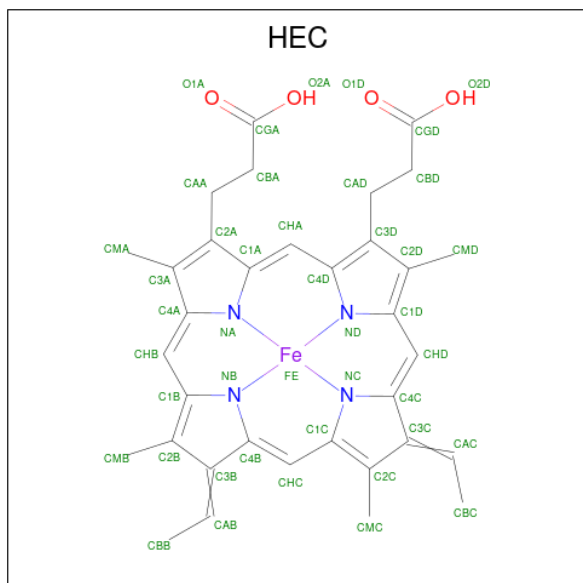
Mol	Chain	Residues	Atoms					AltConf
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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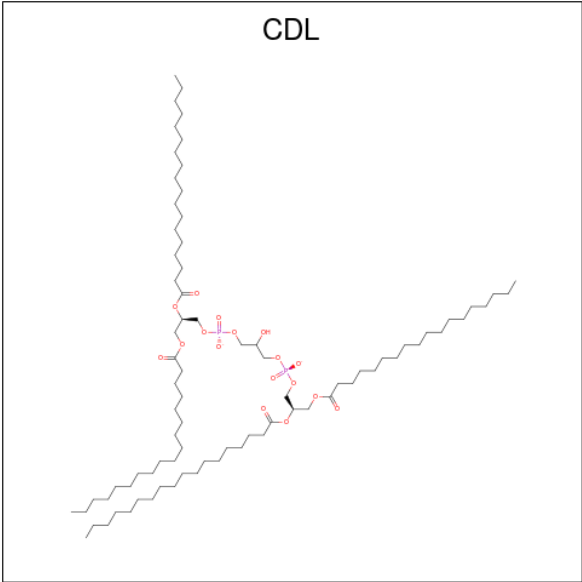
Mol	Chain	Residues	Atoms					AltConf
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



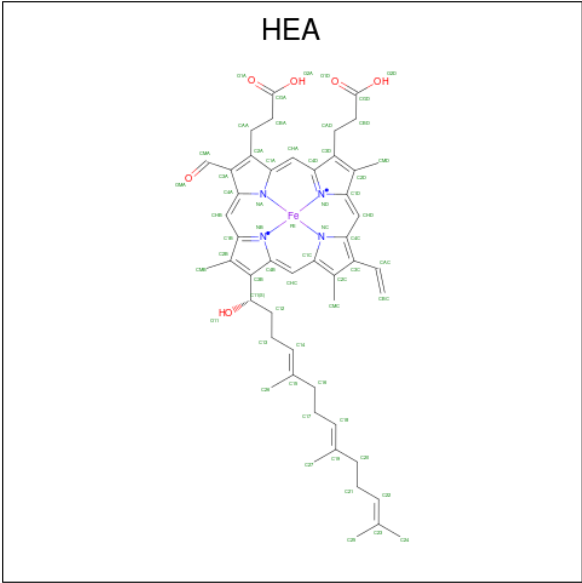
Mol	Chain	Residues	Atoms					AltConf
42	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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

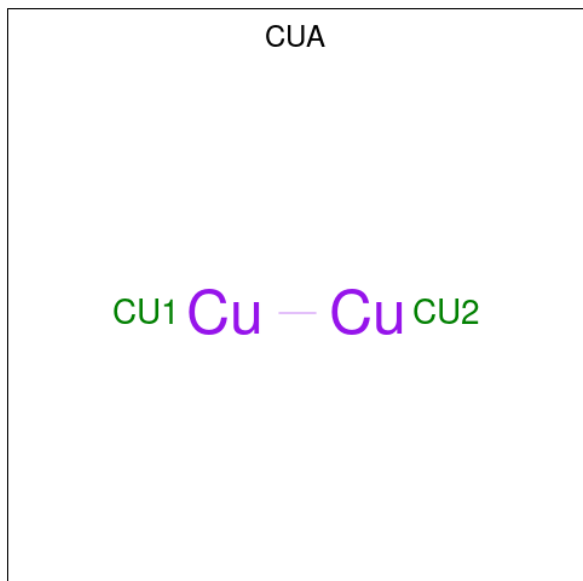
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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: Cu<sub>2</sub>).

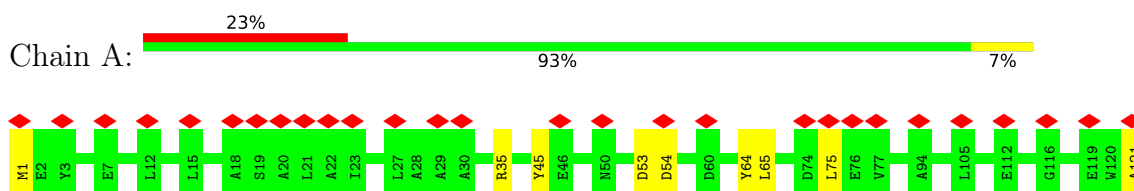


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total	Cu	0
			2	2	

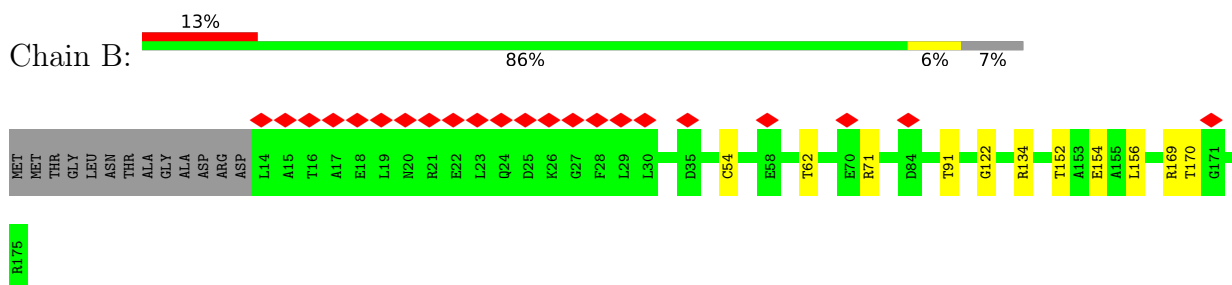
### 3 Residue-property plots [i](#)

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.

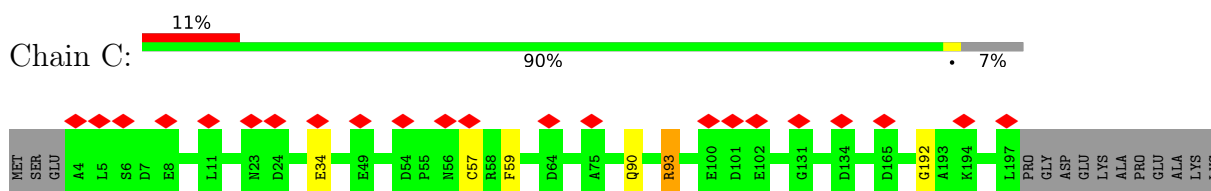
- Molecule 1: NADH-quinone oxidoreductase subunit A



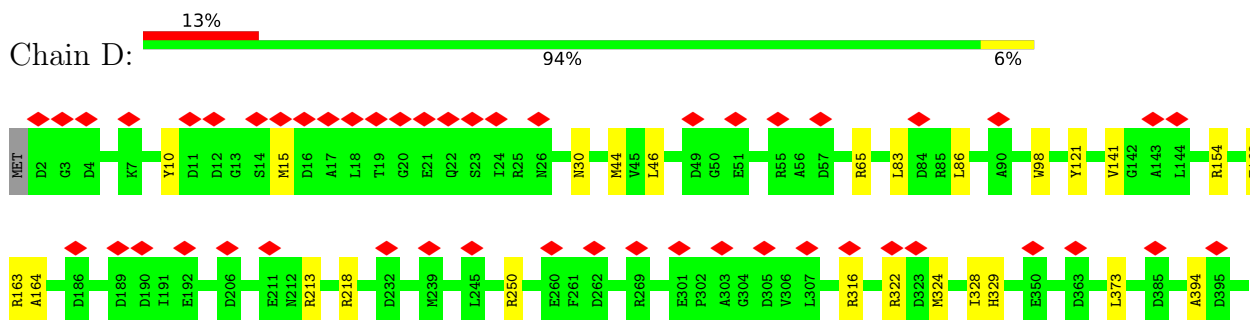
- Molecule 2: NADH-quinone oxidoreductase subunit B

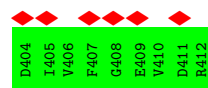


- Molecule 3: NADH-quinone oxidoreductase subunit C

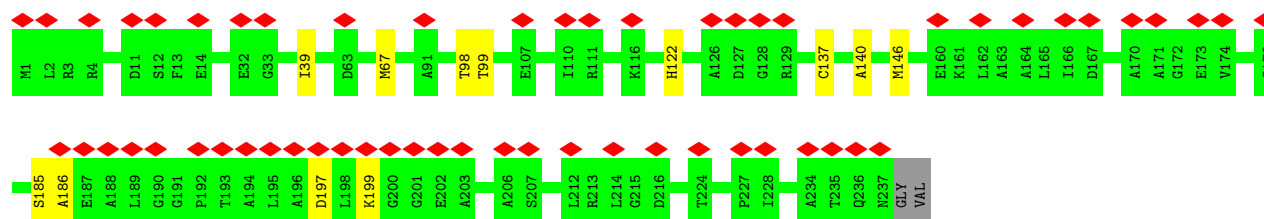
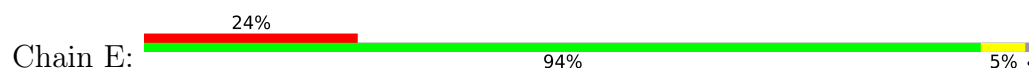


- Molecule 4: NADH-quinone oxidoreductase subunit D

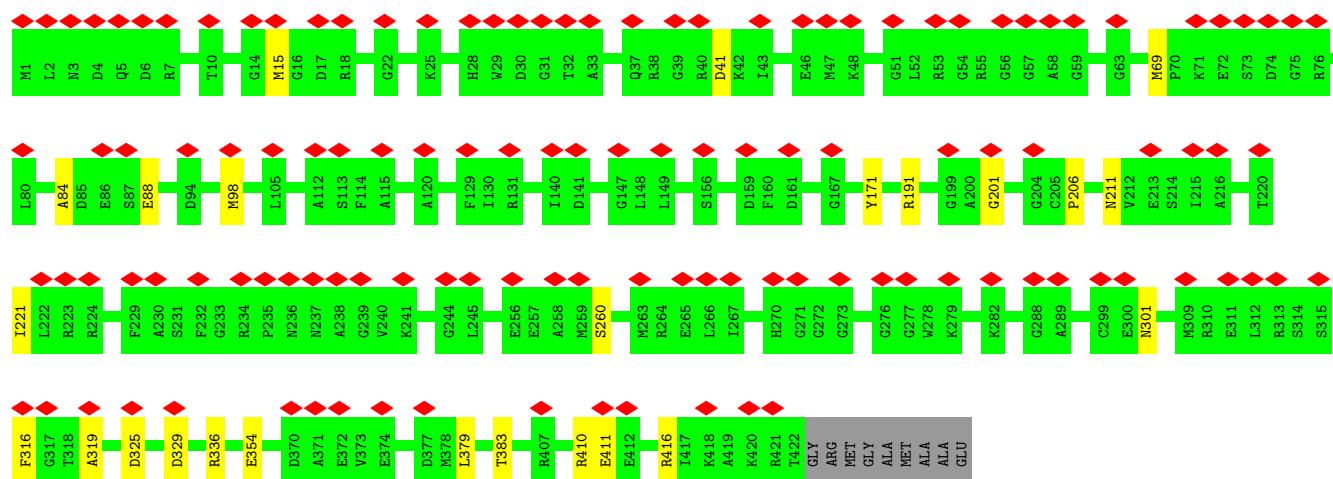
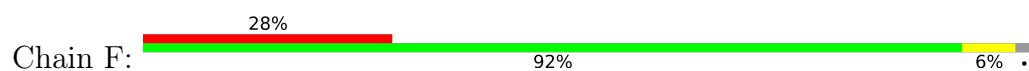




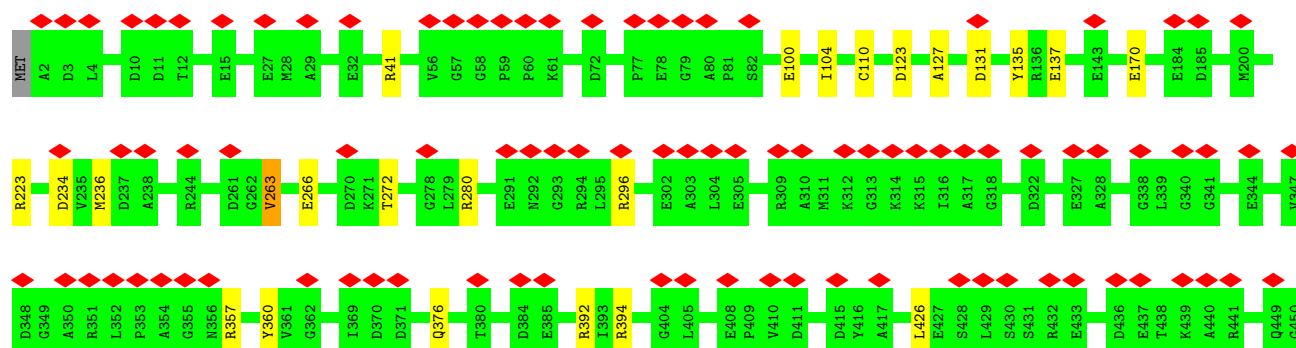
• Molecule 5: NADH dehydrogenase subunit E

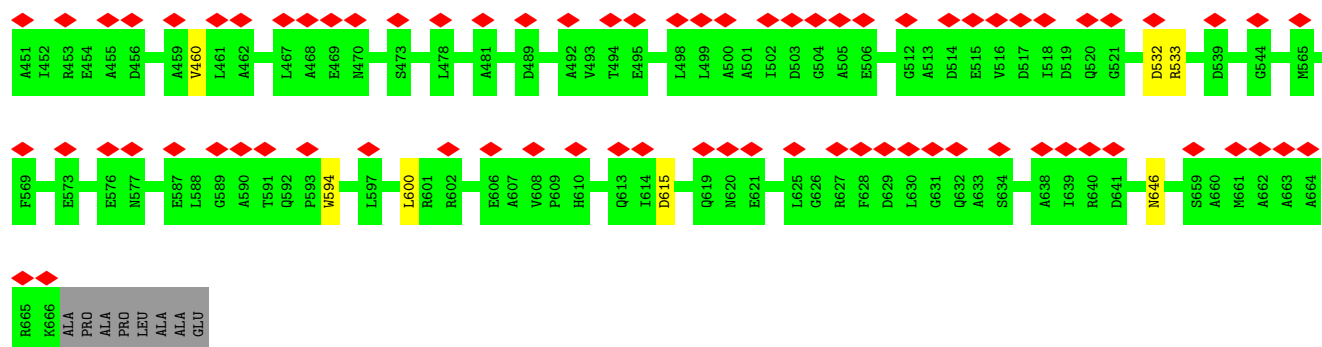


• Molecule 6: NADH-quinone oxidoreductase subunit F



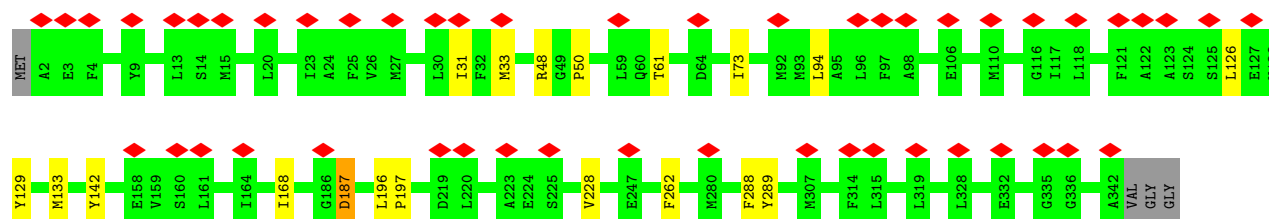
• Molecule 7: NADH-quinone oxidoreductase





• Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H: 14% 93% 5%



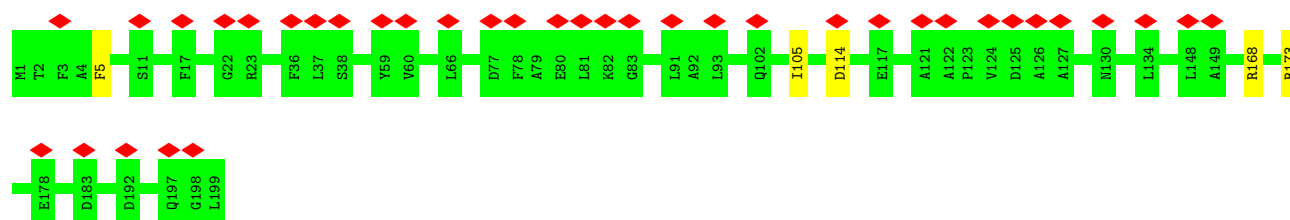
• Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I: 7% 96% 5%



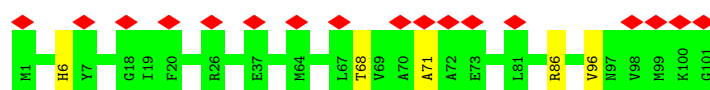
• Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J: 19% 97% 5%

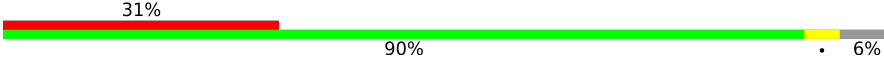


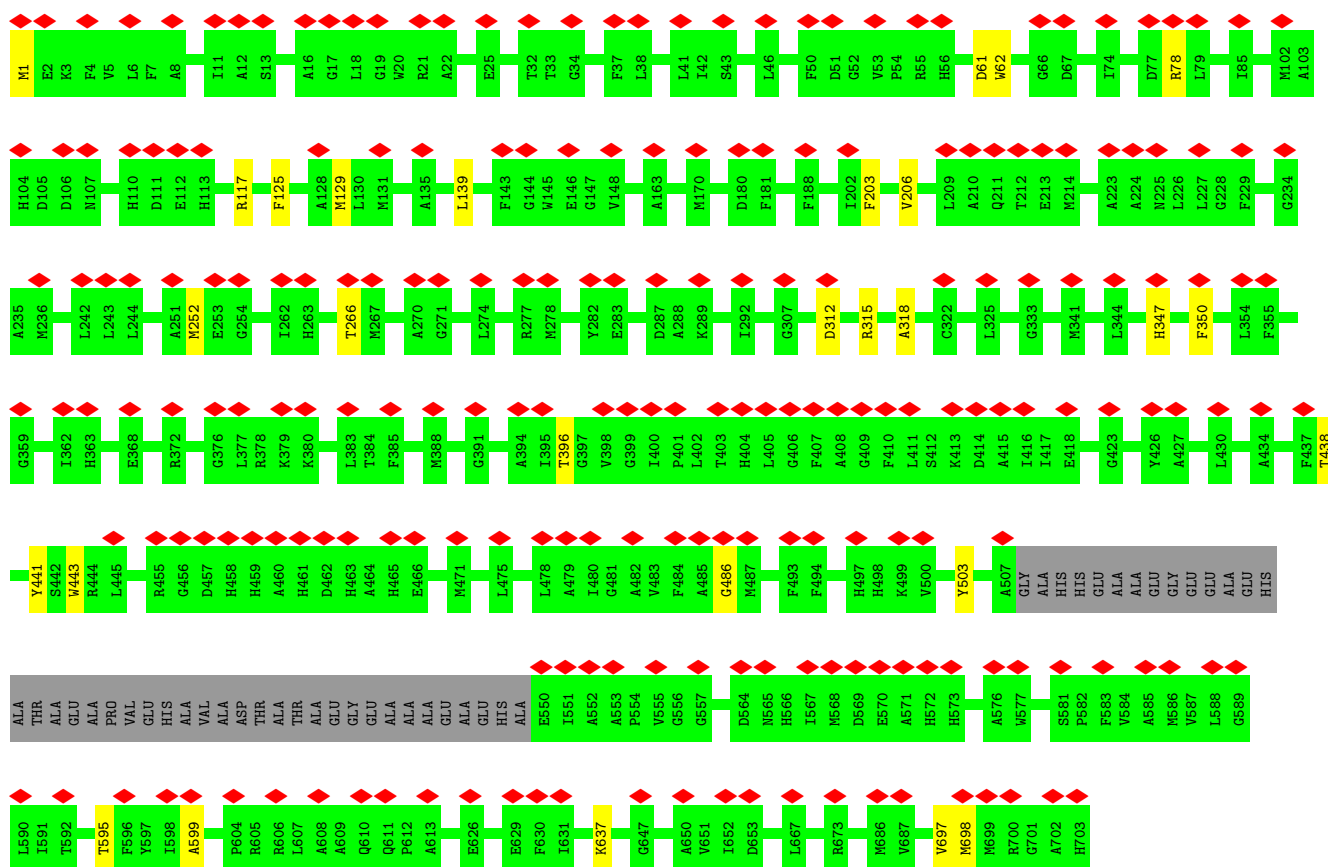
• Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K: 17% 95% 5%

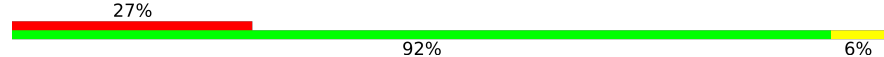


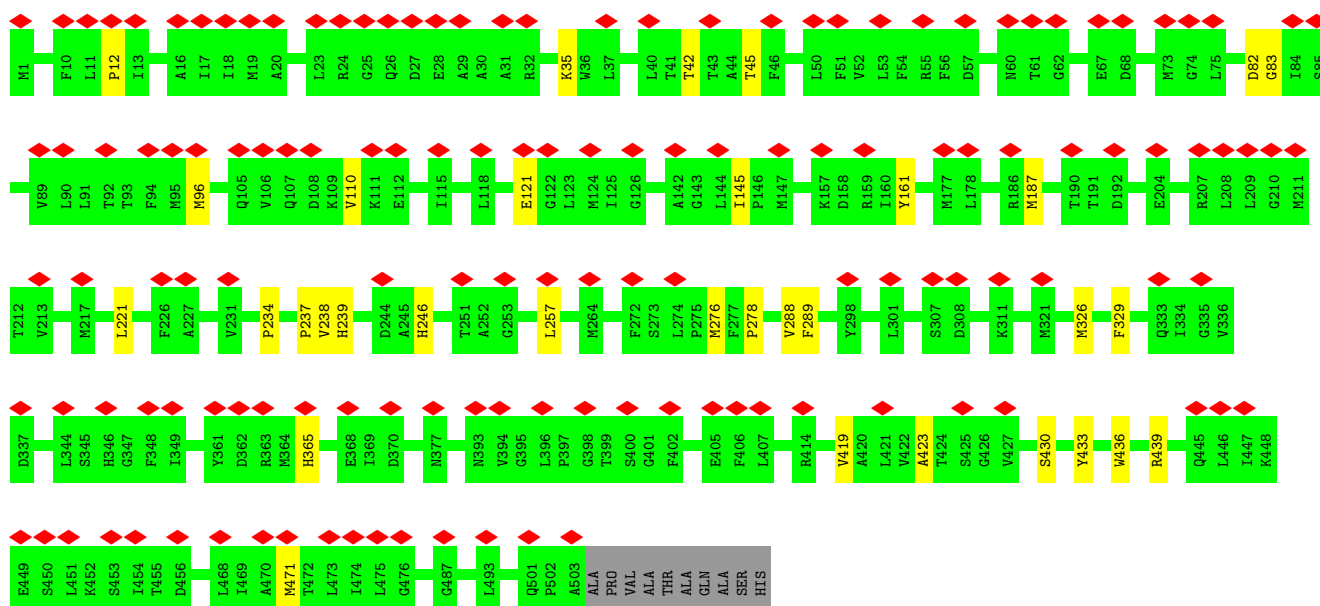
• Molecule 12: NADH dehydrogenase subunit L

Chain L:  31% 90% 6%

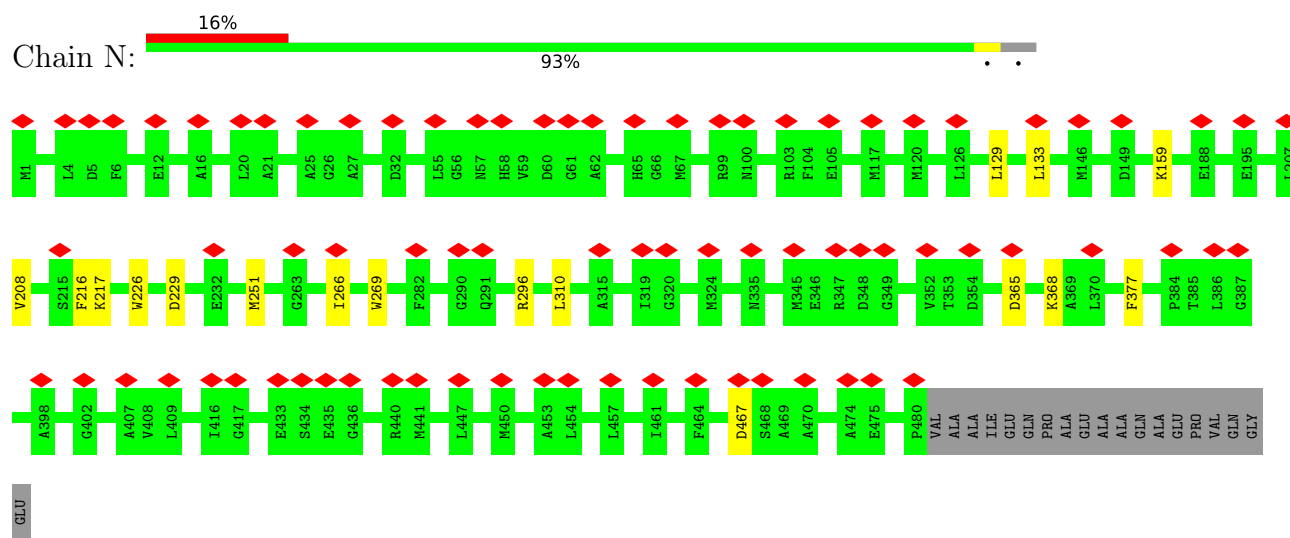


• Molecule 13: NADH dehydrogenase subunit M

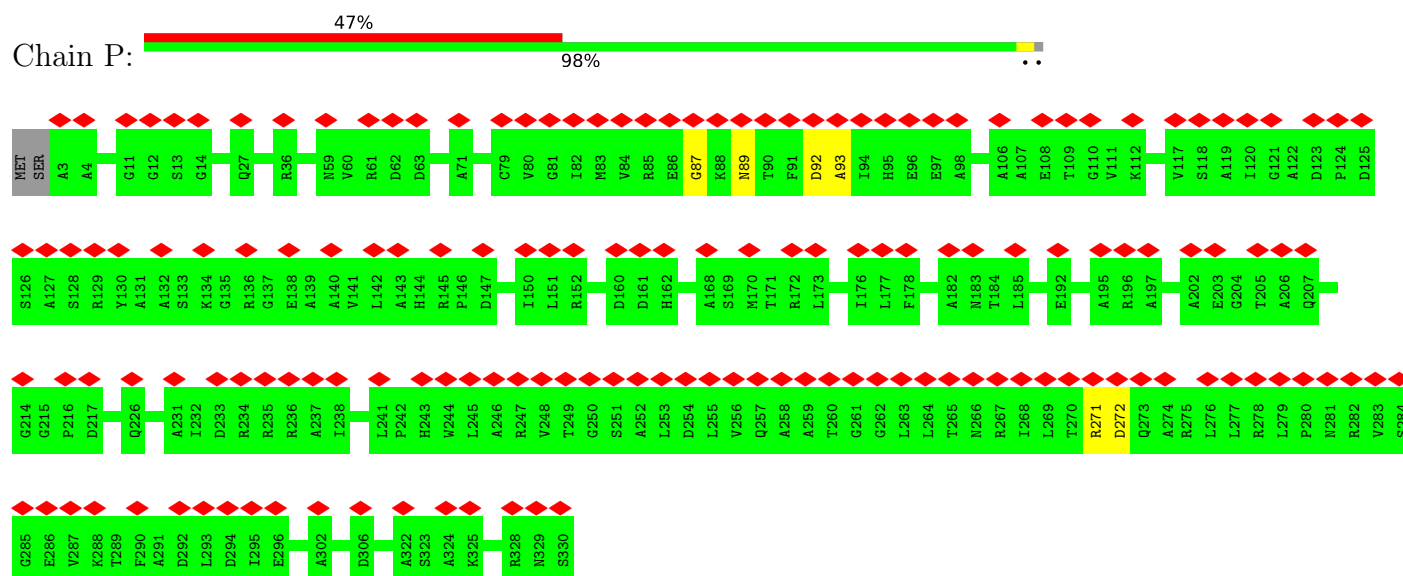
Chain M:  27% 92% 6%



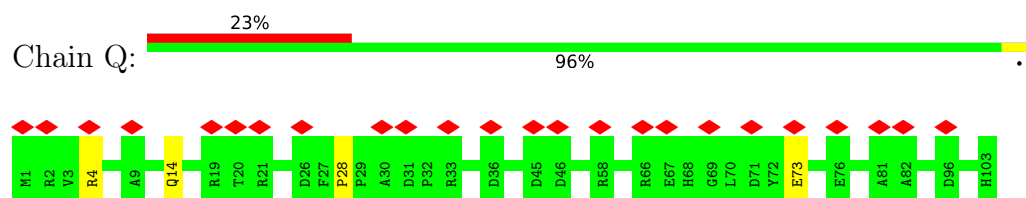
- Molecule 14: NADH-quinone oxidoreductase subunit N



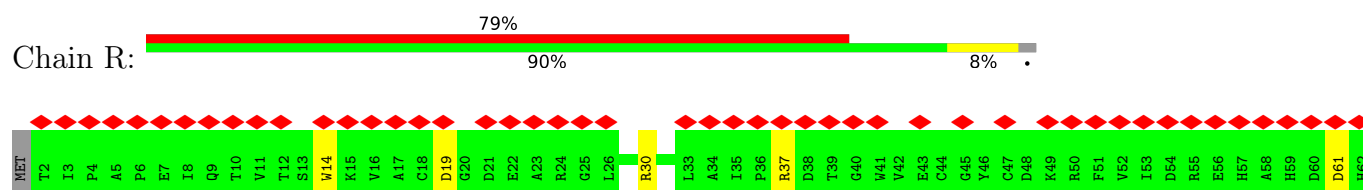
- Molecule 15: NAD-dependent epimerase/dehydratase



- Molecule 16: ETC complex I subunit conserved region

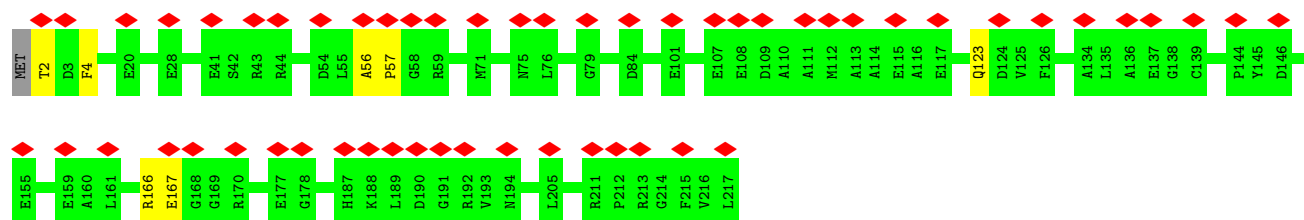


- Molecule 17: Zinc finger CHCC-type domain-containing protein



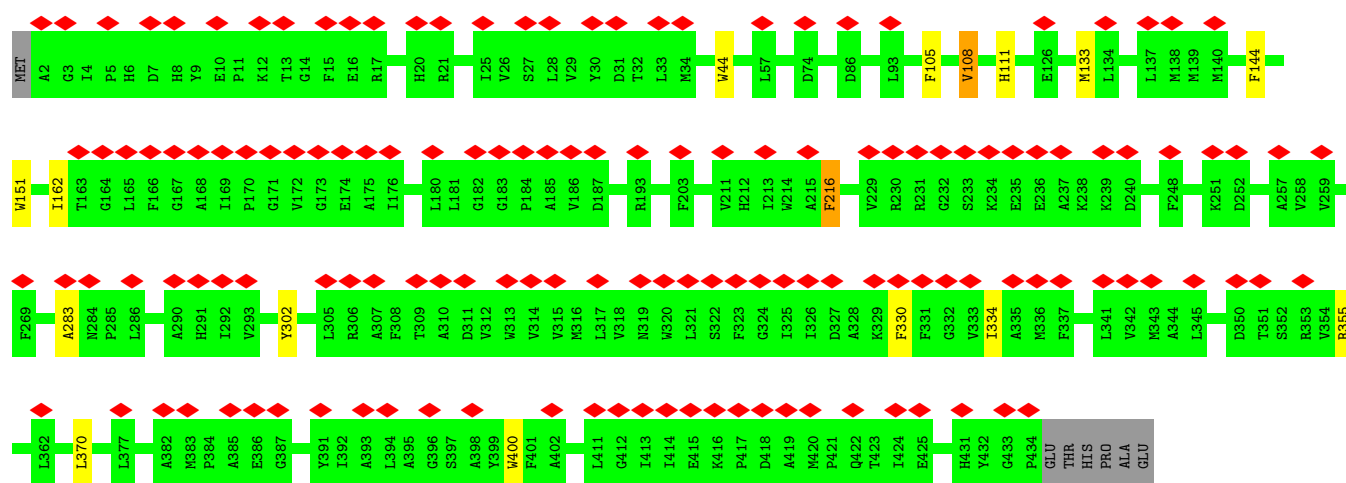
- Molecule 18: Protein-L-isoaspartate O-methyltransferase

Chain Z:  25% 96%

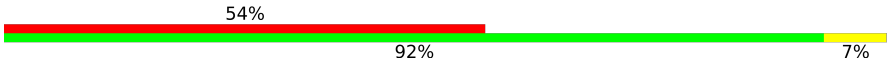


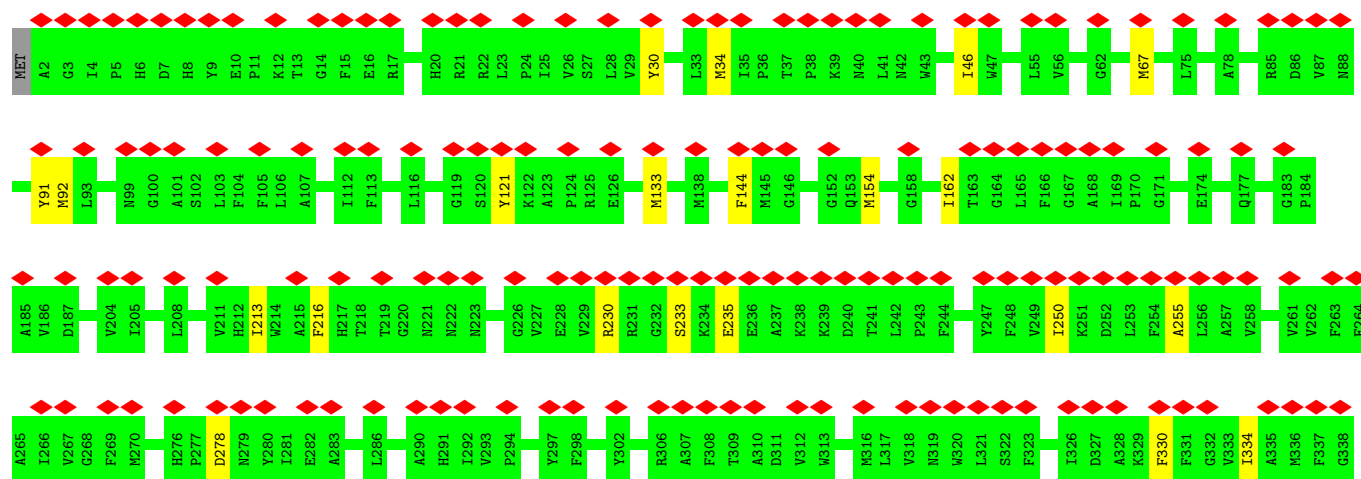
- Molecule 19: Cytochrome b

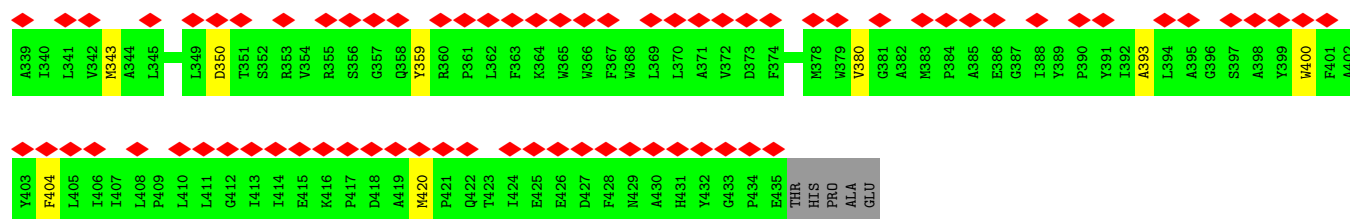
Chain a:  32% 95%



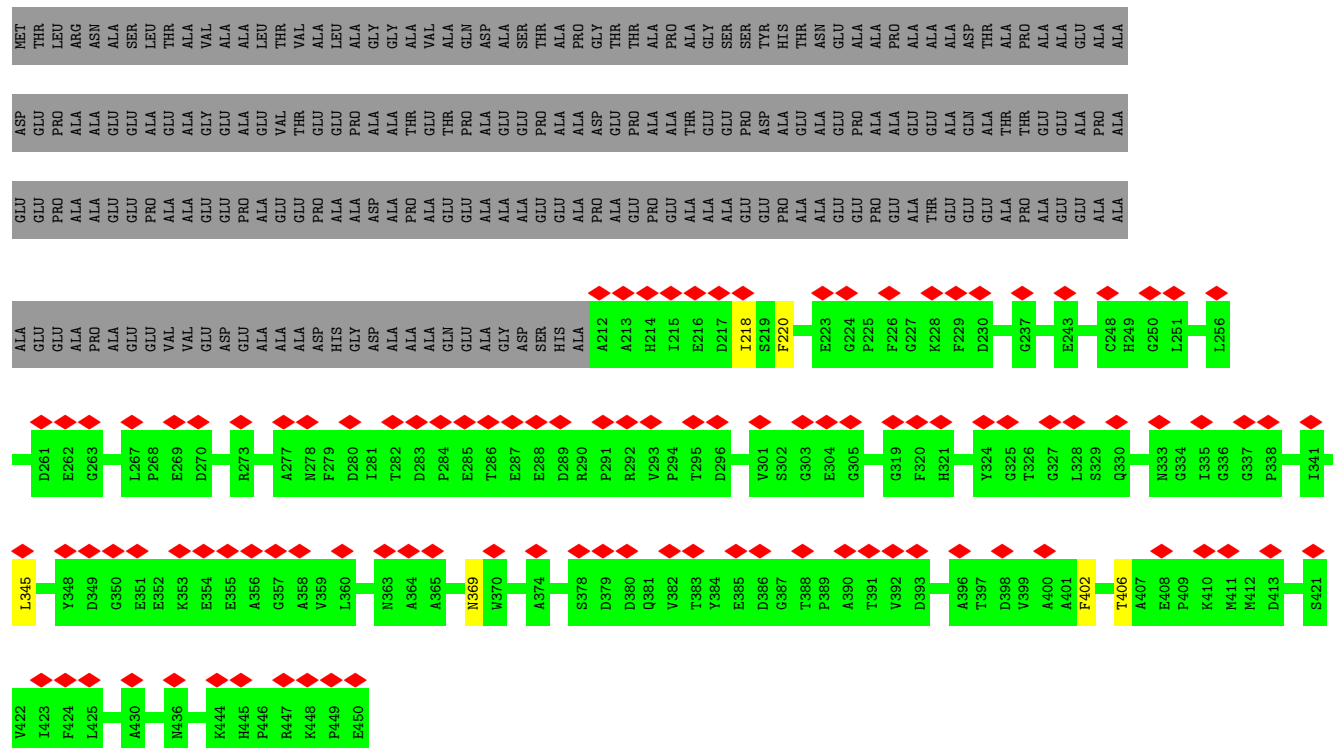
- Molecule 19: Cytochrome b

Chain d:  54% 92% 7%

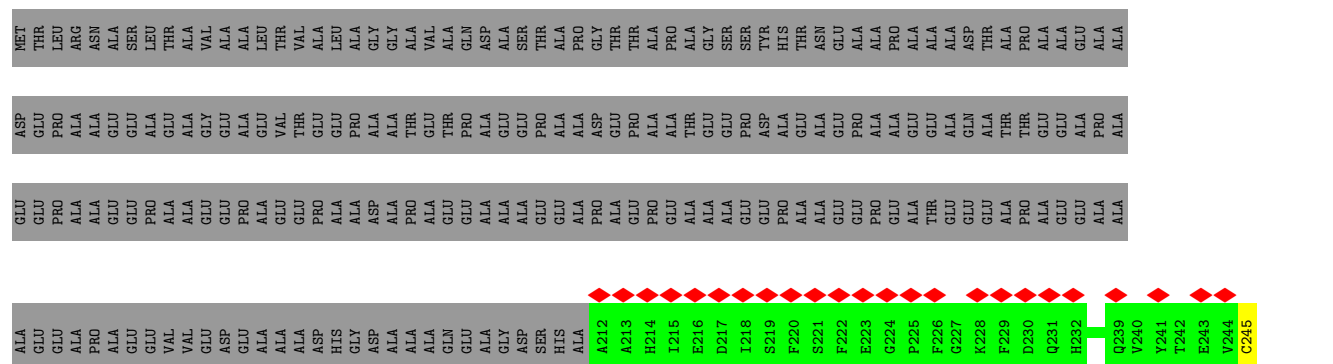


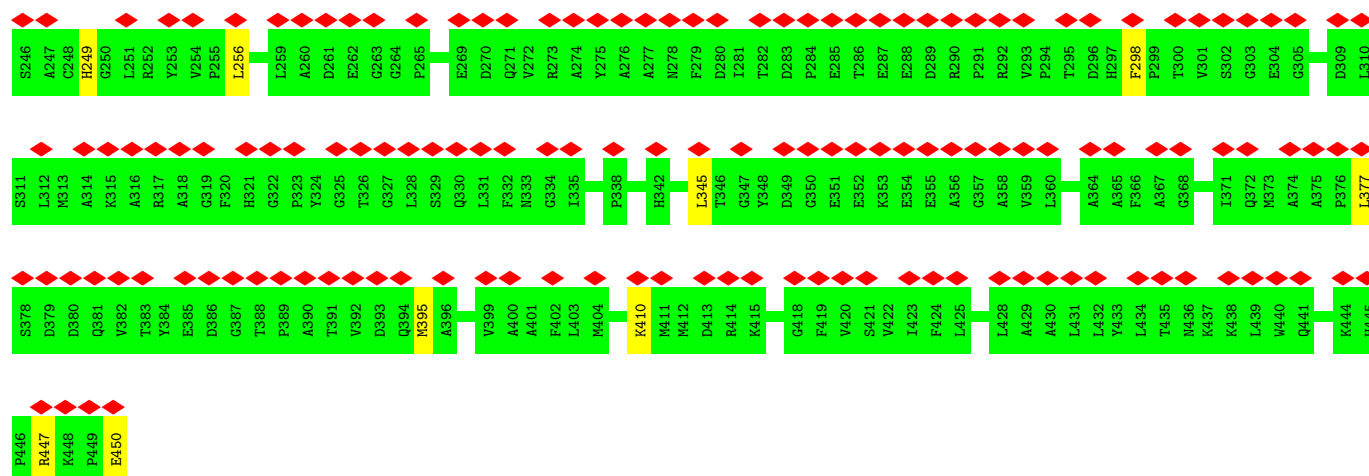


## • Molecule 20: Cytochrome c1

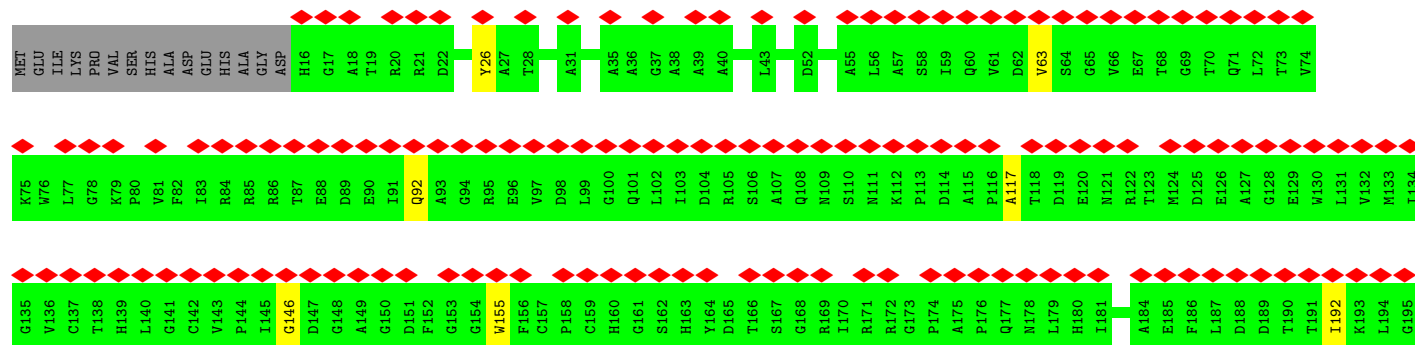
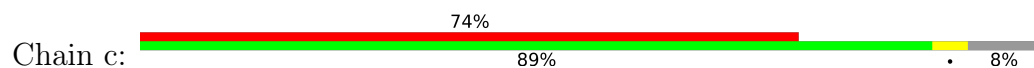


## • Molecule 20: Cytochrome c1

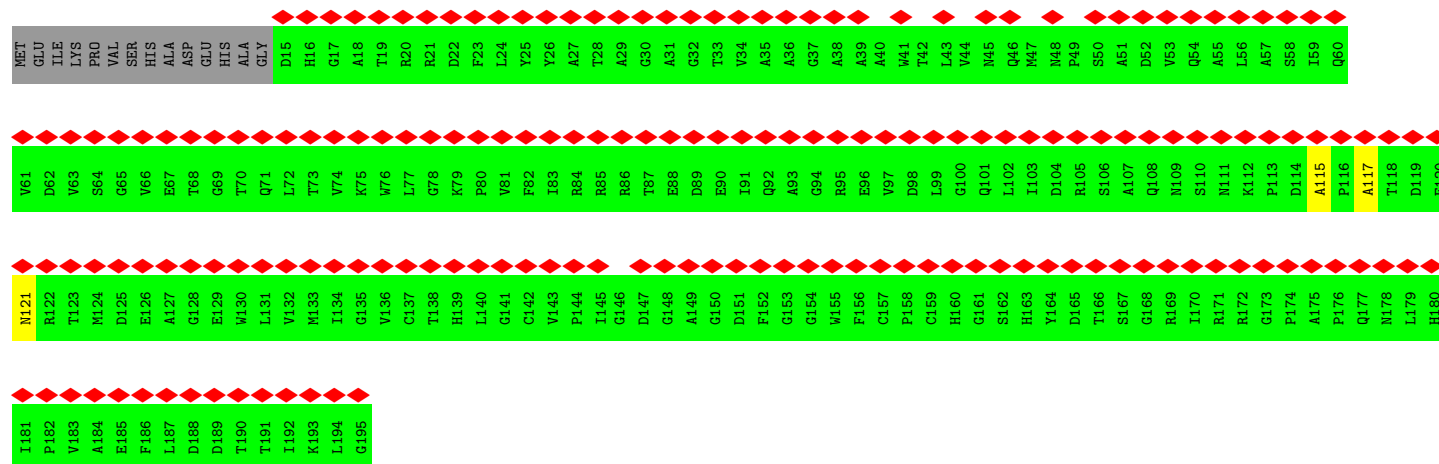
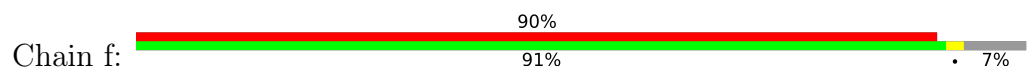




- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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

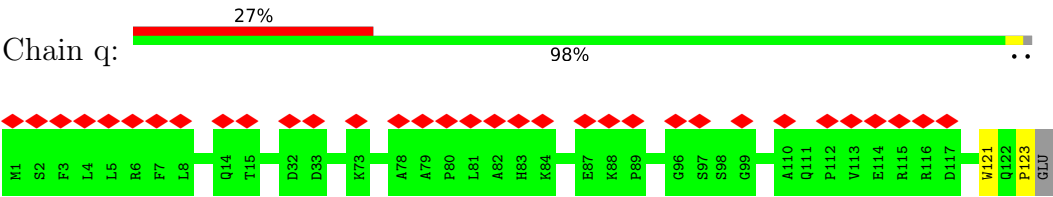


- Molecule 22: Cytochrome c oxidase subunit 1





● Molecule 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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.

All (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
6	F	191	ARG	Sidechain
6	F	410	ARG	Sidechain
7	G	223	ARG	Sidechain
7	G	280	ARG	Sidechain
7	G	394	ARG	Sidechain
9	I	7	ARG	Sidechain
9	I	91	ARG	Sidechain
13	M	439	ARG	Sidechain
14	N	296	ARG	Sidechain
19	a	355	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	d	230	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
7:G:41:ARG:NH2	7:G:266:GLU:OE1	2.28	0.62
7:G:357:ARG:HA	7:G:360:TYR:CE2	2.36	0.61
4:D:86:LEU:HD11	4:D:373:LEU:HD13	1.82	0.61
5:E:98:THR:HG22	5:E:99:THR:H	1.66	0.60
22:g:62:VAL:HG21	22:g:82:PRO:HB3	1.83	0.60
8:H:187:ASP:OD1	8:H:187:ASP:N	2.33	0.60
19:d:380:VAL:HG11	19:d:393:ALA:HB2	1.84	0.59
19:d:144:PHE:HB2	31:d:506:U10:H1M3	1.84	0.59
39:L:806:3PH:H222	24:i:50:TRP:CE2	2.39	0.58
20:b:345:LEU:HD11	42:b:502:HEC:HMB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:i:88:GLN:HA	24:i:91:PHE:CE2	2.40	0.57
12:L:117:ARG:NH1	36:L:801:3PE:O14	2.33	0.56
22:g:91:ILE:HG12	44:g:601:HEA:HBA1	1.87	0.56
20:e:245:CYS:HA	42:e:502:HEC:HMC3	1.87	0.56
13:M:246:HIS:CE1	13:M:257:LEU:HB3	2.41	0.56
1:A:75:LEU:HD13	11:K:68:THR:HA	1.89	0.55
22:g:98:MET:HB3	44:g:601:HEA:CAC	2.37	0.55
7:G:123:ASP:OD2	16:Q:14:GLN:NE2	2.40	0.54
14:N:251:MET:HE1	14:N:310:LEU:HD23	1.89	0.54
4:D:44:MET:HE2	4:D:46:LEU:HD21	1.91	0.53
6:F:329:ASP:CG	6:F:416:ARG:HH22	2.16	0.53
6:F:171:TYR:CE1	35:F:502:FMN:H6	2.44	0.52
31:d:504:U10:H8	31:d:504:U10:H153	1.91	0.52
19:d:121:TYR:OH	19:d:350:ASP:OD2	2.24	0.52
4:D:30:ASN:O	8:H:142:TYR:OH	2.23	0.52
5:E:140:ALA:HB3	5:E:146:MET:SD	2.50	0.51
5:E:39:ILE:HD12	5:E:67:MET:SD	2.49	0.51
5:E:185:SER:OG	5:E:186:ALA:N	2.42	0.51
19:a:144:PHE:HB2	31:a:508:U10:H101	1.90	0.51
22:g:207:MET:HE3	24:i:9:TYR:CD1	2.44	0.51
12:L:203:PHE:HA	12:L:206:VAL:HG23	1.91	0.51
23:h:33:LEU:HD22	23:h:263:VAL:HG11	1.92	0.51
13:M:326:MET:HE1	13:M:423:ALA:HB1	1.93	0.51
24:i:244:GLN:CD	33:i:1005:PC1:H132	2.36	0.51
8:H:94:LEU:HD13	8:H:126:LEU:HB3	1.92	0.51
13:M:35:LYS:HE3	13:M:110:VAL:HG11	1.91	0.51
2:B:62:THR:HG21	2:B:156:LEU:HD23	1.91	0.51
15:P:271:ARG:NE	15:P:272:ASP:OD1	2.38	0.51
22:g:474:ARG:HD2	23:h:248:LEU:HD22	1.93	0.51
22:g:382:LEU:HD13	22:g:418:LEU:HB3	1.92	0.51
19:d:133:MET:HE1	19:d:343:MET:HE3	1.93	0.50
27:q:121:TRP:CH2	27:q:123:PRO:HA	2.46	0.50
1:A:45:TYR:HE2	8:H:228:VAL:HG21	1.76	0.50
13:M:187:MET:HE1	13:M:221:LEU:HD11	1.93	0.50
4:D:121:TYR:OH	4:D:164:ALA:HB2	2.12	0.50
4:D:83:LEU:HG	4:D:98:TRP:HB2	1.92	0.50
13:M:430:SER:HA	13:M:433:TYR:CE2	2.47	0.49
22:g:98:MET:HB3	44:g:601:HEA:HAC	1.92	0.49
1:A:53:ASP:OD1	1:A:54:ASP:N	2.43	0.49
26:o:48:GLN:NE2	26:o:50:TYR:O	2.46	0.49
4:D:322:ARG:HG2	4:D:322:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:44:TRP:CZ2	39:a:503:3PH:H221	2.48	0.48
6:F:329:ASP:OD1	6:F:416:ARG:NH2	2.41	0.48
6:F:211:ASN:ND2	35:F:502:FMN:O2	2.38	0.48
7:G:532:ASP:CG	7:G:533:ARG:H	2.22	0.48
5:E:197:ASP:OD1	5:E:197:ASP:N	2.47	0.48
8:H:48:ARG:NE	33:H:403:PC1:O14	2.45	0.48
12:L:637:LYS:HE2	13:M:436:TRP:CH2	2.49	0.48
14:N:133:LEU:HD21	14:N:217:LYS:HE3	1.94	0.48
19:d:162:ILE:HG13	31:d:506:U10:H3M3	1.96	0.48
12:L:595:THR:HA	12:L:599:ALA:HB3	1.96	0.48
14:N:159:LYS:NZ	14:N:229:ASP:OD2	2.38	0.48
1:A:35:ARG:NH1	8:H:73:ILE:O	2.47	0.48
10:J:114:ASP:N	10:J:114:ASP:OD1	2.46	0.48
12:L:125:PHE:CE1	12:L:266:THR:HG21	2.49	0.48
3:C:59:PHE:CE1	3:C:90:GLN:HG3	2.48	0.47
7:G:135:TYR:CZ	7:G:137:GLU:HB2	2.49	0.47
21:c:26:TYR:CE1	26:p:9:LYS:HE3	2.48	0.47
16:Q:4:ARG:CZ	16:Q:28:PRO:HB3	2.44	0.47
44:g:601:HEA:HHA	44:g:601:HEA:HBD2	1.96	0.47
31:d:506:U10:H102	31:d:506:U10:C1M	2.44	0.47
20:e:377:LEU:HB3	20:e:395:MET:HE3	1.95	0.47
13:M:82:ASP:OD1	13:M:83:GLY:N	2.48	0.47
1:A:75:LEU:CD1	11:K:71:ALA:HB3	2.40	0.47
22:g:220:PHE:HB2	22:g:292:HIS:CD2	2.50	0.47
6:F:379:LEU:O	6:F:383:THR:HG23	2.15	0.46
8:H:168:ILE:HD11	8:H:262:PHE:CE1	2.50	0.46
19:a:330:PHE:CE2	19:a:334:ILE:HD11	2.50	0.46
19:d:30:TYR:CE2	19:d:34:MET:HG3	2.50	0.46
42:e:502:HEC:HHA	42:e:502:HEC:HBD1	1.97	0.46
19:a:370:LEU:HD11	19:a:400:TRP:CE3	2.50	0.46
6:F:69:MET:HE1	6:F:206:PRO:HB2	1.96	0.46
2:B:71:ARG:HA	8:H:50:PRO:HA	1.98	0.46
13:M:12:PRO:HG3	13:M:45:THR:HG21	1.97	0.46
22:g:475:TYR:CZ	23:h:254:ALA:HA	2.51	0.46
14:N:365:ASP:OD2	14:N:368:LYS:NZ	2.44	0.46
19:a:216:PHE:CD1	19:a:216:PHE:C	2.94	0.46
3:C:34:GLU:OE2	3:C:93:ARG:NH1	2.47	0.46
22:g:94:HIS:CE1	44:g:601:HEA:NC	2.84	0.46
22:g:21:ARG:O	22:g:25:SER:HB3	2.16	0.45
19:a:302:TYR:CE1	31:a:508:U10:H3M2	2.51	0.45
19:d:162:ILE:CG1	31:d:506:U10:H3M3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:347:HIS:HA	12:L:350:PHE:CE2	2.52	0.45
10:J:5:PHE:CZ	11:K:6:HIS:HB3	2.51	0.45
3:C:34:GLU:OE2	3:C:93:ARG:NH2	2.49	0.45
7:G:263:VAL:O	7:G:392:ARG:NH1	2.49	0.45
13:M:237:PRO:C	13:M:239:HIS:H	2.25	0.44
20:e:345:LEU:HD11	42:e:502:HEC:HMB3	1.99	0.44
14:N:216:PHE:CE1	14:N:226:TRP:CD1	3.05	0.44
20:e:450:GLU:H	20:e:450:GLU:CD	2.23	0.44
24:i:91:PHE:O	24:i:95:ILE:HG12	2.17	0.44
13:M:234:PRO:HB2	13:M:239:HIS:HA	2.00	0.44
19:a:162:ILE:HD11	31:a:508:U10:C4	2.46	0.44
1:A:121:ALA:OXT	10:J:173:ARG:NH2	2.50	0.44
20:b:218:ILE:HD11	20:b:220:PHE:CZ	2.52	0.44
20:b:345:LEU:HD11	42:b:502:HEC:CMB	2.46	0.44
19:d:213:ILE:HA	19:d:216:PHE:CE2	2.53	0.44
4:D:213:ARG:NH1	33:D:502:PC1:O12	2.40	0.44
14:N:266:ILE:HA	14:N:269:TRP:NE1	2.33	0.44
2:B:169:ARG:HG3	2:B:170:THR:HG23	2.00	0.44
7:G:100:GLU:O	7:G:104:ILE:HG23	2.18	0.44
31:d:504:U10:H1M1	31:d:504:U10:H1O2	2.00	0.44
5:E:199:LYS:HA	6:F:15:MET:SD	2.58	0.43
6:F:354:GLU:HB3	7:G:104:ILE:HD11	2.00	0.43
12:L:697:VAL:HG21	14:N:208:VAL:HG21	2.00	0.43
21:c:146:GLY:HA2	21:c:155:TRP:CD1	2.52	0.43
12:L:62:TRP:CZ3	12:L:139:LEU:HG	2.53	0.43
13:M:288:VAL:HG11	13:M:329:PHE:CD1	2.53	0.43
13:M:289:PHE:HB3	13:M:419:VAL:HG21	2.01	0.43
17:R:19:ASP:OD1	17:R:30:ARG:NE	2.41	0.43
22:g:345:MET:HE1	23:h:121:ILE:HB	1.99	0.43
23:h:150:TRP:CD2	23:h:252:ASN:HB2	2.53	0.43
3:C:192:GLY:HA2	7:G:127:ALA:HB1	2.00	0.43
4:D:324:MET:HE1	7:G:110:CYS:SG	2.59	0.43
8:H:33:MET:HG3	8:H:288:PHE:CZ	2.54	0.43
19:d:154:MET:HG2	19:d:278:ASP:HB2	2.00	0.43
20:e:249:HIS:CE1	42:e:502:HEC:NA	2.86	0.43
24:i:128:TRP:HA	24:i:129:PRO:C	2.44	0.43
23:h:52:ALA:HB2	23:h:61:GLN:CD	2.44	0.43
4:D:329:HIS:CE1	7:G:131:ASP:HA	2.54	0.42
12:L:129:MET:HB2	12:L:266:THR:HG23	2.01	0.42
15:P:92:ASP:OD1	15:P:93:ALA:N	2.52	0.42
19:d:46:ILE:HD12	19:d:255:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:129:TYR:HB3	8:H:133:MET:HE3	2.00	0.42
22:g:417:SER:O	22:g:418:LEU:HD23	2.18	0.42
19:d:91:TYR:CE2	19:d:92:MET:HG2	2.54	0.42
22:g:276:HIS:O	22:g:279:VAL:HG22	2.19	0.42
3:C:57:CYS:HB3	3:C:59:PHE:CD2	2.55	0.42
9:I:26:ARG:HH11	9:I:26:ARG:HB3	1.85	0.42
12:L:78:ARG:HD3	12:L:503:TYR:CZ	2.55	0.42
12:L:312:ASP:OD2	12:L:315:ARG:NH1	2.47	0.42
19:d:359:TYR:CD2	19:d:420:MET:HG2	2.54	0.42
22:g:27:ASN:ND2	22:g:30:ASP:OD2	2.47	0.42
24:i:9:TYR:CE2	25:j:15:MET:HE1	2.54	0.42
24:i:149:LEU:HD23	24:i:149:LEU:HA	1.91	0.42
1:A:64:TYR:CD1	1:A:65:LEU:N	2.87	0.42
4:D:15:MET:HE2	4:D:15:MET:HB2	1.90	0.42
22:g:104:ILE:HB	22:g:105:PRO:HD3	2.02	0.42
23:h:149:GLN:HG2	23:h:150:TRP:CE2	2.55	0.42
7:G:236:MET:SD	7:G:646:ASN:ND2	2.92	0.42
8:H:31:ILE:HA	8:H:61:THR:HG21	2.01	0.42
15:P:89:ASN:ND2	15:P:271:ARG:HH12	2.17	0.42
42:b:502:HEC:HMB3	42:b:502:HEC:HBB3	2.02	0.42
22:g:412:PHE:HA	22:g:415:VAL:HG22	2.02	0.42
4:D:218:ARG:NH2	4:D:394:ALA:O	2.52	0.42
7:G:426:LEU:HD21	7:G:460:VAL:HG13	2.02	0.42
9:I:35:LEU:O	9:I:35:LEU:HD12	2.19	0.42
4:D:10:TYR:HA	10:J:168:ARG:HA	2.02	0.42
6:F:84:ALA:HB1	6:F:98:MET:SD	2.60	0.42
13:M:42:THR:HG22	13:M:121:GLU:OE1	2.20	0.42
18:Z:2:THR:HB	18:Z:4:PHE:CE2	2.55	0.42
19:a:105:PHE:HA	19:a:108:VAL:HG22	2.02	0.42
19:a:151:TRP:CD1	19:a:283:ALA:HB3	2.55	0.42
33:i:1006:PC1:H152	33:j:1001:PC1:H112	2.02	0.42
13:M:276:MET:C	13:M:278:PRO:HD3	2.45	0.41
24:i:147:LEU:HD22	26:p:15:ILE:HG23	2.02	0.41
22:g:16:ARG:HH11	22:g:16:ARG:HG3	1.85	0.41
19:a:111:HIS:CD2	41:a:507:HEM:NC	2.88	0.41
4:D:324:MET:HE2	4:D:328:ILE:HG13	2.02	0.41
8:H:196:LEU:HB3	8:H:197:PRO:HD3	2.02	0.41
12:L:396:THR:HG21	12:L:443:TRP:HE1	1.86	0.41
17:R:14:TRP:CZ3	17:R:37:ARG:HA	2.55	0.41
18:Z:166:ARG:HD2	18:Z:167:GLU:O	2.21	0.41
22:g:299:LYS:HB3	22:g:526:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:p:2:PHE:CG	26:p:3:ASP:N	2.87	0.41
4:D:141:VAL:HG12	4:D:141:VAL:O	2.21	0.41
33:L:802:PC1:H133	13:M:161:TYR:CD1	2.56	0.41
19:d:330:PHE:CE2	19:d:334:ILE:HD11	2.55	0.41
23:h:136:PRO:HD3	23:h:232:TRP:CD1	2.56	0.41
10:J:105:ILE:HG21	12:L:698:MET:HE1	2.02	0.41
20:e:256:LEU:HD23	20:e:298:PHE:CE1	2.56	0.41
6:F:316:PHE:CZ	6:F:319:ALA:HB2	2.55	0.41
7:G:234:ASP:CG	7:G:272:THR:HG23	2.46	0.41
20:b:402:PHE:O	20:b:406:THR:HG23	2.21	0.41
2:B:152:THR:HG22	2:B:154:GLU:H	1.85	0.41
6:F:171:TYR:CZ	35:F:502:FMN:H6	2.56	0.41
6:F:411:GLU:H	6:F:411:GLU:CD	2.27	0.41
12:L:78:ARG:HD2	12:L:503:TYR:O	2.21	0.41
14:N:467:ASP:OD1	14:N:467:ASP:N	2.54	0.41
17:R:14:TRP:CZ3	17:R:37:ARG:HD2	2.56	0.41
21:c:63:VAL:HG11	21:c:192:ILE:HD12	2.02	0.41
22:g:414:TYR:CE2	22:g:460:PHE:HB2	2.56	0.41
23:h:113:VAL:HB	23:h:114:PRO:HD3	2.03	0.41
6:F:41:ASP:OD1	6:F:41:ASP:N	2.54	0.41
21:f:115:ALA:HB1	21:f:121:ASN:ND2	2.36	0.41
4:D:163:ARG:HH11	4:D:163:ARG:HG2	1.85	0.40
6:F:336:ARG:HA	6:F:336:ARG:HD2	1.90	0.40
19:d:91:TYR:CE1	20:e:410:LYS:HD3	2.55	0.40
12:L:252:MET:SD	12:L:318:ALA:HB2	2.62	0.40
19:d:400:TRP:CE2	19:d:404:PHE:HE2	2.39	0.40
33:i:1006:PC1:H11	33:j:1001:PC1:H2	2.03	0.40
7:G:594:TRP:CZ2	7:G:600:LEU:HD13	2.57	0.40
18:Z:56:ALA:HB1	18:Z:57:PRO:HD2	2.03	0.40
22:g:538:PRO:HA	22:g:539:PRO:HD3	1.94	0.40
13:M:145:ILE:HG23	14:N:377:PHE:CZ	2.57	0.40
19:d:233:SER:OG	19:d:235:GLU:OE2	2.35	0.40
22:g:87:TRP:NE1	22:g:91:ILE:HD11	2.36	0.40
4:D:162:GLU:OE2	9:I:45:SER:OG	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS
13	M	238	VAL
15	P	87	GLY
20	b	369	ASN
6	F	201	GLY
17	R	61	ASP
7	G	263	VAL
21	c	117	ALA
21	f	117	ALA
7	G	615	ASP
23	h	184	LEU
5	E	122	HIS
20	e	447	ARG
11	K	96	VAL
2	B	122	GLY
12	L	486	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	91	THR
6	F	88	GLU
6	F	221	ILE
6	F	260	SER
6	F	301	ASN
6	F	325	ASP
7	G	170	GLU
7	G	296	ARG
7	G	376	GLN
8	H	187	ASP
8	H	289	TYR
9	I	116	ASP
12	L	61	ASP
13	M	365	HIS
13	M	471	MET
14	N	129	LEU
16	Q	73	GLU
18	Z	123	GLN
19	a	108	VAL
19	a	133	MET
19	a	216	PHE
21	c	92	GLN
19	d	67	MET
19	d	250	ILE
22	g	29	LYS
22	g	317	ILE
23	h	30	GLN
26	o	24	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	GLN
3	C	38	ASN
3	C	97	GLN
4	D	28	ASN
4	D	59	HIS
4	D	329	HIS
5	E	85	GLN
6	F	5	GLN

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Mol	Chain	Res	Type
6	F	137	GLN
7	G	259	ASN
7	G	472	ASN
7	G	613	GLN
11	K	46	ASN
12	L	198	GLN
12	L	208	GLN
12	L	225	ASN
12	L	241	GLN
12	L	263	HIS
13	M	26	GLN
13	M	333	GLN
13	M	498	ASN
14	N	65	HIS
14	N	291	GLN
14	N	323	ASN
14	N	359	ASN
14	N	445	GLN
15	P	27	GLN
15	P	95	HIS
16	Q	78	HIS
18	Z	78	ASN
19	a	279	ASN
20	b	342	HIS
20	b	436	ASN
20	b	445	HIS
21	c	16	HIS
21	c	45	ASN
21	c	48	ASN
21	c	121	ASN
20	e	416	GLN
20	e	436	ASN
22	g	13	HIS
22	g	59	HIS
22	g	526	HIS
23	h	48	ASN
23	h	202	GLN
23	h	230	GLN
24	i	161	HIS
24	i	165	HIS
24	i	244	GLN
25	j	49	ASN

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Mol	Chain	Res	Type
27	q	65	HIS

### 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
39	c	205	3PH	P-O11	7.14	1.82	1.60
39	L	806	3PH	P-O11	7.09	1.82	1.60
42	e	502	HEC	CAC-C3C	6.46	1.56	1.35
42	b	502	HEC	CAC-C3C	6.39	1.55	1.35
42	e	502	HEC	CAB-C3B	6.22	1.55	1.35
42	b	502	HEC	CAB-C3B	6.05	1.54	1.35
42	e	502	HEC	C3D-C2D	5.16	1.52	1.38
42	b	502	HEC	C3D-C2D	4.98	1.51	1.38
44	g	601	HEA	C3B-C2B	4.25	1.44	1.34
44	g	604	HEA	C3B-C2B	4.18	1.44	1.34
44	g	601	HEA	C3D-C2D	3.69	1.44	1.36
36	L	801	3PE	P-O14	-3.68	1.38	1.50
33	D	502	PC1	P-O14	-3.64	1.38	1.50
36	c	201	3PE	P-O14	-3.62	1.38	1.50
36	d	505	3PE	P-O14	-3.61	1.38	1.50
44	g	604	HEA	C3D-C2D	3.60	1.44	1.36
33	i	1006	PC1	P-O14	-3.59	1.38	1.50
36	H	402	3PE	P-O14	-3.59	1.38	1.50
33	H	403	PC1	P-O14	-3.56	1.38	1.50
33	M	2003	PC1	P-O14	-3.55	1.38	1.50
36	i	1004	3PE	P-O14	-3.54	1.38	1.50
36	b	501	3PE	P-O14	-3.54	1.38	1.50
36	i	1007	3PE	P-O14	-3.53	1.38	1.50
36	I	203	3PE	P-O14	-3.52	1.38	1.50
33	a	502	PC1	P-O14	-3.51	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	804	PGT	P-O2P	-3.50	1.39	1.55
33	i	1005	PC1	P-O14	-3.49	1.38	1.50
33	L	802	PC1	P-O14	-3.49	1.38	1.50
33	a	509	PC1	P-O14	-3.48	1.38	1.50
33	a	504	PC1	P-O14	-3.48	1.38	1.50
33	a	501	PC1	P-O14	-3.47	1.38	1.50
33	i	1001	PC1	P-O14	-3.45	1.38	1.50
28	J	203	PGT	P-O2P	-3.43	1.39	1.55
28	A	1003	PGT	P-O2P	-3.41	1.39	1.55
33	d	507	PC1	P-O14	-3.41	1.39	1.50
33	i	1003	PC1	P-O14	-3.40	1.39	1.50
33	M	2005	PC1	P-O14	-3.39	1.39	1.50
33	j	1001	PC1	P-O14	-3.38	1.39	1.50
28	A	1001	PGT	P-O2P	-3.38	1.39	1.55
28	P	401	PGT	P-O2P	-3.36	1.39	1.55
28	q	1000	PGT	P-O2P	-3.34	1.39	1.55
37	J	201	T7X	P1-O1	3.34	1.69	1.59
33	j	1001	PC1	P-O13	3.34	1.72	1.59
33	a	509	PC1	P-O13	3.30	1.72	1.59
33	D	502	PC1	P-O12	-3.28	1.40	1.55
37	J	201	T7X	P1-O12	-3.28	1.40	1.55
33	L	802	PC1	P-O13	3.27	1.72	1.59
33	a	501	PC1	P-O13	3.27	1.72	1.59
38	L	803	P5S	P12-O15	-3.26	1.40	1.55
33	i	1003	PC1	P-O13	3.24	1.72	1.59
33	i	1001	PC1	P-O13	3.23	1.72	1.59
33	H	403	PC1	P-O12	-3.19	1.40	1.55
33	d	507	PC1	P-O13	3.19	1.71	1.59
33	M	2003	PC1	P-O13	3.18	1.71	1.59
33	a	502	PC1	P-O13	3.18	1.71	1.59
33	M	2003	PC1	P-O12	-3.18	1.40	1.55
33	i	1005	PC1	P-O12	-3.17	1.40	1.55
33	i	1006	PC1	P-O12	-3.16	1.40	1.55
33	a	501	PC1	P-O12	-3.14	1.40	1.55
33	M	2005	PC1	P-O12	-3.12	1.40	1.55
33	L	802	PC1	P-O12	-3.10	1.41	1.55
33	i	1003	PC1	P-O12	-3.10	1.41	1.55
33	i	1001	PC1	P-O12	-3.09	1.41	1.55
33	M	2005	PC1	P-O13	3.08	1.71	1.59
33	a	502	PC1	P-O12	-3.08	1.41	1.55
33	a	504	PC1	P-O12	-3.06	1.41	1.55
33	d	507	PC1	P-O12	-3.06	1.41	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	504	PC1	P-O13	3.05	1.71	1.59
41	a	505	HEM	C3B-C2B	-3.04	1.31	1.37
33	j	1001	PC1	P-O12	-3.03	1.41	1.55
33	i	1005	PC1	P-O13	3.02	1.71	1.59
28	L	804	PGT	P-O1P	-3.02	1.40	1.50
33	a	509	PC1	P-O12	-3.01	1.41	1.55
35	F	502	FMN	C4A-N5	3.00	1.37	1.30
37	J	201	T7X	P1-O11	-3.00	1.40	1.50
33	H	403	PC1	P-O13	2.92	1.70	1.59
36	i	1007	3PE	P-O12	-2.92	1.41	1.55
36	H	402	3PE	P-O12	-2.91	1.41	1.55
36	c	201	3PE	P-O12	-2.90	1.41	1.55
36	L	801	3PE	P-O12	-2.88	1.42	1.55
28	P	401	PGT	P-O1P	-2.86	1.40	1.50
41	d	502	HEM	CAB-C3B	2.84	1.55	1.47
33	i	1006	PC1	P-O13	2.84	1.70	1.59
36	d	505	3PE	P-O12	-2.83	1.42	1.55
28	J	203	PGT	P-O1P	-2.82	1.41	1.50
38	L	803	P5S	P12-O13	-2.82	1.41	1.50
28	A	1001	PGT	P-O1P	-2.81	1.41	1.50
44	g	601	HEA	C11-C3B	-2.80	1.48	1.51
36	i	1004	3PE	P-O12	-2.79	1.42	1.55
36	b	501	3PE	P-O12	-2.78	1.42	1.55
44	g	601	HEA	C3A-C2A	2.77	1.43	1.37
44	g	604	HEA	C3A-C2A	2.77	1.43	1.37
36	I	203	3PE	P-O12	-2.76	1.42	1.55
28	A	1003	PGT	P-O1P	-2.76	1.41	1.50
33	D	502	PC1	P-O13	2.74	1.70	1.59
38	L	803	P5S	P12-O16	2.70	1.70	1.59
39	M	2001	3PH	P-O14	-2.69	1.44	1.54
39	M	2001	3PH	P-O13	-2.66	1.44	1.54
44	g	604	HEA	C4B-C3B	2.66	1.49	1.44
44	g	601	HEA	C1D-ND	-2.65	1.35	1.40
39	c	205	3PH	P-O14	-2.65	1.44	1.54
28	q	1000	PGT	P-O1P	-2.65	1.41	1.50
39	f	202	3PH	P-O14	-2.64	1.45	1.54
39	f	202	3PH	P-O13	-2.63	1.45	1.54
41	a	507	HEM	C2A-C3A	-2.62	1.32	1.38
43	d	501	CDL	OB8-CB7	2.62	1.41	1.33
39	i	1009	3PH	P-O14	-2.62	1.45	1.54
39	i	1009	3PH	P-O13	-2.60	1.45	1.54
41	d	502	HEM	CAC-C3C	2.60	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	501	CDL	OB6-CB4	-2.60	1.40	1.46
39	a	503	3PH	P-O14	-2.60	1.45	1.54
39	L	806	3PH	P-O14	-2.58	1.45	1.54
41	a	507	HEM	FE-NB	2.58	2.02	1.94
36	I	203	3PE	P-O13	2.57	1.69	1.59
43	d	501	CDL	OA8-CA7	2.57	1.40	1.33
39	c	205	3PH	P-O13	-2.56	1.45	1.54
39	L	805	3PH	P-O13	-2.56	1.45	1.54
41	a	505	HEM	C2A-C3A	-2.55	1.32	1.38
36	i	1004	3PE	P-O11	2.55	1.69	1.59
39	L	805	3PH	P-O14	-2.54	1.45	1.54
39	L	806	3PH	P-O13	-2.54	1.45	1.54
41	d	503	HEM	C2A-C3A	-2.53	1.32	1.38
36	I	203	3PE	P-O11	2.52	1.69	1.59
44	g	604	HEA	C1D-ND	-2.51	1.35	1.40
39	L	806	3PH	O11-C1	-2.51	1.35	1.44
41	a	507	HEM	CAB-C3B	2.51	1.54	1.47
28	q	1000	PGT	P-O3P	2.51	1.69	1.59
39	a	503	3PH	P-O13	-2.47	1.45	1.54
39	L	805	3PH	O11-C1	-2.47	1.35	1.44
36	L	801	3PE	P-O13	2.47	1.69	1.59
36	c	201	3PE	P-O11	2.46	1.69	1.59
43	d	501	CDL	OA6-CA5	2.46	1.41	1.34
41	d	503	HEM	C3B-C2B	-2.45	1.32	1.37
41	a	507	HEM	CAC-C3C	2.45	1.53	1.47
41	d	503	HEM	CAC-C3C	2.43	1.53	1.47
28	L	804	PGT	P-O3P	2.41	1.68	1.59
39	M	2001	3PH	P-O12	-2.41	1.43	1.50
41	a	505	HEM	C3C-C2C	-2.41	1.32	1.37
39	c	205	3PH	O11-C1	-2.40	1.35	1.44
36	i	1004	3PE	P-O13	2.39	1.68	1.59
36	b	501	3PE	P-O11	2.38	1.68	1.59
36	d	505	3PE	P-O11	2.37	1.68	1.59
28	A	1001	PGT	P-O3P	2.36	1.68	1.59
36	H	402	3PE	P-O11	2.34	1.68	1.59
36	H	402	3PE	P-O13	2.34	1.68	1.59
41	d	503	HEM	CAB-C3B	2.33	1.53	1.47
39	L	805	3PH	P-O12	-2.32	1.43	1.50
41	a	505	HEM	C3D-C2D	-2.31	1.31	1.36
41	a	507	HEM	C3B-C2B	-2.31	1.32	1.37
28	J	203	PGT	P-O3P	2.30	1.68	1.59
43	d	501	CDL	OA6-CA4	-2.29	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	503	3PH	O11-C1	-2.29	1.35	1.44
36	i	1007	3PE	P-O13	2.29	1.68	1.59
43	d	501	CDL	OB6-CB5	2.28	1.40	1.34
39	M	2001	3PH	O11-C1	-2.27	1.36	1.44
41	a	505	HEM	CAB-C3B	2.27	1.53	1.47
41	d	502	HEM	C2A-C3A	-2.27	1.33	1.38
39	f	202	3PH	O11-C1	-2.26	1.36	1.44
44	g	604	HEA	C4A-NA	-2.26	1.35	1.39
39	c	205	3PH	P-O12	-2.25	1.43	1.50
39	i	1009	3PH	P-O12	-2.25	1.43	1.50
36	d	505	3PE	P-O13	2.25	1.68	1.59
43	d	501	CDL	OB8-CB6	-2.22	1.40	1.45
41	d	502	HEM	C3C-C2C	-2.22	1.32	1.37
41	d	503	HEM	C3C-C2C	-2.21	1.32	1.37
36	b	501	3PE	P-O13	2.21	1.68	1.59
28	q	1000	PGT	P-O4P	2.20	1.68	1.59
28	J	203	PGT	P-O4P	2.20	1.68	1.59
41	a	507	HEM	C3C-C2C	-2.20	1.32	1.37
39	i	1009	3PH	O11-C1	-2.20	1.36	1.44
41	a	505	HEM	CAC-C3C	2.19	1.53	1.47
28	A	1003	PGT	P-O4P	2.19	1.68	1.59
39	a	503	3PH	P-O12	-2.18	1.43	1.50
36	c	201	3PE	P-O13	2.18	1.67	1.59
36	i	1007	3PE	P-O11	2.17	1.67	1.59
39	f	202	3PH	P-O12	-2.16	1.43	1.50
36	L	801	3PE	P-O11	2.15	1.67	1.59
28	P	401	PGT	P-O4P	2.15	1.67	1.59
28	L	804	PGT	P-O4P	2.13	1.67	1.59
28	P	401	PGT	P-O3P	2.13	1.67	1.59
42	e	502	HEC	CMC-C2C	2.10	1.55	1.50
42	e	502	HEC	CMB-C2B	2.09	1.55	1.50
37	J	201	T7X	P1-O13	2.08	1.67	1.59
28	A	1001	PGT	P-O4P	2.07	1.67	1.59
39	L	806	3PH	O31-C31	2.07	1.39	1.33
28	A	1003	PGT	P-O3P	2.07	1.67	1.59
39	L	806	3PH	P-O12	-2.07	1.44	1.50
42	b	502	HEC	CMC-C2C	2.06	1.55	1.50
44	g	601	HEA	C4D-C3D	2.05	1.48	1.45
41	a	507	HEM	C3D-C2D	-2.04	1.32	1.36
42	b	502	HEC	C3B-C2B	-2.03	1.34	1.41
44	g	601	HEA	C1C-C2C	2.03	1.47	1.43
33	H	403	PC1	O13-C11	-2.03	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	g	601	HEA	C1A-NA	-2.02	1.35	1.39
33	j	1001	PC1	P-O11	2.01	1.67	1.59
35	F	502	FMN	C9A-N10	-2.01	1.37	1.41
39	f	202	3PH	O31-C31	2.00	1.39	1.33

All (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
44	g	604	HEA	CAA-CBA-CGA	-5.26	99.72	113.67
42	b	502	HEC	CBC-CAC-C3C	-5.16	117.13	127.43
44	g	601	HEA	C3D-C4D-ND	4.99	115.17	110.35
44	g	601	HEA	C2A-C1A-NA	4.93	115.08	110.32
31	B	1002	U10	C7-C6-C5	-4.93	112.79	118.52
42	e	502	HEC	CBC-CAC-C3C	-4.91	117.62	127.43
31	B	1002	U10	C8-C7-C6	4.89	124.11	112.08
44	g	604	HEA	C2A-C1A-NA	4.86	115.02	110.32
33	D	502	PC1	O12-P-O14	4.74	134.49	112.44
44	g	604	HEA	CMC-C2C-C3C	4.69	137.57	126.55
44	g	604	HEA	C3D-C4D-ND	4.68	114.88	110.35
33	i	1005	PC1	O12-P-O14	4.55	133.60	112.44
33	H	403	PC1	O12-P-O14	4.54	133.57	112.44
33	a	509	PC1	O12-P-O14	4.50	133.39	112.44
33	i	1003	PC1	O12-P-O14	4.47	133.23	112.44
44	g	601	HEA	CMC-C2C-C3C	4.45	137.02	126.55
33	i	1006	PC1	O12-P-O14	4.44	133.11	112.44
36	d	505	3PE	O12-P-O14	4.44	133.09	112.44
33	i	1001	PC1	O12-P-O14	4.40	132.93	112.44
33	M	2005	PC1	O12-P-O14	4.40	132.93	112.44
44	g	604	HEA	CMC-C2C-C1C	-4.40	118.72	125.42
36	L	801	3PE	O12-P-O14	4.37	132.79	112.44
36	b	501	3PE	O12-P-O14	4.37	132.78	112.44
31	d	504	U10	C7-C6-C5	-4.36	113.45	118.52
31	B	1002	U10	C7-C8-C9	-4.34	119.35	126.83
33	a	502	PC1	O12-P-O14	4.33	132.58	112.44
36	i	1007	3PE	O12-P-O14	4.32	132.56	112.44
33	L	802	PC1	O12-P-O14	4.32	132.54	112.44
33	a	501	PC1	O12-P-O14	4.32	132.52	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	M	2003	PC1	O12-P-O14	4.31	132.52	112.44
44	g	604	HEA	CAD-CBD-CGD	-4.30	102.25	113.67
33	d	507	PC1	O12-P-O14	4.29	132.40	112.44
33	j	1001	PC1	O12-P-O14	4.28	132.35	112.44
31	d	504	U10	C6-C1-C2	4.22	122.50	119.17
33	a	504	PC1	O12-P-O14	4.22	132.08	112.44
44	g	604	HEA	CBA-CAA-C2A	4.22	124.19	112.53
44	g	601	HEA	CHA-C1A-C2A	-4.18	118.26	124.86
36	c	201	3PE	O12-P-O14	4.18	131.88	112.44
42	e	502	HEC	CMC-C2C-C1C	-4.17	119.07	125.42
44	g	604	HEA	CMB-C2B-C1B	-4.13	118.58	125.03
36	H	402	3PE	O12-P-O14	4.13	131.66	112.44
36	i	1004	3PE	O12-P-O14	4.09	131.49	112.44
28	L	804	PGT	C3-C2-C1	4.06	121.24	111.78
44	g	601	HEA	C13-C14-C15	-4.05	118.34	127.62
36	I	203	3PE	O12-P-O14	4.05	131.30	112.44
44	g	604	HEA	CHA-C4D-C3D	-4.04	118.89	124.77
44	g	601	HEA	CMD-C2D-C1D	-4.03	118.74	125.03
44	g	601	HEA	C4D-C3D-C2D	-3.98	101.10	106.89
42	b	502	HEC	CMC-C2C-C1C	-3.89	119.49	125.42
44	g	601	HEA	CMC-C2C-C1C	-3.88	119.52	125.42
44	g	601	HEA	C12-C11-C3B	3.85	118.14	112.12
31	a	508	U10	C6-C1-C2	3.79	122.16	119.17
44	g	601	HEA	CAD-C3D-C4D	3.78	131.28	124.70
44	g	601	HEA	CMB-C2B-C1B	-3.74	119.19	125.03
31	B	1002	U10	C6-C1-C2	3.74	122.12	119.17
44	g	601	HEA	CAA-CBA-CGA	-3.68	103.92	113.67
44	g	604	HEA	CAA-C2A-C1A	3.64	132.25	124.85
39	L	805	3PH	O13-P-O11	-3.59	97.31	106.67
39	L	806	3PH	O13-P-O11	-3.58	97.35	106.67
43	d	501	CDL	OA8-CA6-CA4	3.53	118.56	108.40
44	g	604	HEA	C4D-C3D-C2D	-3.52	101.76	106.89
44	g	601	HEA	C13-C12-C11	-3.52	108.77	114.39
36	i	1004	3PE	C2-O21-C21	3.51	126.19	117.80
44	g	604	HEA	CHA-C1A-C2A	-3.48	119.36	124.86
44	g	604	HEA	C26-C15-C16	3.46	121.23	115.23
39	a	503	3PH	O13-P-O11	-3.45	97.67	106.67
44	g	604	HEA	CMD-C2D-C1D	-3.39	119.73	125.03
28	L	804	PGT	C2-O2-C31	-3.38	109.71	117.80
28	P	401	PGT	O2P-P-O1P	3.38	128.15	112.44
28	L	804	PGT	O2-C31-O31	-3.35	115.86	123.70
42	b	502	HEC	CAA-CBA-CGA	-3.35	104.78	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	402	3PE	C2-O21-C21	3.34	125.80	117.80
29	M	2002	DU0	O10-C09-O16	-3.34	101.93	109.88
29	c	204	DU0	C22-C21-C20	3.33	116.37	111.45
28	L	804	PGT	O2P-P-O1P	3.32	127.87	112.44
28	A	1001	PGT	O2P-P-O1P	3.31	127.84	112.44
37	J	201	T7X	O12-P1-O11	3.27	127.66	112.44
28	A	1003	PGT	O2P-P-O1P	3.26	127.61	112.44
44	g	601	HEA	CHA-C4D-C3D	-3.24	120.05	124.77
29	i	1008	DU0	C22-C21-C20	3.21	116.19	111.45
37	J	201	T7X	O1-C1-C6	3.18	115.46	108.73
44	g	601	HEA	C3C-C2C-C1C	-3.14	103.46	107.17
44	g	601	HEA	CMD-C2D-C3D	3.13	134.63	126.15
39	M	2001	3PH	O13-P-O11	-3.13	98.51	106.67
31	a	506	U10	C6-C1-C2	3.11	121.63	119.17
44	g	601	HEA	CAD-CBD-CGD	-3.08	105.50	113.67
39	i	1009	3PH	O13-P-O11	-3.07	98.67	106.67
29	c	204	DU0	C76-C75-C22	3.06	115.33	110.33
41	d	502	HEM	CAA-CBA-CGA	-3.05	105.58	113.67
29	c	202	DU0	C77-C79-C17	-3.02	108.29	112.71
29	i	1008	DU0	C04-C03-C02	-3.01	100.28	103.85
28	J	203	PGT	O2P-P-O1P	2.99	126.34	112.44
29	M	2004	DU0	O10-C09-C15	2.98	113.36	110.76
29	A	1002	DU0	O10-C09-O16	-2.96	102.83	109.88
44	g	604	HEA	C3C-C2C-C1C	-2.95	103.70	107.17
35	F	502	FMN	C4A-C10-N10	2.95	120.70	116.48
43	d	501	CDL	OB6-CB5-C51	2.90	117.76	111.48
28	q	1000	PGT	O2P-P-O1P	2.89	125.88	112.44
44	g	604	HEA	CMD-C2D-C3D	2.89	133.96	126.15
35	F	502	FMN	C4-N3-C2	-2.87	120.54	125.64
31	a	508	U10	C8-C7-C6	2.86	119.13	112.08
44	g	601	HEA	CMB-C2B-C3B	2.85	135.79	130.28
41	a	507	HEM	CAD-CBD-CGD	-2.84	106.14	113.67
29	c	202	DU0	C78-C77-C79	-2.82	108.49	111.66
44	g	601	HEA	C27-C19-C20	2.80	120.09	115.23
36	b	501	3PE	O31-C3-C2	2.78	116.40	108.40
44	g	604	HEA	CMB-C2B-C3B	2.76	135.62	130.28
29	c	202	DU0	C78-C77-C76	2.75	113.61	109.43
38	L	803	P5S	O15-P12-O13	2.74	125.19	112.44
39	c	205	3PH	O13-P-O11	-2.74	99.53	106.67
39	a	503	3PH	O31-C31-O32	-2.72	116.81	123.63
39	i	1009	3PH	O21-C21-O22	-2.72	117.36	123.70
41	d	502	HEM	CAD-CBD-CGD	-2.71	106.48	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	g	604	HEA	CHB-C1B-C2B	-2.71	120.75	125.03
29	H	401	DU0	C22-C21-C20	-2.68	107.49	111.45
42	e	502	HEC	C4D-ND-C1D	2.68	110.19	105.82
39	f	202	3PH	O31-C31-O32	-2.67	116.94	123.63
39	c	205	3PH	O31-C3-C2	2.66	116.07	108.40
36	b	501	3PE	O31-C31-O32	-2.65	117.01	123.63
36	H	402	3PE	O31-C3-C2	-2.62	100.83	108.40
41	a	505	HEM	CBD-CAD-C3D	-2.62	105.28	112.53
39	c	205	3PH	O14-P-O11	-2.62	99.84	106.67
29	M	2004	DU0	C04-C03-C02	-2.62	100.74	103.85
29	i	1008	DU0	C08-C07-C09	-2.61	110.73	114.94
39	L	806	3PH	O14-P-O11	-2.59	99.90	106.67
44	g	604	HEA	C27-C19-C20	2.59	119.72	115.23
44	g	604	HEA	C4B-C3B-C2B	-2.59	103.09	107.44
36	i	1007	3PE	O12-P-O11	-2.58	95.87	107.57
29	c	204	DU0	O10-C09-C15	2.58	113.01	110.76
44	g	601	HEA	CBA-CAA-C2A	2.57	119.64	112.53
33	i	1006	PC1	O31-C31-O32	-2.57	117.20	123.63
42	e	502	HEC	CAA-CBA-CGA	-2.56	106.88	113.67
33	L	802	PC1	C3-C2-C1	-2.56	105.83	111.78
33	i	1005	PC1	O31-C31-O32	-2.56	117.24	123.63
39	M	2001	3PH	O31-C31-O32	-2.55	117.25	123.63
29	c	202	DU0	C08-C07-C09	-2.55	110.83	114.94
44	g	604	HEA	CHC-C1C-C2C	-2.54	120.04	127.43
35	F	502	FMN	C5A-C9A-N10	2.51	120.24	117.97
39	L	806	3PH	O21-C21-O22	-2.51	117.83	123.70
44	g	601	HEA	CAA-C2A-C1A	2.51	129.95	124.85
33	j	1001	PC1	C2-O21-C21	2.50	123.79	117.80
29	c	204	DU0	C04-C03-C02	-2.50	100.88	103.85
28	A	1003	PGT	O2-C31-O31	-2.50	117.86	123.70
42	b	502	HEC	C4D-ND-C1D	2.50	109.89	105.82
31	d	506	U10	C8-C7-C6	2.49	118.21	112.08
36	L	801	3PE	O21-C21-O22	-2.48	117.90	123.70
39	i	1009	3PH	O14-P-O11	-2.48	100.20	106.67
28	P	401	PGT	O2-C31-O31	-2.48	117.91	123.70
42	e	502	HEC	CMB-C2B-C1B	-2.47	121.65	125.42
44	g	604	HEA	C3B-C4B-NB	2.45	112.66	109.84
41	a	507	HEM	CHC-C1C-NC	2.45	127.12	124.45
36	b	501	3PE	O21-C21-O22	-2.43	118.02	123.70
39	c	205	3PH	O31-C31-O32	-2.43	117.55	123.63
29	M	2002	DU0	C18-C17-C79	2.43	112.53	109.72
44	g	604	HEA	CBD-CAD-C3D	2.42	119.22	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M	2002	DU0	C79-C17-C03	-2.41	105.93	109.09
39	L	805	3PH	O31-C31-O32	-2.41	117.59	123.63
29	i	1008	DU0	C18-C17-C79	-2.41	106.94	109.72
44	g	601	HEA	CHB-C1B-C2B	-2.40	121.23	125.03
29	c	204	DU0	C21-C20-C77	2.39	119.48	116.42
36	L	801	3PE	O31-C31-O32	-2.39	117.65	123.63
29	A	1002	DU0	C77-C79-C17	-2.38	109.23	112.71
39	f	202	3PH	O31-C3-C2	2.38	115.26	108.40
44	g	604	HEA	CAD-C3D-C4D	2.38	128.85	124.70
29	J	204	DU0	O10-C11-C12	-2.38	109.12	112.17
31	a	506	U10	C7-C8-C9	-2.38	122.74	126.83
28	L	804	PGT	O3-C11-O11	-2.37	117.70	123.63
28	A	1003	PGT	O3-C3-C2	2.37	115.22	108.40
33	j	1001	PC1	O12-P-O13	-2.36	96.85	107.57
29	M	2002	DU0	C02-C03-C17	-2.36	111.06	114.41
38	L	803	P5S	O37-C38-O47	-2.36	118.19	123.70
39	i	1009	3PH	O31-C31-O32	-2.35	117.75	123.63
35	F	502	FMN	O4-C4-C4A	-2.35	120.34	126.53
29	J	202	DU0	O10-C09-O16	-2.34	104.30	109.88
43	d	501	CDL	OA6-CA5-C11	2.34	116.54	111.48
44	g	601	HEA	O11-C11-C3B	-2.33	106.98	111.26
36	d	505	3PE	O31-C31-O32	-2.31	117.85	123.63
36	b	501	3PE	O21-C21-C22	2.31	116.47	111.48
28	J	203	PGT	O3-C11-O11	-2.30	117.87	123.63
33	j	1001	PC1	O31-C31-O32	-2.30	117.87	123.63
29	A	1002	DU0	O10-C09-C07	2.30	114.12	107.26
39	L	805	3PH	O14-P-O13	2.30	116.42	107.80
33	i	1005	PC1	O12-P-O13	-2.29	97.17	107.57
41	a	505	HEM	CMB-C2B-C1B	2.29	128.61	125.03
35	F	502	FMN	O3P-P-O5'	2.29	112.63	106.67
33	a	504	PC1	O31-C31-O32	-2.28	117.92	123.63
29	A	1002	DU0	C18-C17-C79	-2.28	107.09	109.72
28	J	203	PGT	O3-C3-C2	2.28	114.96	108.40
38	L	803	P5S	O19-C17-O18	-2.27	117.94	123.63
42	b	502	HEC	CHC-C4B-NB	2.26	126.92	124.45
29	M	2004	DU0	C18-C17-C03	-2.26	107.73	110.93
29	J	204	DU0	C77-C79-C17	-2.25	109.42	112.71
39	M	2001	3PH	C2-O21-C21	2.25	123.18	117.80
44	g	604	HEA	C2B-C1B-NB	2.25	112.50	109.90
29	J	204	DU0	O10-C09-O16	-2.25	104.53	109.88
29	c	202	DU0	O10-C09-O16	-2.24	104.54	109.88
33	i	1006	PC1	O12-P-O13	-2.24	97.40	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	J	201	T7X	O3-C3-C2	-2.24	105.09	110.38
39	L	805	3PH	O14-P-O11	-2.24	100.83	106.67
36	L	801	3PE	O12-P-O11	-2.24	97.43	107.57
29	M	2002	DU0	C75-C22-C21	-2.23	107.87	110.97
33	H	403	PC1	O21-C21-O22	-2.23	118.50	123.70
31	B	1002	U10	C15-C14-C16	-2.23	111.36	115.23
33	M	2005	PC1	O12-P-O13	-2.22	97.49	107.57
29	M	2004	DU0	O10-C09-O16	-2.22	104.59	109.88
39	c	205	3PH	O21-C21-O22	-2.21	118.54	123.70
39	L	806	3PH	O14-P-O13	2.21	116.08	107.80
36	b	501	3PE	O12-P-O13	-2.21	97.57	107.57
44	g	601	HEA	C3C-C4C-NC	2.20	111.65	109.80
33	a	501	PC1	O31-C3-C2	2.19	114.72	108.40
39	f	202	3PH	O13-P-O11	-2.19	100.95	106.67
39	c	205	3PH	O14-P-O13	2.19	116.02	107.80
28	A	1001	PGT	C2-O2-C31	2.19	123.03	117.80
29	M	2002	DU0	O10-C09-C07	2.19	113.78	107.26
28	J	203	PGT	O2-C31-O31	-2.18	118.60	123.70
28	A	1003	PGT	O3-C11-O11	-2.18	118.19	123.63
36	H	402	3PE	O12-P-O11	-2.17	97.71	107.57
44	g	604	HEA	CHB-C1B-NB	2.16	126.75	124.42
29	M	2002	DU0	C80-C79-C17	-2.15	108.78	111.78
31	d	506	U10	C41-C39-C38	2.15	126.00	121.17
28	L	804	PGT	O2-C2-C1	2.15	116.06	108.34
35	F	502	FMN	C4A-C4-N3	2.15	118.72	113.25
29	J	204	DU0	C02-C03-C17	-2.15	111.37	114.41
28	P	401	PGT	O3-C11-O11	-2.14	118.27	123.63
44	g	601	HEA	CHB-C1B-NB	2.13	126.72	124.42
28	A	1001	PGT	O3-C3-C2	2.13	114.54	108.40
35	F	502	FMN	C10-C4A-N5	-2.13	120.46	124.81
31	a	508	U10	C1-C6-C5	2.13	121.69	119.62
44	g	601	HEA	CHC-C1C-C2C	-2.13	121.26	127.43
36	i	1004	3PE	O31-C3-C2	-2.13	102.27	108.40
42	b	502	HEC	CBD-CAD-C3D	-2.12	106.66	112.53
41	d	503	HEM	CHD-C4C-NC	2.11	126.75	124.45
42	b	502	HEC	CAD-CBD-CGD	-2.11	108.08	113.67
39	f	202	3PH	O21-C21-O22	-2.10	118.79	123.70
39	L	805	3PH	O21-C21-O22	-2.10	118.80	123.70
43	d	501	CDL	OA8-CA7-C31	2.10	118.24	111.83
42	e	502	HEC	CHA-C1A-NA	2.10	126.74	124.45
41	d	503	HEM	CAA-CBA-CGA	-2.10	108.10	113.67
36	d	505	3PE	O21-C21-O22	-2.10	118.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	i	1004	3PE	O12-P-O11	-2.09	98.07	107.57
31	d	506	U10	C7-C6-C1	-2.09	121.30	124.89
44	g	604	HEA	C13-C12-C11	-2.09	111.06	114.39
28	L	804	PGT	O4P-P-O1P	-2.08	100.68	108.94
43	d	501	CDL	CA6-CA4-CA3	-2.08	106.93	111.78
33	d	507	PC1	C2-O21-C21	2.08	122.77	117.80
39	L	806	3PH	O31-C3-C2	2.07	114.37	108.40
44	g	601	HEA	C3B-C4B-NB	2.07	112.22	109.84
43	d	501	CDL	OB8-CB7-C71	2.07	118.14	111.83
29	c	204	DU0	O16-C05-C06	2.06	107.91	105.12
39	f	202	3PH	O14-P-O13	2.05	115.50	107.80
36	i	1004	3PE	O32-C31-C32	2.05	131.81	123.78
29	c	204	DU0	O10-C11-C12	-2.04	109.55	112.17
33	D	502	PC1	O31-C31-O32	-2.04	118.52	123.63
36	i	1007	3PE	O31-C31-O32	-2.04	118.52	123.63
37	J	201	T7X	C6-C1-C2	-2.04	108.03	110.86
31	a	508	U10	C7-C6-C1	-2.04	121.40	124.89
33	i	1003	PC1	O12-P-O13	-2.03	98.35	107.57
36	c	201	3PE	O21-C21-O22	-2.02	118.97	123.70
41	d	502	HEM	C3B-C2B-C1B	2.02	107.93	106.41
44	g	604	HEA	C16-C15-C14	-2.02	116.63	121.17
36	H	402	3PE	O31-C31-O32	-2.02	118.58	123.63
35	F	502	FMN	C4'-C3'-C2'	-2.02	110.21	113.57
39	M	2001	3PH	O14-P-O13	2.02	115.36	107.80
31	a	506	U10	C7-C6-C1	-2.01	121.44	124.89
44	g	601	HEA	CHA-C1A-NA	2.01	126.64	124.45
39	i	1009	3PH	O14-P-O13	2.01	115.33	107.80
33	d	507	PC1	O12-P-O13	-2.00	98.49	107.57
31	d	506	U10	C46-C44-C43	2.00	125.66	121.17
31	d	506	U10	O2-C2-C3	2.00	125.27	121.03
44	g	601	HEA	O2D-CGD-CBD	2.00	120.32	114.00

There are no chirality outliers.

All (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
28	P	401	PGT	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
28	P	401	PGT	C4-O4P-P-O1P
28	q	1000	PGT	C5-C4-O4P-P
31	B	1002	U10	C1-C6-C7-C8
31	B	1002	U10	C5-C6-C7-C8
31	B	1002	U10	C11-C12-C13-C14
33	D	502	PC1	C11-O13-P-O14
33	D	502	PC1	C11-O13-P-O11
33	D	502	PC1	C12-C11-O13-P
33	D	502	PC1	O13-C11-C12-N
33	H	403	PC1	C11-O13-P-O12
33	H	403	PC1	C11-O13-P-O11
33	L	802	PC1	C11-O13-P-O12
33	L	802	PC1	C11-O13-P-O11
33	M	2003	PC1	C11-O13-P-O12
33	M	2003	PC1	C1-O11-P-O14
33	M	2003	PC1	C12-C11-O13-P
33	M	2003	PC1	C2-C1-O11-P
33	M	2005	PC1	C1-O11-P-O12
33	M	2005	PC1	C1-O11-P-O13
33	M	2005	PC1	O11-C1-C2-O21
33	a	502	PC1	C1-O11-P-O14
33	a	502	PC1	C2-C1-O11-P
33	a	504	PC1	C11-O13-P-O12
33	d	507	PC1	C11-O13-P-O12
33	d	507	PC1	C11-O13-P-O14
33	d	507	PC1	C11-O13-P-O11
33	d	507	PC1	C1-O11-P-O12
33	i	1001	PC1	C11-O13-P-O11
33	i	1001	PC1	O13-C11-C12-N
33	i	1003	PC1	C11-O13-P-O14
33	i	1003	PC1	C1-O11-P-O12
33	i	1003	PC1	C12-C11-O13-P
33	i	1005	PC1	C11-O13-P-O14
33	i	1005	PC1	C1-O11-P-O13
33	i	1006	PC1	C11-O13-P-O14
33	i	1006	PC1	C12-C11-O13-P
36	H	402	3PE	C1-O11-P-O12
36	H	402	3PE	C11-O13-P-O11
36	H	402	3PE	C11-O13-P-O12
36	I	203	3PE	C1-O11-P-O12
36	L	801	3PE	C1-O11-P-O13
36	L	801	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
36	L	801	3PE	C12-C11-O13-P
36	b	501	3PE	C11-O13-P-O11
36	b	501	3PE	C11-O13-P-O12
36	b	501	3PE	C2-C1-O11-P
36	b	501	3PE	C12-C11-O13-P
36	b	501	3PE	O21-C2-C3-O31
36	c	201	3PE	C11-O13-P-O14
36	c	201	3PE	C12-C11-O13-P
36	d	505	3PE	C1-O11-P-O13
36	d	505	3PE	C1-O11-P-O14
36	d	505	3PE	C11-O13-P-O12
36	d	505	3PE	C12-C11-O13-P
36	i	1004	3PE	C2-C1-O11-P
36	i	1007	3PE	C1-O11-P-O12
36	i	1007	3PE	C11-O13-P-O12
36	i	1007	3PE	C12-C11-O13-P
37	J	201	T7X	C6-C1-O1-P1
37	J	201	T7X	O13-C7-C8-O16
37	J	201	T7X	C19-C20-C21-C22
39	L	806	3PH	C1-O11-P-O14
39	i	1009	3PH	C2-C1-O11-P
39	i	1009	3PH	O21-C2-C3-O31
41	a	505	HEM	C2B-C3B-CAB-CBB
41	a	505	HEM	C4B-C3B-CAB-CBB
41	d	502	HEM	C2C-C3C-CAC-CBC
41	d	502	HEM	C4C-C3C-CAC-CBC
41	d	503	HEM	C2B-C3B-CAB-CBB
41	d	503	HEM	C4B-C3B-CAB-CBB
42	b	502	HEC	C2B-C3B-CAB-CBB
42	b	502	HEC	C4B-C3B-CAB-CBB
42	b	502	HEC	C4C-C3C-CAC-CBC
42	e	502	HEC	C2B-C3B-CAB-CBB
42	e	502	HEC	C4B-C3B-CAB-CBB
43	d	501	CDL	CB4-CB3-OB5-PB2
31	B	1002	U10	C40-C39-C41-C42
28	A	1001	PGT	O4P-C4-C5-O5
31	B	1002	U10	C38-C39-C41-C42
31	a	506	U10	C24-C26-C27-C28
31	d	504	U10	C19-C21-C22-C23
31	d	506	U10	C9-C11-C12-C13
31	d	506	U10	C14-C16-C17-C18
31	d	506	U10	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	d	506	U10	C39-C41-C42-C43
28	P	401	PGT	C2-C1-O3P-P
33	a	509	PC1	C2-C1-O11-P
39	L	806	3PH	C21-C22-C23-C24
33	a	501	PC1	C22-C23-C24-C25
28	J	203	PGT	O2-C2-C3-O3
33	i	1005	PC1	C33-C34-C35-C36
31	B	1002	U10	C14-C16-C17-C18
36	i	1007	3PE	C21-C22-C23-C24
28	P	401	PGT	C5-C4-O4P-P
39	f	202	3PH	C2-C1-O11-P
39	M	2001	3PH	C21-C22-C23-C24
33	a	501	PC1	C31-C32-C33-C34
39	L	806	3PH	C2-C3-O31-C31
36	i	1007	3PE	C31-C32-C33-C34
31	d	504	U10	C49-C51-C52-C53
28	J	203	PGT	C2-C1-O3P-P
28	q	1000	PGT	C2-C1-O3P-P
29	c	204	DU0	C75-C22-O23-C24
28	q	1000	PGT	C31-C32-C33-C34
28	L	804	PGT	C11-C12-C13-C14
39	L	805	3PH	C22-C23-C24-C25
33	D	502	PC1	C2D-C2E-C2F-C2G
33	M	2005	PC1	C33-C34-C35-C36
36	L	801	3PE	C35-C36-C37-C38
33	D	502	PC1	C3B-C3C-C3D-C3E
28	L	804	PGT	C35-C36-C37-C38
36	b	501	3PE	C21-C22-C23-C24
38	L	803	P5S	OXT-C-CA-N
33	a	504	PC1	C3A-C3B-C3C-C3D
33	j	1001	PC1	C22-C23-C24-C25
33	a	502	PC1	C25-C26-C27-C28
33	d	507	PC1	C1-C2-C3-O31
36	H	402	3PE	C1-C2-C3-O31
33	D	502	PC1	C2A-C2B-C2C-C2D
33	D	502	PC1	C39-C3A-C3B-C3C
39	L	806	3PH	C3B-C3C-C3D-C3E
36	c	201	3PE	C3D-C3E-C3F-C3G
39	L	806	3PH	C32-C33-C34-C35
39	M	2001	3PH	C2B-C2C-C2D-C2E
33	a	509	PC1	C2B-C2C-C2D-C2E
39	f	202	3PH	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
36	b	501	3PE	C31-C32-C33-C34
36	d	505	3PE	C21-C22-C23-C24
33	D	502	PC1	C34-C35-C36-C37
33	j	1001	PC1	C2-C1-O11-P
36	d	505	3PE	C2-C1-O11-P
36	c	201	3PE	C29-C2A-C2B-C2C
39	L	805	3PH	C3B-C3C-C3D-C3E
33	i	1006	PC1	C29-C2A-C2B-C2C
39	a	503	3PH	C32-C33-C34-C35
39	c	205	3PH	C27-C28-C29-C2A
43	d	501	CDL	C80-C81-C82-C83
33	d	507	PC1	C3E-C3F-C3G-C3H
33	a	502	PC1	C38-C39-C3A-C3B
36	L	801	3PE	C2A-C2B-C2C-C2D
41	d	503	HEM	C2C-C3C-CAC-CBC
33	a	509	PC1	C27-C28-C29-C2A
39	i	1009	3PH	C37-C38-C39-C3A
33	i	1006	PC1	O21-C2-C3-O31
38	L	803	P5S	C42-C43-C44-C45
28	A	1003	PGT	C5-C4-O4P-P
36	H	402	3PE	C2-C1-O11-P
39	a	503	3PH	C2-C1-O11-P
39	M	2001	3PH	C35-C36-C37-C38
36	I	203	3PE	C25-C26-C27-C28
36	i	1007	3PE	C3D-C3E-C3F-C3G
33	L	802	PC1	O11-C1-C2-C3
37	J	201	T7X	O13-C7-C8-C9
43	d	501	CDL	OB5-CB3-CB4-CB6
43	d	501	CDL	C22-C23-C24-C25
44	g	601	HEA	C2D-C3D-CAD-CBD
28	J	203	PGT	C21-C22-C23-C24
36	L	801	3PE	C36-C37-C38-C39
43	d	501	CDL	C17-C18-C19-C20
29	J	204	DU0	C25-C24-O23-C22
44	g	601	HEA	C4D-C3D-CAD-CBD
28	J	203	PGT	C1-C2-C3-O3
39	i	1009	3PH	C1-C2-C3-O31
28	q	1000	PGT	C41-C42-C43-C44
28	L	804	PGT	C42-C43-C44-C45
28	L	804	PGT	C2-C1-O3P-P
29	c	204	DU0	C21-C22-O23-C24
28	J	203	PGT	O4P-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	d	507	PC1	O11-C1-C2-O21
33	j	1001	PC1	O11-C1-C2-O21
33	j	1001	PC1	C3D-C3E-C3F-C3G
33	i	1005	PC1	C2F-C2G-C2H-C2I
33	M	2005	PC1	C2D-C2E-C2F-C2G
28	L	804	PGT	C32-C33-C34-C35
36	b	501	3PE	C23-C24-C25-C26
33	i	1001	PC1	C35-C36-C37-C38
33	a	504	PC1	C2-C1-O11-P
41	a	505	HEM	C2A-CAA-CBA-CGA
33	D	502	PC1	C26-C27-C28-C29
28	J	203	PGT	O3P-C1-C2-C3
33	D	502	PC1	C29-C2A-C2B-C2C
39	L	805	3PH	C2D-C2E-C2F-C2G
36	H	402	3PE	C3F-C3G-C3H-C3I
28	A	1001	PGT	C18-C19-C20-C21
31	B	1002	U10	C25-C24-C26-C27
31	B	1002	U10	C45-C44-C46-C47
33	i	1005	PC1	C3B-C3C-C3D-C3E
31	B	1002	U10	C23-C24-C26-C27
43	d	501	CDL	C15-C16-C17-C18
33	i	1006	PC1	C1-C2-C3-O31
31	B	1002	U10	C43-C44-C46-C47
33	H	403	PC1	O11-C1-C2-O21
39	L	806	3PH	C2C-C2D-C2E-C2F
28	A	1001	PGT	C2-C1-O3P-P
35	F	502	FMN	C4'-C5'-O5'-P
36	c	201	3PE	C2-C1-O11-P
36	c	201	3PE	C32-C33-C34-C35
28	P	401	PGT	O2-C2-C3-O3
39	L	805	3PH	O21-C2-C3-O31
43	d	501	CDL	OA6-CA4-CA6-OA8
33	a	509	PC1	C37-C38-C39-C3A
33	H	403	PC1	C39-C3A-C3B-C3C
36	d	505	3PE	C2A-C2B-C2C-C2D
39	M	2001	3PH	C27-C28-C29-C2A
33	a	504	PC1	C34-C35-C36-C37
28	L	804	PGT	C20-C21-C22-C23
33	i	1003	PC1	C3C-C3D-C3E-C3F
36	i	1007	3PE	C25-C26-C27-C28
28	J	203	PGT	O5-C5-C6-O6
36	H	402	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
33	H	403	PC1	O11-C1-C2-C3
33	M	2005	PC1	O11-C1-C2-C3
33	i	1006	PC1	O11-C1-C2-C3
28	P	401	PGT	C45-C46-C47-C48
33	a	501	PC1	C2-C3-O31-C31
43	d	501	CDL	C13-C14-C15-C16
39	L	806	3PH	C1-O11-P-O13
28	q	1000	PGT	C40-C41-C42-C43
33	a	504	PC1	C24-C25-C26-C27
41	a	505	HEM	C2C-C3C-CAC-CBC
41	a	507	HEM	C2B-C3B-CAB-CBB
41	a	507	HEM	C2C-C3C-CAC-CBC
36	d	505	3PE	C26-C27-C28-C29
43	d	501	CDL	C18-C19-C20-C21
28	J	203	PGT	C4-C5-C6-O6
33	i	1003	PC1	C29-C2A-C2B-C2C
33	a	502	PC1	C34-C35-C36-C37
28	J	203	PGT	O3P-C1-C2-O2
33	L	802	PC1	O11-C1-C2-O21
33	i	1001	PC1	O11-C1-C2-O21
33	i	1006	PC1	O11-C1-C2-O21
39	a	503	3PH	O11-C1-C2-O21
39	i	1009	3PH	O11-C1-C2-O21
43	d	501	CDL	OB5-CB3-CB4-OB6
36	b	501	3PE	C26-C27-C28-C29
31	B	1002	U10	C34-C36-C37-C38
33	a	504	PC1	C1-C2-C3-O31
36	b	501	3PE	C1-C2-C3-O31
39	L	806	3PH	C1-C2-C3-O31
41	d	503	HEM	C4C-C3C-CAC-CBC
33	H	403	PC1	C12-C11-O13-P
33	L	802	PC1	C12-C11-O13-P
33	M	2005	PC1	C12-C11-O13-P
33	a	501	PC1	C12-C11-O13-P
33	a	502	PC1	C12-C11-O13-P
33	a	504	PC1	C12-C11-O13-P
33	i	1001	PC1	C12-C11-O13-P
33	i	1005	PC1	C12-C11-O13-P
33	j	1001	PC1	C12-C11-O13-P
36	H	402	3PE	C12-C11-O13-P
36	I	203	3PE	C12-C11-O13-P
28	P	401	PGT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	a	504	PC1	O21-C2-C3-O31
36	H	402	3PE	O21-C2-C3-O31
31	d	506	U10	C16-C17-C18-C19
33	M	2003	PC1	O13-C11-C12-N
33	a	501	PC1	O13-C11-C12-N
33	a	502	PC1	O13-C11-C12-N
33	a	504	PC1	O13-C11-C12-N
33	a	509	PC1	O13-C11-C12-N
33	d	507	PC1	O13-C11-C12-N
33	i	1005	PC1	O13-C11-C12-N
33	i	1006	PC1	O13-C11-C12-N
33	j	1001	PC1	O13-C11-C12-N
33	i	1003	PC1	C24-C25-C26-C27
33	a	501	PC1	C3B-C3C-C3D-C3E
31	B	1002	U10	C12-C11-C9-C10
28	A	1003	PGT	C18-C19-C20-C21
33	i	1001	PC1	O11-C1-C2-C3
33	j	1001	PC1	O11-C1-C2-C3
36	I	203	3PE	O11-C1-C2-C3
39	a	503	3PH	O11-C1-C2-C3
39	i	1009	3PH	O11-C1-C2-C3
33	i	1001	PC1	C2C-C2D-C2E-C2F
33	M	2005	PC1	C27-C28-C29-C2A
28	A	1001	PGT	C5-C4-O4P-P
33	a	501	PC1	C2-C1-O11-P
43	d	501	CDL	C1-CA2-OA2-PA1
39	f	202	3PH	C2D-C2E-C2F-C2G
36	I	203	3PE	C3B-C3C-C3D-C3E
36	I	203	3PE	O11-C1-C2-O21
33	d	507	PC1	O21-C2-C3-O31
33	i	1006	PC1	C25-C26-C27-C28
31	a	508	U10	C40-C39-C41-C42
36	d	505	3PE	C29-C2A-C2B-C2C
39	c	205	3PH	C29-C2A-C2B-C2C
33	M	2003	PC1	C28-C29-C2A-C2B
28	A	1001	PGT	C1-O3P-P-O4P
28	J	203	PGT	C1-O3P-P-O2P
28	P	401	PGT	C1-O3P-P-O2P
33	H	403	PC1	C11-O13-P-O14
33	L	802	PC1	C11-O13-P-O14
33	M	2003	PC1	C1-O11-P-O13
33	a	502	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
33	a	504	PC1	C11-O13-P-O11
33	a	509	PC1	C1-O11-P-O14
33	i	1001	PC1	C11-O13-P-O14
33	i	1005	PC1	C1-O11-P-O14
33	i	1006	PC1	C11-O13-P-O11
33	i	1006	PC1	C1-O11-P-O14
36	c	201	3PE	C11-O13-P-O11
36	i	1007	3PE	C11-O13-P-O11
36	i	1007	3PE	C11-O13-P-O14
36	c	201	3PE	C28-C29-C2A-C2B
43	d	501	CDL	C42-C43-C44-C45
33	i	1006	PC1	C36-C37-C38-C39
39	L	806	3PH	C3A-C3B-C3C-C3D
33	d	507	PC1	C2-C1-O11-P
43	d	501	CDL	CA4-CA3-OA5-PA1
43	d	501	CDL	C1-CB2-OB2-PB2
39	L	806	3PH	C1-O11-P-O12
39	c	205	3PH	C3A-C3B-C3C-C3D
28	A	1001	PGT	C1-C2-O2-C31
36	i	1004	3PE	C3-C2-O21-C21
43	d	501	CDL	CA3-CA4-OA6-CA5
39	a	503	3PH	C2A-C2B-C2C-C2D
31	B	1002	U10	C9-C11-C12-C13
43	d	501	CDL	C21-C22-C23-C24
33	d	507	PC1	O11-C1-C2-C3
33	a	509	PC1	C33-C34-C35-C36
28	A	1003	PGT	O4P-C4-C5-C6
38	L	803	P5S	O37-C2-C3-O16
36	c	201	3PE	C39-C3A-C3B-C3C
31	a	506	U10	C15-C14-C16-C17
31	a	508	U10	C15-C14-C16-C17
31	B	1002	U10	C12-C11-C9-C8
31	a	508	U10	C2-C3-O3-C3M
31	B	1002	U10	C16-C17-C18-C19
36	I	203	3PE	C2-C1-O11-P
33	a	509	PC1	C26-C27-C28-C29
31	d	506	U10	C44-C46-C47-C48
39	L	805	3PH	C1-C2-C3-O31
39	c	205	3PH	C3C-C3D-C3E-C3F
39	a	503	3PH	C2C-C2D-C2E-C2F
31	d	506	U10	C4-C3-O3-C3M
33	a	504	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
33	i	1003	PC1	C2-C1-O11-P
31	B	1002	U10	C5-C4-O4-C4M
33	M	2005	PC1	C25-C26-C27-C28
39	c	205	3PH	C2-C3-O31-C31
39	f	202	3PH	C2E-C2F-C2G-C2H
33	D	502	PC1	C3A-C3B-C3C-C3D
33	D	502	PC1	C28-C29-C2A-C2B
28	A	1001	PGT	C37-C38-C39-C40
36	b	501	3PE	C39-C3A-C3B-C3C
28	q	1000	PGT	O2-C2-C3-O3
31	a	508	U10	C13-C14-C16-C17
31	a	508	U10	C38-C39-C41-C42
39	M	2001	3PH	C37-C38-C39-C3A
33	D	502	PC1	C2B-C2C-C2D-C2E
33	j	1001	PC1	C27-C28-C29-C2A
31	a	506	U10	C5-C4-O4-C4M
42	b	502	HEC	CAA-CBA-CGA-O1A
42	e	502	HEC	CAA-CBA-CGA-O1A
28	L	804	PGT	C19-C20-C21-C22
31	B	1002	U10	C44-C46-C47-C48
31	a	506	U10	C14-C16-C17-C18
28	J	203	PGT	C40-C41-C42-C43
33	d	507	PC1	C3-C2-O21-C21
33	j	1001	PC1	C1-C2-O21-C21
36	H	402	3PE	C1-C2-O21-C21
39	M	2001	3PH	C1-C2-O21-C21
42	e	502	HEC	CAA-CBA-CGA-O2A
36	H	402	3PE	C3B-C3C-C3D-C3E
42	b	502	HEC	CAA-CBA-CGA-O2A
44	g	601	HEA	CAA-CBA-CGA-O1A
28	J	203	PGT	O4P-C4-C5-O5
44	g	604	HEA	CAD-CBD-CGD-O2D
33	i	1005	PC1	C2-C1-O11-P
28	J	203	PGT	C13-C14-C15-C16
41	d	503	HEM	CAA-CBA-CGA-O2A
31	B	1002	U10	C20-C19-C21-C22
31	a	506	U10	C13-C14-C16-C17
37	J	201	T7X	C38-C39-C40-C41
33	a	504	PC1	C26-C27-C28-C29
42	b	502	HEC	CAD-CBD-CGD-O1D
33	L	802	PC1	O21-C2-C3-O31
44	g	601	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	c	205	3PH	C3B-C3C-C3D-C3E
31	a	506	U10	C30-C29-C31-C32
31	d	506	U10	C45-C44-C46-C47
44	g	601	HEA	C27-C19-C20-C21
36	i	1007	3PE	C28-C29-C2A-C2B
31	d	506	U10	C43-C44-C46-C47
33	j	1001	PC1	C38-C39-C3A-C3B
33	a	504	PC1	C25-C26-C27-C28
41	d	503	HEM	CAA-CBA-CGA-O1A
33	M	2003	PC1	C3A-C3B-C3C-C3D
44	g	604	HEA	CAD-CBD-CGD-O1D
28	P	401	PGT	C38-C39-C40-C41
28	q	1000	PGT	C34-C35-C36-C37
33	d	507	PC1	C3A-C3B-C3C-C3D
31	a	506	U10	C25-C24-C26-C27
28	q	1000	PGT	C39-C40-C41-C42
43	d	501	CDL	C32-C33-C34-C35
31	B	1002	U10	C18-C19-C21-C22
41	d	502	HEM	CAA-CBA-CGA-O2A
42	b	502	HEC	CAD-CBD-CGD-O2D
31	a	506	U10	C28-C29-C31-C32
28	q	1000	PGT	C17-C18-C19-C20
33	i	1001	PC1	C33-C34-C35-C36
37	J	201	T7X	C24-C25-C26-C27
33	H	403	PC1	O31-C31-C32-C33
33	H	403	PC1	C36-C37-C38-C39
39	L	805	3PH	C34-C35-C36-C37
28	A	1003	PGT	C21-C22-C23-C24
36	L	801	3PE	O11-C1-C2-C3
38	L	803	P5S	C1-C2-C3-O16
36	I	203	3PE	O21-C2-C3-O31
41	d	502	HEM	CAD-CBD-CGD-O2D
33	a	509	PC1	C34-C35-C36-C37
31	a	508	U10	C51-C52-C53-C54
39	M	2001	3PH	C33-C34-C35-C36
44	g	604	HEA	CAA-CBA-CGA-O2A
43	d	501	CDL	CA4-CA6-OA8-CA7
33	a	504	PC1	C3E-C3F-C3G-C3H
33	H	403	PC1	C11-C12-N-C14
28	q	1000	PGT	C1-C2-O2-C31
33	j	1001	PC1	C3-C2-O21-C21
39	L	806	3PH	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
41	a	507	HEM	CAA-CBA-CGA-O2A
38	L	803	P5S	C24-C25-C26-C27
36	L	801	3PE	O11-C1-C2-O21
31	B	1002	U10	C31-C32-C33-C34
28	P	401	PGT	C1-C2-C3-O3
41	a	505	HEM	C4C-C3C-CAC-CBC
41	a	507	HEM	C4B-C3B-CAB-CBB
41	a	507	HEM	C4C-C3C-CAC-CBC
33	a	509	PC1	O21-C21-C22-C23
39	a	503	3PH	C3F-C3G-C3H-C3I
33	j	1001	PC1	C23-C24-C25-C26
37	J	201	T7X	O16-C10-C12-C13
41	d	502	HEM	CAA-CBA-CGA-O1A
41	d	502	HEM	CAD-CBD-CGD-O1D
33	a	502	PC1	C33-C34-C35-C36
41	a	507	HEM	CAA-CBA-CGA-O1A
39	c	205	3PH	C25-C26-C27-C28
44	g	604	HEA	CAA-CBA-CGA-O1A
36	H	402	3PE	O21-C21-C22-C23
33	a	504	PC1	C33-C34-C35-C36
31	a	508	U10	C4-C3-O3-C3M
33	a	501	PC1	O31-C31-C32-C33
33	d	507	PC1	O31-C31-C32-C33
43	d	501	CDL	C52-C51-CB5-OB6
33	j	1001	PC1	O31-C31-C32-C33
31	B	1002	U10	C33-C34-C36-C37
33	i	1003	PC1	O22-C21-O21-C2
43	d	501	CDL	C54-C55-C56-C57
37	J	201	T7X	O18-C11-C31-C32
33	H	403	PC1	C11-C12-N-C13
36	I	203	3PE	C28-C29-C2A-C2B
43	d	501	CDL	C12-C13-C14-C15
28	J	203	PGT	C15-C16-C17-C18
28	A	1001	PGT	O3-C11-C12-C13
41	a	507	HEM	CAD-CBD-CGD-O1D
31	a	506	U10	C36-C37-C38-C39
41	a	507	HEM	CAD-CBD-CGD-O2D
39	a	503	3PH	C2B-C2C-C2D-C2E
39	L	805	3PH	O31-C31-C32-C33
43	d	501	CDL	CB3-CB4-CB6-OB8
36	b	501	3PE	C2E-C2F-C2G-C2H
31	B	1002	U10	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
33	a	504	PC1	O21-C21-C22-C23
28	A	1001	PGT	O2-C2-C3-O3
33	j	1001	PC1	O21-C2-C3-O31
39	M	2001	3PH	O21-C2-C3-O31
43	d	501	CDL	OB6-CB4-CB6-OB8
41	a	505	HEM	CAA-CBA-CGA-O1A
36	i	1004	3PE	C3D-C3E-C3F-C3G
33	i	1005	PC1	O21-C21-C22-C23
36	i	1004	3PE	O21-C21-C22-C23
33	a	501	PC1	C2C-C2D-C2E-C2F
28	q	1000	PGT	O3P-C1-C2-C3
29	J	204	DU0	C75-C22-O23-C24
33	H	403	PC1	C38-C39-C3A-C3B
33	i	1001	PC1	O31-C31-C32-C33
33	j	1001	PC1	O21-C21-C22-C23
37	J	201	T7X	C36-C37-C38-C39
33	a	504	PC1	C11-C12-N-C15
33	d	507	PC1	C32-C33-C34-C35
33	D	502	PC1	C23-C24-C25-C26
28	q	1000	PGT	C37-C38-C39-C40
33	j	1001	PC1	C32-C33-C34-C35
41	a	505	HEM	CAA-CBA-CGA-O2A
31	d	506	U10	C35-C34-C36-C37
31	d	506	U10	C50-C49-C51-C52
37	J	201	T7X	O19-C11-C31-C32
39	f	202	3PH	C37-C38-C39-C3A
33	i	1001	PC1	C22-C23-C24-C25
33	L	802	PC1	C32-C33-C34-C35
36	L	801	3PE	O21-C21-C22-C23
36	H	402	3PE	O22-C21-C22-C23
33	i	1003	PC1	C22-C21-O21-C2
33	d	507	PC1	O32-C31-C32-C33
28	A	1003	PGT	O4P-C4-C5-O5
44	g	601	HEA	CAD-CBD-CGD-O2D
33	i	1005	PC1	O32-C31-C32-C33
36	d	505	3PE	O21-C21-C22-C23
29	c	204	DU0	C25-C24-O23-C22
33	a	504	PC1	O22-C21-C22-C23
33	i	1001	PC1	C38-C39-C3A-C3B
38	L	803	P5S	C30-C31-C32-C33
28	q	1000	PGT	O2-C31-C32-C33
33	a	501	PC1	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
33	i	1005	PC1	O22-C21-C22-C23
33	j	1001	PC1	O32-C31-C32-C33
37	J	201	T7X	O17-C10-C12-C13
31	d	504	U10	C40-C39-C41-C42
33	D	502	PC1	C31-C32-C33-C34
33	a	504	PC1	C31-C32-C33-C34
41	d	502	HEM	C2B-C3B-CAB-CBB
33	i	1006	PC1	C11-C12-N-C15
28	A	1001	PGT	O11-C11-C12-C13
33	a	504	PC1	O31-C31-C32-C33
33	j	1001	PC1	O22-C21-C22-C23
39	L	805	3PH	O32-C31-C32-C33
33	D	502	PC1	O11-C1-C2-C3
38	L	803	P5S	O-C-CA-N
37	J	201	T7X	C42-C43-C44-C45
33	d	507	PC1	O21-C21-C22-C23
33	i	1005	PC1	O31-C31-C32-C33
36	L	801	3PE	C3D-C3E-C3F-C3G
36	i	1004	3PE	O22-C21-C22-C23
33	L	802	PC1	C35-C36-C37-C38
36	L	801	3PE	O31-C31-C32-C33

There are no ring outliers.

17 monomers are involved in 35 short contacts:

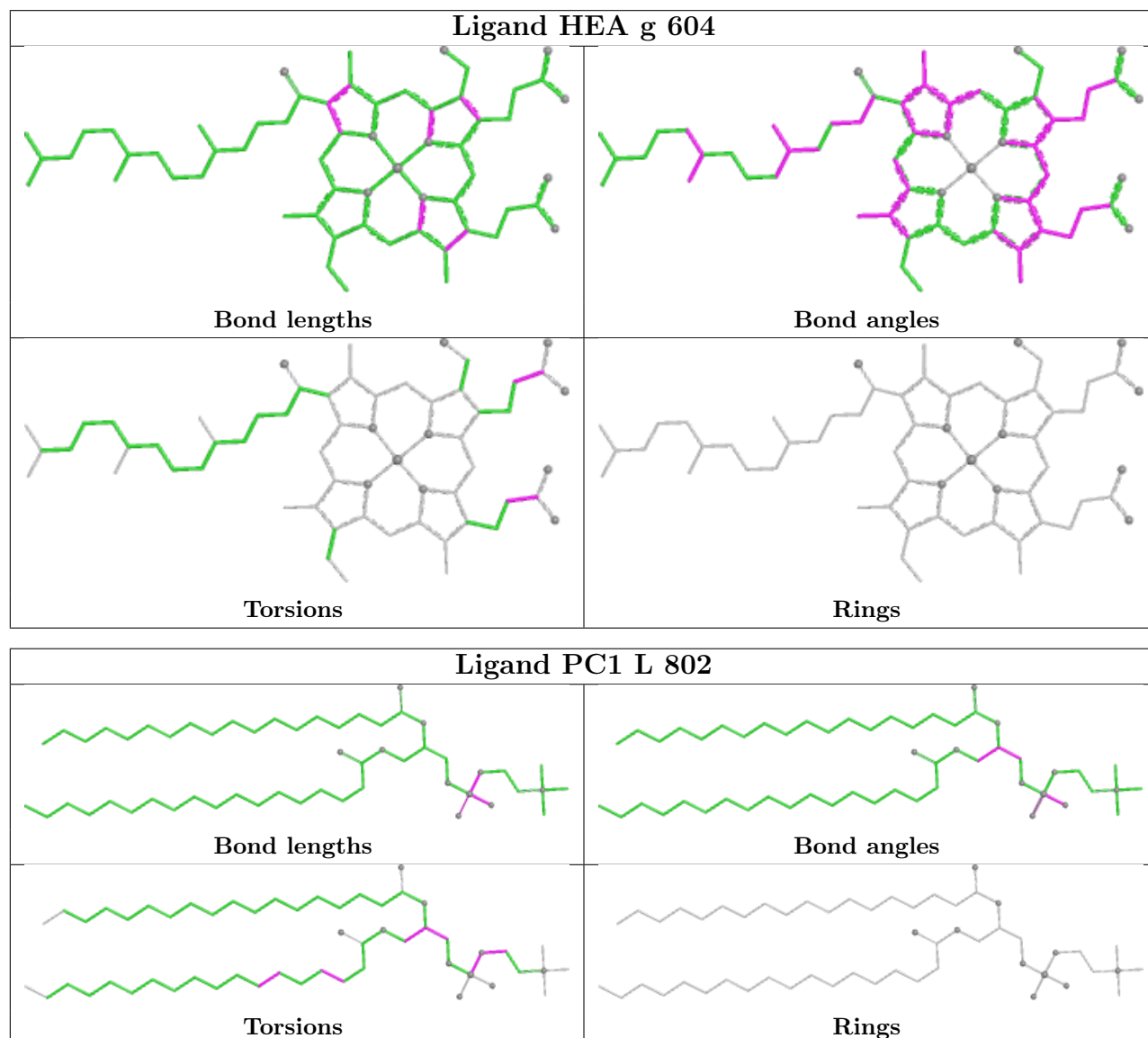
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	L	802	PC1	1	0
33	j	1001	PC1	2	0
33	H	403	PC1	1	0
39	a	503	3PH	1	0
39	L	806	3PH	1	0
41	a	507	HEM	1	0
42	e	502	HEC	4	0
33	D	502	PC1	1	0
42	b	502	HEC	3	0
31	d	504	U10	2	0
35	F	502	FMN	3	0
31	d	506	U10	5	0
33	i	1005	PC1	1	0
33	i	1006	PC1	2	0
36	L	801	3PE	1	0
31	a	508	U10	3	0

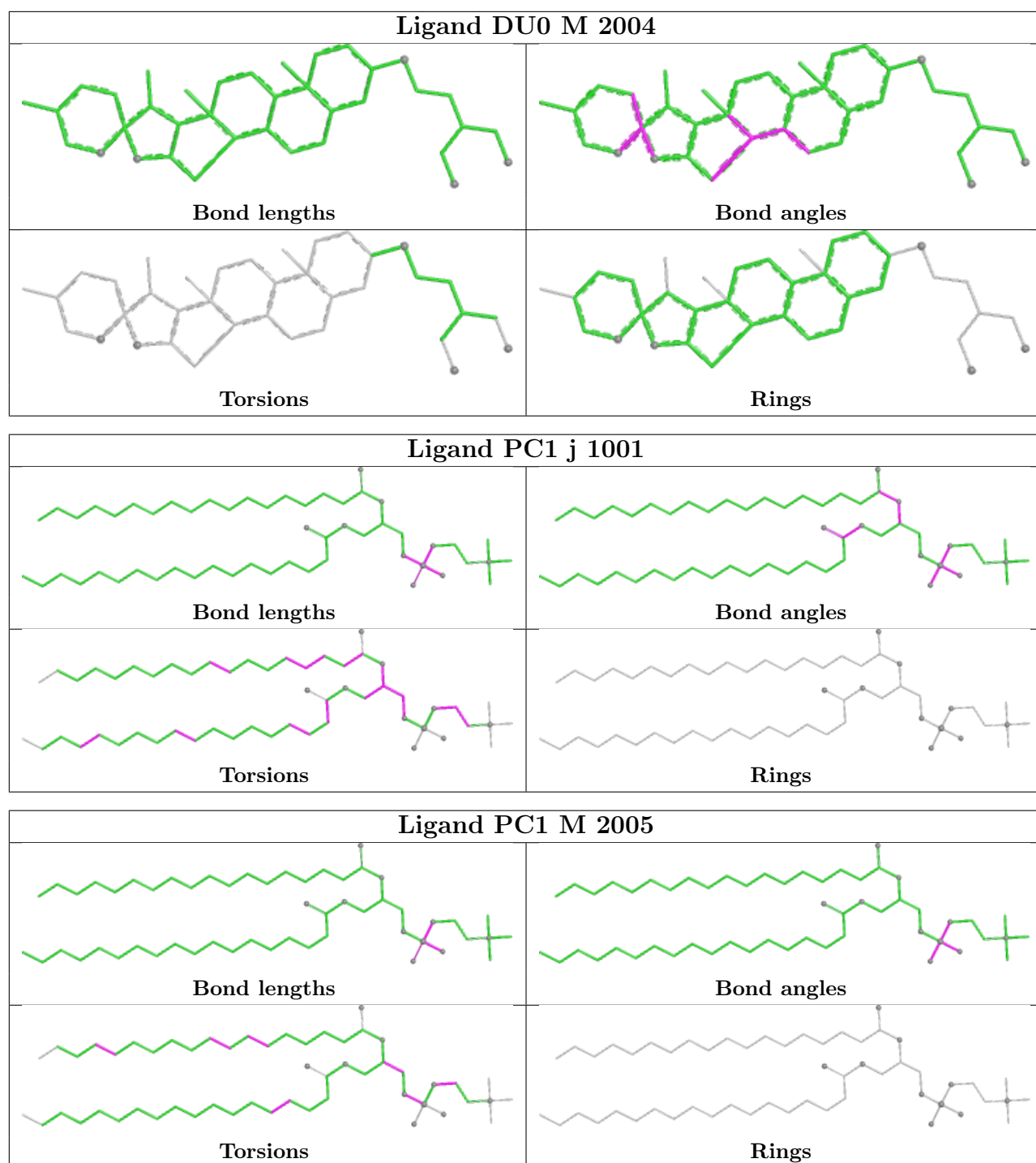
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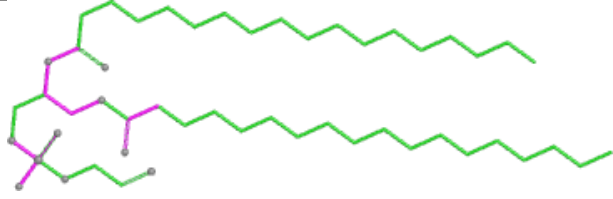
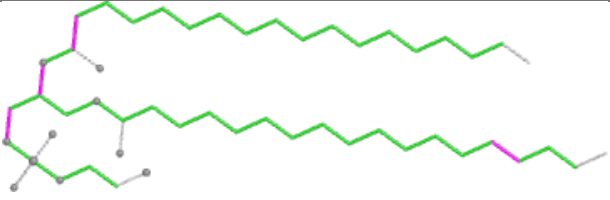
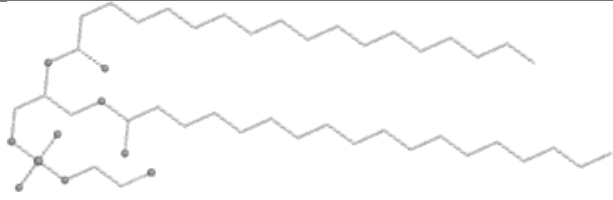
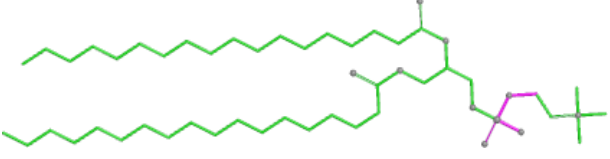
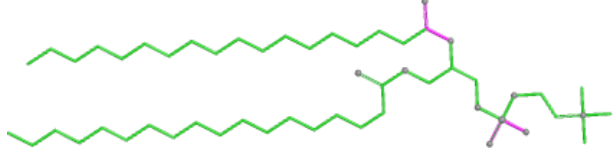
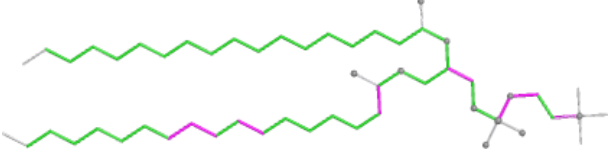
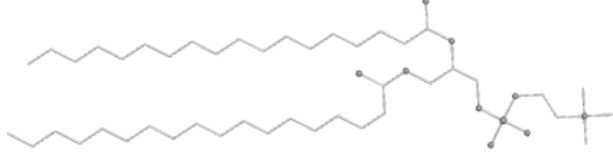
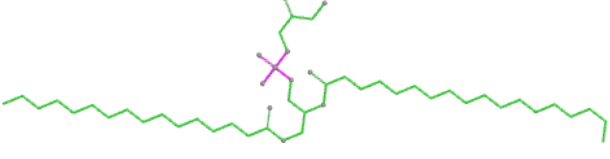
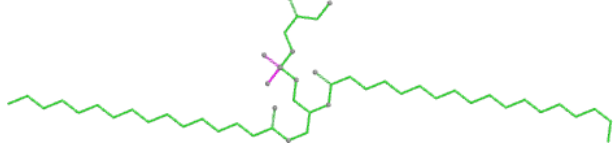
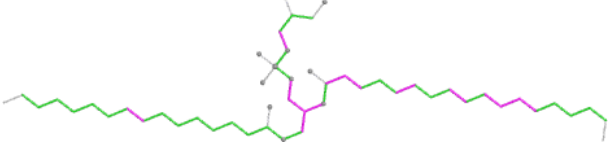
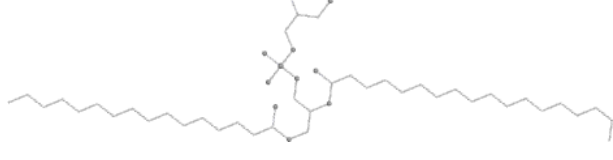
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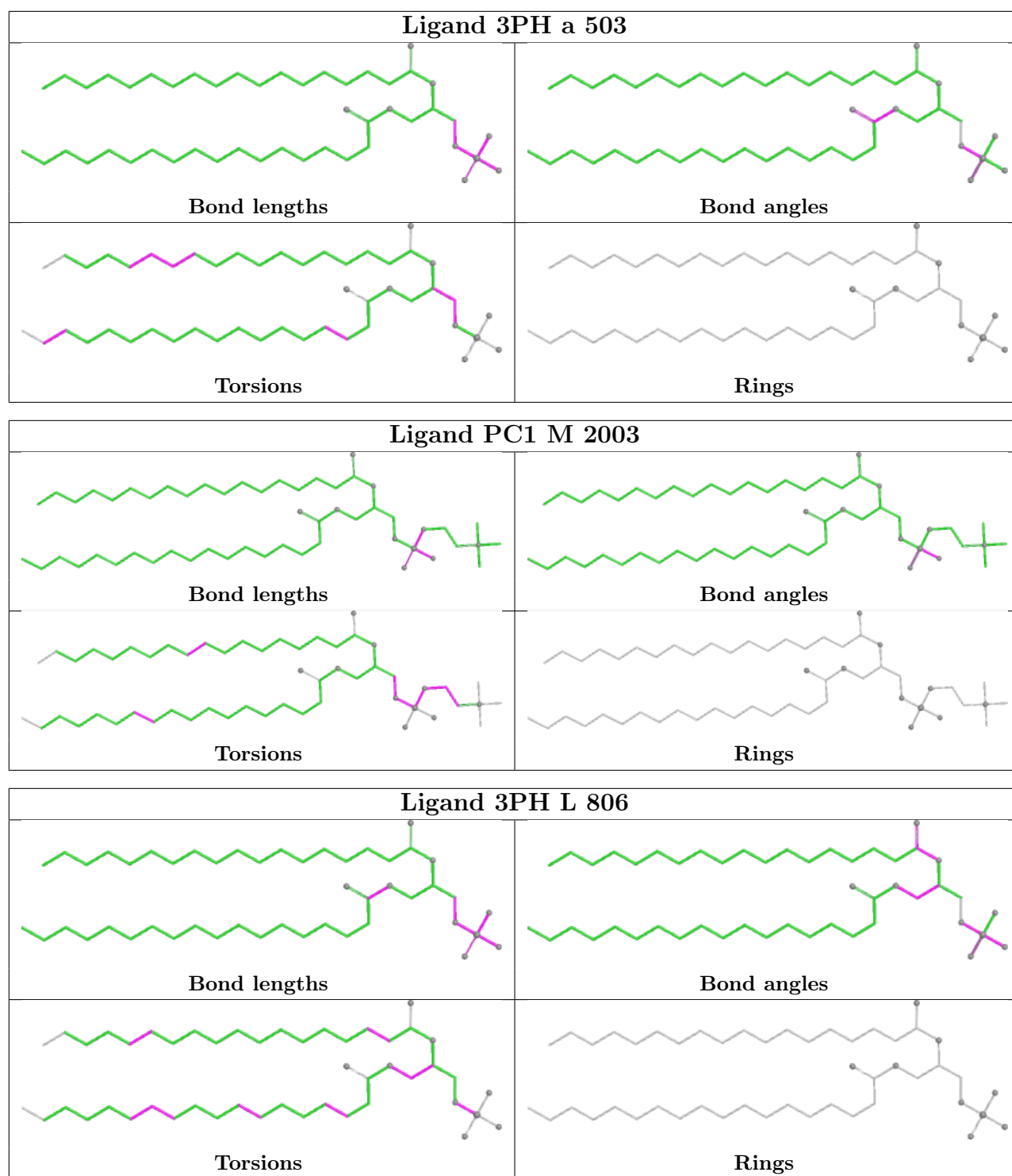
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	g	601	HEA	5	0

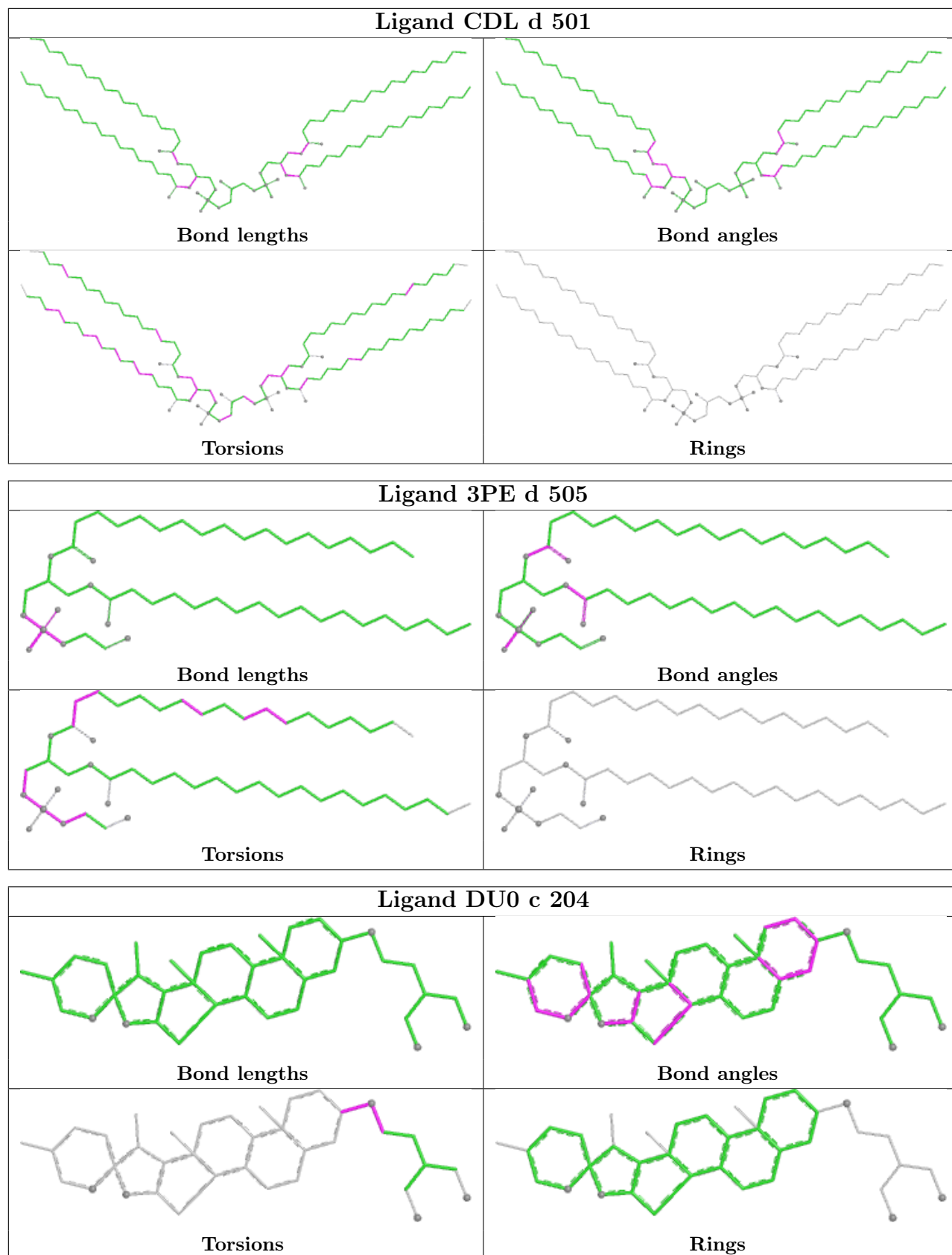
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

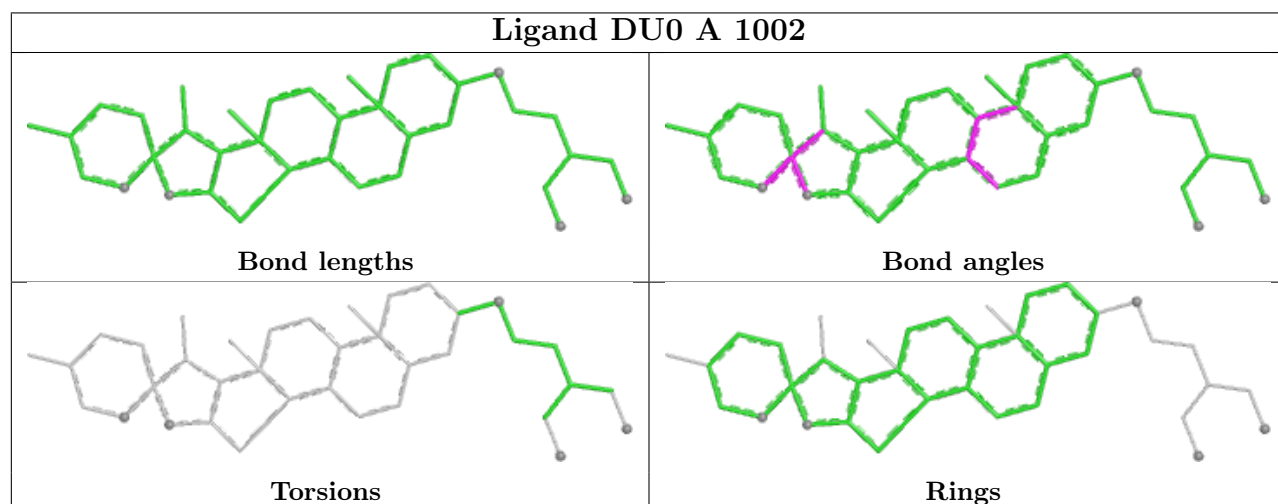
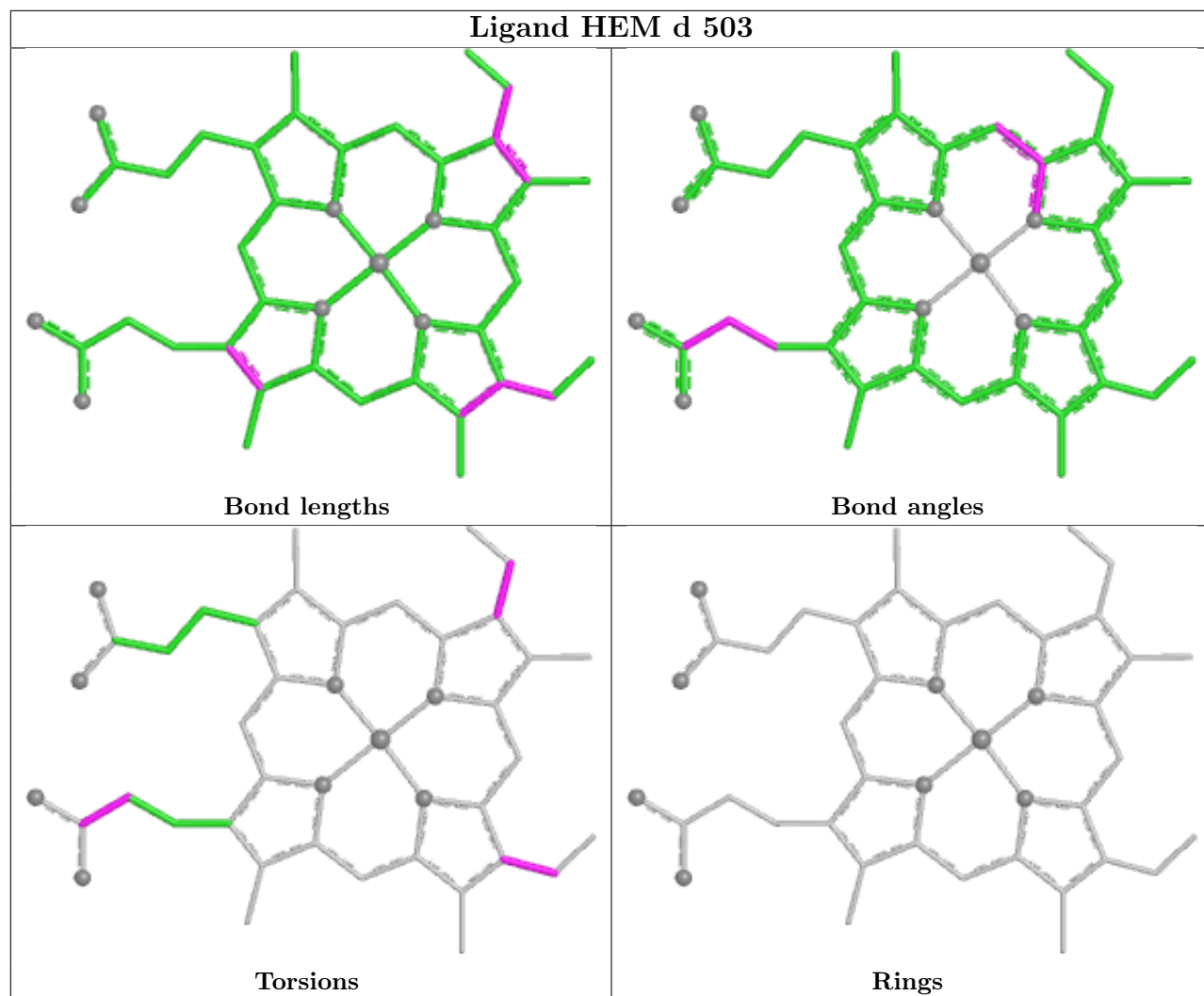


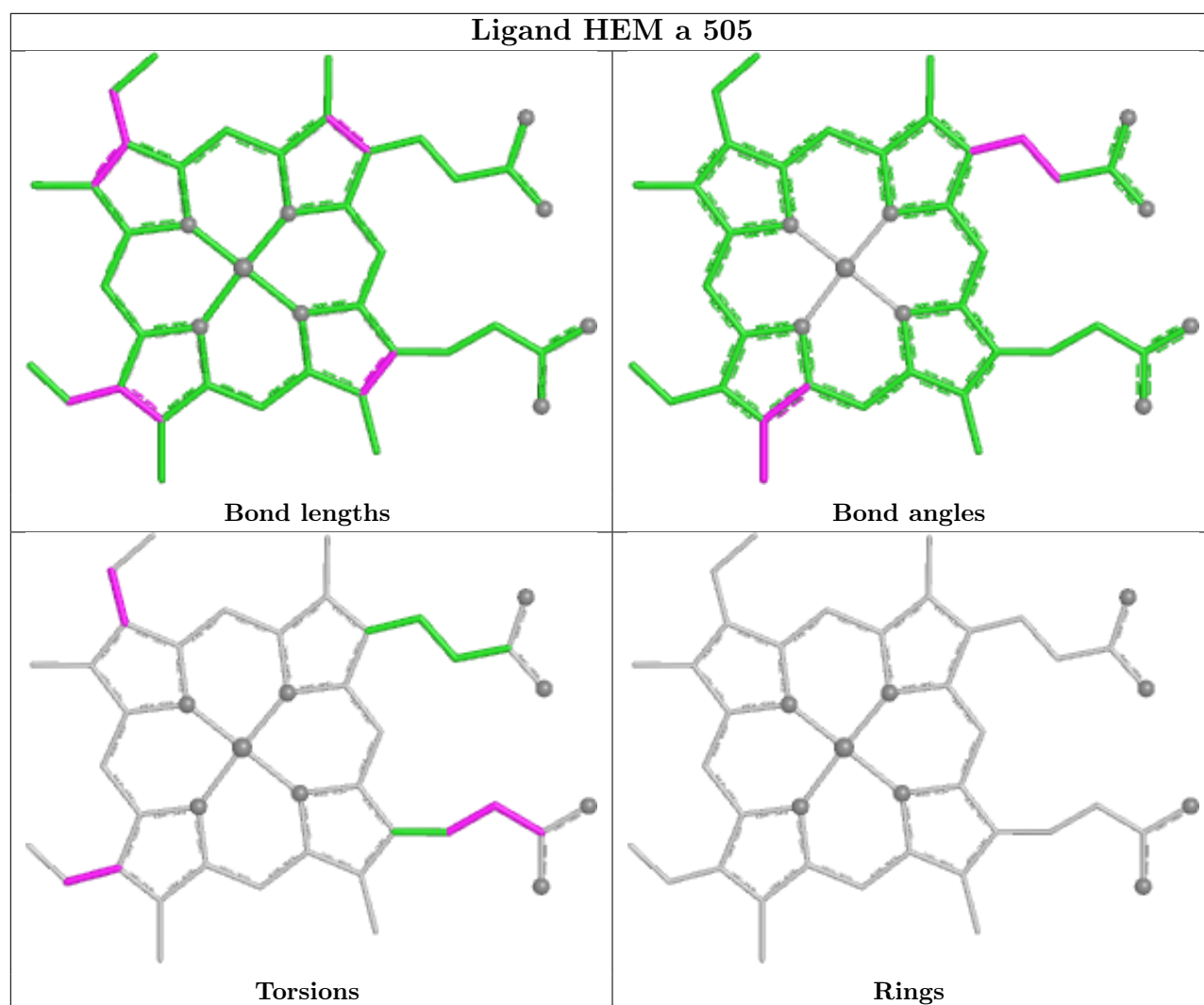
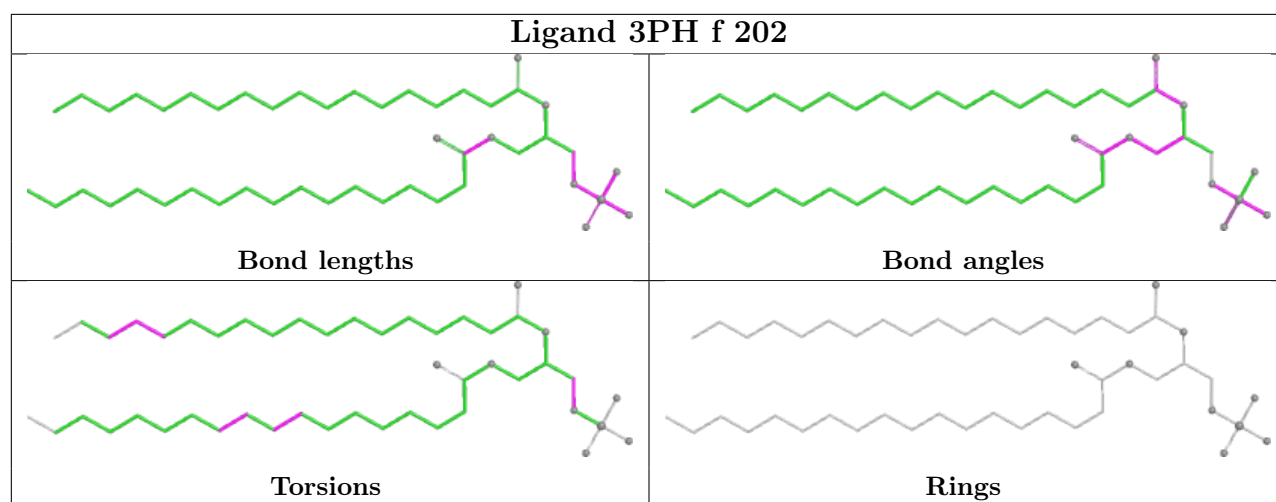


Ligand 3PE i 1004	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PC1 H 403	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PGT q 1000	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

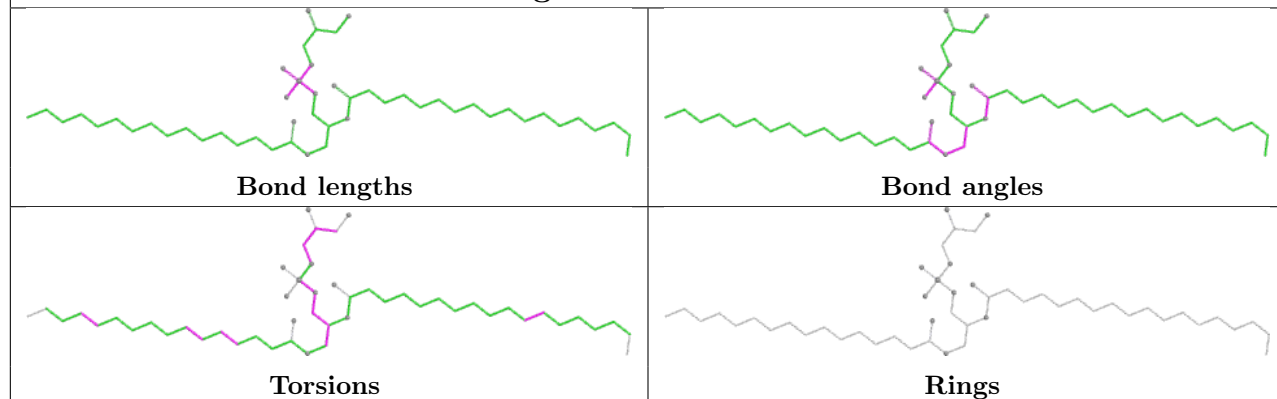




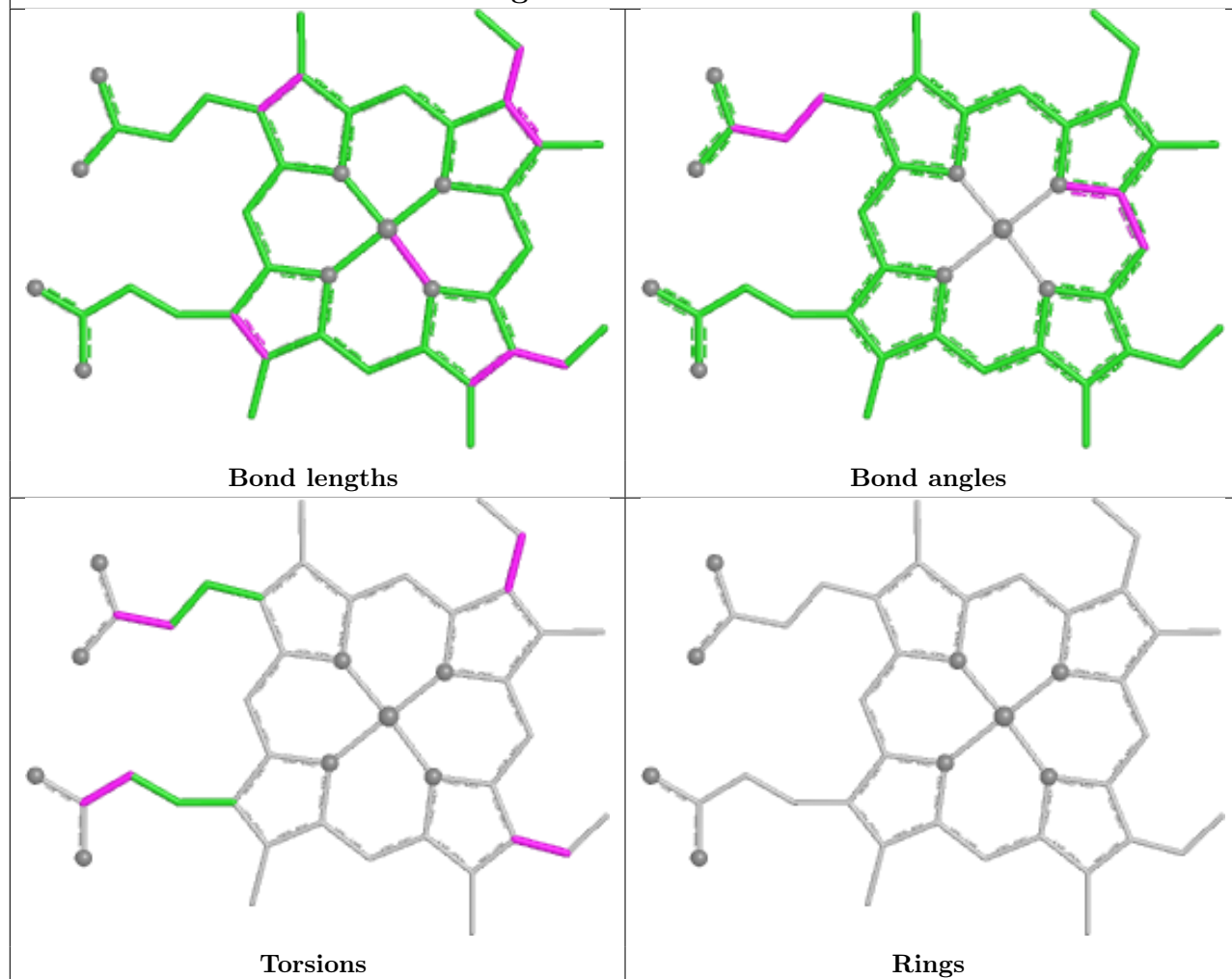


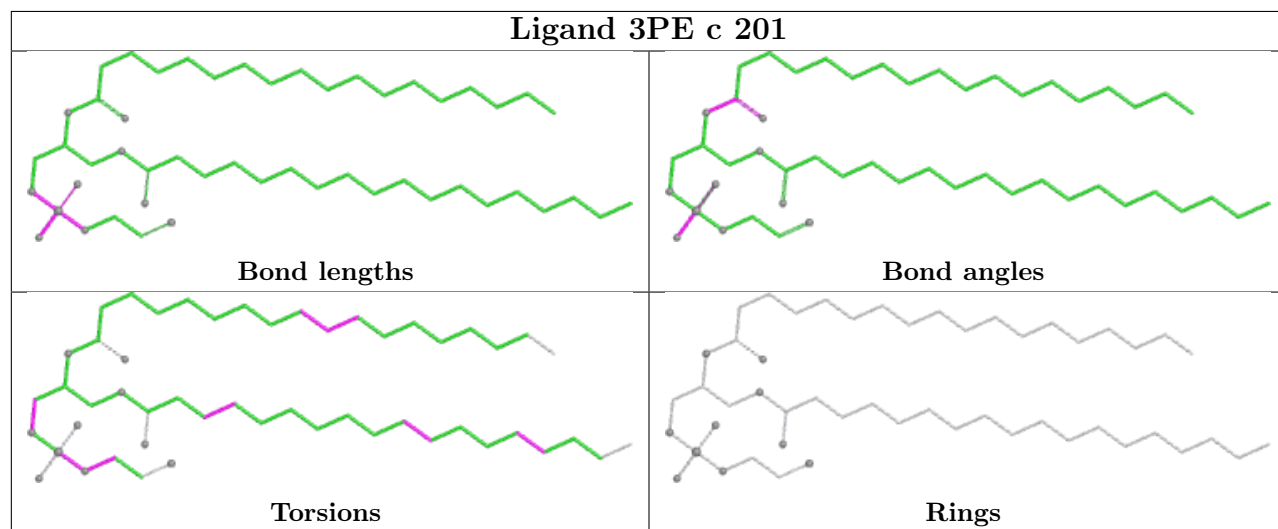
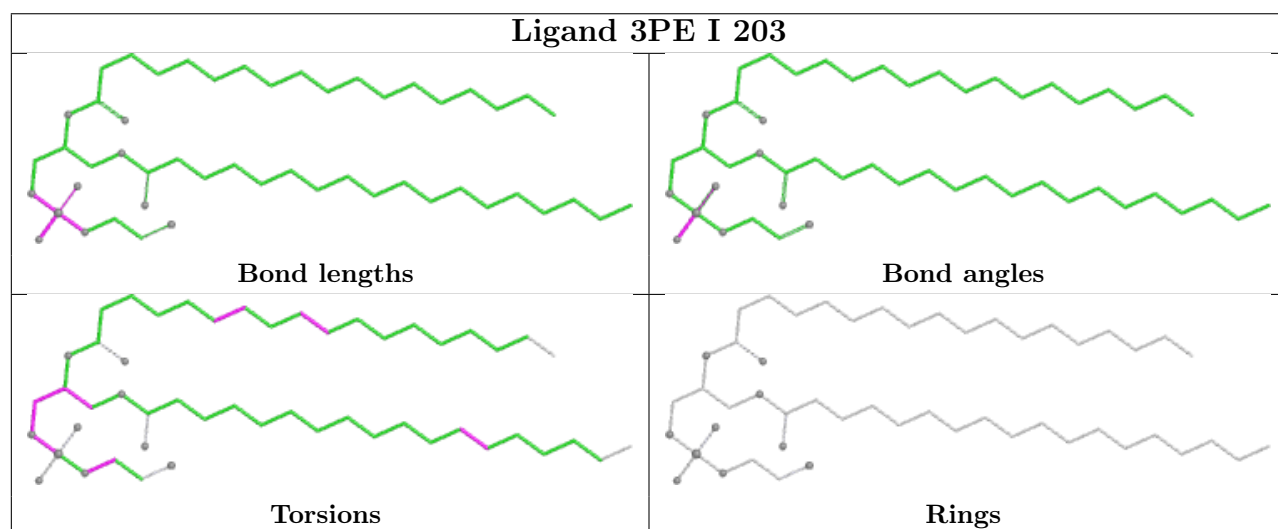
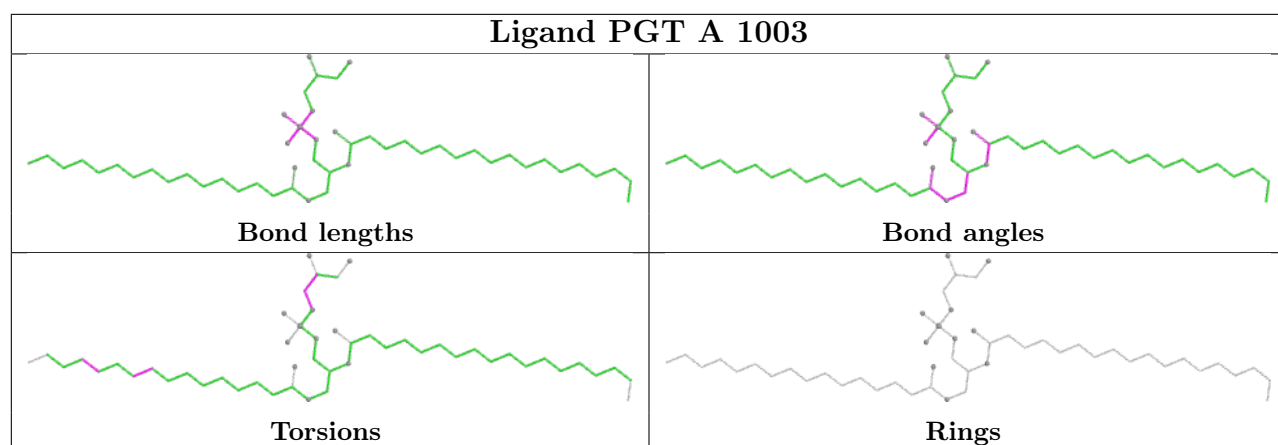


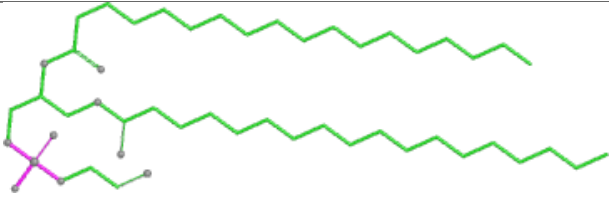
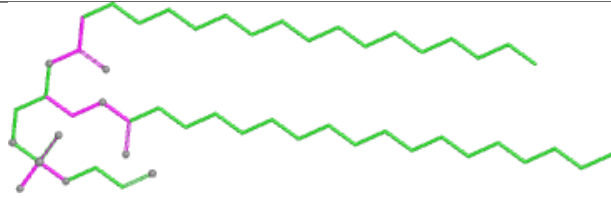
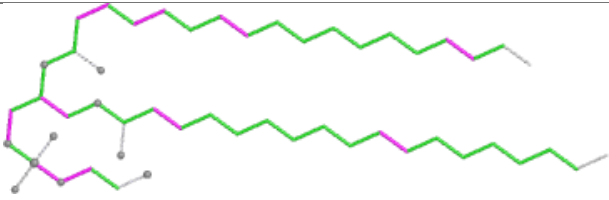
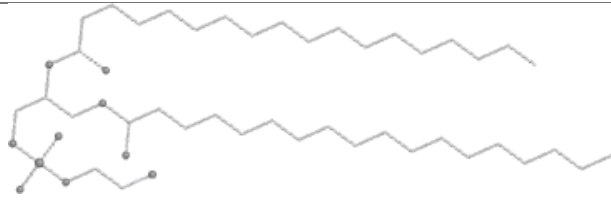
## Ligand PGT J 203

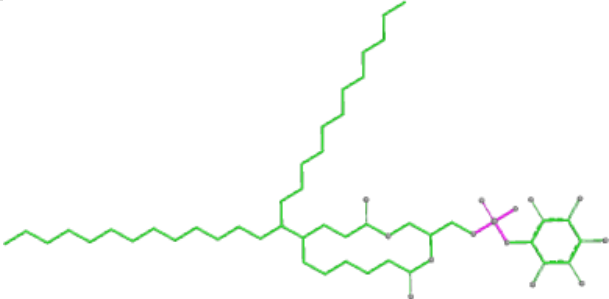
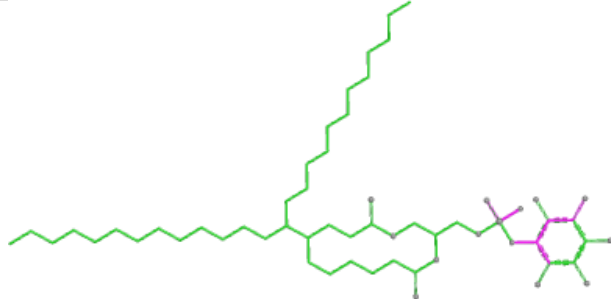
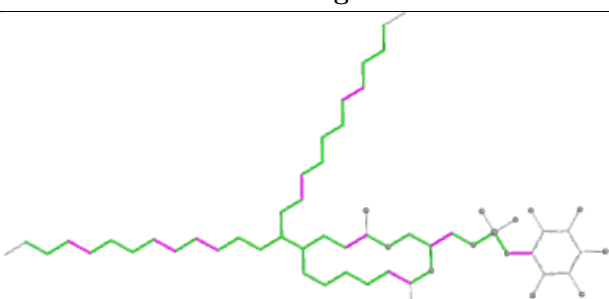
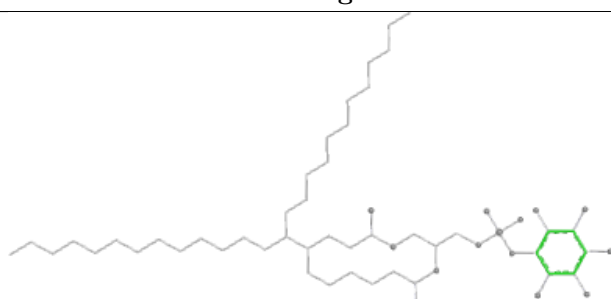


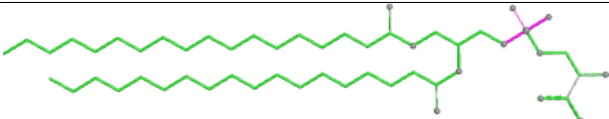
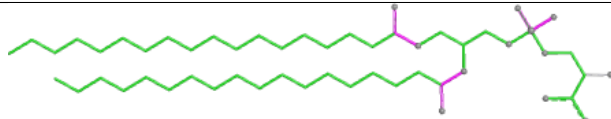
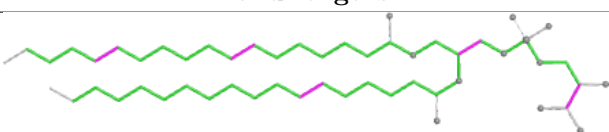
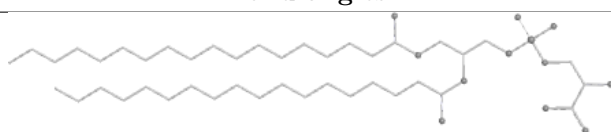
## Ligand HEM a 507



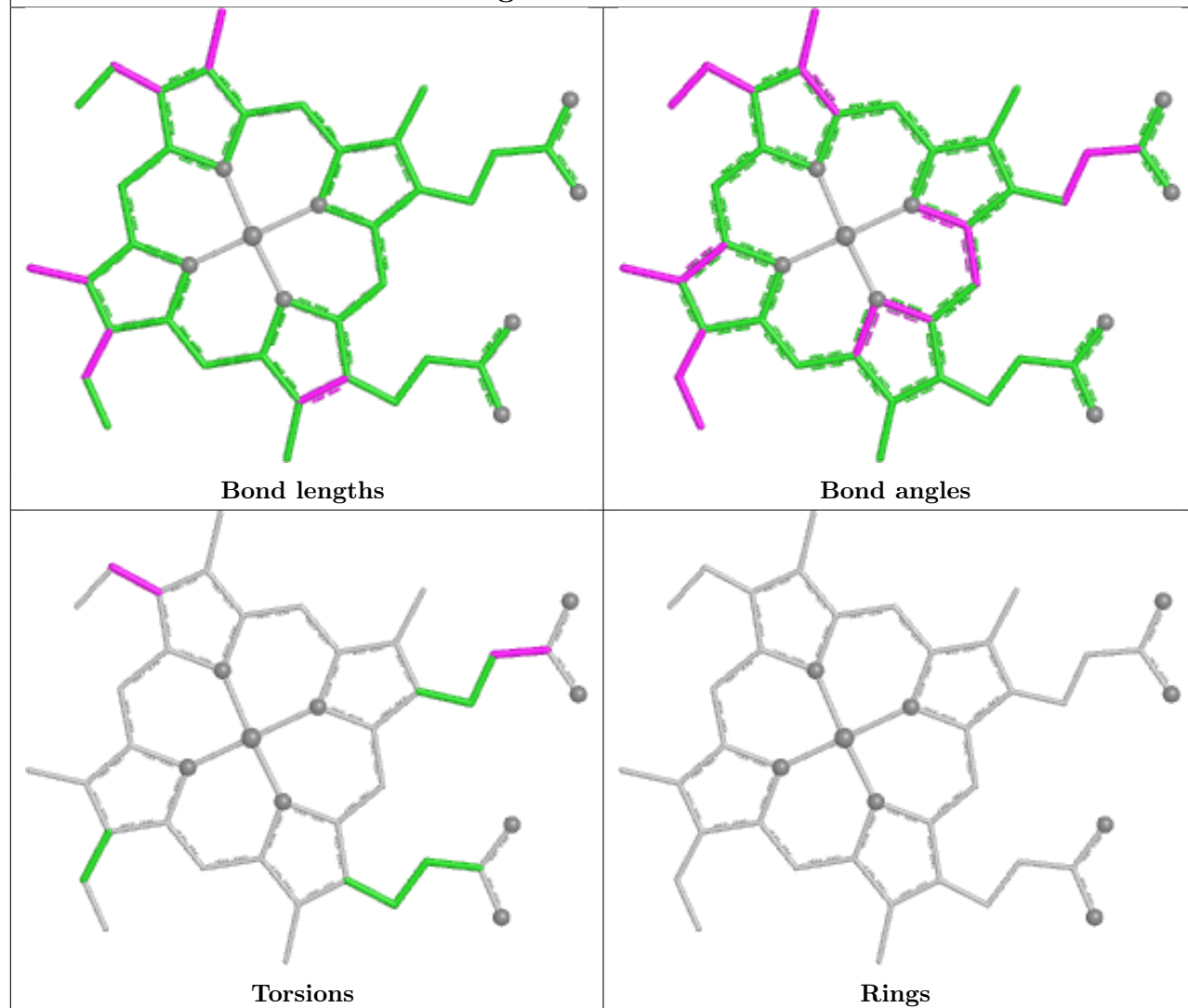


Ligand 3PE b 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

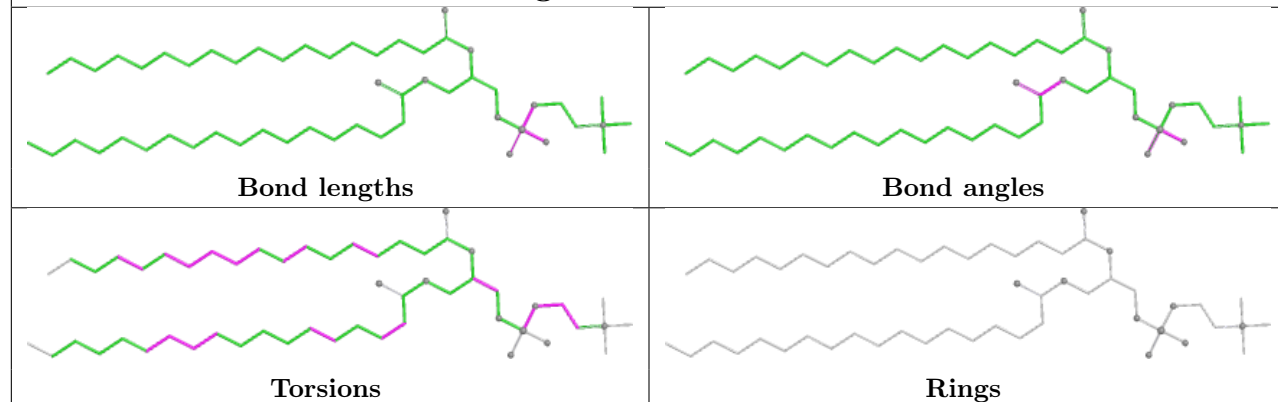
Ligand T7X J 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

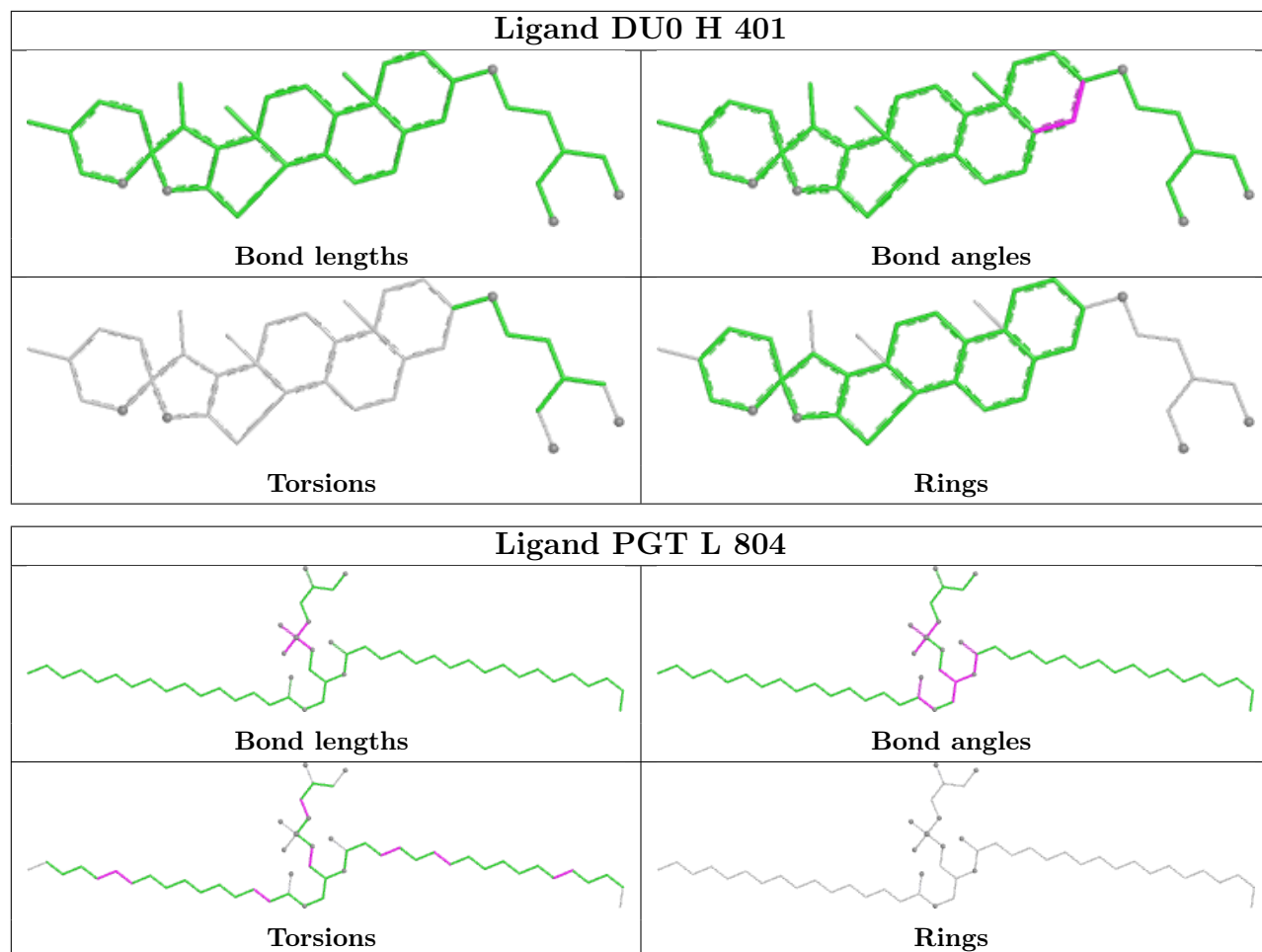
Ligand P5S L 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand HEC e 502

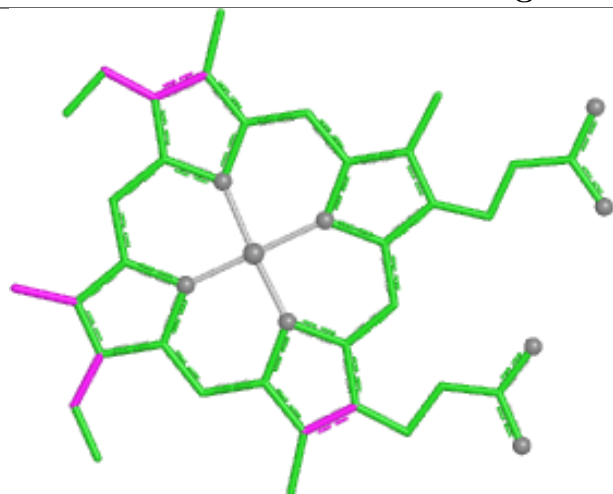


## Ligand PC1 D 502

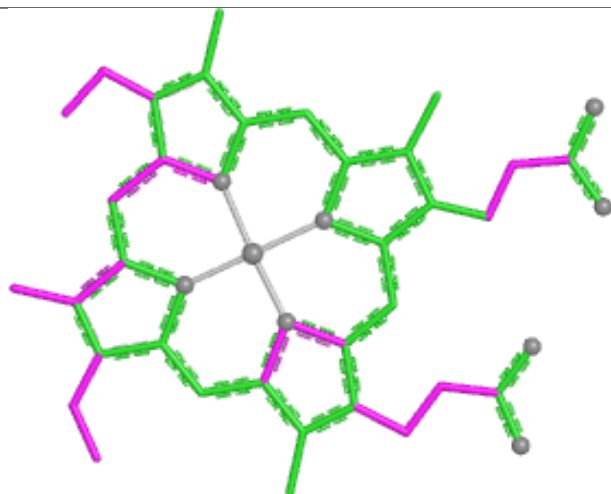




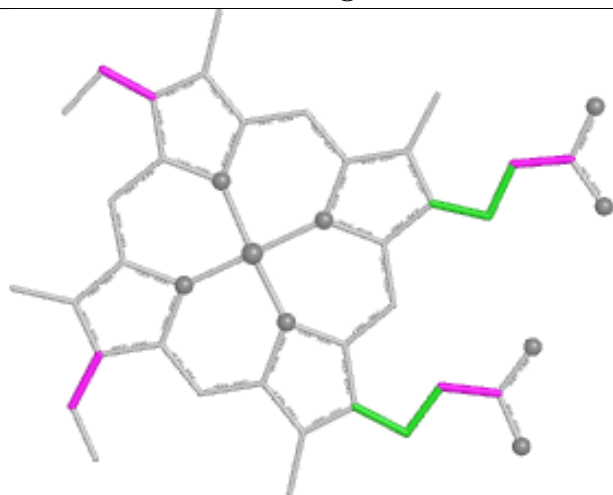
## Ligand HEC b 502



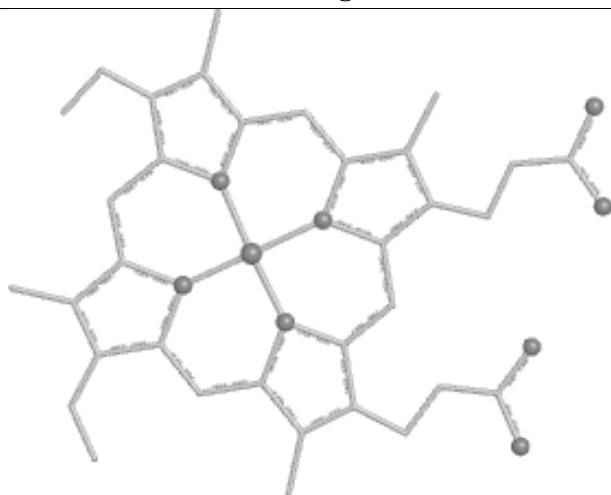
Bond lengths



Bond angles

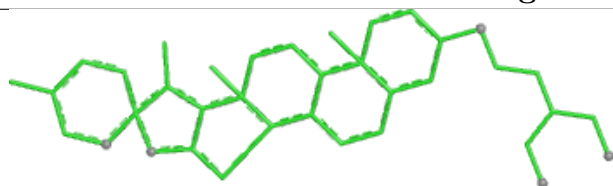


Torsions

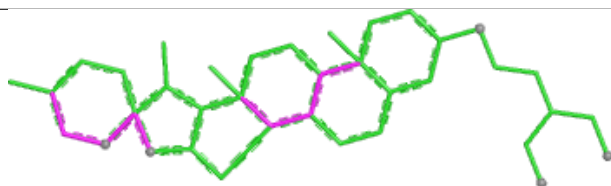


Rings

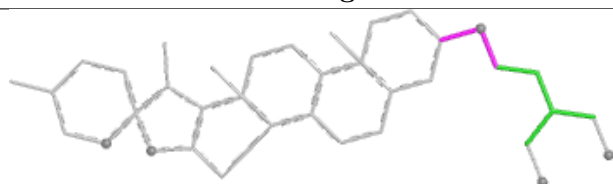
## Ligand DU0 J 204



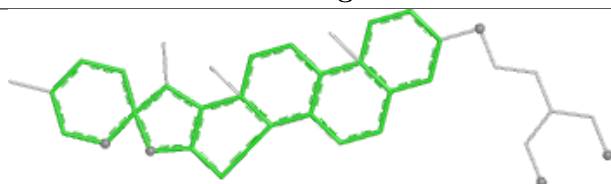
Bond lengths



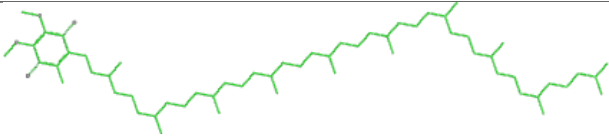
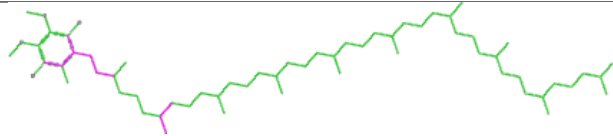
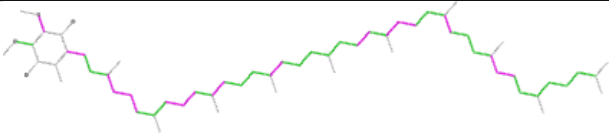

Bond angles

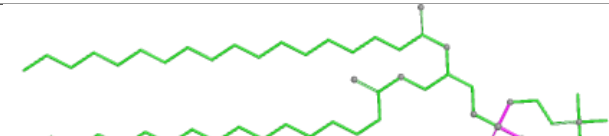
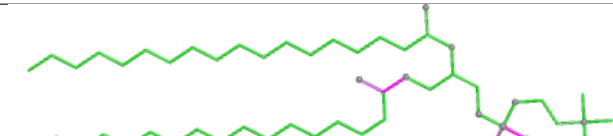
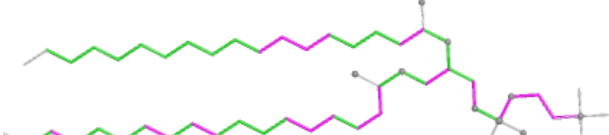
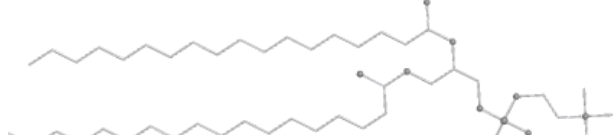


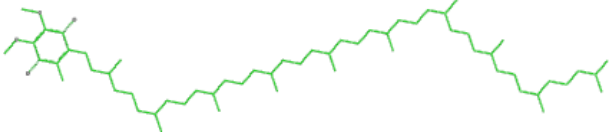

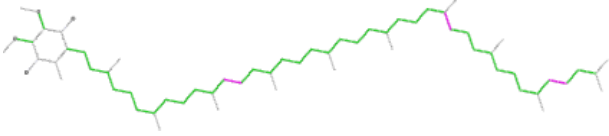

Torsions

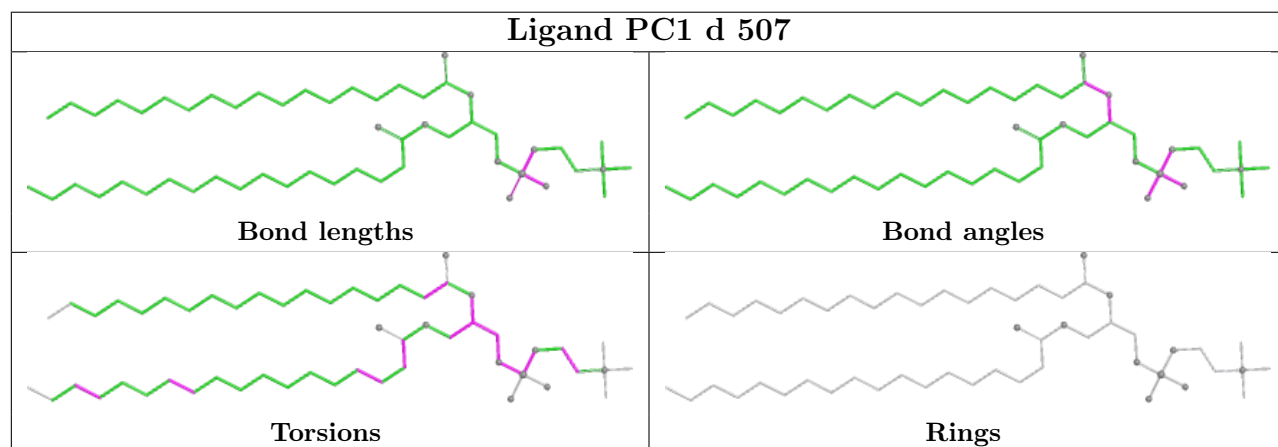
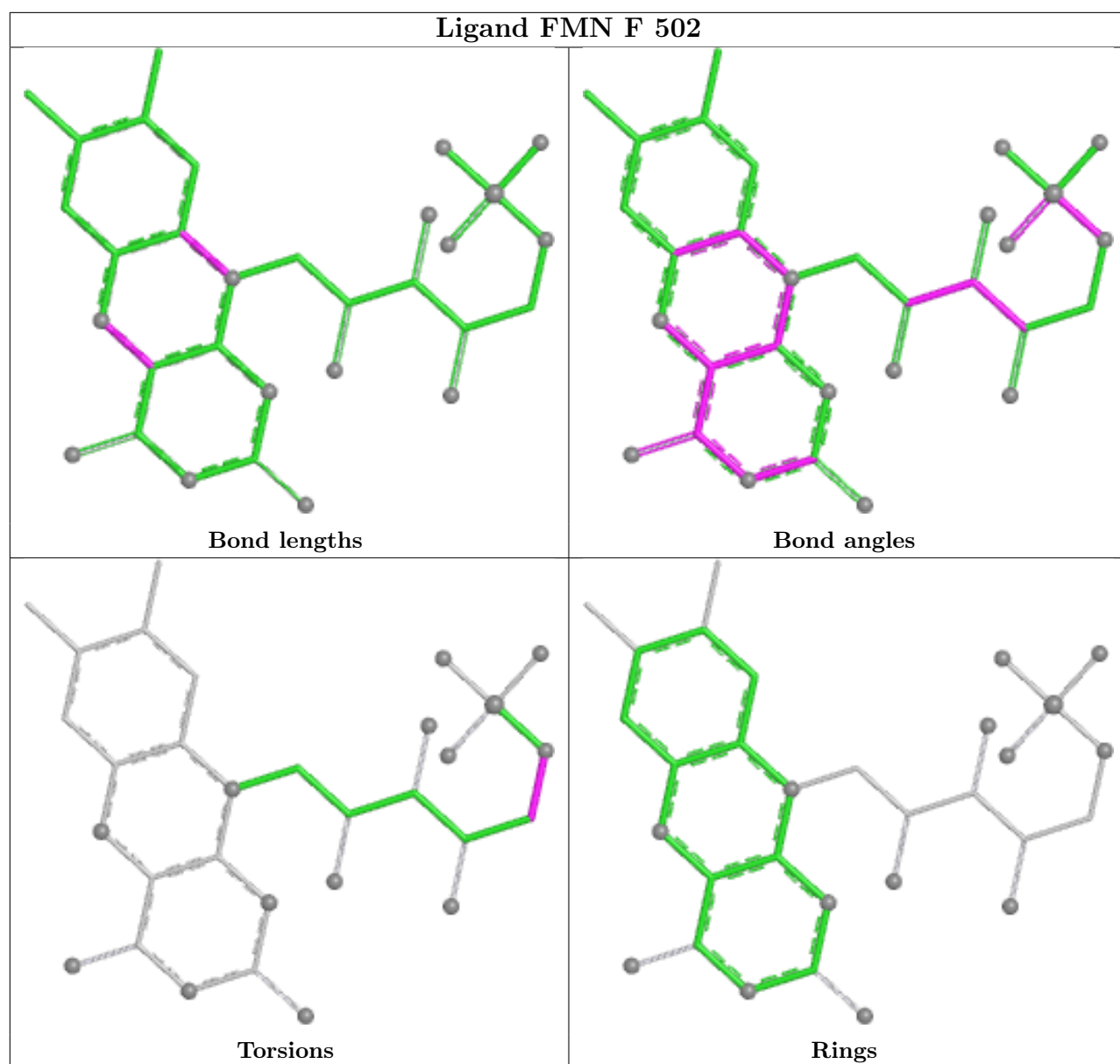


Rings

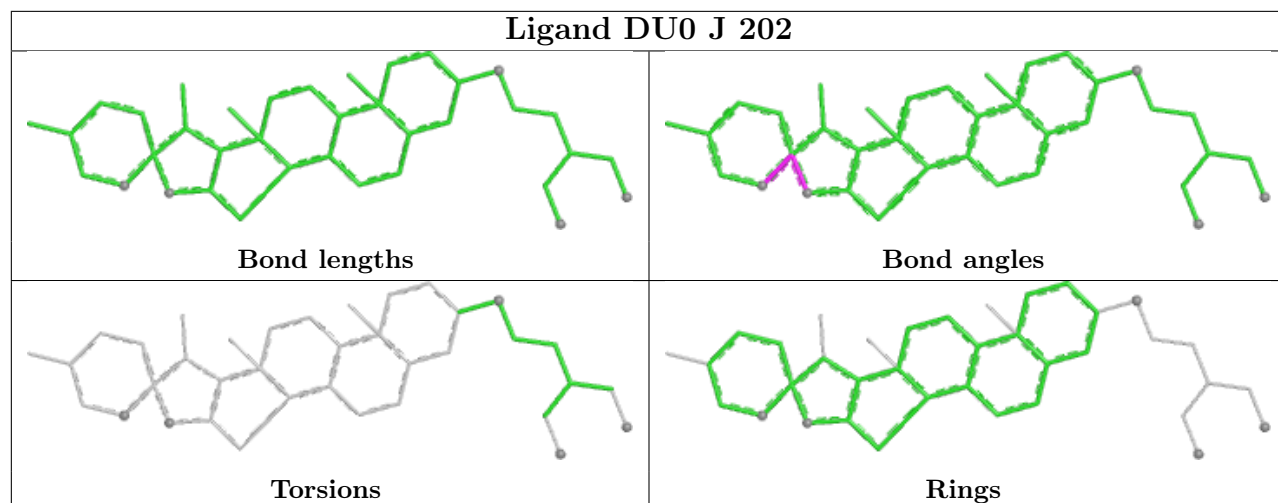
Ligand U10 B 1002	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand PC1 a 504	
	Bond lengths
	Bond angles
	Torsions
	Rings

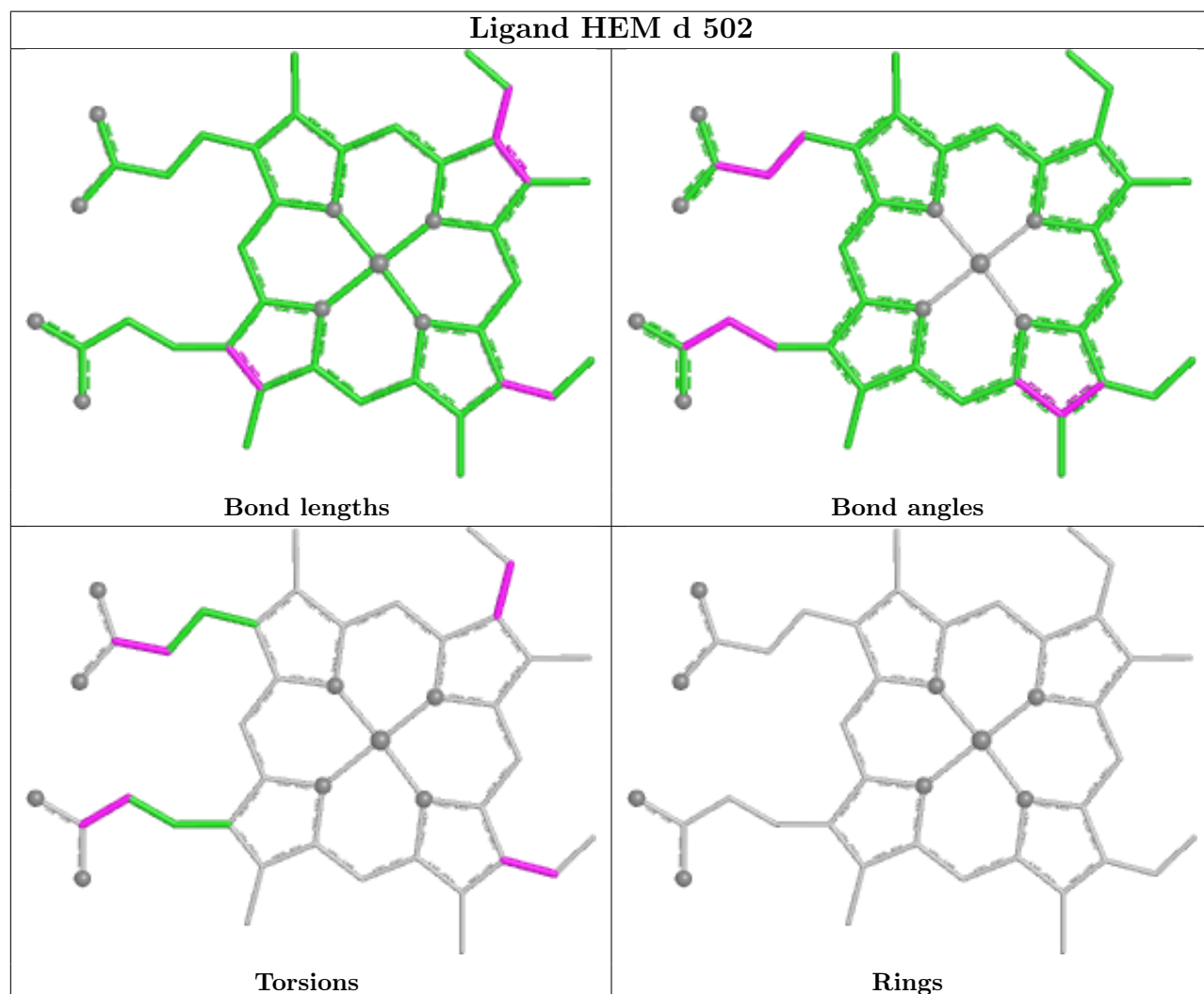
Ligand U10 d 504	
	Bond lengths
	Bond angles
	Torsions
	Rings

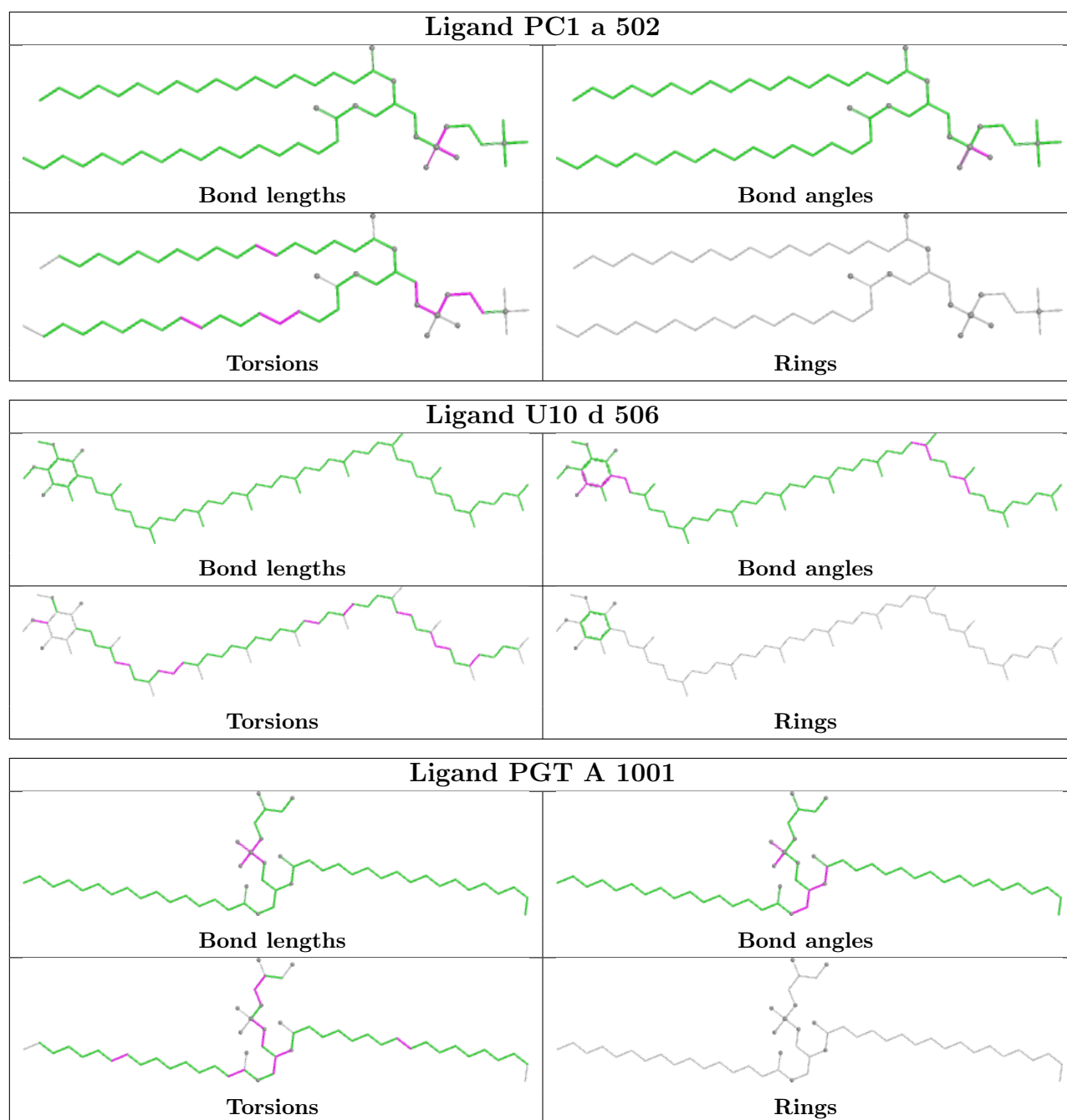


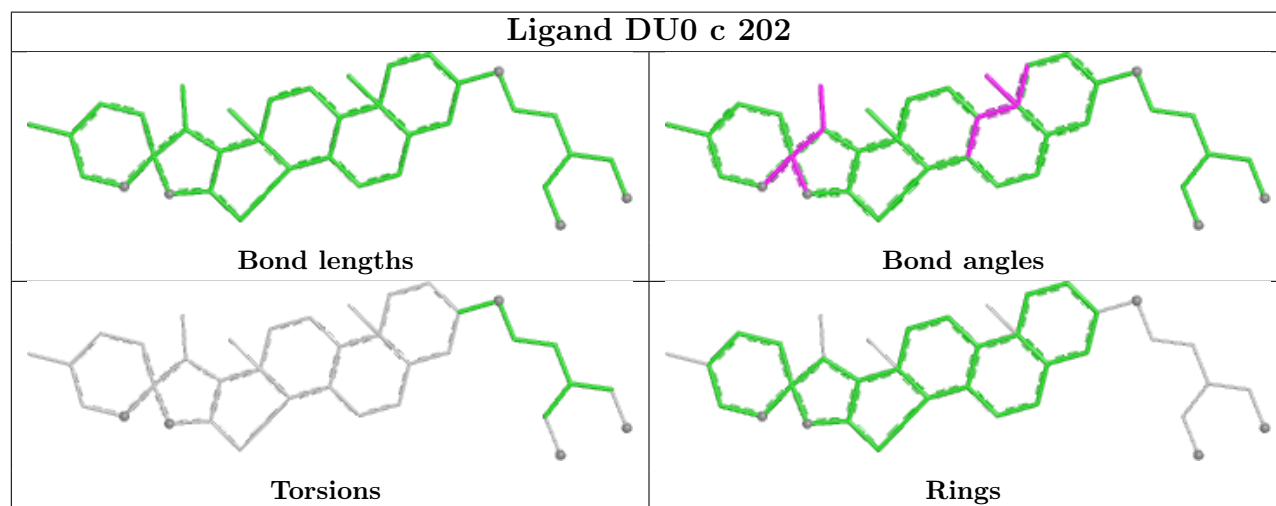
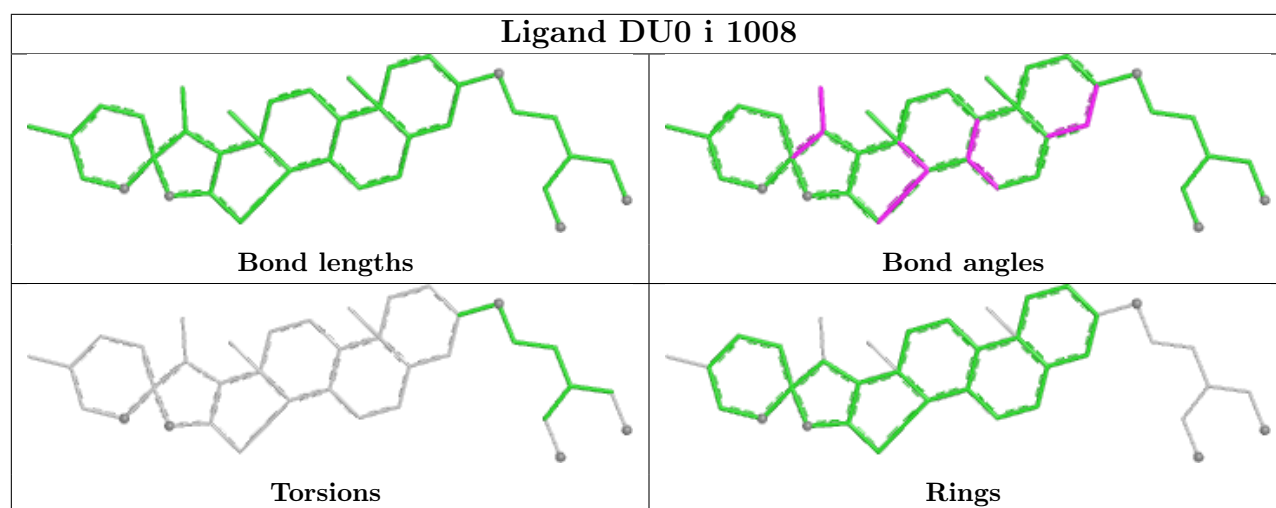
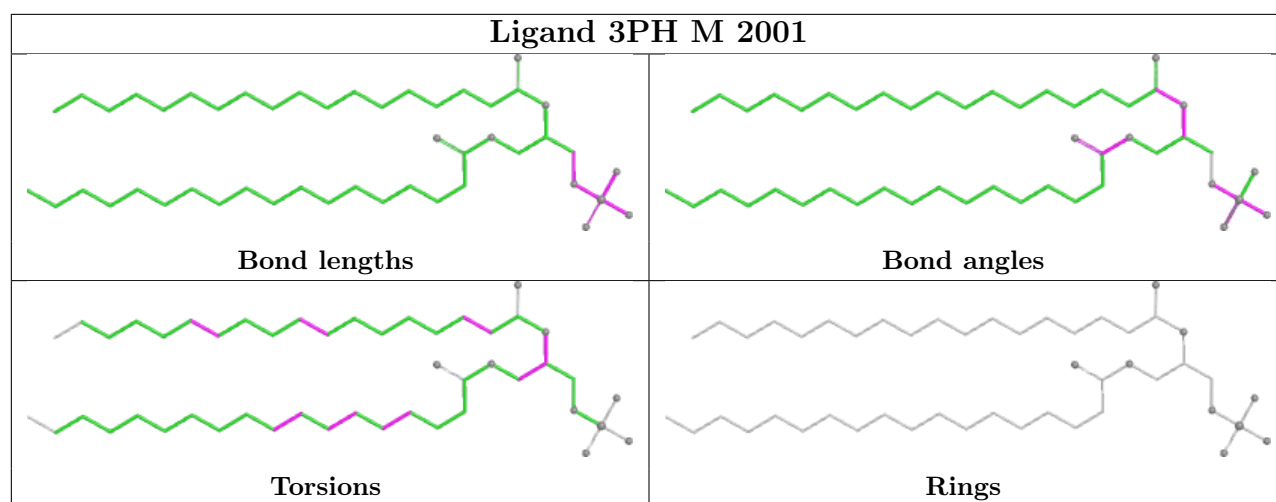
## Ligand DU0 J 202

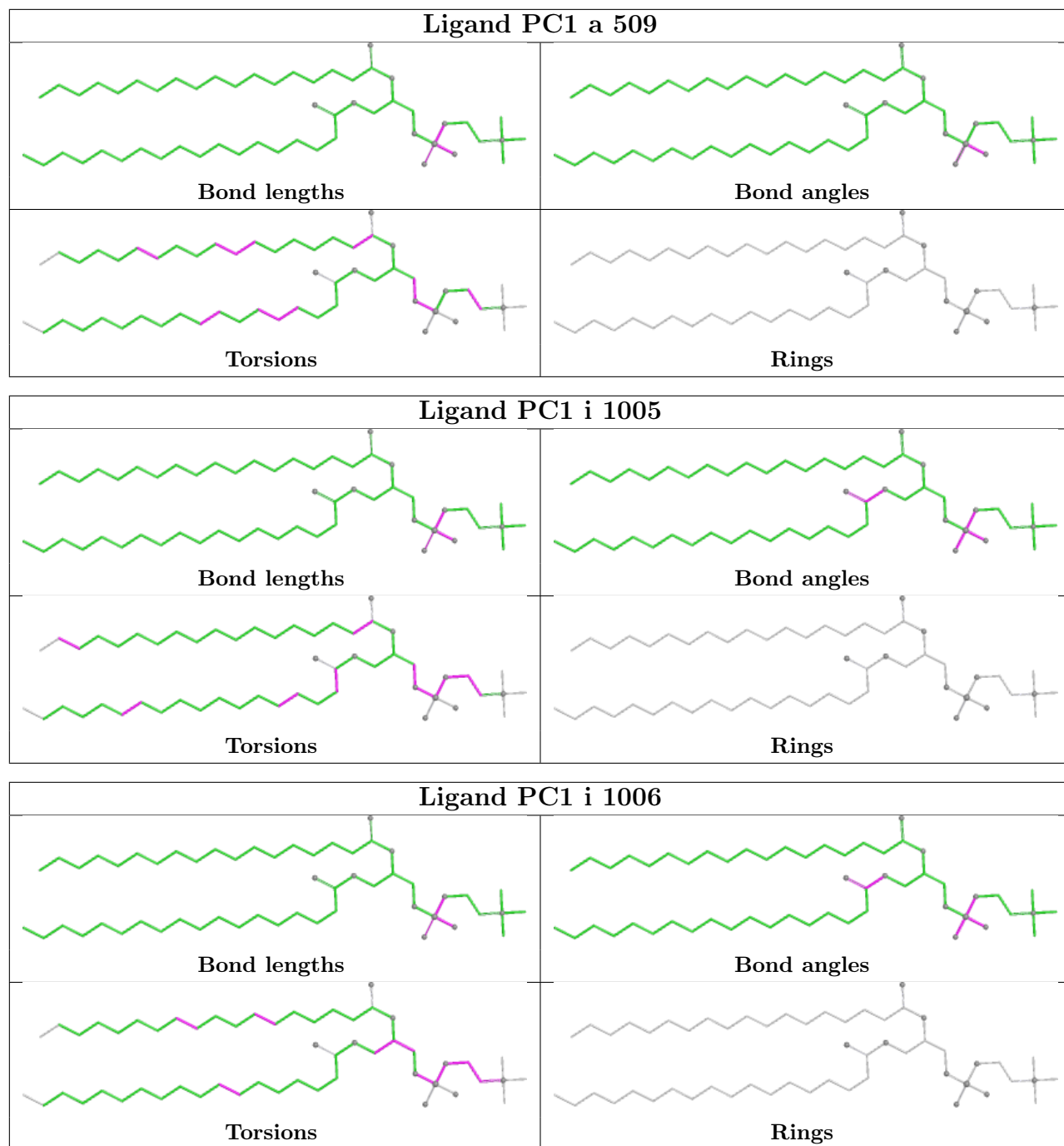


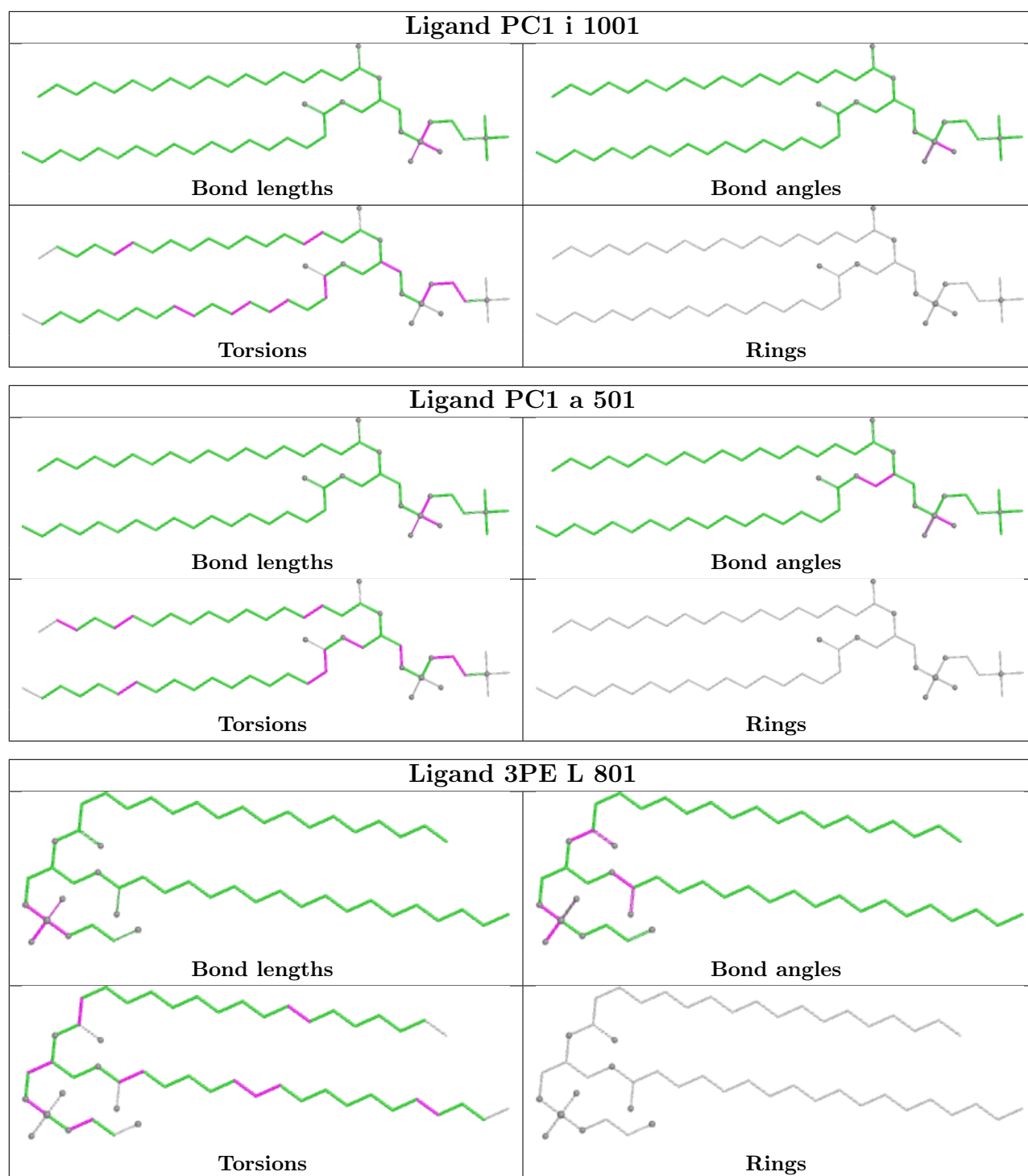
## Ligand HEM d 502

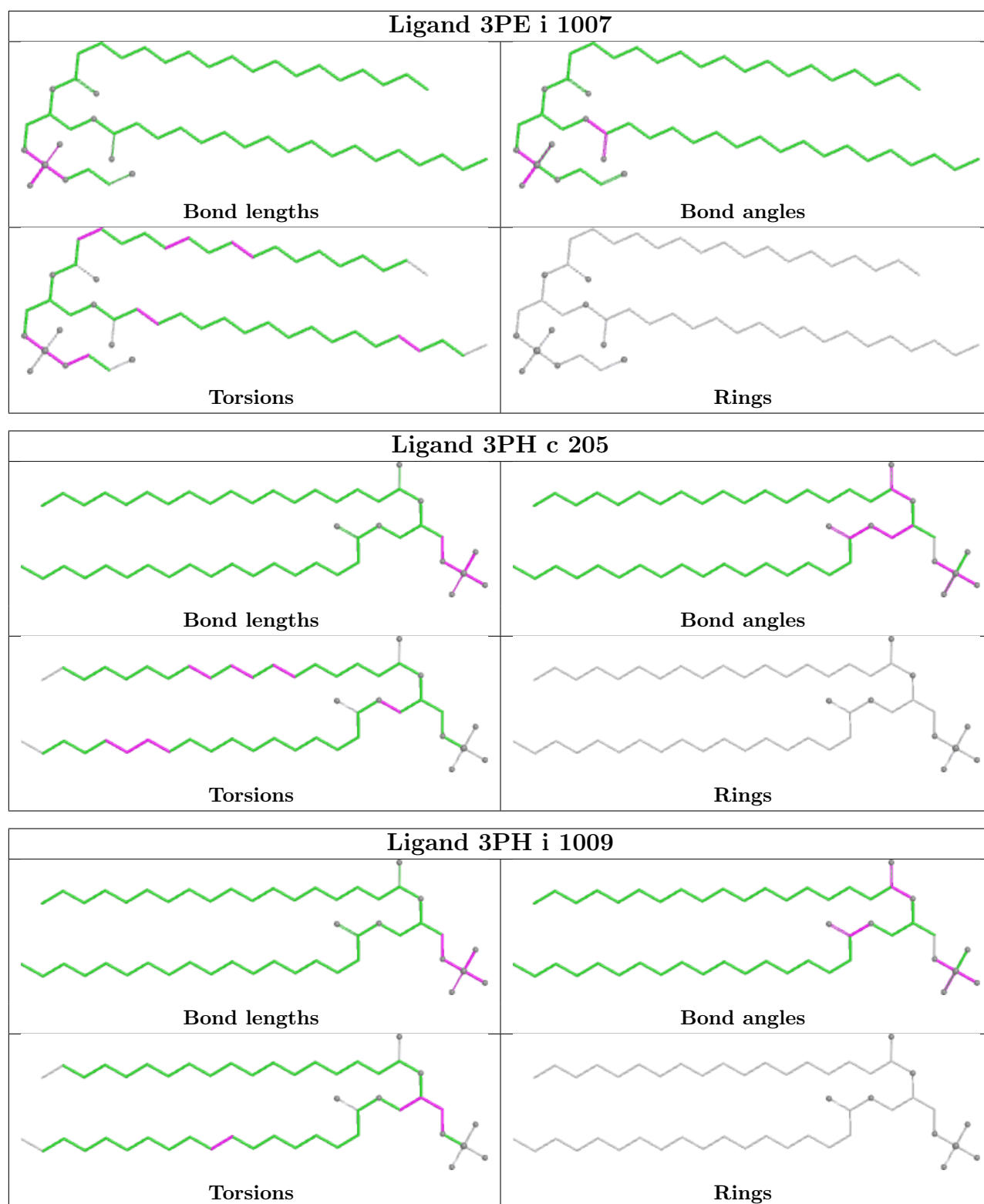


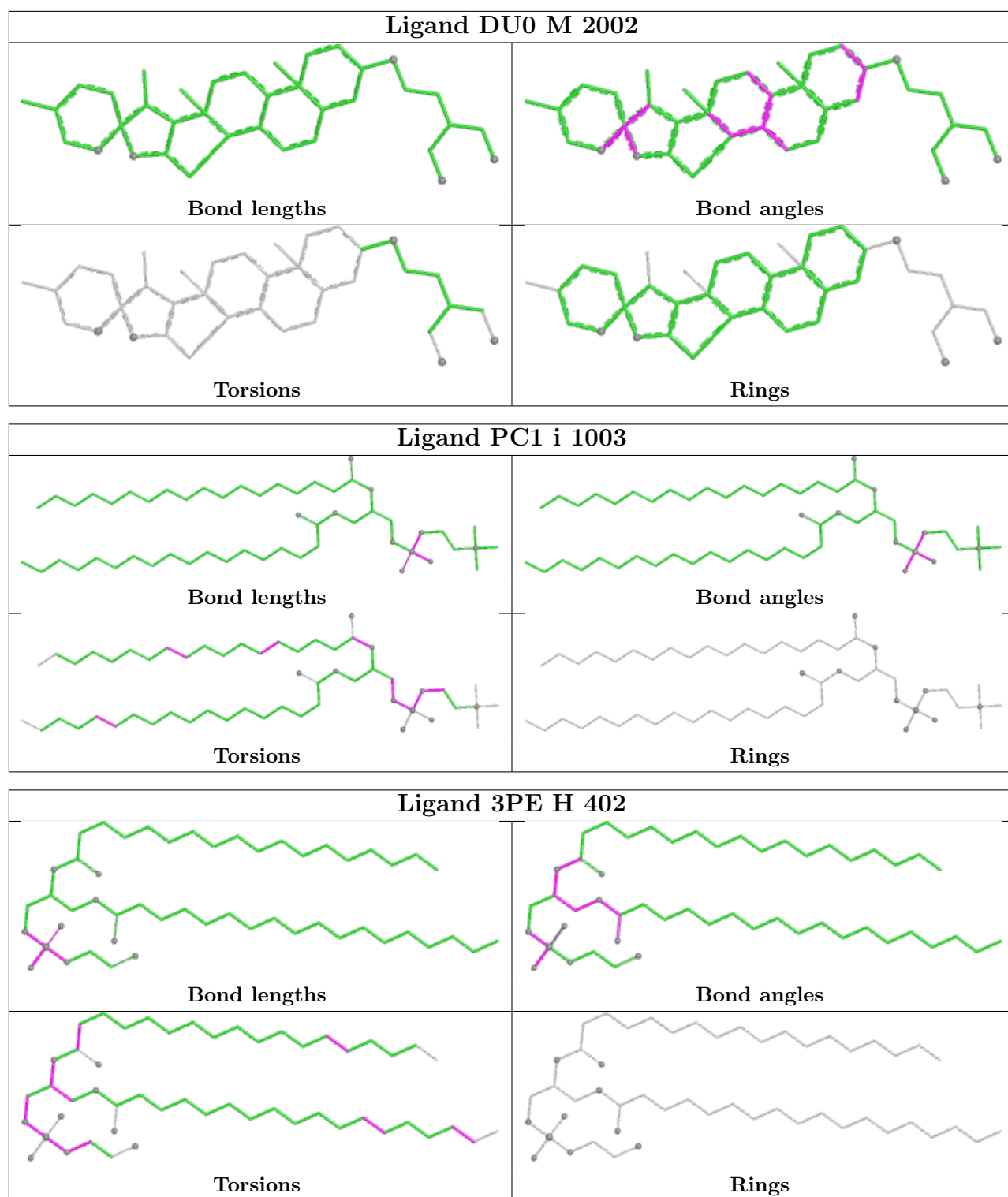


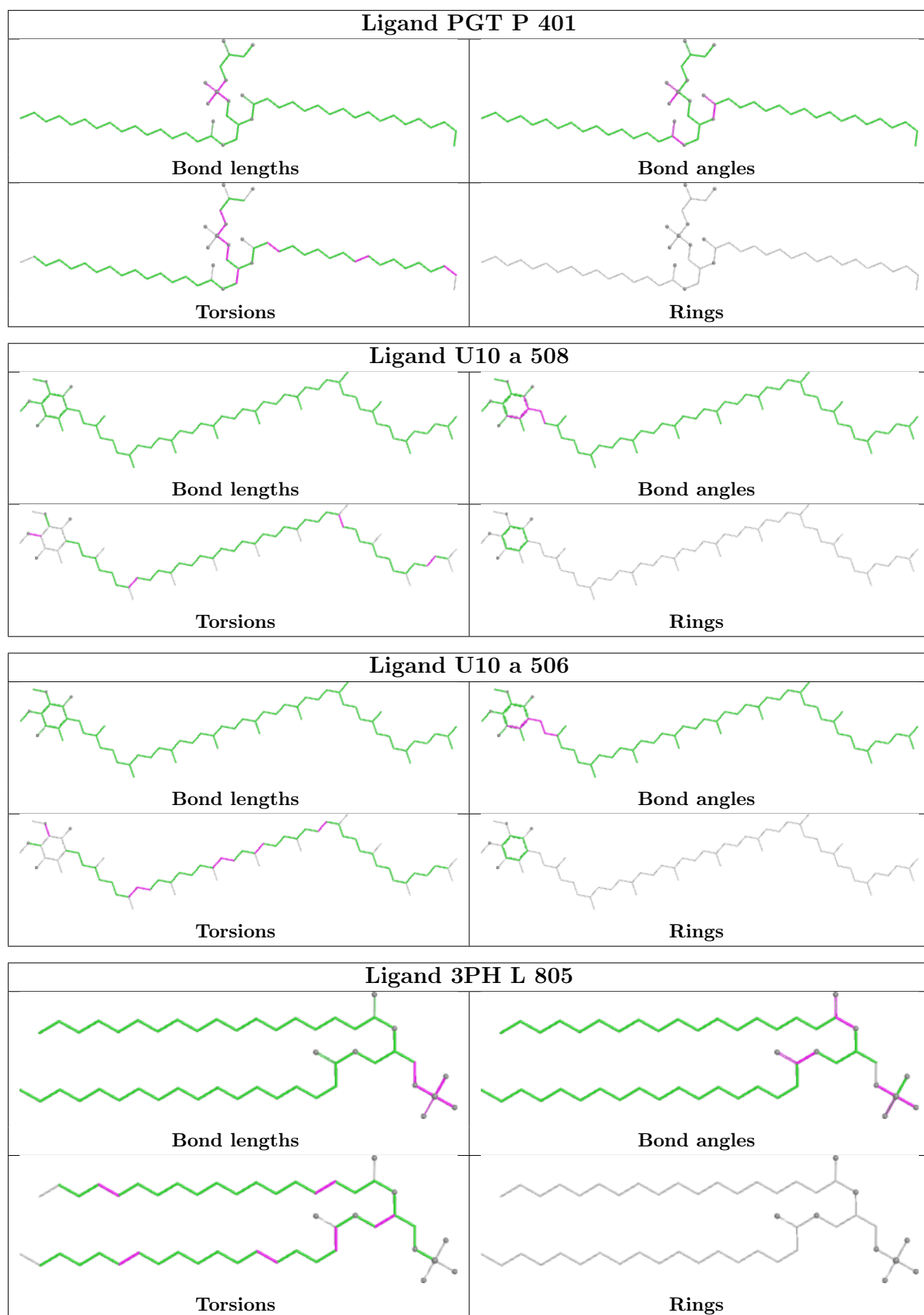


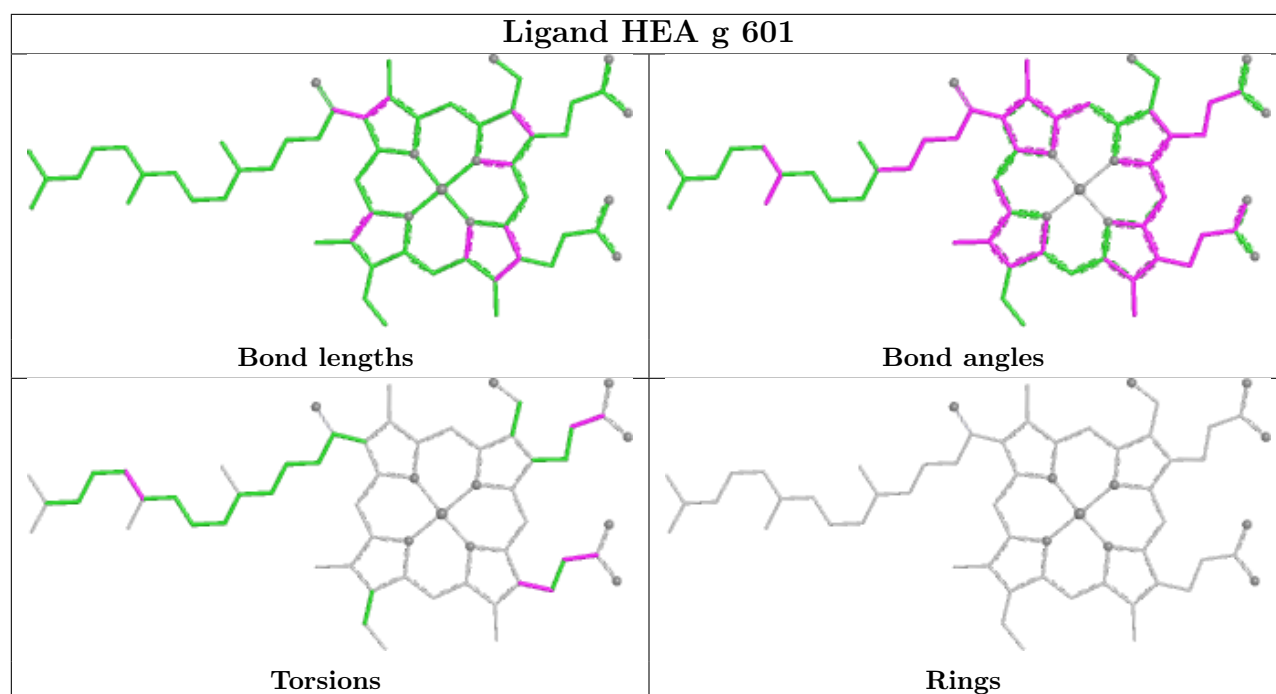












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

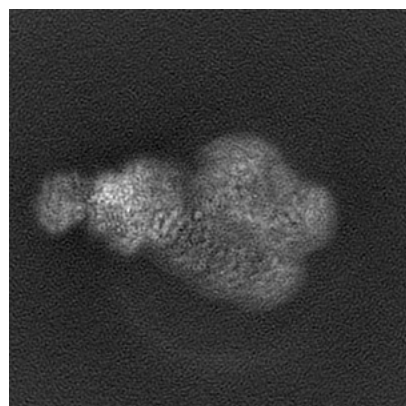
## 6 Map visualisation [i](#)

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.

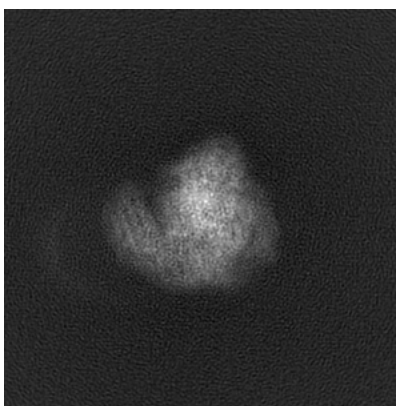
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

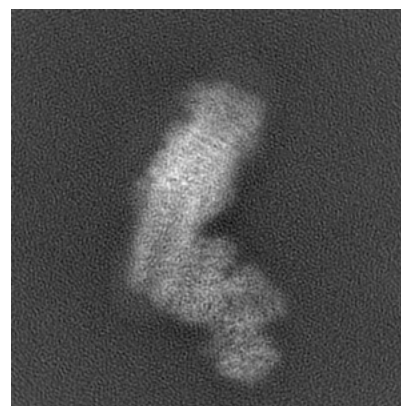
#### 6.1.1 Primary map



X

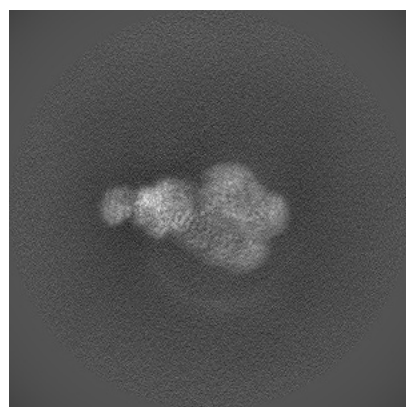


Y

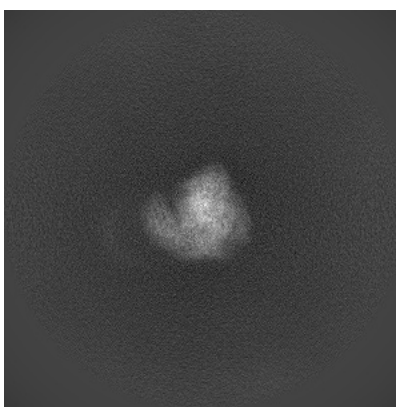


Z

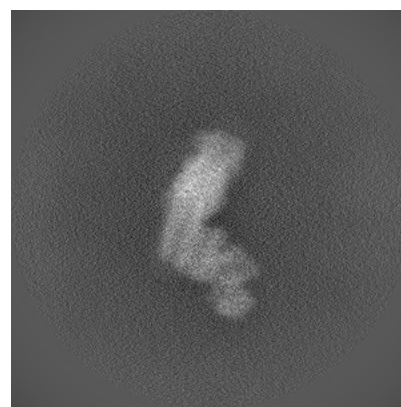
#### 6.1.2 Raw map



X



Y

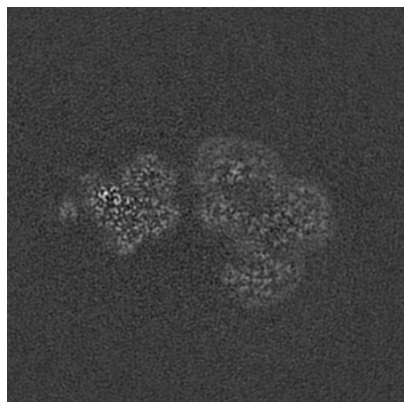


Z

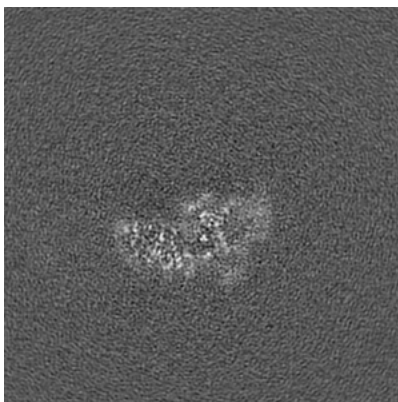
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

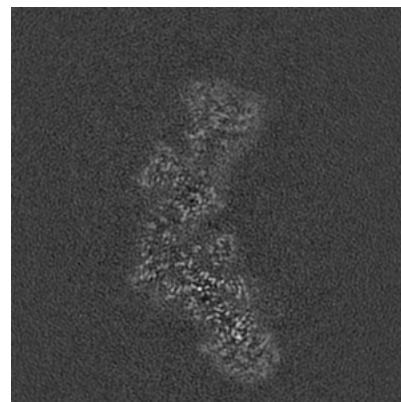
### 6.2.1 Primary map



X Index: 187

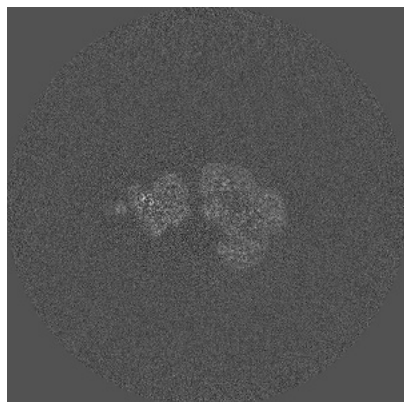


Y Index: 187

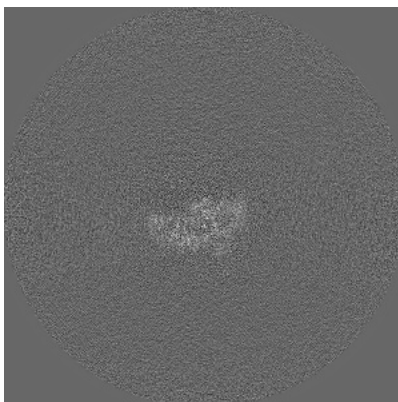


Z Index: 187

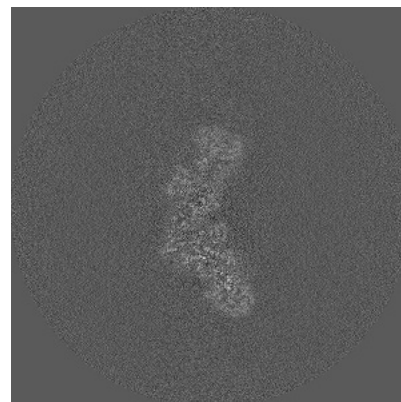
### 6.2.2 Raw map



X Index: 300



Y Index: 300

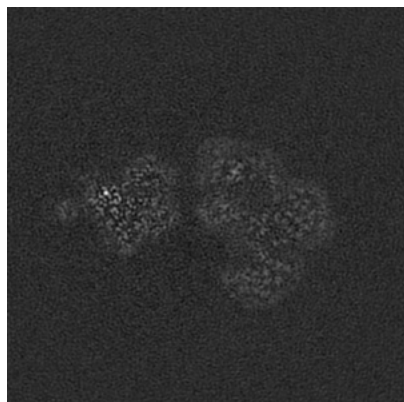


Z Index: 300

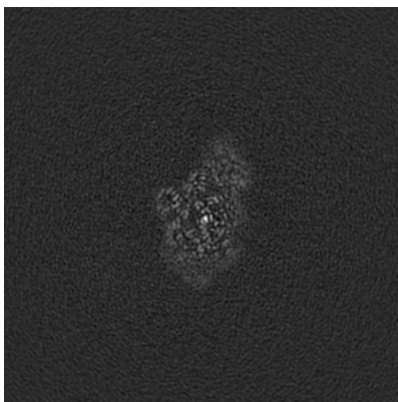
The images above show central slices of the map in three orthogonal directions.

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

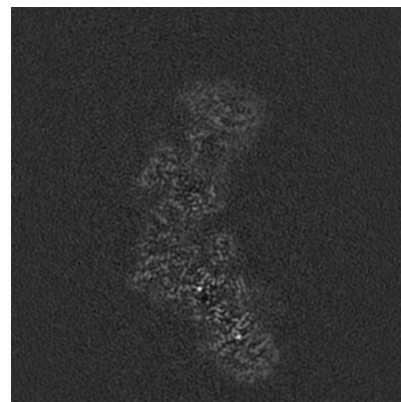
### 6.3.1 Primary map



X Index: 188

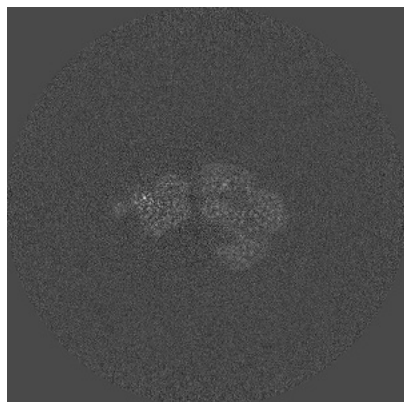


Y Index: 111

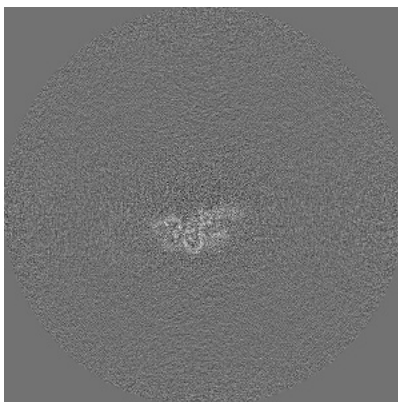


Z Index: 188

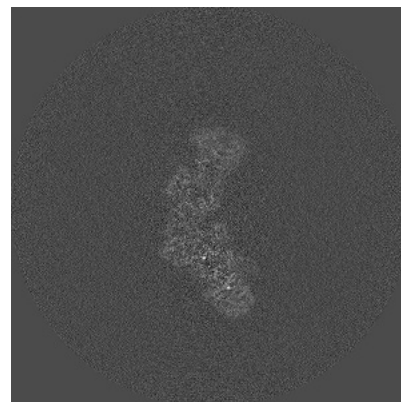
### 6.3.2 Raw map



X Index: 301



Y Index: 289

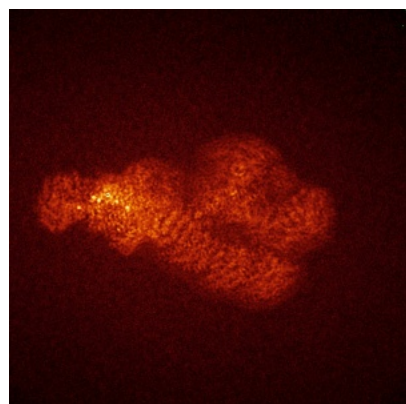


Z Index: 301

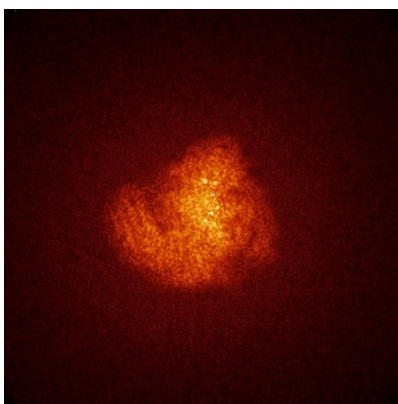
The images above show the largest variance slices of the map in three orthogonal directions.

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

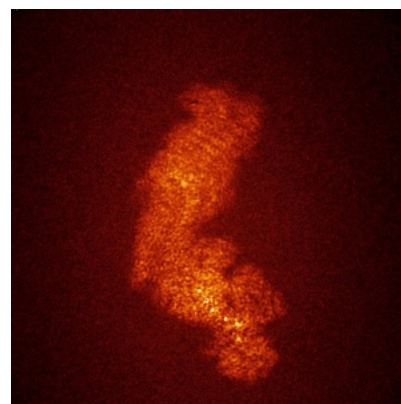
### 6.4.1 Primary map



X

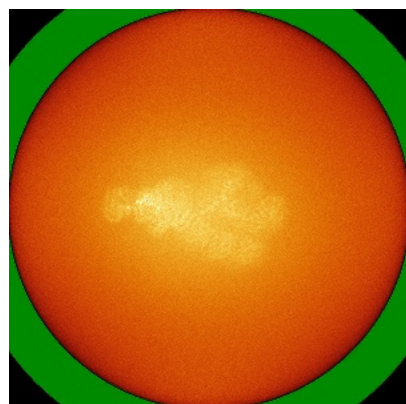


Y

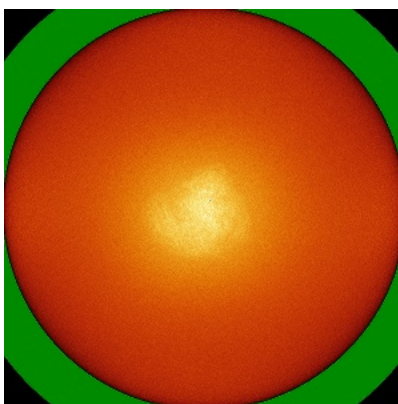


Z

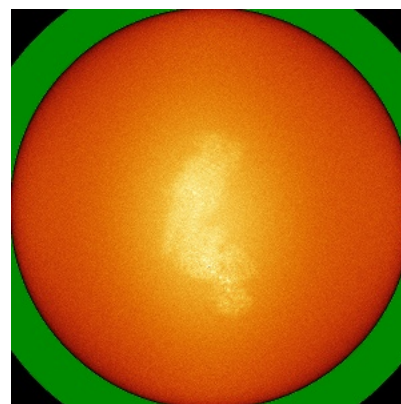
### 6.4.2 Raw map



X



Y

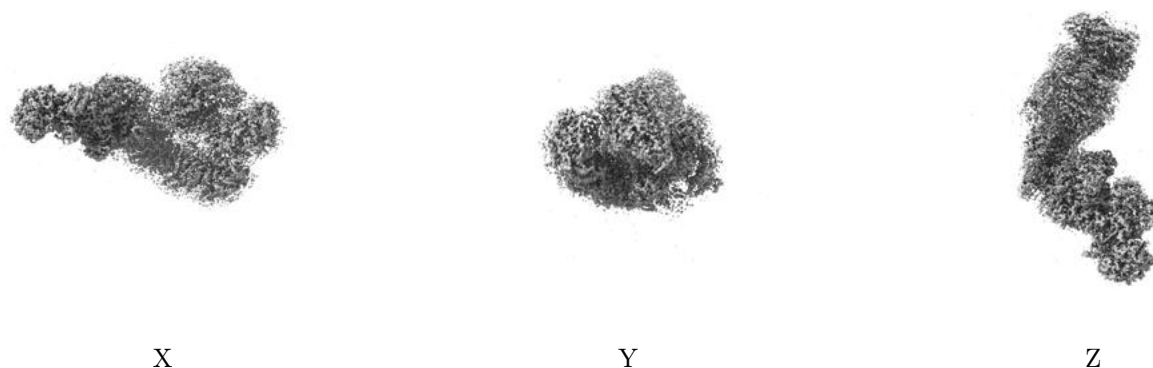


Z

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.

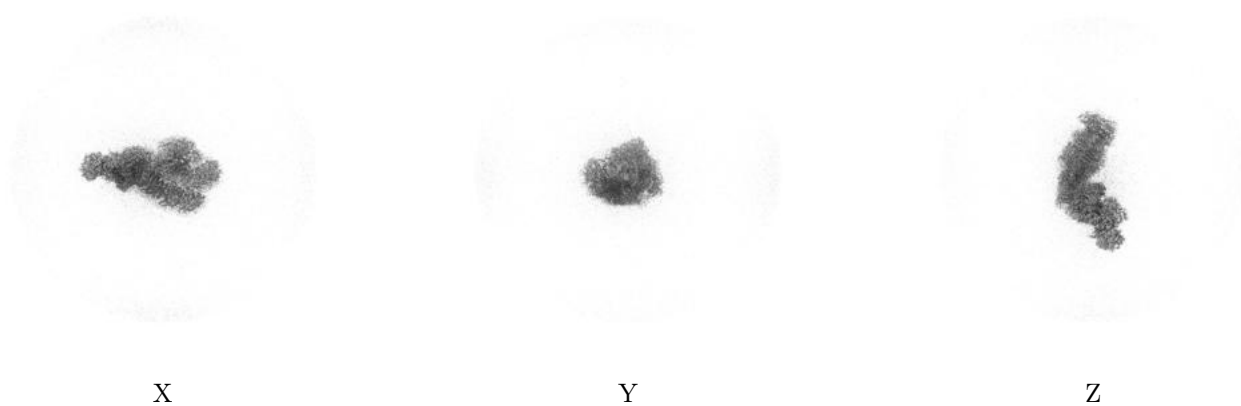
## 6.5 Orthogonal surface views [i](#)

### 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.

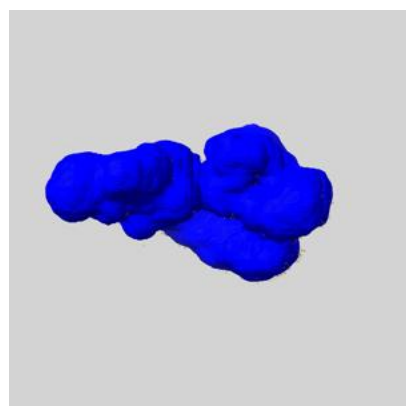
## 6.6 Mask visualisation [i](#)

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

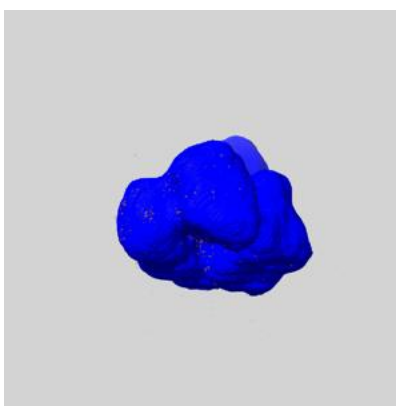
A mask typically either:

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

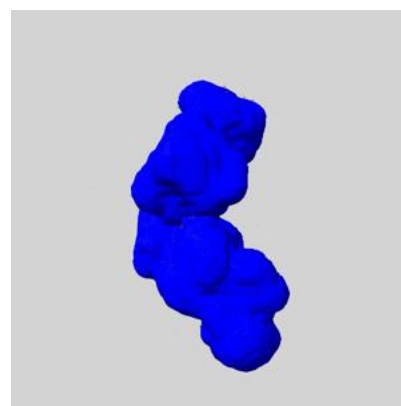
### 6.6.1 emd\_51162\_msk\_1.map [i](#)



X

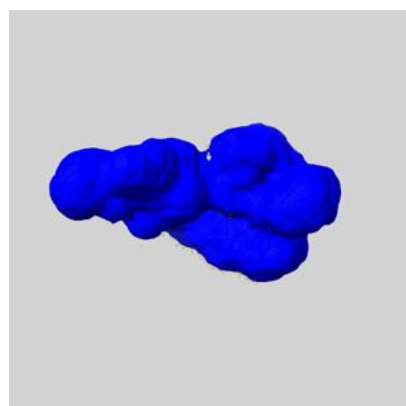


Y

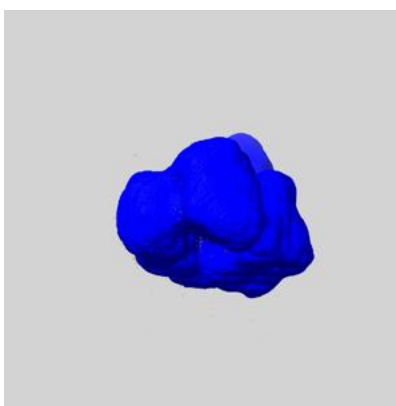


Z

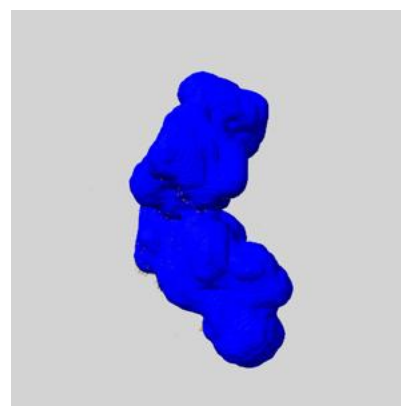
### 6.6.2 emd\_51162\_msk\_2.map [i](#)



X



Y

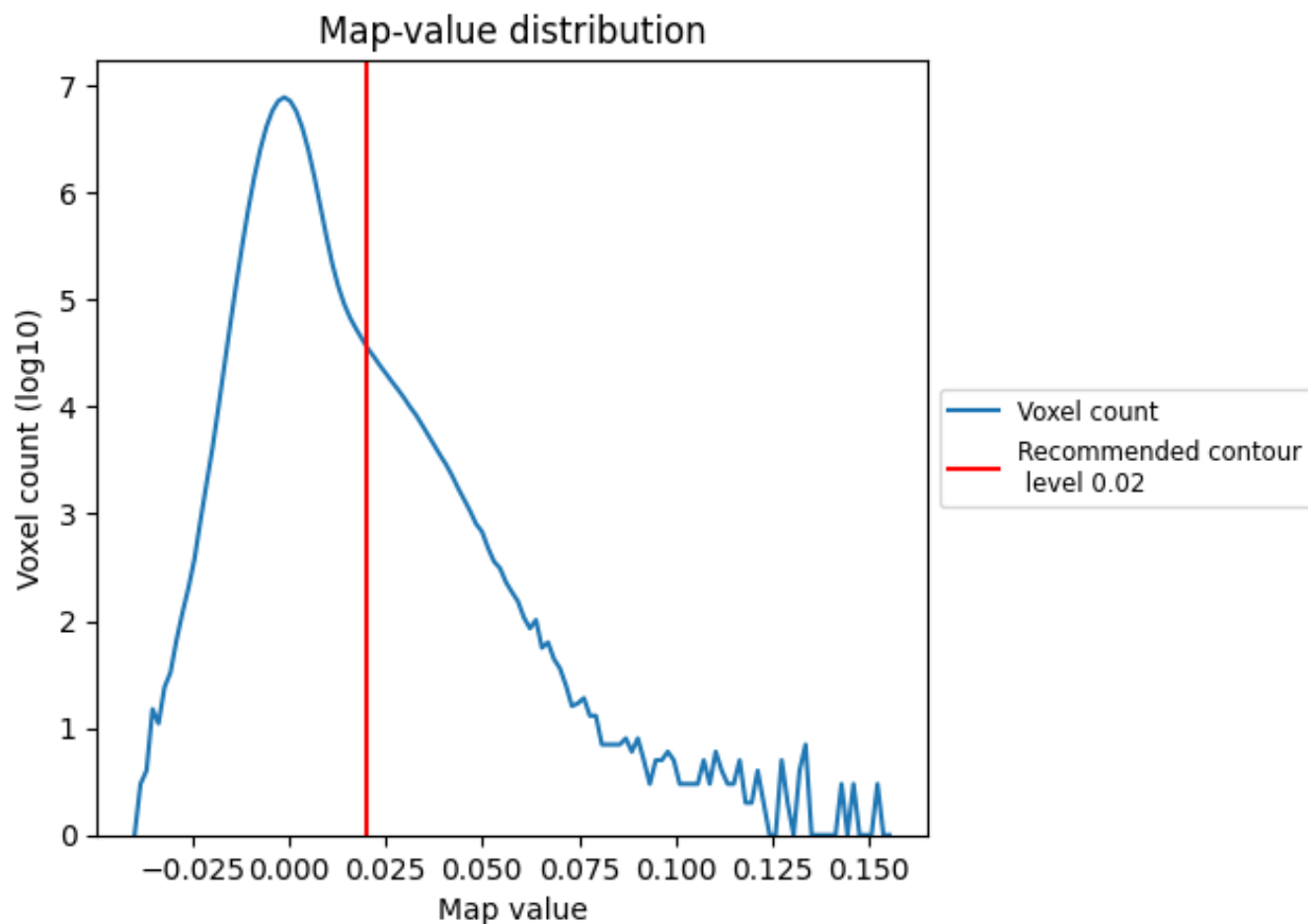


Z

## 7 Map analysis [i](#)

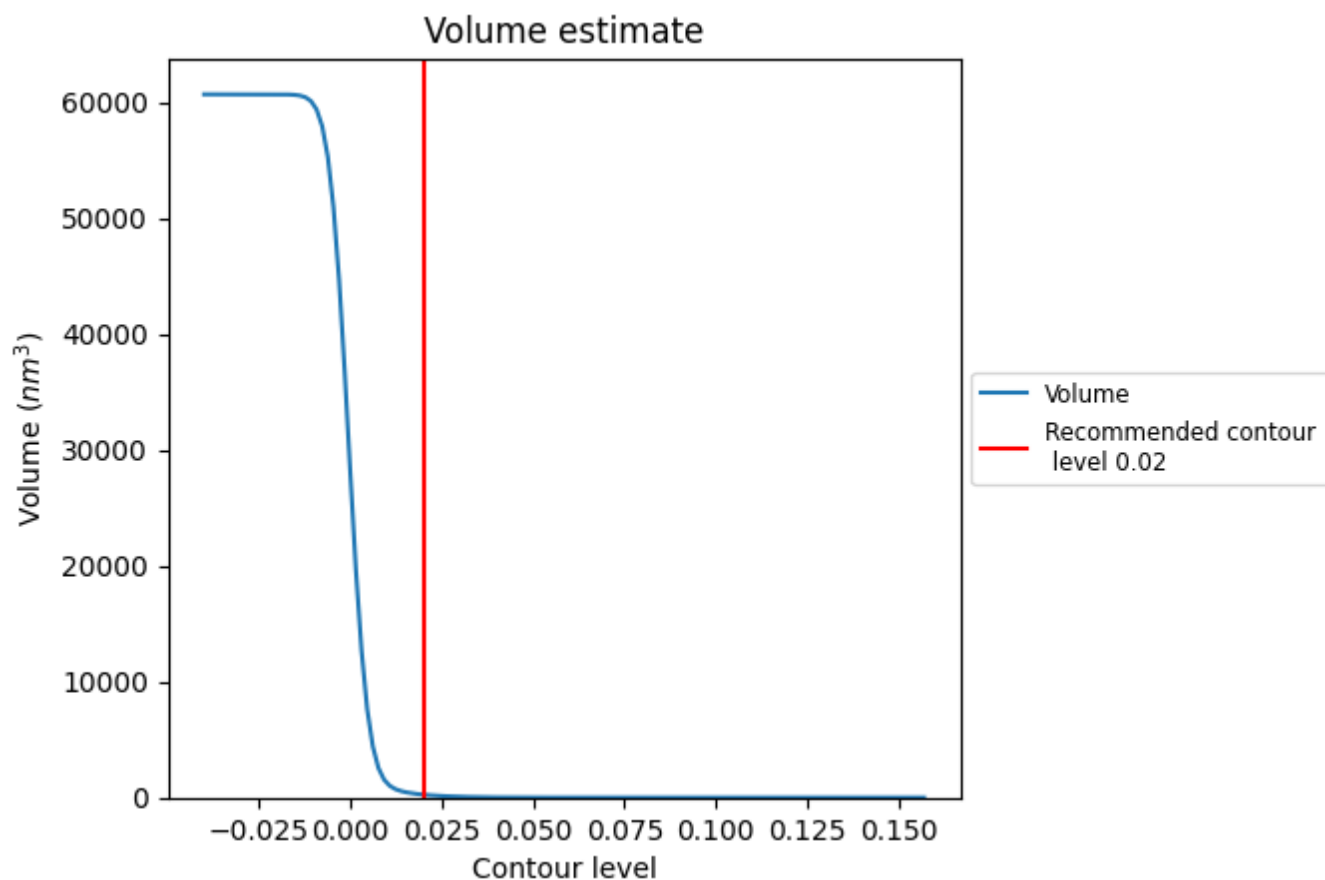
This section contains the results of statistical analysis of the map.

### 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.

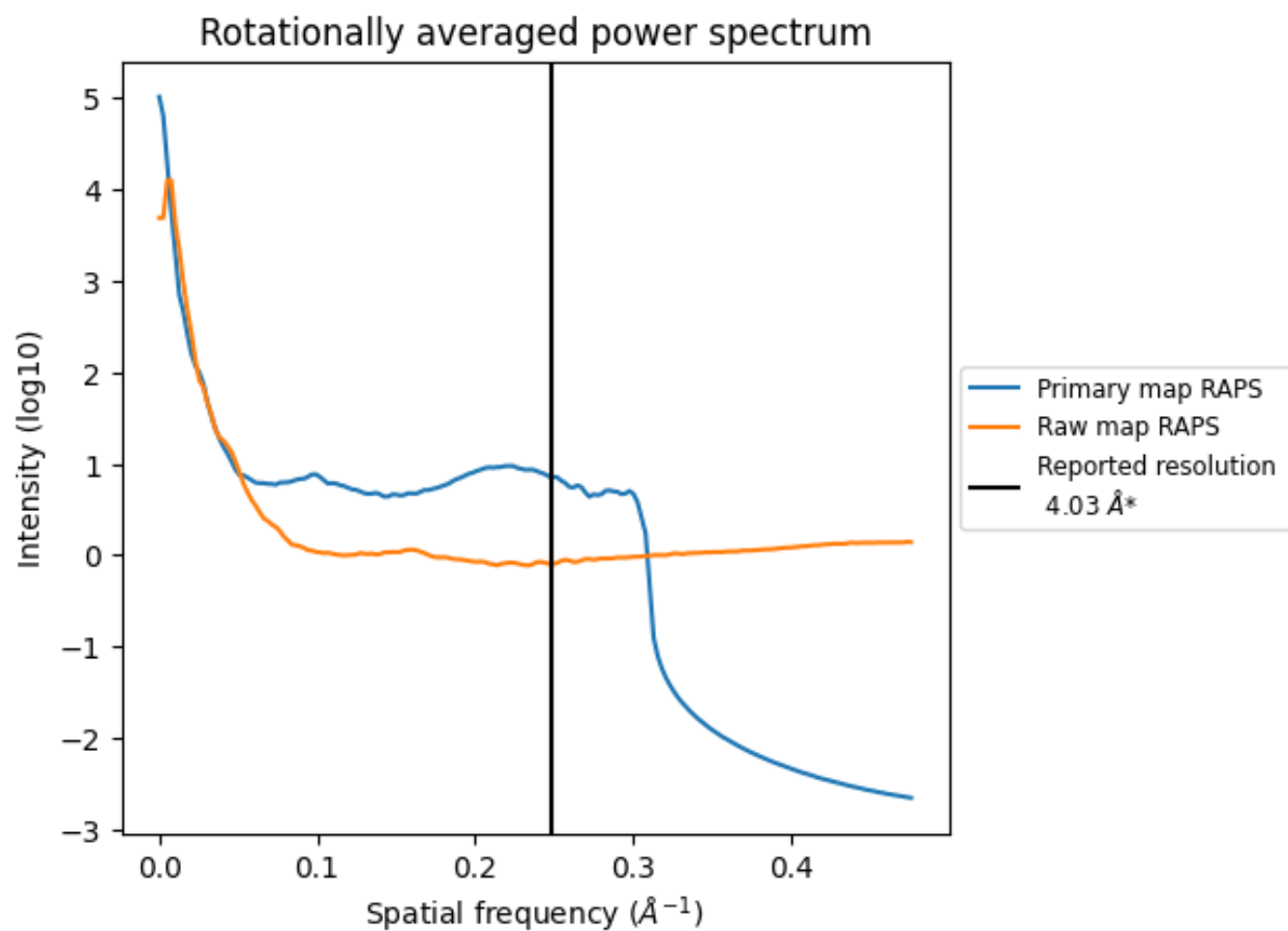
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm<sup>3</sup>; 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 ⓘ

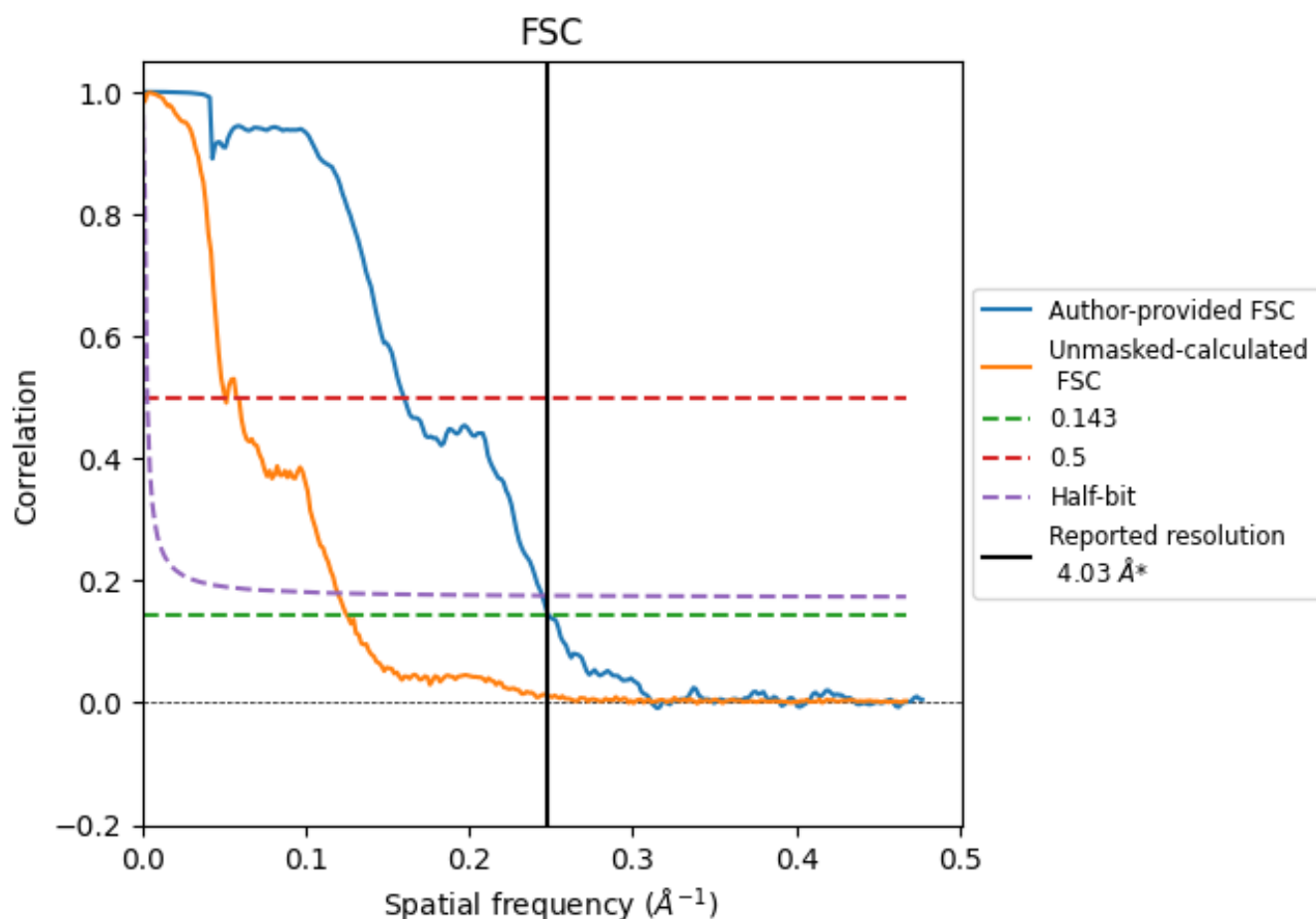


\*Reported resolution corresponds to spatial frequency of 0.248  $\text{\AA}^{-1}$

## 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  $0.248 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

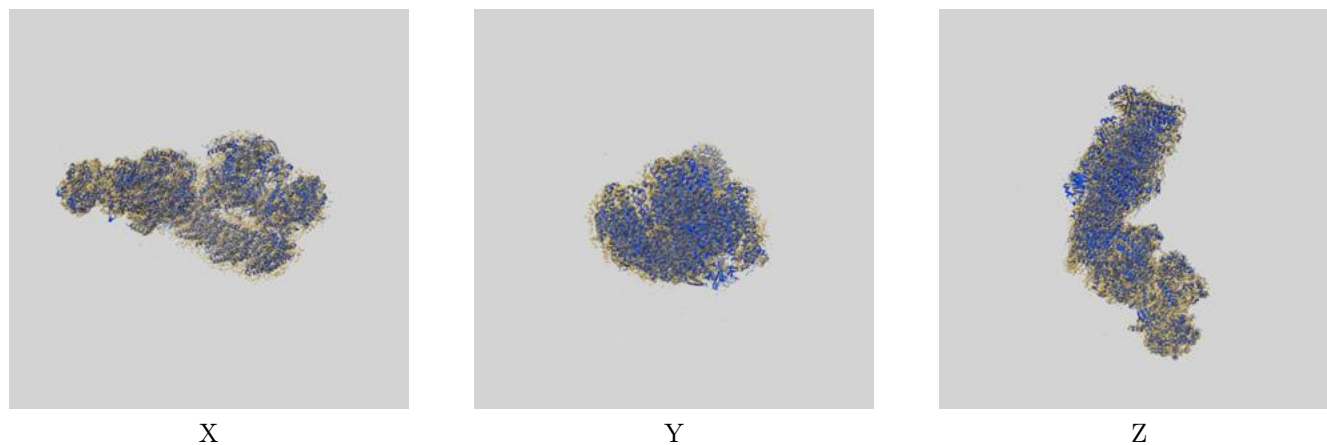
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.02	6.25	4.09
Unmasked-calculated*	7.99	19.72	8.36

\*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](#)

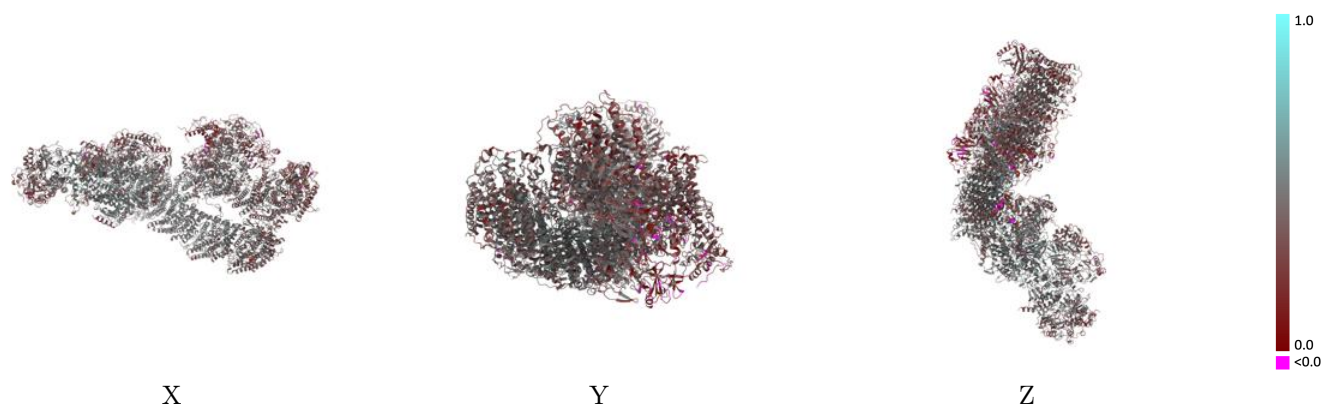
This section contains information regarding the fit between EMDB map EMD-51162 and PDB model 9G9Z. Per-residue inclusion information can be found in section [3](#) on page [22](#).

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



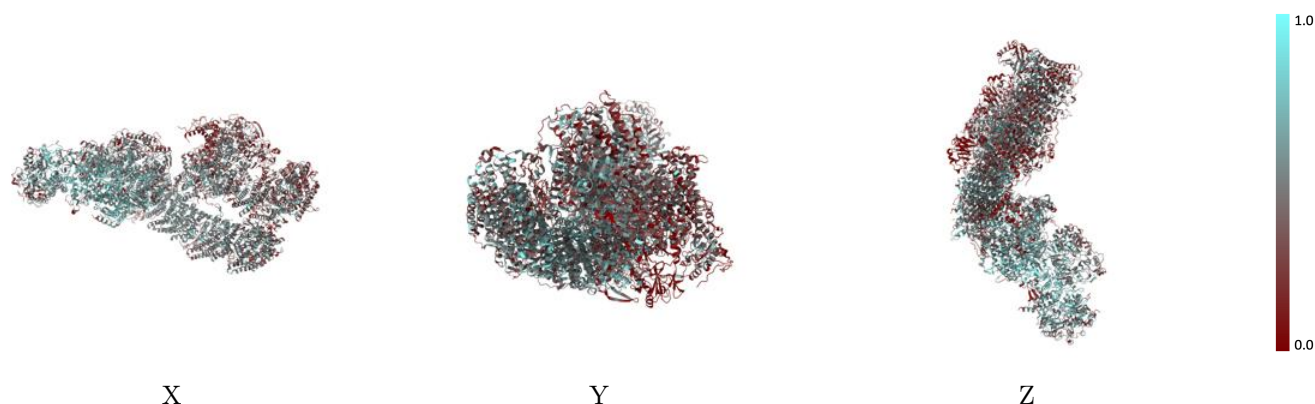
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



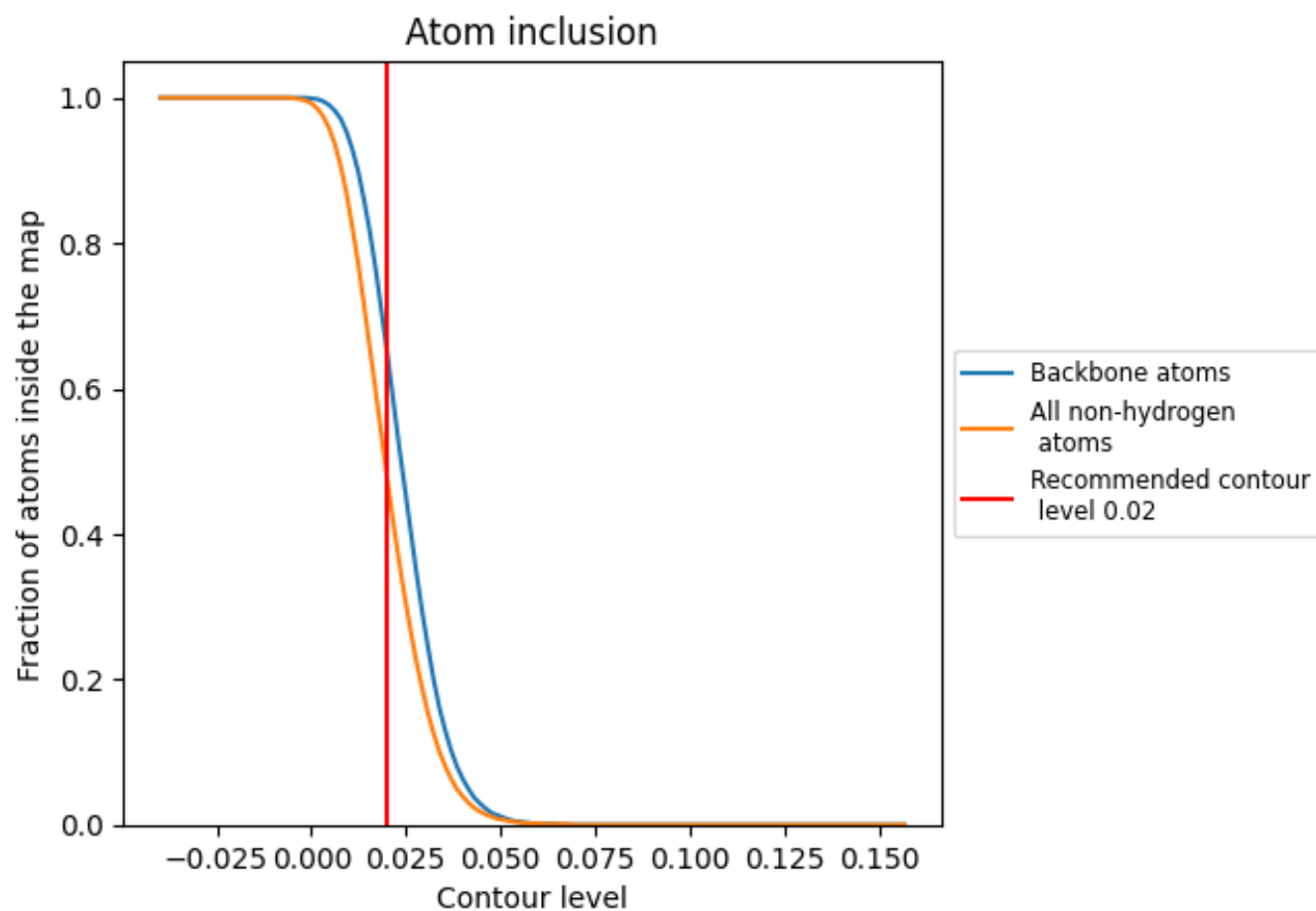
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

