Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 11:14 AM JST

PDB ID	:	8IAO
EMDB ID	:	EMD-35313
Title	:	Respiratory complex CI:CIII2, type I, Wild type mouse under thermoneutral temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	4.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

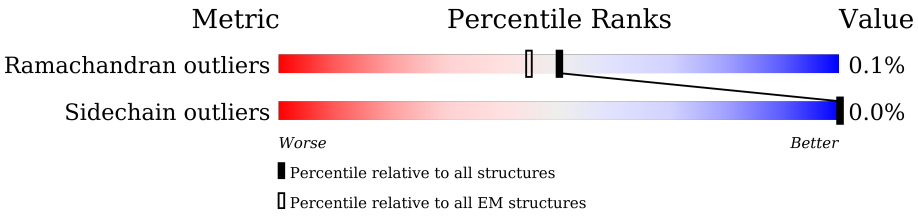
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	115	13% 80% 20%
2	B	224	6% 68% · 30%
3	C	263	8% 75% 25%
4	D	463	9% 90% · 8%
5	E	248	31% 83% · 15%
6	F	464	35% 89% · 8%
7	G	727	37% 92% · 6%
8	H	318	10% 96% ·
9	I	212	6% 83% · 16%

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Mol	Chain	Length	Quality of chain
10	J	172	27% 97%
11	K	98	97%
12	L	607	97%
13	M	459	97%
14	N	345	98%
15	O	355	11% 87% 10%
16	P	377	47% 89% 10%
17	Q	175	23% 65% 33%
18	R	116	24% 72% 28%
19	S	99	48% 83% 16%
20	T	156	36% 47% 52%
20	U	156	54% 44%
21	V	116	23% 93%
22	W	131	35% 86% 13%
23	X	172	98%
24	Y	143	6% 98%
25	Z	144	6% 97%
26	a	70	96%
27	b	84	5% 93% 6%
28	c	76	12% 59% 38%
29	d	120	12% 99%
30	e	106	95%
31	f	57	11% 91% 9%
32	g	151	66% 33%
33	h	189	73% 27%

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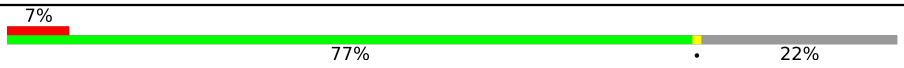
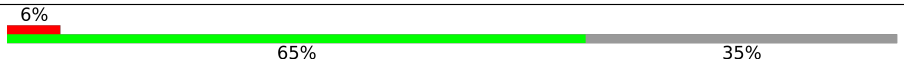
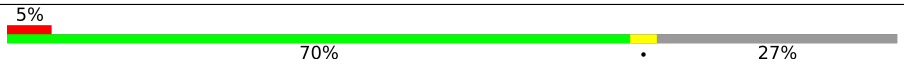
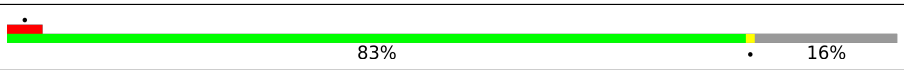
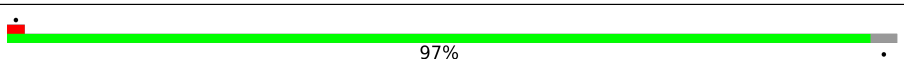
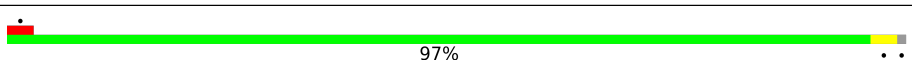
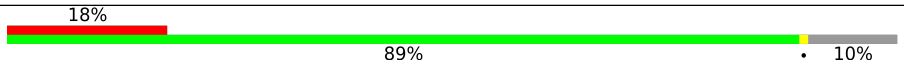
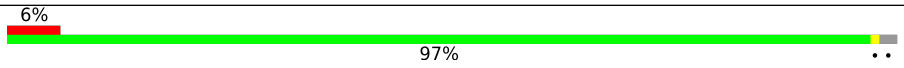
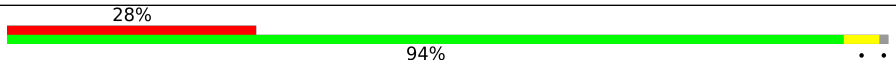
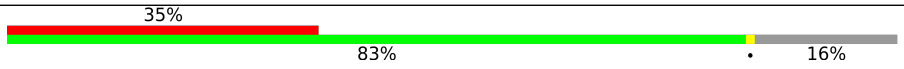
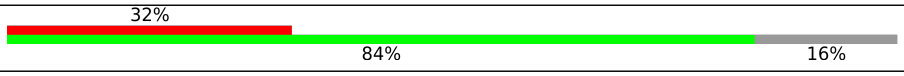
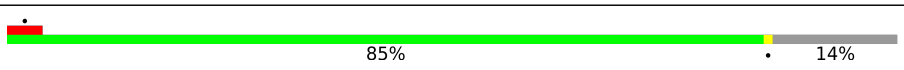
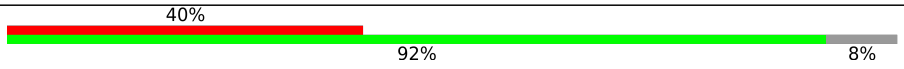
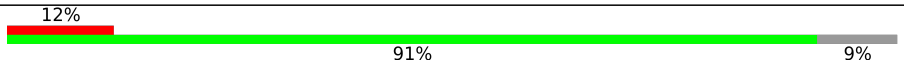
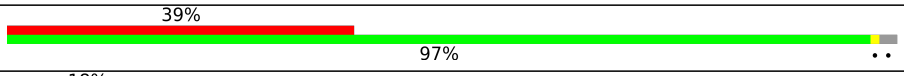
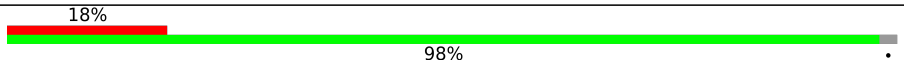
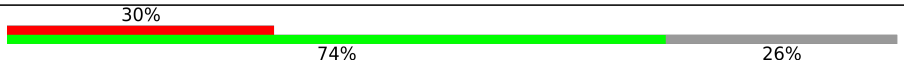
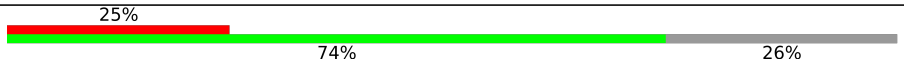
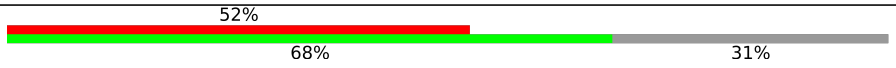
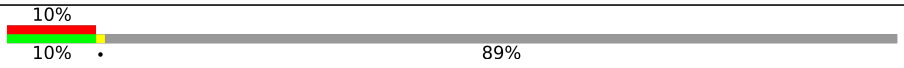
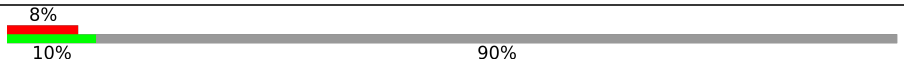
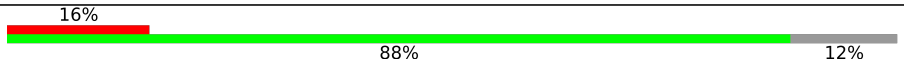
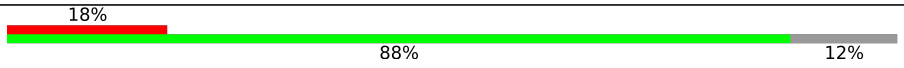
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
49	Ai	274	
50	AF	111	
50	Af	111	

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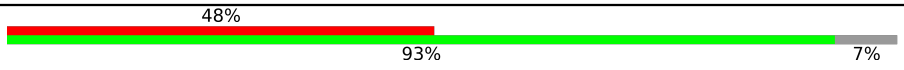
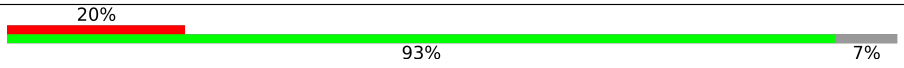
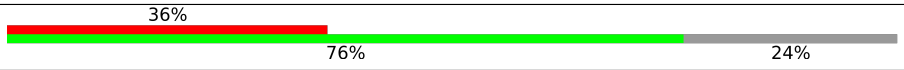
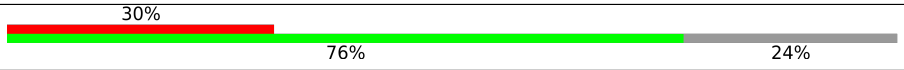
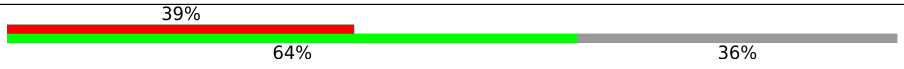
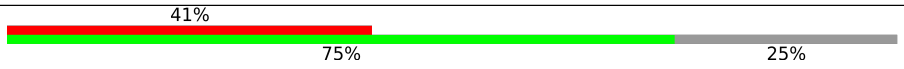
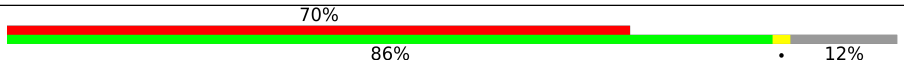
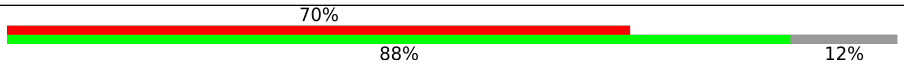
Mol	Chain	Length	Quality of chain
51	AG	82	
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 98999 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	92	754	523	107	119	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1258	802	227	215	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	424	3416	2184	587	621	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total 3288	C 2073	N 588	O 605	S 22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total 5287	C 3316	N 918	O 1012	S 41	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total 2532	C 1702	N 383	O 425	S 22	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total 1431	C 898	N 245	O 276	S 12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total 1287	C 866	N 183	O 223	S 15	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total 729	C 473	N 111	O 135	S 10	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total 4798	C 3181	N 746	O 826	S 45	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			447	290	80	75	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	100	Total	C	N	O	S	0	0
			839	546	146	144	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	68	Total	C	N	O	S	0	0
			578	378	96	103	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	76	Total	C	N	O	S	0	0
			618	410	105	101	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	125	Total	C	N	O	0	0
			1044	673	188	183		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	403	Total	C	N	O	S	0	0
			3153	1970	560	607	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	412	Total 3225	C 2016	N 569	O 624	S 16	0	0

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	418	Total 3137	C 1970	N 552	O 606	S 9	0	0
46	Ab	412	Total 3094	C 1945	N 542	O 598	S 9	0	0

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AC	373	Total 2988	C 2018	N 461	O 489	S 20	0	0
47	Ac	373	Total 2988	C 2018	N 461	O 489	S 20	0	0

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	240	Total 1912	C 1221	N 328	O 349	S 14	0	0
48	Ad	240	Total 1912	C 1221	N 328	O 349	S 14	0	0

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	188	Total 1451	C 916	N 254	O 274	S 7	0	0
49	AI	30	Total 217	C 138	N 42	O 37		0	0
49	Ae	188	Total 1451	C 916	N 254	O 274	S 7	0	0
49	Ai	28	Total 207	C 133	N 40	O 34		0	0

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	68	Total	C	N	O	S	0	0
			562	343	103	111	5		
52	Ah	68	Total	C	N	O	S	0	0
			562	343	103	111	5		

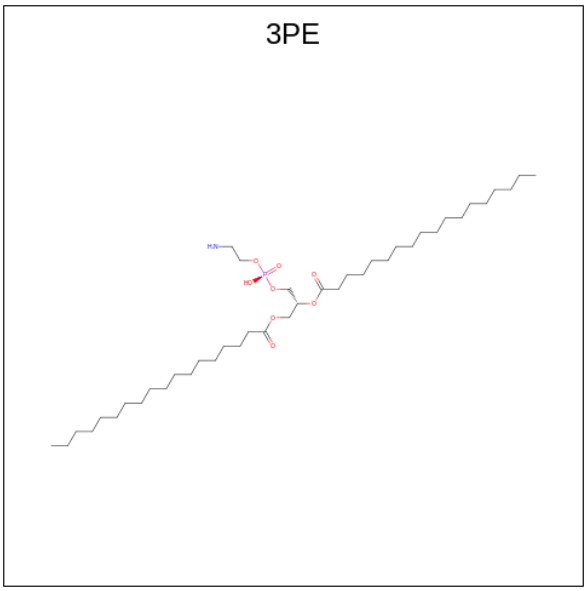
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
53	Aj	48	Total	C	N	O	0	0
			391	257	66	68		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		
54	Ak	49	Total	C	N	O	S	0	0
			401	266	71	63	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
55	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	AC	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	

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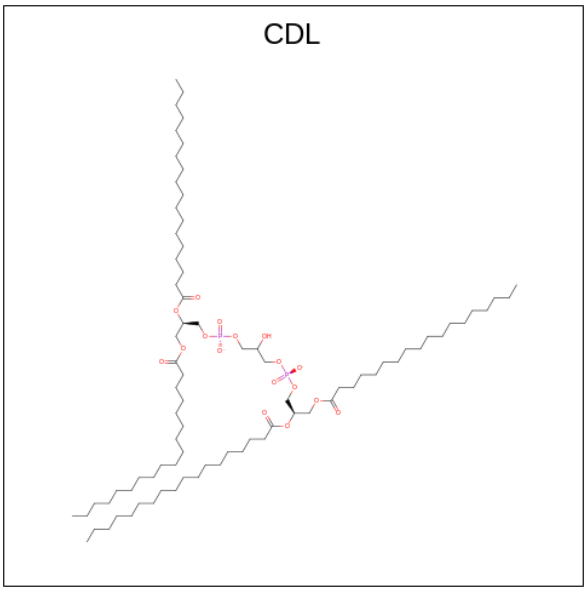
Mol	Chain	Residues	Atoms					AltConf
55	AG	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 56 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	O	P	0
			92	73	17	2	
56	L	1	Total	C	O	P	0
			74	55	17	2	
56	M	1	Total	C	O	P	0
			79	60	17	2	
56	Y	1	Total	C	O	P	0
			81	62	17	2	
56	d	1	Total	C	O	P	0
			84	65	17	2	
56	h	1	Total	C	O	P	0
			93	74	17	2	
56	q	1	Total	C	O	P	0
			57	38	17	2	

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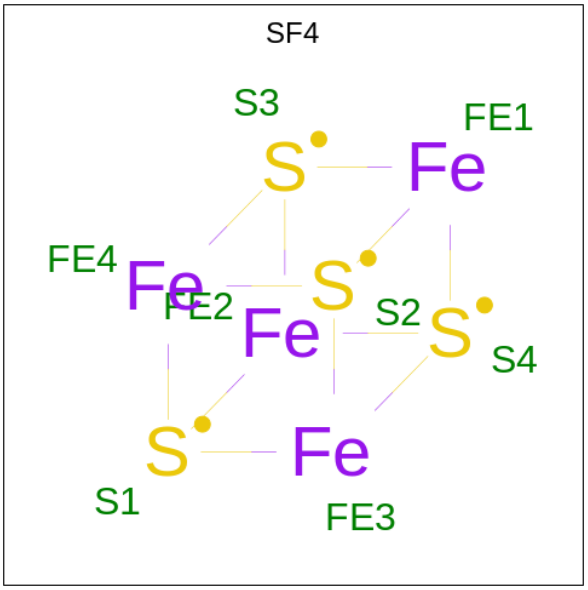
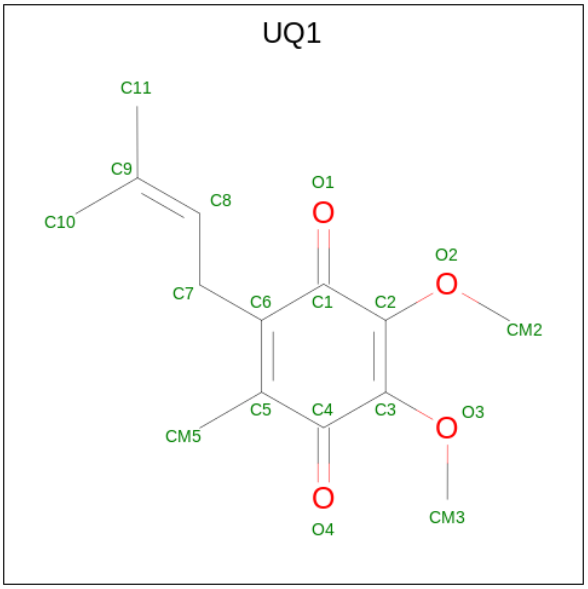
Mol	Chain	Residues	Atoms				AltConf
56	AG	1	Total	C	O	P	0
			42	23	17	2	
56	AG	1	Total	C	O	P	0
			56	37	17	2	
56	Aa	1	Total	C	O	P	0
			46	27	17	2	
56	Ag	1	Total	C	O	P	0
			42	23	17	2	
56	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



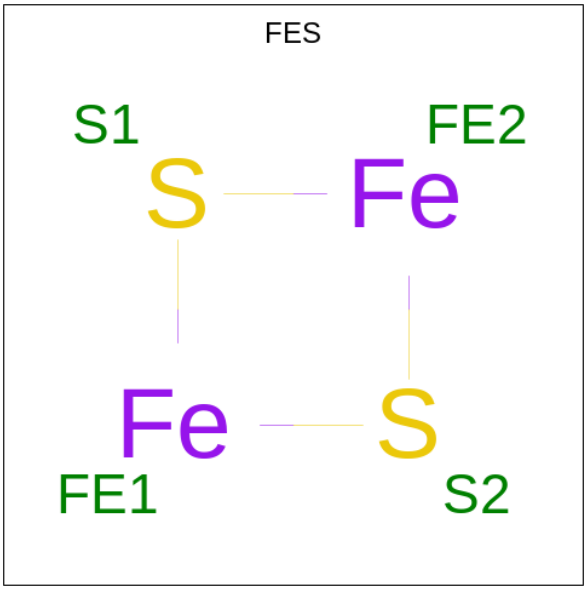
Mol	Chain	Residues	Atoms				AltConf
57	B	1	Total	Fe	S		0
			8	4	4		
57	F	1	Total	Fe	S		0
			8	4	4		
57	G	1	Total	Fe	S		0
			8	4	4		
57	G	1	Total	Fe	S		0
			8	4	4		
57	I	1	Total	Fe	S		0
			8	4	4		
57	I	1	Total	Fe	S		0
			8	4	4		

- Molecule 58 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	D	1	18	14	4	0

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

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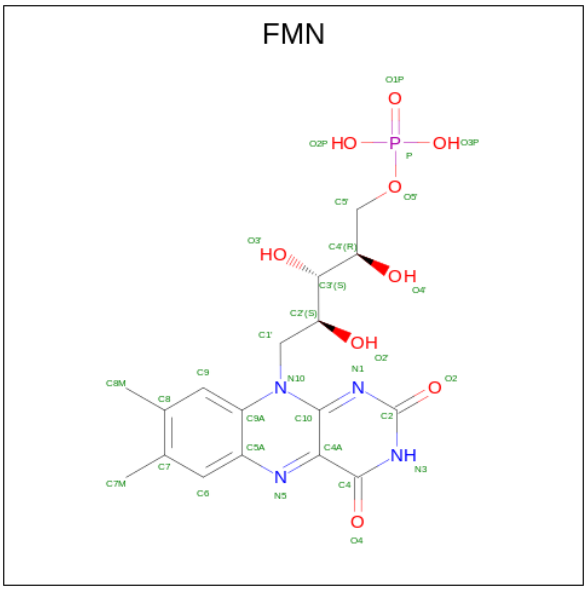
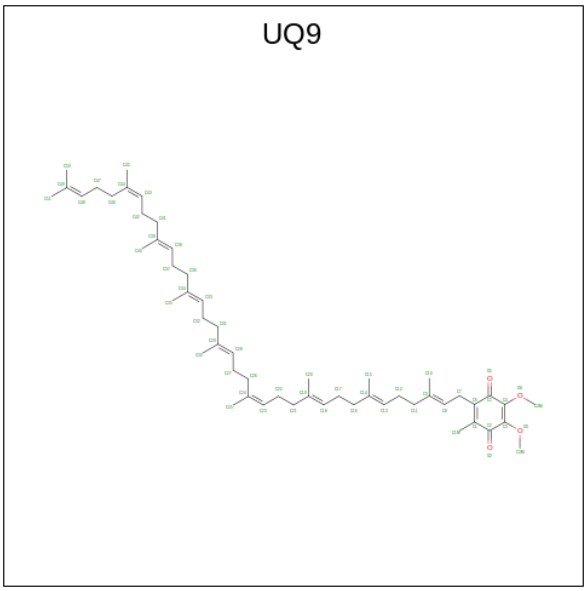
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	G	1	4	2	2	0

- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



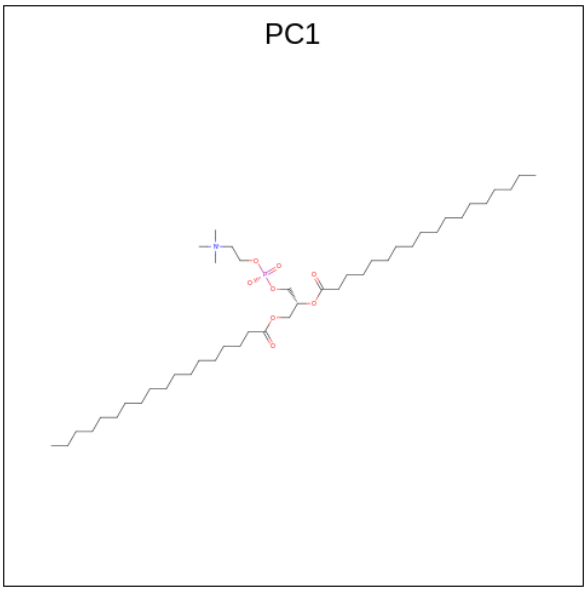
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

- Molecule 61 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
62	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
62	L	1	Total	C	N	O	P	0
			48	38	1	8	1	

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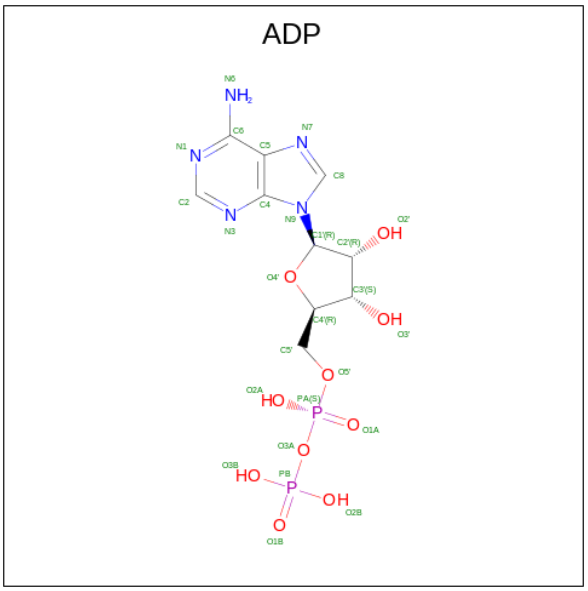
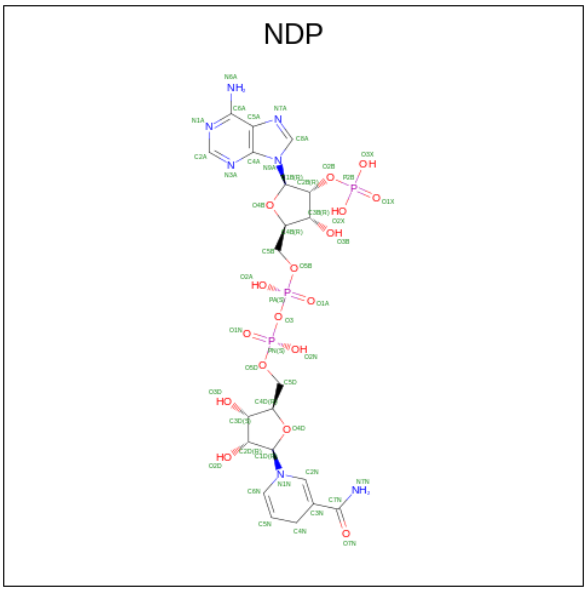
Mol	Chain	Residues	Atoms					AltConf
62	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
62	q	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	Ae	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
63	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 64 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

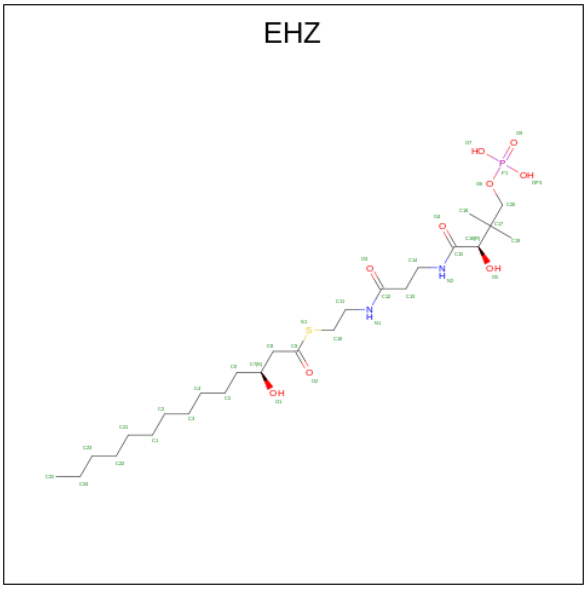


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

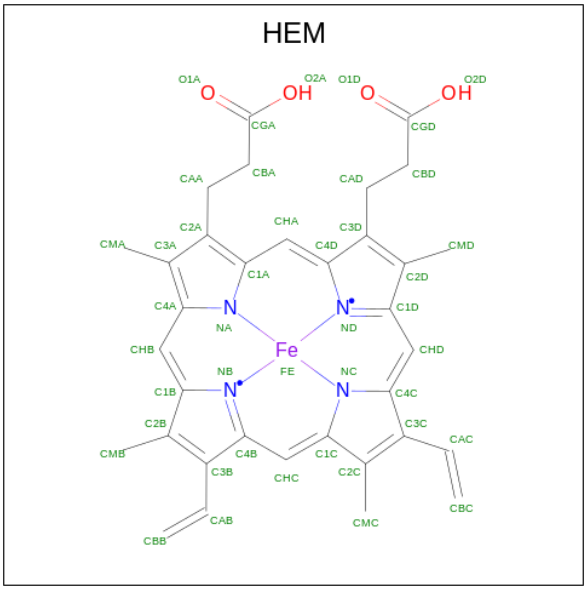
Mol	Chain	Residues	Atoms		AltConf
65	R	1	Total	Zn	0
			1	1	

- Molecule 66 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



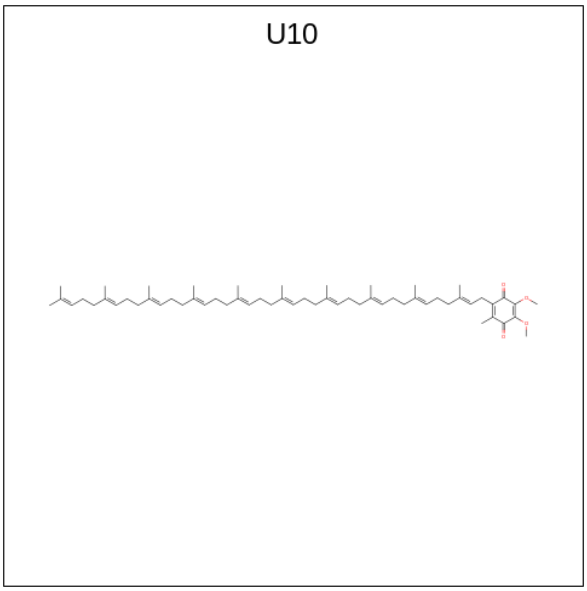
Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



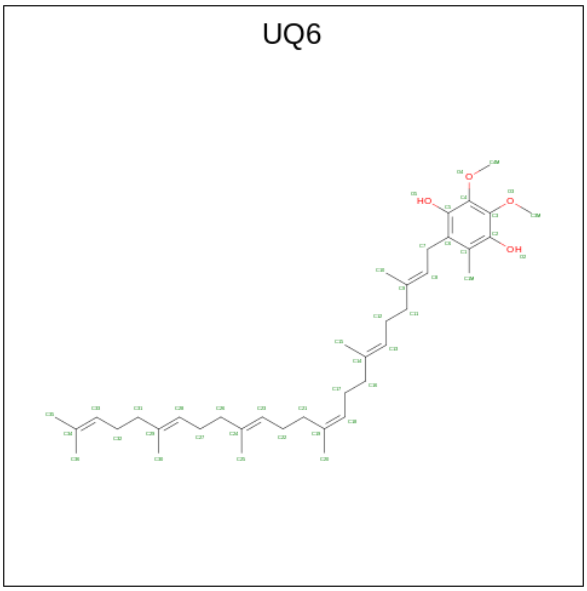
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 68 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			23	19	4	
68	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 69 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	

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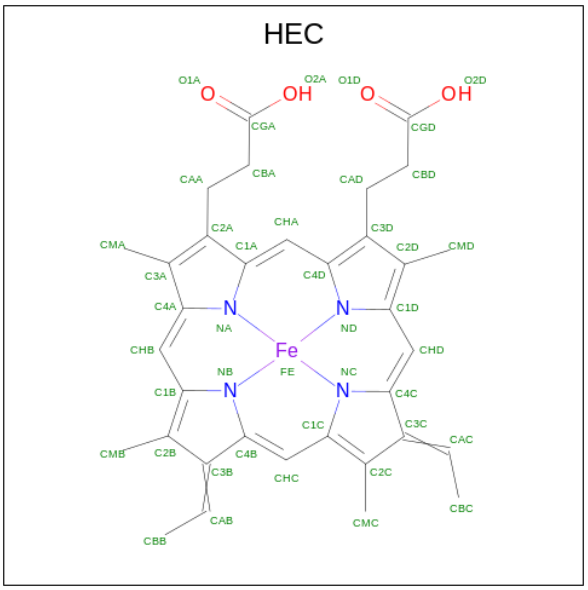
Mol	Chain	Residues	Atoms			AltConf
69	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 70 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

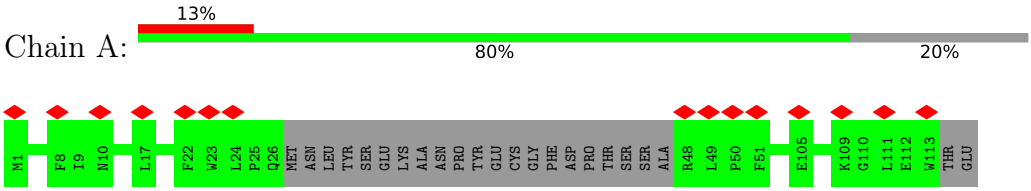


Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

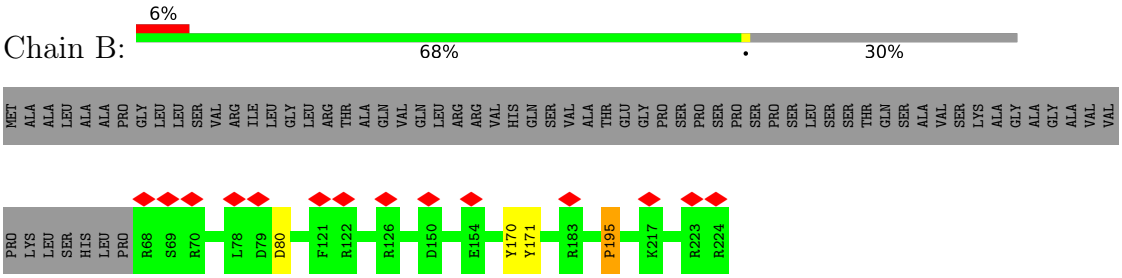
3 Residue-property plots (i)

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.

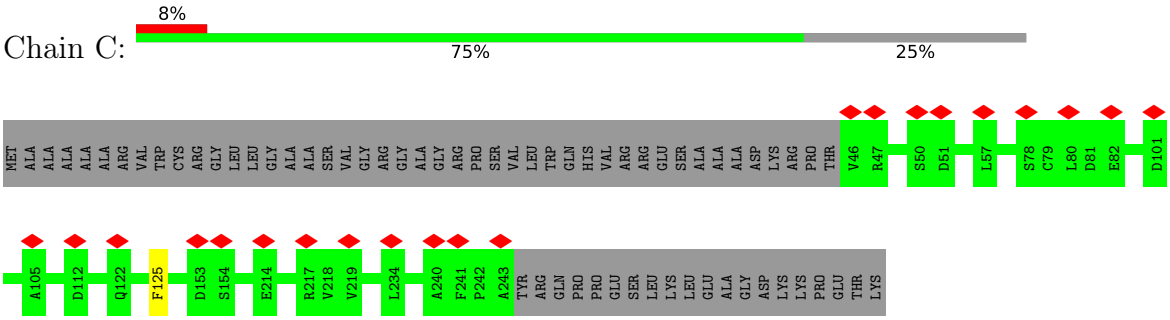
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



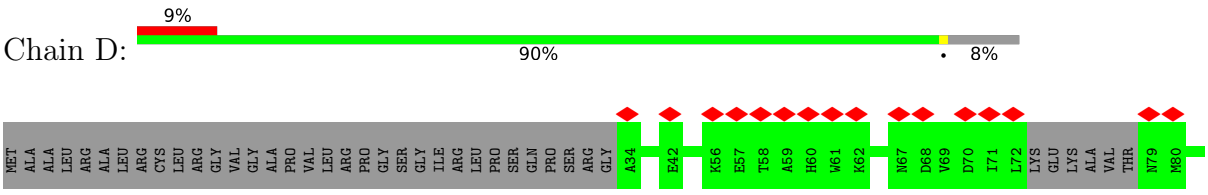
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

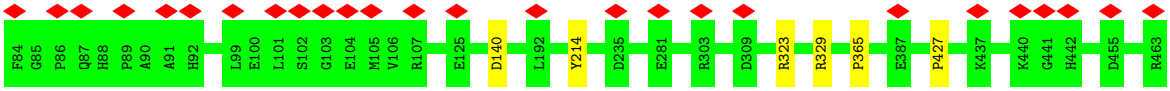


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



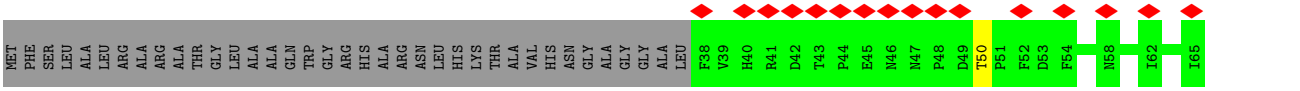
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

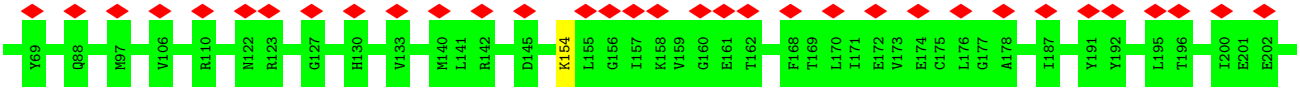


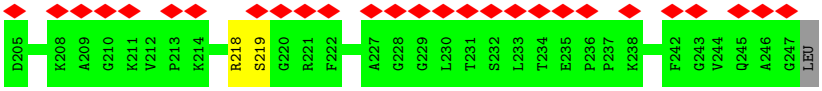


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

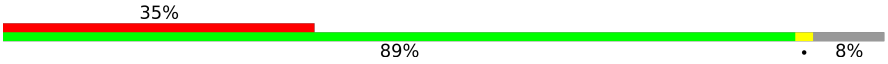


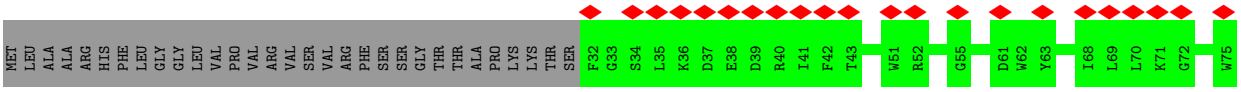


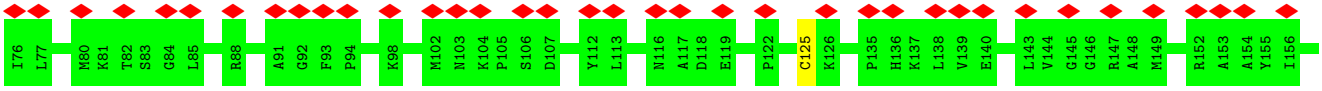


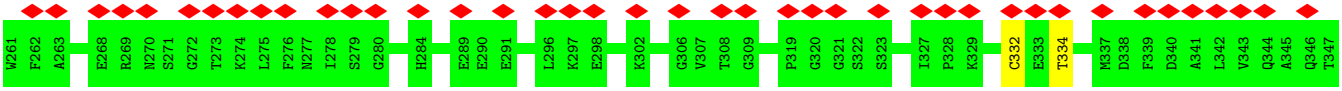
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

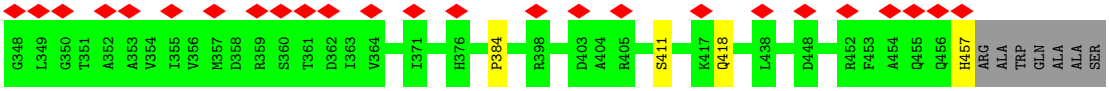
Chain F:





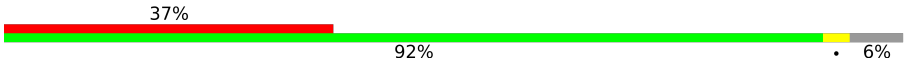


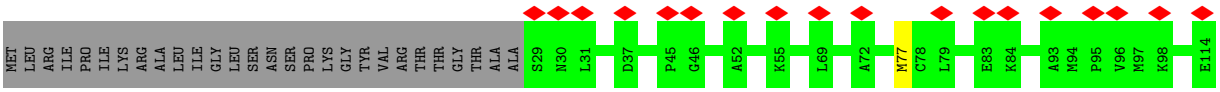


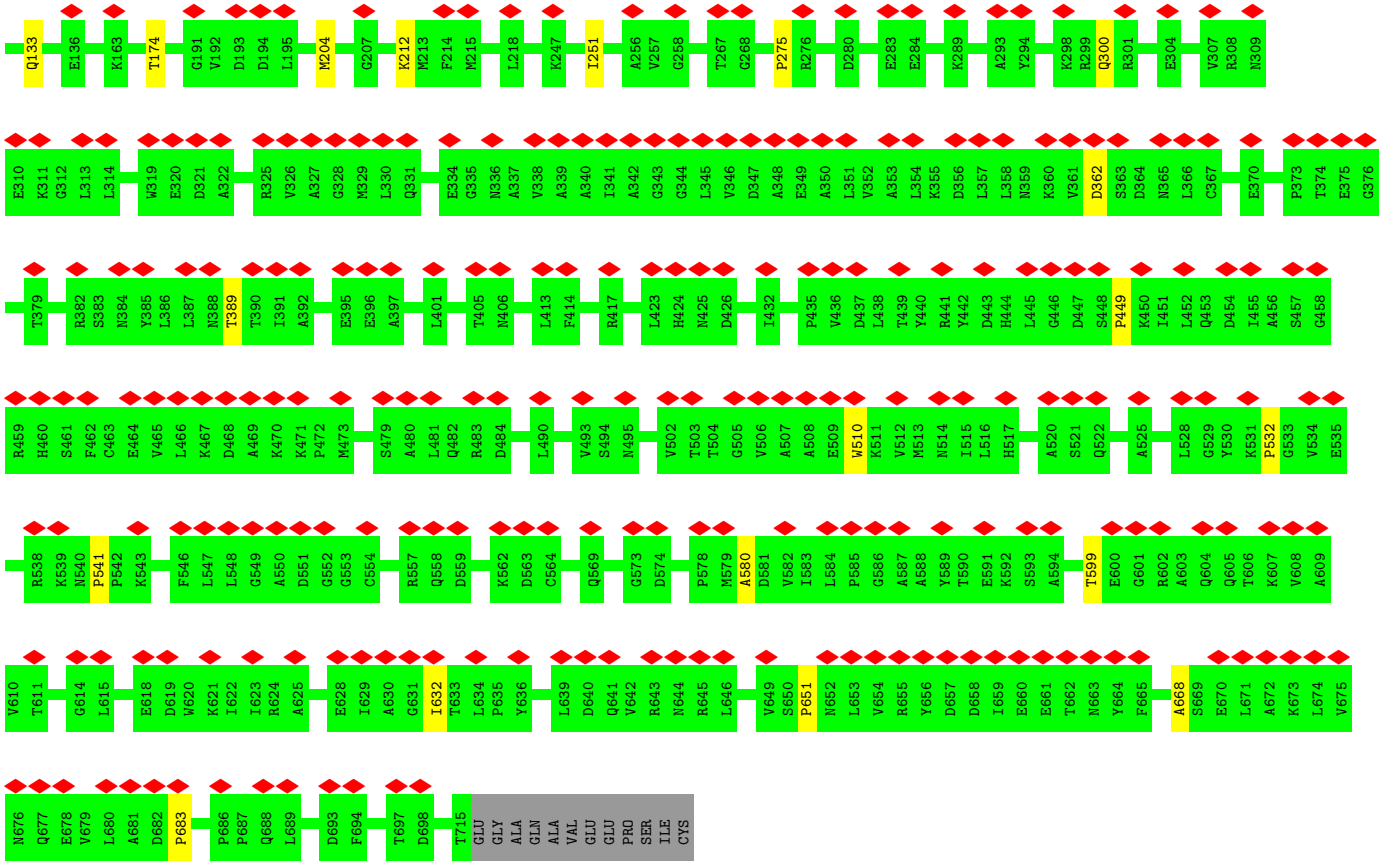


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

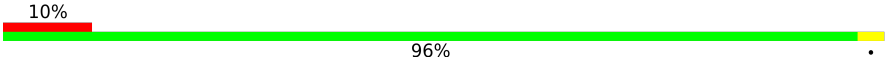


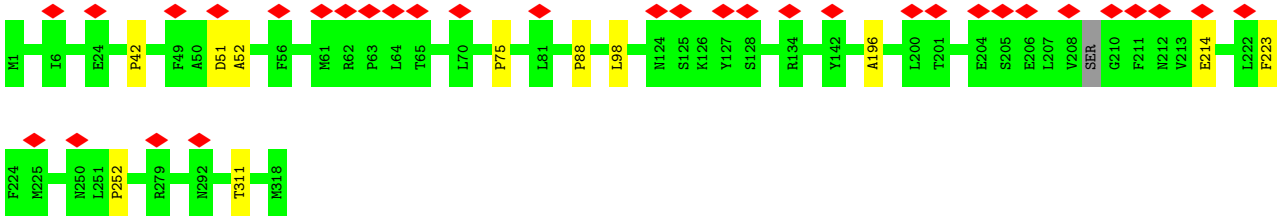




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

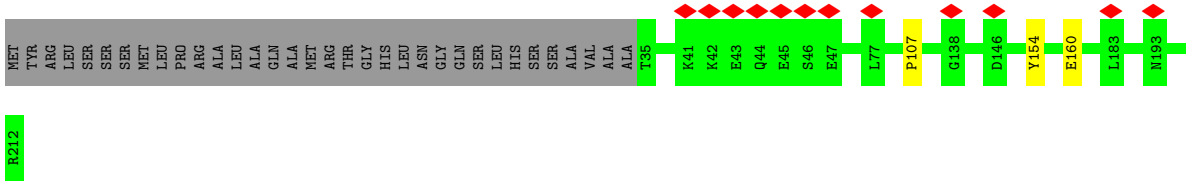
Chain H:





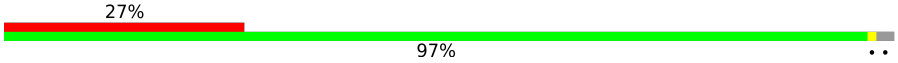
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

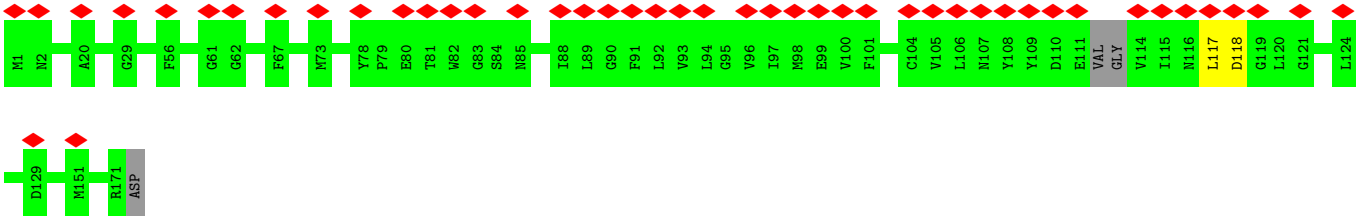
Chain I:



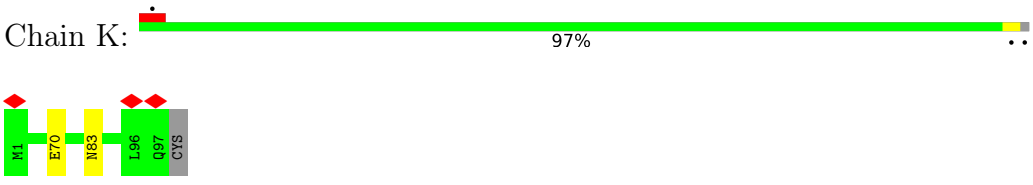
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

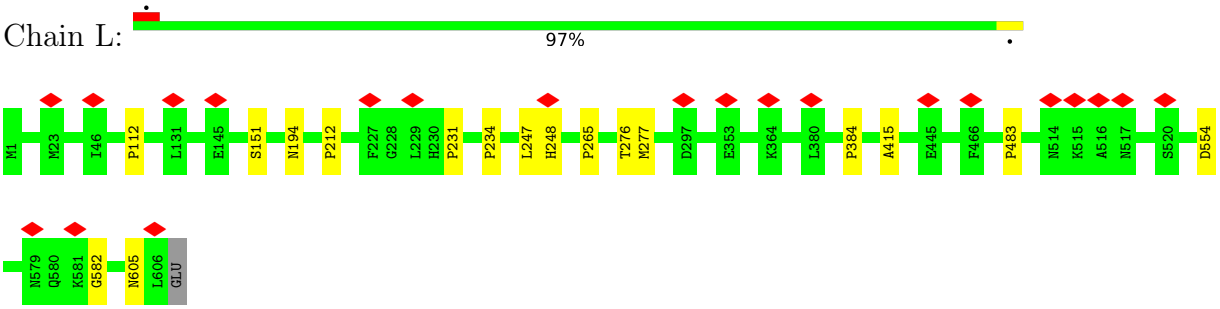




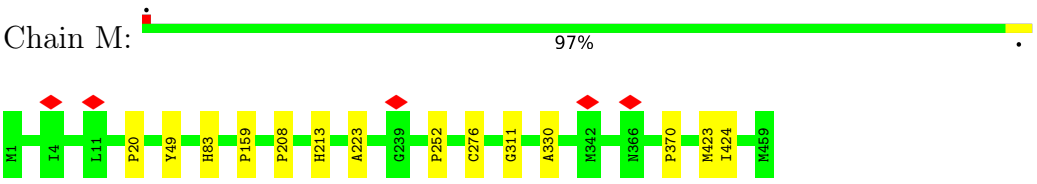
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



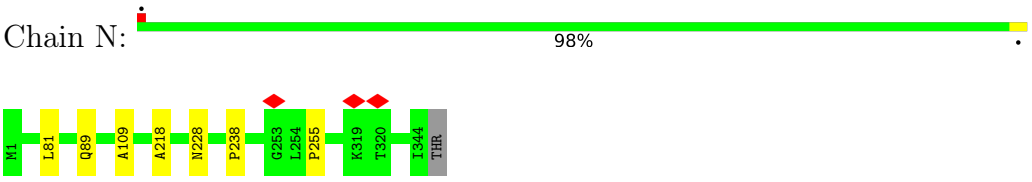
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



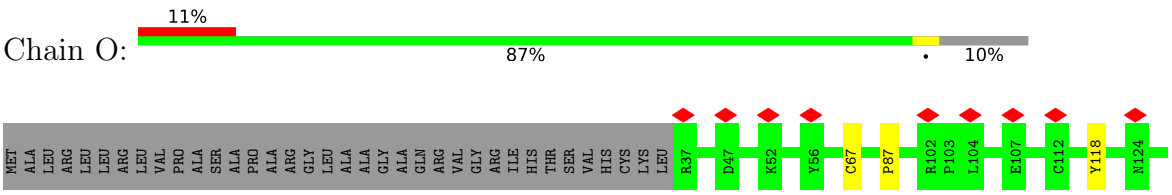
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

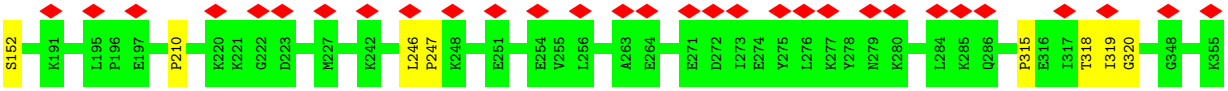


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



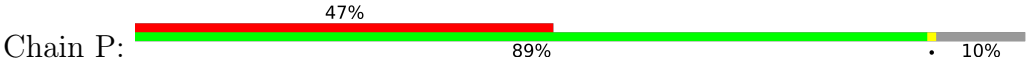
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

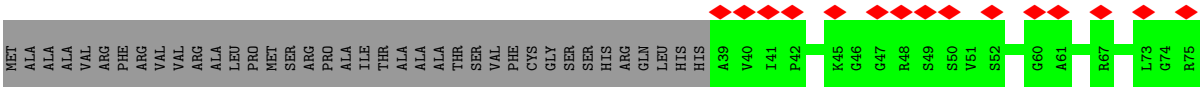


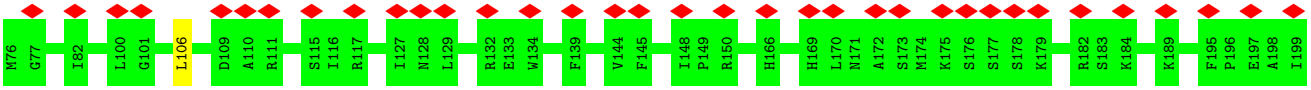


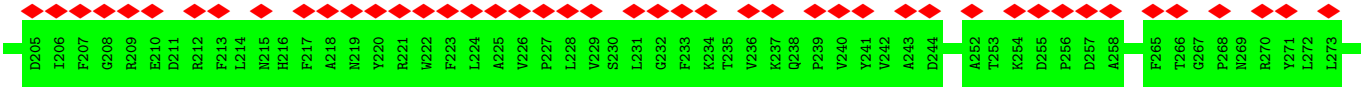
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

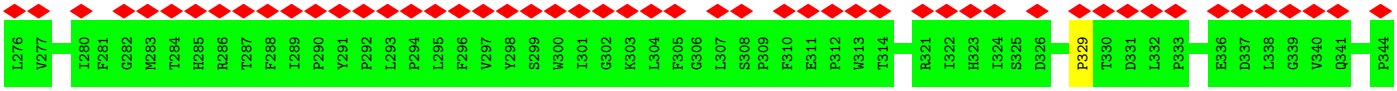
Chain P:

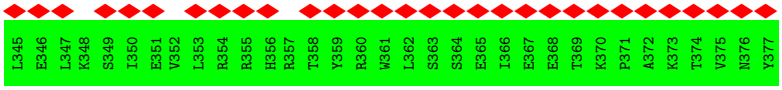






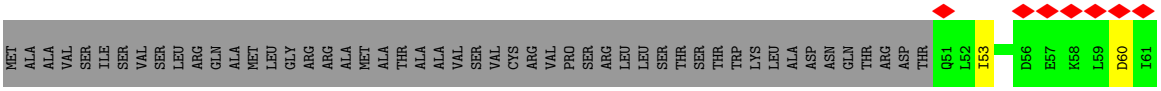


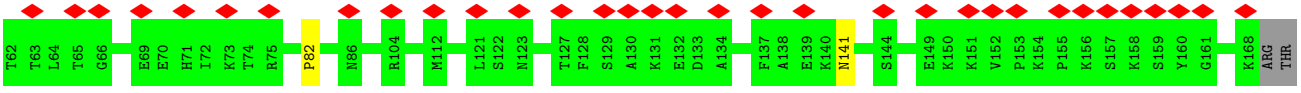




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

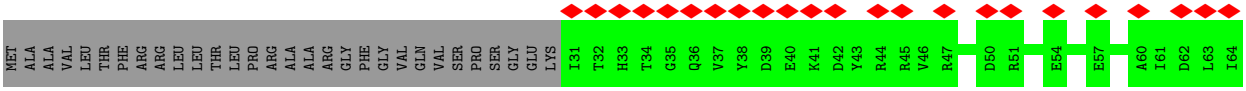
Chain Q:

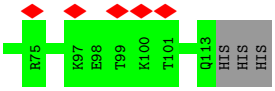




• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

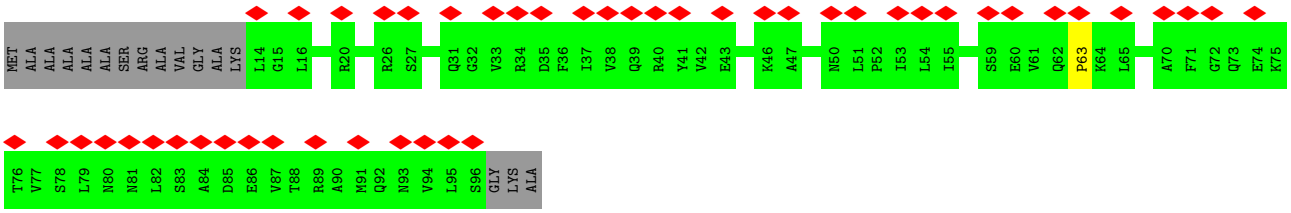
Chain R:





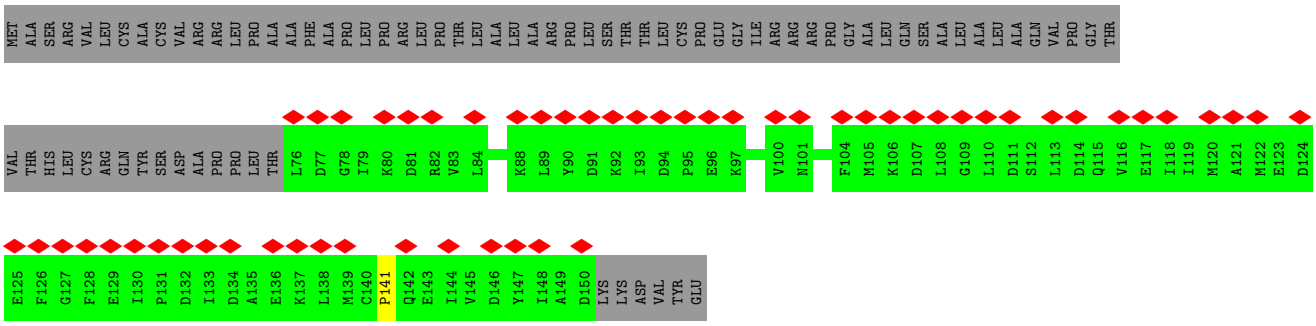
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



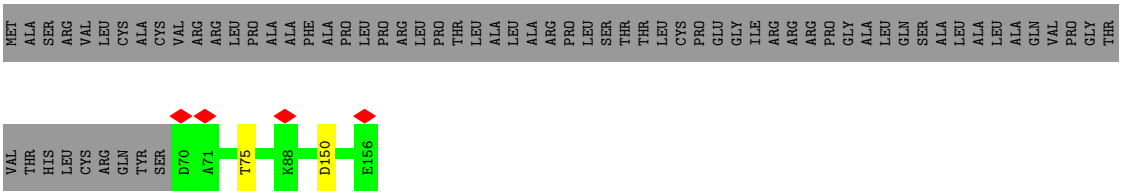
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



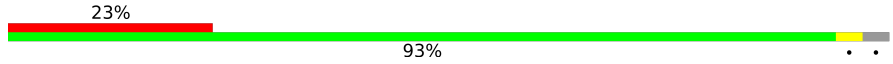
• Molecule 20: Acyl carrier protein, mitochondrial

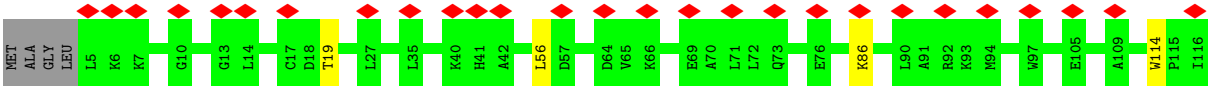
Chain U:



• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

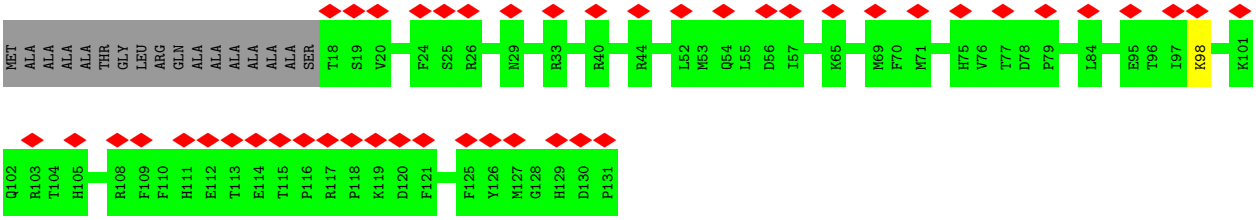
Chain V:



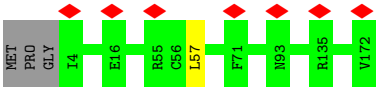


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

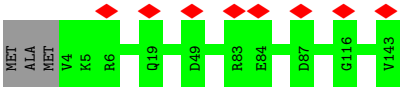
Chain W:



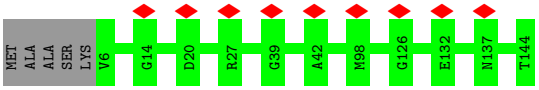
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



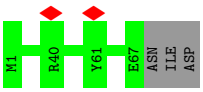
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



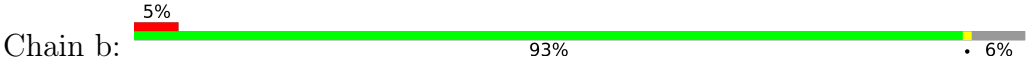
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

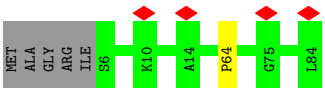


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

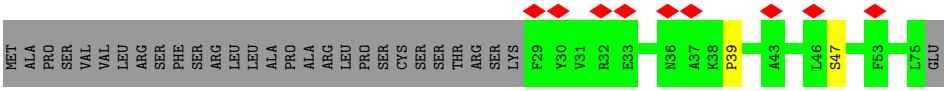


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

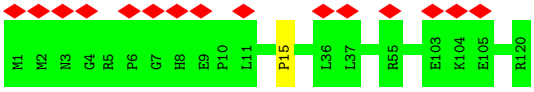




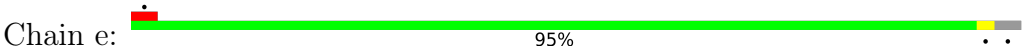
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

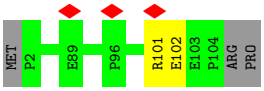


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

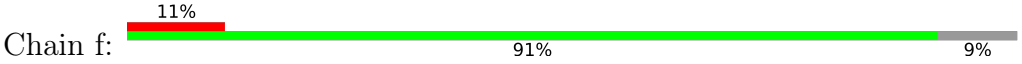


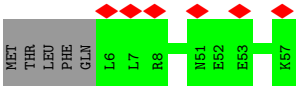
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



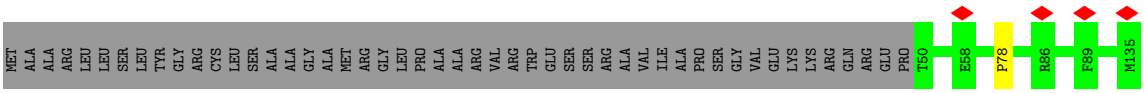


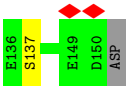
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



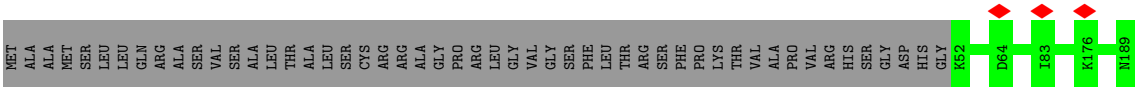


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

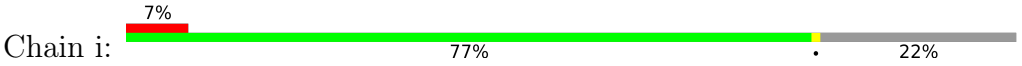


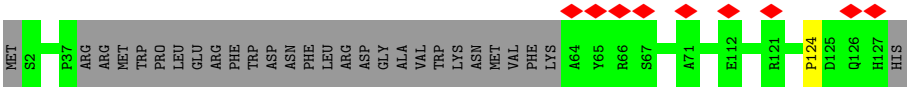


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



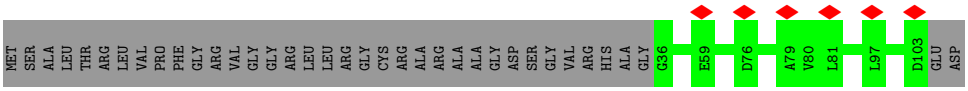
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6





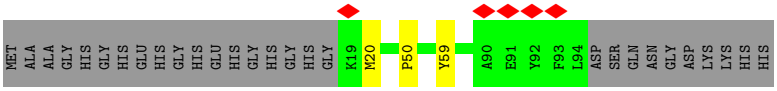
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



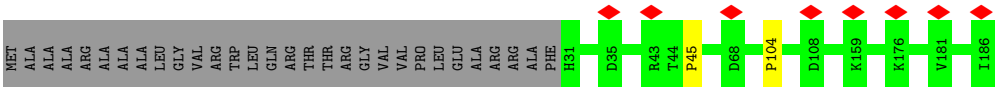
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



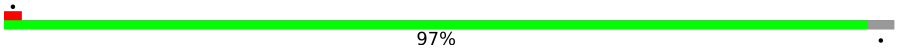
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

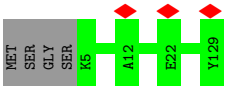
Chain l:



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

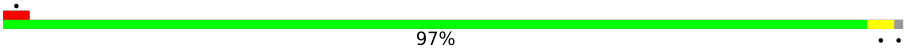
Chain m:

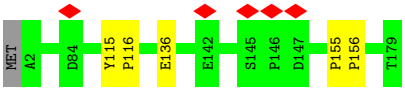




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

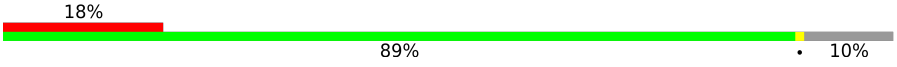
Chain n:

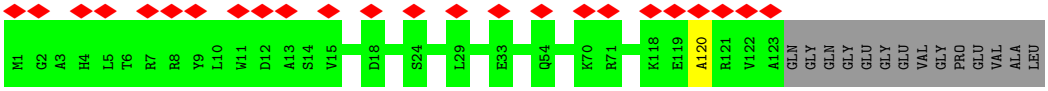




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

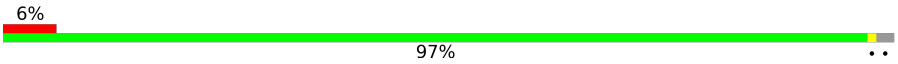
Chain o:

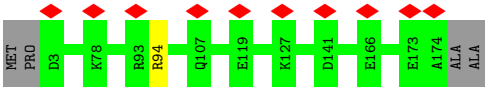




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

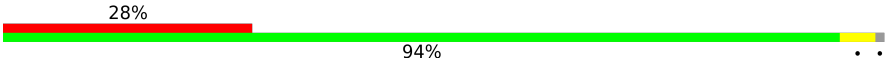
Chain p:

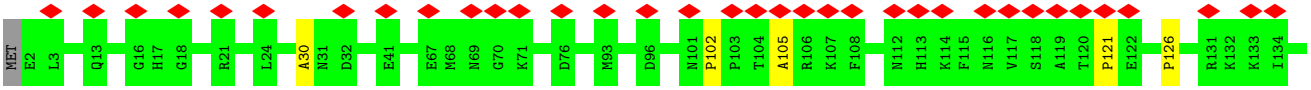


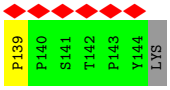


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

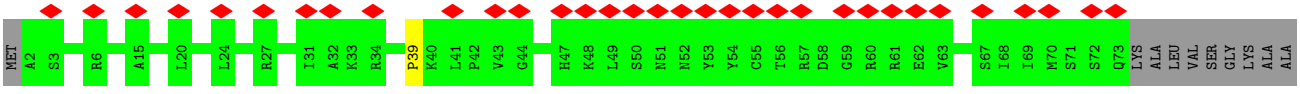


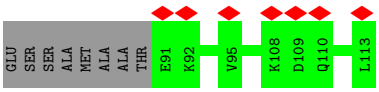




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

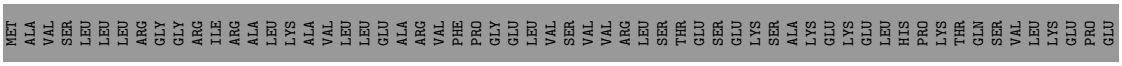
Chain r:

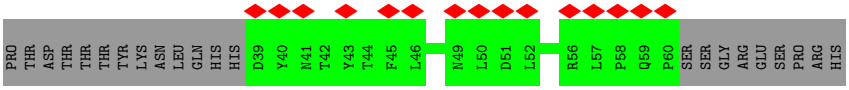




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

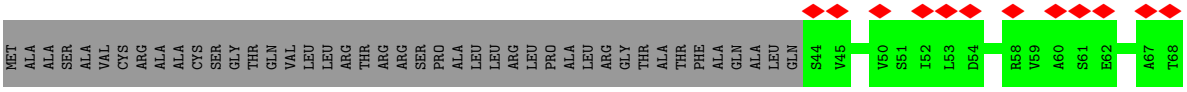
Chain s:

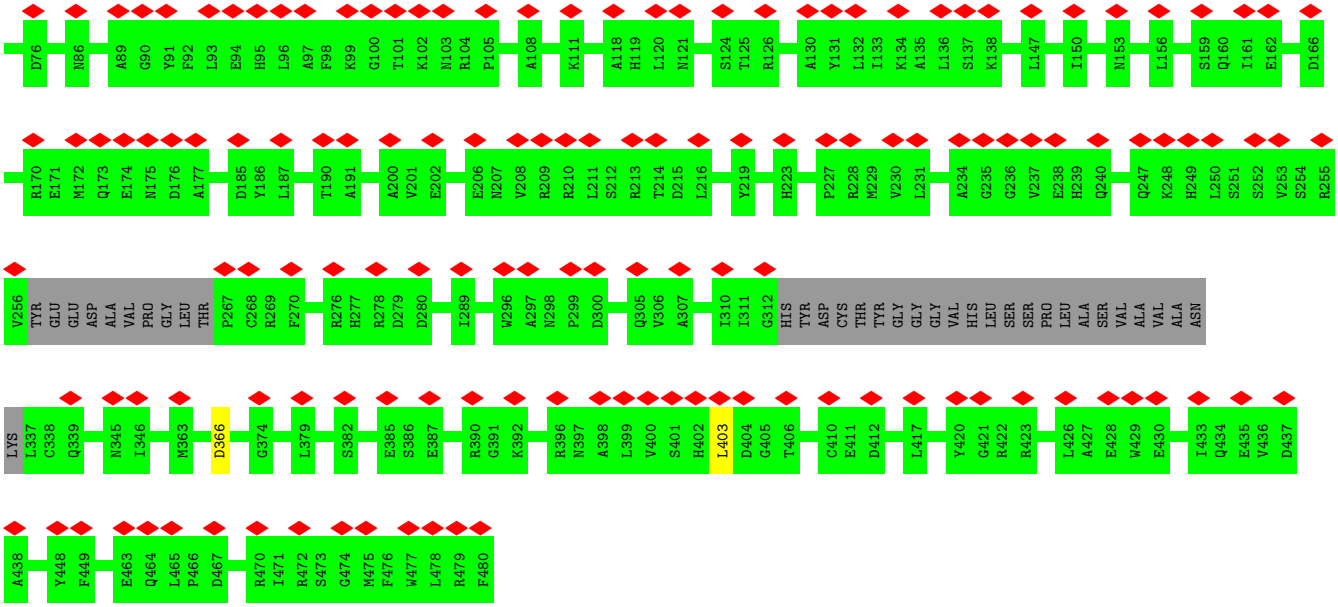




• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

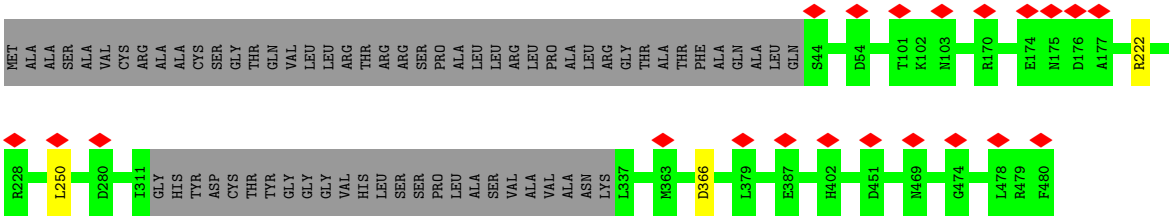
Chain AA:





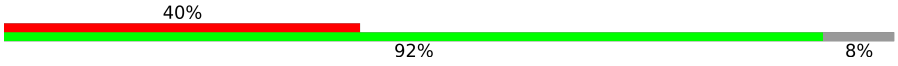
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

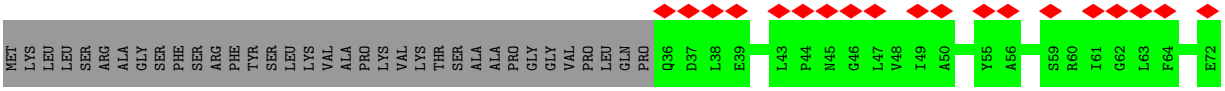
Chain Aa:

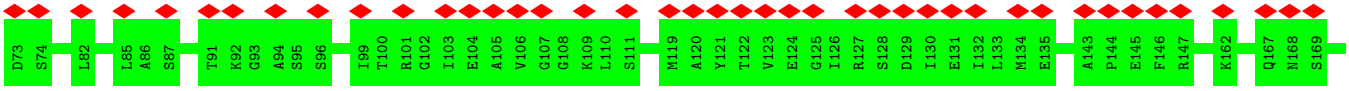


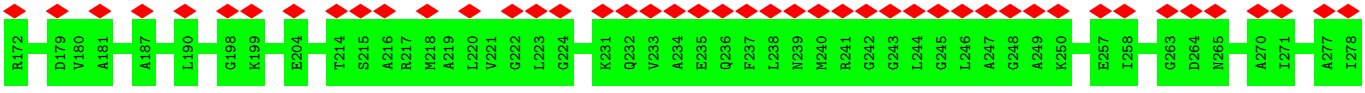
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

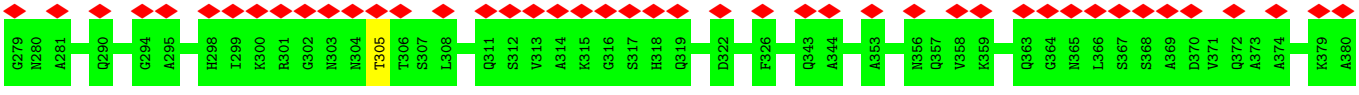
Chain AB:

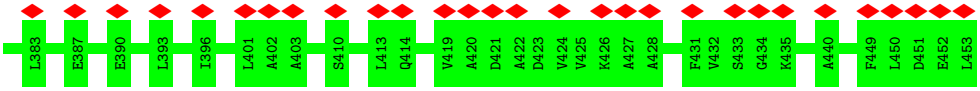






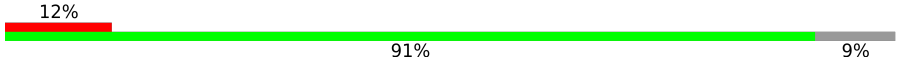


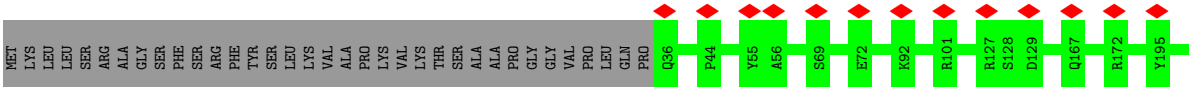


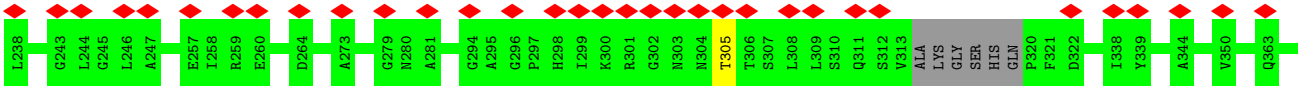


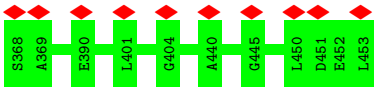
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:



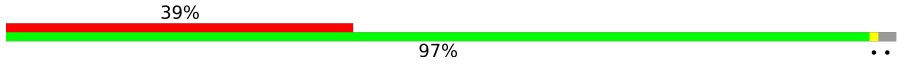


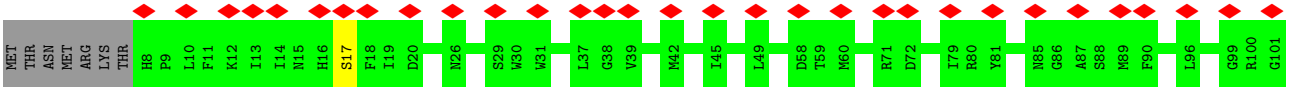


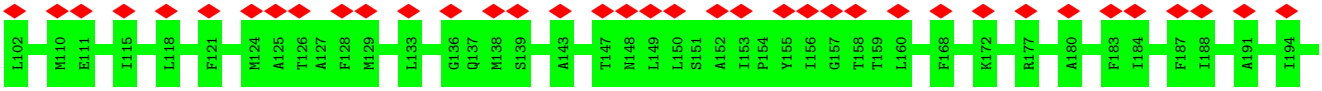


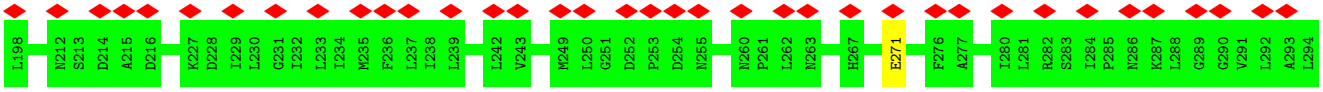
• Molecule 47: Cytochrome b

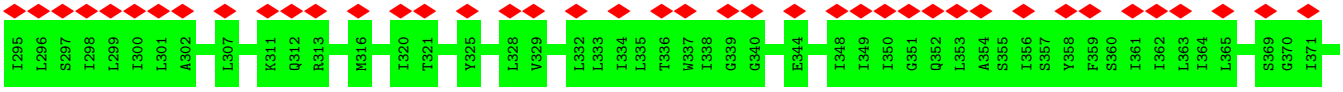
Chain AC:

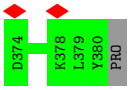






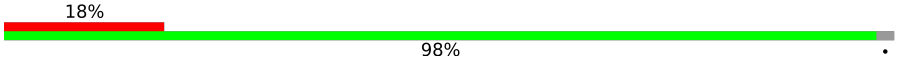


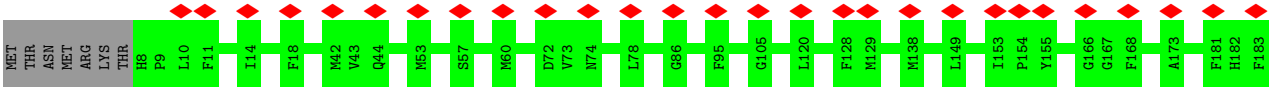


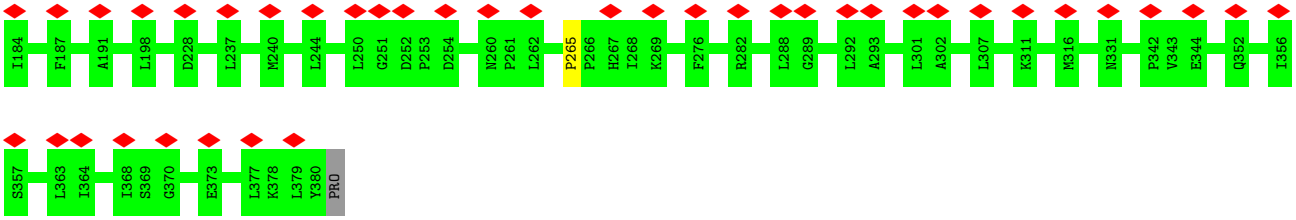


• Molecule 47: Cytochrome b

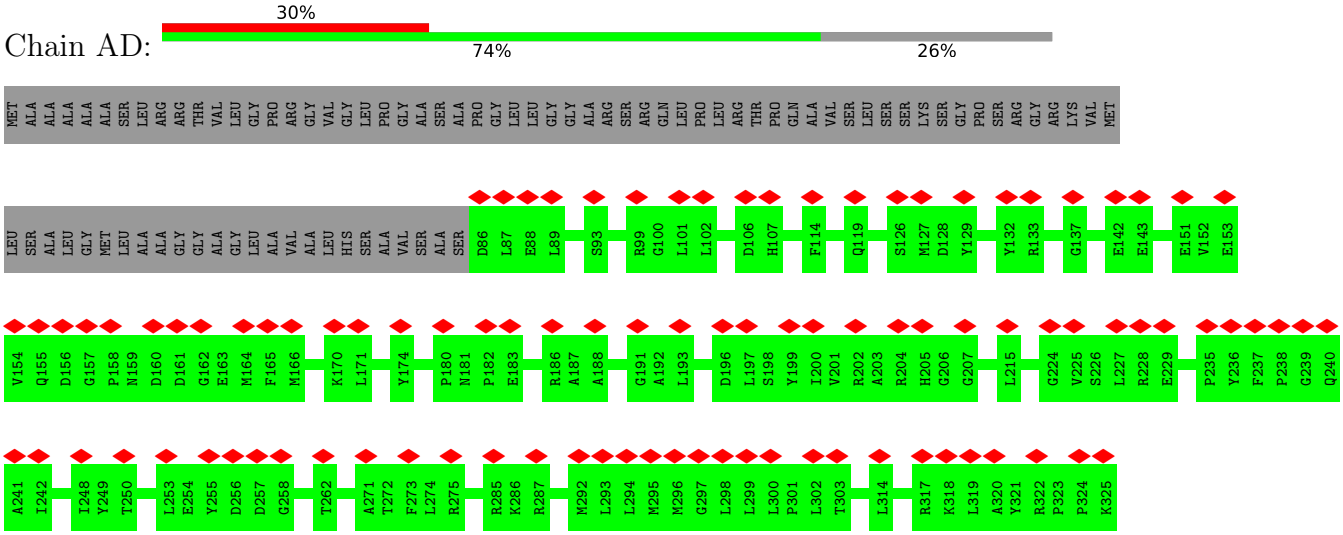
Chain Ac:



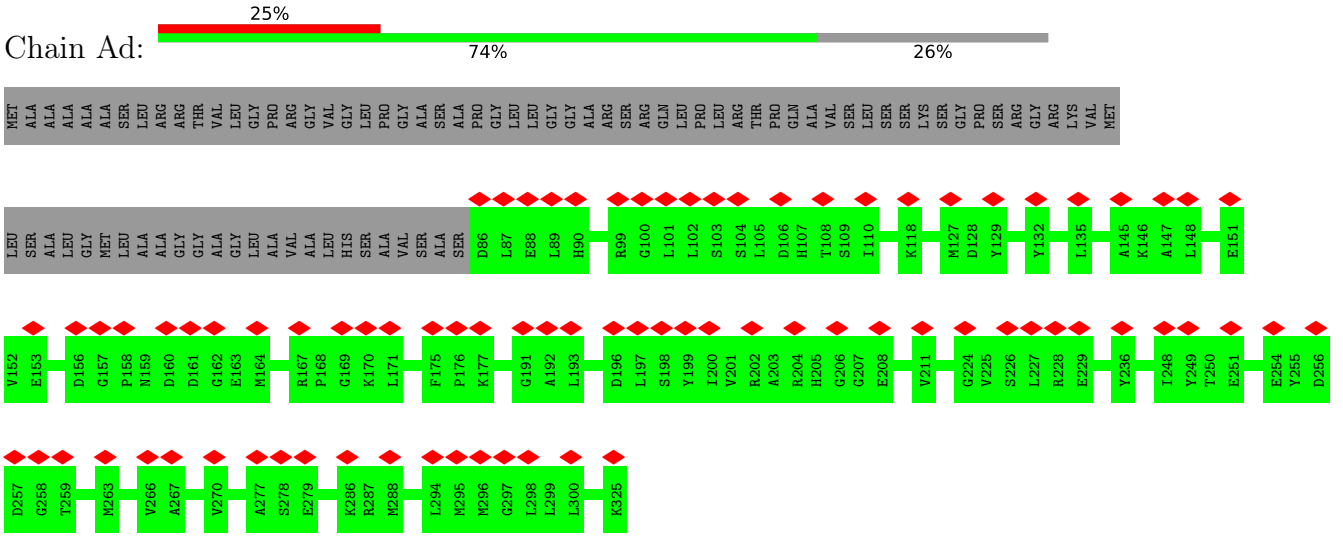




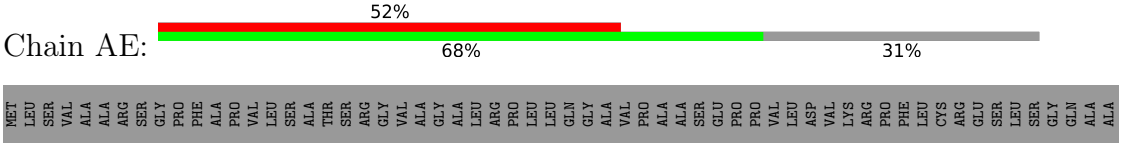
• Molecule 48: Cytochrome c1, heme protein, mitochondrial

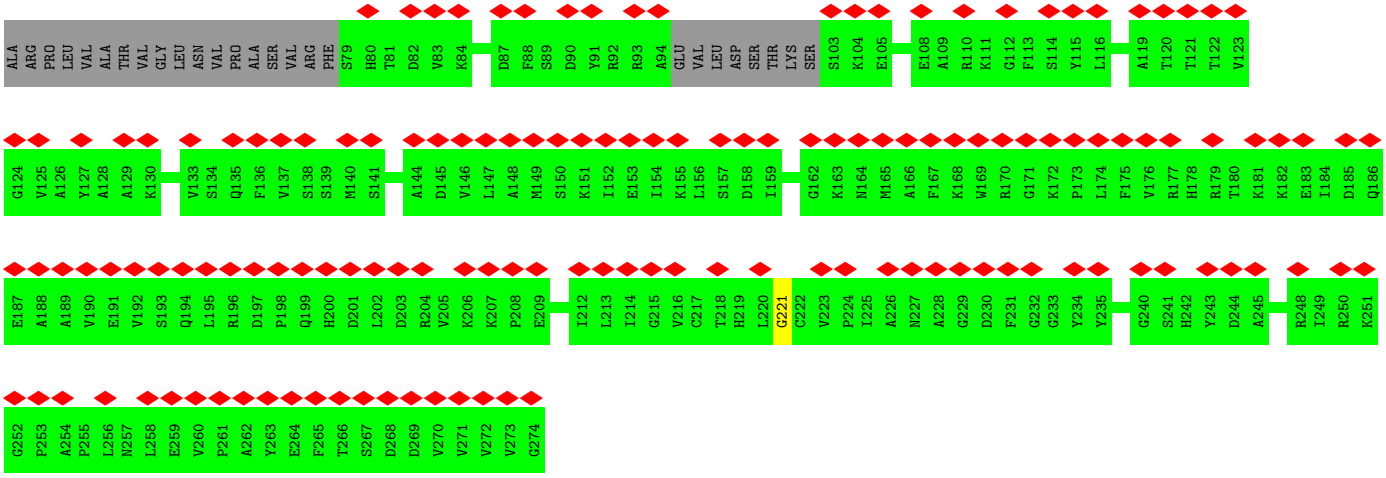


• Molecule 48: Cytochrome c1, heme protein, mitochondrial



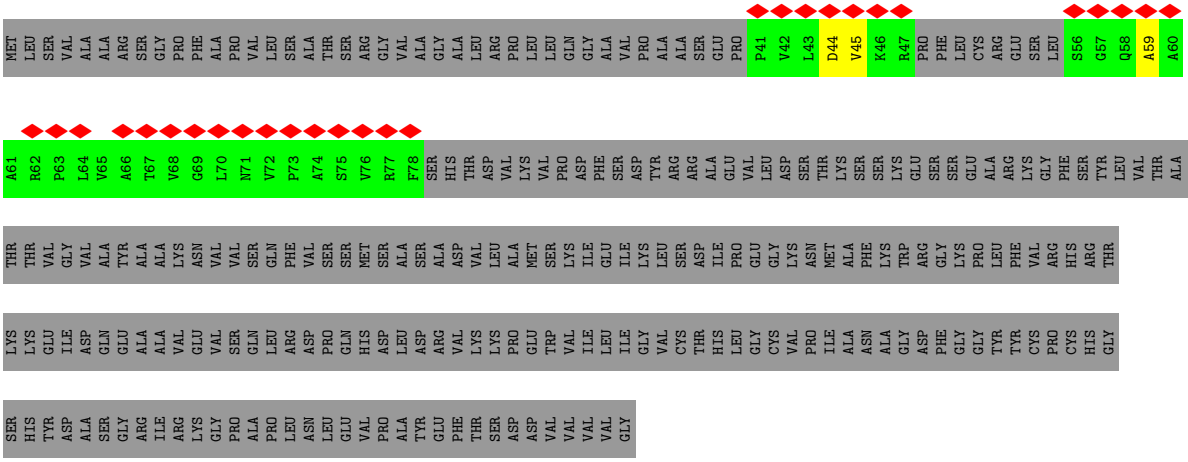
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial





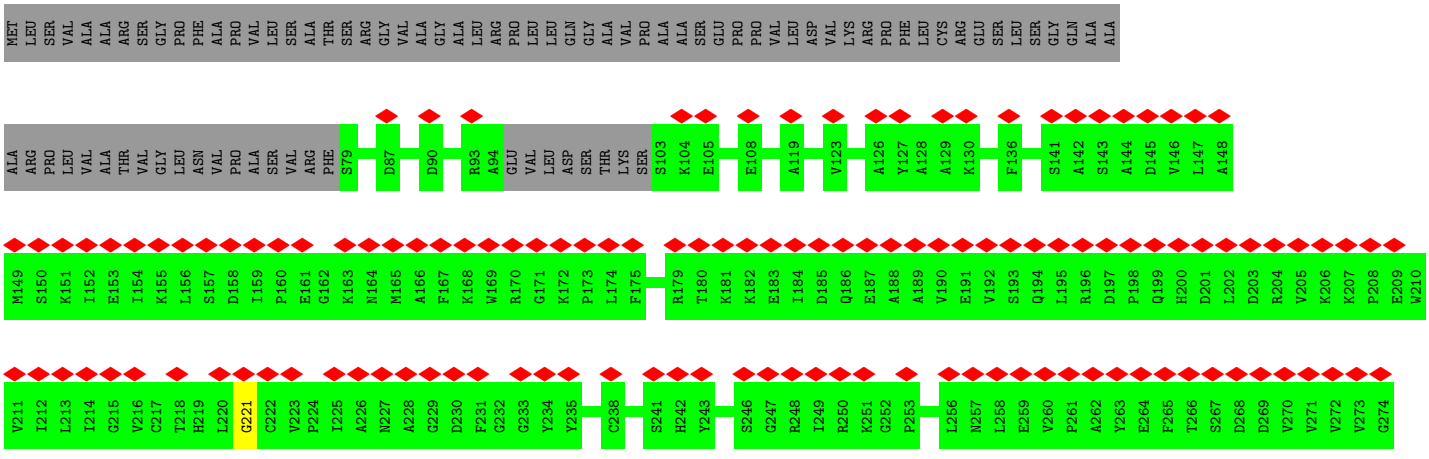
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



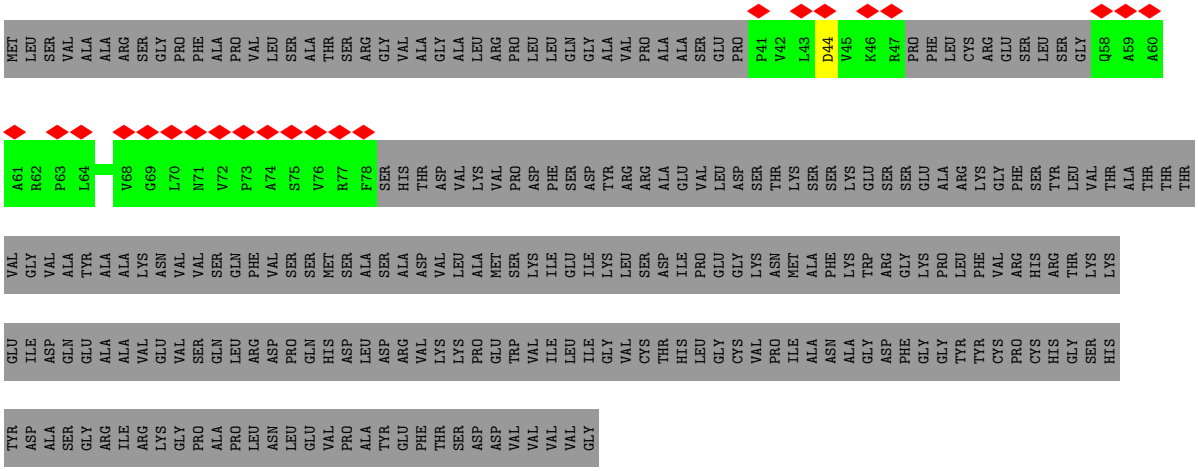
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



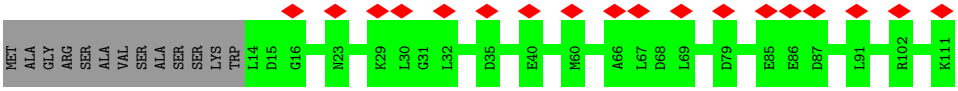
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ai:



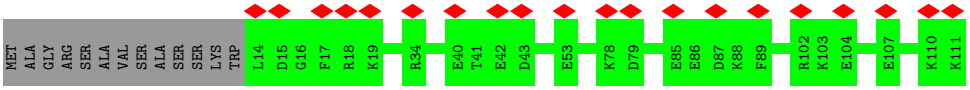
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain AF:



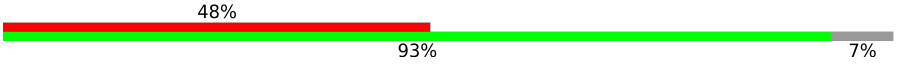
• Molecule 50: Cytochrome b-c1 complex subunit 7

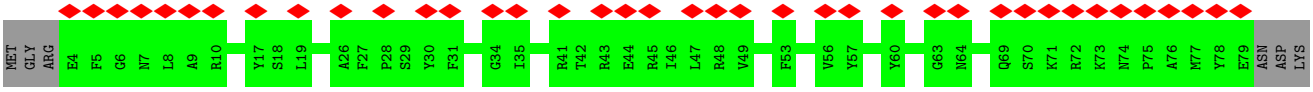
Chain Af:



• Molecule 51: Cytochrome b-c1 complex subunit 8

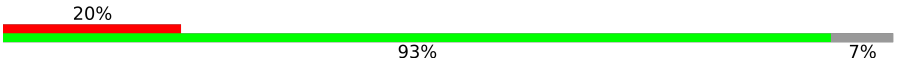
Chain AG:

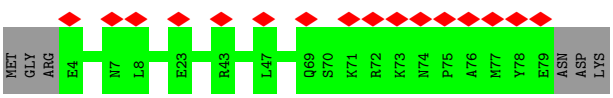




• Molecule 51: Cytochrome b-c1 complex subunit 8

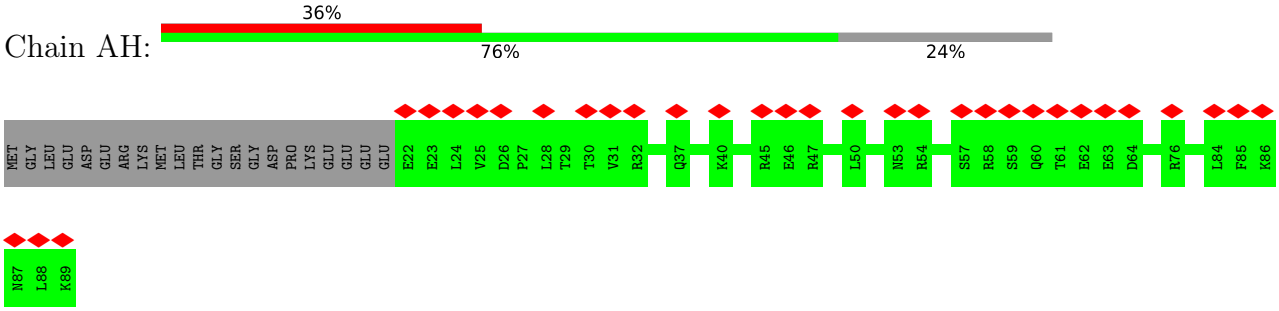
Chain Ag:





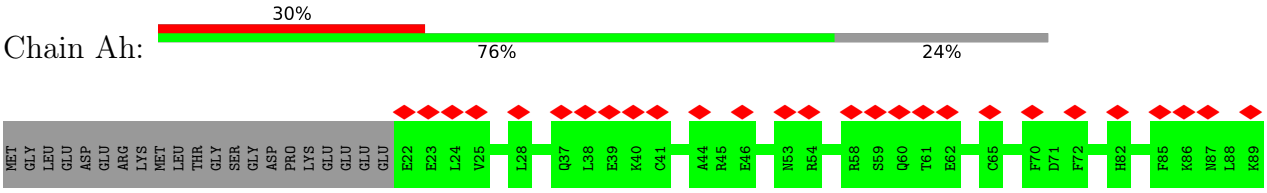
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH:



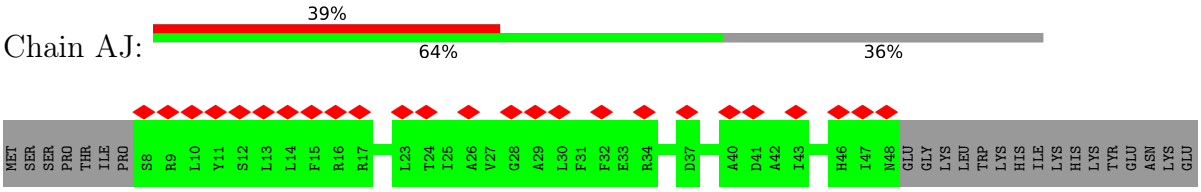
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:



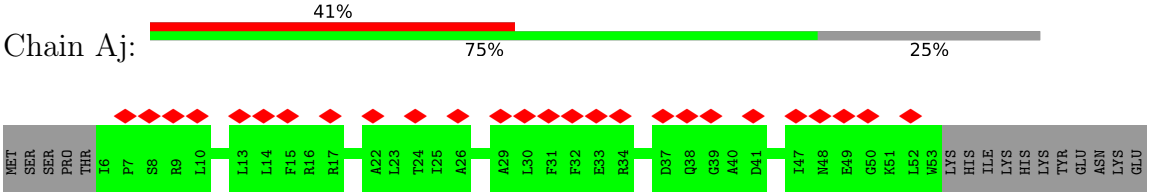
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ:



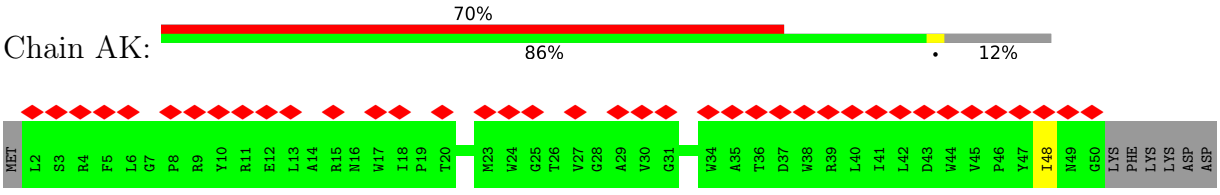
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



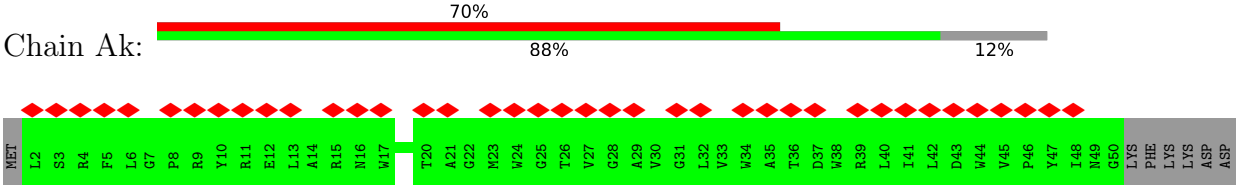
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain AK:



• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28091	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: U10, UQ9, HEM, ADP, ZN, HEC, NDP, CDL, UQ1, UQ6, FMN, EHZ, FES, 3PE, SF4, PC1

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	0.50	0/774	0.66	0/1056
2	B	0.61	0/1289	0.83	2/1744 (0.1%)
3	C	0.55	0/1687	0.78	1/2297 (0.0%)
4	D	0.62	1/3505 (0.0%)	0.90	6/4748 (0.1%)
5	E	0.46	0/1675	0.67	4/2282 (0.2%)
6	F	0.61	4/3363 (0.1%)	0.83	7/4543 (0.2%)
7	G	0.65	5/5374 (0.1%)	0.97	18/7281 (0.2%)
8	H	0.68	3/2608 (0.1%)	0.84	8/3563 (0.2%)
9	I	0.62	1/1461 (0.1%)	0.88	2/1974 (0.1%)
10	J	0.59	2/1318 (0.2%)	0.69	1/1791 (0.1%)
11	K	0.60	0/740	0.83	2/1005 (0.2%)
12	L	0.69	5/4921 (0.1%)	0.90	18/6696 (0.3%)
13	M	0.69	5/3717 (0.1%)	0.91	11/5062 (0.2%)
14	N	0.67	2/2756 (0.1%)	0.85	7/3751 (0.2%)
15	O	0.70	6/2666 (0.2%)	0.79	14/3615 (0.4%)
16	P	0.49	0/2793	0.67	1/3787 (0.0%)
17	Q	0.59	2/980 (0.2%)	0.79	2/1324 (0.2%)
18	R	0.47	0/671	0.58	0/903
19	S	0.64	1/678 (0.1%)	0.85	1/915 (0.1%)
20	T	0.50	1/613 (0.2%)	0.67	1/826 (0.1%)
20	U	0.64	0/712	0.86	2/962 (0.2%)
21	V	0.54	0/937	0.81	4/1270 (0.3%)
22	W	0.50	0/993	0.62	2/1335 (0.1%)
23	X	0.48	0/1422	0.70	0/1921
24	Y	0.53	0/1061	0.64	0/1439
25	Z	0.45	0/1183	0.64	0/1597
26	a	0.55	0/561	0.61	0/755
27	b	0.56	1/643 (0.2%)	0.58	0/884
28	c	0.82	1/400 (0.2%)	0.91	3/544 (0.6%)
29	d	0.61	1/1028 (0.1%)	0.63	2/1387 (0.1%)
30	e	0.57	2/881 (0.2%)	0.65	0/1173
31	f	0.52	0/459	0.53	0/618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.65	1/878 (0.1%)	0.93	3/1196 (0.3%)
33	h	0.52	0/1197	0.75	0/1621
34	i	0.58	1/867 (0.1%)	0.73	0/1179
35	j	0.51	0/603	0.67	0/825
36	k	0.83	2/638 (0.3%)	0.91	3/862 (0.3%)
37	l	0.68	2/1367 (0.1%)	0.76	1/1866 (0.1%)
38	m	0.53	0/1073	0.70	0/1455
39	n	0.66	2/1596 (0.1%)	0.78	2/2162 (0.1%)
40	o	0.54	1/1075 (0.1%)	0.61	0/1442
41	p	0.49	0/1485	0.68	1/2007 (0.0%)
42	q	0.76	4/1234 (0.3%)	0.86	7/1681 (0.4%)
43	r	0.40	0/782	0.59	0/1058
44	s	0.32	0/194	0.57	0/264
45	AA	0.34	0/3213	0.60	1/4355 (0.0%)
45	Aa	0.38	1/3288 (0.0%)	0.60	2/4462 (0.0%)
46	AB	0.32	0/3187	0.57	1/4308 (0.0%)
46	Ab	0.34	0/3142	0.56	1/4246 (0.0%)
47	AC	0.37	1/3089 (0.0%)	0.55	1/4221 (0.0%)
47	Ac	0.38	1/3089 (0.0%)	0.56	0/4221
48	AD	0.33	0/1971	0.53	0/2677
48	Ad	0.37	0/1971	0.50	0/2677
49	AE	0.45	0/1483	0.62	1/2007 (0.0%)
49	AI	0.87	2/219 (0.9%)	0.98	3/296 (1.0%)
49	Ae	0.45	0/1483	0.62	1/2007 (0.0%)
49	Ai	0.65	1/209 (0.5%)	0.72	1/283 (0.4%)
50	AF	0.32	0/884	0.50	0/1184
50	Af	0.33	0/884	0.50	0/1184
51	AG	0.37	0/662	0.55	0/895
51	Ag	0.38	0/662	0.56	0/895
52	AH	0.33	0/569	0.59	0/763
52	Ah	0.33	0/569	0.59	0/763
53	AJ	0.35	0/339	0.48	0/457
53	Aj	0.37	0/401	0.47	0/542
54	AK	0.33	0/416	0.64	1/571 (0.2%)
54	Ak	0.34	0/416	0.52	0/571
All	All	0.55	62/99004 (0.1%)	0.74	149/134251 (0.1%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	247	PRO	N-CD	16.50	1.71	1.47
12	L	265	PRO	N-CD	13.78	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	50	PRO	N-CD	-13.76	1.28	1.47
14	N	255	PRO	N-CD	-13.61	1.28	1.47
42	q	139	PRO	N-CD	-13.44	1.29	1.47
28	c	39	PRO	N-CD	-13.37	1.29	1.47
7	G	532	PRO	N-CD	-12.60	1.30	1.47
15	O	315	PRO	N-CD	-12.14	1.30	1.47
42	q	102	PRO	N-CD	-11.30	1.32	1.47
12	L	234	PRO	N-CD	11.07	1.63	1.47
8	H	42	PRO	N-CD	10.82	1.62	1.47
45	Aa	250	LEU	C-N	10.79	1.58	1.34
13	M	370	PRO	N-CD	-10.74	1.32	1.47
15	O	210	PRO	N-CD	-10.34	1.33	1.47
6	F	227	PRO	N-CD	10.05	1.61	1.47
7	G	275	PRO	N-CD	-9.62	1.34	1.47
8	H	214	GLU	C-N	9.59	1.56	1.34
32	g	78	PRO	N-CD	-9.56	1.34	1.47
29	d	15	PRO	N-CD	-9.51	1.34	1.47
8	H	75	PRO	N-CD	9.19	1.60	1.47
9	I	107	PRO	N-CD	8.59	1.59	1.47
13	M	20	PRO	N-CD	8.55	1.59	1.47
49	AI	45	VAL	C-N	8.53	1.53	1.34
27	b	64	PRO	N-CD	8.47	1.59	1.47
42	q	121	PRO	N-CD	-8.47	1.35	1.47
12	L	212	PRO	N-CD	-8.26	1.36	1.47
47	Ac	265	PRO	N-CD	8.12	1.59	1.47
39	n	155	PRO	N-CD	8.08	1.59	1.47
19	S	63	PRO	N-CD	-8.01	1.36	1.47
49	Ai	44	ASP	C-N	7.84	1.52	1.34
49	AI	44	ASP	C-N	7.84	1.52	1.34
47	AC	271	GLU	C-N	7.81	1.52	1.34
20	T	141	PRO	N-CD	-7.75	1.36	1.47
4	D	365	PRO	N-CD	-7.48	1.37	1.47
37	l	104	PRO	N-CD	-7.38	1.37	1.47
42	q	126	PRO	N-CD	-7.17	1.37	1.47
13	M	208	PRO	N-CD	7.17	1.57	1.47
14	N	238	PRO	N-CD	-7.15	1.37	1.47
6	F	234	GLY	CA-C	-6.90	1.40	1.51
7	G	541	PRO	N-CD	-6.78	1.38	1.47
7	G	449	PRO	N-CD	6.64	1.57	1.47
10	J	118	ASP	C-N	6.50	1.44	1.33
39	n	116	PRO	N-CD	6.45	1.56	1.47
6	F	384	PRO	N-CD	-6.20	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	384	PRO	N-CD	6.13	1.56	1.47
34	i	124	PRO	C-N	6.06	1.48	1.34
12	L	112	PRO	N-CD	6.03	1.56	1.47
15	O	319	ILE	C-N	6.01	1.43	1.33
36	k	20	MET	C-N	5.92	1.47	1.34
37	l	45	PRO	N-CD	-5.89	1.39	1.47
15	O	87	PRO	N-CD	-5.86	1.39	1.47
6	F	235	VAL	N-CA	-5.85	1.34	1.46
13	M	252	PRO	N-CD	-5.70	1.39	1.47
10	J	117	LEU	C-N	-5.64	1.21	1.34
30	e	102	GLU	N-CA	-5.56	1.35	1.46
7	G	683	PRO	N-CD	-5.54	1.40	1.47
15	O	318	THR	C-N	-5.48	1.21	1.34
17	Q	53	ILE	C-O	5.35	1.33	1.23
30	e	101	ARG	CA-C	-5.15	1.39	1.52
40	o	120	ALA	C-N	-5.03	1.22	1.34
13	M	159	PRO	N-CD	5.03	1.54	1.47
17	Q	82	PRO	N-CD	-5.02	1.40	1.47

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	50	PRO	CA-N-CD	9.96	125.64	111.70
14	N	255	PRO	CA-N-CD	9.86	125.51	111.70
42	q	139	PRO	CA-N-CD	9.58	125.11	111.70
45	AA	366	ASP	CB-CG-OD1	9.44	126.79	118.30
45	Aa	366	ASP	CB-CG-OD1	9.42	126.78	118.30
15	O	247	PRO	N-CA-CB	9.13	114.26	103.30
5	E	219	SER	N-CA-CB	9.01	124.01	110.50
6	F	334	THR	N-CA-CB	8.95	127.31	110.30
15	O	247	PRO	CA-N-CD	-8.76	99.23	111.50
15	O	315	PRO	CA-N-CD	8.73	123.93	111.70
7	G	532	PRO	CA-N-CD	8.54	123.66	111.70
7	G	632	ILE	N-CA-C	-8.52	88.01	111.00
36	k	50	PRO	N-CA-CB	-8.15	93.51	103.30
22	W	98	LYS	N-CA-C	-8.15	88.99	111.00
28	c	39	PRO	CA-N-CD	8.15	123.11	111.70
7	G	174	THR	N-CA-C	-8.13	89.04	111.00
17	Q	60	ASP	N-CA-C	-7.65	90.34	111.00
42	q	102	PRO	CA-N-CD	7.64	122.40	111.70
6	F	411	SER	N-CA-CB	7.52	121.78	110.50
12	L	265	PRO	CA-N-CD	-7.40	101.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	204	MET	N-CA-C	-7.22	91.49	111.00
14	N	255	PRO	N-CA-CB	-7.22	94.64	103.30
20	U	75	THR	N-CA-CB	7.12	123.83	110.30
6	F	332	CYS	N-CA-C	7.05	130.05	111.00
32	g	78	PRO	CA-N-CD	6.99	121.49	111.70
12	L	265	PRO	N-CA-CB	6.99	111.69	103.30
15	O	210	PRO	CA-N-CD	6.98	121.47	111.70
28	c	47	SER	N-CA-CB	6.96	120.95	110.50
8	H	311	THR	N-CA-CB	6.95	123.50	110.30
13	M	213	HIS	CB-CA-C	-6.79	96.81	110.40
7	G	300	GLN	N-CA-CB	6.63	122.54	110.60
7	G	275	PRO	CA-N-CD	6.63	120.98	111.70
28	c	39	PRO	N-CA-CB	-6.62	95.32	102.60
15	O	320	GLY	N-CA-C	-6.62	96.56	113.10
29	d	15	PRO	CA-N-CD	6.61	120.95	111.70
16	P	106	LEU	N-CA-C	6.55	128.70	111.00
45	Aa	250	LEU	O-C-N	-6.55	112.22	122.70
36	k	59	TYR	N-CA-CB	-6.55	98.81	110.60
8	H	214	GLU	N-CA-CB	-6.52	98.86	110.60
6	F	125	CYS	N-CA-C	-6.50	93.46	111.00
15	O	318	THR	O-C-N	-6.49	112.31	122.70
4	D	214	TYR	CB-CA-C	-6.38	97.64	110.40
39	n	115	TYR	N-CA-CB	6.38	122.08	110.60
8	H	52	ALA	N-CA-CB	6.37	119.02	110.10
4	D	427	PRO	N-CA-C	-6.37	95.55	112.10
13	M	370	PRO	N-CA-C	6.33	128.56	112.10
9	I	154	TYR	N-CA-CB	-6.32	99.23	110.60
42	q	139	PRO	N-CA-CB	-6.31	95.66	102.60
8	H	196	ALA	N-CA-C	6.28	127.94	111.00
13	M	424	ILE	N-CA-C	-6.25	94.11	111.00
14	N	255	PRO	N-CA-C	6.23	128.31	112.10
13	M	370	PRO	CA-N-CD	6.23	120.42	111.70
49	AI	59	ALA	N-CA-CB	-6.21	101.40	110.10
14	N	81	LEU	N-CA-C	-6.16	94.37	111.00
32	g	137	SER	N-CA-CB	-6.13	101.30	110.50
7	G	133	GLN	N-CA-CB	6.10	121.58	110.60
7	G	212	LYS	N-CA-C	-6.08	94.59	111.00
4	D	140	ASP	N-CA-C	-6.02	94.75	111.00
15	O	315	PRO	N-CA-CB	-6.00	95.99	102.60
42	q	30	ALA	N-CA-CB	6.00	118.50	110.10
12	L	231	PRO	N-CA-C	6.00	127.69	112.10
12	L	234	PRO	CA-N-CD	-5.97	103.15	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	276	THR	N-CA-CB	5.96	121.62	110.30
14	N	218	ALA	N-CA-CB	5.95	118.43	110.10
12	L	554	ASP	N-CA-CB	5.93	121.27	110.60
12	L	605	ASN	N-CA-CB	5.92	121.25	110.60
5	E	50	THR	N-CA-CB	5.92	121.54	110.30
12	L	483	PRO	N-CA-C	-5.90	96.77	112.10
15	O	67	CYS	N-CA-CB	-5.85	100.06	110.60
7	G	389	THR	N-CA-CB	5.85	121.42	110.30
7	G	251	ILE	N-CA-C	5.84	126.78	111.00
8	H	98	LEU	N-CA-CB	-5.79	98.82	110.40
4	D	329	ARG	CB-CA-C	5.78	121.97	110.40
19	S	63	PRO	CA-N-CD	5.77	119.78	111.70
13	M	49	TYR	N-CA-CB	-5.75	100.25	110.60
11	K	83	ASN	N-CA-CB	5.74	120.92	110.60
42	q	102	PRO	N-CA-CB	-5.73	96.29	102.60
20	U	150	ASP	CB-CA-C	5.73	121.86	110.40
7	G	510	TRP	N-CA-CB	5.72	120.89	110.60
29	d	15	PRO	N-CA-CB	-5.72	96.31	102.60
15	O	318	THR	CA-C-N	5.69	129.71	117.20
17	Q	141	ASN	N-CA-CB	5.67	120.81	110.60
8	H	223	PHE	CB-CA-C	-5.65	99.09	110.40
13	M	223	ALA	N-CA-CB	5.65	118.01	110.10
2	B	80	ASP	N-CA-CB	5.64	120.76	110.60
7	G	599	THR	N-CA-C	5.64	126.22	111.00
14	N	89	GLN	N-CA-CB	-5.63	100.46	110.60
47	AC	17	SER	N-CA-CB	-5.62	102.06	110.50
42	q	121	PRO	CA-N-CD	5.61	119.55	111.70
15	O	118	TYR	N-CA-CB	-5.58	100.56	110.60
12	L	415	ALA	N-CA-CB	5.56	117.89	110.10
7	G	580	ALA	N-CA-CB	5.56	117.88	110.10
21	V	56	LEU	CA-CB-CG	5.53	128.03	115.30
3	C	125	PHE	N-CA-CB	-5.53	100.64	110.60
8	H	252	PRO	CA-N-CD	5.52	119.43	111.70
49	AE	221	GLY	N-CA-C	5.51	126.88	113.10
13	M	311	GLY	N-CA-C	-5.51	99.33	113.10
39	n	136	GLU	CB-CA-C	5.50	121.41	110.40
49	Ae	221	GLY	N-CA-C	5.49	126.83	113.10
15	O	118	TYR	N-CA-C	5.48	125.80	111.00
7	G	389	THR	N-CA-C	-5.48	96.20	111.00
21	V	19	THR	N-CA-CB	5.46	120.68	110.30
9	I	160	GLU	N-CA-CB	-5.46	100.77	110.60
12	L	582	GLY	N-CA-C	-5.44	99.50	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	246	LEU	C-N-CD	5.44	139.82	128.40
7	G	651	PRO	CB-CA-C	-5.42	98.45	112.00
42	q	105	ALA	N-CA-CB	5.40	117.66	110.10
21	V	114	TRP	N-CA-CB	5.37	120.26	110.60
13	M	276	CYS	N-CA-CB	5.36	120.25	110.60
13	M	330	ALA	N-CA-CB	5.35	117.59	110.10
6	F	457	HIS	N-CA-CB	-5.35	100.97	110.60
15	O	152	SER	N-CA-CB	5.34	118.52	110.50
54	AK	48	ILE	CB-CA-C	-5.34	100.93	111.60
7	G	362	ASP	N-CA-C	5.33	125.40	111.00
12	L	151	SER	N-CA-CB	5.33	118.50	110.50
12	L	248	HIS	CB-CA-C	5.33	121.07	110.40
49	AI	44	ASP	O-C-N	5.33	131.23	122.70
49	Ai	44	ASP	O-C-N	5.32	131.22	122.70
12	L	194	ASN	N-CA-C	5.31	125.35	111.00
5	E	218	ARG	CB-CA-C	-5.31	99.78	110.40
6	F	418	GLN	N-CA-CB	5.31	120.16	110.60
12	L	212	PRO	N-CA-C	5.25	125.74	112.10
11	K	70	GLU	N-CA-CB	5.24	120.04	110.60
8	H	51	ASP	CB-CA-C	-5.23	99.94	110.40
49	AI	45	VAL	C-N-CA	-5.23	108.62	121.70
12	L	277	MET	CB-CA-C	-5.22	99.96	110.40
13	M	423	MET	N-CA-C	-5.22	96.92	111.00
12	L	234	PRO	N-CA-CB	5.21	109.55	103.30
46	AB	305	THR	N-CA-CB	-5.21	100.41	110.30
46	Ab	305	THR	N-CA-CB	-5.19	100.43	110.30
12	L	212	PRO	CA-N-CD	5.19	118.96	111.70
20	T	141	PRO	N-CA-CB	-5.19	96.89	102.60
2	B	195	PRO	N-CA-C	-5.17	98.66	112.10
37	l	104	PRO	CA-N-CD	5.16	118.92	111.70
10	J	117	LEU	O-C-N	-5.15	114.46	122.70
12	L	247	LEU	N-CA-CB	5.13	120.67	110.40
4	D	365	PRO	CA-N-CD	5.13	118.88	111.70
4	D	323	ARG	N-CA-C	5.11	124.79	111.00
5	E	154	LYS	N-CA-CB	5.09	119.77	110.60
13	M	83	HIS	N-CA-C	-5.09	97.25	111.00
6	F	228	PRO	N-CA-C	-5.08	98.88	112.10
7	G	77	MET	N-CA-C	-5.06	97.35	111.00
41	p	94	ARG	NE-CZ-NH1	5.06	122.83	120.30
15	O	210	PRO	N-CA-CB	-5.05	97.04	102.60
14	N	228	ASN	N-CA-CB	5.05	119.69	110.60
21	V	86	LYS	N-CA-CB	5.04	119.68	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	668	ALA	N-CA-CB	5.04	117.16	110.10
32	g	78	PRO	N-CA-CB	-5.03	97.06	102.60
22	W	98	LYS	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	88/115 (76%)	83 (94%)	5 (6%)	0	100 100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	10 42
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100 100
4	D	420/463 (91%)	401 (96%)	19 (4%)	0	100 100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100 100
6	F	424/464 (91%)	409 (96%)	15 (4%)	0	100 100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100 100
8	H	313/318 (98%)	298 (95%)	14 (4%)	1 (0%)	37 71
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100 100
10	J	165/172 (96%)	157 (95%)	8 (5%)	0	100 100
11	K	95/98 (97%)	93 (98%)	2 (2%)	0	100 100
12	L	604/607 (100%)	571 (94%)	33 (6%)	0	100 100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37 71
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100 100
16	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	37 71
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100 100
18	R	81/116 (70%)	78 (96%)	3 (4%)	0	100 100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100 100
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100 100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100 100
21	V	110/116 (95%)	106 (96%)	4 (4%)	0	100 100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100 100
23	X	167/172 (97%)	154 (92%)	13 (8%)	0	100 100
24	Y	138/143 (96%)	135 (98%)	3 (2%)	0	100 100
25	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100 100
26	a	65/70 (93%)	62 (95%)	3 (5%)	0	100 100
27	b	77/84 (92%)	72 (94%)	5 (6%)	0	100 100
28	c	45/76 (59%)	45 (100%)	0	0	100 100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100 100
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100 100
31	f	50/57 (88%)	50 (100%)	0	0	100 100
32	g	99/151 (66%)	93 (94%)	6 (6%)	0	100 100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100 100
34	i	96/128 (75%)	87 (91%)	9 (9%)	0	100 100
35	j	66/105 (63%)	60 (91%)	6 (9%)	0	100 100
36	k	74/104 (71%)	71 (96%)	3 (4%)	0	100 100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100 100
38	m	123/129 (95%)	116 (94%)	7 (6%)	0	100 100
39	n	176/179 (98%)	167 (95%)	8 (4%)	1 (1%)	22 59
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100 100
41	p	170/176 (97%)	157 (92%)	13 (8%)	0	100 100
42	q	141/145 (97%)	138 (98%)	3 (2%)	0	100 100
43	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	12 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	s	20/104 (19%)	20 (100%)	0	0	100	100
45	AA	397/480 (83%)	388 (98%)	9 (2%)	0	100	100
45	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
46	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
46	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
48	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
48	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
49	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	Ai	24/274 (9%)	23 (96%)	1 (4%)	0	100	100
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	74 (100%)	0	0	100	100
52	AH	66/89 (74%)	66 (100%)	0	0	100	100
52	Ah	66/89 (74%)	66 (100%)	0	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	46 (100%)	0	0	100	100
54	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
54	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	11921/14392 (83%)	11425 (96%)	489 (4%)	7 (0%)	50	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
8	H	88	PRO
16	P	329	PRO
2	B	171	TYR
43	r	39	PRO
39	n	156	PRO

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Mol	Chain	Res	Type
2	B	195	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	79	84
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	366 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	579 (100%)	0	100	100
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/138 (99%)	136 (100%)	0	100	100
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	549 (100%)	0	100	100
13	M	415/415 (100%)	415 (100%)	0	100	100
14	N	307/308 (100%)	307 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	296/325 (91%)	296 (100%)	0	100	100
17	Q	105/153 (69%)	105 (100%)	0	100	100
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	80/135 (59%)	80 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	152/154 (99%)	151 (99%)	1 (1%)	81	86
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	94/120 (78%)	94 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	59/78 (76%)	59 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	112/121 (93%)	112 (100%)	0	100	100
41	p	156/158 (99%)	156 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	85/96 (88%)	85 (100%)	0	100	100
44	s	22/95 (23%)	22 (100%)	0	100	100
45	AA	341/398 (86%)	340 (100%)	1 (0%)	91	92
45	Aa	349/398 (88%)	348 (100%)	1 (0%)	91	92
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	324/356 (91%)	324 (100%)	0	100	100
47	AC	325/333 (98%)	325 (100%)	0	100	100
47	Ac	325/333 (98%)	325 (100%)	0	100	100
48	AD	205/260 (79%)	205 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	158/224 (70%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	AI	23/224 (10%)	23 (100%)	0	100	100
49	Ae	158/224 (70%)	158 (100%)	0	100	100
49	Ai	22/224 (10%)	22 (100%)	0	100	100
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	65/83 (78%)	65 (100%)	0	100	100
52	Ah	65/83 (78%)	65 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	39/46 (85%)	39 (100%)	0	100	100
54	Ak	39/46 (85%)	39 (100%)	0	100	100
All	All	10476/12261 (85%)	10472 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR
23	X	57	LEU
45	AA	403	LEU
45	Aa	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (207) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	108	GLN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	73	GLN
3	C	88	HIS
3	C	104	ASN
3	C	123	ASN
3	C	179	ASN

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Mol	Chain	Res	Type
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	60	HIS
4	D	79	ASN
4	D	83	ASN
4	D	88	HIS
4	D	92	HIS
4	D	112	HIS
4	D	117	HIS
4	D	147	ASN
4	D	160	ASN
4	D	168	GLN
4	D	182	ASN
4	D	270	ASN
4	D	381	HIS
5	E	68	ASN
5	E	132	GLN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	270	ASN
6	F	303	HIS
6	F	346	GLN
6	F	418	GLN
6	F	441	HIS
7	G	74	ASN
7	G	140	GLN
7	G	205	GLN
7	G	260	ASN
7	G	406	ASN
7	G	444	HIS
7	G	495	ASN
7	G	514	ASN
7	G	571	HIS
7	G	666	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	169	GLN
8	H	171	HIS

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Mol	Chain	Res	Type
8	H	287	HIS
8	H	292	ASN
10	J	85	ASN
10	J	107	ASN
11	K	7	ASN
11	K	25	HIS
12	L	2	ASN
12	L	25	ASN
12	L	58	ASN
12	L	135	ASN
12	L	139	GLN
12	L	170	GLN
12	L	194	ASN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	296	ASN
12	L	321	GLN
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	ASN
12	L	572	ASN
12	L	579	ASN
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN
13	M	168	GLN
13	M	170	HIS
13	M	175	ASN
13	M	184	HIS
13	M	192	ASN
13	M	213	HIS
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	349	GLN
13	M	374	ASN
13	M	390	ASN
14	N	120	GLN
14	N	134	GLN

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Mol	Chain	Res	Type
14	N	204	ASN
14	N	273	ASN
14	N	310	ASN
14	N	317	GLN
15	O	71	ASN
15	O	80	GLN
15	O	175	ASN
15	O	219	GLN
15	O	286	GLN
15	O	292	HIS
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	71	ASN
16	P	79	GLN
16	P	102	GLN
16	P	154	GLN
16	P	216	HIS
16	P	251	ASN
16	P	269	ASN
16	P	275	HIS
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	86	ASN
17	Q	88	GLN
18	R	56	ASN
19	S	25	GLN
19	S	48	HIS
21	V	41	HIS
22	W	54	GLN
22	W	94	GLN
22	W	105	HIS
23	X	69	ASN
23	X	73	GLN
23	X	77	HIS
23	X	140	ASN
23	X	151	ASN
24	Y	46	ASN
24	Y	81	GLN
24	Y	91	ASN
24	Y	108	HIS

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Mol	Chain	Res	Type
25	Z	137	ASN
26	a	31	ASN
27	b	83	ASN
29	d	59	HIS
30	e	29	ASN
31	f	10	HIS
32	g	146	GLN
33	h	170	GLN
33	h	181	HIS
34	i	74	HIS
34	i	83	HIS
35	j	41	GLN
36	k	39	GLN
36	k	66	ASN
37	l	91	GLN
37	l	106	HIS
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	13	GLN
39	n	14	GLN
39	n	33	HIS
39	n	53	ASN
39	n	76	HIS
40	o	110	GLN
41	p	23	GLN
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	31	ASN
42	q	52	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS
43	r	21	GLN
43	r	29	GLN
43	r	52	ASN
43	r	110	GLN
44	s	59	GLN
45	AA	87	ASN
45	AA	160	GLN

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Mol	Chain	Res	Type
45	AA	173	GLN
45	AA	181	ASN
45	AA	207	ASN
45	AA	402	HIS
46	AB	167	GLN
46	AB	298	HIS
46	AB	304	ASN
46	AB	415	GLN
47	AC	312	GLN
47	AC	341	GLN
48	AD	115	GLN
49	AE	242	HIS
49	AI	71	ASN
54	AK	16	ASN
45	Aa	87	ASN
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	207	ASN
46	Ab	167	GLN
46	Ab	298	HIS
46	Ab	304	ASN
46	Ab	415	GLN
47	Ac	201	HIS
47	Ac	312	GLN
47	Ac	341	GLN
48	Ad	115	GLN
48	Ad	190	ASN
49	Ae	242	HIS
54	Ak	16	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 61 ligands modelled in this entry, 1 is monoatomic - leaving 60 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	$\#\|Z\| > 2$
56	CDL	A	402	-	91,91,99	0.95	4 (4%)	97,103,111	1.09	6 (6%)
57	SF4	I	303	9	0,12,12	-	-	-		
67	HEM	Ac	402	47	41,50,50	1.25	3 (7%)	45,82,82	1.71	8 (17%)
56	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.25	6 (9%)
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.09	3 (5%)
66	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
56	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
55	3PE	m	202	-	40,40,50	1.01	2 (5%)	43,45,55	1.21	5 (11%)
62	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
57	SF4	B	301	2	0,12,12	-	-	-		
68	U10	AC	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.10	7 (25%)
55	3PE	M	501	-	36,36,50	1.06	2 (5%)	39,41,55	1.07	3 (7%)
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.08	3 (5%)
62	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
55	3PE	L	704	-	37,37,50	1.05	2 (5%)	40,42,55	1.18	4 (10%)
55	3PE	H	402	-	45,45,50	0.92	2 (4%)	48,50,55	1.33	5 (10%)
67	HEM	AC	402	47	41,50,50	1.23	4 (9%)	45,82,82	1.70	8 (17%)
68	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
67	HEM	Ac	401	47	41,50,50	1.22	4 (9%)	45,82,82	1.68	8 (17%)
69	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
55	3PE	Y	201	-	38,38,50	1.03	2 (5%)	41,43,55	1.11	3 (7%)
57	SF4	G	802	7	0,12,12	-	-	-		
57	SF4	I	302	9	0,12,12	-	-	-		
59	FES	G	803	7	0,4,4	-	-	-		
58	UQ1	D	501	-	18,18,18	1.32	3 (16%)	22,25,25	1.61	5 (22%)
66	EHZ	n	201	-	27,31,37	1.88	7 (25%)	37,41,47	1.69	8 (21%)
56	CDL	L	703	-	73,73,99	1.06	4 (5%)	79,85,111	1.15	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	HEC	Ad	401	48	32,50,50	2.17	3 (9%)	24,82,82	1.64	5 (20%)
55	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
56	CDL	h	201	-	92,92,99	0.94	4 (4%)	98,104,111	1.12	6 (6%)
62	PC1	l	201	-	49,49,53	0.96	2 (4%)	55,57,61	1.01	4 (7%)
62	PC1	L	701	-	47,47,53	0.99	2 (4%)	53,55,61	1.09	3 (5%)
55	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.21	3 (8%)
62	PC1	Ae	301	-	34,34,53	1.17	2 (5%)	40,42,61	1.18	4 (10%)
56	CDL	d	201	-	83,83,99	1.00	4 (4%)	89,95,111	1.10	5 (5%)
63	ADP	O	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
64	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.20	4 (7%)
56	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.36	6 (11%)
55	3PE	J	201	-	45,45,50	0.96	2 (4%)	48,50,55	1.08	3 (6%)
55	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
55	3PE	m	201	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	4 (7%)
55	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.73	1 (4%)
56	CDL	AG	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.33	6 (12%)
67	HEM	AC	403	47	41,50,50	1.27	3 (7%)	45,82,82	1.72	9 (20%)
55	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.20	2 (8%)
55	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.14	3 (8%)
56	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.35	6 (12%)
55	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
56	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
56	CDL	M	503	-	78,78,99	1.02	4 (5%)	84,90,111	1.11	6 (7%)
59	FES	E	301	5	0,4,4	-	-	-		
60	FMN	F	501	-	33,33,33	1.38	5 (15%)	48,50,50	1.23	7 (14%)
55	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
70	HEC	AD	401	48	32,50,50	2.16	3 (9%)	24,82,82	1.62	5 (20%)
56	CDL	Y	202	-	80,80,99	1.01	4 (5%)	86,92,111	1.13	6 (6%)
69	UQ6	AC	406	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
61	UQ9	H	401	-	35,35,58	0.84	3 (8%)	42,45,73	0.63	1 (2%)
57	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	i	201	-	39,39,50	1.05	2 (5%)	42,44,55	1.03	2 (4%)
57	SF4	G	801	7	0,12,12	-	-	-		

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
56	CDL	A	402	-	-	24/102/102/110	-
57	SF4	I	303	9	-	-	0/6/5/5
67	HEM	Ac	402	47	-	6/12/54/54	-
56	CDL	AG	102	-	-	15/66/66/110	-
55	3PE	L	702	-	-	14/52/52/54	-
66	EHZ	W	201	-	-	12/39/39/45	-
56	CDL	q	201	-	-	15/67/67/110	-
55	3PE	m	202	-	-	8/44/44/54	-
62	PC1	I	301	-	-	10/50/50/57	-
68	U10	AC	405	-	-	6/15/39/87	0/1/1/1
57	SF4	B	301	2	-	-	0/6/5/5
55	3PE	M	501	-	-	11/40/40/54	-
55	3PE	M	502	-	-	13/54/54/54	-
62	PC1	q	202	-	-	14/38/38/57	-
55	3PE	L	704	-	-	7/41/41/54	-
55	3PE	H	402	-	-	11/49/49/54	-
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
67	HEM	Ac	401	47	-	7/12/54/54	-
55	3PE	Y	201	-	-	5/42/42/54	-
57	SF4	G	802	7	-	-	0/6/5/5
57	SF4	I	302	9	-	-	0/6/5/5
59	FES	G	803	7	-	-	0/1/1/1
58	UQ1	D	501	-	-	6/9/33/33	0/1/1/1
66	EHZ	n	201	-	-	19/39/39/45	-
56	CDL	L	703	-	-	18/84/84/110	-
70	HEC	Ad	401	48	-	0/10/54/54	-
55	3PE	AG	103	-	-	9/54/54/54	-
56	CDL	h	201	-	-	27/103/103/110	-
62	PC1	l	201	-	-	8/53/53/57	-
62	PC1	L	701	-	-	11/51/51/57	-
55	3PE	Ac	403	-	-	3/38/38/54	-
62	PC1	Ae	301	-	-	7/38/38/57	-
56	CDL	d	201	-	-	17/94/94/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	ADP	O	401	-	-	3/12/32/32	0/3/3/3
64	NDP	P	401	-	-	2/30/77/77	0/5/5/5
56	CDL	Aa	502	-	-	13/56/56/110	-
55	3PE	J	201	-	-	12/49/49/54	-
55	3PE	b	201	-	-	10/49/49/54	-
55	3PE	m	201	-	-	14/54/54/54	-
55	3PE	AC	401	-	-	7/26/26/54	-
56	CDL	AG	101	-	-	8/52/52/110	-
67	HEM	AC	403	47	-	6/12/54/54	-
55	3PE	Aa	501	-	-	7/26/26/54	-
55	3PE	AC	404	-	-	1/38/38/54	-
56	CDL	Ag	101	-	-	7/52/52/110	-
55	3PE	Ag	103	-	-	10/54/54/54	-
56	CDL	Ag	102	-	-	13/66/66/110	-
56	CDL	M	503	-	-	26/89/89/110	-
59	FES	E	301	5	-	-	0/1/1/1
57	SF4	F	502	6	-	-	0/6/5/5
60	FMN	F	501	-	-	0/18/18/18	0/3/3/3
55	3PE	A	401	-	-	18/49/49/54	-
70	HEC	AD	401	48	-	0/10/54/54	-
56	CDL	Y	202	-	-	24/91/91/110	-
69	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
61	UQ9	H	401	-	-	15/30/54/81	0/1/1/1
67	HEM	AC	402	47	-	7/12/54/54	-
55	3PE	i	201	-	-	13/43/43/54	-
57	SF4	G	801	7	-	-	0/6/5/5

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	Ad	401	HEC	C3C-C2C	-6.46	1.34	1.40
70	AD	401	HEC	C3C-C2C	-6.40	1.34	1.40
70	Ad	401	HEC	C2B-C3B	-6.15	1.34	1.40
70	AD	401	HEC	C2B-C3B	-6.07	1.34	1.40
70	Ad	401	HEC	C3D-C2D	5.48	1.53	1.37
70	AD	401	HEC	C3D-C2D	5.41	1.53	1.37
66	n	201	EHZ	C15-N2	5.33	1.45	1.33
66	n	201	EHZ	C12-N1	5.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	W	201	EHZ	C15-N2	5.15	1.44	1.33
66	W	201	EHZ	C12-N1	5.03	1.44	1.33
60	F	501	FMN	C9A-C5A	4.80	1.49	1.41
62	L	701	PC1	O31-C31	4.34	1.46	1.33
62	Ae	301	PC1	O31-C31	4.33	1.46	1.33
56	A	402	CDL	OA8-CA7	4.29	1.45	1.33
55	i	201	3PE	O31-C31	4.26	1.45	1.33
55	b	201	3PE	O31-C31	4.26	1.45	1.33
55	M	501	3PE	O31-C31	4.25	1.45	1.33
56	M	503	CDL	OA8-CA7	4.24	1.45	1.33
56	Y	202	CDL	OB8-CB7	4.24	1.45	1.33
56	Aa	502	CDL	OA8-CA7	4.24	1.45	1.33
55	i	201	3PE	O21-C21	4.24	1.46	1.34
56	h	201	CDL	OA8-CA7	4.24	1.45	1.33
56	d	201	CDL	OA8-CA7	4.24	1.45	1.33
56	Aa	502	CDL	OB8-CB7	4.24	1.45	1.33
56	AG	101	CDL	OA8-CA7	4.24	1.45	1.33
55	AC	404	3PE	O31-C31	4.23	1.45	1.33
55	m	201	3PE	O31-C31	4.23	1.45	1.33
55	Aa	501	3PE	O31-C31	4.22	1.45	1.33
55	Ac	403	3PE	O31-C31	4.22	1.45	1.33
62	l	201	PC1	O31-C31	4.21	1.45	1.33
55	J	201	3PE	O31-C31	4.21	1.45	1.33
55	AG	103	3PE	O31-C31	4.21	1.45	1.33
56	L	703	CDL	OB6-CB5	4.21	1.46	1.34
56	Y	202	CDL	OA8-CA7	4.20	1.45	1.33
56	Ag	101	CDL	OB8-CB7	4.20	1.45	1.33
55	m	202	3PE	O31-C31	4.20	1.45	1.33
56	L	703	CDL	OA8-CA7	4.19	1.45	1.33
55	L	704	3PE	O31-C31	4.18	1.45	1.33
56	M	503	CDL	OB8-CB7	4.18	1.45	1.33
56	d	201	CDL	OB8-CB7	4.17	1.45	1.33
55	Y	201	3PE	O31-C31	4.17	1.45	1.33
56	A	402	CDL	OB8-CB7	4.17	1.45	1.33
56	A	402	CDL	OA6-CA5	4.17	1.46	1.34
62	I	301	PC1	O31-C31	4.17	1.45	1.33
56	Ag	101	CDL	OA8-CA7	4.16	1.45	1.33
56	AG	101	CDL	OB8-CB7	4.16	1.45	1.33
56	h	201	CDL	OB8-CB7	4.16	1.45	1.33
56	AG	102	CDL	OB8-CB7	4.16	1.45	1.33
56	q	201	CDL	OB8-CB7	4.15	1.45	1.33
56	AG	102	CDL	OA8-CA7	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Aa	501	3PE	O21-C21	4.14	1.46	1.34
55	AG	103	3PE	O21-C21	4.14	1.46	1.34
56	L	703	CDL	OB8-CB7	4.13	1.45	1.33
56	d	201	CDL	OB6-CB5	4.13	1.45	1.34
56	Aa	502	CDL	OB6-CB5	4.11	1.45	1.34
56	q	201	CDL	OA8-CA7	4.11	1.45	1.33
55	M	502	3PE	O31-C31	4.11	1.45	1.33
62	Ae	301	PC1	O21-C21	4.10	1.45	1.34
55	L	702	3PE	O31-C31	4.10	1.45	1.33
56	AG	101	CDL	OA6-CA5	4.10	1.45	1.34
56	d	201	CDL	OA6-CA5	4.07	1.45	1.34
56	Y	202	CDL	OA6-CA5	4.06	1.45	1.34
62	q	202	PC1	O31-C31	4.06	1.45	1.33
55	M	502	3PE	O21-C21	4.06	1.45	1.34
56	q	201	CDL	OA6-CA5	4.06	1.45	1.34
62	q	202	PC1	O21-C21	4.05	1.45	1.34
56	Ag	101	CDL	OA6-CA5	4.05	1.45	1.34
56	L	703	CDL	OA6-CA5	4.05	1.45	1.34
55	b	201	3PE	O21-C21	4.04	1.45	1.34
55	Y	201	3PE	O21-C21	4.04	1.45	1.34
56	AG	101	CDL	OB6-CB5	4.04	1.45	1.34
56	Ag	101	CDL	OB6-CB5	4.03	1.45	1.34
56	h	201	CDL	OA6-CA5	4.03	1.45	1.34
55	L	704	3PE	O21-C21	4.03	1.45	1.34
55	m	202	3PE	O21-C21	4.02	1.45	1.34
62	I	301	PC1	O21-C21	4.02	1.45	1.34
56	Y	202	CDL	OB6-CB5	4.01	1.45	1.34
56	AG	102	CDL	OA6-CA5	4.01	1.45	1.34
56	Aa	502	CDL	OA6-CA5	4.01	1.45	1.34
56	q	201	CDL	OB6-CB5	4.00	1.45	1.34
56	M	503	CDL	OB6-CB5	4.00	1.45	1.34
62	l	201	PC1	O21-C21	4.00	1.45	1.34
55	m	201	3PE	O21-C21	3.99	1.45	1.34
56	A	402	CDL	OB6-CB5	3.97	1.45	1.34
55	J	201	3PE	O21-C21	3.95	1.45	1.34
56	M	503	CDL	OA6-CA5	3.94	1.45	1.34
55	AC	404	3PE	O21-C21	3.94	1.45	1.34
55	L	702	3PE	O21-C21	3.94	1.45	1.34
55	M	501	3PE	O21-C21	3.93	1.45	1.34
55	Ac	403	3PE	O21-C21	3.93	1.45	1.34
62	L	701	PC1	O21-C21	3.92	1.45	1.34
56	AG	102	CDL	OB6-CB5	3.92	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	D	501	UQ1	C2-C1	-3.91	1.37	1.48
56	h	201	CDL	OB6-CB5	3.88	1.45	1.34
55	H	402	3PE	O21-C21	3.84	1.45	1.34
67	AC	403	HEM	C4D-ND	-3.81	1.33	1.40
67	Ac	402	HEM	C4D-ND	-3.73	1.33	1.40
55	H	402	3PE	O31-C31	3.71	1.44	1.33
67	AC	402	HEM	C4D-ND	-3.67	1.34	1.40
67	Ac	401	HEM	C4D-ND	-3.59	1.34	1.40
55	A	401	3PE	O21-C21	3.26	1.43	1.34
67	AC	403	HEM	C1B-NB	-3.26	1.34	1.40
64	P	401	NDP	C6N-C5N	3.23	1.39	1.33
67	Ac	402	HEM	C1B-NB	-3.21	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.06	1.35	1.40
67	Ac	401	HEM	C1B-NB	-3.06	1.35	1.40
55	A	401	3PE	O31-C31	3.00	1.42	1.33
60	F	501	FMN	C8-C7	2.99	1.48	1.40
69	Ac	405	UQ6	O2-C2	-2.96	1.30	1.37
69	AC	406	UQ6	O2-C2	-2.95	1.30	1.37
68	AC	405	U10	C6-C5	-2.93	1.38	1.46
68	Ac	404	U10	C6-C5	-2.92	1.38	1.46
68	Ac	404	U10	C4-C3	2.90	1.48	1.36
68	AC	405	U10	C4-C3	2.89	1.48	1.36
61	H	401	UQ9	C3-C2	-2.80	1.40	1.48
67	AC	403	HEM	C1D-ND	-2.72	1.33	1.38
67	Ac	402	HEM	C1D-ND	-2.69	1.33	1.38
66	n	201	EHZ	P1-O7	2.62	1.64	1.54
60	F	501	FMN	C4-N3	-2.59	1.34	1.38
67	AC	402	HEM	C1D-ND	-2.55	1.33	1.38
61	H	401	UQ9	C4-C5	-2.52	1.41	1.48
68	Ac	404	U10	C3-C2	-2.50	1.41	1.48
68	AC	405	U10	C3-C2	-2.47	1.41	1.48
58	D	501	UQ1	C3-C4	-2.46	1.41	1.48
67	Ac	401	HEM	C1D-ND	-2.45	1.33	1.38
66	n	201	EHZ	C9-S1	2.44	1.82	1.76
66	W	201	EHZ	O4-C15	-2.44	1.18	1.23
66	n	201	EHZ	O4-C15	-2.39	1.18	1.23
66	W	201	EHZ	O3-C12	-2.38	1.18	1.23
58	D	501	UQ1	C3-C2	2.33	1.45	1.36
63	O	401	ADP	C5-C4	2.29	1.47	1.40
61	H	401	UQ9	C6-C5	-2.28	1.40	1.46
66	n	201	EHZ	P1-OP3	-2.26	1.46	1.54
64	P	401	NDP	C5A-C4A	2.26	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	n	201	EHZ	O3-C12	-2.25	1.18	1.23
60	F	501	FMN	C4A-N5	2.20	1.35	1.30
66	W	201	EHZ	C9-S1	2.20	1.81	1.76
55	A	401	3PE	P-O12	-2.12	1.45	1.55
60	F	501	FMN	C5A-N5	-2.08	1.35	1.39
67	AC	402	HEM	CHB-C1B	2.06	1.40	1.35
55	A	401	3PE	O21-C2	-2.06	1.41	1.46
55	A	401	3PE	O31-C3	-2.06	1.40	1.45
67	Ac	401	HEM	CHB-C1B	2.06	1.40	1.35

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	AC	405	U10	C6-C1-C2	7.80	125.35	119.18
68	Ac	404	U10	C6-C1-C2	7.71	125.28	119.18
66	W	201	EHZ	C8-C9-S1	6.05	121.11	113.63
66	n	201	EHZ	C8-C9-S1	5.26	120.14	113.63
67	AC	402	HEM	CHC-C4B-NB	4.74	129.58	124.43
55	A	401	3PE	O21-C21-C22	4.72	121.67	111.50
58	D	501	UQ1	O1-C1-C2	-4.70	110.95	120.93
67	Ac	401	HEM	CHC-C4B-NB	4.66	129.49	124.43
55	H	402	3PE	O21-C21-C22	4.64	121.50	111.50
67	AC	403	HEM	C4D-ND-C1D	4.47	109.69	105.07
55	AG	103	3PE	O21-C21-C22	4.44	121.07	111.50
67	Ac	402	HEM	C4D-ND-C1D	4.38	109.59	105.07
56	h	201	CDL	OB6-CB5-C51	4.37	120.92	111.50
62	I	301	PC1	O21-C21-C22	4.37	120.91	111.50
56	q	201	CDL	OA6-CA5-C11	4.36	120.90	111.50
56	L	703	CDL	OB6-CB5-C51	4.33	120.84	111.50
56	d	201	CDL	OA6-CA5-C11	4.33	120.83	111.50
56	A	402	CDL	OB6-CB5-C51	4.29	120.74	111.50
55	m	202	3PE	O21-C21-C22	4.28	120.73	111.50
55	L	704	3PE	O21-C21-C22	4.27	120.70	111.50
62	L	701	PC1	O21-C21-C22	4.22	120.59	111.50
67	AC	403	HEM	CHC-C4B-NB	4.20	128.99	124.43
67	Ac	402	HEM	CHC-C4B-NB	4.19	128.99	124.43
55	M	502	3PE	O21-C21-C22	4.17	120.50	111.50
56	Aa	502	CDL	OA6-CA5-C11	4.17	120.49	111.50
56	h	201	CDL	OA6-CA5-C11	4.15	120.45	111.50
68	AC	405	U10	C1-C6-C5	-4.14	115.69	119.58
55	b	201	3PE	O21-C21-C22	4.13	120.41	111.50
68	Ac	404	U10	C1-C6-C5	-4.09	115.73	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	Ac	403	3PE	O21-C21-C22	4.07	120.27	111.50
62	Ae	301	PC1	O21-C21-C22	4.03	120.19	111.50
62	q	202	PC1	O21-C21-C22	4.02	120.17	111.50
55	m	201	3PE	O21-C21-C22	4.00	120.11	111.50
67	Ac	402	HEM	CHB-C1B-NB	3.99	129.31	124.38
56	M	503	CDL	OA6-CA5-C11	3.98	120.09	111.50
56	AG	102	CDL	OA6-CA5-C11	3.97	120.06	111.50
56	AG	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
67	AC	403	HEM	CHB-C1B-NB	3.95	129.26	124.38
67	Ac	401	HEM	CHB-C1B-NB	3.94	129.24	124.38
56	AG	101	CDL	OB6-CB5-C51	3.92	119.94	111.50
64	P	401	NDP	PN-O3-PA	-3.90	119.43	132.83
63	O	401	ADP	PA-O3A-PB	-3.88	119.50	132.83
55	M	501	3PE	O21-C21-C22	3.88	119.86	111.50
67	AC	402	HEM	CHB-C1B-NB	3.87	129.16	124.38
55	J	201	3PE	O21-C21-C22	3.86	119.83	111.50
56	Y	202	CDL	OA6-CA5-C11	3.86	119.82	111.50
56	L	703	CDL	OA6-CA5-C11	3.84	119.78	111.50
55	Y	201	3PE	O21-C21-C22	3.82	119.73	111.50
55	i	201	3PE	O21-C21-C22	3.81	119.71	111.50
56	M	503	CDL	OB6-CB5-C51	3.79	119.68	111.50
70	Ad	401	HEC	CMC-C2C-C1C	-3.79	122.64	128.46
55	L	702	3PE	O21-C21-C22	3.78	119.66	111.50
70	AD	401	HEC	CMC-C2C-C1C	-3.78	122.66	128.46
56	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
55	AC	404	3PE	O21-C21-C22	3.70	119.48	111.50
62	l	201	PC1	O21-C21-C22	3.68	119.42	111.50
56	Y	202	CDL	OB6-CB5-C51	3.64	119.35	111.50
56	q	201	CDL	OB6-CB5-C51	3.63	119.32	111.50
56	d	201	CDL	OB6-CB5-C51	3.59	119.24	111.50
56	A	402	CDL	OA6-CA5-C11	3.50	119.04	111.50
56	Ag	101	CDL	OA6-CA5-C11	3.36	120.17	110.80
56	Aa	502	CDL	OB6-CB5-C51	3.34	120.11	110.80
56	Ag	101	CDL	OB8-CB7-C71	3.33	120.12	111.38
66	n	201	EHZ	C14-C13-C12	-3.32	106.82	112.36
58	D	501	UQ1	C3-C2-C1	-3.31	114.18	120.68
67	AC	402	HEM	C4D-ND-C1D	3.29	108.48	105.07
56	Aa	502	CDL	OB8-CB7-C71	3.29	120.00	111.38
68	Ac	404	U10	C4-C3-C2	-3.28	114.23	120.68
55	Aa	501	3PE	O21-C21-C22	3.27	119.92	110.80
63	O	401	ADP	N3-C2-N1	-3.25	123.60	128.68
68	AC	405	U10	C4-C3-C2	-3.25	114.30	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AC	403	HEM	C1B-NB-C4B	3.23	108.41	105.07
67	AC	403	HEM	CHD-C1D-ND	3.22	127.92	124.43
67	Ac	401	HEM	C4D-ND-C1D	3.21	108.39	105.07
67	Ac	402	HEM	C1B-NB-C4B	3.20	108.38	105.07
55	H	402	3PE	C3-C2-C1	-3.20	104.22	111.79
67	Ac	402	HEM	CHD-C1D-ND	3.17	127.88	124.43
64	P	401	NDP	N3A-C2A-N1A	-3.13	123.79	128.68
56	AG	101	CDL	OA6-CA5-C11	3.12	119.49	110.80
56	AG	101	CDL	OB8-CB7-C71	3.11	119.53	111.38
67	Ac	401	HEM	C1B-NB-C4B	3.09	108.27	105.07
62	q	202	PC1	O31-C31-C32	3.08	121.56	111.91
56	M	503	CDL	CA4-OA6-CA5	-3.07	110.22	117.79
56	A	402	CDL	CB4-OB6-CB5	-3.07	110.23	117.79
67	AC	402	HEM	C1B-NB-C4B	3.07	108.24	105.07
66	n	201	EHZ	C13-C12-N1	2.97	121.42	116.42
56	h	201	CDL	OA8-CA7-C31	2.97	121.23	111.91
62	L	701	PC1	C2-O21-C21	-2.97	110.48	117.79
56	d	201	CDL	OA8-CA7-C31	2.92	121.06	111.91
55	m	202	3PE	O31-C31-C32	2.90	121.02	111.91
56	AG	102	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
67	AC	402	HEM	CHD-C1D-ND	2.87	127.55	124.43
55	i	201	3PE	O31-C31-C32	2.86	120.89	111.91
56	Y	202	CDL	CA4-OA6-CA5	-2.85	110.78	117.79
62	I	301	PC1	O31-C31-C32	2.84	120.83	111.91
67	Ac	401	HEM	CHD-C1D-ND	2.82	127.49	124.43
56	Y	202	CDL	OB8-CB7-C71	2.82	120.74	111.91
56	A	402	CDL	OA8-CA7-C31	2.81	120.72	111.91
62	I	301	PC1	C2-O21-C21	-2.80	110.89	117.79
55	J	201	3PE	O31-C31-C32	2.80	120.68	111.91
55	A	401	3PE	O31-C31-C32	2.79	120.66	111.91
56	AG	102	CDL	CB4-OB6-CB5	-2.79	110.93	117.79
55	M	502	3PE	O31-C31-C32	2.78	120.63	111.91
70	Ad	401	HEC	CMB-C2B-C1B	-2.77	124.20	128.46
56	h	201	CDL	CB4-OB6-CB5	-2.77	110.98	117.79
56	Y	202	CDL	CB4-OB6-CB5	-2.76	110.99	117.79
55	L	702	3PE	C2-O21-C21	-2.75	111.03	117.79
55	m	202	3PE	C2-O21-C21	-2.73	111.06	117.79
56	Aa	502	CDL	CB4-OB6-CB5	-2.73	111.07	117.79
56	L	703	CDL	OB8-CB7-C71	2.73	120.47	111.91
55	Ac	403	3PE	C2-O21-C21	-2.72	111.08	117.79
60	F	501	FMN	C4-C4A-N5	2.71	122.09	118.23
70	AD	401	HEC	CMB-C2B-C1B	-2.70	124.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	q	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
56	Ag	101	CDL	CA4-OA6-CA5	-2.69	111.16	117.79
55	M	502	3PE	C2-O21-C21	-2.68	111.18	117.79
56	M	503	CDL	OA8-CA7-C31	2.68	120.32	111.91
64	P	401	NDP	C4A-C5A-N7A	-2.68	106.61	109.40
55	Ac	403	3PE	O31-C31-C32	2.68	120.31	111.91
56	A	402	CDL	OB8-CB7-C71	2.68	120.31	111.91
56	L	703	CDL	OA8-CA7-C31	2.67	120.27	111.91
55	m	201	3PE	O31-C31-C32	2.66	120.26	111.91
62	Ae	301	PC1	O31-C31-C32	2.66	120.25	111.91
55	J	201	3PE	C2-O21-C21	-2.64	111.28	117.79
68	AC	405	U10	C7-C6-C5	2.64	121.66	118.48
55	AC	404	3PE	O31-C31-C32	2.63	120.17	111.91
56	q	201	CDL	OA8-CA7-C31	2.63	120.16	111.91
61	H	401	UQ9	C1M-C1-C6	-2.63	120.11	124.40
66	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
56	AG	101	CDL	OA8-CA7-C31	2.62	120.11	111.91
56	Aa	502	CDL	CA4-OA6-CA5	-2.61	111.36	117.79
56	AG	101	CDL	CB4-OB6-CB5	-2.60	111.38	117.79
68	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
62	Ae	301	PC1	C2-O21-C21	-2.59	111.42	117.79
55	b	201	3PE	C2-O21-C21	-2.58	111.43	117.79
67	AC	402	HEM	CHA-C4D-ND	2.58	127.57	124.38
56	h	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
55	b	201	3PE	O31-C31-C32	2.57	119.99	111.91
55	L	704	3PE	C2-O21-C21	-2.57	111.47	117.79
56	M	503	CDL	OB8-CB7-C71	2.56	119.94	111.91
60	F	501	FMN	C4A-C10-N1	-2.55	118.81	124.73
68	Ac	404	U10	O4-C4-C5	-2.55	107.94	116.56
56	d	201	CDL	OB8-CB7-C71	2.55	119.90	111.91
68	AC	405	U10	O4-C4-C5	-2.55	107.95	116.56
55	H	402	3PE	O31-C31-C32	2.54	119.88	111.91
55	Aa	501	3PE	O31-C31-C32	2.53	119.85	111.91
55	L	704	3PE	O31-C31-C32	2.52	119.83	111.91
63	O	401	ADP	C3'-C2'-C1'	2.51	104.75	100.98
55	Y	201	3PE	O31-C31-C32	2.51	119.77	111.91
66	n	201	EHZ	OP3-P1-O9	-2.50	100.88	110.68
55	L	702	3PE	O31-C31-C32	2.50	119.74	111.91
56	Ag	101	CDL	OA8-CA7-C31	2.49	119.71	111.91
63	O	401	ADP	C4-C5-N7	-2.47	106.82	109.40
66	W	201	EHZ	C13-C12-N1	2.47	120.58	116.42
55	m	201	3PE	C2-O21-C21	-2.47	111.72	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	l	201	PC1	O31-C31-C32	2.46	119.64	111.91
67	Ac	401	HEM	CHA-C4D-ND	2.46	127.42	124.38
56	AG	102	CDL	OB8-CB7-C71	2.46	119.61	111.91
56	AG	102	CDL	OA8-CA7-C31	2.45	119.59	111.91
56	q	201	CDL	CA4-OA6-CA5	-2.44	111.77	117.79
67	Ac	402	HEM	CHB-C1B-C2B	-2.44	119.98	126.72
66	W	201	EHZ	C14-N2-C15	-2.43	118.25	122.59
67	AC	403	HEM	CHB-C1B-C2B	-2.43	120.00	126.72
55	AG	103	3PE	O31-C31-C32	2.43	119.52	111.91
56	Aa	502	CDL	OA8-CA7-C31	2.42	119.51	111.91
62	L	701	PC1	O31-C31-C32	2.42	119.50	111.91
62	Ae	301	PC1	C11-C12-N	-2.41	107.73	115.78
70	Ad	401	HEC	CBD-CAD-C3D	-2.41	108.51	112.62
67	Ac	401	HEM	C4B-C3B-C2B	-2.37	105.23	107.11
66	n	201	EHZ	C11-N1-C12	-2.37	118.44	122.84
55	AC	404	3PE	C2-O21-C21	-2.37	111.96	117.79
67	AC	402	HEM	C4B-C3B-C2B	-2.37	105.24	107.11
55	M	501	3PE	O31-C31-C32	2.36	119.33	111.91
70	AD	401	HEC	CBD-CAD-C3D	-2.36	108.59	112.62
70	Ad	401	HEC	C1D-C2D-C3D	-2.36	105.35	107.00
55	H	402	3PE	C24-C23-C22	-2.36	104.70	113.19
62	l	201	PC1	C2-O21-C21	-2.36	111.98	117.79
66	W	201	EHZ	O2-C9-S1	-2.35	119.56	122.61
56	Y	202	CDL	OA8-CA7-C31	2.35	119.29	111.91
66	n	201	EHZ	C10-S1-C9	2.35	109.18	101.87
62	q	202	PC1	C2-O21-C21	-2.35	112.01	117.79
67	AC	403	HEM	CHA-C4D-ND	2.31	127.24	124.38
70	AD	401	HEC	C1D-C2D-C3D	-2.31	105.39	107.00
56	AG	101	CDL	CA4-OA6-CA5	-2.29	112.16	117.79
56	q	201	CDL	CB4-OB6-CB5	-2.27	112.19	117.79
56	Ag	101	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
56	h	201	CDL	OB6-CB5-OB7	-2.26	118.24	123.70
55	A	401	3PE	O12-P-O14	-2.26	101.08	112.24
55	Y	201	3PE	C2-O21-C21	-2.25	112.25	117.79
67	Ac	401	HEM	CHB-C1B-C2B	-2.25	120.50	126.72
67	Ac	402	HEM	CHA-C4D-ND	2.25	127.16	124.38
67	AC	402	HEM	CHB-C1B-C2B	-2.24	120.53	126.72
55	AC	401	3PE	C2-O21-C21	2.23	123.29	117.79
66	n	201	EHZ	O2-C9-S1	-2.23	119.72	122.61
55	AG	103	3PE	C2-O21-C21	-2.22	112.31	117.79
60	F	501	FMN	O2-C2-N1	-2.21	118.16	121.83
60	F	501	FMN	C4A-C10-N10	2.19	119.67	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	F	501	FMN	O4-C4-C4A	-2.18	120.82	126.60
58	D	501	UQ1	O1-C1-C6	-2.18	117.73	121.55
56	d	201	CDL	CA4-OA6-CA5	-2.18	112.43	117.79
62	q	202	PC1	O31-C31-O32	-2.14	118.18	123.59
56	M	503	CDL	OA6-CA5-OA7	-2.14	118.54	123.70
58	D	501	UQ1	CM2-O2-C2	2.11	123.93	116.47
66	n	201	EHZ	C14-N2-C15	-2.10	118.84	122.59
55	M	501	3PE	C2-O21-C21	-2.10	112.62	117.79
60	F	501	FMN	C10-N1-C2	2.10	121.10	116.90
55	H	402	3PE	C26-C25-C24	-2.09	103.80	114.42
55	m	202	3PE	O21-C21-O22	-2.09	118.65	123.70
67	AC	403	HEM	CAD-C3D-C4D	2.07	128.28	124.66
70	AD	401	HEC	CAA-CBA-CGA	-2.07	107.96	113.76
55	m	202	3PE	O31-C31-O32	-2.07	118.38	123.59
56	L	703	CDL	OB8-CB7-OB9	-2.05	118.41	123.59
55	L	704	3PE	O21-C21-O22	-2.05	118.75	123.70
64	P	401	NDP	C3D-C2D-C1D	2.05	105.31	101.43
67	Ac	402	HEM	CAD-C3D-C4D	2.04	128.22	124.66
56	A	402	CDL	OB6-CB5-OB7	-2.04	118.78	123.70
68	Ac	404	U10	C3M-O3-C3	2.04	123.69	116.47
62	l	201	PC1	C11-C12-N	-2.04	108.98	115.78
70	Ad	401	HEC	CAA-CBA-CGA	-2.04	108.05	113.76
58	D	501	UQ1	O2-C2-C3	2.04	131.31	123.64
60	F	501	FMN	C4A-C4-N3	2.03	118.35	113.19
68	AC	405	U10	C3M-O3-C3	2.03	123.66	116.47
68	AC	405	U10	O4-C4-C3	2.02	131.26	123.64
55	m	201	3PE	O21-C21-O22	-2.01	118.83	123.70
68	Ac	404	U10	O4-C4-C3	2.00	131.20	123.64
67	AC	403	HEM	CMC-C2C-C3C	2.00	128.42	124.68

There are no chirality outliers.

All (551) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	O22-C21-O21-C2
55	H	402	3PE	C11-O13-P-O11
55	H	402	3PE	C11-O13-P-O12
55	H	402	3PE	C11-O13-P-O14
55	H	402	3PE	O13-C11-C12-N
55	J	201	3PE	C1-O11-P-O12
55	J	201	3PE	C1-O11-P-O13
55	J	201	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
55	J	201	3PE	C11-O13-P-O14
55	L	702	3PE	C1-O11-P-O12
55	L	702	3PE	C1-O11-P-O14
55	L	702	3PE	O22-C21-O21-C2
55	L	702	3PE	C22-C21-O21-C2
55	L	704	3PE	C1-O11-P-O12
55	M	501	3PE	C1-O11-P-O12
55	M	501	3PE	C1-O11-P-O13
55	M	501	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O14
55	M	502	3PE	C11-O13-P-O14
55	Y	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C1-O11-P-O14
55	b	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C1-O11-P-O12
55	i	201	3PE	C1-O11-P-O14
55	m	201	3PE	C11-O13-P-O14
55	m	202	3PE	C11-O13-P-O14
55	AC	401	3PE	C11-O13-P-O12
55	AC	401	3PE	O13-C11-C12-N
55	AG	103	3PE	C1-O11-P-O12
55	AG	103	3PE	C1-O11-P-O13
55	AG	103	3PE	C1-O11-P-O14
55	AG	103	3PE	C11-O13-P-O14
55	Aa	501	3PE	C11-O13-P-O12
55	Ag	103	3PE	C1-O11-P-O12
55	Ag	103	3PE	C1-O11-P-O14
55	Ag	103	3PE	C11-O13-P-O11
55	Ag	103	3PE	O13-C11-C12-N
56	A	402	CDL	CA4-CA3-OA5-PA1
56	A	402	CDL	CB3-OB5-PB2-OB3
56	A	402	CDL	CB3-OB5-PB2-OB4
56	L	703	CDL	CA2-OA2-PA1-OA3
56	L	703	CDL	CB3-OB5-PB2-OB3
56	L	703	CDL	C51-CB5-OB6-CB4
56	M	503	CDL	CA3-OA5-PA1-OA4
56	M	503	CDL	CA4-CA3-OA5-PA1
56	M	503	CDL	CB2-OB2-PB2-OB3
56	M	503	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CB3-OB5-PB2-OB3
56	M	503	CDL	CB3-OB5-PB2-OB4
56	Y	202	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
56	Y	202	CDL	CB2-OB2-PB2-OB4
56	Y	202	CDL	CB3-OB5-PB2-OB4
56	Y	202	CDL	C51-CB5-OB6-CB4
56	d	201	CDL	CA2-OA2-PA1-OA3
56	d	201	CDL	CA2-OA2-PA1-OA4
56	d	201	CDL	C11-CA5-OA6-CA4
56	d	201	CDL	CB2-OB2-PB2-OB3
56	d	201	CDL	CB2-OB2-PB2-OB4
56	d	201	CDL	CB2-OB2-PB2-OB5
56	h	201	CDL	CA2-OA2-PA1-OA4
56	h	201	CDL	C11-CA5-OA6-CA4
56	h	201	CDL	CB2-OB2-PB2-OB3
56	h	201	CDL	OB7-CB5-OB6-CB4
56	q	201	CDL	CA3-OA5-PA1-OA3
56	q	201	CDL	CA3-OA5-PA1-OA4
56	AG	101	CDL	CA2-OA2-PA1-OA4
56	AG	101	CDL	CB2-OB2-PB2-OB3
56	AG	102	CDL	C1-CB2-OB2-PB2
56	AG	102	CDL	CB2-OB2-PB2-OB4
56	AG	102	CDL	CB3-OB5-PB2-OB2
56	AG	102	CDL	CB3-OB5-PB2-OB3
56	AG	102	CDL	CB3-OB5-PB2-OB4
56	Aa	502	CDL	CA2-OA2-PA1-OA5
56	Aa	502	CDL	CA3-OA5-PA1-OA3
56	Aa	502	CDL	CB2-OB2-PB2-OB3
56	Aa	502	CDL	CB2-OB2-PB2-OB4
56	Ag	101	CDL	CB2-OB2-PB2-OB3
56	Ag	101	CDL	CB2-OB2-PB2-OB4
56	Ag	101	CDL	CB2-OB2-PB2-OB5
56	Ag	101	CDL	CB3-OB5-PB2-OB2
56	Ag	101	CDL	CB3-OB5-PB2-OB3
56	Ag	101	CDL	CB3-OB5-PB2-OB4
56	Ag	102	CDL	CB2-OB2-PB2-OB5
56	Ag	102	CDL	CB3-OB5-PB2-OB4
58	D	501	UQ1	C1-C6-C7-C8
58	D	501	UQ1	C5-C6-C7-C8
61	H	401	UQ9	C24-C26-C27-C28
61	H	401	UQ9	C22-C23-C24-C26
61	H	401	UQ9	C22-C23-C24-C25
61	H	401	UQ9	C21-C22-C23-C24
61	H	401	UQ9	C19-C21-C22-C23
61	H	401	UQ9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
61	H	401	UQ9	C17-C18-C19-C20
62	I	301	PC1	C11-O13-P-O12
62	I	301	PC1	C11-O13-P-O14
62	I	301	PC1	C11-O13-P-O11
62	L	701	PC1	C11-O13-P-O12
62	L	701	PC1	C11-O13-P-O14
62	L	701	PC1	C1-O11-P-O12
62	L	701	PC1	C1-O11-P-O14
62	L	701	PC1	C1-O11-P-O13
62	l	201	PC1	C11-O13-P-O14
62	q	202	PC1	C11-O13-P-O14
62	q	202	PC1	C1-O11-P-O12
62	q	202	PC1	C1-O11-P-O14
62	q	202	PC1	C1-O11-P-O13
62	Ae	301	PC1	C1-O11-P-O12
62	Ae	301	PC1	O13-C11-C12-N
63	O	401	ADP	C5'-O5'-PA-O3A
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	O2-C9-S1-C10
66	W	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C6-C7-C8-C9
66	n	201	EHZ	S1-C10-C11-N1
66	n	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C19
66	n	201	EHZ	C15-C16-C17-C20
66	n	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C19
66	n	201	EHZ	O5-C16-C17-C20
66	n	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C20-O6-P1-OP3
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	403	HEM	C2B-C3B-CAB-CBB
67	AC	403	HEM	C4B-C3B-CAB-CBB
67	Ac	401	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
68	AC	405	U10	C7-C8-C9-C10
68	AC	405	U10	C7-C8-C9-C11
68	Ac	404	U10	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
68	Ac	404	U10	C7-C8-C9-C11
69	AC	406	UQ6	C1-C6-C7-C8
69	AC	406	UQ6	C7-C8-C9-C10
69	AC	406	UQ6	C7-C8-C9-C11
69	AC	406	UQ6	C12-C13-C14-C15
69	AC	406	UQ6	C12-C13-C14-C16
69	AC	406	UQ6	C13-C14-C16-C17
69	AC	406	UQ6	C15-C14-C16-C17
69	AC	406	UQ6	C17-C18-C19-C20
69	Ac	405	UQ6	C1-C6-C7-C8
69	Ac	405	UQ6	C7-C8-C9-C10
69	Ac	405	UQ6	C7-C8-C9-C11
69	Ac	405	UQ6	C12-C13-C14-C15
69	Ac	405	UQ6	C12-C13-C14-C16
69	Ac	405	UQ6	C13-C14-C16-C17
69	Ac	405	UQ6	C15-C14-C16-C17
69	Ac	405	UQ6	C17-C18-C19-C20
55	H	402	3PE	O32-C31-O31-C3
56	L	703	CDL	OA9-CA7-OA8-CA6
55	m	202	3PE	C2-C3-O31-C31
55	b	201	3PE	C32-C31-O31-C3
56	L	703	CDL	C31-CA7-OA8-CA6
58	D	501	UQ1	C7-C8-C9-C10
58	D	501	UQ1	C7-C8-C9-C11
68	AC	405	U10	C12-C13-C14-C15
68	AC	405	U10	C12-C13-C14-C16
68	Ac	404	U10	C12-C13-C14-C15
68	Ac	404	U10	C12-C13-C14-C16
55	J	201	3PE	O32-C31-O31-C3
55	Y	201	3PE	O32-C31-O31-C3
55	b	201	3PE	O32-C31-O31-C3
55	m	202	3PE	O32-C31-O31-C3
55	M	502	3PE	O22-C21-O21-C2
56	L	703	CDL	OB7-CB5-OB6-CB4
56	Y	202	CDL	OB7-CB5-OB6-CB4
56	d	201	CDL	OA7-CA5-OA6-CA4
55	H	402	3PE	C32-C31-O31-C3
55	Y	201	3PE	C32-C31-O31-C3
55	m	202	3PE	C32-C31-O31-C3
55	A	401	3PE	C22-C21-O21-C2
55	M	502	3PE	C22-C21-O21-C2
55	Y	201	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
55	b	201	3PE	C22-C21-O21-C2
56	h	201	CDL	C51-CB5-OB6-CB4
55	J	201	3PE	C32-C31-O31-C3
56	h	201	CDL	C31-CA7-OA8-CA6
69	AC	406	UQ6	C17-C18-C19-C21
69	Ac	405	UQ6	C17-C18-C19-C21
61	H	401	UQ9	C7-C8-C9-C10
56	M	503	CDL	OB7-CB5-OB6-CB4
56	h	201	CDL	OA7-CA5-OA6-CA4
62	Ae	301	PC1	O32-C31-O31-C3
62	I	301	PC1	C32-C31-O31-C3
55	Aa	501	3PE	C22-C21-O21-C2
56	M	503	CDL	C51-CB5-OB6-CB4
62	Ae	301	PC1	C32-C31-O31-C3
56	h	201	CDL	OA9-CA7-OA8-CA6
62	I	301	PC1	O32-C31-O31-C3
62	L	701	PC1	O32-C31-O31-C3
61	H	401	UQ9	C9-C11-C12-C13
69	AC	406	UQ6	C9-C11-C12-C13
69	AC	406	UQ6	C14-C16-C17-C18
69	Ac	405	UQ6	C9-C11-C12-C13
69	Ac	405	UQ6	C14-C16-C17-C18
62	L	701	PC1	C32-C31-O31-C3
55	Aa	501	3PE	O22-C21-O21-C2
55	m	201	3PE	C32-C31-O31-C3
56	Y	202	CDL	C71-CB7-OB8-CB6
62	l	201	PC1	C32-C31-O31-C3
55	H	402	3PE	C24-C25-C26-C27
55	A	401	3PE	C32-C31-O31-C3
67	AC	402	HEM	C2A-CAA-CBA-CGA
67	Ac	401	HEM	C2A-CAA-CBA-CGA
55	Ag	103	3PE	C32-C33-C34-C35
66	n	201	EHZ	C5-C6-C7-O1
56	Y	202	CDL	C51-C52-C53-C54
62	q	202	PC1	C2-C1-O11-P
56	Y	202	CDL	OB9-CB7-OB8-CB6
55	m	201	3PE	O32-C31-O31-C3
62	l	201	PC1	O32-C31-O31-C3
56	M	503	CDL	C71-CB7-OB8-CB6
55	A	401	3PE	O32-C31-O31-C3
55	L	702	3PE	C33-C34-C35-C36
56	q	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
56	A	402	CDL	C11-CA5-OA6-CA4
56	A	402	CDL	C51-CB5-OB6-CB4
55	J	201	3PE	C11-O13-P-O11
55	L	702	3PE	C1-O11-P-O13
55	i	201	3PE	C1-O11-P-O13
55	m	201	3PE	C1-O11-P-O13
55	m	201	3PE	C11-O13-P-O11
55	AC	401	3PE	C11-O13-P-O11
55	AG	103	3PE	C11-O13-P-O11
55	Ag	103	3PE	C1-O11-P-O13
56	A	402	CDL	CA3-OA5-PA1-OA2
56	A	402	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CA2-OA2-PA1-OA5
56	M	503	CDL	CA3-OA5-PA1-OA2
56	Y	202	CDL	CB2-OB2-PB2-OB5
56	Y	202	CDL	CB3-OB5-PB2-OB2
56	d	201	CDL	CA2-OA2-PA1-OA5
56	h	201	CDL	CB2-OB2-PB2-OB5
56	h	201	CDL	CB3-OB5-PB2-OB2
56	q	201	CDL	CA3-OA5-PA1-OA2
56	AG	101	CDL	CB2-OB2-PB2-OB5
56	AG	102	CDL	CB2-OB2-PB2-OB5
56	Aa	502	CDL	CB2-OB2-PB2-OB5
56	Aa	502	CDL	CB3-OB5-PB2-OB2
56	Ag	102	CDL	CB3-OB5-PB2-OB2
62	L	701	PC1	C11-O13-P-O11
62	q	202	PC1	C11-O13-P-O11
62	l	201	PC1	C3B-C3C-C3D-C3E
56	A	402	CDL	C71-CB7-OB8-CB6
56	A	402	CDL	OA7-CA5-OA6-CA4
56	A	402	CDL	OB7-CB5-OB6-CB4
55	AG	103	3PE	C32-C33-C34-C35
56	A	402	CDL	C31-CA7-OA8-CA6
55	Ag	103	3PE	C3C-C3D-C3E-C3F
66	W	201	EHZ	C18-C17-C20-O6
66	W	201	EHZ	C19-C17-C20-O6
55	A	401	3PE	C3-C2-O21-C21
56	h	201	CDL	CA3-CA4-OA6-CA5
56	AG	101	CDL	C31-CA7-OA8-CA6
56	Aa	502	CDL	C51-CB5-OB6-CB4
55	Ag	103	3PE	C37-C38-C39-C3A
56	Ag	102	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
55	A	401	3PE	O13-C11-C12-N
55	M	501	3PE	C32-C33-C34-C35
56	A	402	CDL	OA9-CA7-OA8-CA6
56	A	402	CDL	OB9-CB7-OB8-CB6
56	h	201	CDL	C71-CB7-OB8-CB6
56	Y	202	CDL	C73-C74-C75-C76
55	L	704	3PE	C22-C21-O21-C2
56	Y	202	CDL	C11-CA5-OA6-CA4
56	M	503	CDL	OB9-CB7-OB8-CB6
55	L	704	3PE	O22-C21-O21-C2
56	Y	202	CDL	OA7-CA5-OA6-CA4
56	Aa	502	CDL	OB7-CB5-OB6-CB4
61	H	401	UQ9	C7-C8-C9-C11
55	AG	103	3PE	C37-C38-C39-C3A
56	h	201	CDL	OB9-CB7-OB8-CB6
56	AG	101	CDL	OA9-CA7-OA8-CA6
56	L	703	CDL	C71-CB7-OB8-CB6
56	AG	102	CDL	C31-CA7-OA8-CA6
55	i	201	3PE	C32-C31-O31-C3
56	AG	102	CDL	C74-C75-C76-C77
55	m	201	3PE	C22-C21-O21-C2
55	H	402	3PE	C39-C3A-C3B-C3C
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	401	HEM	C4B-C3B-CAB-CBB
55	M	501	3PE	C22-C21-O21-C2
56	AG	102	CDL	C51-CB5-OB6-CB4
56	h	201	CDL	C56-C57-C58-C59
55	m	202	3PE	C11-O13-P-O11
55	Aa	501	3PE	C11-O13-P-O11
56	A	402	CDL	CB2-OB2-PB2-OB5
56	AG	101	CDL	CA2-OA2-PA1-OA5
56	Ag	102	CDL	C1-CB2-OB2-PB2
66	W	201	EHZ	C3-C4-C5-C6
55	M	502	3PE	C3C-C3D-C3E-C3F
56	q	201	CDL	C11-CA5-OA6-CA4
56	AG	102	CDL	OA9-CA7-OA8-CA6
56	M	503	CDL	C43-C44-C45-C46
55	L	702	3PE	C25-C26-C27-C28
56	L	703	CDL	C12-C13-C14-C15
62	L	701	PC1	C33-C34-C35-C36
56	L	703	CDL	OB9-CB7-OB8-CB6
66	n	201	EHZ	O4-C15-C16-O5

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Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C27-C28-C29-C2A
66	W	201	EHZ	C5-C6-C7-O1
56	A	402	CDL	CA3-CA4-OA6-CA5
56	M	503	CDL	CB6-CB4-OB6-CB5
56	M	503	CDL	C11-C12-C13-C14
62	Ae	301	PC1	C2-C1-O11-P
55	i	201	3PE	O32-C31-O31-C3
62	l	201	PC1	C33-C34-C35-C36
55	A	401	3PE	O21-C2-C3-O31
55	m	201	3PE	O22-C21-O21-C2
56	M	503	CDL	C31-C32-C33-C34
55	J	201	3PE	C33-C34-C35-C36
66	W	201	EHZ	C5-C6-C7-C8
66	n	201	EHZ	C5-C6-C7-C8
55	L	702	3PE	C32-C31-O31-C3
56	q	201	CDL	C31-CA7-OA8-CA6
55	L	702	3PE	C31-C32-C33-C34
56	Ag	102	CDL	OB5-CB3-CB4-CB6
56	Aa	502	CDL	C71-CB7-OB8-CB6
56	d	201	CDL	C54-C55-C56-C57
55	M	501	3PE	O22-C21-O21-C2
62	q	202	PC1	C32-C31-O31-C3
56	Y	202	CDL	CA4-CA3-OA5-PA1
56	d	201	CDL	C1-CA2-OA2-PA1
64	P	401	NDP	O4D-C1D-N1N-C6N
56	d	201	CDL	C33-C34-C35-C36
55	L	704	3PE	C1-O11-P-O13
55	M	501	3PE	C11-O13-P-O11
55	M	502	3PE	C11-O13-P-O11
56	A	402	CDL	CA2-OA2-PA1-OA5
56	h	201	CDL	CA2-OA2-PA1-OA5
62	Ae	301	PC1	C1-O11-P-O13
56	M	503	CDL	C34-C35-C36-C37
56	Y	202	CDL	C72-C73-C74-C75
55	A	401	3PE	C37-C38-C39-C3A
56	Ag	102	CDL	OB5-CB3-CB4-OB6
56	AG	102	CDL	OB7-CB5-OB6-CB4
56	q	201	CDL	OB6-CB4-CB6-OB8
55	H	402	3PE	C34-C35-C36-C37
55	M	502	3PE	C36-C37-C38-C39
56	q	201	CDL	OA7-CA5-OA6-CA4
55	L	704	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
56	AG	102	CDL	C1-CA2-OA2-PA1
62	I	301	PC1	C11-C12-N-C15
55	A	401	3PE	C2B-C2C-C2D-C2E
56	L	703	CDL	C31-C32-C33-C34
55	L	702	3PE	O32-C31-O31-C3
56	q	201	CDL	OA9-CA7-OA8-CA6
56	Y	202	CDL	CB7-C71-C72-C73
66	n	201	EHZ	N2-C15-C16-O5
56	h	201	CDL	C73-C74-C75-C76
55	Aa	501	3PE	C3-C2-O21-C21
56	Aa	502	CDL	OB9-CB7-OB8-CB6
56	d	201	CDL	C60-C61-C62-C63
55	i	201	3PE	C1-C2-C3-O31
56	A	402	CDL	CB4-CB3-OB5-PB2
56	q	201	CDL	CB3-CB4-CB6-OB8
56	AG	102	CDL	CB4-CB3-OB5-PB2
62	q	202	PC1	O32-C31-O31-C3
56	Y	202	CDL	OA5-CA3-CA4-OA6
62	I	301	PC1	C11-C12-N-C13
55	m	201	3PE	C33-C34-C35-C36
62	q	202	PC1	C32-C33-C34-C35
55	A	401	3PE	C22-C23-C24-C25
55	H	402	3PE	C1-O11-P-O13
55	b	201	3PE	C1-O11-P-O13
56	d	201	CDL	CA3-OA5-PA1-OA2
62	I	301	PC1	C1-O11-P-O13
56	A	402	CDL	C1-CA2-OA2-PA1
56	q	201	CDL	CA4-CA3-OA5-PA1
56	Ag	102	CDL	CB4-CB3-OB5-PB2
55	J	201	3PE	C1-O11-P-O14
55	L	704	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O12
55	b	201	3PE	C1-O11-P-O12
55	m	201	3PE	C1-O11-P-O14
55	m	201	3PE	C11-O13-P-O12
55	m	202	3PE	C11-O13-P-O12
55	AC	401	3PE	C11-O13-P-O14
55	AG	103	3PE	C11-O13-P-O12
55	Aa	501	3PE	C11-O13-P-O14
55	Ag	103	3PE	C11-O13-P-O12
56	A	402	CDL	CA3-OA5-PA1-OA3
56	M	503	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
56	Y	202	CDL	CA3-OA5-PA1-OA4
56	h	201	CDL	CA2-OA2-PA1-OA3
56	h	201	CDL	CB2-OB2-PB2-OB4
56	h	201	CDL	CB3-OB5-PB2-OB3
56	AG	101	CDL	CA2-OA2-PA1-OA3
56	AG	101	CDL	CB2-OB2-PB2-OB4
56	Aa	502	CDL	CA2-OA2-PA1-OA4
56	Aa	502	CDL	CB3-OB5-PB2-OB3
56	Aa	502	CDL	CB3-OB5-PB2-OB4
56	Ag	102	CDL	CB2-OB2-PB2-OB4
62	q	202	PC1	C11-O13-P-O12
62	Ae	301	PC1	C1-O11-P-O14
63	O	401	ADP	C5'-O5'-PA-O1A
63	O	401	ADP	C5'-O5'-PA-O2A
58	D	501	UQ1	C1-C2-O2-CM2
56	d	201	CDL	C51-C52-C53-C54
55	i	201	3PE	C32-C33-C34-C35
55	m	202	3PE	C22-C21-O21-C2
66	W	201	EHZ	C2-C3-C4-C5
62	L	701	PC1	O13-C11-C12-N
62	l	201	PC1	O13-C11-C12-N
62	q	202	PC1	O13-C11-C12-N
55	J	201	3PE	O22-C21-O21-C2
55	i	201	3PE	O21-C2-C3-O31
56	M	503	CDL	C1-CB2-OB2-PB2
56	q	201	CDL	C1-CB2-OB2-PB2
66	n	201	EHZ	C3-C4-C5-C6
56	h	201	CDL	C53-C54-C55-C56
66	W	201	EHZ	O4-C15-C16-O5
62	I	301	PC1	C11-C12-N-C14
61	H	401	UQ9	C12-C11-C9-C10
55	i	201	3PE	C3-C2-O21-C21
56	L	703	CDL	CB3-CB4-OB6-CB5
55	J	201	3PE	C22-C21-O21-C2
56	q	201	CDL	C1-CA2-OA2-PA1
56	Ag	102	CDL	C1-CA2-OA2-PA1
56	AG	102	CDL	C71-CB7-OB8-CB6
56	AG	102	CDL	OB9-CB7-OB8-CB6
55	A	401	3PE	O11-C1-C2-O21
56	M	503	CDL	C15-C16-C17-C18
55	M	502	3PE	C1-O11-P-O13
55	Y	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
56	L	703	CDL	CA2-OA2-PA1-OA5
56	L	703	CDL	CA3-OA5-PA1-OA2
56	L	703	CDL	CB2-OB2-PB2-OB5
56	L	703	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CB2-OB2-PB2-OB5
56	d	201	CDL	CB3-OB5-PB2-OB2
56	q	201	CDL	CB2-OB2-PB2-OB5
62	l	201	PC1	C11-O13-P-O11
55	L	704	3PE	C21-C22-C23-C24
55	A	401	3PE	C1-C2-C3-O31
55	M	501	3PE	C1-C2-C3-O31
55	A	401	3PE	C25-C26-C27-C28
55	Ag	103	3PE	C35-C36-C37-C38
64	P	401	NDP	PN-O3-PA-O2A
55	AG	103	3PE	C35-C36-C37-C38
55	i	201	3PE	C2-C1-O11-P
55	m	202	3PE	O22-C21-O21-C2
55	J	201	3PE	C23-C24-C25-C26
56	M	503	CDL	C17-C18-C19-C20
56	Y	202	CDL	C53-C54-C55-C56
62	q	202	PC1	O11-C1-C2-C3
61	H	401	UQ9	C14-C16-C17-C18
56	L	703	CDL	C74-C75-C76-C77
56	A	402	CDL	C16-C17-C18-C19
56	Ag	101	CDL	C1-CA2-OA2-PA1
68	AC	405	U10	C12-C11-C9-C10
68	Ac	404	U10	C12-C11-C9-C10
56	h	201	CDL	C79-C80-C81-C82
67	AC	403	HEM	CAD-CBD-CGD-O1D
67	Ac	402	HEM	CAD-CBD-CGD-O1D
55	L	702	3PE	C28-C29-C2A-C2B
56	Y	202	CDL	CA3-CA4-OA6-CA5
55	i	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C25-C26-C27-C28
67	AC	402	HEM	CAD-CBD-CGD-O1D
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAD-CBD-CGD-O2D
56	M	503	CDL	C42-C43-C44-C45
67	AC	402	HEM	CAA-CBA-CGA-O2A
67	Ac	401	HEM	CAA-CBA-CGA-O2A
67	Ac	401	HEM	CAD-CBD-CGD-O1D
56	A	402	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
56	Y	202	CDL	OA5-CA3-CA4-CA6
67	AC	403	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O2D
55	A	401	3PE	C21-C22-C23-C24
67	AC	402	HEM	CAA-CBA-CGA-O1A
67	Ac	401	HEM	CAA-CBA-CGA-O1A
56	h	201	CDL	C16-C17-C18-C19
66	n	201	EHZ	C11-C10-S1-C9
56	d	201	CDL	C36-C37-C38-C39
68	AC	405	U10	C12-C11-C9-C8
68	Ac	404	U10	C12-C11-C9-C8
56	L	703	CDL	C53-C54-C55-C56
69	AC	406	UQ6	C5-C6-C7-C8
69	Ac	405	UQ6	C5-C6-C7-C8
62	q	202	PC1	C34-C35-C36-C37
56	Y	202	CDL	C60-C61-C62-C63
56	Ag	102	CDL	C72-C73-C74-C75
61	H	401	UQ9	C12-C11-C9-C8
62	l	201	PC1	C2-C3-O31-C31
67	AC	403	HEM	CAA-CBA-CGA-O2A
67	Ac	402	HEM	CAA-CBA-CGA-O2A
56	Ag	102	CDL	C52-C51-CB5-OB6
55	b	201	3PE	C2B-C2C-C2D-C2E
62	L	701	PC1	C38-C39-C3A-C3B
66	n	201	EHZ	C20-O6-P1-O7
56	h	201	CDL	CB5-C51-C52-C53
56	A	402	CDL	C59-C60-C61-C62
55	M	502	3PE	O32-C31-O31-C3
55	L	702	3PE	C24-C25-C26-C27
56	h	201	CDL	C39-C40-C41-C42
55	A	401	3PE	C39-C3A-C3B-C3C
55	L	702	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C38-C39-C3A-C3B
67	Ac	402	HEM	CAA-CBA-CGA-O1A
55	M	502	3PE	C2F-C2G-C2H-C2I
55	H	402	3PE	C2F-C2G-C2H-C2I
67	AC	403	HEM	CAA-CBA-CGA-O1A
56	L	703	CDL	C35-C36-C37-C38
66	n	201	EHZ	O1-C7-C8-C9
55	Ac	403	3PE	C23-C24-C25-C26
55	m	201	3PE	C27-C28-C29-C2A
55	i	201	3PE	O21-C21-C22-C23

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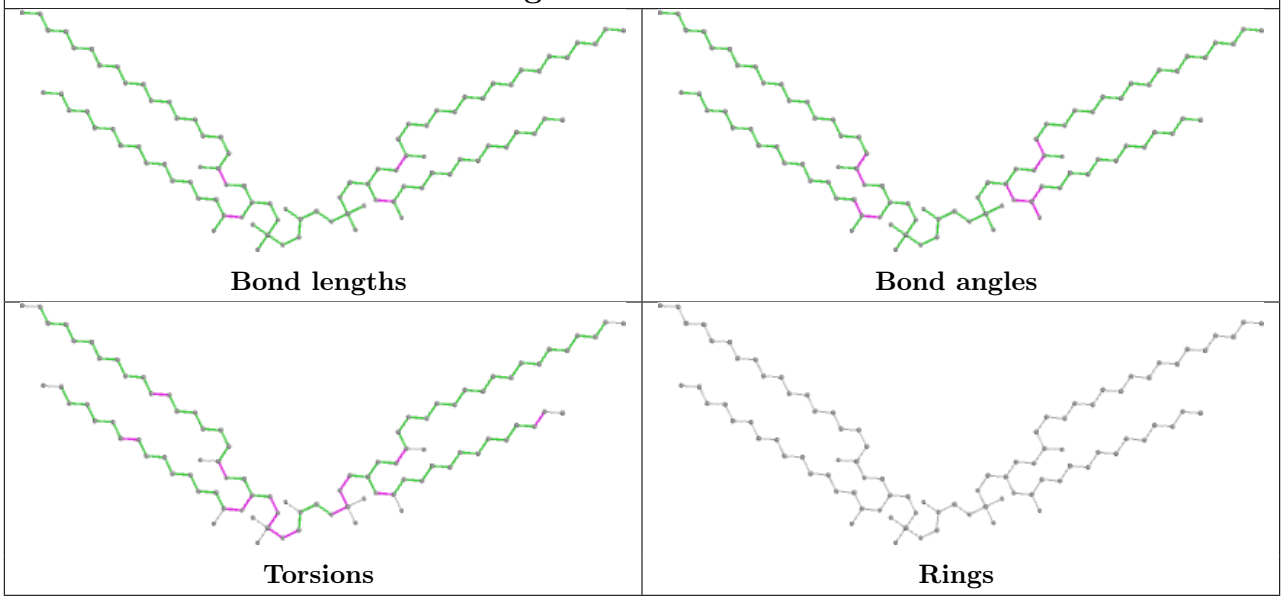
Mol	Chain	Res	Type	Atoms
55	AC	401	3PE	O31-C31-C32-C33
62	q	202	PC1	C11-C12-N-C15
55	M	502	3PE	C32-C31-O31-C3
56	h	201	CDL	C11-C12-C13-C14
61	H	401	UQ9	C23-C24-C26-C27
56	d	201	CDL	OB7-CB5-OB6-CB4
55	M	501	3PE	C33-C34-C35-C36
56	h	201	CDL	C12-C11-CA5-OA6
69	AC	406	UQ6	C6-C7-C8-C9
69	Ac	405	UQ6	C6-C7-C8-C9
55	L	702	3PE	C2B-C2C-C2D-C2E
55	i	201	3PE	O22-C21-C22-C23
55	M	502	3PE	C2-C1-O11-P
56	M	503	CDL	CB4-CB3-OB5-PB2
56	Y	202	CDL	C1-CA2-OA2-PA1
55	m	201	3PE	C36-C37-C38-C39
55	A	401	3PE	C1-O11-P-O14
55	AC	404	3PE	C11-O13-P-O14
55	Aa	501	3PE	C1-O11-P-O14
55	Ac	403	3PE	C11-O13-P-O14
56	A	402	CDL	CA2-OA2-PA1-OA4
56	A	402	CDL	CB2-OB2-PB2-OB3
56	h	201	CDL	C12-C11-CA5-OA7
55	A	401	3PE	O11-C1-C2-C3
56	M	503	CDL	OA5-CA3-CA4-CA6
55	b	201	3PE	C37-C38-C39-C3A
55	m	201	3PE	C2A-C2B-C2C-C2D
56	M	503	CDL	C73-C74-C75-C76
56	q	201	CDL	C18-C19-C20-C21
55	m	201	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C12-C11-O13-P
56	Y	202	CDL	C72-C71-CB7-OB8
56	Ag	102	CDL	CB2-C1-CA2-OA2
61	H	401	UQ9	C25-C24-C26-C27
55	Ac	403	3PE	C22-C23-C24-C25
62	I	301	PC1	C2C-C2D-C2E-C2F
55	AC	401	3PE	O21-C21-C22-C23
55	AC	401	3PE	O32-C31-C32-C33
58	D	501	UQ1	C2-C3-O3-CM3

There are no ring outliers.

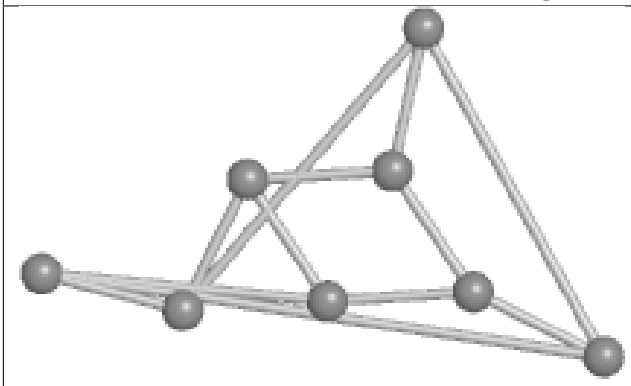
No monomer is involved in short contacts.

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

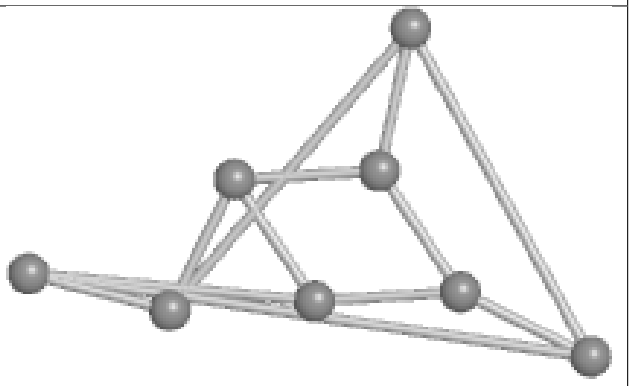
Ligand CDL A 402



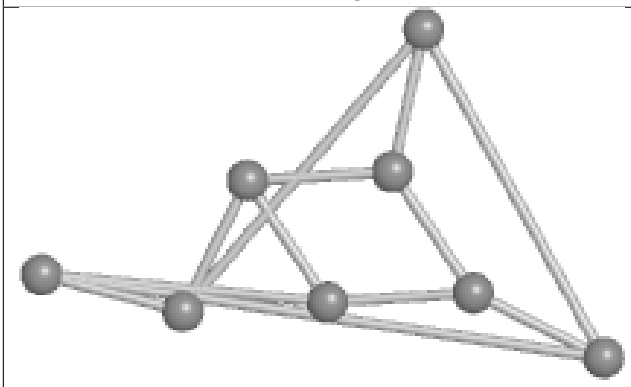
Ligand SF4 I 303



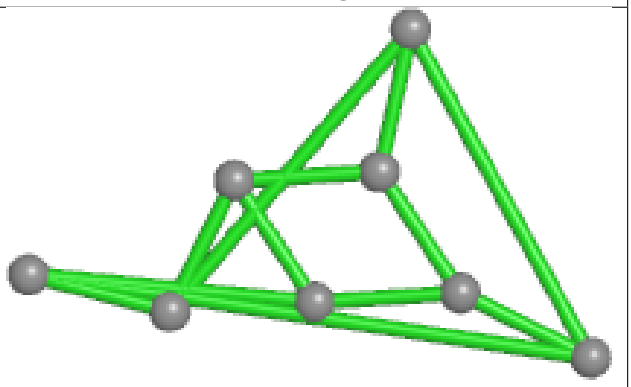
Bond lengths



Bond angles

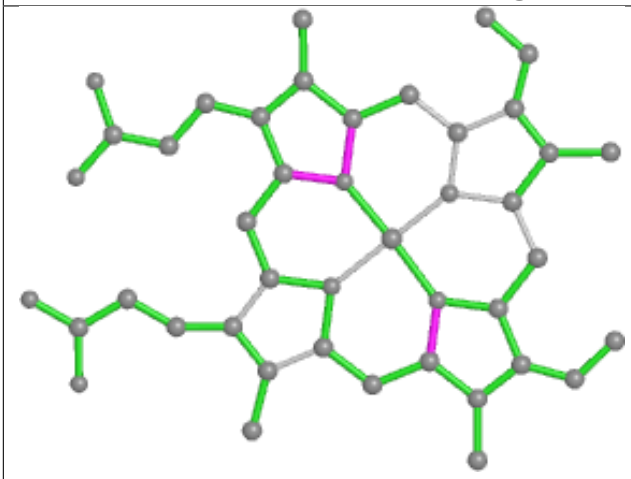


Torsions

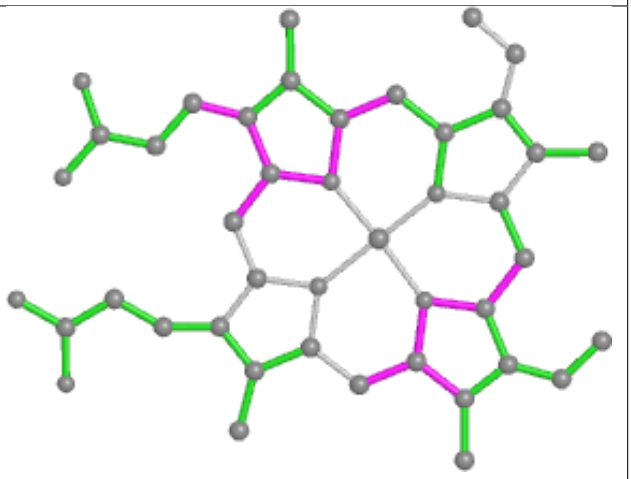


Rings

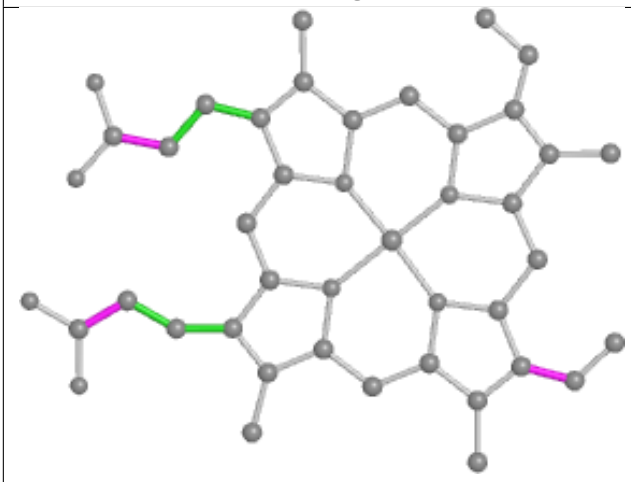
Ligand HEM Ac 402



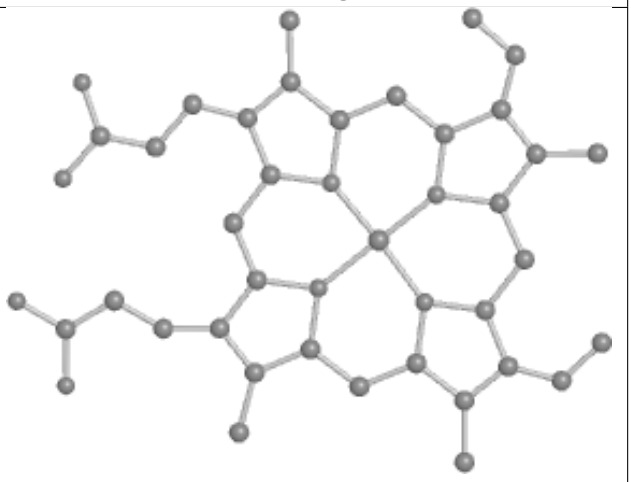
Bond lengths



Bond angles

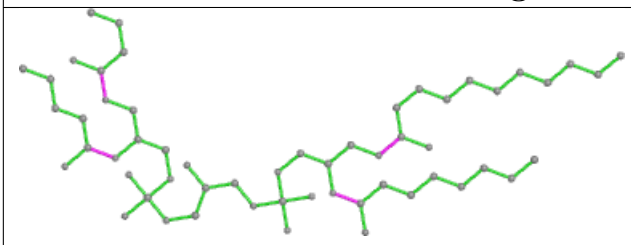


Torsions

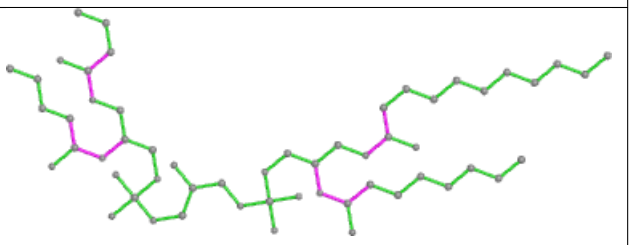


Rings

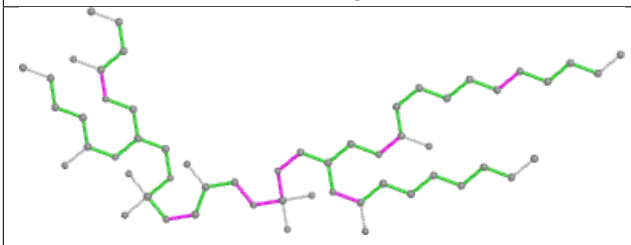
Ligand CDL AG 102



Bond lengths



Bond angles



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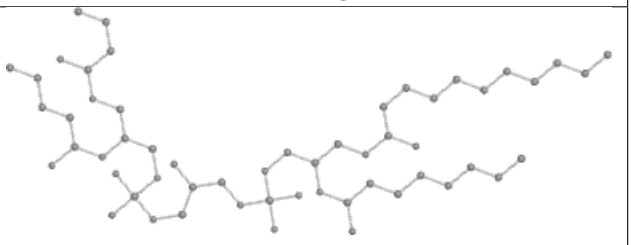
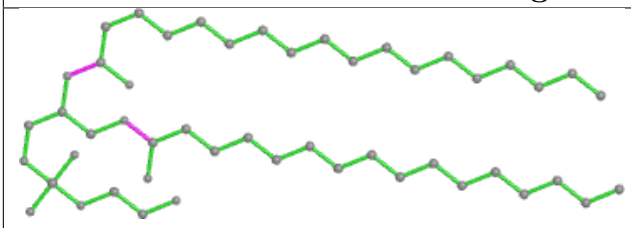
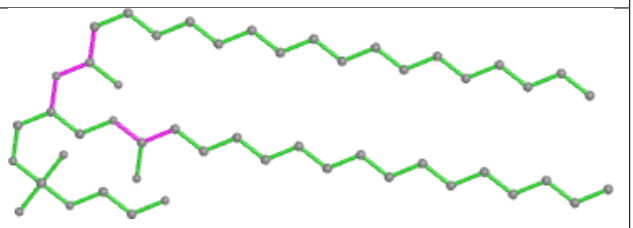


Rings

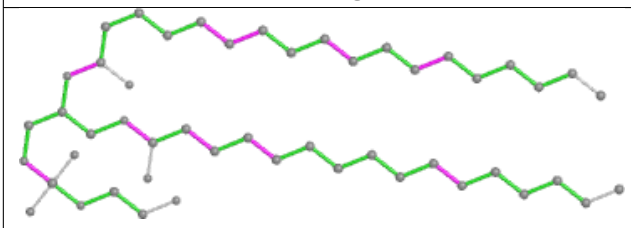
Ligand 3PE L 702



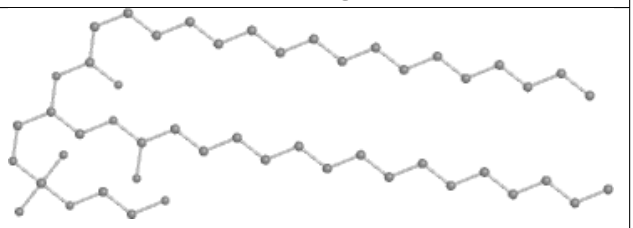
Bond lengths



Bond angles

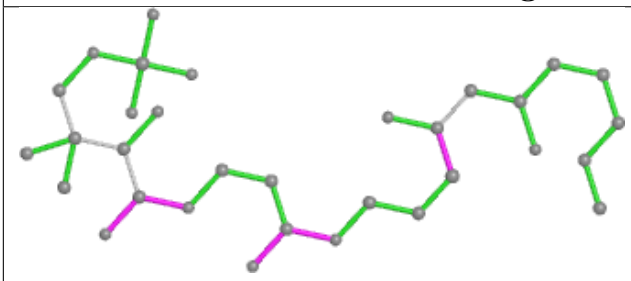


Torsions

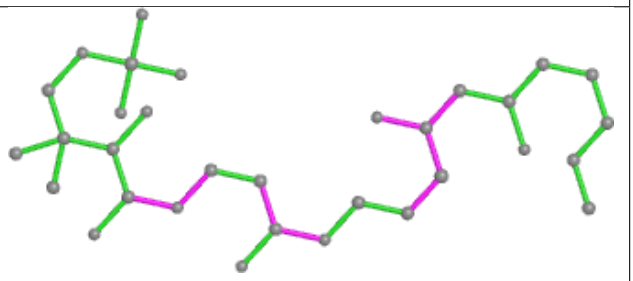


Rings

Ligand EHZ W 201



Bond lengths



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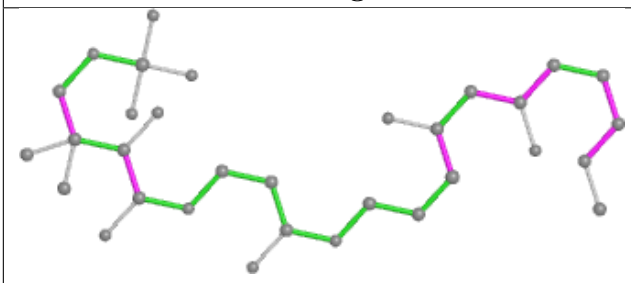

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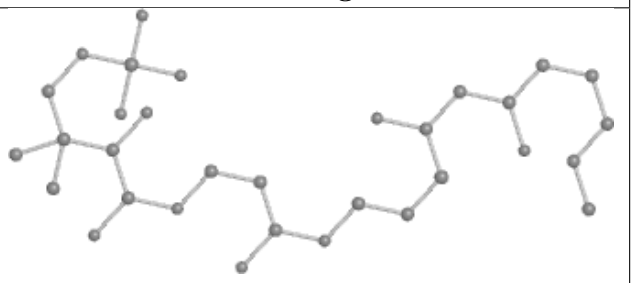
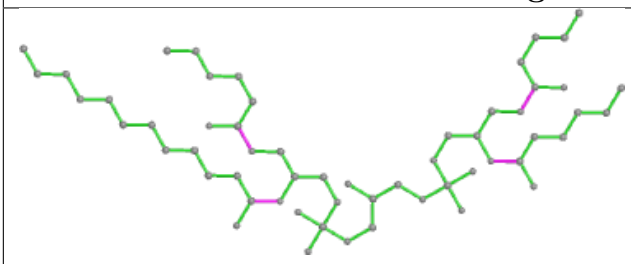


Rings

Ligand CDL q 201



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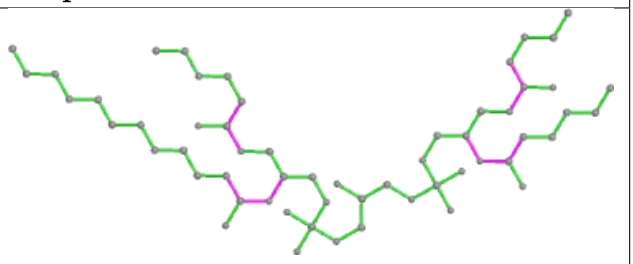
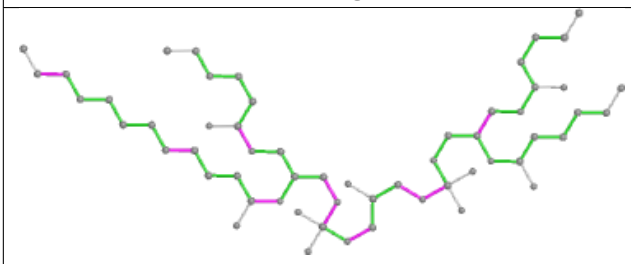


Bond angles



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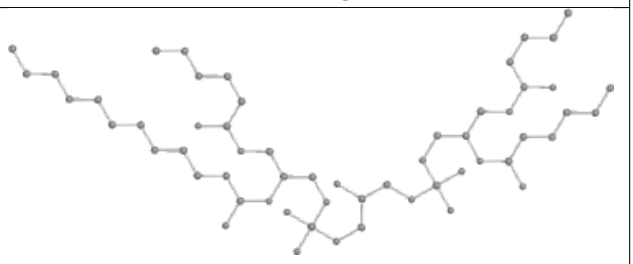
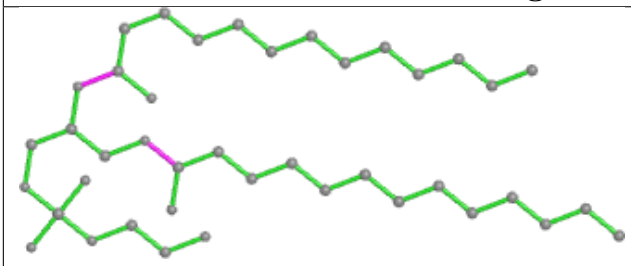


Rings

Ligand 3PE m 202



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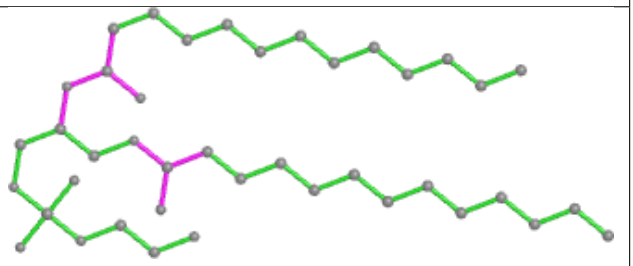

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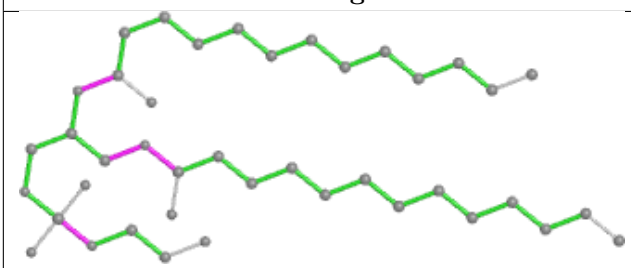
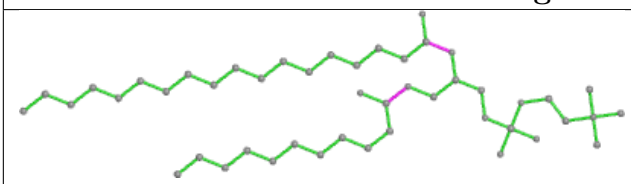


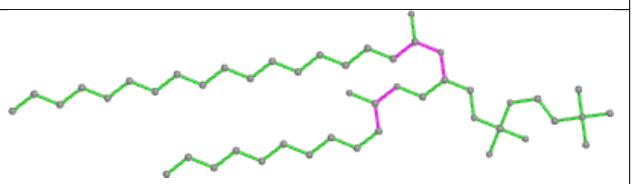
Torsions

Rings

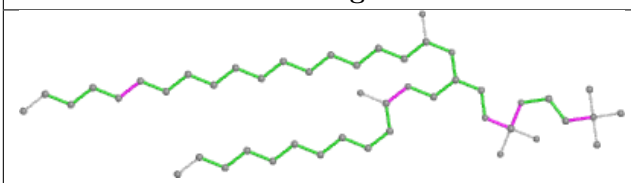
Ligand PC1 I 301



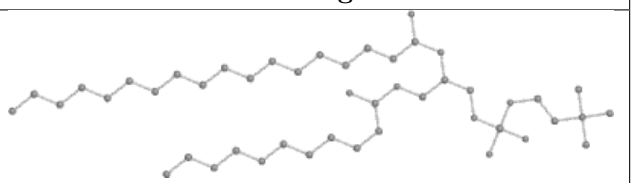
Bond lengths



Bond angles

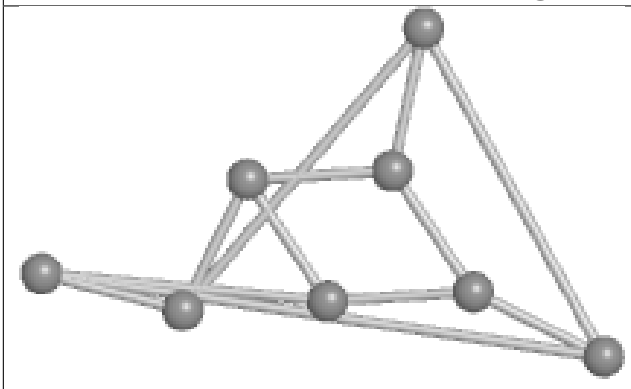


Torsions



Rings

Ligand SF4 B 301



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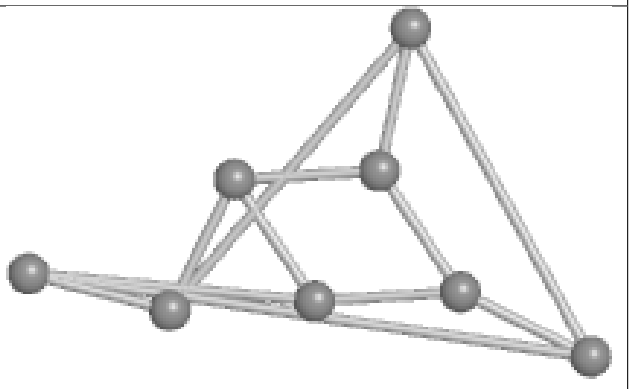
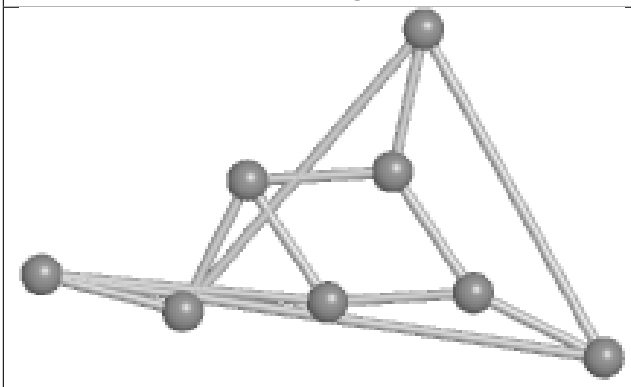


Bond angles



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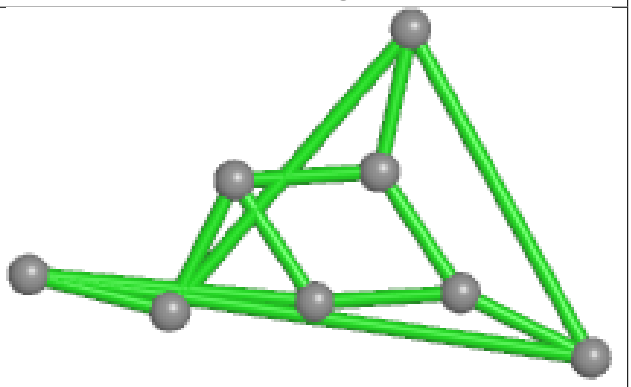
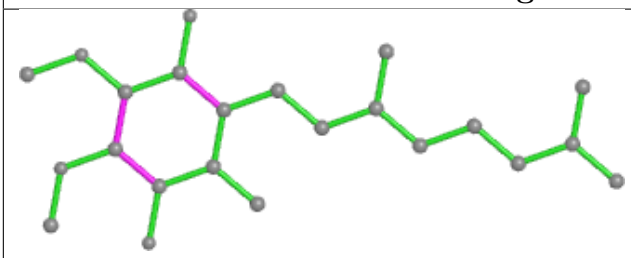


Rings

Ligand U10 AC 405



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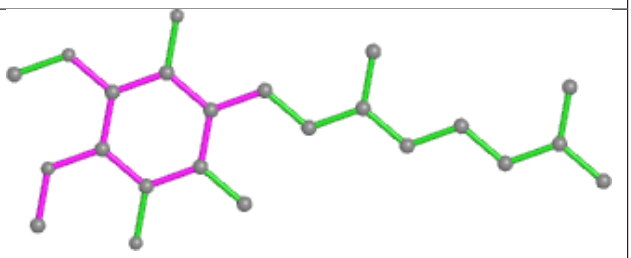
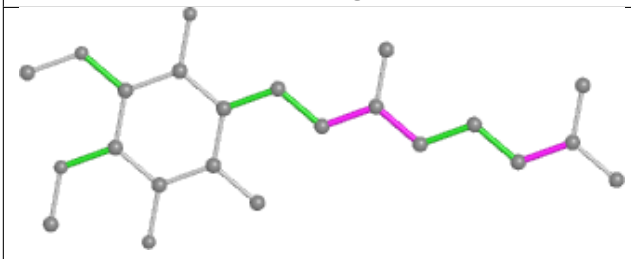


Bond angles



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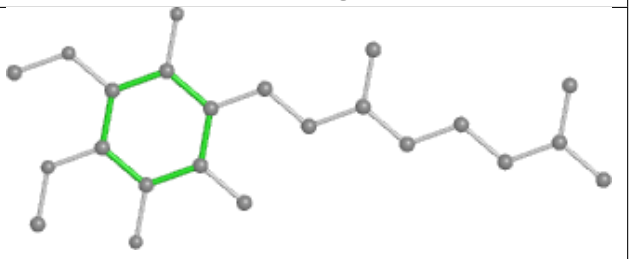
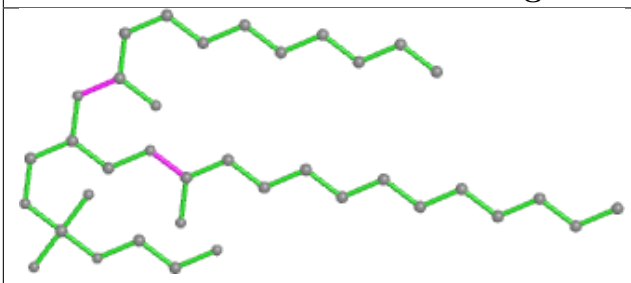


Rings

Ligand 3PE M 501



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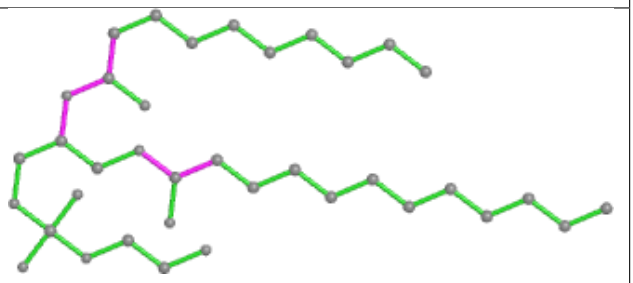
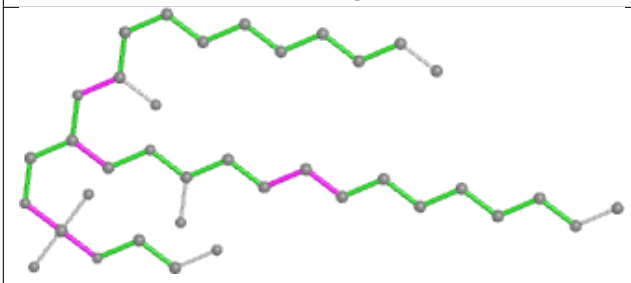
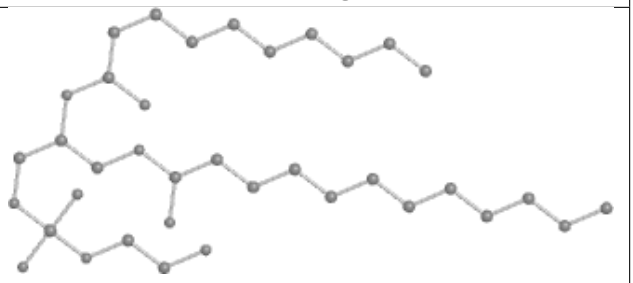


Bond angles

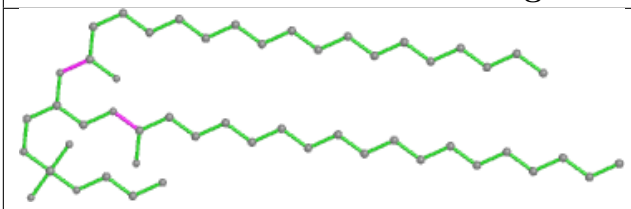


Torsions



Rings

Ligand 3PE M 502



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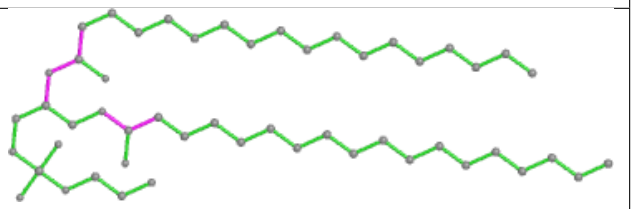
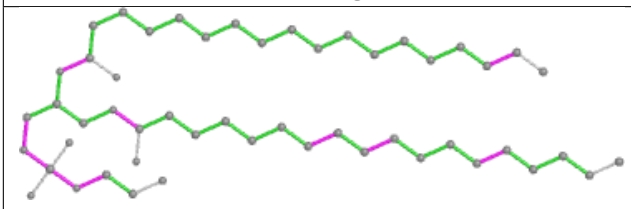


Bond angles



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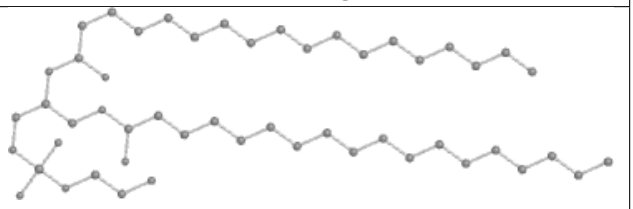
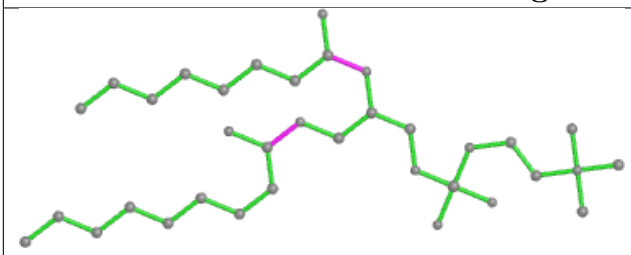


Rings

Ligand PC1 q 202



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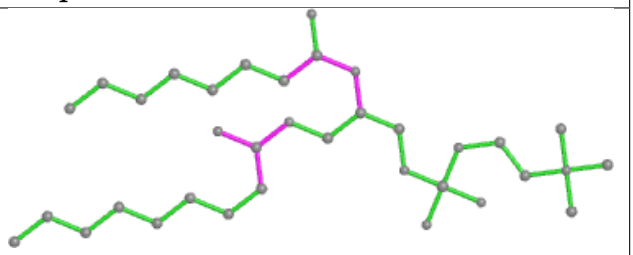
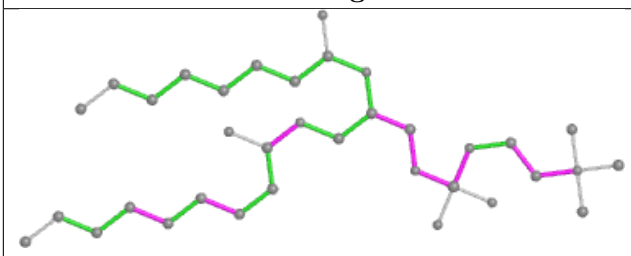


Bond angles



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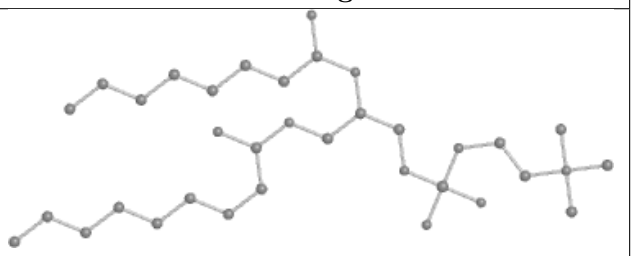
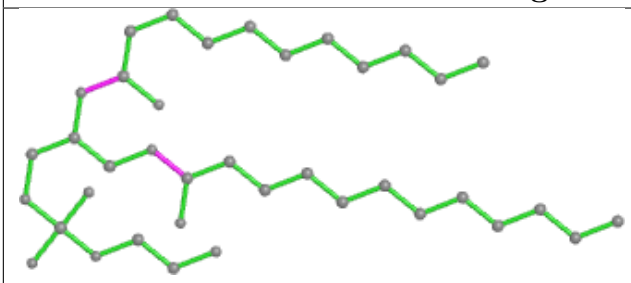


Rings

Ligand 3PE L 704



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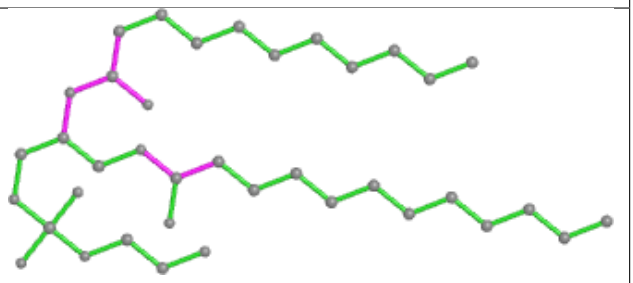
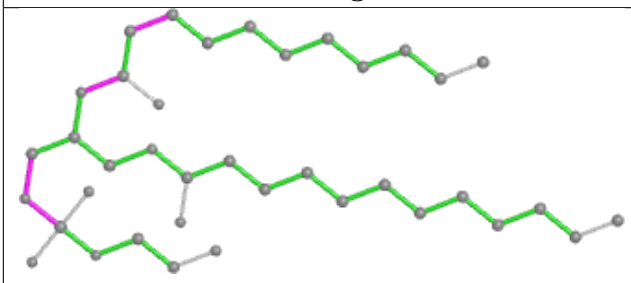


Bond angles



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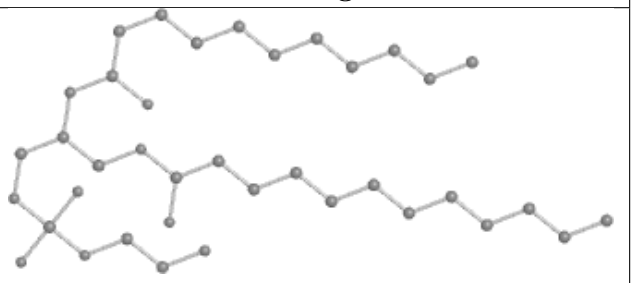
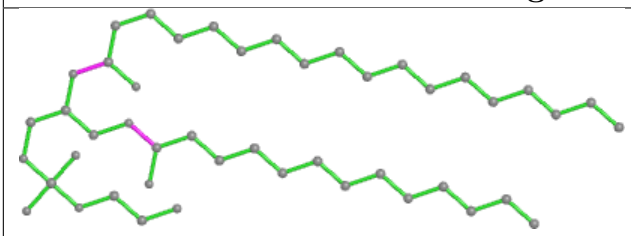


Rings

Ligand 3PE H 402



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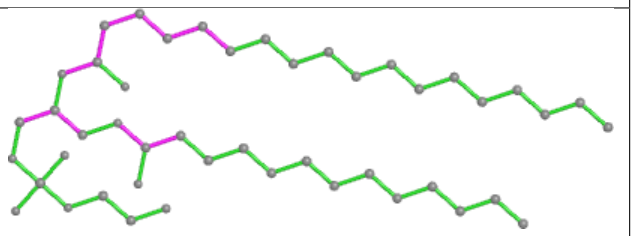
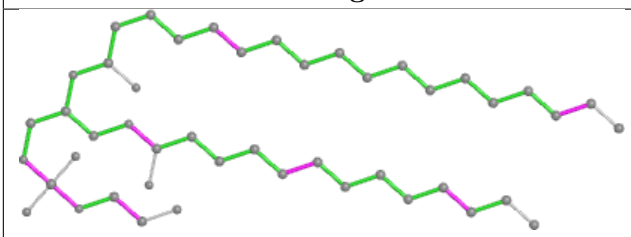


Bond angles



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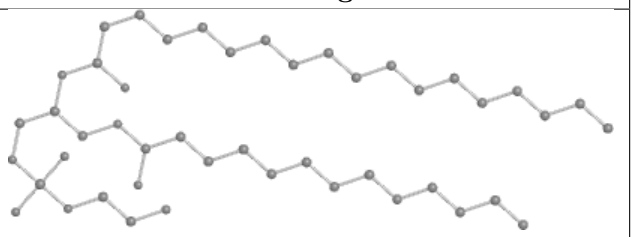
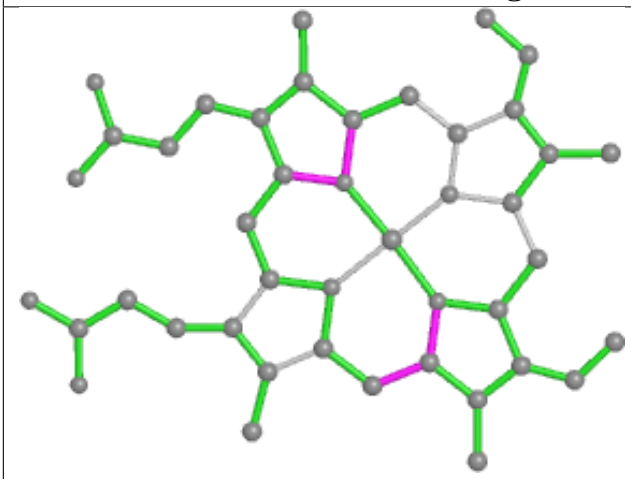


Rings

Ligand HEM AC 402



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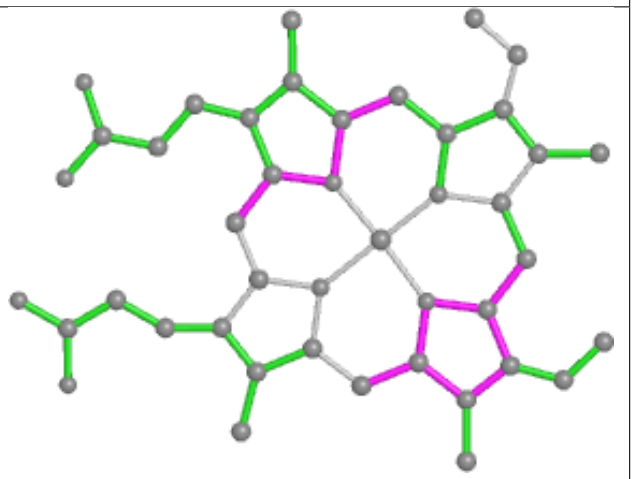
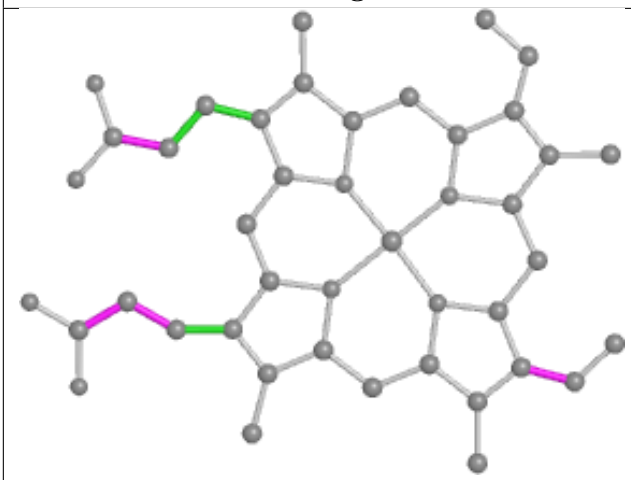
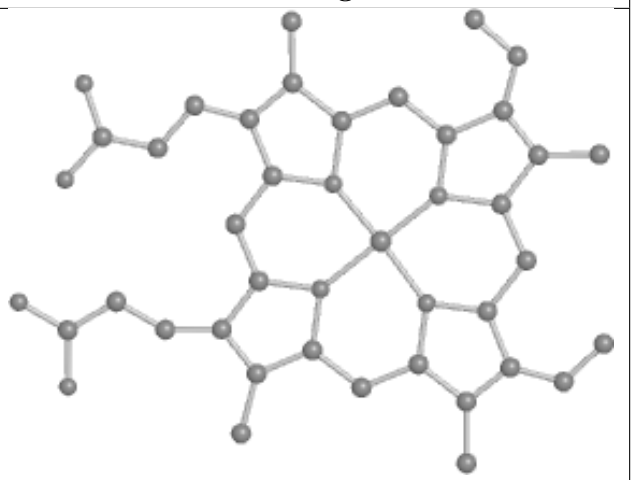


Bond angles

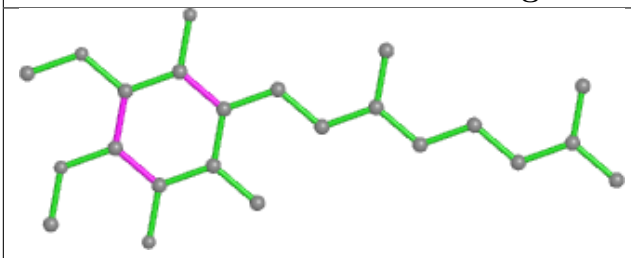


Torsions

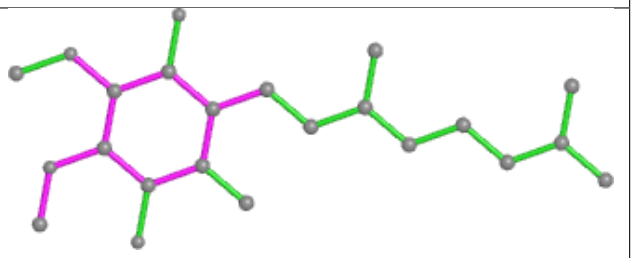


Rings

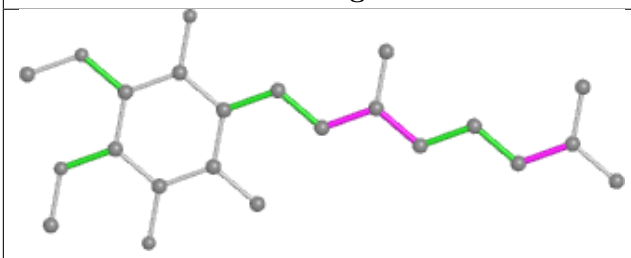
Ligand U10 Ac 404



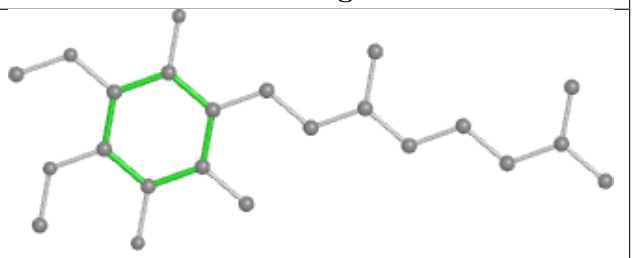
Bond lengths



Bond angles

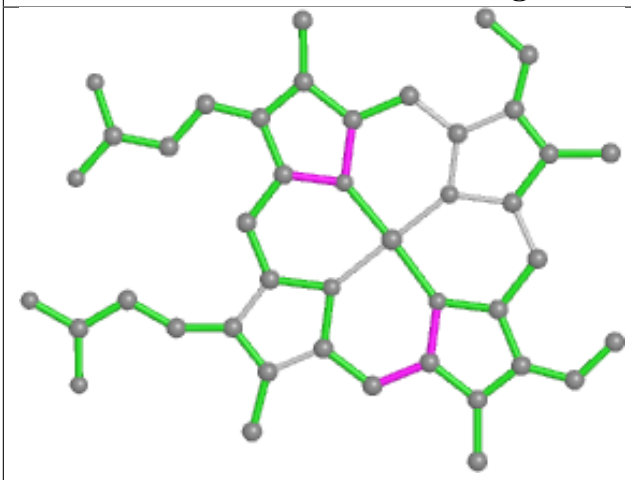


Torsions



Rings

Ligand HEM Ac 401



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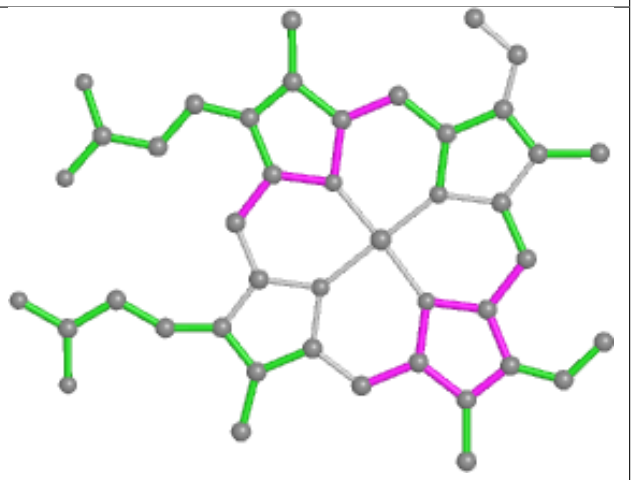
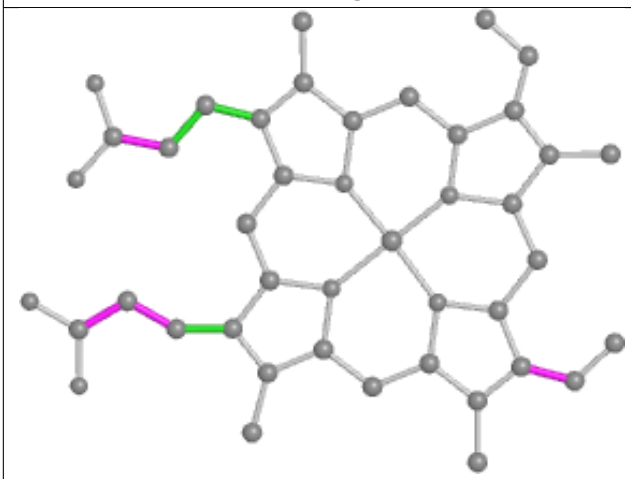


Bond angles



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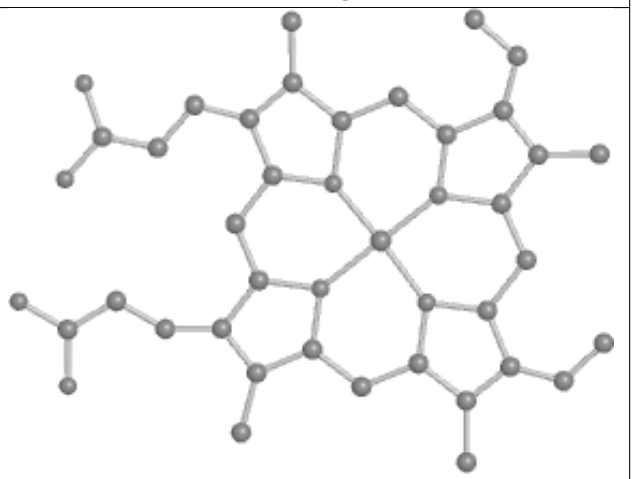
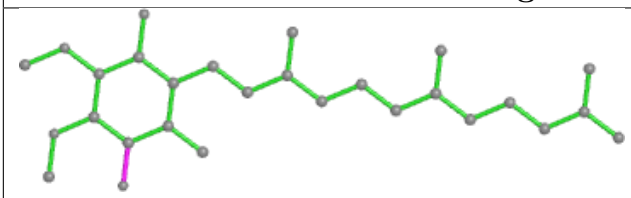


Rings

Ligand UQ6 Ac 405



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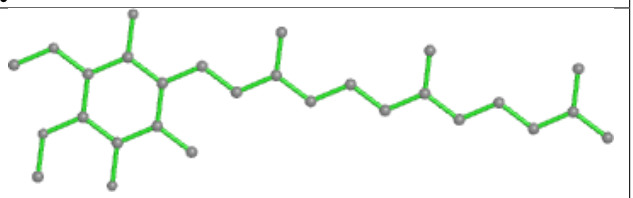
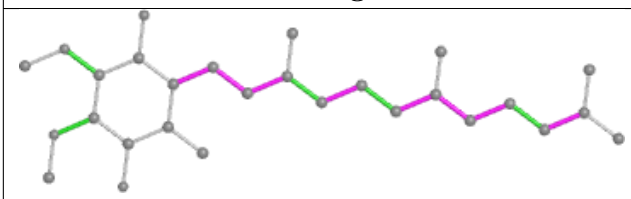


Bond angles



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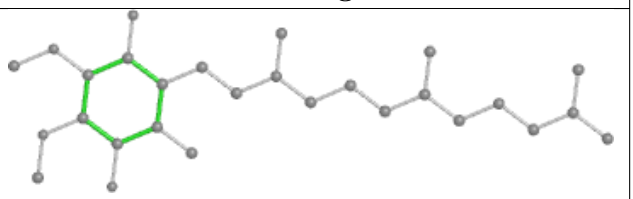
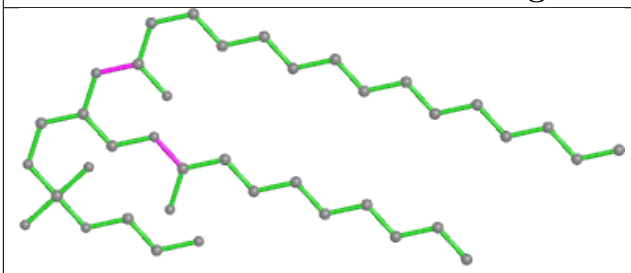


Rings

Ligand 3PE Y 201



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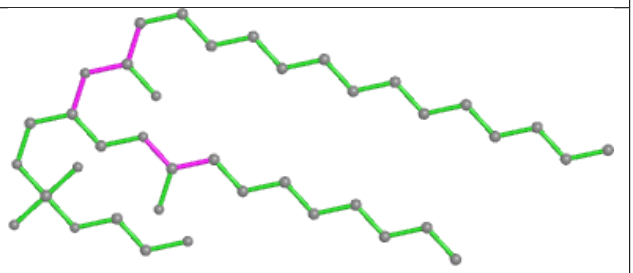
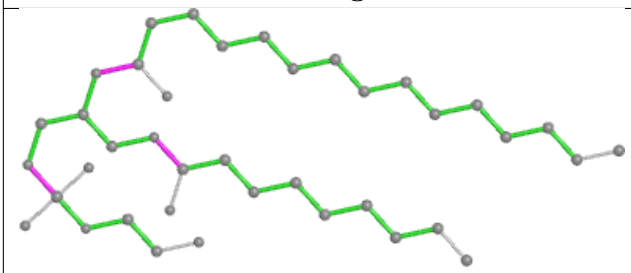


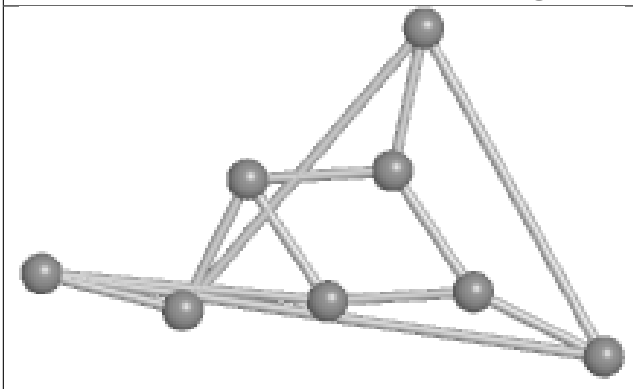
Bond angles



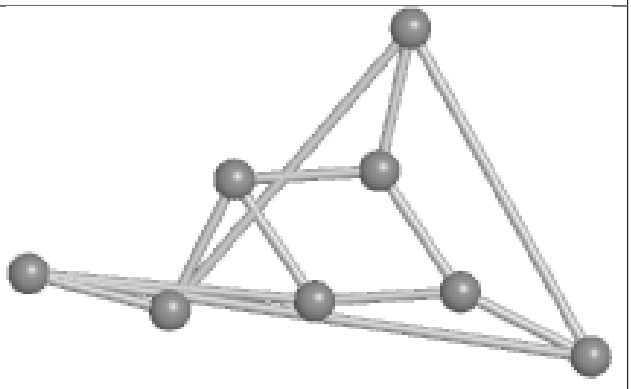
Torsions

Rings

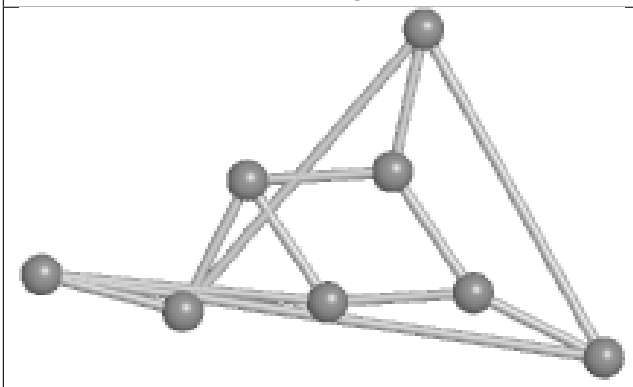
Ligand SF4 G 802



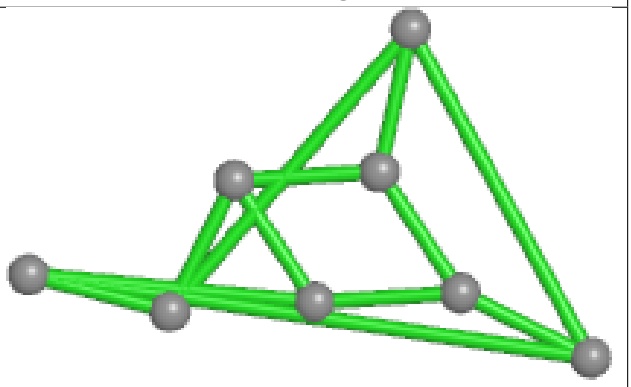
Bond lengths



Bond angles

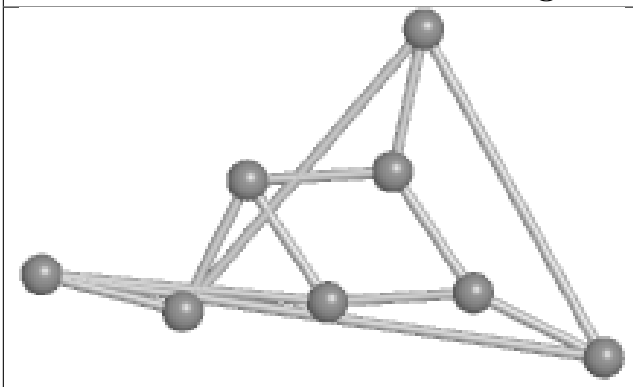


Torsions

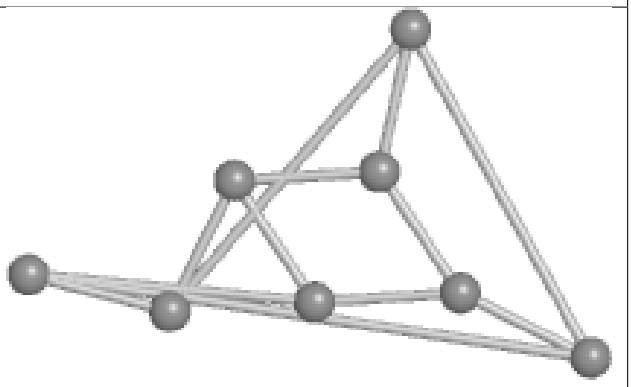


Rings

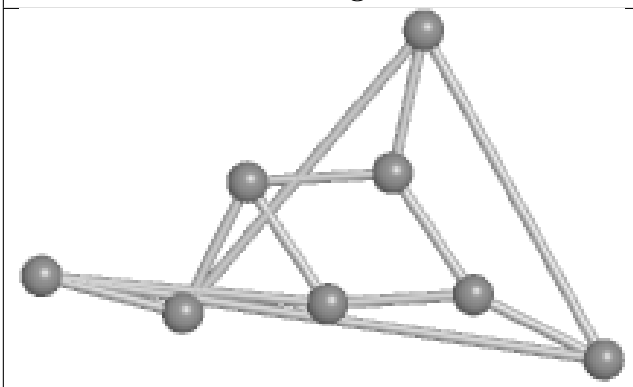
Ligand SF4 I 302



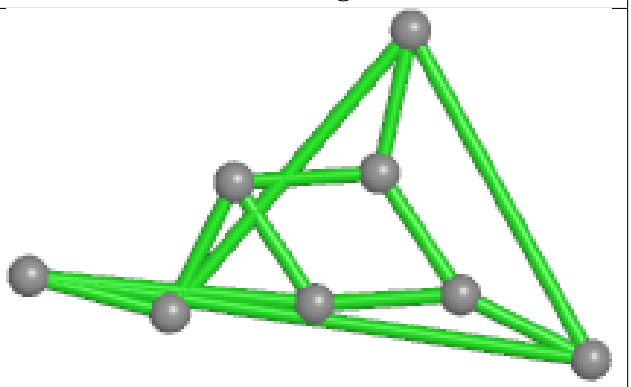
Bond lengths



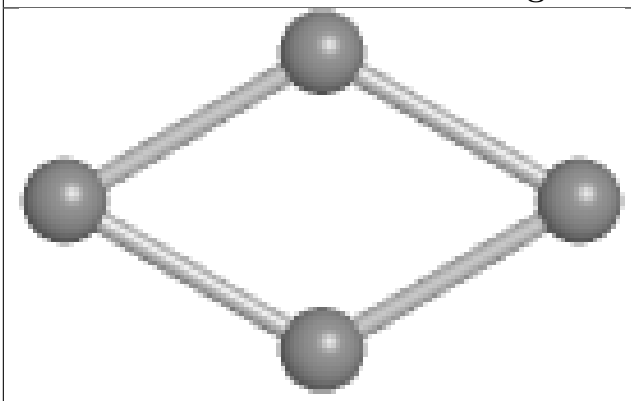
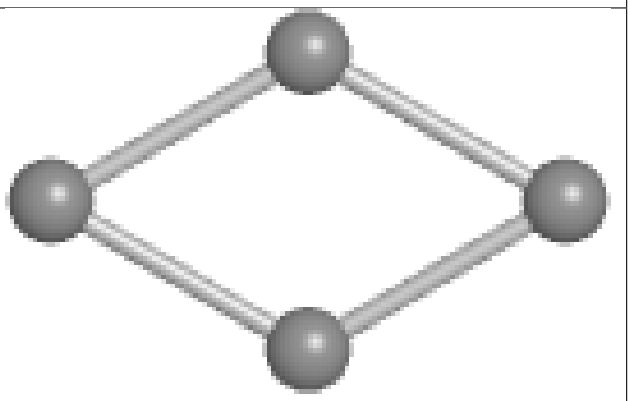
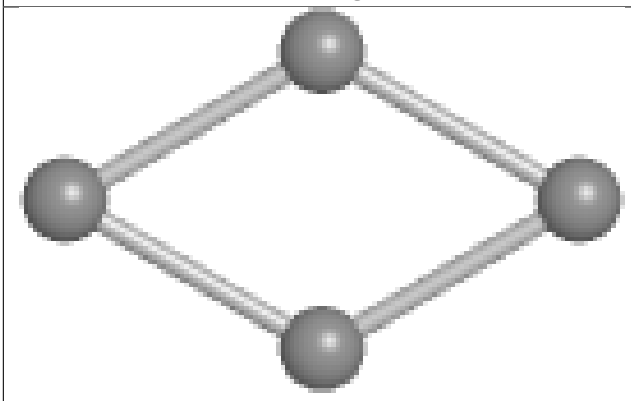
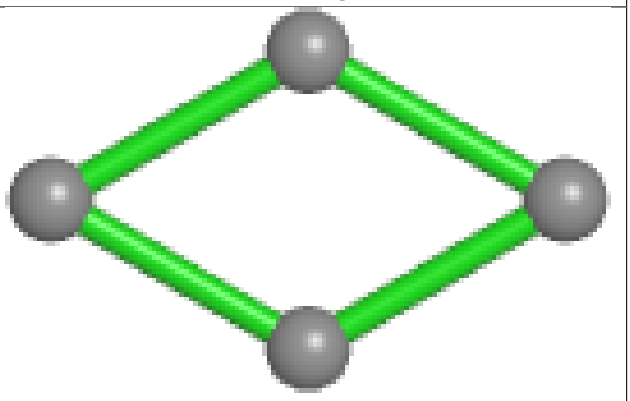
Bond angles



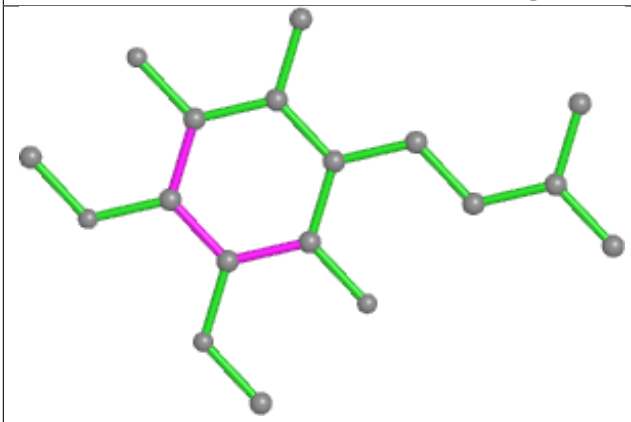
Torsions



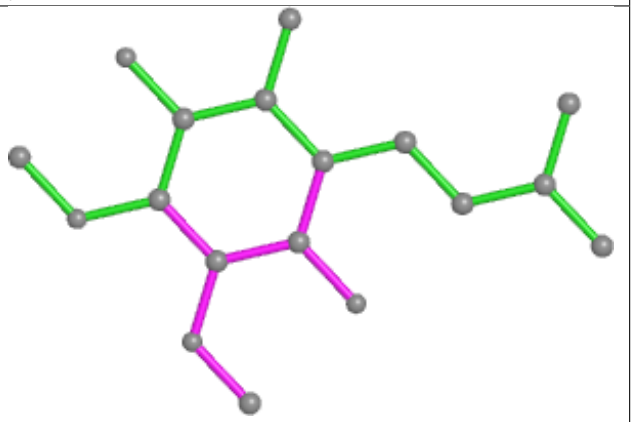
Rings

Ligand FES G 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

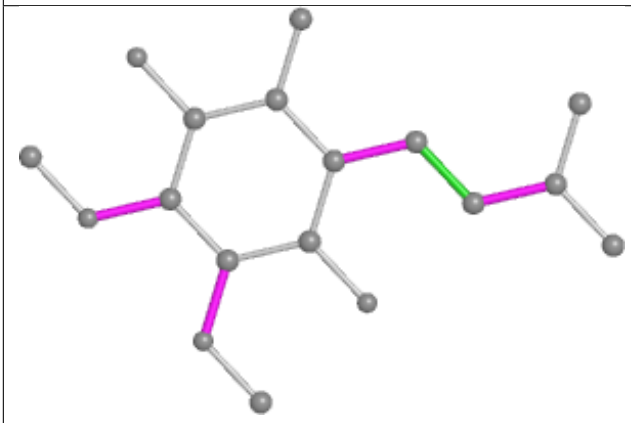
Ligand UQ1 D 501



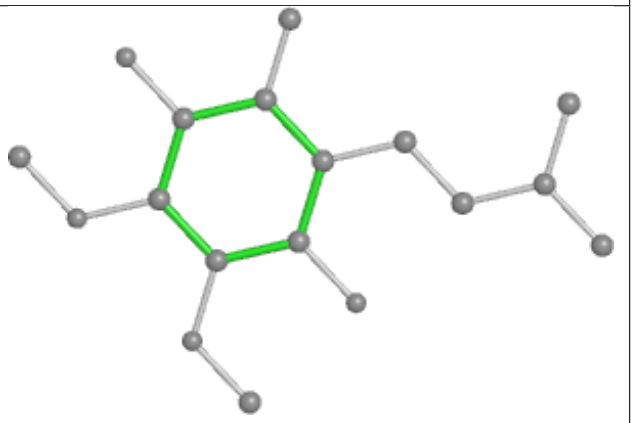
Bond lengths



Bond angles

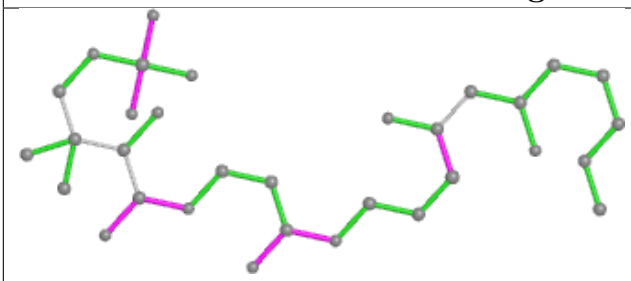


Torsions



Rings

Ligand EHZ n 201



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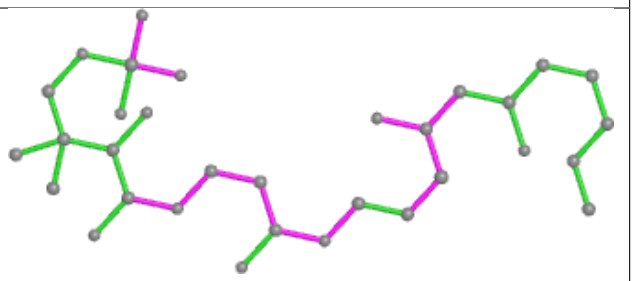
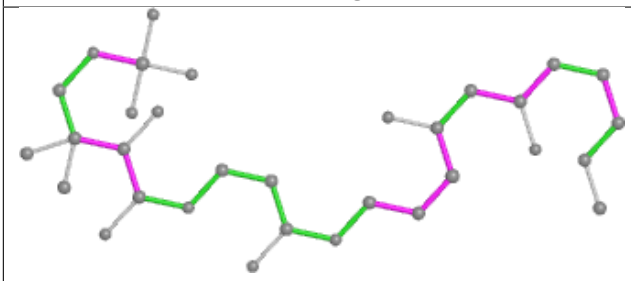


Bond angles



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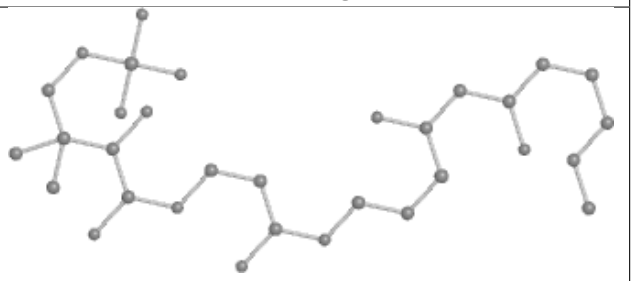
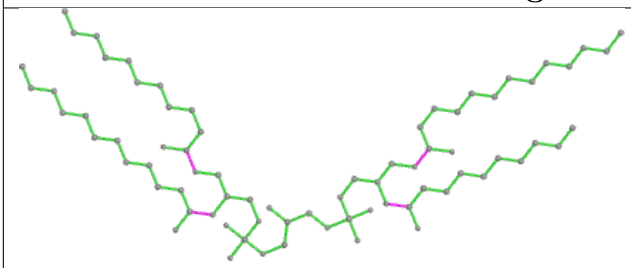


Rings

Ligand CDL L 703



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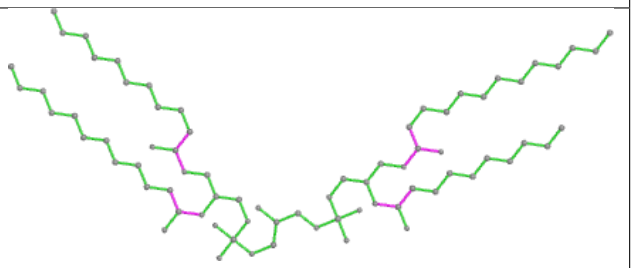
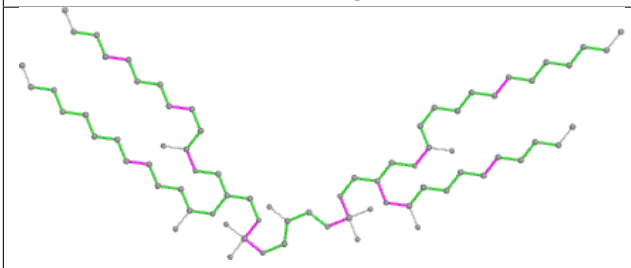


Bond angles



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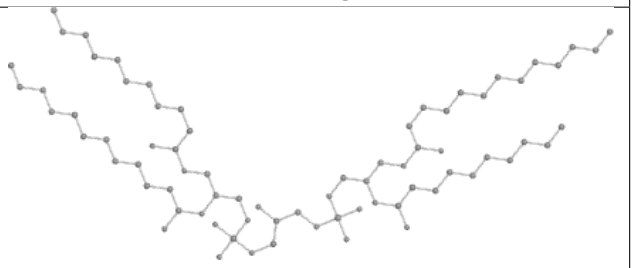
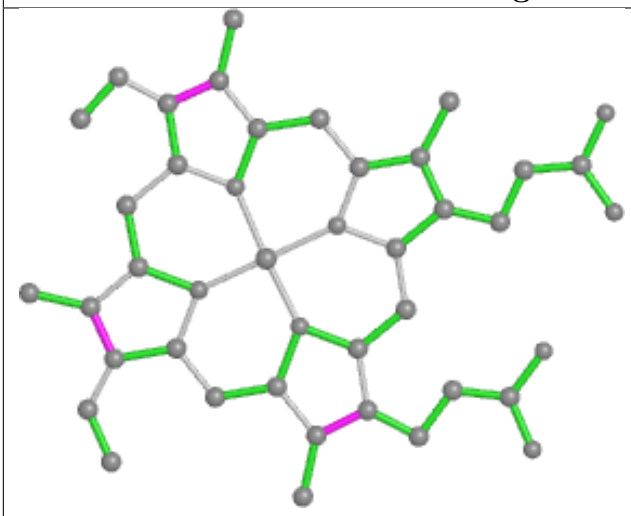


Rings

Ligand HEC Ad 401



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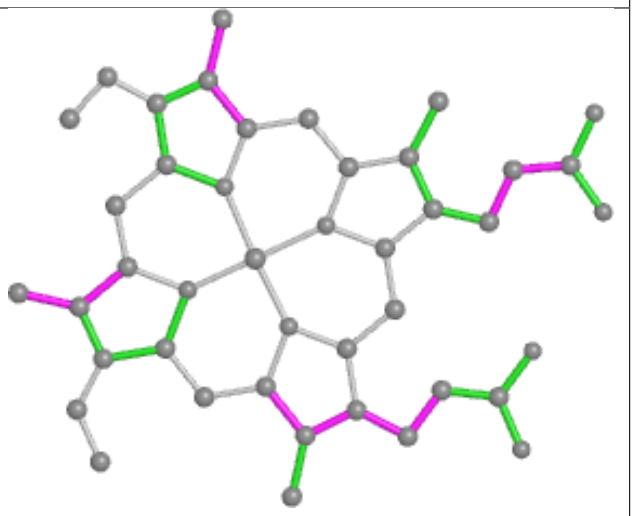
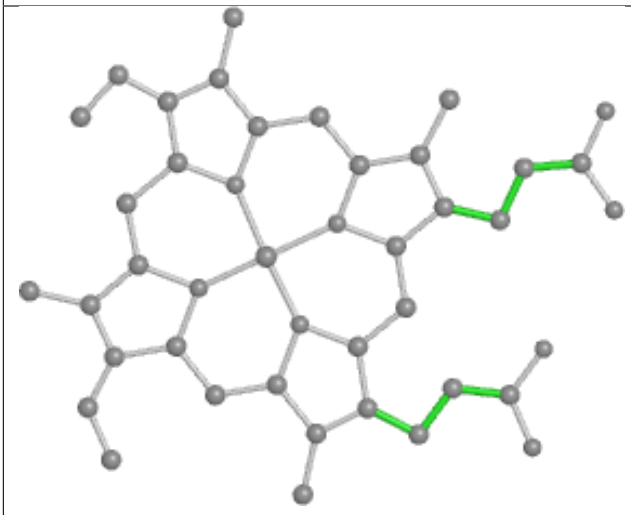


Bond angles



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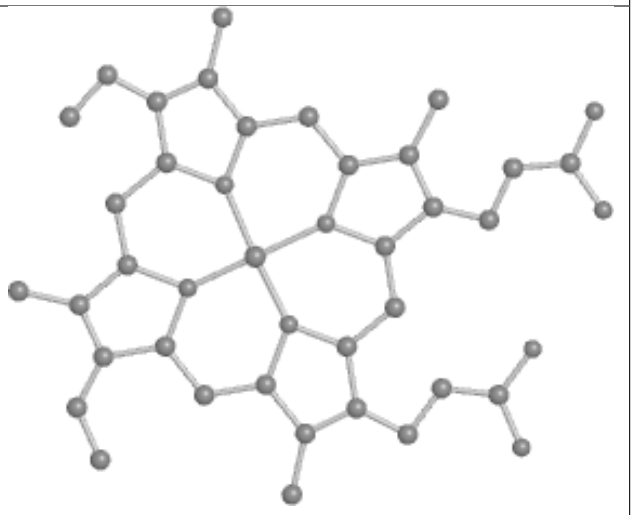

Rings

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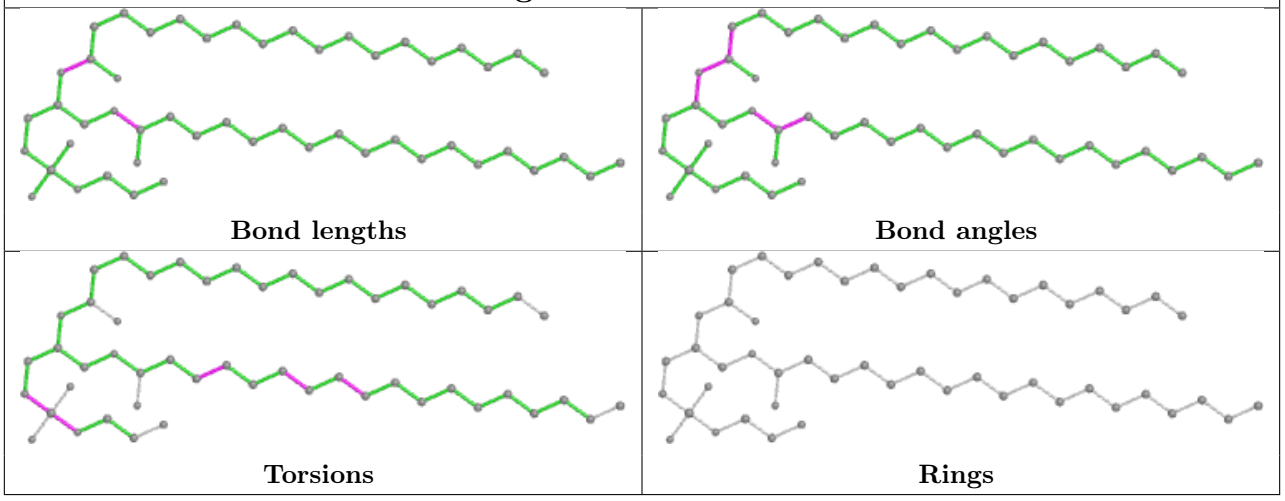

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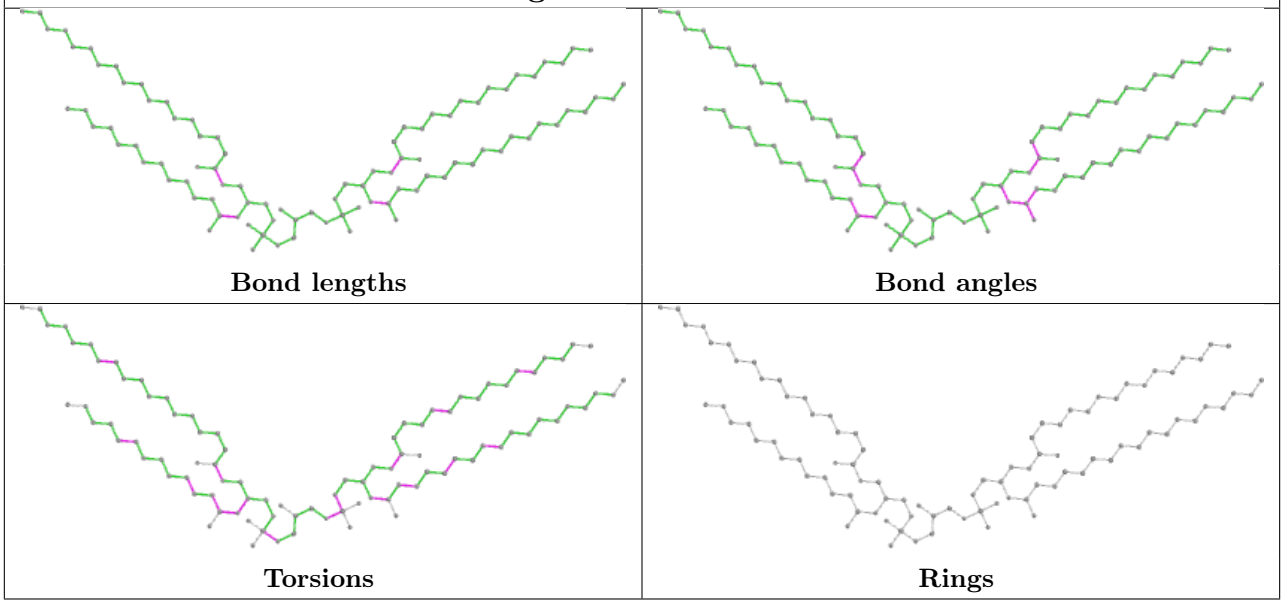

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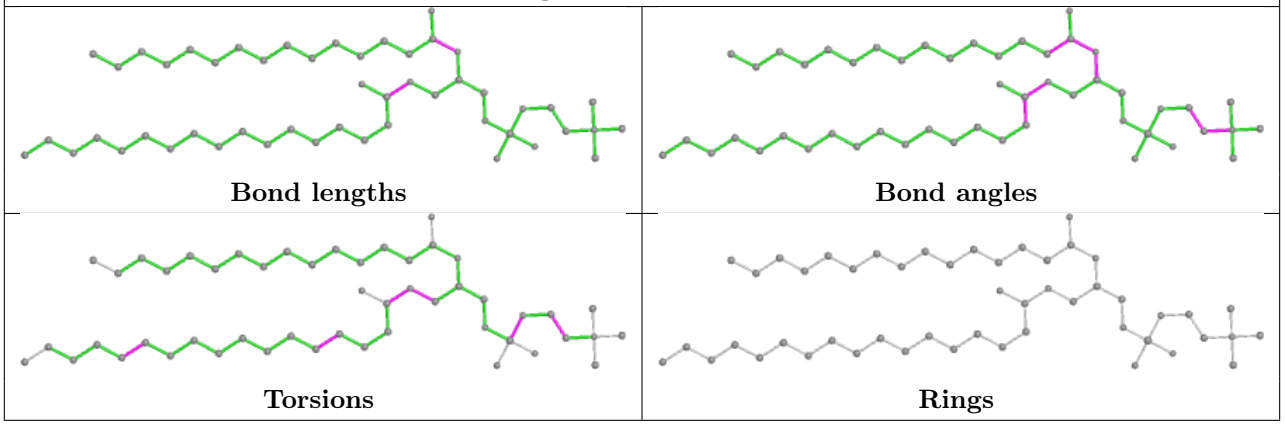

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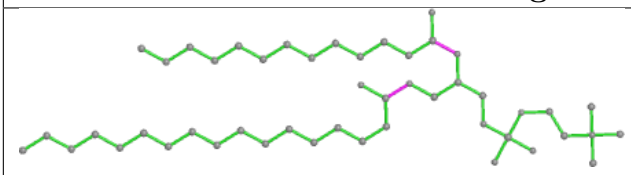
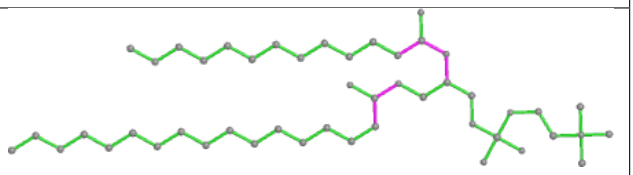
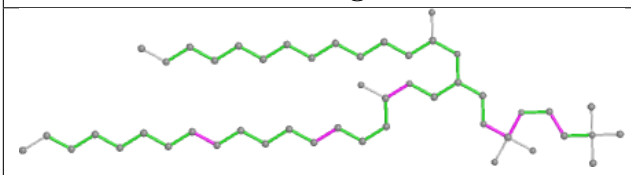


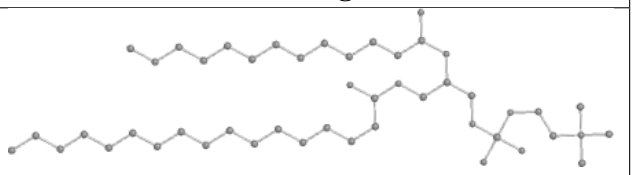
Bond lengths



Bond angles

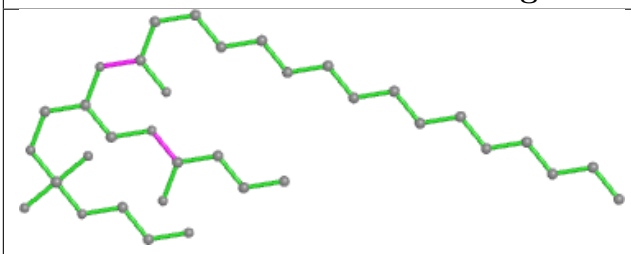


Torsions



Rings

Ligand 3PE Ac 403



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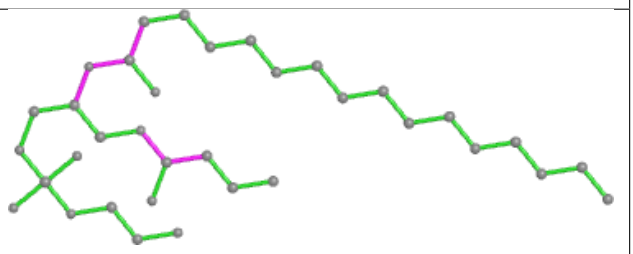
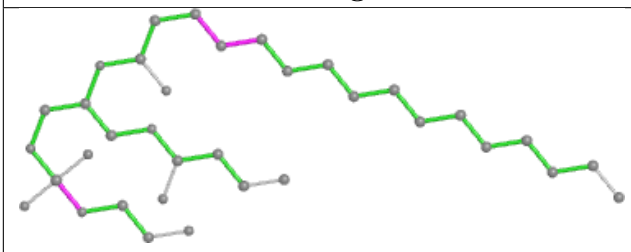
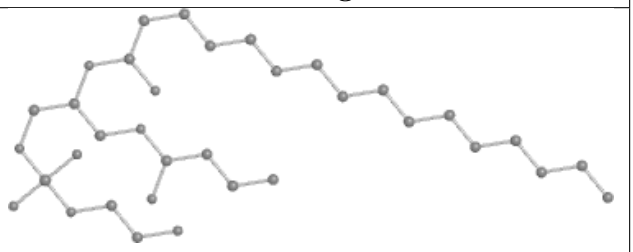


Bond angles

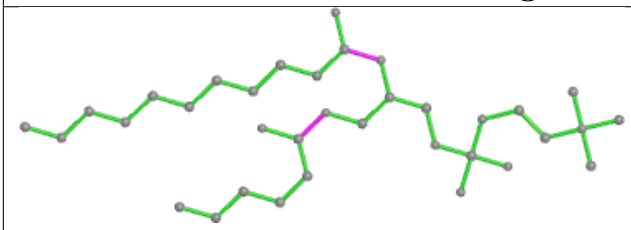


Torsions



Rings

Ligand PC1 Ae 301



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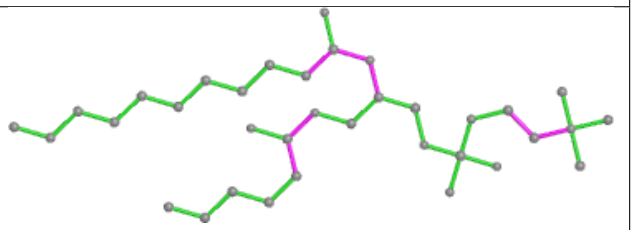

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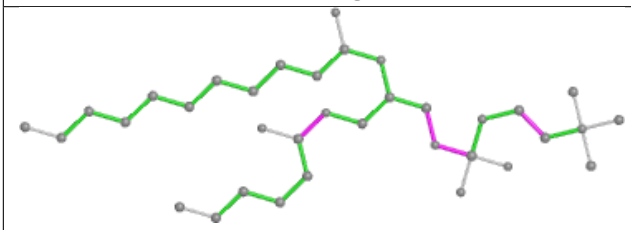

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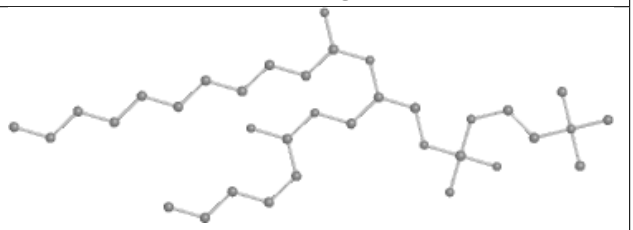
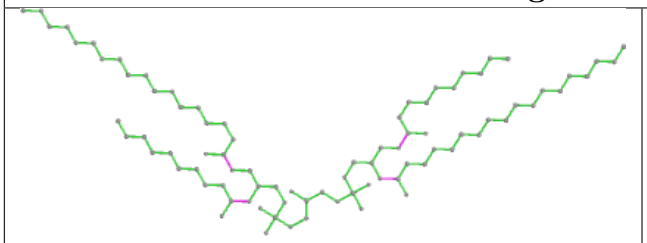


Rings

Ligand CDL d 201



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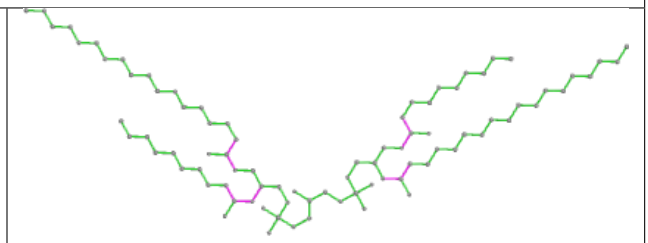
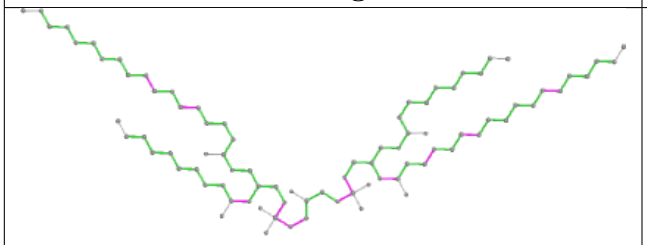


Bond angles



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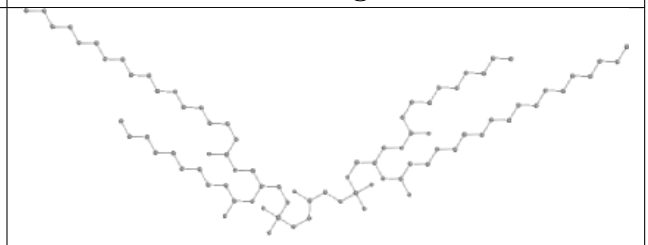
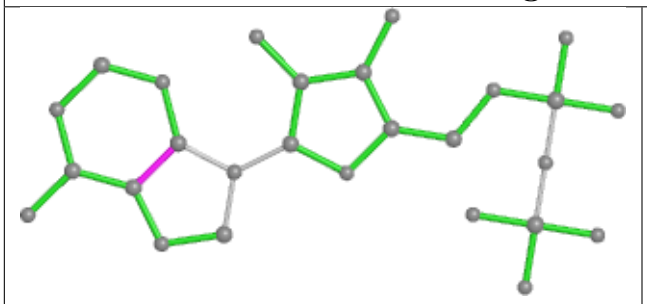


Rings

Ligand ADP O 401



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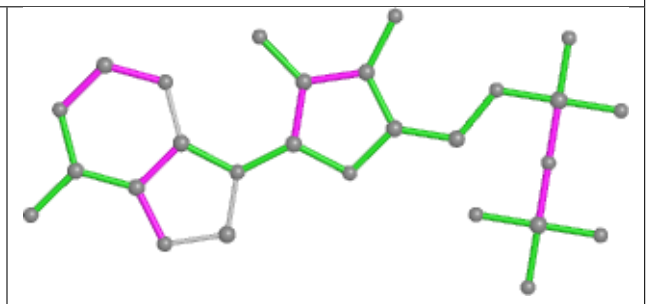
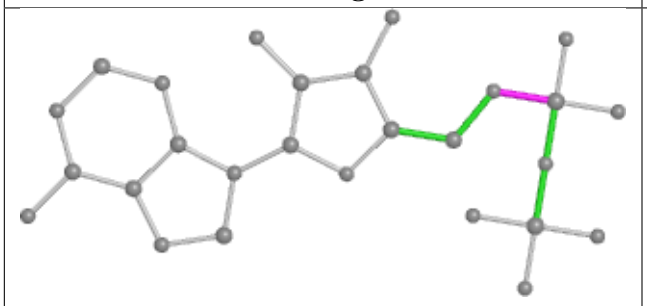


Bond angles



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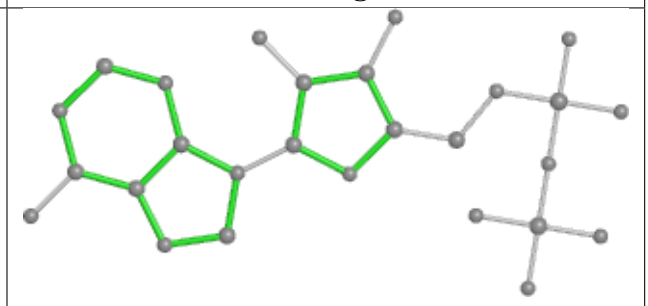
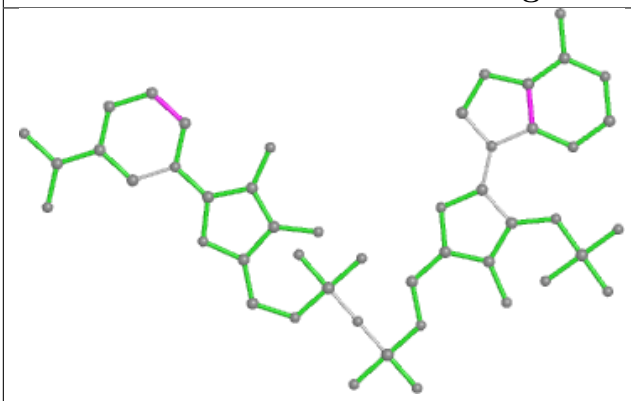


Rings

Ligand NDP P 401



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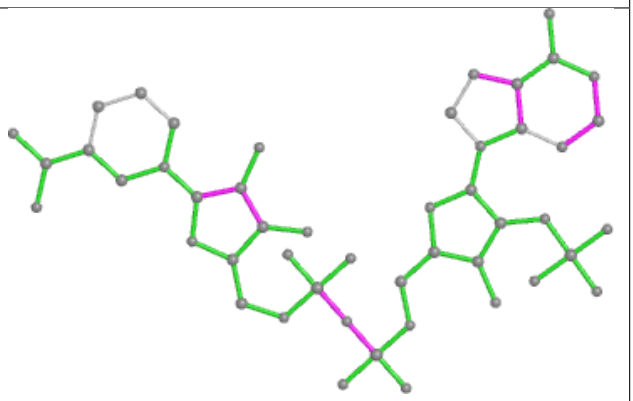

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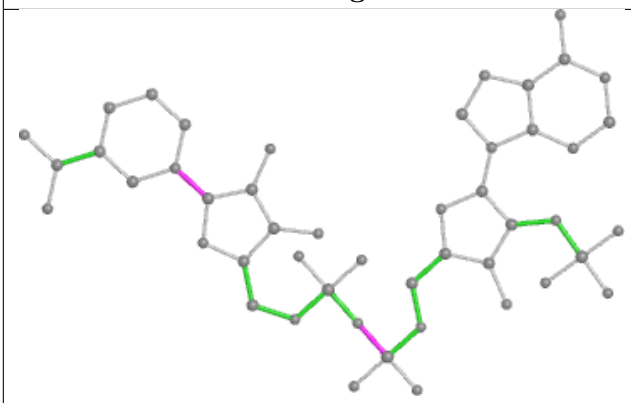

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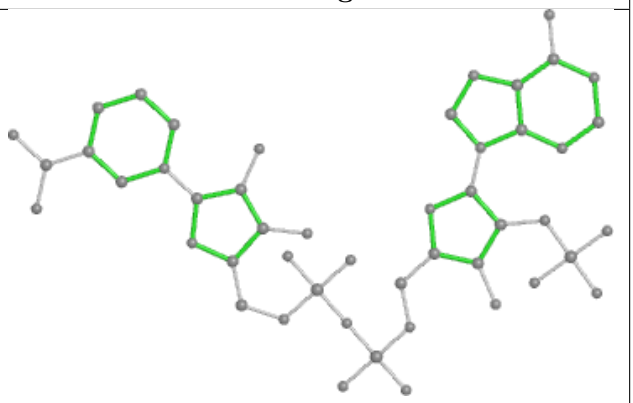
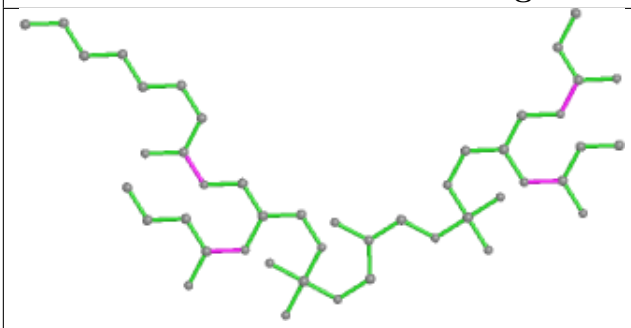


Rings

Ligand CDL Aa 502



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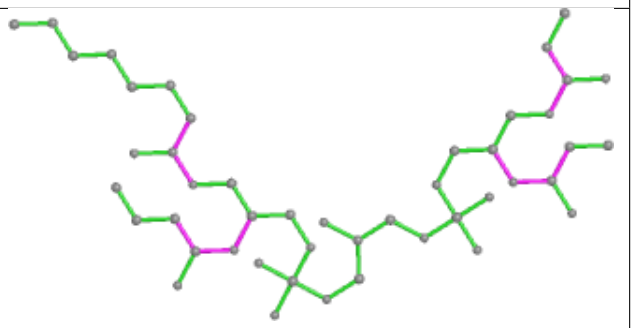
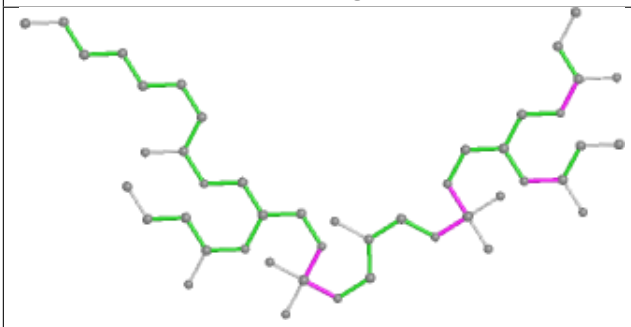


Bond angles



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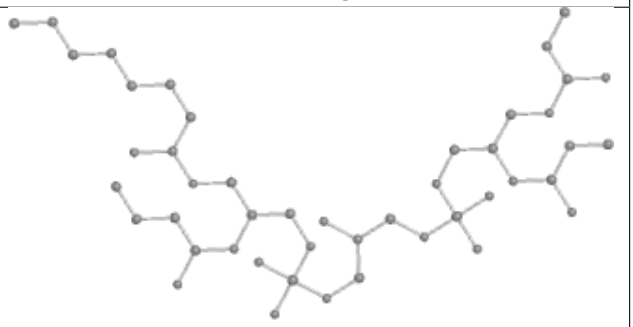
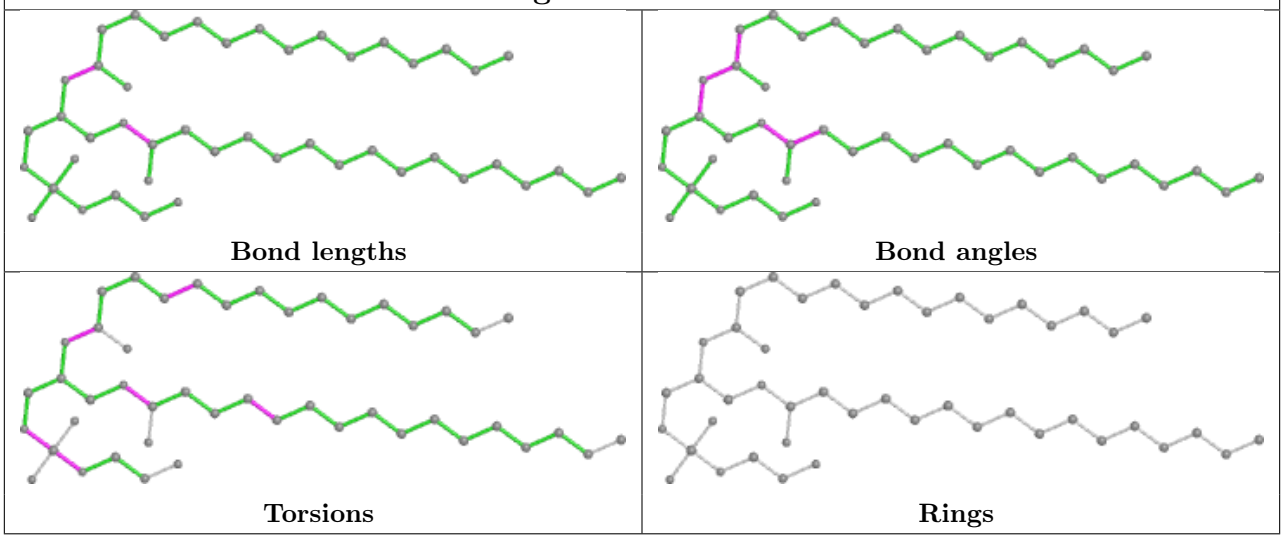
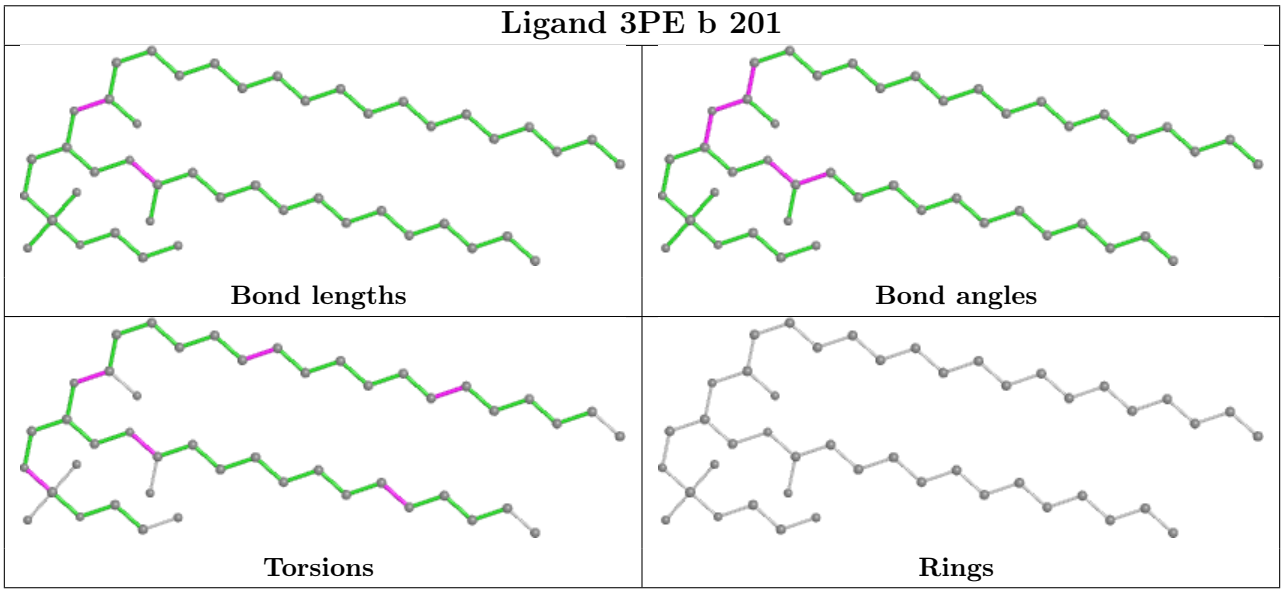


Rings

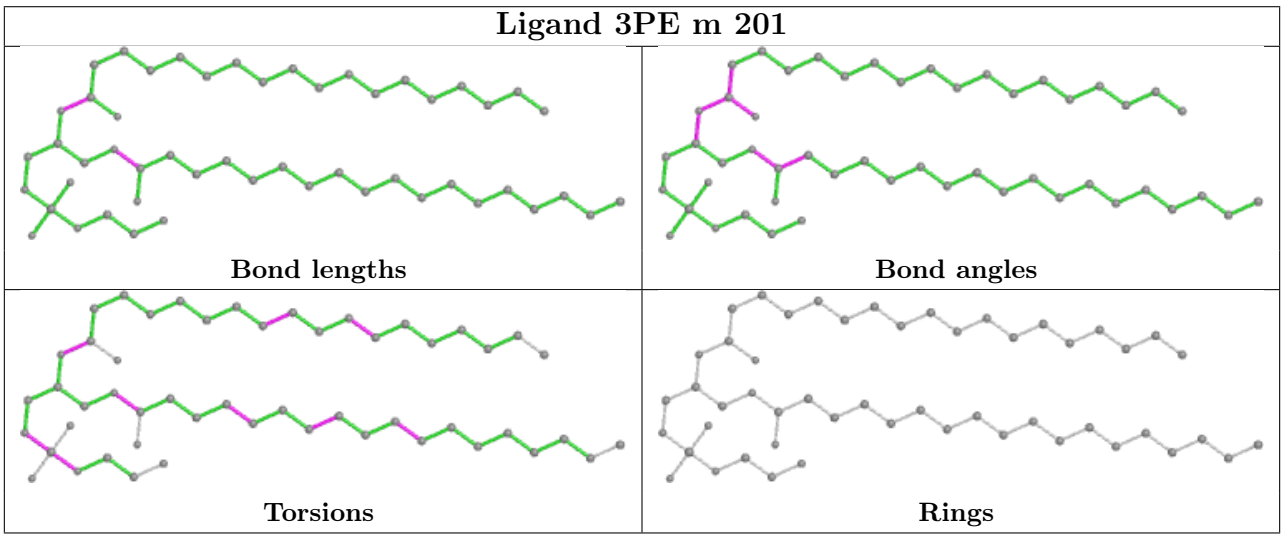
Ligand 3PE J 201



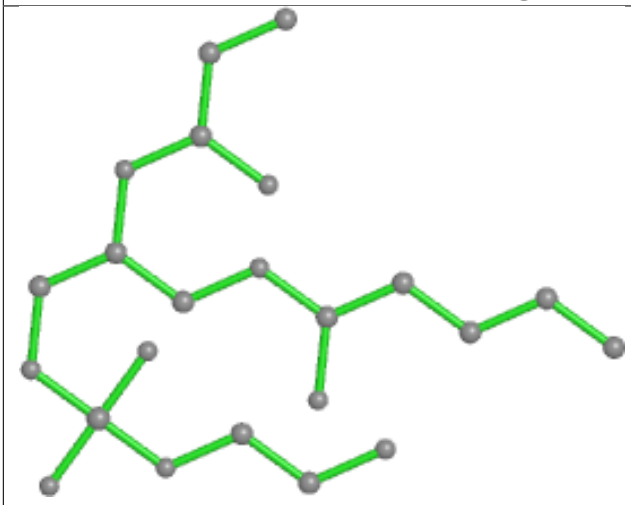
Ligand 3PE b 201



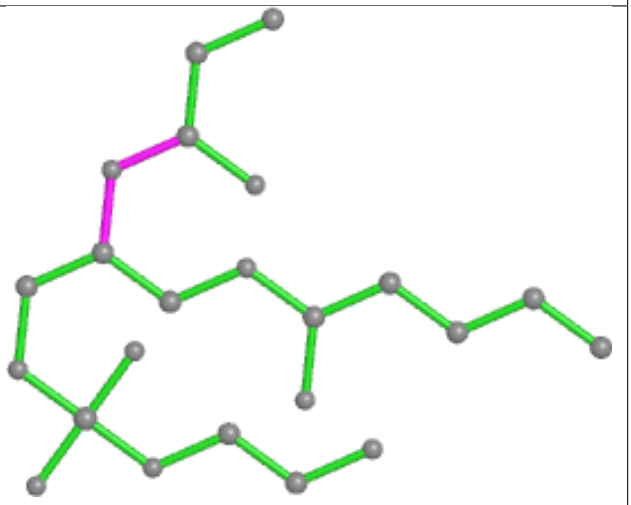
Ligand 3PE m 201



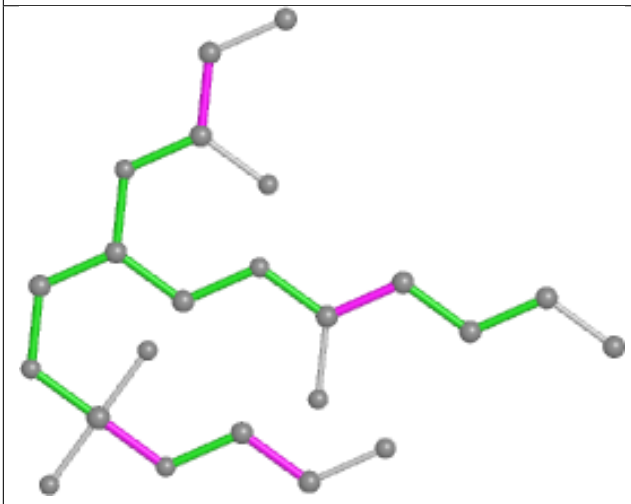
Ligand 3PE AC 401



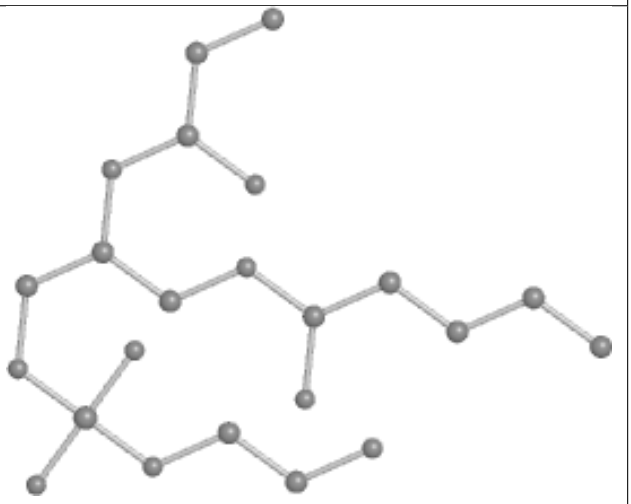
Bond lengths



Bond angles

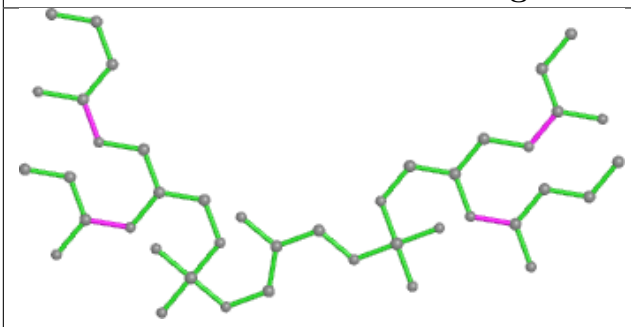


Torsions

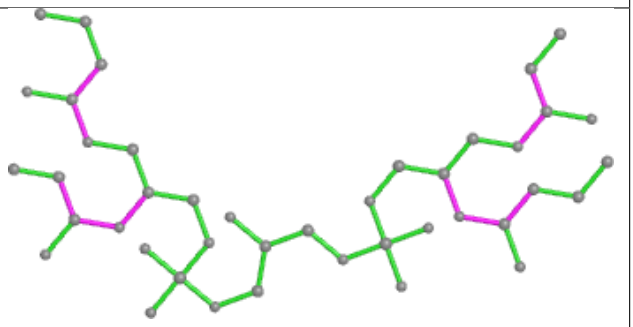


Rings

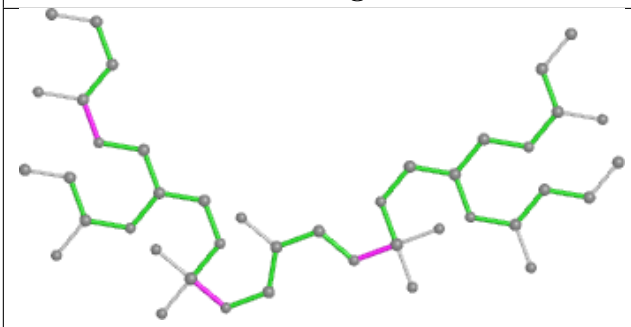
Ligand CDL AG 101



Bond lengths



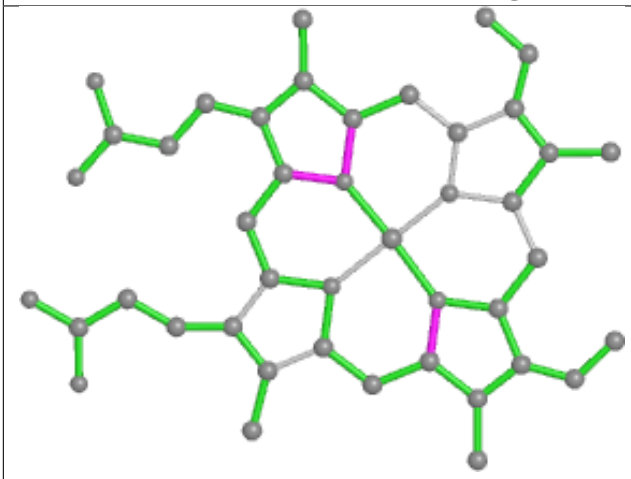
Bond angles



Torsions

Rings

Ligand HEM AC 403



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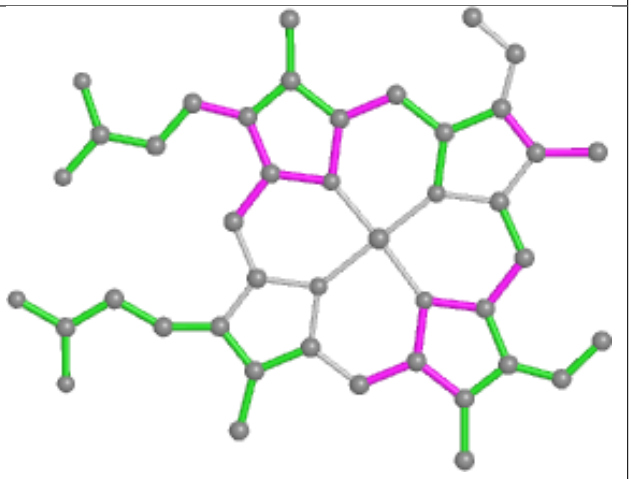
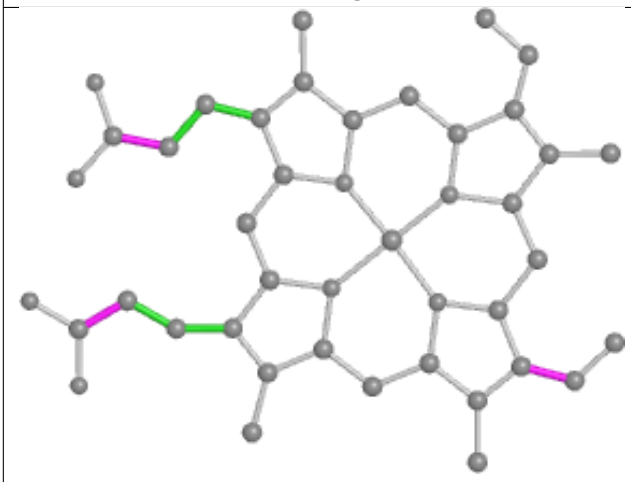
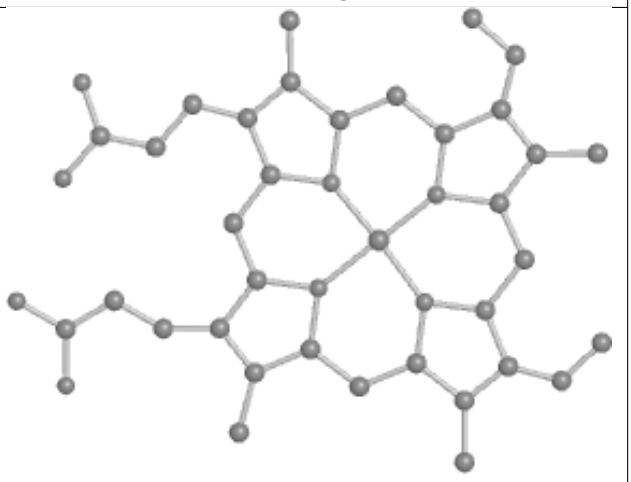


Bond angles

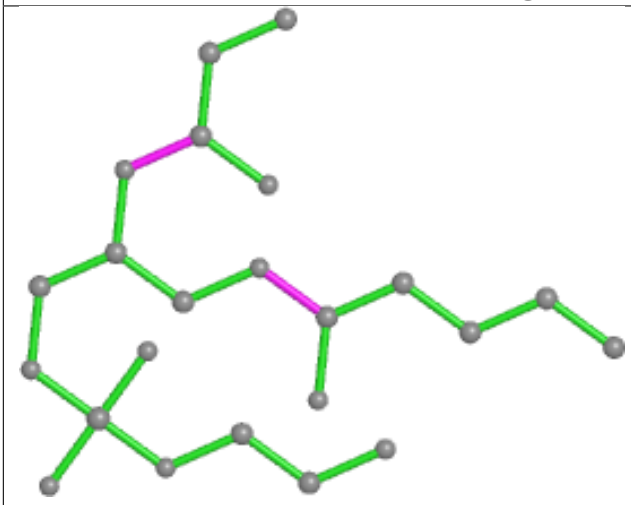


Torsions



Rings

Ligand 3PE Aa 501



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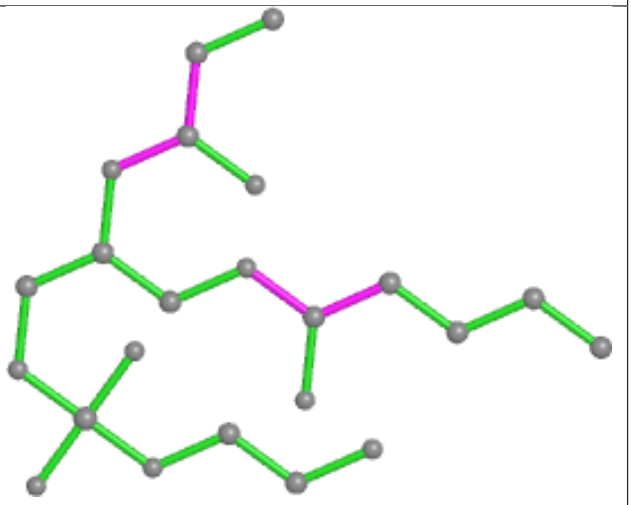
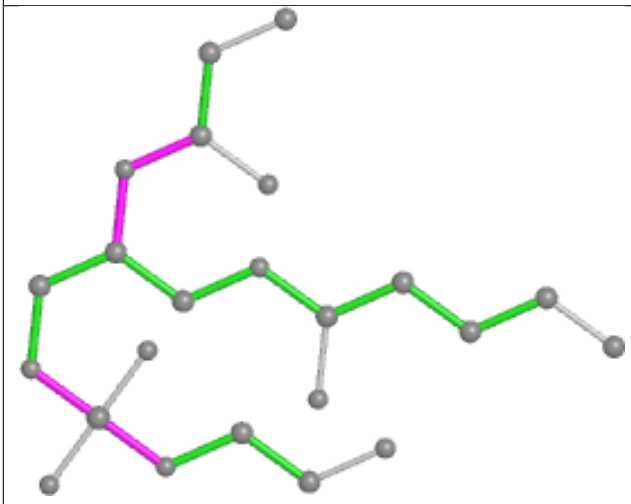
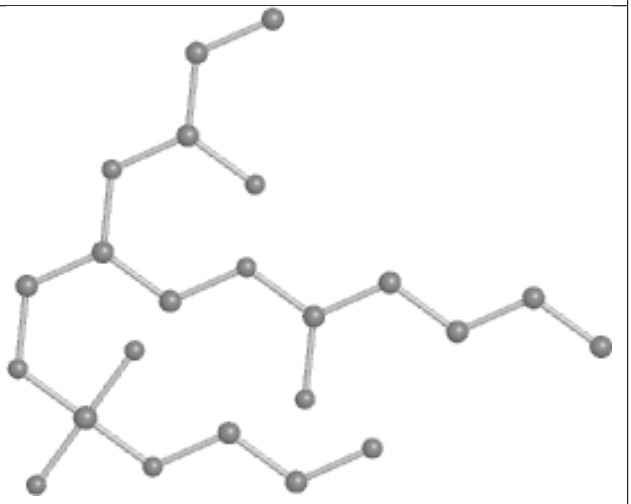


Bond angles

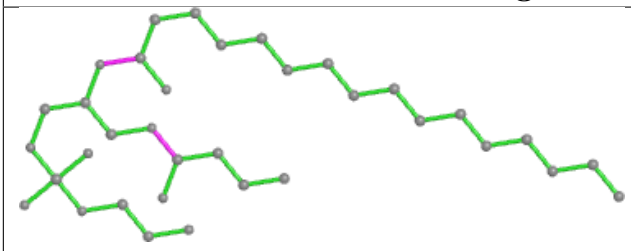


Torsions

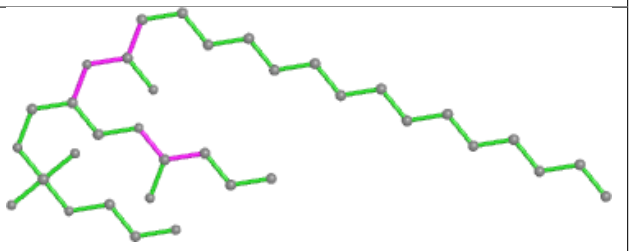


Rings

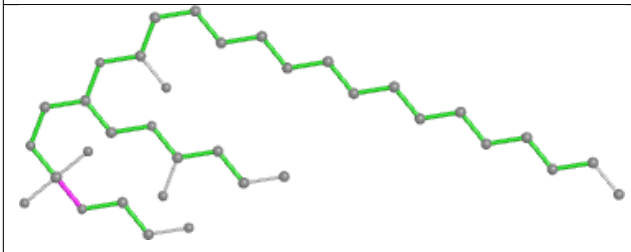
Ligand 3PE AC 404



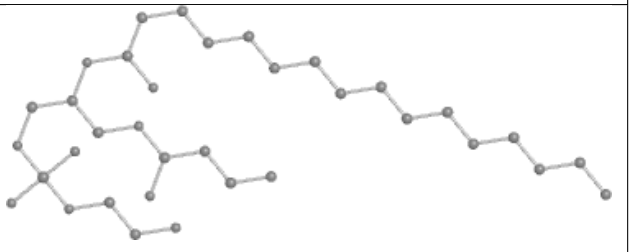
Bond lengths



Bond angles

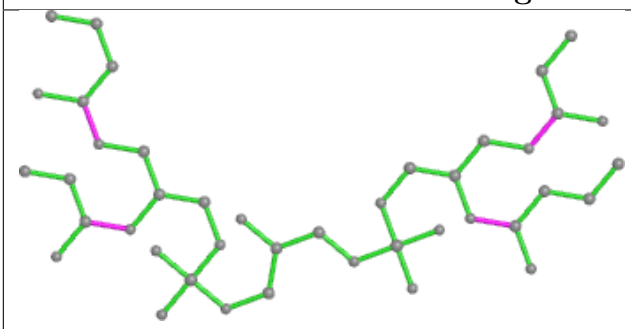


Torsions

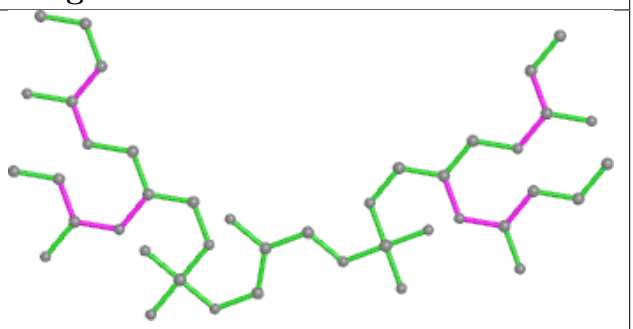


Rings

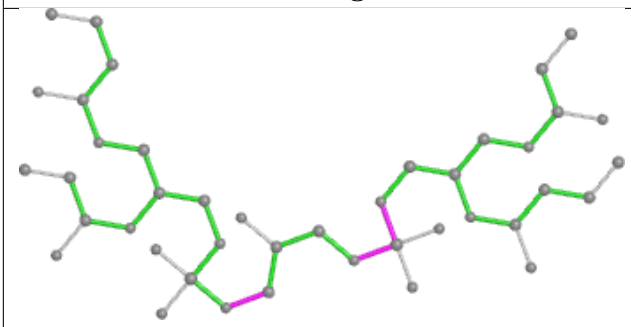
Ligand CDL Ag 101



Bond lengths



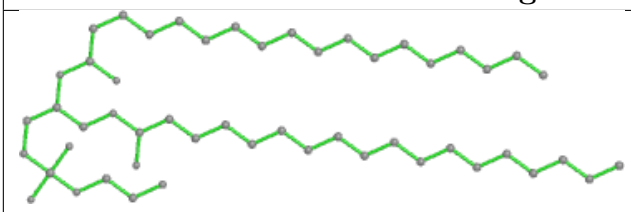
Bond angles



Torsions

Rings

Ligand 3PE Ag 103



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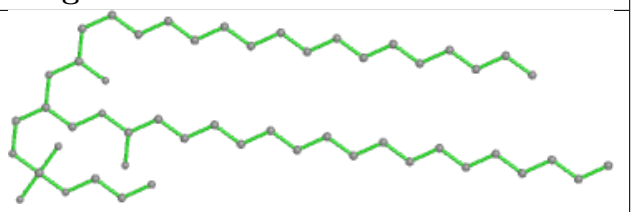
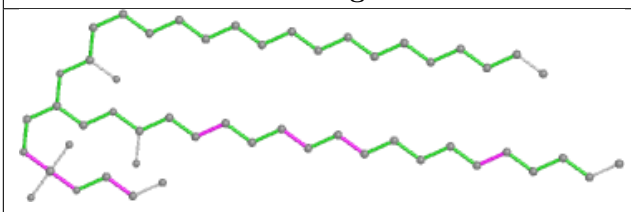
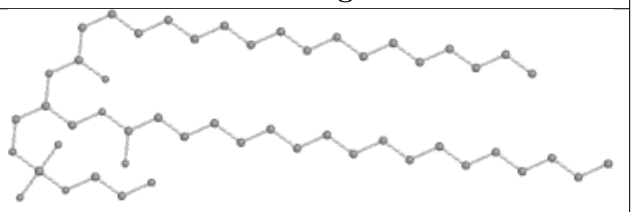


Bond angles

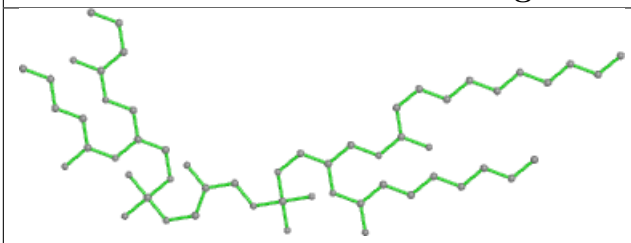


Torsions

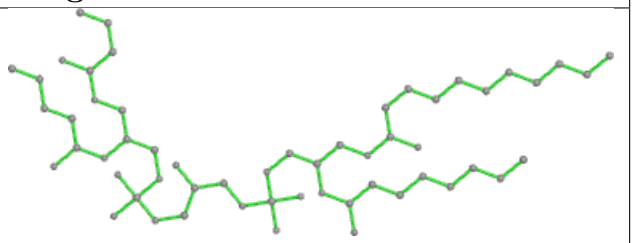


Rings

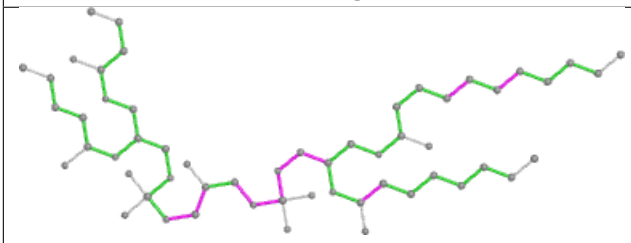
Ligand CDL Ag 102



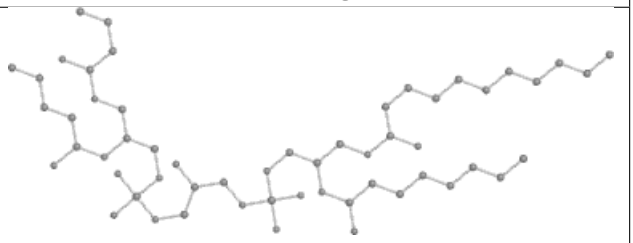
Bond lengths



Bond angles

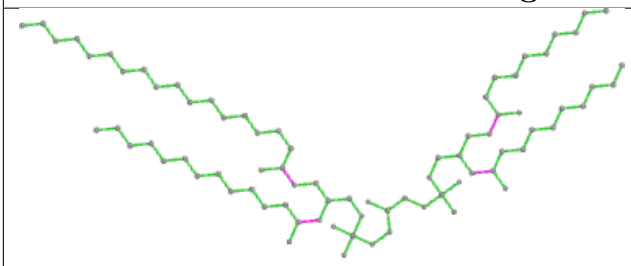


Torsions

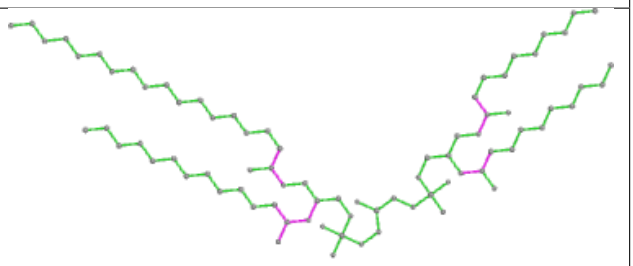


Rings

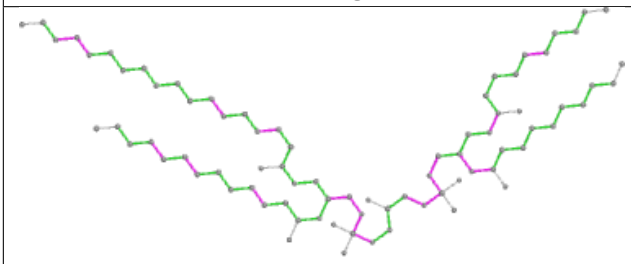
Ligand CDL M 503



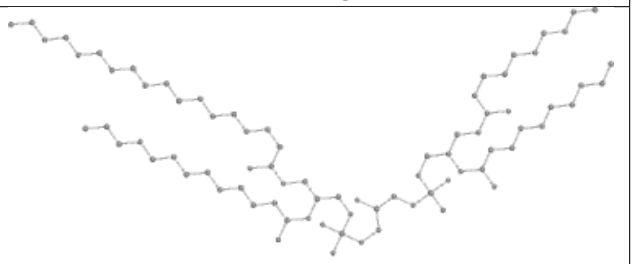
Bond lengths



Bond angles

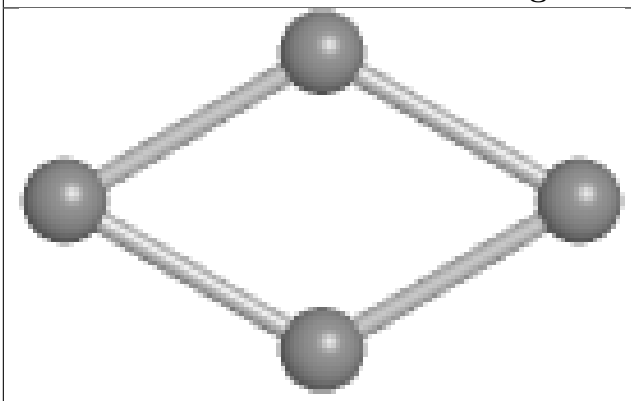


Torsions



Rings

Ligand FES E 301



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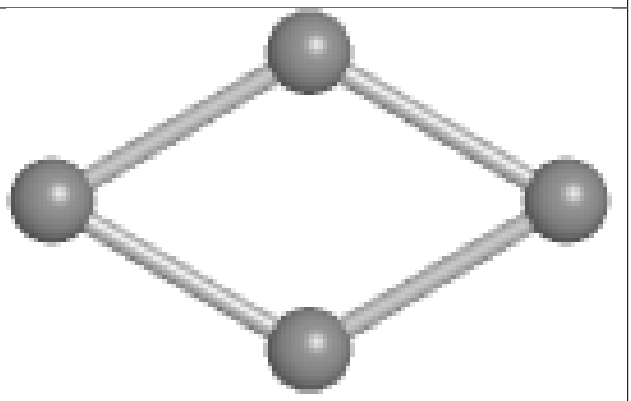
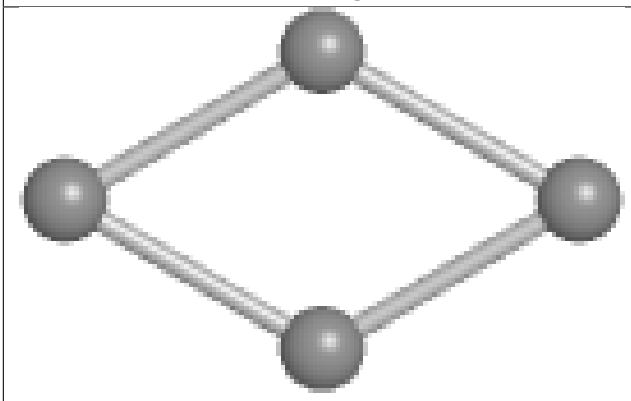
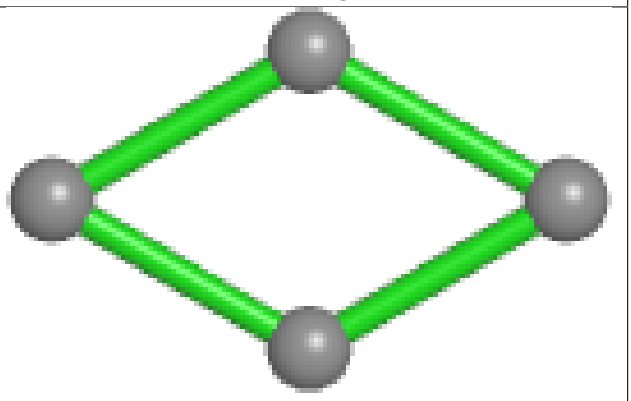


Bond angles

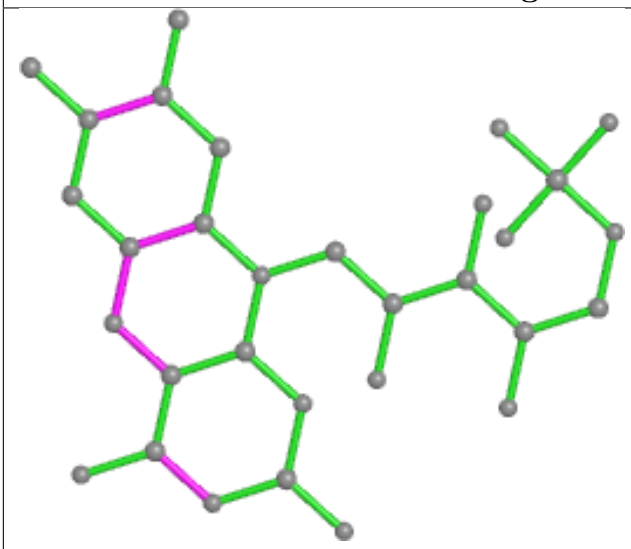


Torsions



Rings

Ligand FMN F 501



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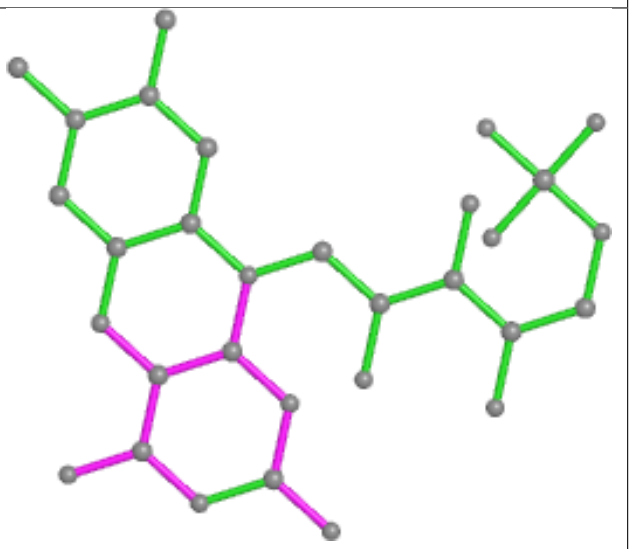
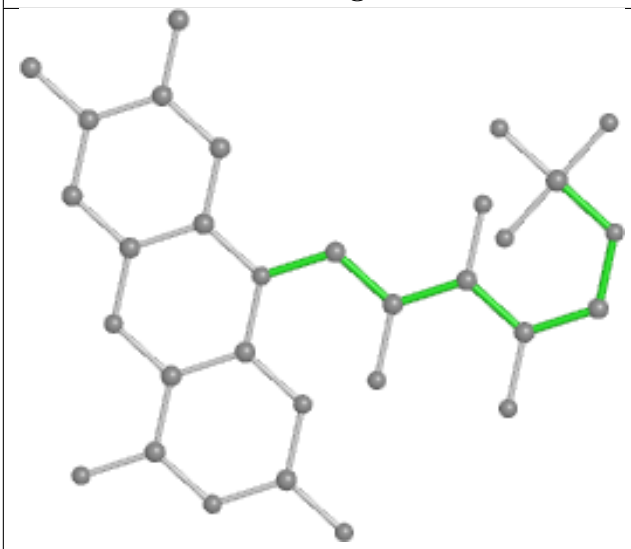
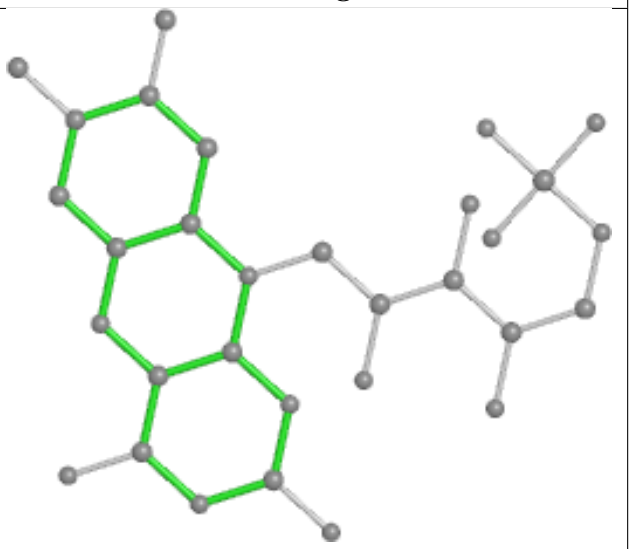


Bond angles

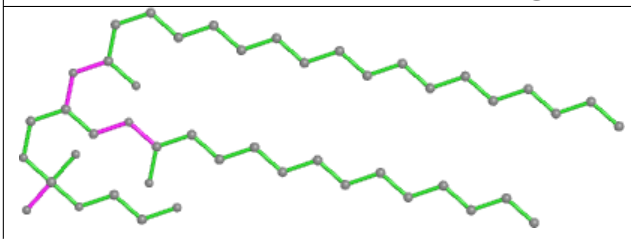


Torsions

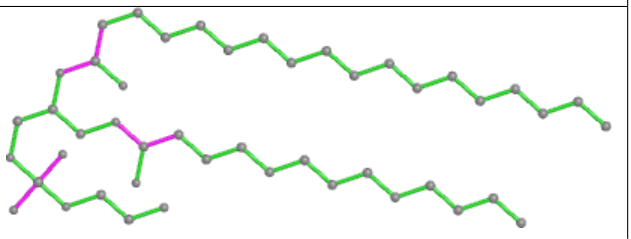


Rings

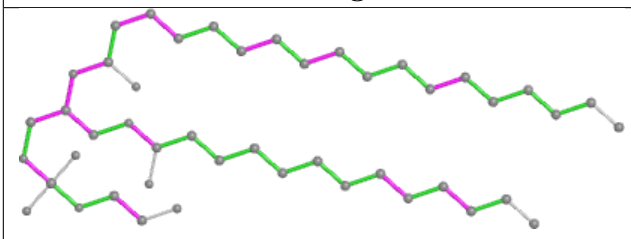
Ligand 3PE A 401



Bond lengths



Bond angles



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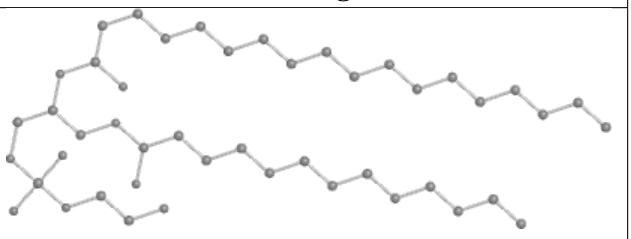
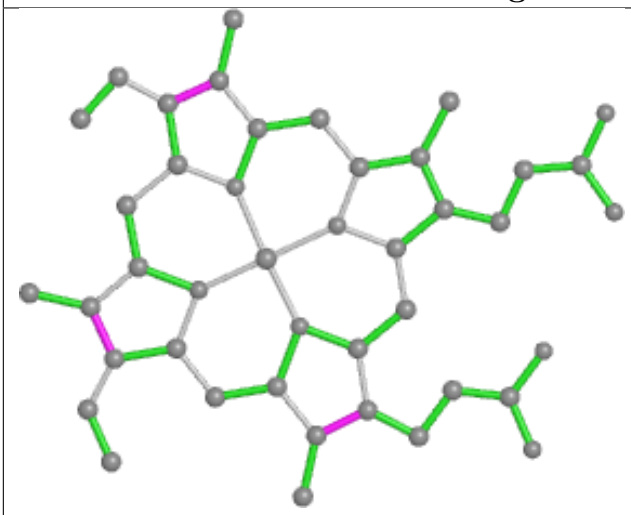
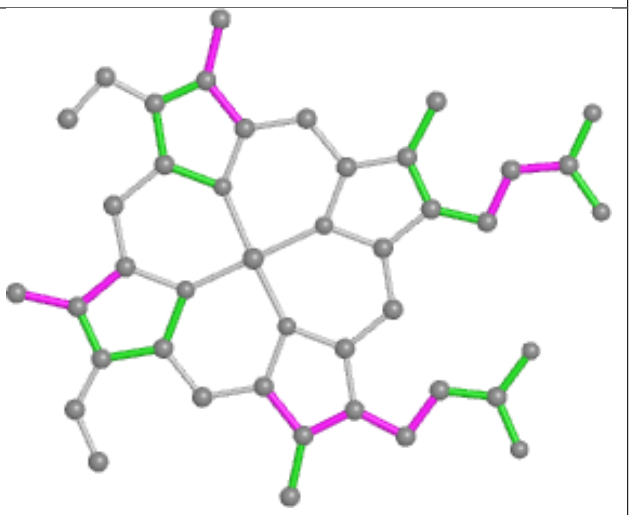


Rings

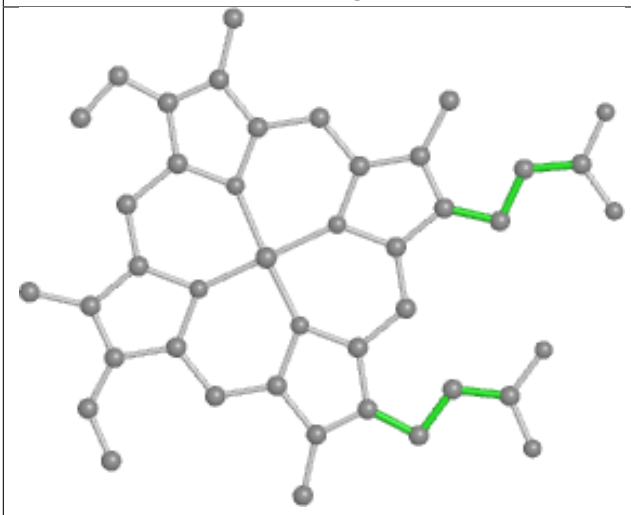
Ligand HEC AD 401



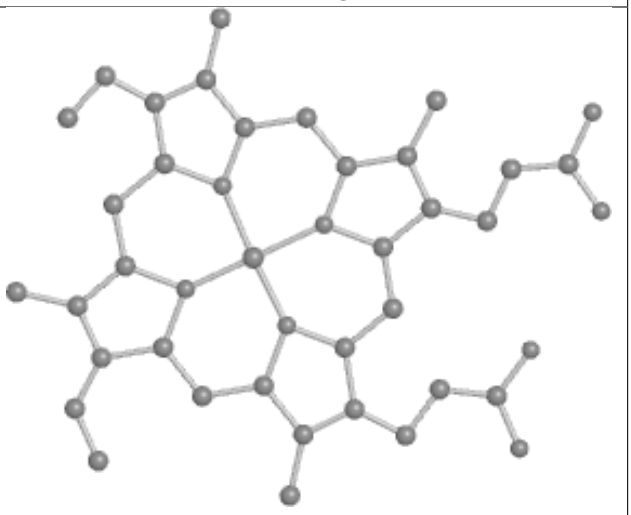
Bond lengths



Bond angles

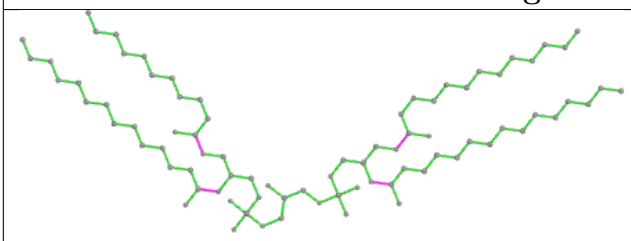


Torsions

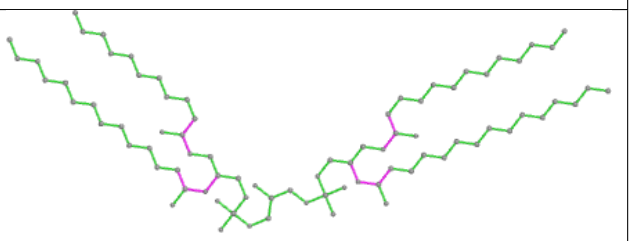


Rings

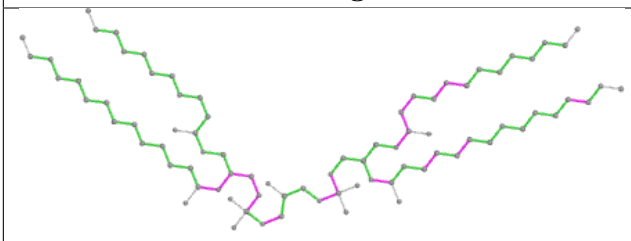
Ligand CDL Y 202



Bond lengths



Bond angles



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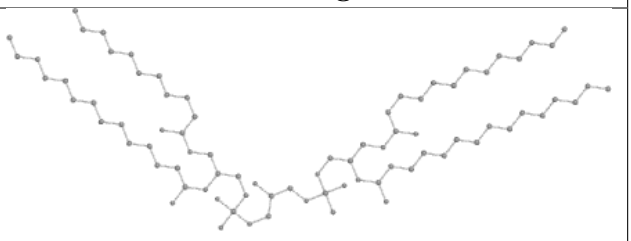
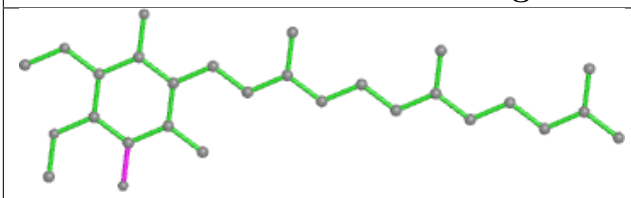
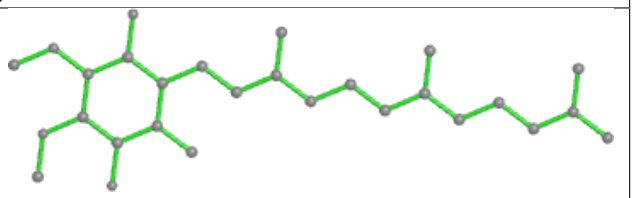


Rings

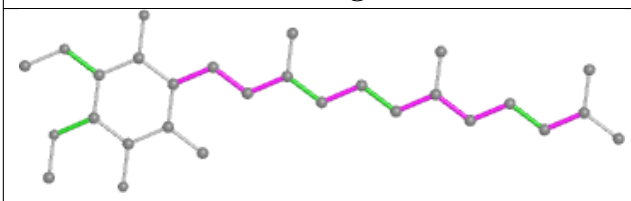
Ligand UQ6 AC 406



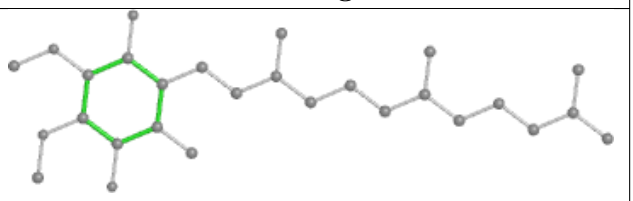
Bond lengths



Bond angles

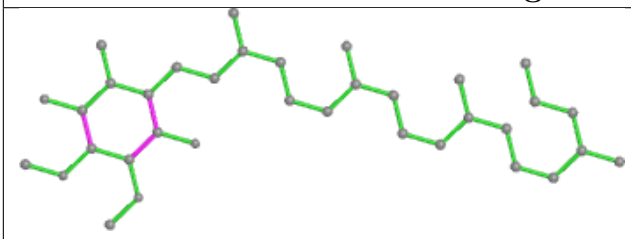


Torsions

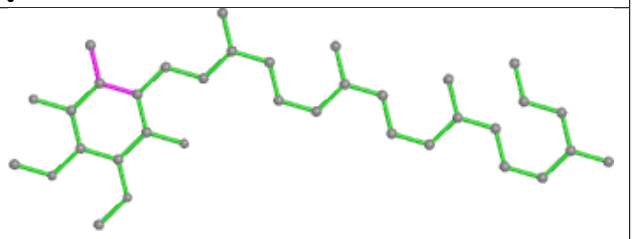


Rings

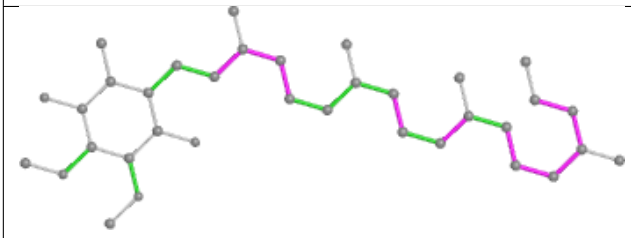
Ligand UQ9 H 401



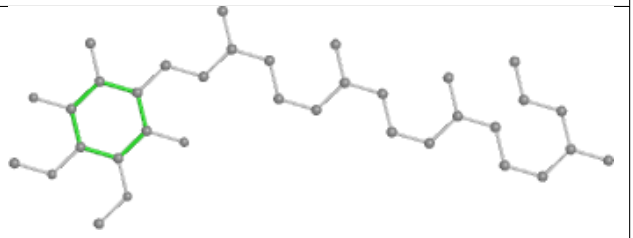
Bond lengths



Bond angles

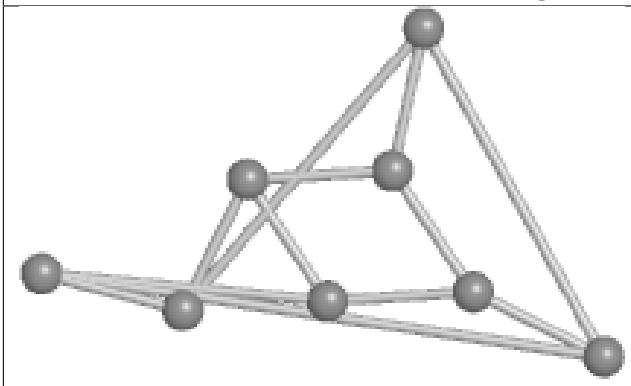


Torsions

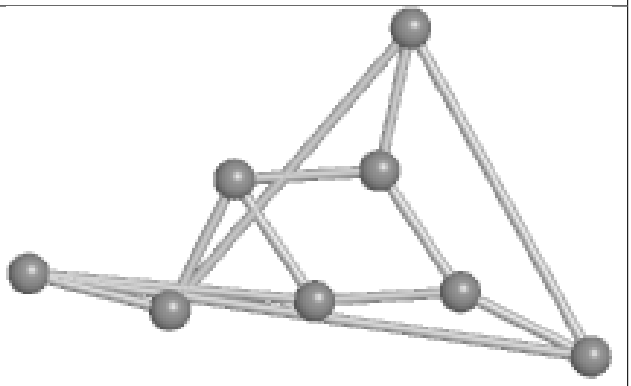


Rings

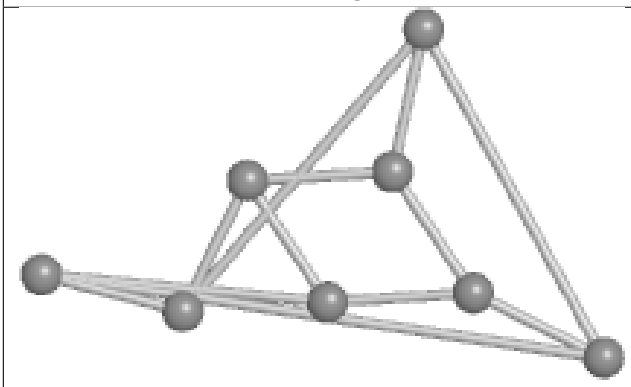
Ligand SF4 F 502



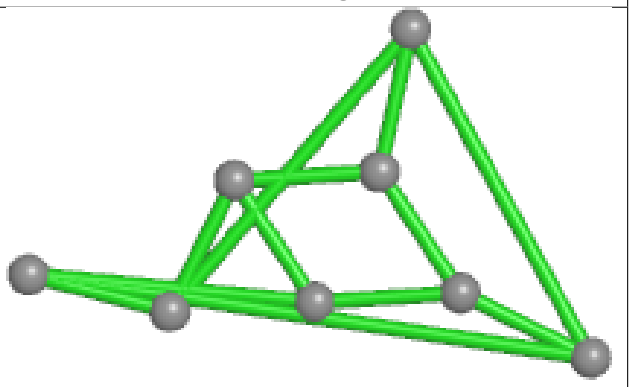
Bond lengths



Bond angles

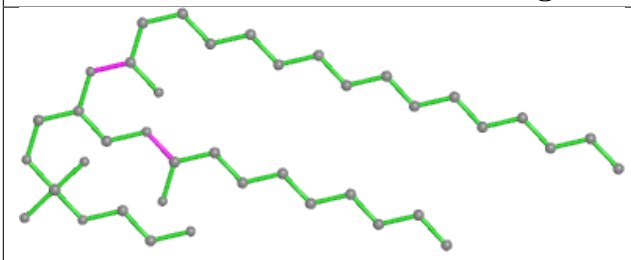


Torsions

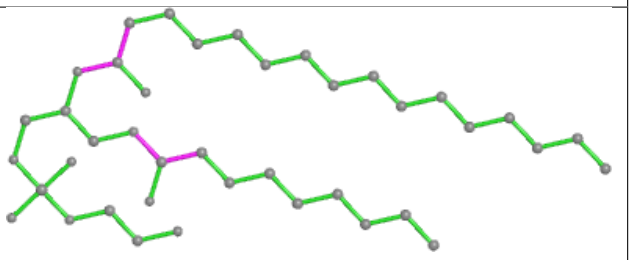


Rings

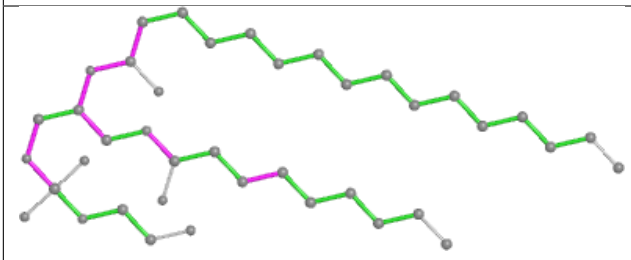
Ligand 3PE i 201



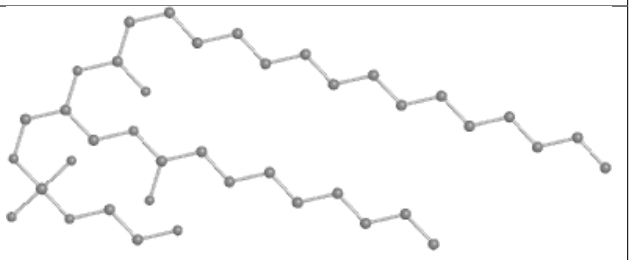
Bond lengths



Bond angles

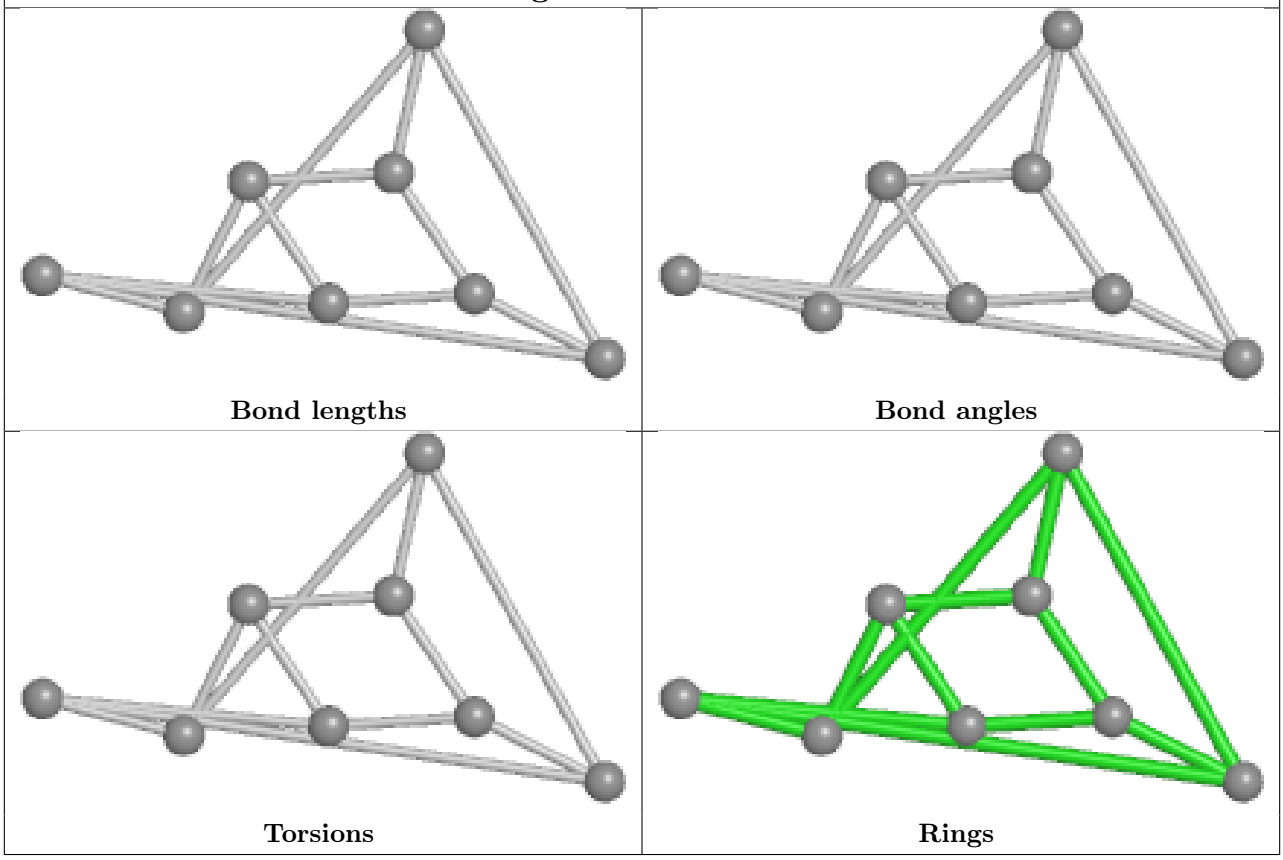


Torsions



Rings

Ligand SF4 G 801



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.

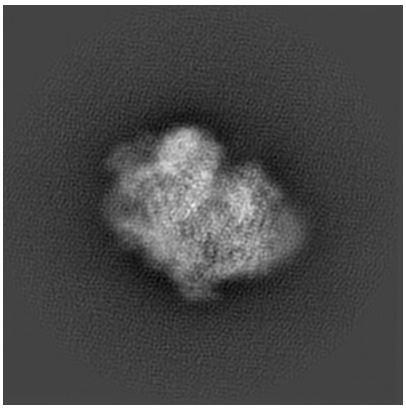
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35313. These allow visual inspection of the internal detail of the map and identification of artifacts.

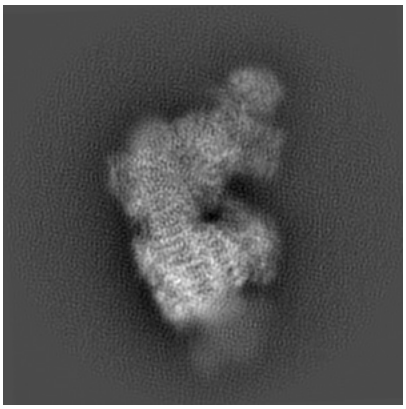
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

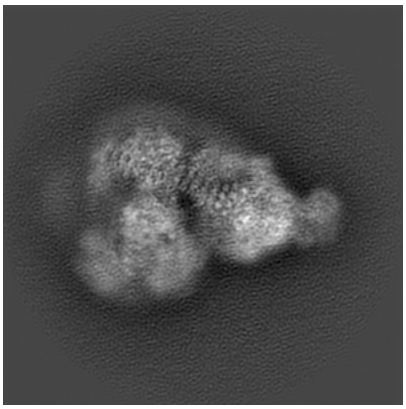
6.1.1 Primary map



X

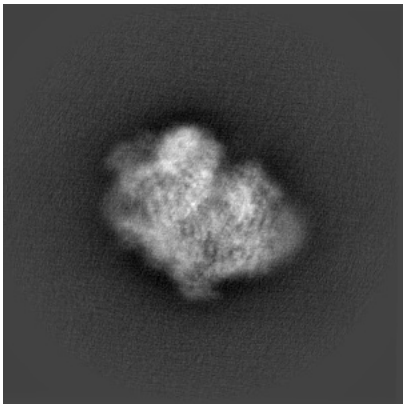


Y

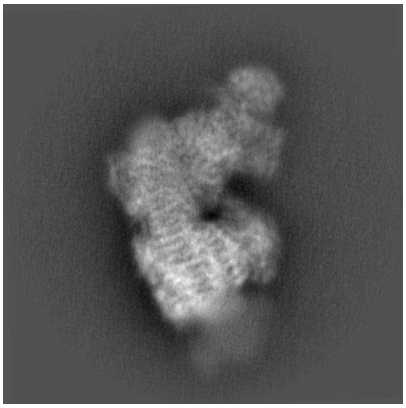


Z

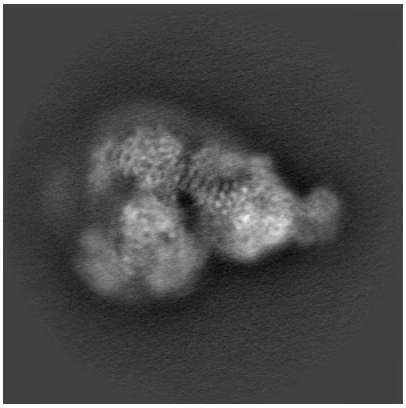
6.1.2 Raw map



X



Y

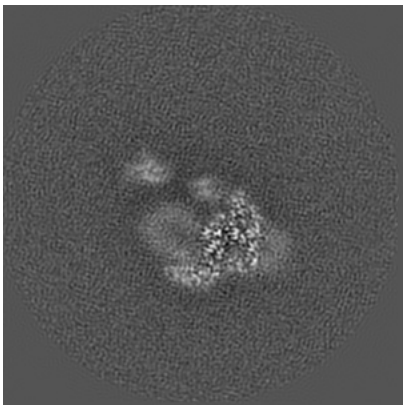


Z

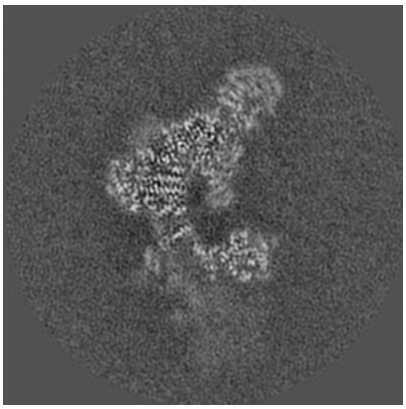
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

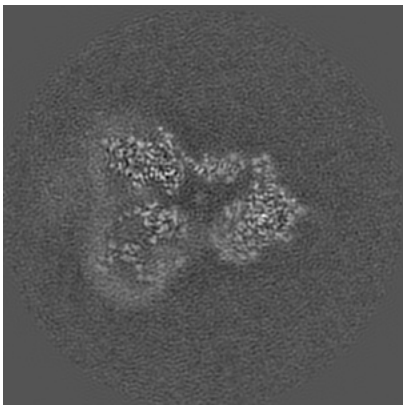
6.2.1 Primary map



X Index: 192

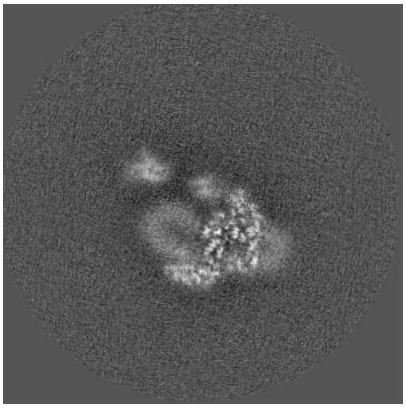


Y Index: 192

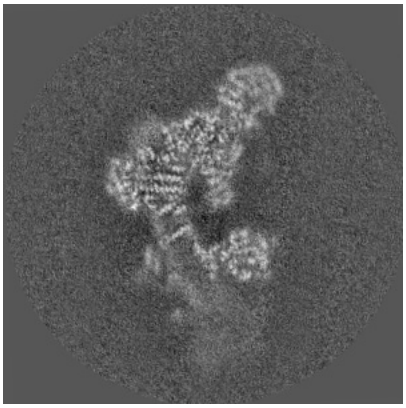


Z Index: 192

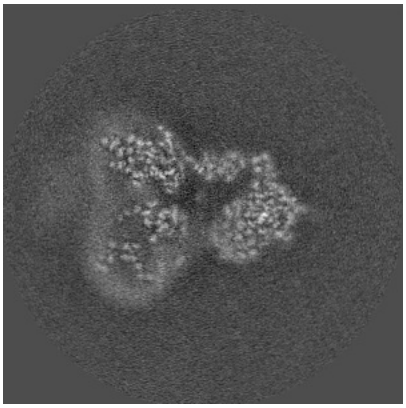
6.2.2 Raw map



X Index: 192



Y Index: 192

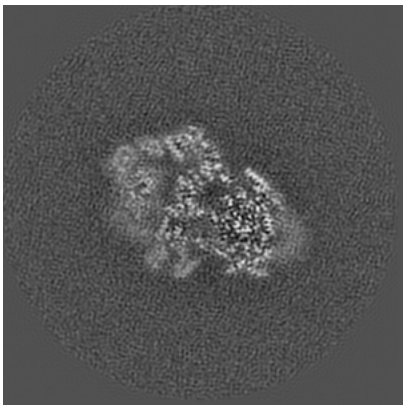


Z Index: 192

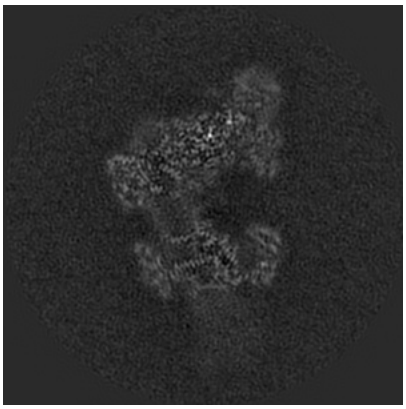
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

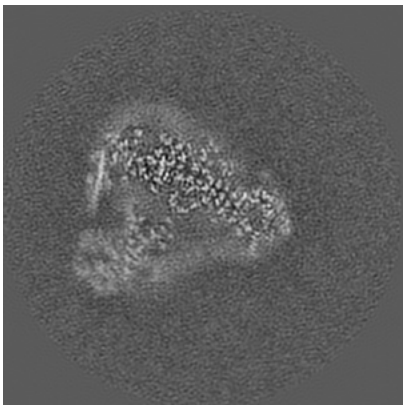
6.3.1 Primary map



X Index: 153

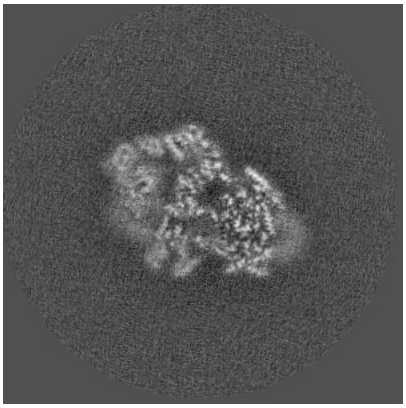


Y Index: 177

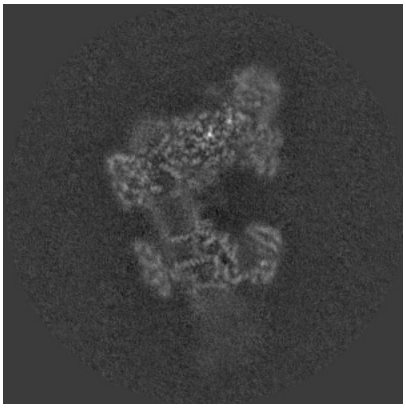


Z Index: 167

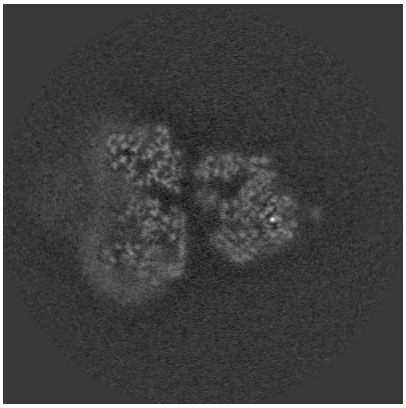
6.3.2 Raw map



X Index: 153



Y Index: 177

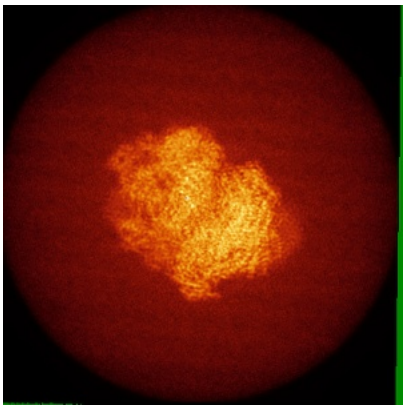


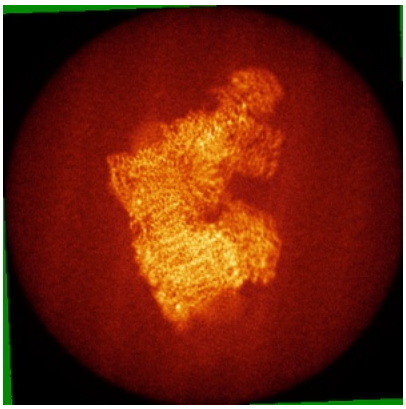
Z Index: 198

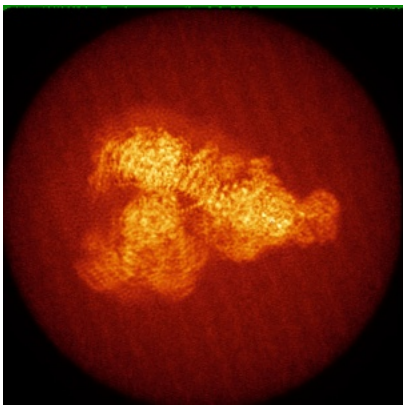
The images above show the largest variance slices of the map in three orthogonal directions.

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

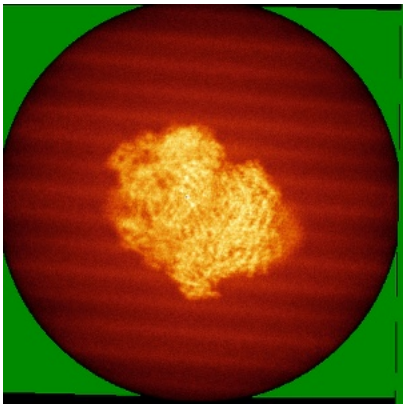
6.4.1 Primary map

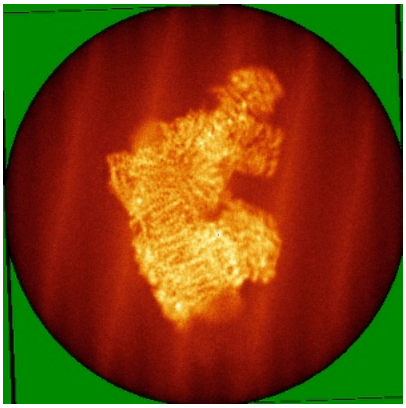

X

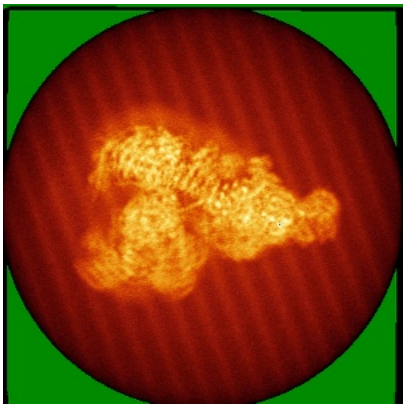

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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

X Y Z

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.

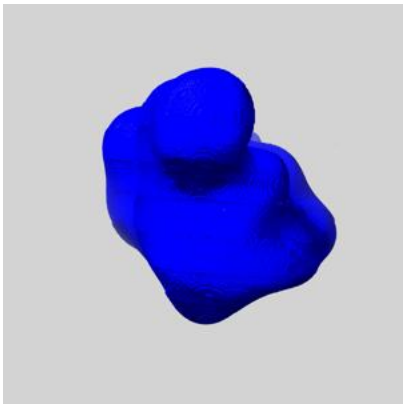
6.6 Mask visualisation

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

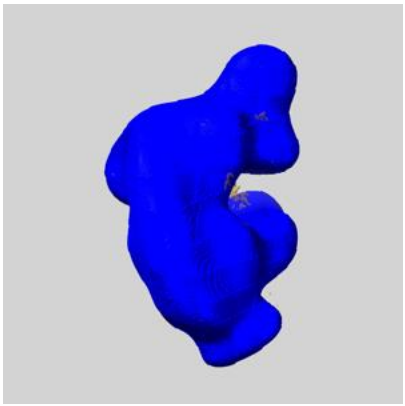
A mask typically either:

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

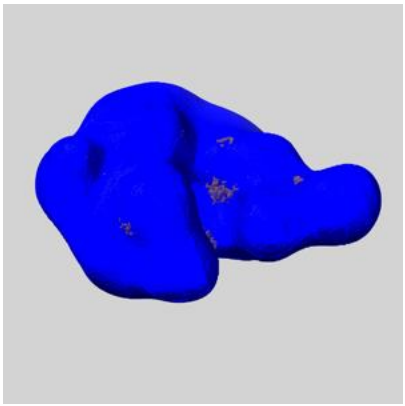
6.6.1 emd_35313_msk_1.map



X



Y

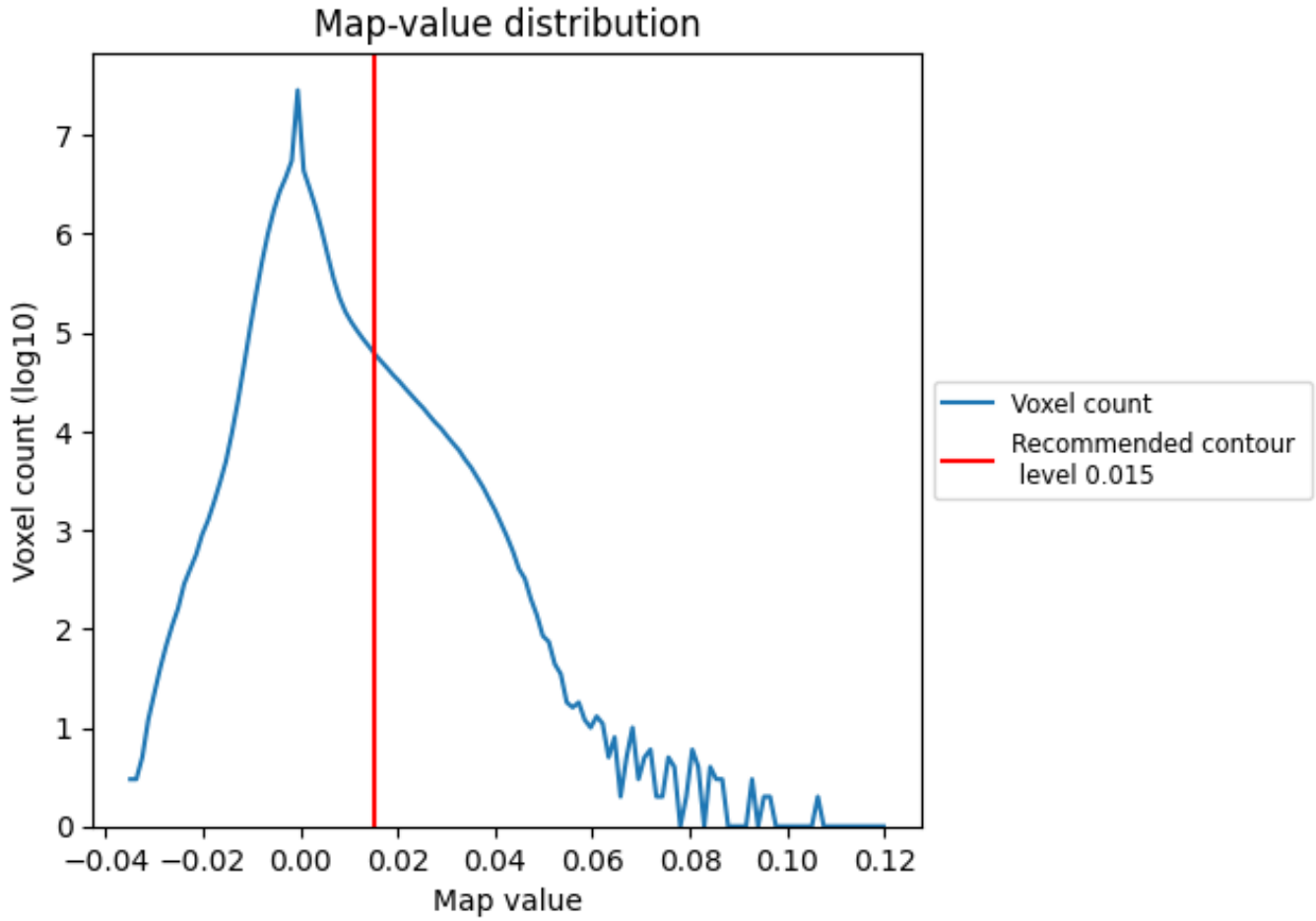


Z

7 Map analysis

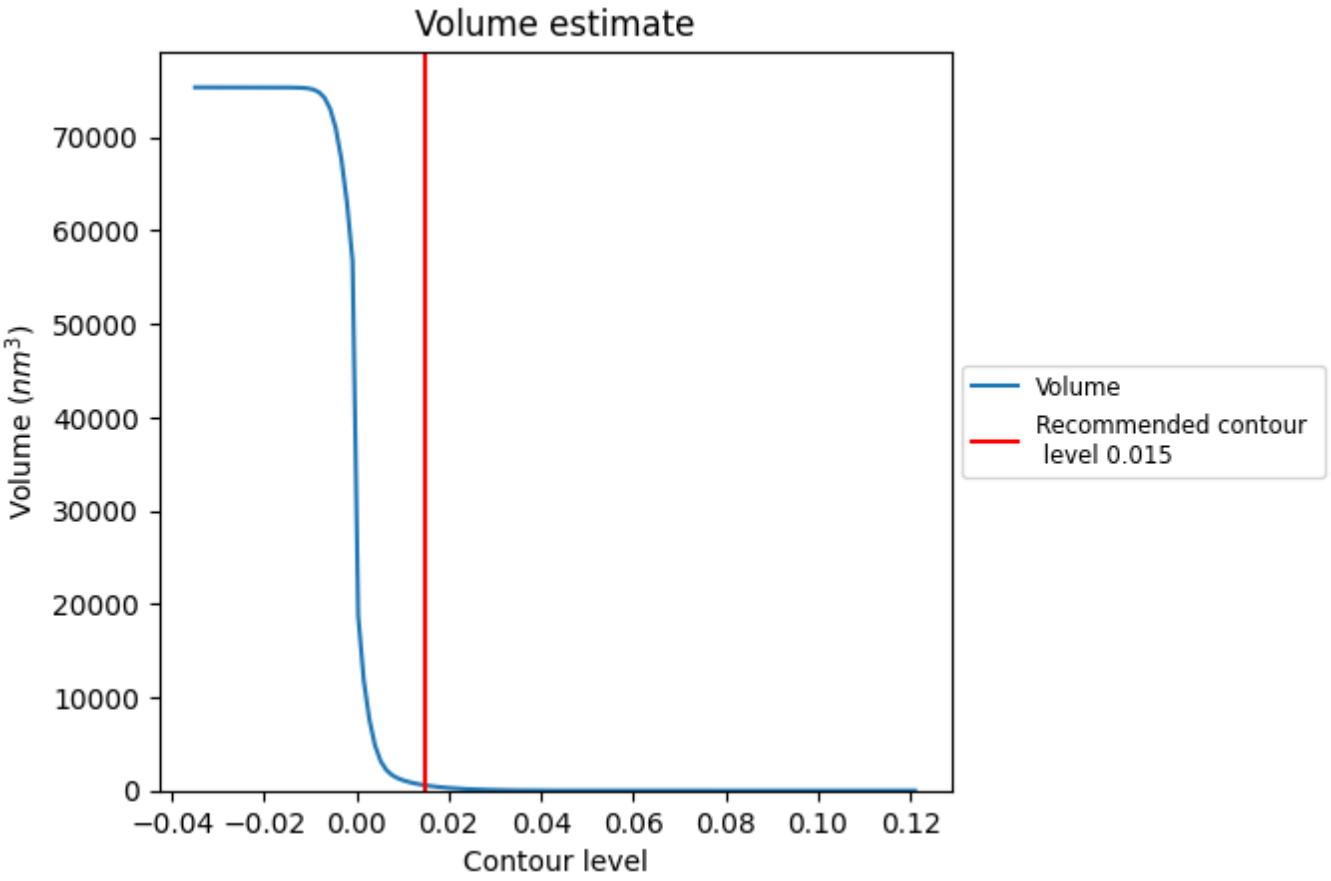
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

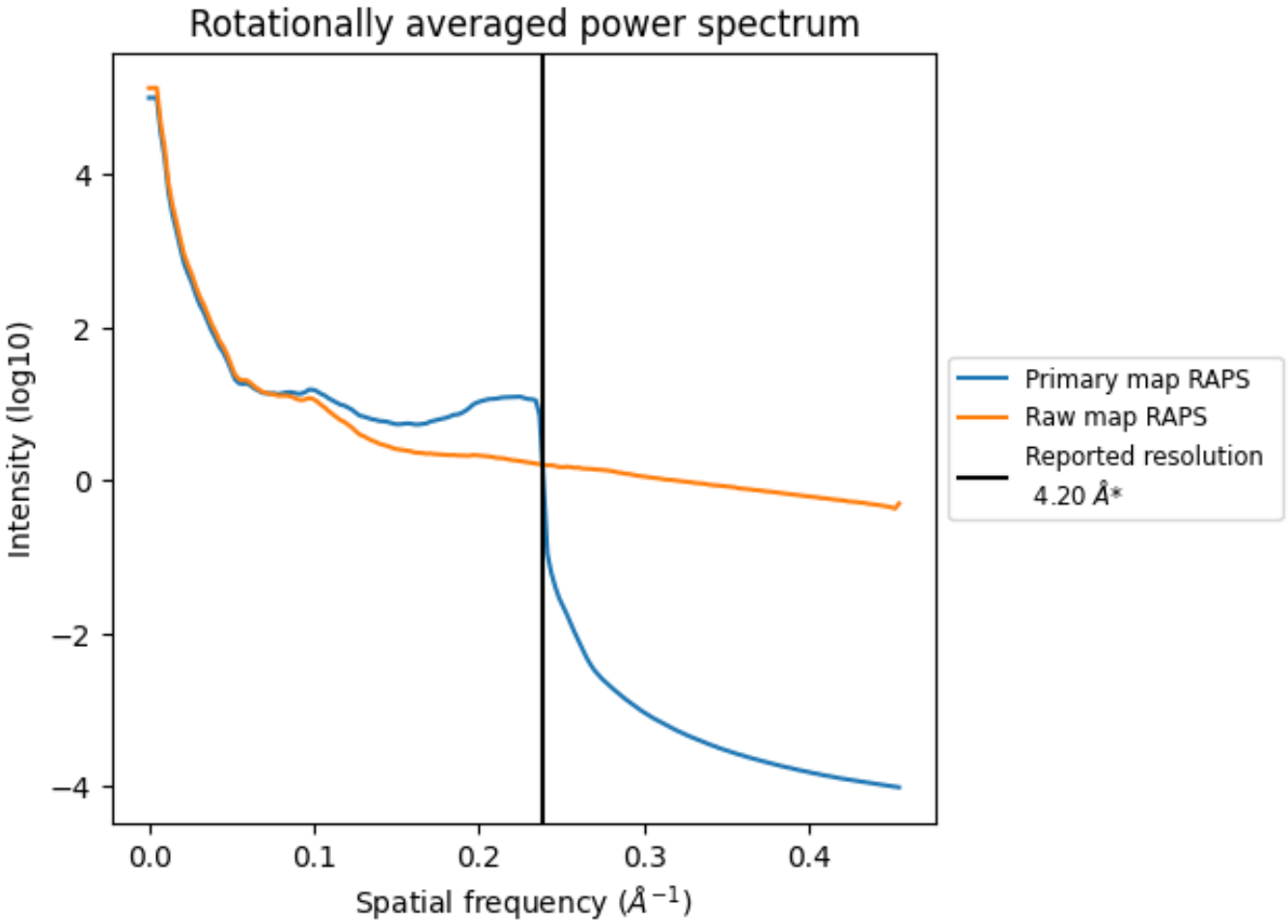
7.2 Volume estimate



The volume at the recommended contour level is 556 nm^3; this corresponds to an approximate mass of 502 kDa.

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

7.3 Rotationally averaged power spectrum (i)

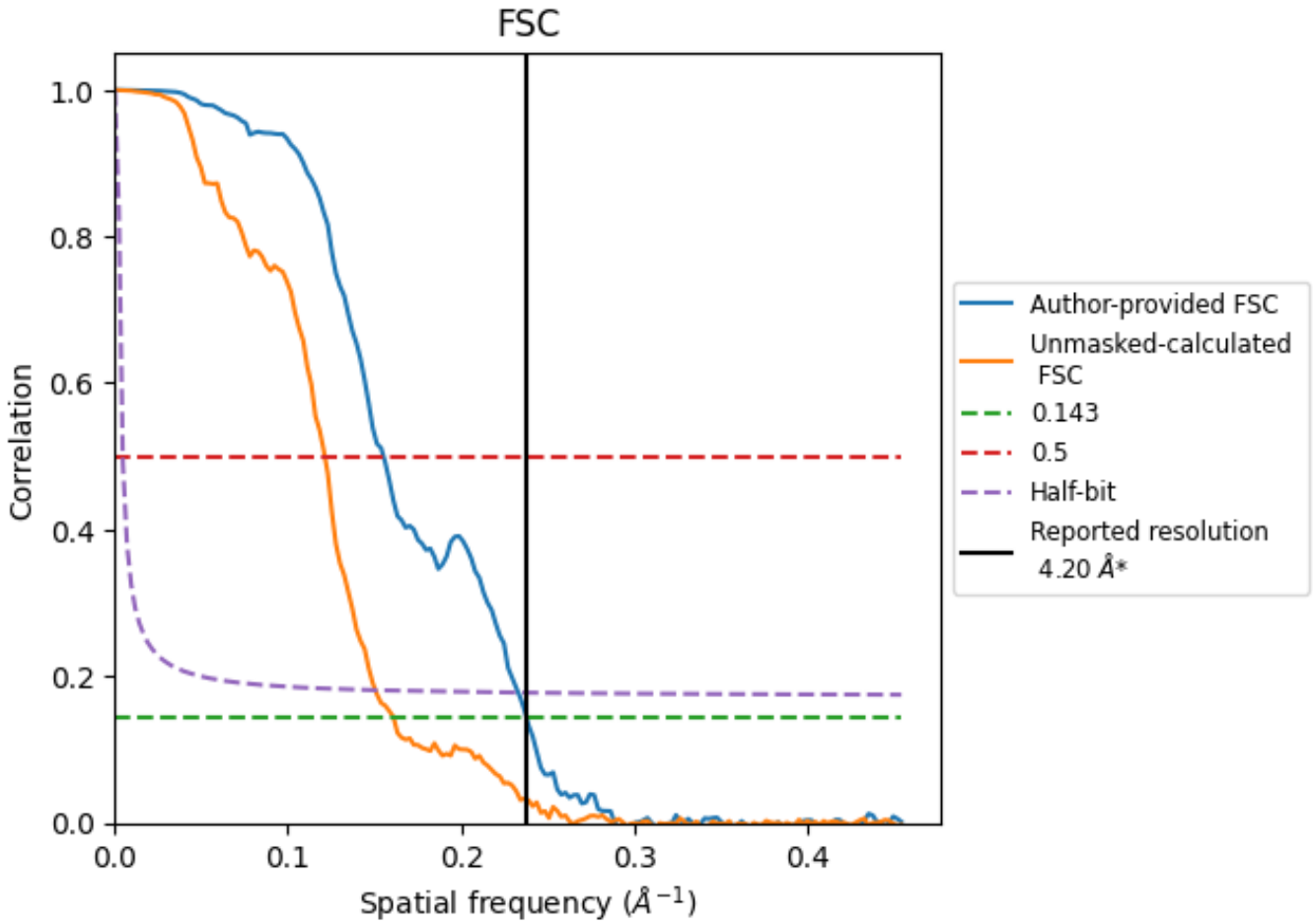


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

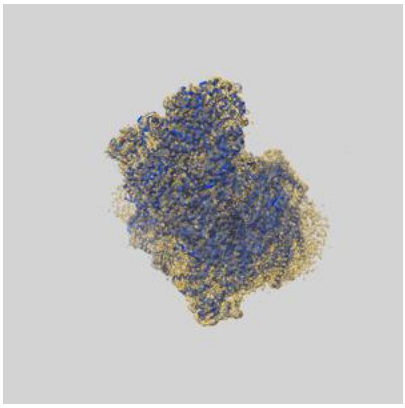
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.44	4.29
Unmasked-calculated*	6.21	8.24	6.64

*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 6.21 differs from the reported value 4.2 by more than 10 %

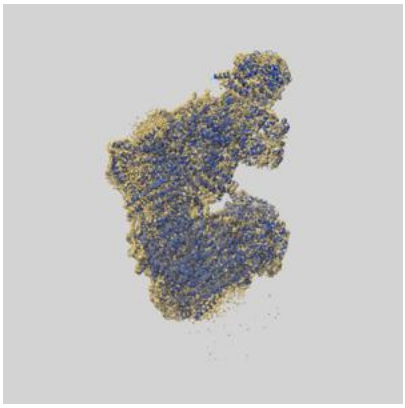
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35313 and PDB model 8IAO. Per-residue inclusion information can be found in section 3 on page 26.

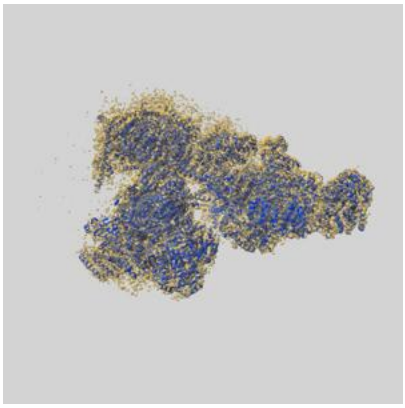
9.1 Map-model overlay



X



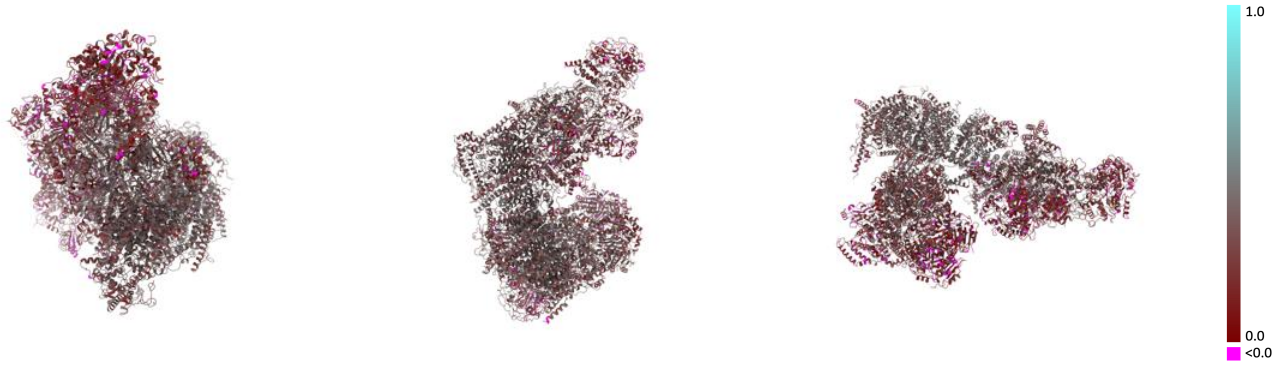
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

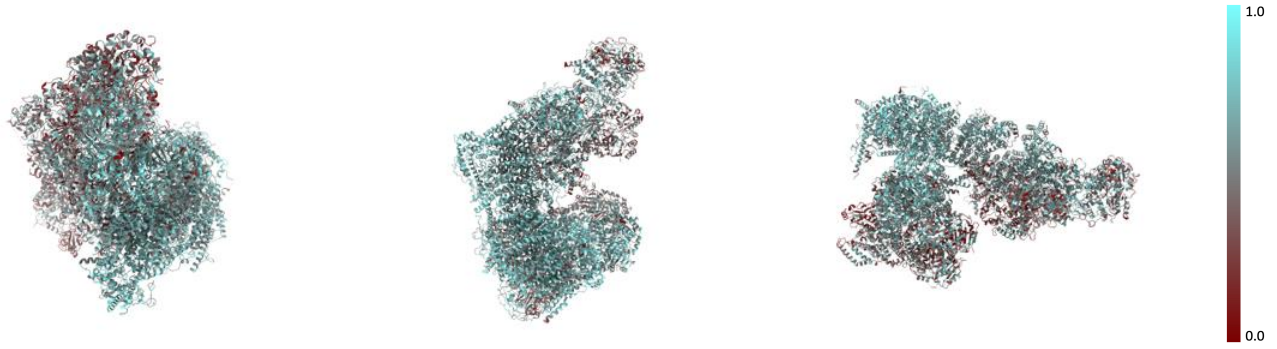
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

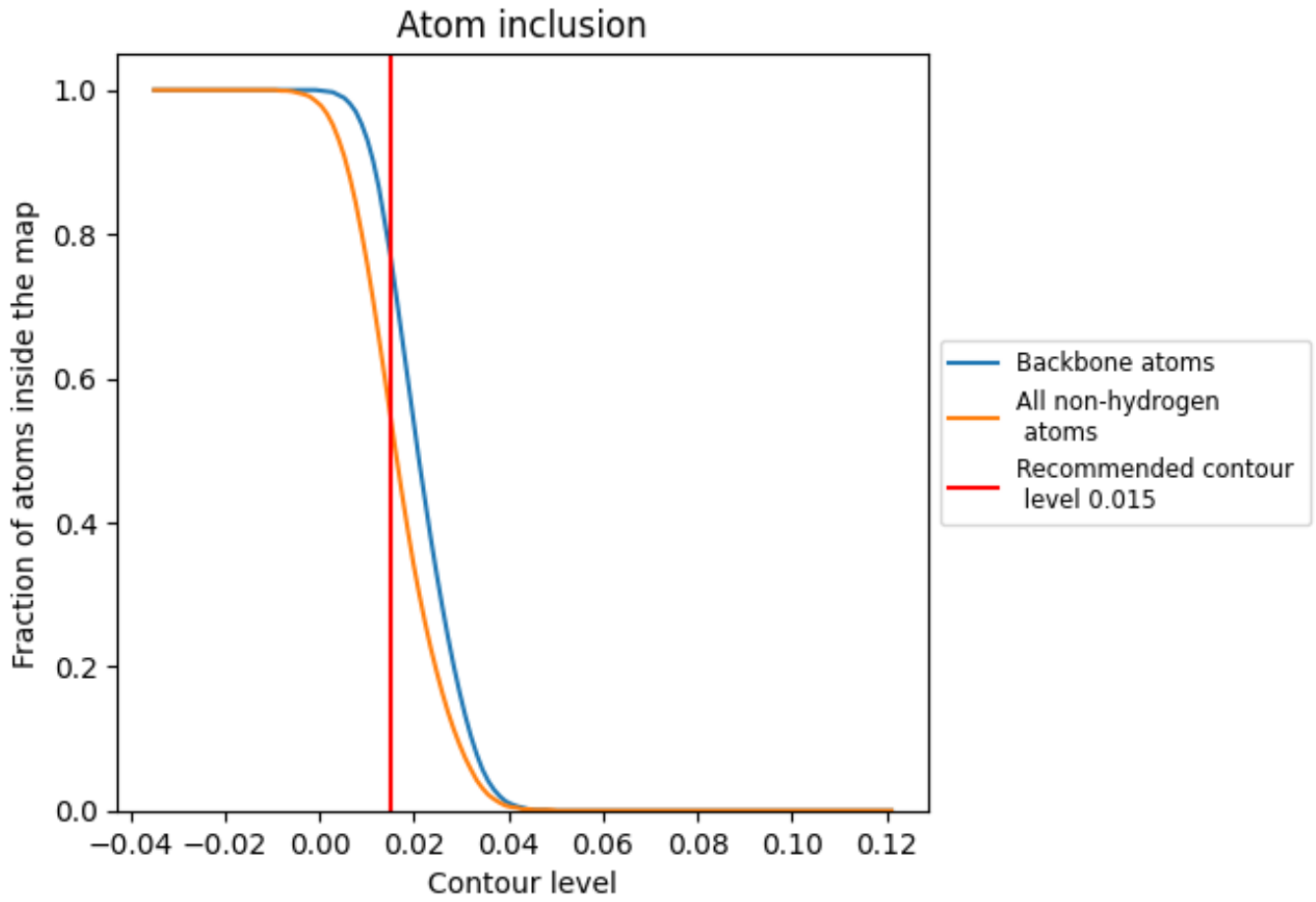
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 55% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.2950
A	0.4860	0.3410
AA	0.4790	0.1900
AB	0.4570	0.2030
AC	0.4580	0.2680
AD	0.4900	0.2020
AE	0.2500	0.1680
AF	0.5790	0.2560
AG	0.3290	0.1880
AH	0.4340	0.1150
AI	0.1140	0.1520
AJ	0.3730	0.2090
AK	0.2270	0.1820
Aa	0.6570	0.3410
Ab	0.6130	0.2800
Ac	0.5380	0.3210
Ad	0.5200	0.2490
Ae	0.2530	0.1840
Af	0.5570	0.2980
Ag	0.4900	0.3220
Ah	0.4380	0.1750
Ai	0.2340	0.2550
Aj	0.3740	0.2260
Ak	0.2810	0.2340
B	0.6520	0.3650
C	0.6110	0.3230
D	0.6340	0.3640
E	0.4710	0.2200
F	0.4780	0.2120
G	0.4680	0.2300
H	0.5830	0.3630
I	0.6470	0.3510
J	0.4890	0.3360
K	0.6140	0.3890
L	0.6360	0.3700

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Chain	Atom inclusion	Q-score
M	0.6520	0.4030
N	0.6470	0.3960
O	0.6120	0.3250
P	0.3820	0.1950
Q	0.4740	0.2750
R	0.4820	0.2780
S	0.3800	0.1320
T	0.2640	0.1360
U	0.6950	0.3650
V	0.5510	0.2390
W	0.4310	0.2360
X	0.6940	0.3350
Y	0.5540	0.3560
Z	0.6820	0.3230
a	0.6990	0.3640
b	0.6520	0.3380
c	0.5850	0.2880
d	0.6340	0.3740
e	0.6710	0.3650
f	0.6220	0.3180
g	0.6470	0.3470
h	0.6460	0.3530
i	0.6530	0.3580
j	0.6570	0.3130
k	0.7120	0.3440
l	0.6680	0.3680
m	0.6300	0.3620
n	0.7200	0.3760
o	0.5940	0.2710
p	0.6840	0.3510
q	0.5190	0.3170
r	0.4450	0.2750
s	0.3350	0.1910