Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 04:41 PM JST

PDB ID	:	8IB4
EMDB ID	:	EMD-35331
Title	:	Respiratory complex CI:CIII2, type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	4.30 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:

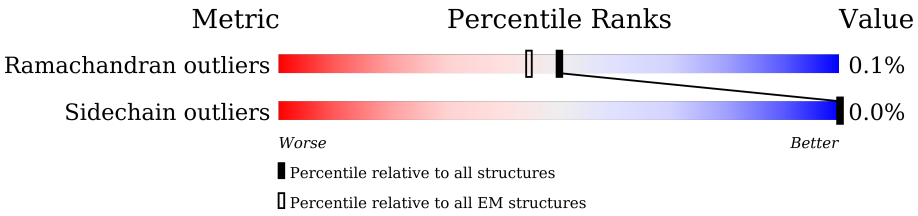
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 4.30 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	11% 80% 20%
2	B	224	6% 67% 30%
3	C	263	25% 75% 25%
4	D	463	13% 90% 8%
5	E	248	73% 81% 15%
6	F	464	69% 89% 8%
7	G	727	55% 92% 6%
8	H	318	8% 95%
9	I	212	5% 81% 18%

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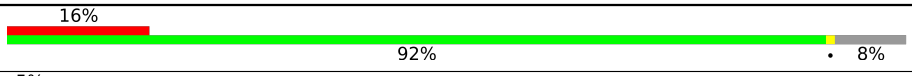
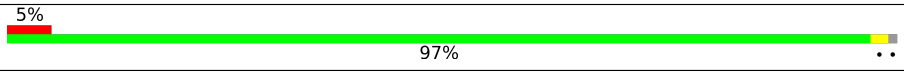
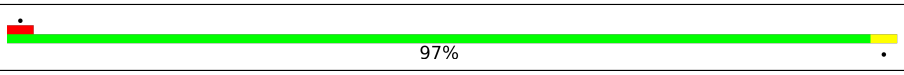
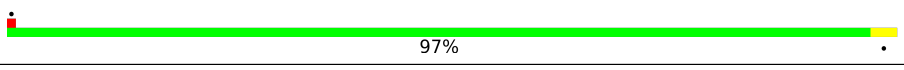
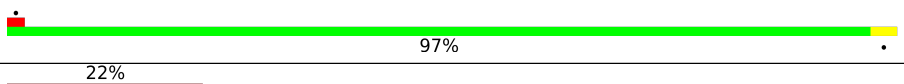
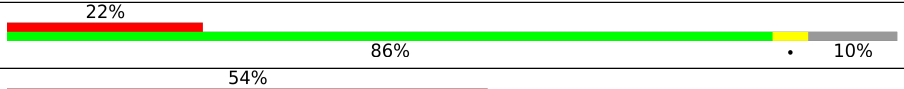
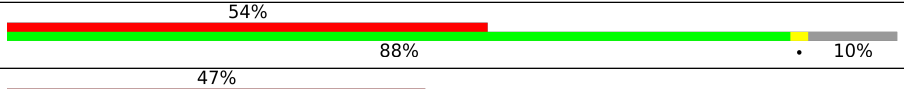
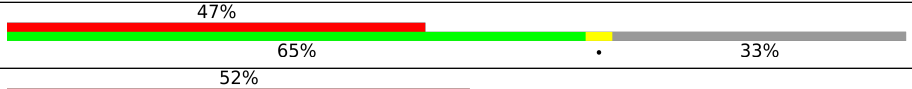
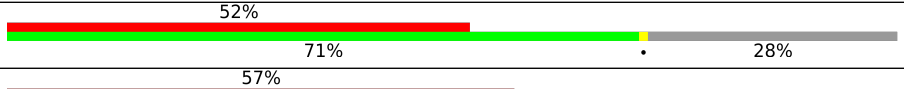
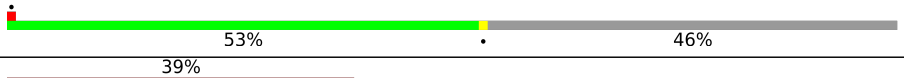
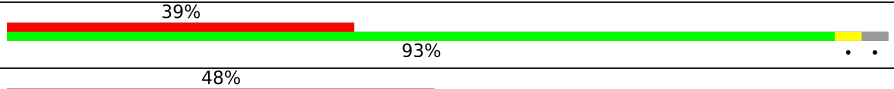
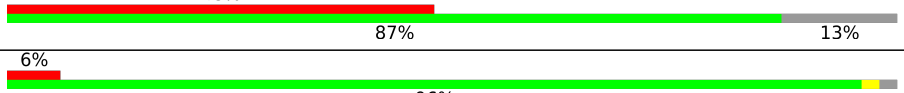
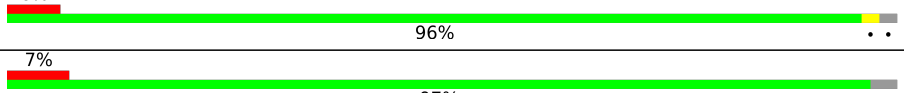
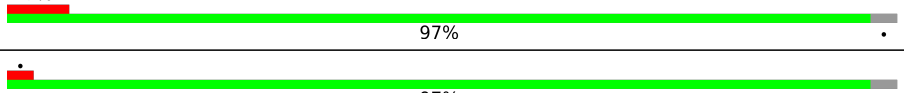
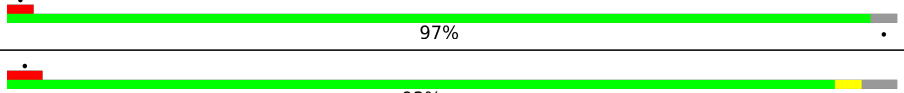
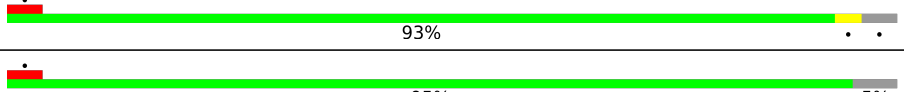
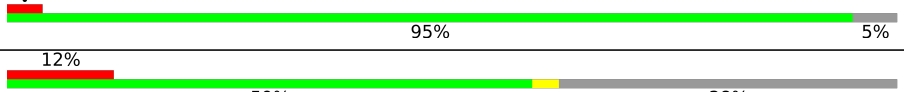
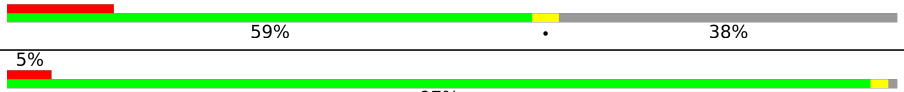
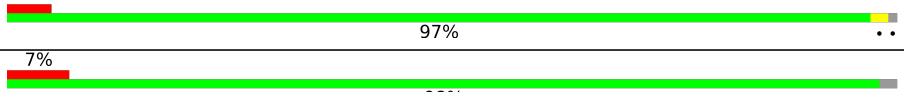
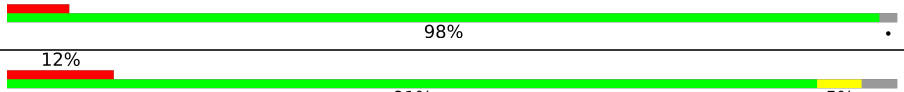
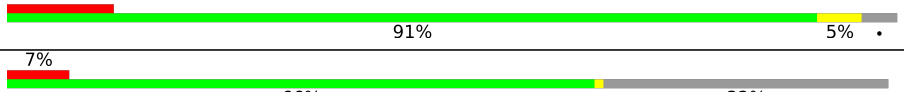
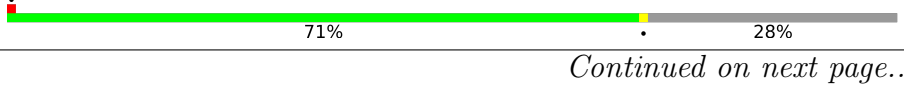
Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

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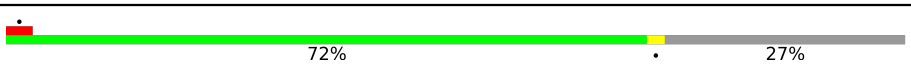
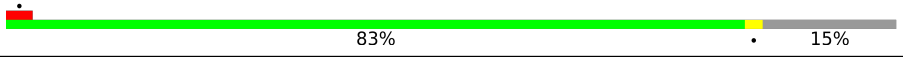
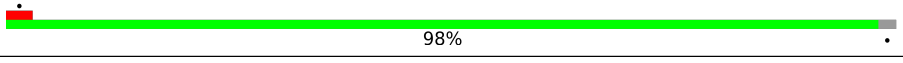
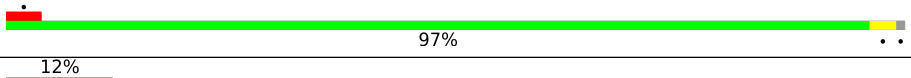
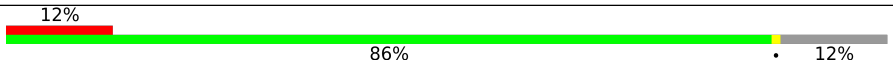
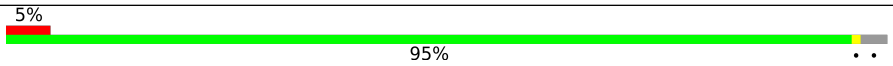
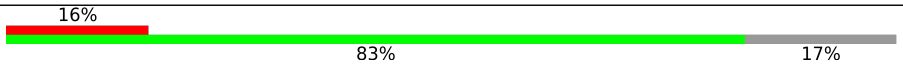
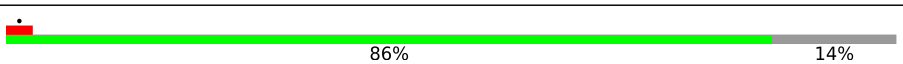
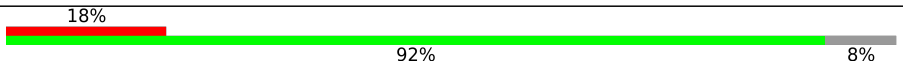
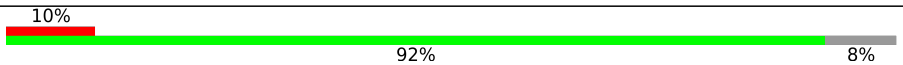
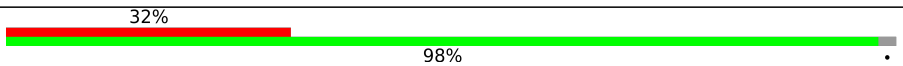
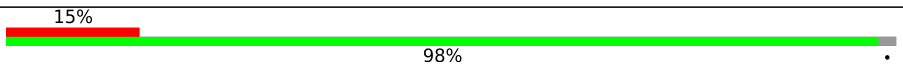
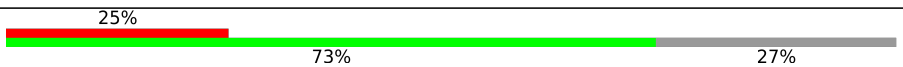
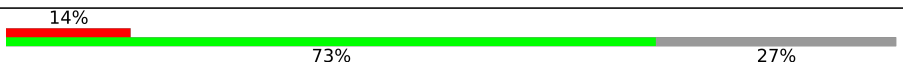
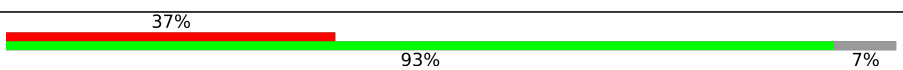
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
50	AF	111	
50	Af	111	
51	AG	82	

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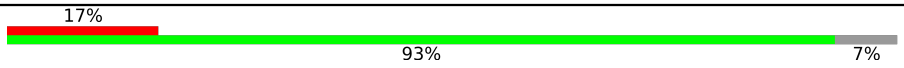
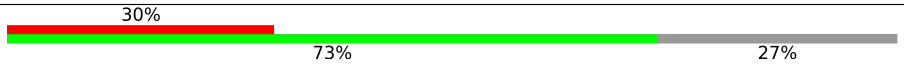
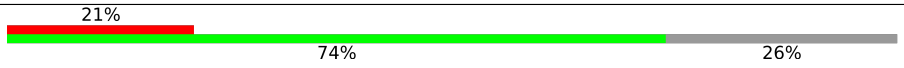
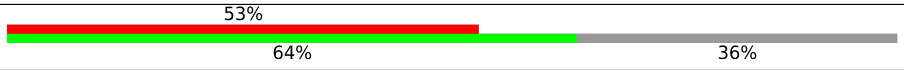
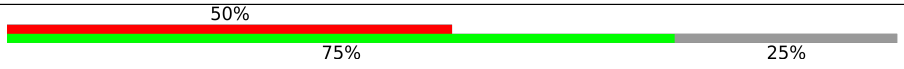
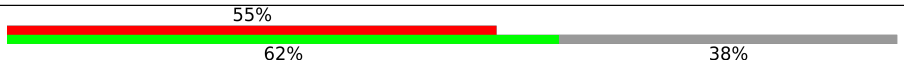
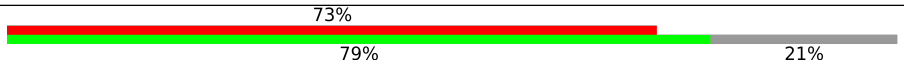
Mol	Chain	Length	Quality of chain
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

2 Entry composition

There are 71 unique types of molecules in this entry. The entry contains 97639 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	3415	2182	587	622	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	C	N	O	S	0	0
			3288	2073	588	605	22		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	314	Total	C	N	O	S	0	0
			2510	1687	380	421	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total	C	N	O	S	0	0
			1398	880	240	266	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	159	Total	C	N	O	S	0	0
			1205	814	171	205	15		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3622	2402	566	615	39		

- 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	340	Total	C	N	O	S	0	0
			2730	1765	479	479	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	84	Total	C	N	O	S	0	0
			678	438	100	135	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	139	Total	C	N	O	S	0	0
			1030	657	174	191	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	80	Total	C	N	O	S	0	0
			628	414	99	111	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	119	Total	C	N	O	S	0	0
			988	646	170	164	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			863	546	158	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	55	Total	C	N	O	S	0	0
			475	310	84	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	136	Total	C	N	O	S	0	0
			1146	754	191	198	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	94	Total	C	N	O	S	0	0
			796	520	139	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	71	Total	C	N	O	S	0	0
			569	375	99	93	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	158	Total	C	N	O	S	0	0
			1328	858	221	238	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	127	Total	C	N	O	0	0
			1054	678	190	186		

- 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	120	Total	C	N	O	S	0	0
			1027	647	192	179	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	904	258	268	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	14	Total	C	N	O	0	0
			115	75	17	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		

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

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

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

- Molecule 47 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
48	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
49	AI	51	Total	C	N	O		0	0
			345	221	64	60			
49	Ae	185	Total	C	N	O	S	0	0
			1432	905	250	270	7		

- 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		

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	65	Total 535	C 327	N 99	O 104	S 5	0	0
52	Ah	66	Total 544	C 333	N 101	O 105	S 5	0	0

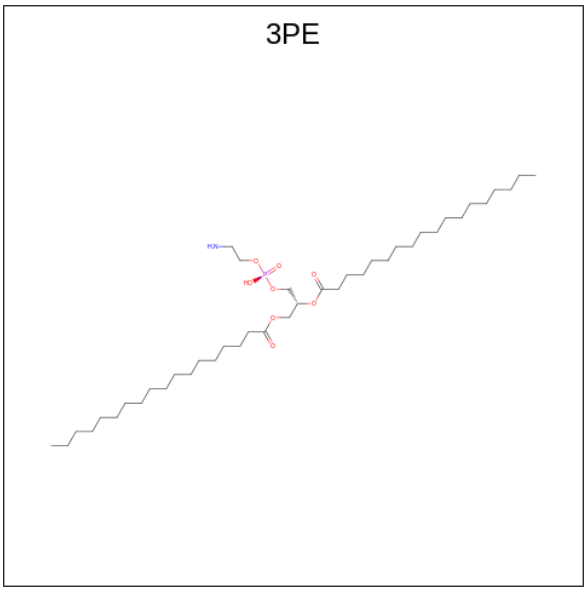
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total 332	C 216	N 57	O 59	0	0
53	Aj	48	Total 392	C 257	N 67	O 68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	35	Total 281	C 184	N 52	O 44	S 1	0	0
54	Ak	44	Total 357	C 236	N 63	O 57	S 1	0	0

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	I	1	Total	C	N	O	P	0
			51	41	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
			42	32	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	L	1	Total	C	N	O	P	0
			45	35	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
			51	41	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
55	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	

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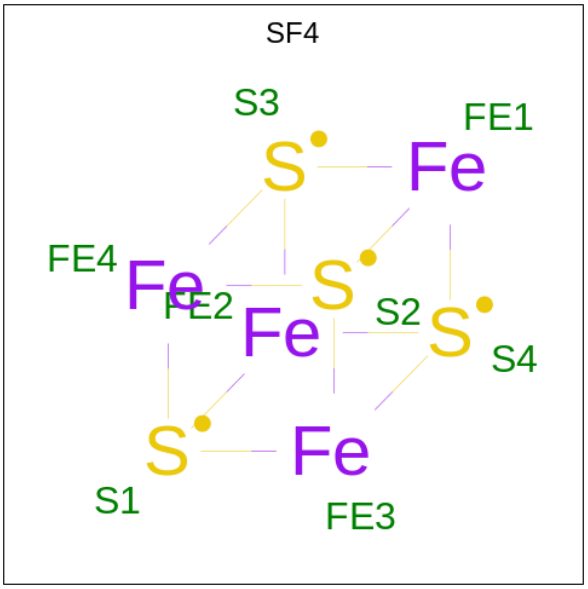
Mol	Chain	Residues	Atoms					AltConf
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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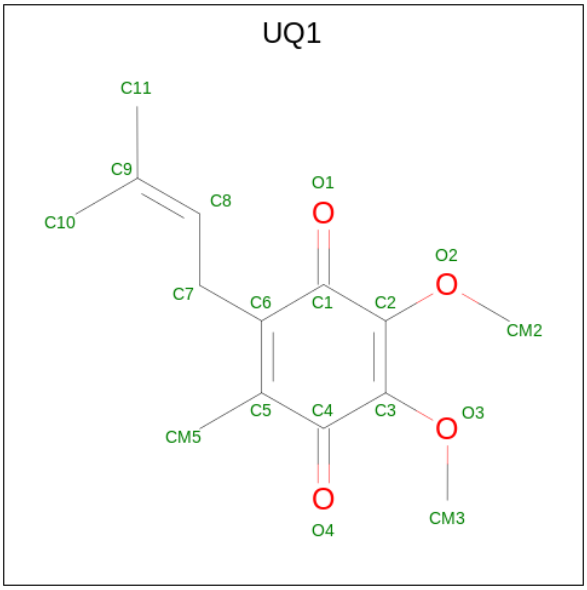
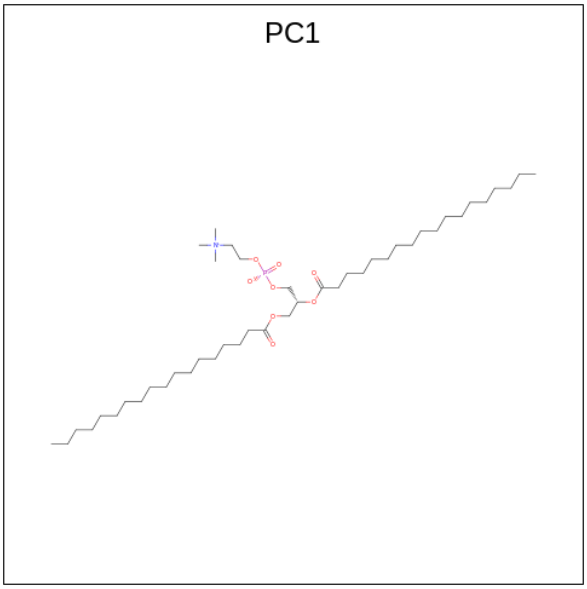
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
56	I	1	8	4	4	0

- Molecule 57 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



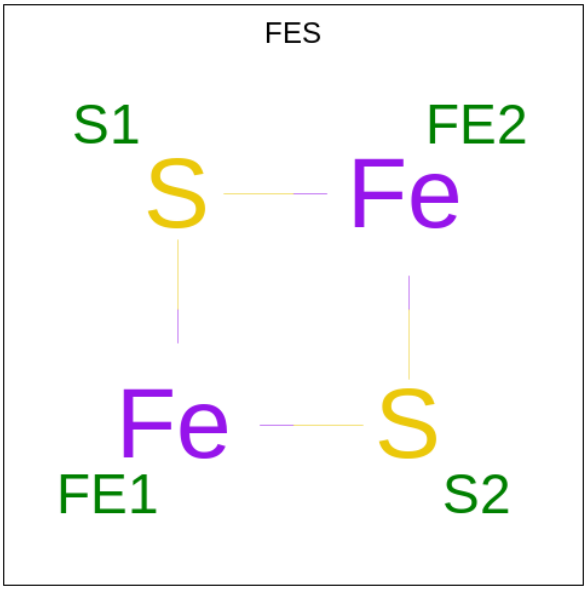
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	B	1	18	14	4	0

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



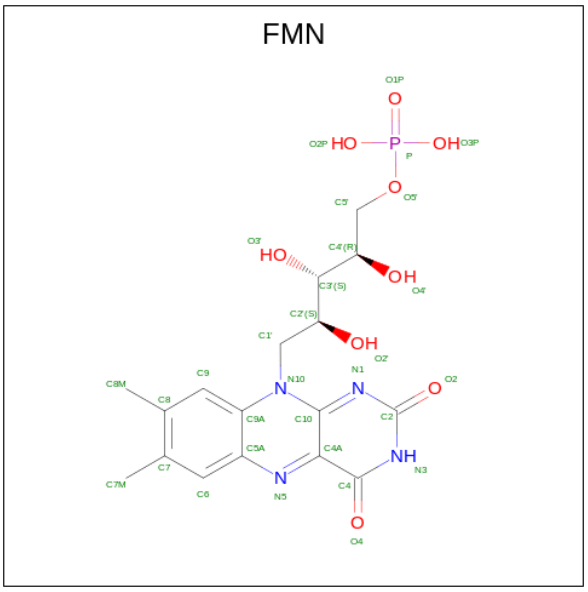
Mol	Chain	Residues	Atoms					AltConf
58	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	J	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



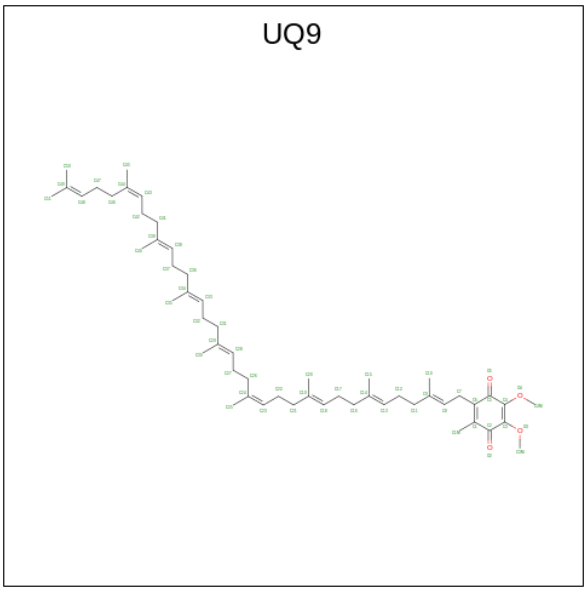
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



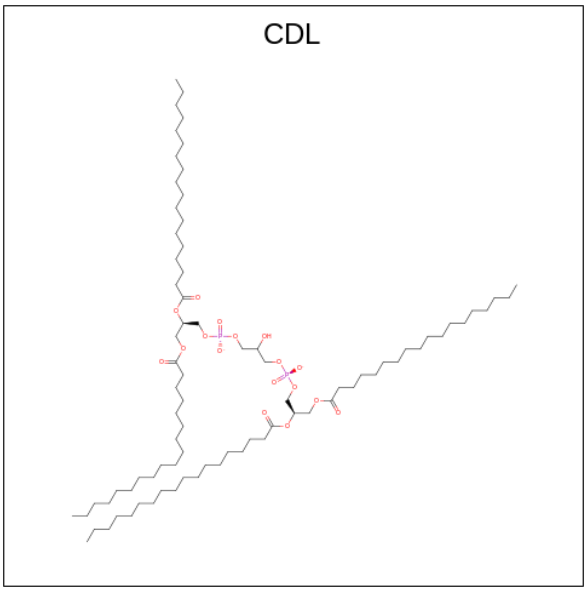
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



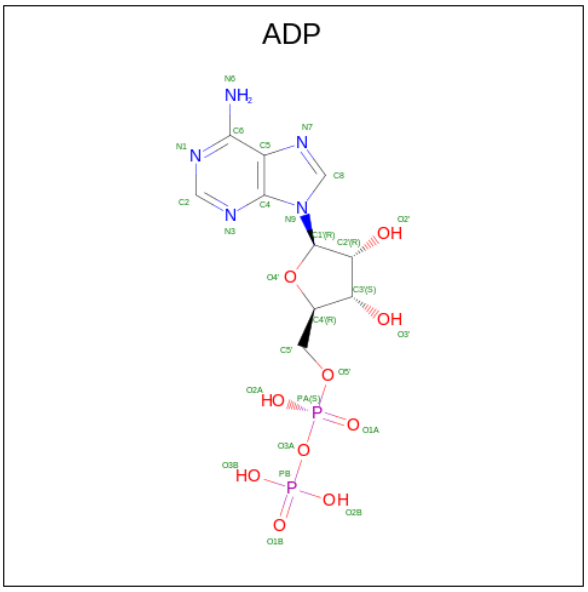
Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



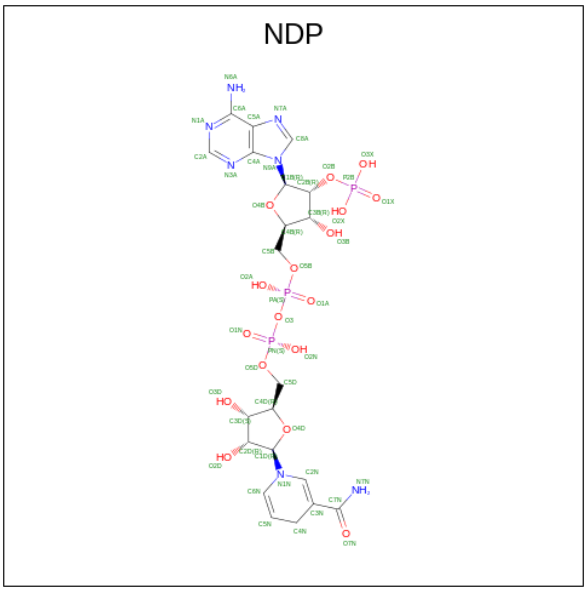
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			77	58	17	2	
62	L	1	Total	C	O	P	0
			86	67	17	2	
62	X	1	Total	C	O	P	0
			67	48	17	2	
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	AC	1	Total	C	O	P	0
			56	37	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ac	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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: $C_{21}H_{30}N_7O_{17}P_3$).

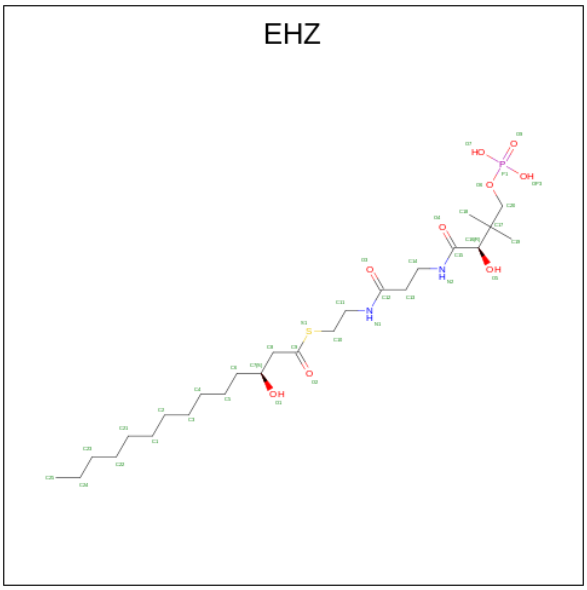


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

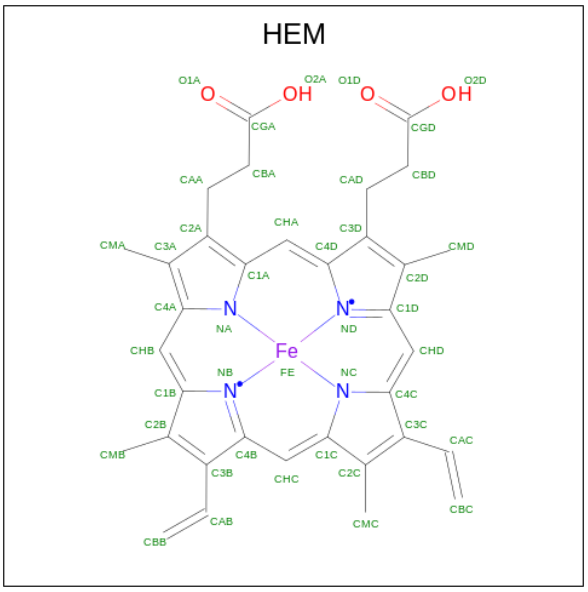
Mol	Chain	Residues	Atoms	AltConf
65	R	1	Total Zn 1 1	0

- 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: $C_{25}H_{49}N_2O_9PS$).



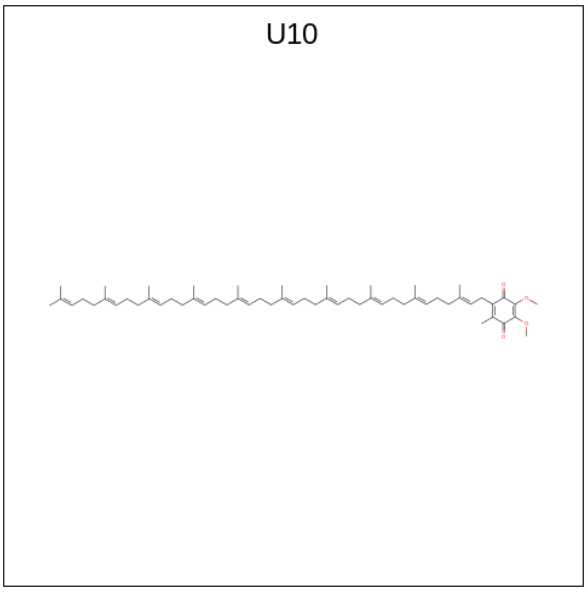
Mol	Chain	Residues	Atoms	AltConf
66	W	1	Total C N O P S 32 19 2 9 1 1	0
66	n	1	Total C N O P S 32 19 2 9 1 1	0

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



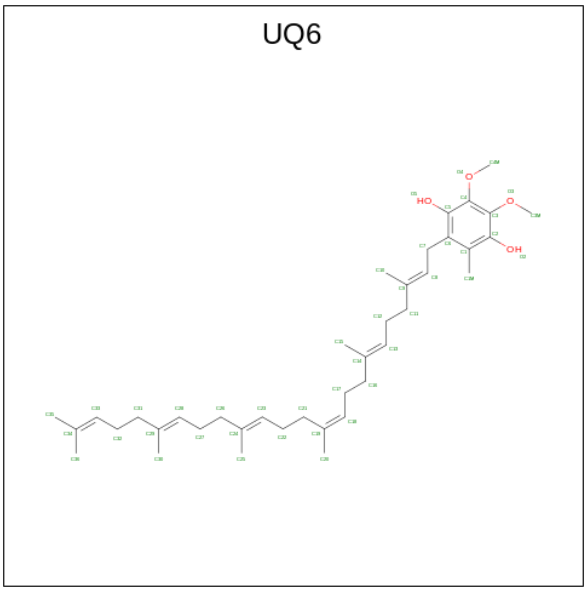
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



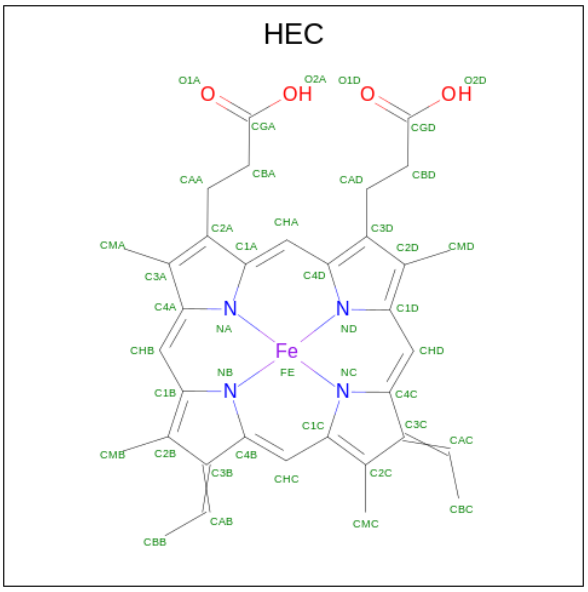
Mol	Chain	Residues	Atoms	AltConf
68	AC	1	Total C O 23 19 4	0
68	Ac	1	Total C O 38 34 4	0

- 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).



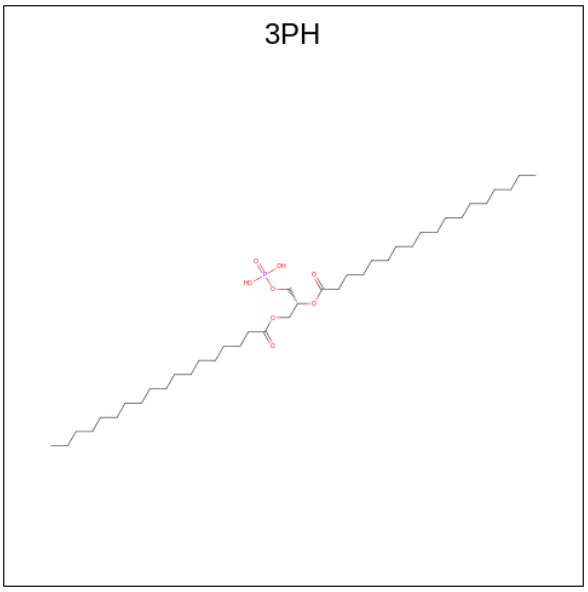
Mol	Chain	Residues	Atoms	AltConf
69	AC	1	Total C O 28 24 4	0
69	Ac	1	Total C O 28 24 4	0

- Molecule 70 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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	

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
71	AD	1	Total	C	O	P	0
			36	27	8	1	

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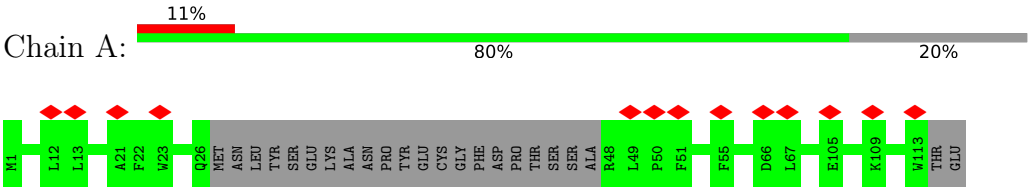
Mol	Chain	Residues	Atoms				AltConf
71	Ad	1	Total	C	O	P	0
			36	27	8	1	

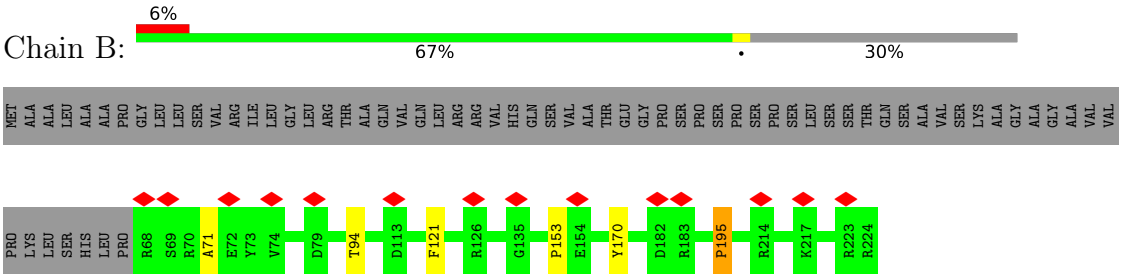
3 Residue-property plots (i)

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.

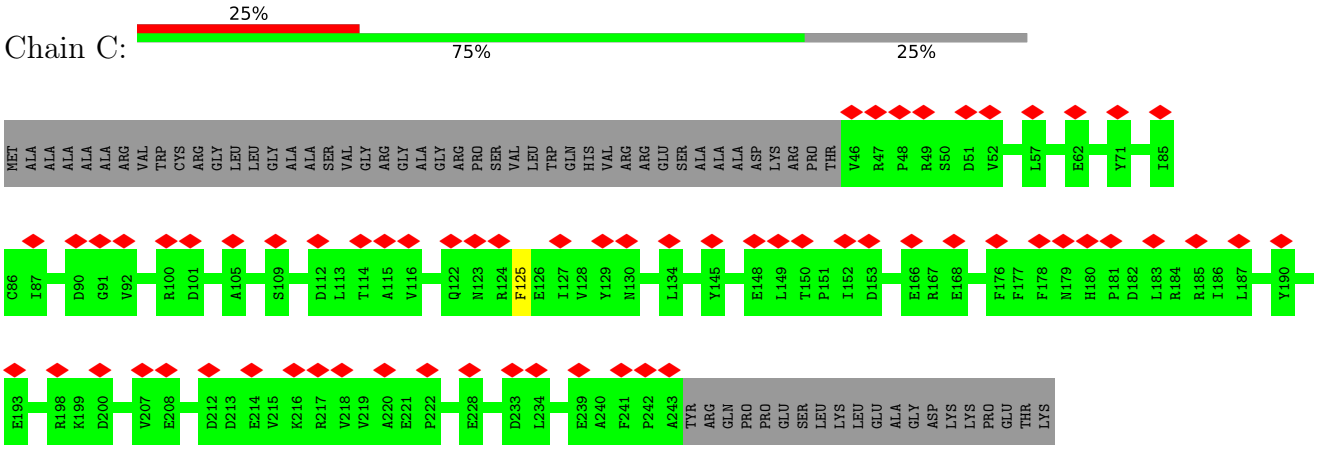
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



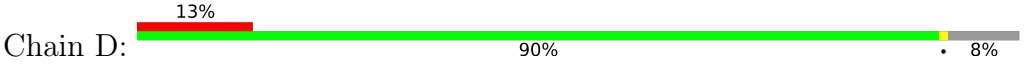
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

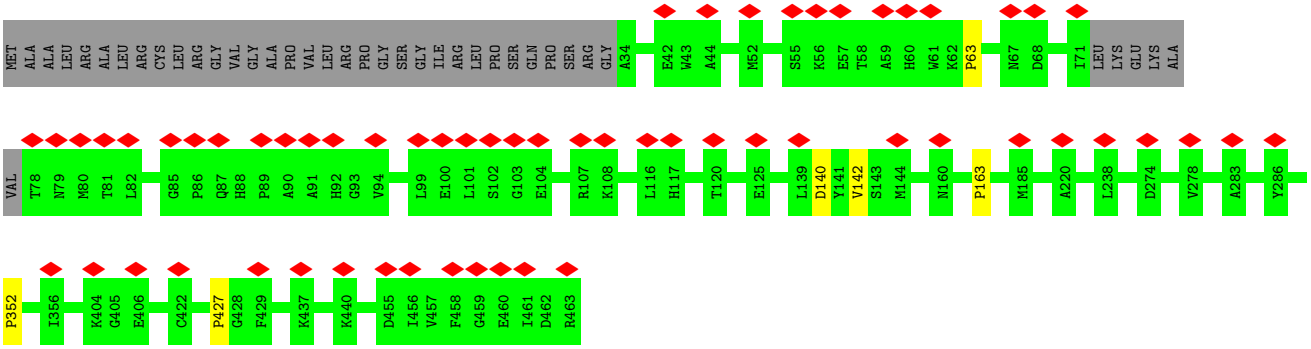


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



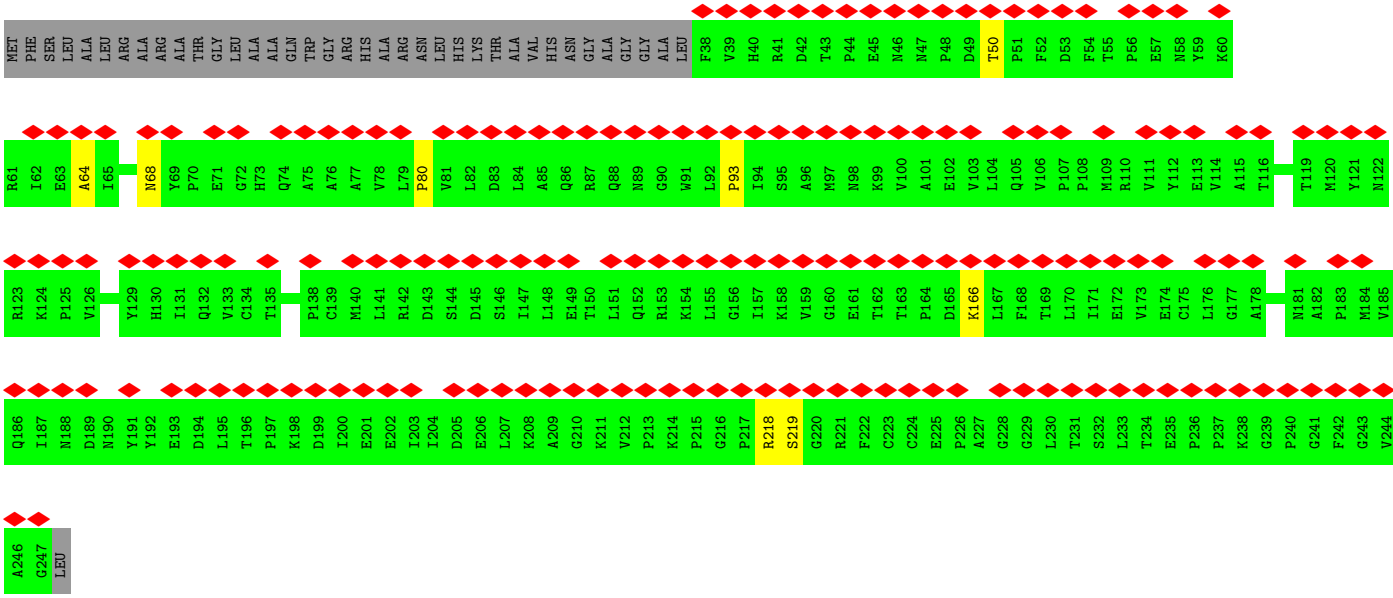
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





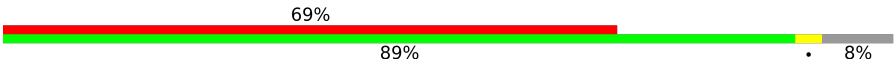
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

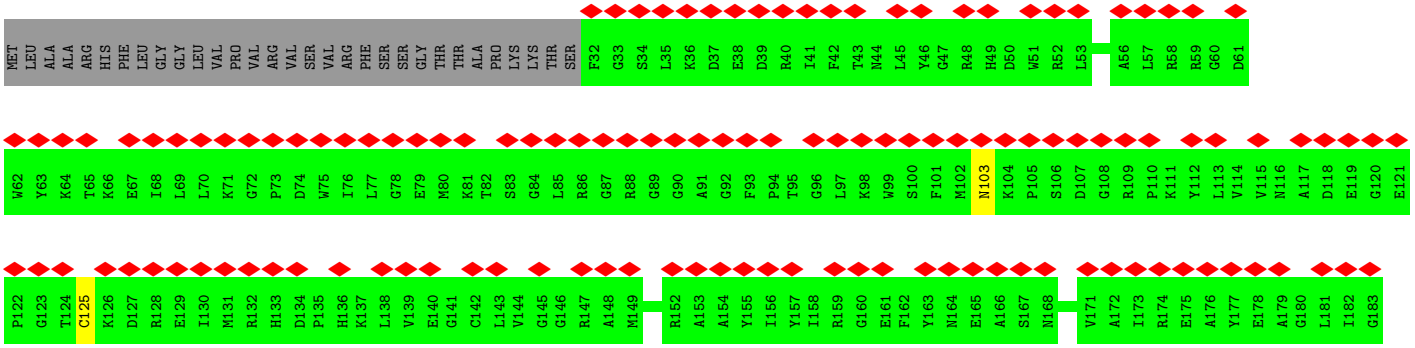
Chain E:

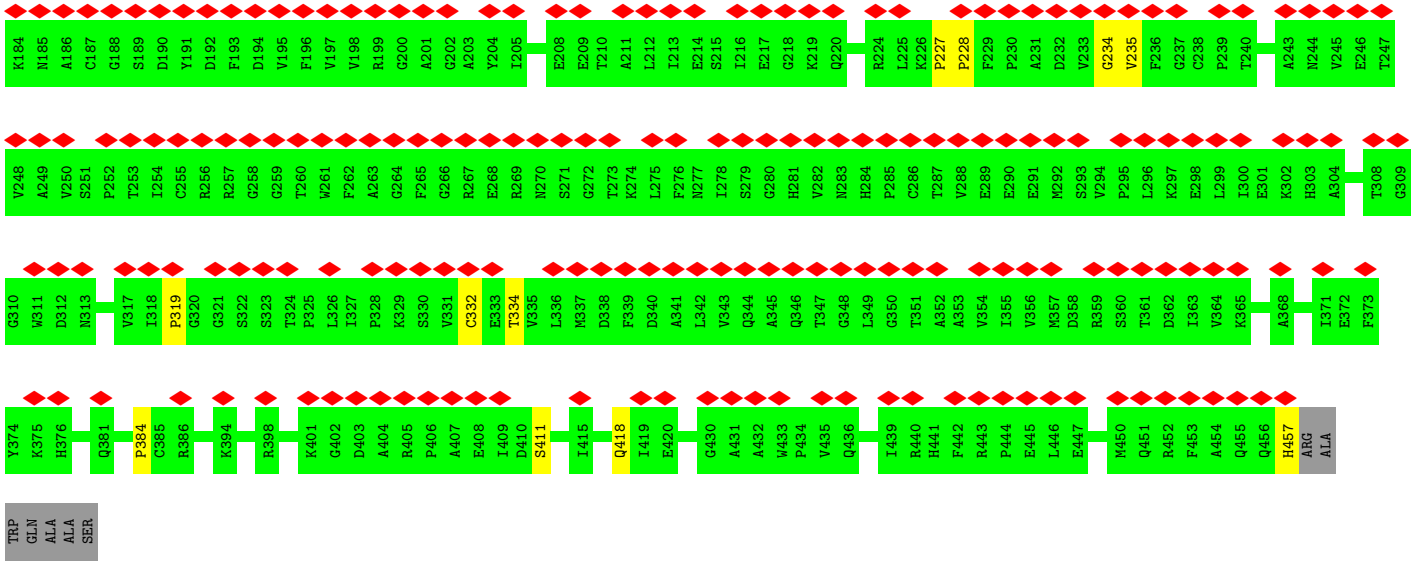


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

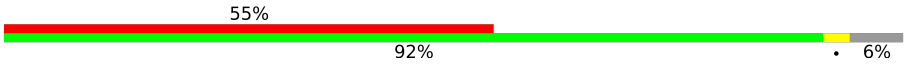


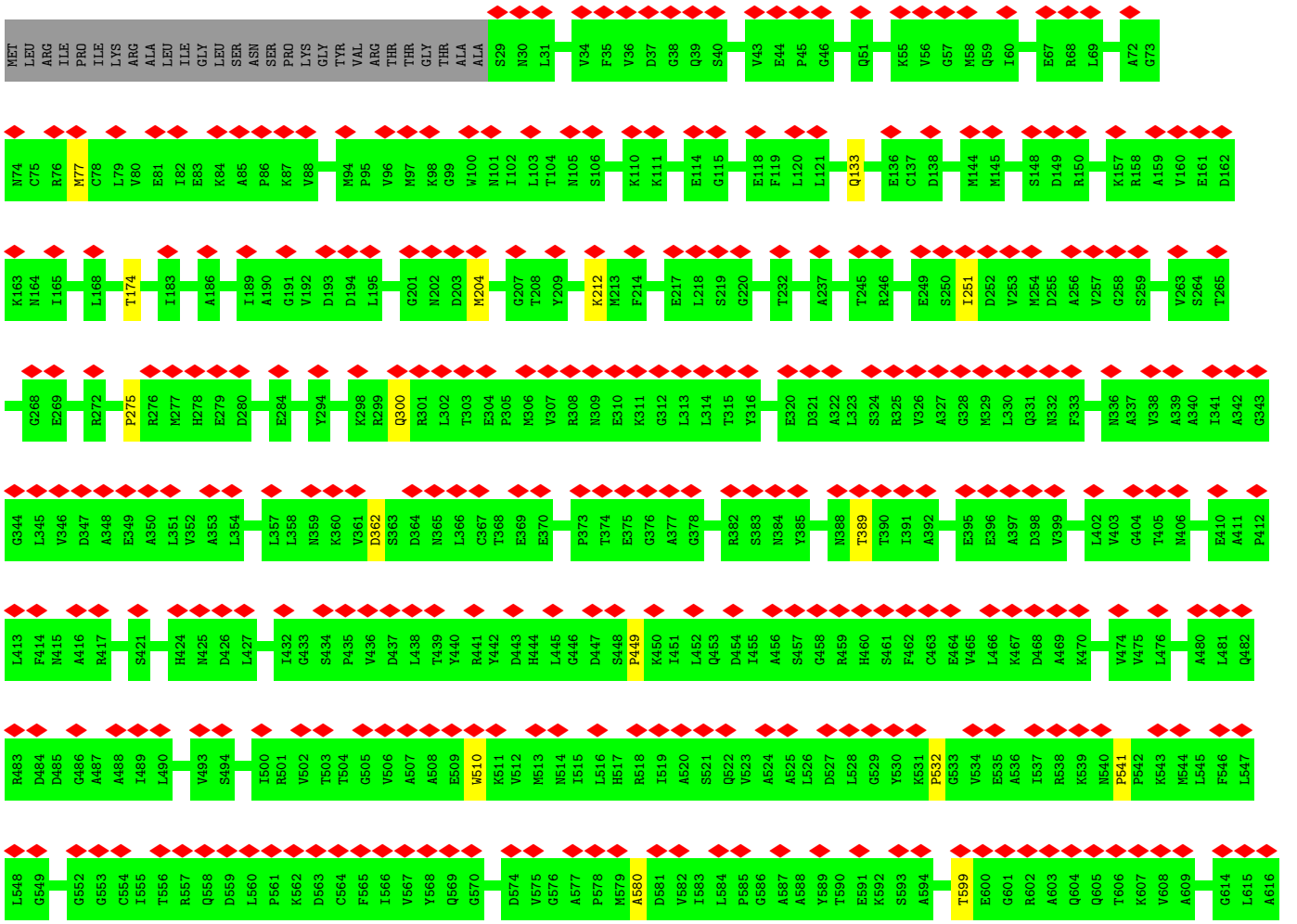


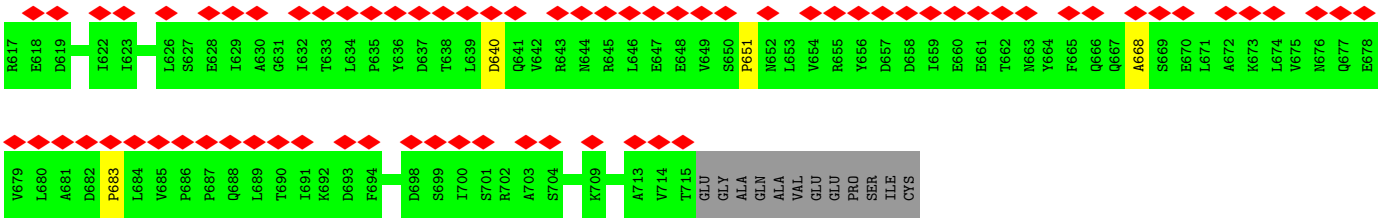


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

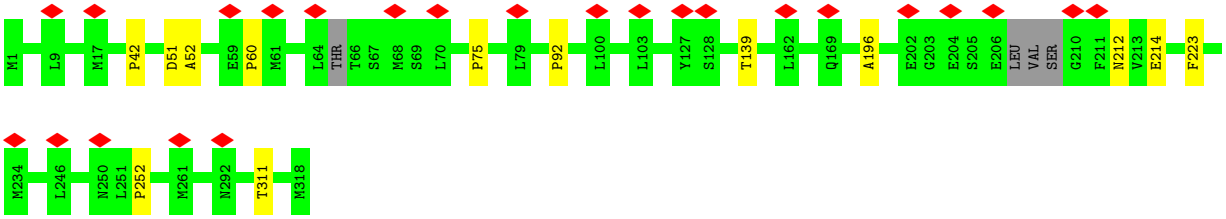
Chain G:



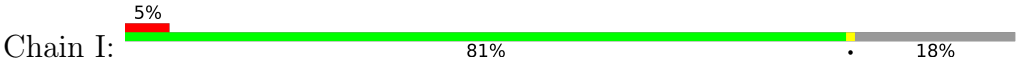


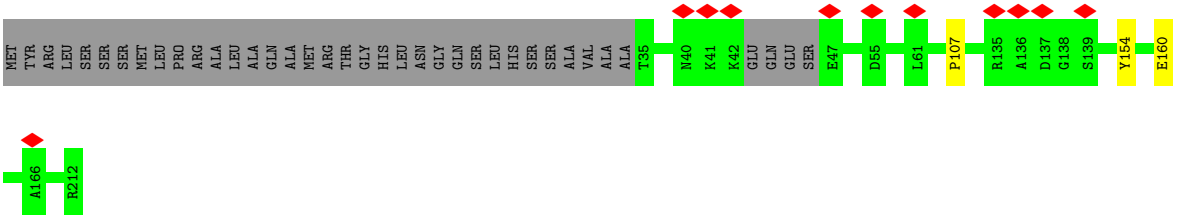


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

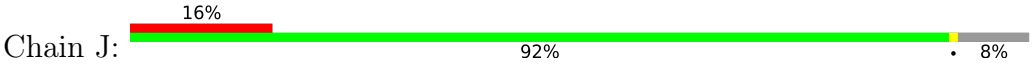


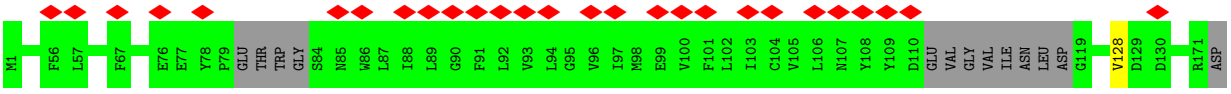
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



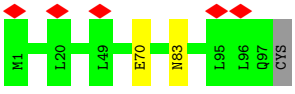


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

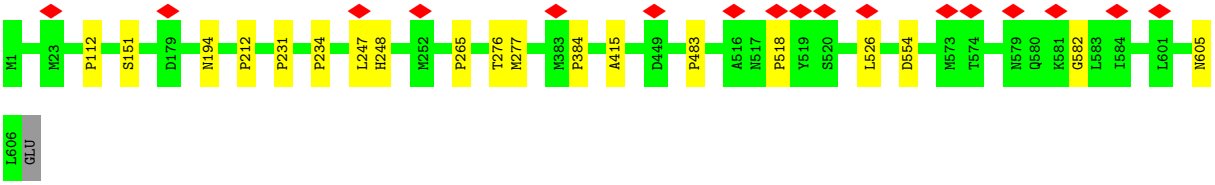




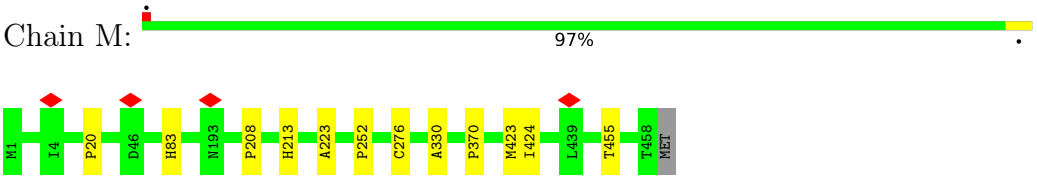
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



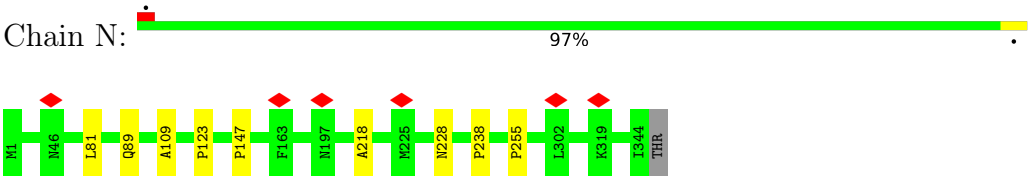
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



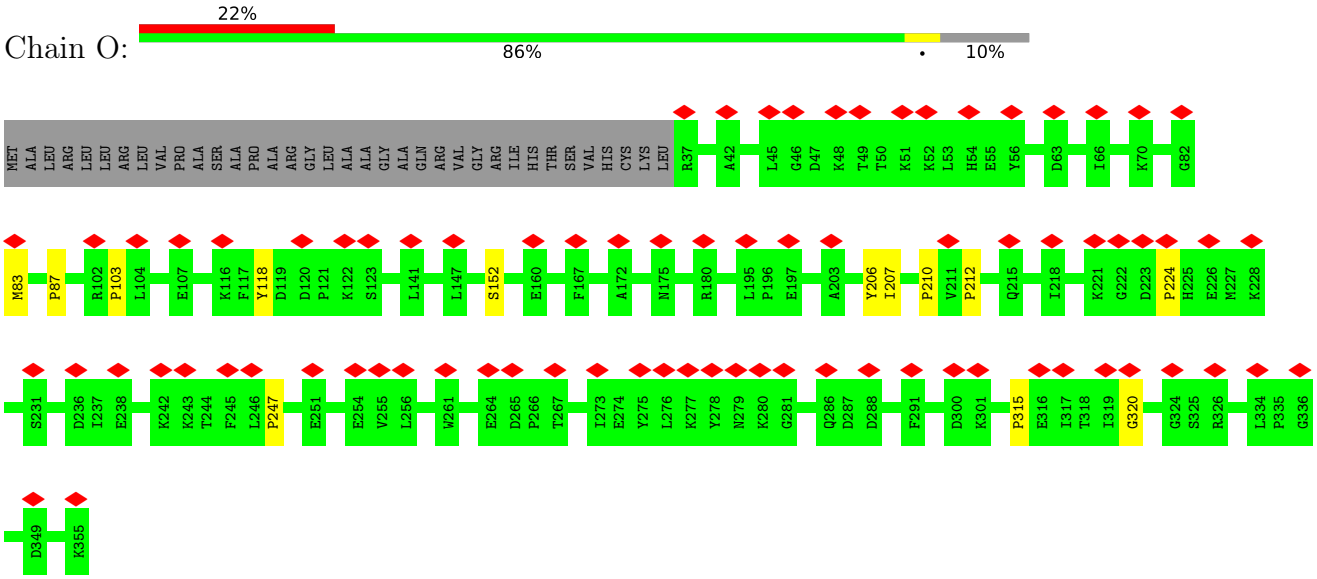
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



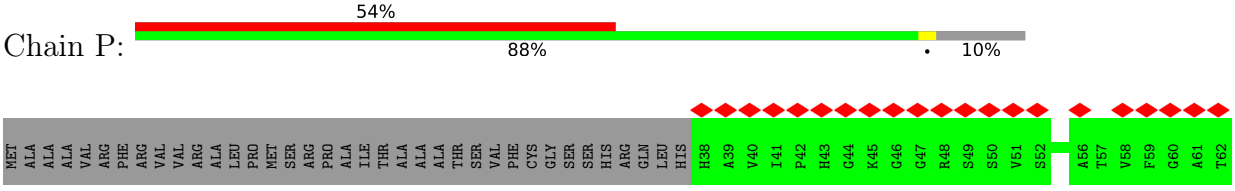
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

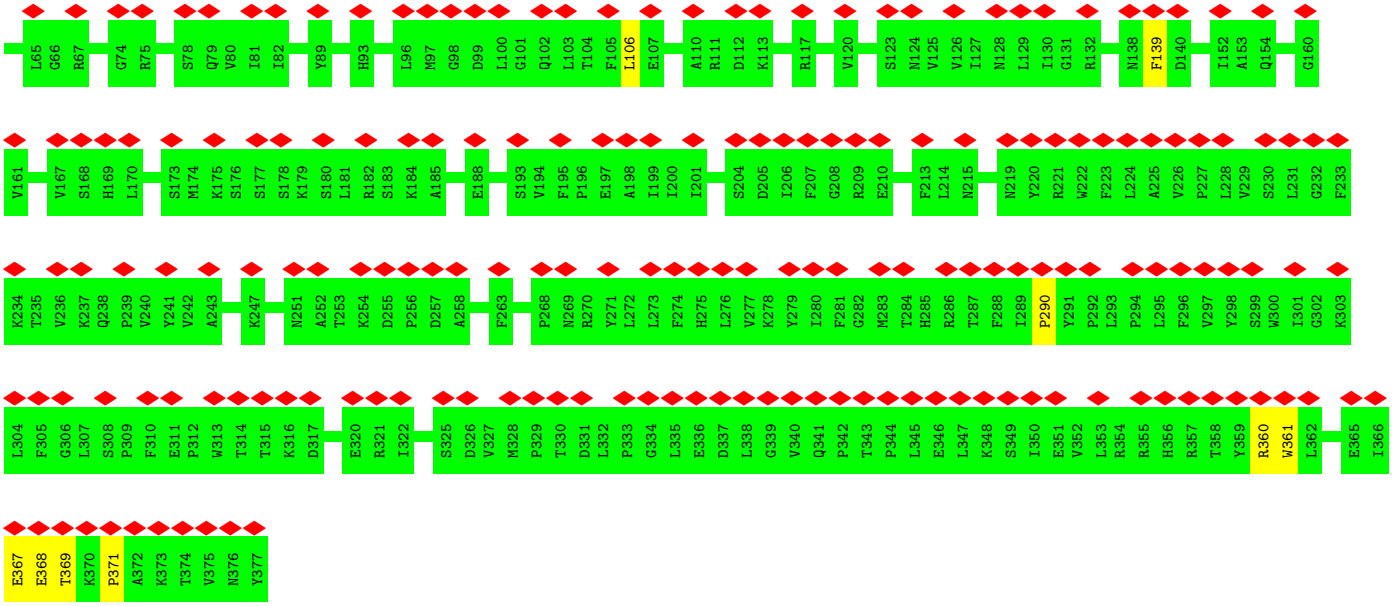


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

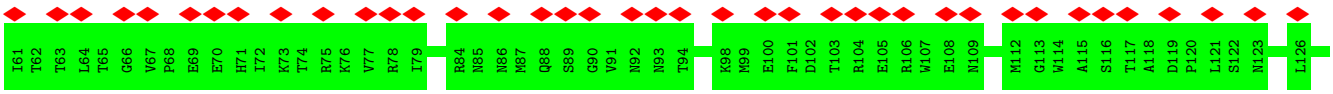


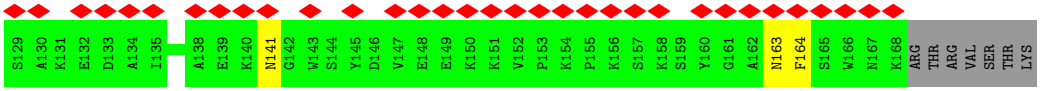
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



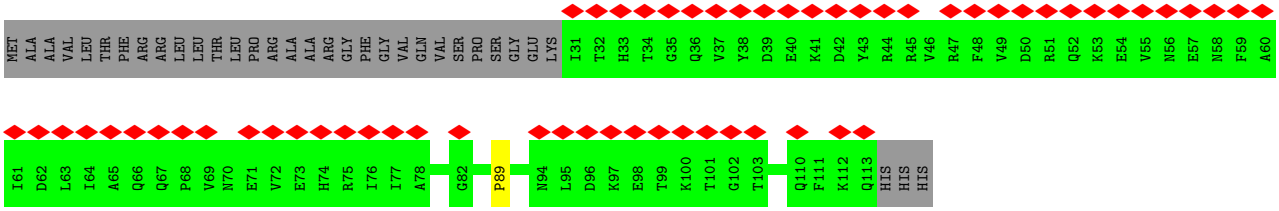


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

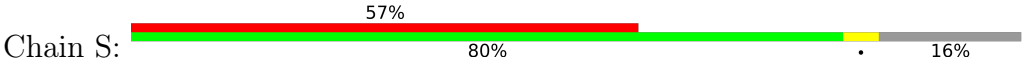


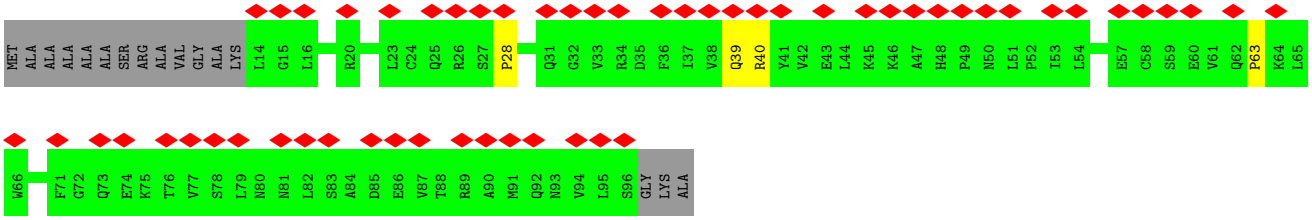


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



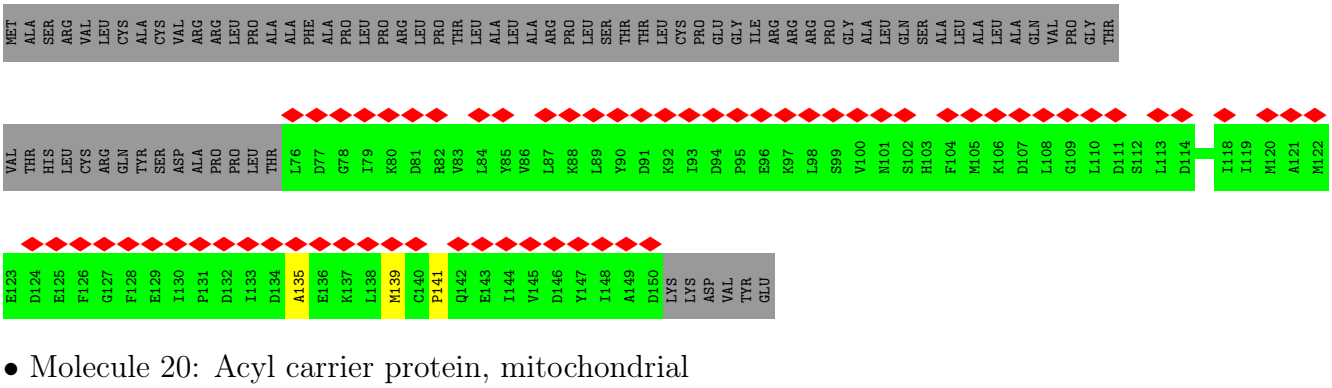
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2





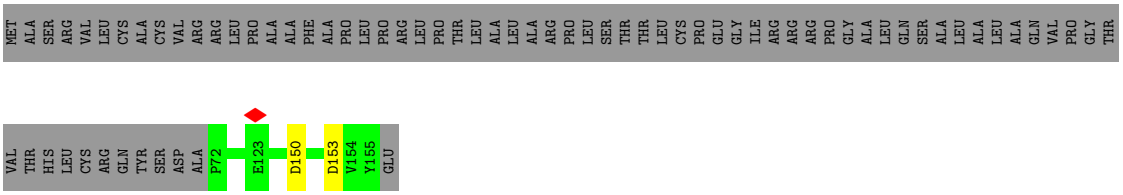
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



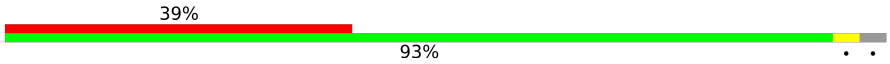
• Molecule 20: Acyl carrier protein, mitochondrial

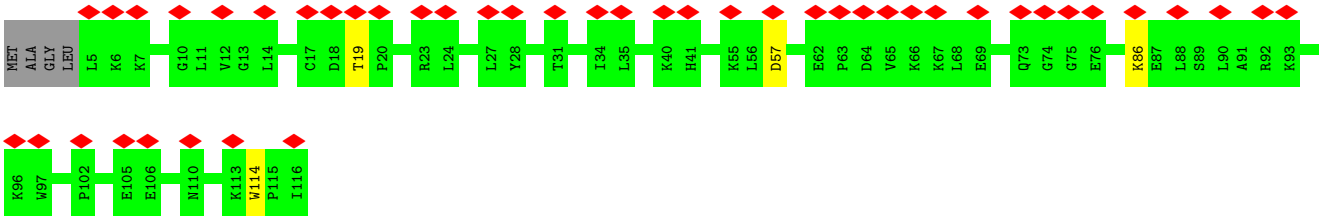
Chain U:



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

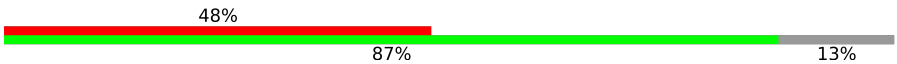
Chain V:

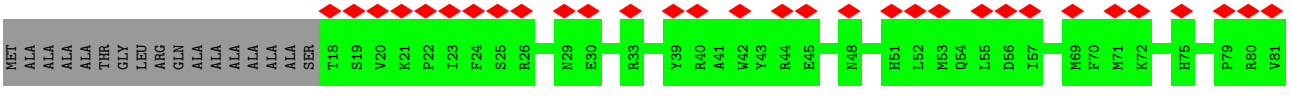


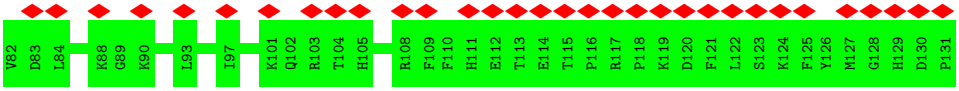


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

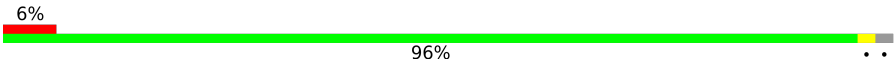


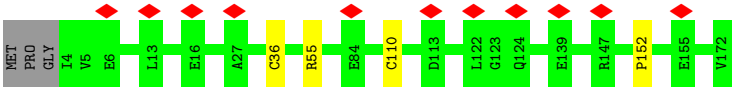




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

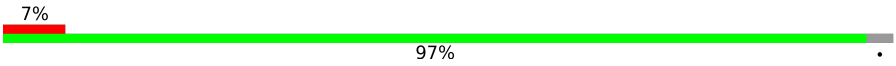
Chain X:

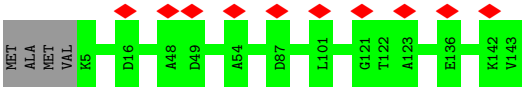




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

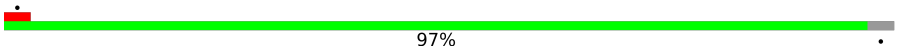
Chain Y:

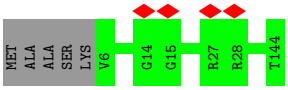




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

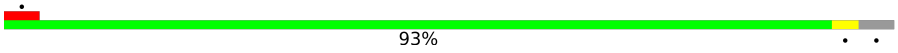
Chain Z:

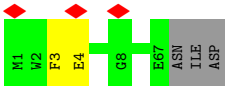




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

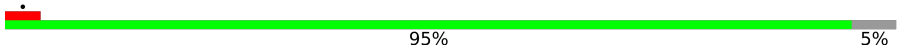
Chain a:

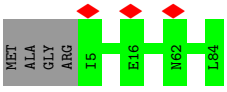




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

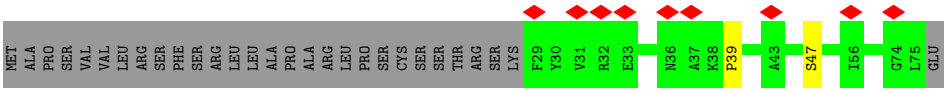
Chain b:





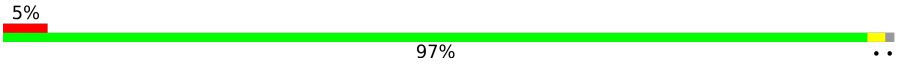
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

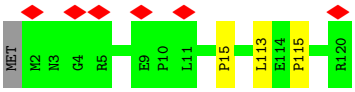
Chain c:



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

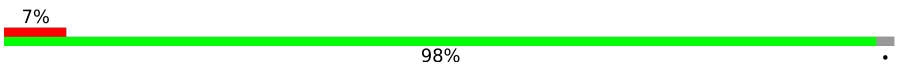
Chain d:

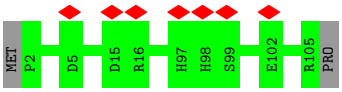




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

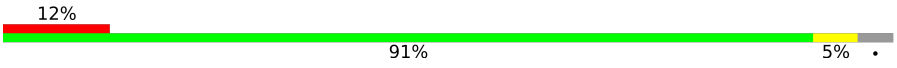
Chain e:

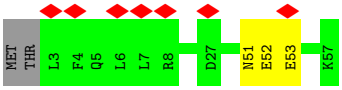




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

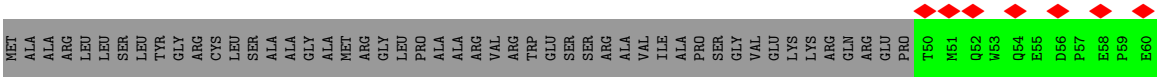
Chain f:





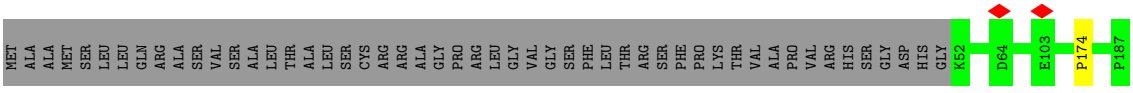
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



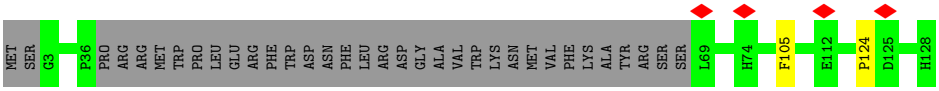
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



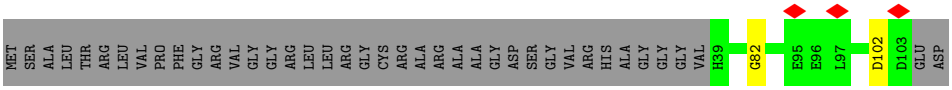
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



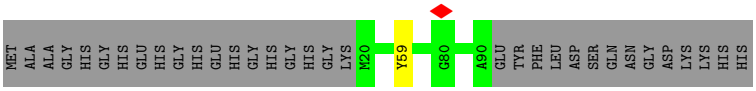
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



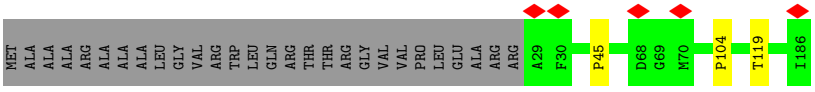
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



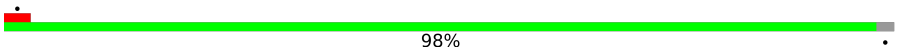
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

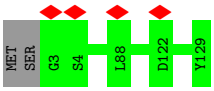
Chain l:



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

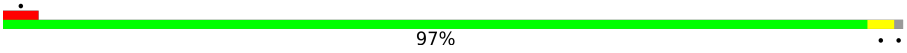
Chain m:

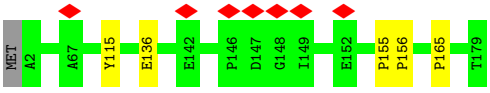




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

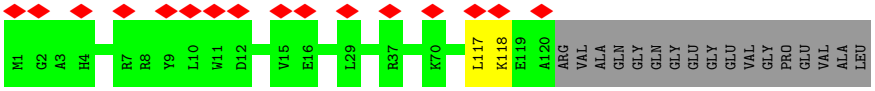
Chain n:





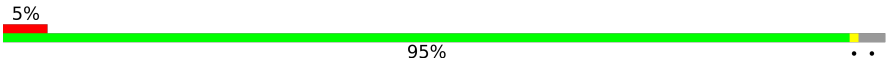
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

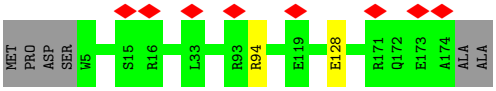
Chain o:



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

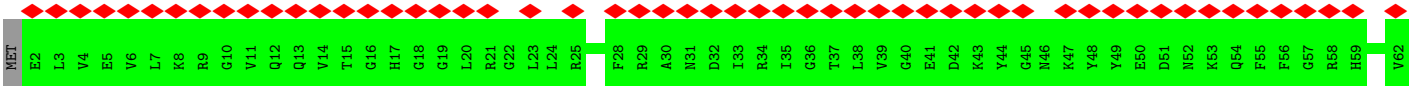
Chain p:

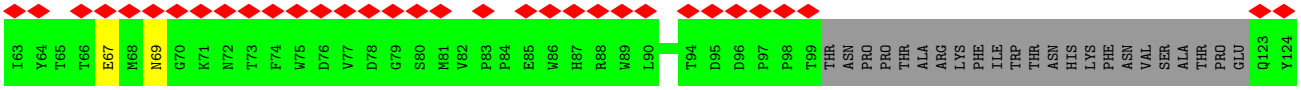


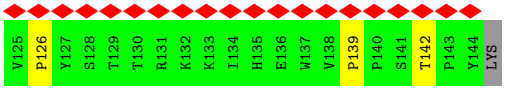


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

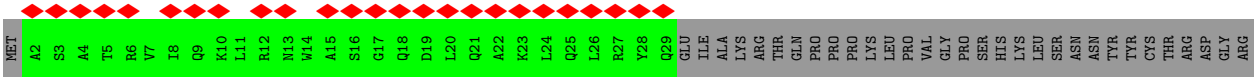


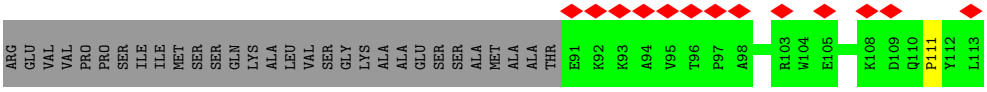




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

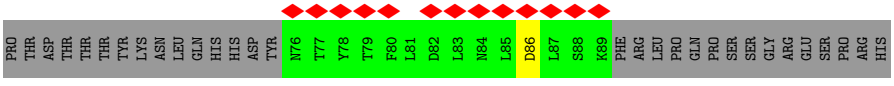
Chain r:





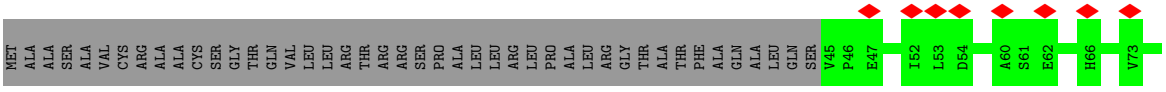
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

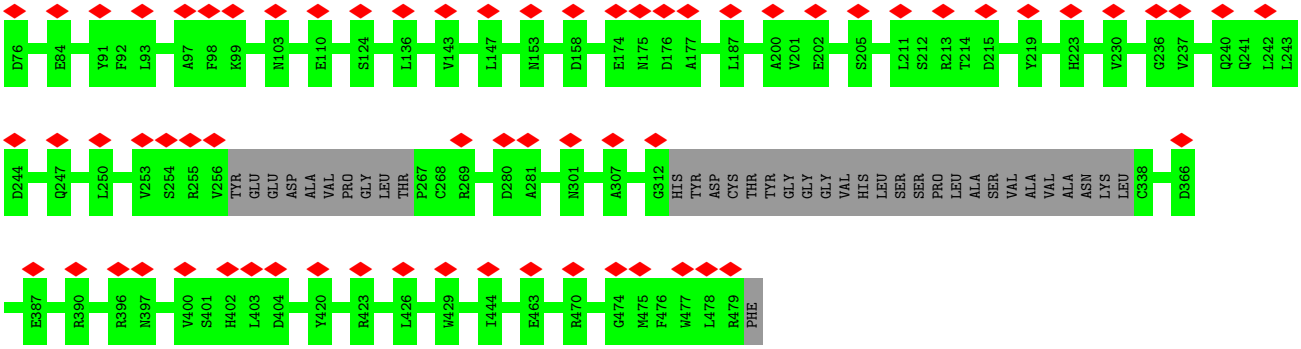
Chain s:



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

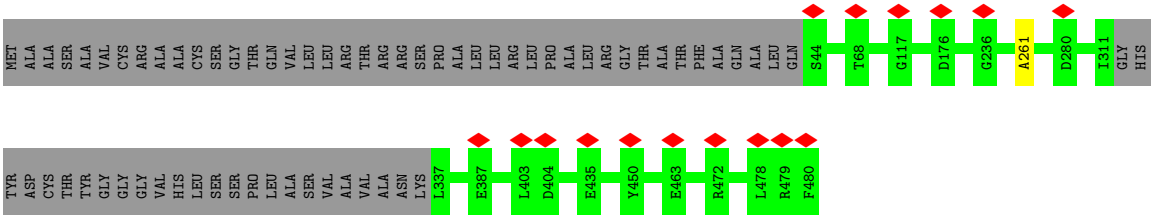
Chain AA:





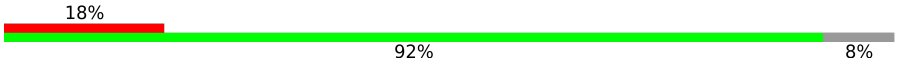
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

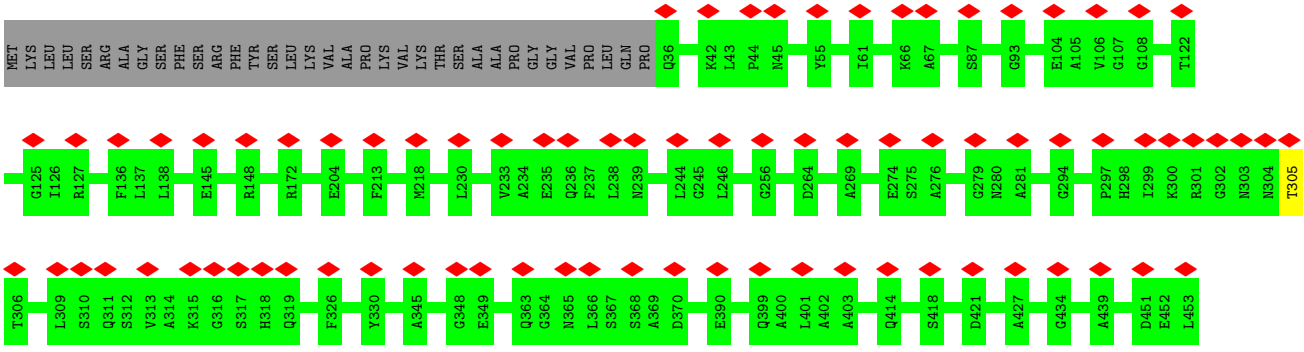
Chain Aa:



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

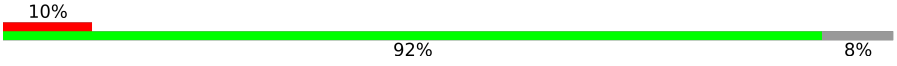
Chain AB:

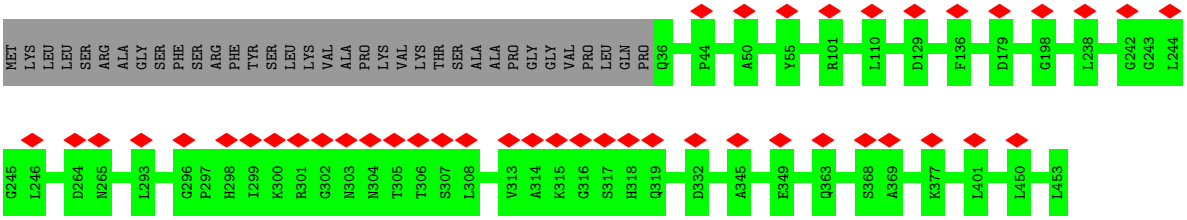




• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

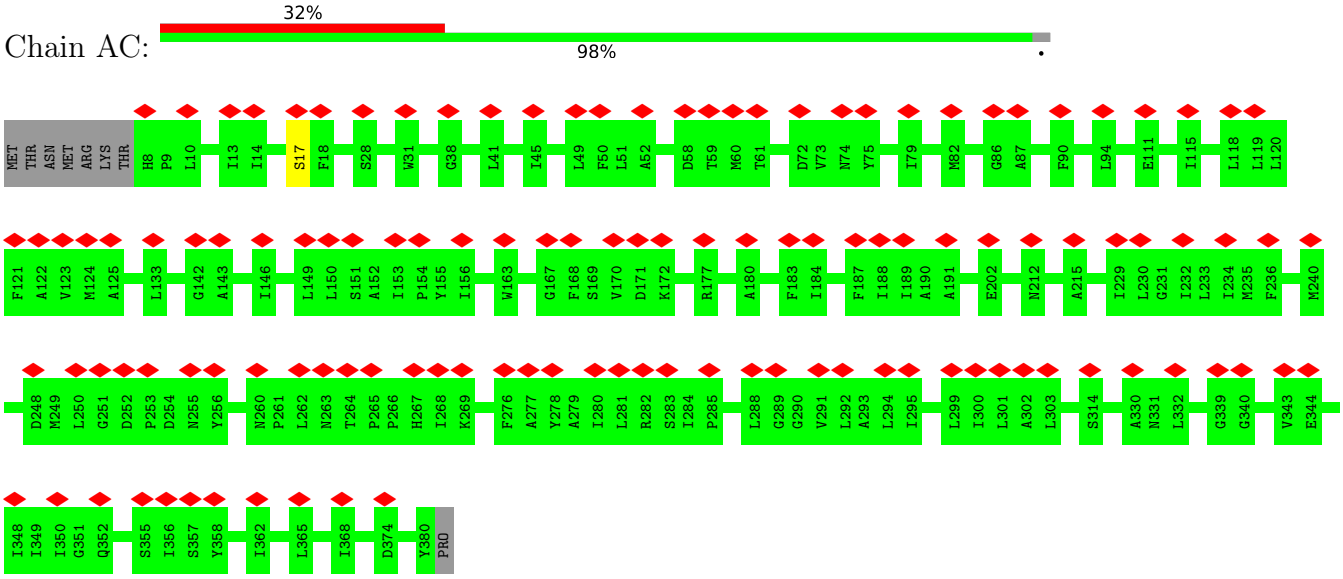
Chain Ab:





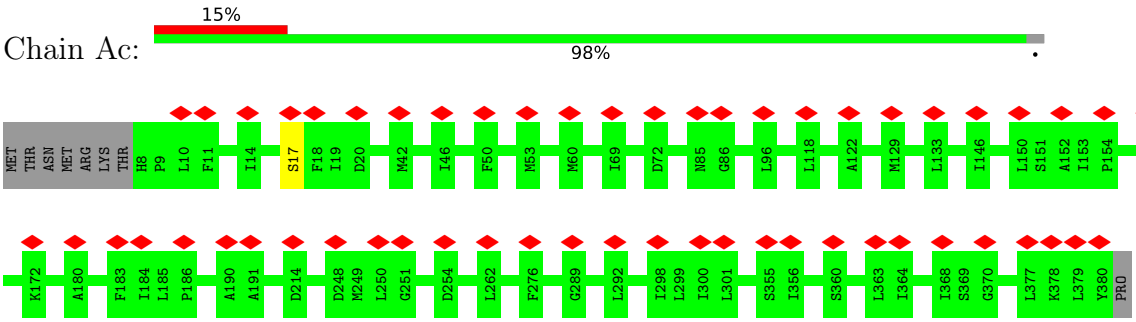
• Molecule 47: Cytochrome b

Chain AC:



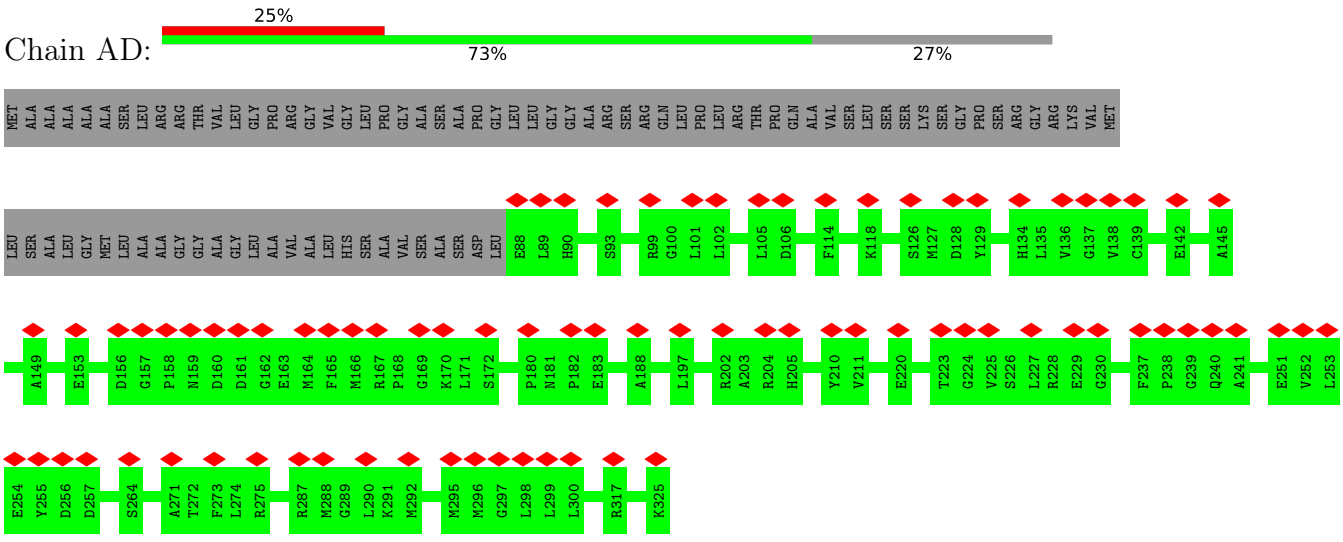
• Molecule 47: Cytochrome b

Chain Ac:



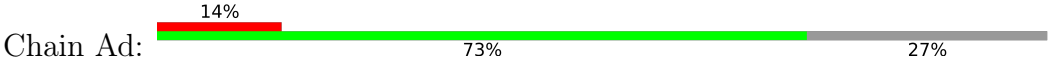
• Molecule 48: Cytochrome c1, heme protein, mitochondrial

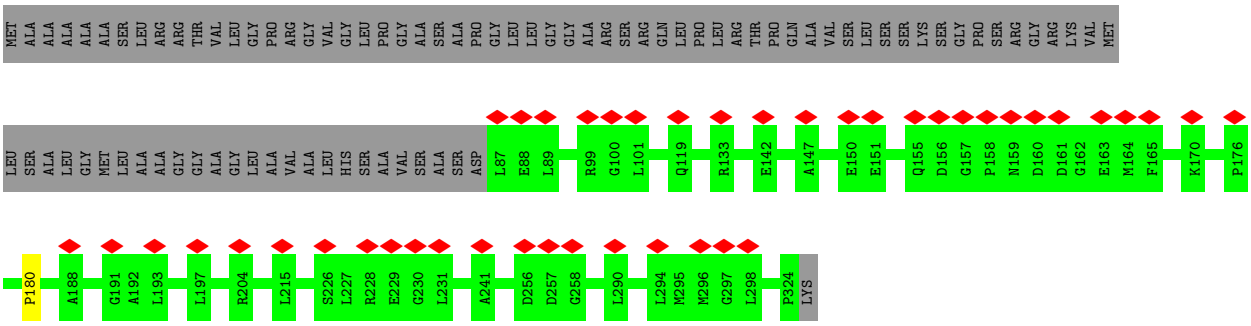
Chain AD:



• Molecule 48: Cytochrome c1, heme protein, mitochondrial

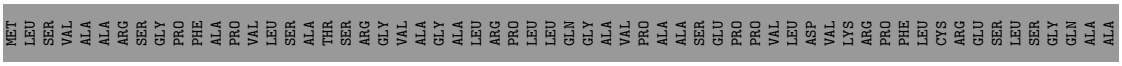
Chain Ad:

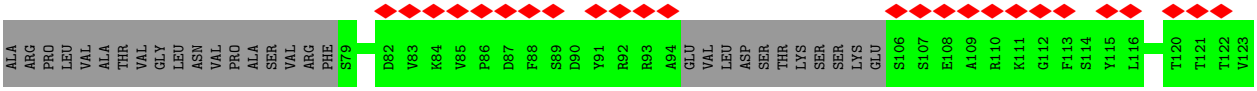


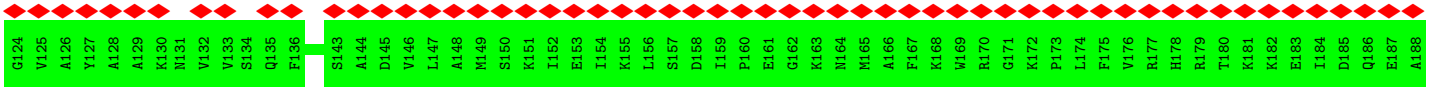


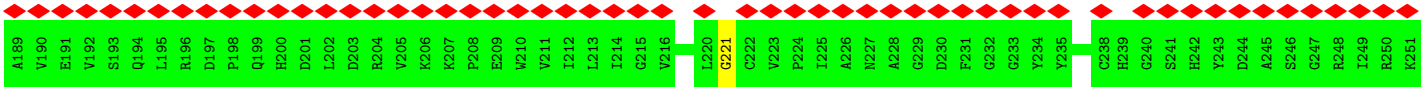
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

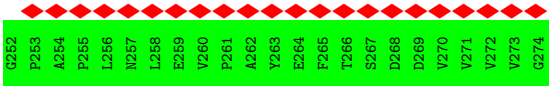
Chain AE:





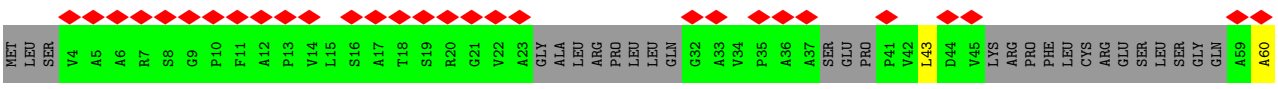


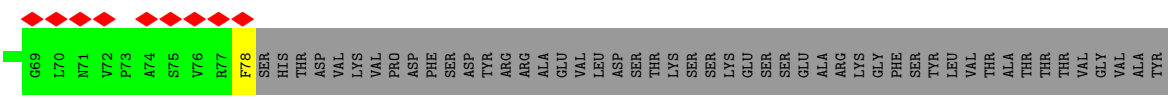


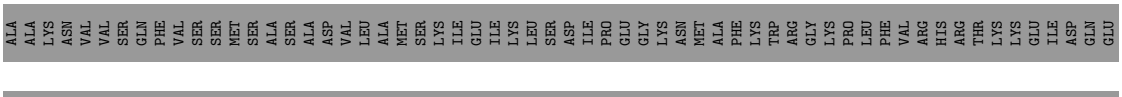


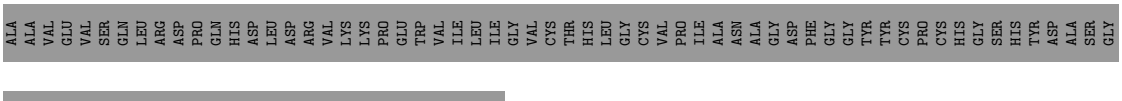
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



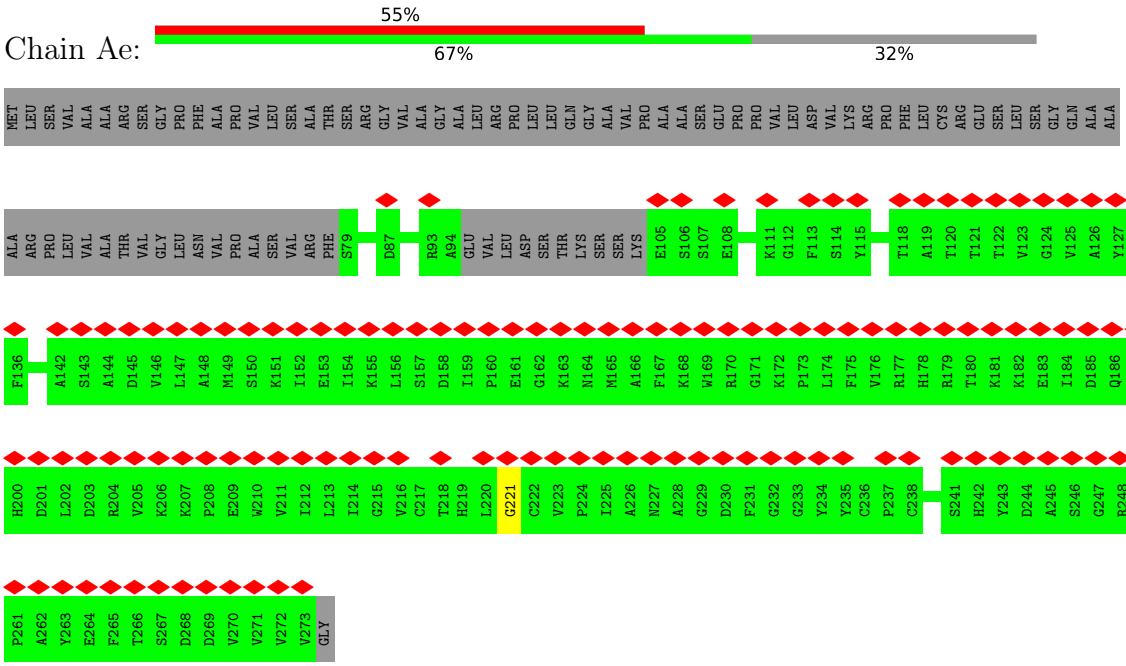






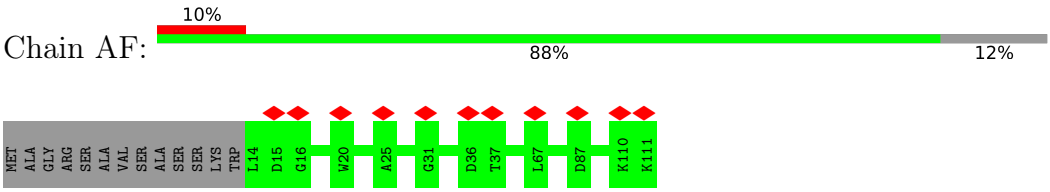
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



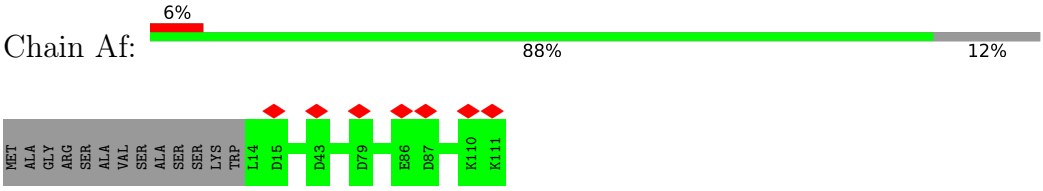
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain AF:



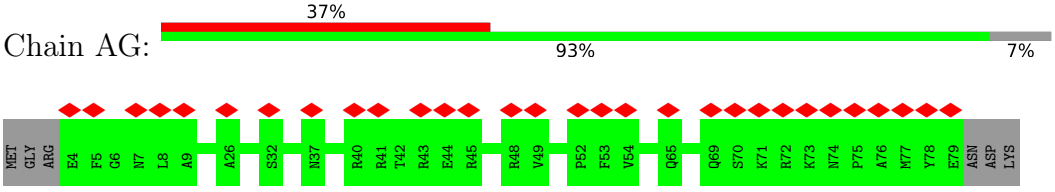
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain Af:



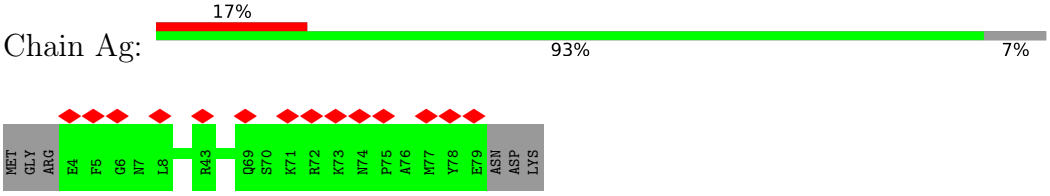
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain AG:



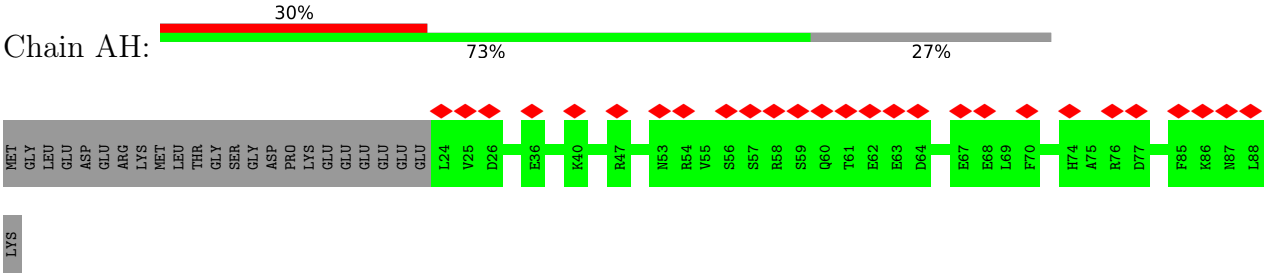
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain Ag:



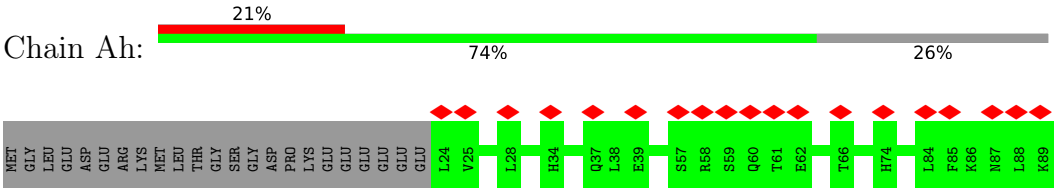
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH:



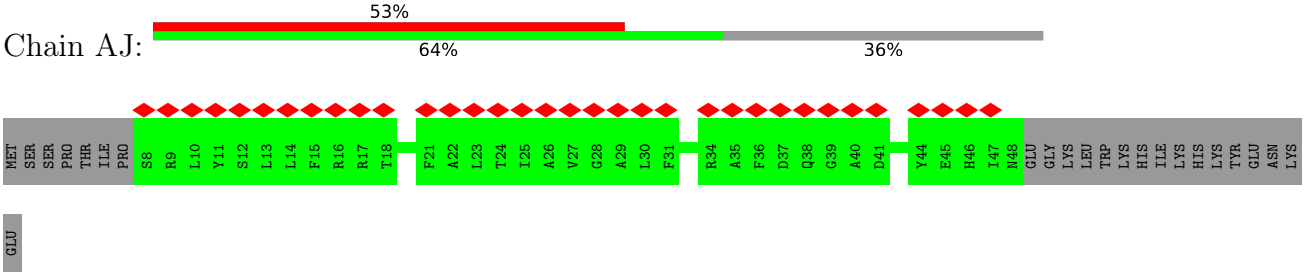
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:



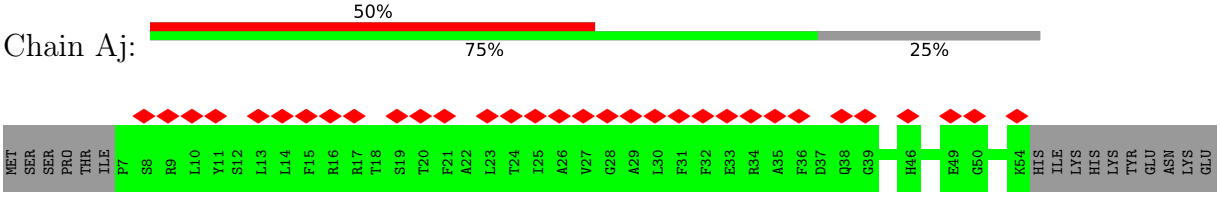
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ:



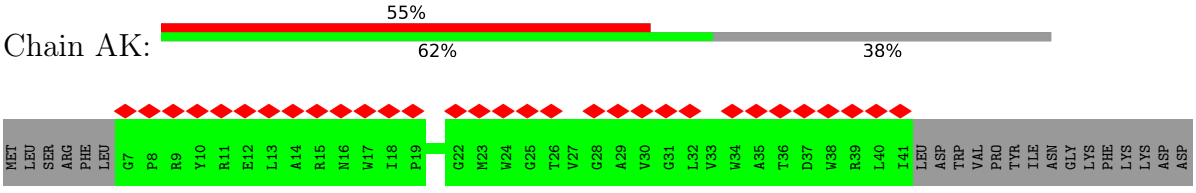
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



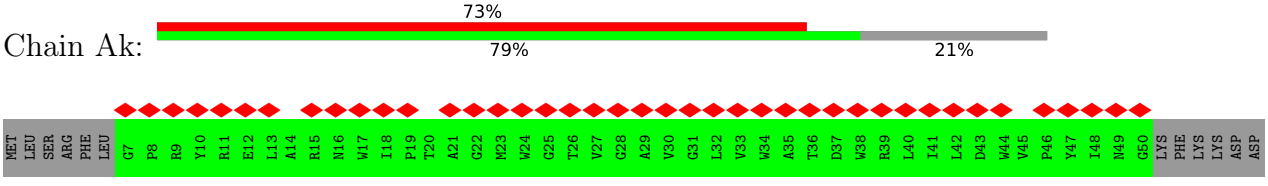
• Molecule 54: Cytochrome b-c1 complex subunit 10

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	49613	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 ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	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

5.1 Standard geometry

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

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	0.54	0/774	0.79	0/1056
2	B	0.63	0/1289	0.94	5/1744 (0.3%)
3	C	0.55	0/1687	0.81	1/2297 (0.0%)
4	D	0.63	3/3504 (0.1%)	0.84	6/4747 (0.1%)
5	E	0.56	2/1675 (0.1%)	0.83	6/2282 (0.3%)
6	F	0.65	5/3363 (0.1%)	0.89	8/4543 (0.2%)
7	G	0.65	5/5374 (0.1%)	0.99	19/7281 (0.3%)
8	H	0.68	3/2585 (0.1%)	0.90	9/3529 (0.3%)
9	I	0.63	1/1427 (0.1%)	0.89	2/1927 (0.1%)
10	J	0.53	0/1233	0.77	1/1672 (0.1%)
11	K	0.59	0/740	0.83	2/1005 (0.2%)
12	L	0.69	5/4921 (0.1%)	0.91	19/6696 (0.3%)
13	M	0.69	4/3709 (0.1%)	0.89	10/5052 (0.2%)
14	N	0.71	4/2756 (0.1%)	0.91	8/3751 (0.2%)
15	O	0.78	7/2666 (0.3%)	0.92	18/3615 (0.5%)
16	P	0.61	2/2804 (0.1%)	0.82	9/3802 (0.2%)
17	Q	0.58	1/980 (0.1%)	0.80	4/1324 (0.3%)
18	R	0.72	1/671 (0.1%)	0.74	1/903 (0.1%)
19	S	0.83	2/678 (0.3%)	1.08	5/915 (0.5%)
20	T	0.75	1/613 (0.2%)	0.90	4/826 (0.5%)
20	U	0.61	0/690	0.90	3/931 (0.3%)
21	V	0.56	0/937	0.85	4/1270 (0.3%)
22	W	0.53	0/993	0.72	0/1335
23	X	0.60	1/1422 (0.1%)	0.88	7/1921 (0.4%)
24	Y	0.53	0/1054	0.59	0/1429
25	Z	0.50	0/1183	0.62	0/1597
26	a	0.54	0/561	0.86	2/755 (0.3%)
27	b	0.47	0/651	0.53	0/895
28	c	0.81	1/400 (0.2%)	0.95	3/544 (0.6%)
29	d	0.77	2/1020 (0.2%)	0.74	5/1377 (0.4%)
30	e	0.44	0/885	0.60	0/1178
31	f	0.59	0/488	0.81	3/657 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.67	1/886 (0.1%)	0.92	3/1207 (0.2%)
33	h	0.54	1/1181 (0.1%)	0.79	0/1599
34	i	0.52	0/823	0.76	1/1119 (0.1%)
35	j	0.56	0/588	0.82	2/805 (0.2%)
36	k	0.58	0/587	0.80	1/794 (0.1%)
37	l	0.68	2/1384 (0.1%)	0.76	2/1889 (0.1%)
38	m	0.54	0/1083	0.73	0/1468
39	n	0.62	1/1596 (0.1%)	0.79	3/2162 (0.1%)
40	o	0.52	0/1052	0.72	3/1411 (0.2%)
41	p	0.50	0/1471	0.73	3/1988 (0.2%)
42	q	0.77	2/1037 (0.2%)	0.97	5/1408 (0.4%)
43	r	0.73	1/426 (0.2%)	0.98	1/573 (0.2%)
44	s	0.64	0/116	1.01	1/157 (0.6%)
45	AA	0.41	0/3187	0.61	0/4320
45	Aa	0.42	0/3288	0.61	1/4462 (0.0%)
46	AB	0.35	0/3187	0.58	1/4308 (0.0%)
46	Ab	0.36	0/3187	0.56	0/4308
47	AC	0.35	0/3089	0.55	1/4221 (0.0%)
47	Ac	0.36	0/3089	0.56	1/4221 (0.0%)
48	AD	0.38	0/1955	0.53	0/2655
48	Ad	0.44	1/1954 (0.1%)	0.55	0/2655
49	AE	0.47	0/1459	0.63	1/1976 (0.1%)
49	AI	0.47	0/349	0.73	3/476 (0.6%)
49	Ae	0.47	0/1464	0.63	1/1983 (0.1%)
50	AF	0.32	0/884	0.50	0/1184
50	Af	0.32	0/884	0.50	0/1184
51	AG	0.37	0/662	0.55	0/895
51	Ag	0.42	0/662	0.53	0/895
52	AH	0.34	0/542	0.61	0/728
52	Ah	0.44	0/551	0.60	0/739
53	AJ	0.35	0/339	0.48	0/457
53	Aj	0.42	0/402	0.61	0/541
54	AK	0.31	0/291	0.49	0/399
54	Ak	0.41	0/371	0.55	0/511
All	All	0.57	59/97759 (0.1%)	0.78	198/132554 (0.1%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	247	PRO	N-CD	16.59	1.71	1.47
18	R	89	PRO	N-CD	-15.12	1.26	1.47
29	d	115	PRO	N-CD	-14.05	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	265	PRO	N-CD	13.77	1.67	1.47
14	N	255	PRO	N-CD	-13.61	1.28	1.47
42	q	139	PRO	N-CD	-13.51	1.28	1.47
28	c	39	PRO	N-CD	-13.39	1.29	1.47
16	P	371	PRO	N-CD	12.85	1.65	1.47
7	G	532	PRO	N-CD	-12.59	1.30	1.47
15	O	315	PRO	N-CD	-12.12	1.30	1.47
19	S	28	PRO	N-CD	-11.98	1.31	1.47
20	T	141	PRO	N-CD	11.68	1.64	1.47
12	L	234	PRO	N-CD	11.10	1.63	1.47
14	N	123	PRO	N-CD	-10.99	1.32	1.47
8	H	42	PRO	N-CD	10.80	1.62	1.47
13	M	370	PRO	N-CD	-10.62	1.32	1.47
15	O	210	PRO	N-CD	-10.56	1.33	1.47
15	O	224	PRO	N-CD	-10.29	1.33	1.47
23	X	152	PRO	N-CD	-10.21	1.33	1.47
6	F	227	PRO	N-CD	9.98	1.61	1.47
32	g	78	PRO	N-CD	-9.59	1.34	1.47
16	P	290	PRO	N-CD	9.55	1.61	1.47
7	G	275	PRO	N-CD	-9.55	1.34	1.47
29	d	15	PRO	N-CD	-9.48	1.34	1.47
8	H	75	PRO	N-CD	9.20	1.60	1.47
6	F	319	PRO	N-CD	9.04	1.60	1.47
15	O	212	PRO	N-CD	-8.96	1.35	1.47
13	M	20	PRO	N-CD	8.53	1.59	1.47
4	D	163	PRO	N-CD	-8.51	1.35	1.47
9	I	107	PRO	N-CD	8.48	1.59	1.47
12	L	212	PRO	N-CD	-8.35	1.36	1.47
48	Ad	180	PRO	N-CD	-8.24	1.36	1.47
39	n	155	PRO	N-CD	8.02	1.59	1.47
4	D	352	PRO	N-CD	-7.97	1.36	1.47
19	S	63	PRO	N-CD	-7.96	1.36	1.47
43	r	111	PRO	N-CD	-7.51	1.37	1.47
37	l	104	PRO	N-CD	-7.29	1.37	1.47
14	N	238	PRO	N-CD	-7.15	1.37	1.47
13	M	208	PRO	N-CD	7.04	1.57	1.47
14	N	147	PRO	N-CD	-6.84	1.38	1.47
7	G	541	PRO	N-CD	-6.82	1.38	1.47
6	F	234	GLY	CA-C	-6.76	1.41	1.51
7	G	449	PRO	N-CD	6.75	1.57	1.47
12	L	384	PRO	N-CD	6.34	1.56	1.47
6	F	384	PRO	N-CD	-6.19	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	93	PRO	N-CD	-5.99	1.39	1.47
37	l	45	PRO	N-CD	-5.90	1.39	1.47
6	F	235	VAL	N-CA	-5.84	1.34	1.46
12	L	112	PRO	N-CD	5.82	1.56	1.47
15	O	87	PRO	N-CD	-5.78	1.39	1.47
8	H	60	PRO	N-CD	5.70	1.55	1.47
13	M	252	PRO	N-CD	-5.68	1.40	1.47
5	E	80	PRO	N-CD	5.62	1.55	1.47
7	G	683	PRO	N-CD	-5.50	1.40	1.47
15	O	103	PRO	N-CD	-5.39	1.40	1.47
42	q	126	PRO	N-CD	5.32	1.55	1.47
17	Q	53	ILE	C-O	5.31	1.33	1.23
33	h	174	PRO	N-CD	-5.22	1.40	1.47
4	D	63	PRO	N-CD	-5.11	1.40	1.47

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	83	MET	O-C-N	11.12	140.50	122.70
26	a	3	PHE	CB-CA-C	-10.42	89.56	110.40
14	N	255	PRO	CA-N-CD	9.91	125.58	111.70
15	O	206	TYR	N-CA-CB	-9.89	92.81	110.60
42	q	139	PRO	CA-N-CD	9.58	125.12	111.70
29	d	115	PRO	CA-N-CD	9.56	125.08	111.70
4	D	142	VAL	N-CA-CB	9.50	132.39	111.50
15	O	247	PRO	N-CA-CB	9.16	114.29	103.30
5	E	219	SER	N-CA-CB	9.05	124.07	110.50
6	F	334	THR	N-CA-CB	8.92	127.25	110.30
35	j	82	GLY	N-CA-C	-8.83	91.03	113.10
15	O	315	PRO	CA-N-CD	8.74	123.93	111.70
15	O	247	PRO	CA-N-CD	-8.73	99.27	111.50
15	O	83	MET	C-N-CA	-8.66	100.06	121.70
15	O	83	MET	CA-C-N	-8.57	98.35	117.20
7	G	532	PRO	CA-N-CD	8.53	123.64	111.70
28	c	39	PRO	CA-N-CD	8.15	123.11	111.70
7	G	174	THR	N-CA-C	-8.12	89.08	111.00
19	S	28	PRO	CA-N-CD	8.12	123.06	111.70
17	Q	60	ASP	N-CA-C	-7.67	90.30	111.00
6	F	411	SER	N-CA-CB	7.54	121.81	110.50
23	X	55	ARG	N-CA-CB	-7.42	97.24	110.60
12	L	265	PRO	CA-N-CD	-7.41	101.13	111.50
15	O	210	PRO	CA-N-CD	7.36	122.01	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	255	PRO	N-CA-CB	-7.26	94.58	103.30
7	G	204	MET	N-CA-C	-7.25	91.43	111.00
2	B	121	PHE	CB-CA-C	7.14	124.69	110.40
16	P	371	PRO	N-CA-CB	7.11	111.84	103.30
32	g	78	PRO	CA-N-CD	7.08	121.61	111.70
6	F	332	CYS	N-CA-C	7.07	130.09	111.00
23	X	55	ARG	N-CA-C	7.06	130.06	111.00
39	n	165	PRO	N-CA-C	7.06	130.45	112.10
12	L	265	PRO	N-CA-CB	6.96	111.66	103.30
8	H	311	THR	N-CA-CB	6.95	123.50	110.30
16	P	369	THR	N-CA-CB	6.95	123.50	110.30
28	c	47	SER	N-CA-CB	6.91	120.87	110.50
15	O	224	PRO	CA-N-CD	6.88	121.34	111.70
4	D	142	VAL	N-CA-C	-6.84	92.53	111.00
29	d	115	PRO	N-CA-CB	-6.83	95.09	102.60
13	M	213	HIS	CB-CA-C	-6.76	96.88	110.40
23	X	152	PRO	CA-N-CD	6.71	121.10	111.70
41	p	128	GLU	N-CA-CB	-6.69	98.56	110.60
28	c	39	PRO	N-CA-CB	-6.65	95.28	102.60
7	G	275	PRO	CA-N-CD	6.62	120.97	111.70
7	G	300	GLN	N-CA-CB	6.61	122.50	110.60
15	O	320	GLY	N-CA-C	-6.59	96.63	113.10
16	P	106	LEU	N-CA-C	6.59	128.79	111.00
23	X	36	CYS	CB-CA-C	-6.58	97.25	110.40
5	E	64	ALA	N-CA-CB	6.57	119.29	110.10
29	d	15	PRO	CA-N-CD	6.56	120.88	111.70
5	E	166	LYS	CB-CA-C	6.54	123.47	110.40
31	f	51	ASN	CB-CA-C	-6.53	97.35	110.40
8	H	214	GLU	N-CA-CB	-6.51	98.89	110.60
36	k	59	TYR	N-CA-CB	-6.50	98.90	110.60
6	F	125	CYS	N-CA-C	-6.50	93.46	111.00
16	P	360	ARG	N-CA-CB	-6.44	99.02	110.60
42	q	139	PRO	N-CA-CB	-6.39	95.57	102.60
8	H	52	ALA	N-CA-CB	6.38	119.03	110.10
4	D	427	PRO	N-CA-C	-6.34	95.62	112.10
9	I	154	TYR	N-CA-CB	-6.34	99.19	110.60
39	n	115	TYR	N-CA-CB	6.33	122.00	110.60
16	P	371	PRO	CA-N-CD	-6.33	102.64	111.50
14	N	255	PRO	N-CA-C	6.31	128.50	112.10
13	M	370	PRO	N-CA-C	6.31	128.50	112.10
8	H	196	ALA	N-CA-C	6.29	127.99	111.00
13	M	424	ILE	N-CA-C	-6.29	94.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	71	ALA	N-CA-CB	-6.25	101.34	110.10
44	s	86	ASP	N-CA-CB	6.24	121.84	110.60
13	M	370	PRO	CA-N-CD	6.20	120.38	111.70
16	P	139	PHE	N-CA-CB	6.17	121.72	110.60
4	D	140	ASP	CB-CA-C	-6.17	98.06	110.40
32	g	137	SER	N-CA-CB	-6.16	101.27	110.50
23	X	36	CYS	CA-CB-SG	6.14	125.06	114.00
14	N	81	LEU	N-CA-C	-6.13	94.44	111.00
20	T	141	PRO	N-CA-CB	6.13	110.66	103.30
20	T	141	PRO	CA-N-CD	-6.12	102.92	111.50
23	X	110	CYS	CA-CB-SG	6.11	125.00	114.00
7	G	212	LYS	N-CA-C	-6.06	94.63	111.00
7	G	133	GLN	N-CA-CB	6.05	121.48	110.60
12	L	231	PRO	N-CA-C	6.02	127.76	112.10
12	L	234	PRO	CA-N-CD	-6.02	103.07	111.50
12	L	605	ASN	N-CA-CB	5.99	121.39	110.60
42	q	69	ASN	N-CA-CB	5.99	121.39	110.60
15	O	315	PRO	N-CA-CB	-5.98	96.02	102.60
12	L	276	THR	N-CA-CB	5.96	121.62	110.30
14	N	218	ALA	N-CA-CB	5.93	118.41	110.10
12	L	554	ASP	N-CA-CB	5.88	121.19	110.60
12	L	483	PRO	N-CA-C	-5.88	96.81	112.10
7	G	389	THR	N-CA-CB	5.87	121.46	110.30
5	E	50	THR	N-CA-CB	5.87	121.45	110.30
7	G	251	ILE	N-CA-C	5.86	126.83	111.00
45	Aa	261	ALA	N-CA-C	-5.85	95.20	111.00
31	f	52	GLU	N-CA-CB	5.83	121.10	110.60
49	AI	60	ALA	N-CA-CB	-5.83	101.94	110.10
6	F	103	ASN	N-CA-CB	5.82	121.08	110.60
19	S	63	PRO	CA-N-CD	5.80	119.82	111.70
20	T	135	ALA	N-CA-CB	5.79	118.21	110.10
5	E	68	ASN	N-CA-CB	5.79	121.02	110.60
20	U	150	ASP	CB-CA-C	5.76	121.93	110.40
13	M	455	THR	N-CA-C	-5.76	95.44	111.00
11	K	83	ASN	N-CA-CB	5.75	120.95	110.60
7	G	510	TRP	N-CA-CB	5.74	120.93	110.60
13	M	223	ALA	N-CA-CB	5.74	118.13	110.10
14	N	123	PRO	CA-N-CD	5.72	119.71	111.70
29	d	15	PRO	N-CA-CB	-5.71	96.32	102.60
12	L	526	LEU	N-CA-CB	-5.70	99.00	110.40
8	H	223	PHE	CB-CA-C	-5.68	99.05	110.40
47	Ac	17	SER	N-CA-CB	-5.66	102.01	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	119	THR	N-CA-C	-5.64	95.76	111.00
12	L	415	ALA	N-CA-CB	5.63	117.99	110.10
17	Q	141	ASN	N-CA-CB	5.63	120.74	110.60
14	N	89	GLN	N-CA-CB	-5.63	100.47	110.60
7	G	599	THR	N-CA-C	5.63	126.19	111.00
21	V	57	ASP	N-CA-CB	5.61	120.70	110.60
47	AC	17	SER	N-CA-CB	-5.61	102.09	110.50
7	G	580	ALA	N-CA-CB	5.57	117.90	110.10
15	O	118	TYR	N-CA-CB	-5.56	100.59	110.60
3	C	125	PHE	N-CA-CB	-5.55	100.61	110.60
17	Q	163	ASN	CB-CA-C	-5.55	99.30	110.40
23	X	152	PRO	N-CA-CB	-5.53	96.52	102.60
40	o	118	LYS	N-CA-CB	5.53	120.55	110.60
15	O	118	TYR	N-CA-C	5.53	125.92	111.00
8	H	252	PRO	CA-N-CD	5.52	119.43	111.70
49	Ae	221	GLY	N-CA-C	5.51	126.87	113.10
8	H	212	ASN	N-CA-CB	5.50	120.50	110.60
49	AE	221	GLY	N-CA-C	5.50	126.85	113.10
21	V	19	THR	N-CA-CB	5.48	120.72	110.30
9	I	160	GLU	N-CA-CB	-5.46	100.77	110.60
7	G	389	THR	N-CA-C	-5.46	96.26	111.00
12	L	582	GLY	N-CA-C	-5.45	99.47	113.10
16	P	367	GLU	CB-CA-C	-5.45	99.51	110.40
15	O	212	PRO	N-CA-C	5.44	126.24	112.10
39	n	136	GLU	CB-CA-C	5.43	121.26	110.40
43	r	111	PRO	CA-N-CD	5.42	119.29	111.70
7	G	651	PRO	CB-CA-C	-5.41	98.48	112.00
42	q	67	GLU	CB-CA-C	-5.40	99.60	110.40
2	B	195	PRO	N-CA-C	-5.39	98.10	112.10
6	F	457	HIS	N-CA-CB	-5.38	100.91	110.60
49	AI	60	ALA	N-CA-C	5.37	125.51	111.00
4	D	140	ASP	N-CA-C	-5.36	96.54	111.00
19	S	28	PRO	N-CA-CB	-5.35	96.71	102.60
15	O	152	SER	N-CA-CB	5.35	118.53	110.50
19	S	39	GLN	N-CA-C	5.35	125.45	111.00
7	G	362	ASP	N-CA-C	5.35	125.44	111.00
21	V	114	TRP	N-CA-CB	5.35	120.22	110.60
8	H	139	THR	N-CA-CB	5.34	120.44	110.30
13	M	276	CYS	N-CA-CB	5.33	120.20	110.60
12	L	151	SER	N-CA-CB	5.33	118.49	110.50
6	F	418	GLN	N-CA-CB	5.32	120.18	110.60
15	O	224	PRO	N-CA-CB	-5.32	96.75	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	218	ARG	CB-CA-C	-5.31	99.78	110.40
34	i	105	PHE	N-CA-CB	-5.31	101.05	110.60
12	L	194	ASN	N-CA-C	5.30	125.31	111.00
12	L	234	PRO	N-CA-CB	5.30	109.66	103.30
10	J	128	VAL	CB-CA-C	-5.29	101.35	111.40
19	S	40	ARG	N-CA-CB	-5.28	101.09	110.60
11	K	70	GLU	N-CA-CB	5.26	120.07	110.60
15	O	212	PRO	CA-N-CD	5.25	119.04	111.70
12	L	212	PRO	N-CA-C	5.24	125.73	112.10
12	L	248	HIS	CB-CA-C	5.24	120.88	110.40
13	M	423	MET	N-CA-C	-5.24	96.86	111.00
35	j	102	ASP	CB-CG-OD2	5.24	123.01	118.30
13	M	330	ALA	N-CA-CB	5.23	117.43	110.10
46	AB	305	THR	N-CA-CB	-5.23	100.36	110.30
29	d	113	LEU	N-CA-CB	-5.23	99.94	110.40
12	L	212	PRO	CA-N-CD	5.22	119.01	111.70
7	G	640	ASP	N-CA-CB	5.21	119.98	110.60
2	B	153	PRO	CB-CA-C	-5.21	98.98	112.00
12	L	277	MET	CB-CA-C	-5.20	100.00	110.40
41	p	128	GLU	N-CA-C	5.20	125.04	111.00
8	H	51	ASP	CB-CA-C	-5.20	100.01	110.40
18	R	89	PRO	CA-N-CD	5.18	118.95	111.70
41	p	94	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	94	THR	CA-CB-CG2	-5.16	105.18	112.40
40	o	117	LEU	CB-CA-C	-5.14	100.43	110.20
37	l	104	PRO	CA-N-CD	5.14	118.89	111.70
16	P	361	TRP	N-CA-CB	5.12	119.82	110.60
31	f	53	GLU	N-CA-CB	-5.12	101.39	110.60
16	P	368	GLU	N-CA-CB	5.12	119.81	110.60
20	U	153	ASP	CB-CA-C	5.11	120.63	110.40
26	a	4	GLU	N-CA-C	5.11	124.81	111.00
12	L	247	LEU	N-CA-CB	5.10	120.60	110.40
13	M	83	HIS	N-CA-C	-5.10	97.23	111.00
17	Q	164	PHE	N-CA-CB	5.10	119.78	110.60
6	F	228	PRO	N-CA-C	-5.09	98.88	112.10
15	O	207	ILE	N-CA-C	-5.08	97.28	111.00
4	D	352	PRO	CA-N-CD	5.07	118.80	111.70
40	o	118	LYS	N-CA-C	-5.07	97.31	111.00
7	G	77	MET	N-CA-C	-5.07	97.31	111.00
32	g	78	PRO	N-CA-CB	-5.06	97.03	102.60
7	G	668	ALA	N-CA-CB	5.05	117.17	110.10
49	AI	43	LEU	CB-CG-CD1	-5.05	102.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	228	ASN	N-CA-CB	5.04	119.68	110.60
42	q	142	THR	N-CA-CB	5.04	119.87	110.30
20	U	153	ASP	N-CA-CB	-5.04	101.54	110.60
21	V	86	LYS	N-CA-CB	5.03	119.66	110.60
7	G	532	PRO	N-CA-CB	-5.01	97.08	102.60
20	T	139	MET	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	22	59
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	420/463 (91%)	391 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	37	72
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	153/172 (89%)	144 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	L	604/607 (100%)	573 (95%)	30 (5%)	1 (0%)	44 78
13	M	456/459 (99%)	438 (96%)	18 (4%)	0	100 100
14	N	342/345 (99%)	330 (96%)	11 (3%)	1 (0%)	37 72
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100 100
16	P	338/377 (90%)	317 (94%)	21 (6%)	0	100 100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100 100
18	R	81/116 (70%)	77 (95%)	4 (5%)	0	100 100
19	S	81/99 (82%)	78 (96%)	3 (4%)	0	100 100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100 100
20	U	82/156 (53%)	76 (93%)	6 (7%)	0	100 100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100 100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100 100
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100 100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100 100
25	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100 100
26	a	65/70 (93%)	57 (88%)	8 (12%)	0	100 100
27	b	78/84 (93%)	68 (87%)	10 (13%)	0	100 100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100 100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100 100
30	e	102/106 (96%)	97 (95%)	5 (5%)	0	100 100
31	f	53/57 (93%)	50 (94%)	3 (6%)	0	100 100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100 100
33	h	134/189 (71%)	127 (95%)	7 (5%)	0	100 100
34	i	90/128 (70%)	76 (84%)	13 (14%)	1 (1%)	12 46
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100 100
36	k	69/104 (66%)	67 (97%)	2 (3%)	0	100 100
37	l	156/186 (84%)	143 (92%)	13 (8%)	0	100 100
38	m	125/129 (97%)	117 (94%)	8 (6%)	0	100 100
39	n	176/179 (98%)	162 (92%)	13 (7%)	1 (1%)	22 59
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100 100
41	p	168/176 (96%)	153 (91%)	15 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	12/104 (12%)	12 (100%)	0	0	100	100
45	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
45	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
46	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
46	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
49	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
49	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
49	Ae	181/274 (66%)	166 (92%)	15 (8%)	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%)	73 (99%)	1 (1%)	0	100	100
52	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
52	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
54	AK	33/56 (59%)	33 (100%)	0	0	100	100
54	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	11769/14118 (83%)	11186 (95%)	577 (5%)	6 (0%)	50	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
14	N	109	ALA
34	i	124	PRO
2	B	195	PRO
39	n	156	PRO

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Mol	Chain	Res	Type
12	L	518	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	85
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	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	127/138 (92%)	127 (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	414/415 (100%)	414 (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	297/325 (91%)	297 (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	78/135 (58%)	78 (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%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (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	71/73 (97%)	71 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	51/53 (96%)	51 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	121/162 (75%)	121 (100%)	0	100	100
34	i	89/120 (74%)	89 (100%)	0	100	100
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	110/121 (91%)	110 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	108/131 (82%)	108 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	14/95 (15%)	14 (100%)	0	100	100
45	AA	338/398 (85%)	338 (100%)	0	100	100
45	Aa	349/398 (88%)	349 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	328 (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	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	203 (100%)	0	100	100
49	AE	155/224 (69%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	AI	34/224 (15%)	33 (97%)	1 (3%)	37 58
49	Ae	156/224 (70%)	156 (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	62/83 (75%)	62 (100%)	0	100 100
52	Ah	63/83 (76%)	63 (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	26/46 (56%)	26 (100%)	0	100 100
54	Ak	34/46 (74%)	34 (100%)	0	100 100
All	All	10334/12037 (86%)	10332 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR
49	AI	78	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	36	GLN
4	D	117	HIS

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Mol	Chain	Res	Type
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	233	HIS
4	D	265	ASN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	277	ASN
6	F	346	GLN
6	F	441	HIS
7	G	59	GLN
7	G	74	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	406	ASN
7	G	444	HIS
7	G	495	ASN
7	G	514	ASN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	169	GLN
8	H	171	HIS
8	H	292	ASN
10	J	3	ASN
10	J	107	ASN
11	K	7	ASN
12	L	2	ASN
12	L	25	ASN
12	L	56	HIS

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Mol	Chain	Res	Type
12	L	102	GLN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	296	ASN
12	L	321	GLN
12	L	328	HIS
12	L	332	HIS
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	ASN
12	L	517	ASN
12	L	579	ASN
13	M	26	ASN
13	M	44	GLN
13	M	51	ASN
13	M	81	GLN
13	M	92	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
13	M	415	GLN
14	N	120	GLN
14	N	150	ASN
14	N	204	ASN
14	N	273	ASN
15	O	132	GLN
15	O	175	ASN
15	O	235	GLN
15	O	292	HIS

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Mol	Chain	Res	Type
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	71	ASN
16	P	79	GLN
16	P	169	HIS
16	P	216	HIS
16	P	251	ASN
16	P	269	ASN
16	P	275	HIS
16	P	341	GLN
17	Q	51	GLN
17	Q	88	GLN
19	S	25	GLN
20	U	101	ASN
21	V	41	HIS
21	V	50	GLN
22	W	54	GLN
23	X	30	HIS
23	X	151	ASN
24	Y	19	GLN
24	Y	21	HIS
24	Y	91	ASN
26	a	58	ASN
27	b	69	HIS
27	b	83	ASN
29	d	59	HIS
30	e	34	HIS
31	f	5	GLN
31	f	10	HIS
31	f	13	HIS
32	g	52	GLN
33	h	170	GLN
33	h	181	HIS
34	i	83	HIS
35	j	83	HIS
36	k	39	GLN
36	k	66	ASN
37	l	31	HIS
37	l	91	GLN
37	l	106	HIS
37	l	154	GLN

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Mol	Chain	Res	Type
38	m	75	ASN
38	m	79	ASN
39	n	13	GLN
39	n	14	GLN
39	n	33	HIS
39	n	53	ASN
40	o	85	HIS
41	p	100	GLN
41	p	124	ASN
42	q	13	GLN
42	q	31	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS
43	r	21	GLN
43	r	110	GLN
44	s	84	ASN
45	AA	87	ASN
45	AA	103	ASN
45	AA	173	GLN
45	AA	207	ASN
45	AA	286	HIS
45	AA	342	GLN
45	AA	397	ASN
45	AA	402	HIS
46	AB	167	GLN
46	AB	304	ASN
46	AB	415	GLN
47	AC	201	HIS
47	AC	341	GLN
48	AD	189	ASN
48	AD	190	ASN
49	AE	131	ASN
49	AE	135	GLN
49	AE	242	HIS
54	AK	16	ASN
45	Aa	87	ASN
45	Aa	103	ASN
45	Aa	119	HIS
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	207	ASN

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Mol	Chain	Res	Type
46	Ab	284	ASN
46	Ab	290	GLN
46	Ab	291	HIS
46	Ab	304	ASN
46	Ab	415	GLN
47	Ac	148	ASN
47	Ac	312	GLN
47	Ac	341	GLN
48	Ad	115	GLN
48	Ad	155	GLN
48	Ad	190	ASN
49	Ae	131	ASN
49	Ae	135	GLN
49	Ae	242	HIS
51	Ag	24	GLN
52	Ah	60	GLN
52	Ah	82	HIS
53	Aj	48	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

Of 60 ligands modelled in this entry, 1 is monoatomic - leaving 59 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	$\#\|Z\| > 2$
55	3PE	M	502	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	4 (7%)
55	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
70	HEC	AD	401	48	32,50,50	2.16	10 (31%)	24,82,82	2.57	6 (25%)
69	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
55	3PE	L	701	-	41,41,50	0.99	2 (4%)	44,46,55	1.03	2 (4%)
62	CDL	X	201	-	66,66,99	1.09	4 (6%)	72,78,111	1.26	6 (8%)
55	3PE	L	703	-	50,50,50	0.90	2 (4%)	53,55,55	1.12	3 (5%)
55	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0
55	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
64	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.21	4 (7%)
68	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
69	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
55	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
55	3PE	M	501	-	50,50,50	0.91	2 (4%)	53,55,55	1.11	4 (7%)
56	SF4	I	304	9	0,12,12	-	-	-		
62	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
56	SF4	G	801	7	0,12,12	-	-	-		
58	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
67	HEM	AC	402	47	41,50,50	1.47	8 (19%)	45,82,82	2.43	16 (35%)
55	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
55	3PE	Y	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.14	3 (7%)
55	3PE	J	202	-	45,45,50	0.96	2 (4%)	48,50,55	1.06	3 (6%)
55	3PE	M	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
67	HEM	AC	401	47	41,50,50	1.36	5 (12%)	45,82,82	1.88	10 (22%)
61	UQ9	H	400	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
55	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
55	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
55	3PE	L	704	-	46,46,50	0.95	2 (4%)	49,51,55	1.08	3 (6%)
60	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
55	3PE	L	707	-	44,44,50	0.96	2 (4%)	47,49,55	1.08	3 (6%)
66	EHZ	n	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.85	11 (29%)
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
67	HEM	Ac	403	47	41,50,50	1.42	6 (14%)	45,82,82	1.84	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
59	FES	G	803	7	0,4,4	-	-	-		
68	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
62	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
58	PC1	J	201	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)
62	CDL	L	706	-	85,85,99	0.99	4 (4%)	91,97,111	1.13	5 (5%)
62	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
63	ADP	O	402	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
56	SF4	F	502	6	0,12,12	-	-	-		
56	SF4	G	802	7	0,12,12	-	-	-		
70	HEC	Ad	401	48	32,50,50	2.18	11 (34%)	24,82,82	2.45	6 (25%)
55	3PE	N	401	-	36,36,50	1.06	2 (5%)	39,41,55	1.18	4 (10%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
66	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
55	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
57	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
62	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
56	SF4	I	303	9	0,12,12	-	-	-		
62	CDL	L	705	-	76,76,99	1.02	4 (5%)	82,88,111	1.17	5 (6%)
59	FES	E	301	5	0,4,4	-	-	-		
71	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
55	3PE	L	702	-	39,39,50	1.03	2 (5%)	42,44,55	1.10	4 (9%)
67	HEM	Ac	402	47	41,50,50	1.42	6 (14%)	45,82,82	2.15	11 (24%)
55	3PE	O	401	-	30,30,50	1.16	2 (6%)	33,35,55	1.27	3 (9%)
56	SF4	B	301	2	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
55	3PE	M	502	-	-	14/54/54/54	-
55	3PE	I	301	-	-	17/54/54/54	-
70	HEC	AD	401	48	-	3/10/54/54	-
69	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3PE	L	701	-	-	13/45/45/54	-
62	CDL	X	201	-	-	27/77/77/110	-
55	3PE	L	703	-	-	13/54/54/54	-
55	3PE	Ac	401	-	-	10/26/26/54	-
55	3PE	Ac	404	-	-	8/38/38/54	-
64	NDP	P	401	-	-	6/30/77/77	0/5/5/5
68	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
55	3PE	AC	403	-	-	12/38/38/54	-
55	3PE	M	501	-	-	15/54/54/54	-
56	SF4	I	304	9	-	-	0/6/5/5
62	CDL	Ag	101	-	-	12/66/66/110	-
56	SF4	G	801	7	-	-	0/6/5/5
58	PC1	B	303	-	-	11/38/38/57	-
67	HEM	AC	402	47	-	4/12/54/54	-
55	3PE	A	401	-	-	14/49/49/54	-
55	3PE	Y	201	-	-	5/43/43/54	-
55	3PE	J	202	-	-	12/49/49/54	-
55	3PE	M	503	-	-	17/54/54/54	-
67	HEM	AC	401	47	-	6/12/54/54	-
61	UQ9	H	400	-	-	13/30/54/81	0/1/1/1
55	3PE	AF	201	-	-	9/45/45/54	-
55	3PE	Ag	102	-	-	5/42/42/54	-
55	3PE	L	704	-	-	13/50/50/54	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
55	3PE	L	707	-	-	13/48/48/54	-
66	EHZ	n	201	-	-	21/39/39/45	-
62	CDL	a	101	-	-	14/67/67/110	-
67	HEM	Ac	403	47	-	8/12/54/54	-
58	PC1	I	302	-	-	13/50/50/57	-
68	U10	AC	404	-	-	0/15/39/87	0/1/1/1
59	FES	G	803	7	-	-	0/1/1/1
62	CDL	Ac	407	-	-	11/52/52/110	-
58	PC1	J	201	-	-	14/45/45/57	-
62	CDL	L	706	-	-	27/96/96/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	CDL	AC	406	-	-	18/66/66/110	-
63	ADP	O	402	-	-	4/12/32/32	0/3/3/3
71	3PH	Ad	402	-	-	8/37/37/49	-
70	HEC	Ad	401	48	-	2/10/54/54	-
56	SF4	F	502	6	-	-	0/6/5/5
55	3PE	N	401	-	-	8/40/40/54	-
56	SF4	G	802	7	-	-	0/6/5/5
62	CDL	h	201	-	-	23/80/80/110	-
66	EHZ	W	201	-	-	22/39/39/45	-
55	3PE	b	201	-	-	8/49/49/54	-
57	UQ1	B	302	-	-	3/9/33/33	0/1/1/1
62	CDL	Aa	501	-	-	16/56/56/110	-
56	SF4	I	303	9	-	-	0/6/5/5
62	CDL	L	705	-	-	24/87/87/110	-
71	3PH	AD	402	-	-	8/37/37/49	-
59	FES	E	301	5	-	-	0/1/1/1
55	3PE	L	702	-	-	8/43/43/54	-
67	HEM	Ac	402	47	-	3/12/54/54	-
55	3PE	O	401	-	-	10/34/34/54	-
56	SF4	B	301	2	-	-	0/6/5/5

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	404	U10	C6-C1	7.59	1.49	1.35
68	Ac	405	U10	C6-C1	7.42	1.48	1.35
70	Ad	401	HEC	C3C-C2C	6.23	1.47	1.40
69	AC	405	UQ6	C2-C3	5.95	1.49	1.39
69	Ac	406	UQ6	C2-C3	5.90	1.49	1.39
69	Ac	406	UQ6	C5-C4	5.87	1.48	1.39
69	Ac	406	UQ6	C5-C6	5.87	1.49	1.40
70	AD	401	HEC	C2B-C3B	5.76	1.46	1.40
69	AC	405	UQ6	C5-C4	5.67	1.48	1.39
70	Ad	401	HEC	C2B-C3B	5.65	1.46	1.40
69	AC	405	UQ6	C5-C6	5.60	1.48	1.40
69	AC	405	UQ6	C6-C1	5.57	1.49	1.40
69	Ac	406	UQ6	C6-C1	5.46	1.49	1.40
70	AD	401	HEC	C3C-C2C	5.42	1.46	1.40
66	W	201	EHZ	C15-N2	5.38	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	n	201	EHZ	C15-N2	5.37	1.45	1.33
66	n	201	EHZ	C12-N1	5.19	1.45	1.33
66	W	201	EHZ	C12-N1	5.11	1.45	1.33
60	F	501	FMN	C9A-C5A	4.79	1.49	1.41
69	Ac	406	UQ6	C4-C3	4.68	1.49	1.39
69	AC	405	UQ6	C4-C3	4.53	1.48	1.39
69	AC	405	UQ6	C2-C1	4.40	1.49	1.40
62	AC	406	CDL	OB8-CB7	4.34	1.46	1.33
55	M	503	3PE	O31-C31	4.31	1.45	1.33
62	Ag	101	CDL	OB8-CB7	4.27	1.45	1.33
55	J	202	3PE	O31-C31	4.26	1.45	1.33
62	L	706	CDL	OB8-CB7	4.26	1.45	1.33
62	Ac	407	CDL	OA8-CA7	4.26	1.45	1.33
62	Ac	407	CDL	OB8-CB7	4.26	1.45	1.33
69	Ac	406	UQ6	C2-C1	4.25	1.48	1.40
71	AD	402	3PH	O31-C31	4.24	1.45	1.33
62	L	705	CDL	OB8-CB7	4.24	1.45	1.33
55	L	702	3PE	O31-C31	4.24	1.45	1.33
58	J	201	PC1	O31-C31	4.24	1.45	1.33
71	Ad	402	3PH	O31-C31	4.23	1.45	1.33
55	Y	201	3PE	O31-C31	4.22	1.45	1.33
55	Ag	102	3PE	O31-C31	4.22	1.45	1.33
62	a	101	CDL	OB8-CB7	4.20	1.45	1.33
55	Ac	404	3PE	O31-C31	4.20	1.45	1.33
55	M	501	3PE	O31-C31	4.19	1.45	1.33
55	L	704	3PE	O31-C31	4.18	1.45	1.33
62	L	706	CDL	OA8-CA7	4.18	1.45	1.33
55	AF	201	3PE	O31-C31	4.18	1.45	1.33
58	B	303	PC1	O31-C31	4.17	1.45	1.33
58	I	302	PC1	O31-C31	4.17	1.45	1.33
62	X	201	CDL	OB6-CB5	4.17	1.46	1.34
55	L	707	3PE	O31-C31	4.16	1.45	1.33
55	AC	403	3PE	O31-C31	4.15	1.45	1.33
55	O	401	3PE	O31-C31	4.15	1.45	1.33
55	M	502	3PE	O31-C31	4.14	1.45	1.33
62	a	101	CDL	OB6-CB5	4.14	1.46	1.34
55	b	201	3PE	O31-C31	4.14	1.45	1.33
55	L	701	3PE	O31-C31	4.13	1.45	1.33
62	L	706	CDL	OB6-CB5	4.11	1.45	1.34
62	a	101	CDL	OA8-CA7	4.11	1.45	1.33
62	h	201	CDL	OA8-CA7	4.11	1.45	1.33
62	h	201	CDL	OB8-CB7	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	L	705	CDL	OA8-CA7	4.11	1.45	1.33
55	A	401	3PE	O31-C31	4.10	1.45	1.33
55	L	701	3PE	O21-C21	4.10	1.45	1.34
58	J	201	PC1	O21-C21	4.10	1.45	1.34
58	I	302	PC1	O21-C21	4.09	1.45	1.34
62	AC	406	CDL	OA8-CA7	4.09	1.45	1.33
62	L	706	CDL	OA6-CA5	4.08	1.45	1.34
55	N	401	3PE	O21-C21	4.08	1.45	1.34
62	X	201	CDL	OB8-CB7	4.08	1.45	1.33
62	h	201	CDL	OB6-CB5	4.08	1.45	1.34
55	I	301	3PE	O31-C31	4.08	1.45	1.33
55	N	401	3PE	O31-C31	4.07	1.45	1.33
55	M	503	3PE	O21-C21	4.06	1.45	1.34
55	AF	201	3PE	O21-C21	4.05	1.45	1.34
62	X	201	CDL	OA8-CA7	4.05	1.45	1.33
62	a	101	CDL	OA6-CA5	4.05	1.45	1.34
55	L	702	3PE	O21-C21	4.05	1.45	1.34
62	AC	406	CDL	OB6-CB5	4.04	1.45	1.34
62	Ag	101	CDL	OA8-CA7	4.04	1.45	1.33
62	Ag	101	CDL	OB6-CB5	4.04	1.45	1.34
58	B	303	PC1	O21-C21	4.04	1.45	1.34
55	L	703	3PE	O21-C21	4.03	1.45	1.34
62	Ac	407	CDL	OA6-CA5	4.03	1.45	1.34
55	L	704	3PE	O21-C21	4.02	1.45	1.34
62	h	201	CDL	OA6-CA5	4.02	1.45	1.34
55	b	201	3PE	O21-C21	4.01	1.45	1.34
55	AC	403	3PE	O21-C21	4.01	1.45	1.34
55	Ag	102	3PE	O21-C21	4.00	1.45	1.34
55	L	703	3PE	O31-C31	4.00	1.45	1.33
55	J	202	3PE	O21-C21	3.99	1.45	1.34
55	O	401	3PE	O21-C21	3.99	1.45	1.34
62	L	705	CDL	OB6-CB5	3.98	1.45	1.34
55	I	301	3PE	O21-C21	3.97	1.45	1.34
55	A	401	3PE	O21-C21	3.96	1.45	1.34
67	Ac	403	HEM	C1B-NB	-3.95	1.33	1.40
55	M	501	3PE	O21-C21	3.95	1.45	1.34
62	Ag	101	CDL	OA6-CA5	3.95	1.45	1.34
55	L	707	3PE	O21-C21	3.94	1.45	1.34
62	Ac	407	CDL	OB6-CB5	3.93	1.45	1.34
55	Y	201	3PE	O21-C21	3.93	1.45	1.34
71	AD	402	3PH	O21-C21	3.91	1.45	1.34
67	AC	402	HEM	C1B-NB	-3.91	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	Ad	402	3PH	O21-C21	3.91	1.45	1.34
62	X	201	CDL	OA6-CA5	3.90	1.45	1.34
55	Ac	404	3PE	O21-C21	3.89	1.45	1.34
62	AC	406	CDL	OA6-CA5	3.89	1.45	1.34
55	M	502	3PE	O21-C21	3.86	1.45	1.34
67	Ac	402	HEM	C1B-NB	-3.80	1.33	1.40
62	L	705	CDL	OA6-CA5	3.73	1.44	1.34
67	Ac	403	HEM	C4D-ND	-3.66	1.34	1.40
67	AC	402	HEM	C4D-ND	-3.55	1.34	1.40
67	AC	401	HEM	C4D-ND	-3.44	1.34	1.40
67	AC	401	HEM	C1B-NB	-3.43	1.34	1.40
67	Ac	402	HEM	C4D-ND	-3.39	1.34	1.40
64	P	401	NDP	C6N-C5N	3.26	1.39	1.33
70	AD	401	HEC	C2A-C3A	3.26	1.47	1.37
70	Ad	401	HEC	C2A-C3A	3.23	1.47	1.37
70	AD	401	HEC	C3D-C2D	3.22	1.47	1.37
60	F	501	FMN	C8-C7	3.15	1.48	1.40
70	Ad	401	HEC	C3D-C2D	3.15	1.47	1.37
67	Ac	402	HEM	FE-NB	3.14	2.12	1.96
68	AC	404	U10	C4-C3	3.08	1.48	1.36
68	Ac	405	U10	C4-C3	3.04	1.48	1.36
70	AD	401	HEC	C3C-C4C	3.03	1.48	1.43
70	AD	401	HEC	C2A-C1A	3.01	1.49	1.42
67	AC	402	HEM	C4B-NB	-2.98	1.32	1.38
57	B	302	UQ1	C3-C4	-2.96	1.40	1.48
67	AC	402	HEM	C1B-C2B	-2.94	1.38	1.44
70	AD	401	HEC	C4B-C3B	2.85	1.48	1.43
67	AC	401	HEM	FE-NB	2.84	2.10	1.96
70	Ad	401	HEC	C3C-C4C	2.83	1.48	1.43
67	Ac	403	HEM	FE-NB	2.78	2.10	1.96
70	Ad	401	HEC	C3A-C4A	2.75	1.48	1.42
60	F	501	FMN	C4-N3	-2.75	1.33	1.38
67	Ac	402	HEM	CHB-C1B	2.71	1.41	1.35
70	AD	401	HEC	C3A-C4A	2.71	1.48	1.42
70	Ad	401	HEC	C2A-C1A	2.70	1.48	1.42
61	H	400	UQ9	C4-C5	-2.68	1.41	1.48
61	H	400	UQ9	C3-C2	-2.61	1.41	1.48
66	n	201	EHZ	P1-O7	2.55	1.64	1.54
66	W	201	EHZ	P1-O7	2.55	1.64	1.54
70	AD	401	HEC	C1D-CHD	2.53	1.48	1.41
66	W	201	EHZ	O4-C15	-2.48	1.18	1.23
63	O	402	ADP	C5-C4	2.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AC	402	HEM	FE-NB	2.47	2.09	1.96
70	Ad	401	HEC	C1B-CHB	2.46	1.47	1.41
66	n	201	EHZ	O4-C15	-2.44	1.18	1.23
60	F	501	FMN	C5A-N5	-2.41	1.34	1.39
66	W	201	EHZ	C9-S1	2.40	1.81	1.76
57	B	302	UQ1	C2-C1	-2.40	1.42	1.48
70	Ad	401	HEC	C4B-C3B	2.39	1.47	1.43
66	n	201	EHZ	C9-S1	2.38	1.81	1.76
66	n	201	EHZ	O3-C12	-2.38	1.18	1.23
67	Ac	403	HEM	C4B-NB	-2.36	1.33	1.38
70	AD	401	HEC	C4D-CHA	2.36	1.47	1.41
66	W	201	EHZ	O3-C12	-2.33	1.18	1.23
67	AC	402	HEM	C1D-ND	-2.29	1.34	1.38
64	P	401	NDP	C5A-C4A	2.29	1.47	1.40
66	n	201	EHZ	P1-OP3	-2.27	1.46	1.54
70	Ad	401	HEC	C4D-CHA	2.27	1.47	1.41
66	W	201	EHZ	P1-OP3	-2.22	1.46	1.54
67	Ac	402	HEM	C1D-ND	-2.22	1.34	1.38
67	Ac	403	HEM	C1D-ND	-2.20	1.34	1.38
67	AC	402	HEM	FE-ND	-2.14	1.86	1.96
67	Ac	402	HEM	C3B-C4B	2.14	1.49	1.44
67	AC	401	HEM	C4B-NB	-2.13	1.34	1.38
67	AC	402	HEM	C3B-C2B	-2.11	1.33	1.37
70	Ad	401	HEC	C1C-CHC	2.08	1.46	1.41
67	AC	401	HEM	C1D-ND	-2.06	1.34	1.38
60	F	501	FMN	C4A-N5	2.05	1.34	1.30
67	Ac	403	HEM	FE-ND	-2.04	1.86	1.96

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	AD	401	HEC	CMC-C2C-C3C	7.21	134.30	125.82
67	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
70	Ad	401	HEC	C1D-C2D-C3D	-6.40	102.54	107.00
66	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
66	n	201	EHZ	C8-C9-S1	6.30	121.43	113.63
67	AC	402	HEM	CHC-C4B-NB	6.27	131.24	124.43
70	AD	401	HEC	C1D-C2D-C3D	-6.03	102.80	107.00
69	AC	405	UQ6	C7-C8-C9	-5.55	118.63	127.24
67	AC	401	HEM	CHC-C4B-NB	5.47	130.37	124.43
70	Ad	401	HEC	CBD-CAD-C3D	-5.09	103.93	112.62
62	X	201	CDL	OA6-CA5-C11	5.01	122.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	Ac	402	HEM	C3B-C2B-C1B	4.83	110.07	106.49
67	AC	402	HEM	CHD-C1D-ND	4.79	129.63	124.43
67	AC	402	HEM	C3B-C2B-C1B	-4.70	103.00	106.49
67	AC	402	HEM	CHB-C1B-NB	4.65	130.13	124.38
67	AC	401	HEM	CHD-C1D-ND	4.54	129.36	124.43
55	M	503	3PE	O21-C21-C22	4.50	121.20	111.50
70	Ad	401	HEC	CMC-C2C-C3C	4.47	131.08	125.82
62	h	201	CDL	OB6-CB5-C51	4.46	121.11	111.50
67	Ac	403	HEM	CHC-C4B-NB	4.42	129.23	124.43
67	Ac	402	HEM	CHD-C1D-ND	4.42	129.23	124.43
55	N	401	3PE	O21-C21-C22	4.37	120.92	111.50
55	M	502	3PE	O21-C21-C22	4.37	120.91	111.50
55	L	703	3PE	O21-C21-C22	4.35	120.89	111.50
67	AC	402	HEM	C4B-C3B-C2B	4.35	110.57	107.11
62	a	101	CDL	OA6-CA5-C11	4.33	120.84	111.50
55	O	401	3PE	O21-C21-C22	4.32	120.80	111.50
67	Ac	403	HEM	CHD-C1D-ND	4.30	129.11	124.43
58	I	302	PC1	O21-C21-C22	4.23	120.61	111.50
62	X	201	CDL	OB6-CB5-C51	4.23	120.61	111.50
55	Ac	404	3PE	O21-C21-C22	4.22	120.61	111.50
62	L	706	CDL	OA6-CA5-C11	4.20	120.56	111.50
62	L	706	CDL	OB6-CB5-C51	4.20	120.55	111.50
70	AD	401	HEC	CMB-C2B-C3B	4.15	130.70	125.82
55	Ag	102	3PE	O21-C21-C22	4.11	120.36	111.50
62	a	101	CDL	OB6-CB5-C51	4.07	120.28	111.50
67	Ac	403	HEM	CHA-C4D-ND	4.06	129.39	124.38
67	Ac	402	HEM	CHC-C4B-NB	4.05	128.83	124.43
68	AC	404	U10	C7-C8-C9	-4.04	120.07	126.79
62	Ag	101	CDL	OA6-CA5-C11	4.02	120.17	111.50
55	J	202	3PE	O21-C21-C22	4.01	120.14	111.50
58	J	201	PC1	O21-C21-C22	4.01	120.13	111.50
62	Ac	407	CDL	OB6-CB5-C51	4.00	120.12	111.50
62	h	201	CDL	OA6-CA5-C11	3.96	120.03	111.50
62	Ag	101	CDL	OB6-CB5-C51	3.95	120.01	111.50
67	AC	402	HEM	CHA-C4D-ND	3.92	129.23	124.38
55	M	501	3PE	O21-C21-C22	3.86	119.82	111.50
67	AC	401	HEM	CHA-C4D-ND	3.84	129.12	124.38
55	AC	403	3PE	O21-C21-C22	3.84	119.77	111.50
58	B	303	PC1	O21-C21-C22	3.81	119.71	111.50
67	AC	402	HEM	CMA-C3A-C4A	-3.80	122.63	128.46
55	A	401	3PE	O21-C21-C22	3.76	119.61	111.50
62	AC	406	CDL	OA6-CA5-C11	3.76	119.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	L	704	3PE	O21-C21-C22	3.75	119.58	111.50
55	Y	201	3PE	O21-C21-C22	3.75	119.58	111.50
68	Ac	405	U10	C22-C23-C24	-3.74	118.65	127.66
70	Ad	401	HEC	CMD-C2D-C3D	3.74	131.99	124.94
67	AC	401	HEM	C1B-NB-C4B	3.72	108.92	105.07
62	AC	406	CDL	OB6-CB5-C51	3.72	119.52	111.50
68	Ac	405	U10	C12-C13-C14	-3.71	118.72	127.66
62	X	201	CDL	CA4-OA6-CA5	-3.71	108.67	117.79
55	I	301	3PE	O21-C21-C22	3.68	119.43	111.50
67	AC	401	HEM	CHB-C1B-NB	3.67	128.91	124.38
67	AC	402	HEM	CHB-C1B-C2B	-3.65	116.61	126.72
55	L	707	3PE	O21-C21-C22	3.64	119.34	111.50
55	L	701	3PE	O21-C21-C22	3.62	119.30	111.50
69	AC	405	UQ6	C15-C14-C16	3.60	121.33	115.27
55	L	702	3PE	O21-C21-C22	3.58	119.22	111.50
62	L	705	CDL	OA6-CA5-C11	3.58	119.22	111.50
64	P	401	NDP	PN-O3-PA	-3.56	120.62	132.83
67	Ac	403	HEM	CHB-C1B-NB	3.55	128.77	124.38
71	AD	402	3PH	O21-C21-C22	3.54	119.13	111.50
67	Ac	402	HEM	CHA-C4D-ND	3.54	128.76	124.38
55	b	201	3PE	O21-C21-C22	3.51	119.07	111.50
70	AD	401	HEC	CBD-CAD-C3D	-3.50	106.65	112.62
55	b	201	3PE	C2-O21-C21	-3.48	109.22	117.79
63	O	402	ADP	C3'-C2'-C1'	3.44	106.15	100.98
71	Ad	402	3PH	O21-C21-C22	3.44	118.91	111.50
62	L	705	CDL	CA4-OA6-CA5	-3.41	109.40	117.79
62	Ac	407	CDL	OA6-CA5-C11	3.41	120.31	110.80
69	Ac	406	UQ6	C7-C8-C9	-3.40	121.97	127.24
62	L	705	CDL	OB6-CB5-C51	3.38	118.79	111.50
62	Ac	407	CDL	OB8-CB7-C71	3.38	120.24	111.38
67	Ac	403	HEM	C1B-NB-C4B	3.34	108.53	105.07
55	AF	201	3PE	O21-C21-C22	3.33	118.67	111.50
55	M	502	3PE	C2-O21-C21	-3.33	109.60	117.79
70	Ad	401	HEC	CMB-C2B-C3B	3.21	129.59	125.82
63	O	402	ADP	N3-C2-N1	-3.18	123.71	128.68
67	AC	402	HEM	C1B-NB-C4B	3.17	108.35	105.07
70	AD	401	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
64	P	401	NDP	N3A-C2A-N1A	-3.14	123.78	128.68
68	Ac	405	U10	C15-C14-C16	3.11	120.51	115.27
68	AC	404	U10	C10-C9-C11	3.11	120.50	115.27
66	W	201	EHZ	C13-C12-N1	3.10	121.64	116.42
66	n	201	EHZ	C13-C12-N1	3.09	121.62	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	M	501	3PE	O31-C31-C32	3.08	121.58	111.91
62	L	705	CDL	OB8-CB7-C71	3.07	121.55	111.91
63	O	402	ADP	PA-O3A-PB	-3.07	122.31	132.83
67	Ac	402	HEM	C1B-NB-C4B	3.05	108.22	105.07
68	Ac	405	U10	C10-C9-C11	3.04	120.39	115.27
67	Ac	402	HEM	CHD-C1D-C2D	-3.04	120.23	124.98
66	n	201	EHZ	C14-C13-C12	-3.03	107.31	112.36
67	AC	402	HEM	C4D-ND-C1D	3.03	108.20	105.07
66	W	201	EHZ	C14-C13-C12	-3.02	107.33	112.36
55	M	503	3PE	O31-C31-C32	3.02	121.38	111.91
55	L	702	3PE	O31-C31-C32	3.02	121.37	111.91
62	Ag	101	CDL	CA4-OA6-CA5	-3.02	110.37	117.79
55	Ac	404	3PE	C2-O21-C21	-3.00	110.40	117.79
68	Ac	405	U10	C20-C19-C21	2.96	120.25	115.27
67	Ac	402	HEM	CHC-C4B-C3B	-2.94	120.07	124.57
68	Ac	405	U10	C1M-C1-C6	-2.92	119.63	124.40
55	O	401	3PE	O31-C31-C32	2.91	121.04	111.91
66	W	201	EHZ	OP3-P1-O9	-2.90	99.33	110.68
66	n	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
66	W	201	EHZ	C7-C8-C9	-2.89	107.30	113.89
67	AC	402	HEM	C2B-C1B-NB	2.89	113.26	109.84
66	n	201	EHZ	C7-C8-C9	-2.88	107.33	113.89
55	Ag	102	3PE	O31-C31-C32	2.86	120.89	111.91
55	M	501	3PE	C2-O21-C21	-2.86	110.76	117.79
68	Ac	405	U10	C17-C18-C19	-2.85	120.80	127.66
69	AC	405	UQ6	C10-C9-C11	2.85	120.06	115.27
55	N	401	3PE	O31-C31-C32	2.84	120.82	111.91
58	I	302	PC1	C2-O21-C21	-2.83	110.83	117.79
55	AC	403	3PE	C2-O21-C21	-2.82	110.85	117.79
71	AD	402	3PH	O31-C31-C32	2.81	120.74	111.91
62	L	706	CDL	OB8-CB7-C71	2.81	120.73	111.91
62	h	201	CDL	OB8-CB7-C71	2.81	120.72	111.91
63	O	402	ADP	C4-C5-N7	-2.80	106.48	109.40
62	L	706	CDL	OA8-CA7-C31	2.80	120.69	111.91
58	B	303	PC1	O31-C31-C32	2.78	120.62	111.91
62	Ac	407	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
69	Ac	406	UQ6	C10-C9-C11	2.77	119.92	115.27
69	Ac	406	UQ6	C4M-O4-C4	2.76	122.35	114.78
62	Ac	407	CDL	CB4-OB6-CB5	-2.75	111.01	117.79
69	AC	405	UQ6	C12-C13-C14	-2.75	121.03	127.66
55	J	202	3PE	C2-O21-C21	-2.75	111.03	117.79
67	AC	402	HEM	CHD-C1D-C2D	-2.74	120.69	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	a	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
62	a	101	CDL	CA4-OA6-CA5	-2.74	111.06	117.79
55	Y	201	3PE	O31-C31-C32	2.73	120.49	111.91
55	L	703	3PE	O31-C31-C32	2.73	120.47	111.91
67	Ac	403	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
64	P	401	NDP	C4A-C5A-N7A	-2.70	106.59	109.40
58	B	303	PC1	C2-O21-C21	-2.69	111.16	117.79
67	AC	402	HEM	CBD-CAD-C3D	-2.69	105.15	112.63
55	L	701	3PE	O31-C31-C32	2.69	120.34	111.91
71	Ad	402	3PH	C2-O21-C21	-2.68	111.19	117.79
55	I	301	3PE	O31-C31-C32	2.67	120.28	111.91
55	L	704	3PE	O31-C31-C32	2.66	120.26	111.91
69	Ac	406	UQ6	C6-C7-C8	-2.65	107.97	112.17
60	F	501	FMN	C4A-C10-N1	-2.63	118.62	124.73
55	Y	201	3PE	C2-O21-C21	-2.63	111.32	117.79
62	AC	406	CDL	OB8-CB7-C71	2.62	120.13	111.91
62	h	201	CDL	CA4-OA6-CA5	-2.61	111.38	117.79
62	L	705	CDL	OA8-CA7-C31	2.60	120.07	111.91
62	X	201	CDL	OA8-CA7-C31	2.60	120.06	111.91
67	Ac	403	HEM	CBD-CAD-C3D	-2.60	105.41	112.63
58	I	302	PC1	O31-C31-C32	2.59	120.04	111.91
55	L	707	3PE	C2-O21-C21	-2.58	111.43	117.79
55	AC	403	3PE	O31-C31-C32	2.58	119.99	111.91
67	AC	401	HEM	C4D-ND-C1D	2.57	107.73	105.07
55	A	401	3PE	O31-C31-C32	2.56	119.95	111.91
67	Ac	403	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
67	AC	402	HEM	CBA-CAA-C2A	-2.56	108.26	112.62
67	Ac	403	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
69	Ac	406	UQ6	C17-C18-C19	-2.55	119.05	127.75
55	Ac	404	3PE	O31-C31-C32	2.54	119.88	111.91
55	L	704	3PE	C2-O21-C21	-2.54	111.53	117.79
69	Ac	406	UQ6	C21-C19-C20	2.54	120.22	114.60
62	Ag	101	CDL	OA8-CA7-C31	2.54	119.87	111.91
60	F	501	FMN	O4-C4-C4A	-2.53	119.90	126.60
62	Ag	101	CDL	CB4-OB6-CB5	-2.52	111.59	117.79
71	Ad	402	3PH	O31-C31-C32	2.52	119.81	111.91
62	h	201	CDL	CB4-OB6-CB5	-2.51	111.62	117.79
55	b	201	3PE	O31-C31-C32	2.49	119.74	111.91
62	h	201	CDL	OA8-CA7-C31	2.49	119.73	111.91
55	AF	201	3PE	O31-C31-C32	2.49	119.73	111.91
68	Ac	405	U10	C27-C28-C29	-2.48	119.27	127.75
69	AC	405	UQ6	C21-C19-C20	2.47	120.06	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AC	401	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
64	P	401	NDP	C3D-C2D-C1D	2.47	106.11	101.43
68	AC	404	U10	C16-C14-C15	2.45	120.02	114.60
62	Ag	101	CDL	OB8-CB7-C71	2.45	119.59	111.91
62	Ac	407	CDL	OA8-CA7-C31	2.45	119.59	111.91
55	M	502	3PE	O31-C31-C32	2.43	119.54	111.91
66	W	201	EHZ	C5-C6-C7	-2.39	107.98	114.85
62	a	101	CDL	OB8-CB7-C71	2.39	119.40	111.91
68	AC	404	U10	C1M-C1-C6	-2.38	120.52	124.40
71	AD	402	3PH	C2-O21-C21	-2.37	111.94	117.79
66	n	201	EHZ	C5-C6-C7	-2.37	108.02	114.85
62	AC	406	CDL	OA8-CA7-C31	2.37	119.34	111.91
67	AC	401	HEM	CHA-C4D-C3D	-2.37	120.88	125.33
69	AC	405	UQ6	C4M-O4-C4	2.36	121.25	114.78
62	L	706	CDL	CB4-OB6-CB5	-2.35	112.01	117.79
62	X	201	CDL	OA6-CA5-OA7	-2.34	118.05	123.70
58	J	201	PC1	C2-O21-C21	-2.33	112.04	117.79
58	J	201	PC1	O31-C31-C32	2.33	119.23	111.91
67	Ac	403	HEM	CHB-C1B-C2B	-2.32	120.29	126.72
62	AC	406	CDL	CB4-OB6-CB5	-2.32	112.07	117.79
67	Ac	402	HEM	C4A-C3A-C2A	2.32	108.61	107.00
67	Ac	402	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
67	Ac	402	HEM	CHB-C1B-NB	2.30	127.23	124.38
55	J	202	3PE	O31-C31-C32	2.30	119.13	111.91
69	AC	405	UQ6	C7-C6-C5	-2.30	117.80	120.82
68	Ac	405	U10	C31-C29-C30	2.30	119.68	114.60
67	Ac	403	HEM	C4D-ND-C1D	2.28	107.43	105.07
66	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
55	L	703	3PE	O21-C21-O22	-2.26	118.24	123.70
66	n	201	EHZ	C10-S1-C9	2.26	108.91	101.87
55	M	502	3PE	O21-C21-O22	-2.25	118.26	123.70
55	N	401	3PE	C2-O21-C21	-2.25	112.26	117.79
55	L	707	3PE	O31-C31-C32	2.25	118.95	111.91
68	AC	404	U10	C12-C13-C14	-2.23	120.11	127.75
69	AC	405	UQ6	C17-C18-C19	-2.23	120.11	127.75
62	a	101	CDL	CB4-OB6-CB5	-2.23	112.30	117.79
62	X	201	CDL	OB8-CB7-C71	2.22	118.87	111.91
67	AC	402	HEM	CMA-C3A-C2A	2.21	129.10	124.94
60	F	501	FMN	C4-C4A-N5	2.19	121.35	118.23
66	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
67	AC	401	HEM	CHB-C1B-C2B	-2.17	120.71	126.72
55	O	401	3PE	C2-O21-C21	-2.16	112.47	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	AD	401	HEC	C3B-C4B-NB	2.15	115.00	110.94
62	AC	406	CDL	CA4-OA6-CA5	-2.14	112.52	117.79
70	Ad	401	HEC	CAA-CBA-CGA	-2.14	107.76	113.76
66	n	201	EHZ	C11-N1-C12	-2.14	118.86	122.84
55	M	503	3PE	O21-C21-O22	-2.13	118.56	123.70
60	F	501	FMN	C4A-C10-N10	2.12	119.58	116.48
66	W	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
66	n	201	EHZ	O3-C12-N1	-2.11	119.02	123.01
69	AC	405	UQ6	C1M-C1-C6	-2.11	117.37	120.42
62	Ac	407	CDL	OB6-CB5-OB7	-2.10	118.62	123.70
66	W	201	EHZ	O6-P1-O9	2.10	112.36	106.47
66	n	201	EHZ	O6-P1-O9	2.10	112.36	106.47
55	N	401	3PE	O31-C31-O32	-2.10	118.30	123.59
55	Ag	102	3PE	C2-O21-C21	-2.09	112.63	117.79
68	Ac	405	U10	C7-C6-C5	2.09	121.00	118.48
68	Ac	405	U10	C25-C24-C26	2.09	118.78	115.27
66	n	201	EHZ	O2-C9-S1	-2.09	119.91	122.61
55	L	702	3PE	O21-C21-O22	-2.08	118.66	123.70
69	AC	405	UQ6	C1M-C1-C2	2.08	124.03	120.50
69	Ac	406	UQ6	C7-C6-C5	-2.08	118.09	120.82
67	AC	402	HEM	CMB-C2B-C1B	2.08	128.20	125.04
66	W	201	EHZ	O3-C12-N1	-2.07	119.11	123.01
60	F	501	FMN	O2-C2-N1	-2.06	118.41	121.83
55	L	702	3PE	C2-O21-C21	-2.06	112.72	117.79
60	F	501	FMN	C10-N1-C2	2.06	121.02	116.90
55	Ac	404	3PE	O21-C21-O22	-2.06	118.73	123.70
55	M	501	3PE	O21-C21-O22	-2.05	118.76	123.70
69	Ac	406	UQ6	C3M-O3-C3	2.04	120.38	114.78
69	Ac	406	UQ6	C17-C16-C14	-2.04	106.26	112.98
68	Ac	405	U10	C7-C8-C9	-2.04	123.40	126.79
67	AC	401	HEM	CAA-CBA-CGA	-2.03	108.07	113.76
55	I	301	3PE	O31-C31-O32	-2.03	118.47	123.59
58	J	201	PC1	C11-C12-N	-2.01	109.05	115.78
55	Ag	102	3PE	O31-C31-O32	-2.01	118.52	123.59
55	I	301	3PE	C2-O21-C21	-2.01	112.85	117.79
60	F	501	FMN	C4A-C4-N3	2.00	118.28	113.19

There are no chirality outliers.

All (568) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
55	A	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C32-C31-O31-C3
55	I	301	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O12
55	L	701	3PE	C1-O11-P-O13
55	L	701	3PE	C1-O11-P-O14
55	L	702	3PE	C11-O13-P-O14
55	L	703	3PE	C1-O11-P-O14
55	L	703	3PE	O22-C21-O21-C2
55	L	703	3PE	C22-C21-O21-C2
55	L	704	3PE	C1-O11-P-O12
55	L	707	3PE	C11-O13-P-O11
55	L	707	3PE	C11-O13-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-O11
55	M	501	3PE	C11-O13-P-O12
55	M	501	3PE	C11-O13-P-O14
55	M	502	3PE	C11-O13-P-O12
55	M	502	3PE	C11-O13-P-O14
55	M	503	3PE	C1-O11-P-O12
55	M	503	3PE	C1-O11-P-O13
55	M	503	3PE	C1-O11-P-O14
55	M	503	3PE	C11-O13-P-O12
55	M	503	3PE	C11-O13-P-O14
55	M	503	3PE	C22-C21-O21-C2
55	N	401	3PE	C11-O13-P-O11
55	N	401	3PE	C11-O13-P-O12
55	N	401	3PE	C11-O13-P-O14
55	O	401	3PE	C11-O13-P-O12
55	O	401	3PE	C11-O13-P-O14
55	O	401	3PE	C22-C21-O21-C2
55	b	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C22-C21-O21-C2
55	AC	403	3PE	C1-O11-P-O12
55	AC	403	3PE	C1-O11-P-O13
55	AC	403	3PE	C1-O11-P-O14
55	AC	403	3PE	C11-O13-P-O12
55	AC	403	3PE	C11-O13-P-O14
55	Ac	401	3PE	C1-O11-P-O12
55	Ac	401	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
55	Ag	102	3PE	C11-O13-P-O11
55	Ag	102	3PE	C11-O13-P-O12
55	Ag	102	3PE	C11-O13-P-O14
57	B	302	UQ1	C7-C8-C9-C11
58	B	303	PC1	C1-O11-P-O12
58	B	303	PC1	C1-O11-P-O14
58	B	303	PC1	C1-O11-P-O13
58	B	303	PC1	C22-C21-O21-C2
58	I	302	PC1	C11-O13-P-O12
58	I	302	PC1	C11-O13-P-O14
58	I	302	PC1	C11-O13-P-O11
58	I	302	PC1	C1-O11-P-O12
58	J	201	PC1	C11-O13-P-O12
58	J	201	PC1	C11-O13-P-O14
58	J	201	PC1	C1-O11-P-O12
58	J	201	PC1	C1-O11-P-O13
58	J	201	PC1	C12-C11-O13-P
60	F	501	FMN	N10-C1'-C2'-O2'
60	F	501	FMN	C5'-O5'-P-O1P
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C22-C23-C24-C26
61	H	400	UQ9	C22-C23-C24-C25
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C7-C8-C9-C11
61	H	400	UQ9	C7-C8-C9-C10
62	L	705	CDL	CA2-OA2-PA1-OA4
62	L	705	CDL	CA3-OA5-PA1-OA3
62	L	705	CDL	C11-CA5-OA6-CA4
62	L	705	CDL	C51-CB5-OB6-CB4
62	L	706	CDL	C11-CA5-OA6-CA4
62	L	706	CDL	CB2-OB2-PB2-OB4
62	L	706	CDL	OB7-CB5-OB6-CB4
62	L	706	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CB3-OB5-PB2-OB3
62	X	201	CDL	CB3-OB5-PB2-OB4
62	X	201	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	C71-CB7-OB8-CB6
62	a	101	CDL	CA3-OA5-PA1-OA2
62	a	101	CDL	CA3-OA5-PA1-OA3
62	a	101	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB2-OB2-PB2-OB3
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	AC	406	CDL	CA2-OA2-PA1-OA4
62	AC	406	CDL	CA3-OA5-PA1-OA3
62	AC	406	CDL	CA3-OA5-PA1-OA4
62	AC	406	CDL	C31-CA7-OA8-CA6
62	Aa	501	CDL	CA3-OA5-PA1-OA2
62	Aa	501	CDL	CB4-CB3-OB5-PB2
62	Ac	407	CDL	CB2-OB2-PB2-OB3
62	Ac	407	CDL	CB2-OB2-PB2-OB4
62	Ac	407	CDL	CB2-OB2-PB2-OB5
62	Ac	407	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
63	O	402	ADP	C5'-O5'-PA-O2A
63	O	402	ADP	C5'-O5'-PA-O3A
64	P	401	NDP	C2N-C3N-C7N-N7N
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C7-C8-C9-S1
66	W	201	EHZ	S1-C10-C11-N1
66	W	201	EHZ	C11-C10-S1-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	C20-O6-P1-O7
66	W	201	EHZ	C20-O6-P1-O9
66	W	201	EHZ	C20-O6-P1-OP3
66	n	201	EHZ	O1-C7-C8-C9
66	n	201	EHZ	C6-C7-C8-C9
66	n	201	EHZ	C7-C8-C9-S1
66	n	201	EHZ	S1-C10-C11-N1
66	n	201	EHZ	C11-C10-S1-C9
66	n	201	EHZ	C16-C17-C20-O6
66	n	201	EHZ	C20-O6-P1-O7
66	n	201	EHZ	C20-O6-P1-O9
66	n	201	EHZ	C20-O6-P1-OP3

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Mol	Chain	Res	Type	Atoms
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	403	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C4B-C3B-CAB-CBB
68	Ac	405	U10	C5-C6-C7-C8
69	AC	405	UQ6	C13-C14-C16-C17
69	AC	405	UQ6	C15-C14-C16-C17
69	Ac	406	UQ6	C1-C6-C7-C8
69	Ac	406	UQ6	C13-C14-C16-C17
69	Ac	406	UQ6	C15-C14-C16-C17
70	AD	401	HEC	C1A-C2A-CAA-CBA
71	Ad	402	3PH	C22-C21-O21-C2
55	O	401	3PE	O32-C31-O31-C3
58	I	302	PC1	O32-C31-O31-C3
62	AC	406	CDL	OA9-CA7-OA8-CA6
55	O	401	3PE	C32-C31-O31-C3
58	I	302	PC1	C32-C31-O31-C3
55	AF	201	3PE	O32-C31-O31-C3
58	J	201	PC1	O32-C31-O31-C3
62	L	705	CDL	OA9-CA7-OA8-CA6
55	M	503	3PE	O22-C21-O21-C2
55	O	401	3PE	O22-C21-O21-C2
55	Ac	401	3PE	O22-C21-O21-C2
58	B	303	PC1	O22-C21-O21-C2
62	L	705	CDL	OA7-CA5-OA6-CA4
62	L	705	CDL	OB7-CB5-OB6-CB4
62	L	706	CDL	OA7-CA5-OA6-CA4
62	X	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
62	AC	406	CDL	OA7-CA5-OA6-CA4
71	Ad	402	3PH	O22-C21-O21-C2
55	M	502	3PE	C32-C31-O31-C3
58	J	201	PC1	C32-C31-O31-C3
55	J	202	3PE	C22-C21-O21-C2
68	Ac	405	U10	C25-C24-C26-C27
61	H	400	UQ9	C18-C19-C21-C22
55	AF	201	3PE	C32-C31-O31-C3
62	L	705	CDL	C31-CA7-OA8-CA6
62	X	201	CDL	C31-CA7-OA8-CA6
55	Y	201	3PE	O32-C31-O31-C3
55	AC	403	3PE	O32-C31-O31-C3
55	Y	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
55	AC	403	3PE	C32-C31-O31-C3
55	M	502	3PE	O32-C31-O31-C3
62	X	201	CDL	OA9-CA7-OA8-CA6
62	AC	406	CDL	C11-CA5-OA6-CA4
57	B	302	UQ1	C7-C8-C9-C10
55	J	202	3PE	O22-C21-O21-C2
62	h	201	CDL	CA4-CA3-OA5-PA1
62	Ag	101	CDL	CB4-CB3-OB5-PB2
61	H	400	UQ9	C25-C24-C26-C27
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C23-C24-C26-C27
61	H	400	UQ9	C13-C14-C16-C17
62	AC	406	CDL	OB9-CB7-OB8-CB6
62	AC	406	CDL	C71-CB7-OB8-CB6
55	A	401	3PE	C22-C21-O21-C2
62	Aa	501	CDL	CA2-C1-CB2-OB2
58	J	201	PC1	C11-C12-N-C13
55	I	301	3PE	C32-C31-O31-C3
55	b	201	3PE	C32-C31-O31-C3
62	Aa	501	CDL	O1-C1-CB2-OB2
71	AD	402	3PH	O21-C2-C3-O31
55	Y	201	3PE	C23-C24-C25-C26
62	a	101	CDL	C12-C13-C14-C15
62	L	705	CDL	C13-C14-C15-C16
62	h	201	CDL	C71-CB7-OB8-CB6
67	Ac	402	HEM	C2A-CAA-CBA-CGA
67	Ac	403	HEM	C2A-CAA-CBA-CGA
70	AD	401	HEC	C2A-CAA-CBA-CGA
62	Ag	101	CDL	C31-CA7-OA8-CA6
58	I	302	PC1	C11-C12-N-C15
67	Ac	403	HEM	C3D-CAD-CBD-CGD
55	I	301	3PE	O32-C31-O31-C3
55	b	201	3PE	O32-C31-O31-C3
61	H	400	UQ9	C19-C21-C22-C23
69	Ac	406	UQ6	C9-C11-C12-C13
55	A	401	3PE	O22-C21-O21-C2
62	Ag	101	CDL	OA9-CA7-OA8-CA6
55	M	501	3PE	C22-C21-O21-C2
55	A	401	3PE	C11-O13-P-O11
55	I	301	3PE	C1-O11-P-O13
55	I	301	3PE	C11-O13-P-O11
55	J	202	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
55	L	702	3PE	C11-O13-P-O11
55	L	703	3PE	C1-O11-P-O13
55	L	704	3PE	C1-O11-P-O13
55	M	502	3PE	C11-O13-P-O11
55	M	503	3PE	C11-O13-P-O11
55	O	401	3PE	C11-O13-P-O11
55	AC	403	3PE	C11-O13-P-O11
55	AF	201	3PE	C1-O11-P-O13
55	AF	201	3PE	C11-O13-P-O11
58	I	302	PC1	C1-O11-P-O13
58	J	201	PC1	C11-O13-P-O11
62	L	705	CDL	CA2-OA2-PA1-OA5
62	L	706	CDL	CA2-OA2-PA1-OA5
62	L	706	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CB3-OB5-PB2-OB2
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2
62	AC	406	CDL	CA2-OA2-PA1-OA5
62	AC	406	CDL	CA3-OA5-PA1-OA2
62	AC	406	CDL	CB2-OB2-PB2-OB5
62	Ac	407	CDL	CB3-OB5-PB2-OB2
55	L	703	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
68	Ac	405	U10	C23-C24-C26-C27
58	J	201	PC1	C11-C12-N-C15
55	L	703	3PE	C24-C25-C26-C27
62	Aa	501	CDL	C11-CA5-OA6-CA4
55	AF	201	3PE	C34-C35-C36-C37
62	h	201	CDL	C18-C19-C20-C21
62	h	201	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	CB6-CB4-OB6-CB5
55	M	501	3PE	O22-C21-O21-C2
62	Aa	501	CDL	OA7-CA5-OA6-CA4
68	Ac	405	U10	C12-C11-C9-C10
68	Ac	405	U10	C20-C19-C21-C22
62	X	201	CDL	C61-C62-C63-C64
55	M	502	3PE	O13-C11-C12-N
55	L	703	3PE	O32-C31-O31-C3
62	a	101	CDL	OA9-CA7-OA8-CA6
68	Ac	405	U10	C12-C11-C9-C8
55	M	501	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
58	I	302	PC1	C11-C12-N-C13
58	J	201	PC1	C11-C12-N-C14
62	Ag	101	CDL	C74-C75-C76-C77
55	L	702	3PE	C22-C21-O21-C2
68	Ac	405	U10	C18-C19-C21-C22
55	Ac	401	3PE	O21-C21-C22-C23
62	Aa	501	CDL	C72-C71-CB7-OB8
55	Ac	404	3PE	C32-C31-O31-C3
62	L	706	CDL	CB5-C51-C52-C53
55	M	503	3PE	C39-C3A-C3B-C3C
55	A	401	3PE	C31-C32-C33-C34
62	X	201	CDL	C11-CA5-OA6-CA4
62	a	101	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	OA7-CA5-OA6-CA4
62	a	101	CDL	OB7-CB5-OB6-CB4
62	AC	406	CDL	OB6-CB4-CB6-OB8
58	I	302	PC1	C11-C12-N-C14
71	Ad	402	3PH	C25-C26-C27-C28
55	L	704	3PE	C27-C28-C29-C2A
55	M	501	3PE	C3C-C3D-C3E-C3F
55	L	702	3PE	O22-C21-O21-C2
55	I	301	3PE	C22-C21-O21-C2
55	AC	403	3PE	C22-C21-O21-C2
55	Ac	404	3PE	C22-C21-O21-C2
55	AC	403	3PE	C22-C23-C24-C25
62	L	705	CDL	CA3-OA5-PA1-OA2
62	L	706	CDL	CB2-OB2-PB2-OB5
62	h	201	CDL	CB3-OB5-PB2-OB2
71	AD	402	3PH	C1-C2-C3-O31
71	Ad	402	3PH	C1-C2-C3-O31
68	Ac	405	U10	C1-C6-C7-C8
62	L	706	CDL	C72-C73-C74-C75
55	L	704	3PE	C31-C32-C33-C34
55	Ac	404	3PE	O32-C31-O31-C3
55	L	704	3PE	C38-C39-C3A-C3B
55	Y	201	3PE	C2A-C2B-C2C-C2D
55	N	401	3PE	C37-C38-C39-C3A
55	L	707	3PE	C32-C31-O31-C3
62	L	705	CDL	CB6-CB4-OB6-CB5
62	AC	406	CDL	CA6-CA4-OA6-CA5
55	M	503	3PE	C2C-C2D-C2E-C2F
62	L	706	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
62	L	705	CDL	C56-C57-C58-C59
55	I	301	3PE	C24-C25-C26-C27
55	b	201	3PE	C2A-C2B-C2C-C2D
55	M	503	3PE	C2D-C2E-C2F-C2G
55	I	301	3PE	O22-C21-O21-C2
55	AC	403	3PE	O22-C21-O21-C2
55	N	401	3PE	C32-C33-C34-C35
55	J	202	3PE	C32-C31-O31-C3
58	B	303	PC1	C2-C1-O11-P
58	B	303	PC1	C32-C33-C34-C35
71	AD	402	3PH	C32-C31-O31-C3
62	AC	406	CDL	CB3-CB4-CB6-OB8
66	W	201	EHZ	N2-C15-C16-C17
66	n	201	EHZ	N2-C15-C16-C17
62	h	201	CDL	CB2-OB2-PB2-OB5
66	W	201	EHZ	C3-C4-C5-C6
55	Ag	102	3PE	C32-C31-O31-C3
55	L	707	3PE	O32-C31-O31-C3
66	n	201	EHZ	C3-C4-C5-C6
62	L	706	CDL	OA9-CA7-OA8-CA6
66	W	201	EHZ	C5-C6-C7-O1
66	n	201	EHZ	C5-C6-C7-O1
55	J	202	3PE	O21-C2-C3-O31
71	Ad	402	3PH	O21-C2-C3-O31
58	B	303	PC1	C32-C31-O31-C3
55	Ac	404	3PE	O22-C21-O21-C2
62	L	705	CDL	C1-CA2-OA2-PA1
62	Aa	501	CDL	C1-CB2-OB2-PB2
62	h	201	CDL	C14-C15-C16-C17
66	W	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	O2-C9-S1-C10
63	O	402	ADP	PB-O3A-PA-O5'
55	L	703	3PE	C28-C29-C2A-C2B
55	J	202	3PE	C22-C23-C24-C25
55	L	704	3PE	C22-C21-O21-C2
62	Ac	407	CDL	C51-CB5-OB6-CB4
69	Ac	406	UQ6	C5-C6-C7-C8
55	N	401	3PE	C32-C31-O31-C3
70	Ad	401	HEC	C3D-CAD-CBD-CGD
55	A	401	3PE	C3-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5
67	AC	401	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
55	L	704	3PE	C22-C23-C24-C25
62	L	705	CDL	C16-C17-C18-C19
55	J	202	3PE	C25-C26-C27-C28
55	L	701	3PE	C2-C1-O11-P
62	L	705	CDL	CA4-CA3-OA5-PA1
62	h	201	CDL	CB4-CB3-OB5-PB2
55	L	704	3PE	O22-C21-O21-C2
71	AD	402	3PH	O32-C31-O31-C3
55	L	701	3PE	O21-C2-C3-O31
55	J	202	3PE	O32-C31-O31-C3
64	P	401	NDP	C2B-O2B-P2B-O2X
55	Ag	102	3PE	O32-C31-O31-C3
58	B	303	PC1	O32-C31-O31-C3
62	Ac	407	CDL	OB7-CB5-OB6-CB4
55	Ac	404	3PE	C23-C24-C25-C26
71	Ad	402	3PH	C2-C3-O31-C31
55	O	401	3PE	C1-O11-P-O13
55	Ac	401	3PE	C1-O11-P-O13
62	L	705	CDL	CB2-OB2-PB2-OB5
55	A	401	3PE	C2E-C2F-C2G-C2H
55	L	701	3PE	C24-C25-C26-C27
55	A	401	3PE	C2-C1-O11-P
62	L	706	CDL	C1-CA2-OA2-PA1
62	a	101	CDL	CA4-CA3-OA5-PA1
62	AC	406	CDL	CA4-CA3-OA5-PA1
55	N	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C11-O13-P-O14
55	I	301	3PE	C1-O11-P-O12
55	I	301	3PE	C1-O11-P-O14
55	I	301	3PE	C11-O13-P-O14
55	J	202	3PE	C11-O13-P-O14
55	L	702	3PE	C11-O13-P-O12
55	L	703	3PE	C1-O11-P-O12
55	L	704	3PE	C1-O11-P-O14
55	L	707	3PE	C11-O13-P-O14
55	AF	201	3PE	C1-O11-P-O14
55	AF	201	3PE	C11-O13-P-O12
55	AF	201	3PE	C11-O13-P-O14
55	Ac	401	3PE	C1-O11-P-O14
58	J	201	PC1	C1-O11-P-O14
62	L	705	CDL	CA2-OA2-PA1-OA3
62	L	705	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
62	L	706	CDL	CA2-OA2-PA1-OA3
62	L	706	CDL	CA2-OA2-PA1-OA4
62	L	706	CDL	CA3-OA5-PA1-OA4
62	L	706	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CA2-OA2-PA1-OA4
62	X	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	AC	406	CDL	CB2-OB2-PB2-OB3
62	Aa	501	CDL	CA3-OA5-PA1-OA4
62	Ac	407	CDL	CB3-OB5-PB2-OB4
62	Ag	101	CDL	CB2-OB2-PB2-OB4
55	A	401	3PE	O11-C1-C2-C3
55	L	703	3PE	C34-C35-C36-C37
55	J	202	3PE	C12-C11-O13-P
55	M	502	3PE	C12-C11-O13-P
62	X	201	CDL	C59-C60-C61-C62
62	L	705	CDL	C77-C78-C79-C80
55	A	401	3PE	O11-C1-C2-O21
55	L	701	3PE	C1-C2-C3-O31
58	B	303	PC1	O13-C11-C12-N
58	J	201	PC1	O13-C11-C12-N
62	Ag	101	CDL	C54-C55-C56-C57
70	AD	401	HEC	C3A-C2A-CAA-CBA
55	I	301	3PE	O21-C2-C3-O31
62	L	706	CDL	C56-C57-C58-C59
55	AF	201	3PE	C35-C36-C37-C38
55	O	401	3PE	C2-C1-O11-P
55	Ac	401	3PE	C2-C1-O11-P
69	Ac	406	UQ6	C3-C4-O4-C4M
66	W	201	EHZ	O4-C15-C16-O5
66	n	201	EHZ	O4-C15-C16-O5
55	M	503	3PE	C21-C22-C23-C24
55	L	703	3PE	C3C-C3D-C3E-C3F
66	W	201	EHZ	C19-C17-C20-O6
66	n	201	EHZ	C19-C17-C20-O6
62	L	706	CDL	C71-CB7-OB8-CB6
55	M	503	3PE	C32-C31-O31-C3
55	L	707	3PE	C36-C37-C38-C39
55	O	401	3PE	C32-C33-C34-C35
55	L	707	3PE	C22-C21-O21-C2
55	b	201	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
55	M	503	3PE	O32-C31-O31-C3
55	L	707	3PE	C1-O11-P-O13
55	M	502	3PE	C1-O11-P-O13
62	X	201	CDL	CB2-OB2-PB2-OB5
62	a	101	CDL	CB2-OB2-PB2-OB5
55	M	503	3PE	C26-C27-C28-C29
62	L	705	CDL	C33-C34-C35-C36
71	AD	402	3PH	C2-C3-O31-C31
55	J	202	3PE	C1-C2-C3-O31
66	W	201	EHZ	C2-C3-C4-C5
66	n	201	EHZ	C2-C3-C4-C5
64	P	401	NDP	O4D-C1D-N1N-C6N
62	L	706	CDL	OB9-CB7-OB8-CB6
57	B	302	UQ1	C1-C2-O2-CM2
55	L	704	3PE	C29-C2A-C2B-C2C
55	L	704	3PE	C32-C33-C34-C35
62	X	201	CDL	CB4-CB3-OB5-PB2
62	a	101	CDL	C1-CB2-OB2-PB2
62	AC	406	CDL	CB4-CB3-OB5-PB2
62	Ac	407	CDL	C1-CA2-OA2-PA1
58	B	303	PC1	C34-C35-C36-C37
67	Ac	403	HEM	CAD-CBD-CGD-O1D
71	AD	402	3PH	C25-C26-C27-C28
55	M	501	3PE	C2B-C2C-C2D-C2E
55	M	501	3PE	O11-C1-C2-O21
62	L	705	CDL	OB9-CB7-OB8-CB6
62	Aa	501	CDL	CA4-CA6-OA8-CA7
62	L	706	CDL	C74-C75-C76-C77
55	M	502	3PE	C34-C35-C36-C37
55	J	202	3PE	C28-C29-C2A-C2B
55	L	707	3PE	O21-C2-C3-O31
62	L	706	CDL	CB4-CB3-OB5-PB2
55	M	503	3PE	C38-C39-C3A-C3B
55	L	707	3PE	O22-C21-O21-C2
64	P	401	NDP	C2D-C1D-N1N-C6N
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	AC	401	HEM	CAD-CBD-CGD-O1D
62	Aa	501	CDL	C33-C34-C35-C36
55	AC	403	3PE	C24-C25-C26-C27
55	L	707	3PE	C1-C2-C3-O31
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
55	I	301	3PE	C37-C38-C39-C3A
55	L	702	3PE	C38-C39-C3A-C3B
55	L	701	3PE	C3-C2-O21-C21
62	Aa	501	CDL	CA6-CA4-OA6-CA5
62	L	705	CDL	C71-CB7-OB8-CB6
58	J	201	PC1	C34-C35-C36-C37
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	AC	402	HEM	CAD-CBD-CGD-O1D
62	h	201	CDL	C31-CA7-OA8-CA6
55	M	502	3PE	C25-C26-C27-C28
55	Y	201	3PE	C27-C28-C29-C2A
55	b	201	3PE	C24-C25-C26-C27
55	M	501	3PE	C26-C27-C28-C29
58	I	302	PC1	C2E-C2F-C2G-C2H
67	AC	401	HEM	CAA-CBA-CGA-O2A
67	Ac	403	HEM	CAD-CBD-CGD-O2D
64	P	401	NDP	PN-O3-PA-O2A
62	h	201	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C12-C11-C9-C10
71	Ad	402	3PH	C37-C38-C39-C3A
67	Ac	402	HEM	CAD-CBD-CGD-O2D
55	I	301	3PE	C35-C36-C37-C38
55	I	301	3PE	C33-C34-C35-C36
55	M	501	3PE	O11-C1-C2-C3
55	L	701	3PE	C36-C37-C38-C39
62	Ag	101	CDL	C11-C12-C13-C14
63	O	402	ADP	O4'-C4'-C5'-O5'
60	F	501	FMN	C5'-O5'-P-O2P
66	W	201	EHZ	N2-C15-C16-O5
66	n	201	EHZ	N2-C15-C16-O5
71	AD	402	3PH	C1-O11-P-O13
55	M	503	3PE	C33-C34-C35-C36
66	W	201	EHZ	C18-C17-C20-O6
66	n	201	EHZ	C18-C17-C20-O6
55	L	701	3PE	C32-C31-O31-C3
55	L	703	3PE	C3D-C3E-C3F-C3G
62	X	201	CDL	C12-C11-CA5-OA6
55	Ac	401	3PE	C1-C2-O21-C21
66	W	201	EHZ	C8-C9-S1-C10
55	N	401	3PE	C33-C34-C35-C36
62	L	706	CDL	C34-C35-C36-C37
55	M	502	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
62	L	706	CDL	C52-C51-CB5-OB6
68	Ac	405	U10	C5-C4-O4-C4M
69	AC	405	UQ6	C14-C16-C17-C18
62	L	706	CDL	C19-C20-C21-C22
55	L	704	3PE	C2-C1-O11-P
62	L	706	CDL	C55-C56-C57-C58
71	AD	402	3PH	O22-C21-O21-C2
55	Ac	404	3PE	O21-C21-C22-C23
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	403	HEM	CAA-CBA-CGA-O1A
66	W	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C18
62	X	201	CDL	OA6-CA4-CA6-OA8
62	Aa	501	CDL	C72-C71-CB7-OB9
67	Ac	403	HEM	CAA-CBA-CGA-O2A
64	P	401	NDP	C2B-O2B-P2B-O3X
66	W	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C18
55	L	701	3PE	O32-C31-O31-C3
62	X	201	CDL	C52-C51-CB5-OB6
69	Ac	406	UQ6	C5-C4-O4-C4M
55	L	707	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C39-C3A-C3B-C3C
62	a	101	CDL	C32-C31-CA7-OA8
55	M	502	3PE	C22-C21-O21-C2
62	X	201	CDL	C12-C11-CA5-OA7
55	L	703	3PE	C39-C3A-C3B-C3C
61	H	400	UQ9	C12-C11-C9-C8
55	M	502	3PE	O22-C21-C22-C23
55	Ac	404	3PE	O22-C21-C22-C23
55	M	501	3PE	C39-C3A-C3B-C3C
62	L	706	CDL	C52-C51-CB5-OB7
55	Ac	401	3PE	O22-C21-C22-C23
62	Ac	407	CDL	C71-CB7-OB8-CB6
55	I	301	3PE	C1-C2-C3-O31
55	L	702	3PE	C1-O11-P-O13
62	Aa	501	CDL	O1-C1-CA2-OA2
55	Ac	404	3PE	C2-C3-O31-C31
55	L	702	3PE	C1-O11-P-O14
62	X	201	CDL	CA2-OA2-PA1-OA3
62	Aa	501	CDL	CB3-OB5-PB2-OB3
55	A	401	3PE	O13-C11-C12-N

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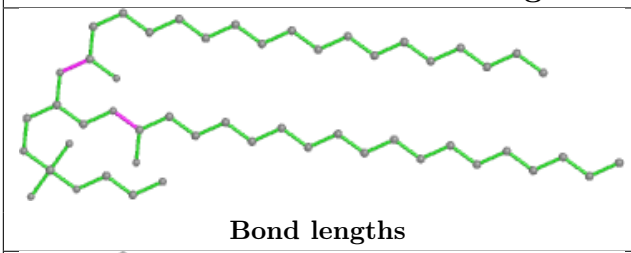
Mol	Chain	Res	Type	Atoms
55	L	701	3PE	O13-C11-C12-N
55	Ac	401	3PE	C3-C2-O21-C21
58	I	302	PC1	C12-C11-O13-P
66	W	201	EHZ	O4-C15-C16-C17
66	n	201	EHZ	O4-C15-C16-C17
62	X	201	CDL	CA5-C11-C12-C13
62	L	705	CDL	C20-C21-C22-C23
55	L	704	3PE	C2B-C2C-C2D-C2E
71	Ad	402	3PH	C23-C24-C25-C26
62	X	201	CDL	C52-C51-CB5-OB7
62	a	101	CDL	OA7-CA5-OA6-CA4
55	I	301	3PE	C2-C1-O11-P
55	L	701	3PE	O21-C21-C22-C23
62	h	201	CDL	C72-C71-CB7-OB8
62	Ac	407	CDL	OB9-CB7-OB8-CB6
55	L	707	3PE	C2B-C2C-C2D-C2E
62	a	101	CDL	C32-C31-CA7-OA9
70	Ad	401	HEC	CAA-CBA-CGA-O2A
55	b	201	3PE	C39-C3A-C3B-C3C
58	I	302	PC1	C2C-C2D-C2E-C2F
62	Aa	501	CDL	C12-C11-CA5-OA6

There are no ring outliers.

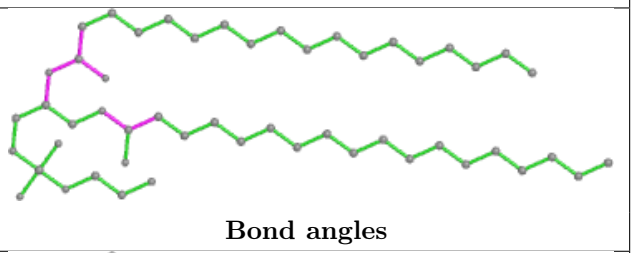
No monomer is involved in short contacts.

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.

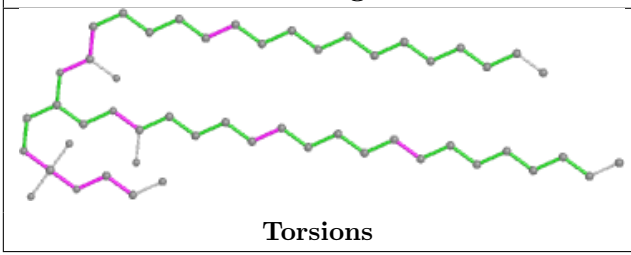
Ligand 3PE M 502



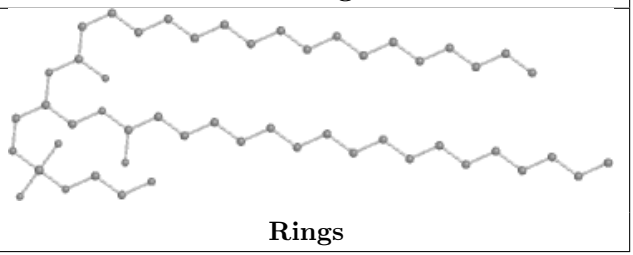
Bond lengths



Bond angles

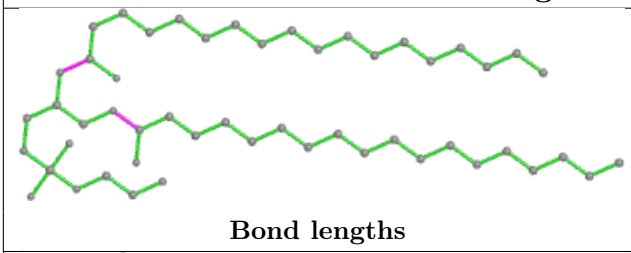


Torsions

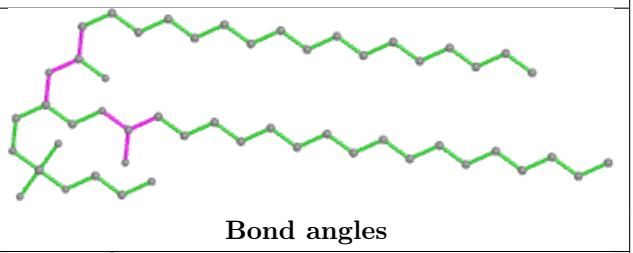


Rings

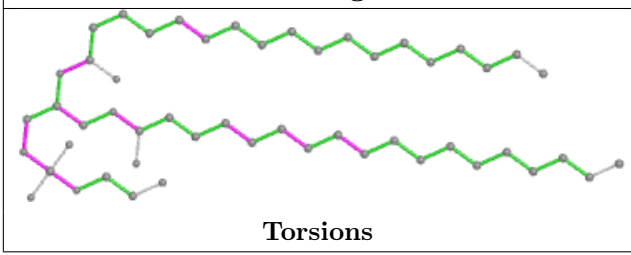
Ligand 3PE I 301



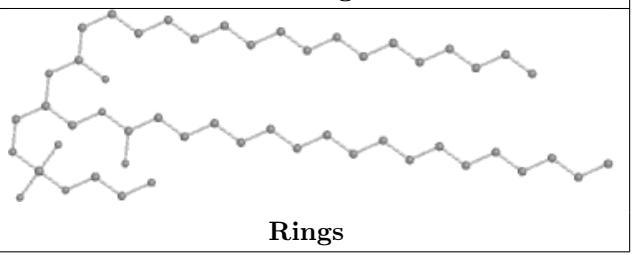
Bond lengths



Bond angles

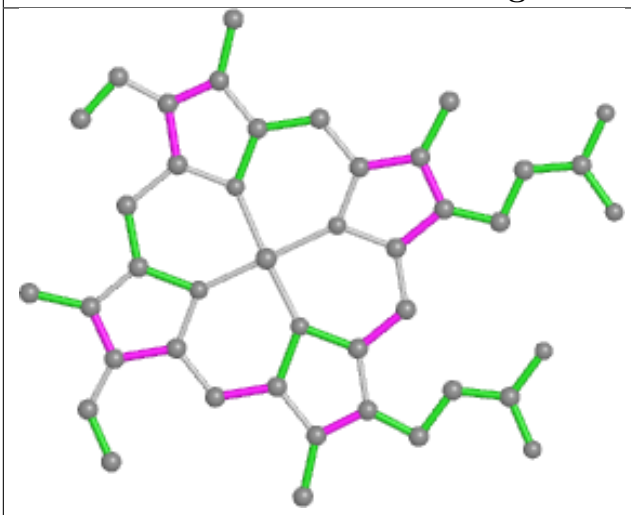


Torsions

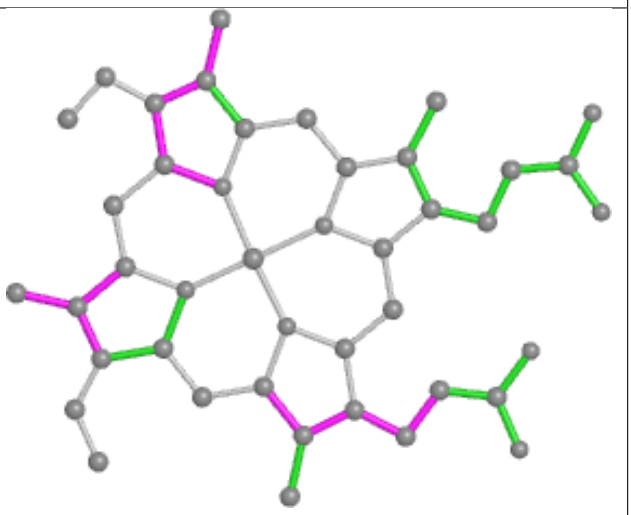


Rings

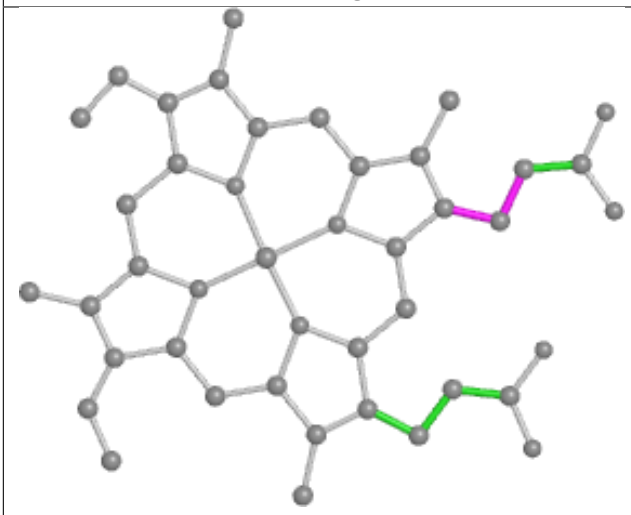
Ligand HEC AD 401



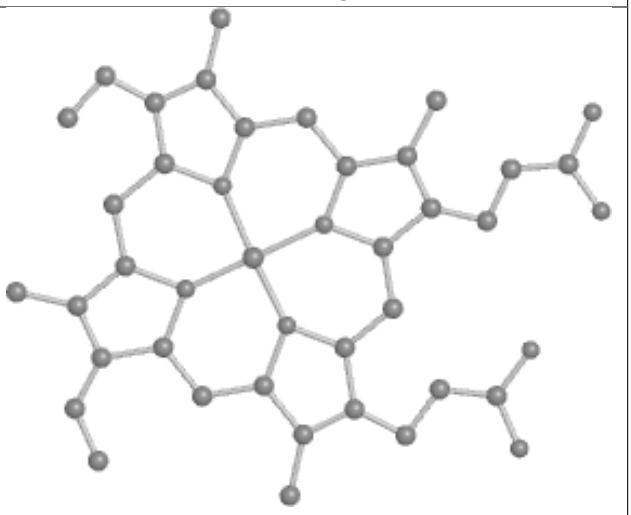
Bond lengths



Bond angles

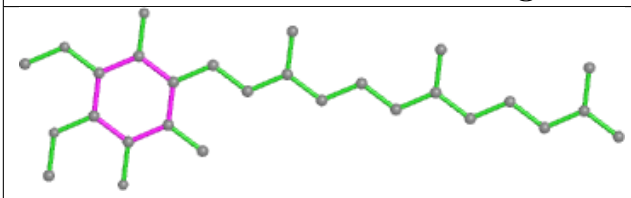


Torsions

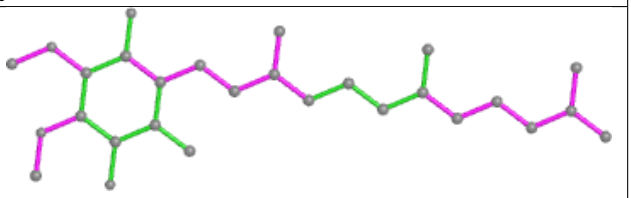


Rings

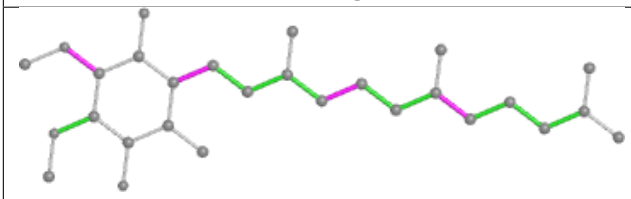
Ligand UQ6 Ac 406



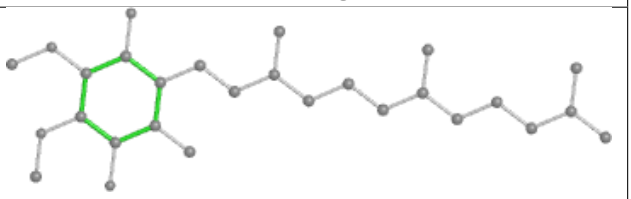
Bond lengths



Bond angles

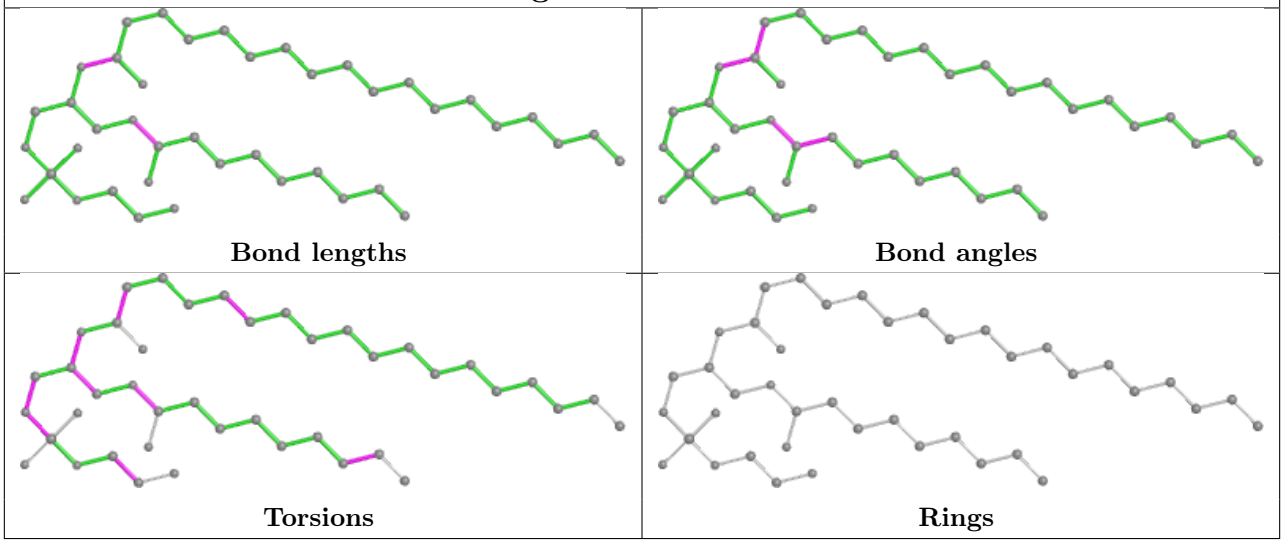


Torsions

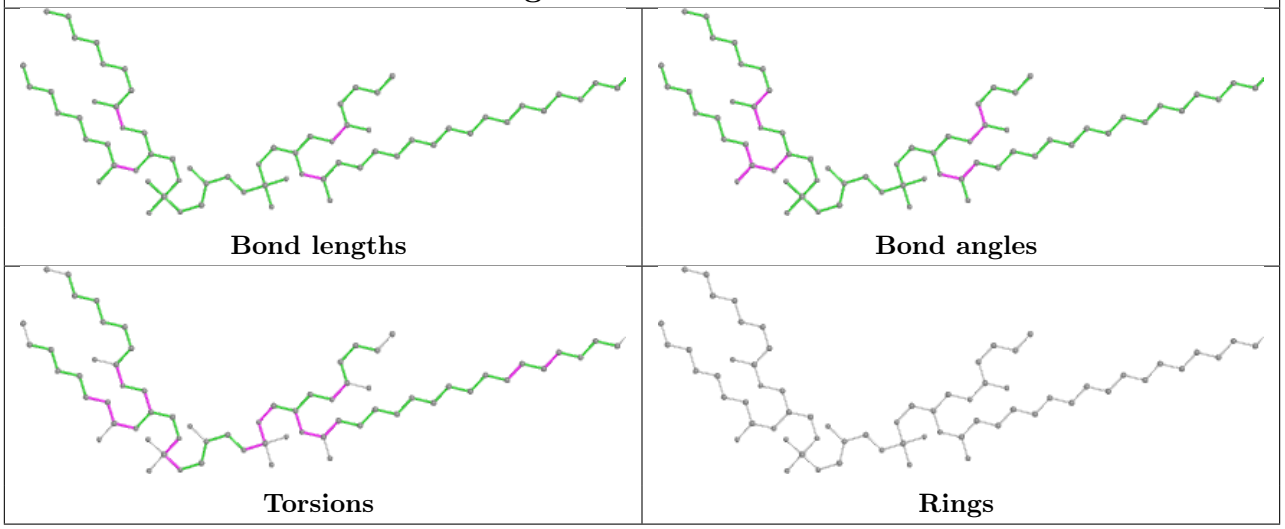


Rings

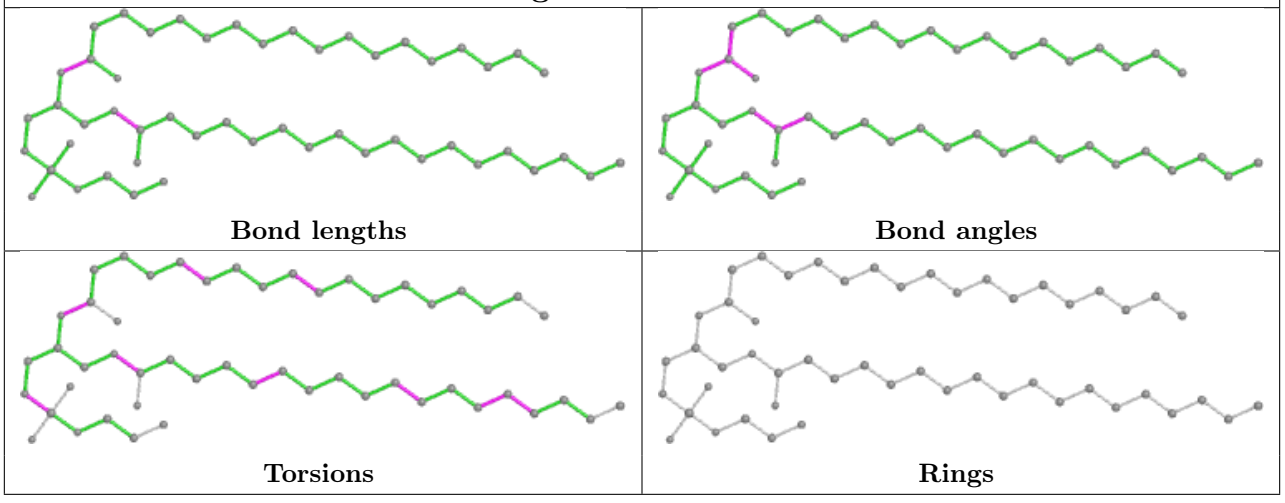
Ligand 3PE L 701



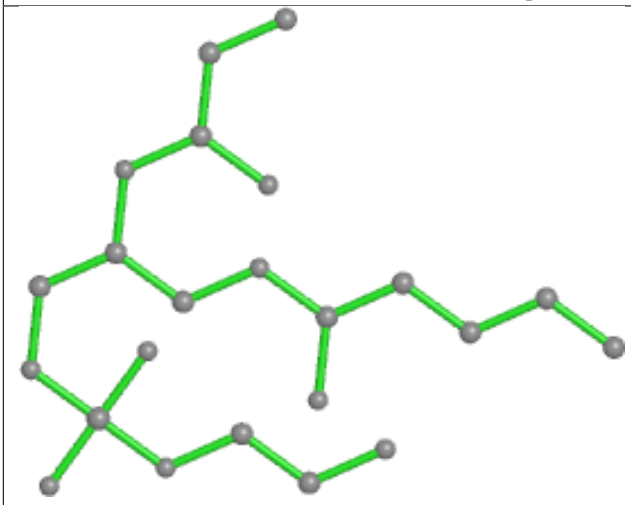
Ligand CDL X 201



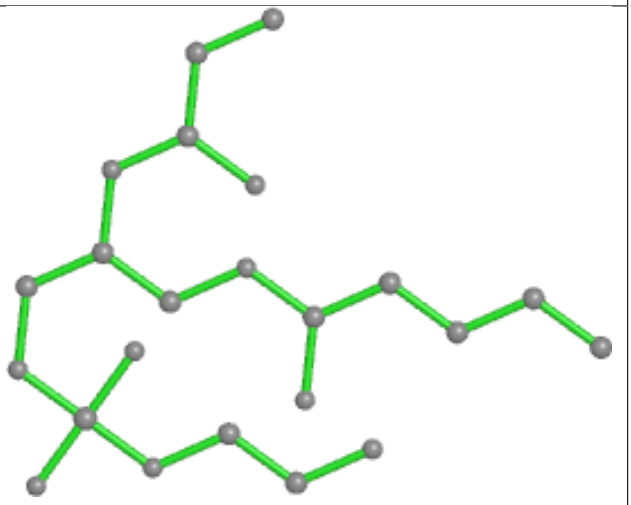
Ligand 3PE L 703



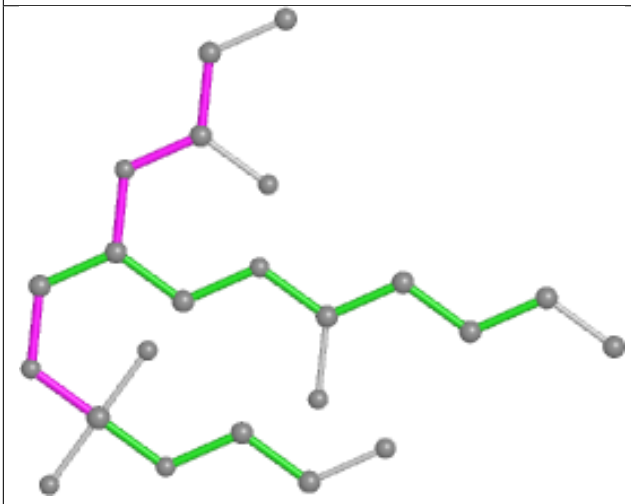
Ligand 3PE Ac 401



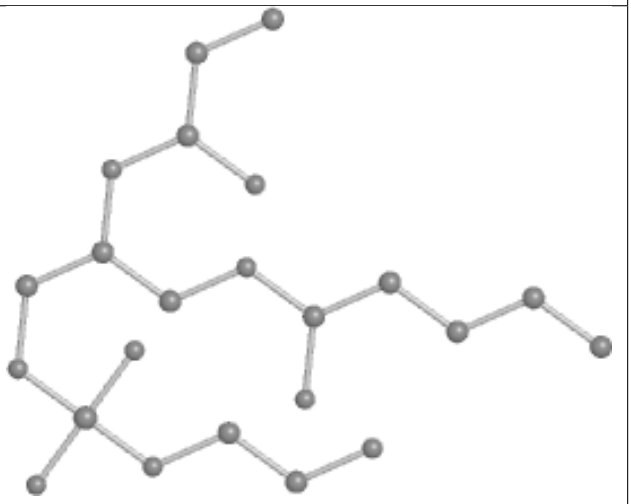
Bond lengths



Bond angles

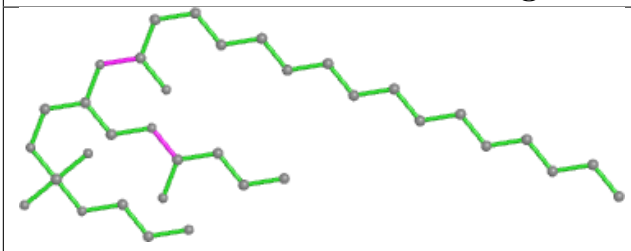


Torsions

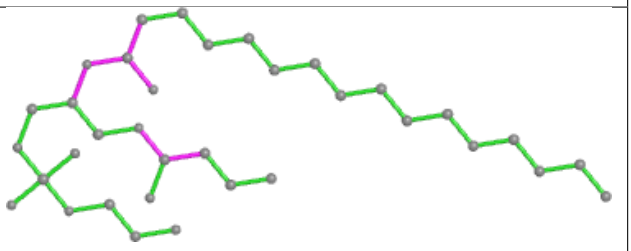


Rings

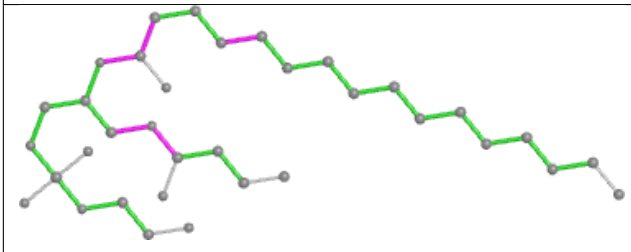
Ligand 3PE Ac 404



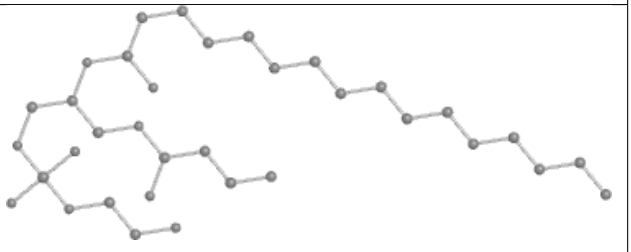
Bond lengths



Bond angles

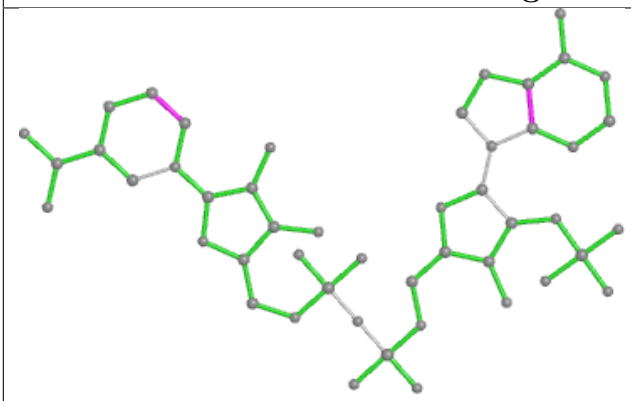


Torsions

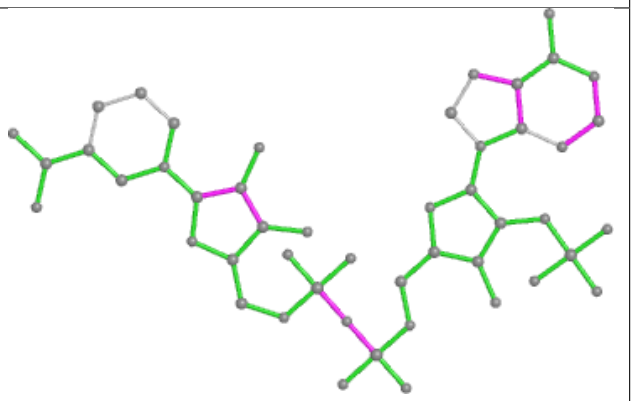


Rings

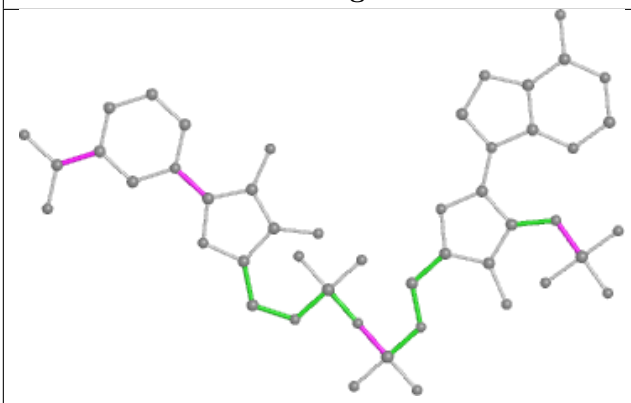
Ligand NDP P 401



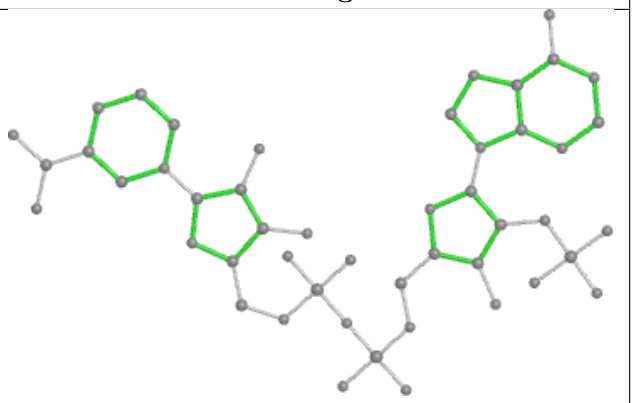
Bond lengths



Bond angles

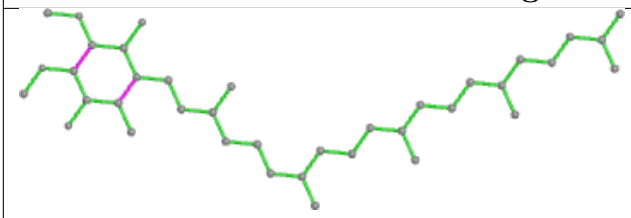


Torsions

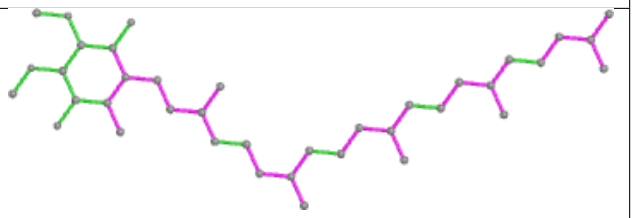


Rings

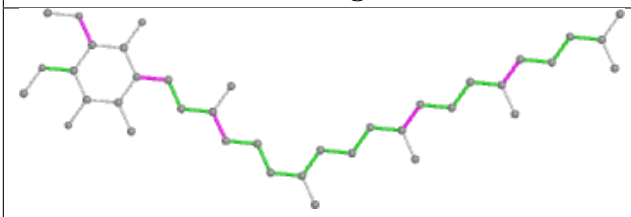
Ligand U10 Ac 405



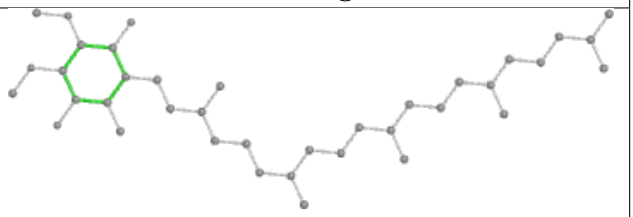
Bond lengths



Bond angles

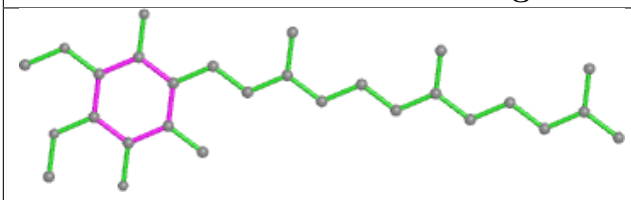


Torsions

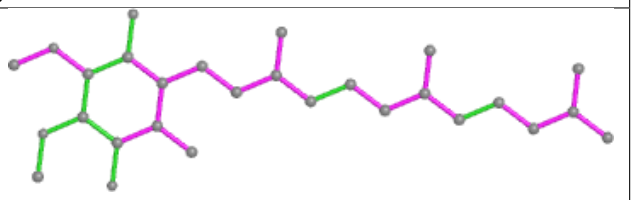


Rings

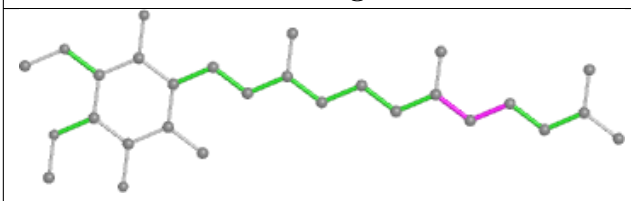
Ligand UQ6 AC 405



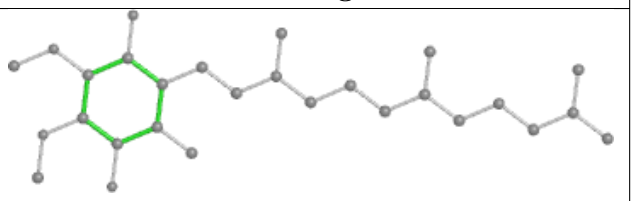
Bond lengths



Bond angles

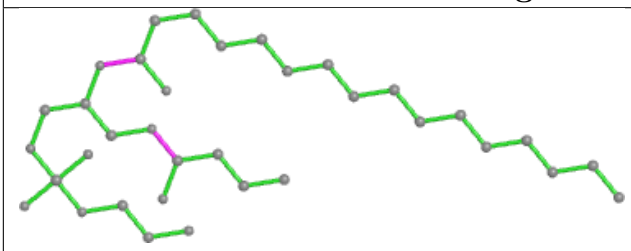


Torsions

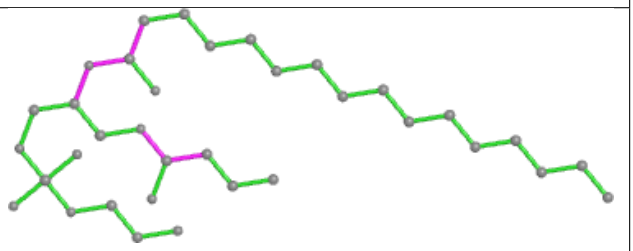


Rings

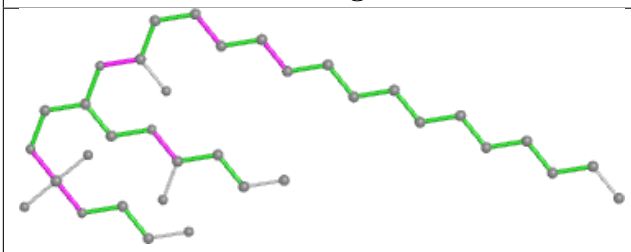
Ligand 3PE AC 403



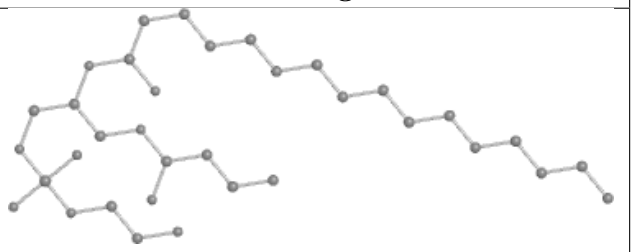
Bond lengths



Bond angles

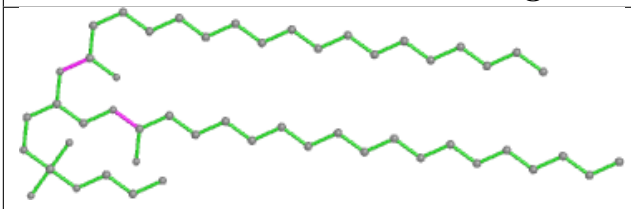


Torsions

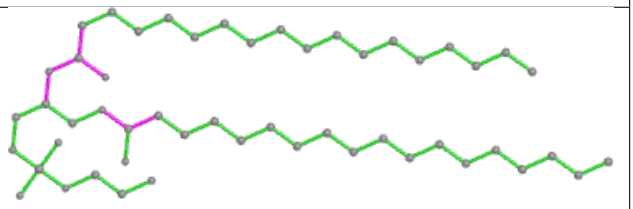


Rings

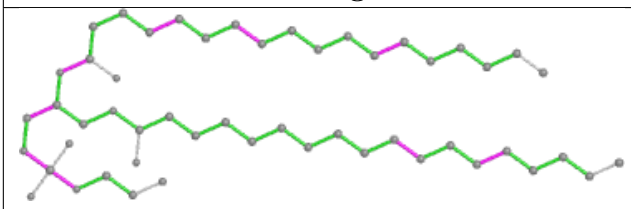
Ligand 3PE M 501



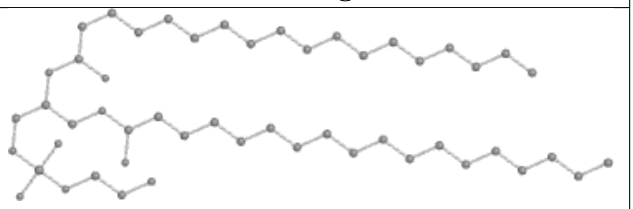
Bond lengths



Bond angles

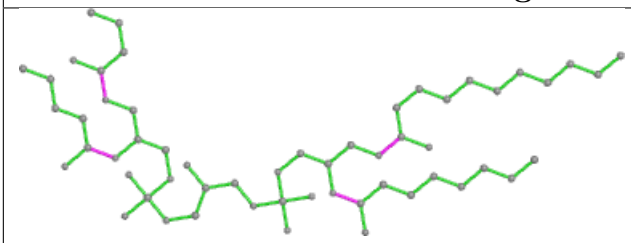


Torsions

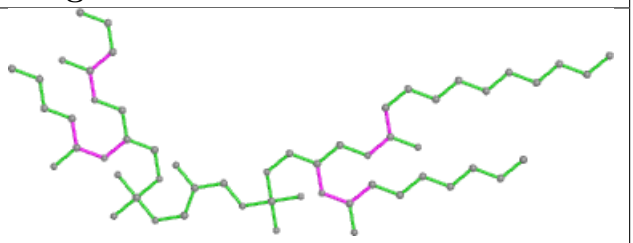


Rings

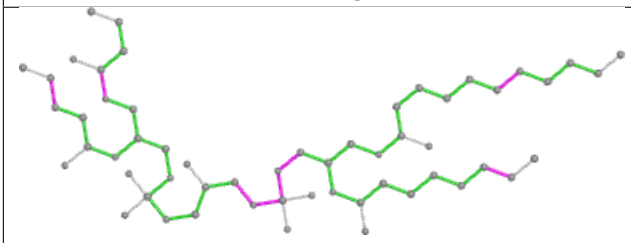
Ligand CDL Ag 101



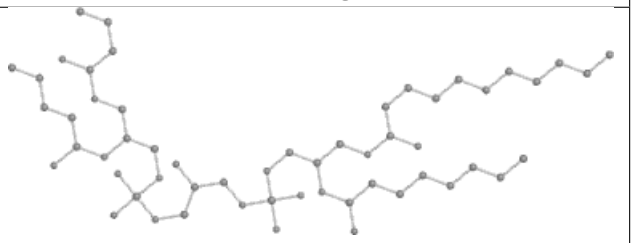
Bond lengths



Bond angles

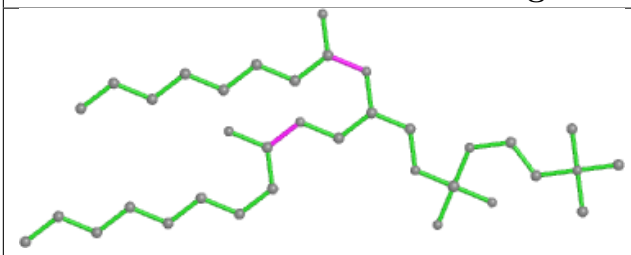


Torsions

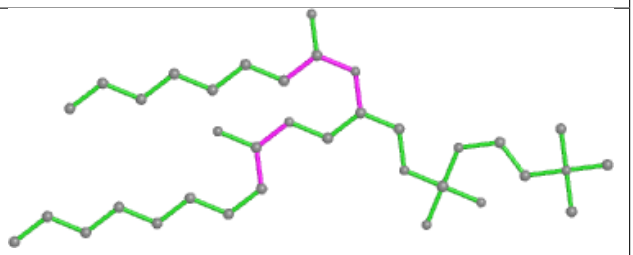


Rings

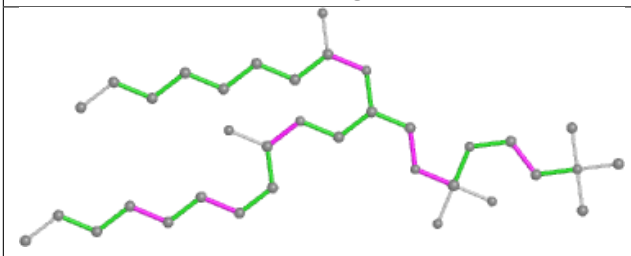
Ligand PC1 B 303



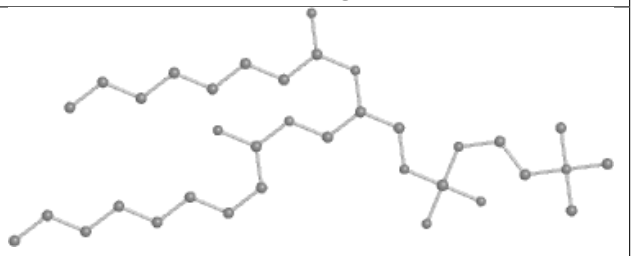
Bond lengths



Bond angles

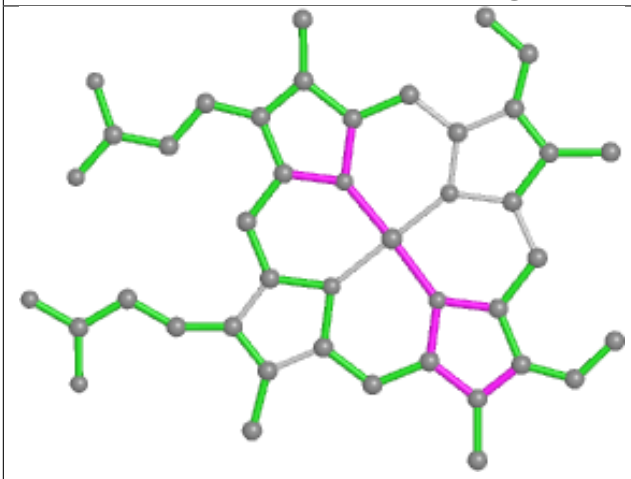


Torsions

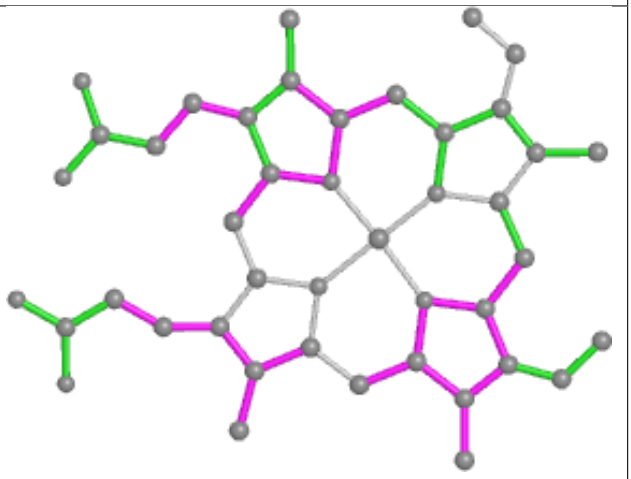


Rings

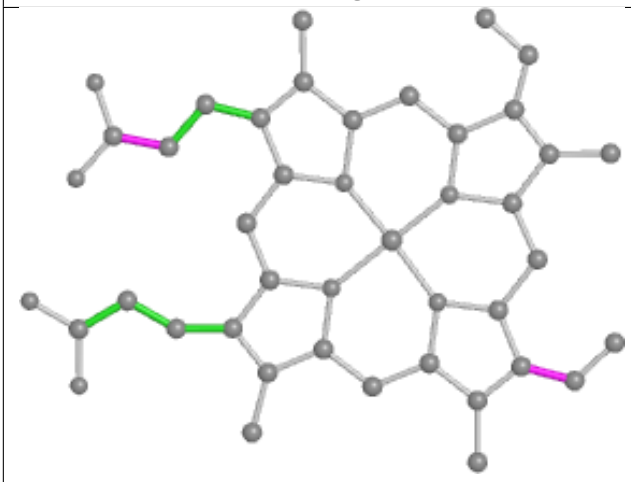
Ligand HEM AC 402



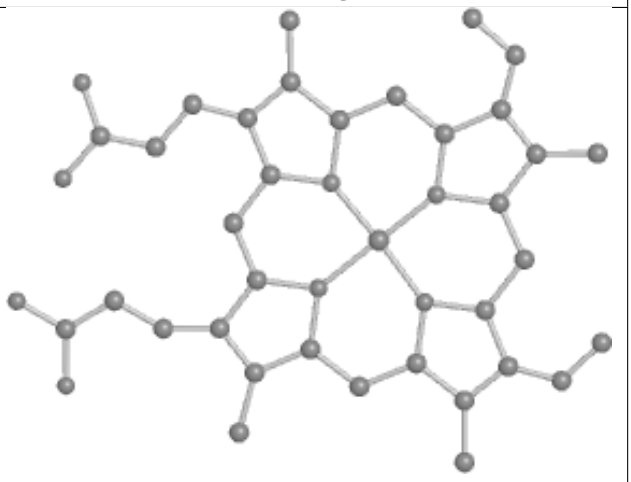
Bond lengths



Bond angles

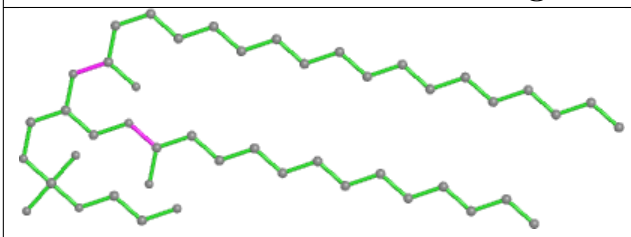


Torsions

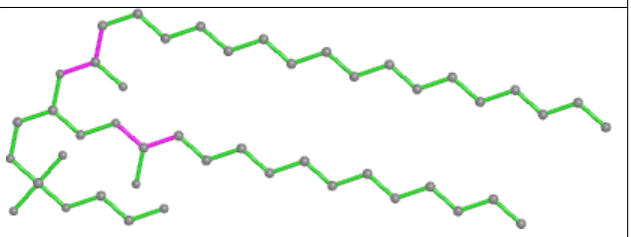


Rings

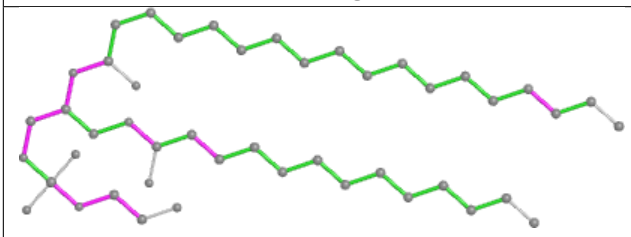
Ligand 3PE A 401



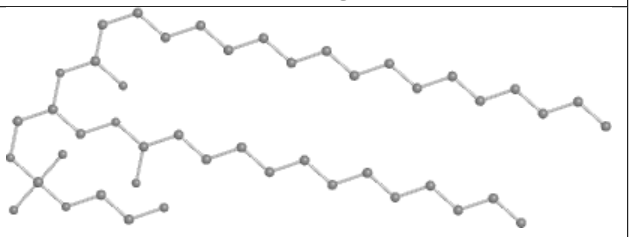
Bond lengths



Bond angles

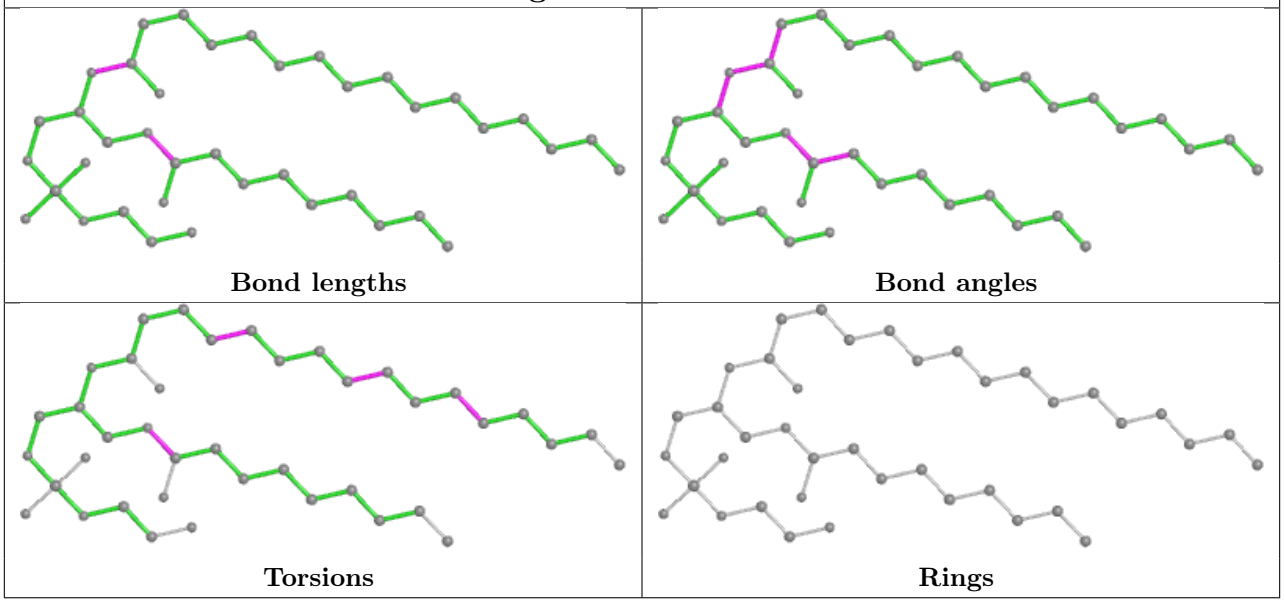


Torsions

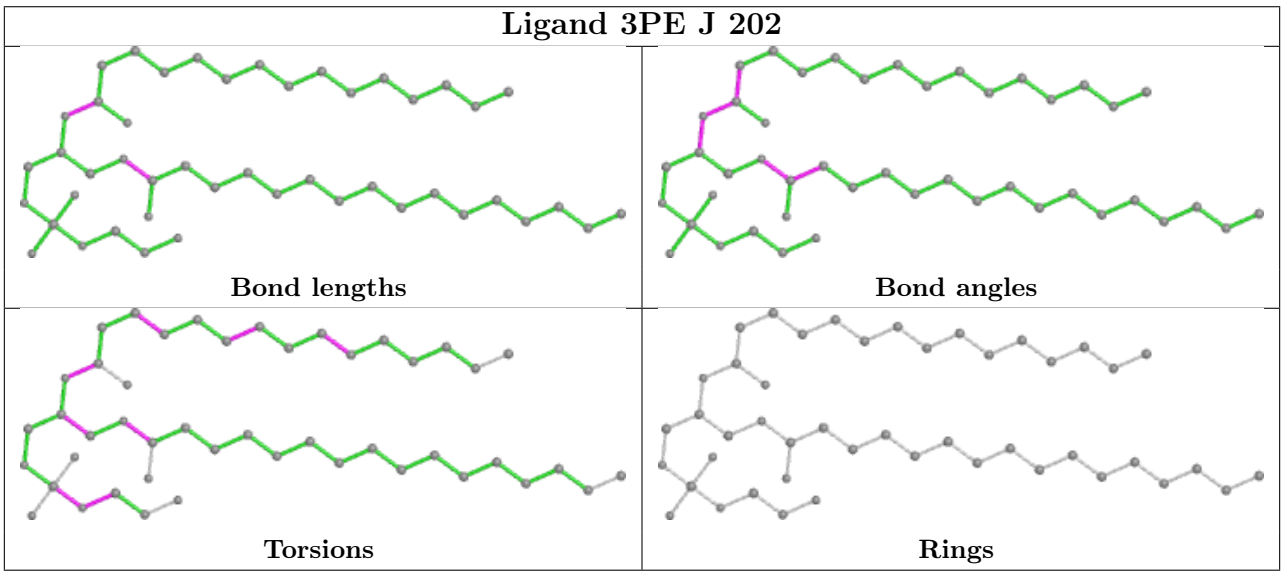


Rings

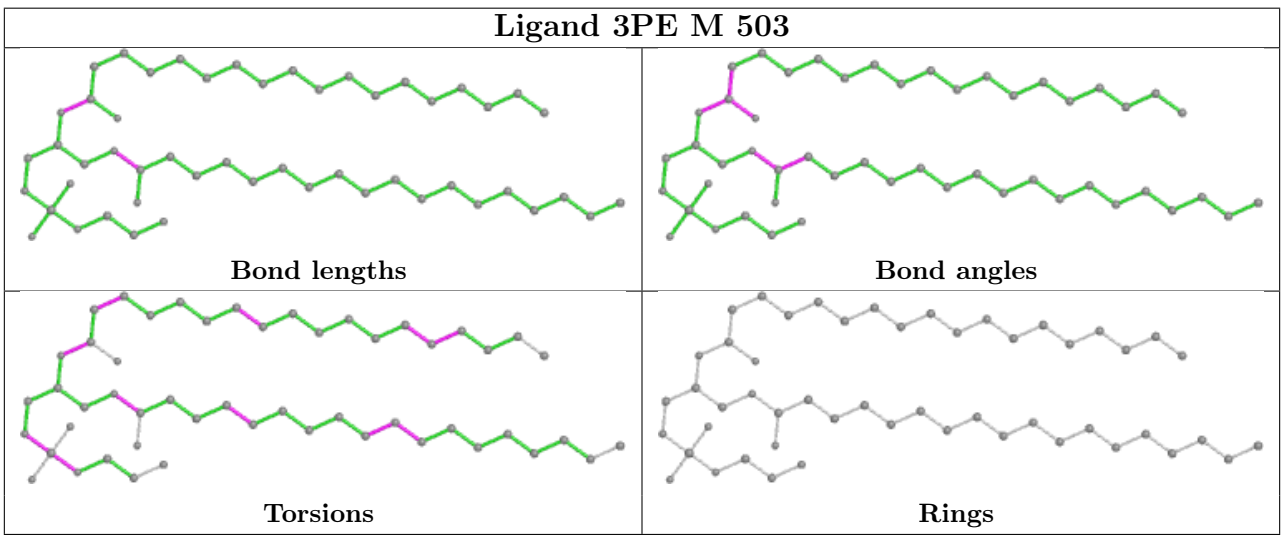
Ligand 3PE Y 201



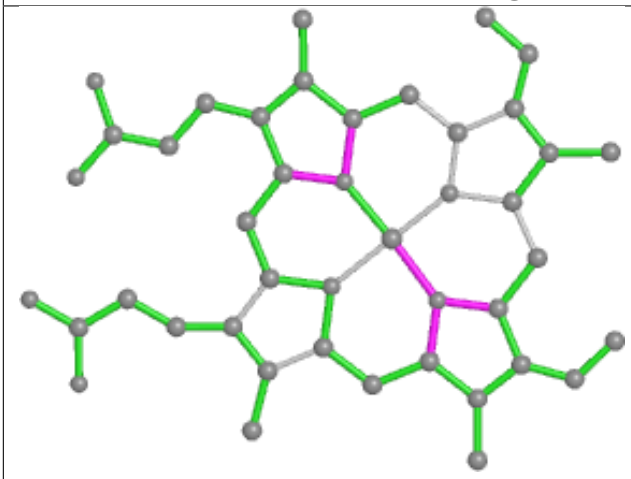
Ligand 3PE J 202



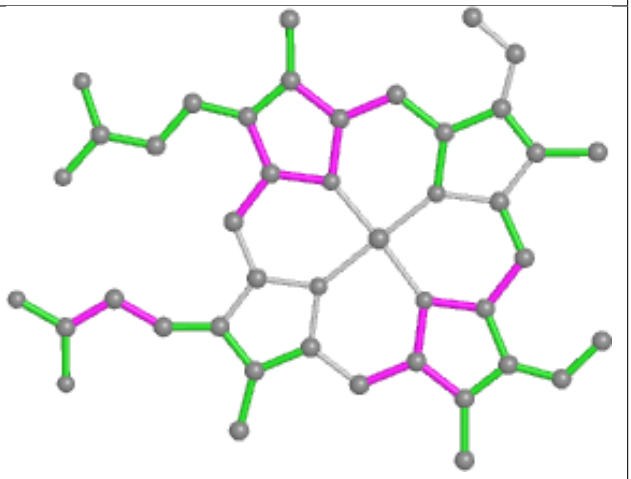
Ligand 3PE M 503



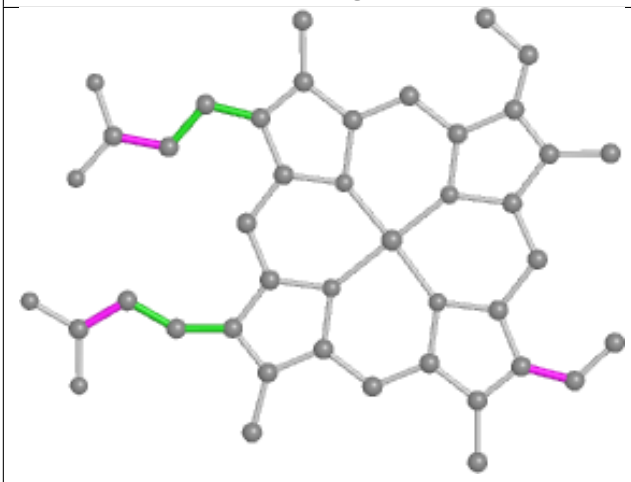
Ligand HEM AC 401



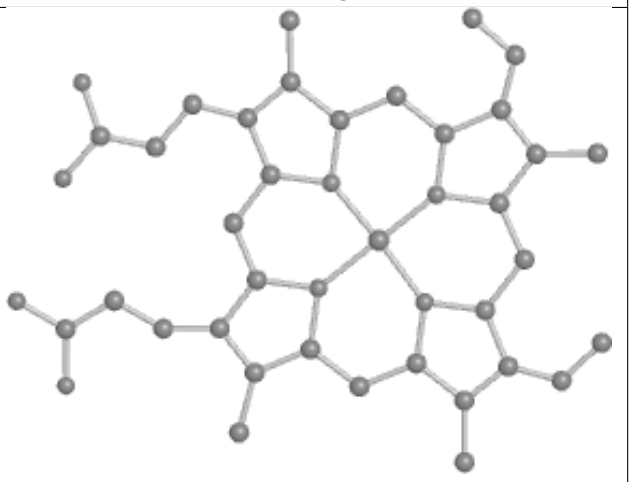
Bond lengths



Bond angles

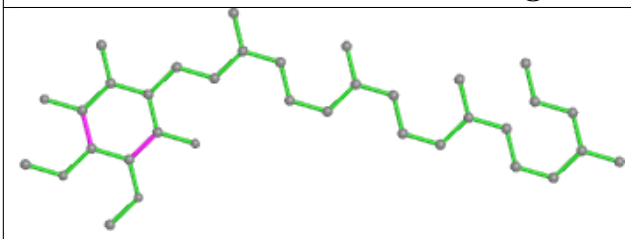


Torsions

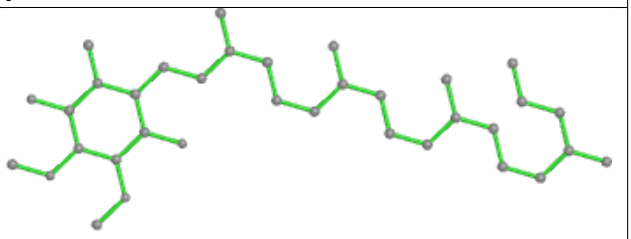


Rings

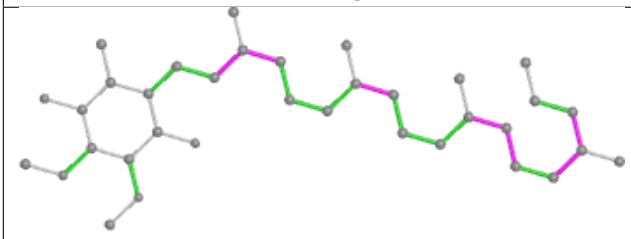
Ligand UQ9 H 400



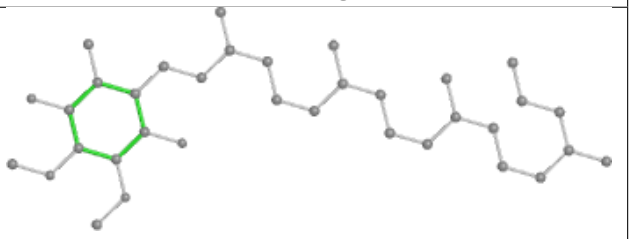
Bond lengths



Bond angles

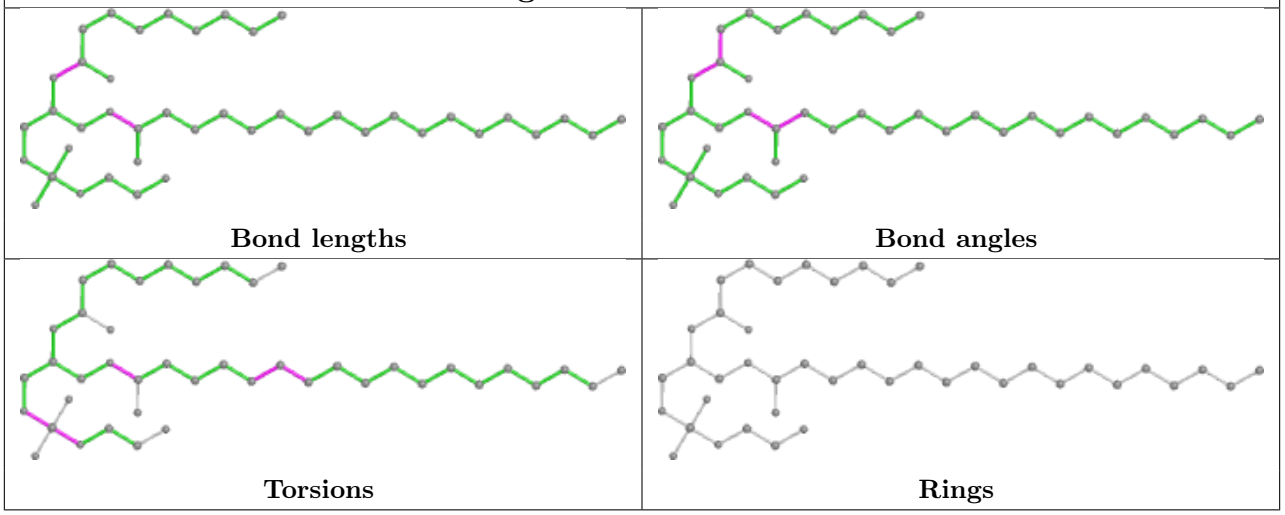


Torsions

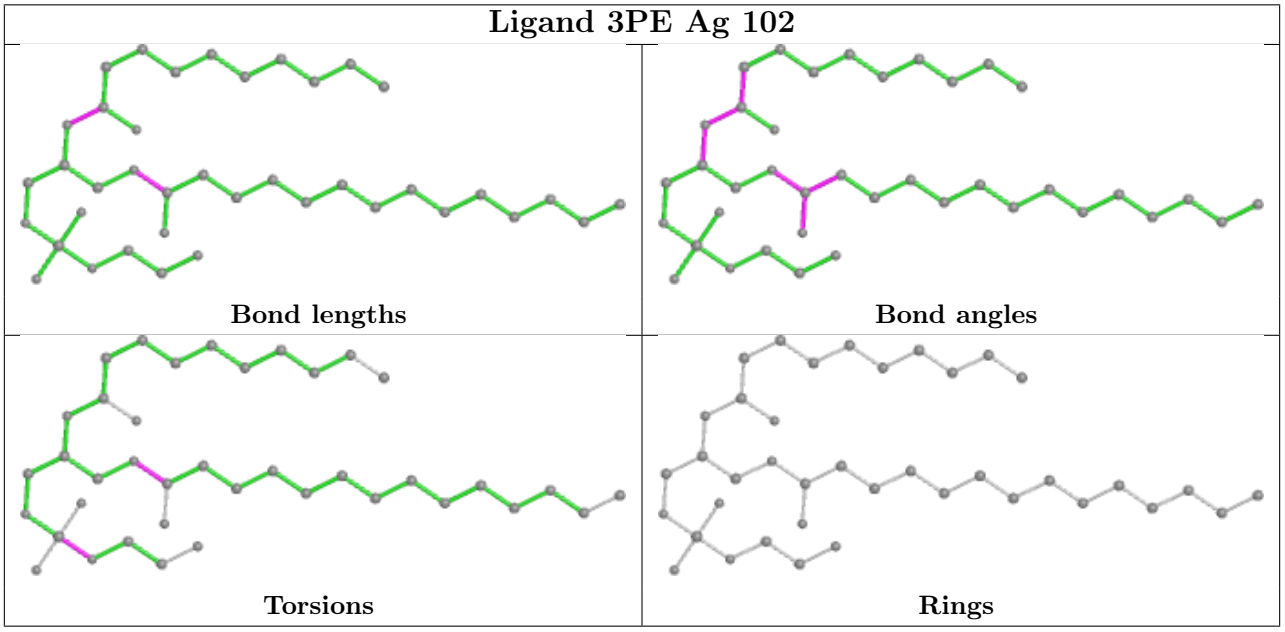


Rings

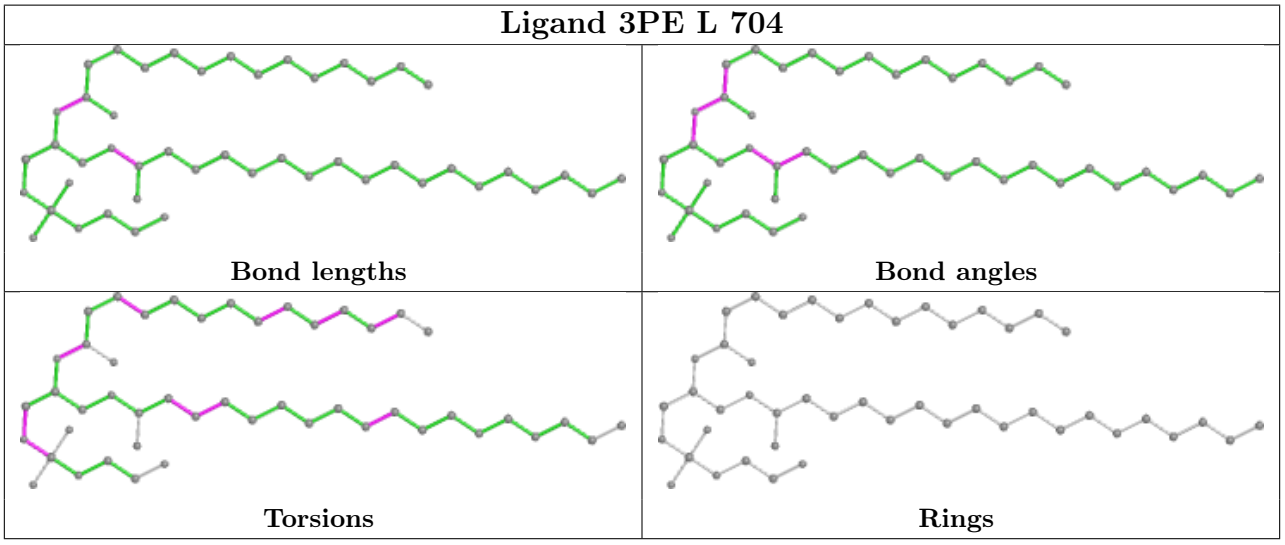
Ligand 3PE AF 201



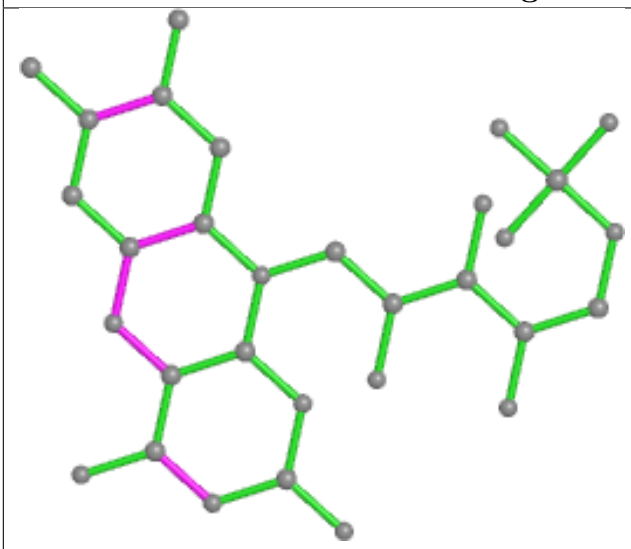
Ligand 3PE Ag 102



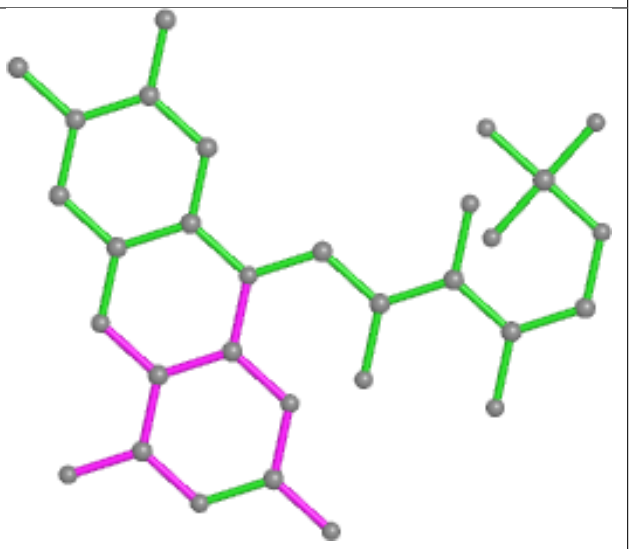
Ligand 3PE L 704



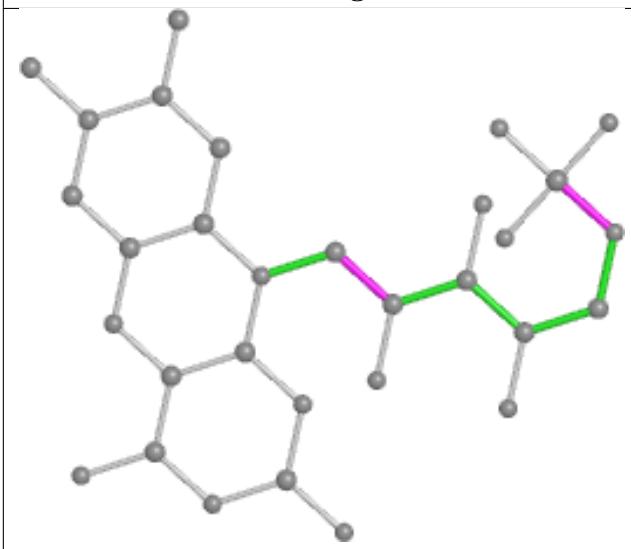
Ligand FMN F 501



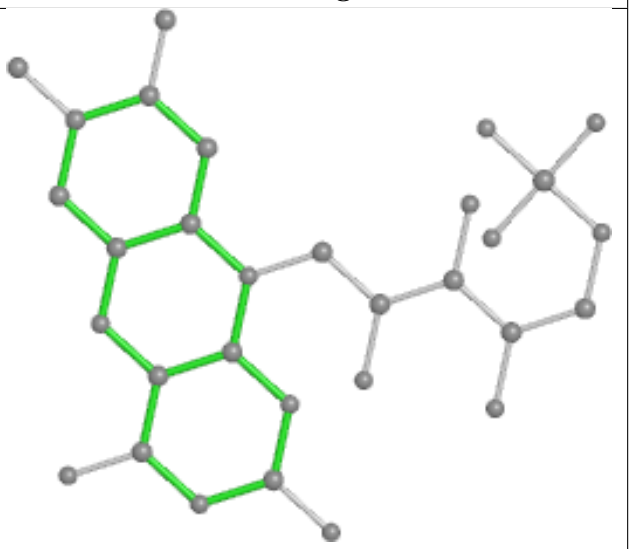
Bond lengths



Bond angles

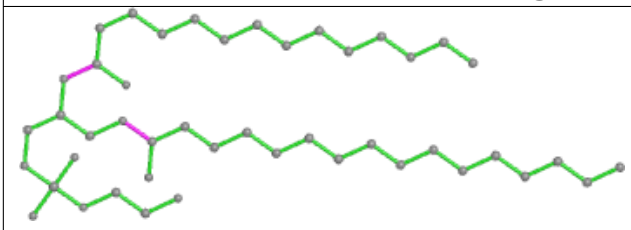


Torsions

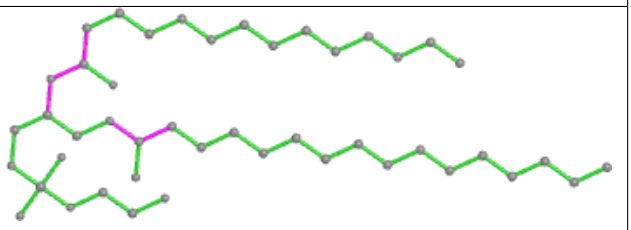


Rings

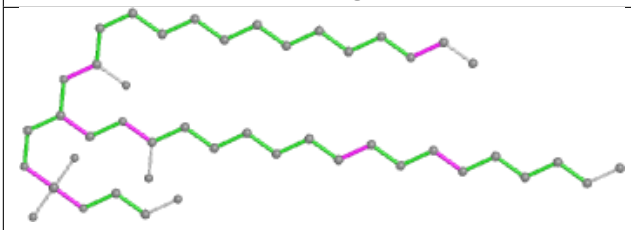
Ligand 3PE L 707



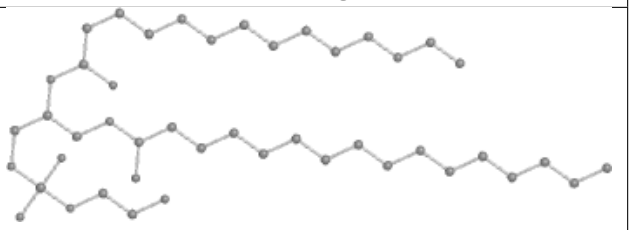
Bond lengths



Bond angles

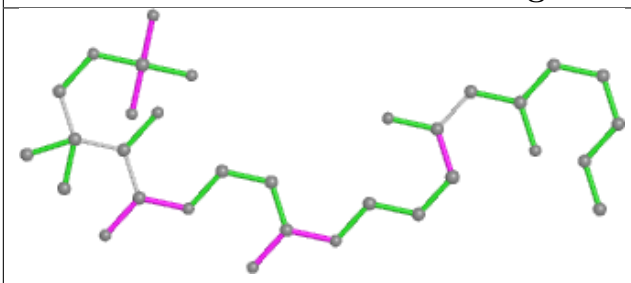


Torsions

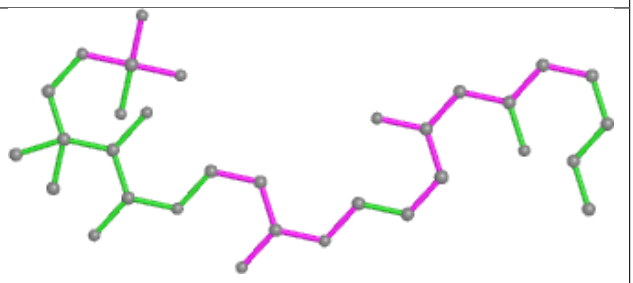


Rings

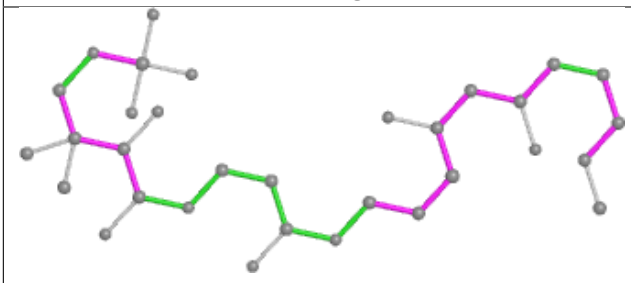
Ligand EHZ n 201



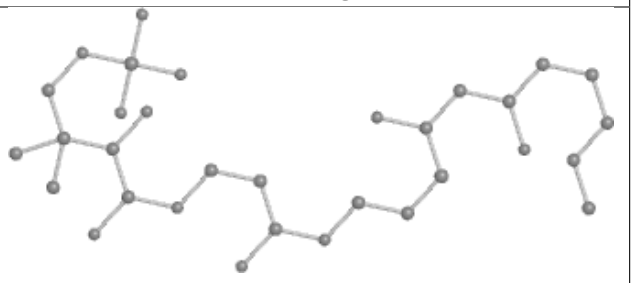
Bond lengths



Bond angles

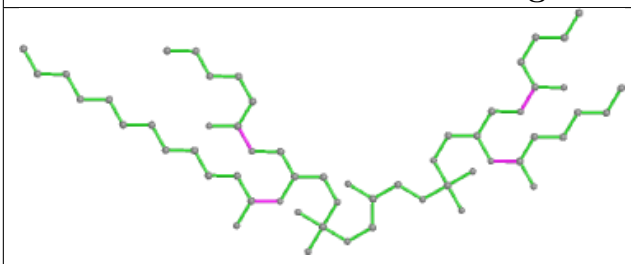


Torsions

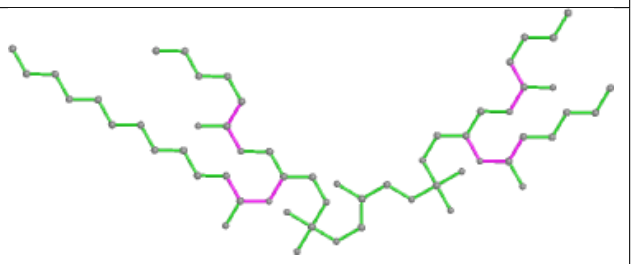


Rings

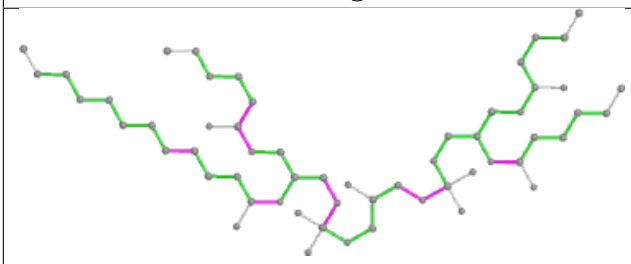
Ligand CDL a 101



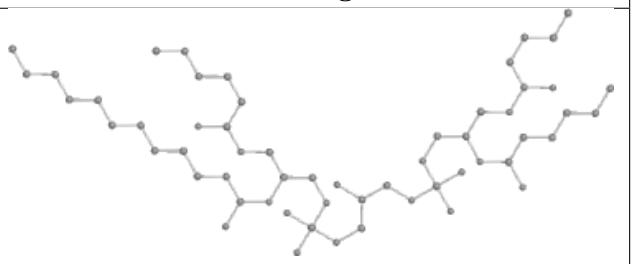
Bond lengths



Bond angles

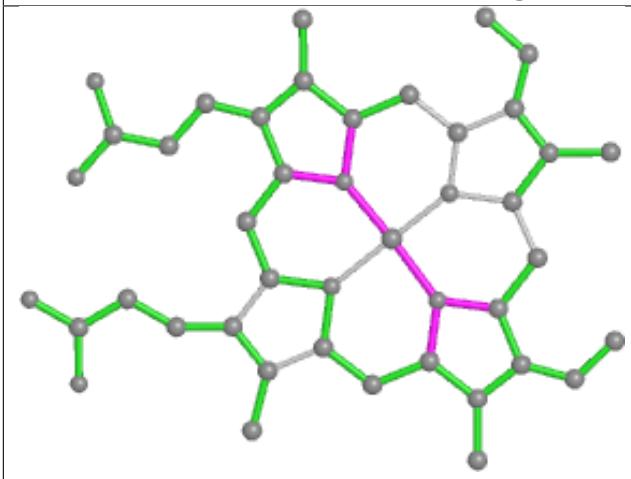


Torsions

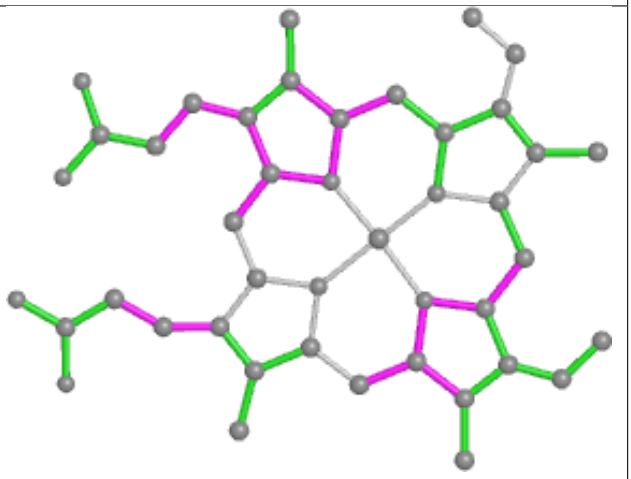


Rings

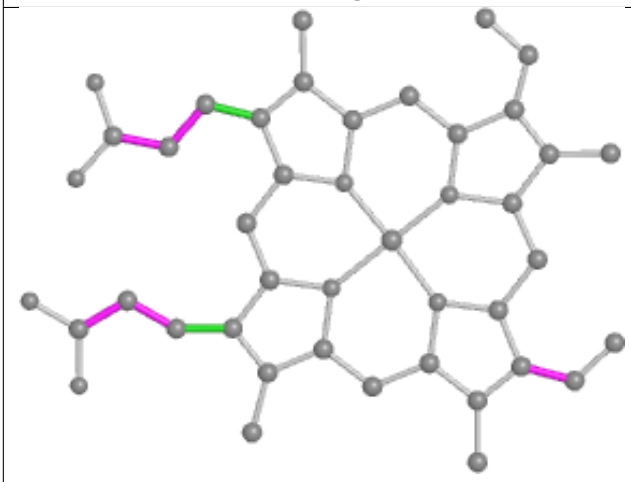
Ligand HEM Ac 403



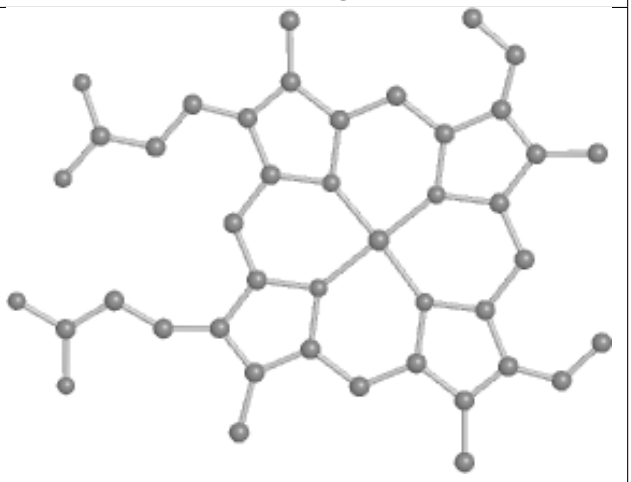
Bond lengths



Bond angles

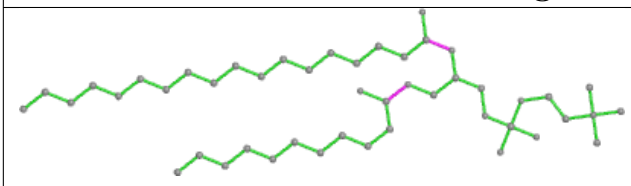


Torsions

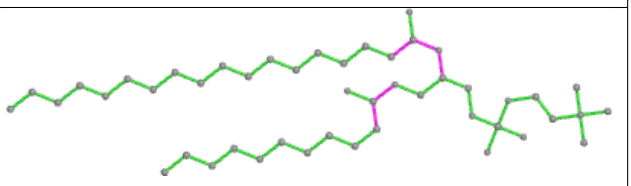


Rings

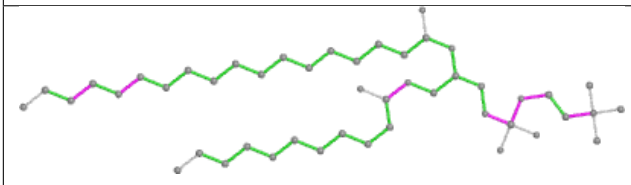
Ligand PC1 I 302



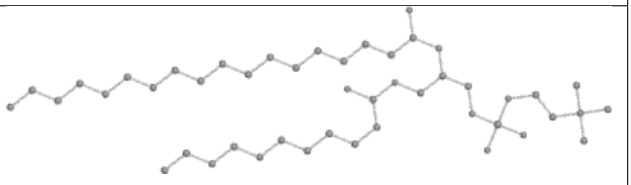
Bond lengths



Bond angles

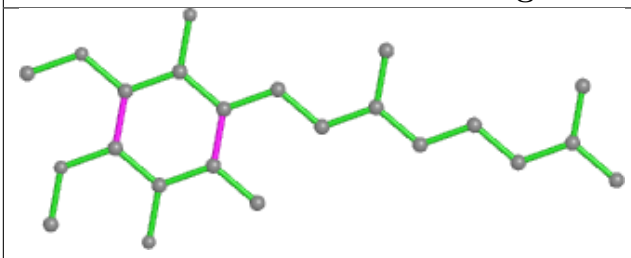


Torsions

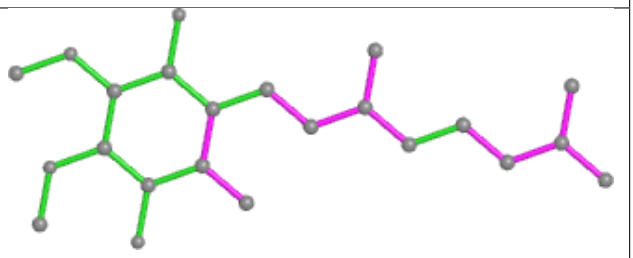


Rings

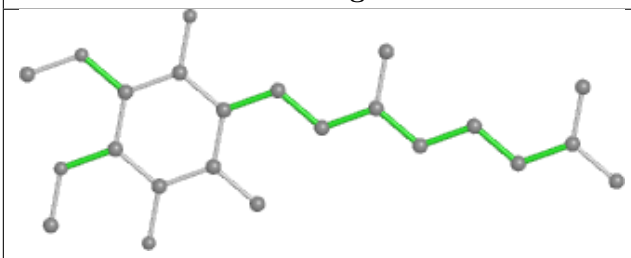
Ligand U10 AC 404



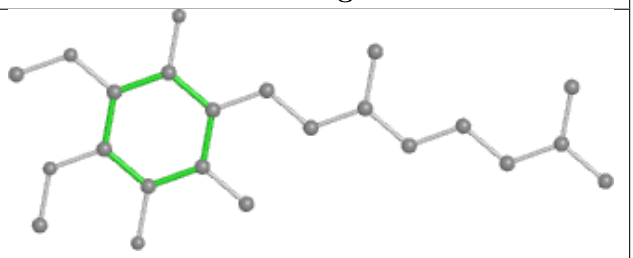
Bond lengths



Bond angles

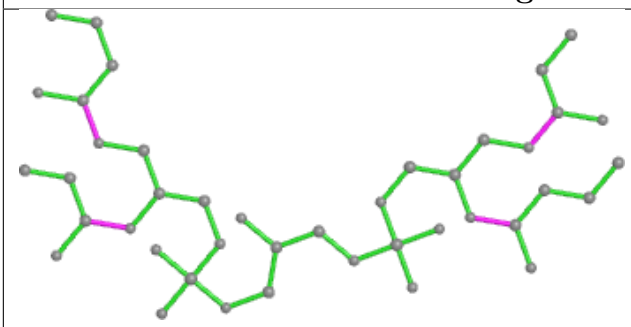


Torsions

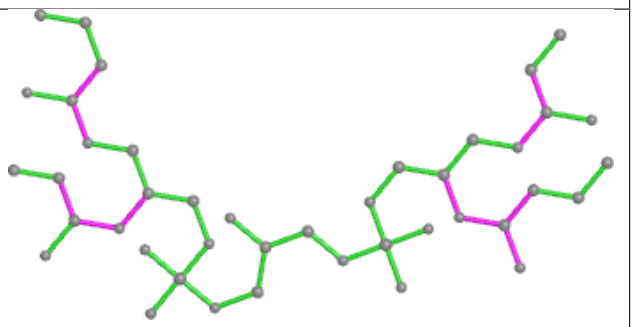


Rings

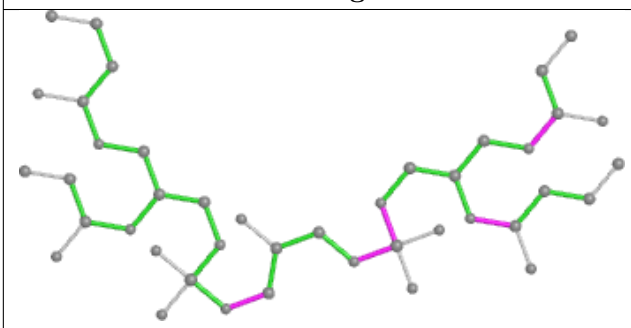
Ligand CDL Ac 407



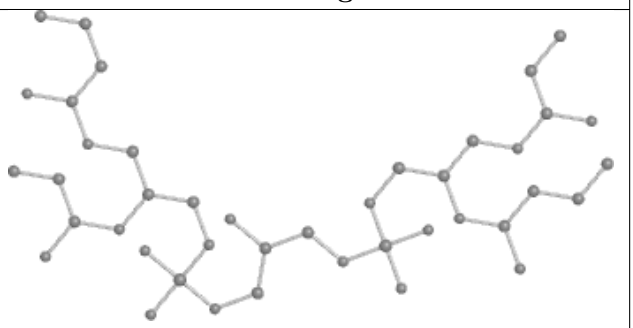
Bond lengths



Bond angles

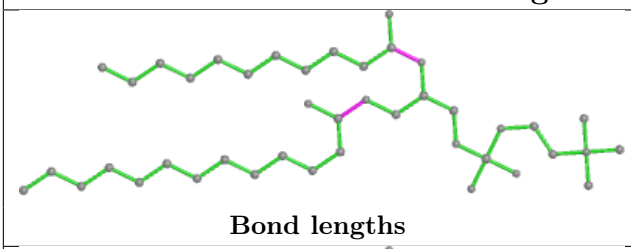


Torsions



Rings

Ligand PC1 J 201



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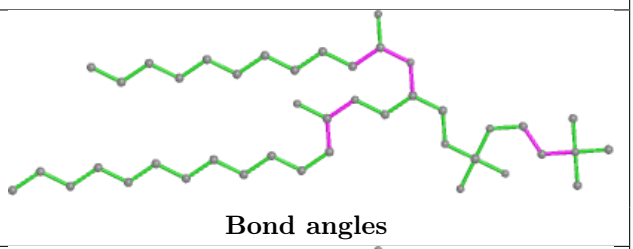
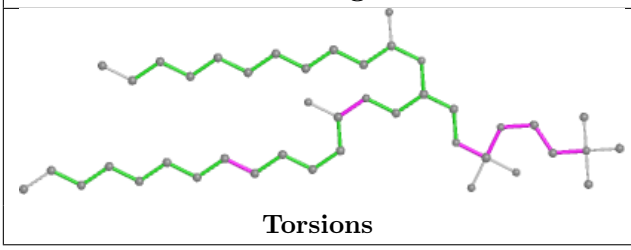
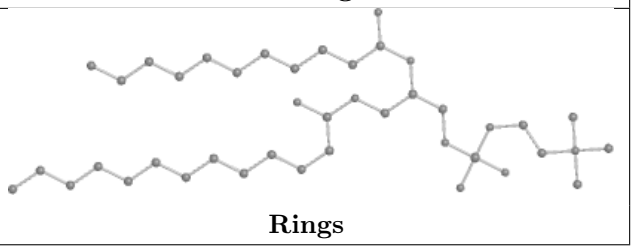


Bond angles

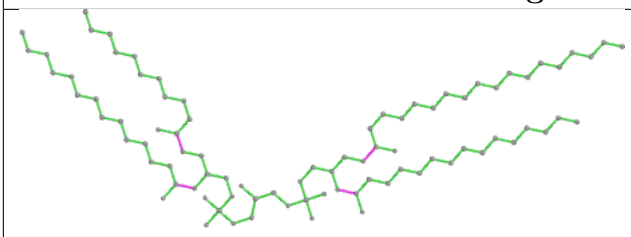


Torsions

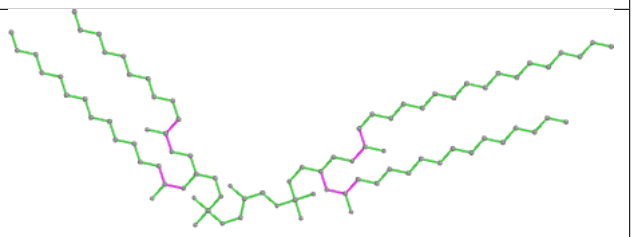


Rings

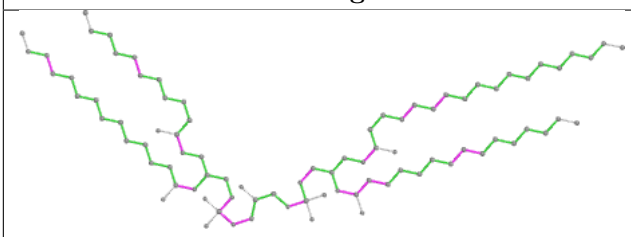
Ligand CDL L 706



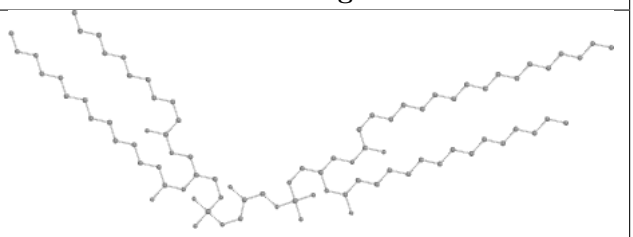
Bond lengths



Bond angles

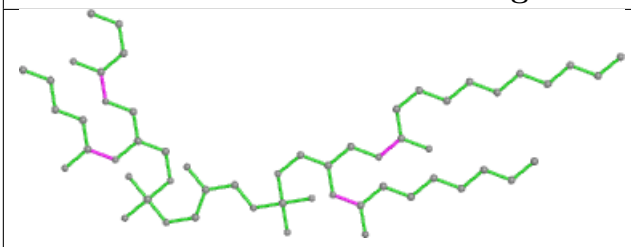


Torsions

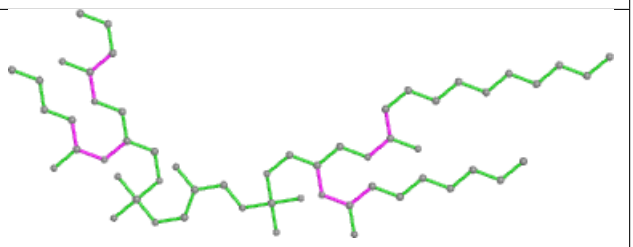


Rings

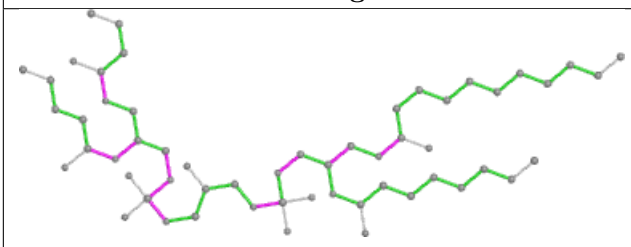
Ligand CDL AC 406



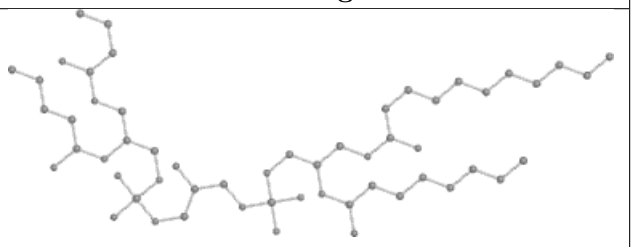
Bond lengths



Bond angles

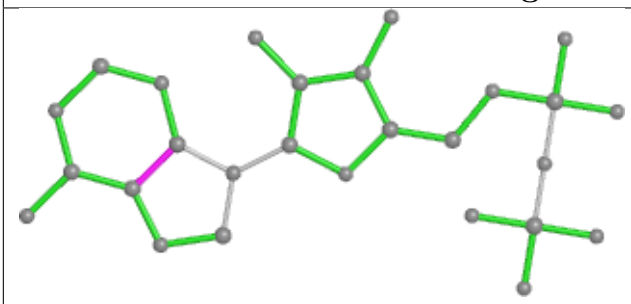


Torsions

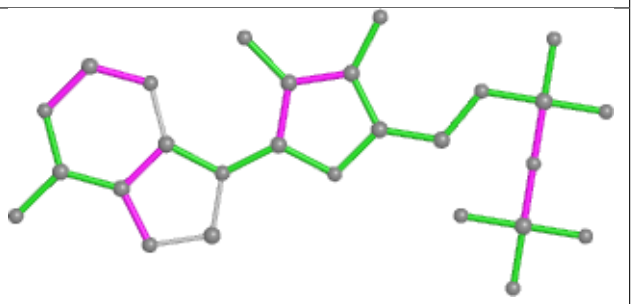


Rings

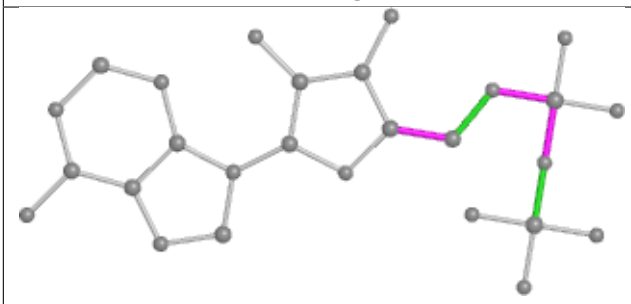
Ligand ADP O 402



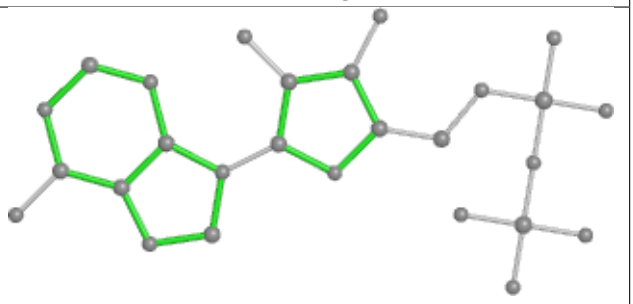
Bond lengths



Bond angles

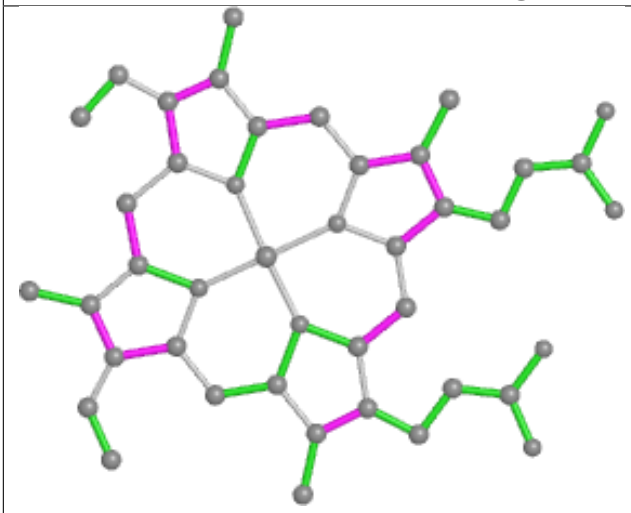


Torsions

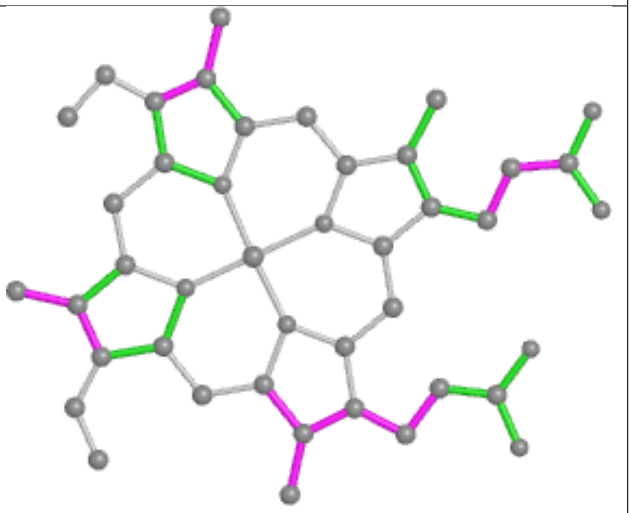


Rings

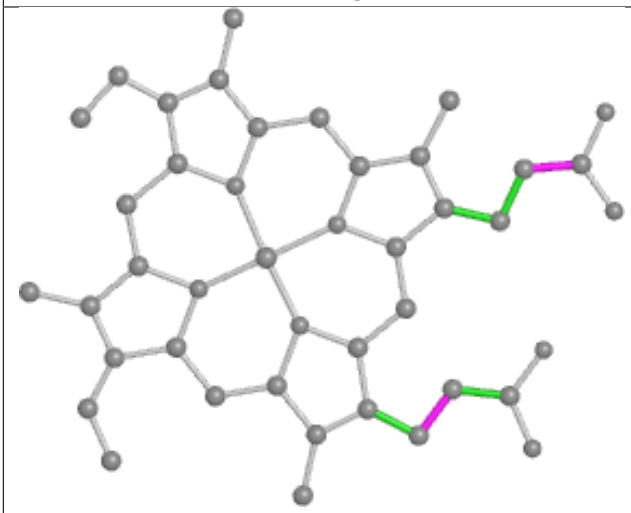
Ligand HEC Ad 401



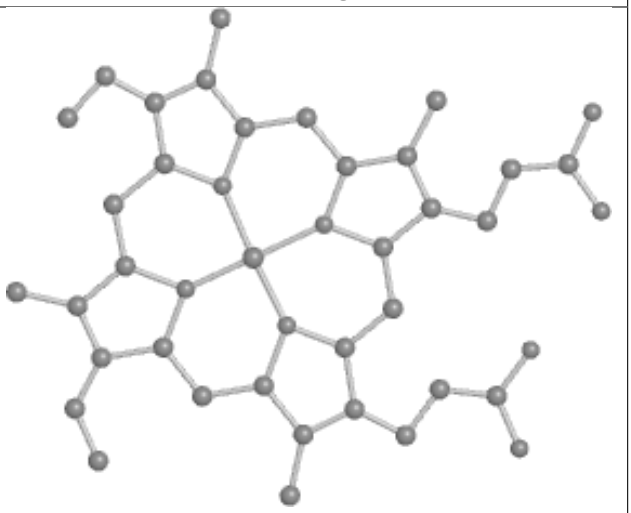
Bond lengths



Bond angles

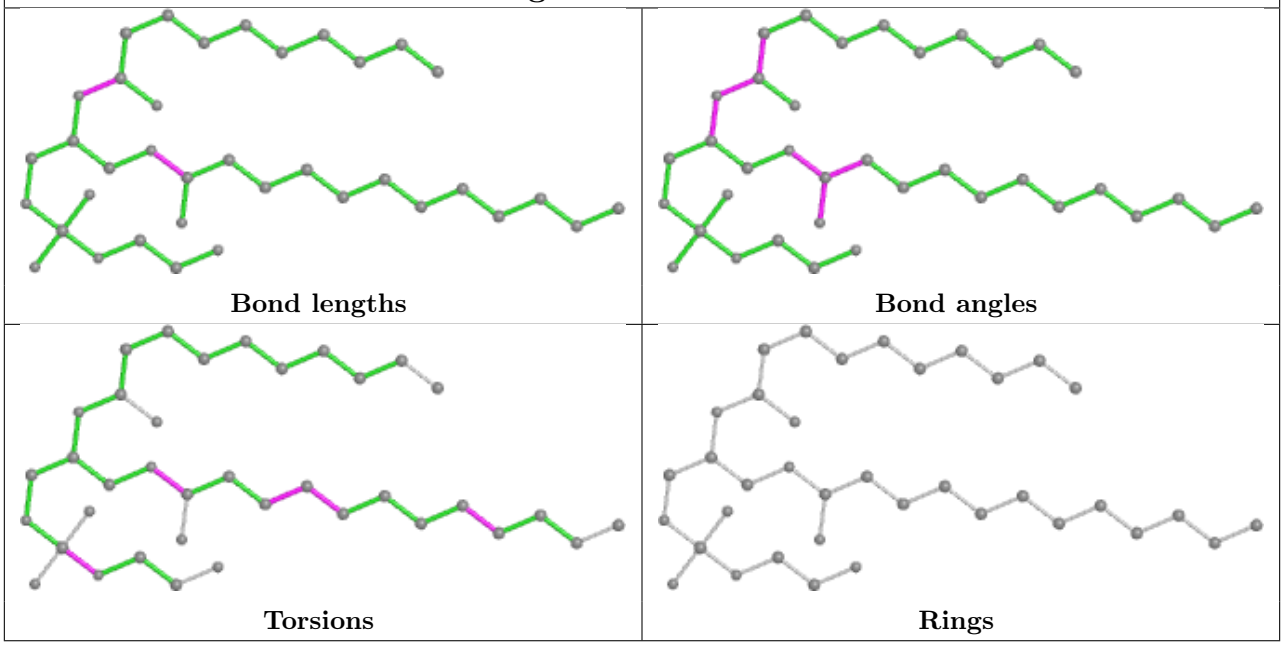


Torsions

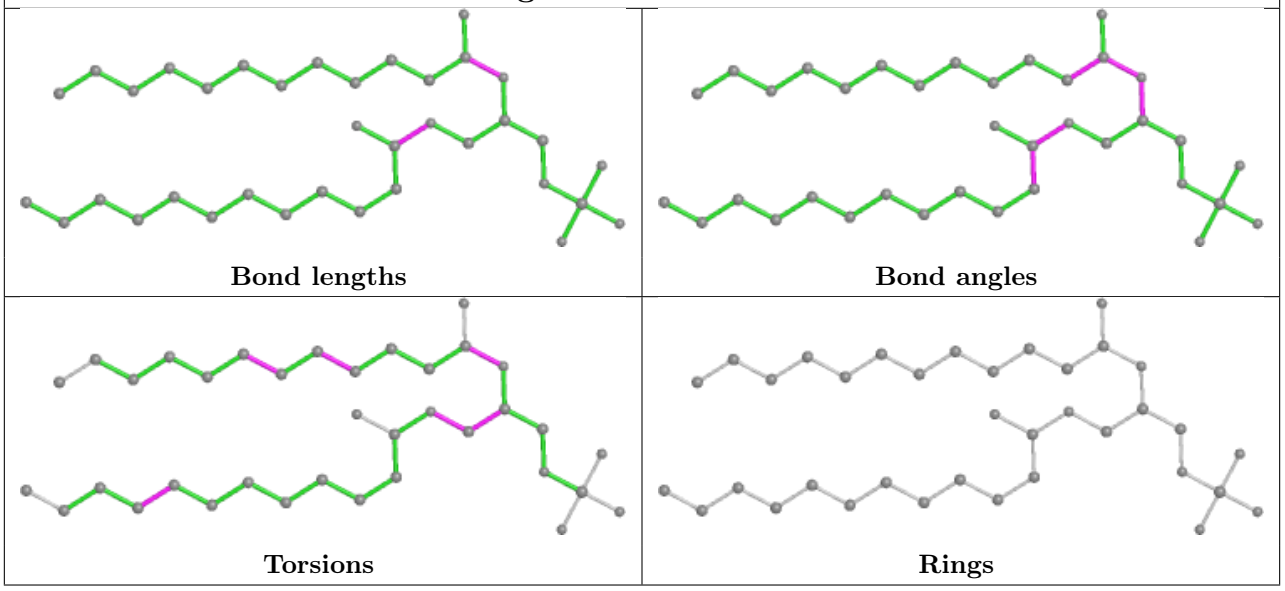


Rings

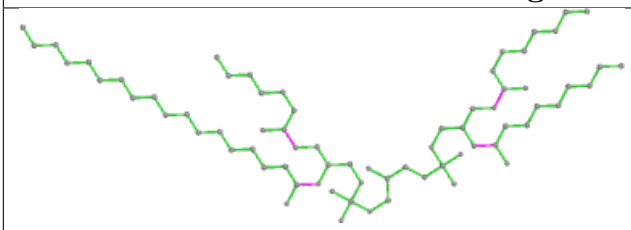
Ligand 3PE N 401



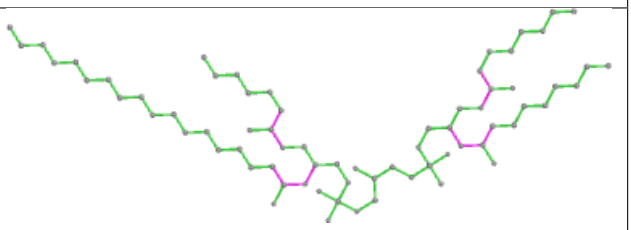
Ligand 3PH Ad 402



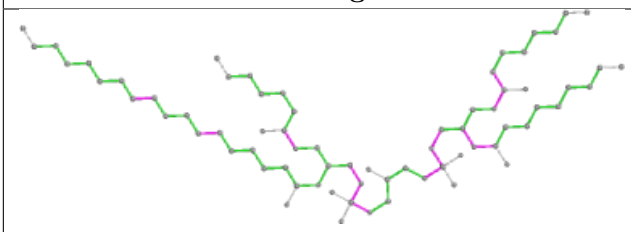
Ligand CDL h 201



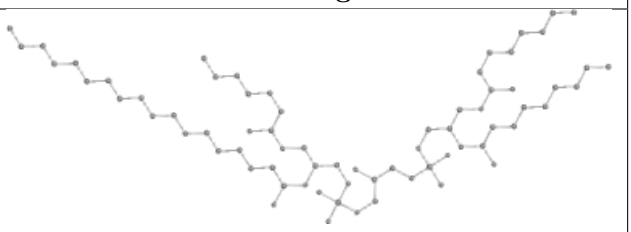
Bond lengths



Bond angles

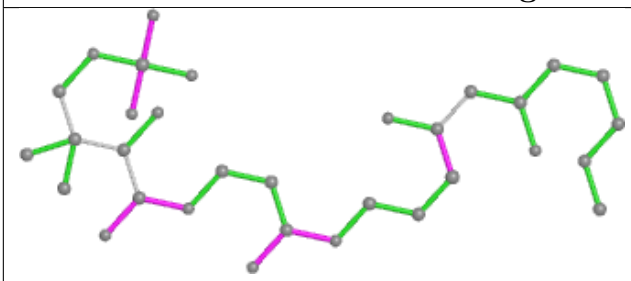


Torsions

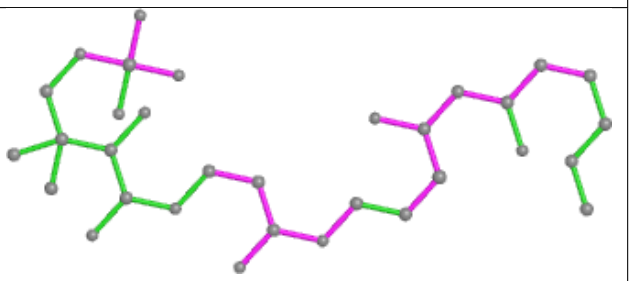


Rings

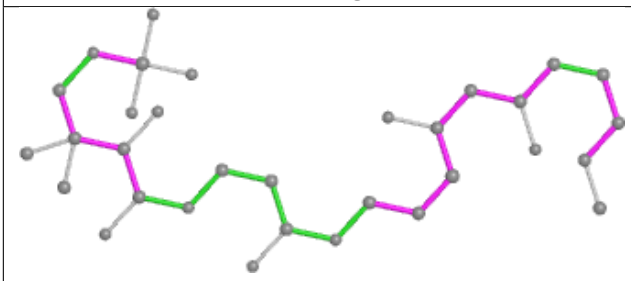
Ligand EHZ W 201



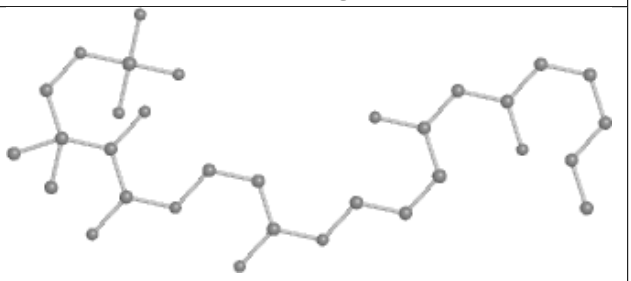
Bond lengths



Bond angles

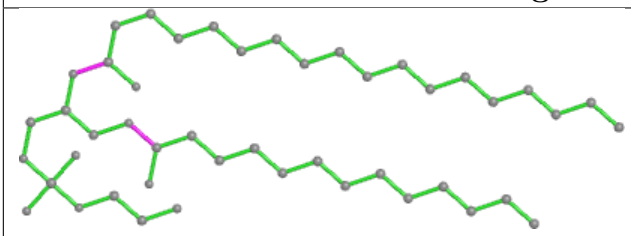


Torsions

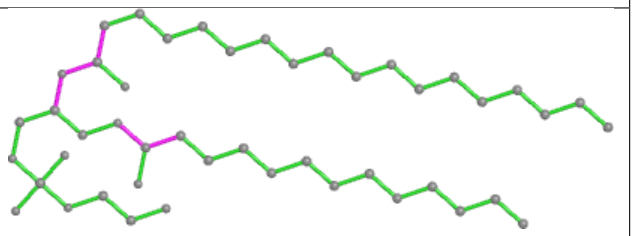


Rings

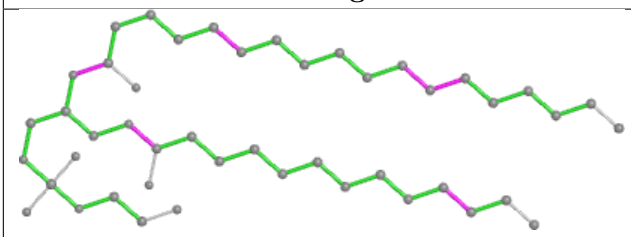
Ligand 3PE b 201



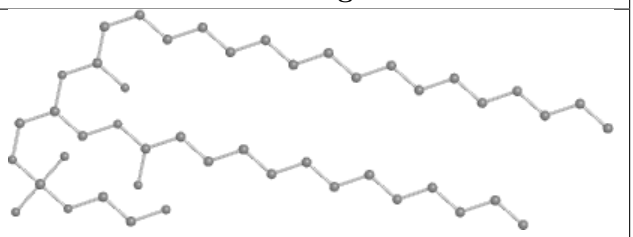
Bond lengths



Bond angles

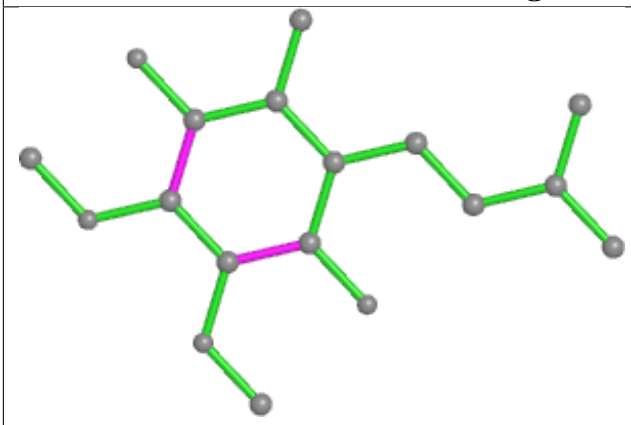


Torsions

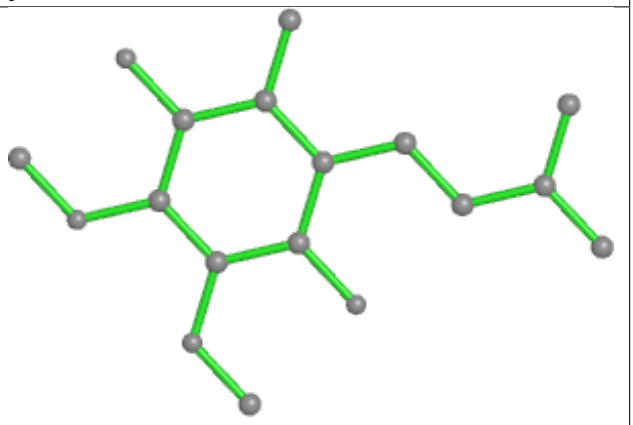


Rings

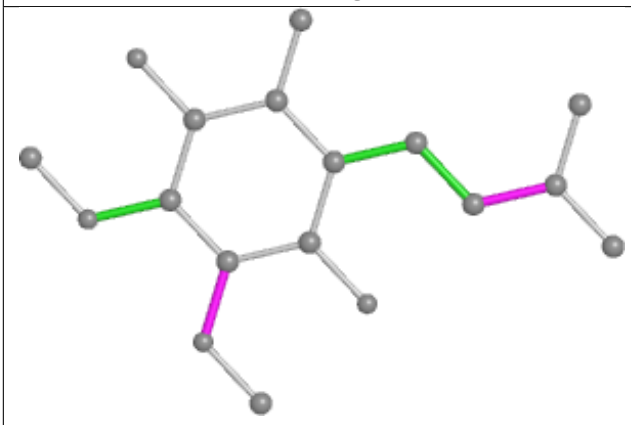
Ligand UQ1 B 302



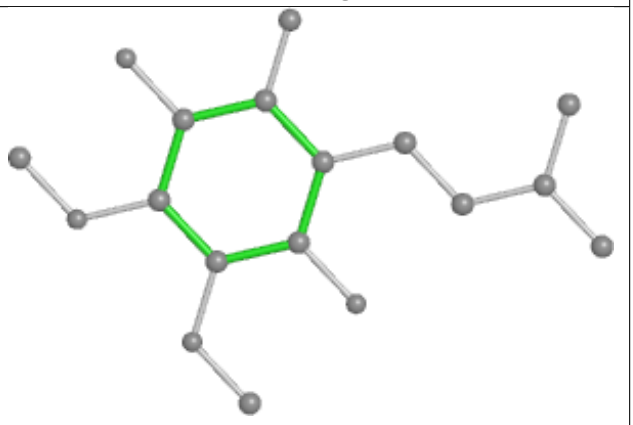
Bond lengths



Bond angles

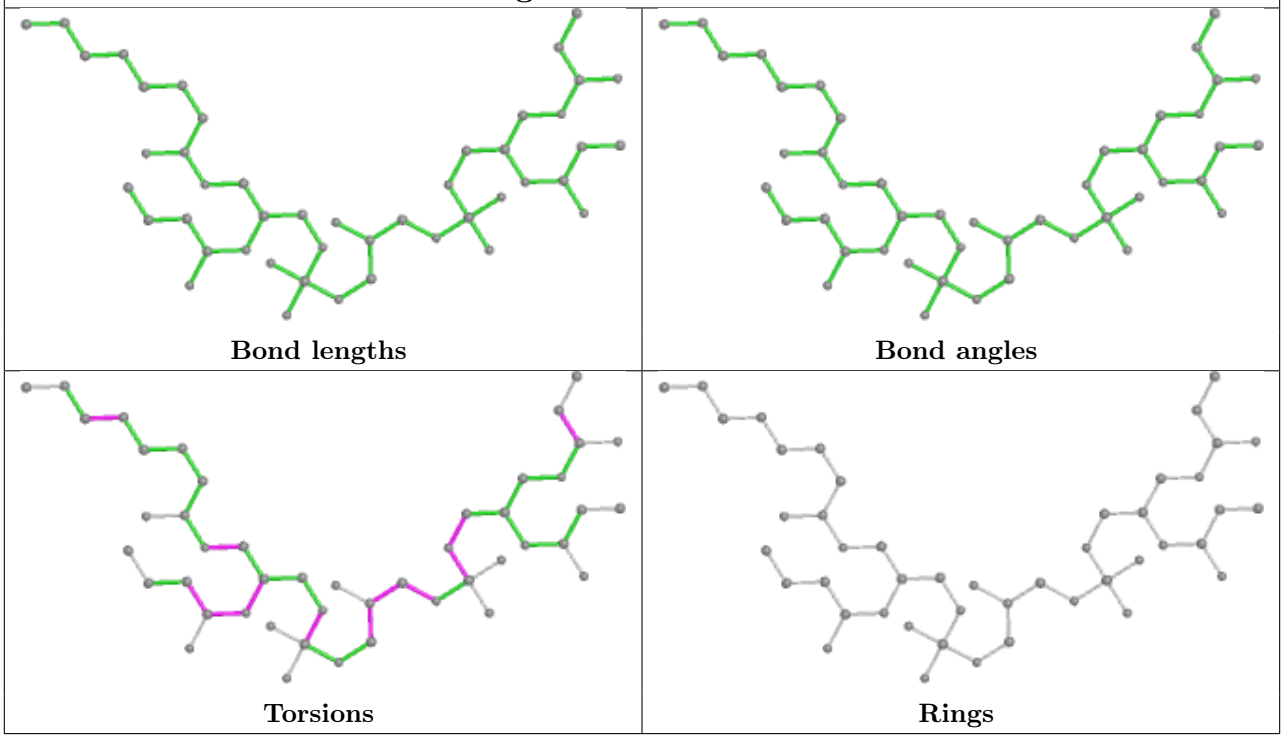


Torsions

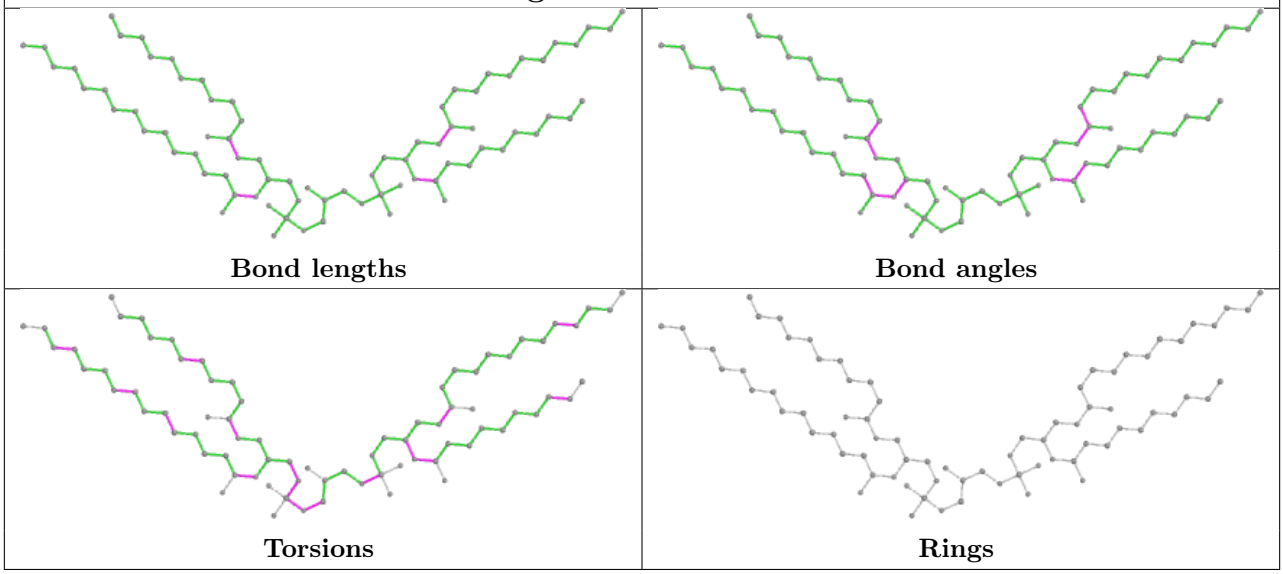


Rings

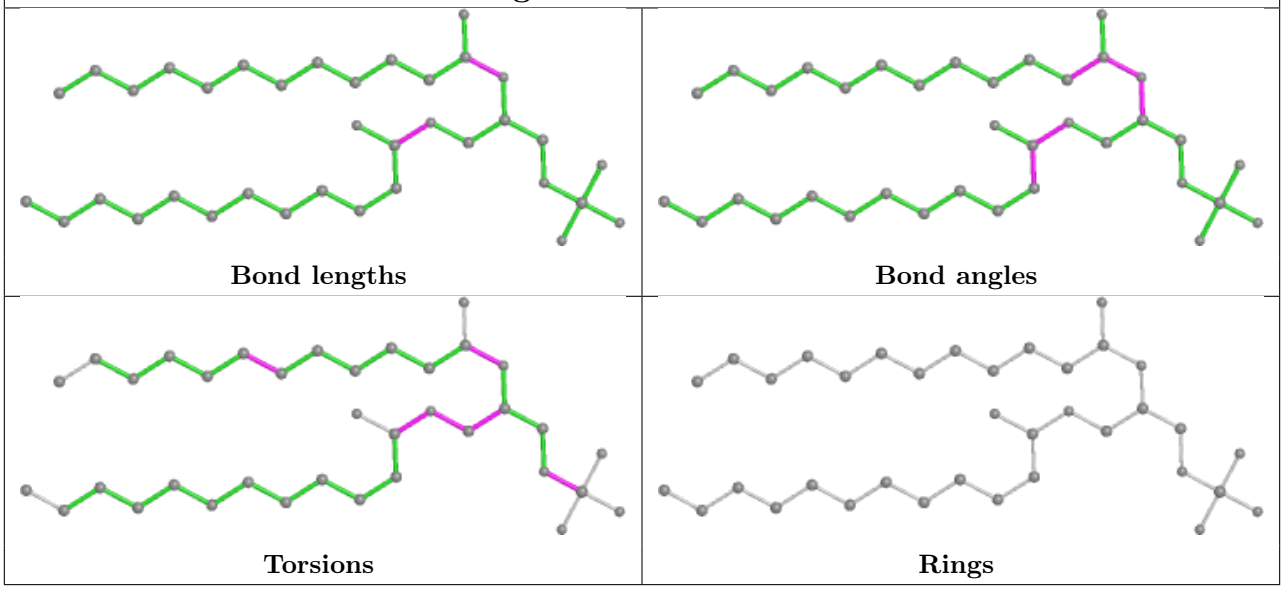
Ligand CDL Aa 501



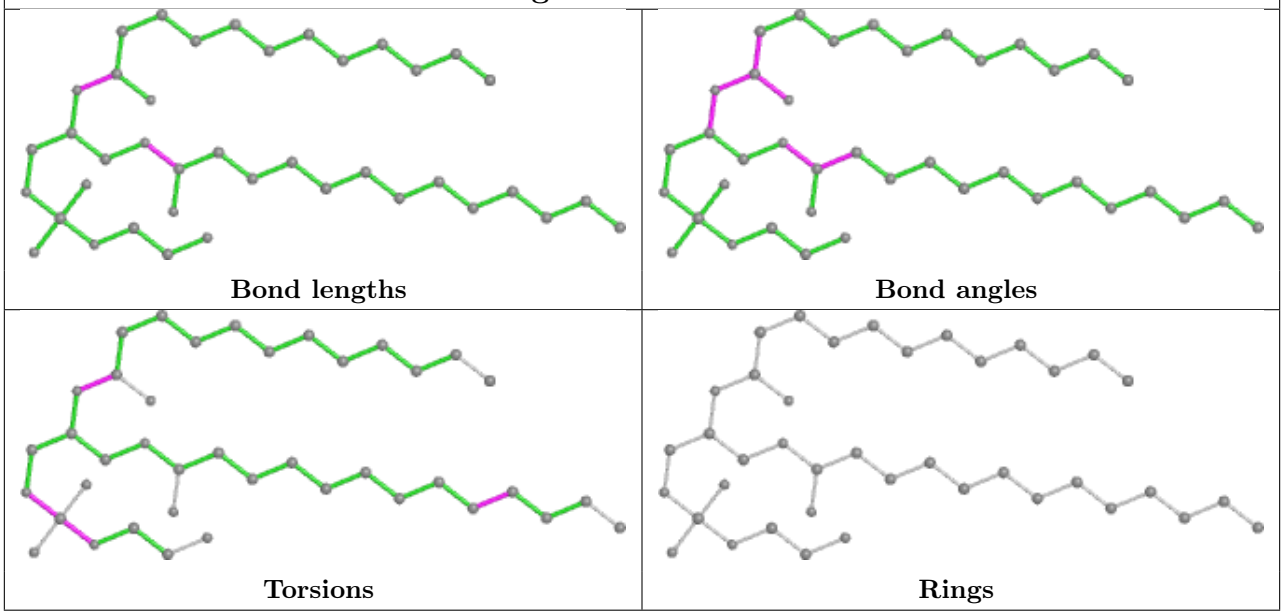
Ligand CDL L 705



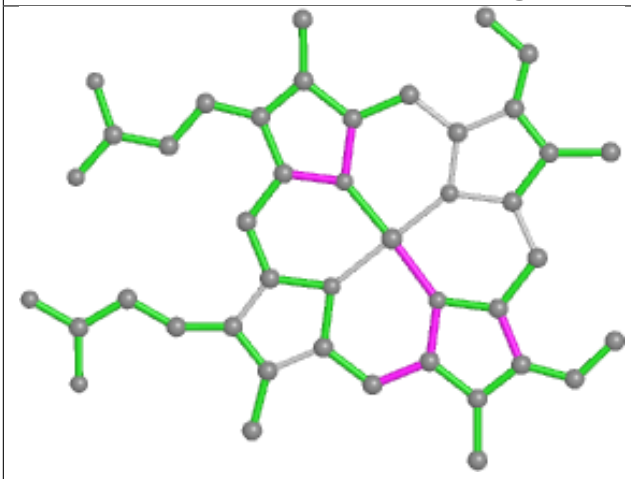
Ligand 3PH AD 402



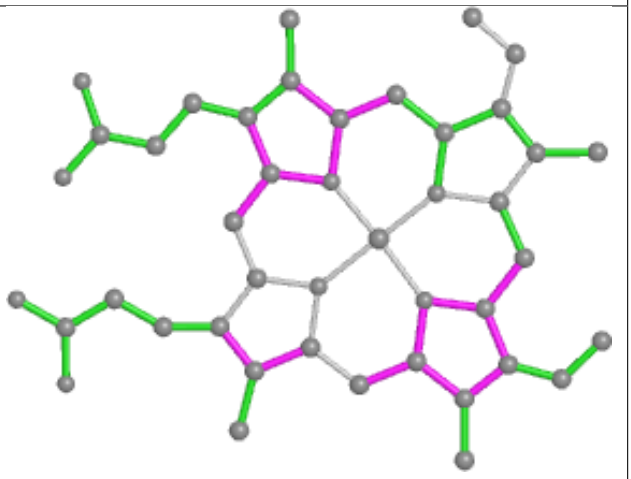
Ligand 3PE L 702



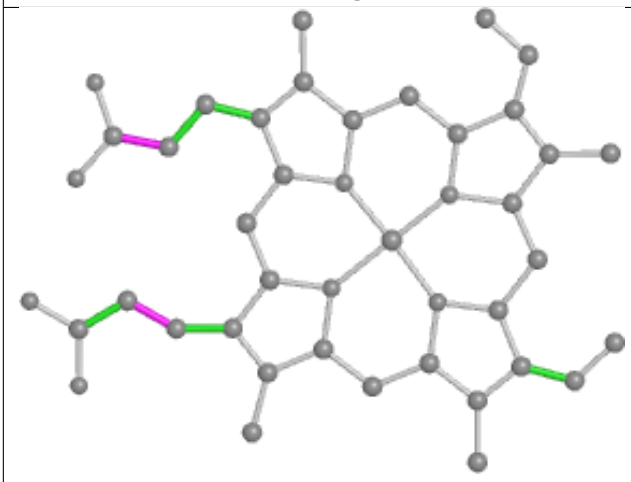
Ligand HEM Ac 402



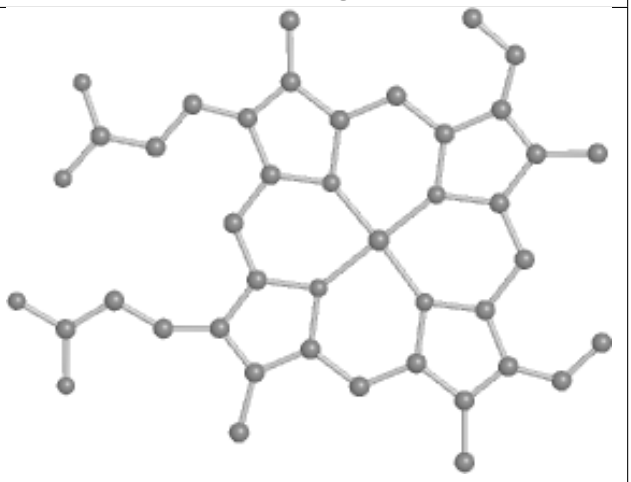
Bond lengths



Bond angles

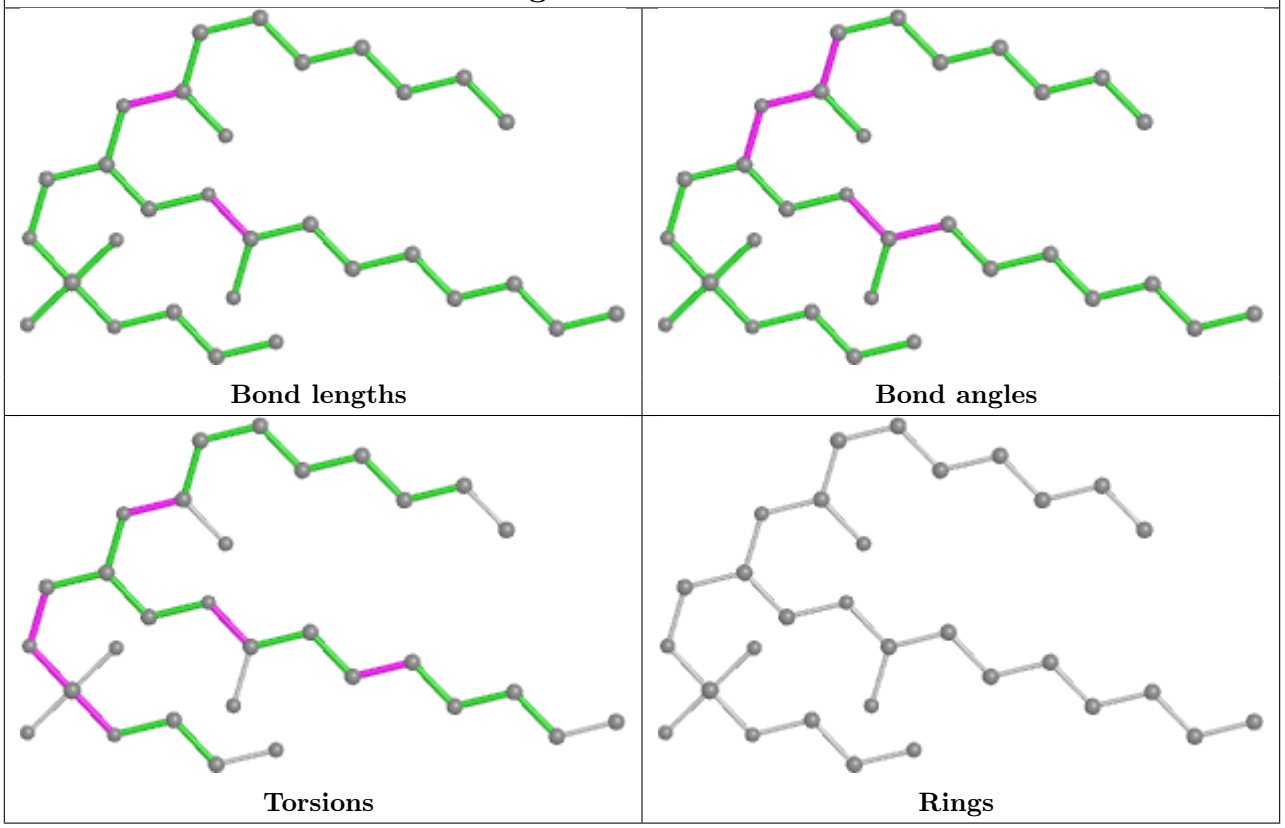


Torsions



Rings

Ligand 3PE O 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

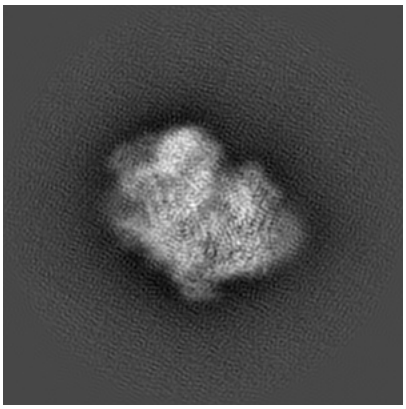
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35331. These allow visual inspection of the internal detail of the map and identification of artifacts.

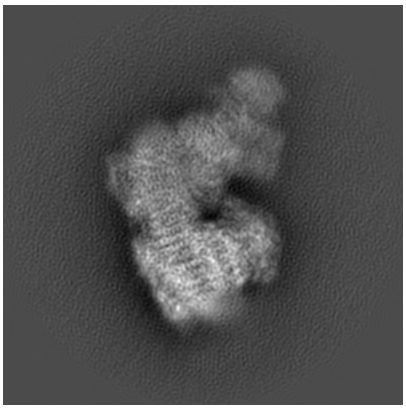
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

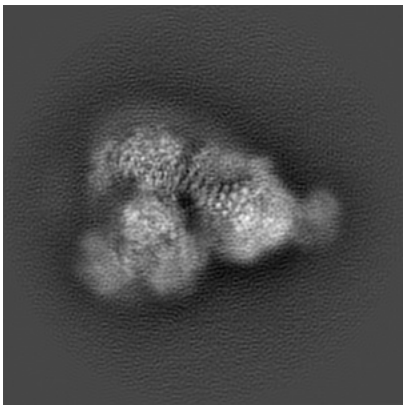
6.1.1 Primary map



X

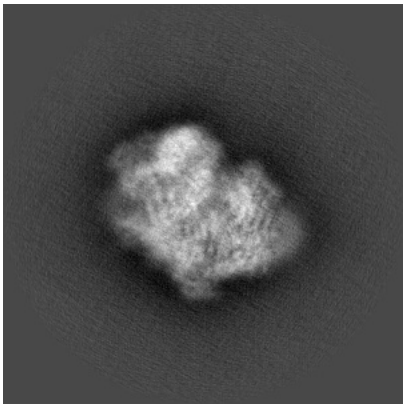


Y

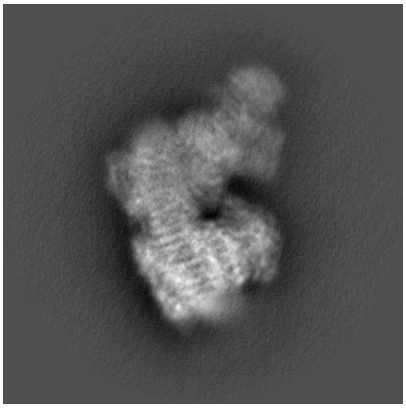


Z

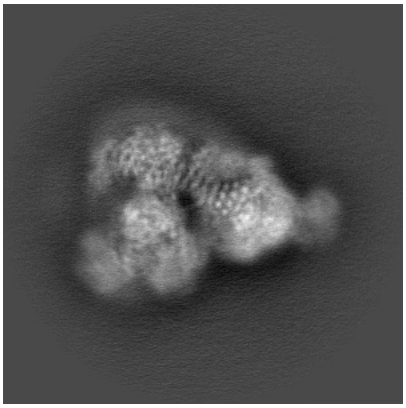
6.1.2 Raw map



X



Y

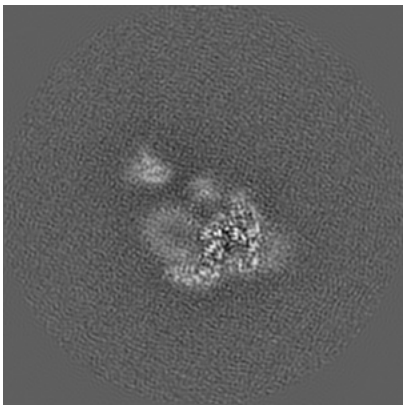


Z

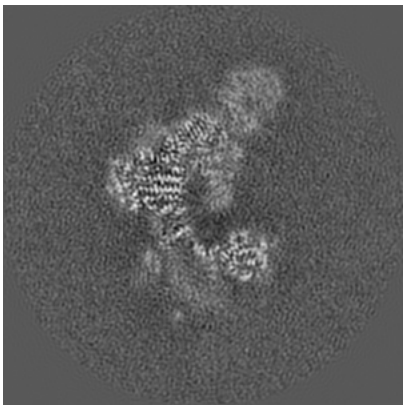
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

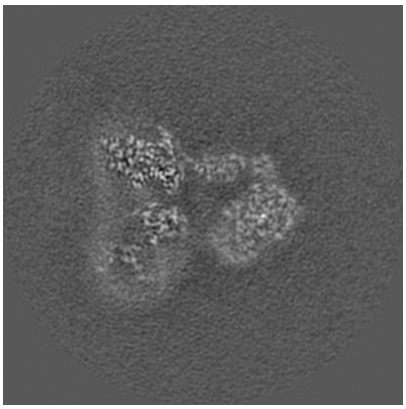
6.2.1 Primary map



X Index: 192

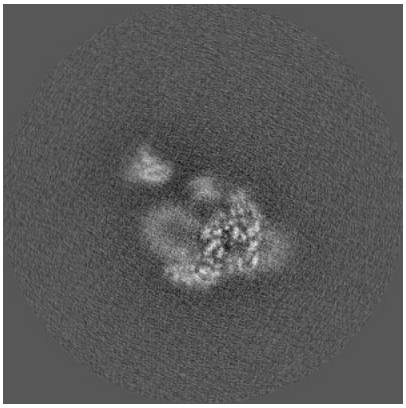


Y Index: 192

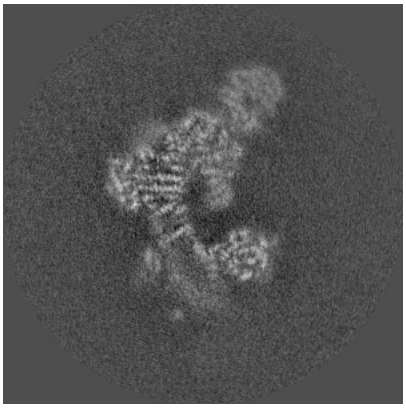


Z Index: 192

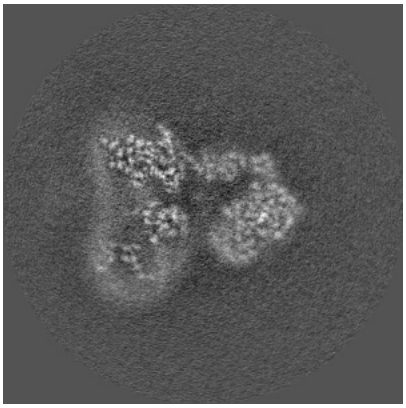
6.2.2 Raw map



X Index: 192



Y Index: 192

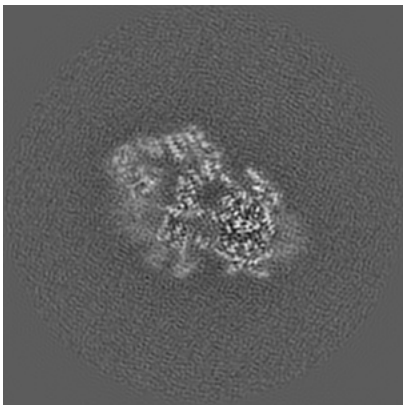


Z Index: 192

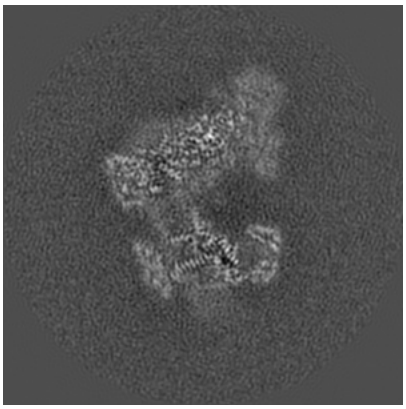
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

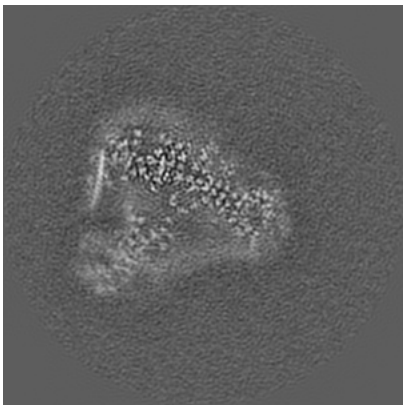
6.3.1 Primary map



X Index: 154

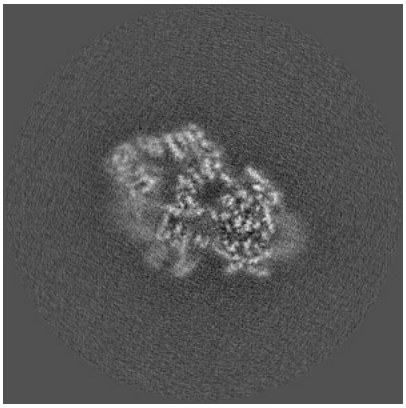


Y Index: 177

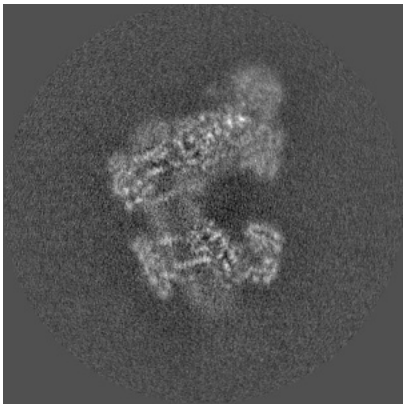


Z Index: 167

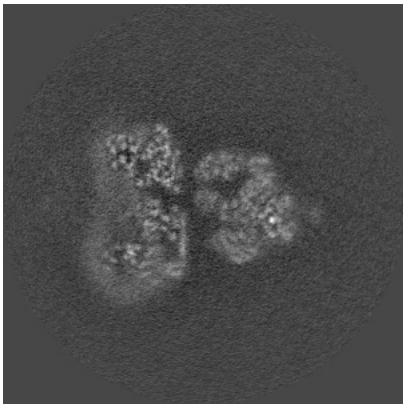
6.3.2 Raw map



X Index: 154



Y Index: 174

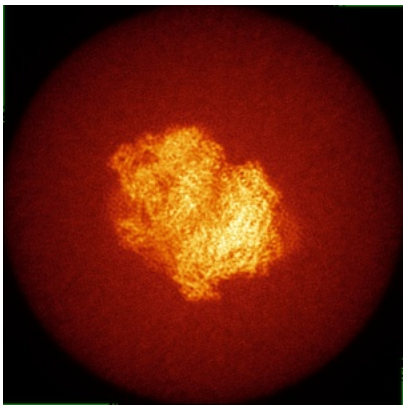


Z Index: 198

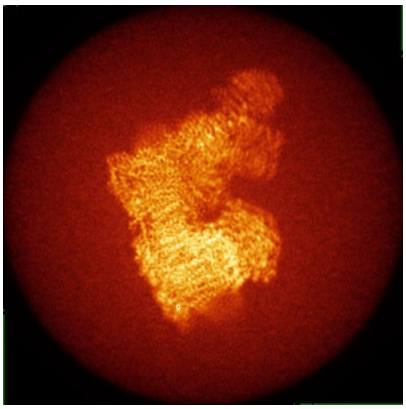
The images above show the largest variance slices of the map in three orthogonal directions.

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

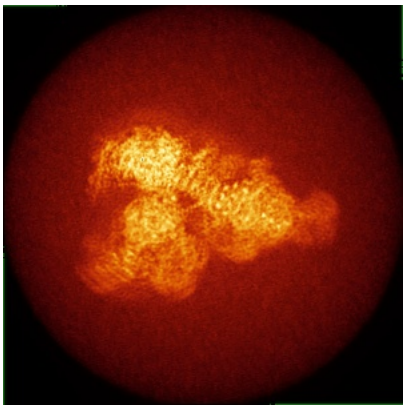
6.4.1 Primary map



X

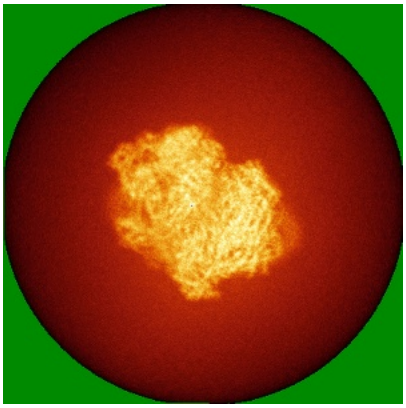


Y

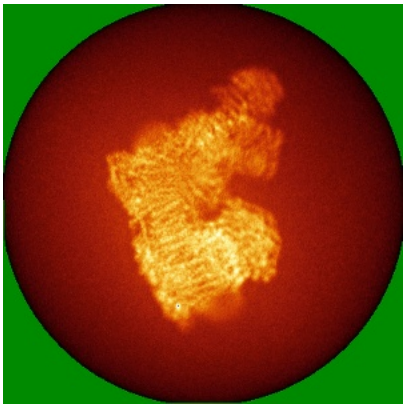


Z

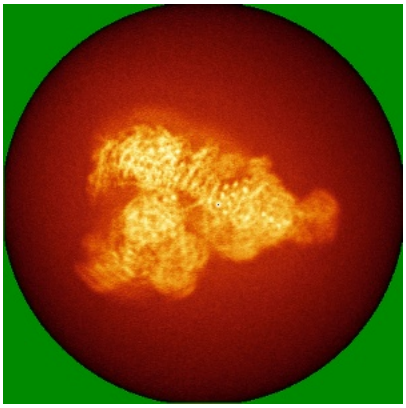
6.4.2 Raw map



X



Y

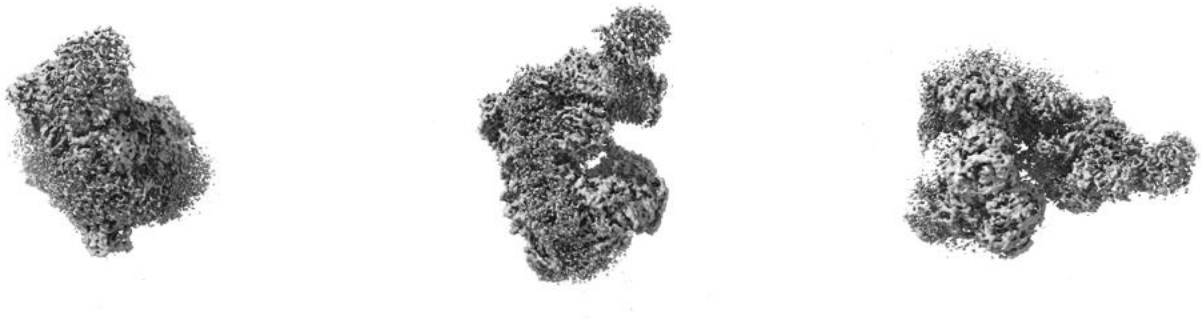


Z

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)

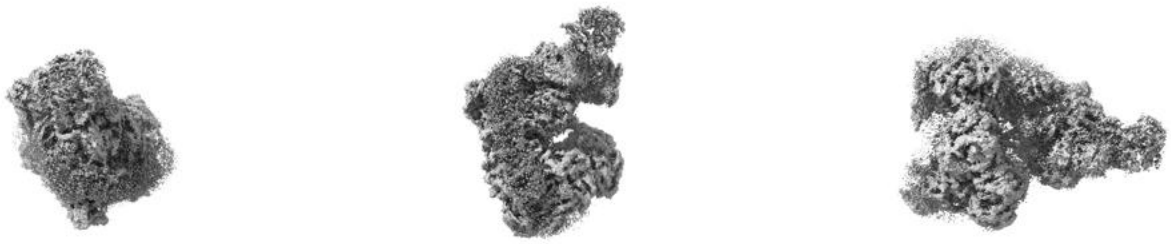
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

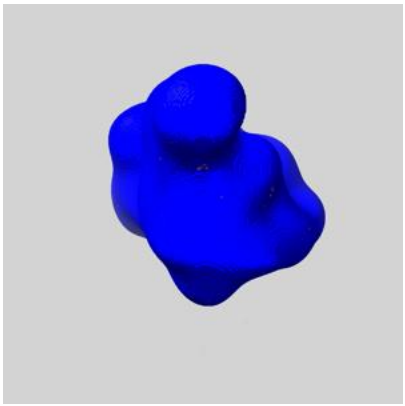
6.6 Mask visualisation (i)

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

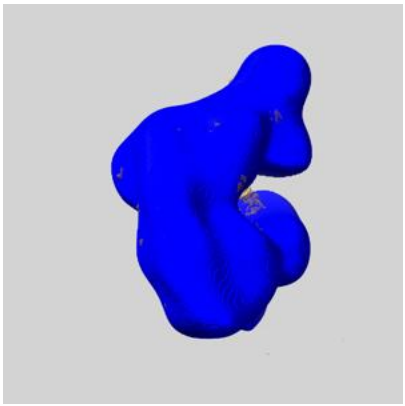
A mask typically either:

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

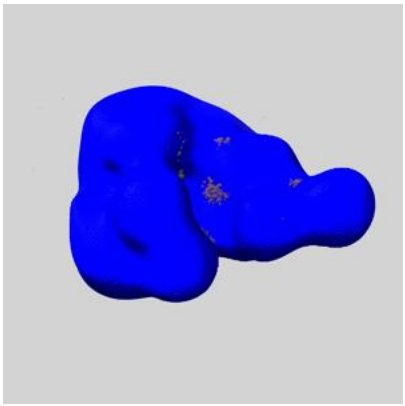
6.6.1 emd_35331_msk_1.map (i)



X



Y

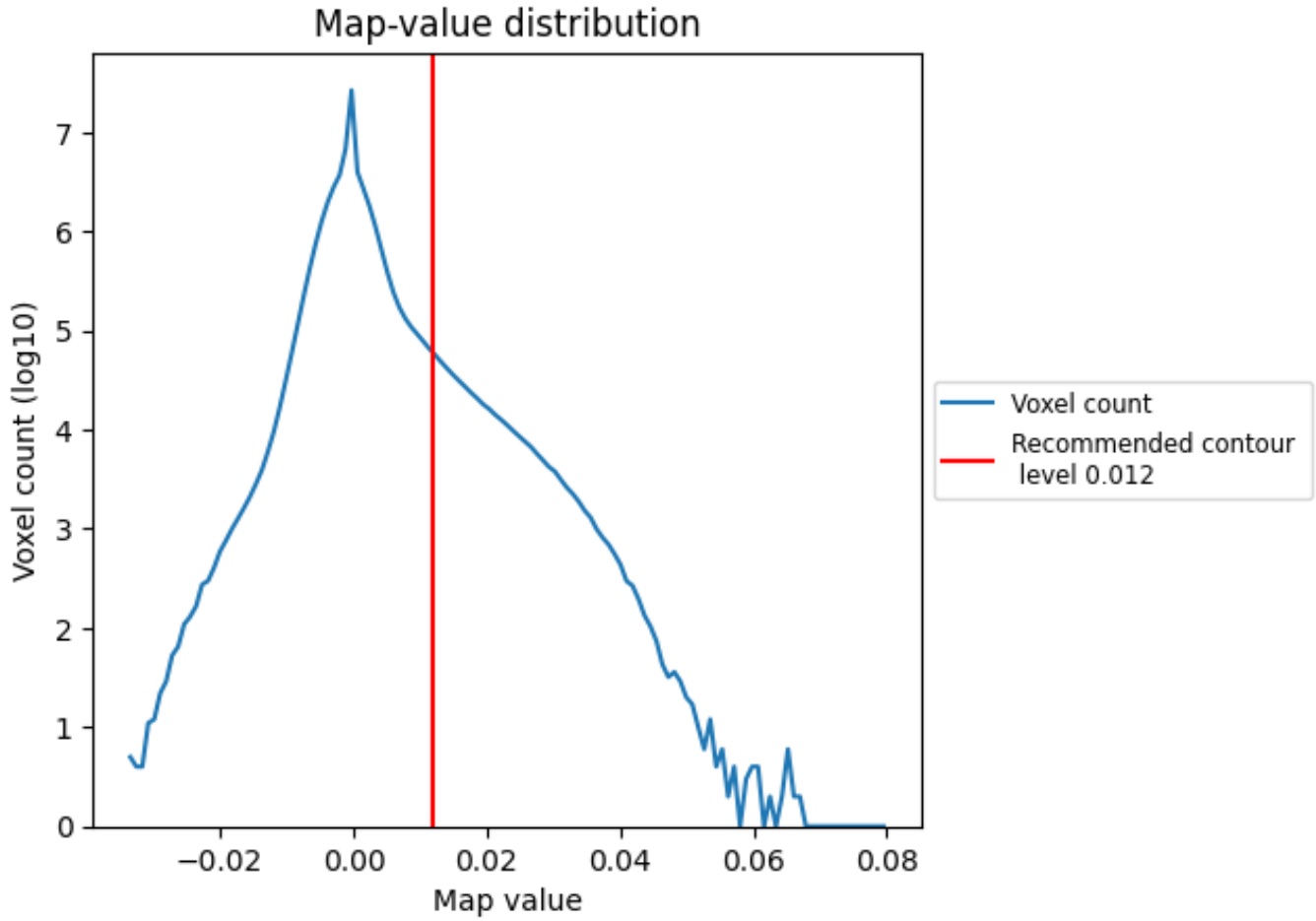


Z

7 Map analysis

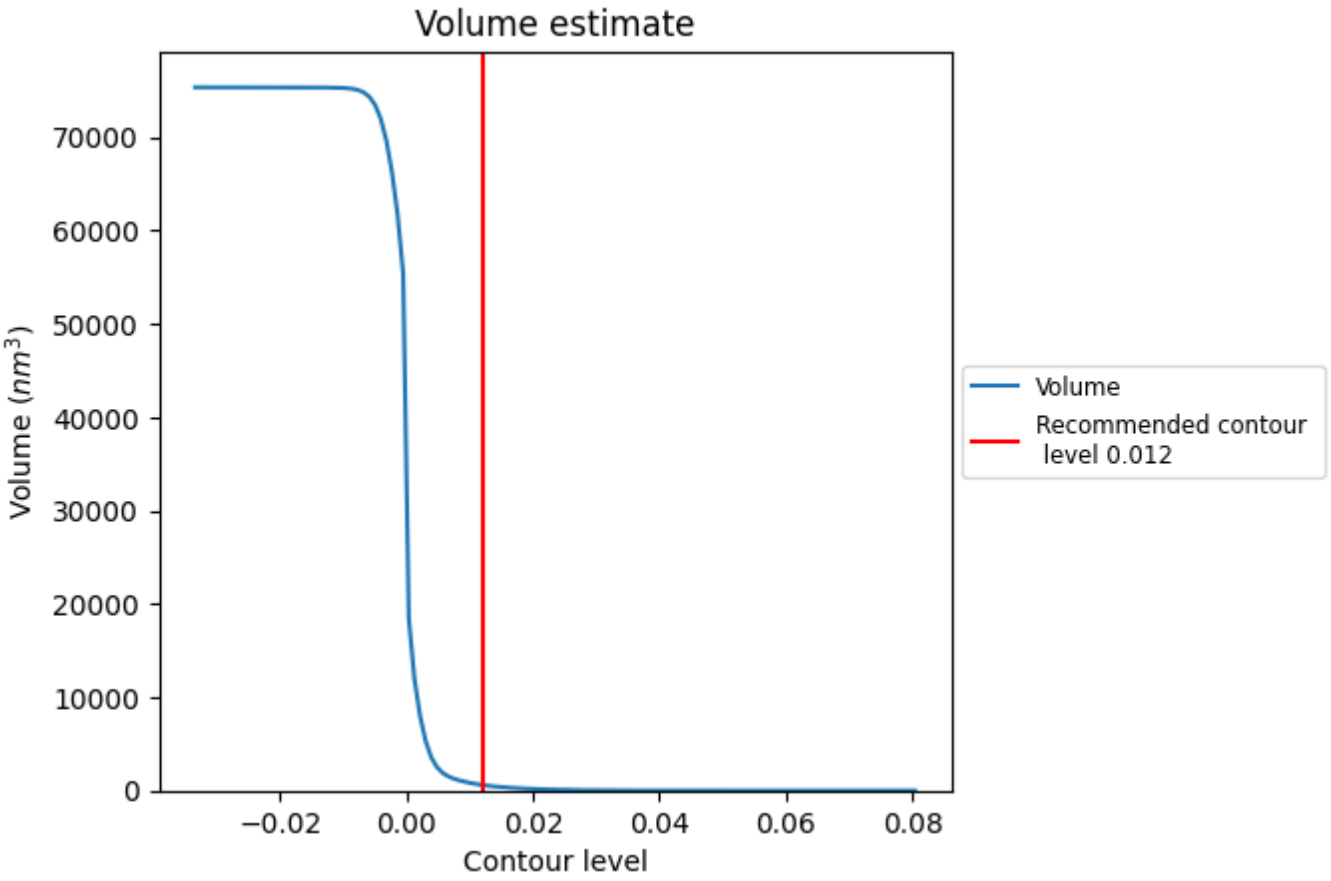
This section contains the results of statistical analysis of the map.

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.

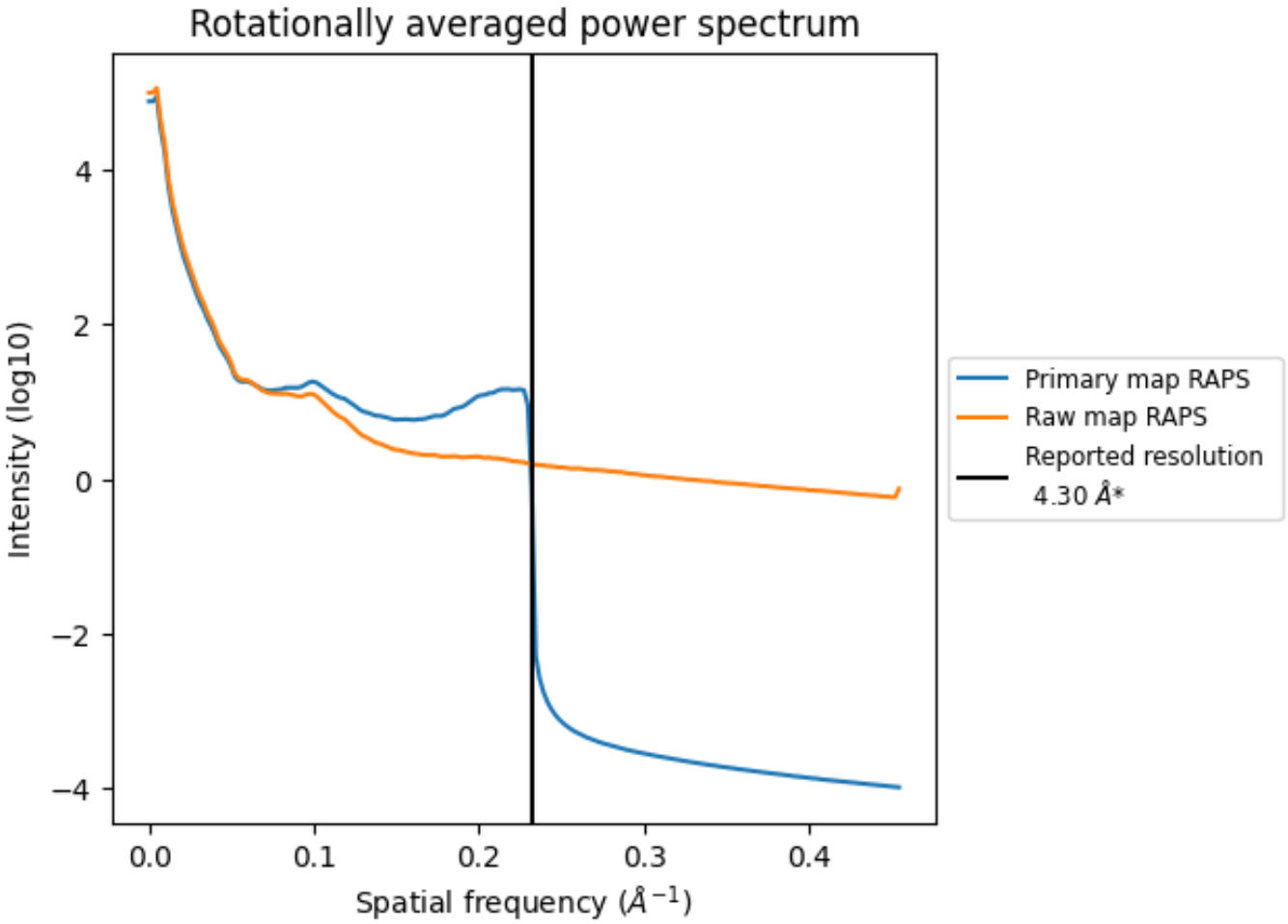
7.2 Volume estimate



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 536 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)

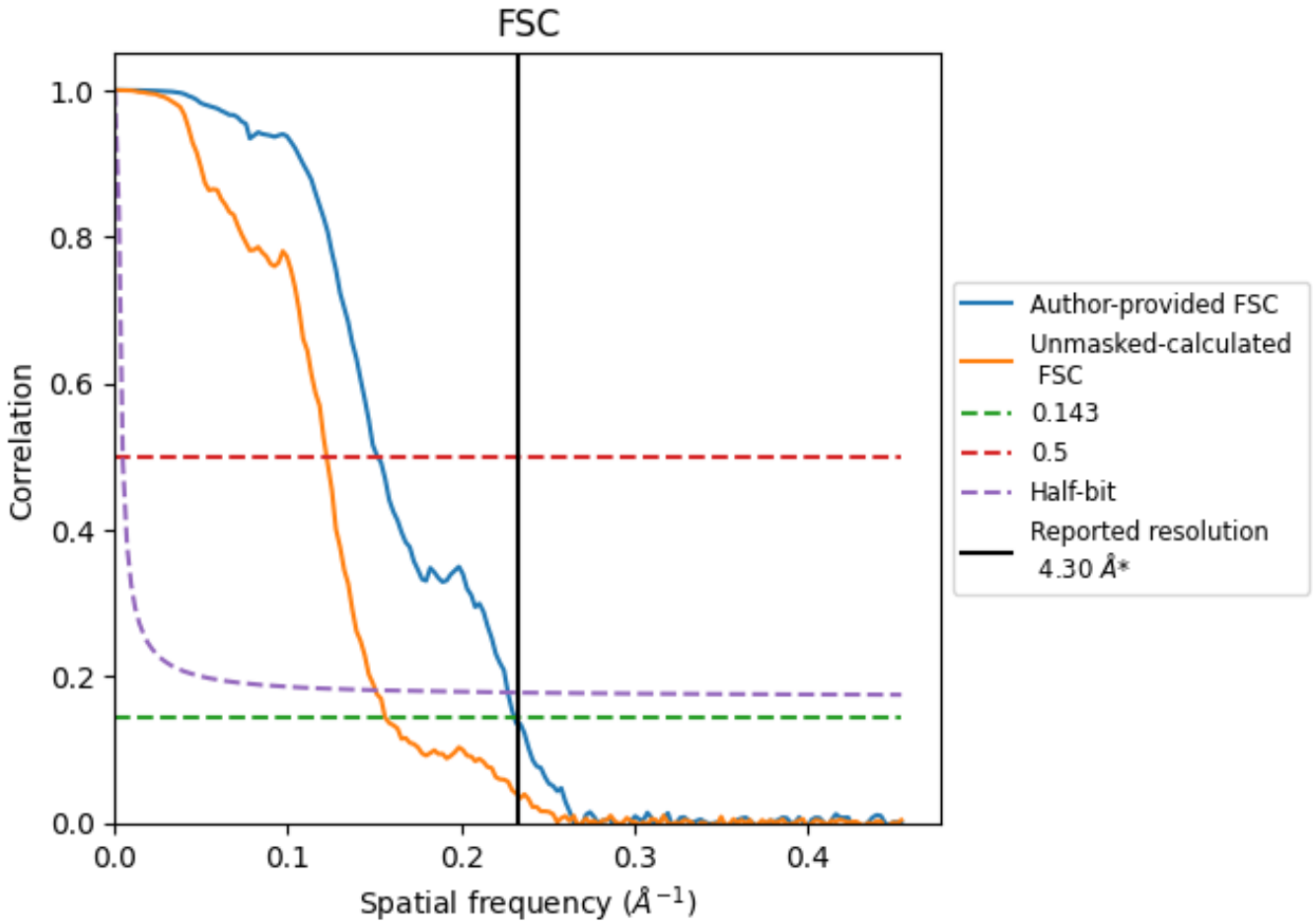


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

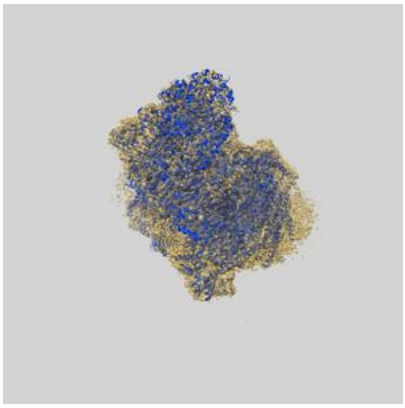
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.59	4.40
Unmasked-calculated*	6.39	8.17	6.64

*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 6.39 differs from the reported value 4.3 by more than 10 %

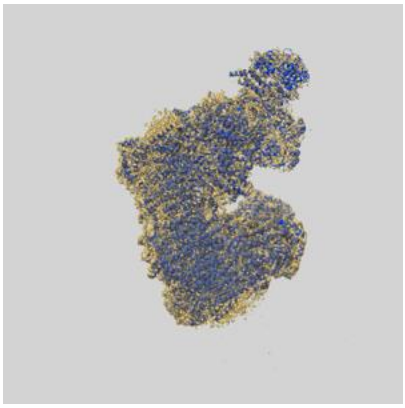
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35331 and PDB model 8IB4. Per-residue inclusion information can be found in section 3 on page 27.

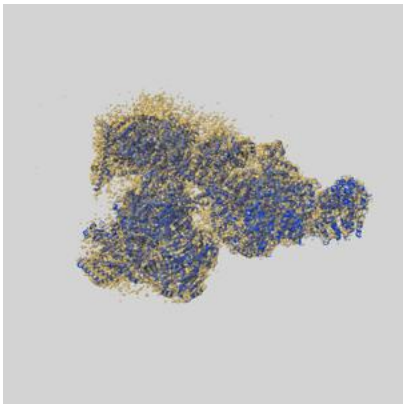
9.1 Map-model overlay



X



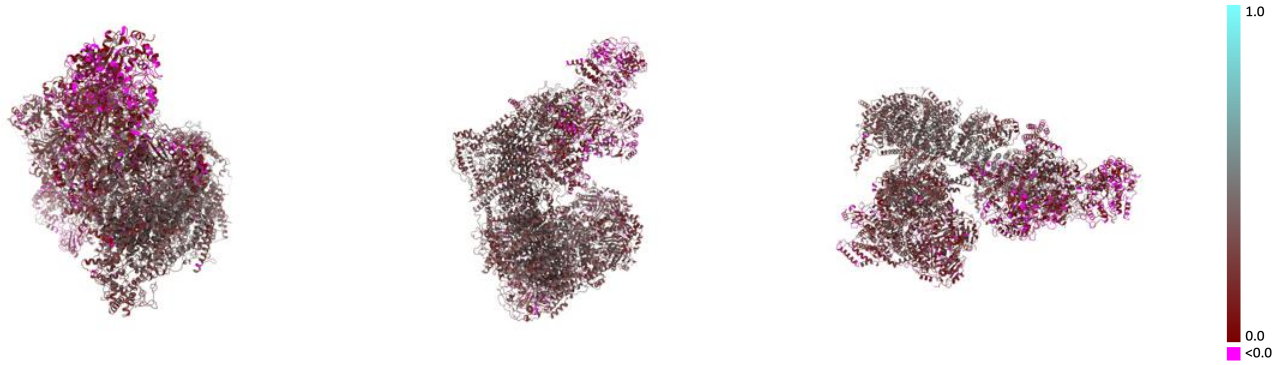
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

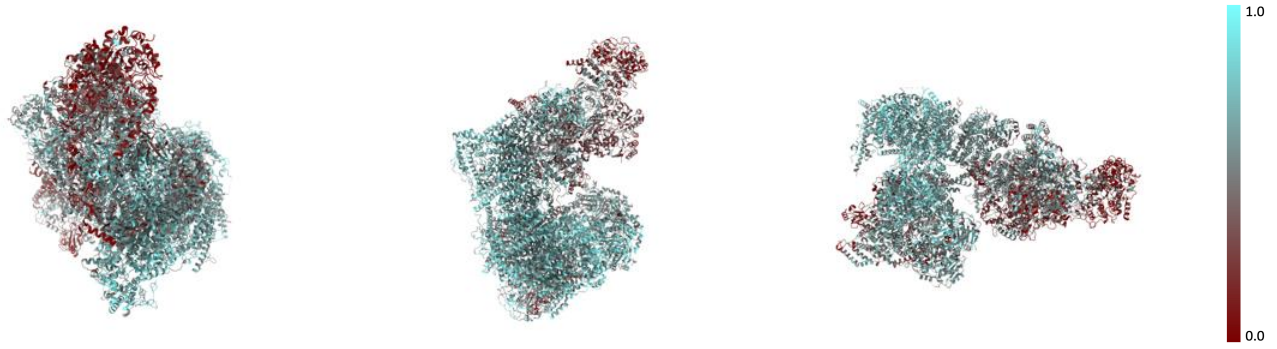
9.2 Q-score mapped to coordinate model



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.

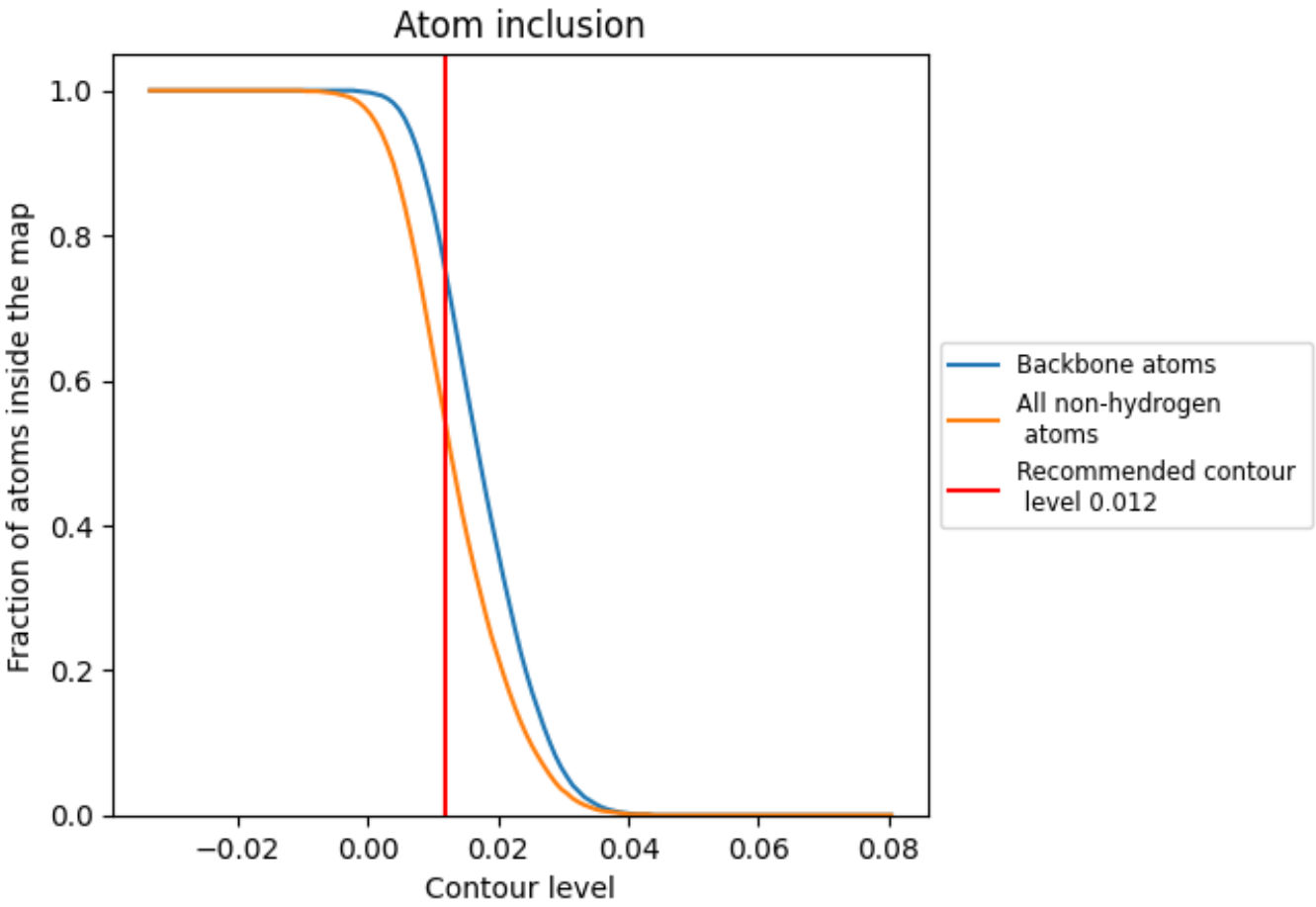
9.3 Atom inclusion mapped to coordinate model



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 54% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5370	0.2580
A	0.5630	0.3210
AA	0.5930	0.2210
AB	0.5900	0.2290
AC	0.4970	0.2570
AD	0.5020	0.1900
AE	0.1630	0.1300
AF	0.6180	0.2580
AG	0.4350	0.1990
AH	0.4400	0.1220
AI	0.2820	0.2100
AJ	0.1830	0.1680
AK	0.1720	0.1620
Aa	0.6900	0.3210
Ab	0.6560	0.2690
Ac	0.5620	0.2860
Ad	0.5900	0.2170
Ae	0.1790	0.1480
Af	0.6290	0.2990
Ag	0.5350	0.2910
Ah	0.5510	0.1690
Aj	0.3540	0.2340
Ak	0.1580	0.1740
B	0.6170	0.3110
C	0.5140	0.2050
D	0.6100	0.3010
E	0.1830	0.0850
F	0.2410	0.1140
G	0.3630	0.1480
H	0.6240	0.3380
I	0.6400	0.2880
J	0.5270	0.2930
K	0.6230	0.3560
L	0.6340	0.3490
M	0.6740	0.3770

Continued on next page...

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Chain	Atom inclusion	Q-score
N	0.6600	0.3700
O	0.5300	0.2840
P	0.3430	0.1390
Q	0.3060	0.1770
R	0.2130	0.1200
S	0.2980	0.1030
T	0.2020	0.0800
U	0.7410	0.3560
V	0.4580	0.1640
W	0.3570	0.1420
X	0.6760	0.2990
Y	0.6030	0.3310
Z	0.6950	0.3090
a	0.6500	0.3120
b	0.6520	0.2950
c	0.5930	0.2730
d	0.7040	0.3470
e	0.6680	0.3140
f	0.6080	0.2920
g	0.6530	0.3140
h	0.6790	0.3300
i	0.7090	0.3220
j	0.6840	0.3020
k	0.7380	0.3450
l	0.7390	0.3840
m	0.7130	0.3500
n	0.7500	0.3470
o	0.6400	0.2640
p	0.7140	0.3320
q	0.1600	0.1780
r	0.2320	0.1530
s	0.1050	0.0160