Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 06:41 PM JST

PDB ID	:	8IB9
EMDB ID	:	EMD-35336
Title	:	Respiratory complex CI:CIII2, type IB, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
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:

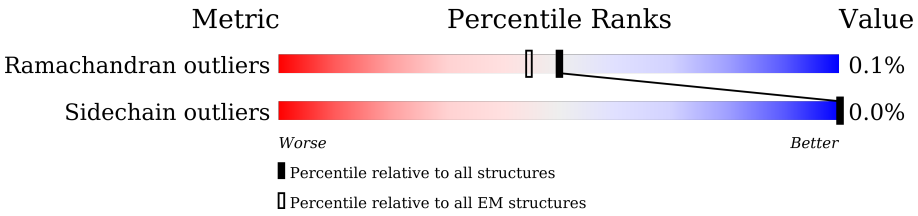
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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	8% 81% 19%
2	B	224	68% 30%
3	C	263	10% 74% 25%
4	D	463	8% 91% 8%
5	E	248	46% 82% 15%
6	F	464	47% 89% 8%
7	G	727	36% 92% 6%
8	H	318	6% 96%
9	I	212	81% 18%

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Mol	Chain	Length	Quality of chain
10	J	172	12% 91% 9%
11	K	98	97%
12	L	607	97%
13	M	459	97%
14	N	345	98%
15	O	355	15% 88% 10%
16	P	377	44% 89% 10%
17	Q	175	28% 64% 33%
18	R	116	47% 70% 28%
19	S	99	46% 83% 16%
20	T	156	31% 46% 52%
20	U	156	55% 44%
21	V	116	16% 93%
22	W	131	24% 85% 13%
23	X	172	98%
24	Y	143	8% 97%
25	Z	144	96%
26	a	70	93%
27	b	84	94% 6%
28	c	76	7% 59% 38%
29	d	120	7% 98%
30	e	106	97%
31	f	57	5% 89% 9%
32	g	151	65% 34%
33	h	189	73% 27%

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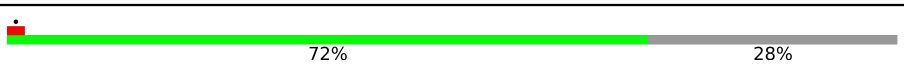
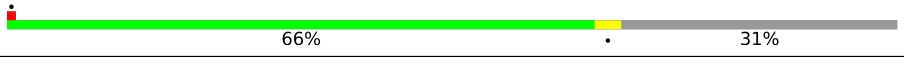
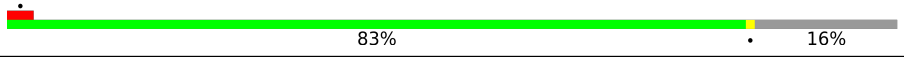
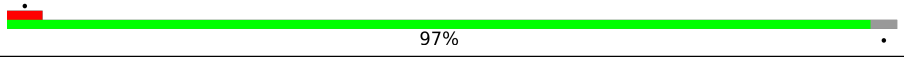
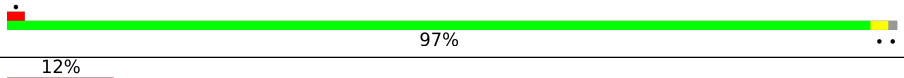
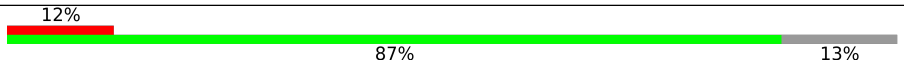
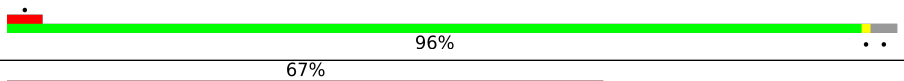
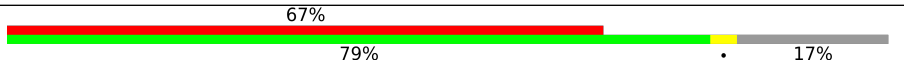
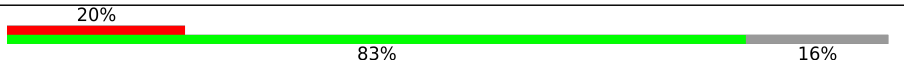
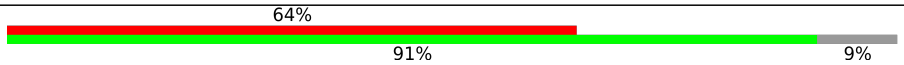
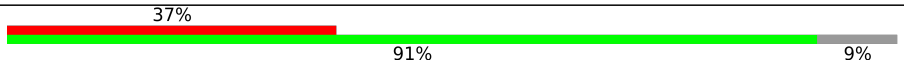
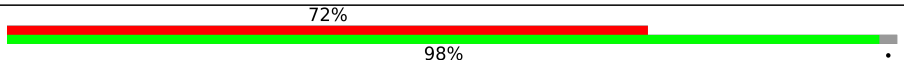
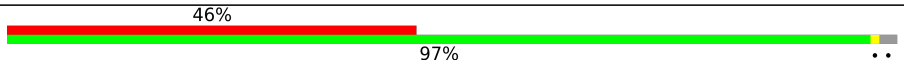
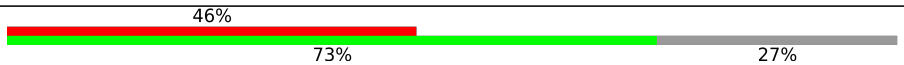
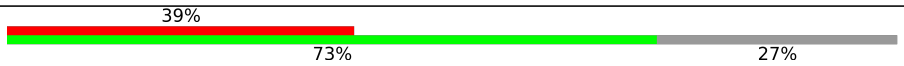
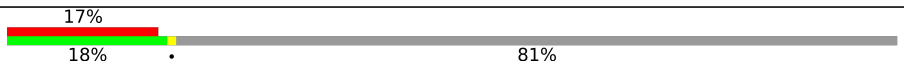
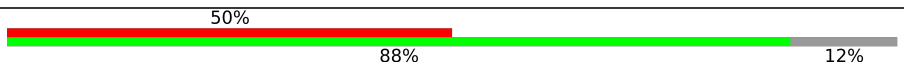
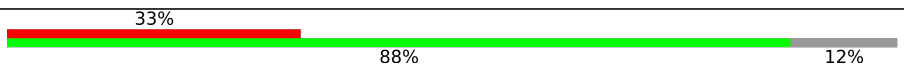
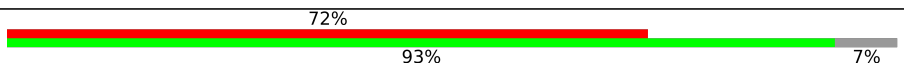
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
50	AF	111	
50	Af	111	
51	AG	82	

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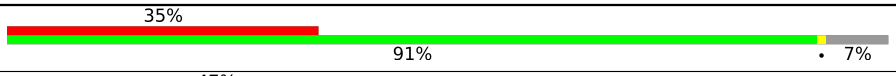
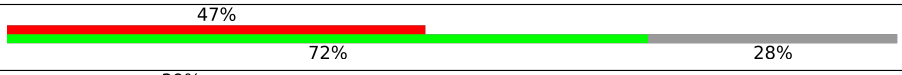
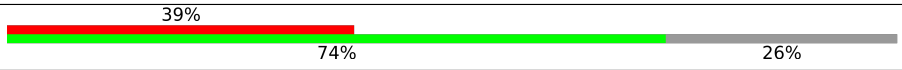
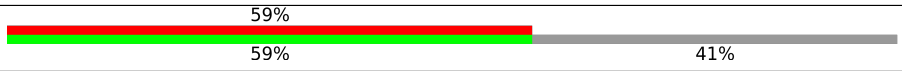
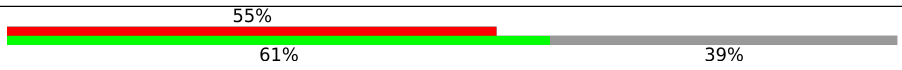
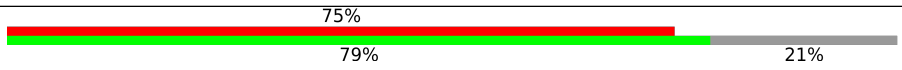
Mol	Chain	Length	Quality of chain
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 97317 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	93	762	528	108	120	6	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	156	1247	796	223	214	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	425	3423	2188	588	623	24	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	316	Total 2525	C 1698	N 382	O 423	S 22	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total 1193	C 806	N 169	O 203	S 15	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	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	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	100	Total	C	N	O	S	0	0
			842	545	135	158	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	92	Total	C	N	O	S	0	0
			773	506	132	132	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	70	Total	C	N	O	S	0	0
			587	383	98	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	72	Total	C	N	O	S	0	0
			578	381	101	94	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	119	Total	C	N	O	S	0	0
			1019	642	191	178	8		

- 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	50	Total	C	N	O	S	0	0
			413	263	77	72	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	26	Total	C	N	O	0	0
			226	147	38	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	399	Total	C	N	O	S	0	0
			3117	1943	554	604	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	401	Total	C	N	O	S	0	0
			3131	1955	555	605	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	414	Total	C	N	O	S	0	0
			3107	1954	546	598	9		
46	Ab	413	Total	C	N	O	S	0	0
			3101	1948	543	601	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
			347	221	65	61			
49	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	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	64	Total 527	C 321	N 98	O 103	S 5	0	0
52	Ah	66	Total 544	C 333	N 101	O 105	S 5	0	0

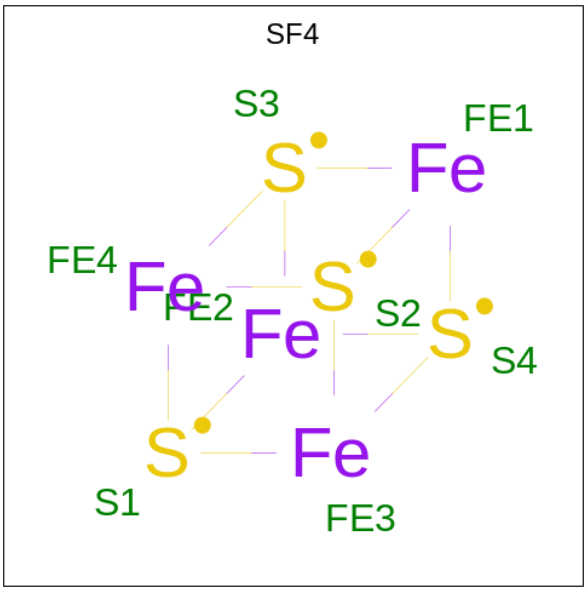
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	38	Total 307	C 201	N 51	O 55	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.

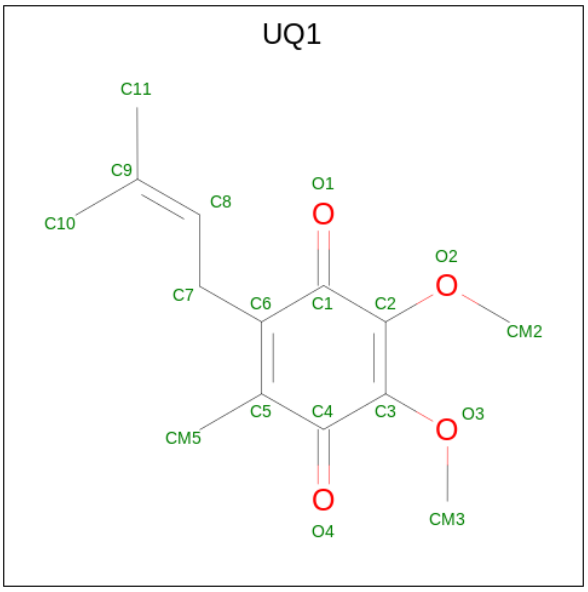
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	34	Total 278	C 183	N 51	O 43	S 1	0	0
54	Ak	44	Total 357	C 236	N 63	O 57	S 1	0	0

- Molecule 55 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



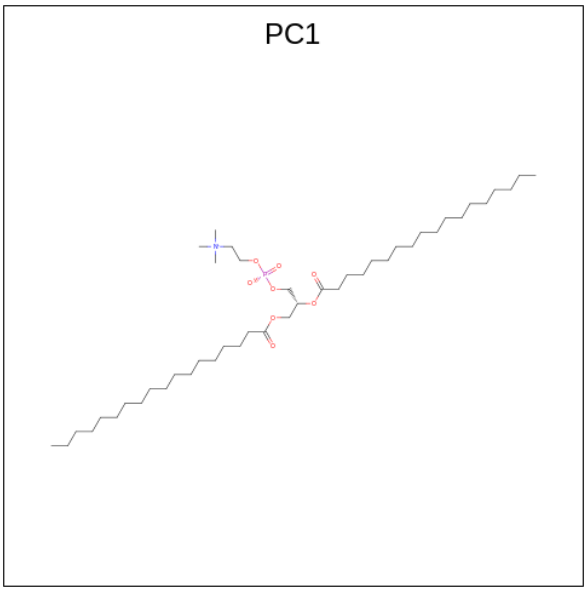
Mol	Chain	Residues	Atoms			AltConf
55	B	1	Total	Fe	S	0
			8	4	4	
55	F	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 56 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 57 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
57	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
57	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

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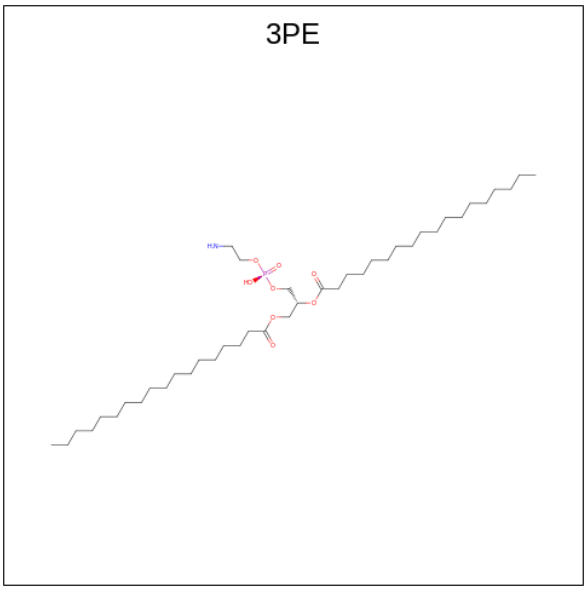
Mol	Chain	Residues	Atoms					AltConf
57	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
58	I	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
58	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
58	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
58	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	M	1	Total	C	N	O	P	0
			51	41	1	8	1	

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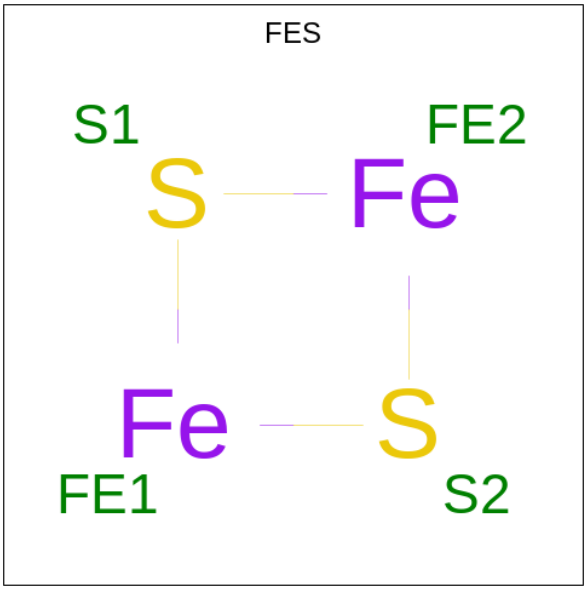
Mol	Chain	Residues	Atoms					AltConf
58	O	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	j	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
58	AC	1	Total	C	N	O	P	0
			25	15	1	8	1	
58	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	

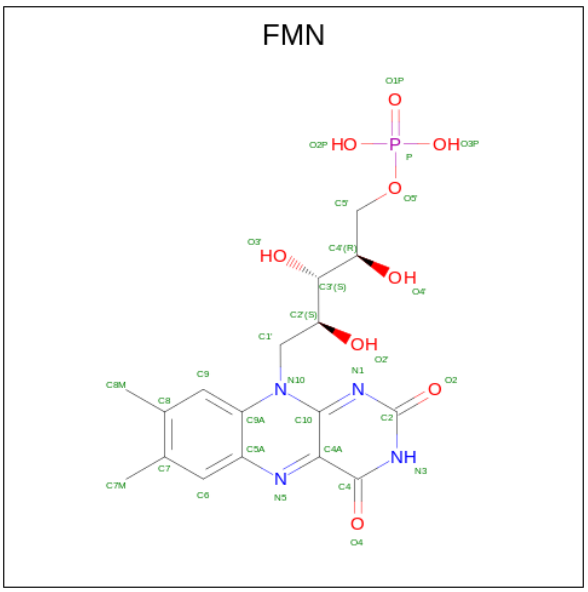
- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

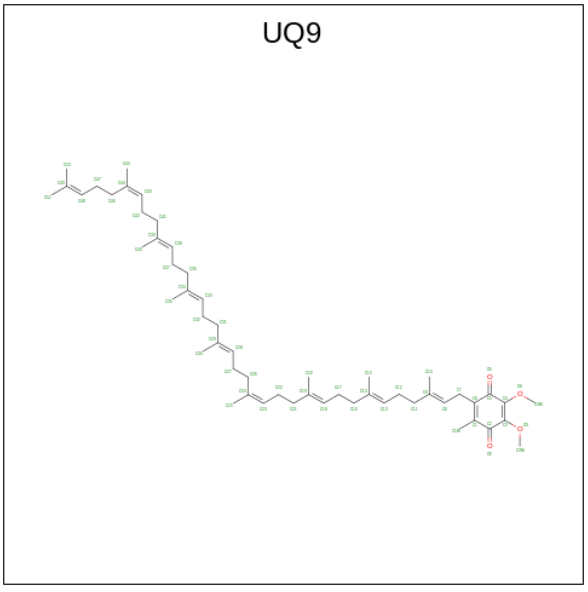
- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$)

(labeled as "Ligand of Interest" by depositor).



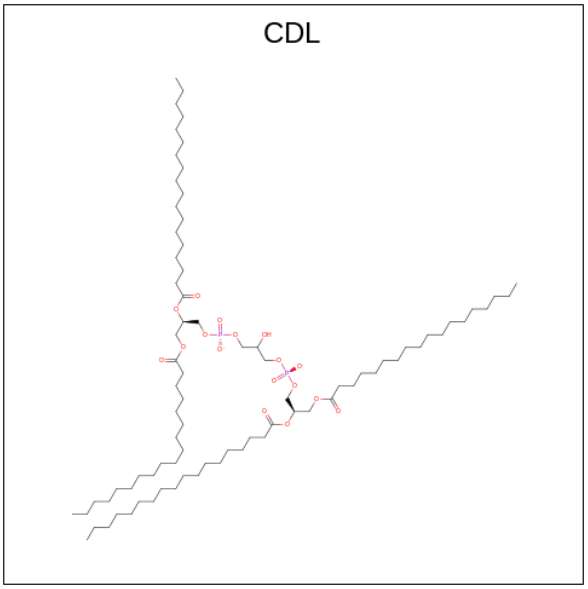
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



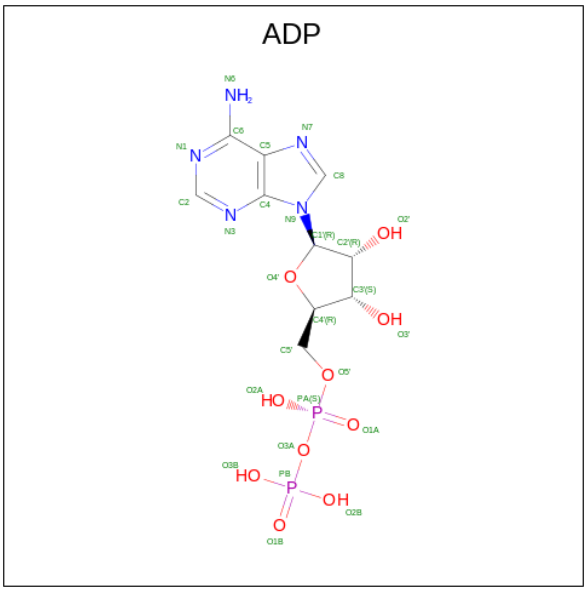
Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



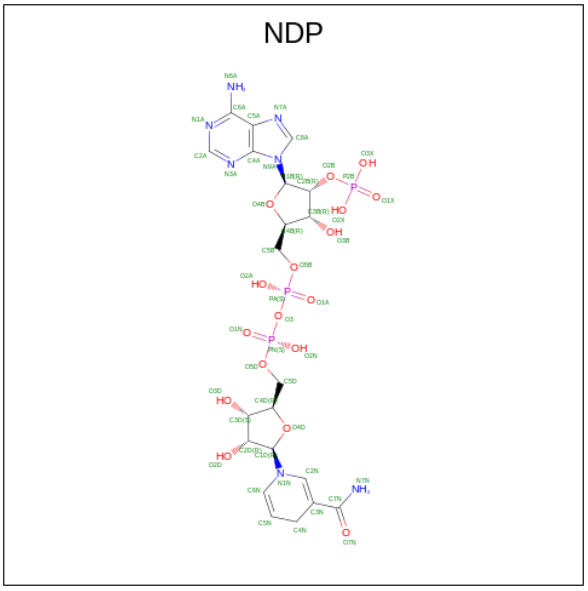
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			77	58	17	2	
62	L	1	Total	C	O	P	0
			81	62	17	2	
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	d	1	Total	C	O	P	0
			67	48	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ac	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

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



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

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



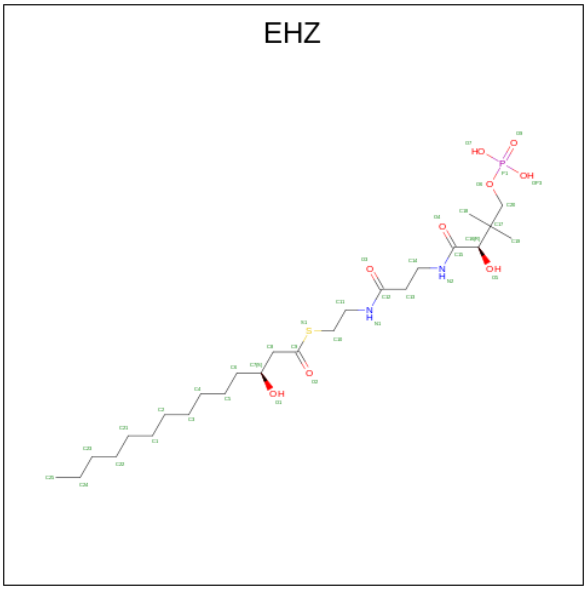
Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

Interest" by depositor).

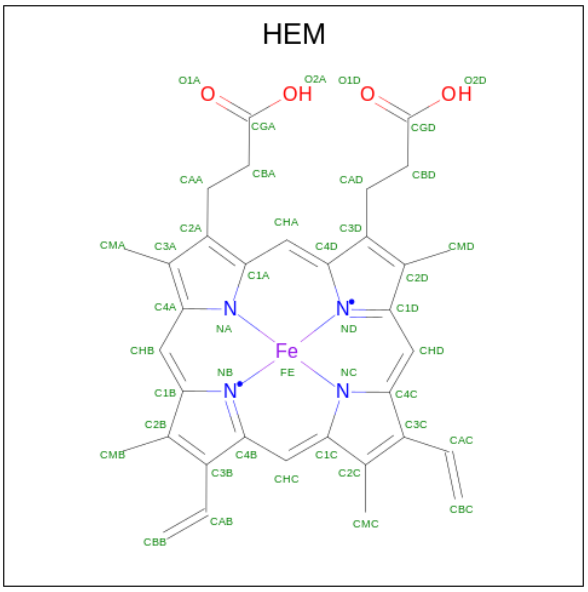
Mol	Chain	Residues	Atoms	AltConf
65	R	1	Total Zn 1 1	0

- 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: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



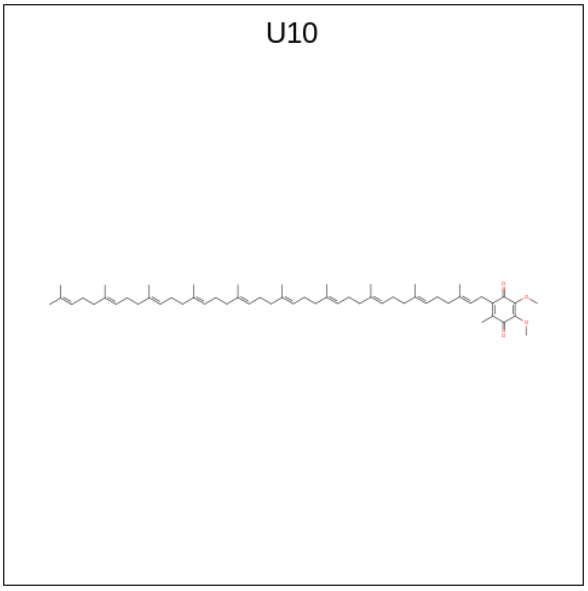
Mol	Chain	Residues	Atoms	AltConf
66	W	1	Total C N O P S 32 19 2 9 1 1	0
66	n	1	Total C N O P S 32 19 2 9 1 1	0

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



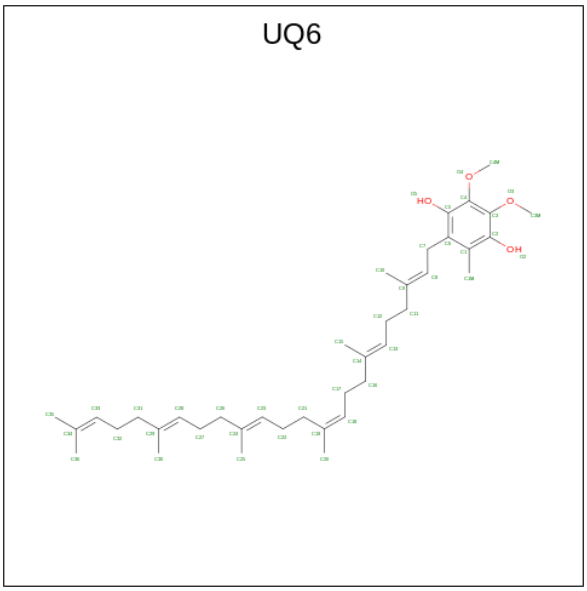
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



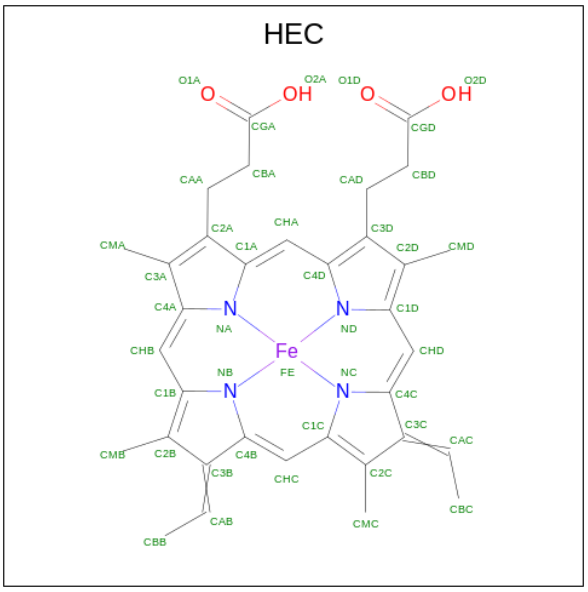
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total 23	C 19	O 4	0
68	Ac	1	Total 23	C 19	O 4	0

- 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 28	C 24	O 4	0
69	Ac	1	Total 28	C 24	O 4	0

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

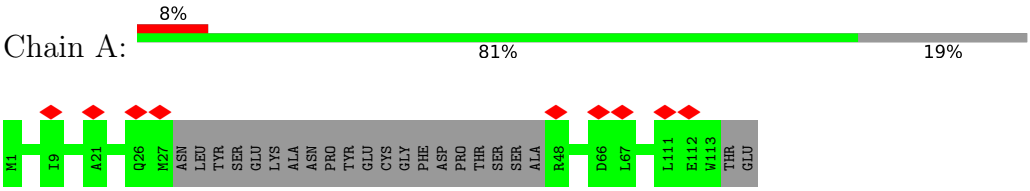


Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

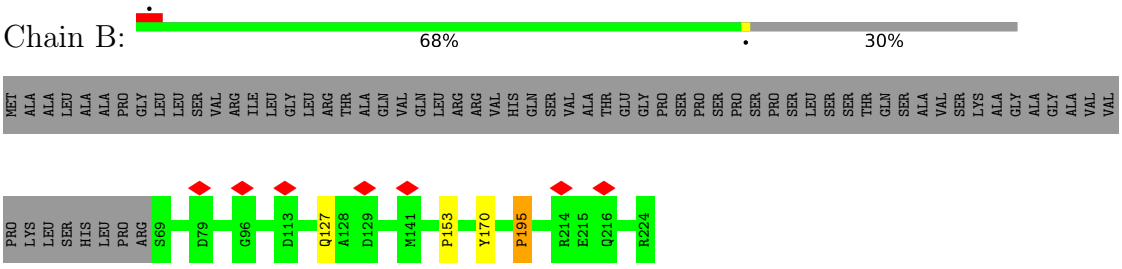
3 Residue-property plots (i)

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

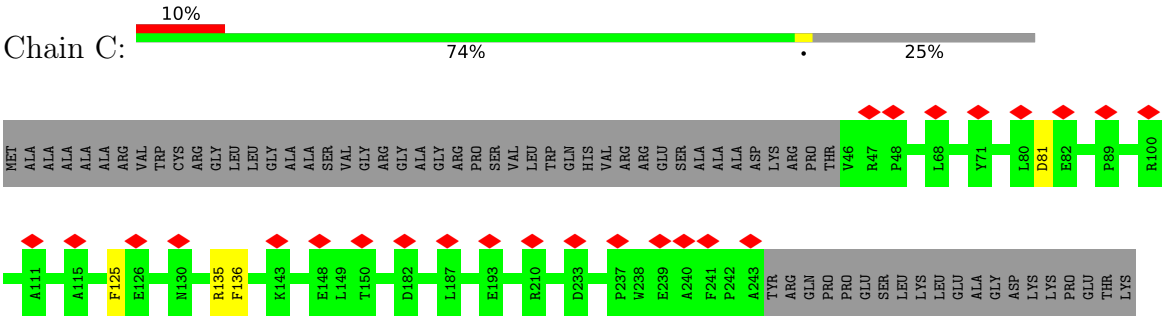
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



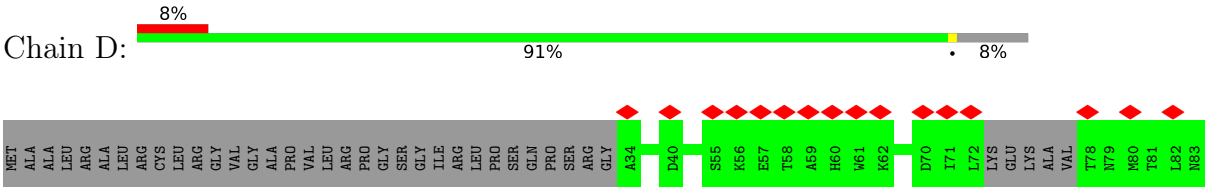
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

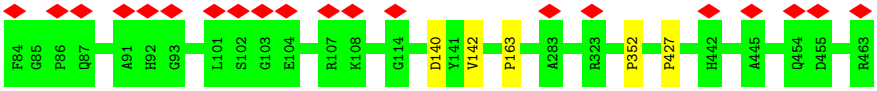


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

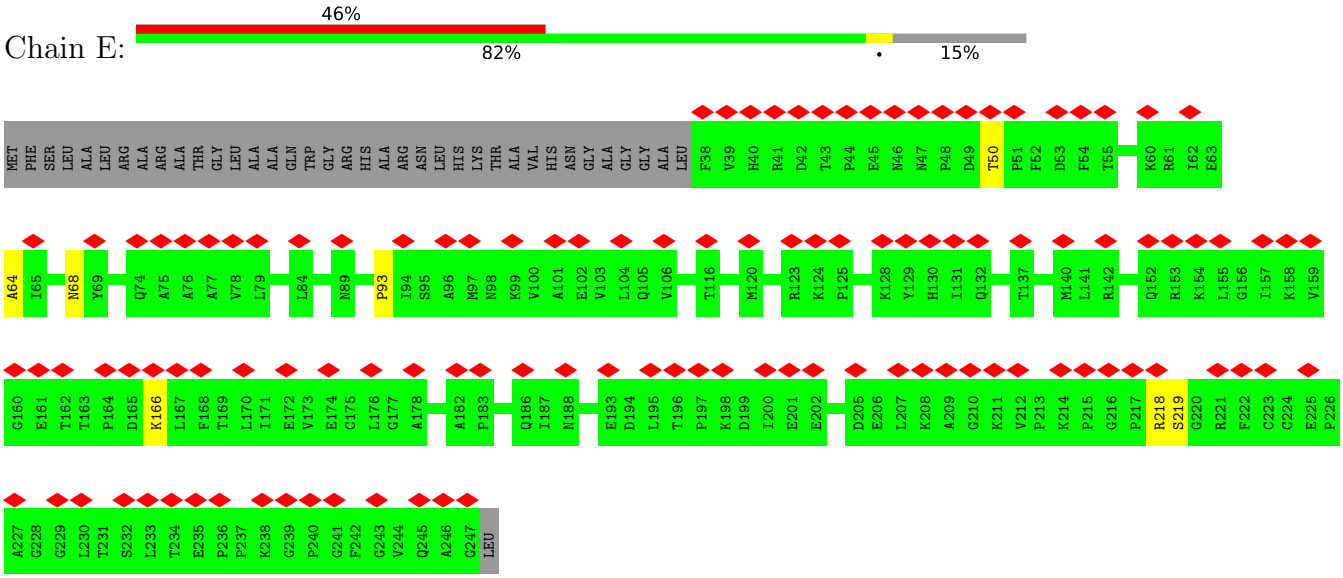


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

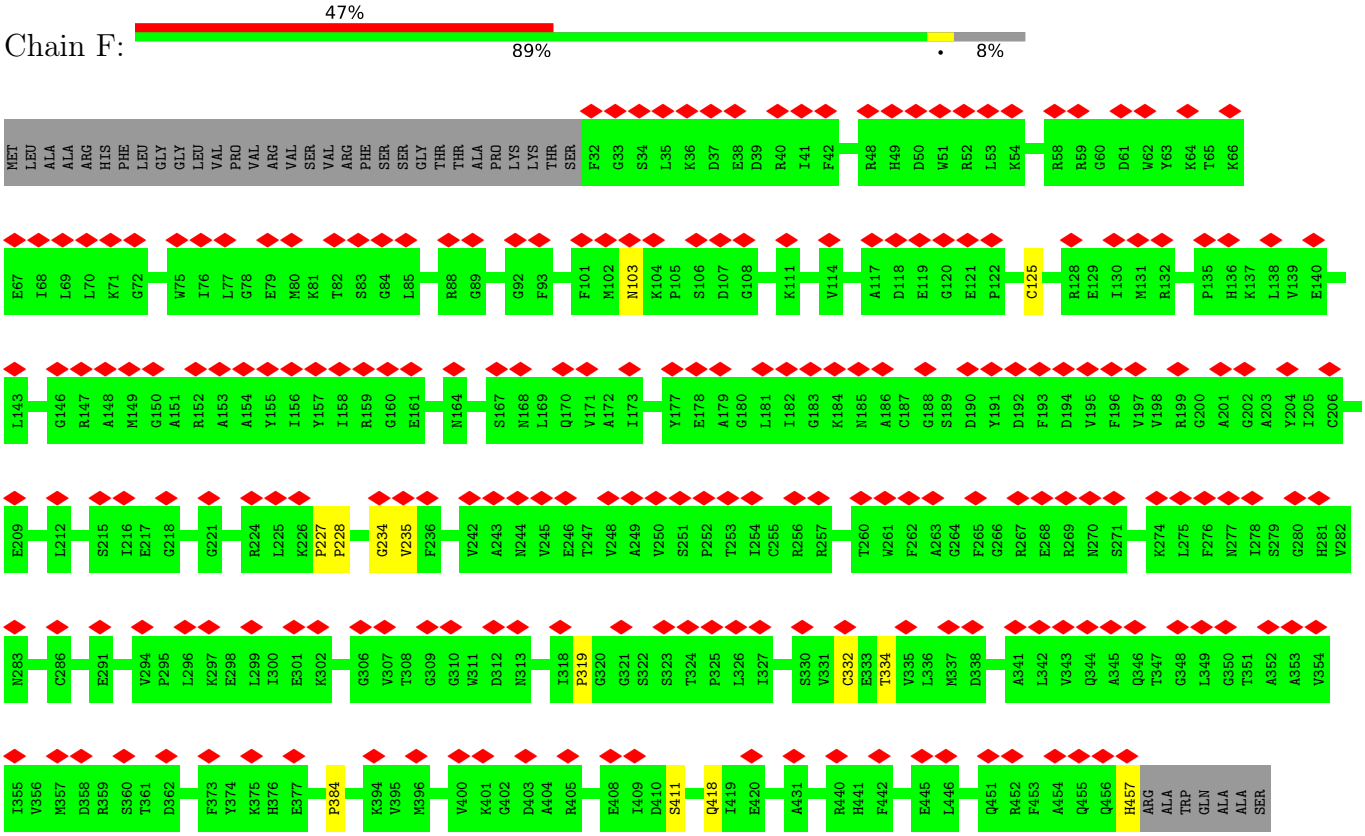




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

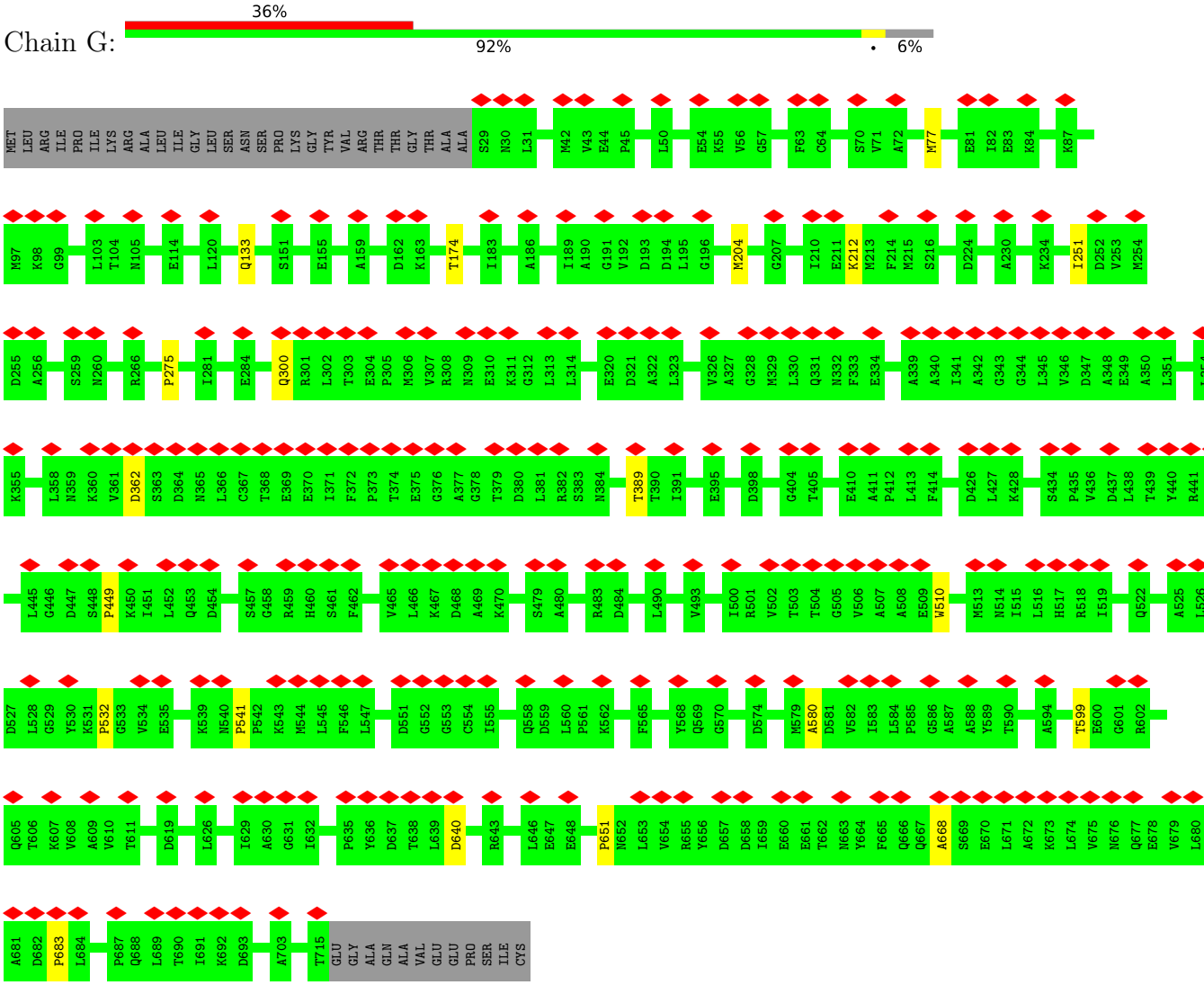


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



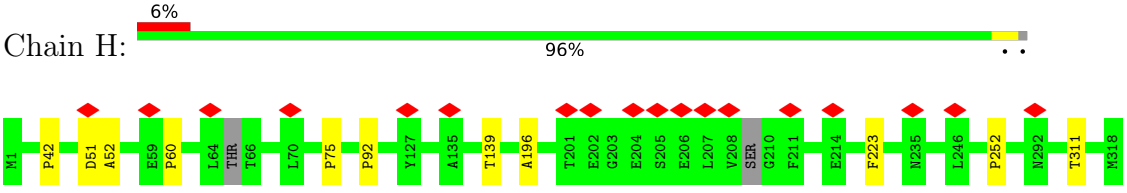
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



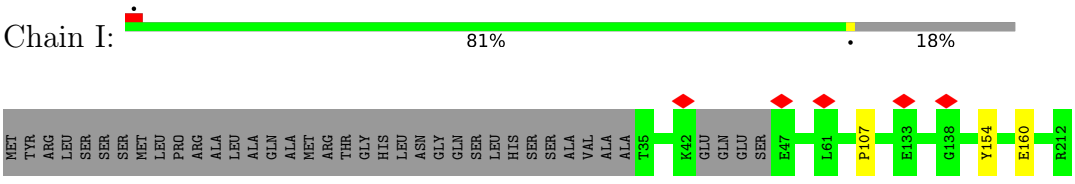
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



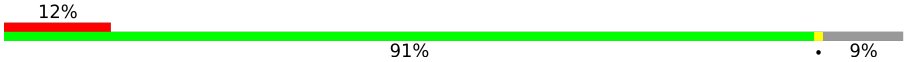
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

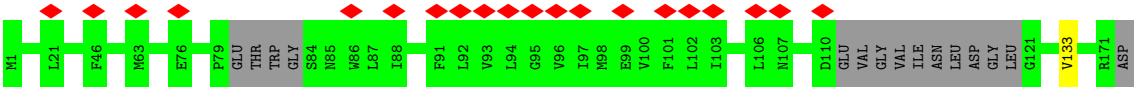
Chain I:



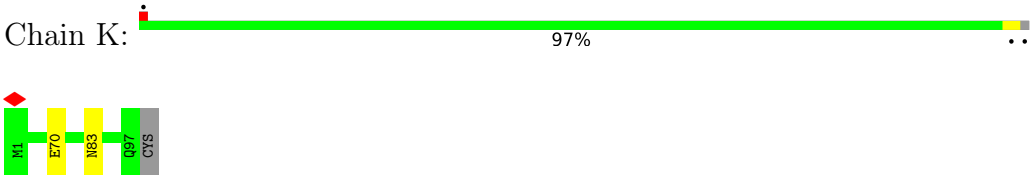
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

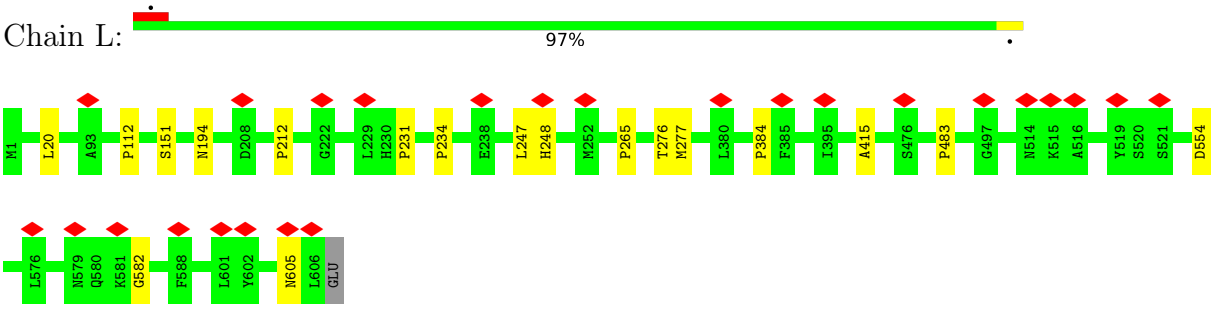




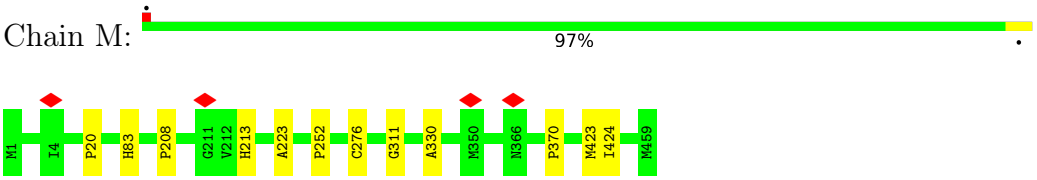
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



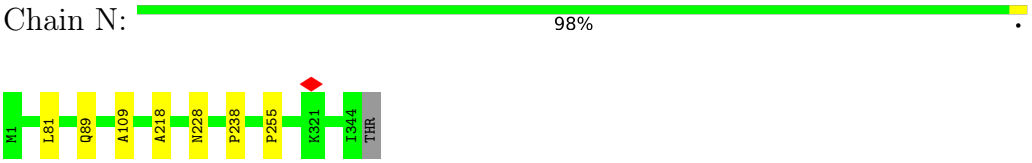
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



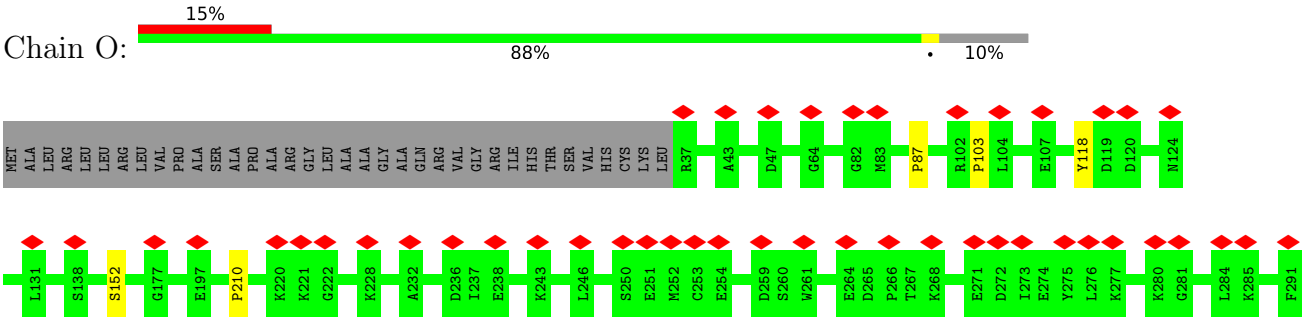
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

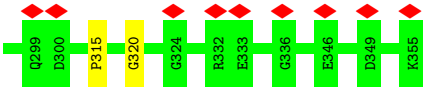


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



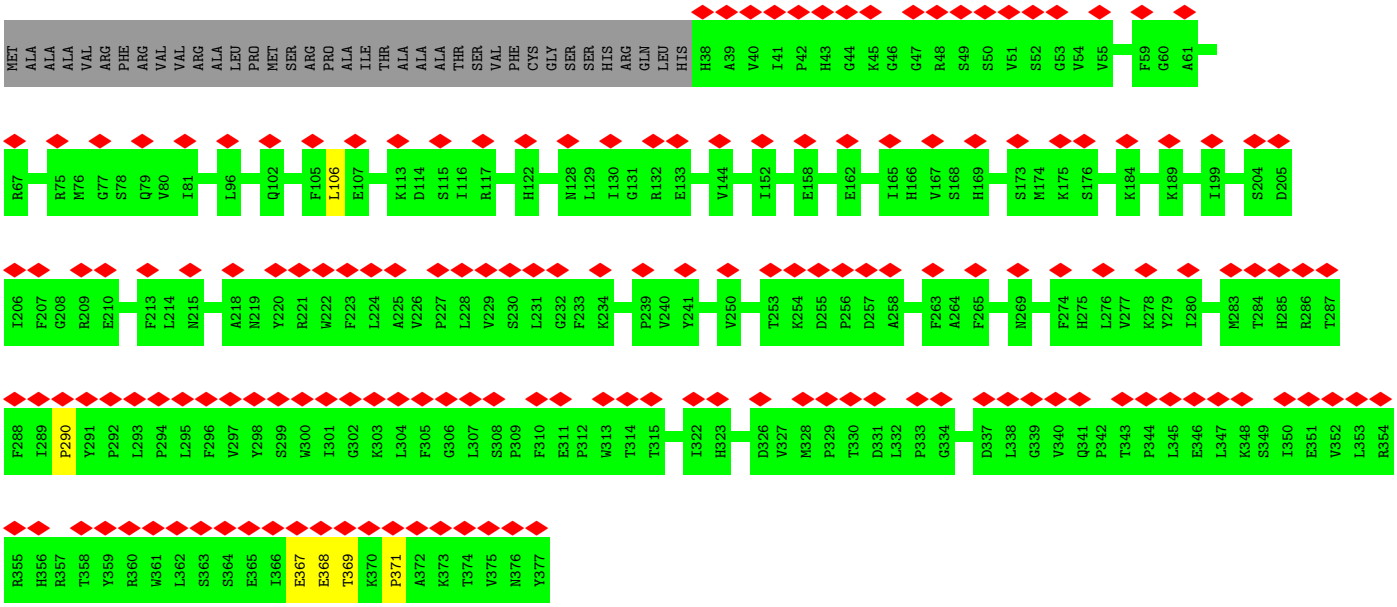
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





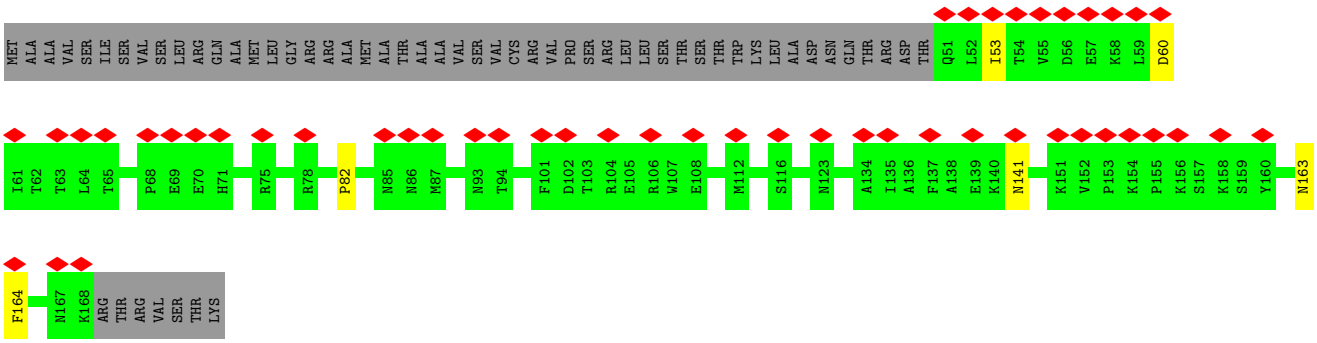
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



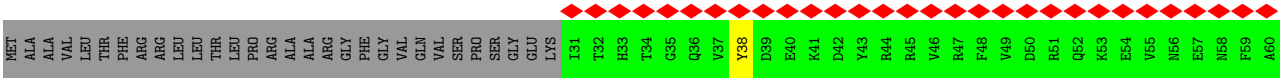
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

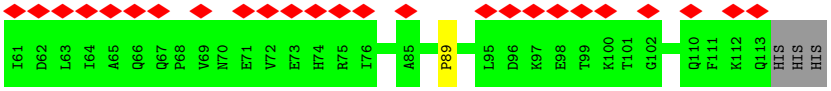
Chain Q:



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

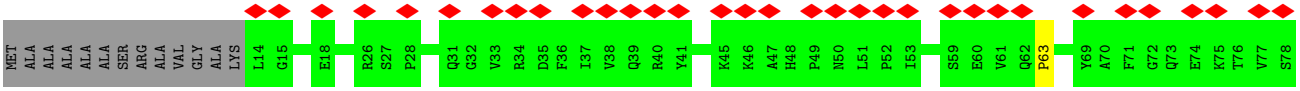
Chain R:

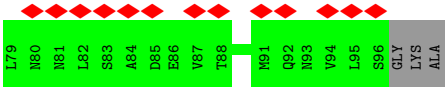




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

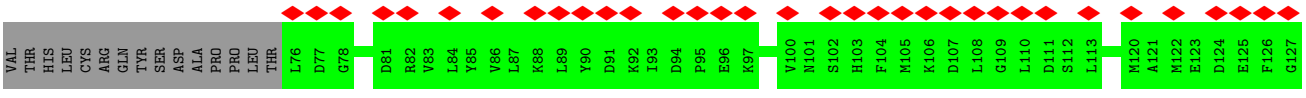
Chain S:

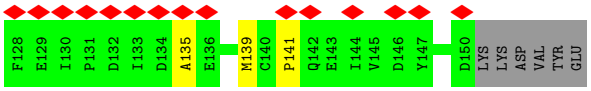




• Molecule 20: Acyl carrier protein, mitochondrial

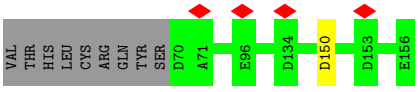
Chain T:





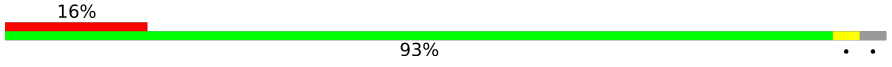
• Molecule 20: Acyl carrier protein, mitochondrial

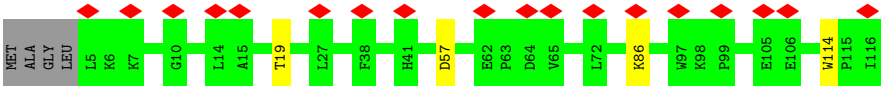
Chain U:



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

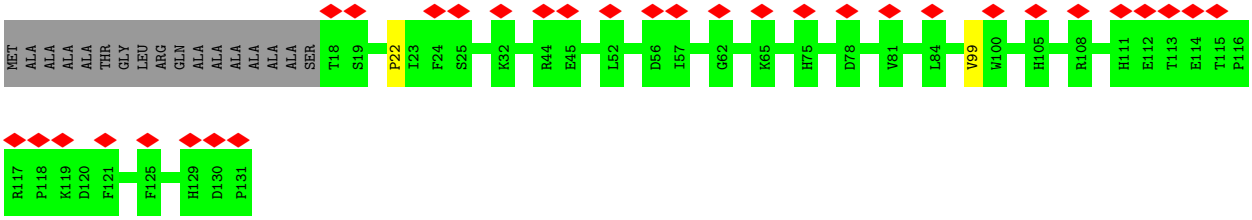
Chain V:



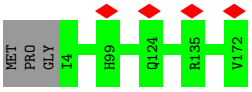


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

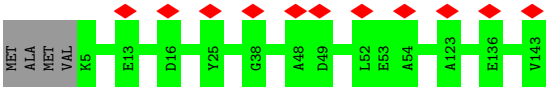
Chain W:



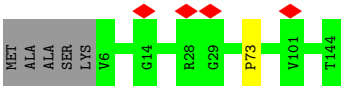
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



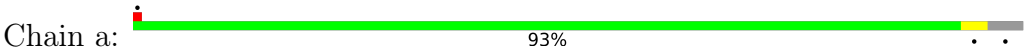
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

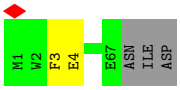


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

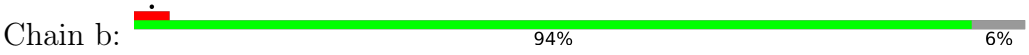


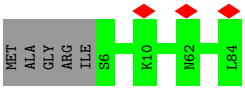
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



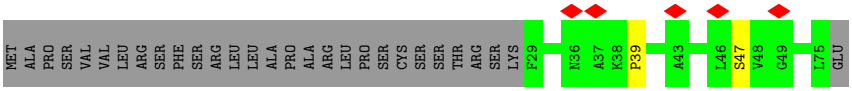


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



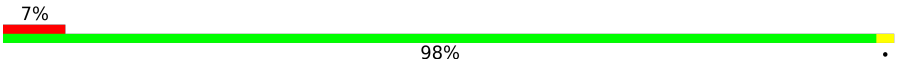


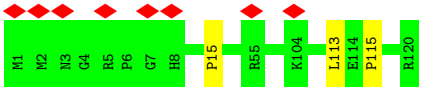
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

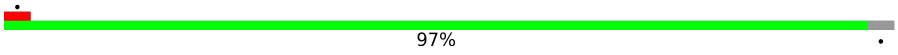
Chain d:

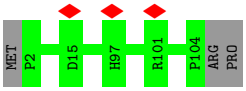




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

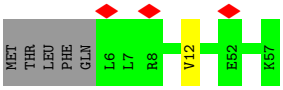
Chain e:





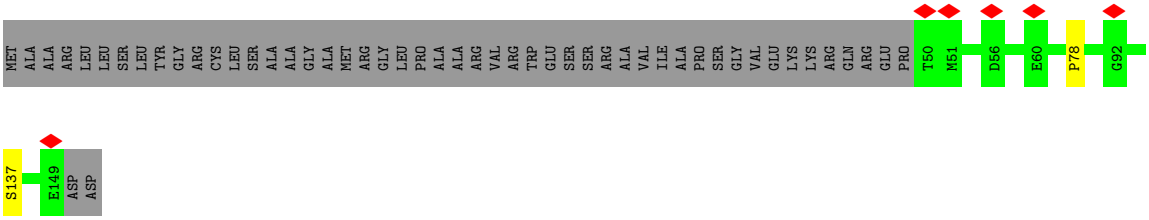
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



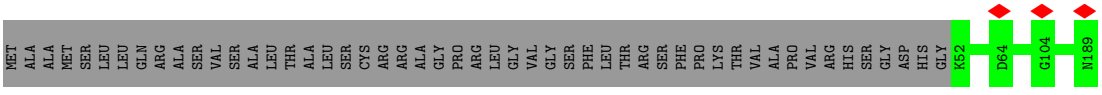
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



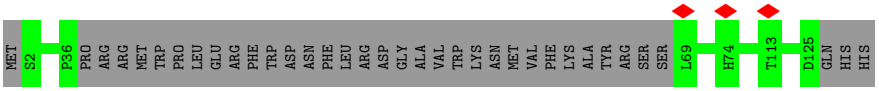
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



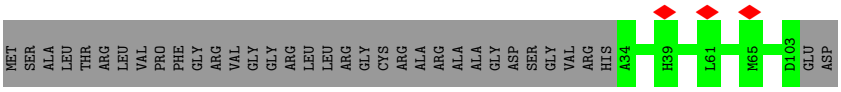
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



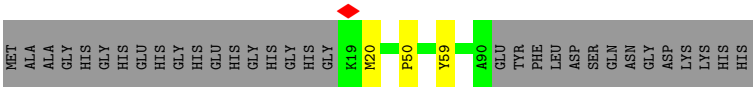
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



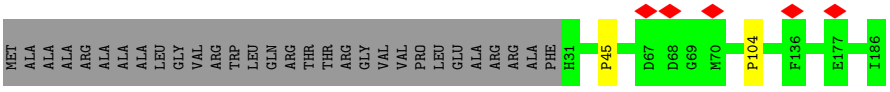
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



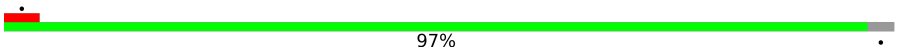
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

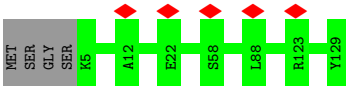
Chain l:



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

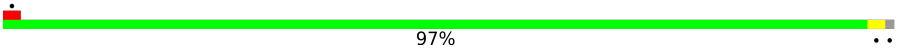
Chain m:

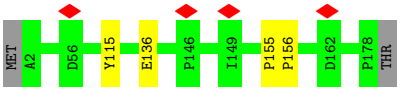




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

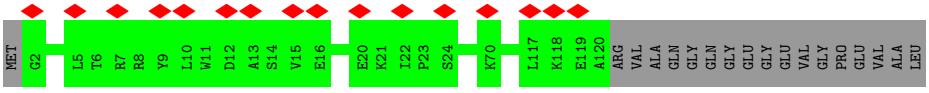
Chain n:





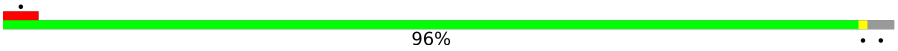
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

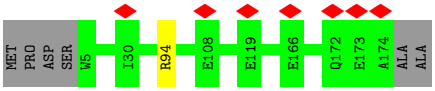
Chain o:



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

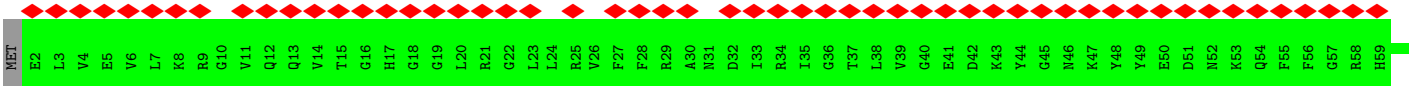
Chain p:

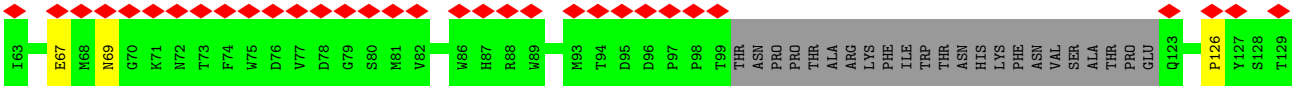


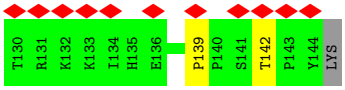


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

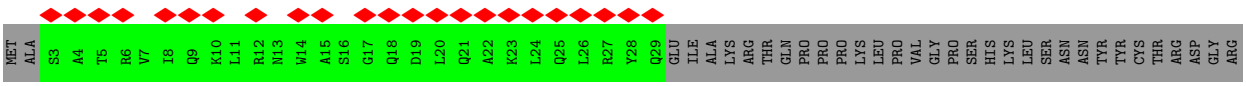


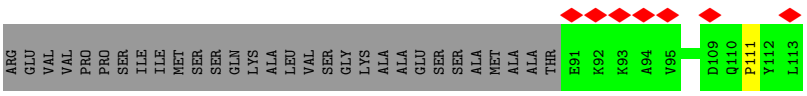




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

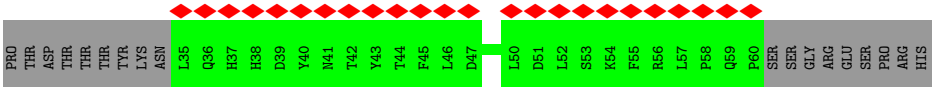
Chain r:





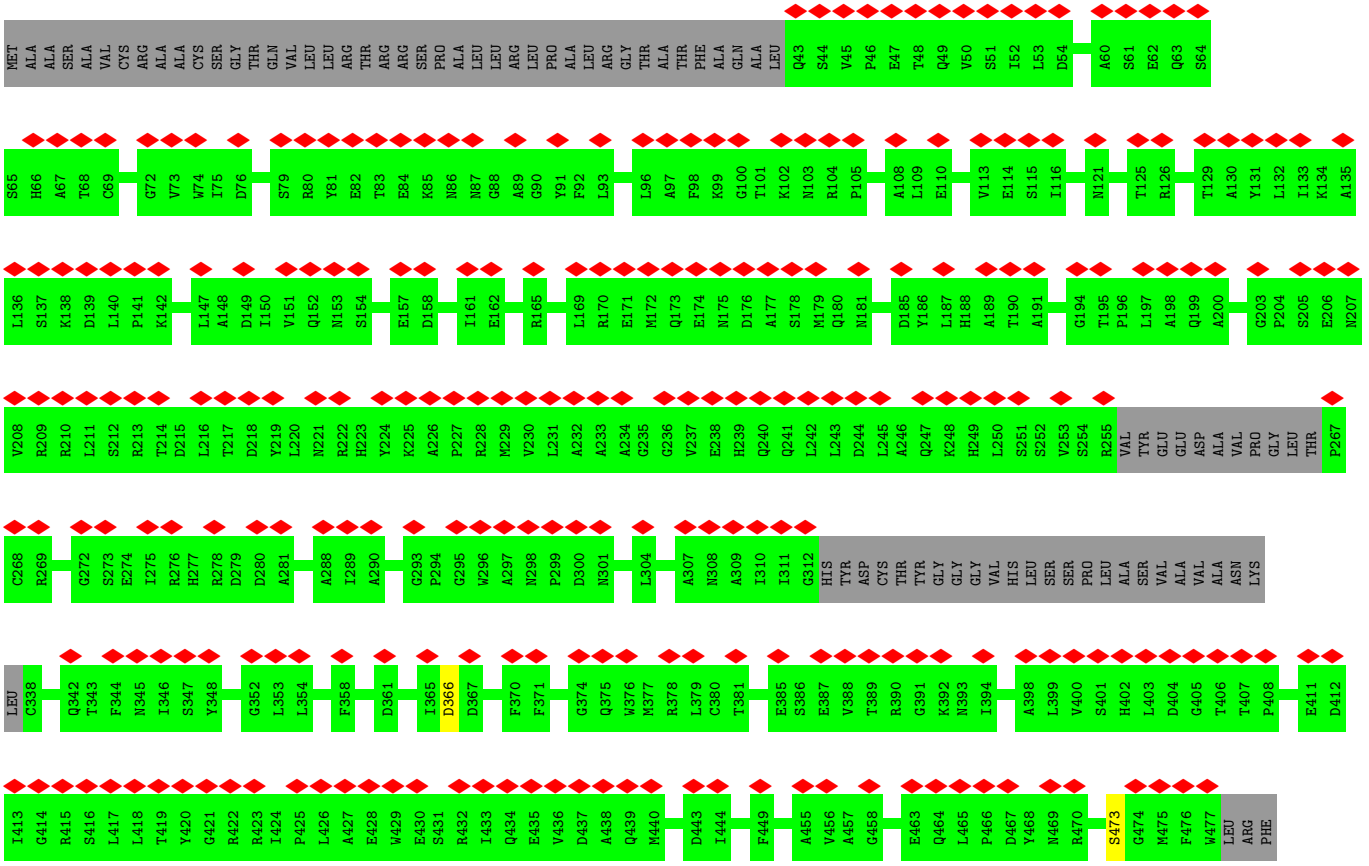
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



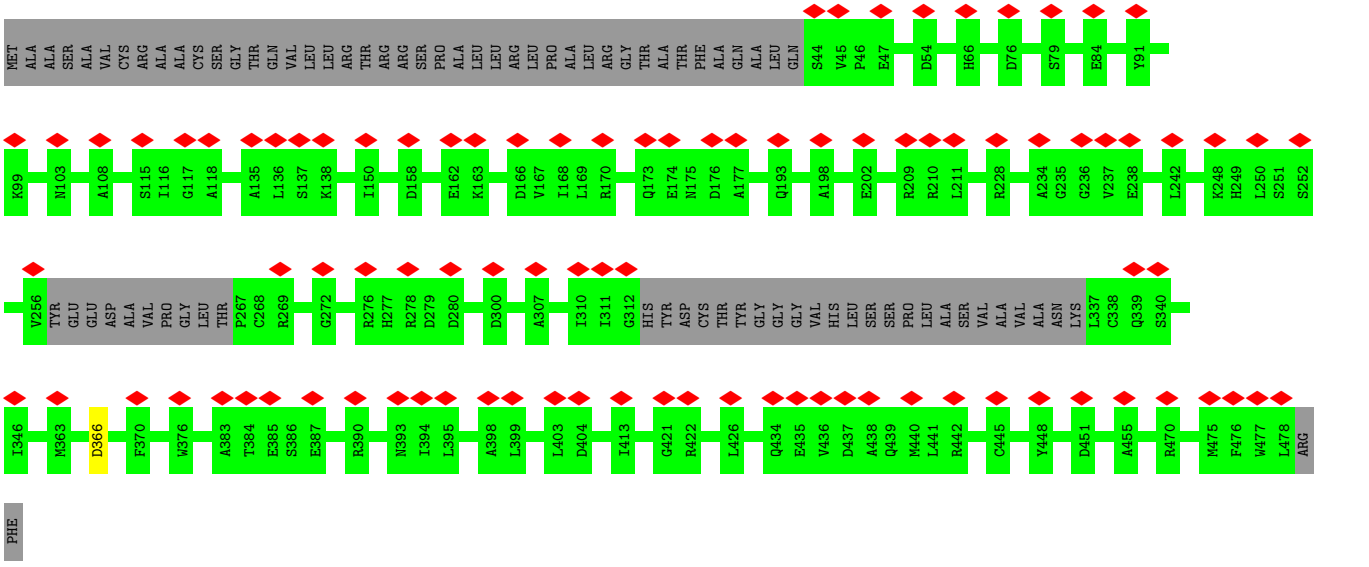
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AA:



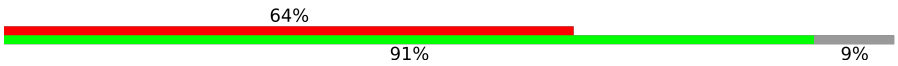
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

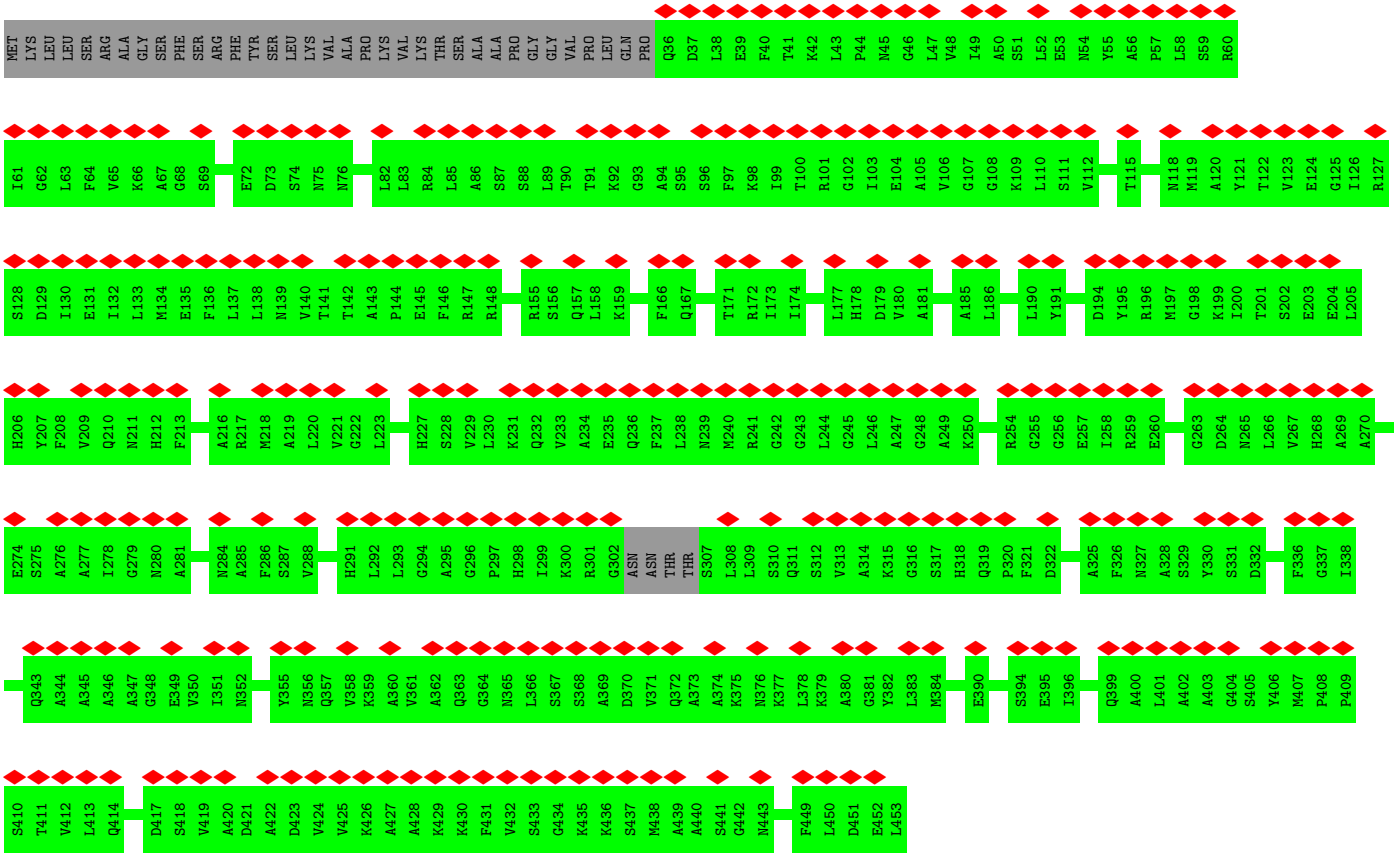
Chain Aa:



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

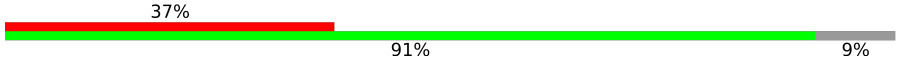
Chain AB:

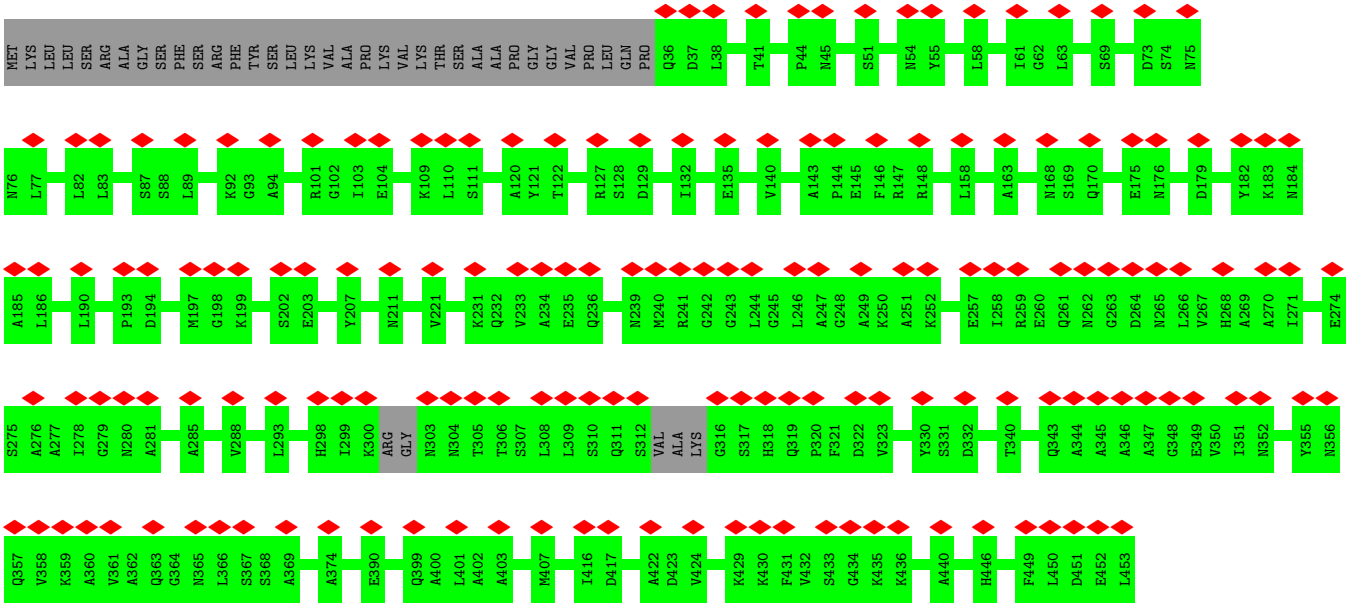




• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

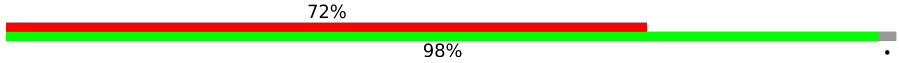
Chain Ab:

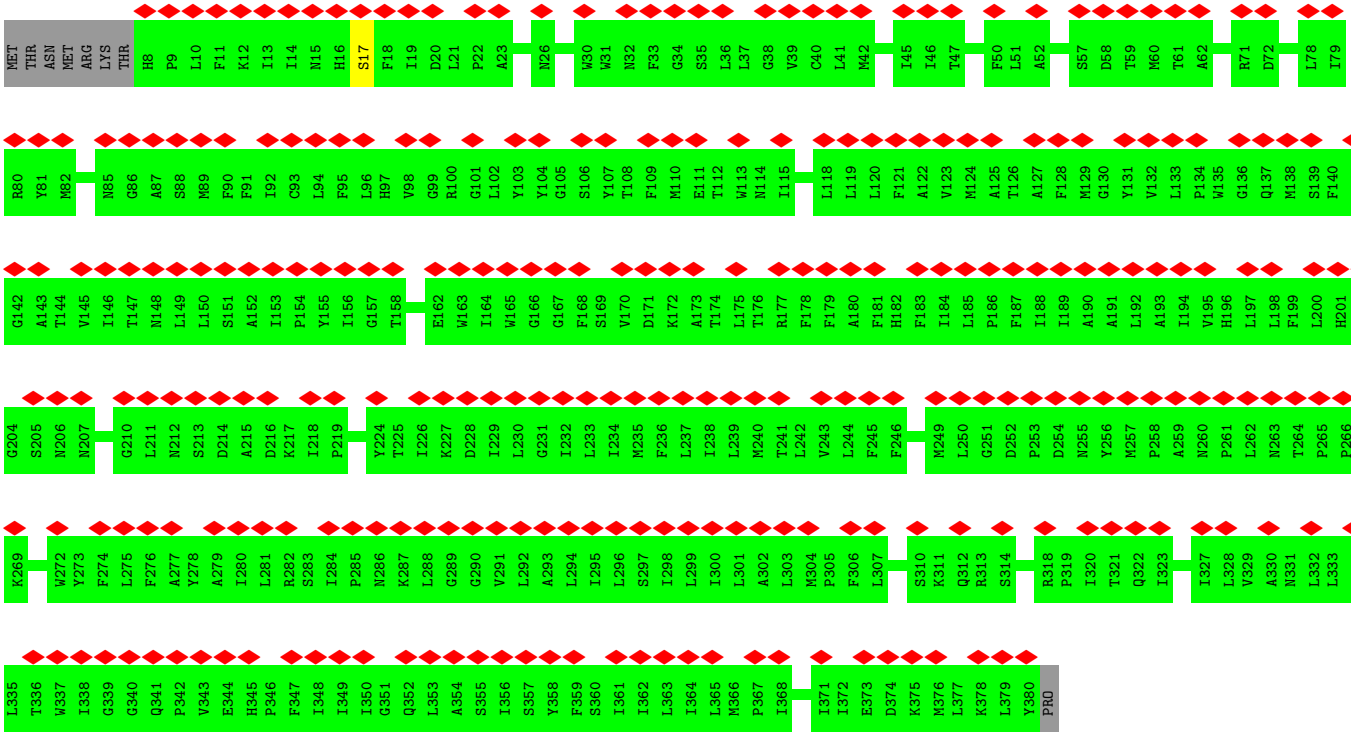




• Molecule 47: Cytochrome b

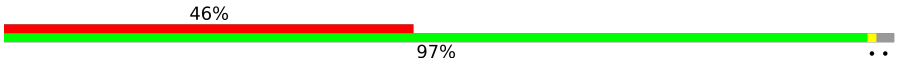
Chain AC:

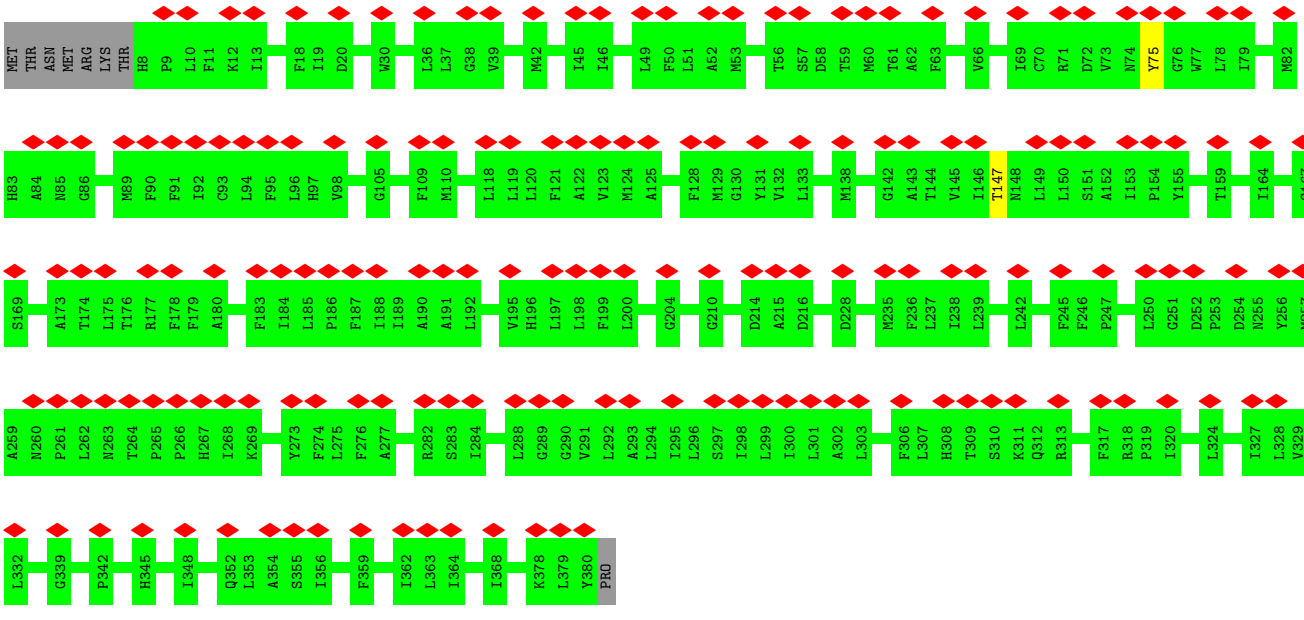




• Molecule 47: Cytochrome b

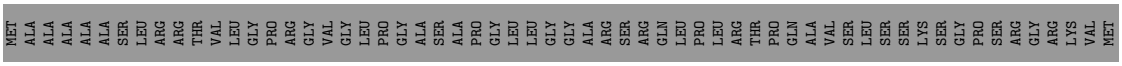
Chain Ac:

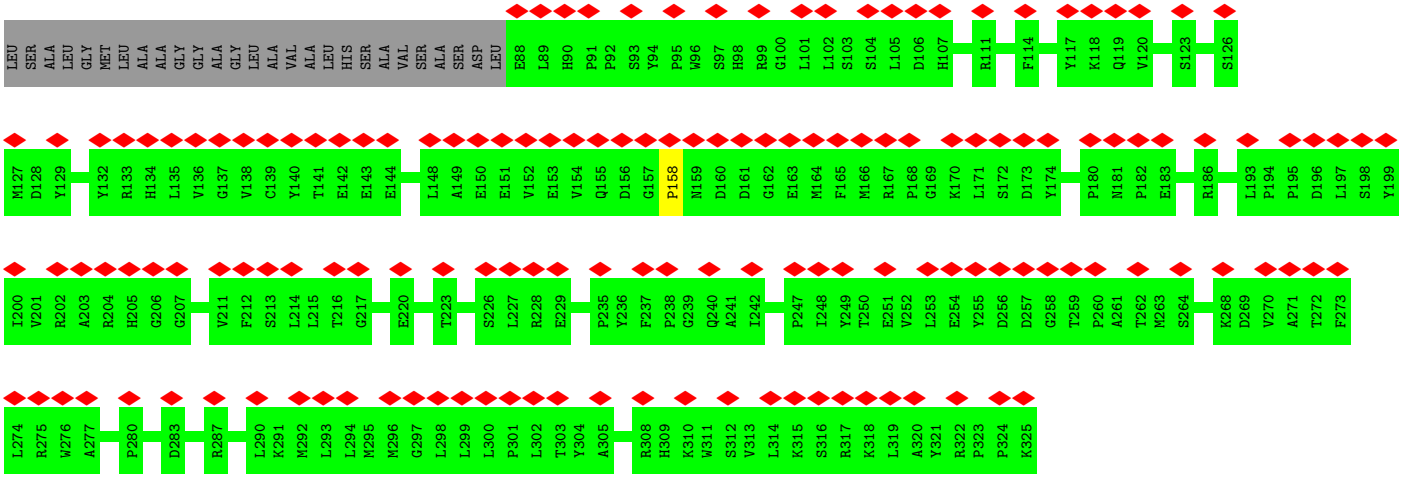




• Molecule 48: Cytochrome c1, heme protein, mitochondrial

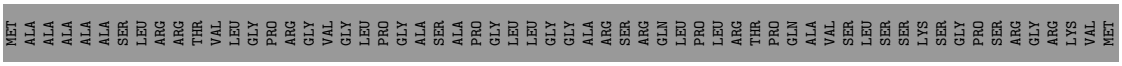
Chain AD:

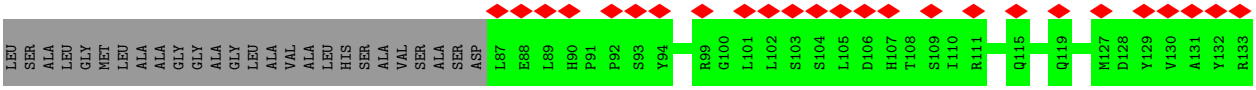


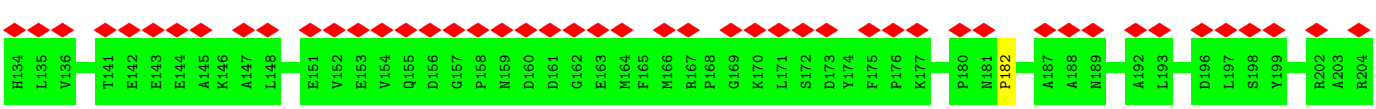


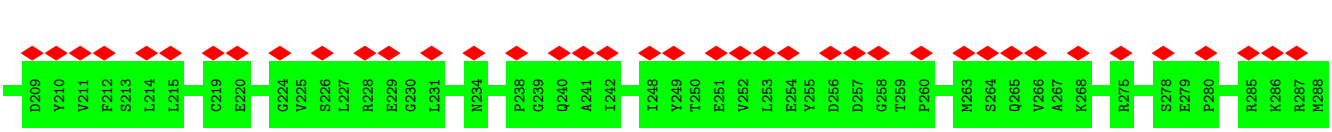
• Molecule 48: Cytochrome c1, heme protein, mitochondrial

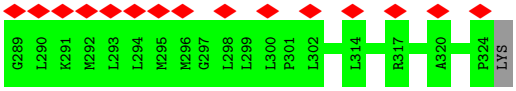
Chain Ad:





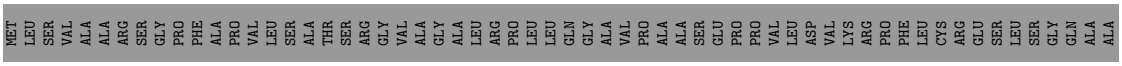


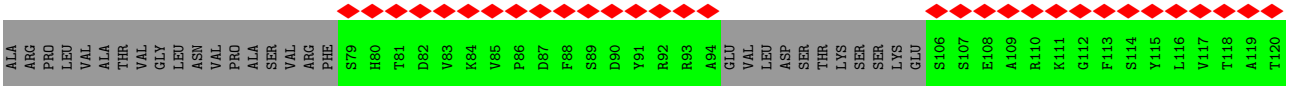


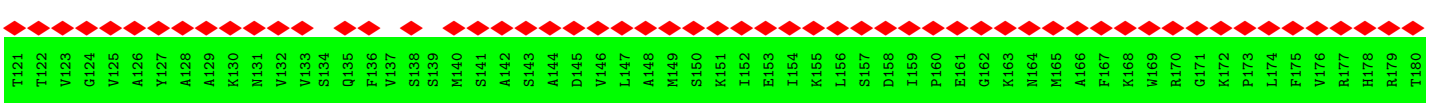


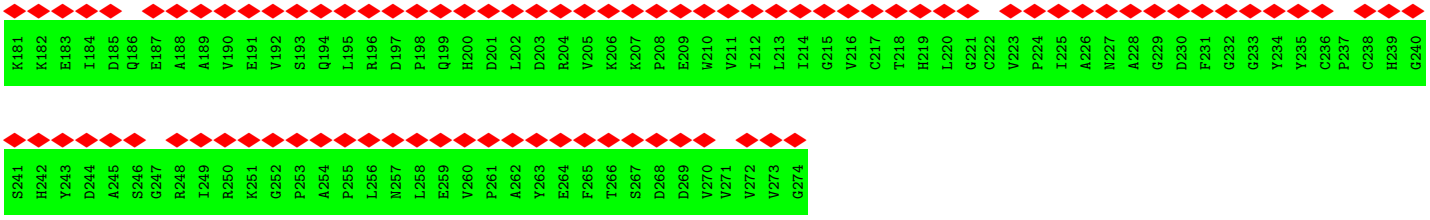
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:



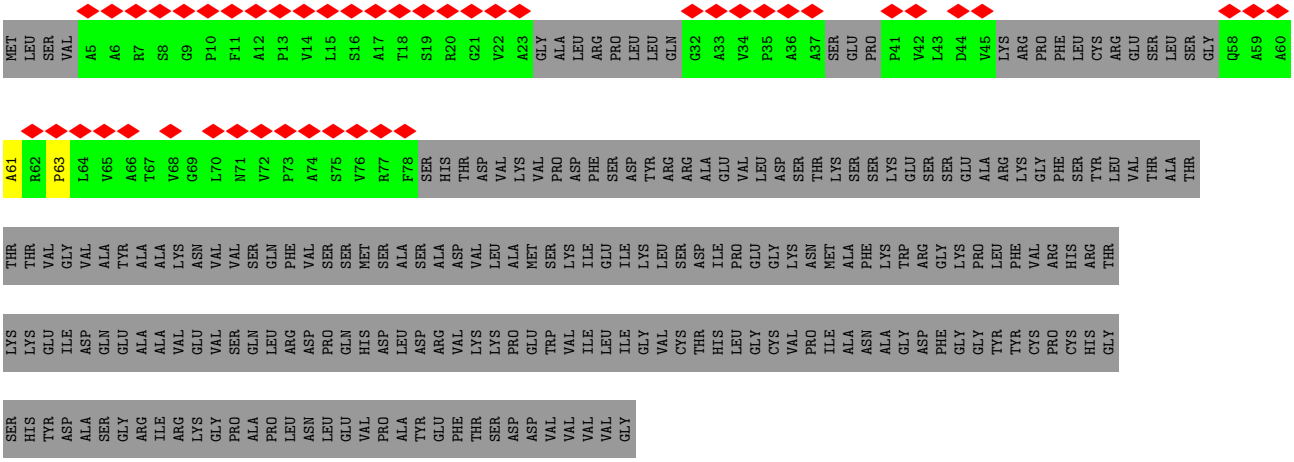






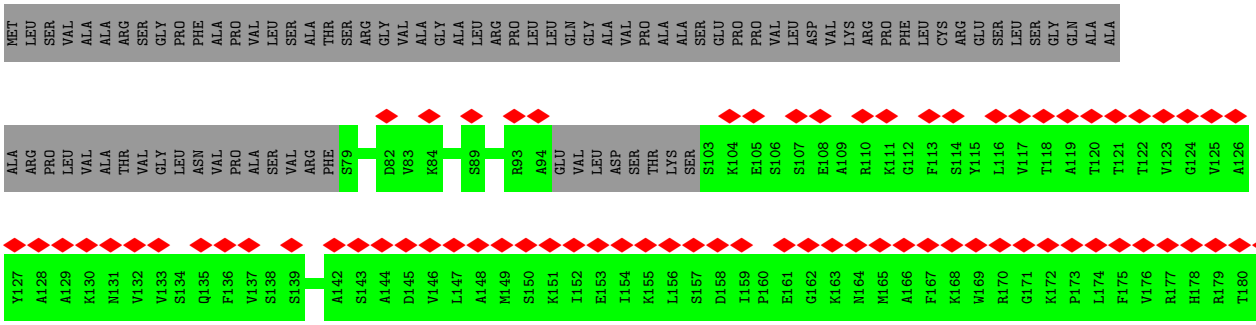
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

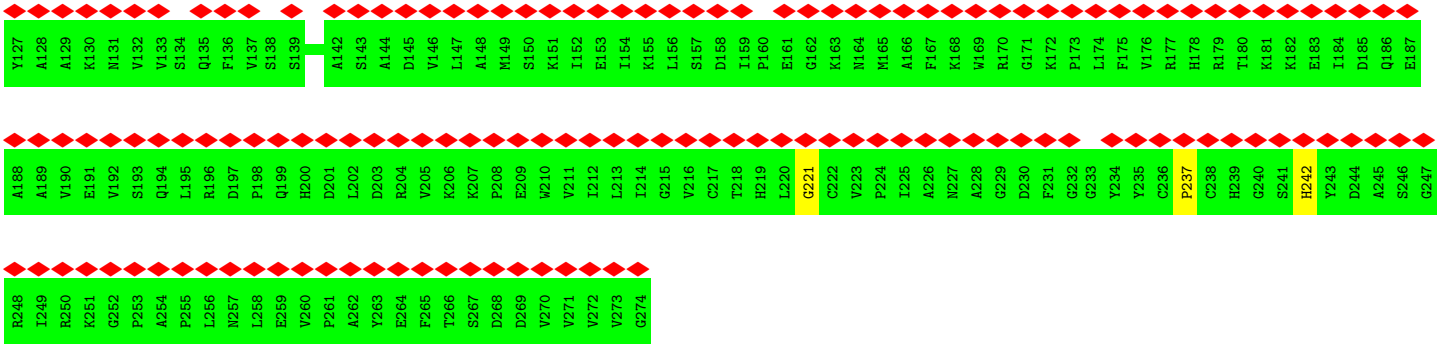
Chain AI:



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

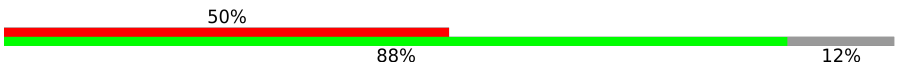
Chain Ae:

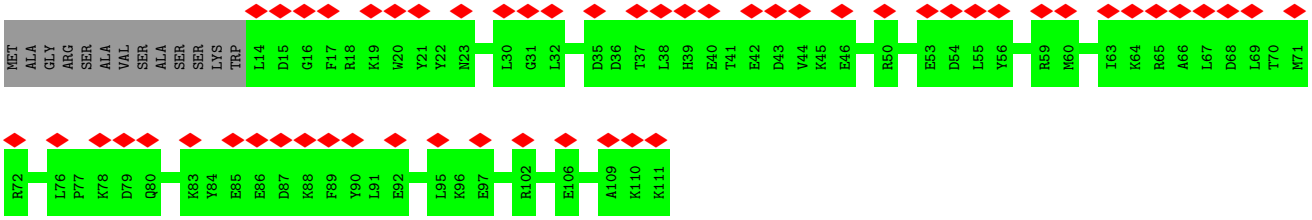




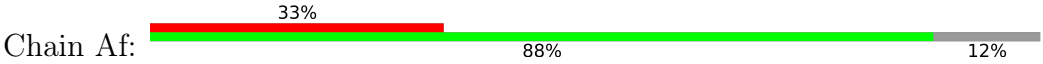
• Molecule 50: Cytochrome b-c1 complex subunit 7

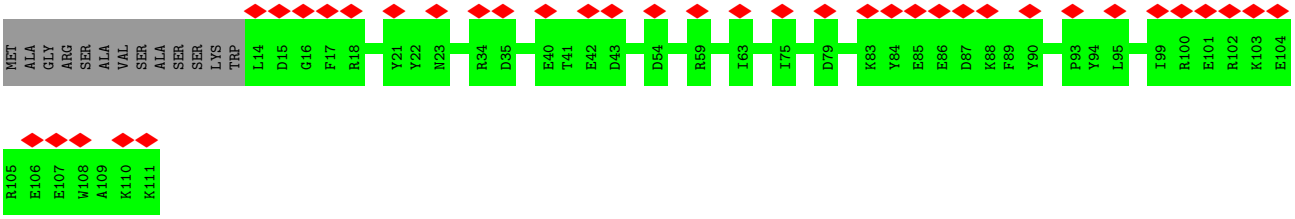
Chain AF:



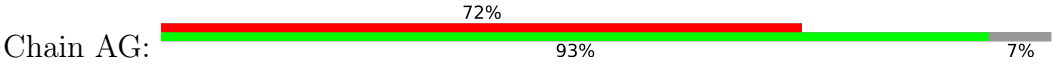


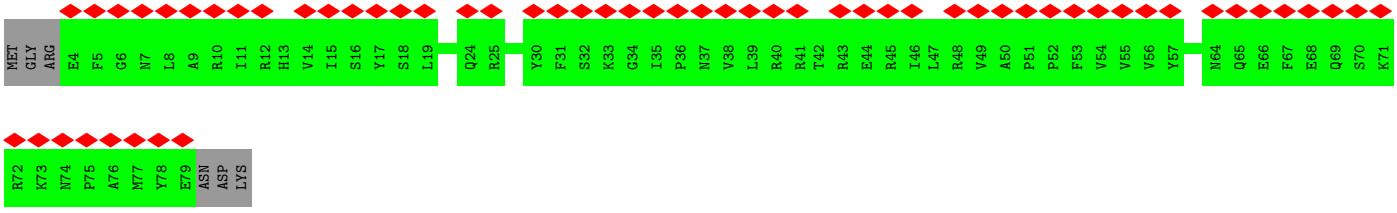
• Molecule 50: Cytochrome b-c1 complex subunit 7



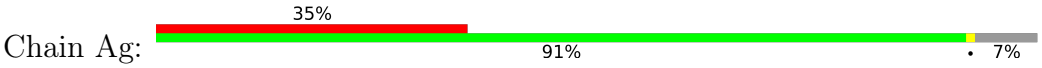


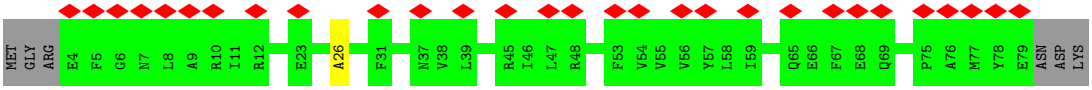
• Molecule 51: Cytochrome b-c1 complex subunit 8



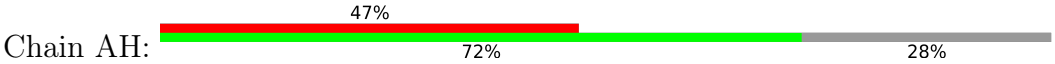


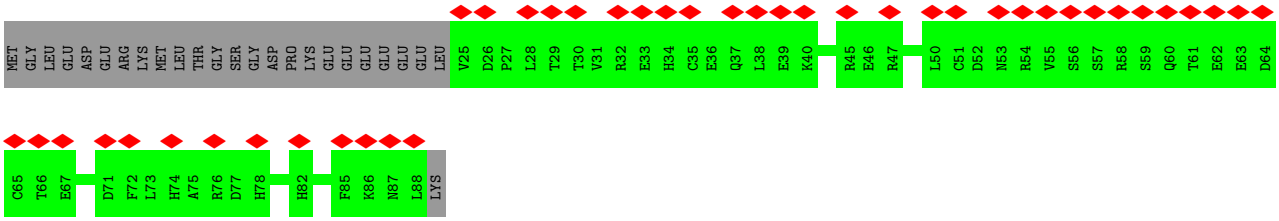
• Molecule 51: Cytochrome b-c1 complex subunit 8





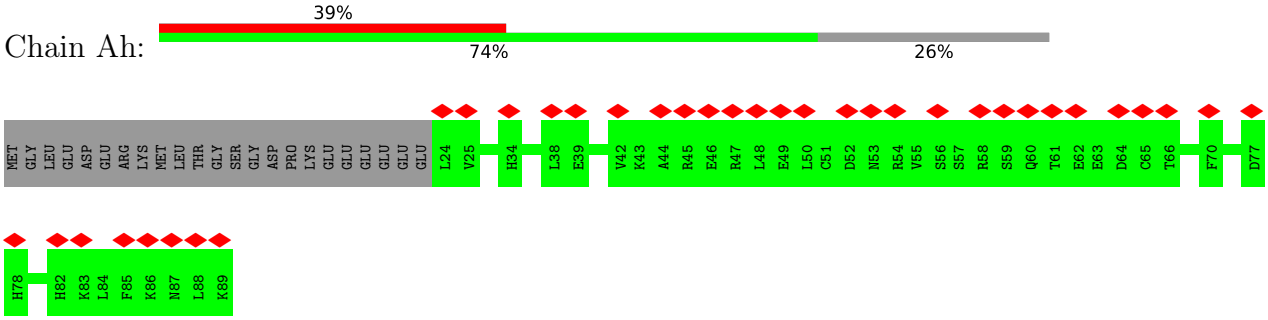
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial





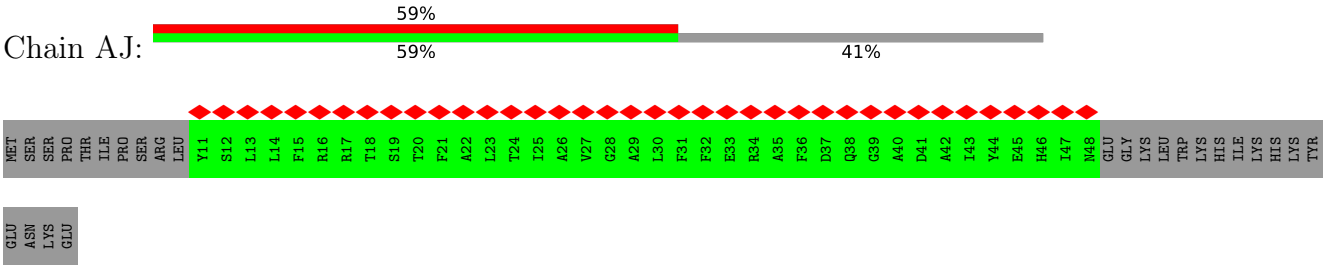
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:



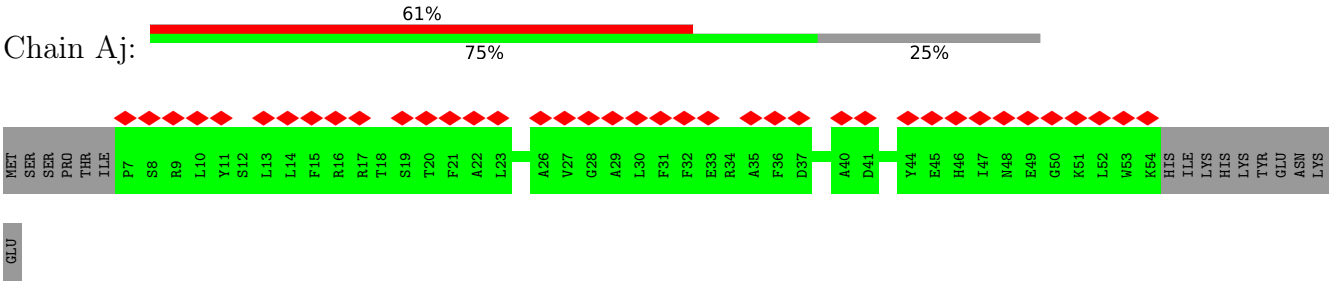
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ:



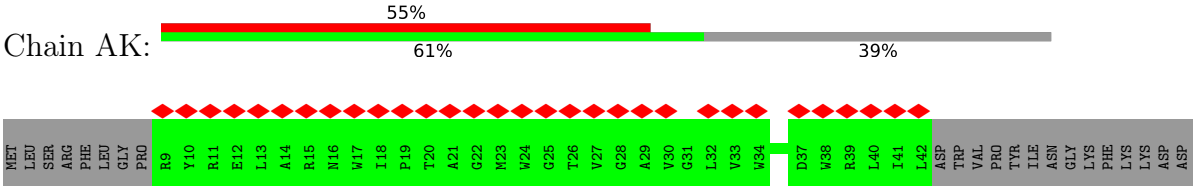
• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



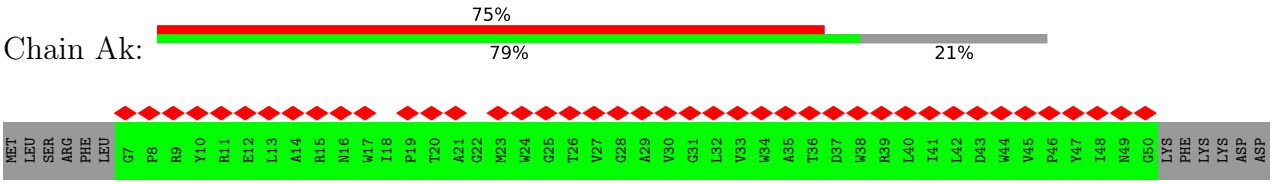
• Molecule 54: Cytochrome b-c1 complex subunit 10

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	37608	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	0.096	Depositor
Minimum map value	-0.037	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 (i)

5.1 Standard geometry (i)

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

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	0.51	0/782	0.70	0/1066
2	B	0.62	0/1278	0.85	2/1730 (0.1%)
3	C	0.59	0/1687	0.82	2/2297 (0.1%)
4	D	0.62	2/3512 (0.1%)	0.84	6/4758 (0.1%)
5	E	0.53	1/1675 (0.1%)	0.79	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	0.67	3/2600 (0.1%)	0.88	7/3550 (0.2%)
9	I	0.63	1/1427 (0.1%)	0.89	2/1927 (0.1%)
10	J	0.54	0/1221	0.73	1/1656 (0.1%)
11	K	0.60	0/740	0.82	2/1005 (0.2%)
12	L	0.68	5/4921 (0.1%)	0.90	19/6696 (0.3%)
13	M	0.69	4/3717 (0.1%)	0.90	10/5062 (0.2%)
14	N	0.67	2/2756 (0.1%)	0.85	7/3751 (0.2%)
15	O	0.63	4/2666 (0.2%)	0.75	8/3615 (0.2%)
16	P	0.59	2/2804 (0.1%)	0.74	6/3802 (0.2%)
17	Q	0.58	2/980 (0.2%)	0.80	4/1324 (0.3%)
18	R	0.80	1/671 (0.1%)	0.85	2/903 (0.2%)
19	S	0.64	1/678 (0.1%)	0.90	1/915 (0.1%)
20	T	0.76	1/613 (0.2%)	0.90	4/826 (0.5%)
20	U	0.65	0/712	0.82	1/962 (0.1%)
21	V	0.56	0/937	0.85	4/1270 (0.3%)
22	W	0.55	1/993 (0.1%)	0.58	0/1335
23	X	0.51	0/1422	0.75	0/1921
24	Y	0.52	0/1054	0.60	0/1429
25	Z	0.56	1/1183 (0.1%)	0.69	0/1597
26	a	0.57	0/561	0.81	2/755 (0.3%)
27	b	0.47	0/643	0.54	0/884
28	c	0.81	1/400 (0.2%)	0.91	3/544 (0.6%)
29	d	0.77	2/1028 (0.2%)	0.75	5/1387 (0.4%)
30	e	0.50	0/881	0.64	0/1173
31	f	0.57	0/459	0.77	1/618 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.64	1/870 (0.1%)	0.94	3/1185 (0.3%)
33	h	0.52	0/1197	0.75	0/1621
34	i	0.56	0/798	0.76	0/1085
35	j	0.57	0/612	0.74	0/837
36	k	0.86	2/596 (0.3%)	0.94	3/805 (0.4%)
37	l	0.69	2/1367 (0.1%)	0.77	1/1866 (0.1%)
38	m	0.57	0/1073	0.75	0/1455
39	n	0.65	1/1589 (0.1%)	0.77	2/2152 (0.1%)
40	o	0.53	0/1044	0.62	0/1401
41	p	0.53	0/1471	0.71	1/1988 (0.1%)
42	q	0.71	2/1037 (0.2%)	0.92	5/1408 (0.4%)
43	r	0.66	1/421 (0.2%)	0.87	1/566 (0.2%)
44	s	0.30	0/233	0.56	0/317
45	AA	0.41	0/3176	0.62	2/4305 (0.0%)
45	Aa	0.37	0/3190	0.62	1/4325 (0.0%)
46	AB	0.36	0/3156	0.56	0/4263
46	Ab	0.35	0/3149	0.56	0/4255
47	AC	0.34	0/3089	0.56	1/4221 (0.0%)
47	Ac	0.37	0/3089	0.57	1/4221 (0.0%)
48	AD	0.38	0/1955	0.50	0/2655
48	Ad	0.49	1/1954 (0.1%)	0.57	2/2655 (0.1%)
49	AE	0.33	0/1459	0.53	0/1976
49	AI	0.84	1/351 (0.3%)	0.92	3/478 (0.6%)
49	Ae	0.36	0/1483	0.61	2/2007 (0.1%)
50	AF	0.33	0/884	0.50	0/1184
50	Af	0.45	0/884	0.48	0/1184
51	AG	0.37	0/662	0.56	0/895
51	Ag	0.39	0/662	0.60	1/895 (0.1%)
52	AH	0.34	0/534	0.56	0/717
52	Ah	0.41	0/551	0.52	0/739
53	AJ	0.33	0/314	0.41	0/424
53	Aj	0.38	0/402	0.50	0/541
54	AK	0.31	0/287	0.54	0/393
54	Ak	0.33	0/371	0.47	0/511
All	All	0.56	55/97648 (0.1%)	0.75	161/132394 (0.1%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	89	PRO	N-CD	-15.19	1.26	1.47
29	d	115	PRO	N-CD	-14.18	1.28	1.47
12	L	265	PRO	N-CD	13.75	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	50	PRO	N-CD	-13.70	1.28	1.47
14	N	255	PRO	N-CD	-13.65	1.28	1.47
49	AI	63	PRO	N-CD	-13.60	1.28	1.47
42	q	139	PRO	N-CD	-13.43	1.29	1.47
28	c	39	PRO	N-CD	-13.33	1.29	1.47
16	P	371	PRO	N-CD	12.88	1.65	1.47
7	G	532	PRO	N-CD	-12.64	1.30	1.47
15	O	315	PRO	N-CD	-12.14	1.30	1.47
20	T	141	PRO	N-CD	11.77	1.64	1.47
48	Ad	182	PRO	N-CD	-11.74	1.31	1.47
15	O	210	PRO	N-CD	-11.46	1.31	1.47
12	L	234	PRO	N-CD	11.10	1.63	1.47
8	H	42	PRO	N-CD	10.78	1.62	1.47
13	M	370	PRO	N-CD	-10.67	1.32	1.47
6	F	227	PRO	N-CD	10.00	1.61	1.47
32	g	78	PRO	N-CD	-9.59	1.34	1.47
7	G	275	PRO	N-CD	-9.55	1.34	1.47
16	P	290	PRO	N-CD	9.54	1.61	1.47
29	d	15	PRO	N-CD	-9.45	1.34	1.47
8	H	75	PRO	N-CD	9.15	1.60	1.47
6	F	319	PRO	N-CD	9.00	1.60	1.47
9	I	107	PRO	N-CD	8.52	1.59	1.47
4	D	163	PRO	N-CD	-8.48	1.35	1.47
13	M	20	PRO	N-CD	8.47	1.59	1.47
12	L	212	PRO	N-CD	-8.28	1.36	1.47
25	Z	73	PRO	N-CD	8.08	1.59	1.47
4	D	352	PRO	N-CD	-8.02	1.36	1.47
39	n	155	PRO	N-CD	8.00	1.59	1.47
19	S	63	PRO	N-CD	-7.95	1.36	1.47
43	r	111	PRO	N-CD	-7.52	1.37	1.47
37	l	104	PRO	N-CD	-7.28	1.37	1.47
13	M	208	PRO	N-CD	7.07	1.57	1.47
14	N	238	PRO	N-CD	-7.07	1.38	1.47
7	G	541	PRO	N-CD	-6.81	1.38	1.47
6	F	234	GLY	CA-C	-6.81	1.41	1.51
7	G	449	PRO	N-CD	6.71	1.57	1.47
6	F	384	PRO	N-CD	-6.25	1.39	1.47
12	L	384	PRO	N-CD	6.21	1.56	1.47
5	E	93	PRO	N-CD	-5.95	1.39	1.47
12	L	112	PRO	N-CD	5.94	1.56	1.47
36	k	20	MET	C-N	5.90	1.47	1.34
6	F	235	VAL	N-CA	-5.86	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	l	45	PRO	N-CD	-5.84	1.39	1.47
15	O	87	PRO	N-CD	-5.79	1.39	1.47
8	H	60	PRO	N-CD	5.76	1.55	1.47
13	M	252	PRO	N-CD	-5.65	1.40	1.47
22	W	22	PRO	N-CD	5.59	1.55	1.47
7	G	683	PRO	N-CD	-5.49	1.40	1.47
17	Q	53	ILE	C-O	5.38	1.33	1.23
15	O	103	PRO	N-CD	-5.31	1.40	1.47
42	q	126	PRO	N-CD	5.25	1.55	1.47
17	Q	82	PRO	N-CD	-5.04	1.40	1.47

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	3	PHE	CB-CA-C	-10.40	89.60	110.40
14	N	255	PRO	CA-N-CD	9.91	125.58	111.70
36	k	50	PRO	CA-N-CD	9.90	125.56	111.70
42	q	139	PRO	CA-N-CD	9.60	125.14	111.70
29	d	115	PRO	CA-N-CD	9.59	125.12	111.70
45	AA	366	ASP	CB-CG-OD1	9.56	126.90	118.30
4	D	142	VAL	N-CA-CB	9.52	132.44	111.50
45	Aa	366	ASP	CB-CG-OD1	9.47	126.83	118.30
49	AI	63	PRO	CA-N-CD	9.36	124.81	111.70
5	E	219	SER	N-CA-CB	8.99	123.99	110.50
6	F	334	THR	N-CA-CB	8.95	127.31	110.30
15	O	315	PRO	CA-N-CD	8.71	123.90	111.70
48	Ad	182	PRO	CA-N-CD	8.60	123.75	111.70
7	G	532	PRO	CA-N-CD	8.56	123.69	111.70
36	k	50	PRO	N-CA-CB	-8.17	93.50	103.30
7	G	174	THR	N-CA-C	-8.15	89.00	111.00
28	c	39	PRO	CA-N-CD	8.12	123.07	111.70
49	AI	63	PRO	N-CA-CB	-7.88	93.84	103.30
15	O	210	PRO	CA-N-CD	7.83	122.66	111.70
17	Q	60	ASP	N-CA-C	-7.66	90.32	111.00
6	F	411	SER	N-CA-CB	7.53	121.80	110.50
12	L	265	PRO	CA-N-CD	-7.41	101.13	111.50
14	N	255	PRO	N-CA-CB	-7.25	94.60	103.30
7	G	204	MET	N-CA-C	-7.24	91.46	111.00
15	O	210	PRO	N-CA-CB	-7.23	94.62	103.30
16	P	371	PRO	N-CA-CB	7.14	111.86	103.30
6	F	332	CYS	N-CA-C	7.03	129.99	111.00
32	g	78	PRO	CA-N-CD	7.01	121.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	265	PRO	N-CA-CB	6.97	111.66	103.30
8	H	311	THR	N-CA-CB	6.94	123.48	110.30
16	P	369	THR	N-CA-CB	6.93	123.47	110.30
29	d	115	PRO	N-CA-CB	-6.91	95.00	102.60
28	c	47	SER	N-CA-CB	6.87	120.80	110.50
4	D	142	VAL	N-CA-C	-6.84	92.53	111.00
13	M	213	HIS	CB-CA-C	-6.79	96.81	110.40
49	AI	61	ALA	CB-CA-C	-6.68	100.07	110.10
7	G	275	PRO	CA-N-CD	6.63	120.98	111.70
28	c	39	PRO	N-CA-CB	-6.62	95.32	102.60
15	O	320	GLY	N-CA-C	-6.60	96.59	113.10
7	G	300	GLN	N-CA-CB	6.60	122.47	110.60
29	d	15	PRO	CA-N-CD	6.56	120.89	111.70
16	P	106	LEU	N-CA-C	6.56	128.70	111.00
5	E	166	LYS	CB-CA-C	6.55	123.49	110.40
36	k	59	TYR	N-CA-CB	-6.54	98.83	110.60
5	E	64	ALA	N-CA-CB	6.50	119.20	110.10
6	F	125	CYS	N-CA-C	-6.49	93.48	111.00
39	n	115	TYR	N-CA-CB	6.39	122.11	110.60
42	q	139	PRO	N-CA-CB	-6.37	95.59	102.60
8	H	52	ALA	N-CA-CB	6.36	119.01	110.10
16	P	371	PRO	CA-N-CD	-6.35	102.61	111.50
9	I	154	TYR	N-CA-CB	-6.34	99.19	110.60
4	D	427	PRO	N-CA-C	-6.30	95.71	112.10
13	M	370	PRO	N-CA-C	6.30	128.48	112.10
8	H	196	ALA	N-CA-C	6.29	127.99	111.00
13	M	424	ILE	N-CA-C	-6.28	94.03	111.00
14	N	255	PRO	N-CA-C	6.26	128.38	112.10
13	M	370	PRO	CA-N-CD	6.22	120.41	111.70
4	D	140	ASP	CB-CA-C	-6.16	98.08	110.40
14	N	81	LEU	N-CA-C	-6.14	94.43	111.00
32	g	137	SER	N-CA-CB	-6.12	101.32	110.50
20	T	141	PRO	CA-N-CD	-6.12	102.94	111.50
20	T	141	PRO	N-CA-CB	6.10	110.62	103.30
7	G	212	LYS	N-CA-C	-6.08	94.58	111.00
7	G	133	GLN	N-CA-CB	6.08	121.54	110.60
47	Ac	147	THR	N-CA-CB	6.04	121.77	110.30
12	L	231	PRO	N-CA-C	6.00	127.71	112.10
12	L	234	PRO	CA-N-CD	-5.99	103.11	111.50
15	O	315	PRO	N-CA-CB	-5.98	96.03	102.60
12	L	276	THR	N-CA-CB	5.96	121.62	110.30
42	q	69	ASN	N-CA-CB	5.96	121.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	218	ALA	N-CA-CB	5.95	118.43	110.10
12	L	554	ASP	N-CA-CB	5.92	121.26	110.60
12	L	605	ASN	N-CA-CB	5.91	121.23	110.60
12	L	483	PRO	N-CA-C	-5.90	96.75	112.10
5	E	50	THR	N-CA-CB	5.88	121.47	110.30
48	Ad	182	PRO	N-CA-CB	-5.88	96.14	102.60
7	G	251	ILE	N-CA-C	5.87	126.84	111.00
7	G	389	THR	N-CA-CB	5.86	121.43	110.30
5	E	68	ASN	N-CA-CB	5.84	121.11	110.60
6	F	103	ASN	N-CA-CB	5.80	121.05	110.60
11	K	83	ASN	N-CA-CB	5.77	120.98	110.60
19	S	63	PRO	CA-N-CD	5.76	119.77	111.70
20	U	150	ASP	CB-CA-C	5.75	121.90	110.40
20	T	135	ALA	N-CA-CB	5.73	118.13	110.10
7	G	510	TRP	N-CA-CB	5.72	120.90	110.60
13	M	223	ALA	N-CA-CB	5.71	118.10	110.10
31	f	12	VAL	N-CA-CB	5.68	124.01	111.50
29	d	15	PRO	N-CA-CB	-5.67	96.37	102.60
17	Q	141	ASN	N-CA-CB	5.66	120.79	110.60
8	H	223	PHE	CB-CA-C	-5.66	99.09	110.40
14	N	89	GLN	N-CA-CB	-5.65	100.43	110.60
7	G	599	THR	N-CA-C	5.62	126.17	111.00
47	AC	17	SER	N-CA-CB	-5.59	102.12	110.50
12	L	415	ALA	N-CA-CB	5.58	117.91	110.10
21	V	57	ASP	N-CA-CB	5.58	120.64	110.60
7	G	580	ALA	N-CA-CB	5.57	117.90	110.10
15	O	118	TYR	N-CA-CB	-5.57	100.57	110.60
3	C	125	PHE	N-CA-CB	-5.55	100.60	110.60
17	Q	163	ASN	CB-CA-C	-5.55	99.30	110.40
8	H	252	PRO	CA-N-CD	5.55	119.47	111.70
13	M	311	GLY	N-CA-C	-5.52	99.30	113.10
15	O	118	TYR	N-CA-C	5.51	125.86	111.00
21	V	19	THR	N-CA-CB	5.48	120.72	110.30
39	n	136	GLU	CB-CA-C	5.48	121.37	110.40
49	Ae	221	GLY	N-CA-C	5.48	126.81	113.10
7	G	389	THR	N-CA-C	-5.46	96.26	111.00
9	I	160	GLU	N-CA-CB	-5.46	100.77	110.60
16	P	367	GLU	CB-CA-C	-5.44	99.53	110.40
12	L	582	GLY	N-CA-C	-5.43	99.52	113.10
43	r	111	PRO	CA-N-CD	5.43	119.31	111.70
18	R	38	TYR	N-CA-C	-5.43	96.34	111.00
7	G	651	PRO	CB-CA-C	-5.42	98.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	457	HIS	N-CA-CB	-5.40	100.87	110.60
42	q	67	GLU	CB-CA-C	-5.40	99.60	110.40
21	V	114	TRP	N-CA-CB	5.39	120.31	110.60
2	B	195	PRO	N-CA-C	-5.39	98.08	112.10
4	D	140	ASP	N-CA-C	-5.38	96.47	111.00
15	O	152	SER	N-CA-CB	5.37	118.56	110.50
13	M	276	CYS	N-CA-CB	5.35	120.22	110.60
7	G	362	ASP	N-CA-C	5.34	125.42	111.00
12	L	194	ASN	N-CA-C	5.33	125.40	111.00
8	H	139	THR	N-CA-CB	5.32	120.42	110.30
49	Ae	242	HIS	N-CA-C	5.32	125.36	111.00
6	F	418	GLN	N-CA-CB	5.31	120.16	110.60
12	L	151	SER	N-CA-CB	5.30	118.45	110.50
5	E	218	ARG	CB-CA-C	-5.29	99.81	110.40
10	J	133	VAL	N-CA-C	-5.29	96.73	111.00
45	AA	473	SER	N-CA-CB	-5.28	102.58	110.50
13	M	330	ALA	N-CA-CB	5.27	117.48	110.10
12	L	234	PRO	N-CA-CB	5.27	109.62	103.30
12	L	248	HIS	CB-CA-C	5.26	120.91	110.40
11	K	70	GLU	N-CA-CB	5.25	120.06	110.60
3	C	136	PHE	N-CA-C	-5.25	96.84	111.00
12	L	212	PRO	N-CA-C	5.24	125.73	112.10
12	L	212	PRO	CA-N-CD	5.24	119.03	111.70
29	d	113	LEU	N-CA-CB	-5.24	99.93	110.40
8	H	51	ASP	CB-CA-C	-5.21	99.98	110.40
2	B	153	PRO	CB-CA-C	-5.21	98.98	112.00
12	L	277	MET	CB-CA-C	-5.21	99.98	110.40
13	M	423	MET	N-CA-C	-5.21	96.95	111.00
7	G	640	ASP	N-CA-CB	5.20	119.97	110.60
41	p	94	ARG	NE-CZ-NH1	5.18	122.89	120.30
18	R	89	PRO	CA-N-CD	5.16	118.93	111.70
51	Ag	26	ALA	N-CA-CB	-5.15	102.89	110.10
37	l	104	PRO	CA-N-CD	5.12	118.87	111.70
17	Q	164	PHE	N-CA-CB	5.11	119.81	110.60
16	P	368	GLU	N-CA-CB	5.11	119.80	110.60
26	a	4	GLU	N-CA-C	5.11	124.80	111.00
12	L	247	LEU	N-CA-CB	5.10	120.60	110.40
13	M	83	HIS	N-CA-C	-5.10	97.24	111.00
4	D	352	PRO	CA-N-CD	5.08	118.81	111.70
6	F	228	PRO	N-CA-C	-5.08	98.89	112.10
32	g	78	PRO	N-CA-CB	-5.07	97.02	102.60
7	G	77	MET	N-CA-C	-5.07	97.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	228	ASN	N-CA-CB	5.06	119.71	110.60
21	V	86	LYS	N-CA-CB	5.04	119.67	110.60
7	G	668	ALA	N-CA-CB	5.04	117.15	110.10
42	q	142	THR	N-CA-CB	5.03	119.86	110.30
7	G	532	PRO	N-CA-CB	-5.03	97.07	102.60
12	L	20	LEU	CB-CA-C	-5.01	100.68	110.20
20	T	139	MET	N-CA-C	-5.01	97.48	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	89/115 (77%)	82 (92%)	7 (8%)	0	100	100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	10	42
3	C	196/263 (74%)	186 (95%)	8 (4%)	2 (1%)	13	48
4	D	421/463 (91%)	392 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	191 (92%)	17 (8%)	0	100	100
6	F	424/464 (91%)	406 (96%)	18 (4%)	0	100	100
7	G	685/727 (94%)	631 (92%)	54 (8%)	0	100	100
8	H	310/318 (98%)	291 (94%)	18 (6%)	1 (0%)	37	72
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	151/172 (88%)	140 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37	72
15	O	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
16	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	110 (98%)	1 (1%)	1 (1%)	14	50
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%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
28	c	45/76 (59%)	45 (100%)	0	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	f	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	g	98/151 (65%)	92 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	88/128 (69%)	79 (90%)	9 (10%)	0	100	100
35	j	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
36	k	70/104 (67%)	67 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	22	59
40	o	117/137 (85%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	168/176 (96%)	150 (89%)	18 (11%)	0	100	100
42	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
43	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
44	s	24/104 (23%)	24 (100%)	0	0	100	100
45	AA	393/480 (82%)	378 (96%)	15 (4%)	0	100	100
45	Aa	395/480 (82%)	384 (97%)	11 (3%)	0	100	100
46	AB	410/453 (90%)	400 (98%)	10 (2%)	0	100	100
46	Ab	407/453 (90%)	397 (98%)	10 (2%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	362 (98%)	8 (2%)	1 (0%)	37	72
48	AD	236/325 (73%)	229 (97%)	6 (2%)	1 (0%)	30	67
48	Ad	236/325 (73%)	224 (95%)	12 (5%)	0	100	100
49	AE	181/274 (66%)	168 (93%)	13 (7%)	0	100	100
49	AI	43/274 (16%)	41 (95%)	2 (5%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	12 (6%)	1 (0%)	25	63
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	62/89 (70%)	62 (100%)	0	0	100	100
52	Ah	64/89 (72%)	63 (98%)	1 (2%)	0	100	100
53	AJ	36/64 (56%)	36 (100%)	0	0	100	100
53	Aj	46/64 (72%)	45 (98%)	1 (2%)	0	100	100
54	AK	32/56 (57%)	31 (97%)	1 (3%)	0	100	100
54	Ak	42/56 (75%)	41 (98%)	1 (2%)	0	100	100
All	All	11748/14118 (83%)	11208 (95%)	529 (4%)	11 (0%)	50	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
3	C	135	ARG
8	H	92	PRO

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Mol	Chain	Res	Type
14	N	109	ALA
3	C	81	ASP
22	W	99	VAL
47	Ac	75	TYR
48	AD	158	PRO
2	B	195	PRO
39	n	156	PRO
49	Ae	237	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	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	79	85
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	367/395 (93%)	367 (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	278/280 (99%)	278 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	126/138 (91%)	126 (100%)	0	100	100
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	549 (100%)	0	100	100
13	M	415/415 (100%)	415 (100%)	0	100	100
14	N	307/308 (100%)	307 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	297/325 (91%)	297 (100%)	0	100	100
17	Q	105/153 (69%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	80/135 (59%)	80 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
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	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	91/129 (70%)	91 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	87/120 (72%)	87 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	109/121 (90%)	109 (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	26/95 (27%)	26 (100%)	0	100	100
45	AA	337/398 (85%)	337 (100%)	0	100	100
45	Aa	339/398 (85%)	339 (100%)	0	100	100
46	AB	324/356 (91%)	324 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Ab	325/356 (91%)	325 (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
49	AI	34/224 (15%)	34 (100%)	0	100	100
49	Ae	158/224 (70%)	158 (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	61/83 (74%)	61 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	30/55 (54%)	30 (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	10324/12037 (86%)	10323 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	108	GLN
2	B	151	GLN
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS

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Mol	Chain	Res	Type
3	C	123	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	60	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	233	HIS
4	D	265	ASN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
5	E	132	GLN
5	E	152	GLN
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	260	ASN
7	G	406	ASN
7	G	444	HIS
7	G	460	HIS
7	G	495	ASN
7	G	514	ASN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
8	H	5	ASN
8	H	32	GLN

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Mol	Chain	Res	Type
8	H	47	GLN
8	H	93	HIS
8	H	169	GLN
8	H	171	HIS
8	H	287	HIS
8	H	292	ASN
11	K	7	ASN
11	K	25	HIS
12	L	2	ASN
12	L	25	ASN
12	L	58	ASN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	194	ASN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	296	ASN
12	L	321	GLN
12	L	328	HIS
12	L	332	HIS
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	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	168	GLN
13	M	170	HIS
13	M	175	ASN
13	M	184	HIS
13	M	192	ASN
13	M	213	HIS
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	349	GLN

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Mol	Chain	Res	Type
13	M	374	ASN
13	M	390	ASN
13	M	415	GLN
14	N	120	GLN
14	N	134	GLN
14	N	204	ASN
14	N	273	ASN
14	N	310	ASN
15	O	54	HIS
15	O	80	GLN
15	O	175	ASN
15	O	219	GLN
15	O	292	HIS
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	71	ASN
16	P	79	GLN
16	P	154	GLN
16	P	216	HIS
16	P	251	ASN
16	P	269	ASN
16	P	275	HIS
16	P	323	HIS
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	88	GLN
18	R	56	ASN
21	V	41	HIS
21	V	50	GLN
22	W	54	GLN
22	W	105	HIS
23	X	30	HIS
23	X	77	HIS
23	X	151	ASN
24	Y	19	GLN
24	Y	91	ASN
25	Z	112	HIS
26	a	31	ASN
27	b	52	ASN
27	b	69	HIS

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Mol	Chain	Res	Type
27	b	83	ASN
29	d	59	HIS
30	e	97	HIS
33	h	170	GLN
33	h	181	HIS
34	i	83	HIS
35	j	41	GLN
36	k	39	GLN
36	k	66	ASN
37	l	91	GLN
37	l	106	HIS
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	14	GLN
39	n	33	HIS
39	n	53	ASN
39	n	76	HIS
40	o	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	104	ASN
41	p	124	ASN
42	q	12	GLN
42	q	31	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS
43	r	110	GLN
44	s	59	GLN
45	AA	43	GLN
45	AA	55	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	402	HIS
46	AB	167	GLN
46	AB	415	GLN

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Mol	Chain	Res	Type
47	AC	341	GLN
48	AD	98	HIS
48	AD	189	ASN
48	AD	190	ASN
51	AG	69	GLN
52	AH	34	HIS
52	AH	37	GLN
52	AH	82	HIS
45	Aa	87	ASN
45	Aa	119	HIS
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	193	GLN
45	Aa	207	ASN
46	Ab	227	HIS
46	Ab	284	ASN
46	Ab	298	HIS
46	Ab	304	ASN
46	Ab	311	GLN
46	Ab	343	GLN
46	Ab	415	GLN
47	Ac	148	ASN
47	Ac	341	GLN
48	Ad	155	GLN
48	Ad	190	ASN
49	Ae	242	HIS
50	Af	80	GLN
51	Ag	24	GLN
52	Ah	82	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 1 is monoatomic - leaving 54 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	$\#\|Z\| > 2$
62	CDL	Ag	101	62	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
55	SF4	G	802	7	0,12,12	-	-	-		
62	CDL	Ac	406	62	41,41,99	1.39	4 (9%)	47,53,111	1.45	7 (14%)
67	HEM	AC	402	47	41,50,50	1.36	6 (14%)	45,82,82	1.95	9 (20%)
58	3PE	m	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.06	4 (7%)
56	UQ1	B	302	-	18,18,18	1.94	2 (11%)	22,25,25	1.35	3 (13%)
60	FMN	F	501	-	33,33,33	1.38	4 (12%)	48,50,50	1.21	6 (12%)
58	3PE	j	700	-	39,39,50	1.02	2 (5%)	42,44,55	1.23	4 (9%)
57	PC1	L	706	-	49,49,53	0.97	2 (4%)	55,57,61	1.09	3 (5%)
58	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	3 (5%)
55	SF4	I	303	9	0,12,12	-	-	-		
67	HEM	Ac	402	47	41,50,50	1.32	4 (9%)	45,82,82	1.94	10 (22%)
68	U10	AC	404	-	23,23,63	1.75	2 (8%)	28,31,79	1.70	7 (25%)
62	CDL	d	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
58	3PE	L	702	-	38,38,50	1.06	2 (5%)	41,43,55	1.15	2 (4%)
58	3PE	M	501	-	36,36,50	1.07	2 (5%)	39,41,55	1.21	3 (7%)
55	SF4	B	301	2	0,12,12	-	-	-		
58	3PE	b	201	-	45,45,50	1.11	5 (11%)	48,50,55	1.23	3 (6%)
62	CDL	L	705	-	80,80,99	1.01	4 (5%)	86,92,111	1.12	7 (8%)
55	SF4	I	304	9	0,12,12	-	-	-		
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
62	CDL	Aa	501	-	45,45,99	1.34	4 (8%)	51,57,111	1.32	6 (11%)
59	FES	E	301	5	0,4,4	-	-	-		
66	EHZ	n	201	-	27,31,37	1.85	7 (25%)	37,41,47	1.99	11 (29%)
58	3PE	m	202	-	40,40,50	1.00	2 (5%)	43,45,55	1.12	3 (6%)
70	HEC	AD	401	48	32,50,50	2.24	12 (37%)	24,82,82	2.28	6 (25%)
57	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	CDL	L	704	-	76,76,99	1.03	4 (5%)	82,88,111	1.17	5 (6%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
58	3PE	L	701	-	48,48,50	0.91	2 (4%)	51,53,55	1.13	4 (7%)
69	UQ6	AC	405	-	28,28,43	2.44	6 (21%)	33,37,55	1.65	8 (24%)
70	HEC	Ad	401	48	32,50,50	2.18	11 (34%)	24,82,82	2.94	8 (33%)
66	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
67	HEM	Ac	401	47	41,50,50	1.37	5 (12%)	45,82,82	1.91	11 (24%)
58	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.06	2 (4%)
64	NDP	P	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.19	4 (7%)
58	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.20	3 (8%)
67	HEM	AC	401	47	41,50,50	1.38	6 (14%)	45,82,82	2.08	13 (28%)
55	SF4	G	801	7	0,12,12	-	-	-		
55	SF4	F	502	6	0,12,12	-	-	-		
58	3PE	D	501	-	37,37,50	1.05	2 (5%)	40,42,55	1.16	3 (7%)
57	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.13	2 (5%)
58	3PE	O	401	-	43,43,50	0.99	2 (4%)	46,48,55	1.04	3 (6%)
63	ADP	O	402	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
59	FES	G	803	7	0,4,4	-	-	-		
61	UQ9	H	400	-	35,35,58	0.83	2 (5%)	42,45,73	0.52	0
58	3PE	I	301	-	45,45,50	0.98	2 (4%)	48,50,55	1.08	3 (6%)
58	3PE	J	401	-	45,45,50	1.12	5 (11%)	48,50,55	1.19	3 (6%)
58	3PE	M	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.05	4 (7%)
58	3PE	L	703	-	46,46,50	0.95	2 (4%)	49,51,55	1.03	3 (6%)
68	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.09	7 (25%)
58	3PE	AC	403	-	24,24,50	1.30	2 (8%)	27,29,55	1.17	2 (7%)
58	3PE	K	101	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
69	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0

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
62	CDL	Ag	101	62	-	22/66/66/110	-
62	CDL	Ac	406	62	-	18/52/52/110	-
55	SF4	G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	HEM	AC	402	47	-	7/12/54/54	-
58	3PE	m	201	-	-	13/54/54/54	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
60	FMN	F	501	-	-	3/18/18/18	0/3/3/3
58	3PE	j	700	-	-	6/43/43/54	-
57	PC1	L	706	-	-	10/53/53/57	-
58	3PE	M	502	-	-	16/54/54/54	-
55	SF4	I	303	9	-	-	0/6/5/5
67	HEM	Ac	402	47	-	6/12/54/54	-
68	U10	AC	404	-	-	5/15/39/87	0/1/1/1
62	CDL	d	201	-	-	27/77/77/110	-
58	3PE	L	702	-	-	16/42/42/54	-
58	3PE	M	501	-	-	8/40/40/54	-
58	3PE	b	201	-	-	19/49/49/54	-
62	CDL	L	705	-	-	21/91/91/110	-
62	CDL	a	101	-	-	18/67/67/110	-
62	CDL	Aa	501	-	-	12/56/56/110	-
55	SF4	B	301	2	-	-	0/6/5/5
55	SF4	I	304	9	-	-	0/6/5/5
66	EHZ	n	201	-	-	14/39/39/45	-
59	FES	E	301	5	-	-	0/1/1/1
58	3PE	m	202	-	-	7/44/44/54	-
70	HEC	AD	401	48	-	3/10/54/54	-
57	PC1	I	302	-	-	10/50/50/57	-
62	CDL	L	704	-	-	27/87/87/110	-
62	CDL	h	201	-	-	23/80/80/110	-
58	3PE	L	701	-	-	13/52/52/54	-
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
70	HEC	Ad	401	48	-	2/10/54/54	-
66	EHZ	W	201	-	-	21/39/39/45	-
67	HEM	Ac	401	47	-	7/12/54/54	-
58	3PE	i	201	-	-	12/43/43/54	-
64	NDP	P	401	-	-	3/30/77/77	0/5/5/5
58	3PE	Ac	403	-	-	3/38/38/54	-
67	HEM	AC	401	47	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	3PE	D	501	-	-	10/41/41/54	-
55	SF4	F	502	6	-	-	0/6/5/5
55	SF4	G	801	7	-	-	0/6/5/5
57	PC1	B	303	-	-	8/38/38/57	-
58	3PE	O	401	-	-	9/47/47/54	-
63	ADP	O	402	-	-	1/12/32/32	0/3/3/3
59	FES	G	803	7	-	-	0/1/1/1
61	UQ9	H	400	-	-	14/30/54/81	0/1/1/1
58	3PE	I	301	-	-	12/49/49/54	-
58	3PE	J	401	-	-	18/49/49/54	-
58	3PE	M	503	-	-	8/54/54/54	-
58	3PE	L	703	-	-	10/50/50/54	-
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
58	3PE	AC	403	-	-	7/28/28/54	-
58	3PE	K	101	-	-	14/49/49/54	-
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	B	302	UQ1	C6-C5	7.36	1.48	1.35
68	AC	404	U10	C6-C1	7.36	1.48	1.35
70	AD	401	HEC	C3C-C2C	6.33	1.47	1.40
70	AD	401	HEC	C2B-C3B	6.19	1.47	1.40
69	AC	405	UQ6	C2-C3	5.91	1.49	1.39
70	Ad	401	HEC	C2B-C3B	5.86	1.46	1.40
69	AC	405	UQ6	C5-C4	5.85	1.48	1.39
70	Ad	401	HEC	C3C-C2C	5.84	1.46	1.40
69	AC	405	UQ6	C5-C6	5.74	1.48	1.40
66	W	201	EHZ	C15-N2	5.38	1.45	1.33
66	n	201	EHZ	C15-N2	5.24	1.45	1.33
66	W	201	EHZ	C12-N1	5.16	1.45	1.33
69	AC	405	UQ6	C6-C1	4.98	1.48	1.40
66	n	201	EHZ	C12-N1	4.92	1.44	1.33
60	F	501	FMN	C9A-C5A	4.82	1.49	1.41
69	AC	405	UQ6	C4-C3	4.58	1.48	1.39
57	L	706	PC1	O31-C31	4.31	1.45	1.33
58	L	702	3PE	O31-C31	4.30	1.45	1.33
58	O	401	3PE	O31-C31	4.30	1.45	1.33
58	i	201	3PE	O31-C31	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	M	501	3PE	O31-C31	4.25	1.45	1.33
58	I	301	3PE	O31-C31	4.25	1.45	1.33
62	d	201	CDL	OB8-CB7	4.25	1.45	1.33
58	L	703	3PE	O31-C31	4.23	1.45	1.33
62	Aa	501	CDL	OA8-CA7	4.23	1.45	1.33
62	L	704	CDL	OB6-CB5	4.23	1.46	1.34
58	i	201	3PE	O21-C21	4.23	1.46	1.34
62	Ac	406	CDL	OB8-CB7	4.22	1.45	1.33
58	j	700	3PE	O31-C31	4.22	1.45	1.33
58	K	101	3PE	O31-C31	4.21	1.45	1.33
58	Ac	403	3PE	O31-C31	4.20	1.45	1.33
58	I	301	3PE	O21-C21	4.20	1.46	1.34
62	a	101	CDL	OA8-CA7	4.19	1.45	1.33
62	L	705	CDL	OA8-CA7	4.19	1.45	1.33
62	Ag	101	CDL	OB8-CB7	4.19	1.45	1.33
62	Aa	501	CDL	OB8-CB7	4.19	1.45	1.33
58	M	503	3PE	O31-C31	4.19	1.45	1.33
58	m	202	3PE	O31-C31	4.18	1.45	1.33
57	B	303	PC1	O31-C31	4.18	1.45	1.33
62	d	201	CDL	OA8-CA7	4.18	1.45	1.33
58	D	501	3PE	O31-C31	4.18	1.45	1.33
62	h	201	CDL	OA8-CA7	4.17	1.45	1.33
58	m	201	3PE	O31-C31	4.17	1.45	1.33
58	AC	403	3PE	O31-C31	4.17	1.45	1.33
62	a	101	CDL	OB8-CB7	4.17	1.45	1.33
62	L	705	CDL	OB8-CB7	4.17	1.45	1.33
57	I	302	PC1	O31-C31	4.16	1.45	1.33
62	Ag	101	CDL	OA8-CA7	4.14	1.45	1.33
62	L	704	CDL	OB8-CB7	4.12	1.45	1.33
58	M	502	3PE	O31-C31	4.11	1.45	1.33
62	h	201	CDL	OB8-CB7	4.10	1.45	1.33
62	h	201	CDL	OB6-CB5	4.10	1.45	1.34
62	Aa	501	CDL	OB6-CB5	4.10	1.45	1.34
58	L	702	3PE	O21-C21	4.10	1.45	1.34
57	B	303	PC1	O21-C21	4.10	1.45	1.34
62	Ac	406	CDL	OA8-CA7	4.10	1.45	1.33
62	Aa	501	CDL	OA6-CA5	4.09	1.45	1.34
69	AC	405	UQ6	C2-C1	4.08	1.48	1.40
62	a	101	CDL	OA6-CA5	4.07	1.45	1.34
57	L	706	PC1	O21-C21	4.07	1.45	1.34
62	L	705	CDL	OA6-CA5	4.07	1.45	1.34
58	L	703	3PE	O21-C21	4.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	L	704	CDL	OA8-CA7	4.05	1.45	1.33
62	Ac	406	CDL	OA6-CA5	4.05	1.45	1.34
62	a	101	CDL	OB6-CB5	4.05	1.45	1.34
58	L	701	3PE	O31-C31	4.04	1.45	1.33
57	I	302	PC1	O21-C21	4.03	1.45	1.34
62	Ag	101	CDL	OA6-CA5	4.02	1.45	1.34
58	Ac	403	3PE	O21-C21	4.02	1.45	1.34
58	AC	403	3PE	O21-C21	4.01	1.45	1.34
58	M	501	3PE	O21-C21	4.00	1.45	1.34
58	D	501	3PE	O21-C21	3.99	1.45	1.34
62	L	705	CDL	OB6-CB5	3.98	1.45	1.34
62	Ag	101	CDL	OB6-CB5	3.98	1.45	1.34
58	j	700	3PE	O21-C21	3.98	1.45	1.34
62	h	201	CDL	OA6-CA5	3.98	1.45	1.34
62	Ac	406	CDL	OB6-CB5	3.97	1.45	1.34
58	M	502	3PE	O21-C21	3.97	1.45	1.34
62	d	201	CDL	OA6-CA5	3.96	1.45	1.34
58	L	701	3PE	O21-C21	3.95	1.45	1.34
58	m	202	3PE	O21-C21	3.94	1.45	1.34
58	M	503	3PE	O21-C21	3.94	1.45	1.34
58	O	401	3PE	O21-C21	3.93	1.45	1.34
62	d	201	CDL	OB6-CB5	3.92	1.45	1.34
58	K	101	3PE	O21-C21	3.91	1.45	1.34
62	L	704	CDL	OA6-CA5	3.89	1.45	1.34
67	AC	402	HEM	C4D-ND	-3.85	1.33	1.40
58	m	201	3PE	O21-C21	3.82	1.45	1.34
67	AC	401	HEM	C1B-NB	-3.79	1.33	1.40
67	Ac	401	HEM	C4D-ND	-3.55	1.34	1.40
67	Ac	402	HEM	C1B-NB	-3.51	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.47	1.34	1.40
67	AC	401	HEM	C4D-ND	-3.46	1.34	1.40
64	P	401	NDP	C6N-C5N	3.35	1.39	1.33
67	Ac	401	HEM	C1B-NB	-3.28	1.34	1.40
70	Ad	401	HEC	C2A-C3A	3.27	1.47	1.37
70	Ad	401	HEC	C3D-C2D	3.25	1.47	1.37
70	AD	401	HEC	C2A-C3A	3.23	1.47	1.37
58	J	401	3PE	O21-C21	3.18	1.43	1.34
67	Ac	402	HEM	C4D-ND	-3.18	1.34	1.40
68	AC	404	U10	C4-C3	3.14	1.49	1.36
58	b	201	3PE	O21-C21	3.13	1.43	1.34
70	AD	401	HEC	C3D-C2D	3.12	1.46	1.37
60	F	501	FMN	C8-C7	3.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	B	302	UQ1	C3-C2	3.03	1.48	1.36
58	b	201	3PE	O31-C31	3.01	1.42	1.33
58	J	401	3PE	O31-C31	3.01	1.42	1.33
70	Ad	401	HEC	C4B-C3B	2.95	1.48	1.43
69	Ac	405	UQ6	O2-C2	-2.92	1.30	1.37
68	Ac	404	U10	C6-C5	-2.92	1.38	1.46
70	Ad	401	HEC	C2A-C1A	2.87	1.49	1.42
67	Ac	401	HEM	FE-NB	2.87	2.11	1.96
68	Ac	404	U10	C4-C3	2.86	1.48	1.36
70	AD	401	HEC	C4B-C3B	2.81	1.48	1.43
61	H	400	UQ9	C3-C2	-2.78	1.40	1.48
70	AD	401	HEC	C3A-C4A	2.77	1.48	1.42
70	AD	401	HEC	C3C-C4C	2.77	1.48	1.43
67	Ac	402	HEM	FE-NB	2.77	2.10	1.96
70	AD	401	HEC	C2A-C1A	2.75	1.48	1.42
70	Ad	401	HEC	C3C-C4C	2.73	1.48	1.43
67	AC	402	HEM	FE-NB	2.68	2.10	1.96
60	F	501	FMN	C4-N3	-2.67	1.33	1.38
67	AC	401	HEM	FE-NB	2.64	2.09	1.96
66	n	201	EHZ	P1-O7	2.59	1.64	1.54
66	W	201	EHZ	P1-O7	2.57	1.64	1.54
61	H	400	UQ9	C4-C5	-2.52	1.41	1.48
66	W	201	EHZ	O4-C15	-2.52	1.18	1.23
68	Ac	404	U10	C3-C2	-2.50	1.41	1.48
66	n	201	EHZ	O4-C15	-2.48	1.18	1.23
70	Ad	401	HEC	C3A-C4A	2.48	1.48	1.42
70	Ad	401	HEC	C1C-CHC	2.46	1.47	1.41
70	Ad	401	HEC	C1D-CHD	2.45	1.47	1.41
66	W	201	EHZ	C9-S1	2.43	1.82	1.76
70	Ad	401	HEC	C4D-CHA	2.39	1.47	1.41
66	W	201	EHZ	O3-C12	-2.39	1.18	1.23
66	n	201	EHZ	O3-C12	-2.39	1.18	1.23
70	AD	401	HEC	C1B-CHB	2.38	1.47	1.41
67	Ac	401	HEM	C1D-ND	-2.34	1.34	1.38
66	n	201	EHZ	P1-OP3	-2.33	1.45	1.54
70	AD	401	HEC	C1D-CHD	2.31	1.47	1.41
70	AD	401	HEC	C4D-CHA	2.30	1.47	1.41
66	n	201	EHZ	C9-S1	2.30	1.81	1.76
60	F	501	FMN	C5A-N5	-2.29	1.35	1.39
63	O	402	ADP	C5-C4	2.27	1.46	1.40
70	AD	401	HEC	C1C-CHC	2.27	1.47	1.41
58	b	201	3PE	O21-C2	-2.27	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	P	401	NDP	C5A-C4A	2.26	1.46	1.40
66	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
58	J	401	3PE	O31-C3	-2.20	1.40	1.45
58	J	401	3PE	O21-C2	-2.19	1.41	1.46
67	Ac	401	HEM	C4B-NB	-2.15	1.34	1.38
58	b	201	3PE	O31-C3	-2.15	1.40	1.45
67	AC	402	HEM	C1D-ND	-2.12	1.34	1.38
58	J	401	3PE	P-O12	-2.12	1.45	1.55
67	AC	401	HEM	C1D-ND	-2.11	1.34	1.38
67	AC	401	HEM	C4B-NB	-2.10	1.34	1.38
58	b	201	3PE	P-O12	-2.09	1.45	1.55
67	AC	402	HEM	FE-ND	-2.08	1.86	1.96
67	Ac	402	HEM	C4B-NB	-2.03	1.34	1.38
67	AC	401	HEM	FE-ND	-2.02	1.86	1.96
67	AC	402	HEM	C4B-NB	-2.01	1.34	1.38

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	Ad	401	HEC	CMB-C2B-C3B	9.37	136.84	125.82
68	Ac	404	U10	C6-C1-C2	7.85	125.39	119.18
70	AD	401	HEC	C1D-C2D-C3D	-6.39	102.55	107.00
66	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
67	AC	401	HEM	CHC-C4B-NB	6.03	130.98	124.43
70	Ad	401	HEC	C1D-C2D-C3D	-5.89	102.90	107.00
67	AC	402	HEM	CHC-C4B-NB	5.74	130.67	124.43
66	n	201	EHZ	C8-C9-S1	5.63	120.59	113.63
67	Ac	402	HEM	CHC-C4B-NB	5.37	130.26	124.43
67	Ac	401	HEM	CHC-C4B-NB	5.19	130.07	124.43
67	Ac	402	HEM	CHD-C1D-ND	5.10	129.97	124.43
66	n	201	EHZ	C14-C13-C12	-4.98	104.06	112.36
67	AC	401	HEM	CHD-C1D-ND	4.85	129.70	124.43
67	AC	402	HEM	CHD-C1D-ND	4.72	129.56	124.43
68	AC	404	U10	C7-C8-C9	-4.63	119.08	126.79
70	AD	401	HEC	CMC-C2C-C3C	4.59	131.22	125.82
62	Ac	406	CDL	OB6-CB5-C51	4.56	121.32	111.50
58	j	700	3PE	O21-C21-C22	4.54	121.28	111.50
70	Ad	401	HEC	CBD-CAD-C3D	-4.52	104.91	112.62
62	d	201	CDL	OA6-CA5-C11	4.50	121.20	111.50
62	h	201	CDL	OB6-CB5-C51	4.45	121.08	111.50
62	L	704	CDL	OB6-CB5-C51	4.43	121.05	111.50
57	L	706	PC1	O21-C21-C22	4.37	120.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AC	401	HEM	CHB-C1B-NB	4.36	129.77	124.38
58	I	301	3PE	O21-C21-C22	4.36	120.90	111.50
62	d	201	CDL	OB6-CB5-C51	4.32	120.82	111.50
62	a	101	CDL	OA6-CA5-C11	4.26	120.69	111.50
67	Ac	402	HEM	CHA-C4D-ND	4.26	129.65	124.38
67	Ac	401	HEM	CHD-C1D-ND	4.26	129.06	124.43
58	M	501	3PE	O21-C21-C22	4.25	120.66	111.50
58	J	401	3PE	O21-C21-C22	4.25	120.65	111.50
70	AD	401	HEC	CMB-C2B-C3B	4.14	130.69	125.82
69	AC	405	UQ6	C7-C8-C9	-4.10	120.89	127.24
57	B	303	PC1	O21-C21-C22	4.08	120.30	111.50
70	Ad	401	HEC	CMB-C2B-C1B	-4.08	122.20	128.46
68	Ac	404	U10	C1-C6-C5	-4.07	115.75	119.58
62	Aa	501	CDL	OA6-CA5-C11	4.06	120.26	111.50
62	L	705	CDL	OB6-CB5-C51	4.05	120.24	111.50
58	i	201	3PE	O21-C21-C22	4.05	120.24	111.50
58	b	201	3PE	O21-C21-C22	4.05	120.22	111.50
58	M	502	3PE	O21-C21-C22	4.03	120.19	111.50
58	L	702	3PE	O21-C21-C22	4.03	120.18	111.50
58	L	701	3PE	O21-C21-C22	3.99	120.11	111.50
58	Ac	403	3PE	O21-C21-C22	3.99	120.11	111.50
62	h	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
62	L	704	CDL	OA6-CA5-C11	3.97	120.05	111.50
57	I	302	PC1	O21-C21-C22	3.97	120.05	111.50
68	AC	404	U10	C1M-C1-C6	-3.95	117.95	124.40
58	D	501	3PE	O21-C21-C22	3.95	120.01	111.50
67	AC	401	HEM	C1B-NB-C4B	3.94	109.14	105.07
67	AC	402	HEM	CHA-C4D-ND	3.90	129.20	124.38
62	a	101	CDL	OB6-CB5-C51	3.90	119.90	111.50
58	K	101	3PE	O21-C21-C22	3.86	119.83	111.50
67	AC	402	HEM	C1B-NB-C4B	3.86	109.06	105.07
67	AC	402	HEM	CBD-CAD-C3D	-3.85	101.92	112.63
67	Ac	402	HEM	C1B-NB-C4B	3.85	109.05	105.07
67	AC	401	HEM	CHA-C4D-ND	3.78	129.05	124.38
62	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
67	Ac	401	HEM	CHB-C1B-NB	3.75	129.01	124.38
58	O	401	3PE	O21-C21-C22	3.73	119.54	111.50
62	L	705	CDL	OA6-CA5-C11	3.73	119.54	111.50
62	Ag	101	CDL	OA6-CA5-C11	3.73	119.53	111.50
67	Ac	401	HEM	CHA-C4D-ND	3.72	128.98	124.38
58	m	201	3PE	O21-C21-C22	3.72	119.51	111.50
67	Ac	401	HEM	C1B-NB-C4B	3.71	108.91	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	m	202	3PE	O21-C21-C22	3.66	119.38	111.50
64	P	401	NDP	PN-O3-PA	-3.65	120.29	132.83
58	M	503	3PE	O21-C21-C22	3.59	119.25	111.50
70	Ad	401	HEC	CMC-C2C-C3C	3.58	130.03	125.82
63	O	402	ADP	PA-O3A-PB	-3.57	120.57	132.83
70	AD	401	HEC	CBD-CAD-C3D	-3.56	106.54	112.62
67	Ac	402	HEM	CHB-C1B-NB	3.56	128.78	124.38
67	AC	402	HEM	CHB-C1B-NB	3.55	128.77	124.38
69	AC	405	UQ6	C12-C13-C14	-3.55	119.12	127.66
66	n	201	EHZ	C13-C12-N1	3.54	122.37	116.42
58	AC	403	3PE	O21-C21-C22	3.49	119.02	111.50
58	L	703	3PE	O21-C21-C22	3.47	118.98	111.50
62	Ac	406	CDL	OB8-CB7-C71	3.46	120.46	111.38
66	n	201	EHZ	C14-N2-C15	-3.34	116.63	122.59
62	Aa	501	CDL	OB6-CB5-C51	3.32	120.07	110.80
62	Aa	501	CDL	OB8-CB7-C71	3.32	120.09	111.38
63	O	402	ADP	N3-C2-N1	-3.32	123.49	128.68
64	P	401	NDP	N3A-C2A-N1A	-3.25	123.59	128.68
62	Ac	406	CDL	CB4-OB6-CB5	-3.24	109.81	117.79
62	Ac	406	CDL	OA6-CA5-C11	3.24	119.83	110.80
69	AC	405	UQ6	C15-C14-C16	3.23	120.70	115.27
68	Ac	404	U10	C4-C3-C2	-3.22	114.35	120.68
67	Ac	401	HEM	CBA-CAA-C2A	-3.21	107.15	112.62
58	M	501	3PE	C2-O21-C21	-3.16	110.02	117.79
66	n	201	EHZ	C11-N1-C12	-3.14	117.00	122.84
58	K	101	3PE	C2-O21-C21	-3.13	110.08	117.79
62	d	201	CDL	CA4-OA6-CA5	-3.11	110.15	117.79
58	j	700	3PE	C2-O21-C21	-3.10	110.16	117.79
66	W	201	EHZ	C13-C12-N1	3.08	121.60	116.42
66	W	201	EHZ	C14-C13-C12	-3.04	107.30	112.36
58	L	702	3PE	O31-C31-C32	3.03	121.43	111.91
58	m	202	3PE	C2-O21-C21	-3.02	110.36	117.79
67	Ac	402	HEM	C4D-ND-C1D	2.99	108.16	105.07
58	M	502	3PE	C2-O21-C21	-2.95	110.52	117.79
67	AC	401	HEM	C4D-ND-C1D	2.91	108.08	105.07
57	B	303	PC1	O31-C31-C32	2.91	121.04	111.91
66	W	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
58	m	201	3PE	C2-O21-C21	-2.86	110.75	117.79
66	W	201	EHZ	C7-C8-C9	-2.85	107.37	113.89
62	h	201	CDL	OB8-CB7-C71	2.85	120.84	111.91
67	AC	401	HEM	CHD-C1D-C2D	-2.84	120.54	124.98
58	i	201	3PE	O31-C31-C32	2.83	120.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	Ac	401	HEM	CAD-CBD-CGD	-2.80	107.57	113.60
62	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
58	Ac	403	3PE	O31-C31-C32	2.78	120.64	111.91
67	AC	402	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
56	B	302	UQ1	CM5-C5-C6	-2.77	119.88	124.40
62	a	101	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
62	L	705	CDL	OB8-CB7-C71	2.76	120.57	111.91
62	L	704	CDL	OB8-CB7-C71	2.73	120.46	111.91
68	AC	404	U10	C12-C13-C14	-2.72	118.47	127.75
58	j	700	3PE	O31-C31-C32	2.71	120.42	111.91
62	d	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
58	K	101	3PE	O31-C31-C32	2.69	120.35	111.91
57	I	302	PC1	C2-O21-C21	-2.69	111.17	117.79
62	L	705	CDL	CA4-OA6-CA5	-2.69	111.17	117.79
62	d	201	CDL	OA8-CA7-C31	2.68	120.32	111.91
56	B	302	UQ1	C11-C9-C10	2.68	120.52	114.60
58	M	502	3PE	O31-C31-C32	2.68	120.31	111.91
62	Ag	101	CDL	CB4-OB6-CB5	-2.66	111.23	117.79
68	AC	404	U10	C10-C9-C11	2.66	119.74	115.27
58	m	202	3PE	O31-C31-C32	2.65	120.23	111.91
58	O	401	3PE	C2-O21-C21	-2.65	111.27	117.79
58	M	503	3PE	O31-C31-C32	2.64	120.21	111.91
69	AC	405	UQ6	C10-C9-C11	2.64	119.71	115.27
58	m	201	3PE	O31-C31-C32	2.64	120.18	111.91
66	n	201	EHZ	OP3-P1-O9	-2.63	100.37	110.68
58	L	701	3PE	O31-C31-C32	2.63	120.17	111.91
69	AC	405	UQ6	C6-C7-C8	-2.63	108.01	112.17
62	L	705	CDL	CB4-OB6-CB5	-2.62	111.34	117.79
62	Aa	501	CDL	OA8-CA7-C31	2.62	120.12	111.91
58	M	503	3PE	C2-O21-C21	-2.61	111.37	117.79
67	AC	402	HEM	CHA-C4D-C3D	-2.60	120.44	125.33
62	h	201	CDL	CA4-OA6-CA5	-2.60	111.39	117.79
58	Ac	403	3PE	C2-O21-C21	-2.59	111.42	117.79
62	L	705	CDL	OA8-CA7-C31	2.58	120.02	111.91
62	a	101	CDL	OB8-CB7-C71	2.58	120.00	111.91
60	F	501	FMN	C4A-C10-N1	-2.57	118.76	124.73
57	L	706	PC1	O31-C31-C32	2.57	119.97	111.91
68	Ac	404	U10	O4-C4-C5	-2.57	107.88	116.56
64	P	401	NDP	C4A-C5A-N7A	-2.56	106.73	109.40
67	AC	401	HEM	C4B-C3B-C2B	-2.56	105.08	107.11
58	M	501	3PE	O31-C31-C32	2.56	119.94	111.91
67	Ac	401	HEM	CHD-C1D-C2D	-2.56	120.99	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	AC	405	UQ6	C21-C19-C20	2.55	120.24	114.60
58	AC	403	3PE	O31-C31-C32	2.54	119.89	111.91
62	Ag	101	CDL	OA8-CA7-C31	2.54	119.89	111.91
58	O	401	3PE	O31-C31-C32	2.53	119.84	111.91
67	Ac	402	HEM	CHD-C1D-C2D	-2.53	121.03	124.98
58	L	703	3PE	O31-C31-C32	2.52	119.81	111.91
62	L	704	CDL	OA8-CA7-C31	2.52	119.81	111.91
58	J	401	3PE	O31-C31-C32	2.52	119.81	111.91
57	L	706	PC1	C2-O21-C21	-2.51	111.61	117.79
58	D	501	3PE	C2-O21-C21	-2.50	111.63	117.79
58	b	201	3PE	O31-C31-C32	2.50	119.76	111.91
62	L	704	CDL	CA4-OA6-CA5	-2.50	111.64	117.79
68	Ac	404	U10	C7-C6-C5	2.50	121.48	118.48
58	L	703	3PE	C2-O21-C21	-2.49	111.67	117.79
58	D	501	3PE	O31-C31-C32	2.49	119.71	111.91
67	AC	401	HEM	CMC-C2C-C3C	2.48	129.32	124.68
62	h	201	CDL	OA8-CA7-C31	2.47	119.67	111.91
66	n	201	EHZ	C10-S1-C9	2.47	109.56	101.87
58	L	701	3PE	C2-O21-C21	-2.47	111.72	117.79
63	O	402	ADP	C3'-C2'-C1'	2.47	104.69	100.98
62	Ac	406	CDL	OA8-CA7-C31	2.46	119.63	111.91
62	h	201	CDL	CB4-OB6-CB5	-2.46	111.74	117.79
67	AC	401	HEM	C3B-C2B-C1B	2.43	108.29	106.49
58	I	301	3PE	C2-O21-C21	-2.43	111.80	117.79
69	AC	405	UQ6	C4M-O4-C4	2.43	121.44	114.78
67	AC	401	HEM	CBD-CAD-C3D	-2.42	105.89	112.63
70	Ad	401	HEC	CBA-CAA-C2A	-2.42	108.53	112.60
67	AC	401	HEM	CHC-C4B-C3B	-2.41	120.88	124.57
67	Ac	402	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
60	F	501	FMN	O4-C4-C4A	-2.40	120.23	126.60
57	I	302	PC1	O31-C31-C32	2.39	119.41	111.91
60	F	501	FMN	C4-C4A-N5	2.39	121.63	118.23
66	W	201	EHZ	C5-C6-C7	-2.38	107.99	114.85
63	O	402	ADP	C4-C5-N7	-2.38	106.92	109.40
62	Aa	501	CDL	CA4-OA6-CA5	-2.36	111.98	117.79
66	n	201	EHZ	O2-C9-S1	-2.36	119.55	122.61
62	a	101	CDL	CB4-OB6-CB5	-2.36	111.99	117.79
67	Ac	401	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
68	AC	404	U10	C16-C14-C15	2.35	119.79	114.60
56	B	302	UQ1	C7-C8-C9	-2.34	119.92	127.26
70	Ad	401	HEC	CMA-C3A-C2A	2.33	129.34	124.94
62	Ag	101	CDL	OB8-CB7-C71	2.33	119.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
62	Aa	501	CDL	CB4-OB6-CB5	-2.25	112.26	117.79
67	Ac	401	HEM	C4D-ND-C1D	2.24	107.39	105.07
67	Ac	402	HEM	CBD-CAD-C3D	-2.22	106.45	112.63
58	I	301	3PE	O31-C31-C32	2.22	118.89	111.91
60	F	501	FMN	O2-C2-N1	-2.22	118.15	121.83
66	n	201	EHZ	O3-C12-N1	-2.22	118.83	123.01
60	F	501	FMN	C4A-C10-N10	2.21	119.70	116.48
64	P	401	NDP	C3D-C2D-C1D	2.20	105.60	101.43
66	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
58	b	201	3PE	O12-P-O14	-2.17	101.49	112.24
70	Ad	401	HEC	CMD-C2D-C3D	2.17	129.04	124.94
66	W	201	EHZ	O2-C9-S1	-2.17	119.80	122.61
67	AC	402	HEM	C4D-ND-C1D	2.17	107.31	105.07
62	Ag	101	CDL	CA4-OA6-CA5	-2.17	112.46	117.79
69	AC	405	UQ6	C17-C18-C19	-2.16	120.35	127.75
62	Ac	406	CDL	OB6-CB5-OB7	-2.16	118.49	123.70
58	m	201	3PE	O21-C21-O22	-2.14	118.54	123.70
60	F	501	FMN	C10-N1-C2	2.13	121.16	116.90
67	Ac	401	HEM	CHB-C1B-C2B	-2.13	120.83	126.72
66	W	201	EHZ	O6-P1-O9	2.12	112.42	106.47
62	d	201	CDL	OB6-CB5-OB7	-2.12	118.58	123.70
62	L	705	CDL	OA6-CA5-OA7	-2.11	118.60	123.70
67	AC	401	HEM	CHB-C1B-C2B	-2.11	120.89	126.72
66	W	201	EHZ	O3-C12-N1	-2.10	119.04	123.01
70	AD	401	HEC	CAA-CBA-CGA	-2.10	107.88	113.76
68	AC	404	U10	C7-C6-C5	2.08	120.99	118.48
66	n	201	EHZ	C5-C6-C7	-2.08	108.87	114.85
58	L	701	3PE	O21-C21-O22	-2.08	118.68	123.70
58	J	401	3PE	O12-P-O14	-2.06	102.07	112.24
58	j	700	3PE	O21-C21-O22	-2.05	118.74	123.70
67	Ac	402	HEM	CHB-C1B-C2B	-2.04	121.07	126.72
70	AD	401	HEC	CMA-C3A-C2A	2.04	128.79	124.94
68	Ac	404	U10	O4-C4-C3	2.04	131.32	123.64
58	M	503	3PE	O21-C21-O22	-2.03	118.78	123.70
68	AC	404	U10	C6-C1-C2	2.03	120.79	119.18
66	n	201	EHZ	C16-C15-N2	2.03	120.62	116.58
68	Ac	404	U10	C3M-O3-C3	2.02	123.64	116.47
62	d	201	CDL	OA6-CA5-OA7	-2.01	118.84	123.70
62	Ac	406	CDL	CA4-OA6-CA5	-2.01	112.85	117.79

There are no chirality outliers.

All (511) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	I	302	PC1	C11-O13-P-O14
57	L	706	PC1	C1-O11-P-O14
57	L	706	PC1	C22-C21-O21-C2
57	L	706	PC1	O32-C31-O31-C3
57	L	706	PC1	C32-C31-O31-C3
58	D	501	3PE	C1-O11-P-O12
58	I	301	3PE	C1-O11-P-O12
58	I	301	3PE	C22-C21-O21-C2
58	J	401	3PE	C11-O13-P-O12
58	J	401	3PE	C11-O13-P-O14
58	J	401	3PE	C12-C11-O13-P
58	J	401	3PE	O32-C31-O31-C3
58	J	401	3PE	C32-C31-O31-C3
58	K	101	3PE	C11-O13-P-O12
58	L	701	3PE	C1-O11-P-O12
58	L	701	3PE	O22-C21-O21-C2
58	L	701	3PE	C22-C21-O21-C2
58	L	702	3PE	C1-O11-P-O13
58	L	702	3PE	C1-O11-P-O14
58	L	702	3PE	C11-O13-P-O11
58	L	702	3PE	C11-O13-P-O12
58	L	702	3PE	C11-O13-P-O14
58	L	702	3PE	O32-C31-O31-C3
58	L	702	3PE	C32-C31-O31-C3
58	L	702	3PE	C22-C21-O21-C2
58	M	502	3PE	C1-O11-P-O12
58	M	502	3PE	C1-O11-P-O13
58	M	502	3PE	C1-O11-P-O14
58	M	502	3PE	C11-O13-P-O11
58	M	502	3PE	C11-O13-P-O12
58	M	502	3PE	C11-O13-P-O14
58	b	201	3PE	C1-O11-P-O12
58	b	201	3PE	C1-O11-P-O14
58	b	201	3PE	O22-C21-O21-C2
58	i	201	3PE	C1-O11-P-O12
58	m	201	3PE	C11-O13-P-O12
58	m	202	3PE	C1-O11-P-O12
58	m	202	3PE	C1-O11-P-O14
58	m	202	3PE	C22-C21-O21-C2
58	AC	403	3PE	C1-O11-P-O12
58	Ac	403	3PE	C1-O11-P-O12
60	F	501	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C19-C21-C22-C23
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C18-C19-C21-C22
61	H	400	UQ9	C17-C18-C19-C21
61	H	400	UQ9	C17-C18-C19-C20
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C12-C13-C14-C16
61	H	400	UQ9	C12-C13-C14-C15
62	L	704	CDL	CA2-OA2-PA1-OA3
62	L	704	CDL	CA2-OA2-PA1-OA4
62	L	704	CDL	CA2-OA2-PA1-OA5
62	L	704	CDL	CB2-OB2-PB2-OB3
62	L	704	CDL	C51-CB5-OB6-CB4
62	L	705	CDL	CA2-OA2-PA1-OA3
62	L	705	CDL	CA2-OA2-PA1-OA4
62	L	705	CDL	CB3-OB5-PB2-OB2
62	L	705	CDL	CB3-OB5-PB2-OB3
62	L	705	CDL	CB3-OB5-PB2-OB4
62	a	101	CDL	CA3-OA5-PA1-OA2
62	a	101	CDL	CA3-OA5-PA1-OA3
62	a	101	CDL	CA3-OA5-PA1-OA4
62	d	201	CDL	CA2-C1-CB2-OB2
62	d	201	CDL	CA3-OA5-PA1-OA2
62	d	201	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	CB2-OB2-PB2-OB3
62	d	201	CDL	CB2-OB2-PB2-OB5
62	d	201	CDL	C51-CB5-OB6-CB4
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	Aa	501	CDL	CA3-OA5-PA1-OA3
62	Aa	501	CDL	CB2-OB2-PB2-OB4
62	Ac	406	CDL	CA2-OA2-PA1-OA3
62	Ac	406	CDL	CA2-OA2-PA1-OA4
62	Ac	406	CDL	CB2-OB2-PB2-OB3
62	Ac	406	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
64	P	401	NDP	C2B-O2B-P2B-O2X
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	C6-C7-C8-C9
66	n	201	EHZ	S1-C10-C11-N1
66	n	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C19
66	n	201	EHZ	C15-C16-C17-C20
66	n	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C19
66	n	201	EHZ	O5-C16-C17-C20
66	n	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	C8-C9-S1-C10
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	401	HEM	C2A-CAA-CBA-CGA
67	Ac	402	HEM	C1A-C2A-CAA-CBA
67	Ac	402	HEM	C3A-C2A-CAA-CBA
68	Ac	404	U10	C7-C8-C9-C10
68	Ac	404	U10	C7-C8-C9-C11
69	Ac	405	UQ6	C1-C6-C7-C8
69	Ac	405	UQ6	C7-C8-C9-C10
69	Ac	405	UQ6	C7-C8-C9-C11
69	Ac	405	UQ6	C12-C13-C14-C15
69	Ac	405	UQ6	C12-C13-C14-C16
69	Ac	405	UQ6	C13-C14-C16-C17
69	Ac	405	UQ6	C15-C14-C16-C17
69	Ac	405	UQ6	C17-C18-C19-C20
68	Ac	404	U10	C12-C13-C14-C15
68	Ac	404	U10	C12-C13-C14-C16
57	I	302	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
58	K	101	3PE	O32-C31-O31-C3
58	M	503	3PE	O32-C31-O31-C3
58	j	700	3PE	O32-C31-O31-C3
62	Ac	406	CDL	OB9-CB7-OB8-CB6
58	I	301	3PE	O22-C21-O21-C2
58	L	702	3PE	O22-C21-O21-C2
58	m	201	3PE	O22-C21-O21-C2
58	m	202	3PE	O22-C21-O21-C2
62	L	704	CDL	OB7-CB5-OB6-CB4
62	d	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
57	I	302	PC1	C32-C31-O31-C3
58	j	700	3PE	C32-C31-O31-C3
62	L	704	CDL	C31-CA7-OA8-CA6
62	L	705	CDL	C71-CB7-OB8-CB6
62	Ac	406	CDL	C71-CB7-OB8-CB6
58	b	201	3PE	C22-C21-O21-C2
58	m	201	3PE	C22-C21-O21-C2
69	Ac	405	UQ6	C17-C18-C19-C21
61	H	400	UQ9	C24-C26-C27-C28
68	AC	404	U10	C12-C11-C9-C10
68	AC	404	U10	C12-C11-C9-C8
58	I	301	3PE	C32-C31-O31-C3
58	K	101	3PE	C32-C31-O31-C3
58	M	503	3PE	C32-C31-O31-C3
61	H	400	UQ9	C22-C23-C24-C25
57	L	706	PC1	O22-C21-O21-C2
61	H	400	UQ9	C22-C23-C24-C26
58	m	202	3PE	O32-C31-O31-C3
62	L	704	CDL	OA9-CA7-OA8-CA6
62	Aa	501	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	O1-C1-CB2-OB2
58	O	401	3PE	C32-C31-O31-C3
58	AC	403	3PE	C32-C31-O31-C3
62	Aa	501	CDL	C71-CB7-OB8-CB6
62	L	705	CDL	OB9-CB7-OB8-CB6
58	D	501	3PE	C22-C21-O21-C2
58	J	401	3PE	C22-C21-O21-C2
58	L	703	3PE	C22-C21-O21-C2
62	L	705	CDL	C11-CA5-OA6-CA4
58	m	202	3PE	C32-C31-O31-C3
62	h	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
58	I	301	3PE	O32-C31-O31-C3
58	AC	403	3PE	O32-C31-O31-C3
61	H	400	UQ9	C13-C14-C16-C17
58	O	401	3PE	O32-C31-O31-C3
61	H	400	UQ9	C9-C11-C12-C13
69	Ac	405	UQ6	C9-C11-C12-C13
69	Ac	405	UQ6	C14-C16-C17-C18
58	L	703	3PE	C32-C31-O31-C3
62	Ac	406	CDL	CB4-CB6-OB8-CB7
58	b	201	3PE	C2B-C2C-C2D-C2E
58	J	401	3PE	O22-C21-O21-C2
58	L	703	3PE	O32-C31-O31-C3
58	b	201	3PE	C32-C31-O31-C3
62	d	201	CDL	C31-CA7-OA8-CA6
62	Aa	501	CDL	C31-CA7-OA8-CA6
58	b	201	3PE	C39-C3A-C3B-C3C
62	d	201	CDL	OA6-CA4-CA6-OA8
58	L	703	3PE	O22-C21-O21-C2
62	a	101	CDL	C12-C13-C14-C15
58	b	201	3PE	O32-C31-O31-C3
62	d	201	CDL	OA9-CA7-OA8-CA6
62	h	201	CDL	C71-CB7-OB8-CB6
67	AC	402	HEM	C2A-CAA-CBA-CGA
58	m	201	3PE	C32-C31-O31-C3
58	M	501	3PE	C2-C3-O31-C31
58	M	501	3PE	C32-C33-C34-C35
62	Ag	101	CDL	CA4-CA3-OA5-PA1
62	Aa	501	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C14-C16-C17-C18
58	D	501	3PE	O22-C21-O21-C2
62	L	705	CDL	OA7-CA5-OA6-CA4
58	m	201	3PE	O32-C31-O31-C3
58	AC	403	3PE	C22-C21-O21-C2
58	I	301	3PE	C1-O11-P-O13
58	J	401	3PE	C11-O13-P-O11
58	L	701	3PE	C1-O11-P-O13
58	O	401	3PE	C1-O11-P-O13
58	b	201	3PE	C1-O11-P-O13
58	i	201	3PE	C1-O11-P-O13
58	m	201	3PE	C1-O11-P-O13
58	m	201	3PE	C11-O13-P-O11
58	m	202	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
58	AC	403	3PE	C1-O11-P-O13
62	L	705	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2
62	Aa	501	CDL	CA3-OA5-PA1-OA2
62	Ac	406	CDL	CA2-OA2-PA1-OA5
62	Ac	406	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CA2-OA2-PA1-OA5
62	Ag	101	CDL	CA3-OA5-PA1-OA2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
58	M	501	3PE	C32-C31-O31-C3
62	L	704	CDL	C17-C18-C19-C20
58	M	502	3PE	C22-C21-O21-C2
58	M	501	3PE	C23-C24-C25-C26
62	h	201	CDL	C18-C19-C20-C21
62	h	201	CDL	OB9-CB7-OB8-CB6
58	M	502	3PE	O22-C21-O21-C2
58	AC	403	3PE	O22-C21-O21-C2
58	L	703	3PE	C21-C22-C23-C24
62	L	704	CDL	C52-C53-C54-C55
58	m	201	3PE	C24-C25-C26-C27
62	L	704	CDL	C12-C13-C14-C15
62	L	704	CDL	C71-CB7-OB8-CB6
58	O	401	3PE	C22-C21-O21-C2
62	L	704	CDL	C11-CA5-OA6-CA4
58	M	501	3PE	O32-C31-O31-C3
62	Ag	101	CDL	C74-C75-C76-C77
62	L	704	CDL	OA7-CA5-OA6-CA4
58	L	703	3PE	C22-C23-C24-C25
57	B	303	PC1	C22-C21-O21-C2
62	L	705	CDL	C51-CB5-OB6-CB4
58	b	201	3PE	C27-C28-C29-C2A
62	L	705	CDL	C72-C73-C74-C75
62	L	704	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	OA7-CA5-OA6-CA4
62	Ac	406	CDL	OA7-CA5-OA6-CA4
62	d	201	CDL	C71-CB7-OB8-CB6
67	Ac	401	HEM	C2B-C3B-CAB-CBB
58	M	502	3PE	C3C-C3D-C3E-C3F
58	K	101	3PE	C22-C21-O21-C2
62	d	201	CDL	C11-CA5-OA6-CA4
62	Ac	406	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	B	303	PC1	O22-C21-O21-C2
58	O	401	3PE	O22-C21-O21-C2
62	L	705	CDL	OB7-CB5-OB6-CB4
58	K	101	3PE	O22-C21-O21-C2
58	I	301	3PE	C11-O13-P-O11
58	K	101	3PE	C11-O13-P-O11
58	M	501	3PE	C1-O11-P-O13
62	h	201	CDL	CB3-OB5-PB2-OB2
62	Aa	501	CDL	CB2-OB2-PB2-OB5
58	J	401	3PE	C37-C38-C39-C3A
58	K	101	3PE	C22-C23-C24-C25
58	D	501	3PE	C24-C25-C26-C27
62	a	101	CDL	C11-CA5-OA6-CA4
58	b	201	3PE	C1-C2-C3-O31
62	d	201	CDL	CA3-CA4-CA6-OA8
58	L	701	3PE	C24-C25-C26-C27
62	a	101	CDL	C71-CB7-OB8-CB6
66	n	201	EHZ	C3-C4-C5-C6
58	AC	403	3PE	C23-C24-C25-C26
62	Ag	101	CDL	C31-CA7-OA8-CA6
62	L	705	CDL	C12-C13-C14-C15
58	J	401	3PE	C3-C2-O21-C21
60	F	501	FMN	C5'-O5'-P-O1P
58	i	201	3PE	C32-C33-C34-C35
62	d	201	CDL	OB9-CB7-OB8-CB6
58	M	503	3PE	C24-C25-C26-C27
58	K	101	3PE	C21-C22-C23-C24
58	L	701	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
58	b	201	3PE	O11-C1-C2-C3
58	M	503	3PE	C28-C29-C2A-C2B
58	m	201	3PE	C23-C24-C25-C26
58	L	702	3PE	C2-C1-O11-P
62	d	201	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB4-CB3-OB5-PB2
58	L	702	3PE	C34-C35-C36-C37
58	L	702	3PE	C24-C25-C26-C27
58	i	201	3PE	C1-C2-C3-O31
66	W	201	EHZ	N2-C15-C16-C17
58	I	301	3PE	C23-C24-C25-C26
58	M	502	3PE	C23-C24-C25-C26
62	a	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
62	Ag	101	CDL	OA9-CA7-OA8-CA6
58	b	201	3PE	C24-C25-C26-C27
57	I	302	PC1	C11-O13-P-O11
62	L	705	CDL	CA3-OA5-PA1-OA2
62	h	201	CDL	CB2-OB2-PB2-OB5
66	W	201	EHZ	C3-C4-C5-C6
62	a	101	CDL	OA9-CA7-OA8-CA6
58	I	301	3PE	C21-C22-C23-C24
66	W	201	EHZ	C5-C6-C7-O1
58	i	201	3PE	O21-C2-C3-O31
57	B	303	PC1	C32-C31-O31-C3
62	d	201	CDL	C52-C53-C54-C55
68	AC	404	U10	C9-C11-C12-C13
62	a	101	CDL	OA7-CA5-OA6-CA4
69	AC	405	UQ6	C15-C14-C16-C17
62	h	201	CDL	C14-C15-C16-C17
62	L	704	CDL	CA4-CA3-OA5-PA1
62	L	705	CDL	CA4-CA3-OA5-PA1
58	M	502	3PE	C32-C31-O31-C3
66	W	201	EHZ	O2-C9-S1-C10
62	Ag	101	CDL	C51-CB5-OB6-CB4
62	L	704	CDL	OB5-CB3-CB4-CB6
58	J	401	3PE	C2A-C2B-C2C-C2D
58	L	702	3PE	C25-C26-C27-C28
62	h	201	CDL	CB3-CB4-OB6-CB5
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
58	J	401	3PE	C2-C1-O11-P
58	O	401	3PE	C2-C1-O11-P
58	i	201	3PE	C2-C1-O11-P
62	a	101	CDL	CB3-CB4-CB6-OB8
62	d	201	CDL	CB4-CB3-OB5-PB2
62	h	201	CDL	CB4-CB3-OB5-PB2
58	b	201	3PE	O11-C1-C2-O21
62	L	704	CDL	OB5-CB3-CB4-OB6
67	Ac	401	HEM	C4B-C3B-CAB-CBB
66	n	201	EHZ	O1-C7-C8-C9
58	L	701	3PE	O32-C31-O31-C3
58	M	502	3PE	O32-C31-O31-C3
62	a	101	CDL	OB6-CB4-CB6-OB8
58	L	701	3PE	C28-C29-C2A-C2B
58	L	702	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
62	L	705	CDL	C57-C58-C59-C60
62	Ac	406	CDL	OB7-CB5-OB6-CB4
62	Ag	101	CDL	OB7-CB5-OB6-CB4
57	B	303	PC1	O32-C31-O31-C3
58	O	401	3PE	C36-C37-C38-C39
62	L	704	CDL	C71-C72-C73-C74
62	Ac	406	CDL	C51-CB5-OB6-CB4
57	I	302	PC1	C1-O11-P-O13
58	M	503	3PE	C11-O13-P-O11
58	b	201	3PE	C11-O13-P-O11
62	L	704	CDL	CB4-CB3-OB5-PB2
62	a	101	CDL	CA4-CA3-OA5-PA1
62	Ag	101	CDL	C1-CA2-OA2-PA1
58	I	301	3PE	C11-O13-P-O12
58	I	301	3PE	C11-O13-P-O14
58	K	101	3PE	C11-O13-P-O14
58	O	401	3PE	C1-O11-P-O12
58	O	401	3PE	C1-O11-P-O14
58	b	201	3PE	C11-O13-P-O12
58	m	201	3PE	C1-O11-P-O12
58	m	201	3PE	C1-O11-P-O14
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	Aa	501	CDL	CA3-OA5-PA1-OA4
62	Aa	501	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CA2-OA2-PA1-OA3
62	Ag	101	CDL	CA3-OA5-PA1-OA3
62	Ag	101	CDL	CA3-OA5-PA1-OA4
58	m	201	3PE	C2E-C2F-C2G-C2H
62	Ag	101	CDL	C71-CB7-OB8-CB6
58	L	701	3PE	C25-C26-C27-C28
58	L	703	3PE	C29-C2A-C2B-C2C
64	P	401	NDP	O4D-C1D-N1N-C6N
57	B	303	PC1	C11-C12-N-C15
57	I	302	PC1	C11-C12-N-C15
57	L	706	PC1	O13-C11-C12-N
58	b	201	3PE	O21-C2-C3-O31
58	m	201	3PE	C33-C34-C35-C36
58	j	700	3PE	C22-C21-O21-C2
62	L	705	CDL	C56-C57-C58-C59
66	W	201	EHZ	O4-C15-C16-O5
62	Ag	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
58	M	503	3PE	C34-C35-C36-C37
57	L	706	PC1	C3B-C3C-C3D-C3E
66	W	201	EHZ	C19-C17-C20-O6
58	b	201	3PE	C3-C2-O21-C21
62	L	704	CDL	CB6-CB4-OB6-CB5
62	Ac	406	CDL	CA6-CA4-OA6-CA5
58	D	501	3PE	C32-C31-O31-C3
57	I	302	PC1	C11-C12-N-C13
58	j	700	3PE	O22-C21-O21-C2
70	AD	401	HEC	C3D-CAD-CBD-CGD
57	L	706	PC1	C1-O11-P-O13
58	M	503	3PE	C1-O11-P-O13
58	j	700	3PE	C1-O11-P-O13
62	L	704	CDL	CA3-OA5-PA1-OA2
62	L	704	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CB2-OB2-PB2-OB5
62	d	201	CDL	CA2-OA2-PA1-OA5
62	d	201	CDL	CB3-OB5-PB2-OB2
62	Aa	501	CDL	CA2-OA2-PA1-OA5
58	D	501	3PE	C32-C33-C34-C35
58	L	701	3PE	C33-C34-C35-C36
66	W	201	EHZ	C2-C3-C4-C5
64	P	401	NDP	PN-O3-PA-O2A
58	j	700	3PE	C2-C1-O11-P
62	Aa	501	CDL	CA4-CA3-OA5-PA1
58	D	501	3PE	O32-C31-O31-C3
58	J	401	3PE	C2B-C2C-C2D-C2E
57	B	303	PC1	C11-C12-N-C14
67	Ac	401	HEM	CAA-CBA-CGA-O1A
58	J	401	3PE	C28-C29-C2A-C2B
67	AC	402	HEM	CAD-CBD-CGD-O1D
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	AC	402	HEM	CAA-CBA-CGA-O2A
67	Ac	402	HEM	CAD-CBD-CGD-O1D
67	AC	401	HEM	CAD-CBD-CGD-O1D
67	AC	402	HEM	CAA-CBA-CGA-O1A
58	i	201	3PE	O22-C21-O21-C2
58	M	503	3PE	C23-C24-C25-C26
68	Ac	404	U10	C12-C11-C9-C10
67	AC	401	HEM	CAA-CBA-CGA-O2A
58	i	201	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
57	B	303	PC1	C11-C12-N-C13
57	I	302	PC1	C11-C12-N-C14
58	M	502	3PE	C39-C3A-C3B-C3C
67	Ac	401	HEM	CAD-CBD-CGD-O2D
62	a	101	CDL	C1-CA2-OA2-PA1
58	J	401	3PE	O11-C1-C2-O21
67	Ac	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAD-CBD-CGD-O1D
62	d	201	CDL	C59-C60-C61-C62
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAA-CBA-CGA-O2A
66	n	201	EHZ	C11-C10-S1-C9
62	h	201	CDL	C31-CA7-OA8-CA6
68	Ac	404	U10	C12-C11-C9-C8
58	L	702	3PE	C23-C24-C25-C26
67	AC	401	HEM	CAD-CBD-CGD-O2D
62	L	704	CDL	C14-C15-C16-C17
62	Ac	406	CDL	CA4-CA3-OA5-PA1
69	Ac	405	UQ6	C5-C6-C7-C8
58	J	401	3PE	C25-C26-C27-C28
66	n	201	EHZ	C2-C3-C4-C5
68	AC	404	U10	C1-C6-C7-C8
62	h	201	CDL	OA9-CA7-OA8-CA6
62	L	704	CDL	OA5-CA3-CA4-OA6
57	I	302	PC1	C2C-C2D-C2E-C2F
57	L	706	PC1	C2-C3-O31-C31
58	J	401	3PE	O11-C1-C2-C3
69	AC	405	UQ6	C13-C14-C16-C17
66	W	201	EHZ	N2-C15-C16-O5
58	b	201	3PE	C25-C26-C27-C28
66	W	201	EHZ	C18-C17-C20-O6
57	I	302	PC1	C2E-C2F-C2G-C2H
68	AC	404	U10	C5-C6-C7-C8
58	D	501	3PE	C34-C35-C36-C37
70	AD	401	HEC	CAA-CBA-CGA-O2A
70	Ad	401	HEC	CAA-CBA-CGA-O2A
62	L	705	CDL	C52-C53-C54-C55
58	i	201	3PE	O21-C21-C22-C23
58	K	101	3PE	O11-C1-C2-O21
58	J	401	3PE	C33-C34-C35-C36
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
58	M	502	3PE	C26-C27-C28-C29
66	W	201	EHZ	C15-C16-C17-C18
70	AD	401	HEC	CAA-CBA-CGA-O1A
70	Ad	401	HEC	CAA-CBA-CGA-O1A
66	W	201	EHZ	O5-C16-C17-C18
58	L	701	3PE	C39-C3A-C3B-C3C
58	M	501	3PE	C24-C25-C26-C27
58	K	101	3PE	C24-C25-C26-C27
62	L	705	CDL	CA7-C31-C32-C33
58	M	502	3PE	C36-C37-C38-C39
58	K	101	3PE	C36-C37-C38-C39
62	L	704	CDL	C53-C54-C55-C56
69	AC	405	UQ6	C1-C6-C7-C8
62	a	101	CDL	C32-C31-CA7-OA8
62	d	201	CDL	C12-C11-CA5-OA6
58	K	101	3PE	C23-C24-C25-C26
58	i	201	3PE	O22-C21-C22-C23
69	Ac	405	UQ6	C6-C7-C8-C9
58	L	701	3PE	C34-C35-C36-C37
62	a	101	CDL	C1-CB2-OB2-PB2
62	Ac	406	CDL	C1-CA2-OA2-PA1
58	D	501	3PE	C1-O11-P-O14
58	L	703	3PE	C1-O11-P-O14
58	M	501	3PE	C1-O11-P-O14
58	Ac	403	3PE	C1-O11-P-O14
62	L	705	CDL	CA3-OA5-PA1-OA4
62	d	201	CDL	CA2-OA2-PA1-OA3
62	d	201	CDL	CB3-OB5-PB2-OB3
63	O	402	ADP	C5'-O5'-PA-O1A
62	a	101	CDL	C32-C31-CA7-OA9
62	Ac	406	CDL	C52-C51-CB5-OB6
58	i	201	3PE	C32-C31-O31-C3
58	K	101	3PE	O13-C11-C12-N
58	L	701	3PE	C2B-C2C-C2D-C2E
58	M	502	3PE	C2B-C2C-C2D-C2E
58	D	501	3PE	C12-C11-O13-P
58	I	301	3PE	C1-C2-O21-C21
58	L	703	3PE	C12-C11-O13-P
66	W	201	EHZ	O4-C15-C16-C17
58	i	201	3PE	O32-C31-O31-C3
58	L	702	3PE	O21-C21-C22-C23
58	Ac	403	3PE	C23-C24-C25-C26

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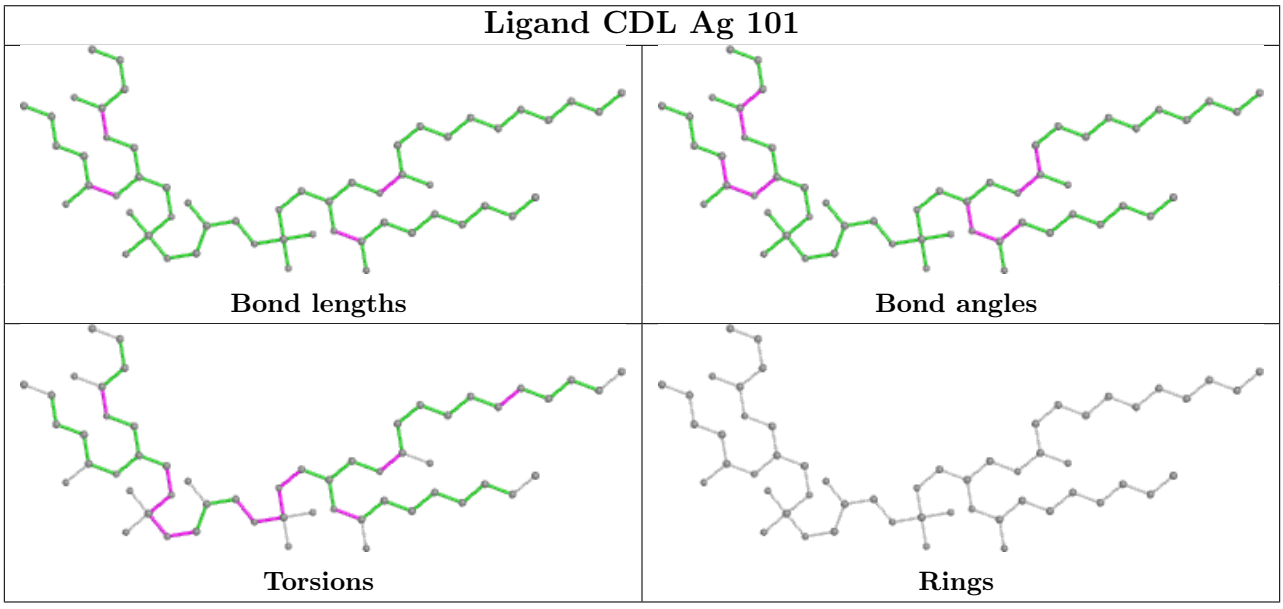
Mol	Chain	Res	Type	Atoms
57	L	706	PC1	C27-C28-C29-C2A
58	L	703	3PE	C24-C25-C26-C27
57	B	303	PC1	O21-C21-C22-C23
62	h	201	CDL	C72-C71-CB7-OB8
62	d	201	CDL	C11-C12-C13-C14
62	d	201	CDL	C12-C11-CA5-OA7
62	Ac	406	CDL	C52-C51-CB5-OB7

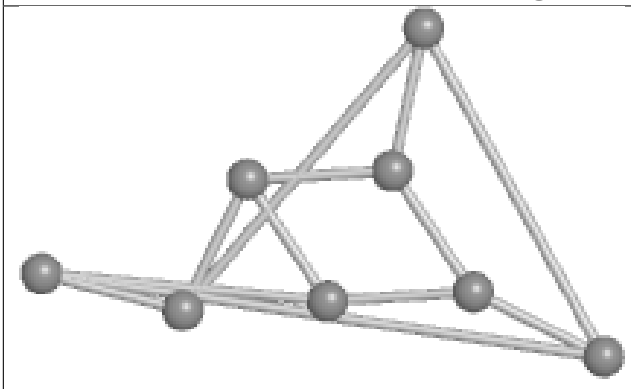
There are no ring outliers.

No monomer is involved in short contacts.

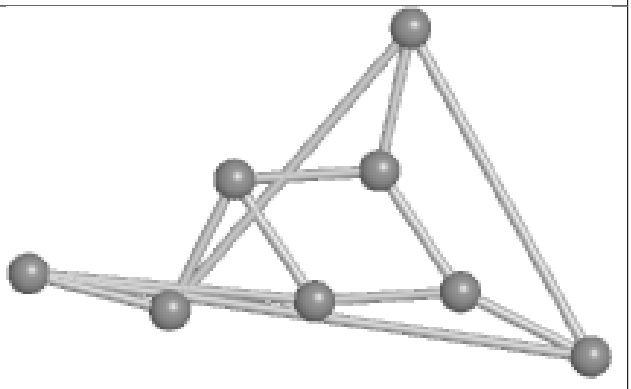
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



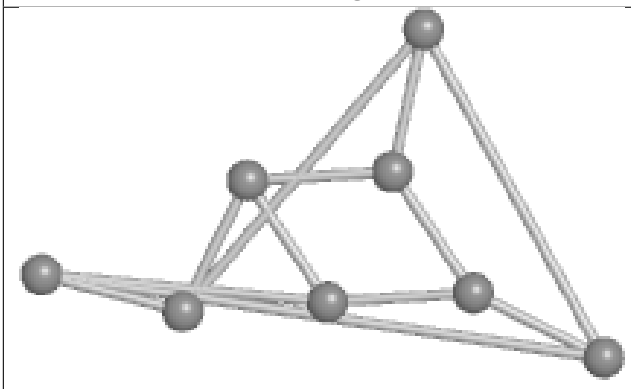
Ligand SF4 G 802



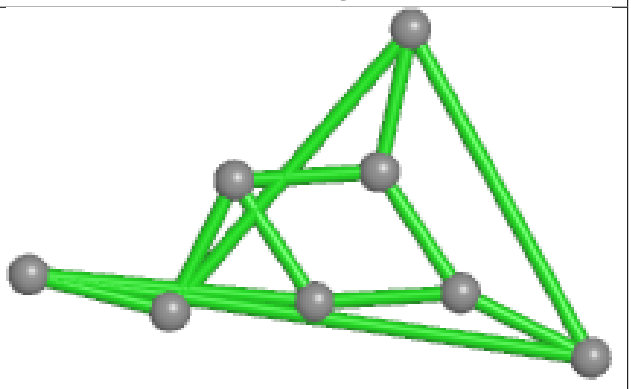
Bond lengths



Bond angles

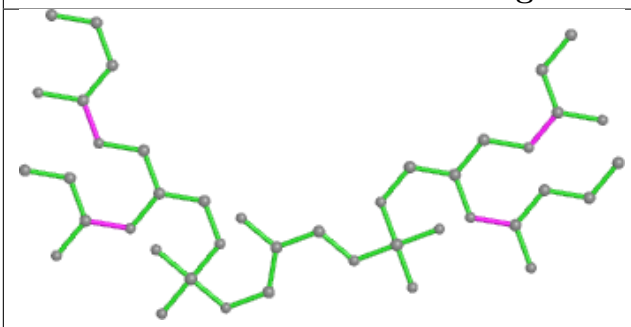


Torsions



Rings

Ligand CDL Ac 406



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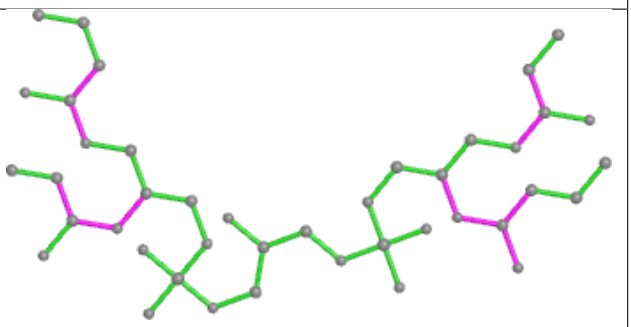
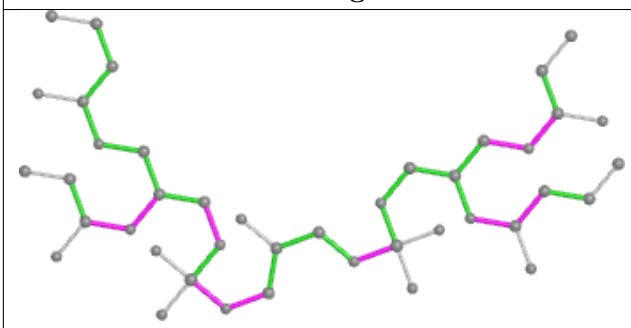
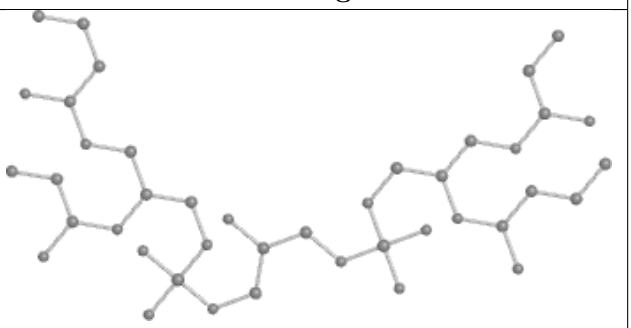


Bond angles

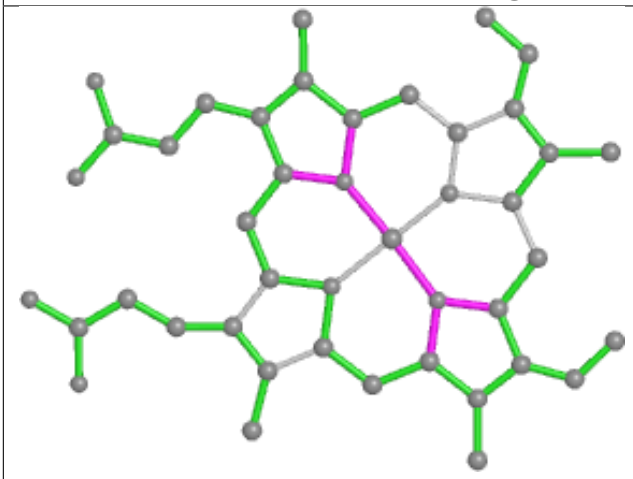


Torsions

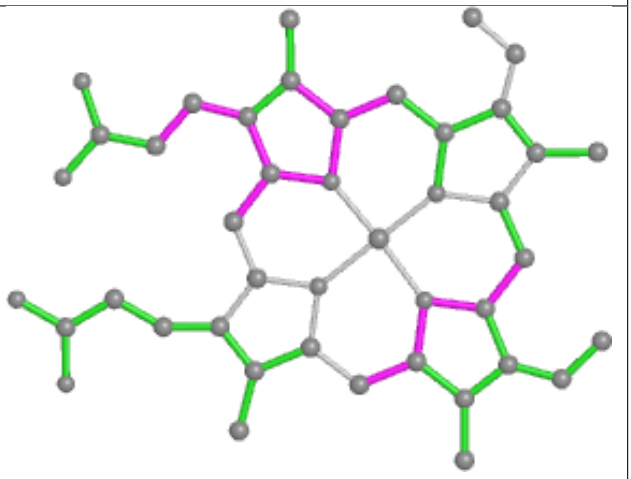


Rings

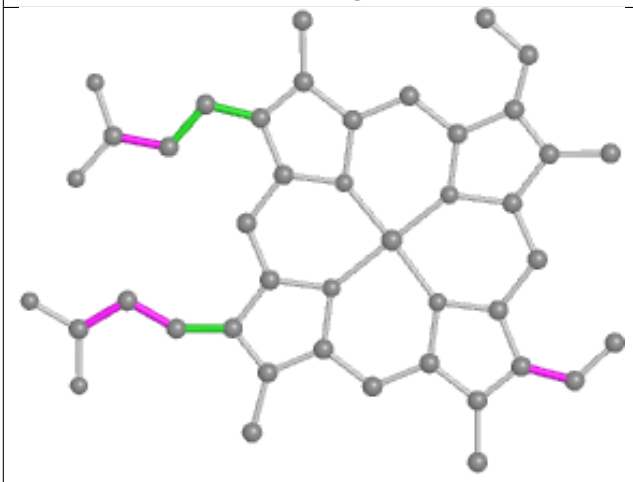
Ligand HEM AC 402



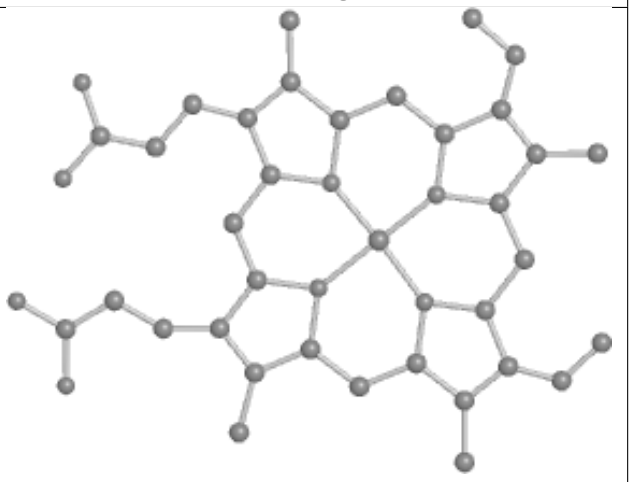
Bond lengths



Bond angles

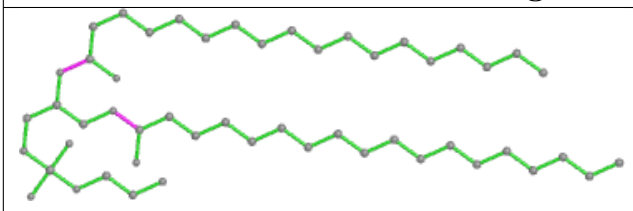


Torsions

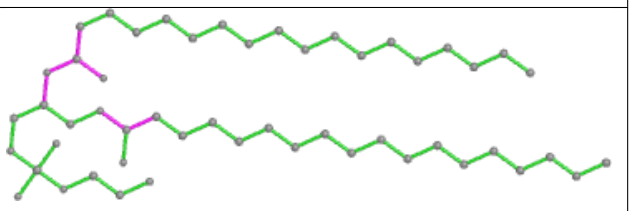


Rings

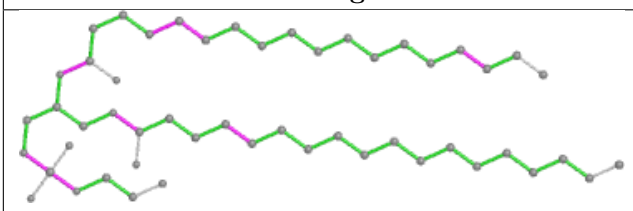
Ligand 3PE m 201



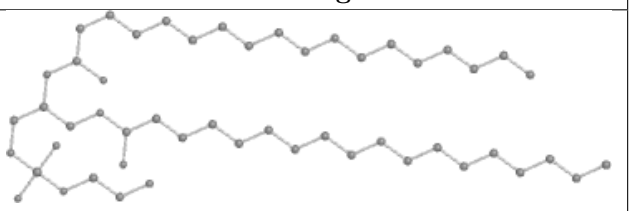
Bond lengths



Bond angles

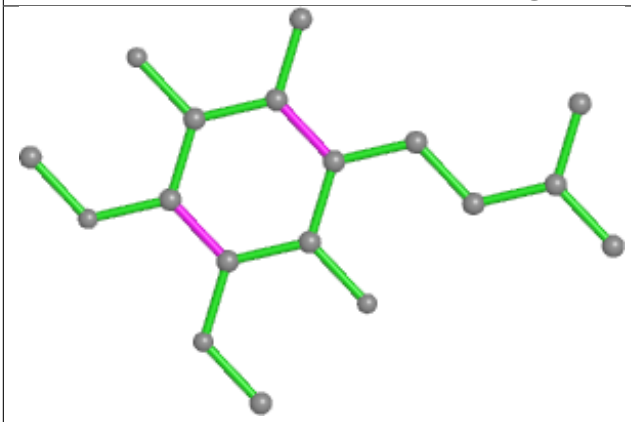


Torsions

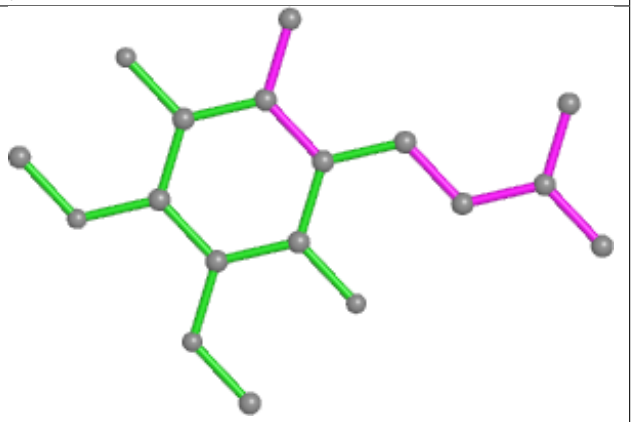


Rings

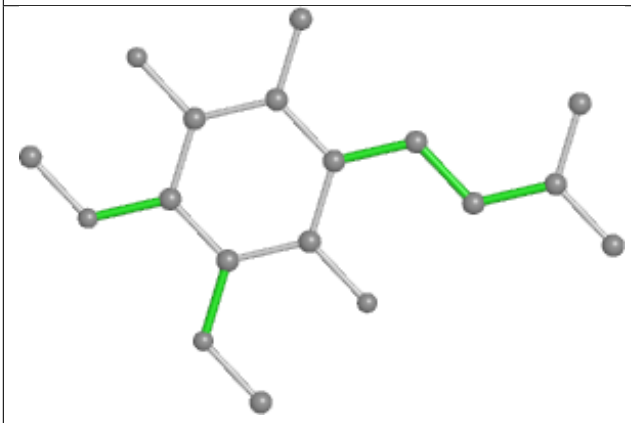
Ligand UQ1 B 302



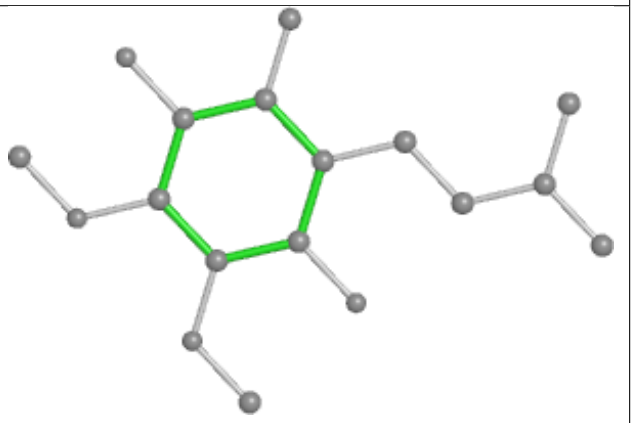
Bond lengths



Bond angles

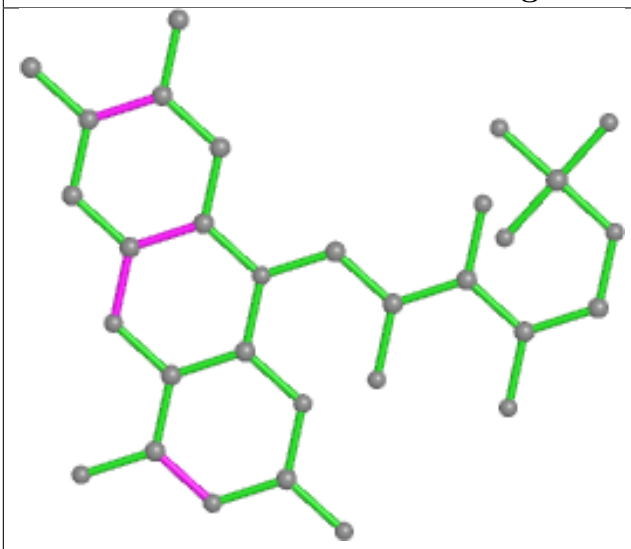


Torsions

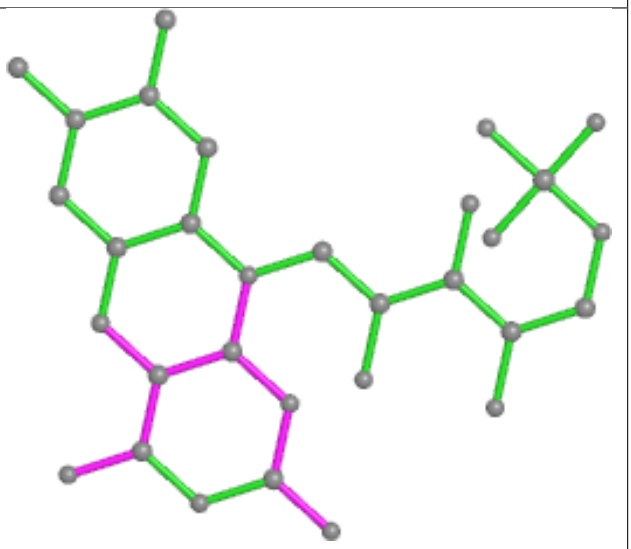


Rings

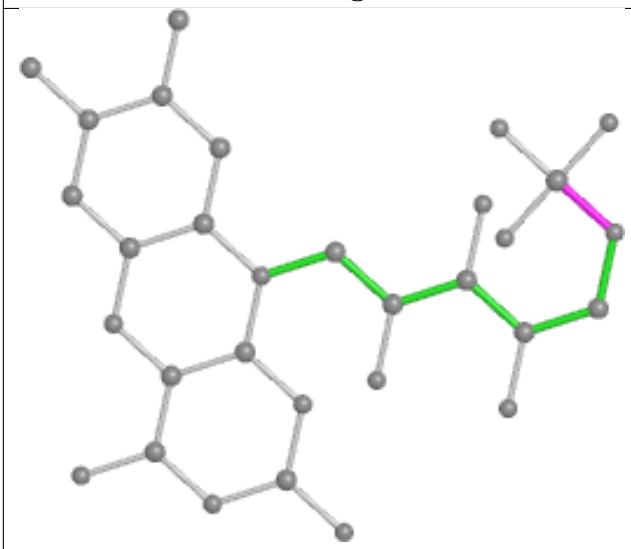
Ligand FMN F 501



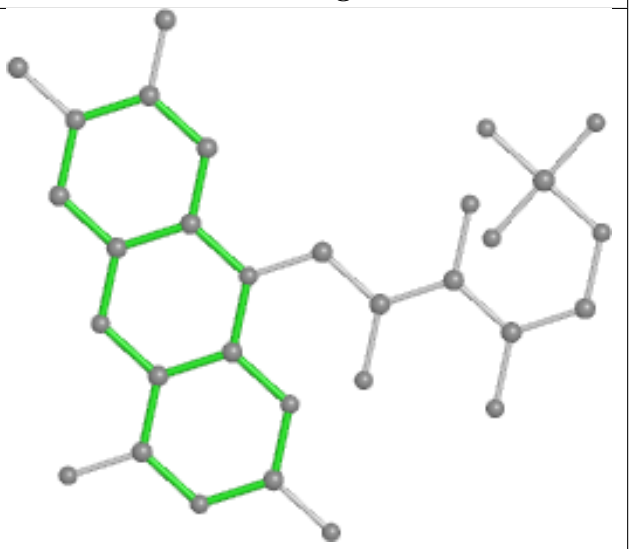
Bond lengths



Bond angles

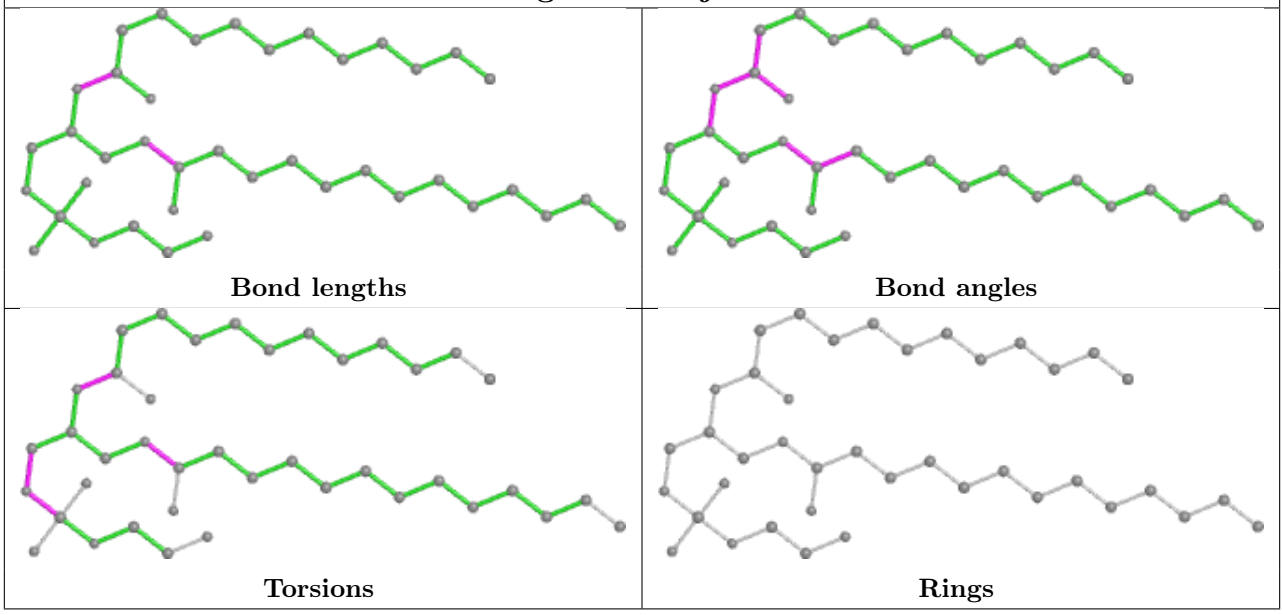


Torsions

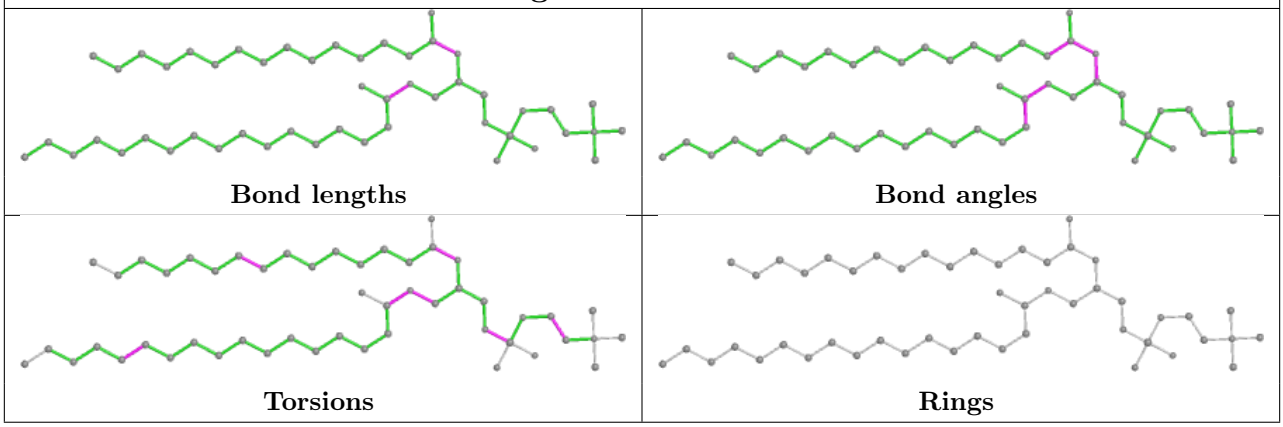


Rings

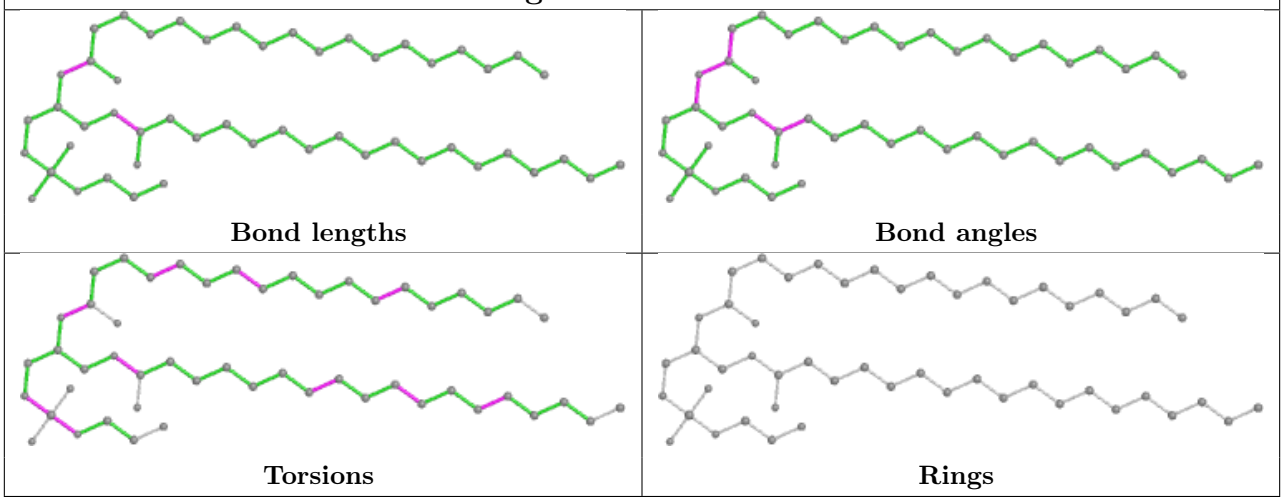
Ligand 3PE j 700



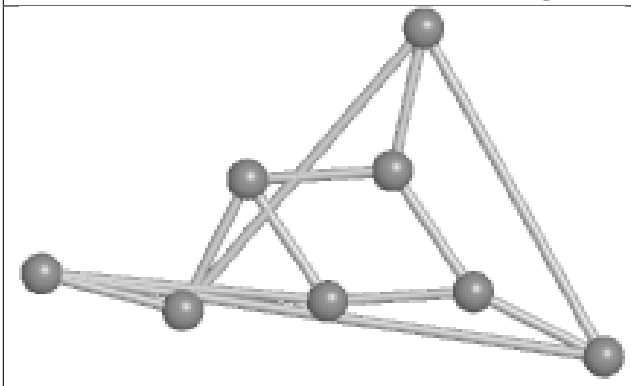
Ligand PC1 L 706



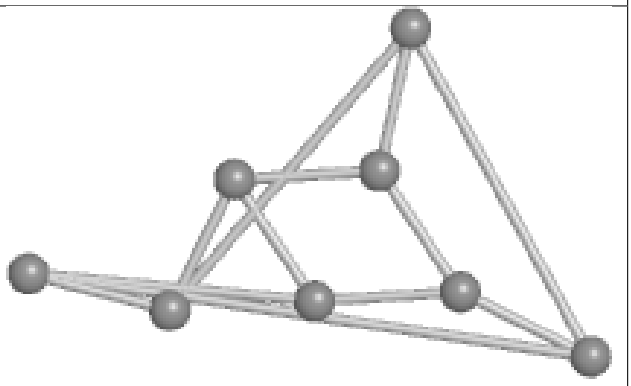
Ligand 3PE M 502



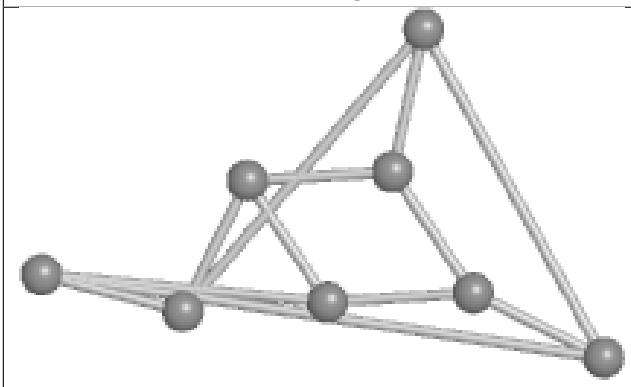
Ligand SF4 I 303



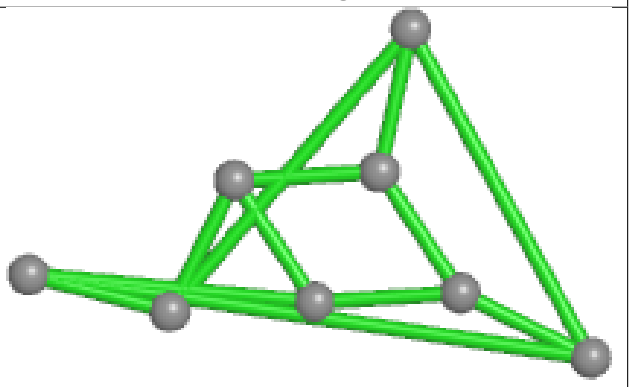
Bond lengths



Bond angles

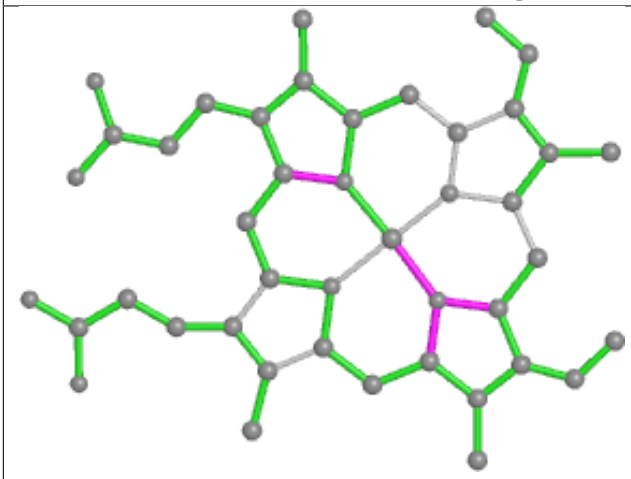


Torsions

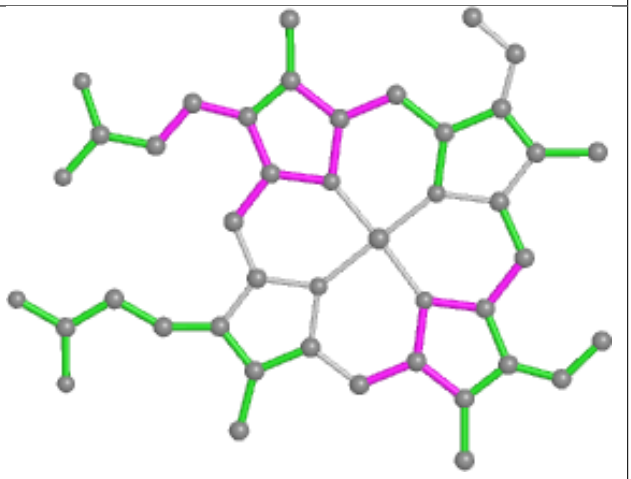


Rings

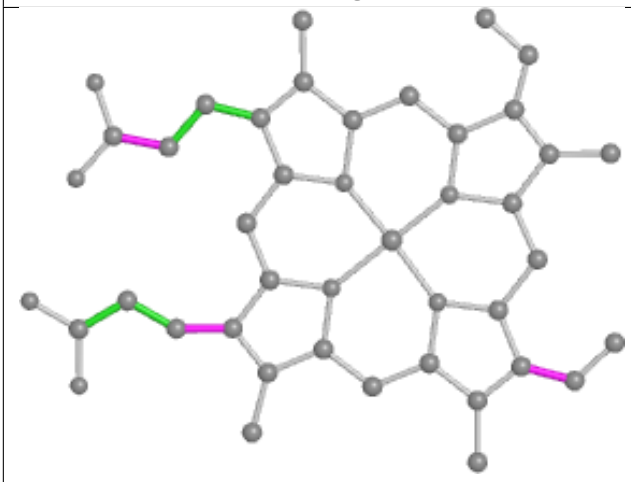
Ligand HEM Ac 402



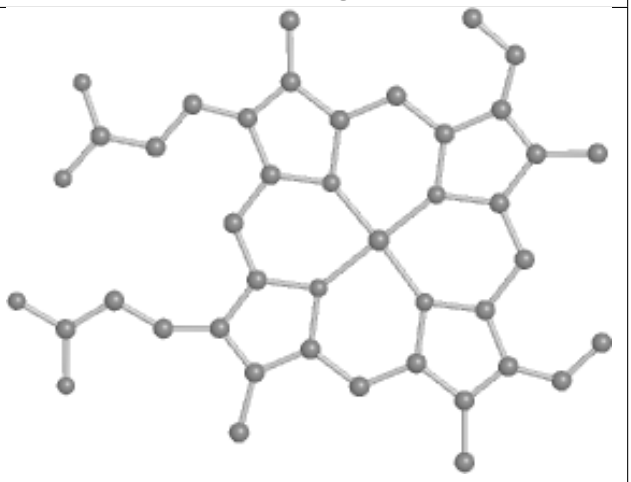
Bond lengths



Bond angles

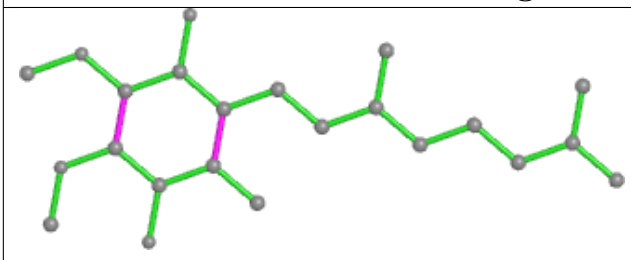


Torsions

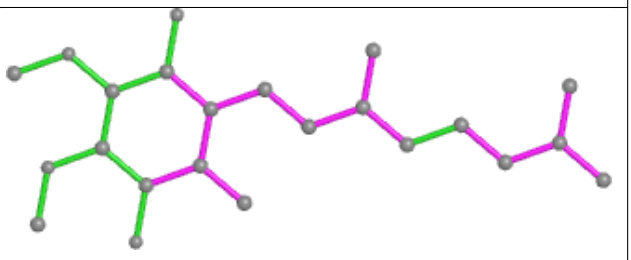


Rings

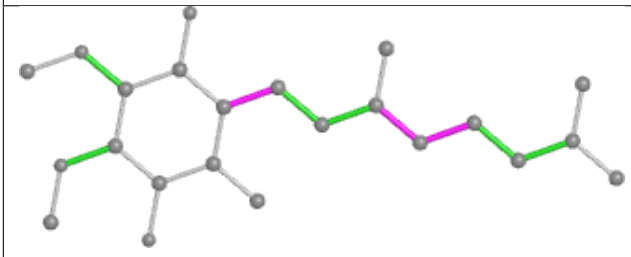
Ligand U10 AC 404



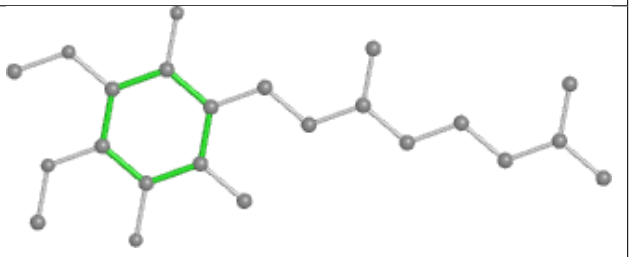
Bond lengths



Bond angles

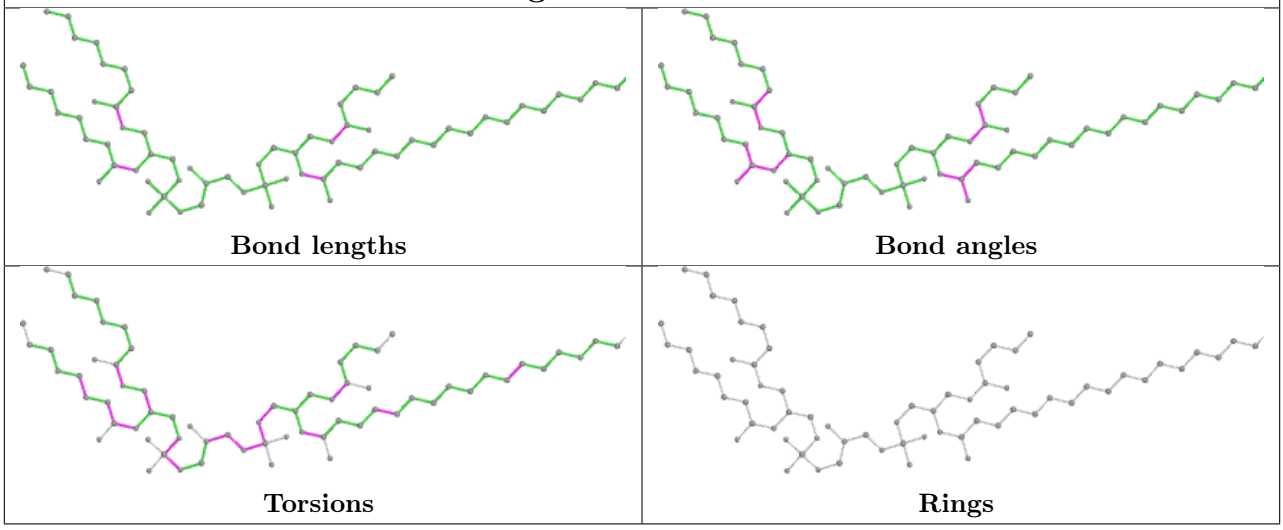


Torsions

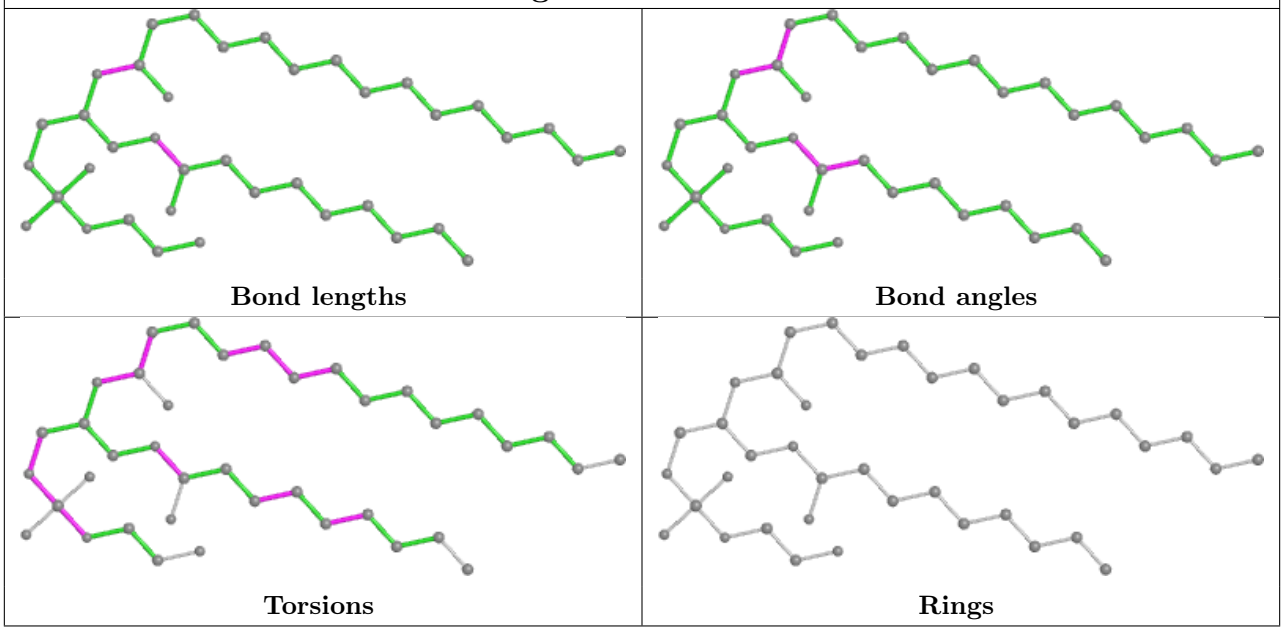


Rings

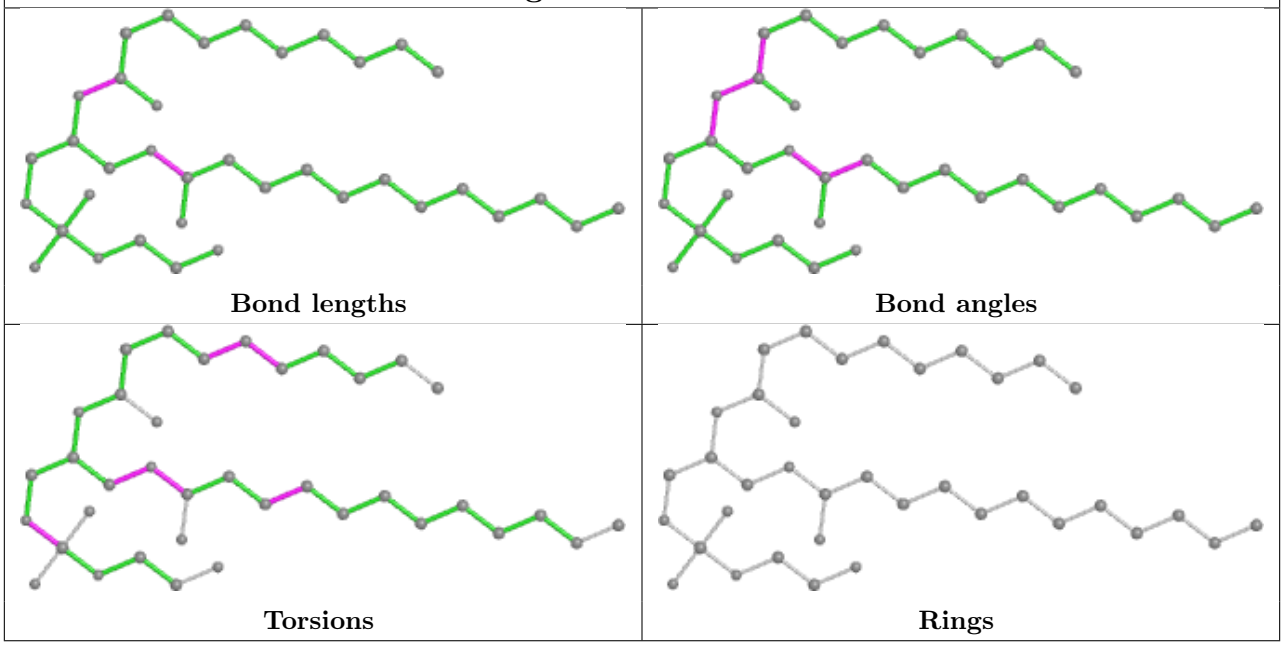
Ligand CDL d 201



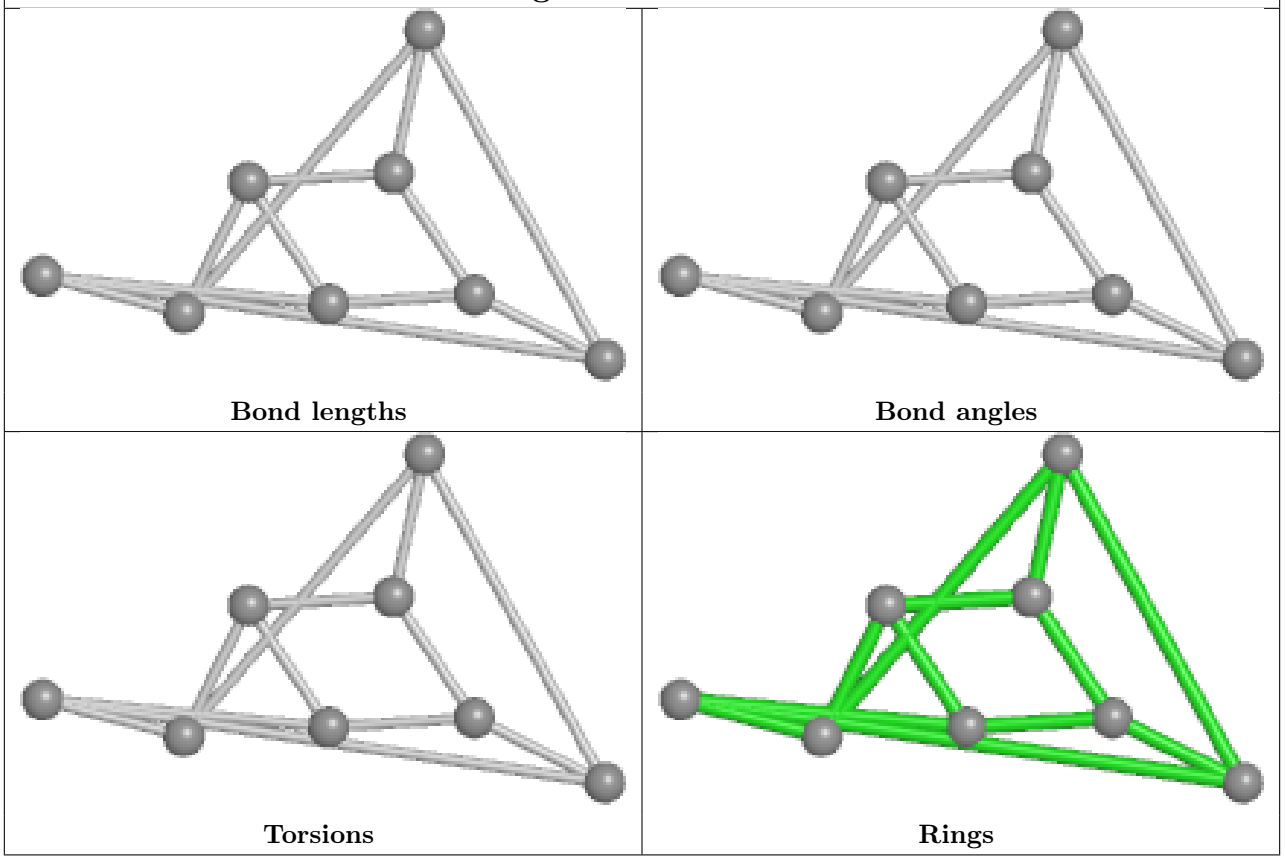
Ligand 3PE L 702



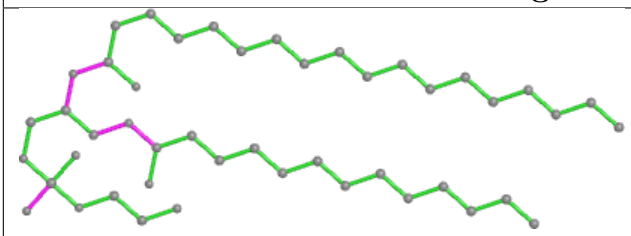
Ligand 3PE M 501



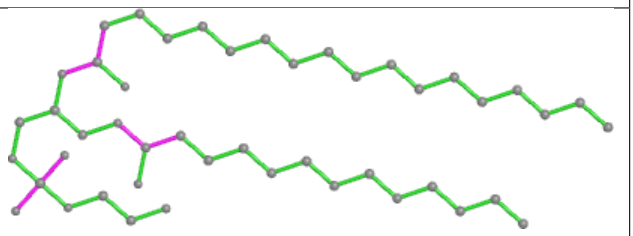
Ligand SF4 B 301



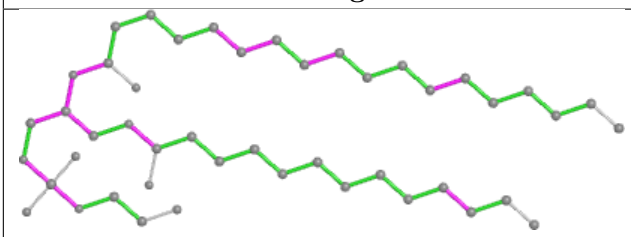
Ligand 3PE b 201



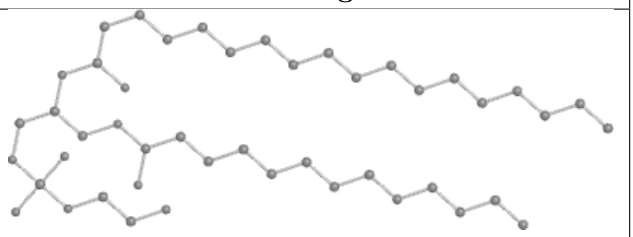
Bond lengths



Bond angles

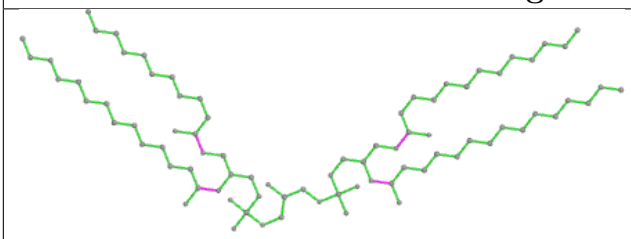


Torsions

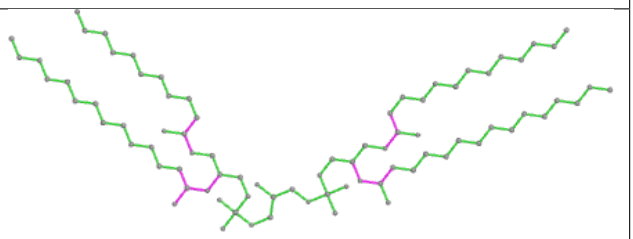


Rings

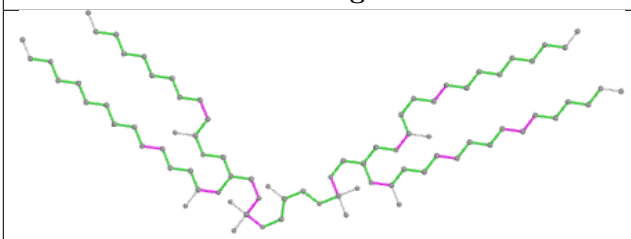
Ligand CDL L 705



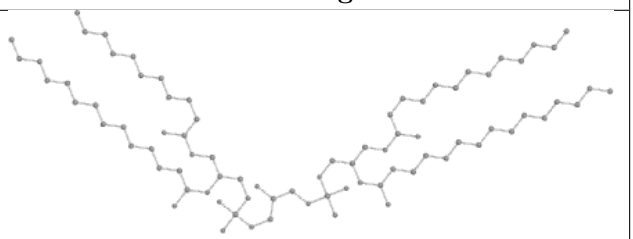
Bond lengths



Bond angles

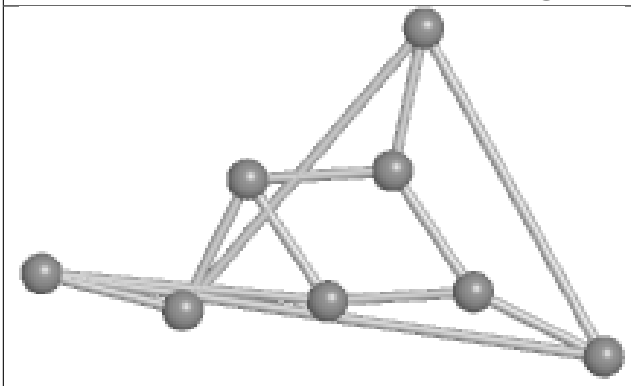


Torsions

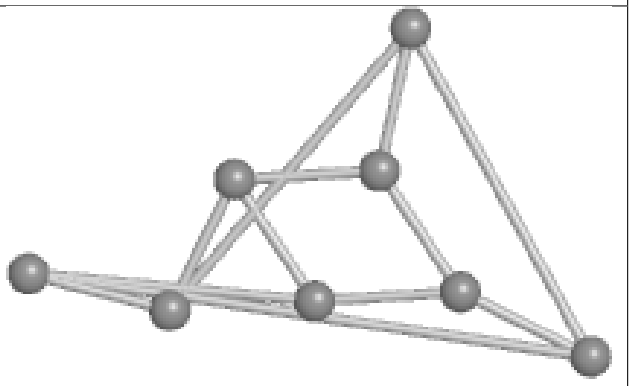


Rings

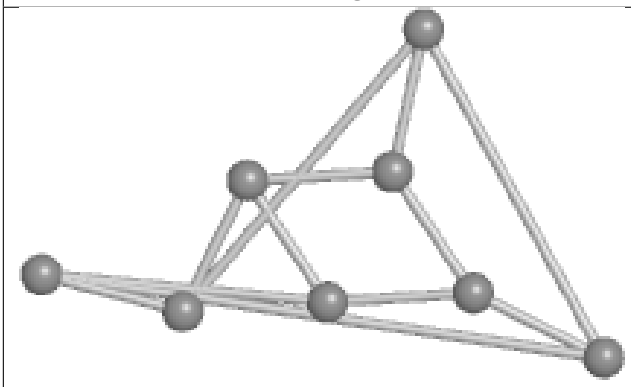
Ligand SF4 I 304



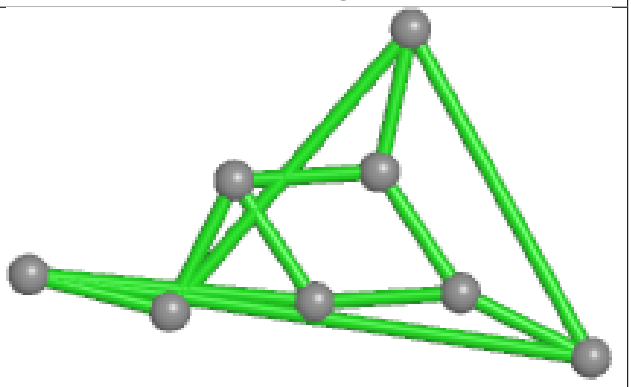
Bond lengths



Bond angles

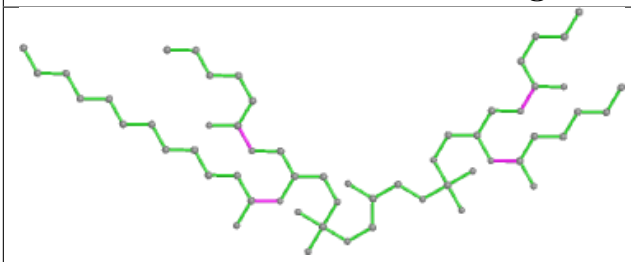


Torsions

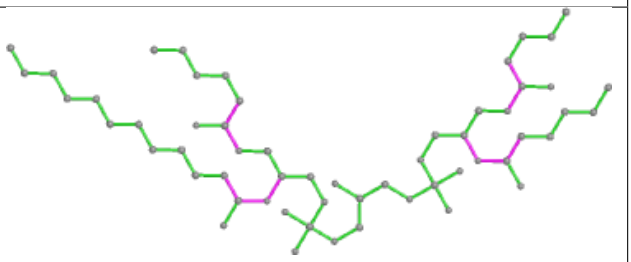


Rings

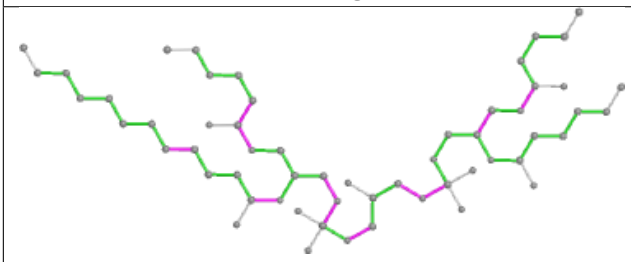
Ligand CDL a 101



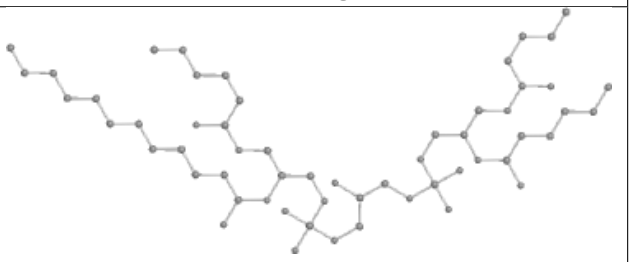
Bond lengths



Bond angles

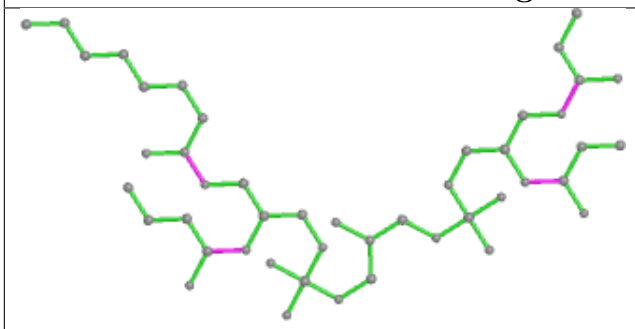


Torsions

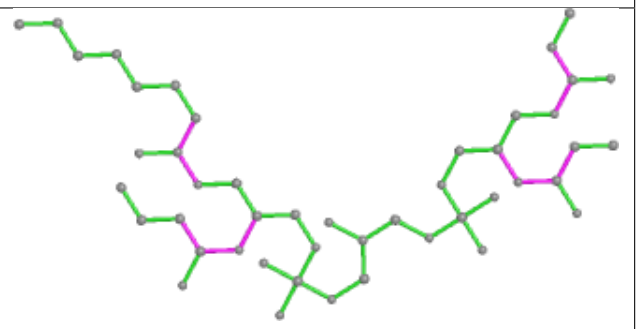


Rings

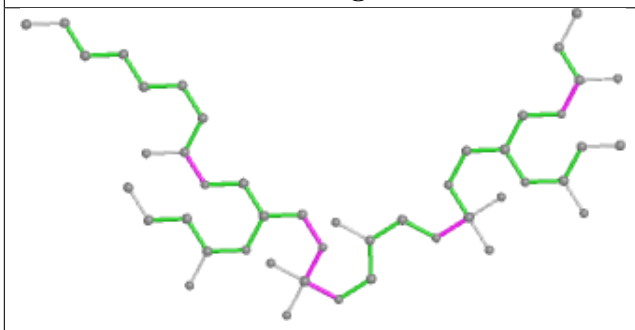
Ligand CDL Aa 501



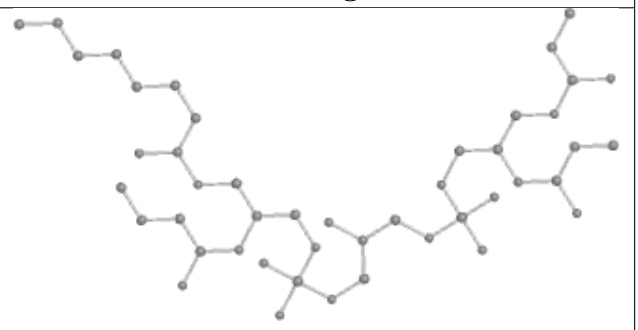
Bond lengths



Bond angles

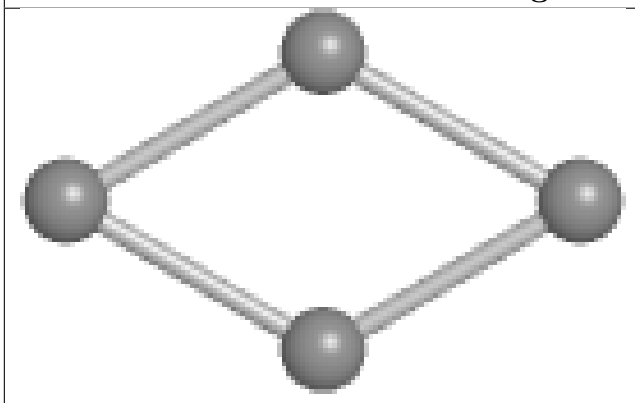


Torsions



Rings

Ligand FES E 301



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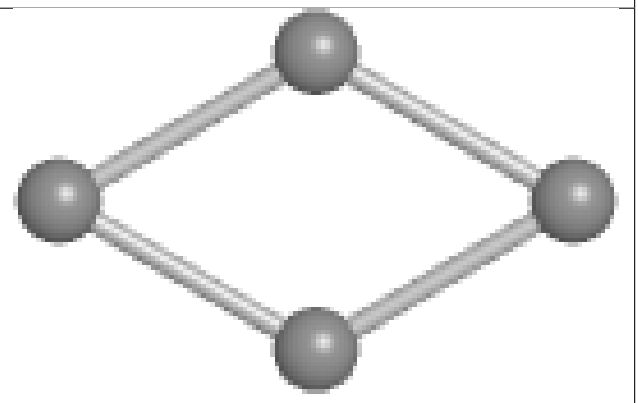
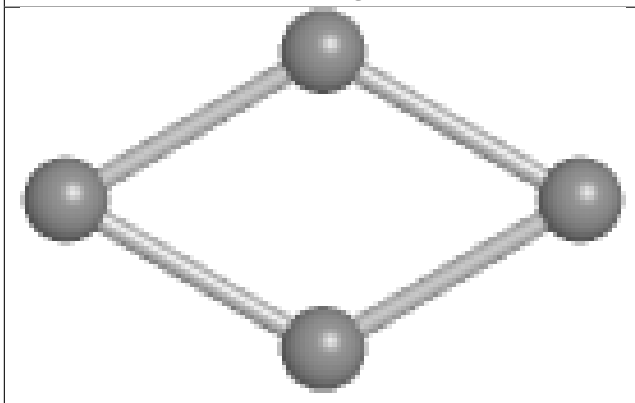
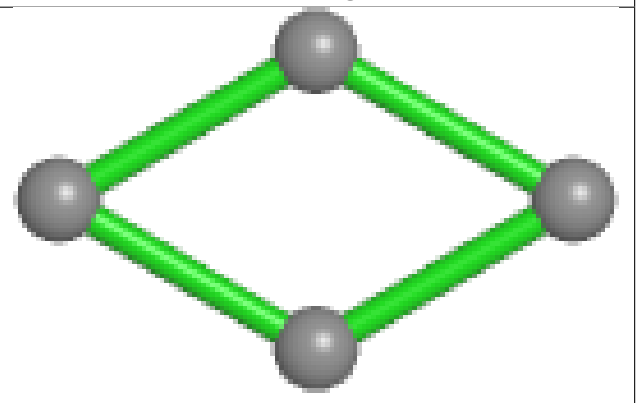


Bond angles

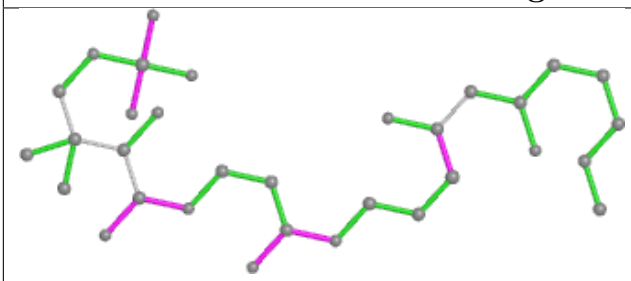


Torsions



Rings

Ligand EHZ n 201



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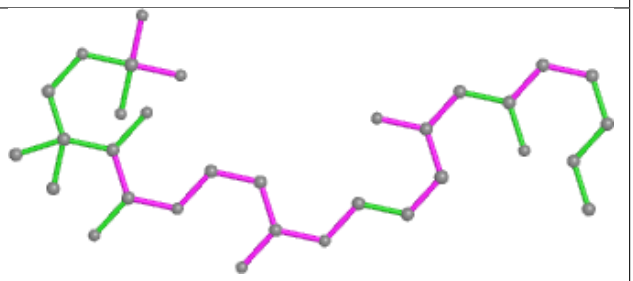
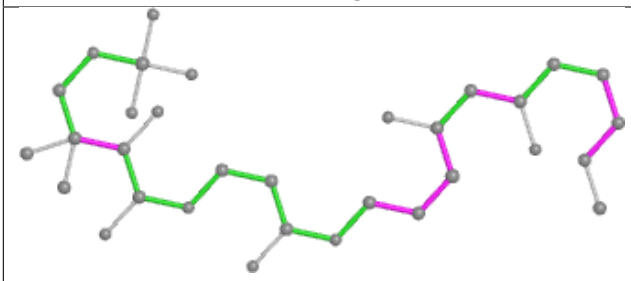
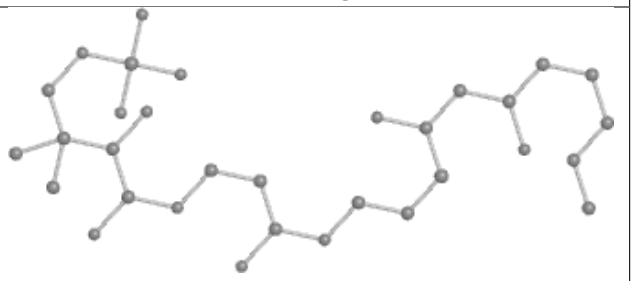


Bond angles

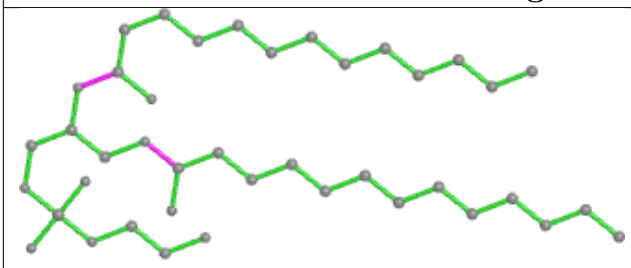


Torsions



Rings

Ligand 3PE m 202



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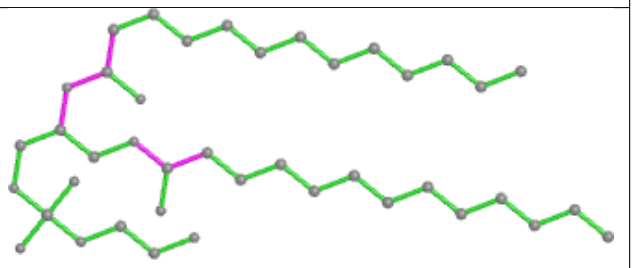
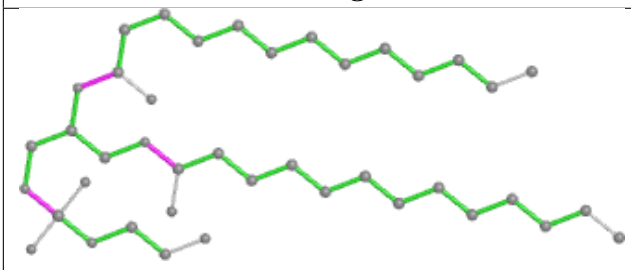


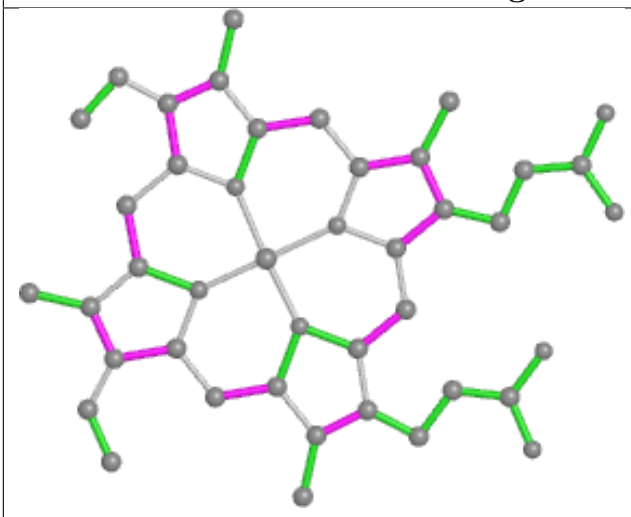
Bond angles



Torsions

Rings

Ligand HEC AD 401



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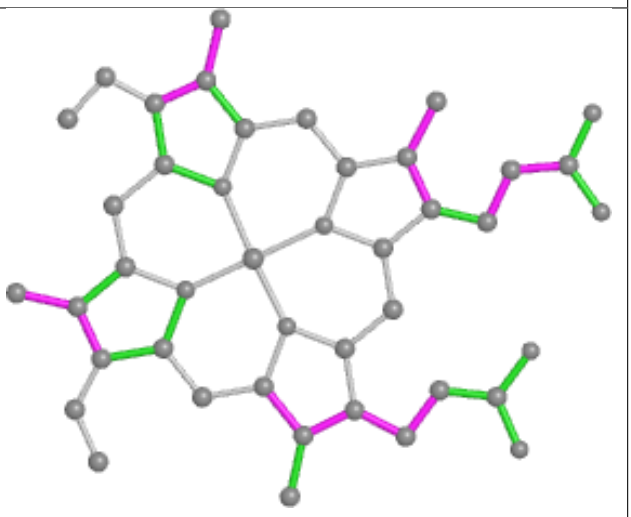
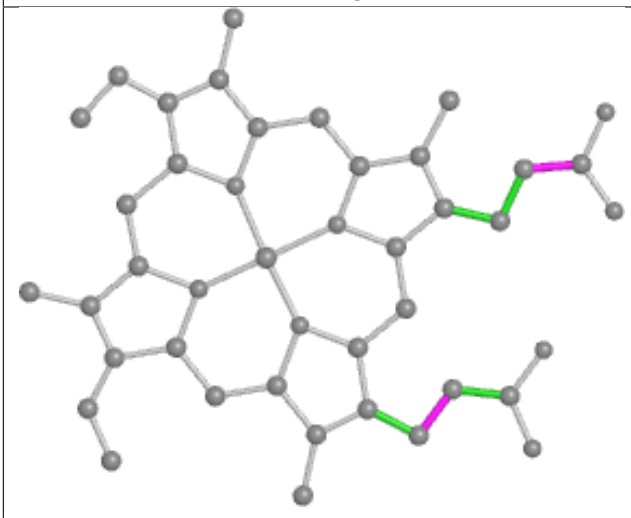


Bond angles



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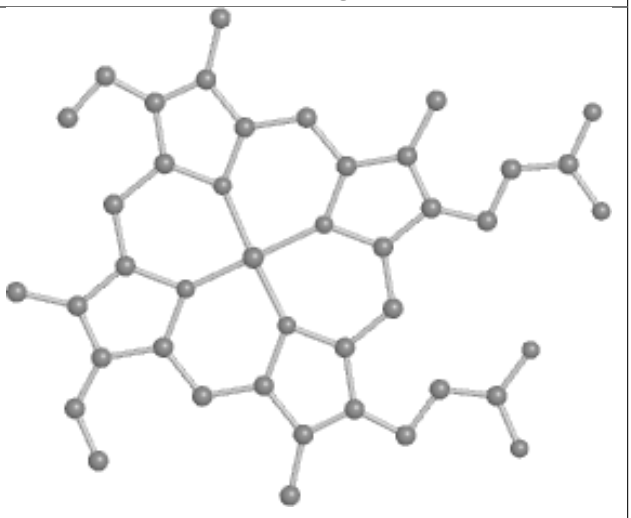
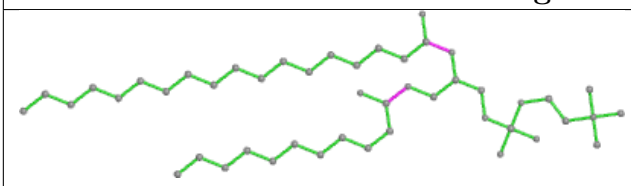


Rings

Ligand PC1 I 302



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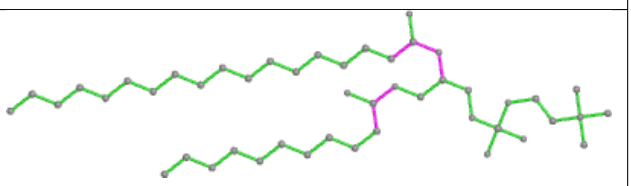
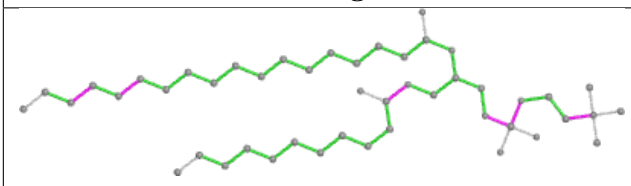
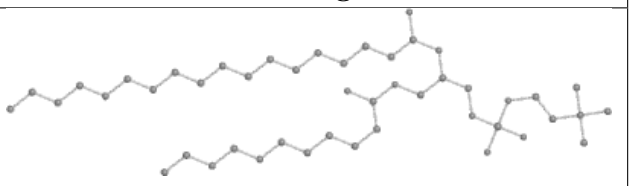


Bond angles

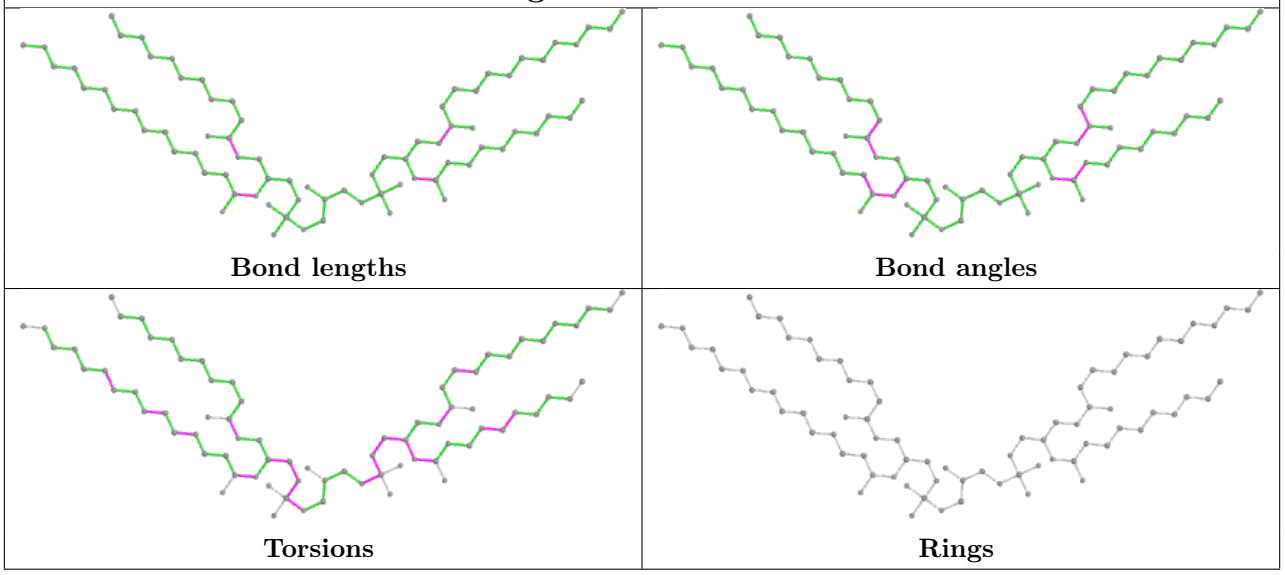


Torsions

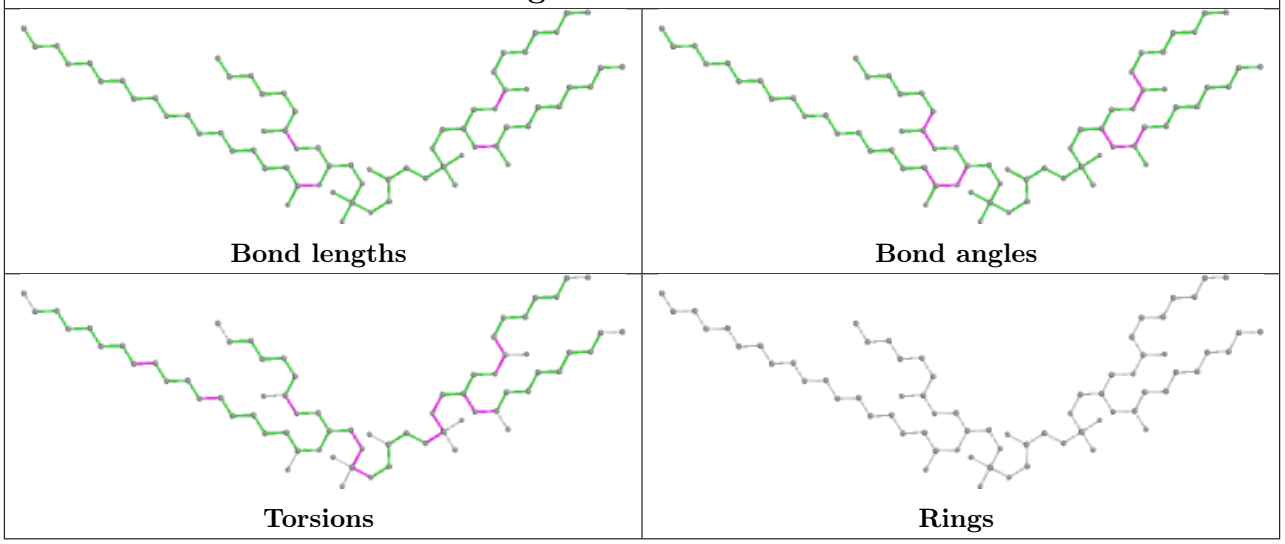


Rings

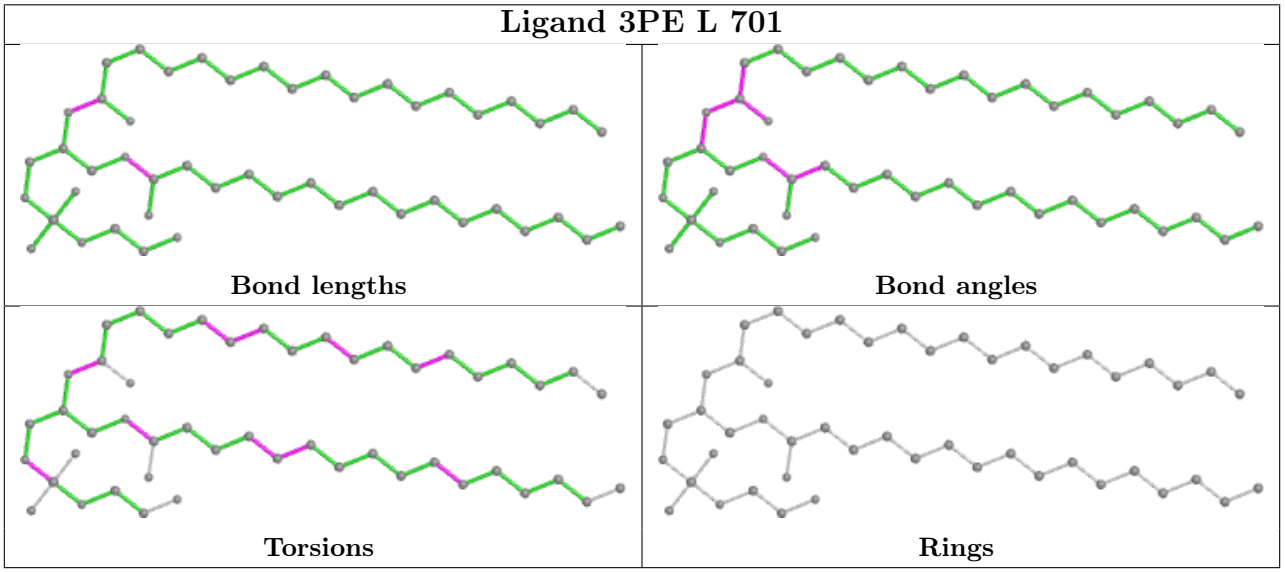
Ligand CDL L 704



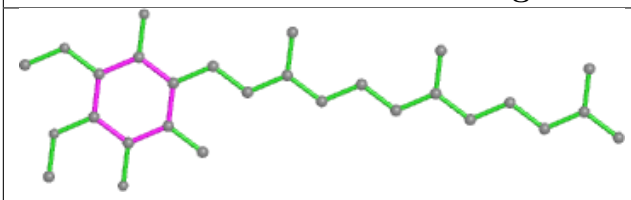
Ligand CDL h 201



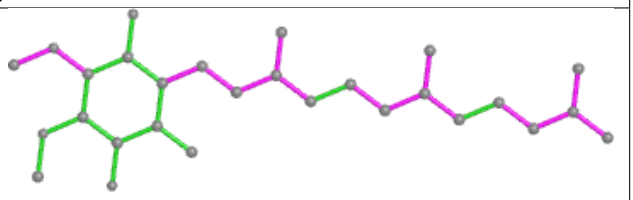
Ligand 3PE L 701



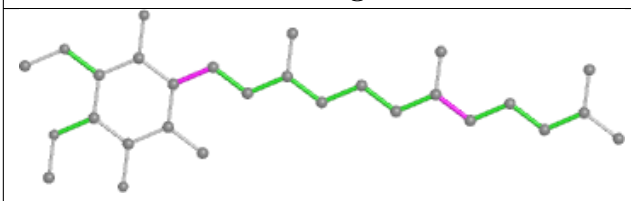
Ligand UQ6 AC 405



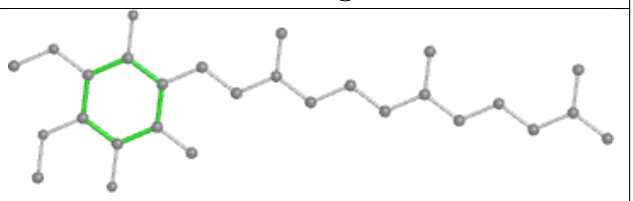
Bond lengths



Bond angles

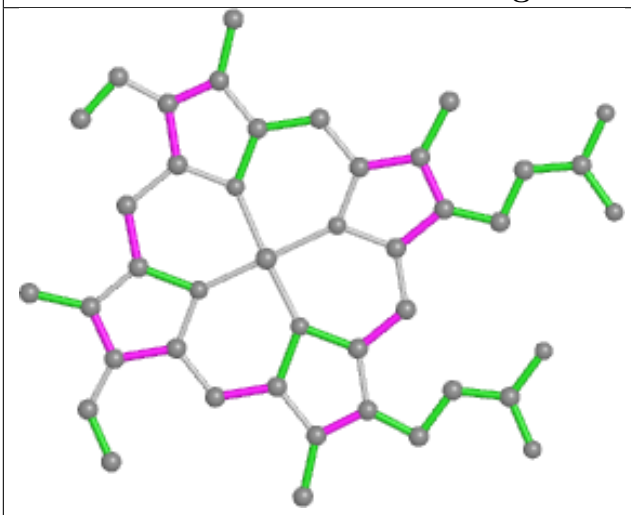


Torsions



Rings

Ligand HEC Ad 401



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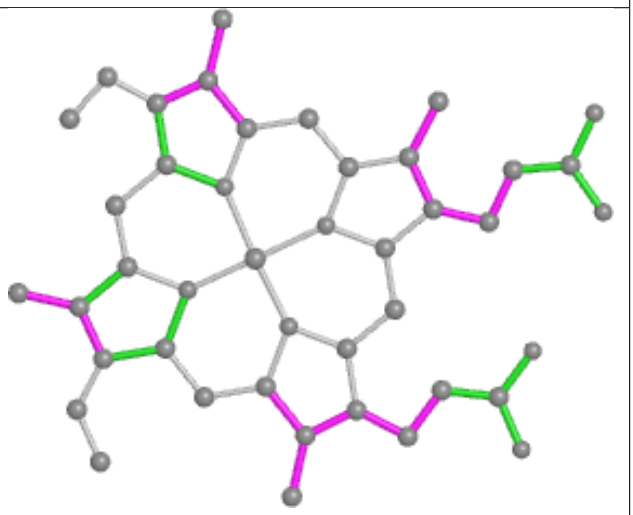
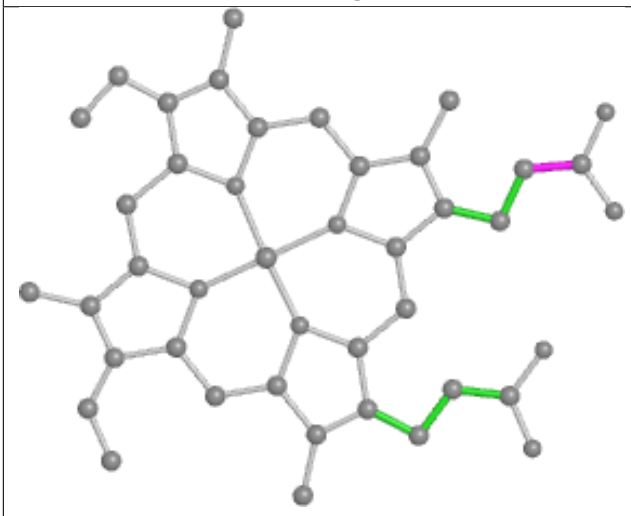
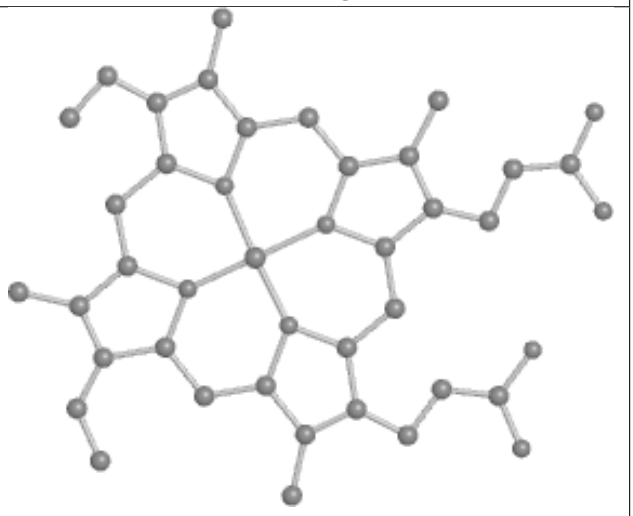


Bond angles

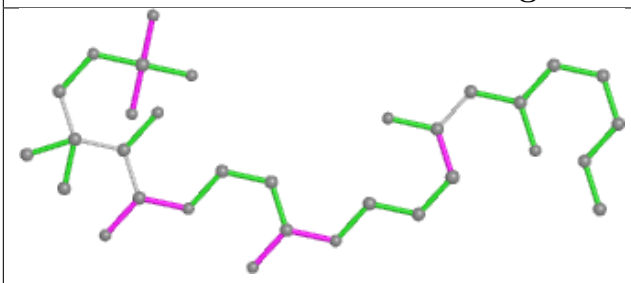


Torsions



Rings

Ligand EHZ W 201



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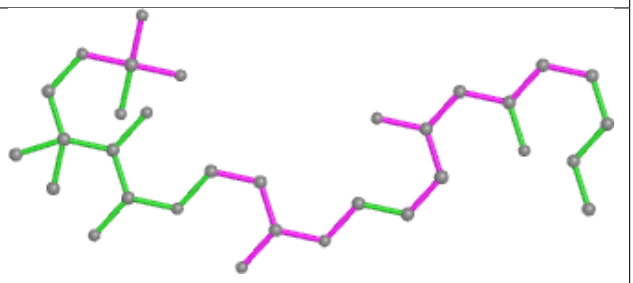
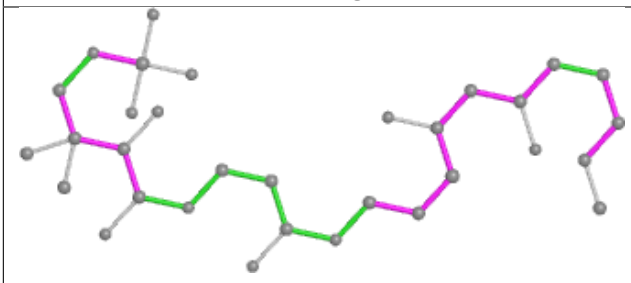


Bond angles



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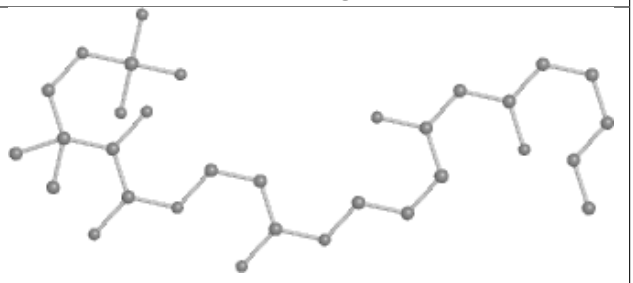
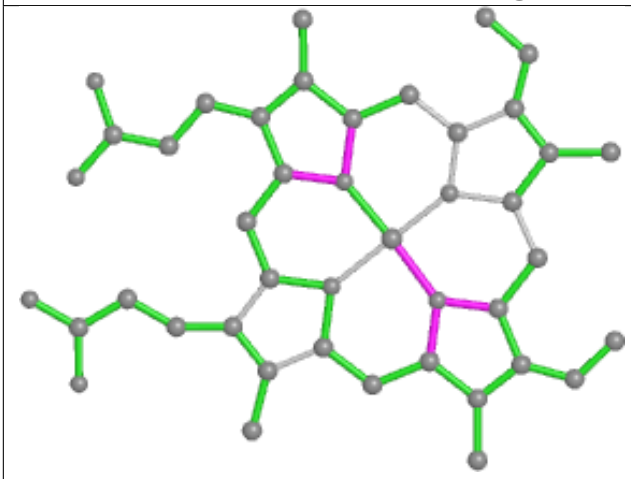


Rings

Ligand HEM Ac 401



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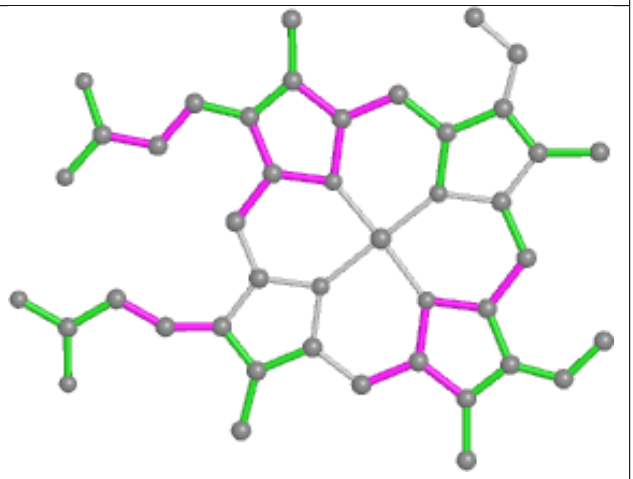
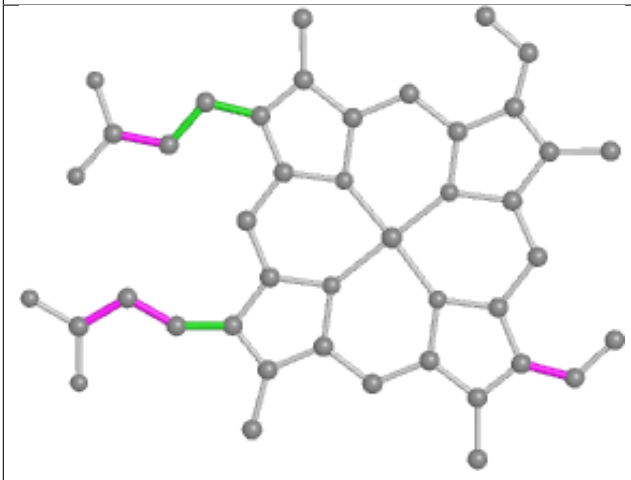


Bond angles



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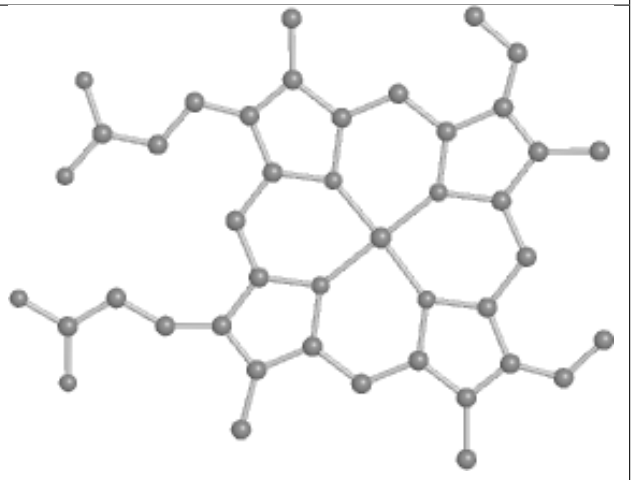
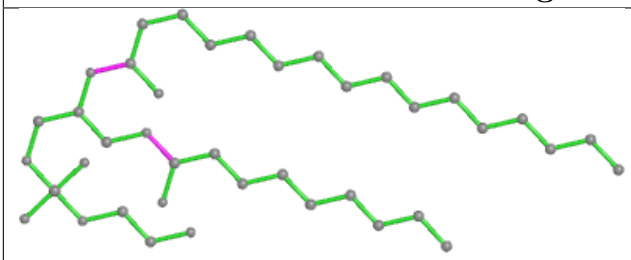


Rings

Ligand 3PE i 201



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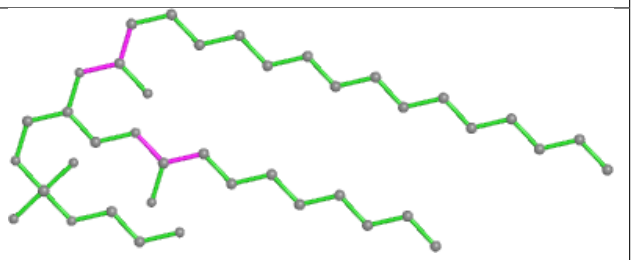
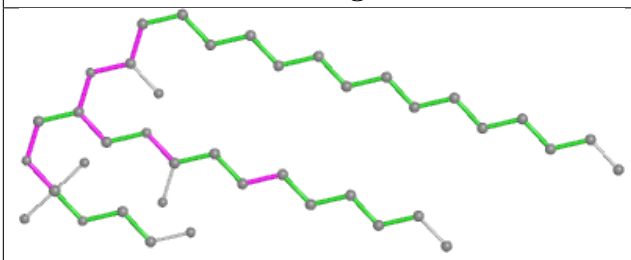
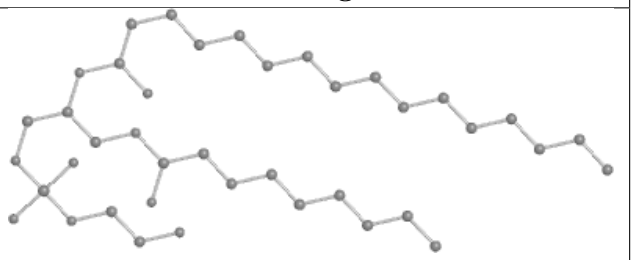


Bond angles

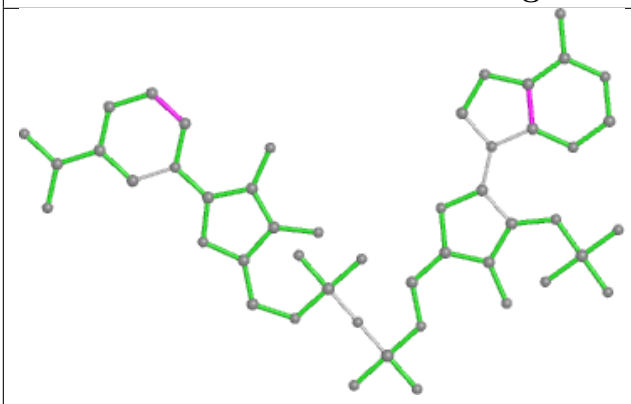


Torsions

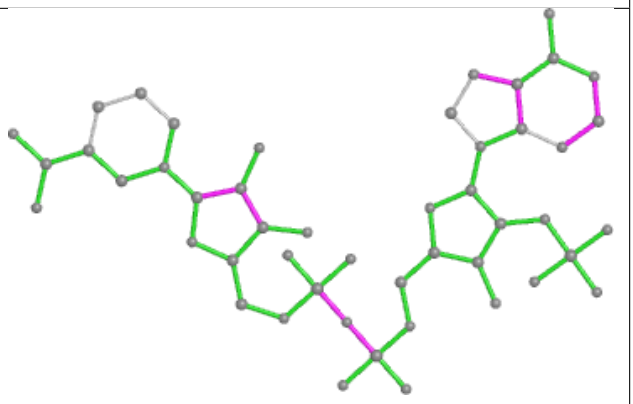


Rings

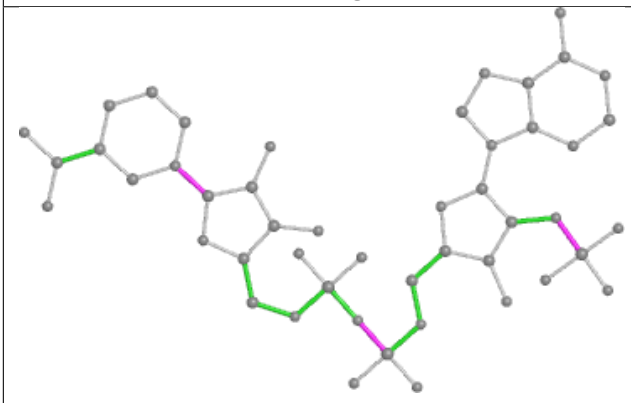
Ligand NDP P 401



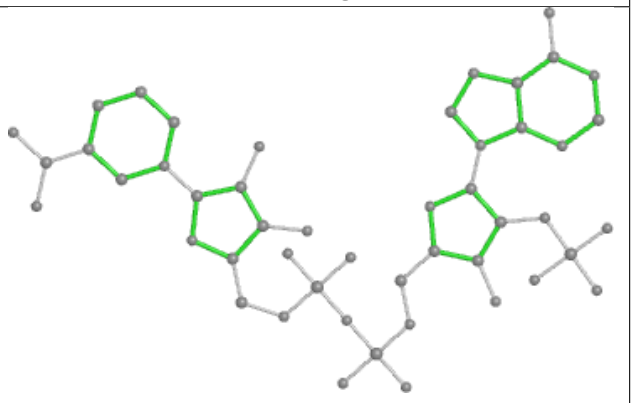
Bond lengths



Bond angles

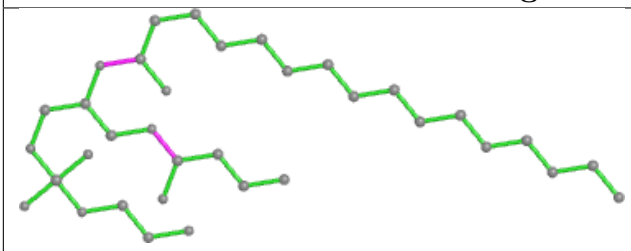


Torsions

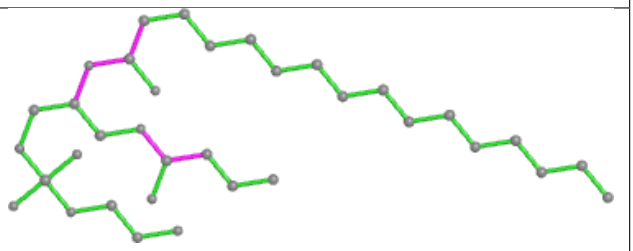


Rings

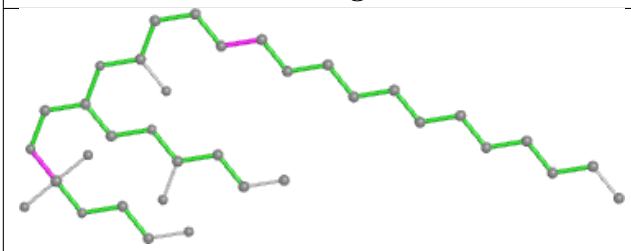
Ligand 3PE Ac 403



Bond lengths



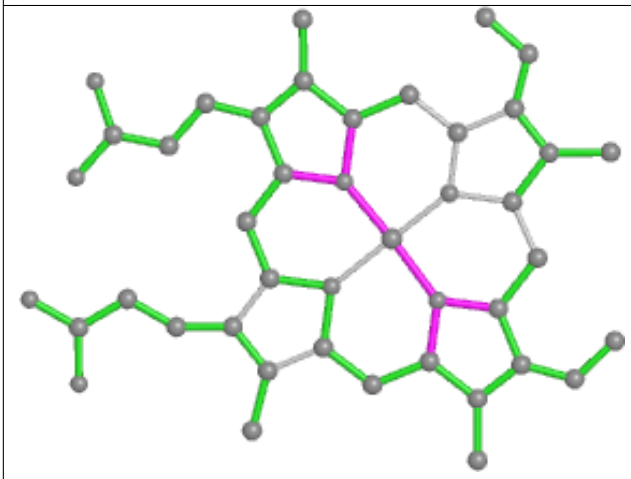
Bond angles



Torsions

Rings

Ligand HEM AC 401



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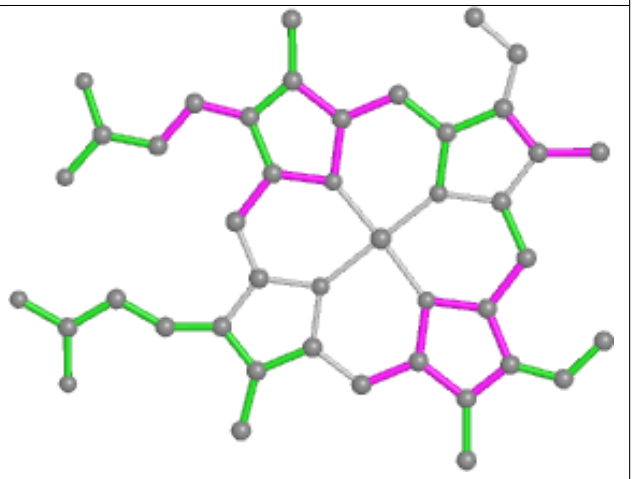
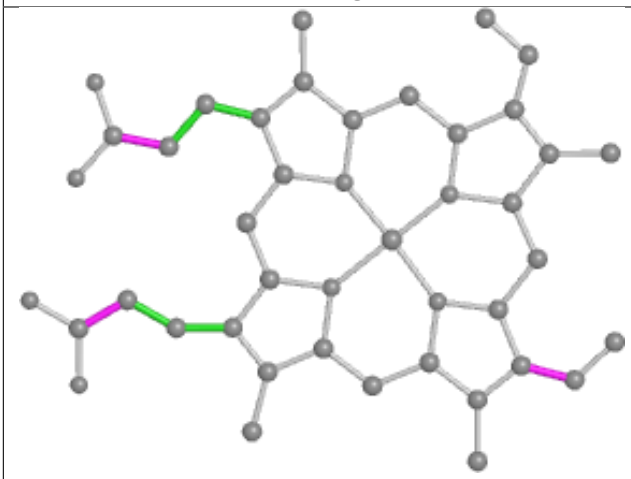
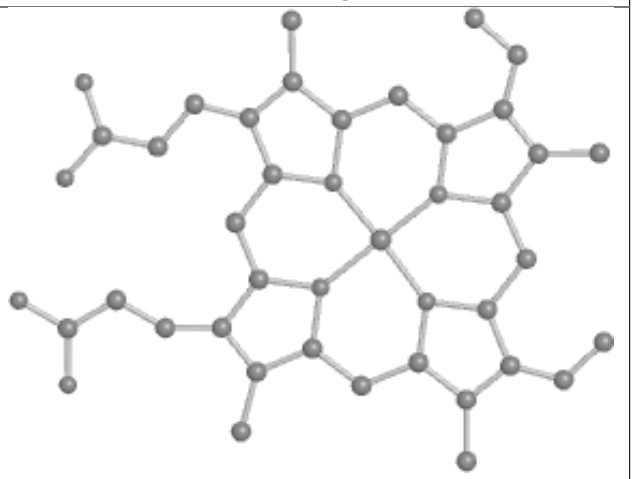


Bond angles

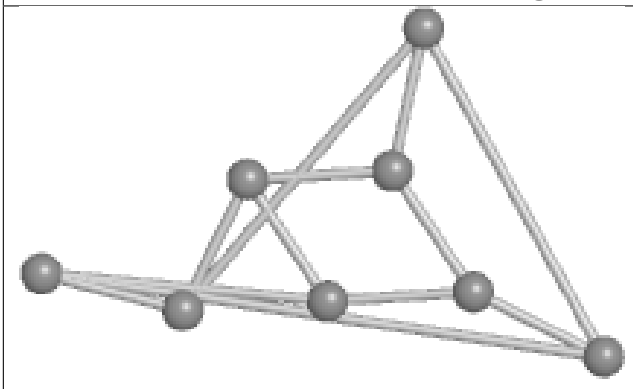


Torsions

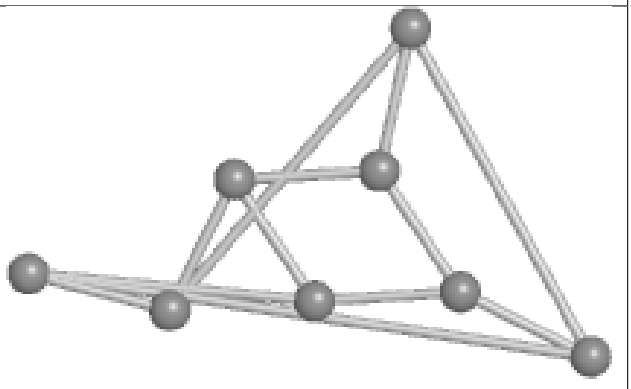


Rings

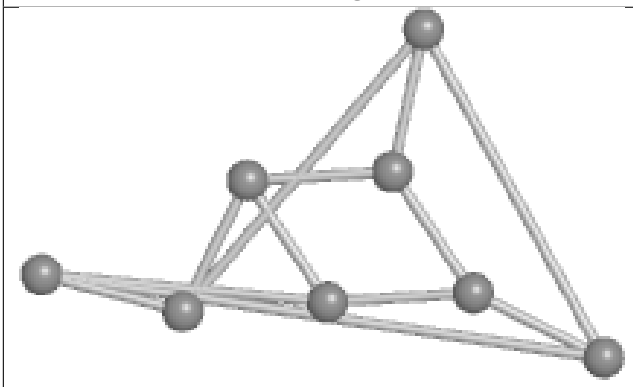
Ligand SF4 G 801



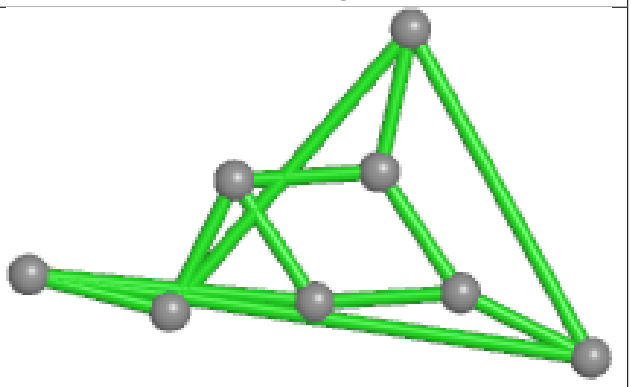
Bond lengths



Bond angles

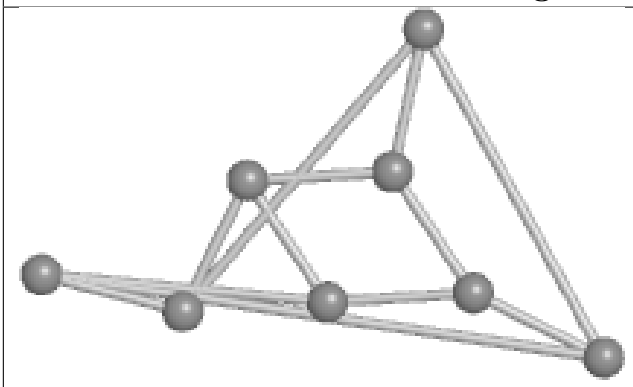


Torsions

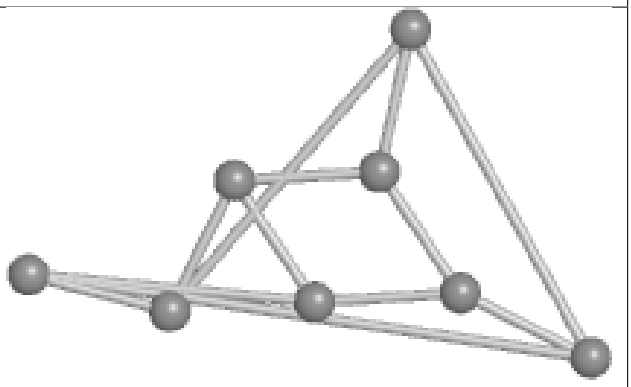


Rings

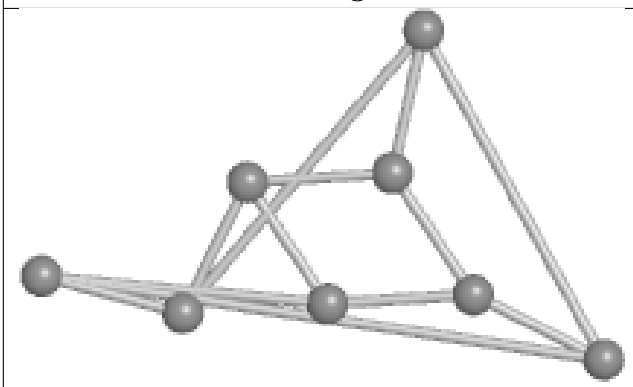
Ligand SF4 F 502



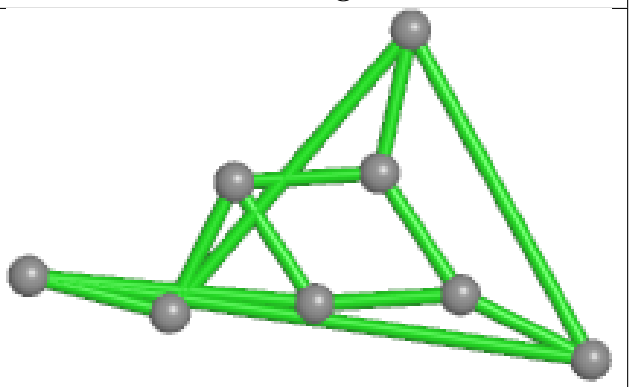
Bond lengths



Bond angles

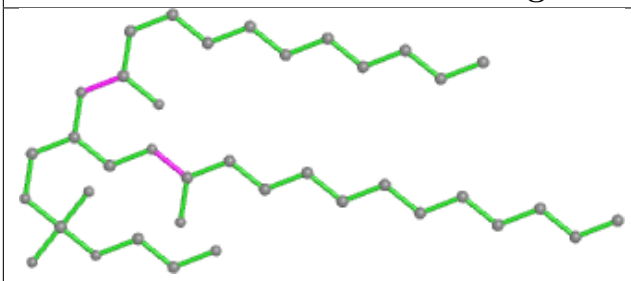


Torsions

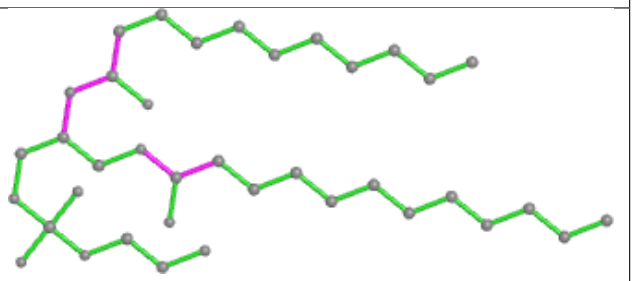


Rings

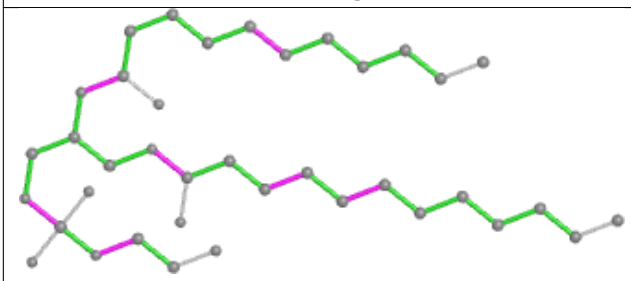
Ligand 3PE D 501



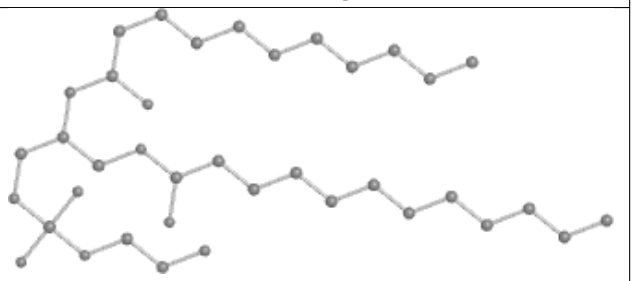
Bond lengths



Bond angles

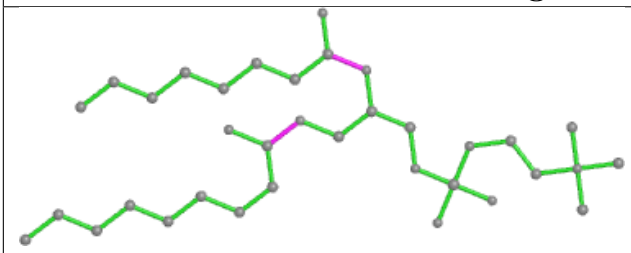


Torsions

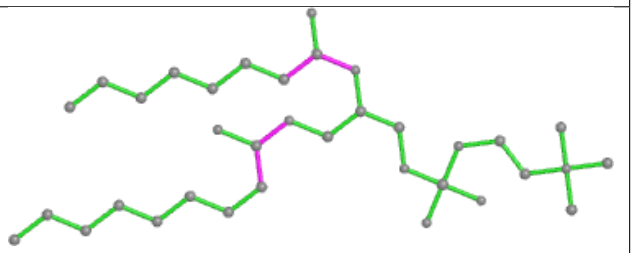


Rings

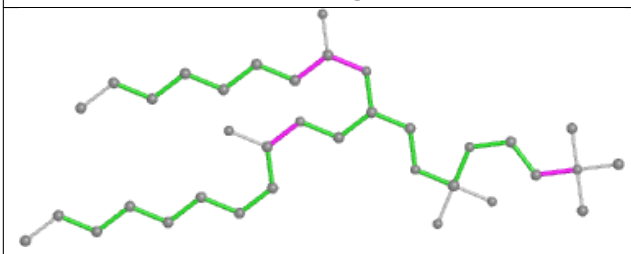
Ligand PC1 B 303



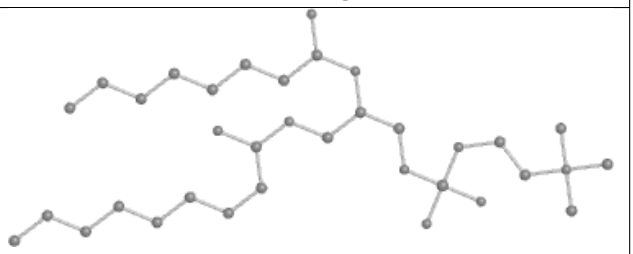
Bond lengths



Bond angles

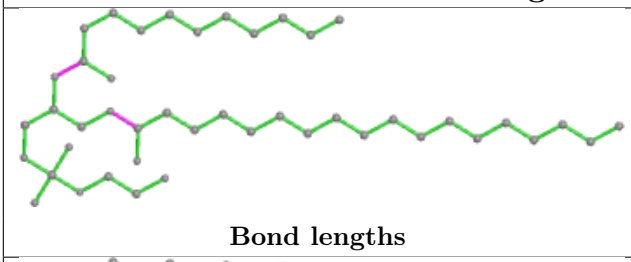


Torsions



Rings

Ligand 3PE O 401



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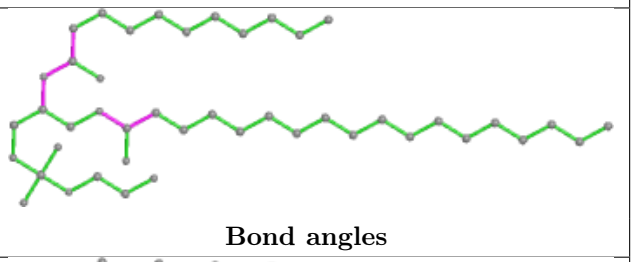
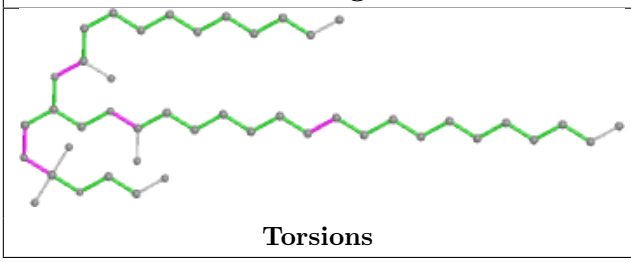
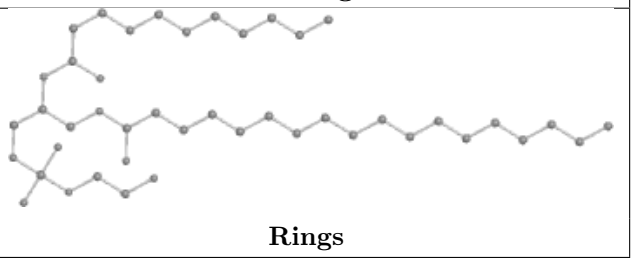


Bond angles

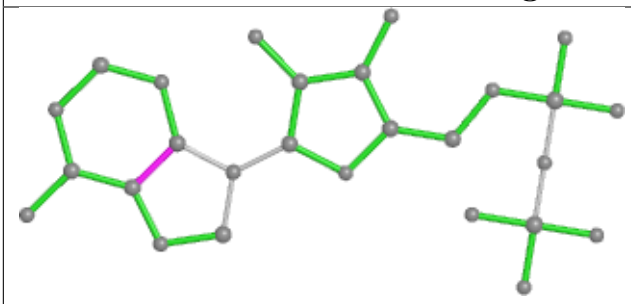


Torsions

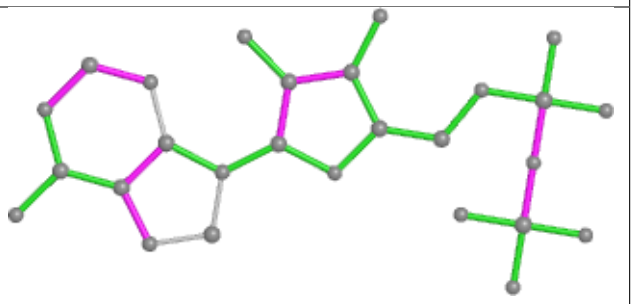


Rings

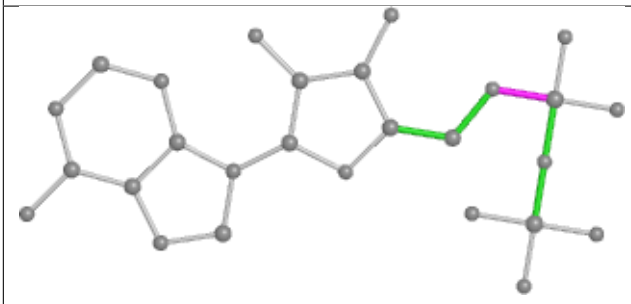
Ligand ADP O 402



Bond lengths



Bond angles



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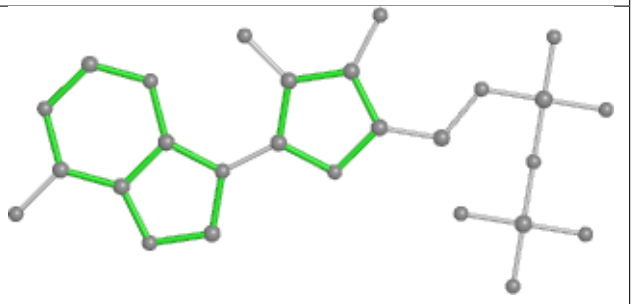
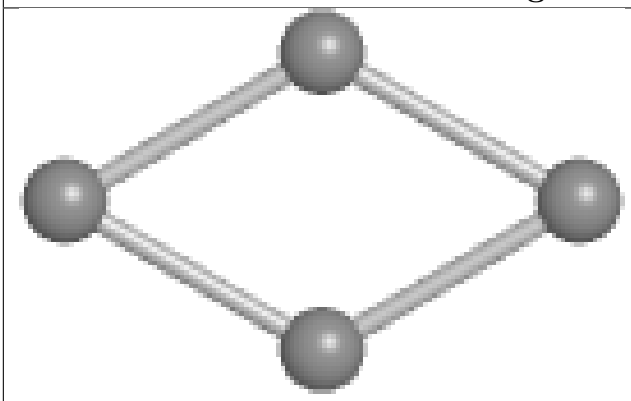
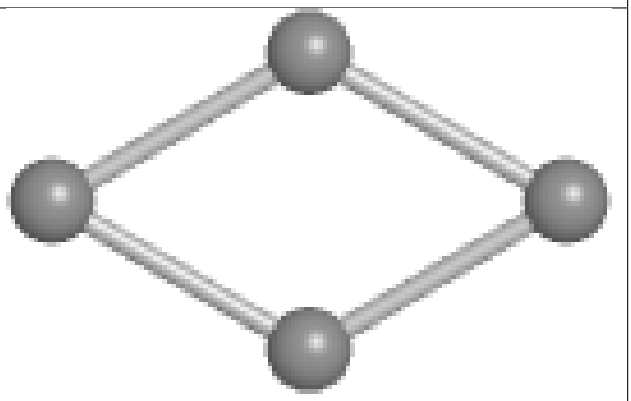


Rings

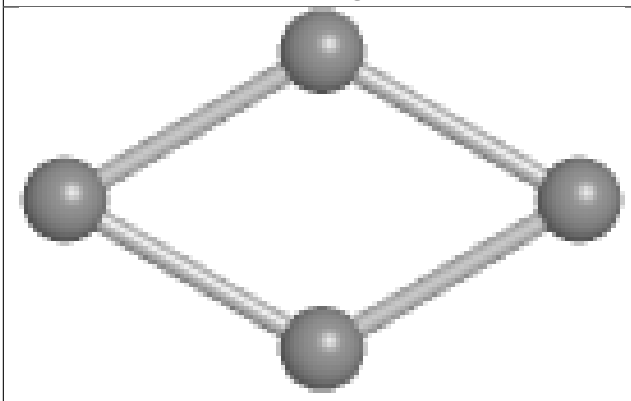
Ligand FES G 803



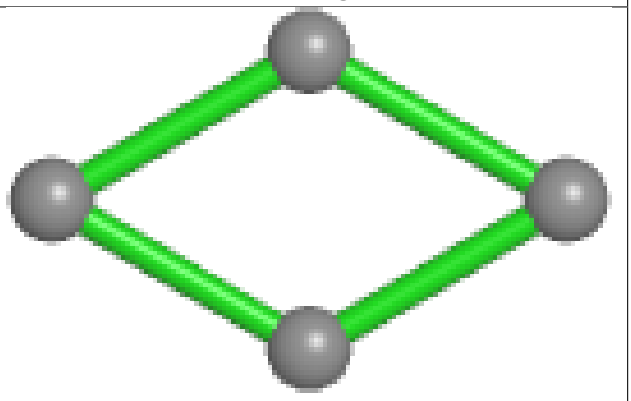
Bond lengths



Bond angles

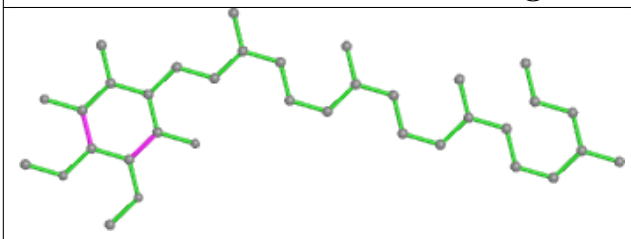


Torsions

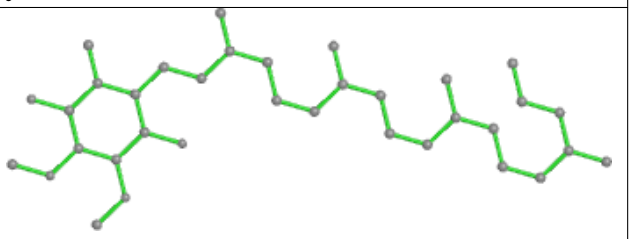


Rings

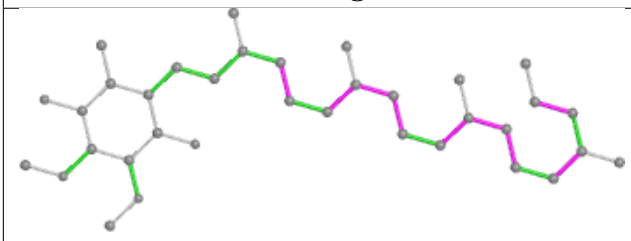
Ligand UQ9 H 400



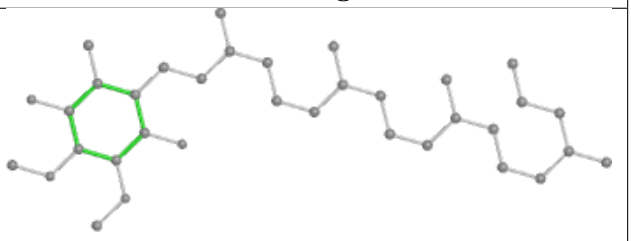
Bond lengths



Bond angles

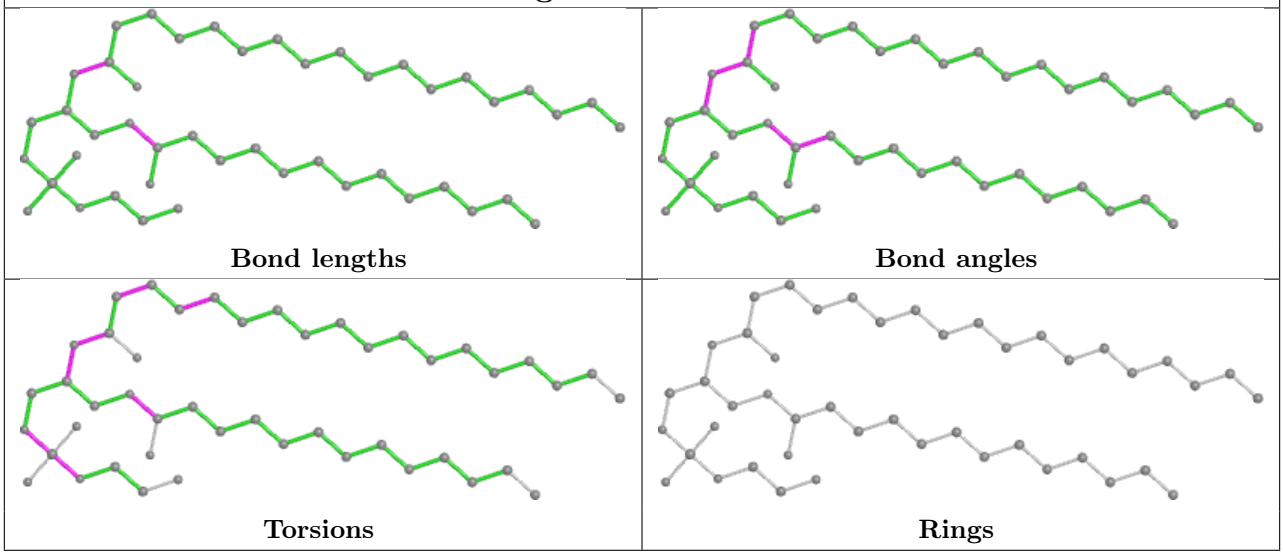


Torsions

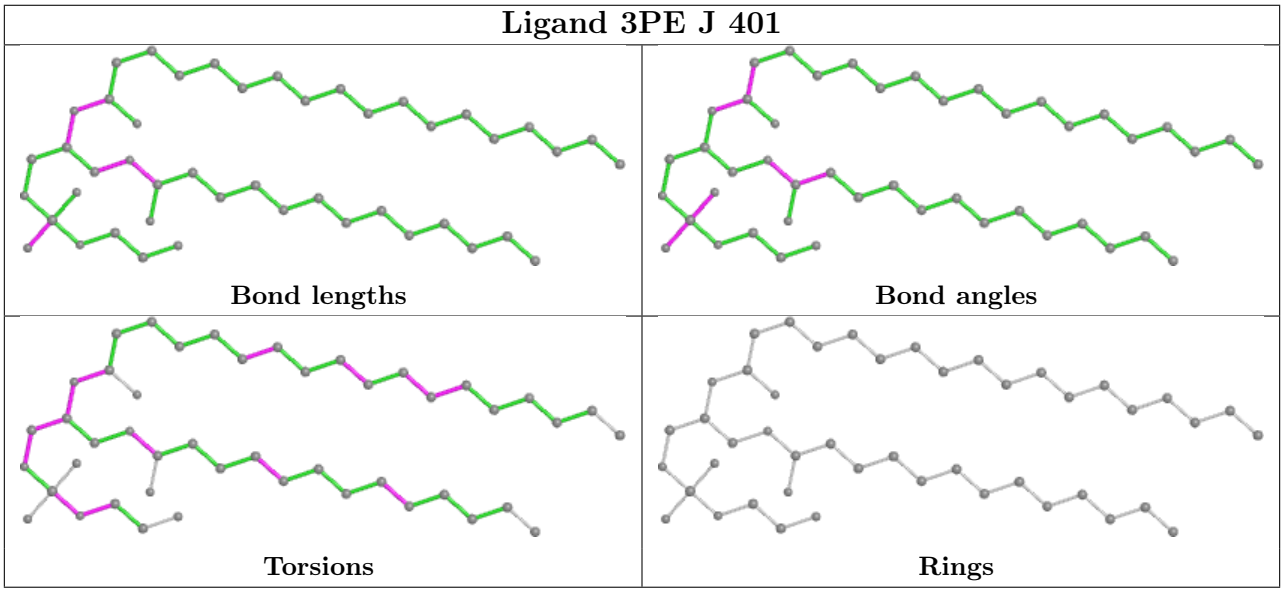


Rings

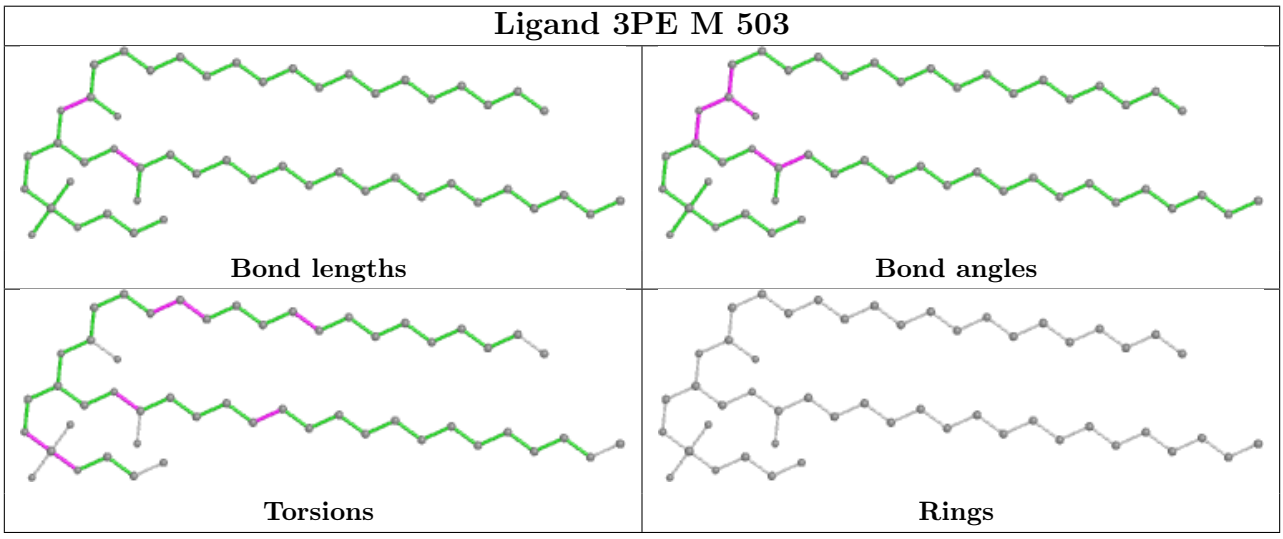
Ligand 3PE I 301

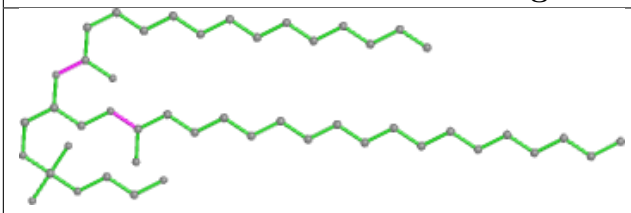
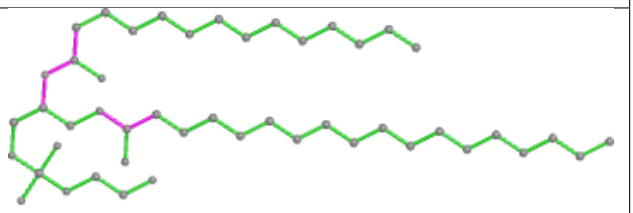
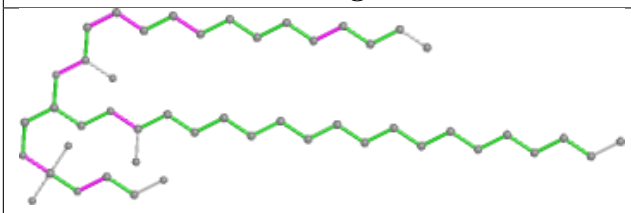
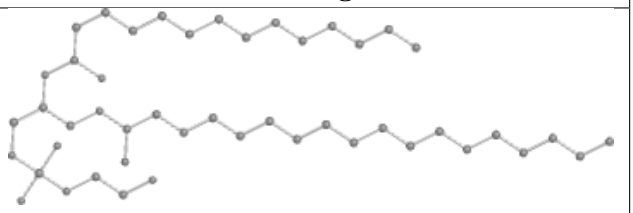


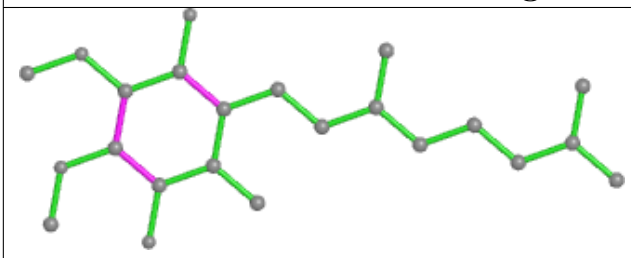
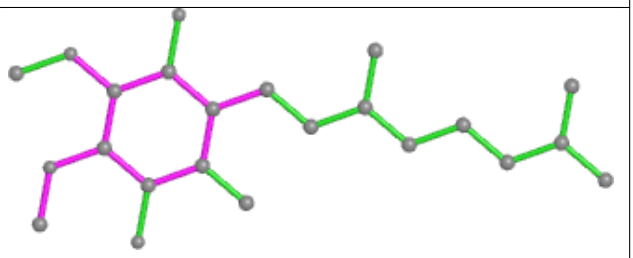
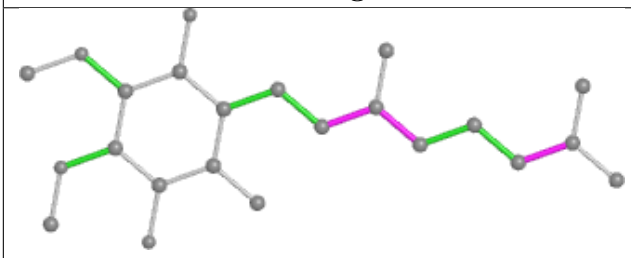
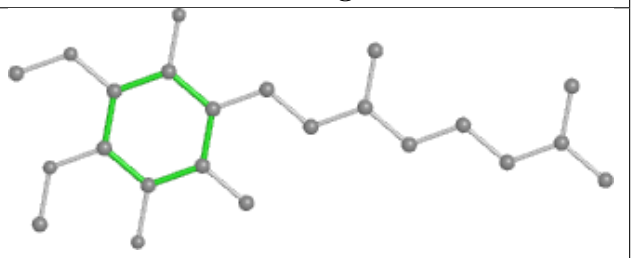
Ligand 3PE J 401



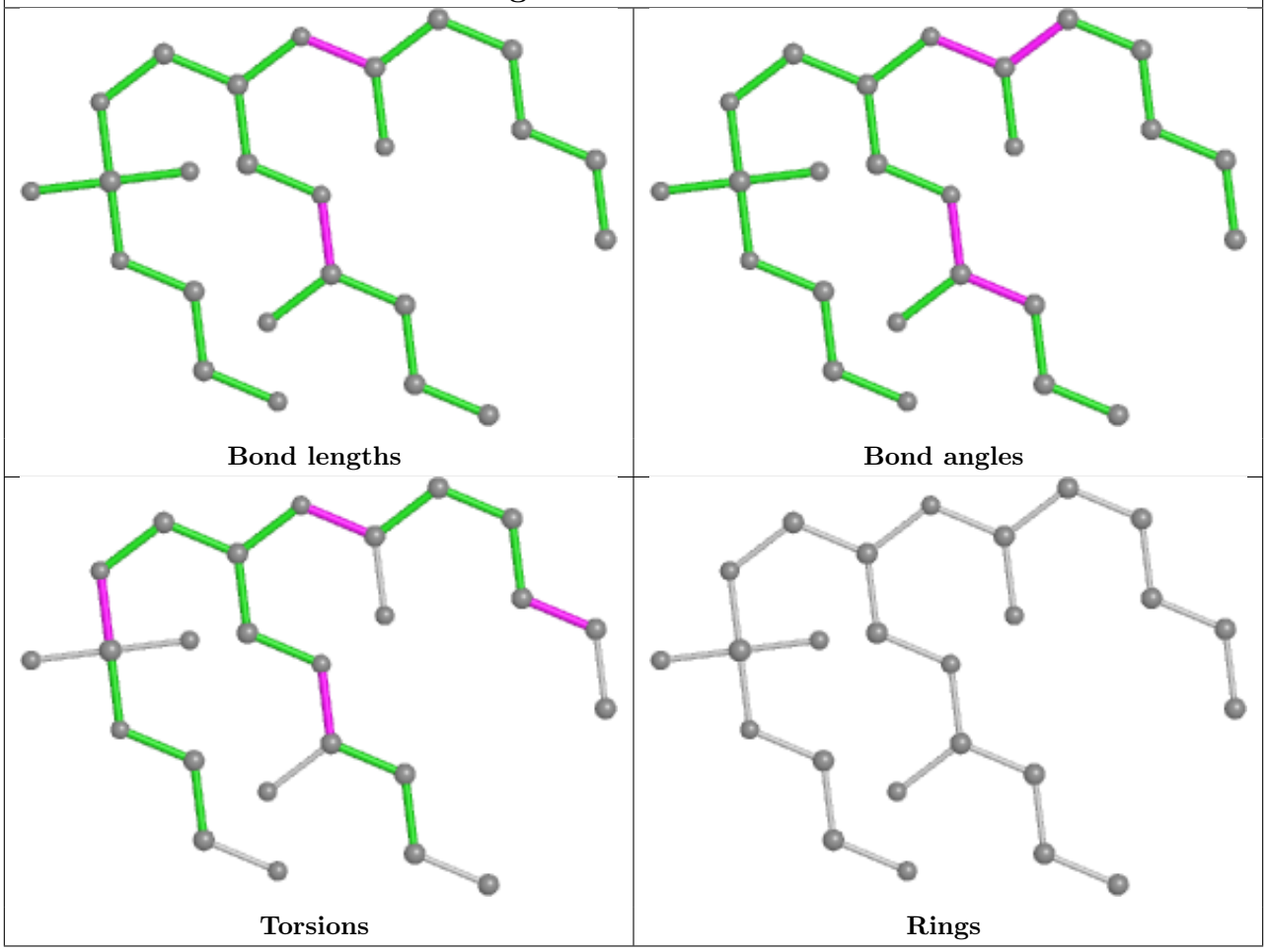
Ligand 3PE M 503



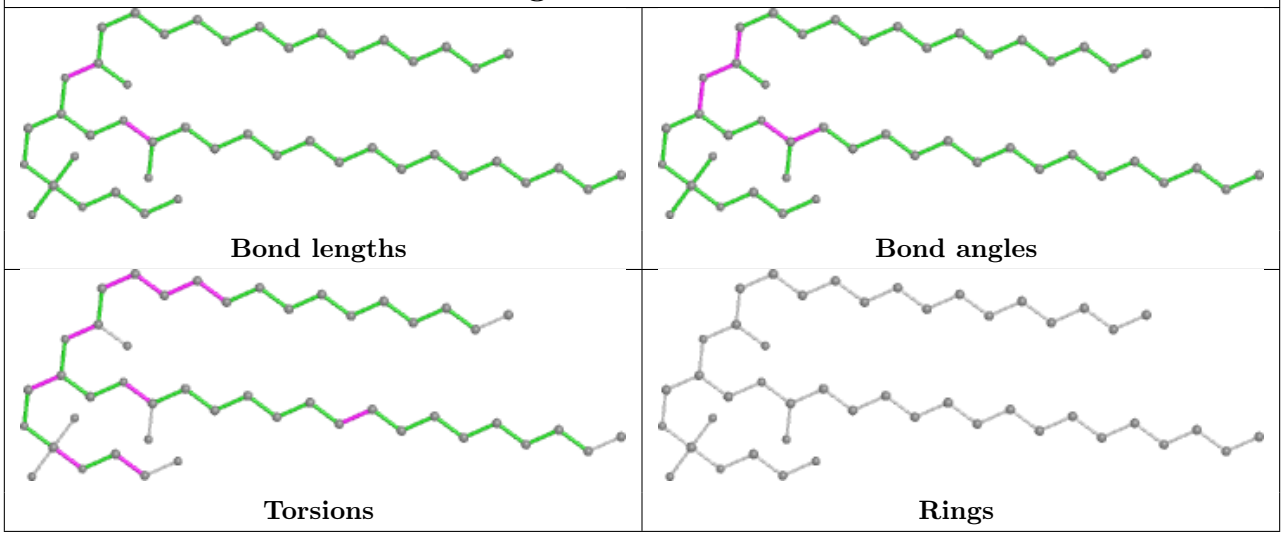
Ligand 3PE L 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

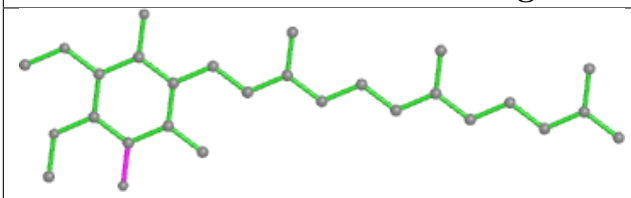
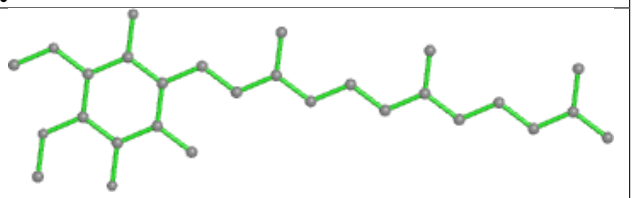
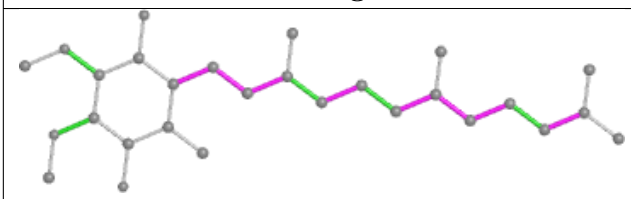
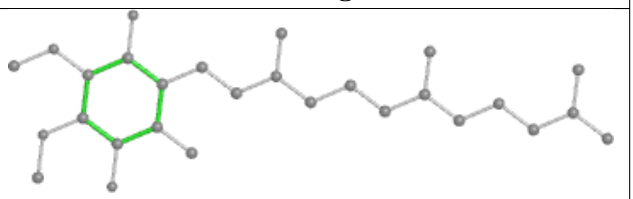
Ligand U10 Ac 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE AC 403



Ligand 3PE K 101



Ligand UQ6 Ac 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

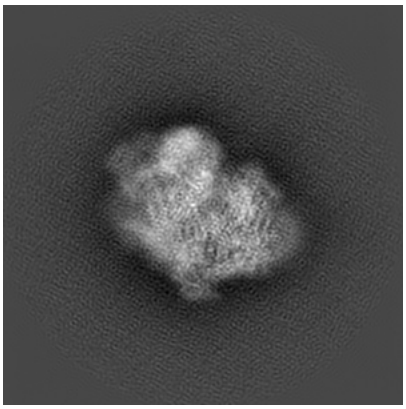
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35336. These allow visual inspection of the internal detail of the map and identification of artifacts.

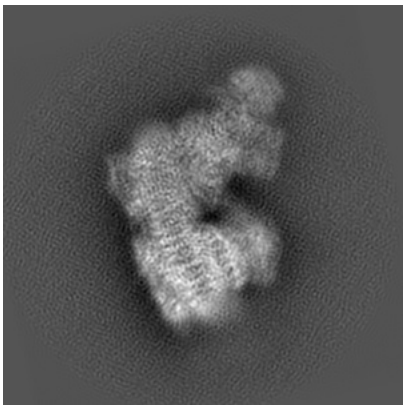
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

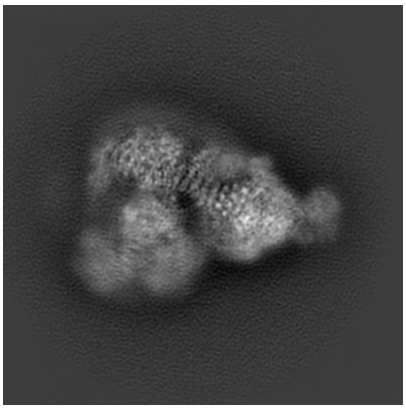
6.1.1 Primary map



X

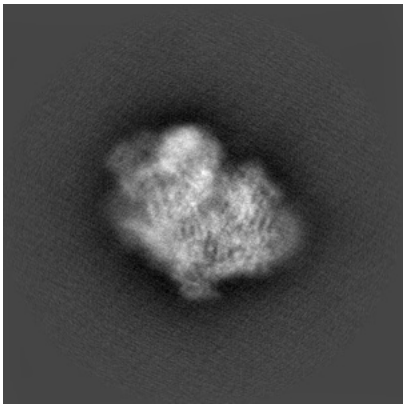


Y

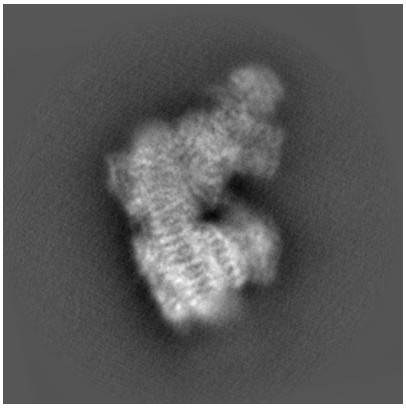


Z

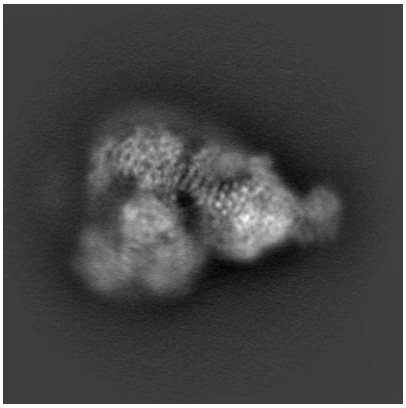
6.1.2 Raw map



X



Y

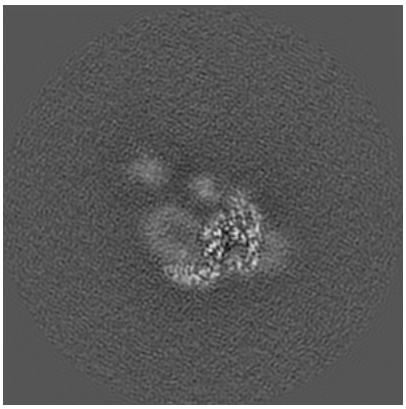


Z

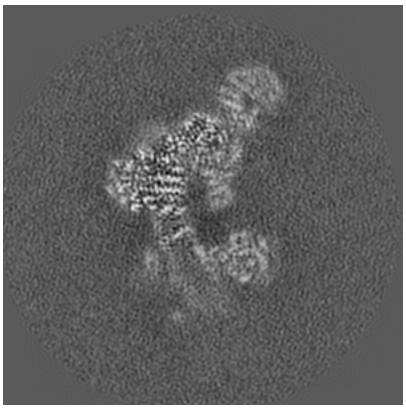
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

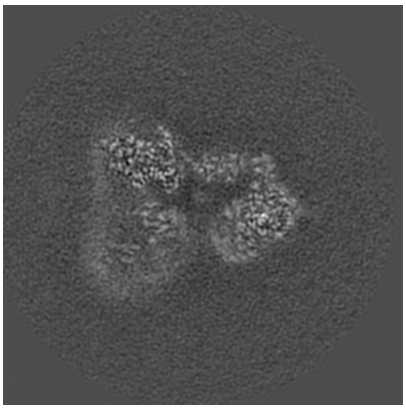
6.2.1 Primary map



X Index: 192

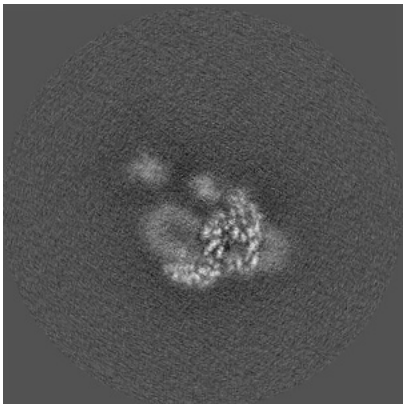


Y Index: 192

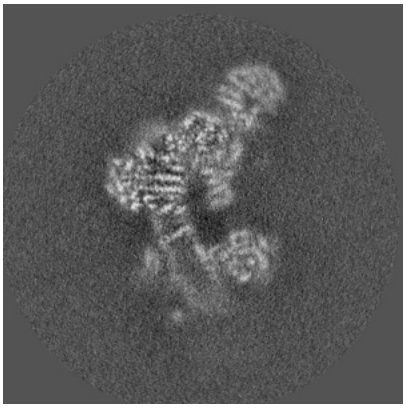


Z Index: 192

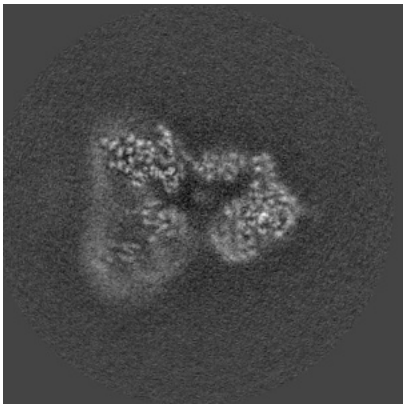
6.2.2 Raw map



X Index: 192



Y Index: 192

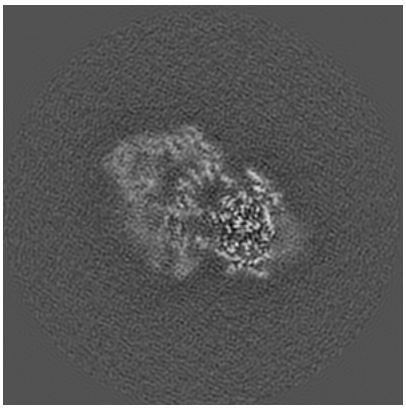


Z Index: 192

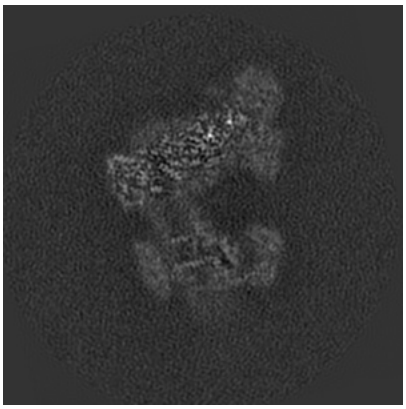
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

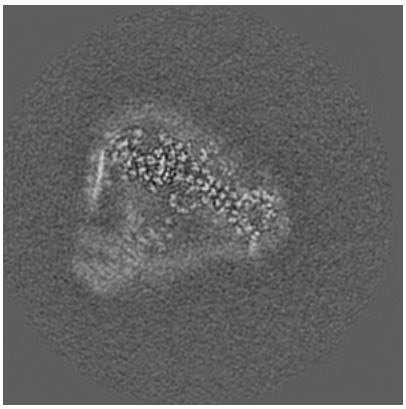
6.3.1 Primary map



X Index: 154

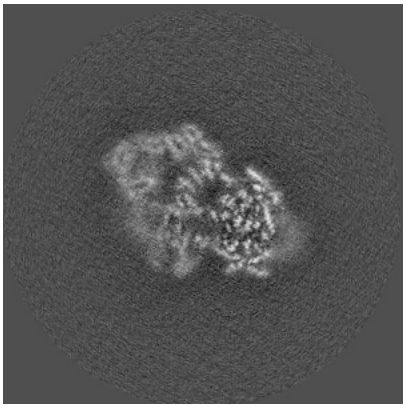


Y Index: 177

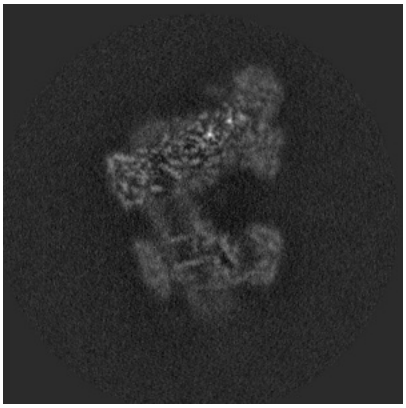


Z Index: 167

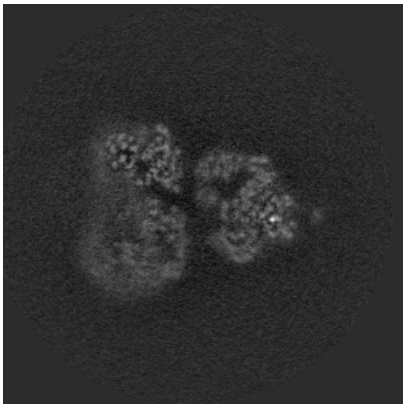
6.3.2 Raw map



X Index: 154



Y Index: 177

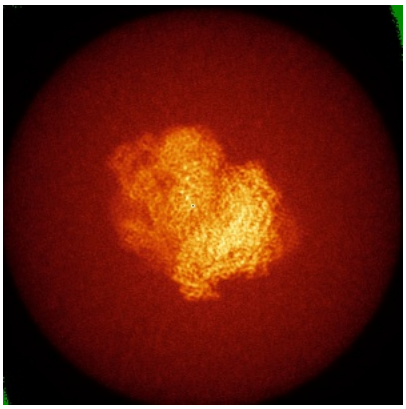


Z Index: 198

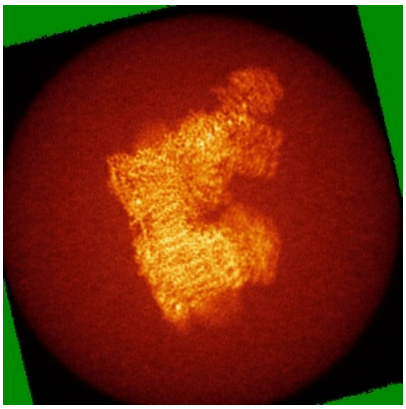
The images above show the largest variance slices of the map in three orthogonal directions.

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

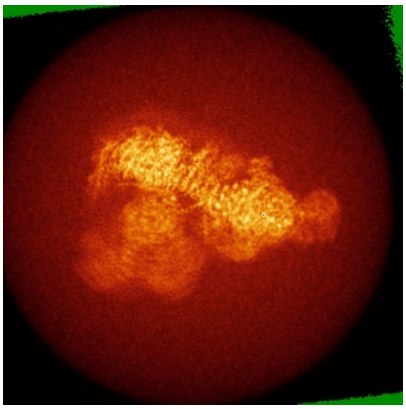
6.4.1 Primary map



X

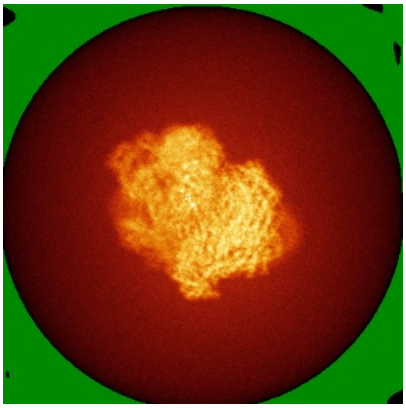


Y

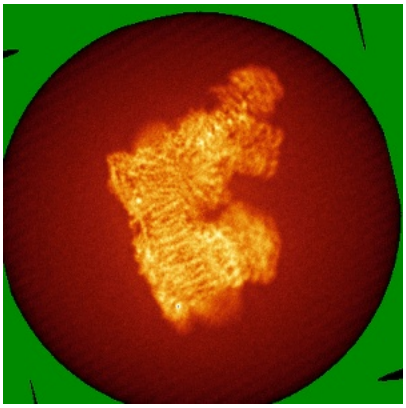


Z

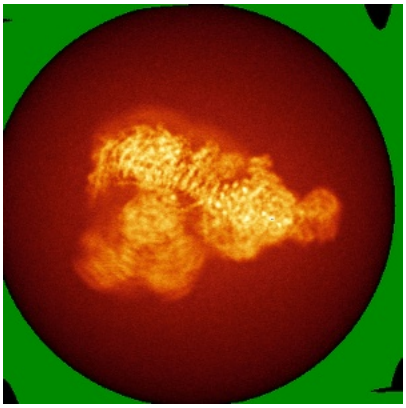
6.4.2 Raw map



X



Y



Z

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

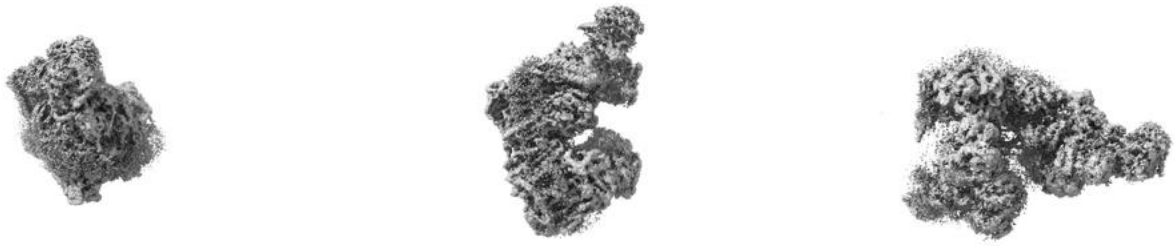
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

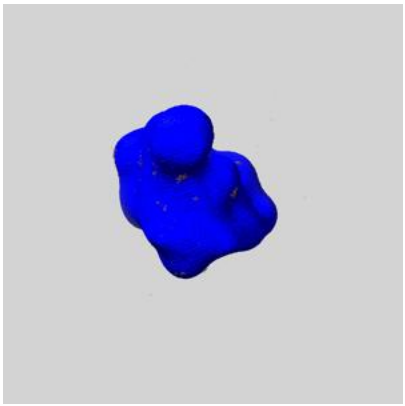
6.6 Mask visualisation (i)

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

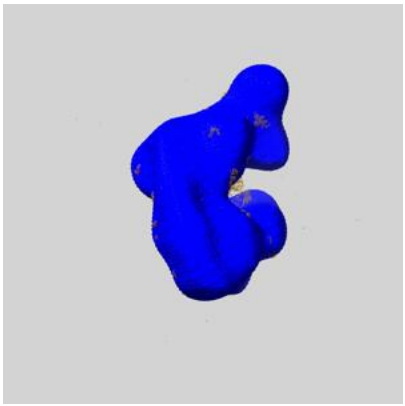
A mask typically either:

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

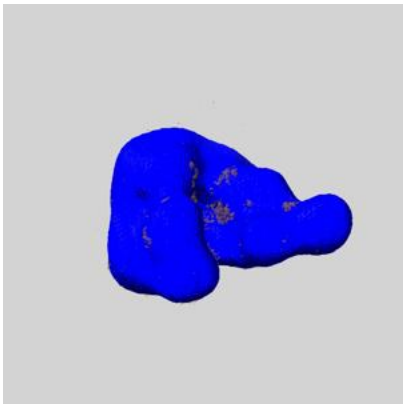
6.6.1 emd_35336_msk_1.map (i)



X



Y

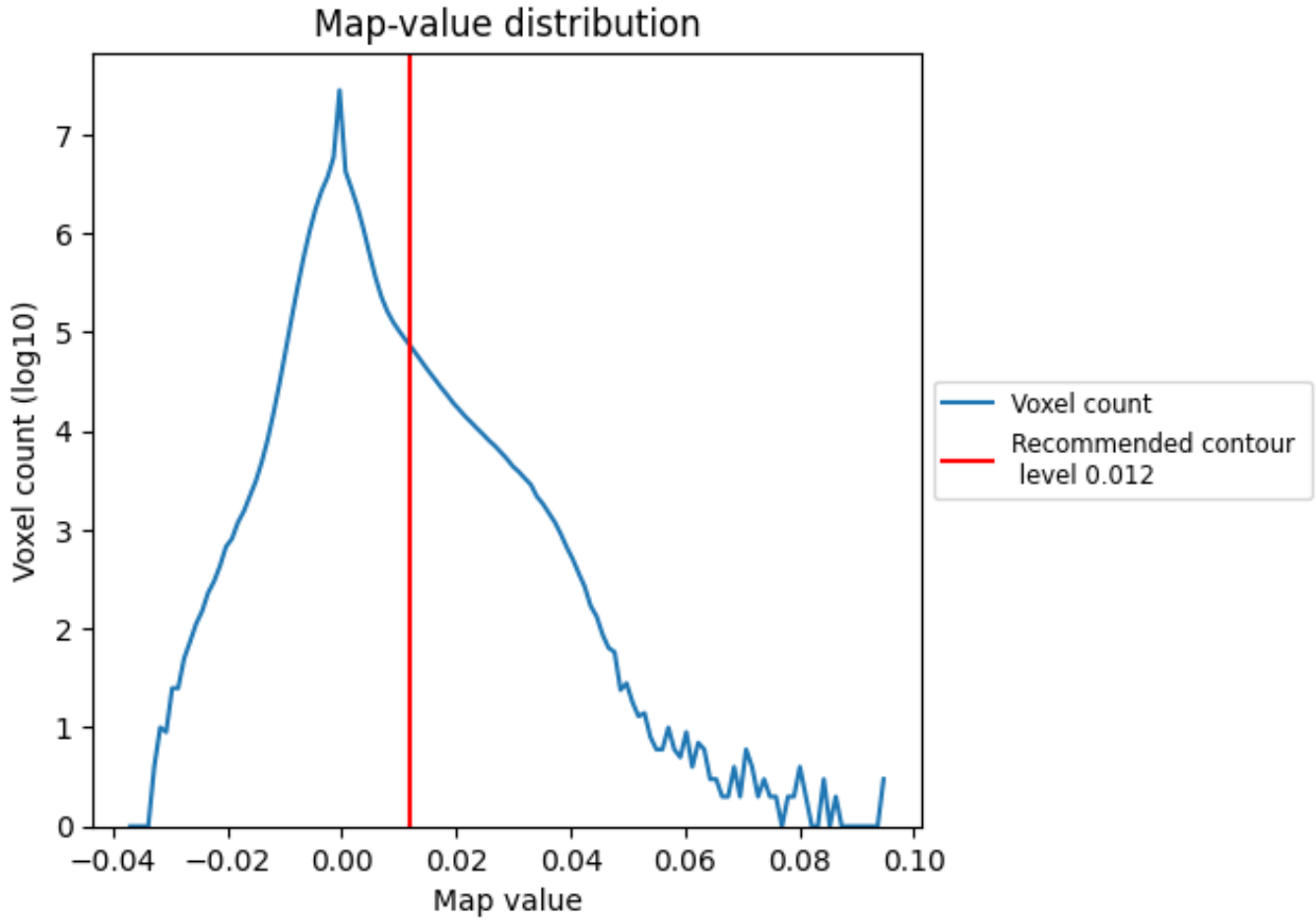


Z

7 Map analysis

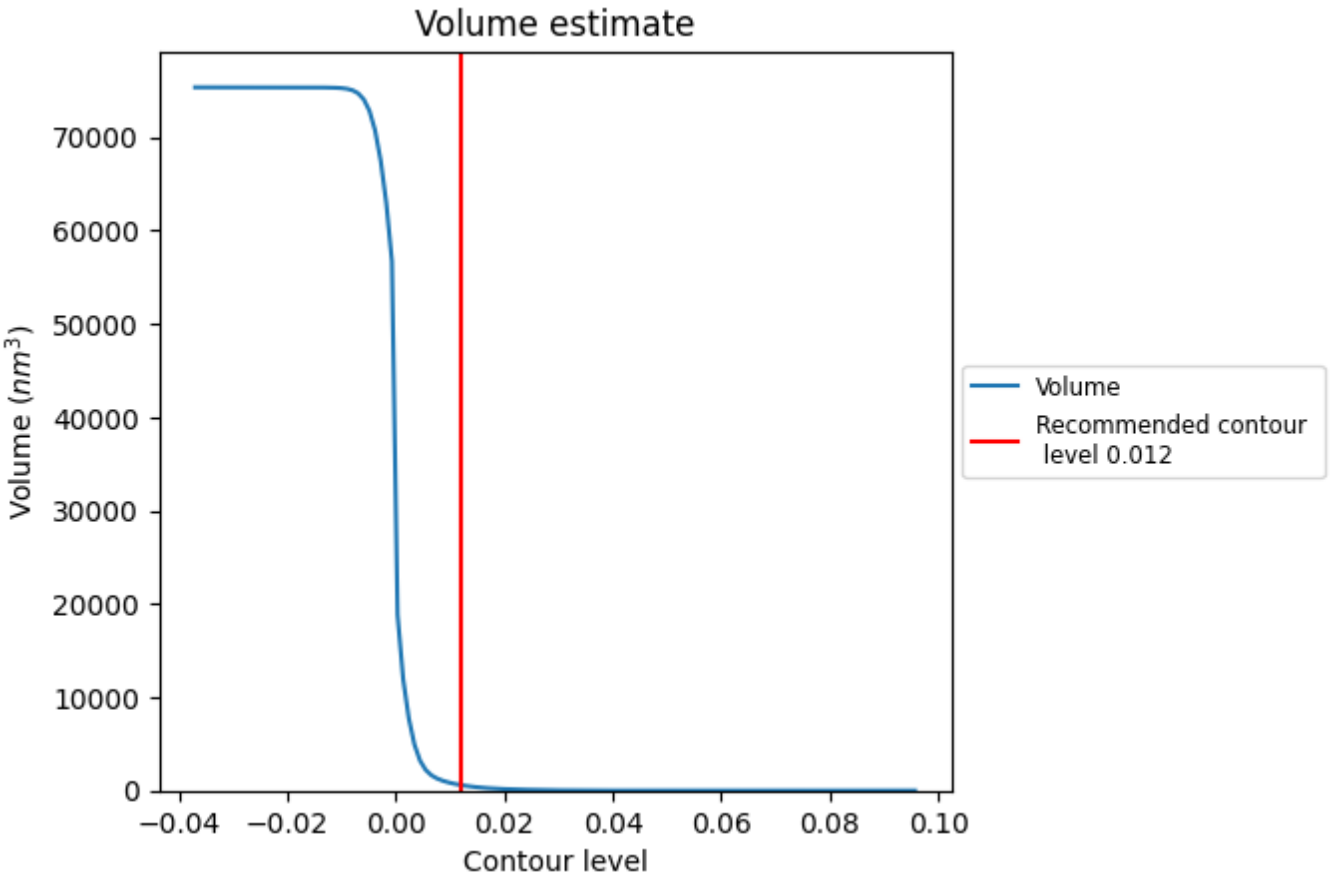
This section contains the results of statistical analysis of the map.

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.

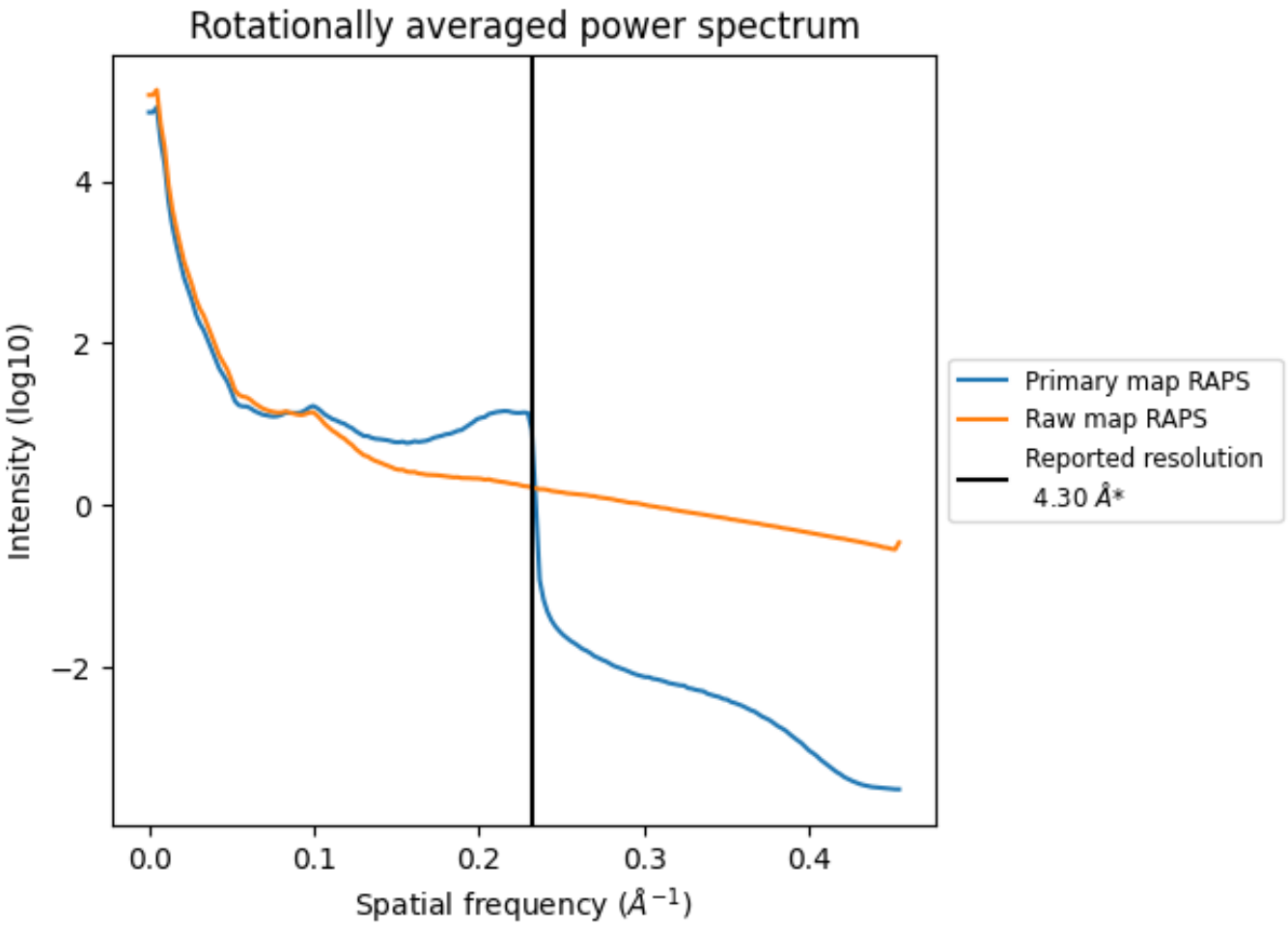
7.2 Volume estimate



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 535 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)

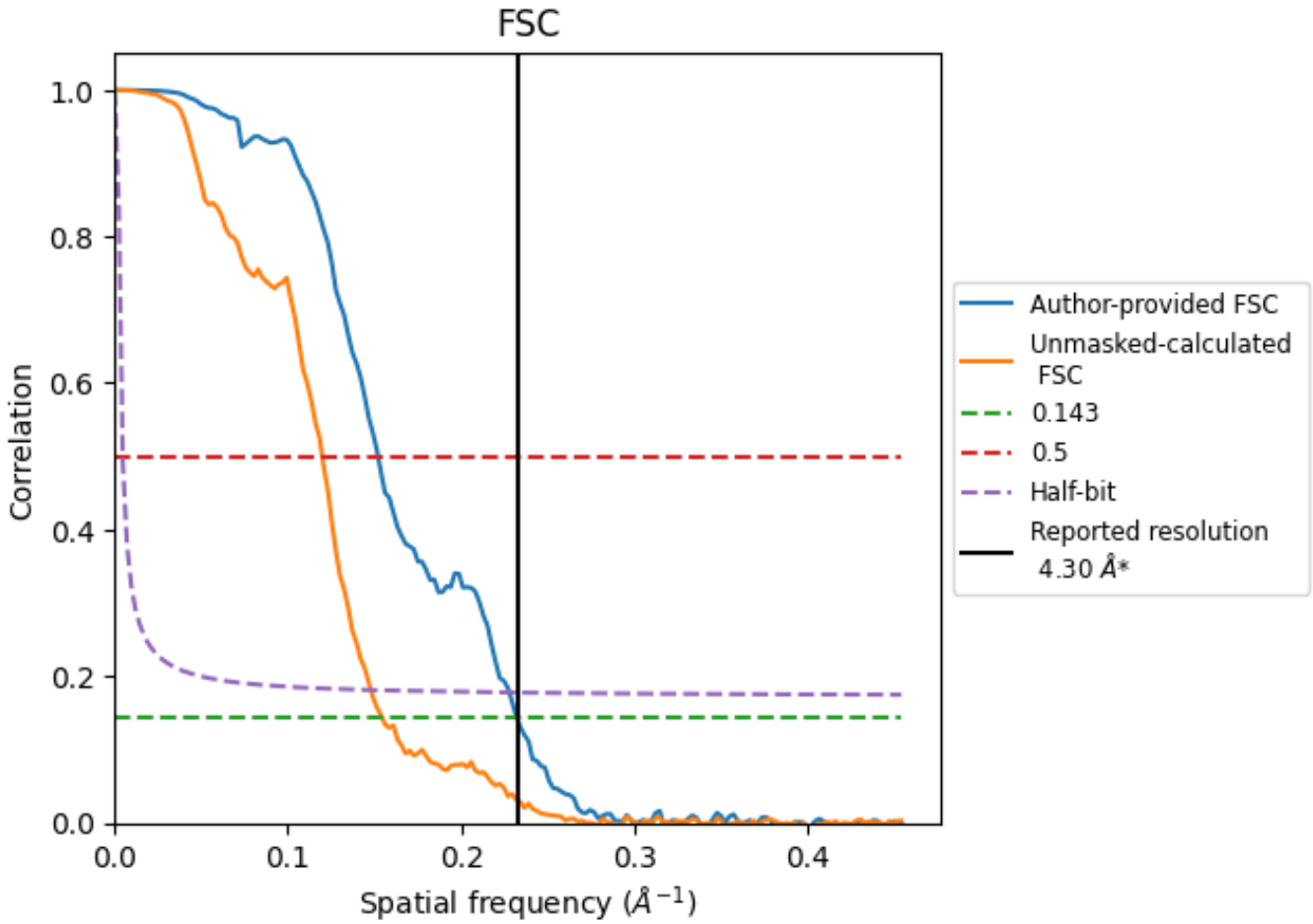


*Reported resolution corresponds to spatial frequency of 0.233 $Å^{-1}$

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)

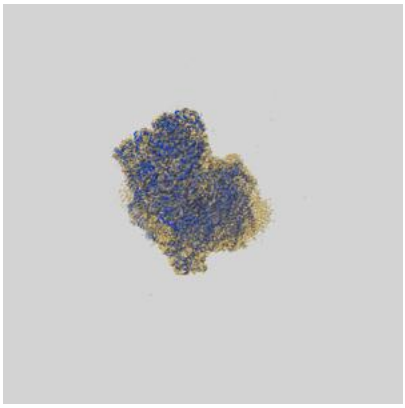
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.30	6.57	4.39
Unmasked-calculated*	6.47	8.34	6.76

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

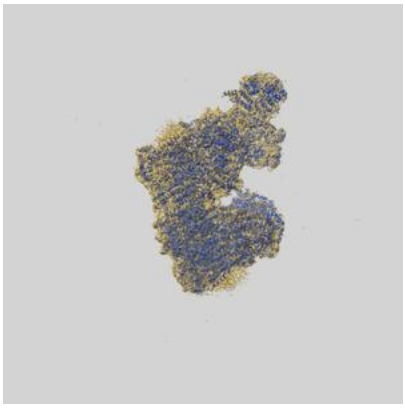
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35336 and PDB model 8IB9. Per-residue inclusion information can be found in section 3 on page 26.

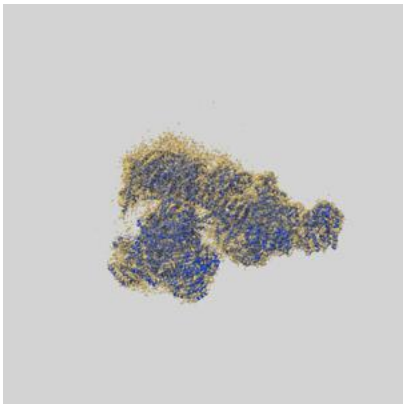
9.1 Map-model overlay



X



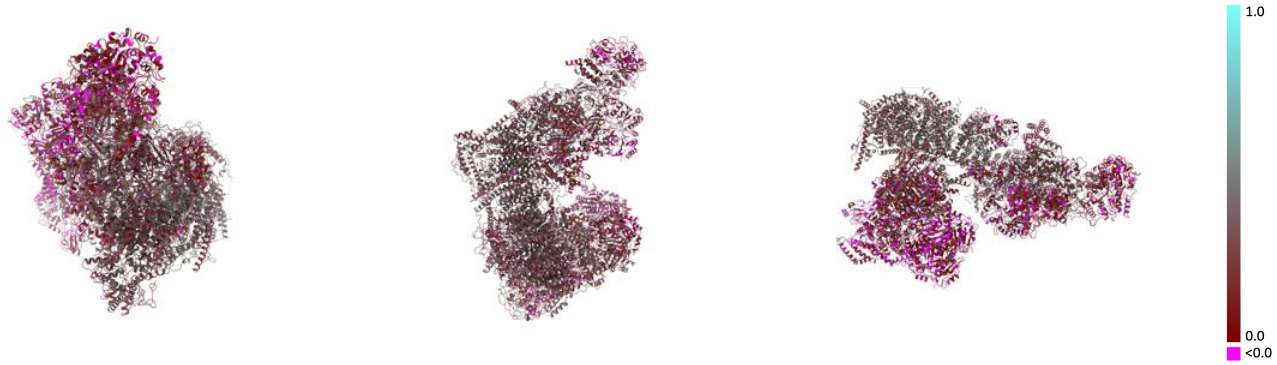
Y



Z

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

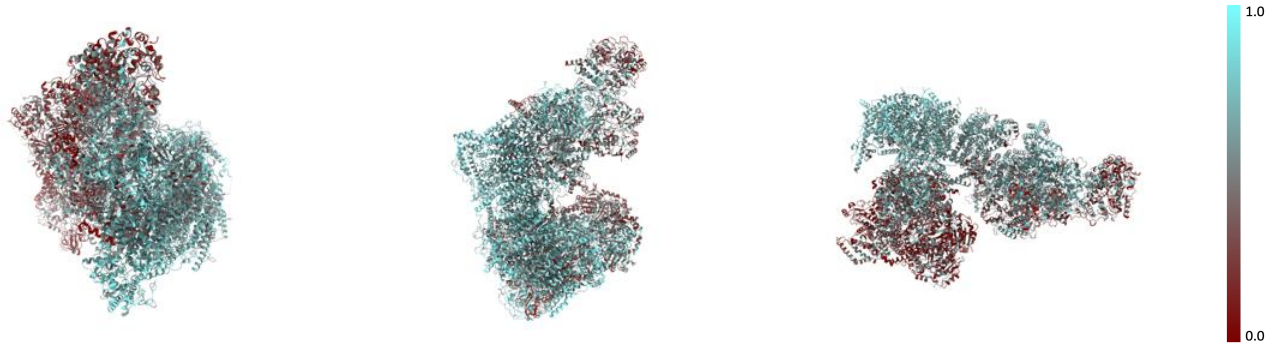
9.2 Q-score mapped to coordinate model (i)



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.

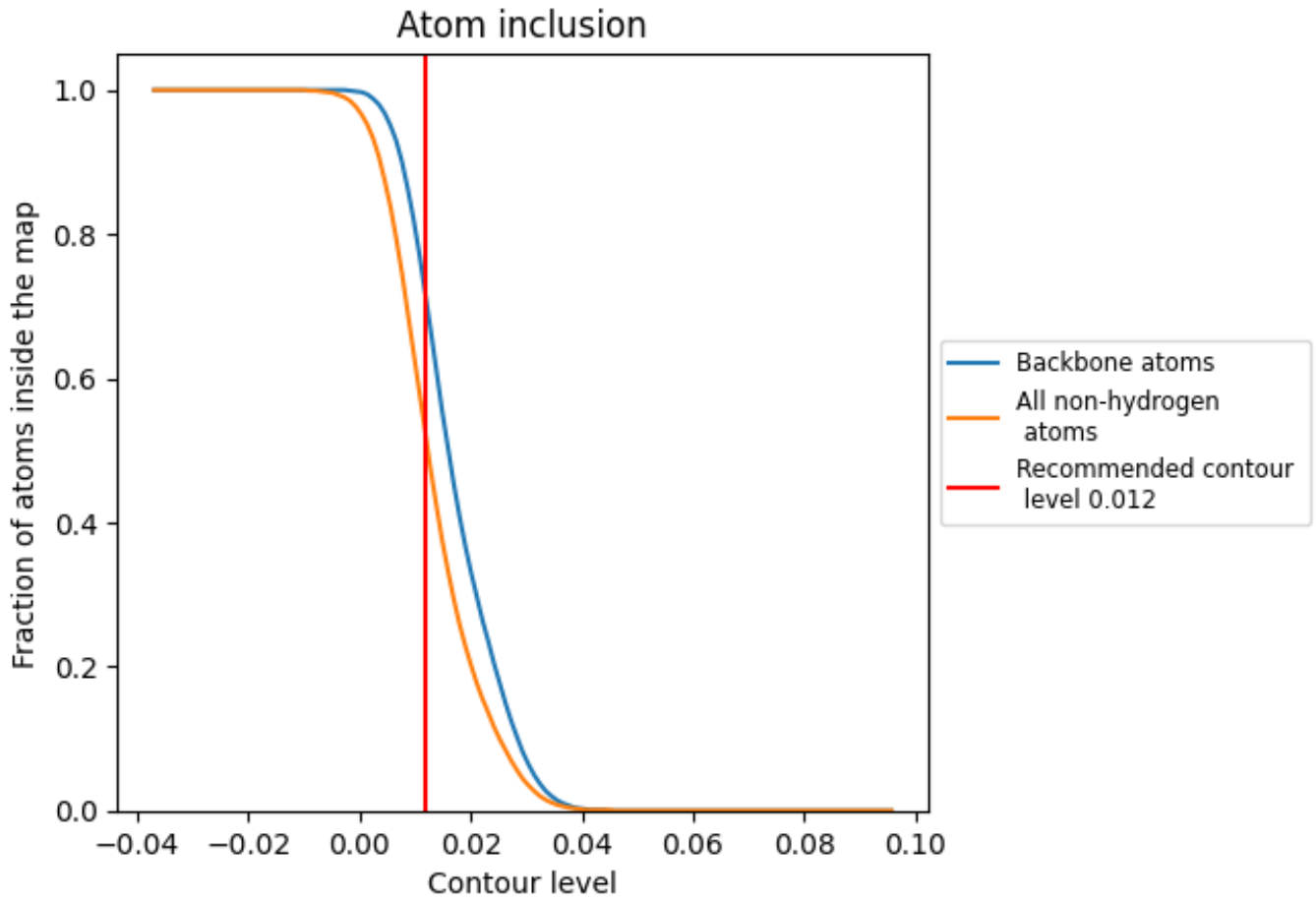
9.3 Atom inclusion mapped to coordinate model (i)



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, 71% of all backbone atoms, 51% 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	0.5140	0.2380
A	0.5960	0.3270
AA	0.3290	0.1030
AB	0.2800	0.0900
AC	0.2780	0.1230
AD	0.3430	0.0940
AE	0.0840	0.0530
AF	0.3680	0.1070
AG	0.2370	0.0720
AH	0.3380	0.0940
AI	0.1240	0.0610
AJ	0.0640	0.0090
AK	0.1170	0.0500
Aa	0.5520	0.2310
Ab	0.4690	0.1540
Ac	0.4130	0.2080
Ad	0.4000	0.1620
Ae	0.1310	0.0920
Af	0.4420	0.2140
Ag	0.4580	0.2400
Ah	0.4290	0.1560
Aj	0.2020	0.1590
Ak	0.1080	0.0950
B	0.6790	0.3330
C	0.6230	0.2680
D	0.6690	0.3310
E	0.3600	0.1540
F	0.4060	0.1480
G	0.4830	0.1870
H	0.6610	0.3420
I	0.6850	0.3280
J	0.5890	0.3280
K	0.6280	0.3540
L	0.6350	0.3430
M	0.6780	0.3790

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N	0.6860	0.3750
O	0.5860	0.2720
P	0.4300	0.1700
Q	0.4520	0.2360
R	0.2640	0.1660
S	0.3870	0.0920
T	0.3070	0.1080
U	0.7020	0.3260
V	0.5970	0.2090
W	0.5010	0.1940
X	0.7410	0.3300
Y	0.6210	0.3320
Z	0.7270	0.3200
a	0.6720	0.3210
b	0.6520	0.2910
c	0.6350	0.2860
d	0.6950	0.3610
e	0.7320	0.3330
f	0.6430	0.2960
g	0.6770	0.3440
h	0.6950	0.3330
i	0.6980	0.3340
j	0.6830	0.3100
k	0.7330	0.3390
l	0.7130	0.3600
m	0.6280	0.3340
n	0.7510	0.3480
o	0.6680	0.2740
p	0.7220	0.3290
q	0.2190	0.2020
r	0.3220	0.1890
s	0.1130	0.0810