Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 06:41 PM JST

PDB ID	:	8IBD
EMDB ID	:	EMD-35340
Title	:	Respiratory complex CI:CIII2, type II, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	4.20 Å(reported)

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

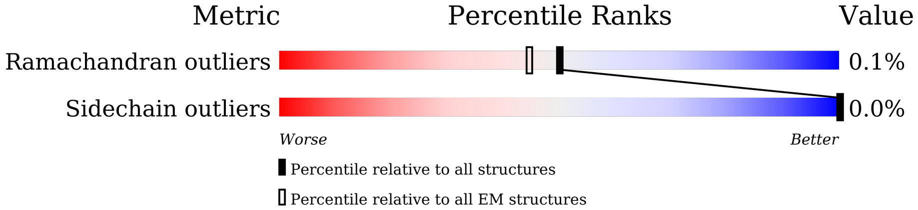
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

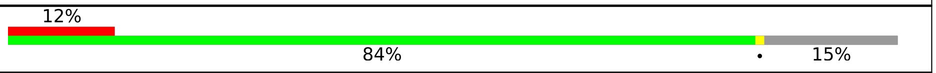
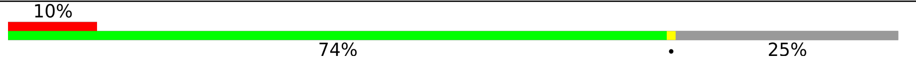
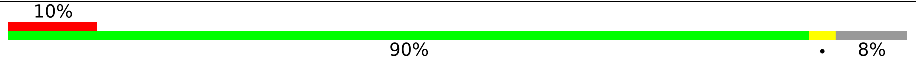
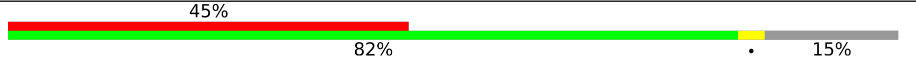
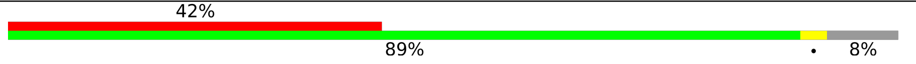
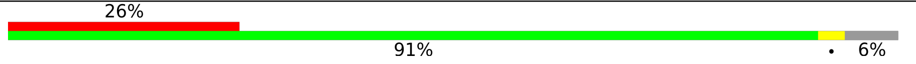
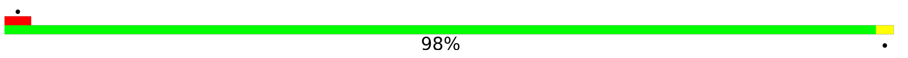
The reported resolution of this entry is 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	224	
3	C	263	
4	D	463	
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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Mol	Chain	Length	Quality of chain
10	J	172	20% 94% • 5%
11	K	98	6% 97% • •
12	L	607	• 97% •
13	M	459	• 97% •
14	N	345	• 98% •
15	O	355	31% 86% • 10%
16	P	377	33% 88% • 10%
17	Q	175	22% 64% • 34%
18	R	116	45% 72% 28%
19	S	99	37% 80% • 16%
20	T	156	34% 48% 52%
20	U	156	• 56% • 43%
21	V	116	25% 97% •
22	W	131	33% 86% • 13%
23	X	172	• 98% • •
24	Y	143	13% 97% •
25	Z	144	• 92% • •
26	a	70	• 93% • •
27	b	84	• 93% • 5%
28	c	76	9% 59% • 38%
29	d	120	5% 98% •
30	e	106	5% 98% ••
31	f	57	5% 84% 5% 11%
32	g	151	6% 66% • 32%
33	h	189	• 72% • 27%

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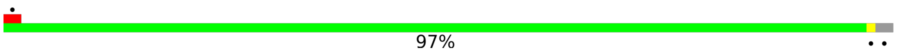
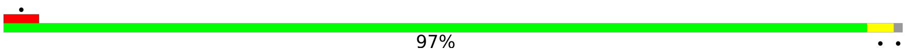
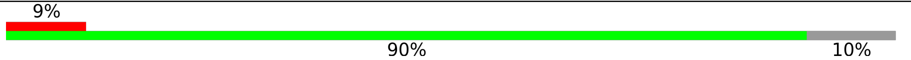
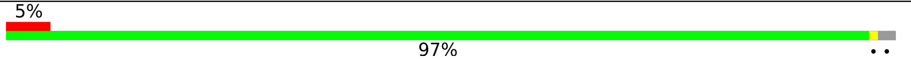
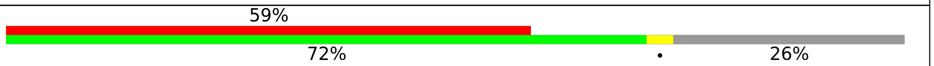
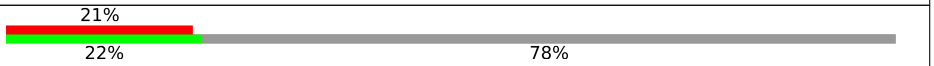
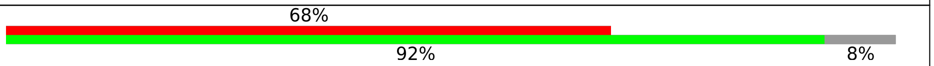
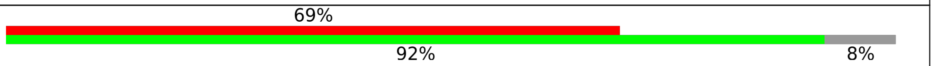
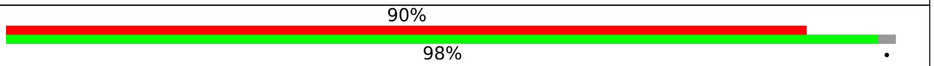
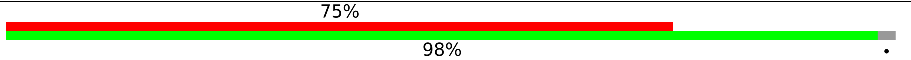
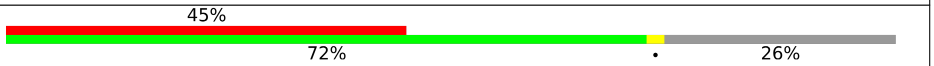
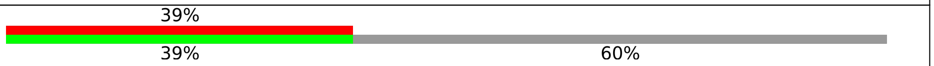
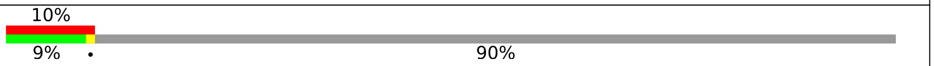
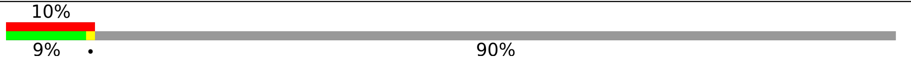
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
49	Ai	274	
50	AF	111	
50	Af	111	

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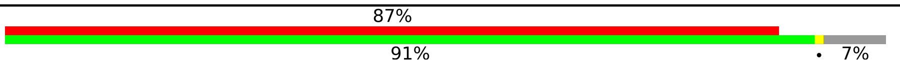
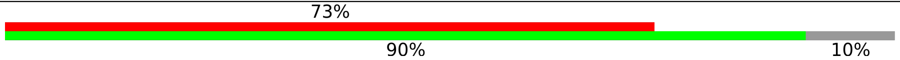
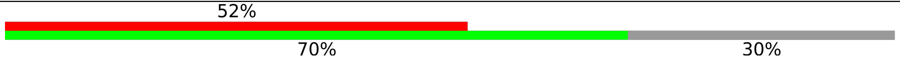
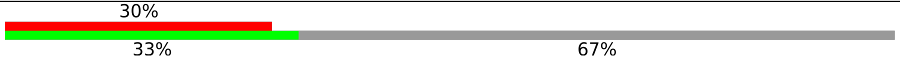
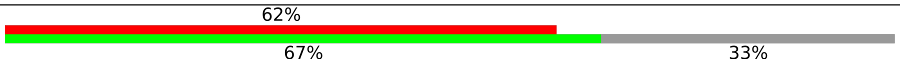
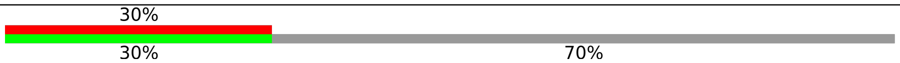
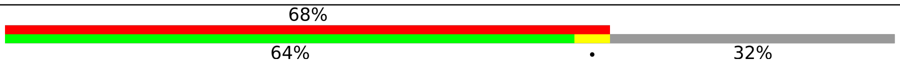
Mol	Chain	Length	Quality of chain
51	AG	82	
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

2 Entry composition ⓘ

There are 71 unique types of molecules in this entry. The entry contains 96599 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	98	799	552	112	130	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	793	222	212	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	1643	1061	279	300	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	427	3438	2197	591	626	24	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total 1380	C 869	N 237	O 262	S 12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	163	Total 1229	C 828	N 175	O 211	S 15	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	116	LEU	ASN	conflict	UNP P03925
J	117	GLY	LEU	conflict	UNP P03925

- 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
			Total	C	N	O	S		
12	L	606	4798	3181	746	826	45	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	116	940	598	161	177	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total 604	C 388	N 89	O 122	S 5	0	0
20	U	89	Total 718	C 462	N 105	O 146	S 5	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	139	Total 1030	C 657	N 174	O 191	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total 1145	C 736	N 203	O 198	S 8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total 628	C 414	N 99	O 111	S 4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total 877	C 555	N 162	O 152	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total 439	C 284	N 79	O 74	S 2	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	95	802	523	140	136	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	73	582	383	102	95	2	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	126	Total	C	N	O	0	0
			1050	676	189	185		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	123	Total	C	N	O	S	0	0
			1025	658	181	182	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	84	Total	C	N	O	S	0	0
			686	435	128	121	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	23	Total 193	C 126	N 30	O 37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	395	Total 3077	C 1918	N 545	O 598	S 16	0	0
45	Aa	394	Total 3076	C 1923	N 545	O 592	S 16	0	0

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

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

- Molecule 47 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	236	Total 1878	C 1200	N 323	O 341	S 14	0	0
48	Ad	239	Total 1903	C 1215	N 326	O 348	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	109	Total 830	C 525	N 152	O 147	S 6	0	0
49	AI	28	Total 200	C 129	N 37	O 34		0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
49	Ae	188	Total C N O S 1451 916 254 274 7	0	0
49	Ai	28	Total C N O 204 130 40 34	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
50	AF	97	Total C N O S 855 546 152 154 3	0	0
50	Af	98	Total C N O S 864 552 154 155 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 C N O S 643 418 116 108 1	0	0
51	Ag	74	Total C N O S 622 404 114 103 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 C N O S 527 321 98 103 5	0	0
52	Ah	62	Total C N O S 512 316 93 98 5	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
53	AJ	21	Total C N O 165 109 27 29	0	0
53	Aj	43	Total C N O 345 223 59 63	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
54	AK	17	Total C N O S 118 77 19 21 1	0	0

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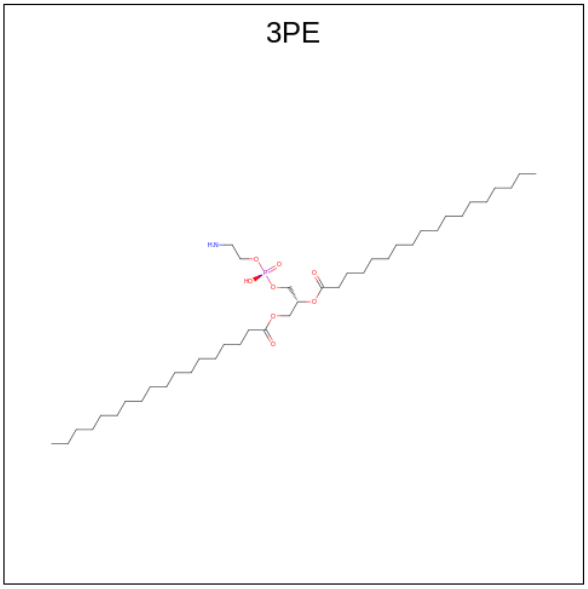
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Ak	38	309	202	58	48	1	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	A	1	42	32	1	8	1	0
55	H	1	48	38	1	8	1	0
55	I	1	51	41	1	8	1	0
55	K	1	46	36	1	8	1	0
55	L	1	40	30	1	8	1	0
55	L	1	49	39	1	8	1	0
55	L	1	40	30	1	8	1	0
55	L	1	38	28	1	8	1	0
55	M	1	37	27	1	8	1	0
55	M	1	51	41	1	8	1	0

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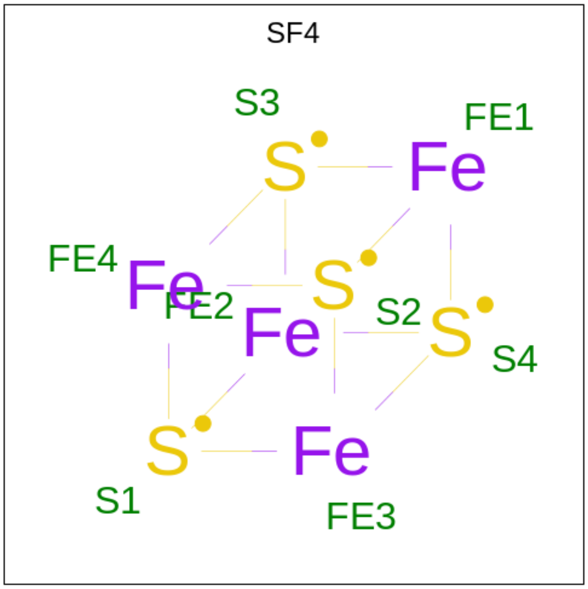
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	N	1	51	41	1	8	1	0
55	Y	1	41	31	1	8	1	0
55	d	1	31	21	1	8	1	0
55	i	1	40	30	1	8	1	0
55	m	1	47	37	1	8	1	0
55	m	1	51	41	1	8	1	0
55	m	1	41	31	1	8	1	0
55	Aa	1	23	13	1	8	1	0
55	Ac	1	35	25	1	8	1	0
55	Ag	1	38	28	1	8	1	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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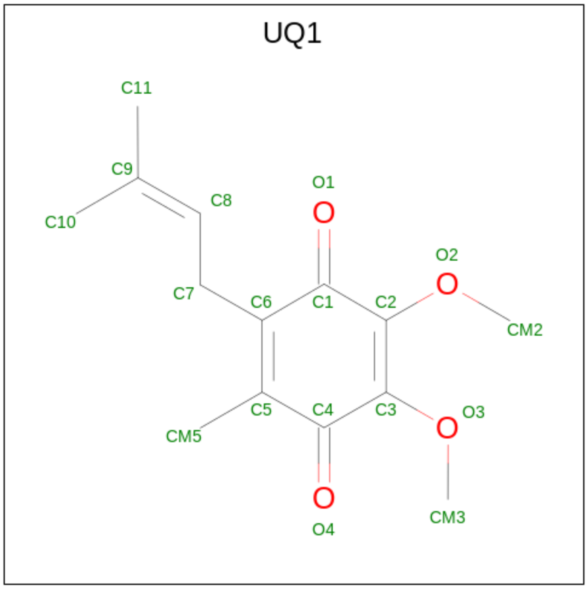
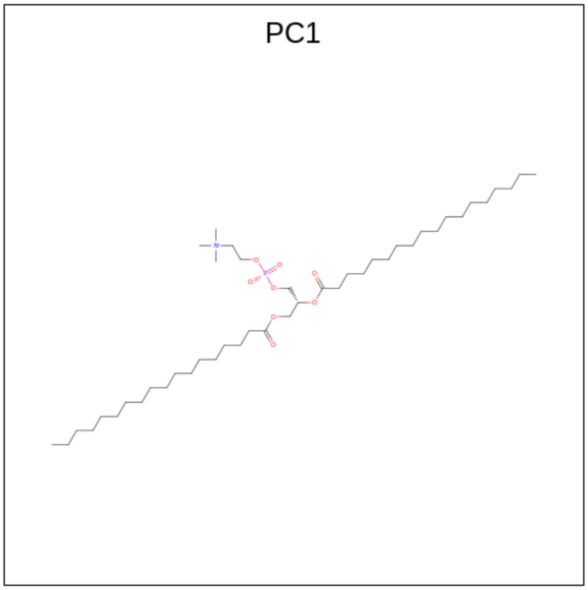
Mol	Chain	Residues	Atoms	AltConf
56	F	1	Total Fe S 8 4 4	0
56	G	1	Total Fe S 8 4 4	0
56	G	1	Total Fe S 8 4 4	0
56	I	1	Total Fe S 8 4 4	0
56	I	1	Total Fe S 8 4 4	0

- Molecule 57 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



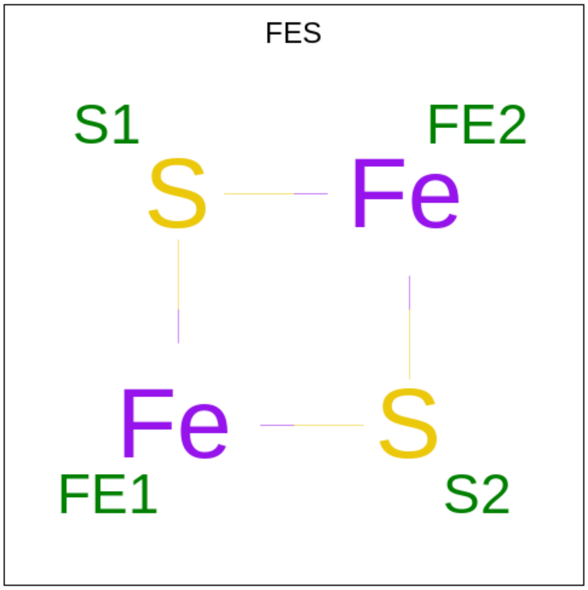
Mol	Chain	Residues	Atoms	AltConf
57	B	1	Total C O 18 14 4	0

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total C N O P 35 25 1 8 1	0
58	B	1	Total C N O P 43 33 1 8 1	0

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



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

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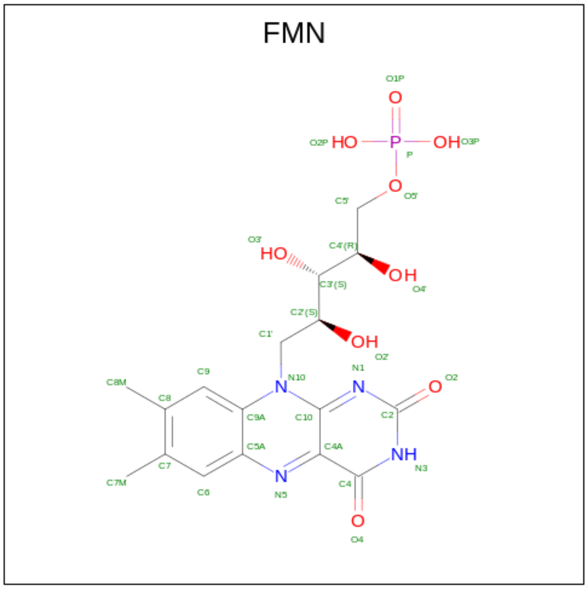
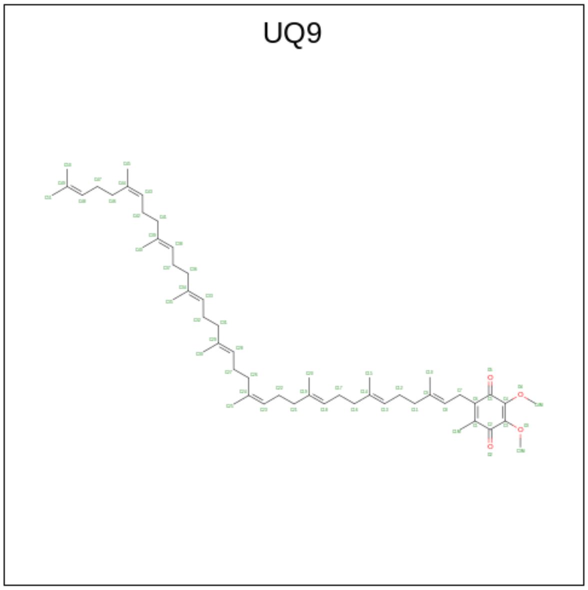
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	G	1	4	2	2	0

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



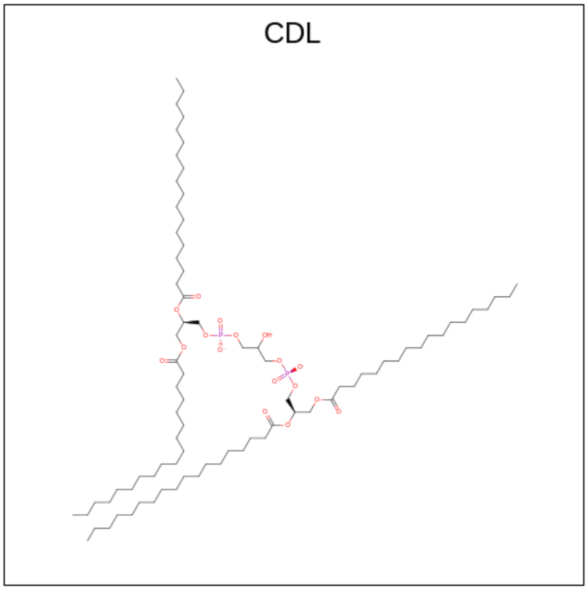
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

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



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

- 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
			Total	C	O	P	
62	L	1	78	59	17	2	0
62	X	1	67	48	17	2	0

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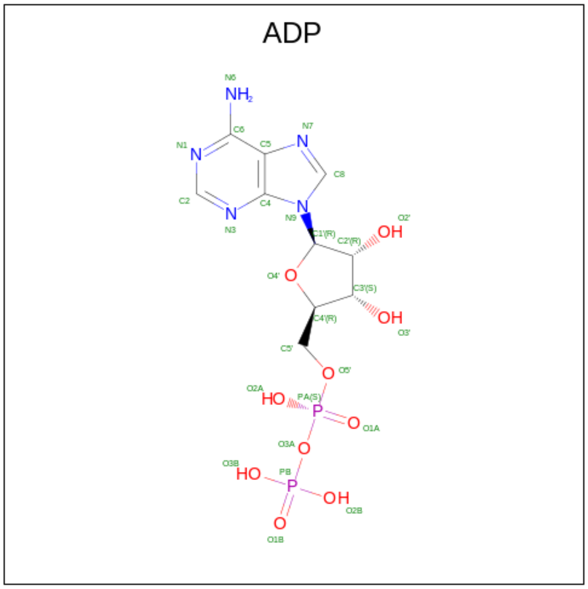
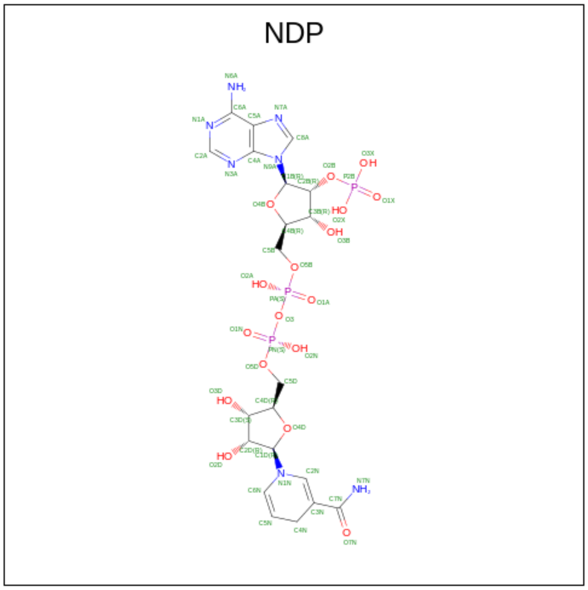
Mol	Chain	Residues	Atoms	AltConf
62	a	1	Total C O P 57 38 17 2	0
62	h	1	Total C O P 70 51 17 2	0
62	Ag	1	Total C O P 42 23 17 2	0
62	Ag	1	Total C O P 56 37 17 2	0

- 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 27 10 5 10 2	0

- 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).

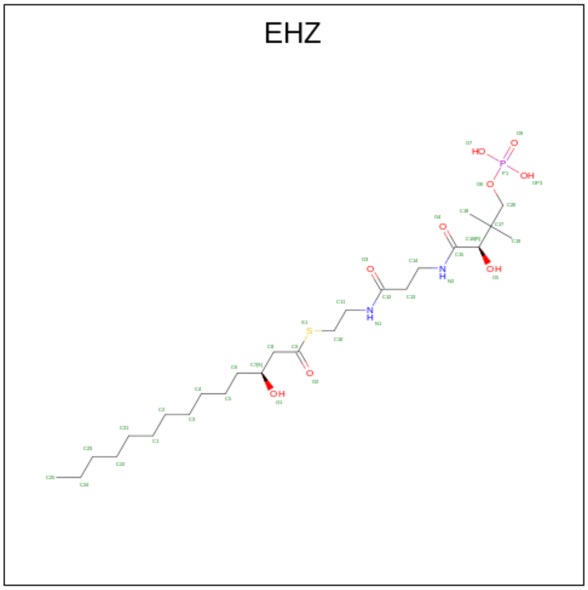


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	P	1	48	21	7	17	3	0

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

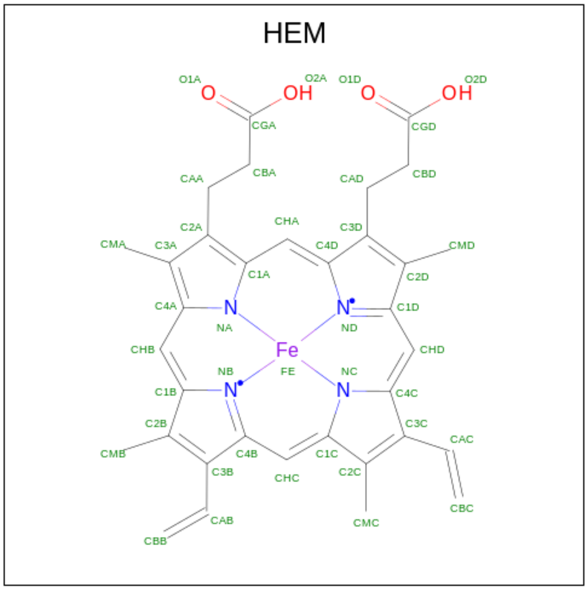
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	R	1	1	1	0

- 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 32	C 19	N 2	O 9	P 1	S 1	0
66	n	1	Total 32	C 19	N 2	O 9	P 1	S 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 43	C 34	Fe 1	N 4	O 4	0

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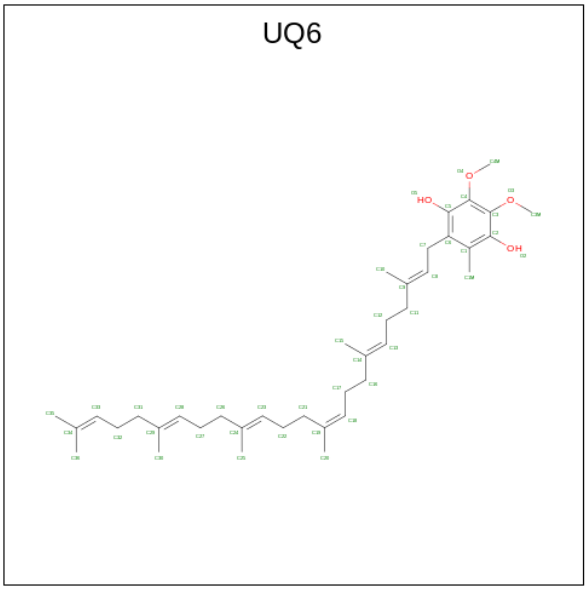
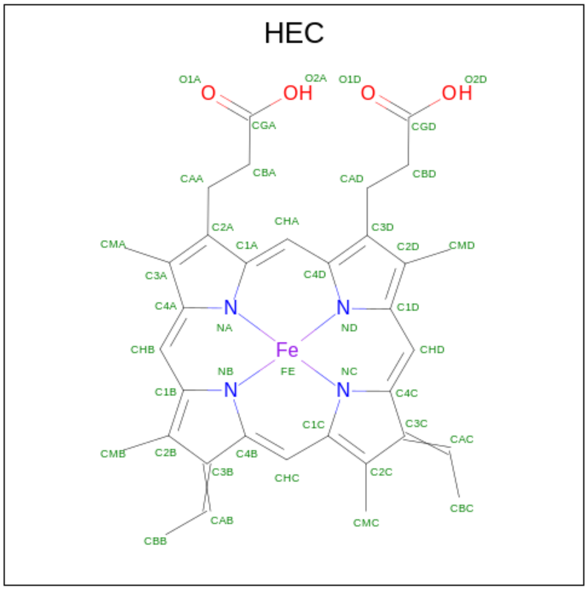
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
67	Ac	1	Total 43	C 34	Fe 1	N 4	O 4	0
67	Ac	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 68 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).



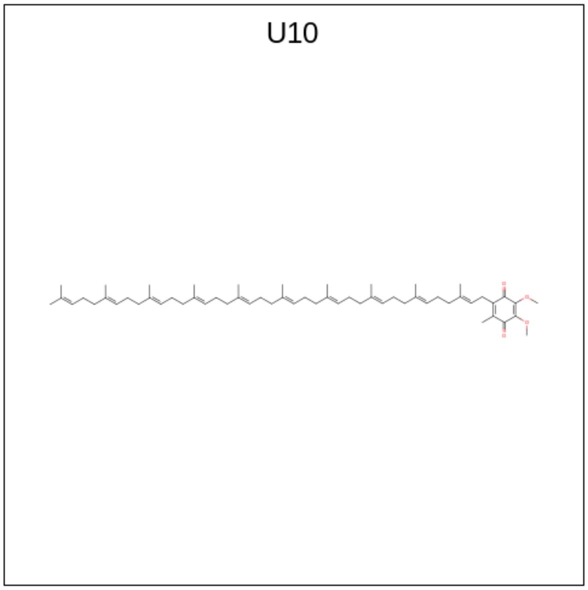
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total 28	C 24	O 4	0
68	Ac	1	Total 28	C 24	O 4	0

- Molecule 69 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



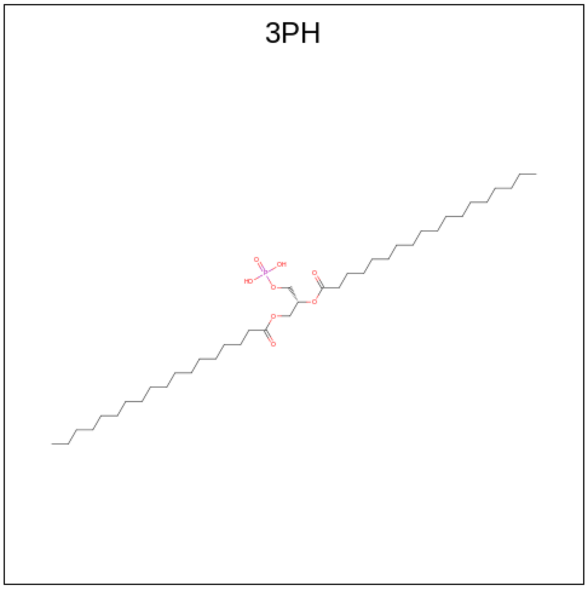
Mol	Chain	Residues	Atoms	AltConf
69	AD	1	Total C Fe N O 43 34 1 4 4	0
69	Ad	1	Total C Fe N O 43 34 1 4 4	0

- Molecule 70 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
70	Ac	1	Total C O 23 19 4	0

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).

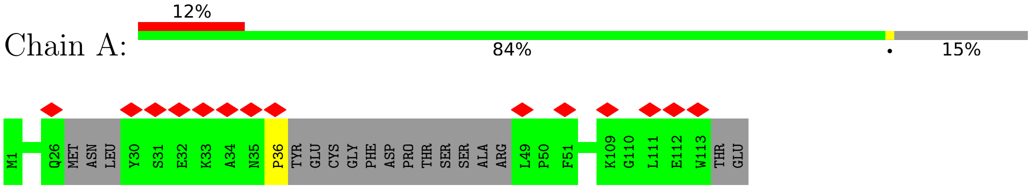


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
71	Ad	1	36	27	8	1	0

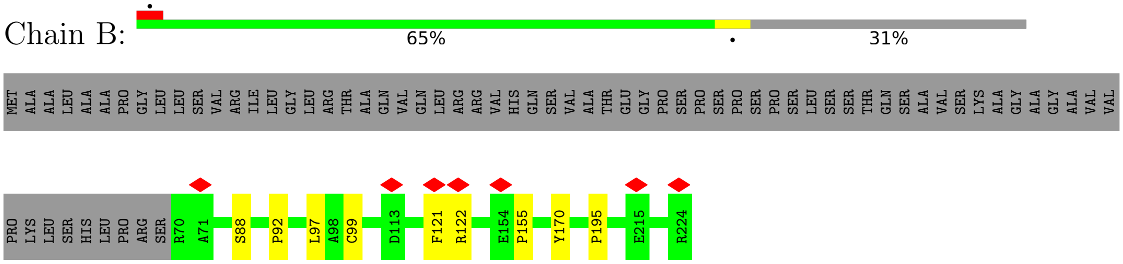
3 Residue-property plots ⓘ

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

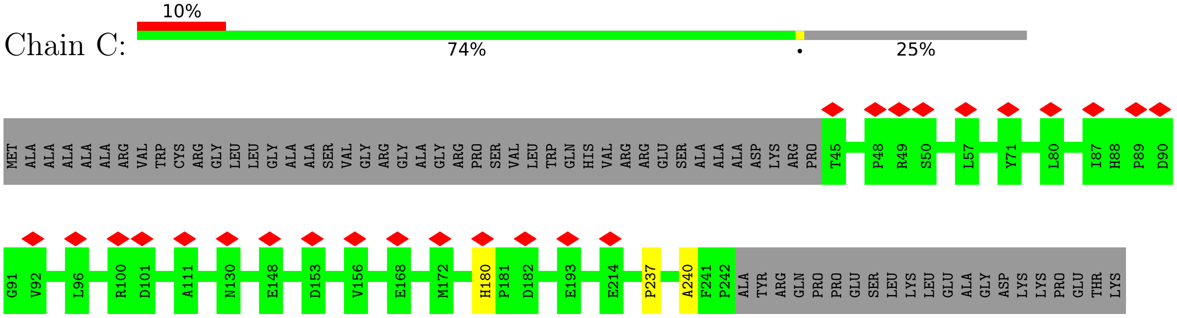
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



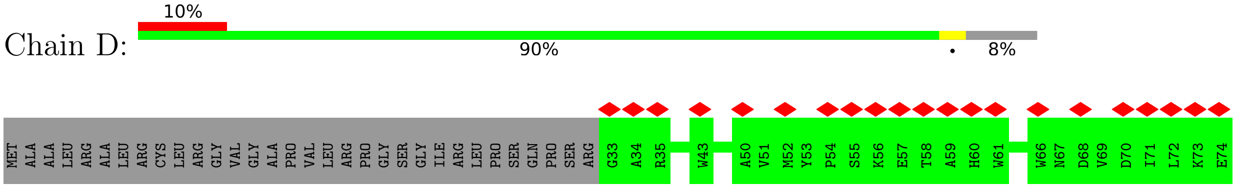
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

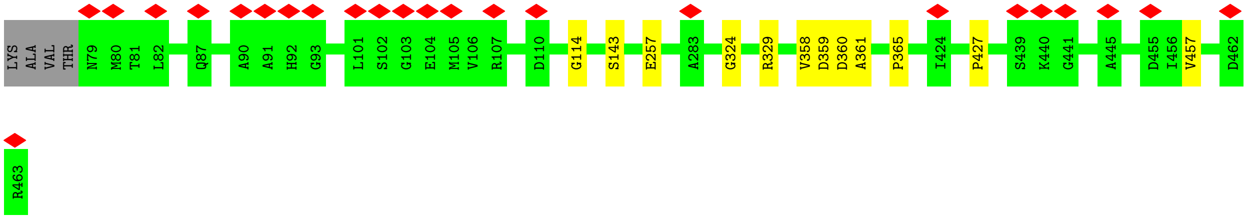


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



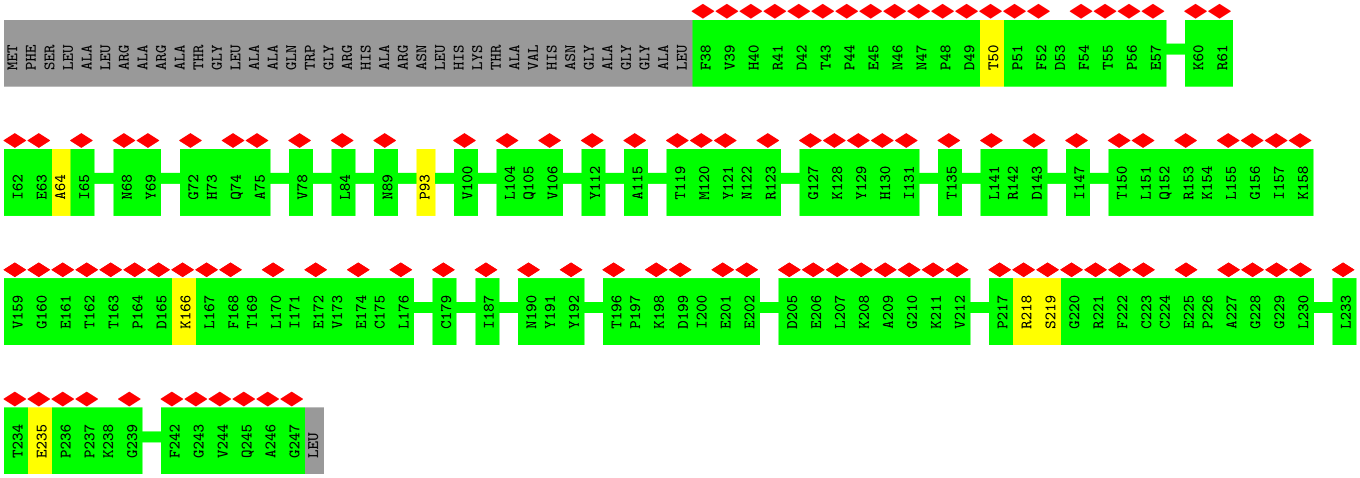
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





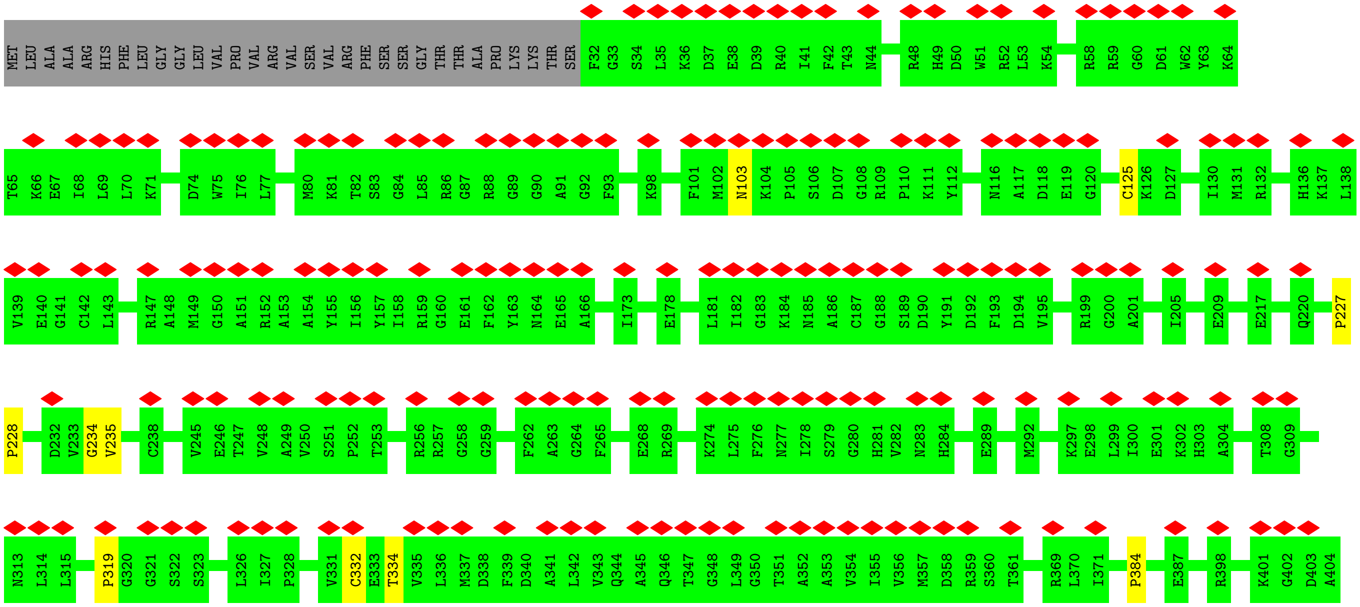
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

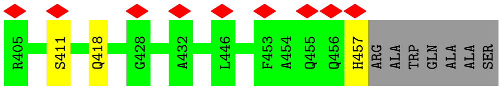
Chain E:



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

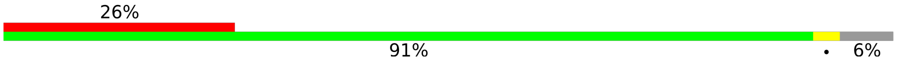
Chain F:

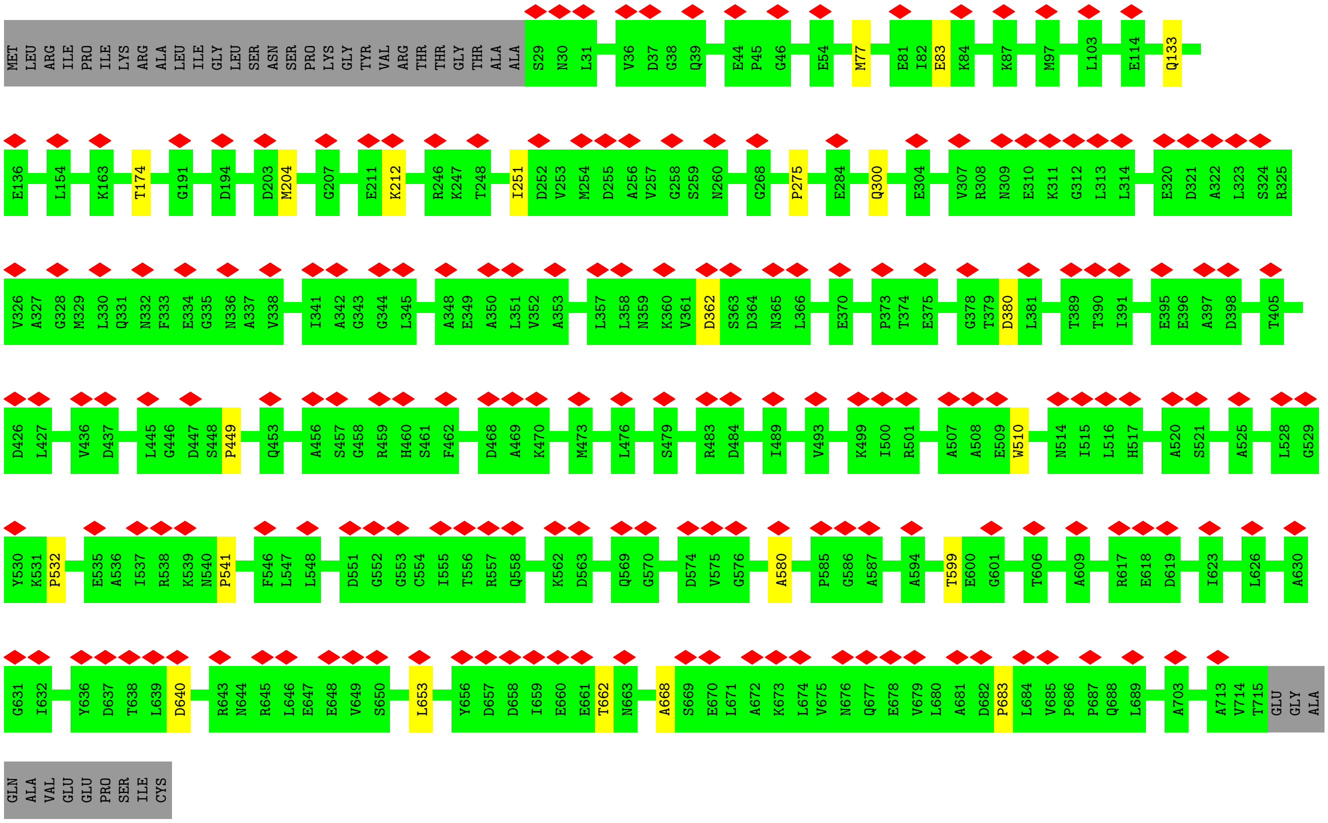




- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

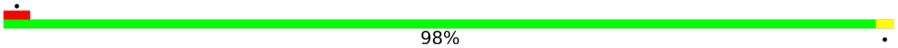
Chain G:

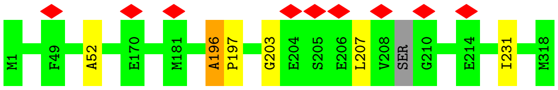




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

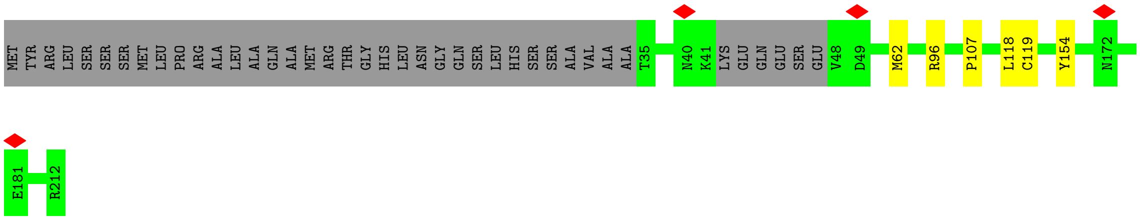
Chain H:



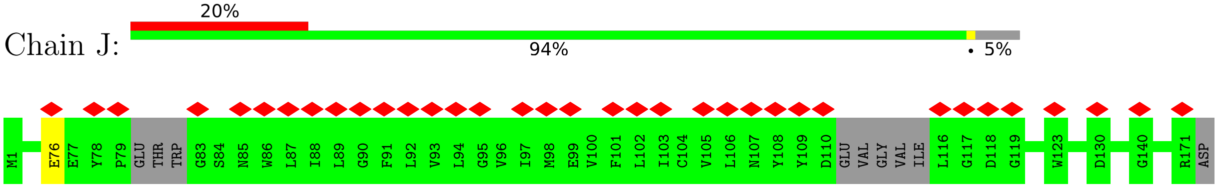


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

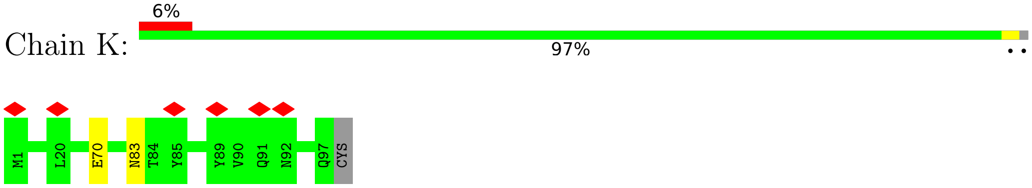
Chain I:



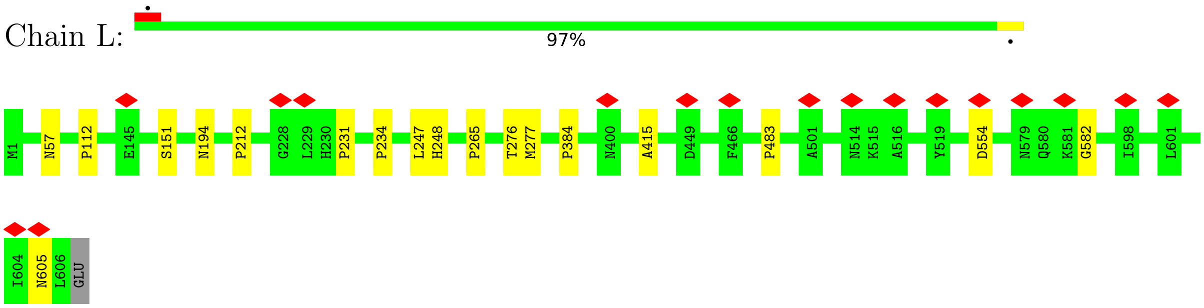
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



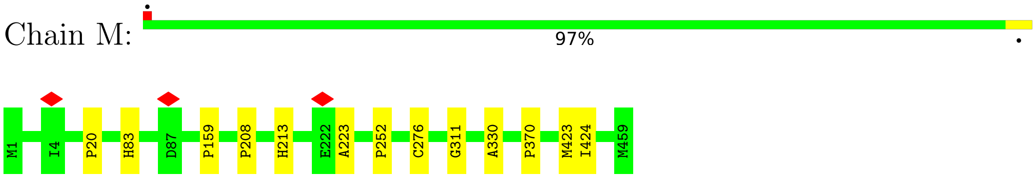
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



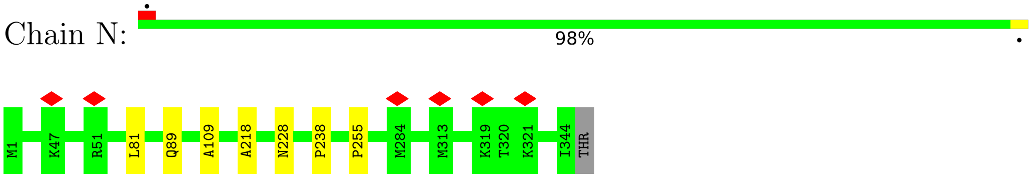
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



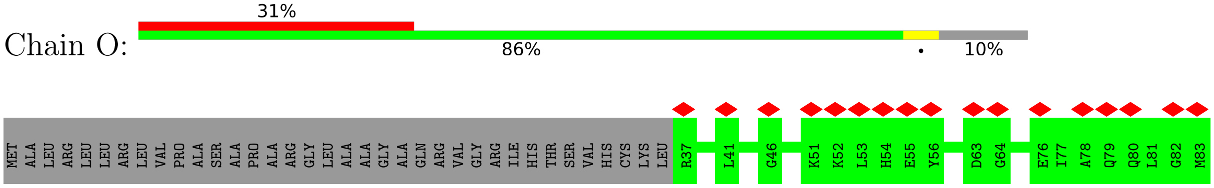
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

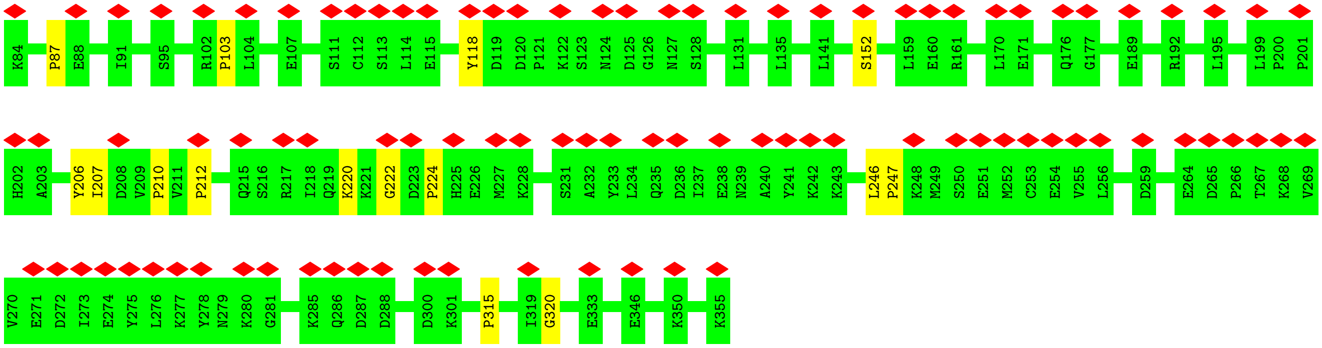


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



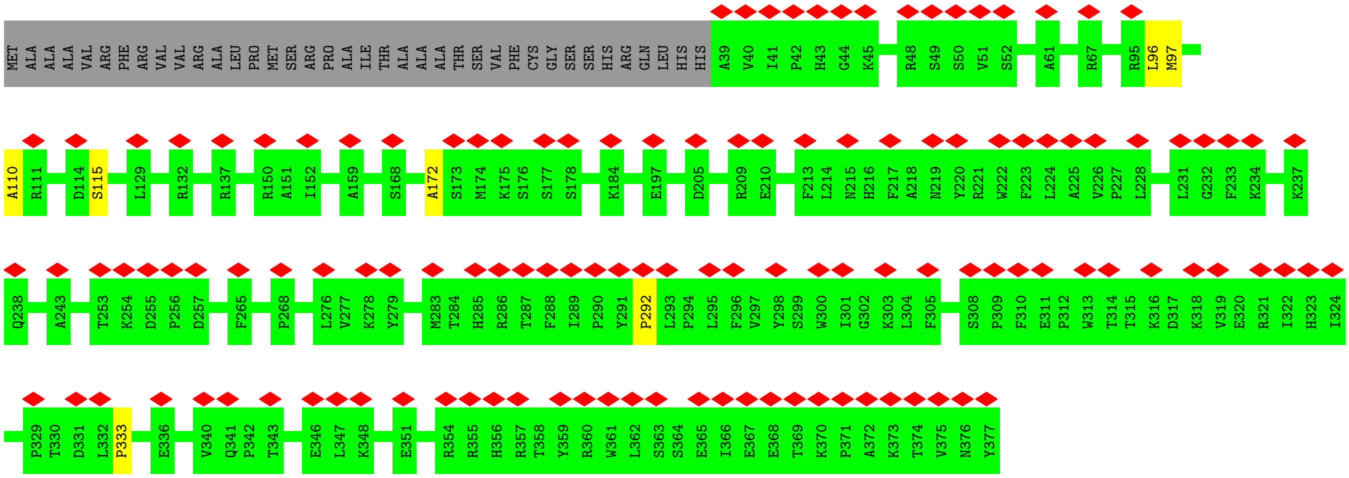
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





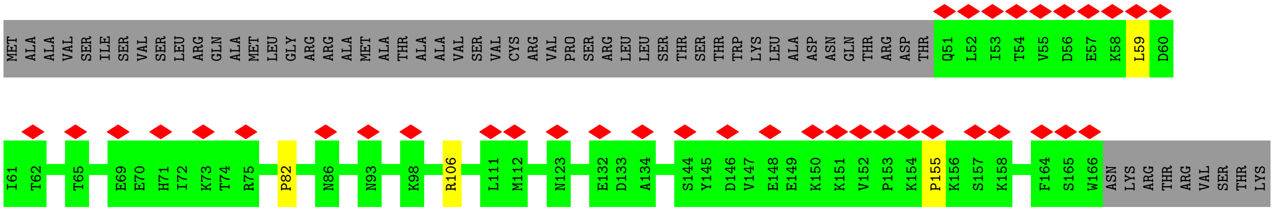
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



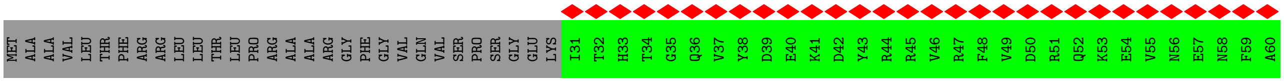
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

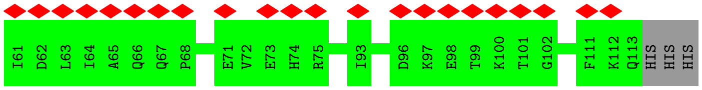
Chain Q:



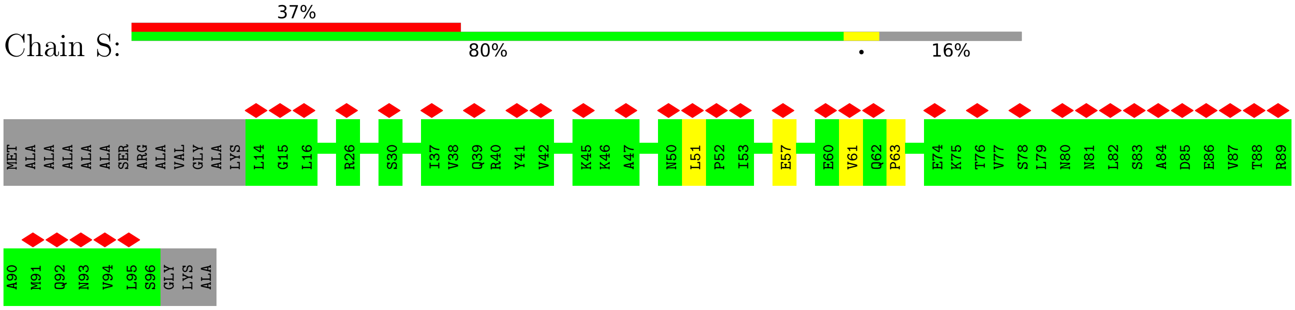
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:

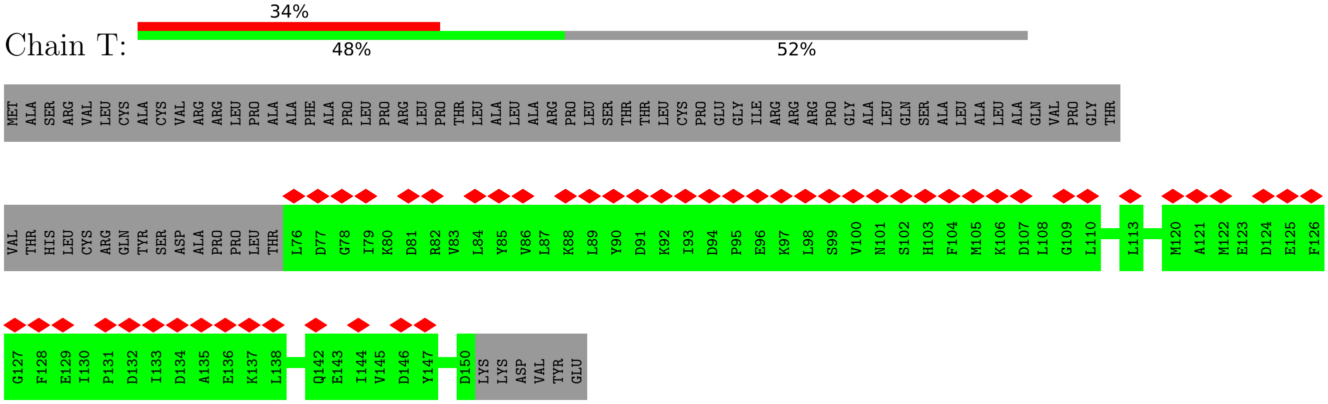




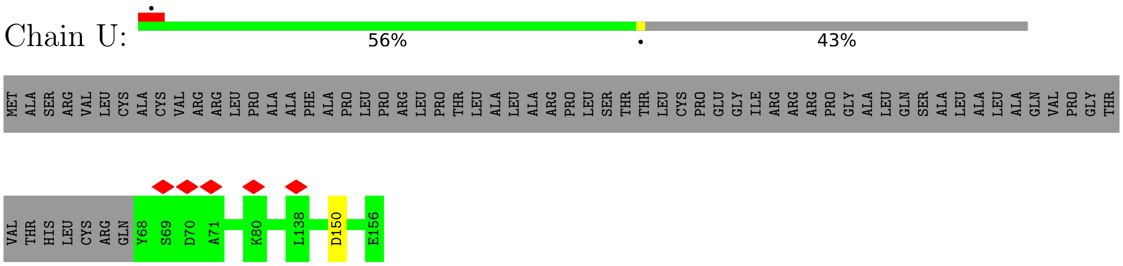
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



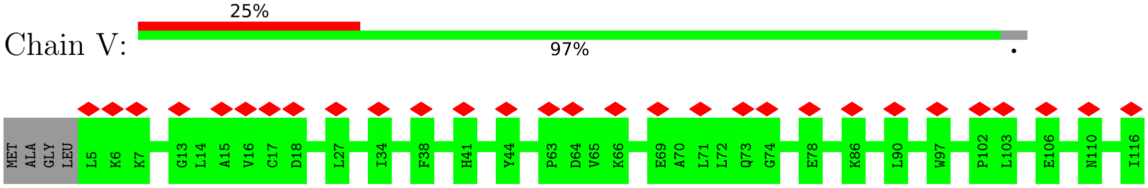
- Molecule 20: Acyl carrier protein, mitochondrial



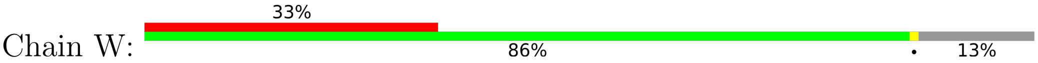
- Molecule 20: Acyl carrier protein, mitochondrial

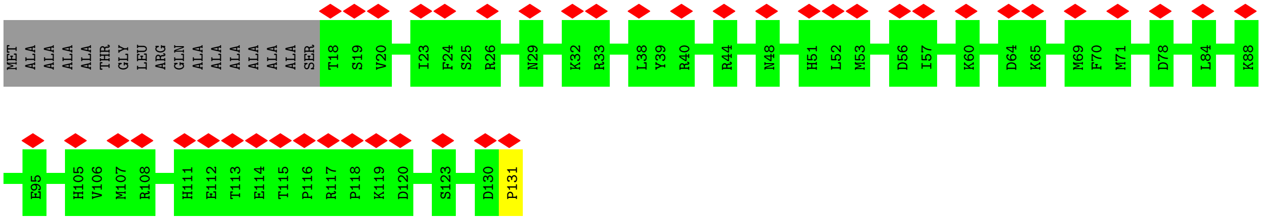


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



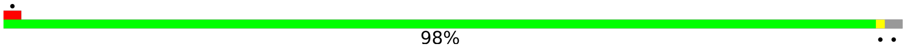
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

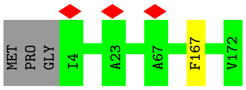




- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

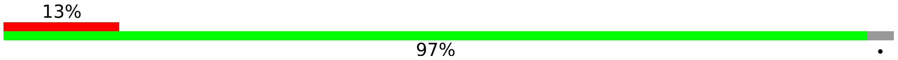
Chain X:

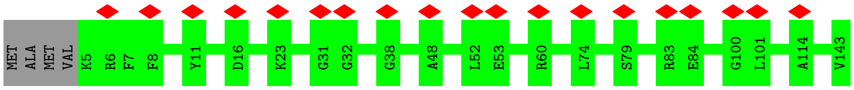




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

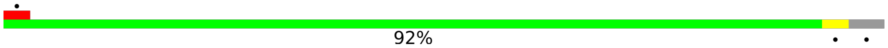
Chain Y:

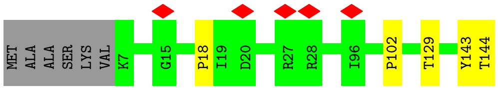




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

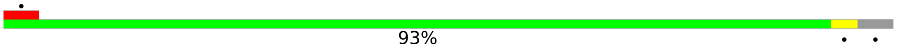
Chain Z:

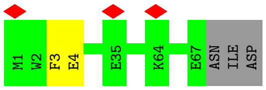




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

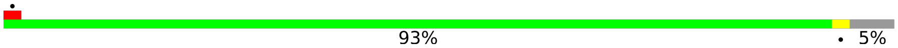
Chain a:

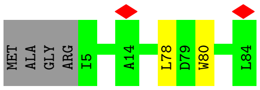




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

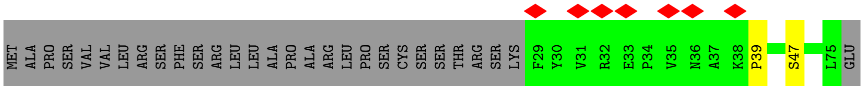
Chain b:





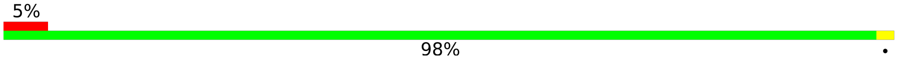
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

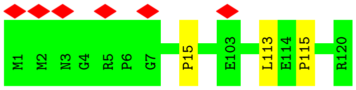
Chain c:



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

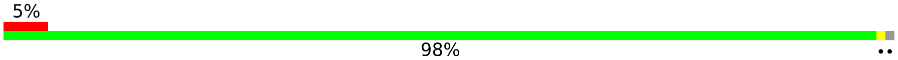
Chain d:

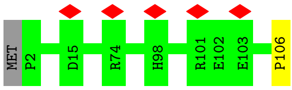




- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

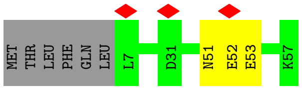
Chain e:





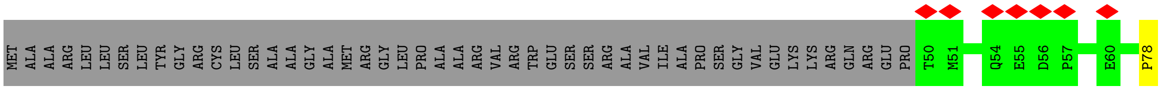
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

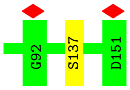
Chain f:



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

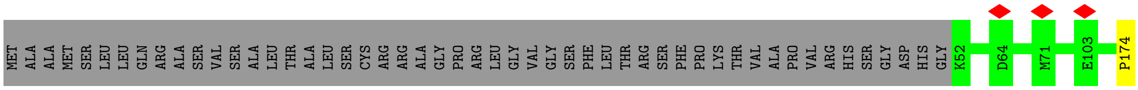
Chain g:

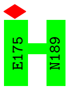




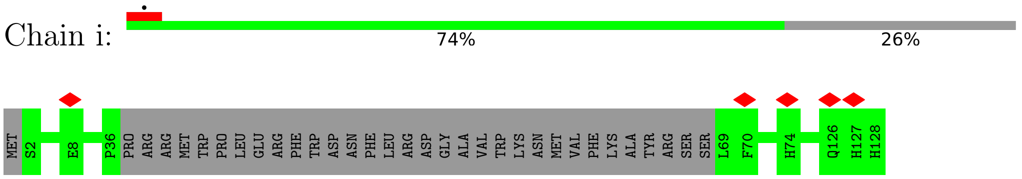
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

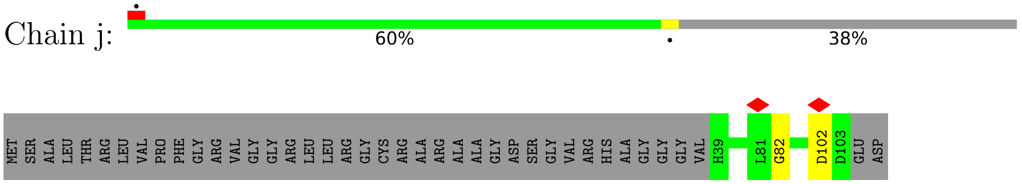




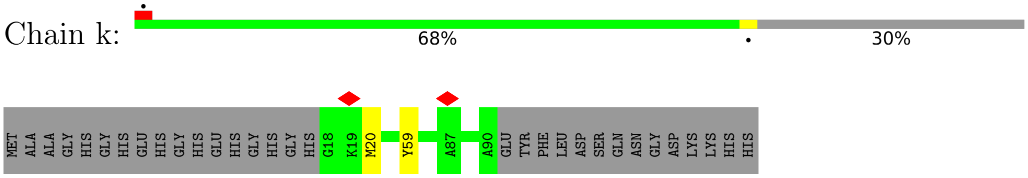
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



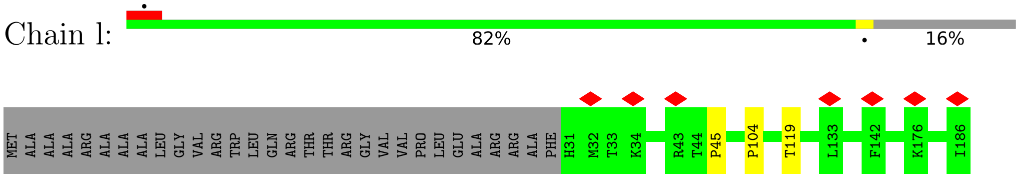
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



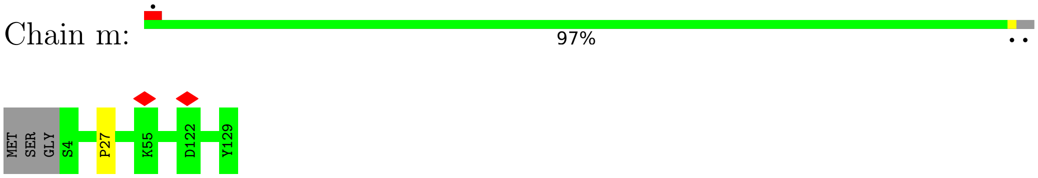
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



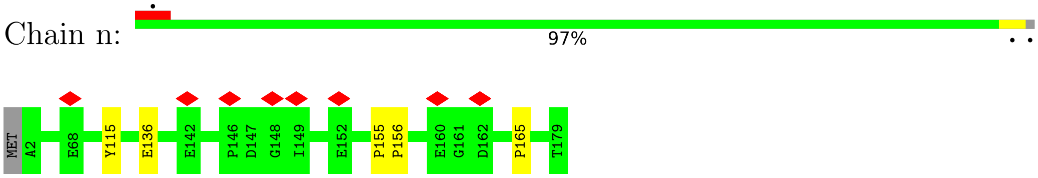
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



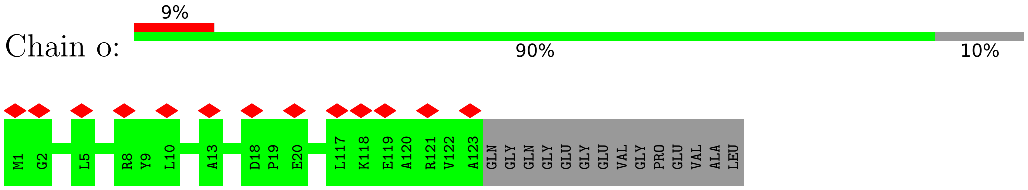
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



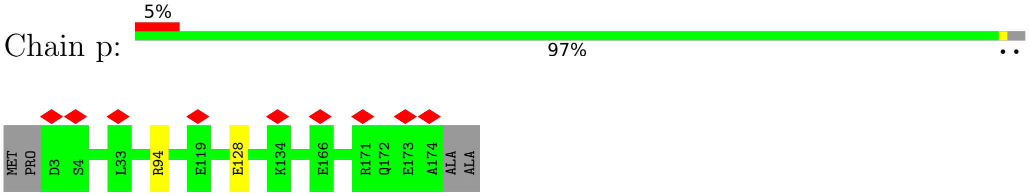
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



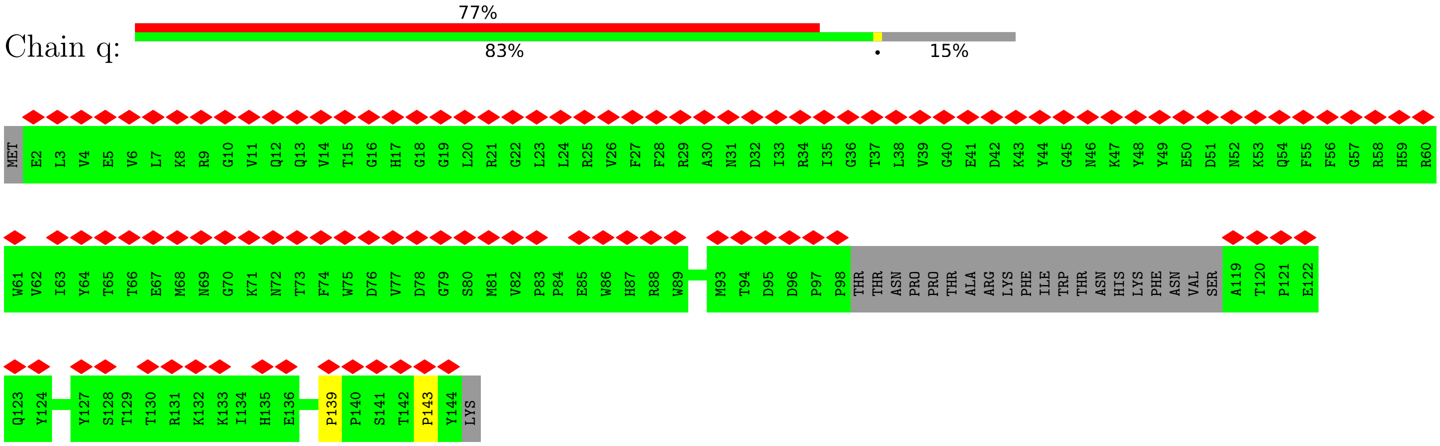
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



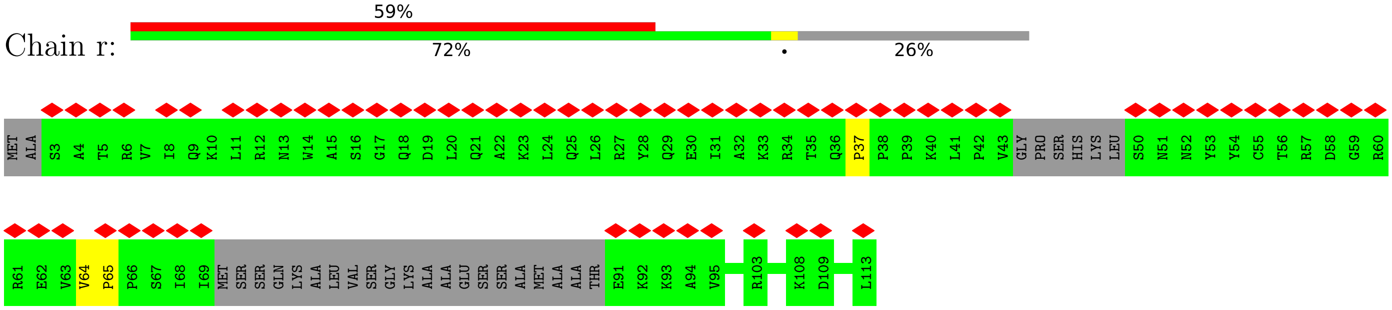
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



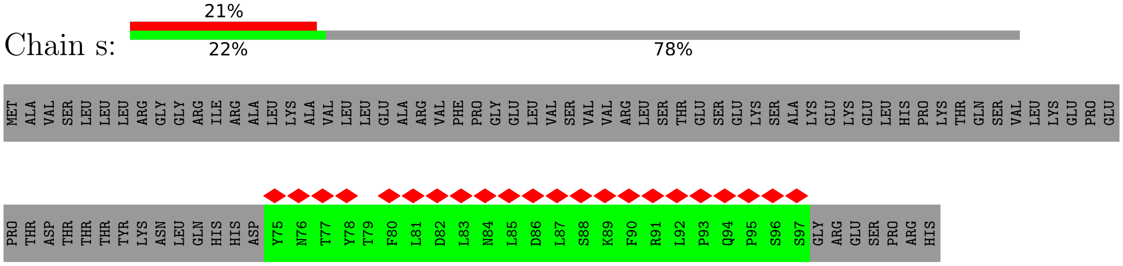
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

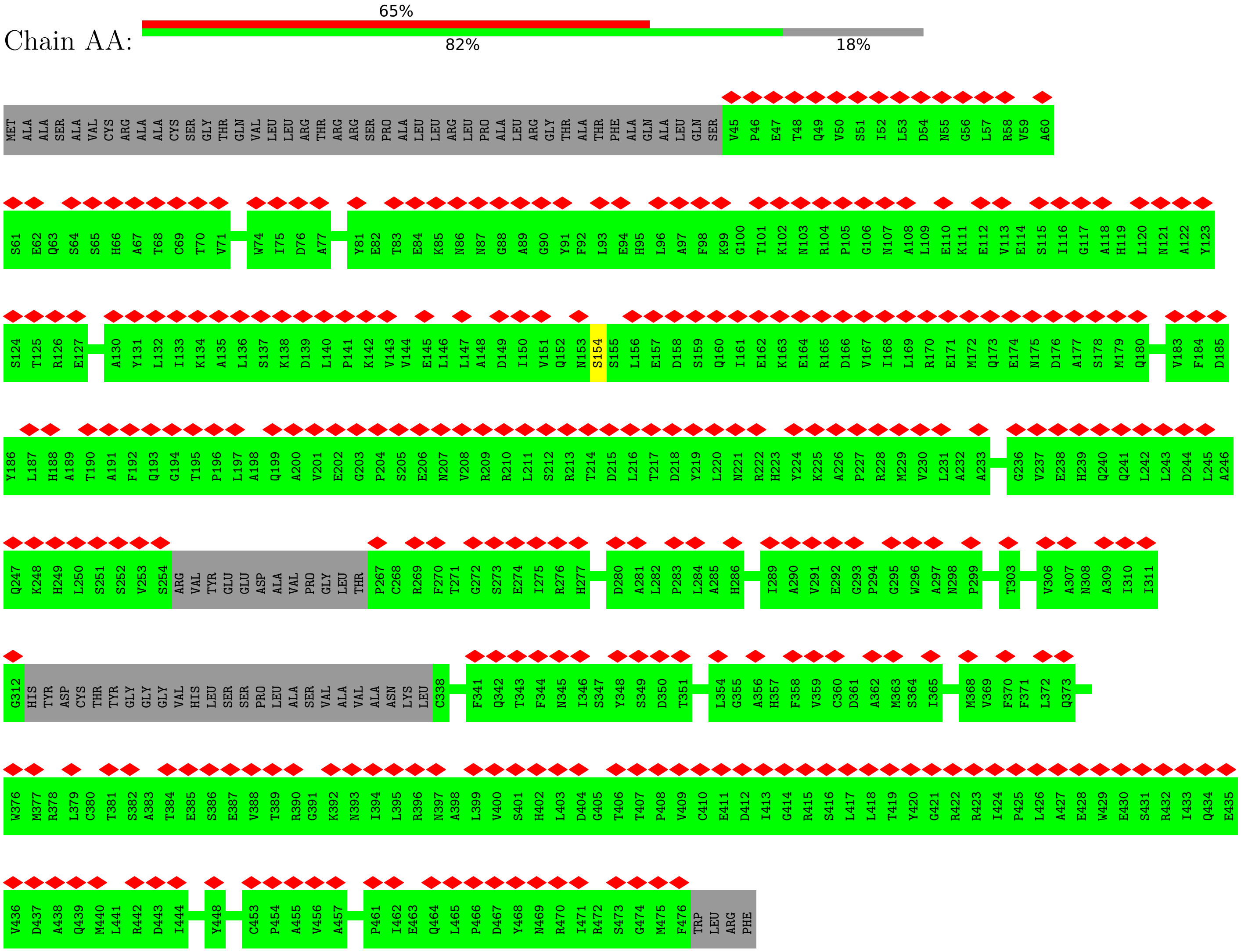


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



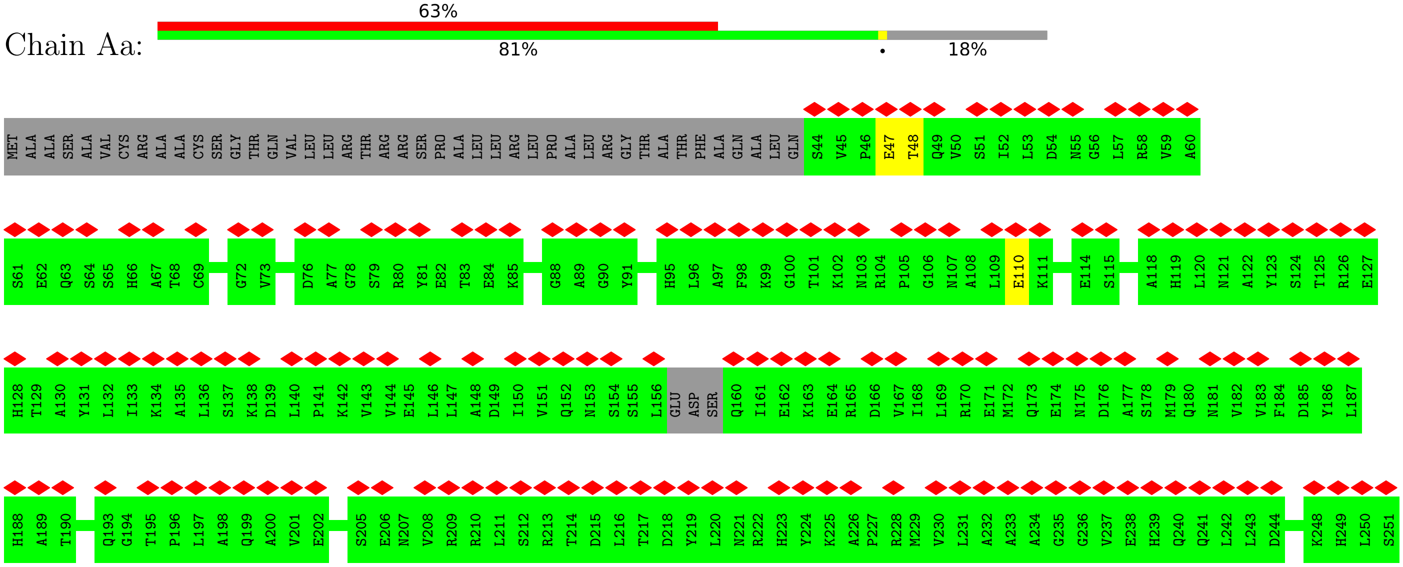
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

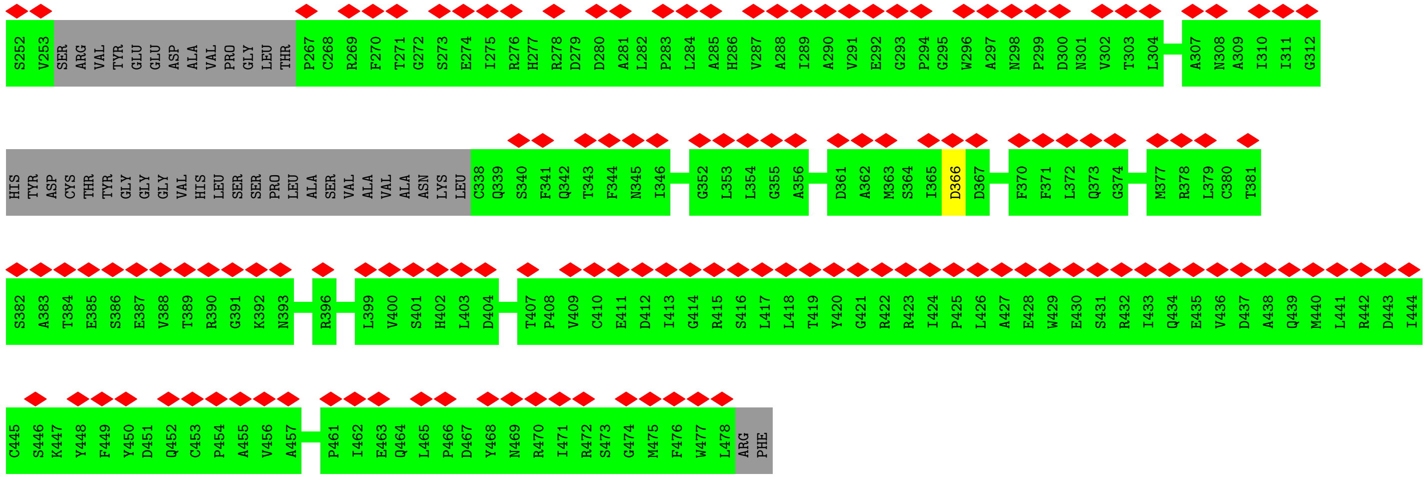
Chain AA:



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

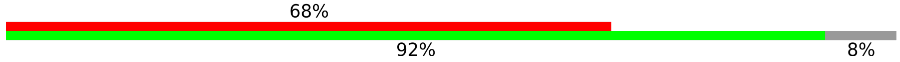
Chain Aa:

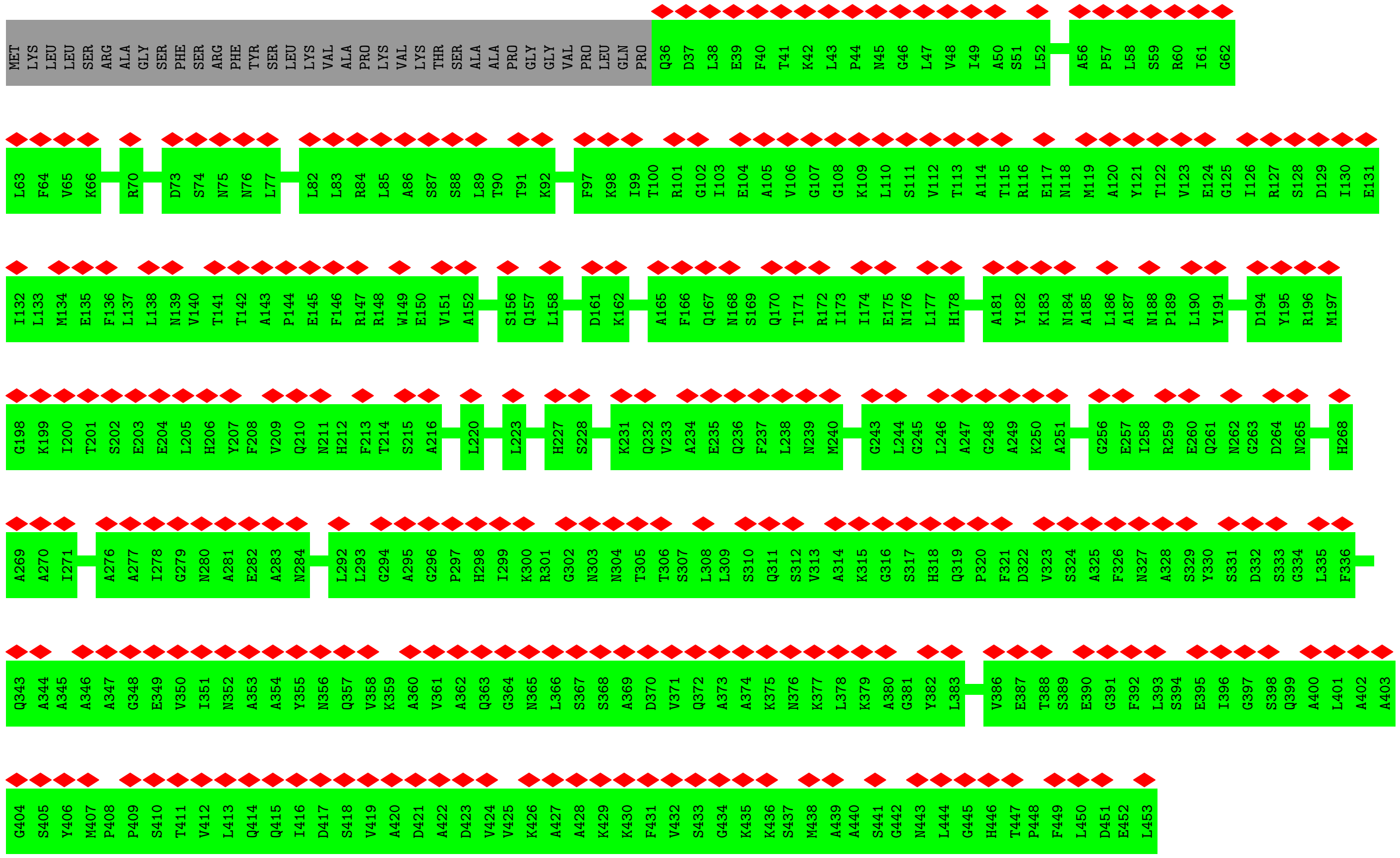




- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

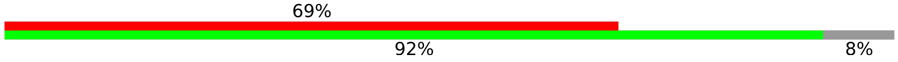
Chain AB:

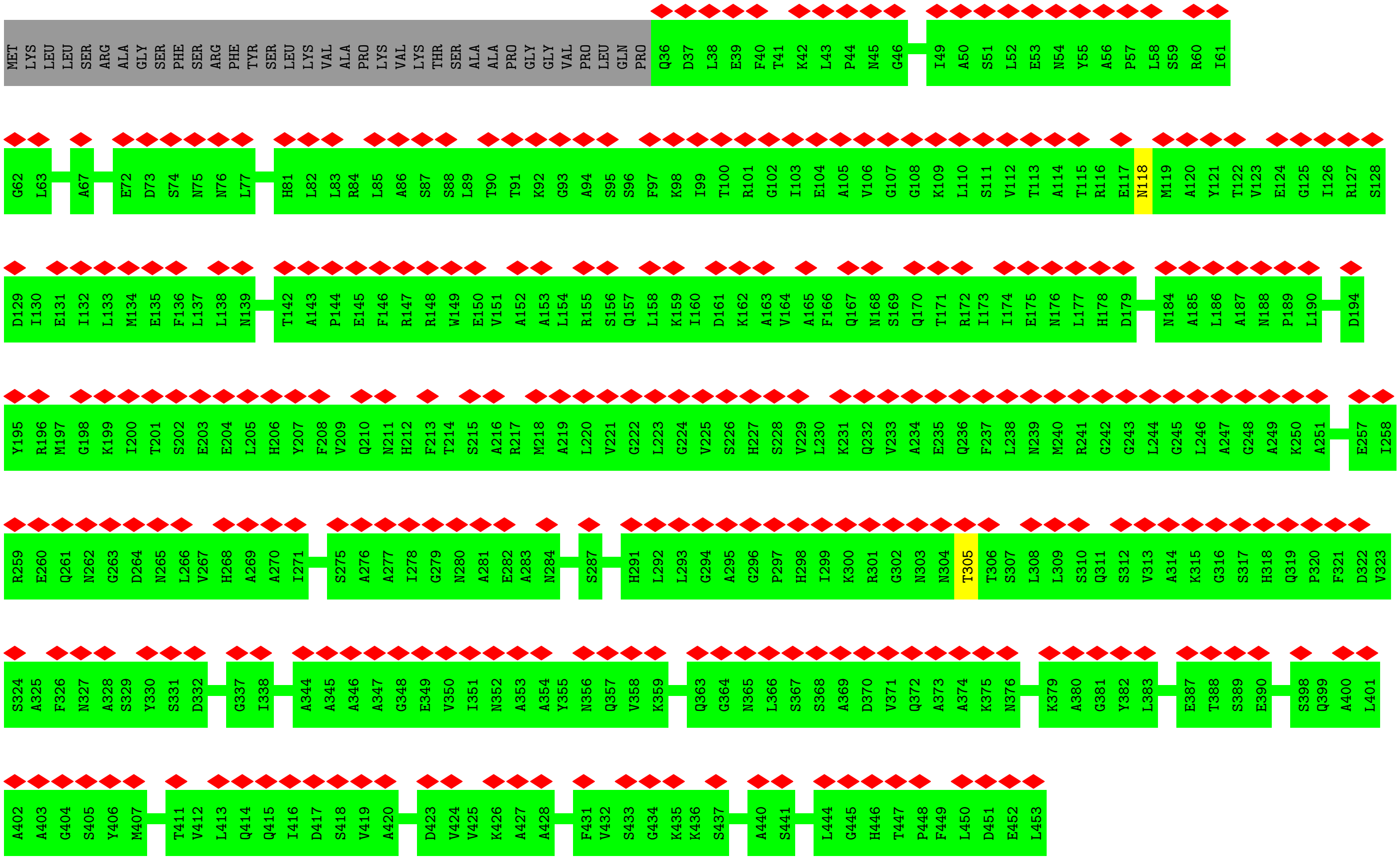




- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

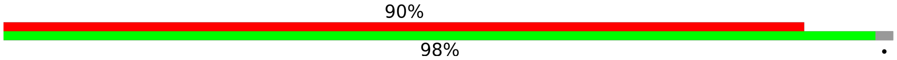
Chain Ab:

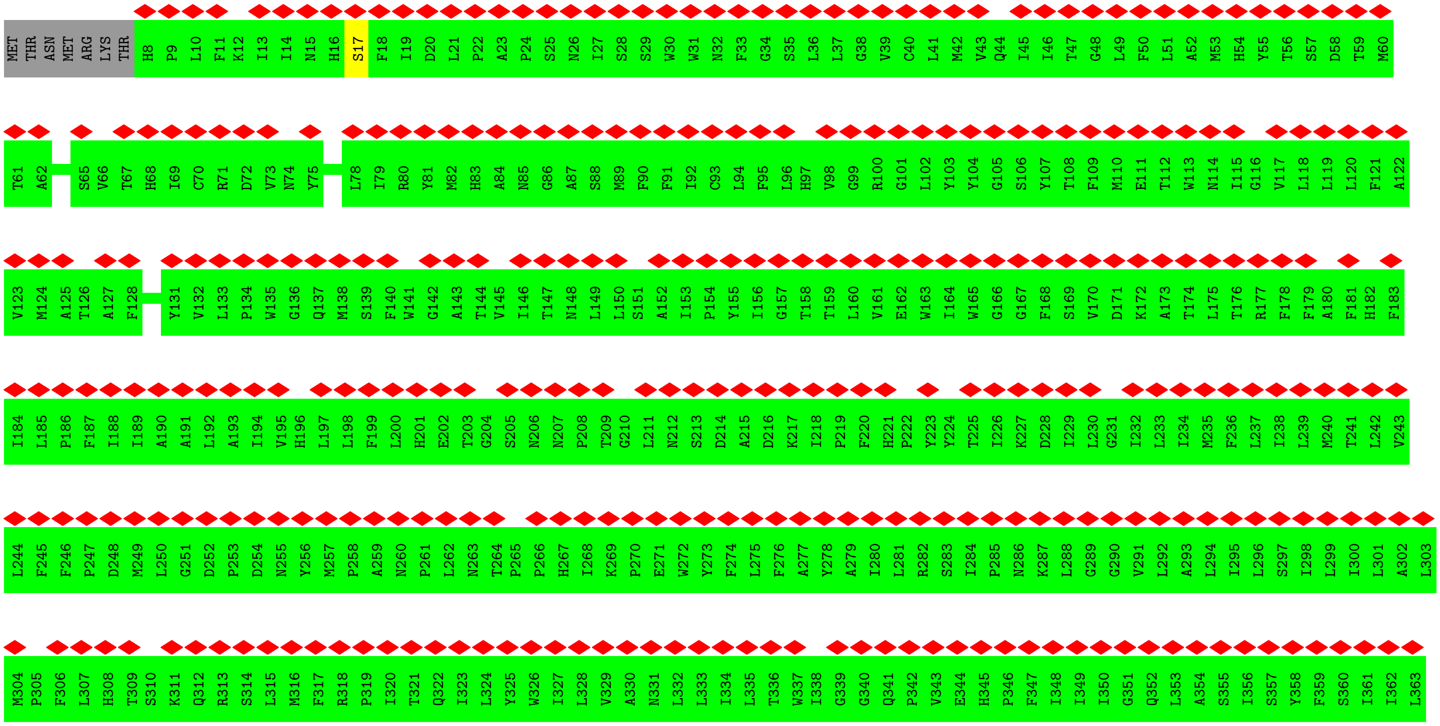


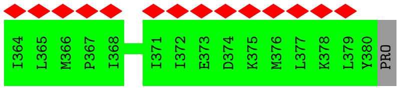


- Molecule 47: Cytochrome b

Chain AC:

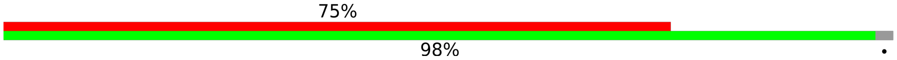


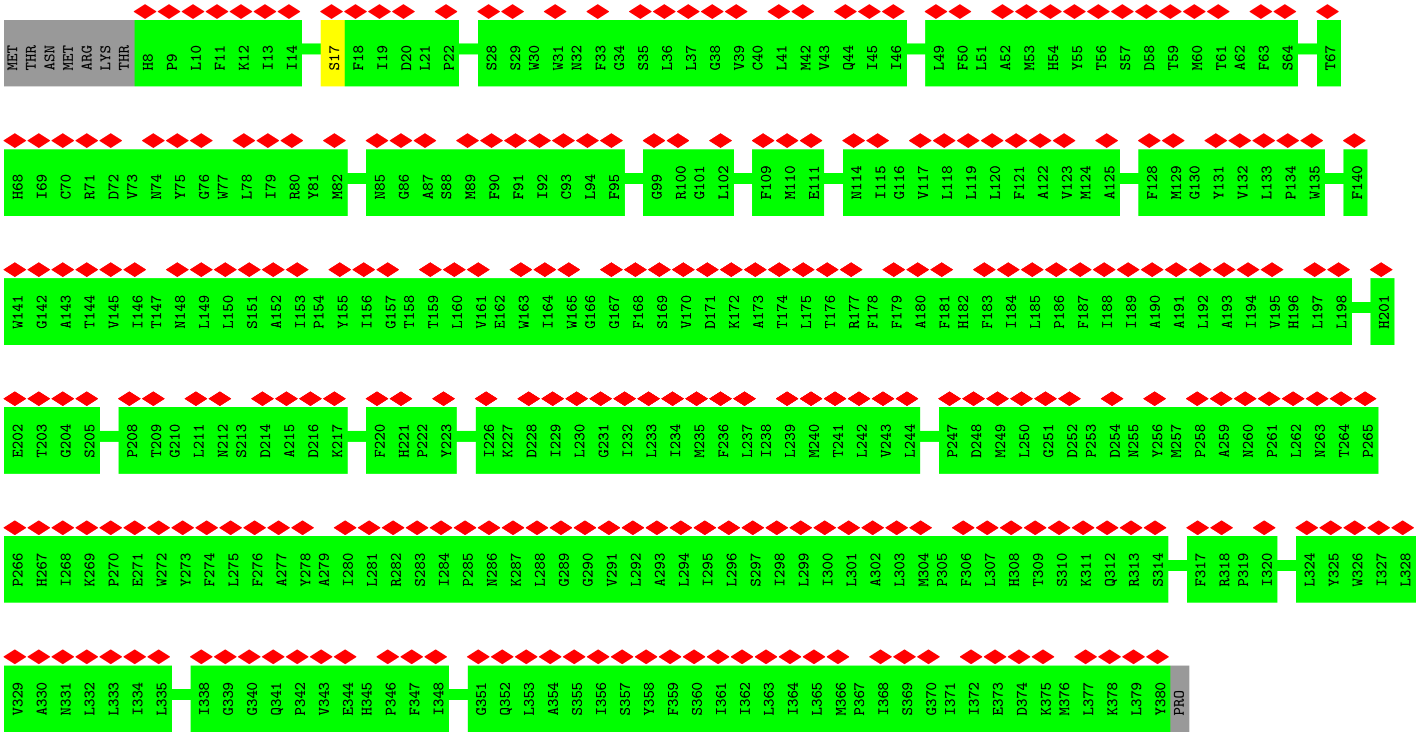




- Molecule 47: Cytochrome b

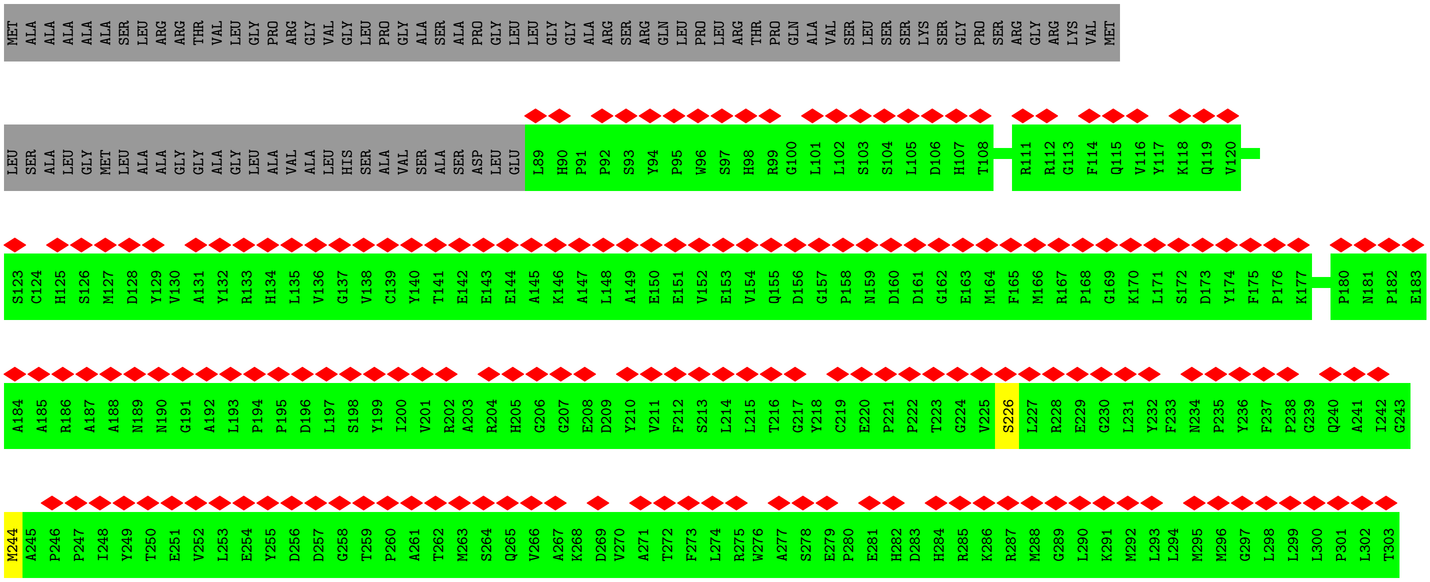
Chain Ac:

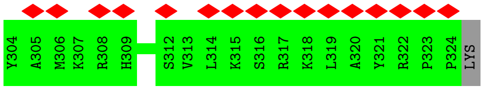




- Molecule 48: Cytochrome c1, heme protein, mitochondrial

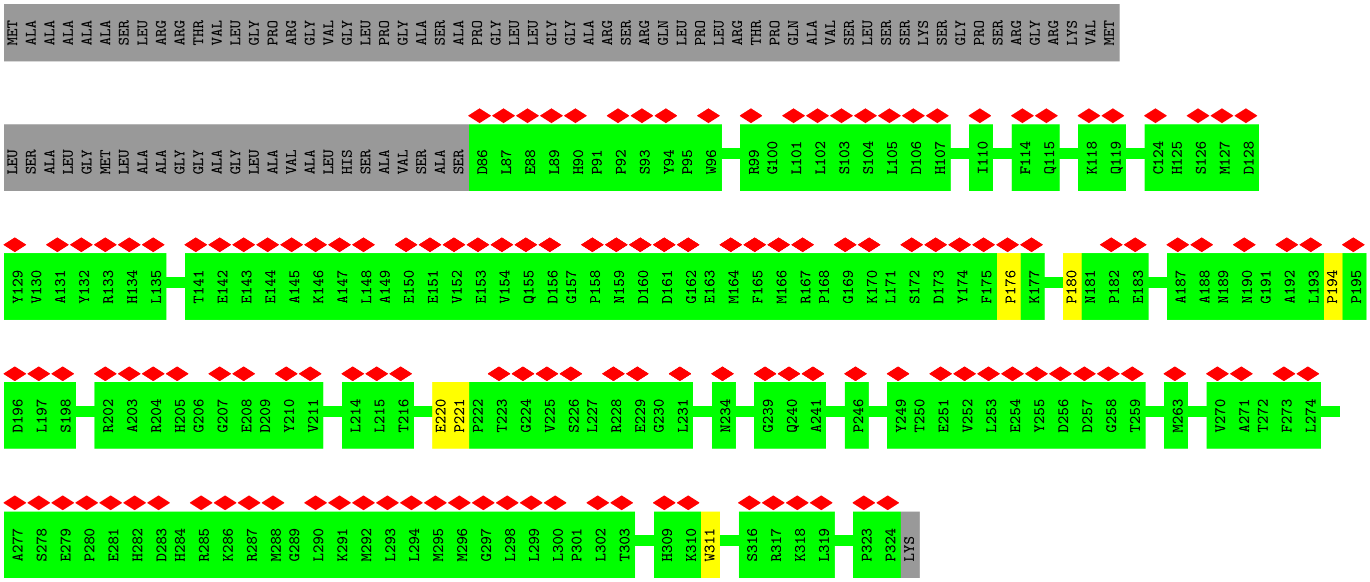
Chain AD:





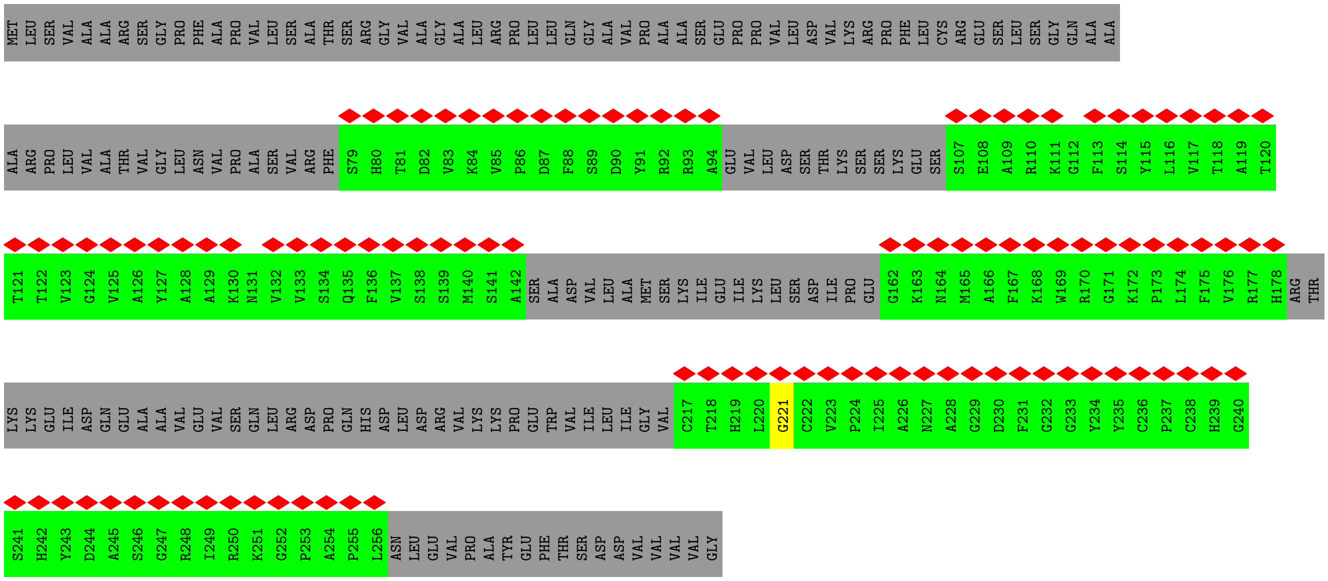
- Molecule 48: Cytochrome c1, heme protein, mitochondrial

Chain Ad:



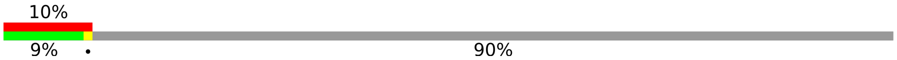
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

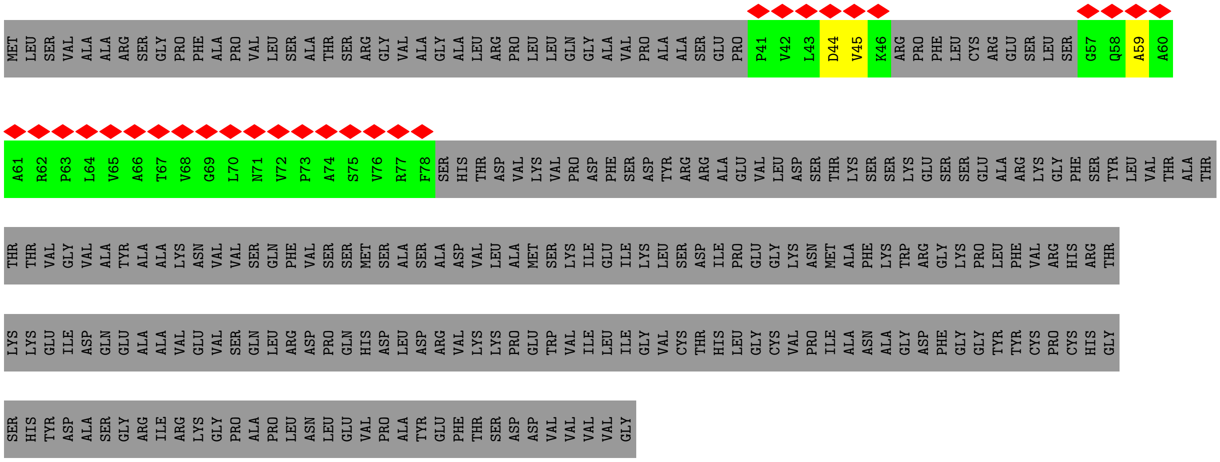
Chain AE:



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

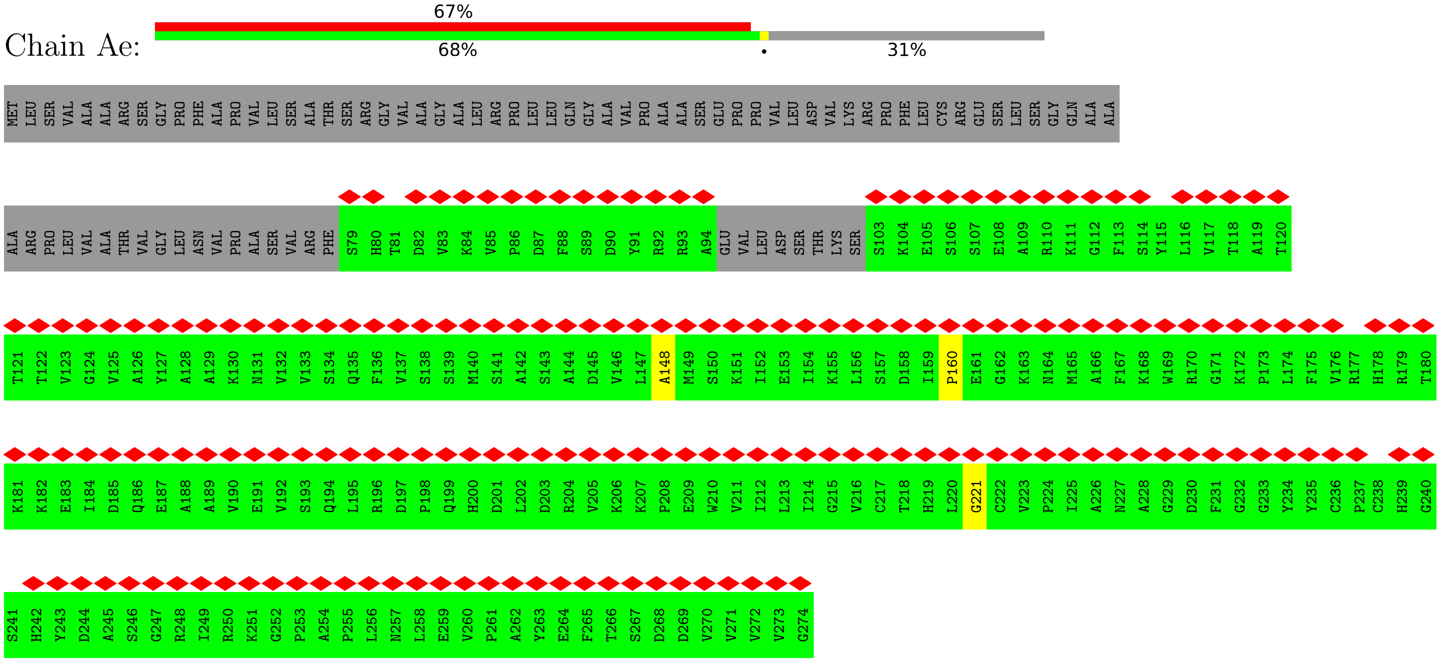
Chain AI:





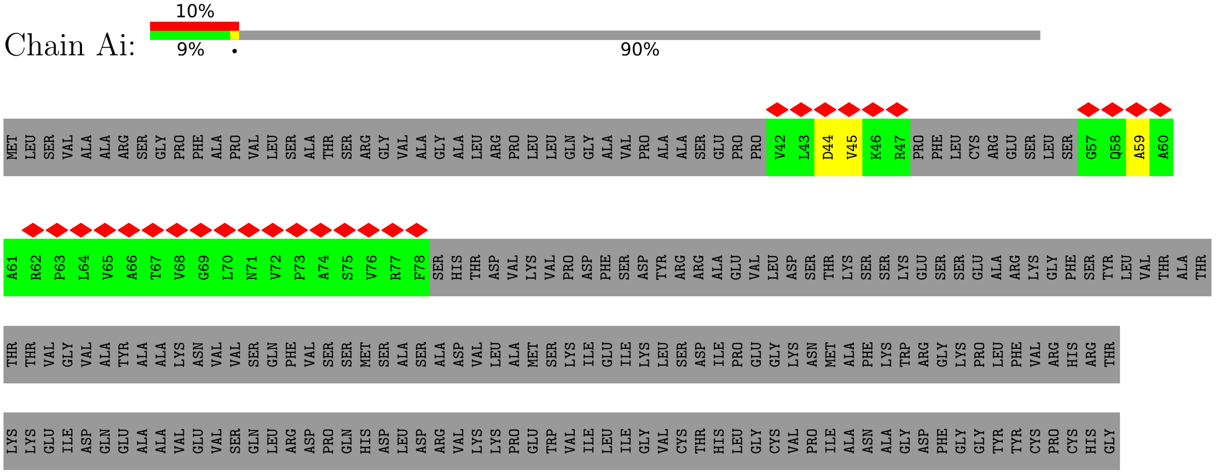
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



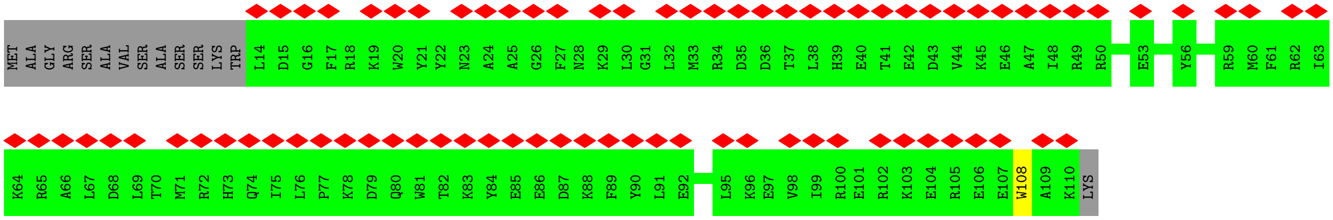
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ai:



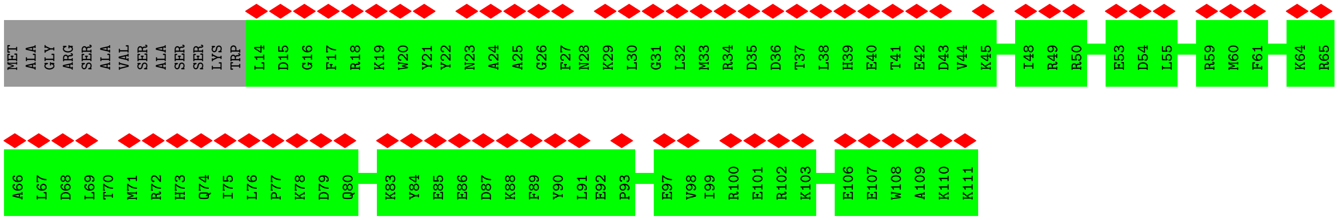
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain AF:



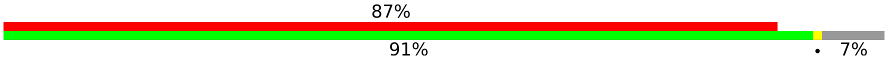
- Molecule 50: Cytochrome b-c1 complex subunit 7

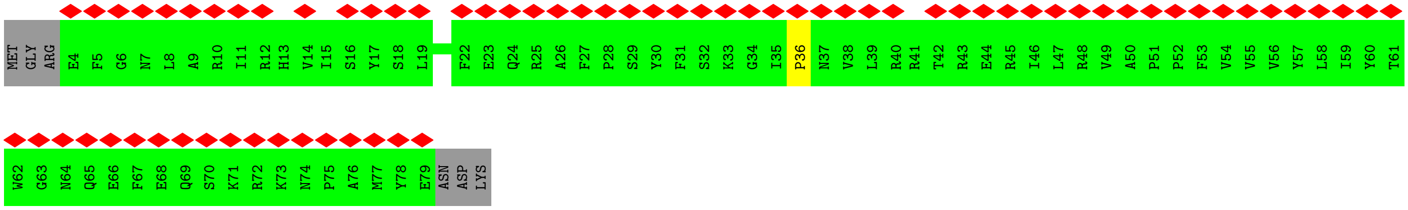
Chain Af:



- Molecule 51: Cytochrome b-c1 complex subunit 8

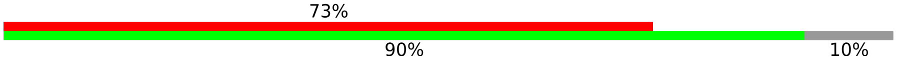
Chain AG:

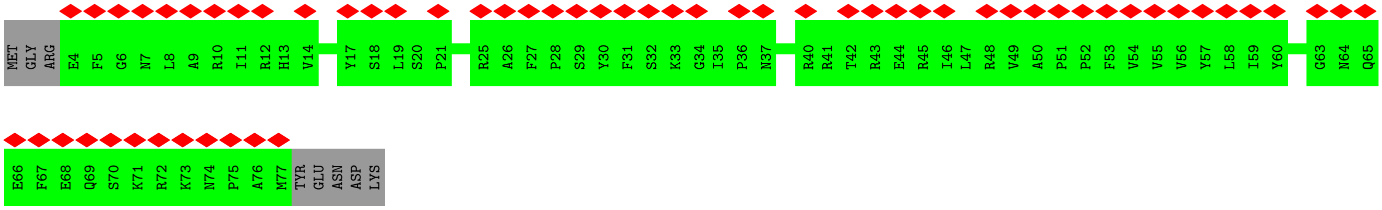




- Molecule 51: Cytochrome b-c1 complex subunit 8

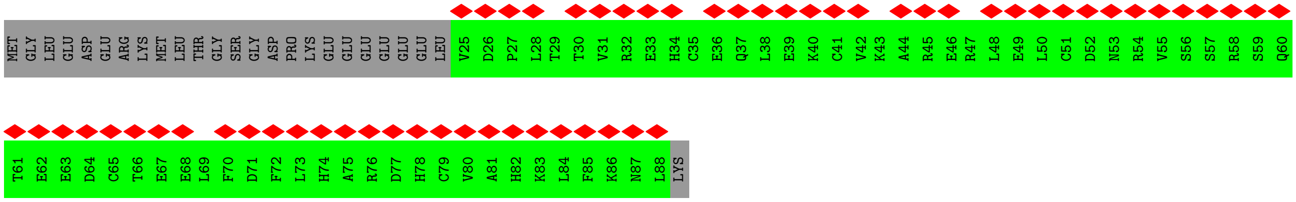
Chain Ag:





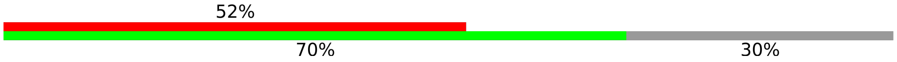
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

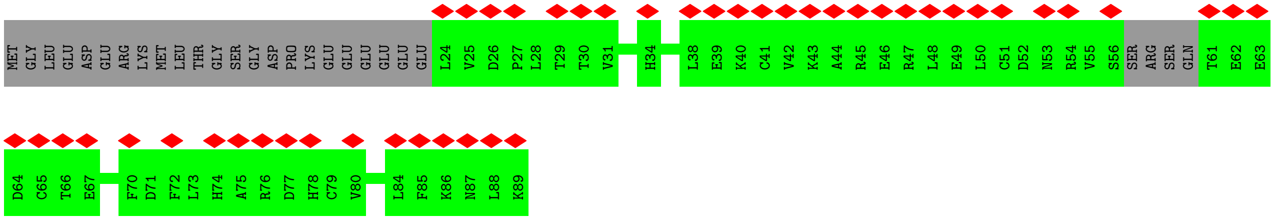
Chain AH:



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

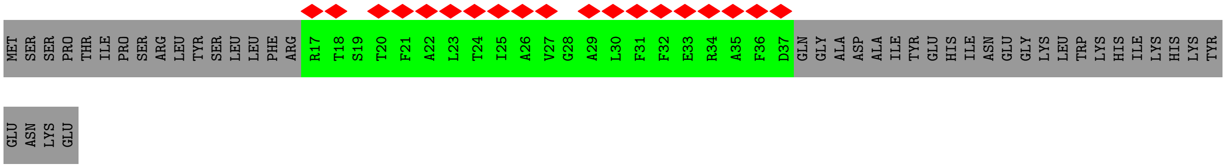
Chain Ah:





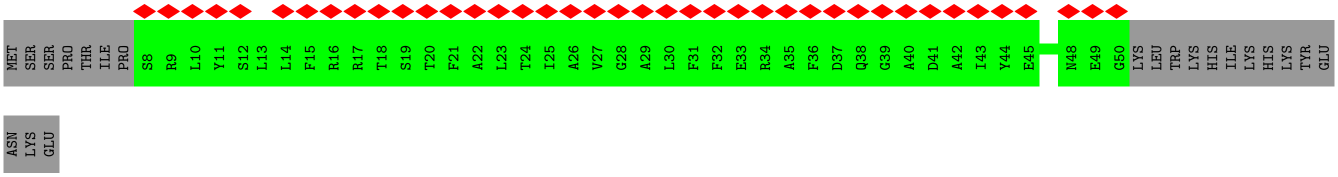
- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ:



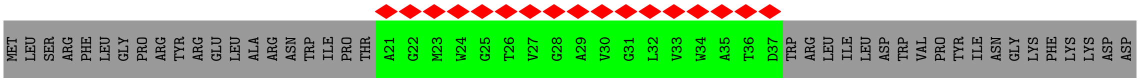
- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



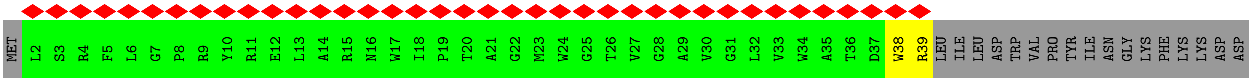
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain AK:



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain Ak:


MET
L2
S3
R4
F5
L6
G7
P8
R9
Y10
R11
E12
L13
A14
R15
N16
W17
I18
P19
T20
A21
G22
M23
W24
G25
T26
V27
G28
A29
V30
G31
L32
V33
W34
A35
T36
D37
W38
R39
LEU
ILE
LEU
ASP
TRP
VAL
PRO
TYR
ILE
ASN
GLY
LYS
PHE
LYS
LYS
ASP
ASP

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62294	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 $(e^-/\text{Å}^2)$	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	0.114	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.67	1/820 (0.1%)	0.77	2/1118 (0.2%)
2	B	0.82	4/1272 (0.3%)	1.04	10/1722 (0.6%)
3	C	0.66	0/1689	0.90	3/2300 (0.1%)
4	D	0.65	1/3527 (0.0%)	0.91	11/4776 (0.2%)
5	E	0.53	1/1675 (0.1%)	0.81	6/2282 (0.3%)
6	F	0.65	5/3363 (0.1%)	0.90	8/4543 (0.2%)
7	G	0.66	5/5374 (0.1%)	0.99	20/7281 (0.3%)
8	H	0.56	0/2608	0.79	8/3563 (0.2%)
9	I	0.65	2/1409 (0.1%)	0.92	5/1904 (0.3%)
10	J	0.55	0/1257	0.72	1/1704 (0.1%)
11	K	0.59	0/740	0.83	2/1005 (0.2%)
12	L	0.69	6/4921 (0.1%)	0.90	18/6696 (0.3%)
13	M	0.69	5/3717 (0.1%)	0.90	10/5062 (0.2%)
14	N	0.67	2/2756 (0.1%)	0.86	7/3751 (0.2%)
15	O	0.77	7/2666 (0.3%)	0.89	19/3615 (0.5%)
16	P	0.55	2/2793 (0.1%)	0.76	6/3787 (0.2%)
17	Q	0.66	3/963 (0.3%)	0.87	2/1302 (0.2%)
18	R	0.45	0/671	0.70	0/903
19	S	0.58	1/678 (0.1%)	0.91	4/915 (0.4%)
20	T	0.47	0/613	0.62	0/826
20	U	0.62	0/731	0.79	1/988 (0.1%)
21	V	0.54	0/937	0.71	0/1270
22	W	0.65	1/993 (0.1%)	0.66	2/1335 (0.1%)
23	X	0.47	0/1422	0.65	0/1921
24	Y	0.52	0/1054	0.59	0/1429
25	Z	0.58	1/1176 (0.1%)	0.82	5/1587 (0.3%)
26	a	0.58	0/561	0.95	2/755 (0.3%)
27	b	0.52	0/651	0.69	2/895 (0.2%)
28	c	0.81	1/400 (0.2%)	0.96	3/544 (0.6%)
29	d	0.77	2/1028 (0.2%)	0.75	5/1387 (0.4%)
30	e	0.50	1/900 (0.1%)	0.65	0/1199
31	f	0.62	0/451	0.85	3/607 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.67	1/886 (0.1%)	0.92	3/1207 (0.2%)
33	h	0.55	1/1197 (0.1%)	0.78	0/1621
34	i	0.56	0/829	0.74	0/1127
35	j	0.55	0/588	0.82	2/805 (0.2%)
36	k	0.64	1/600 (0.2%)	0.83	1/810 (0.1%)
37	l	0.67	2/1367 (0.1%)	0.75	2/1866 (0.1%)
38	m	0.68	1/1079 (0.1%)	0.80	2/1463 (0.1%)
39	n	0.64	1/1596 (0.1%)	0.80	3/2162 (0.1%)
40	o	0.54	0/1075	0.63	0/1442
41	p	0.52	0/1485	0.73	3/2007 (0.1%)
42	q	0.65	2/1059 (0.2%)	0.82	3/1439 (0.2%)
43	r	0.67	2/701 (0.3%)	0.95	1/948 (0.1%)
44	s	0.81	0/198	1.04	0/269
45	AA	0.42	0/3134	0.62	1/4248 (0.0%)
45	Aa	0.41	0/3134	0.66	4/4248 (0.1%)
46	AB	0.35	0/3187	0.56	0/4308
46	Ab	0.40	0/3187	0.61	2/4308 (0.0%)
47	AC	0.37	0/3089	0.58	1/4221 (0.0%)
47	Ac	0.35	0/3089	0.56	1/4221 (0.0%)
48	AD	0.36	0/1937	0.61	3/2632 (0.1%)
48	Ad	0.68	3/1962 (0.2%)	0.65	3/2666 (0.1%)
49	AE	0.37	0/851	0.59	1/1146 (0.1%)
49	AI	0.90	2/202 (1.0%)	0.96	3/274 (1.1%)
49	Ae	0.44	0/1483	0.68	2/2007 (0.1%)
49	Ai	0.89	2/205 (1.0%)	1.02	3/277 (1.1%)
50	AF	0.41	0/875	0.55	1/1173 (0.1%)
50	Af	0.33	0/884	0.50	0/1184
51	AG	0.42	1/662 (0.2%)	0.63	0/895
51	Ag	0.39	0/640	0.57	0/865
52	AH	0.33	0/534	0.48	0/717
52	Ah	0.46	0/518	0.68	0/694
53	AJ	0.30	0/168	0.41	0/226
53	Aj	0.39	0/352	0.51	0/474
54	AK	0.33	0/121	0.58	0/166
54	Ak	0.32	0/320	0.74	2/437 (0.5%)
All	All	0.58	70/97010 (0.1%)	0.78	212/131525 (0.2%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Ad	221	PRO	N-CD	18.44	1.73	1.47
15	O	247	PRO	N-CD	16.58	1.71	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	115	PRO	N-CD	-14.22	1.27	1.47
12	L	265	PRO	N-CD	13.77	1.67	1.47
14	N	255	PRO	N-CD	-13.72	1.28	1.47
28	c	39	PRO	N-CD	-13.29	1.29	1.47
38	m	27	PRO	N-CD	-13.01	1.29	1.47
7	G	532	PRO	N-CD	-12.70	1.30	1.47
22	W	131	PRO	N-CD	-12.46	1.30	1.47
15	O	315	PRO	N-CD	-12.11	1.30	1.47
48	Ad	180	PRO	N-CD	11.20	1.63	1.47
1	A	36	PRO	N-CD	-11.16	1.32	1.47
12	L	234	PRO	N-CD	11.08	1.63	1.47
42	q	143	PRO	N-CD	-10.60	1.33	1.47
15	O	210	PRO	N-CD	-10.54	1.33	1.47
13	M	370	PRO	N-CD	-10.53	1.33	1.47
15	O	224	PRO	N-CD	-10.28	1.33	1.47
16	P	333	PRO	N-CD	-10.22	1.33	1.47
6	F	227	PRO	N-CD	10.06	1.61	1.47
4	D	365	PRO	N-CD	-9.68	1.34	1.47
32	g	78	PRO	N-CD	-9.64	1.34	1.47
7	G	275	PRO	N-CD	-9.47	1.34	1.47
29	d	15	PRO	N-CD	-9.44	1.34	1.47
2	B	92	PRO	N-CD	9.34	1.60	1.47
6	F	319	PRO	N-CD	8.96	1.60	1.47
15	O	212	PRO	N-CD	-8.90	1.35	1.47
25	Z	102	PRO	N-CD	-8.83	1.35	1.47
49	Ai	45	VAL	C-N	8.57	1.53	1.34
13	M	20	PRO	N-CD	8.54	1.59	1.47
9	I	107	PRO	N-CD	8.53	1.59	1.47
49	AI	45	VAL	C-N	8.51	1.53	1.34
12	L	212	PRO	N-CD	-8.33	1.36	1.47
42	q	139	PRO	N-CD	-8.02	1.36	1.47
39	n	155	PRO	N-CD	8.01	1.59	1.47
49	AI	44	ASP	C-N	7.88	1.52	1.34
49	Ai	44	ASP	C-N	7.81	1.52	1.34
37	l	104	PRO	N-CD	-7.24	1.37	1.47
43	r	65	PRO	N-CD	7.10	1.57	1.47
14	N	238	PRO	N-CD	-7.09	1.38	1.47
13	M	208	PRO	N-CD	7.08	1.57	1.47
7	G	541	PRO	N-CD	-6.89	1.38	1.47
7	G	449	PRO	N-CD	6.78	1.57	1.47
6	F	234	GLY	CA-C	-6.76	1.41	1.51
48	Ad	176	PRO	N-CD	-6.69	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	e	106	PRO	N-CD	6.64	1.57	1.47
51	AG	36	PRO	N-CD	6.51	1.56	1.47
17	Q	155	PRO	N-CD	-6.40	1.38	1.47
9	I	154	TYR	C-O	6.25	1.35	1.23
12	L	57	ASN	C-O	-6.22	1.11	1.23
6	F	384	PRO	N-CD	-6.21	1.39	1.47
2	B	121	PHE	C-O	-6.21	1.11	1.23
16	P	292	PRO	N-CD	-6.20	1.39	1.47
12	L	384	PRO	N-CD	6.16	1.56	1.47
5	E	93	PRO	N-CD	-6.03	1.39	1.47
36	k	20	MET	C-N	5.92	1.47	1.34
6	F	235	VAL	N-CA	-5.88	1.34	1.46
12	L	112	PRO	N-CD	5.87	1.56	1.47
15	O	87	PRO	N-CD	-5.81	1.39	1.47
37	l	45	PRO	N-CD	-5.80	1.39	1.47
2	B	122	ARG	CA-CB	-5.73	1.41	1.53
17	Q	106	ARG	C-O	5.72	1.34	1.23
19	S	63	PRO	N-CD	-5.71	1.39	1.47
17	Q	82	PRO	N-CD	-5.65	1.40	1.47
13	M	252	PRO	N-CD	-5.61	1.40	1.47
2	B	170	TYR	CB-CG	-5.54	1.43	1.51
7	G	683	PRO	N-CD	-5.46	1.40	1.47
15	O	103	PRO	N-CD	-5.38	1.40	1.47
43	r	37	PRO	N-CD	5.34	1.55	1.47
33	h	174	PRO	N-CD	-5.21	1.40	1.47
13	M	159	PRO	N-CD	5.01	1.54	1.47

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	122	ARG	N-CA-CB	-13.93	85.52	110.60
26	a	3	PHE	CB-CA-C	-10.35	89.71	110.40
14	N	255	PRO	CA-N-CD	9.94	125.61	111.70
15	O	206	TYR	N-CA-CB	-9.90	92.77	110.60
29	d	115	PRO	CA-N-CD	9.63	125.18	111.70
45	Aa	366	ASP	CB-CG-OD1	9.48	126.83	118.30
2	B	121	PHE	N-CA-C	-9.17	86.23	111.00
15	O	247	PRO	N-CA-CB	9.17	114.30	103.30
5	E	219	SER	N-CA-CB	9.03	124.04	110.50
6	F	334	THR	N-CA-CB	8.96	127.31	110.30
38	m	27	PRO	CA-N-CD	8.95	124.24	111.70
35	j	82	GLY	N-CA-C	-8.82	91.04	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	247	PRO	CA-N-CD	-8.76	99.23	111.50
15	O	315	PRO	CA-N-CD	8.73	123.93	111.70
8	H	197	PRO	N-CA-CB	8.69	113.73	103.30
4	D	360	ASP	N-CA-C	-8.62	87.74	111.00
7	G	532	PRO	CA-N-CD	8.56	123.69	111.70
22	W	131	PRO	CA-N-CD	8.54	123.65	111.70
25	Z	102	PRO	N-CA-CB	-8.41	93.20	103.30
8	H	196	ALA	N-CA-C	8.14	132.97	111.00
28	c	39	PRO	CA-N-CD	8.13	123.08	111.70
7	G	174	THR	N-CA-C	-8.12	89.07	111.00
25	Z	144	THR	N-CA-CB	-8.03	95.05	110.30
4	D	359	ASP	CB-CA-C	-7.85	94.71	110.40
2	B	170	TYR	N-CA-C	-7.80	89.93	111.00
1	A	36	PRO	CA-N-CD	7.73	122.52	111.70
2	B	122	ARG	CB-CA-C	7.57	125.53	110.40
6	F	411	SER	N-CA-CB	7.53	121.79	110.50
1	A	36	PRO	N-CA-CB	-7.52	94.28	103.30
8	H	231	ILE	N-CA-C	-7.42	90.97	111.00
15	O	210	PRO	CA-N-CD	7.40	122.06	111.70
12	L	265	PRO	CA-N-CD	-7.40	101.14	111.50
19	S	51	LEU	N-CA-C	-7.38	91.07	111.00
8	H	52	ALA	N-CA-CB	7.36	120.40	110.10
46	Ab	118	ASN	N-CA-CB	-7.30	97.45	110.60
7	G	204	MET	N-CA-C	-7.26	91.41	111.00
14	N	255	PRO	N-CA-CB	-7.25	94.61	103.30
2	B	99	CYS	N-CA-C	-7.24	91.45	111.00
15	O	220	LYS	CB-CA-C	-7.09	96.22	110.40
6	F	332	CYS	N-CA-C	7.08	130.11	111.00
32	g	78	PRO	CA-N-CD	7.07	121.60	111.70
39	n	165	PRO	N-CA-C	7.04	130.41	112.10
8	H	231	ILE	N-CA-CB	7.01	126.93	110.80
16	P	333	PRO	CA-N-CD	6.99	121.49	111.70
9	I	62	MET	N-CA-C	-6.99	92.12	111.00
25	Z	102	PRO	N-CA-C	6.94	130.15	112.10
12	L	265	PRO	N-CA-CB	6.93	111.62	103.30
29	d	115	PRO	N-CA-CB	-6.92	94.99	102.60
28	c	47	SER	N-CA-CB	6.90	120.84	110.50
15	O	224	PRO	CA-N-CD	6.87	121.32	111.70
54	Ak	39	ARG	N-CA-CB	6.87	122.97	110.60
25	Z	143	TYR	N-CA-C	6.84	129.48	111.00
7	G	380	ASP	N-CA-C	6.79	129.32	111.00
13	M	213	HIS	CB-CA-C	-6.78	96.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	r	64	VAL	N-CA-CB	-6.76	96.63	111.50
4	D	365	PRO	CA-N-CD	6.71	121.09	111.70
41	p	128	GLU	N-CA-CB	-6.70	98.54	110.60
7	G	275	PRO	CA-N-CD	6.66	121.02	111.70
15	O	222	GLY	N-CA-C	6.65	129.73	113.10
28	c	39	PRO	N-CA-CB	-6.61	95.33	102.60
7	G	300	GLN	N-CA-CB	6.59	122.46	110.60
38	m	27	PRO	N-CA-CB	-6.58	95.36	102.60
42	q	143	PRO	CA-N-CD	6.58	120.91	111.70
5	E	64	ALA	N-CA-CB	6.57	119.30	110.10
29	d	15	PRO	CA-N-CD	6.57	120.89	111.70
15	O	320	GLY	N-CA-C	-6.57	96.69	113.10
5	E	166	LYS	CB-CA-C	6.56	123.52	110.40
22	W	131	PRO	N-CA-CB	-6.54	95.40	102.60
31	f	51	ASN	CB-CA-C	-6.54	97.33	110.40
36	k	59	TYR	N-CA-CB	-6.51	98.87	110.60
6	F	125	CYS	N-CA-C	-6.51	93.43	111.00
5	E	235	GLU	N-CA-CB	6.46	122.23	110.60
27	b	78	LEU	CB-CA-C	-6.40	98.04	110.20
4	D	427	PRO	N-CA-C	-6.38	95.52	112.10
8	H	203	GLY	N-CA-C	-6.35	97.22	113.10
8	H	196	ALA	C-N-CD	6.34	141.72	128.40
39	n	115	TYR	N-CA-CB	6.33	122.00	110.60
2	B	155	PRO	N-CA-C	-6.32	95.68	112.10
13	M	370	PRO	N-CA-C	6.30	128.48	112.10
13	M	424	ILE	N-CA-C	-6.30	93.99	111.00
14	N	255	PRO	N-CA-C	6.27	128.39	112.10
13	M	370	PRO	CA-N-CD	6.21	120.39	111.70
49	AI	59	ALA	N-CA-CB	-6.21	101.41	110.10
49	Ai	59	ALA	N-CA-CB	-6.17	101.47	110.10
32	g	137	SER	N-CA-CB	-6.16	101.27	110.50
14	N	81	LEU	N-CA-C	-6.14	94.42	111.00
7	G	212	LYS	N-CA-C	-6.09	94.56	111.00
7	G	83	GLU	N-CA-C	6.09	127.43	111.00
50	AF	108	TRP	N-CA-CB	6.08	121.54	110.60
7	G	133	GLN	N-CA-CB	6.04	121.48	110.60
49	Ae	148	ALA	N-CA-CB	6.04	118.56	110.10
8	H	207	LEU	N-CA-C	-6.02	94.75	111.00
15	O	315	PRO	N-CA-CB	-6.01	95.99	102.60
12	L	231	PRO	N-CA-C	6.01	127.72	112.10
45	AA	154	SER	N-CA-C	-6.00	94.79	111.00
12	L	234	PRO	CA-N-CD	-6.00	103.10	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	110	ALA	N-CA-CB	-6.00	101.70	110.10
12	L	276	THR	N-CA-CB	5.95	121.61	110.30
16	P	97	MET	N-CA-CB	5.95	121.32	110.60
45	Aa	48	THR	N-CA-CB	5.95	121.61	110.30
14	N	218	ALA	N-CA-CB	5.93	118.41	110.10
12	L	554	ASP	N-CA-CB	5.93	121.28	110.60
12	L	605	ASN	N-CA-CB	5.93	121.27	110.60
12	L	483	PRO	N-CA-C	-5.88	96.81	112.10
5	E	50	THR	N-CA-CB	5.88	121.47	110.30
9	I	119	CYS	N-CA-C	5.88	126.86	111.00
48	AD	226	SER	N-CA-C	5.88	126.87	111.00
31	f	52	GLU	N-CA-CB	5.87	121.16	110.60
7	G	251	ILE	N-CA-C	5.85	126.79	111.00
9	I	118	LEU	N-CA-C	5.84	126.77	111.00
4	D	358	VAL	N-CA-C	-5.83	95.26	111.00
4	D	361	ALA	N-CA-CB	-5.81	101.97	110.10
16	P	172	ALA	N-CA-CB	5.79	118.21	110.10
6	F	103	ASN	N-CA-CB	5.79	121.03	110.60
4	D	329	ARG	CB-CA-C	5.77	121.95	110.40
42	q	143	PRO	N-CA-CB	-5.76	96.26	102.60
11	K	83	ASN	N-CA-CB	5.73	120.92	110.60
20	U	150	ASP	CB-CA-C	5.73	121.86	110.40
7	G	510	TRP	N-CA-CB	5.72	120.90	110.60
13	M	223	ALA	N-CA-CB	5.71	118.09	110.10
47	Ac	17	SER	N-CA-CB	-5.66	102.01	110.50
14	N	89	GLN	N-CA-CB	-5.65	100.43	110.60
3	C	180	HIS	N-CA-C	-5.64	95.76	111.00
37	l	119	THR	N-CA-C	-5.64	95.78	111.00
4	D	143	SER	CB-CA-C	5.63	120.80	110.10
17	Q	59	LEU	N-CA-CB	-5.63	99.13	110.40
29	d	15	PRO	N-CA-CB	-5.63	96.40	102.60
12	L	415	ALA	N-CA-CB	5.63	117.98	110.10
47	AC	17	SER	N-CA-CB	-5.62	102.06	110.50
7	G	599	THR	N-CA-C	5.61	126.14	111.00
7	G	580	ALA	N-CA-CB	5.59	117.93	110.10
15	O	118	TYR	N-CA-CB	-5.58	100.56	110.60
54	Ak	38	TRP	N-CA-C	5.58	126.05	111.00
3	C	240	ALA	N-CA-CB	-5.57	102.30	110.10
19	S	57	GLU	N-CA-C	5.56	126.02	111.00
25	Z	102	PRO	CA-N-CD	5.54	119.46	111.70
48	Ad	220	GLU	C-N-CD	5.54	140.03	128.40
19	S	61	VAL	N-CA-C	-5.54	96.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	96	LEU	CB-CA-C	-5.53	99.70	110.20
7	G	653	LEU	N-CA-CB	5.52	121.45	110.40
49	Ae	221	GLY	N-CA-C	5.52	126.90	113.10
49	AE	221	GLY	N-CA-C	5.52	126.90	113.10
15	O	118	TYR	N-CA-C	5.51	125.88	111.00
13	M	311	GLY	N-CA-C	-5.51	99.33	113.10
9	I	119	CYS	N-CA-CB	-5.50	100.70	110.60
4	D	257	GLU	N-CA-CB	5.49	120.48	110.60
48	AD	226	SER	N-CA-CB	-5.49	102.27	110.50
39	n	136	GLU	CB-CA-C	5.46	121.31	110.40
15	O	212	PRO	N-CA-C	5.45	126.26	112.10
12	L	582	GLY	N-CA-C	-5.43	99.52	113.10
4	D	114	GLY	N-CA-C	-5.43	99.53	113.10
15	O	246	LEU	C-N-CD	5.40	139.74	128.40
7	G	662	THR	N-CA-C	-5.39	96.45	111.00
45	Aa	47	GLU	N-CA-C	5.38	125.53	111.00
45	Aa	110	GLU	N-CA-CB	5.38	120.28	110.60
42	q	139	PRO	CA-N-CD	5.38	119.23	111.70
6	F	457	HIS	N-CA-CB	-5.36	100.95	110.60
49	Ai	44	ASP	O-C-N	5.36	131.27	122.70
15	O	152	SER	N-CA-CB	5.34	118.52	110.50
13	M	276	CYS	N-CA-CB	5.34	120.21	110.60
7	G	362	ASP	N-CA-C	5.34	125.41	111.00
48	Ad	180	PRO	CA-N-CD	-5.33	104.03	111.50
12	L	151	SER	N-CA-CB	5.33	118.50	110.50
12	L	194	ASN	N-CA-C	5.31	125.34	111.00
15	O	224	PRO	N-CA-CB	-5.31	96.76	102.60
6	F	418	GLN	N-CA-CB	5.30	120.14	110.60
2	B	121	PHE	CA-C-O	-5.26	109.04	120.10
5	E	218	ARG	CB-CA-C	-5.26	99.87	110.40
12	L	234	PRO	N-CA-CB	5.26	109.61	103.30
46	Ab	305	THR	N-CA-CB	-5.25	100.32	110.30
49	Ai	45	VAL	C-N-CA	-5.25	108.56	121.70
12	L	212	PRO	N-CA-C	5.25	125.76	112.10
13	M	330	ALA	N-CA-CB	5.25	117.45	110.10
19	S	61	VAL	N-CA-CB	5.25	123.05	111.50
41	p	128	GLU	N-CA-C	5.25	125.17	111.00
17	Q	155	PRO	N-CA-CB	-5.24	96.83	102.60
7	G	640	ASP	N-CA-CB	5.24	120.03	110.60
12	L	248	HIS	CB-CA-C	5.24	120.88	110.40
11	K	70	GLU	N-CA-CB	5.24	120.03	110.60
49	AI	45	VAL	C-N-CA	-5.24	108.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	113	LEU	N-CA-CB	-5.23	99.93	110.40
41	p	94	ARG	NE-CZ-NH1	5.23	122.92	120.30
13	M	423	MET	N-CA-C	-5.23	96.89	111.00
4	D	457	VAL	N-CA-C	-5.22	96.90	111.00
48	Ad	180	PRO	N-CA-CB	5.22	109.56	103.30
12	L	277	MET	CB-CA-C	-5.21	99.97	110.40
49	AI	44	ASP	O-C-N	5.21	131.04	122.70
12	L	212	PRO	CA-N-CD	5.21	118.99	111.70
35	j	102	ASP	CB-CG-OD2	5.20	122.98	118.30
15	O	212	PRO	CA-N-CD	5.20	118.98	111.70
2	B	122	ARG	N-CA-C	5.17	124.96	111.00
15	O	220	LYS	N-CA-C	5.15	124.92	111.00
10	J	76	GLU	N-CA-C	-5.15	97.09	111.00
37	l	104	PRO	CA-N-CD	5.14	118.89	111.70
31	f	53	GLU	N-CA-CB	-5.13	101.37	110.60
26	a	4	GLU	N-CA-C	5.11	124.79	111.00
32	g	78	PRO	N-CA-CB	-5.11	96.98	102.60
12	L	247	LEU	N-CA-CB	5.10	120.61	110.40
6	F	228	PRO	N-CA-C	-5.10	98.85	112.10
13	M	83	HIS	N-CA-C	-5.09	97.25	111.00
2	B	88	SER	N-CA-CB	5.09	118.14	110.50
15	O	207	ILE	N-CA-C	-5.09	97.27	111.00
48	AD	244	MET	N-CA-C	-5.08	97.28	111.00
7	G	77	MET	N-CA-C	-5.08	97.29	111.00
2	B	97	LEU	CA-CB-CG	5.07	126.96	115.30
27	b	80	TRP	N-CA-CB	5.06	119.72	110.60
14	N	228	ASN	N-CA-CB	5.06	119.71	110.60
3	C	237	PRO	N-CD-CG	-5.05	95.62	103.20
16	P	115	SER	N-CA-C	-5.04	97.38	111.00
9	I	96	ARG	NE-CZ-NH1	-5.03	117.78	120.30
7	G	668	ALA	N-CA-CB	5.03	117.14	110.10
7	G	532	PRO	N-CA-CB	-5.00	97.10	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
2	B	153/224 (68%)	141 (92%)	11 (7%)	1 (1%)	19	56
3	C	196/263 (74%)	189 (96%)	7 (4%)	0	100	100
4	D	423/463 (91%)	398 (94%)	24 (6%)	1 (0%)	44	77
5	E	208/248 (84%)	194 (93%)	14 (7%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	635 (93%)	50 (7%)	0	100	100
8	H	313/318 (98%)	281 (90%)	31 (10%)	1 (0%)	37	71
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	J	157/172 (91%)	148 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	573 (95%)	31 (5%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37	71
15	O	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
16	P	337/377 (89%)	309 (92%)	28 (8%)	0	100	100
17	Q	114/175 (65%)	100 (88%)	14 (12%)	0	100	100
18	R	81/116 (70%)	72 (89%)	9 (11%)	0	100	100
19	S	81/99 (82%)	74 (91%)	7 (9%)	0	100	100
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
20	U	87/156 (56%)	81 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	167/172 (97%)	148 (89%)	19 (11%)	0	100	100
24	Y	137/143 (96%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	136/144 (94%)	129 (95%)	5 (4%)	2 (2%)	8	40
26	a	65/70 (93%)	59 (91%)	6 (9%)	0	100	100
27	b	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	i	91/128 (71%)	81 (89%)	10 (11%)	0	100	100
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	71/104 (68%)	68 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	176/179 (98%)	165 (94%)	10 (6%)	1 (1%)	22	59
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
41	p	170/176 (97%)	153 (90%)	17 (10%)	0	100	100
42	q	119/145 (82%)	110 (92%)	9 (8%)	0	100	100
43	r	78/113 (69%)	75 (96%)	3 (4%)	0	100	100
44	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
45	AA	389/480 (81%)	372 (96%)	17 (4%)	0	100	100
45	Aa	386/480 (80%)	369 (96%)	17 (4%)	0	100	100
46	AB	416/453 (92%)	408 (98%)	8 (2%)	0	100	100
46	Ab	416/453 (92%)	396 (95%)	20 (5%)	0	100	100
47	AC	371/381 (97%)	361 (97%)	10 (3%)	0	100	100
47	Ac	371/381 (97%)	366 (99%)	5 (1%)	0	100	100
48	AD	234/325 (72%)	213 (91%)	21 (9%)	0	100	100
48	Ad	237/325 (73%)	224 (94%)	12 (5%)	1 (0%)	30	67
49	AE	101/274 (37%)	95 (94%)	6 (6%)	0	100	100
49	AI	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
49	Ae	184/274 (67%)	168 (91%)	15 (8%)	1 (0%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Ai	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
50	AF	95/111 (86%)	94 (99%)	1 (1%)	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
51	Ag	72/82 (88%)	72 (100%)	0	0	100	100
52	AH	62/89 (70%)	61 (98%)	1 (2%)	0	100	100
52	Ah	58/89 (65%)	55 (95%)	3 (5%)	0	100	100
53	AJ	19/64 (30%)	19 (100%)	0	0	100	100
53	Aj	41/64 (64%)	40 (98%)	1 (2%)	0	100	100
54	AK	15/56 (27%)	15 (100%)	0	0	100	100
54	Ak	36/56 (64%)	34 (94%)	2 (6%)	0	100	100
All	All	11672/14392 (81%)	11022 (94%)	641 (6%)	9 (0%)	50	82

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	324	GLY
8	H	196	ALA
14	N	109	ALA
25	Z	129	THR
2	B	195	PRO
25	Z	18	PRO
39	n	156	PRO
49	Ae	160	PRO
48	Ad	194	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	89/104 (86%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	131/185 (71%)	131 (100%)	0	100	100
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	368/395 (93%)	368 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	579 (100%)	0	100	100
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	146/178 (82%)	146 (100%)	0	100	100
10	J	129/137 (94%)	129 (100%)	0	100	100
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	549 (100%)	0	100	100
13	M	415/415 (100%)	415 (100%)	0	100	100
14	N	307/308 (100%)	307 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	296/325 (91%)	296 (100%)	0	100	100
17	Q	103/153 (67%)	103 (100%)	0	100	100
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	82/135 (61%)	82 (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%)	151 (99%)	1 (1%)	81	86
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	119/123 (97%)	119 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	47/53 (89%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	90/120 (75%)	90 (100%)	0	100	100
35	j	61/87 (70%)	61 (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	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	112/121 (93%)	112 (100%)	0	100	100
41	p	156/158 (99%)	156 (100%)	0	100	100
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	76/96 (79%)	76 (100%)	0	100	100
44	s	23/95 (24%)	23 (100%)	0	100	100
45	AA	333/398 (84%)	333 (100%)	0	100	100
45	Aa	332/398 (83%)	332 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	328 (100%)	0	100	100
47	AC	325/333 (98%)	325 (100%)	0	100	100
47	Ac	325/333 (98%)	325 (100%)	0	100	100
48	AD	201/260 (77%)	201 (100%)	0	100	100
48	Ad	204/260 (78%)	203 (100%)	1 (0%)	86	90
49	AE	86/224 (38%)	86 (100%)	0	100	100
49	AI	21/224 (9%)	21 (100%)	0	100	100
49	Ae	158/224 (70%)	158 (100%)	0	100	100
49	Ai	21/224 (9%)	21 (100%)	0	100	100
50	AF	89/99 (90%)	89 (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	67/74 (90%)	67 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	59/83 (71%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	AJ	16/55 (29%)	16 (100%)	0	100	100
53	Aj	34/55 (62%)	34 (100%)	0	100	100
54	AK	10/46 (22%)	10 (100%)	0	100	100
54	Ak	29/46 (63%)	29 (100%)	0	100	100
All	All	10260/12260 (84%)	10258 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
23	X	167	PHE
48	Ad	311	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	209	GLN
3	C	88	HIS
3	C	102	HIS
3	C	130	ASN
3	C	195	HIS
4	D	36	GLN
4	D	79	ASN
4	D	87	GLN
4	D	117	HIS
4	D	147	ASN
4	D	149	GLN
4	D	168	GLN
4	D	182	ASN
4	D	234	GLN
4	D	270	ASN
4	D	285	ASN
4	D	313	GLN
4	D	381	HIS
5	E	152	GLN
5	E	245	GLN
6	F	277	ASN
6	F	346	GLN
6	F	441	HIS
7	G	51	GLN

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Mol	Chain	Res	Type
7	G	59	GLN
7	G	74	ASN
7	G	140	GLN
7	G	205	GLN
7	G	384	ASN
7	G	388	ASN
7	G	444	HIS
7	G	495	ASN
7	G	514	ASN
7	G	571	HIS
7	G	572	HIS
7	G	605	GLN
7	G	667	GLN
8	H	124	ASN
8	H	171	HIS
8	H	235	ASN
8	H	284	GLN
8	H	287	HIS
8	H	292	ASN
9	I	172	ASN
9	I	180	HIS
11	K	7	ASN
12	L	2	ASN
12	L	25	ASN
12	L	56	HIS
12	L	58	ASN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	296	ASN
12	L	321	GLN
12	L	328	HIS
12	L	332	HIS
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	ASN
12	L	505	ASN
12	L	579	ASN

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Mol	Chain	Res	Type
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN
13	M	168	GLN
13	M	170	HIS
13	M	175	ASN
13	M	184	HIS
13	M	192	ASN
13	M	213	HIS
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	349	GLN
13	M	374	ASN
13	M	390	ASN
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	155	GLN
15	O	175	ASN
15	O	235	GLN
15	O	286	GLN
15	O	292	HIS
15	O	306	ASN
15	O	323	GLN
16	P	79	GLN
16	P	102	GLN
16	P	128	ASN
16	P	166	HIS
16	P	251	ASN
16	P	285	HIS
17	Q	86	ASN
17	Q	88	GLN
19	S	22	HIS
19	S	25	GLN
19	S	48	HIS

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Mol	Chain	Res	Type
19	S	81	ASN
19	S	92	GLN
20	U	101	ASN
21	V	50	GLN
21	V	110	ASN
22	W	54	GLN
22	W	61	GLN
22	W	102	GLN
22	W	105	HIS
22	W	129	HIS
23	X	64	ASN
23	X	99	HIS
23	X	151	ASN
24	Y	19	GLN
24	Y	91	ASN
25	Z	8	GLN
25	Z	24	ASN
25	Z	90	ASN
25	Z	137	ASN
27	b	46	ASN
29	d	59	HIS
30	e	98	HIS
31	f	13	HIS
33	h	170	GLN
33	h	181	HIS
33	h	189	ASN
34	i	83	HIS
34	i	127	HIS
34	i	128	HIS
35	j	83	HIS
36	k	39	GLN
36	k	66	ASN
37	l	91	GLN
37	l	106	HIS
37	l	115	ASN
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	13	GLN
39	n	14	GLN
39	n	33	HIS
39	n	53	ASN

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Mol	Chain	Res	Type
40	o	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	17	HIS
42	q	91	HIS
43	r	18	GLN
43	r	21	GLN
45	AA	103	ASN
45	AA	152	GLN
45	AA	173	GLN
45	AA	249	HIS
45	AA	286	HIS
45	AA	342	GLN
45	AA	397	ASN
45	AA	402	HIS
46	AB	167	GLN
46	AB	415	GLN
47	AC	341	GLN
48	AD	189	ASN
48	AD	240	GLN
48	AD	284	HIS
49	AE	135	GLN
49	AE	227	ASN
49	AE	242	HIS
50	AF	39	HIS
50	AF	74	GLN
50	AF	80	GLN
51	AG	7	ASN
51	AG	24	GLN
51	AG	37	ASN
51	AG	69	GLN
52	AH	37	GLN
52	AH	82	HIS
49	AI	71	ASN
45	Aa	49	GLN
45	Aa	87	ASN
45	Aa	95	HIS
45	Aa	173	GLN
45	Aa	207	ASN
45	Aa	286	HIS

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Mol	Chain	Res	Type
45	Aa	342	GLN
45	Aa	397	ASN
45	Aa	402	HIS
46	Ab	211	ASN
46	Ab	212	HIS
46	Ab	304	ASN
46	Ab	415	GLN
47	Ac	221	HIS
47	Ac	312	GLN
47	Ac	341	GLN
48	Ad	115	GLN
48	Ad	309	HIS
49	Ae	131	ASN
49	Ae	164	ASN
49	Ae	200	HIS
49	Ae	219	HIS
49	Ae	239	HIS
51	Ag	69	GLN
52	Ah	53	ASN
52	Ah	82	HIS
54	Ak	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 1 is monoatomic - leaving 53 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	$\#\|Z\| > 2$
66	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
69	HEC	Ad	401	48	32,50,50	2.15	3 (9%)	24,82,82	1.61	5 (20%)
55	3PE	i	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.05	2 (4%)
55	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.10	4 (8%)
62	CDL	Ag	102	-	55,55,99	1.21	4 (7%)	61,67,111	1.24	6 (9%)
63	ADP	O	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
55	3PE	m	201	-	46,46,50	0.96	2 (4%)	49,51,55	1.11	3 (6%)
59	FES	E	301	5	0,4,4	-	-	-		
55	3PE	A	201	-	41,41,50	1.01	2 (4%)	44,46,55	1.09	2 (4%)
55	3PE	H	401	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	3 (6%)
67	HEM	AC	401	47	41,50,50	1.36	4 (9%)	45,82,82	1.74	8 (17%)
56	SF4	G	801	7	0,12,12	-	-	-		
55	3PE	I	301	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	2 (3%)
62	CDL	X	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.27	7 (9%)
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.13	4 (7%)
59	FES	G	803	7	0,4,4	-	-	-		
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.15	4 (7%)
56	SF4	I	302	9	0,12,12	-	-	-		
55	3PE	d	201	-	30,30,50	1.14	2 (6%)	33,35,55	1.31	5 (15%)
56	SF4	G	802	-	0,12,12	-	-	-		
56	SF4	B	301	2	0,12,12	-	-	-		
57	UQ1	B	302	-	18,18,18	1.96	2 (11%)	22,25,25	1.25	4 (18%)
68	UQ6	Ac	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.51	6 (18%)
55	3PE	N	401	-	50,50,50	0.91	2 (4%)	53,55,55	1.06	4 (7%)
58	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.11	3 (7%)
66	EHZ	n	201	-	27,31,37	1.87	7 (25%)	37,41,47	1.58	6 (16%)
67	HEM	Ac	401	47	41,50,50	1.23	5 (12%)	45,82,82	1.71	8 (17%)
55	3PE	Ag	103	-	37,37,50	1.06	2 (5%)	40,42,55	1.20	3 (7%)
55	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.20	3 (7%)
68	UQ6	AC	403	-	28,28,43	2.47	6 (21%)	33,37,55	1.67	10 (30%)
69	HEC	AD	401	48	32,50,50	2.24	11 (34%)	24,82,82	2.40	6 (25%)
55	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.14	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
56	SF4	I	303	9	0,12,12	-	-	-		
55	3PE	m	203	-	40,40,50	1.00	2 (5%)	43,45,55	1.12	3 (6%)
62	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
56	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	L	705	-	37,37,50	1.03	2 (5%)	40,42,55	1.13	3 (7%)
70	U10	Ac	404	-	23,23,63	1.25	3 (13%)	28,31,79	2.09	7 (25%)
58	PC1	B	304	-	42,42,53	1.04	2 (4%)	48,50,61	1.01	3 (6%)
55	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.14	3 (7%)
62	CDL	L	704	-	77,77,99	1.01	4 (5%)	83,89,111	1.13	6 (7%)
67	HEM	AC	402	47	41,50,50	1.38	5 (12%)	45,82,82	1.98	10 (22%)
61	UQ9	H	400	-	35,35,58	0.80	2 (5%)	42,45,73	0.47	0
55	3PE	Aa	501	-	22,22,50	1.36	2 (9%)	25,27,55	1.20	3 (12%)
55	3PE	Y	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.17	5 (11%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.20	6 (9%)
55	3PE	L	703	-	39,39,50	1.02	2 (5%)	42,44,55	1.15	3 (7%)
67	HEM	Ac	402	47	41,50,50	1.37	5 (12%)	45,82,82	1.97	12 (26%)
60	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.19	6 (12%)
55	3PE	m	202	-	50,50,50	0.91	2 (4%)	53,55,55	1.14	4 (7%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.26	4 (10%)
64	NDP	P	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.20	4 (7%)

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
66	EHZ	W	201	-	-	12/39/39/45	-
69	HEC	Ad	401	48	-	0/10/54/54	-
55	3PE	i	201	-	-	16/43/43/54	-
55	3PE	K	101	-	-	17/49/49/54	-
62	CDL	Ag	102	-	-	18/66/66/110	-
63	ADP	O	401	-	-	2/12/32/32	0/3/3/3
55	3PE	m	201	-	-	10/50/50/54	-
59	FES	E	301	5	-	-	0/1/1/1
55	3PE	A	201	-	-	12/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3PE	H	401	-	-	13/51/51/54	-
67	HEM	AC	401	47	-	7/12/54/54	-
56	SF4	G	801	7	-	-	0/6/5/5
55	3PE	I	301	-	-	17/54/54/54	-
62	CDL	X	201	-	-	25/77/77/110	-
55	3PE	L	702	-	-	13/52/52/54	-
59	FES	G	803	7	-	-	0/1/1/1
55	3PE	M	502	-	-	13/54/54/54	-
56	SF4	I	302	9	-	-	0/6/5/5
55	3PE	d	201	-	-	8/34/34/54	-
56	SF4	G	802	-	-	-	0/6/5/5
68	UQ6	Ac	405	-	-	5/21/21/39	0/1/1/1
57	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
56	SF4	B	301	2	-	-	0/6/5/5
55	3PE	N	401	-	-	11/54/54/54	-
58	PC1	B	303	-	-	13/38/38/57	-
66	EHZ	n	201	-	-	13/39/39/45	-
67	HEM	Ac	401	47	-	7/12/54/54	-
55	3PE	Ag	103	-	-	8/41/41/54	-
55	3PE	M	501	-	-	14/40/40/54	-
68	UQ6	AC	403	-	-	3/21/21/39	0/1/1/1
69	HEC	AD	401	48	-	4/10/54/54	-
55	3PE	Ac	403	-	-	2/38/38/54	-
56	SF4	I	303	9	-	-	0/6/5/5
55	3PE	m	203	-	-	7/44/44/54	-
62	CDL	Ag	101	-	-	11/52/52/110	-
56	SF4	F	502	6	-	-	0/6/5/5
55	3PE	L	705	-	-	14/41/41/54	-
70	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
58	PC1	B	304	-	-	14/46/46/57	-
55	3PE	L	701	-	-	5/43/43/54	-
62	CDL	L	704	-	-	28/88/88/110	-
67	HEM	AC	402	47	-	4/12/54/54	-
61	UQ9	H	400	-	-	16/30/54/81	0/1/1/1
55	3PE	Aa	501	-	-	5/26/26/54	-
55	3PE	Y	201	-	-	10/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	CDL	h	201	-	-	23/80/80/110	-
62	CDL	a	101	-	-	18/67/67/110	-
55	3PE	L	703	-	-	7/43/43/54	-
67	HEM	Ac	402	47	-	4/12/54/54	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
55	3PE	m	202	-	-	8/54/54/54	-
71	3PH	Ad	402	-	-	9/37/37/49	-
64	NDP	P	401	-	-	6/30/77/77	0/5/5/5

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	302	UQ1	C6-C5	7.34	1.48	1.35
69	Ad	401	HEC	C3C-C2C	-6.36	1.34	1.40
69	AD	401	HEC	C3C-C2C	6.26	1.47	1.40
69	AD	401	HEC	C2B-C3B	6.15	1.47	1.40
69	Ad	401	HEC	C2B-C3B	-6.06	1.34	1.40
68	AC	403	UQ6	C5-C4	5.98	1.49	1.39
68	Ac	405	UQ6	C5-C6	5.97	1.49	1.40
68	Ac	405	UQ6	C2-C3	5.90	1.49	1.39
68	AC	403	UQ6	C2-C3	5.86	1.48	1.39
68	Ac	405	UQ6	C5-C4	5.82	1.48	1.39
68	AC	403	UQ6	C5-C6	5.79	1.48	1.40
69	Ad	401	HEC	C3D-C2D	5.38	1.53	1.37
66	n	201	EHZ	C15-N2	5.24	1.45	1.33
66	W	201	EHZ	C15-N2	5.16	1.44	1.33
66	n	201	EHZ	C12-N1	5.13	1.45	1.33
68	Ac	405	UQ6	C6-C1	5.12	1.49	1.40
68	AC	403	UQ6	C6-C1	5.05	1.48	1.40
66	W	201	EHZ	C12-N1	5.03	1.44	1.33
60	F	501	FMN	C9A-C5A	4.84	1.49	1.41
68	Ac	405	UQ6	C4-C3	4.64	1.49	1.39
68	AC	403	UQ6	C4-C3	4.59	1.49	1.39
62	a	101	CDL	OA8-CA7	4.31	1.45	1.33
55	A	201	3PE	O31-C31	4.28	1.45	1.33
68	Ac	405	UQ6	C2-C1	4.27	1.49	1.40
62	X	201	CDL	OB8-CB7	4.27	1.45	1.33
62	Ag	101	CDL	OA8-CA7	4.26	1.45	1.33
62	Ag	101	CDL	OB8-CB7	4.25	1.45	1.33
55	K	101	3PE	O31-C31	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	m	202	3PE	O31-C31	4.23	1.45	1.33
55	N	401	3PE	O31-C31	4.23	1.45	1.33
55	m	201	3PE	O31-C31	4.22	1.45	1.33
55	m	201	3PE	O21-C21	4.21	1.46	1.34
55	i	201	3PE	O31-C31	4.21	1.45	1.33
62	X	201	CDL	OA8-CA7	4.20	1.45	1.33
58	B	303	PC1	O31-C31	4.20	1.45	1.33
55	Aa	501	3PE	O31-C31	4.20	1.45	1.33
55	M	501	3PE	O21-C21	4.20	1.46	1.34
55	M	501	3PE	O31-C31	4.19	1.45	1.33
55	L	703	3PE	O31-C31	4.19	1.45	1.33
68	AC	403	UQ6	C2-C1	4.18	1.48	1.40
62	L	704	CDL	OB8-CB7	4.18	1.45	1.33
55	L	701	3PE	O31-C31	4.17	1.45	1.33
55	Y	201	3PE	O21-C21	4.17	1.46	1.34
55	m	203	3PE	O31-C31	4.17	1.45	1.33
55	Ag	103	3PE	O31-C31	4.17	1.45	1.33
58	B	304	PC1	O31-C31	4.16	1.45	1.33
55	Ag	103	3PE	O21-C21	4.16	1.46	1.34
62	a	101	CDL	OB8-CB7	4.16	1.45	1.33
58	B	304	PC1	O21-C21	4.16	1.46	1.34
55	I	301	3PE	O31-C31	4.15	1.45	1.33
55	L	705	3PE	O31-C31	4.15	1.45	1.33
62	Ag	102	CDL	OB8-CB7	4.14	1.45	1.33
55	Y	201	3PE	O31-C31	4.13	1.45	1.33
55	M	502	3PE	O31-C31	4.13	1.45	1.33
55	L	701	3PE	O21-C21	4.13	1.45	1.34
62	h	201	CDL	OA8-CA7	4.13	1.45	1.33
55	H	401	3PE	O31-C31	4.12	1.45	1.33
62	Ag	102	CDL	OA8-CA7	4.12	1.45	1.33
62	h	201	CDL	OB8-CB7	4.11	1.45	1.33
55	Ac	403	3PE	O31-C31	4.11	1.45	1.33
62	L	704	CDL	OB6-CB5	4.11	1.45	1.34
55	i	201	3PE	O21-C21	4.11	1.45	1.34
71	Ad	402	3PH	O21-C21	4.08	1.45	1.34
55	I	301	3PE	O21-C21	4.08	1.45	1.34
62	h	201	CDL	OB6-CB5	4.07	1.45	1.34
55	H	401	3PE	O21-C21	4.06	1.45	1.34
55	A	201	3PE	O21-C21	4.06	1.45	1.34
55	d	201	3PE	O31-C31	4.05	1.45	1.33
62	a	101	CDL	OA6-CA5	4.04	1.45	1.34
62	Ag	101	CDL	OA6-CA5	4.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	h	201	CDL	OA6-CA5	4.03	1.45	1.34
55	L	702	3PE	O31-C31	4.03	1.45	1.33
62	Ag	102	CDL	OA6-CA5	4.02	1.45	1.34
55	Aa	501	3PE	O21-C21	4.01	1.45	1.34
62	Ag	102	CDL	OB6-CB5	3.99	1.45	1.34
62	L	704	CDL	OA8-CA7	3.99	1.45	1.33
55	m	202	3PE	O21-C21	3.98	1.45	1.34
62	X	201	CDL	OB6-CB5	3.97	1.45	1.34
55	L	703	3PE	O21-C21	3.97	1.45	1.34
71	Ad	402	3PH	O31-C31	3.97	1.44	1.33
55	K	101	3PE	O21-C21	3.96	1.45	1.34
55	d	201	3PE	O21-C21	3.96	1.45	1.34
55	L	702	3PE	O21-C21	3.95	1.45	1.34
58	B	303	PC1	O21-C21	3.94	1.45	1.34
62	X	201	CDL	OA6-CA5	3.93	1.45	1.34
55	N	401	3PE	O21-C21	3.93	1.45	1.34
62	a	101	CDL	OB6-CB5	3.93	1.45	1.34
55	m	203	3PE	O21-C21	3.92	1.45	1.34
55	Ac	403	3PE	O21-C21	3.92	1.45	1.34
62	Ag	101	CDL	OB6-CB5	3.91	1.45	1.34
55	M	502	3PE	O21-C21	3.91	1.45	1.34
55	L	705	3PE	O21-C21	3.88	1.45	1.34
67	AC	402	HEM	C4D-ND	-3.83	1.33	1.40
67	AC	401	HEM	C1B-NB	-3.81	1.33	1.40
62	L	704	CDL	OA6-CA5	3.81	1.45	1.34
67	Ac	401	HEM	C4D-ND	-3.67	1.34	1.40
67	Ac	402	HEM	C4D-ND	-3.52	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.37	1.34	1.40
67	Ac	402	HEM	C1B-NB	-3.35	1.34	1.40
64	P	401	NDP	C6N-C5N	3.25	1.39	1.33
69	AD	401	HEC	C2A-C3A	3.25	1.47	1.37
69	AD	401	HEC	C4B-C3B	3.23	1.48	1.43
67	AC	401	HEM	C4D-ND	-3.18	1.34	1.40
60	F	501	FMN	C8-C7	3.11	1.48	1.40
69	AD	401	HEC	C3D-C2D	3.09	1.46	1.37
57	B	302	UQ1	C3-C2	3.09	1.48	1.36
67	Ac	401	HEM	C1B-NB	-3.05	1.35	1.40
67	AC	401	HEM	FE-NB	3.02	2.11	1.96
70	Ac	404	U10	C4-C3	2.94	1.48	1.36
70	Ac	404	U10	C6-C5	-2.91	1.38	1.46
69	AD	401	HEC	C2A-C1A	2.84	1.49	1.42
67	AC	402	HEM	FE-NB	2.84	2.10	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	F	501	FMN	C4-N3	-2.76	1.33	1.38
67	Ac	402	HEM	C1D-ND	-2.76	1.33	1.38
67	Ac	402	HEM	FE-NB	2.69	2.10	1.96
61	H	400	UQ9	C3-C2	-2.66	1.41	1.48
69	AD	401	HEC	C3A-C4A	2.61	1.48	1.42
69	AD	401	HEC	C3C-C4C	2.61	1.47	1.43
66	n	201	EHZ	P1-O7	2.60	1.64	1.54
70	Ac	404	U10	C3-C2	-2.56	1.41	1.48
69	AD	401	HEC	C1C-CHC	2.54	1.48	1.41
61	H	400	UQ9	C4-C5	-2.53	1.41	1.48
67	Ac	401	HEM	C1D-ND	-2.46	1.33	1.38
66	n	201	EHZ	O4-C15	-2.45	1.18	1.23
66	n	201	EHZ	C9-S1	2.45	1.82	1.76
66	W	201	EHZ	O4-C15	-2.44	1.18	1.23
69	AD	401	HEC	C4D-CHA	2.40	1.47	1.41
60	F	501	FMN	C5A-N5	-2.38	1.34	1.39
66	W	201	EHZ	O3-C12	-2.37	1.18	1.23
66	n	201	EHZ	P1-OP3	-2.30	1.46	1.54
69	AD	401	HEC	C1D-CHD	2.29	1.47	1.41
66	n	201	EHZ	O3-C12	-2.28	1.18	1.23
63	O	401	ADP	C5-C4	2.24	1.46	1.40
66	W	201	EHZ	C9-S1	2.23	1.81	1.76
64	P	401	NDP	C5A-C4A	2.19	1.46	1.40
67	AC	402	HEM	C1D-ND	-2.16	1.34	1.38
67	Ac	401	HEM	C4B-NB	-2.08	1.34	1.38
67	Ac	402	HEM	CHB-C1B	2.08	1.40	1.35
60	F	501	FMN	C4A-N5	2.06	1.34	1.30
67	AC	401	HEM	CHB-C1B	2.05	1.40	1.35
67	Ac	401	HEM	CHB-C1B	2.04	1.40	1.35
67	AC	402	HEM	FE-ND	-2.01	1.87	1.96

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	Ac	404	U10	C6-C1-C2	7.78	125.33	119.18
69	AD	401	HEC	CMB-C2B-C3B	6.74	133.74	125.82
67	Ac	402	HEM	CHC-C4B-NB	6.07	131.03	124.43
66	W	201	EHZ	C8-C9-S1	6.03	121.09	113.63
69	AD	401	HEC	C1D-C2D-C3D	-5.97	102.84	107.00
67	AC	402	HEM	CHC-C4B-NB	5.75	130.67	124.43
67	AC	401	HEM	CHC-C4B-NB	5.11	129.98	124.43
66	n	201	EHZ	C8-C9-S1	5.01	119.83	113.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AC	402	HEM	CHD-C1D-ND	4.79	129.63	124.43
67	Ac	401	HEM	CHC-C4B-NB	4.70	129.53	124.43
55	m	201	3PE	O21-C21-C22	4.69	121.62	111.50
55	Ag	103	3PE	O21-C21-C22	4.69	121.61	111.50
55	M	501	3PE	O21-C21-C22	4.65	121.52	111.50
55	m	202	3PE	O21-C21-C22	4.44	121.07	111.50
62	h	201	CDL	OB6-CB5-C51	4.43	121.06	111.50
62	X	201	CDL	OB6-CB5-C51	4.35	120.88	111.50
55	M	502	3PE	O21-C21-C22	4.28	120.72	111.50
62	L	704	CDL	OA6-CA5-C11	4.27	120.69	111.50
67	Ac	402	HEM	C1B-NB-C4B	4.22	109.43	105.07
62	X	201	CDL	OA6-CA5-C11	4.22	120.60	111.50
62	a	101	CDL	OA6-CA5-C11	4.21	120.58	111.50
67	Ac	402	HEM	CHB-C1B-NB	4.16	129.52	124.38
55	Y	201	3PE	O21-C21-C22	4.16	120.46	111.50
68	AC	403	UQ6	C10-C9-C11	4.14	122.23	115.27
70	Ac	404	U10	C1-C6-C5	-4.13	115.69	119.58
55	K	101	3PE	O21-C21-C22	4.12	120.38	111.50
55	I	301	3PE	O21-C21-C22	4.10	120.34	111.50
62	Ag	101	CDL	OB6-CB5-C51	4.10	120.33	111.50
67	AC	402	HEM	CBA-CAA-C2A	-4.06	105.68	112.62
55	L	703	3PE	O21-C21-C22	4.05	120.22	111.50
55	H	401	3PE	O21-C21-C22	4.05	120.22	111.50
64	P	401	NDP	PN-O3-PA	-4.05	118.94	132.83
71	Ad	402	3PH	O21-C21-C22	4.03	120.19	111.50
55	L	702	3PE	O21-C21-C22	4.00	120.13	111.50
67	Ac	401	HEM	CHB-C1B-NB	4.00	129.32	124.38
67	AC	401	HEM	C1B-NB-C4B	4.00	109.20	105.07
62	Ag	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
62	h	201	CDL	OA6-CA5-C11	3.96	120.04	111.50
68	Ac	405	UQ6	C7-C8-C9	-3.96	121.10	127.24
62	Ag	102	CDL	OA6-CA5-C11	3.96	120.03	111.50
58	B	304	PC1	O21-C21-C22	3.96	120.03	111.50
67	AC	401	HEM	CHB-C1B-NB	3.93	129.24	124.38
55	A	201	3PE	O21-C21-C22	3.92	119.96	111.50
55	d	201	3PE	O21-C21-C22	3.92	119.94	111.50
55	L	701	3PE	O21-C21-C22	3.88	119.86	111.50
55	N	401	3PE	O21-C21-C22	3.78	119.64	111.50
55	i	201	3PE	O21-C21-C22	3.77	119.62	111.50
62	L	704	CDL	OB6-CB5-C51	3.77	119.62	111.50
67	AC	402	HEM	C1B-NB-C4B	3.75	108.94	105.07
69	Ad	401	HEC	CMC-C2C-C1C	-3.73	122.73	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	L	705	3PE	O21-C21-C22	3.71	119.50	111.50
68	AC	403	UQ6	C7-C8-C9	-3.68	121.53	127.24
58	B	303	PC1	O21-C21-C22	3.67	119.42	111.50
55	Ac	403	3PE	O21-C21-C22	3.67	119.42	111.50
55	m	203	3PE	O21-C21-C22	3.63	119.33	111.50
69	AD	401	HEC	CMC-C2C-C3C	3.61	130.07	125.82
67	AC	402	HEM	CHB-C1B-NB	3.59	128.82	124.38
68	AC	403	UQ6	C6-C7-C8	-3.55	106.55	112.17
67	Ac	402	HEM	CHA-C4D-ND	3.53	128.75	124.38
62	a	101	CDL	OB6-CB5-C51	3.53	119.11	111.50
63	O	401	ADP	PA-O3A-PB	-3.52	120.75	132.83
62	Ag	101	CDL	OB8-CB7-C71	3.45	120.42	111.38
63	O	401	ADP	N3-C2-N1	-3.42	123.34	128.68
67	Ac	401	HEM	C4D-ND-C1D	3.32	108.51	105.07
68	Ac	405	UQ6	C12-C13-C14	-3.31	119.68	127.66
62	Ag	101	CDL	OA6-CA5-C11	3.31	120.03	110.80
67	Ac	402	HEM	CHD-C1D-ND	3.25	127.97	124.43
70	Ac	404	U10	C4-C3-C2	-3.25	114.30	120.68
64	P	401	NDP	N3A-C2A-N1A	-3.24	123.61	128.68
55	Aa	501	3PE	O21-C21-C22	3.22	119.78	110.80
67	Ac	401	HEM	C1B-NB-C4B	3.17	108.35	105.07
67	AC	402	HEM	CHA-C4D-ND	3.15	128.27	124.38
55	M	502	3PE	C2-O21-C21	-3.15	110.04	117.79
55	d	201	3PE	O31-C31-C32	3.09	121.60	111.91
66	n	201	EHZ	C10-S1-C9	3.08	111.46	101.87
55	m	202	3PE	C2-O21-C21	-3.08	110.22	117.79
62	Ag	101	CDL	CB4-OB6-CB5	-3.07	110.22	117.79
55	d	201	3PE	C2-O21-C21	-3.07	110.24	117.79
69	AD	401	HEC	CBA-CAA-C2A	-3.06	107.44	112.60
62	X	201	CDL	CA4-OA6-CA5	-3.06	110.26	117.79
67	AC	402	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
55	m	203	3PE	C2-O21-C21	-3.02	110.35	117.79
55	M	502	3PE	O31-C31-C32	3.00	121.32	111.91
71	Ad	402	3PH	O31-C31-C32	2.98	121.27	111.91
55	K	101	3PE	C2-O21-C21	-2.90	110.64	117.79
55	H	401	3PE	O31-C31-C32	2.88	120.94	111.91
55	Y	201	3PE	O31-C31-C32	2.87	120.93	111.91
67	Ac	402	HEM	CHD-C1D-C2D	-2.85	120.52	124.98
67	Ac	401	HEM	CHD-C1D-ND	2.85	127.53	124.43
55	m	202	3PE	O31-C31-C32	2.84	120.81	111.91
55	i	201	3PE	O31-C31-C32	2.84	120.81	111.91
62	Ag	102	CDL	CA4-OA6-CA5	-2.84	110.81	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	302	UQ1	CM5-C5-C6	-2.82	119.80	124.40
58	B	303	PC1	O31-C31-C32	2.81	120.73	111.91
63	O	401	ADP	C3'-C2'-C1'	2.80	105.20	100.98
67	Ac	402	HEM	CBA-CAA-C2A	-2.80	107.84	112.62
62	h	201	CDL	OB8-CB7-C71	2.80	120.70	111.91
62	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
55	m	201	3PE	O31-C31-C32	2.79	120.67	111.91
55	N	401	3PE	C2-O21-C21	-2.78	110.95	117.79
67	AC	402	HEM	CBD-CAD-C3D	-2.77	104.94	112.63
68	Ac	405	UQ6	C15-C14-C16	2.77	119.92	115.27
62	L	704	CDL	CA4-OA6-CA5	-2.75	111.03	117.79
67	Ac	402	HEM	CHA-C4D-C3D	-2.73	120.21	125.33
69	Ad	401	HEC	CMB-C2B-C1B	-2.70	124.32	128.46
68	Ac	405	UQ6	C10-C9-C11	2.69	119.79	115.27
62	X	201	CDL	OB8-CB7-C71	2.69	120.34	111.91
62	Ag	102	CDL	CB4-OB6-CB5	-2.67	111.21	117.79
62	L	704	CDL	OB8-CB7-C71	2.67	120.30	111.91
55	m	203	3PE	O31-C31-C32	2.66	120.27	111.91
55	A	201	3PE	O31-C31-C32	2.65	120.23	111.91
55	L	702	3PE	O31-C31-C32	2.65	120.23	111.91
55	K	101	3PE	O31-C31-C32	2.65	120.22	111.91
62	L	704	CDL	OA8-CA7-C31	2.65	120.22	111.91
58	B	303	PC1	C2-O21-C21	-2.64	111.29	117.79
55	L	703	3PE	O31-C31-C32	2.62	120.13	111.91
66	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
55	L	701	3PE	O31-C31-C32	2.62	120.12	111.91
55	Ag	103	3PE	O31-C31-C32	2.61	120.10	111.91
62	h	201	CDL	CA4-OA6-CA5	-2.60	111.38	117.79
70	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
68	AC	403	UQ6	C12-C13-C14	-2.59	121.42	127.66
68	AC	403	UQ6	C15-C14-C16	2.59	119.62	115.27
55	N	401	3PE	O31-C31-C32	2.59	120.03	111.91
63	O	401	ADP	C4-C5-N7	-2.59	106.70	109.40
62	X	201	CDL	OA8-CA7-C31	2.58	120.00	111.91
67	AC	401	HEM	O2A-CGA-CBA	2.58	122.31	114.03
67	AC	401	HEM	O2D-CGD-CBD	2.57	122.30	114.03
55	L	703	3PE	C2-O21-C21	-2.57	111.47	117.79
70	Ac	404	U10	O4-C4-C5	-2.54	107.96	116.56
67	Ac	401	HEM	CHA-C4D-ND	2.54	127.52	124.38
62	Ag	102	CDL	OA8-CA7-C31	2.53	119.84	111.91
55	Ac	403	3PE	O31-C31-C32	2.52	119.83	111.91
55	I	301	3PE	O31-C31-C32	2.50	119.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	F	501	FMN	C4A-C10-N1	-2.50	118.92	124.73
55	Y	201	3PE	C2-O21-C21	-2.49	111.67	117.79
62	h	201	CDL	OA8-CA7-C31	2.48	119.70	111.91
60	F	501	FMN	O4-C4-C4A	-2.48	120.02	126.60
64	P	401	NDP	C4A-C5A-N7A	-2.48	106.81	109.40
66	n	201	EHZ	OP3-P1-O9	-2.48	100.97	110.68
66	W	201	EHZ	C13-C12-N1	2.48	120.59	116.42
67	Ac	402	HEM	C2C-C3C-C4C	2.48	108.63	106.90
62	h	201	CDL	CB4-OB6-CB5	-2.47	111.70	117.79
62	Ag	101	CDL	OA8-CA7-C31	2.47	119.65	111.91
62	Ag	101	CDL	CA4-OA6-CA5	-2.46	111.73	117.79
68	AC	403	UQ6	C17-C18-C19	-2.45	119.36	127.75
62	a	101	CDL	OB8-CB7-C71	2.45	119.60	111.91
55	Aa	501	3PE	O31-C31-C32	2.45	119.60	111.91
67	AC	401	HEM	CHD-C1D-ND	2.45	127.09	124.43
55	L	702	3PE	C2-O21-C21	-2.45	111.77	117.79
66	W	201	EHZ	C14-N2-C15	-2.44	118.24	122.59
67	Ac	401	HEM	C4B-C3B-C2B	-2.44	105.18	107.11
55	L	705	3PE	C2-O21-C21	-2.43	111.80	117.79
55	Ag	103	3PE	C2-O21-C21	-2.42	111.84	117.79
55	M	501	3PE	C2-O21-C21	-2.41	111.86	117.79
57	B	302	UQ1	C11-C9-C10	2.41	119.92	114.60
55	Ac	403	3PE	C2-O21-C21	-2.40	111.88	117.79
68	Ac	405	UQ6	C21-C19-C20	2.39	119.88	114.60
68	AC	403	UQ6	C21-C19-C20	2.37	119.84	114.60
69	Ad	401	HEC	CBD-CAD-C3D	-2.37	108.58	112.62
58	B	304	PC1	O31-C31-C32	2.36	119.33	111.91
67	Ac	402	HEM	C3C-C4C-NC	-2.35	106.51	110.94
66	W	201	EHZ	O2-C9-S1	-2.34	119.58	122.61
60	F	501	FMN	C4-C4A-N5	2.31	121.53	118.23
55	L	705	3PE	O31-C31-C32	2.31	119.17	111.91
66	n	201	EHZ	C10-C11-N1	-2.30	107.58	112.42
55	K	101	3PE	O21-C21-O22	-2.29	118.17	123.70
71	Ad	402	3PH	C2-O21-C21	-2.27	112.19	117.79
67	Ac	402	HEM	CBD-CAD-C3D	-2.26	106.34	112.63
67	Ac	402	HEM	CHB-C1B-C2B	-2.26	120.47	126.72
71	Ad	402	3PH	O31-C31-O32	-2.25	117.91	123.59
55	d	201	3PE	O31-C31-O32	-2.25	117.92	123.59
55	Aa	501	3PE	C2-O21-C21	-2.24	112.27	117.79
62	Ag	101	CDL	OB6-CB5-OB7	-2.23	118.31	123.70
67	AC	402	HEM	C4D-ND-C1D	2.23	107.38	105.07
67	Ac	401	HEM	CHB-C1B-C2B	-2.23	120.56	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Ac	405	UQ6	C17-C18-C19	-2.21	120.18	127.75
62	Ag	102	CDL	OB8-CB7-C71	2.21	118.84	111.91
55	M	502	3PE	O21-C21-O22	-2.21	118.36	123.70
55	Y	201	3PE	O21-C21-O22	-2.21	118.37	123.70
55	m	202	3PE	O21-C21-O22	-2.21	118.37	123.70
69	AD	401	HEC	CAD-CBD-CGD	-2.20	107.58	113.76
69	Ad	401	HEC	C1D-C2D-C3D	-2.19	105.47	107.00
55	N	401	3PE	O21-C21-O22	-2.18	118.44	123.70
62	a	101	CDL	CB4-OB6-CB5	-2.16	112.47	117.79
67	AC	401	HEM	CHB-C1B-C2B	-2.14	120.79	126.72
55	M	501	3PE	O31-C31-C32	2.14	118.62	111.91
68	AC	403	UQ6	C4M-O4-C4	2.14	120.64	114.78
66	n	201	EHZ	C5-C6-C7	-2.14	108.69	114.85
58	B	304	PC1	C2-O21-C21	-2.13	112.53	117.79
57	B	302	UQ1	C7-C8-C9	-2.13	120.60	127.26
62	X	201	CDL	CB6-CB4-CB3	-2.12	106.78	111.79
55	d	201	3PE	O21-C21-O22	-2.12	118.59	123.70
69	AD	401	HEC	CMA-C3A-C2A	2.11	128.92	124.94
62	a	101	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
64	P	401	NDP	C3D-C2D-C1D	2.09	105.39	101.43
55	L	702	3PE	O21-C21-O22	-2.06	118.71	123.70
55	Y	201	3PE	O31-C31-O32	-2.06	118.41	123.59
62	X	201	CDL	OB6-CB5-OB7	-2.05	118.74	123.70
60	F	501	FMN	C4A-C10-N10	2.04	119.46	116.48
67	AC	402	HEM	CHB-C1B-C2B	-2.03	121.09	126.72
70	Ac	404	U10	C3M-O3-C3	2.03	123.67	116.47
57	B	302	UQ1	C8-C7-C6	-2.03	106.57	112.05
68	AC	403	UQ6	C10-C9-C8	-2.03	118.47	123.68
60	F	501	FMN	C4A-C4-N3	2.03	118.34	113.19
69	Ad	401	HEC	CAA-CBA-CGA	-2.02	108.09	113.76
60	F	501	FMN	C10-N1-C2	2.02	120.94	116.90
70	Ac	404	U10	O4-C4-C3	2.02	131.26	123.64
55	L	701	3PE	C2-O21-C21	-2.02	112.83	117.79
62	L	704	CDL	OA6-CA5-OA7	-2.01	118.84	123.70
55	m	201	3PE	O21-C21-O22	-2.01	118.84	123.70
68	AC	403	UQ6	C3M-O3-C3	2.01	120.28	114.78
66	n	201	EHZ	C14-C13-C12	-2.00	109.02	112.36
55	H	401	3PE	O21-C21-O22	-2.00	118.86	123.70
67	AC	401	HEM	C4B-C3B-C2B	-2.00	105.53	107.11

There are no chirality outliers.

All (462) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	201	3PE	C1-O11-P-O14
55	A	201	3PE	C11-O13-P-O11
55	A	201	3PE	C11-O13-P-O14
55	A	201	3PE	C22-C21-O21-C2
55	H	401	3PE	C1-O11-P-O14
55	H	401	3PE	C11-O13-P-O14
55	H	401	3PE	O22-C21-O21-C2
55	H	401	3PE	C22-C21-O21-C2
55	I	301	3PE	C1-O11-P-O14
55	I	301	3PE	C11-O13-P-O12
55	K	101	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O13
55	L	701	3PE	C2-C1-O11-P
55	L	702	3PE	C1-O11-P-O12
55	L	702	3PE	O22-C21-O21-C2
55	L	702	3PE	C22-C21-O21-C2
55	L	703	3PE	C11-O13-P-O11
55	L	703	3PE	C11-O13-P-O12
55	L	703	3PE	C11-O13-P-O14
55	L	705	3PE	C1-O11-P-O12
55	L	705	3PE	C1-O11-P-O14
55	L	705	3PE	C11-O13-P-O12
55	L	705	3PE	C11-O13-P-O14
55	M	501	3PE	C1-O11-P-O12
55	M	501	3PE	C1-O11-P-O13
55	M	501	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O11
55	M	501	3PE	C11-O13-P-O12
55	M	501	3PE	C11-O13-P-O14
55	M	502	3PE	C1-O11-P-O12
55	M	502	3PE	C11-O13-P-O14
55	N	401	3PE	C11-O13-P-O11
55	N	401	3PE	C11-O13-P-O12
55	Y	201	3PE	C1-O11-P-O12
55	d	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C1-O11-P-O12
55	i	201	3PE	C1-O11-P-O13
55	i	201	3PE	C1-O11-P-O14
55	i	201	3PE	C11-O13-P-O12
55	m	201	3PE	C1-O11-P-O14
55	m	201	3PE	C22-C21-O21-C2
55	m	202	3PE	C22-C21-O21-C2
55	m	203	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
55	m	203	3PE	C1-O11-P-O14
55	m	203	3PE	C22-C21-O21-C2
55	Aa	501	3PE	C22-C21-O21-C2
55	Ag	103	3PE	C1-O11-P-O14
55	Ag	103	3PE	C11-O13-P-O12
55	Ag	103	3PE	C11-O13-P-O14
58	B	303	PC1	C11-O13-P-O14
58	B	303	PC1	C22-C21-O21-C2
58	B	304	PC1	C1-O11-P-O14
58	B	304	PC1	C22-C21-O21-C2
60	F	501	FMN	C5'-O5'-P-O2P
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C22-C23-C24-C26
61	H	400	UQ9	C22-C23-C24-C25
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C18-C19-C21-C22
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C13-C14-C16-C17
61	H	400	UQ9	C12-C13-C14-C16
61	H	400	UQ9	C12-C13-C14-C15
61	H	400	UQ9	C11-C12-C13-C14
62	L	704	CDL	CA2-OA2-PA1-OA3
62	L	704	CDL	CB2-OB2-PB2-OB4
62	L	704	CDL	CB3-OB5-PB2-OB3
62	L	704	CDL	CB3-OB5-PB2-OB4
62	L	704	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CA3-OA5-PA1-OA3
62	X	201	CDL	CA3-OA5-PA1-OA4
62	X	201	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CB2-OB2-PB2-OB5
62	X	201	CDL	CB3-OB5-PB2-OB3
62	X	201	CDL	C51-CB5-OB6-CB4
62	a	101	CDL	CA2-OA2-PA1-OA4
62	a	101	CDL	OA7-CA5-OA6-CA4
62	a	101	CDL	C11-CA5-OA6-CA4
62	a	101	CDL	CB2-OB2-PB2-OB3
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

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Mol	Chain	Res	Type	Atoms
62	h	201	CDL	C51-CB5-OB6-CB4
62	Ag	101	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	C1-CB2-OB2-PB2
62	Ag	102	CDL	CB2-OB2-PB2-OB4
62	Ag	102	CDL	CB3-OB5-PB2-OB3
62	Ag	102	CDL	C51-CB5-OB6-CB4
64	P	401	NDP	C5D-O5D-PN-O1N
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	O2-C9-S1-C10
66	W	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C12-C13-C14-N2
66	n	201	EHZ	N2-C15-C16-O5
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
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	Ac	401	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
68	Ac	405	UQ6	C1-C6-C7-C8
68	Ac	405	UQ6	C13-C14-C16-C17
68	Ac	405	UQ6	C15-C14-C16-C17
70	Ac	404	U10	C7-C8-C9-C10
70	Ac	404	U10	C7-C8-C9-C11
71	Ad	402	3PH	C1-O11-P-O13
71	Ad	402	3PH	O21-C2-C3-O31
70	Ac	404	U10	C12-C13-C14-C15
70	Ac	404	U10	C12-C13-C14-C16
58	B	304	PC1	O32-C31-O31-C3
62	L	704	CDL	OA9-CA7-OA8-CA6
55	A	201	3PE	O22-C21-O21-C2
55	m	202	3PE	O22-C21-O21-C2
55	m	203	3PE	O22-C21-O21-C2
55	Aa	501	3PE	O22-C21-O21-C2
58	B	303	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
58	B	304	PC1	O22-C21-O21-C2
62	L	704	CDL	OB7-CB5-OB6-CB4
62	X	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
62	Ag	102	CDL	OB7-CB5-OB6-CB4
55	K	101	3PE	C32-C31-O31-C3
58	B	304	PC1	C32-C31-O31-C3
55	d	201	3PE	C22-C21-O21-C2
68	AC	403	UQ6	C15-C14-C16-C17
55	I	301	3PE	C32-C31-O31-C3
55	N	401	3PE	C32-C31-O31-C3
62	L	704	CDL	C31-CA7-OA8-CA6
71	Ad	402	3PH	C35-C36-C37-C38
55	m	201	3PE	O22-C21-O21-C2
55	H	401	3PE	O32-C31-O31-C3
55	I	301	3PE	O32-C31-O31-C3
55	N	401	3PE	O32-C31-O31-C3
55	m	203	3PE	O32-C31-O31-C3
62	X	201	CDL	O1-C1-CB2-OB2
55	H	401	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
55	K	101	3PE	O32-C31-O31-C3
55	I	301	3PE	C22-C21-O21-C2
55	L	705	3PE	C22-C21-O21-C2
62	L	704	CDL	C11-CA5-OA6-CA4
55	m	203	3PE	C32-C31-O31-C3
62	h	201	CDL	CA4-CA3-OA5-PA1
62	a	101	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C9-C11-C12-C13
61	H	400	UQ9	C17-C18-C19-C20
55	I	301	3PE	O22-C21-O21-C2
55	L	705	3PE	O22-C21-O21-C2
61	H	400	UQ9	C17-C18-C19-C21
58	B	303	PC1	C11-C12-N-C13
55	i	201	3PE	C32-C31-O31-C3
62	X	201	CDL	C31-CA7-OA8-CA6
71	Ad	402	3PH	C31-C32-C33-C34
55	M	501	3PE	C32-C33-C34-C35
68	AC	403	UQ6	C13-C14-C16-C17
55	m	202	3PE	C32-C31-O31-C3
62	h	201	CDL	C71-CB7-OB8-CB6
67	Ac	401	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
62	X	201	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C19-C21-C22-C23
62	L	704	CDL	OA7-CA5-OA6-CA4
55	i	201	3PE	O32-C31-O31-C3
55	m	202	3PE	O32-C31-O31-C3
68	Ac	405	UQ6	C5-C6-C7-C8
55	I	301	3PE	C1-O11-P-O13
55	I	301	3PE	C11-O13-P-O11
55	K	101	3PE	C1-O11-P-O13
55	L	702	3PE	C1-O11-P-O13
55	L	705	3PE	C1-O11-P-O13
55	L	705	3PE	C11-O13-P-O11
55	M	502	3PE	C11-O13-P-O11
55	Y	201	3PE	C1-O11-P-O13
55	Y	201	3PE	C11-O13-P-O11
55	i	201	3PE	C11-O13-P-O11
55	m	203	3PE	C1-O11-P-O13
55	Ag	103	3PE	C1-O11-P-O13
55	Ag	103	3PE	C11-O13-P-O11
58	B	303	PC1	C11-O13-P-O11
58	B	303	PC1	C1-O11-P-O13
62	L	704	CDL	CA2-OA2-PA1-OA5
62	L	704	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	102	CDL	CB2-OB2-PB2-OB5
62	Ag	102	CDL	CB3-OB5-PB2-OB2
62	X	201	CDL	CA2-C1-CB2-OB2
58	B	303	PC1	C11-C12-N-C14
55	M	502	3PE	C22-C21-O21-C2
55	I	301	3PE	C32-C33-C34-C35
62	h	201	CDL	C18-C19-C20-C21
66	W	201	EHZ	C18-C17-C20-O6
66	W	201	EHZ	C19-C17-C20-O6
55	d	201	3PE	C32-C31-O31-C3
55	M	502	3PE	O22-C21-O21-C2
55	L	703	3PE	C25-C26-C27-C28
62	X	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
62	h	201	CDL	OB9-CB7-OB8-CB6
55	Aa	501	3PE	C32-C31-O31-C3
55	K	101	3PE	C22-C23-C24-C25
62	X	201	CDL	C71-CB7-OB8-CB6
67	AC	401	HEM	C2A-CAA-CBA-CGA
69	AD	401	HEC	C2A-CAA-CBA-CGA
55	m	201	3PE	C26-C27-C28-C29
55	M	501	3PE	C32-C31-O31-C3
62	Ag	102	CDL	C74-C75-C76-C77
55	d	201	3PE	O32-C31-O31-C3
55	Aa	501	3PE	O32-C31-O31-C3
58	B	303	PC1	C11-C12-N-C15
55	m	201	3PE	C32-C31-O31-C3
62	Ag	102	CDL	C31-CA7-OA8-CA6
62	Ag	101	CDL	C51-CB5-OB6-CB4
55	M	502	3PE	C23-C24-C25-C26
62	L	704	CDL	C55-C56-C57-C58
55	m	201	3PE	O32-C31-O31-C3
62	X	201	CDL	OB9-CB7-OB8-CB6
71	Ad	402	3PH	C22-C21-O21-C2
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
55	M	501	3PE	O32-C31-O31-C3
62	Ag	102	CDL	OA9-CA7-OA8-CA6
55	M	502	3PE	C3C-C3D-C3E-C3F
62	Ag	101	CDL	OB7-CB5-OB6-CB4
71	Ad	402	3PH	O22-C21-O21-C2
62	a	101	CDL	C13-C14-C15-C16
55	d	201	3PE	C11-O13-P-O11
58	B	304	PC1	C1-O11-P-O13
62	h	201	CDL	CB3-OB5-PB2-OB2
55	Y	201	3PE	C2-C1-O11-P
62	a	101	CDL	C14-C15-C16-C17
55	K	101	3PE	C33-C34-C35-C36
55	N	401	3PE	C24-C25-C26-C27
66	W	201	EHZ	C3-C4-C5-C6
71	Ad	402	3PH	C1-C2-C3-O31
55	L	702	3PE	C24-C25-C26-C27
66	n	201	EHZ	O4-C15-C16-O5
66	W	201	EHZ	C5-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
71	Ad	402	3PH	C34-C35-C36-C37
55	L	703	3PE	C32-C31-O31-C3
71	Ad	402	3PH	C36-C37-C38-C39
55	H	401	3PE	C3-C2-O21-C21
62	L	704	CDL	CB6-CB4-OB6-CB5
55	H	401	3PE	C2-C1-O11-P
60	F	501	FMN	C5'-O5'-P-O1P
62	L	704	CDL	OB5-CB3-CB4-OB6
55	I	301	3PE	C3B-C3C-C3D-C3E
55	L	702	3PE	C32-C31-O31-C3
62	L	704	CDL	C71-CB7-OB8-CB6
66	W	201	EHZ	C5-C6-C7-C8
55	Ac	403	3PE	C22-C21-O21-C2
55	L	705	3PE	C32-C31-O31-C3
55	Ag	103	3PE	C39-C3A-C3B-C3C
61	H	400	UQ9	C14-C16-C17-C18
55	m	201	3PE	C27-C28-C29-C2A
55	K	101	3PE	C36-C37-C38-C39
55	L	703	3PE	O32-C31-O31-C3
55	i	201	3PE	C22-C21-O21-C2
58	B	303	PC1	C2-C1-O11-P
62	Ag	102	CDL	CB4-CB3-OB5-PB2
55	A	201	3PE	C1-C2-C3-O31
62	X	201	CDL	CA3-CA4-CA6-OA8
55	H	401	3PE	C2B-C2C-C2D-C2E
55	M	501	3PE	C2-C3-O31-C31
62	h	201	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	C32-C33-C34-C35
55	K	101	3PE	O11-C1-C2-O21
55	Ac	403	3PE	O22-C21-O21-C2
66	n	201	EHZ	C3-C4-C5-C6
62	L	704	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	OA6-CA4-CA6-OA8
55	i	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C2-C1-O11-P
62	X	201	CDL	C1-CA2-OA2-PA1
62	h	201	CDL	C14-C15-C16-C17
66	n	201	EHZ	O2-C9-S1-C10
58	B	304	PC1	C38-C39-C3A-C3B
55	L	705	3PE	O32-C31-O31-C3
62	L	704	CDL	C12-C13-C14-C15
55	H	401	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
55	Y	201	3PE	C22-C21-O21-C2
62	X	201	CDL	C11-CA5-OA6-CA4
64	P	401	NDP	C2B-O2B-P2B-O1X
55	Y	201	3PE	C32-C31-O31-C3
55	i	201	3PE	C1-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5
66	n	201	EHZ	C8-C9-S1-C10
62	h	201	CDL	CB4-CB3-OB5-PB2
55	L	702	3PE	O32-C31-O31-C3
55	M	501	3PE	O11-C1-C2-O21
63	O	401	ADP	PA-O3A-PB-O3B
58	B	303	PC1	C31-C32-C33-C34
55	L	702	3PE	C28-C29-C2A-C2B
55	Y	201	3PE	O22-C21-O21-C2
62	X	201	CDL	OA7-CA5-OA6-CA4
64	P	401	NDP	PN-O3-PA-O2A
55	M	502	3PE	C1-O11-P-O13
62	L	704	CDL	CA3-OA5-PA1-OA2
64	P	401	NDP	O4D-C1D-N1N-C6N
55	K	101	3PE	C2-C1-O11-P
62	a	101	CDL	CB4-CB3-OB5-PB2
55	I	301	3PE	C1-O11-P-O12
55	I	301	3PE	C11-O13-P-O14
55	K	101	3PE	C1-O11-P-O12
55	K	101	3PE	C1-O11-P-O14
55	L	701	3PE	C1-O11-P-O12
55	M	502	3PE	C11-O13-P-O12
55	N	401	3PE	C11-O13-P-O14
55	Y	201	3PE	C11-O13-P-O12
55	Y	201	3PE	C11-O13-P-O14
55	i	201	3PE	C11-O13-P-O14
55	Ag	103	3PE	C1-O11-P-O12
58	B	303	PC1	C11-O13-P-O12
58	B	303	PC1	C1-O11-P-O14
58	B	304	PC1	C1-O11-P-O12
62	L	704	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	CB3-OB5-PB2-OB4
55	Y	201	3PE	O32-C31-O31-C3
55	N	401	3PE	C12-C11-O13-P
55	d	201	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
62	Ag	102	CDL	C51-C52-C53-C54
60	F	501	FMN	N10-C1'-C2'-O2'
55	L	702	3PE	C25-C26-C27-C28
66	W	201	EHZ	C2-C3-C4-C5
58	B	304	PC1	C11-C12-N-C14
61	H	400	UQ9	C12-C11-C9-C10
66	W	201	EHZ	O4-C15-C16-O5
62	X	201	CDL	C52-C53-C54-C55
66	n	201	EHZ	C2-C3-C4-C5
55	m	201	3PE	C1-C2-O21-C21
62	X	201	CDL	CB6-CB4-OB6-CB5
55	M	501	3PE	O11-C1-C2-C3
62	L	704	CDL	OB5-CB3-CB4-CB6
55	L	701	3PE	C26-C27-C28-C29
55	A	201	3PE	O21-C2-C3-O31
55	A	201	3PE	C1-O11-P-O13
55	H	401	3PE	C11-O13-P-O11
55	K	101	3PE	C11-O13-P-O11
55	N	401	3PE	C1-O11-P-O13
62	X	201	CDL	CA2-OA2-PA1-OA5
62	X	201	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CB3-OB5-PB2-OB2
55	m	202	3PE	C32-C33-C34-C35
55	L	702	3PE	C33-C34-C35-C36
55	N	401	3PE	C34-C35-C36-C37
55	d	201	3PE	C24-C25-C26-C27
55	L	705	3PE	C2-C1-O11-P
62	L	704	CDL	CA4-CA3-OA5-PA1
62	L	704	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	C1-CA2-OA2-PA1
62	Ag	102	CDL	C1-CA2-OA2-PA1
55	m	202	3PE	C23-C24-C25-C26
55	N	401	3PE	C28-C29-C2A-C2B
55	M	501	3PE	O13-C11-C12-N
62	L	704	CDL	C34-C35-C36-C37
55	i	201	3PE	C24-C25-C26-C27
62	a	101	CDL	C71-CB7-OB8-CB6
67	AC	401	HEM	CAA-CBA-CGA-O2A
70	Ac	404	U10	C12-C11-C9-C10
61	H	400	UQ9	C12-C11-C9-C8
67	Ac	402	HEM	CAD-CBD-CGD-O2D
62	Ag	101	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
67	AC	402	HEM	CAD-CBD-CGD-O1D
55	i	201	3PE	C2B-C2C-C2D-C2E
55	L	705	3PE	C24-C25-C26-C27
67	AC	401	HEM	CAD-CBD-CGD-O1D
67	Ac	401	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O1D
55	Aa	501	3PE	C1-C2-O21-C21
55	M	502	3PE	C2B-C2C-C2D-C2E
67	Ac	401	HEM	CAD-CBD-CGD-O1D
55	m	201	3PE	C1-O11-P-O13
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	Ac	401	HEM	CAA-CBA-CGA-O2A
58	B	304	PC1	C2-C1-O11-P
55	H	401	3PE	C31-C32-C33-C34
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAA-CBA-CGA-O1A
55	A	201	3PE	C23-C24-C25-C26
55	I	301	3PE	O11-C1-C2-C3
62	Ag	101	CDL	OB9-CB7-OB8-CB6
62	h	201	CDL	C31-CA7-OA8-CA6
67	AC	402	HEM	CAD-CBD-CGD-O2D
62	Ag	102	CDL	C11-C12-C13-C14
70	Ac	404	U10	C12-C11-C9-C8
62	a	101	CDL	OB9-CB7-OB8-CB6
64	P	401	NDP	PN-O3-PA-O1A
62	a	101	CDL	C15-C16-C17-C18
55	A	201	3PE	C39-C3A-C3B-C3C
62	h	201	CDL	OA9-CA7-OA8-CA6
55	K	101	3PE	C26-C27-C28-C29
55	M	502	3PE	C39-C3A-C3B-C3C
55	K	101	3PE	O11-C1-C2-C3
55	L	705	3PE	C34-C35-C36-C37
62	X	201	CDL	C59-C60-C61-C62
58	B	304	PC1	C11-C12-N-C13
55	N	401	3PE	C23-C24-C25-C26
55	A	201	3PE	C35-C36-C37-C38
69	AD	401	HEC	CAA-CBA-CGA-O2A
55	I	301	3PE	C31-C32-C33-C34
58	B	304	PC1	C3A-C3B-C3C-C3D
55	m	202	3PE	O11-C1-C2-O21
58	B	304	PC1	C11-C12-N-C15
63	O	401	ADP	PA-O3A-PB-O2B

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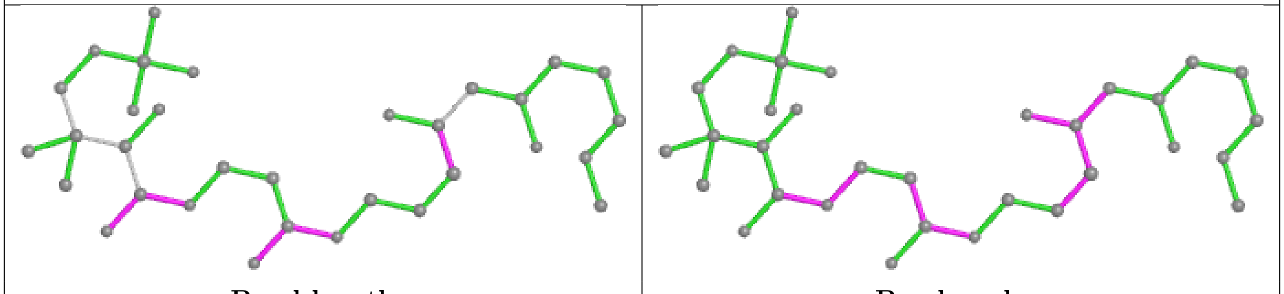
Mol	Chain	Res	Type	Atoms
62	Ag	102	CDL	OA6-CA4-CA6-OA8
55	L	702	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C3A-C3B-C3C-C3D
64	P	401	NDP	C5D-O5D-PN-O3
62	Ag	102	CDL	C53-C54-C55-C56
68	AC	403	UQ6	C14-C16-C17-C18
55	Ag	103	3PE	O21-C21-C22-C23
55	H	401	3PE	C37-C38-C39-C3A
55	L	705	3PE	C33-C34-C35-C36
62	L	704	CDL	C11-C12-C13-C14
62	Ag	102	CDL	C52-C53-C54-C55
69	AD	401	HEC	CAA-CBA-CGA-O1A
62	a	101	CDL	C18-C19-C20-C21
68	Ac	405	UQ6	C6-C7-C8-C9
55	L	702	3PE	C34-C35-C36-C37
62	L	704	CDL	C77-C78-C79-C80
55	i	201	3PE	O21-C21-C22-C23
55	K	101	3PE	C2A-C2B-C2C-C2D
55	L	701	3PE	C38-C39-C3A-C3B
55	K	101	3PE	C11-O13-P-O14
55	M	502	3PE	C1-O11-P-O14
55	d	201	3PE	C11-O13-P-O14
55	m	201	3PE	C1-O11-P-O12
55	m	202	3PE	C1-O11-P-O14
62	a	101	CDL	CB3-OB5-PB2-OB3
55	A	201	3PE	C25-C26-C27-C28
55	L	702	3PE	C2B-C2C-C2D-C2E
55	I	301	3PE	C12-C11-O13-P
55	M	501	3PE	C12-C11-O13-P
58	B	303	PC1	C33-C34-C35-C36
62	a	101	CDL	C12-C11-CA5-OA7
58	B	304	PC1	C3F-C3G-C3H-C3I
55	I	301	3PE	O31-C31-C32-C33
62	a	101	CDL	C12-C11-CA5-OA6
62	Ag	101	CDL	C72-C71-CB7-OB8
55	i	201	3PE	O22-C21-C22-C23
55	K	101	3PE	C27-C28-C29-C2A
62	h	201	CDL	C72-C71-CB7-OB8
55	I	301	3PE	O32-C31-C32-C33
55	L	703	3PE	C22-C23-C24-C25
69	AD	401	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

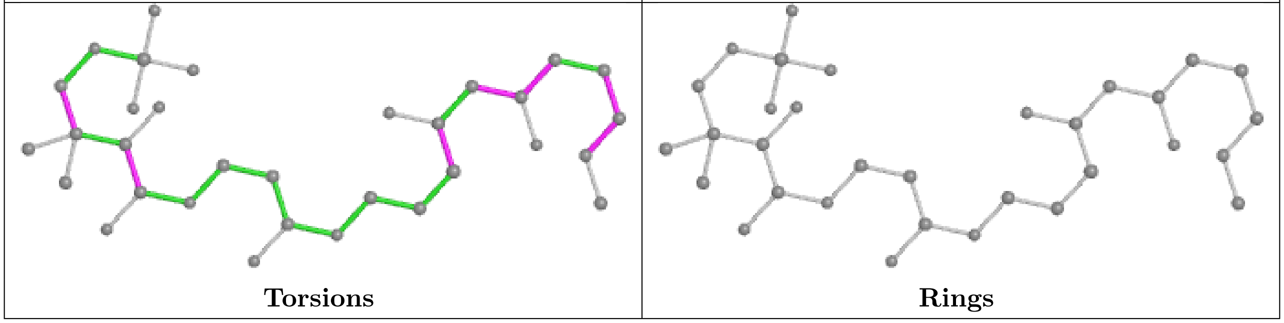
No monomer is involved in short contacts.

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 EHZ W 201

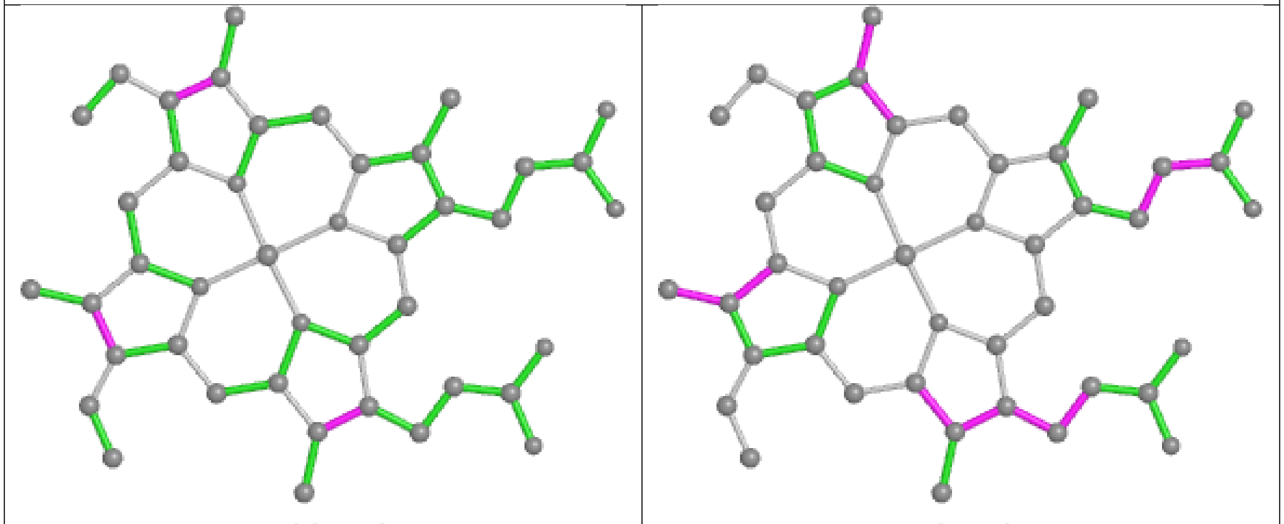


Bond lengths **Bond angles**

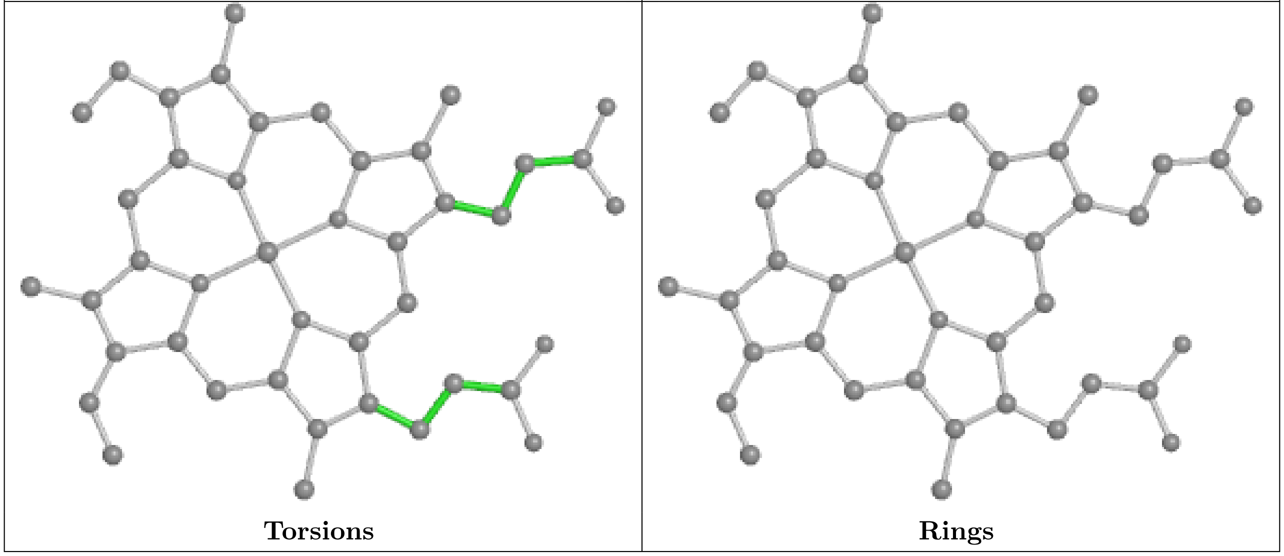


Torsions **Rings**

Ligand HEC Ad 401

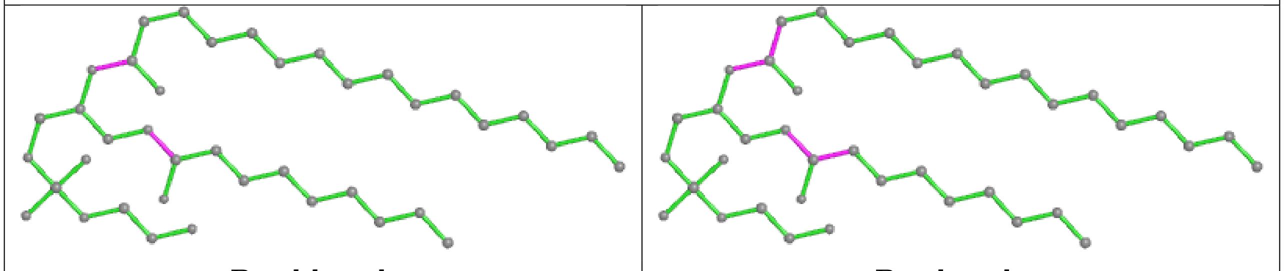


Bond lengths **Bond angles**

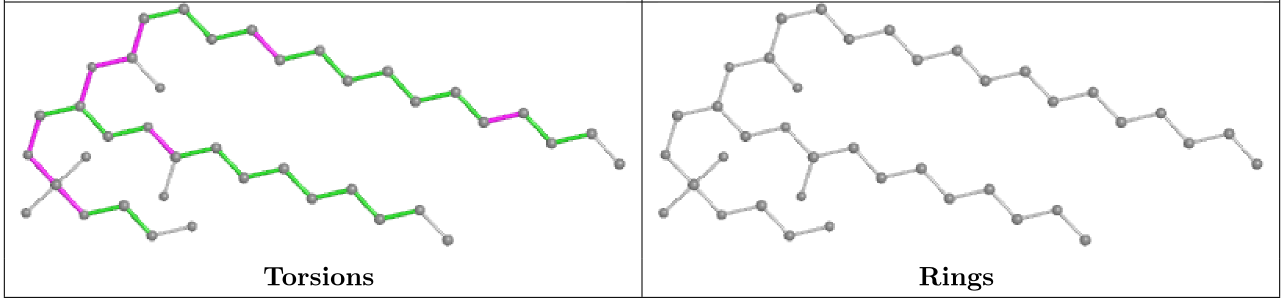


Torsions **Rings**

Ligand 3PE i 201

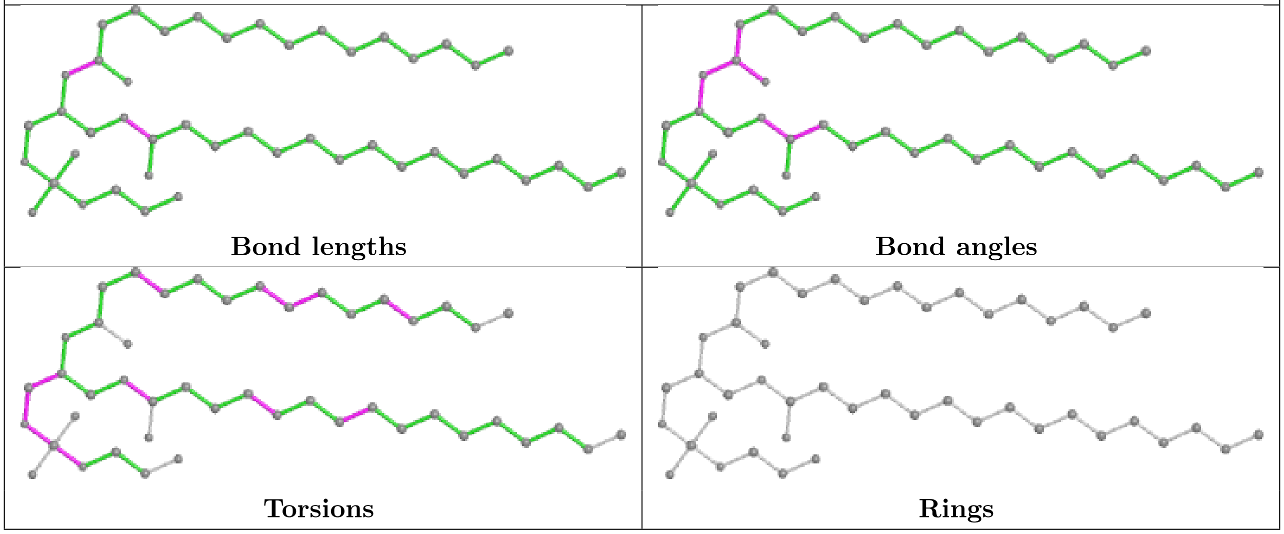


Bond lengths **Bond angles**

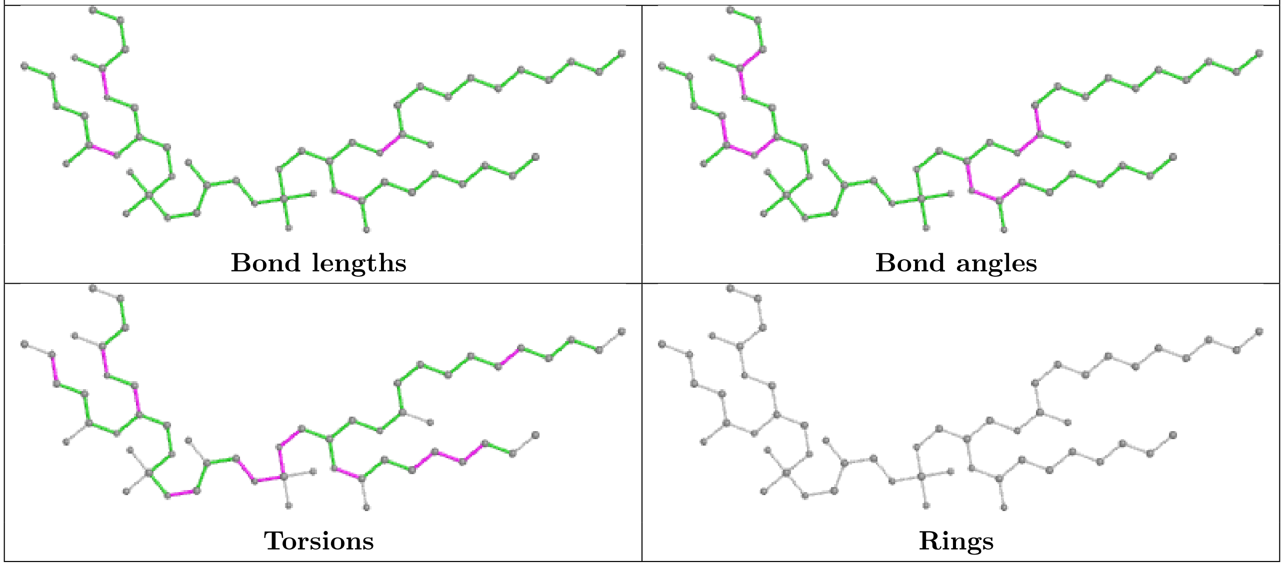


Torsions **Rings**

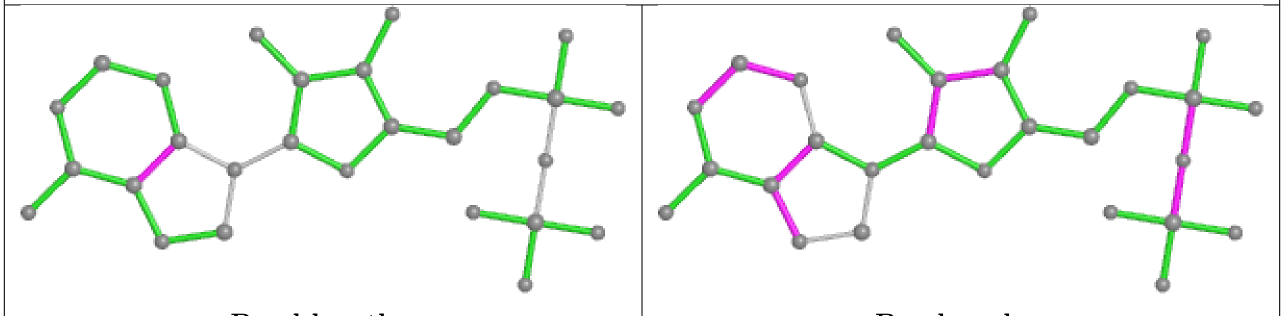
Ligand 3PE K 101



Ligand CDL Ag 102

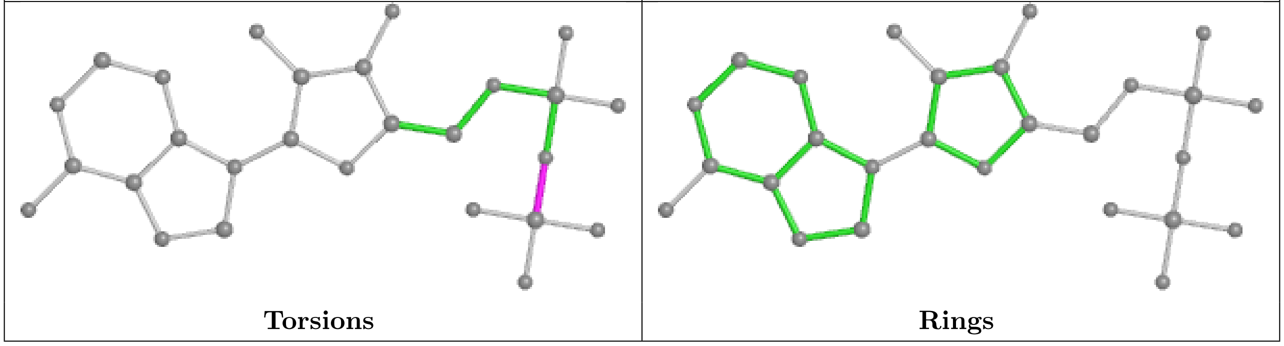


Ligand ADP O 401



Bond lengths

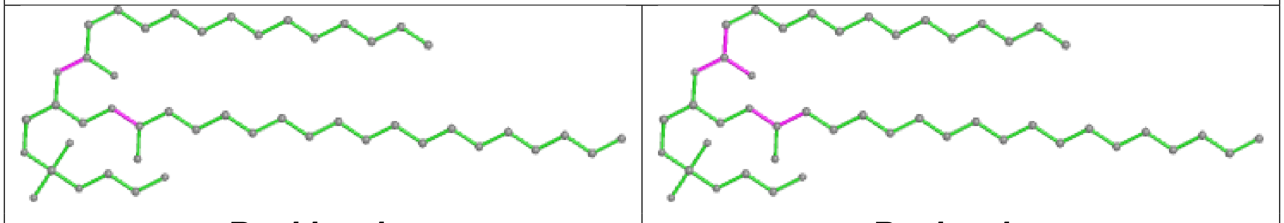
Bond angles



Torsions

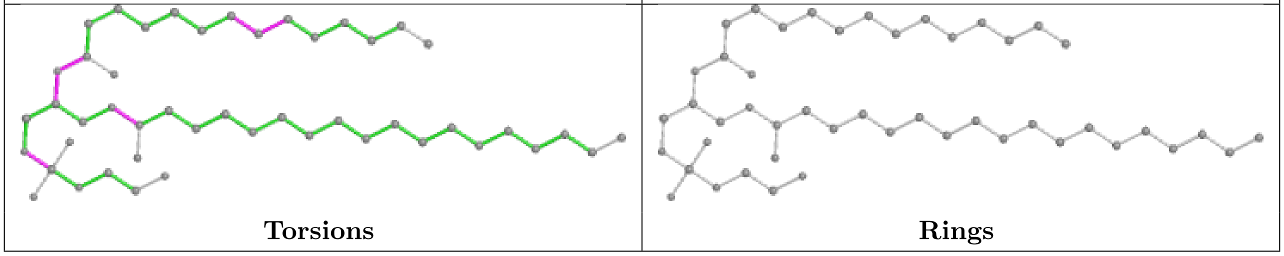
Rings

Ligand 3PE m 201



Bond lengths

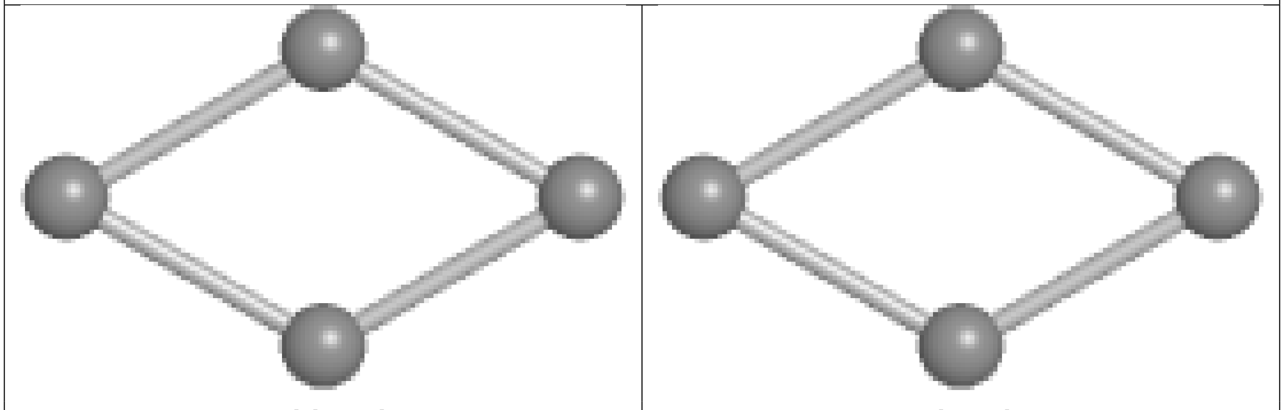
Bond angles



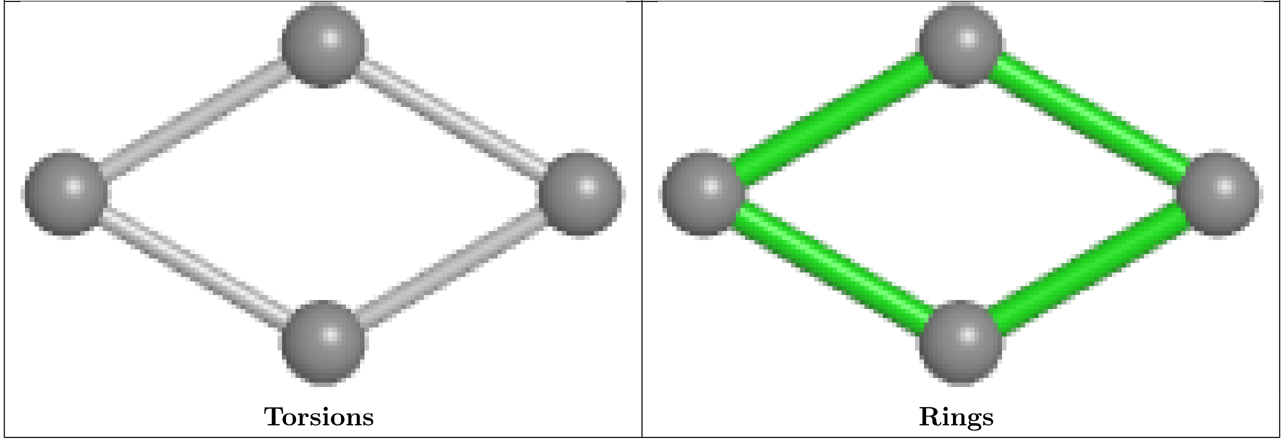
Torsions

Rings

Ligand FES E 301

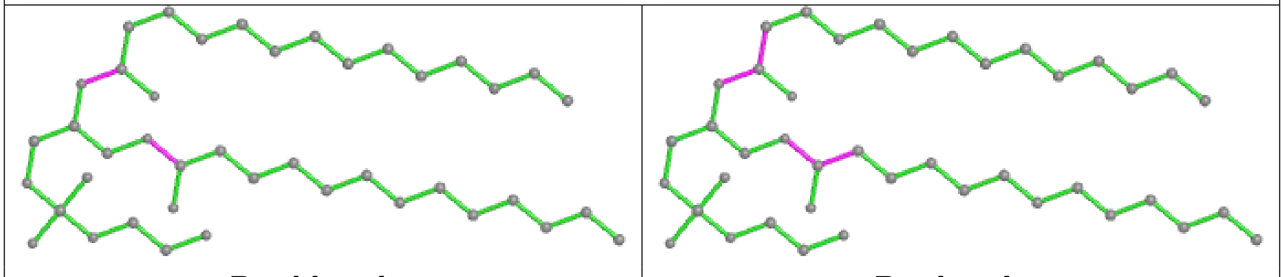


Bond lengths **Bond angles**

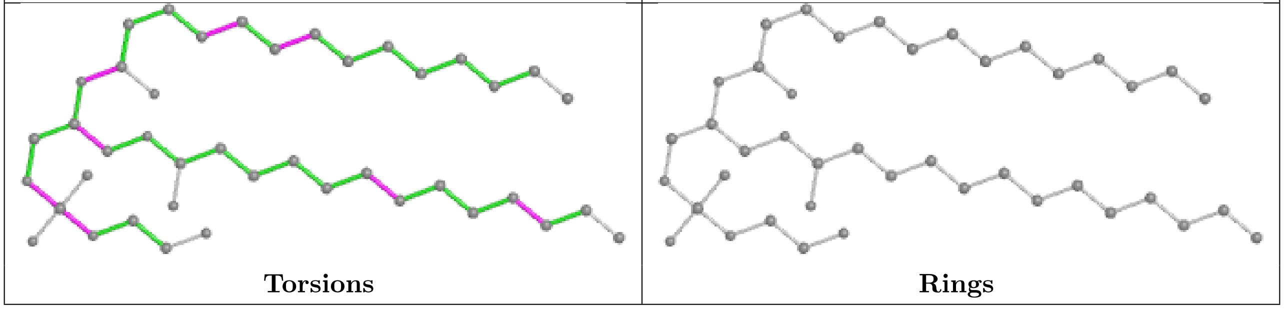


Torsions **Rings**

Ligand 3PE A 201

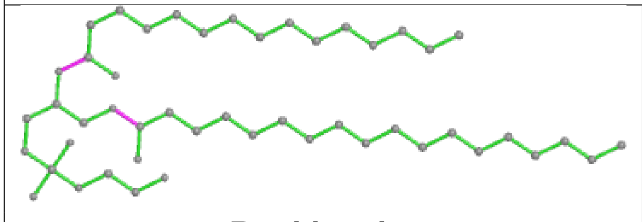


Bond lengths **Bond angles**

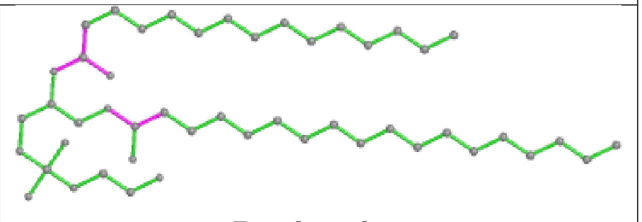


Torsions **Rings**

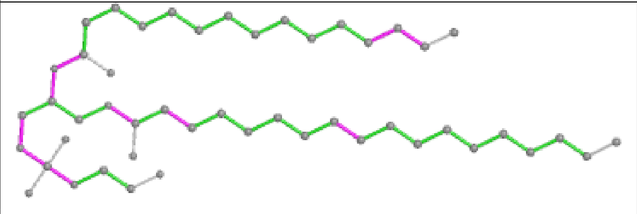
Ligand 3PE H 401



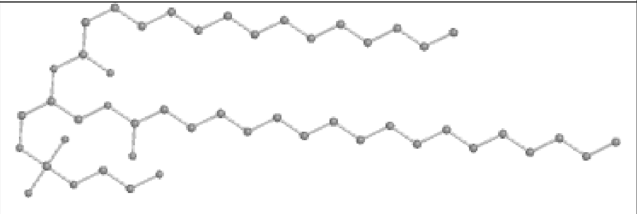
Bond lengths



Bond angles

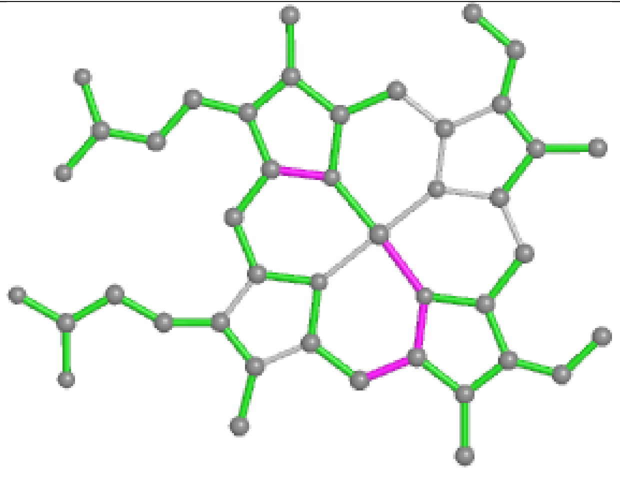


Torsions

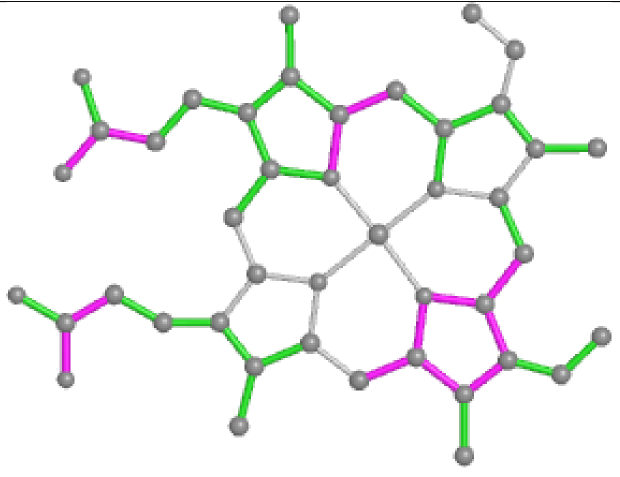


Rings

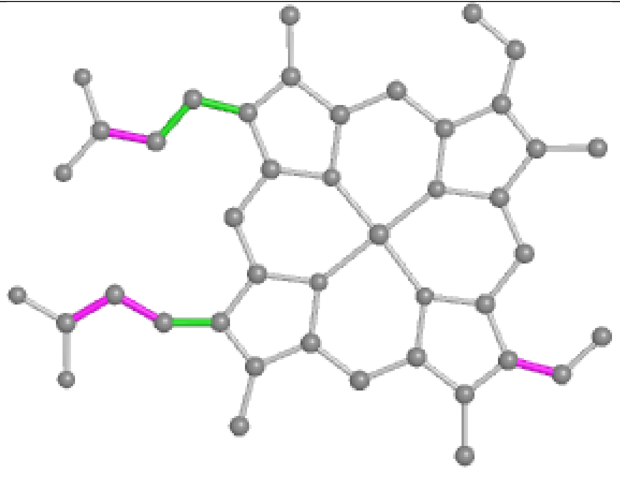
Ligand HEM AC 401



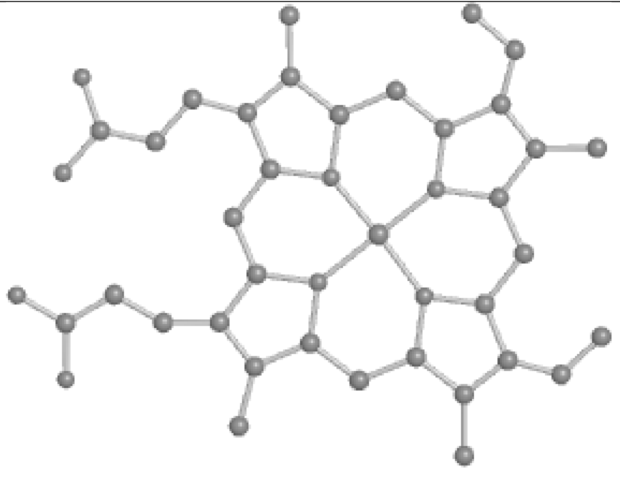
Bond lengths



Bond angles

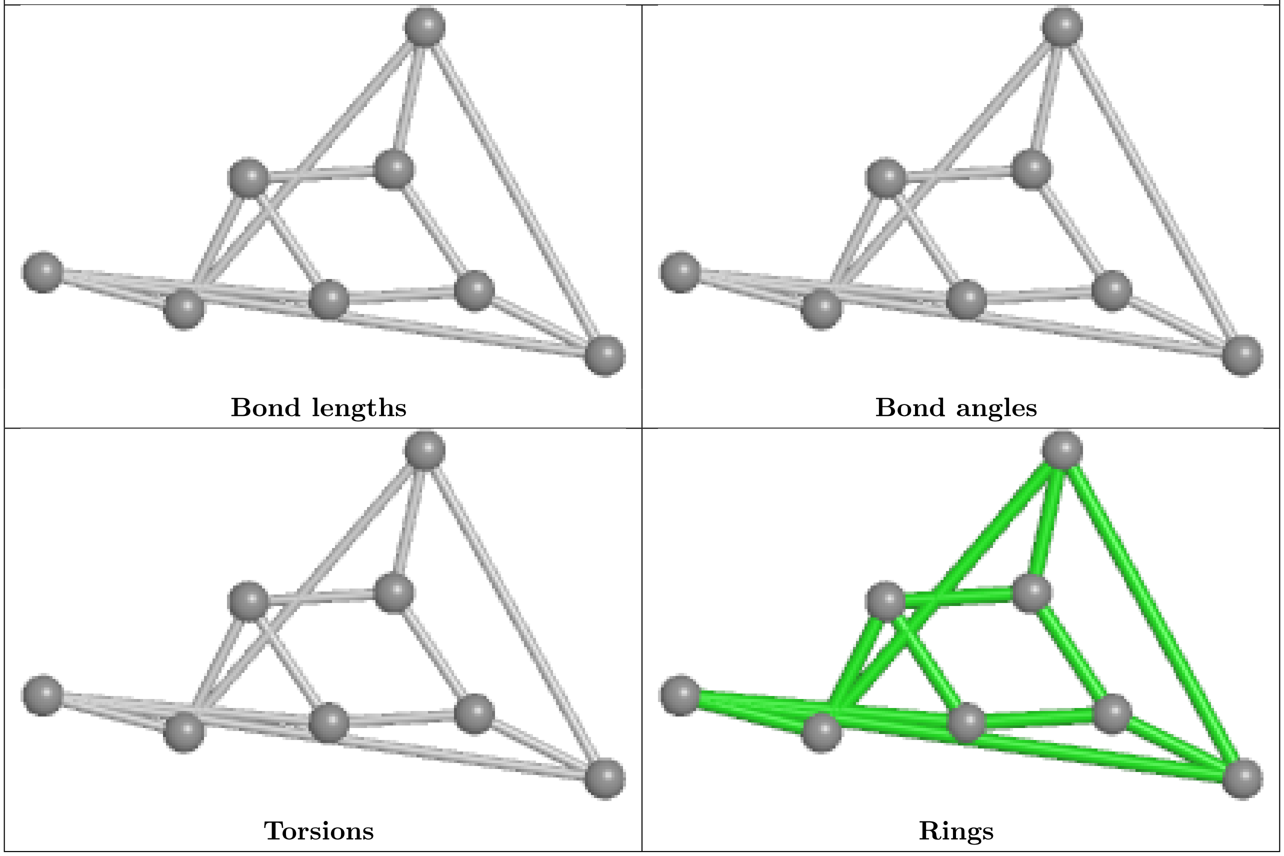


Torsions



Rings

Ligand SF4 G 801



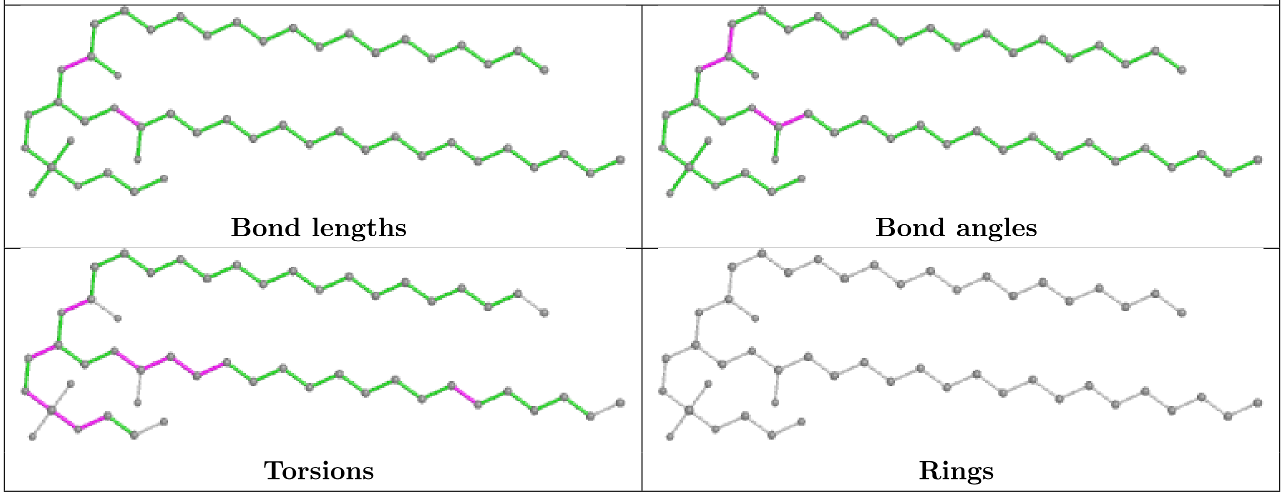
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE I 301



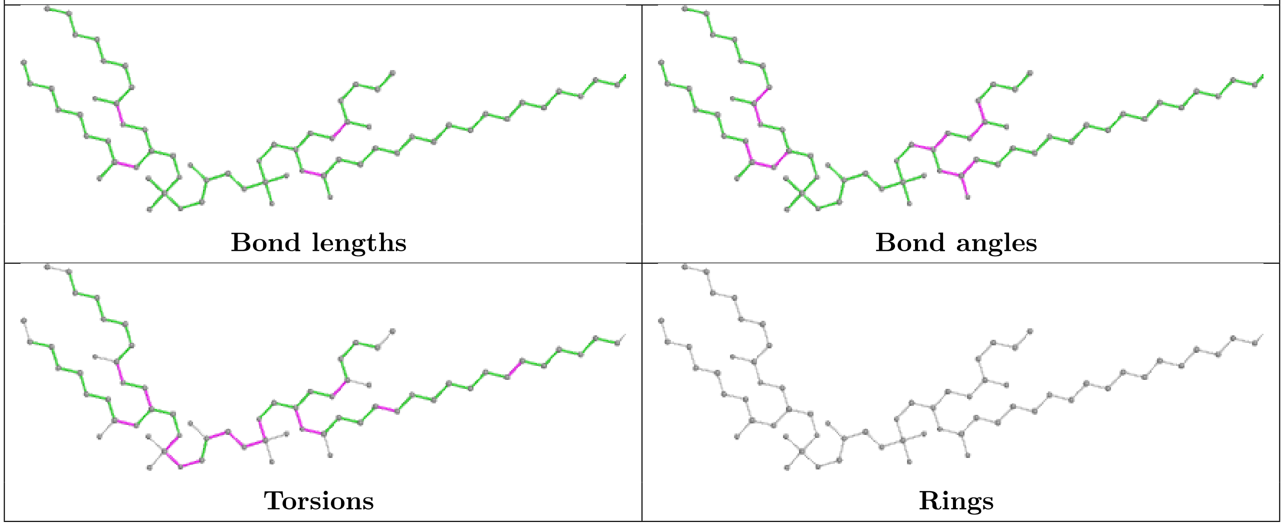
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL X 201



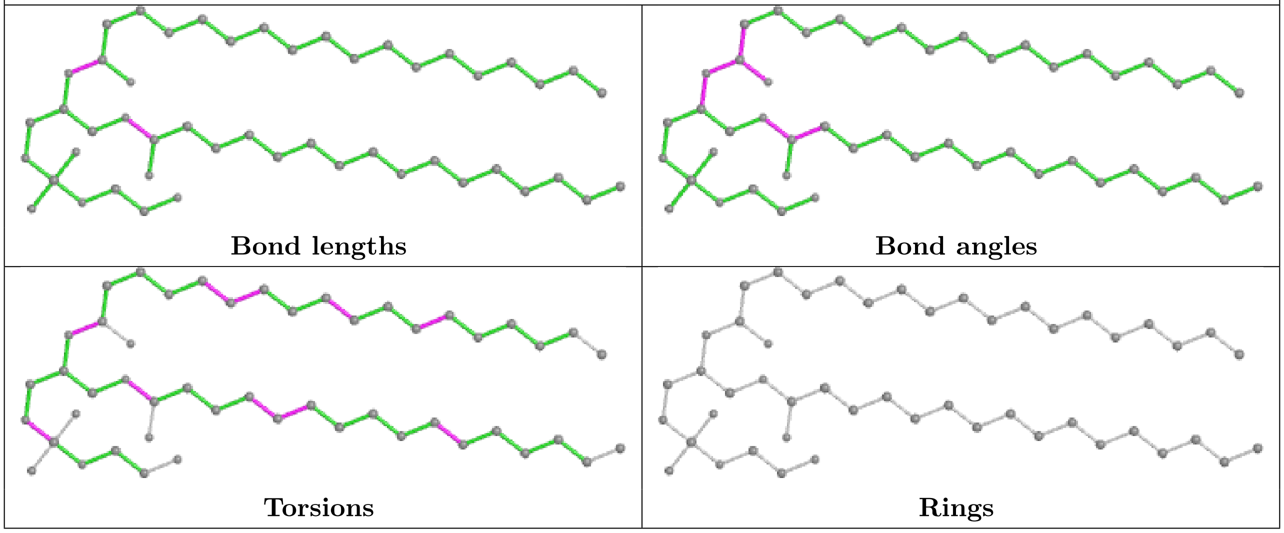
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE L 702



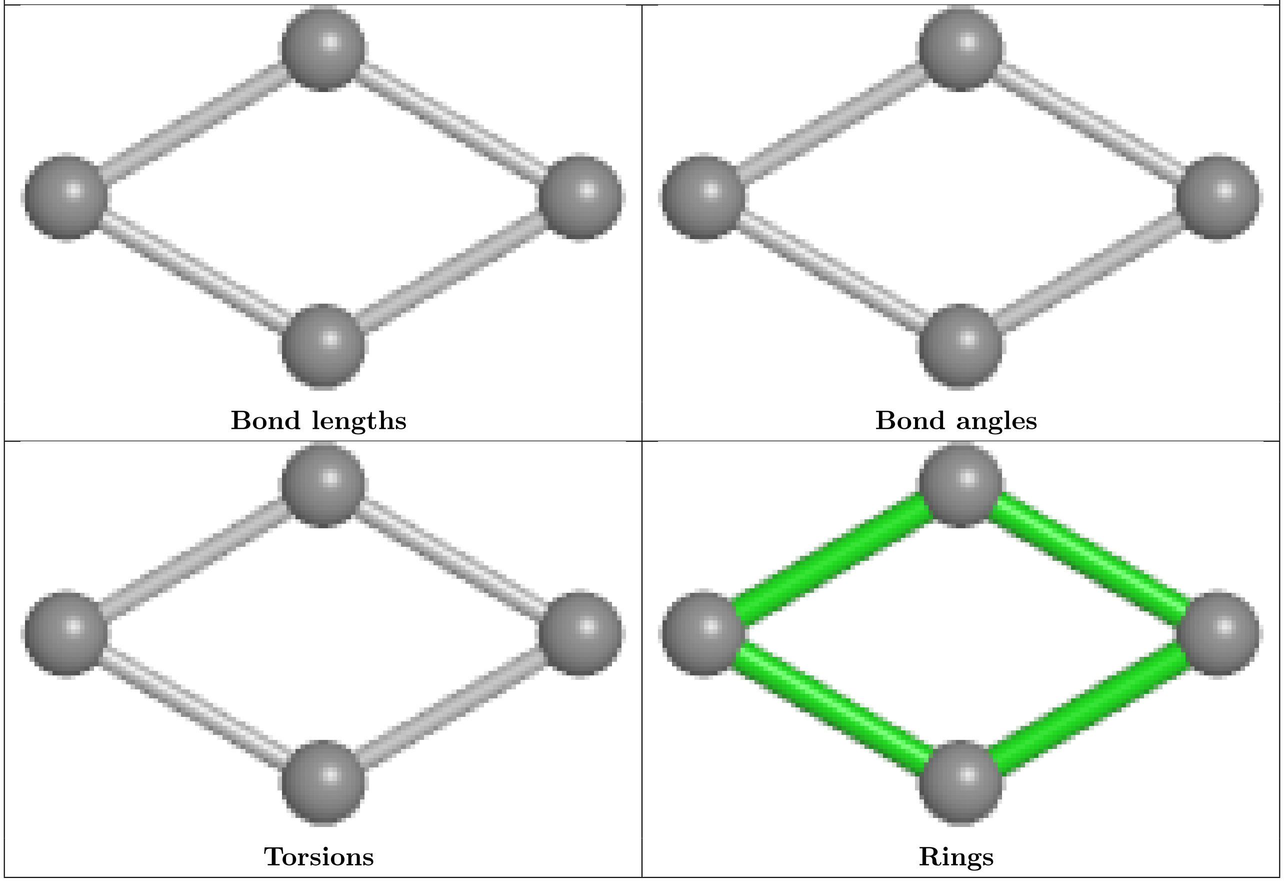
Bond lengths

Bond angles

Torsions

Rings

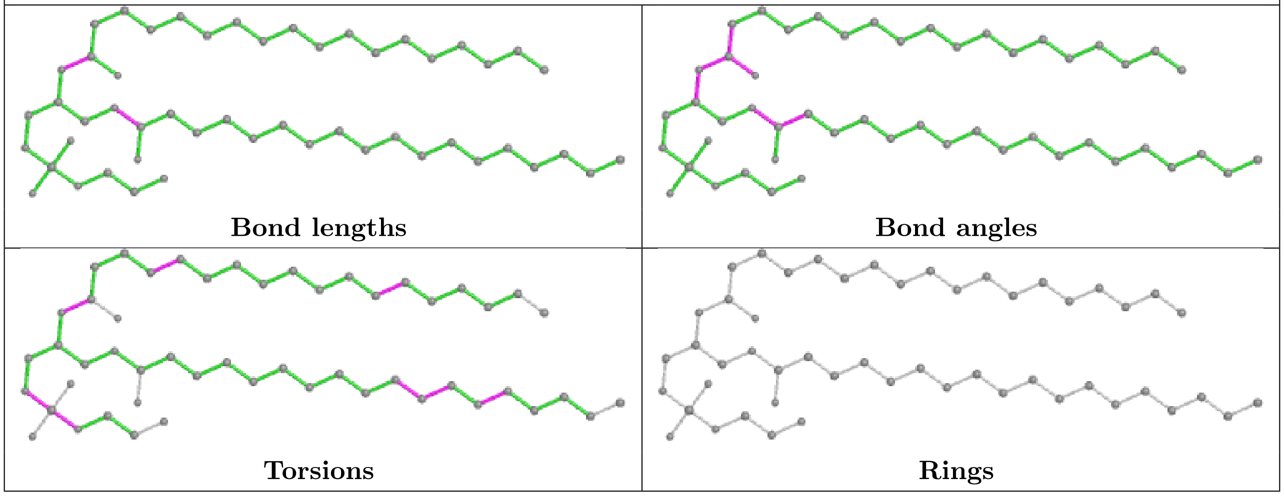
Ligand FES G 803



Bond lengths Bond angles

Torsions Rings

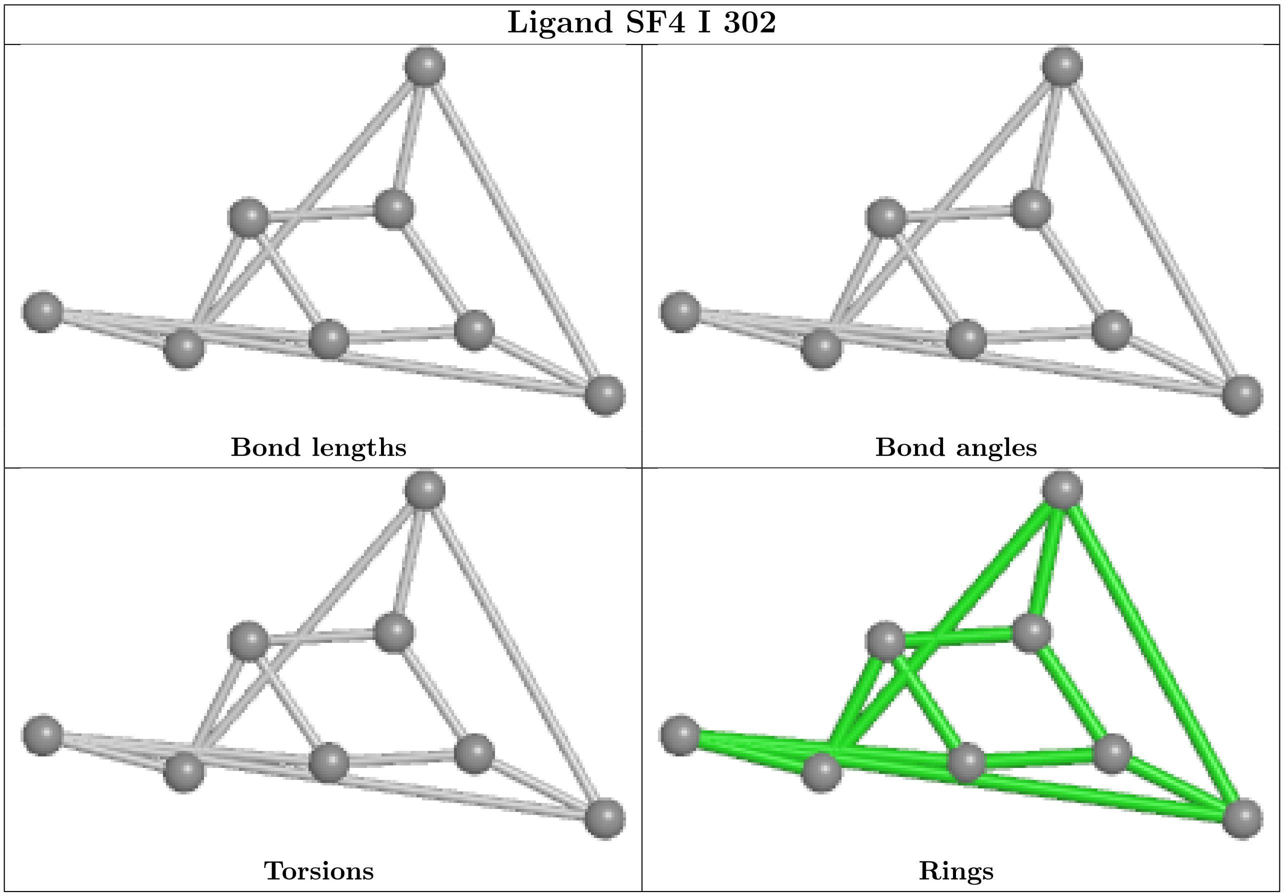
Ligand 3PE M 502



Bond lengths Bond angles

Torsions Rings

Ligand SF4 I 302



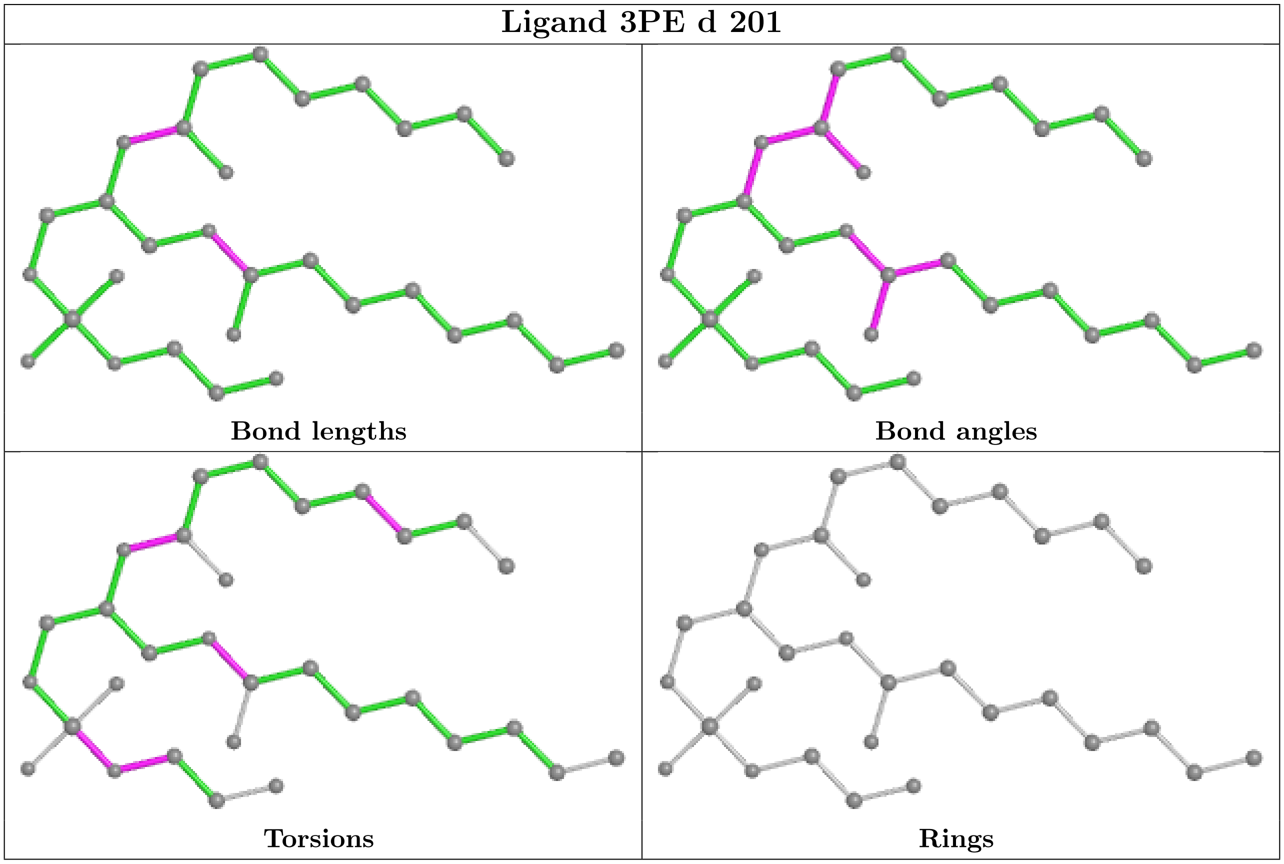
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE d 201



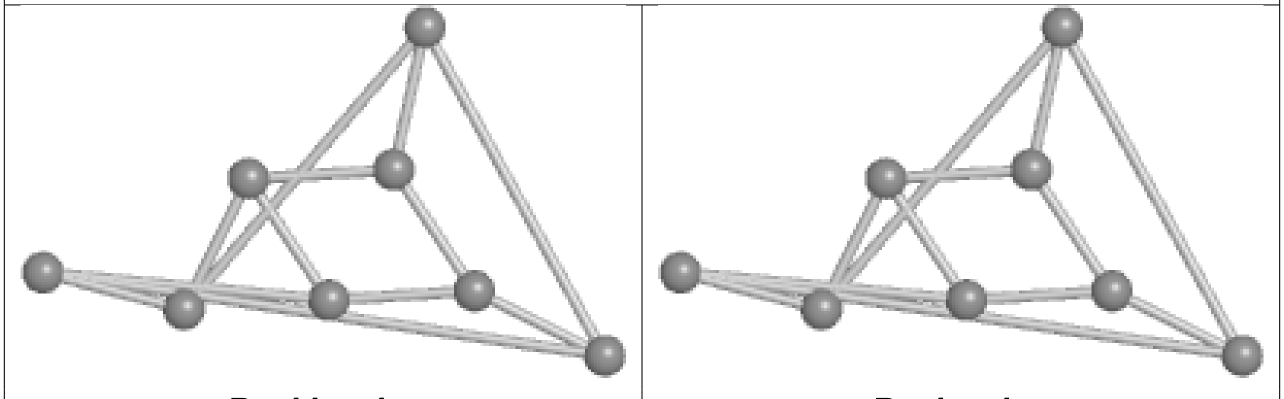
Bond lengths

Bond angles

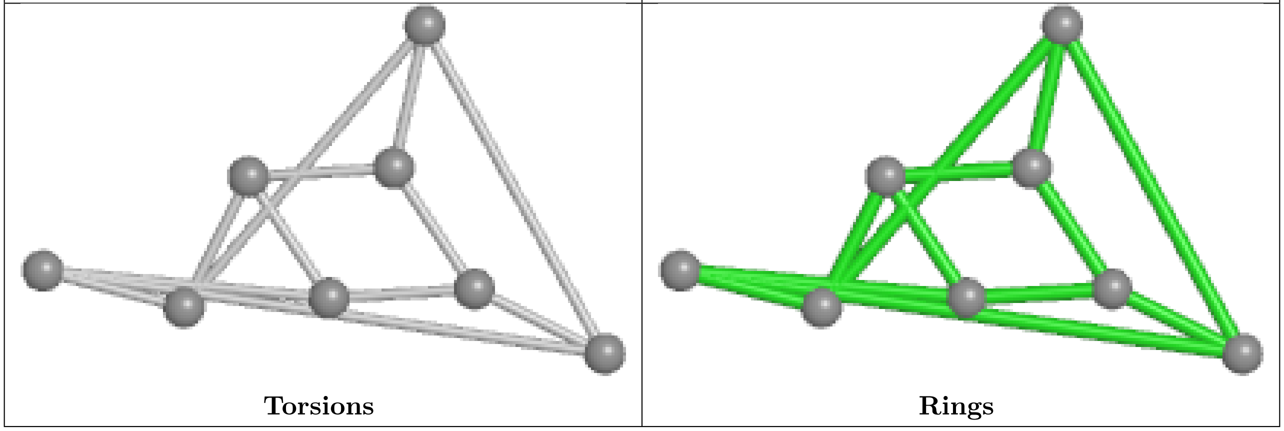
Torsions

Rings

Ligand SF4 G 802

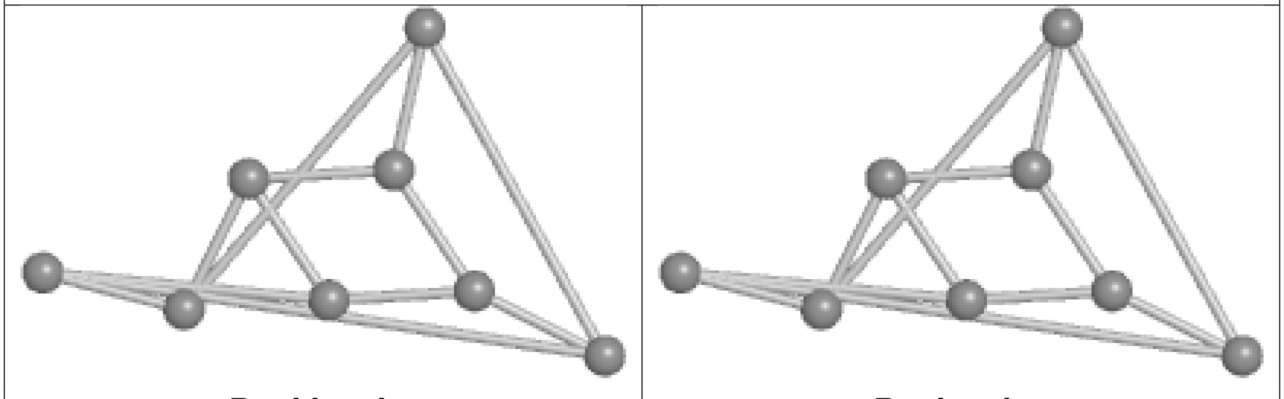


Bond lengths Bond angles

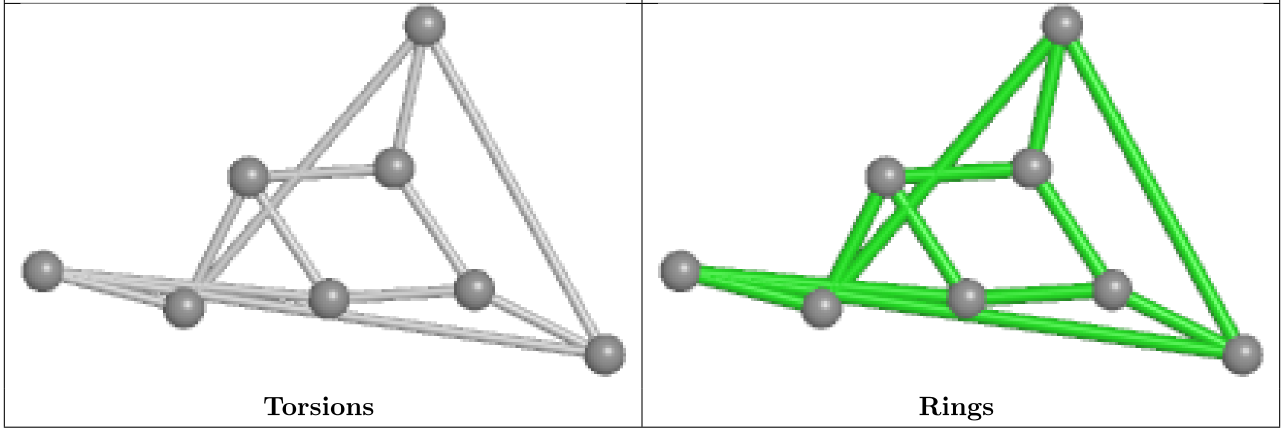


Torsions Rings

Ligand SF4 B 301

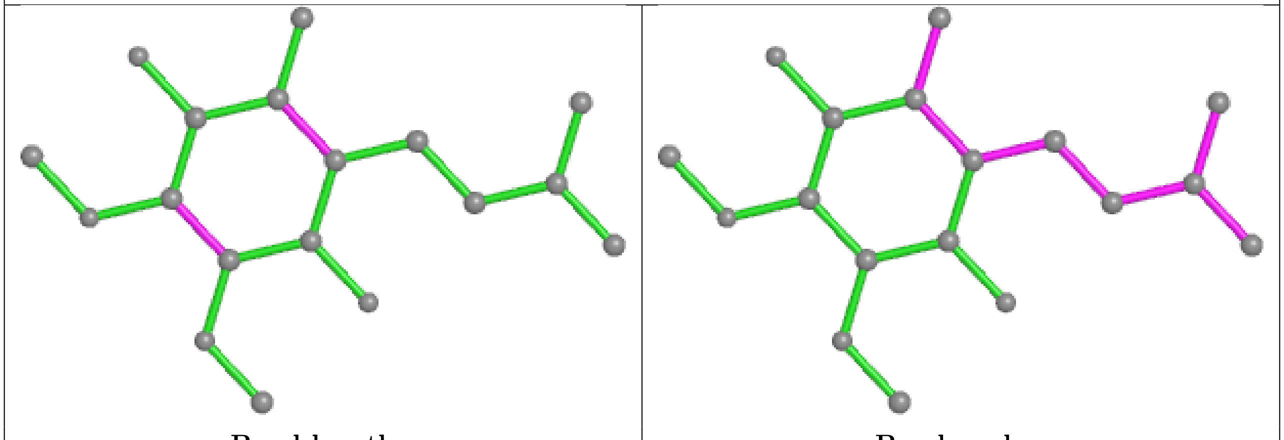


Bond lengths Bond angles

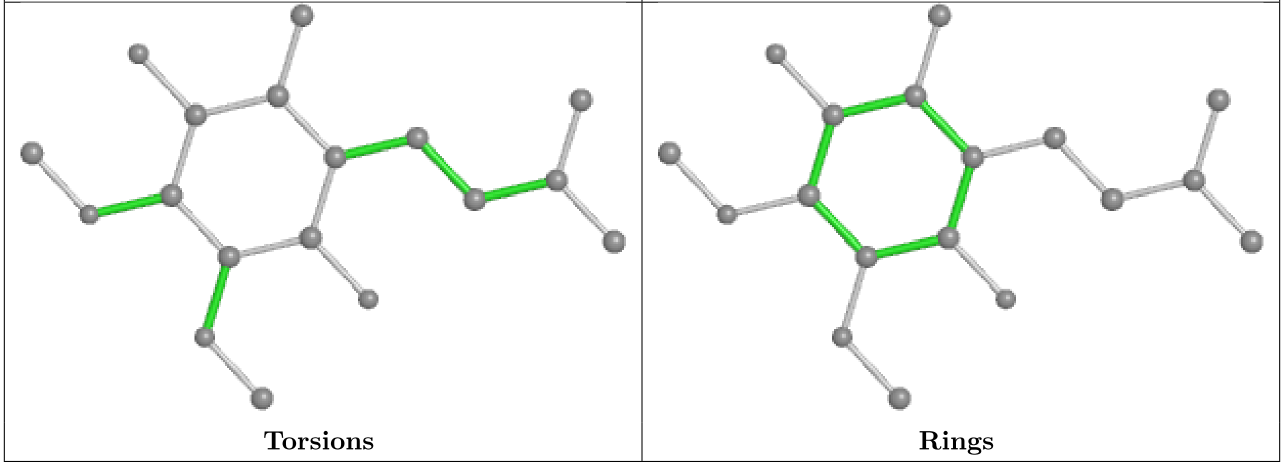


Torsions Rings

Ligand UQ1 B 302

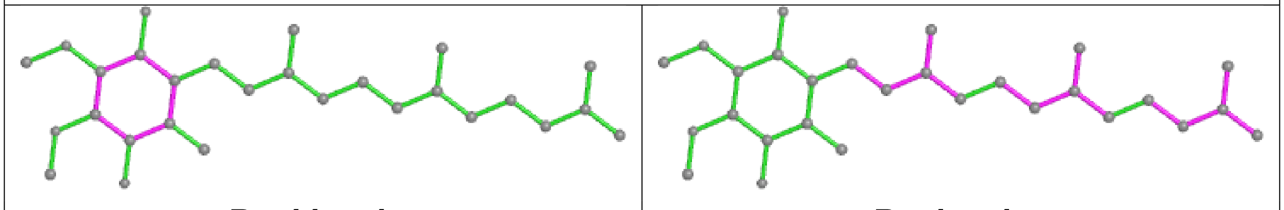


Bond lengths **Bond angles**

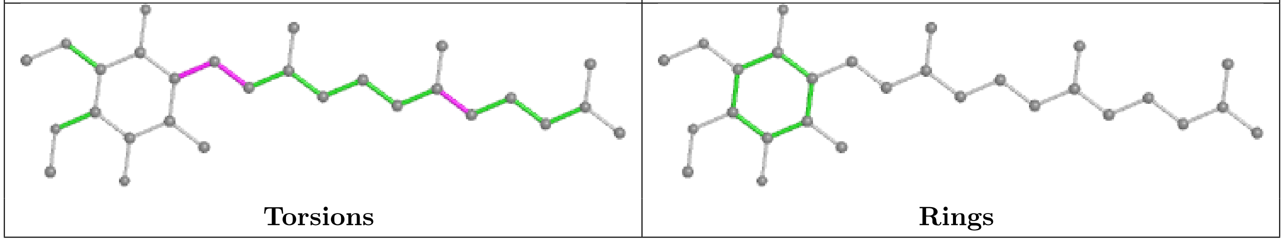


Torsions **Rings**

Ligand UQ6 Ac 405

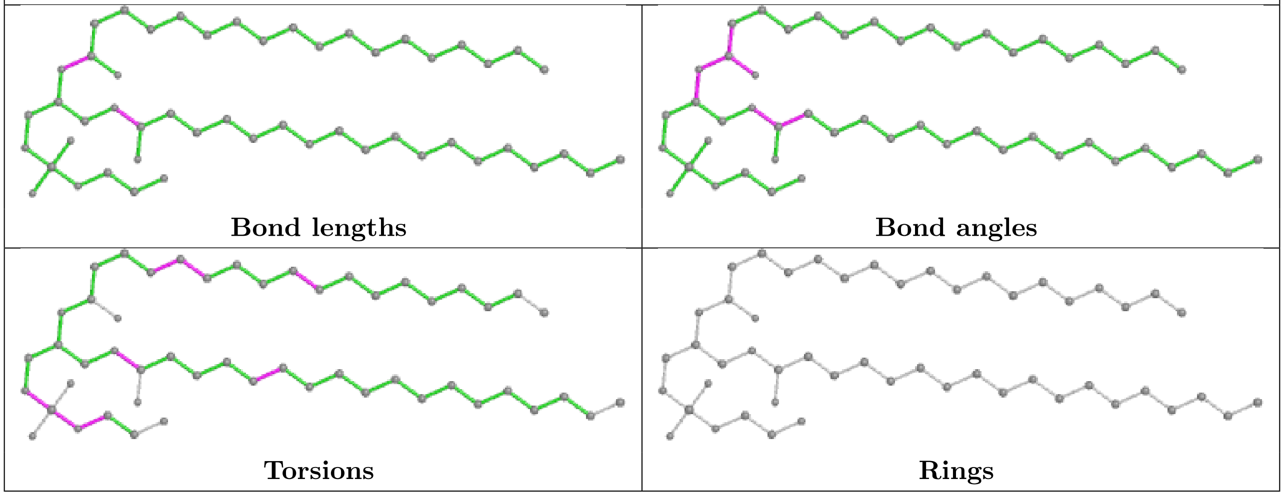


Bond lengths **Bond angles**



Torsions **Rings**

Ligand 3PE N 401



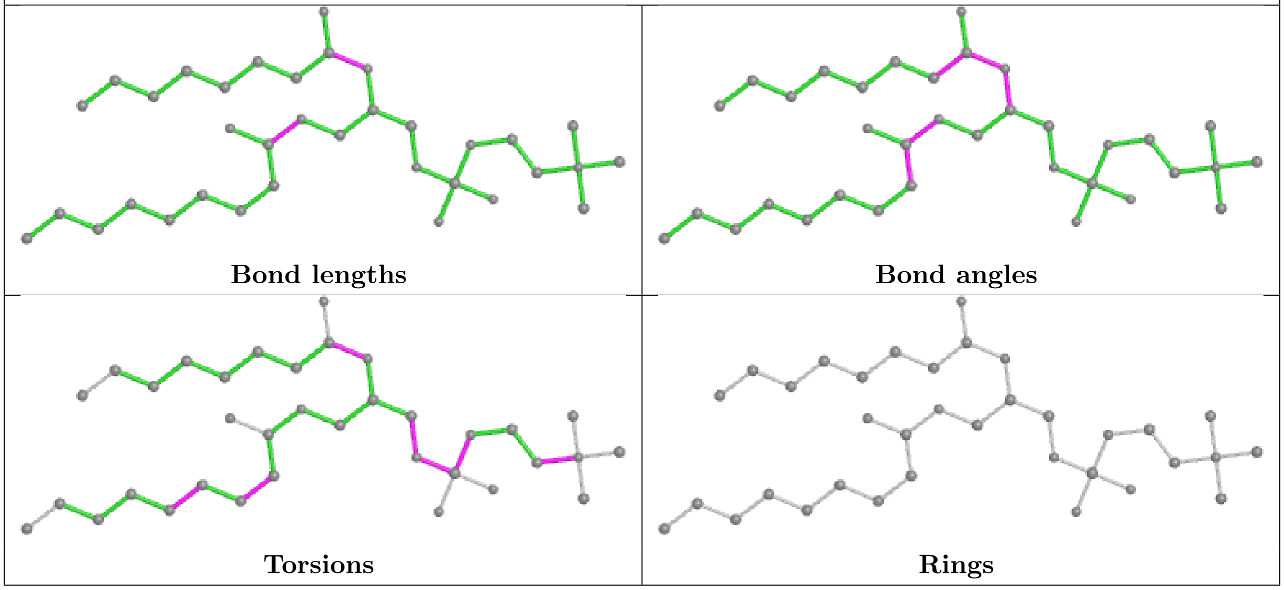
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 303



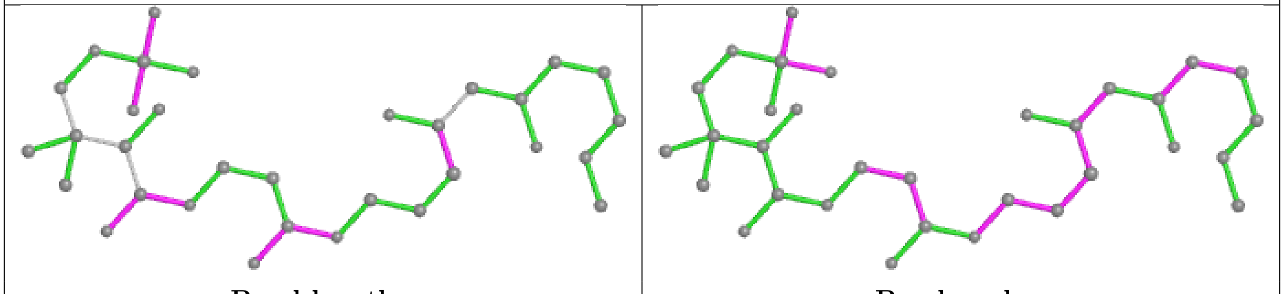
Bond lengths

Bond angles

Torsions

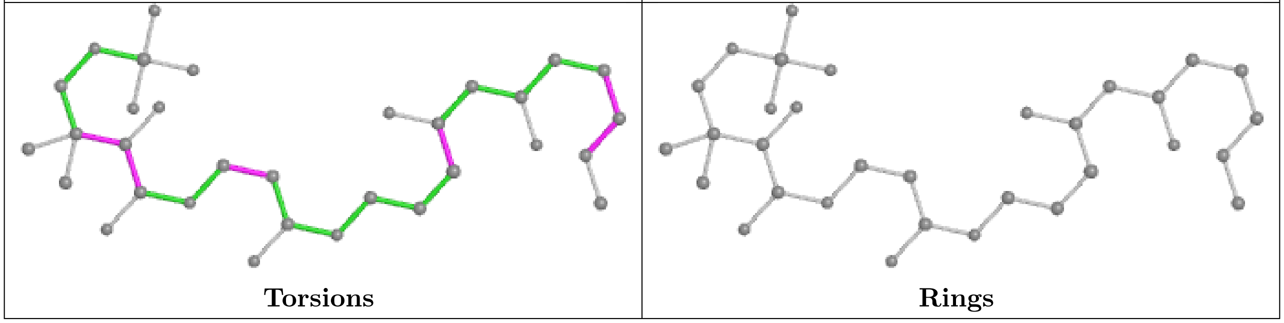
Rings

Ligand EHZ n 201



Bond lengths

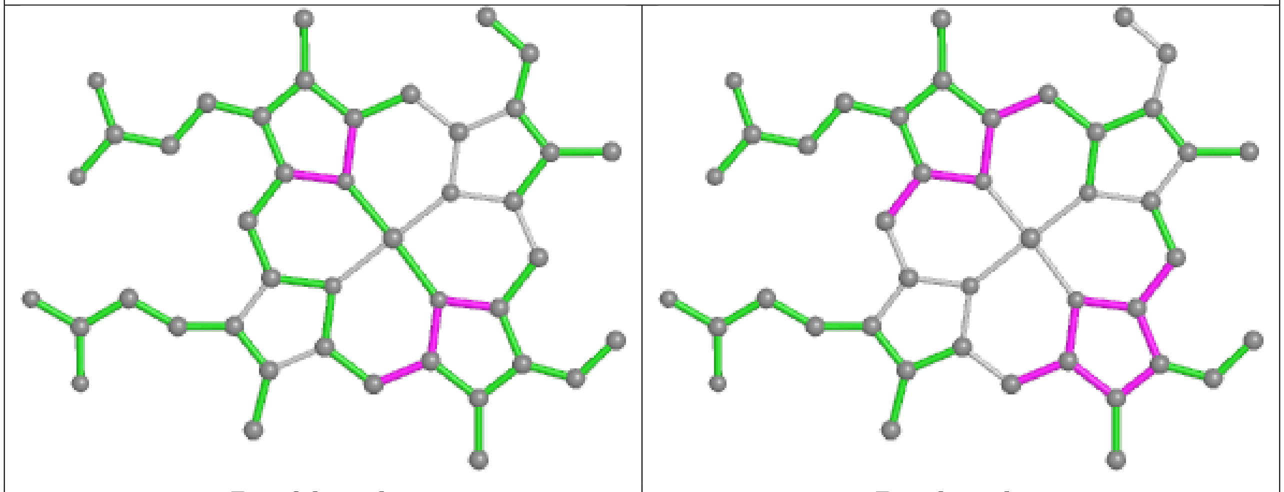
Bond angles



Torsions

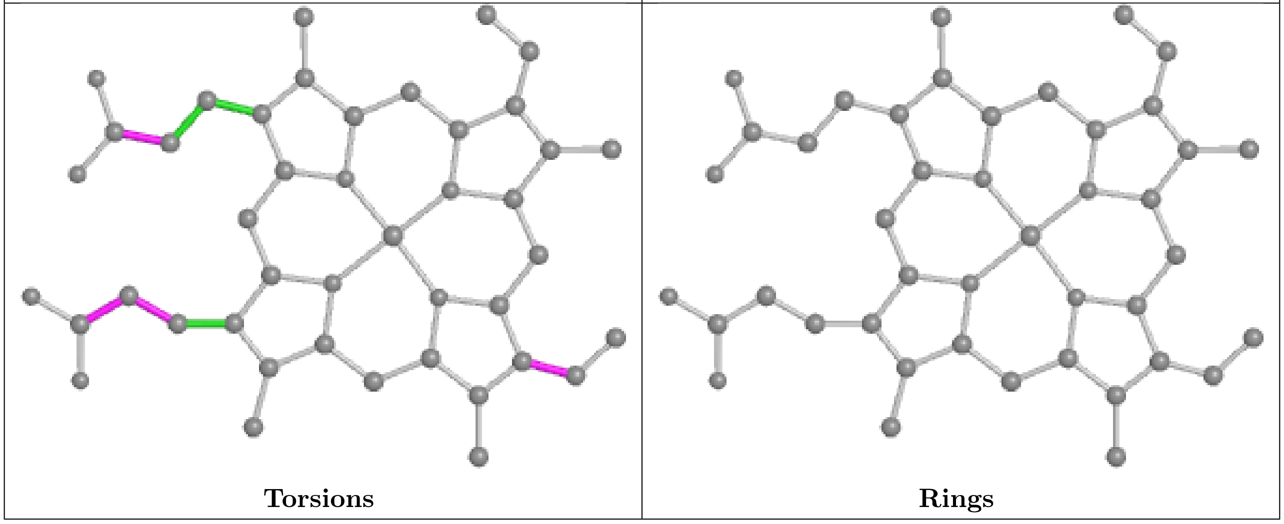
Rings

Ligand HEM Ac 401



Bond lengths

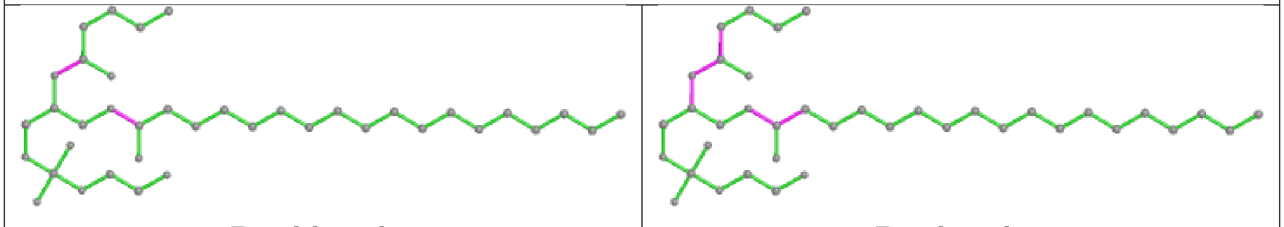
Bond angles



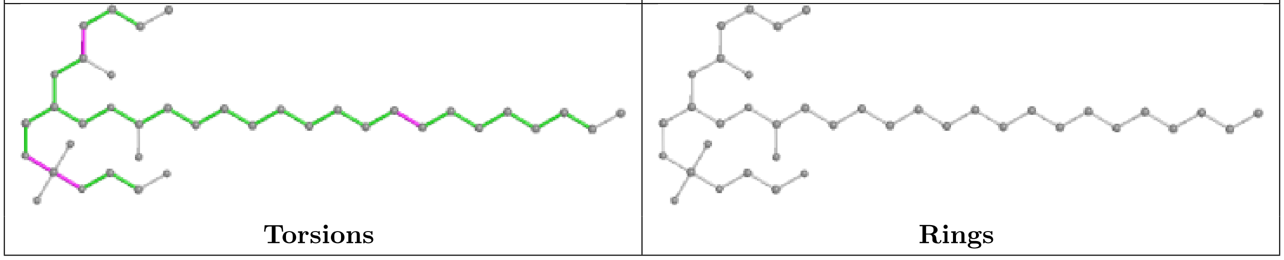
Torsions

Rings

Ligand 3PE Ag 103

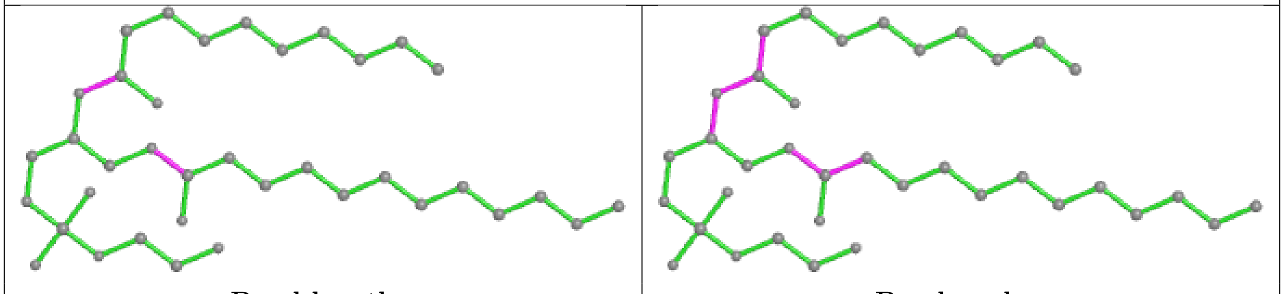


Bond lengths Bond angles

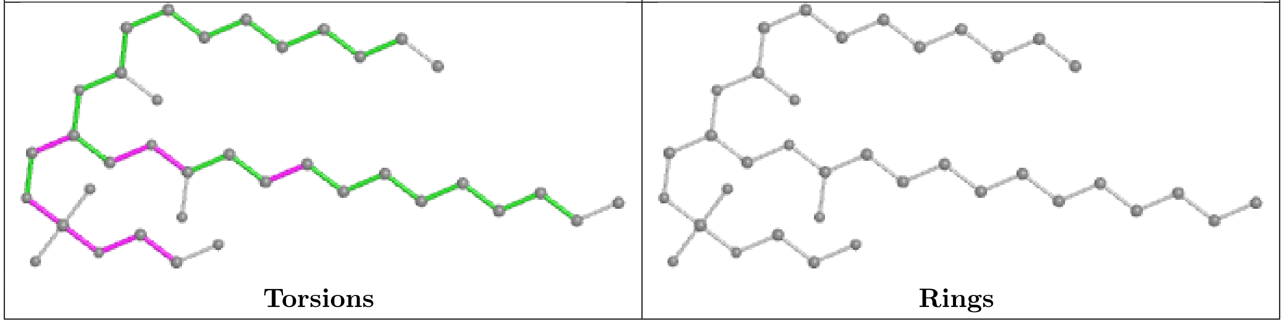


Torsions Rings

Ligand 3PE M 501

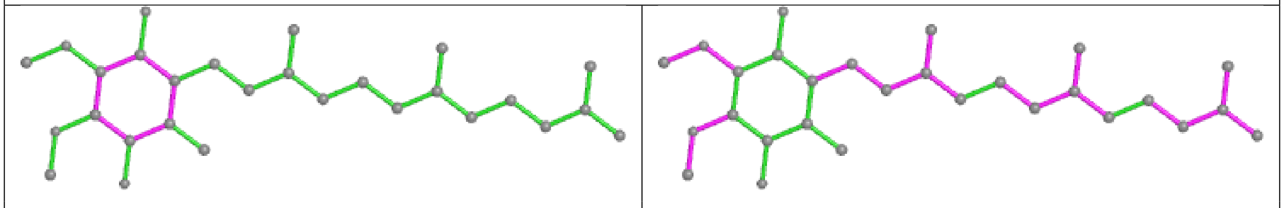


Bond lengths Bond angles

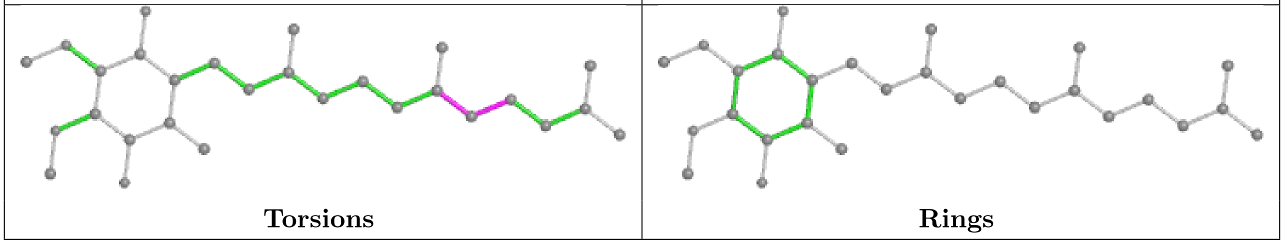


Torsions Rings

Ligand UQ6 AC 403

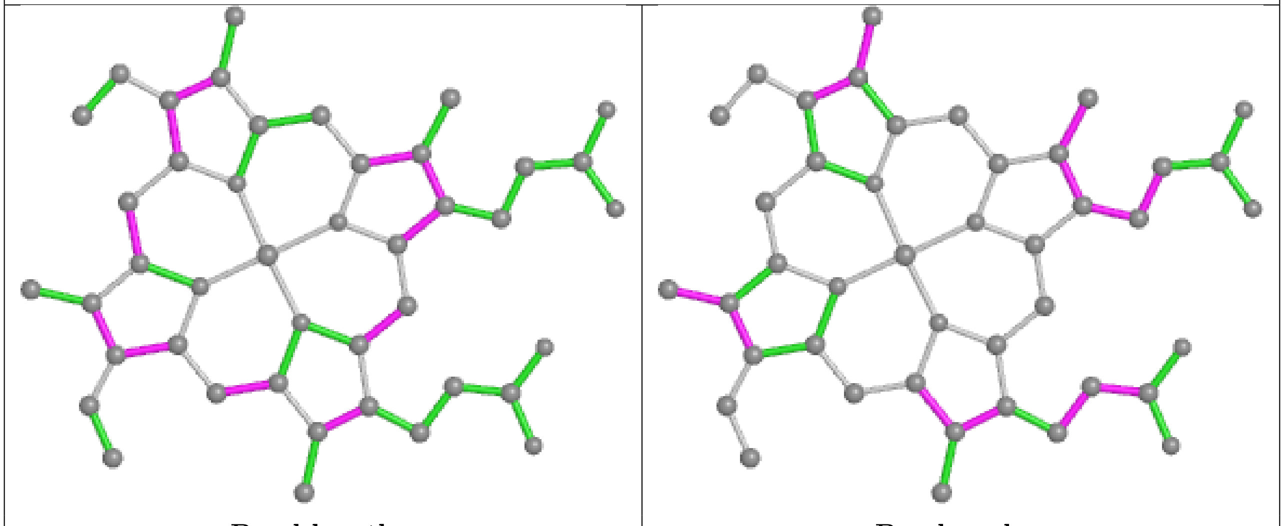


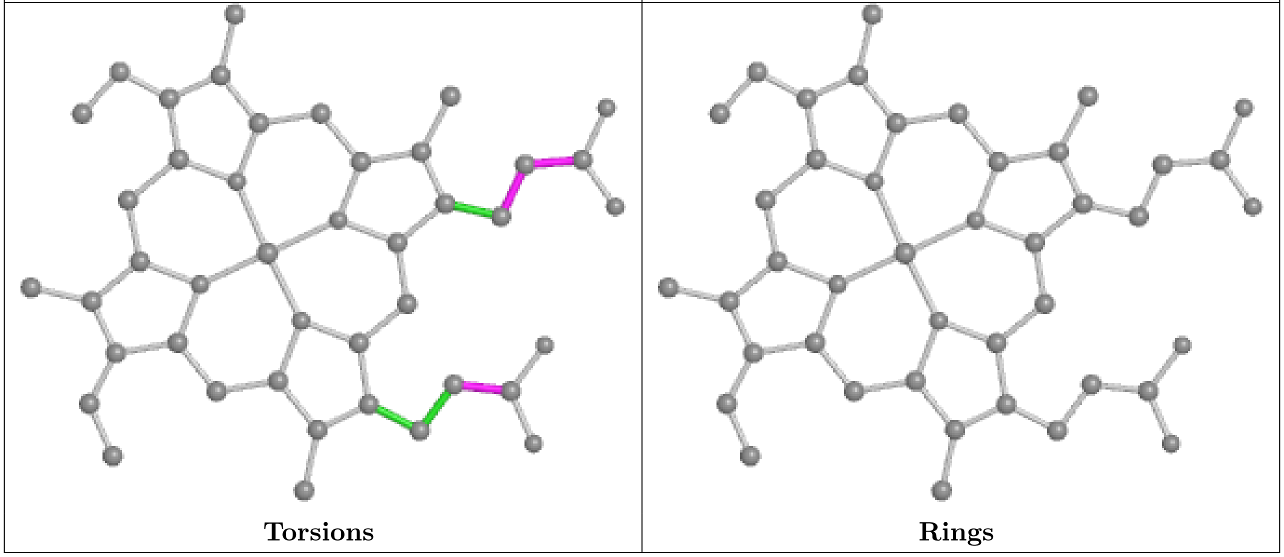
Bond lengths Bond angles



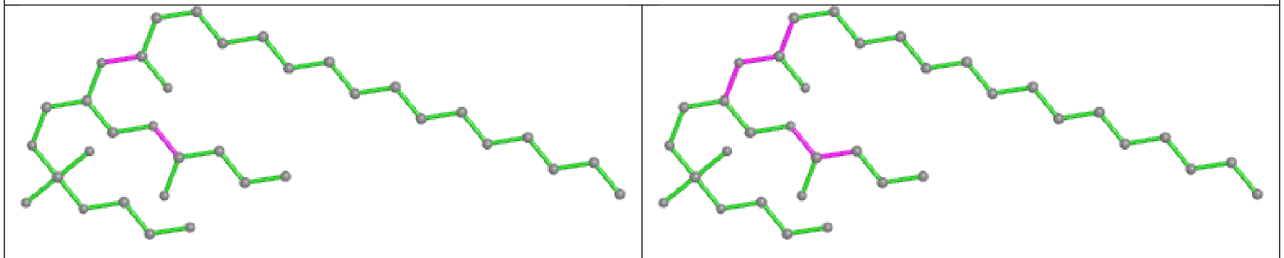
Torsions Rings

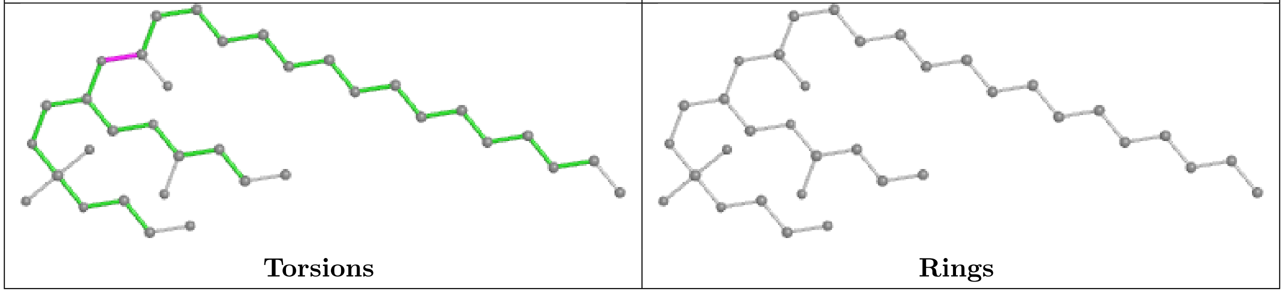
Ligand HEC AD 401


Bond lengths Bond angles

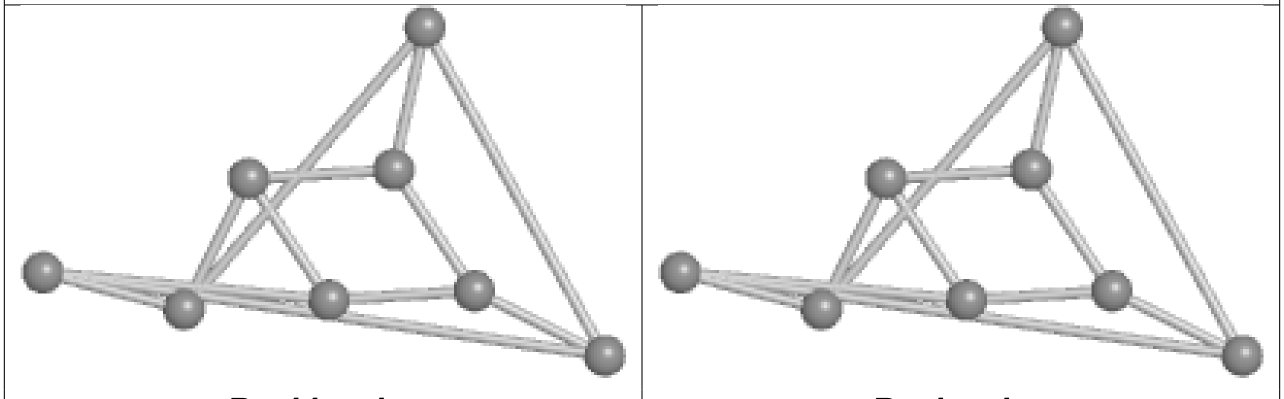

Torsions Rings

Ligand 3PE Ac 403


Bond lengths Bond angles

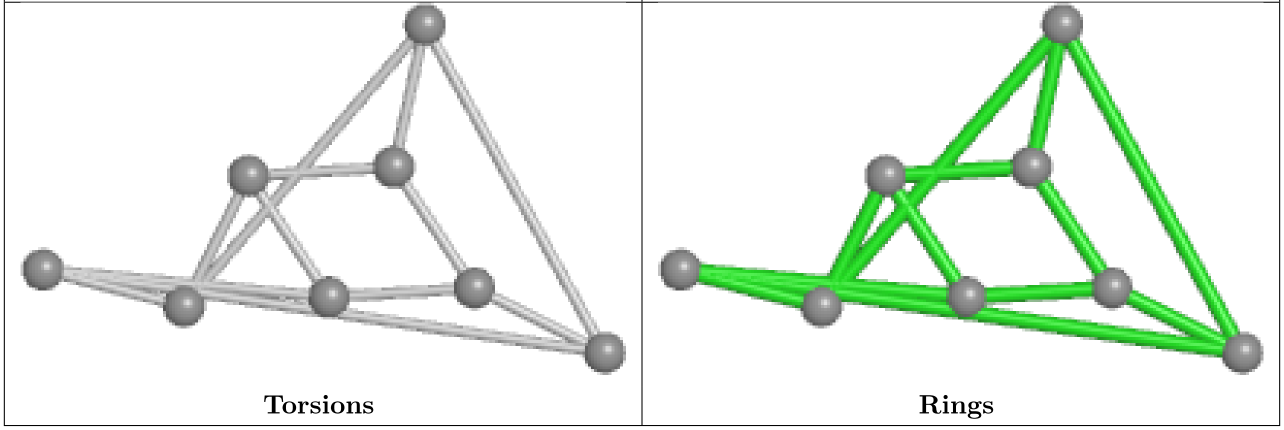

Torsions Rings

Ligand SF4 I 303



Bond lengths

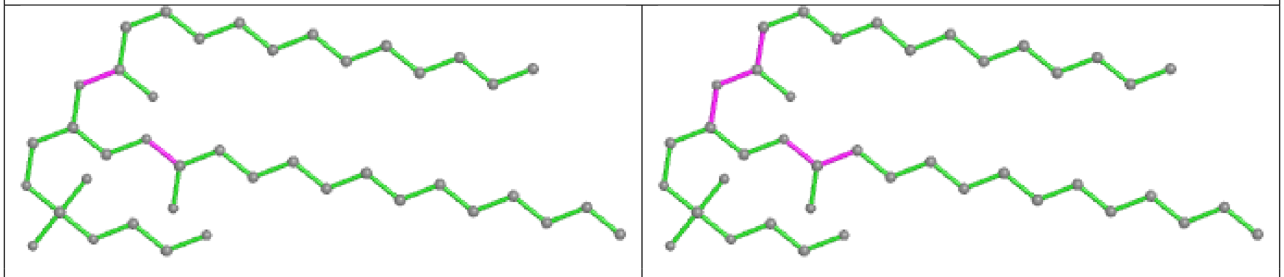
Bond angles



Torsions

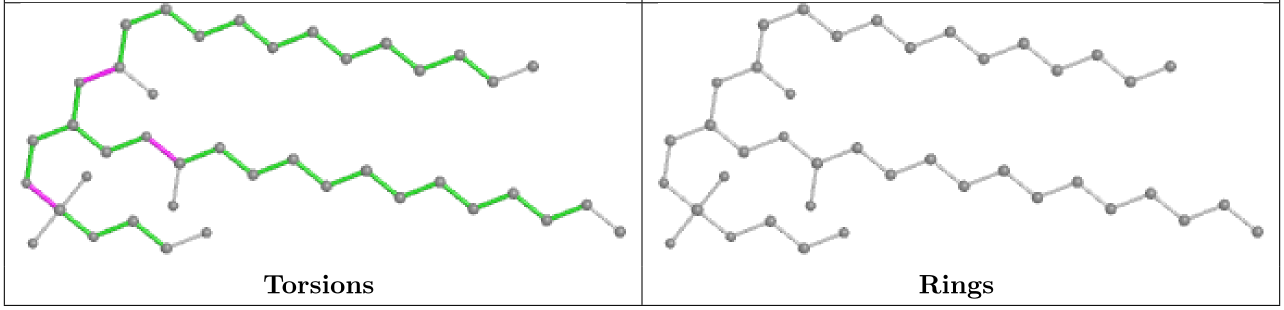
Rings

Ligand 3PE m 203



Bond lengths

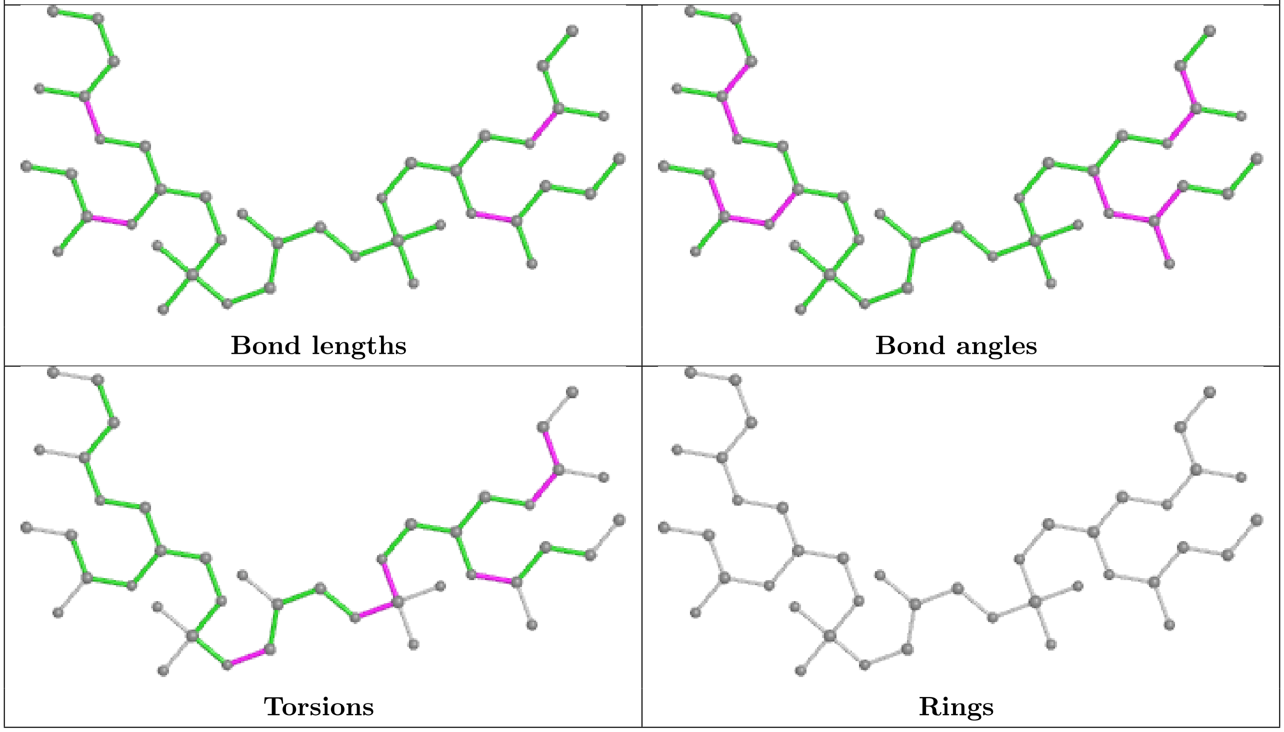
Bond angles



Torsions

Rings

Ligand CDL Ag 101



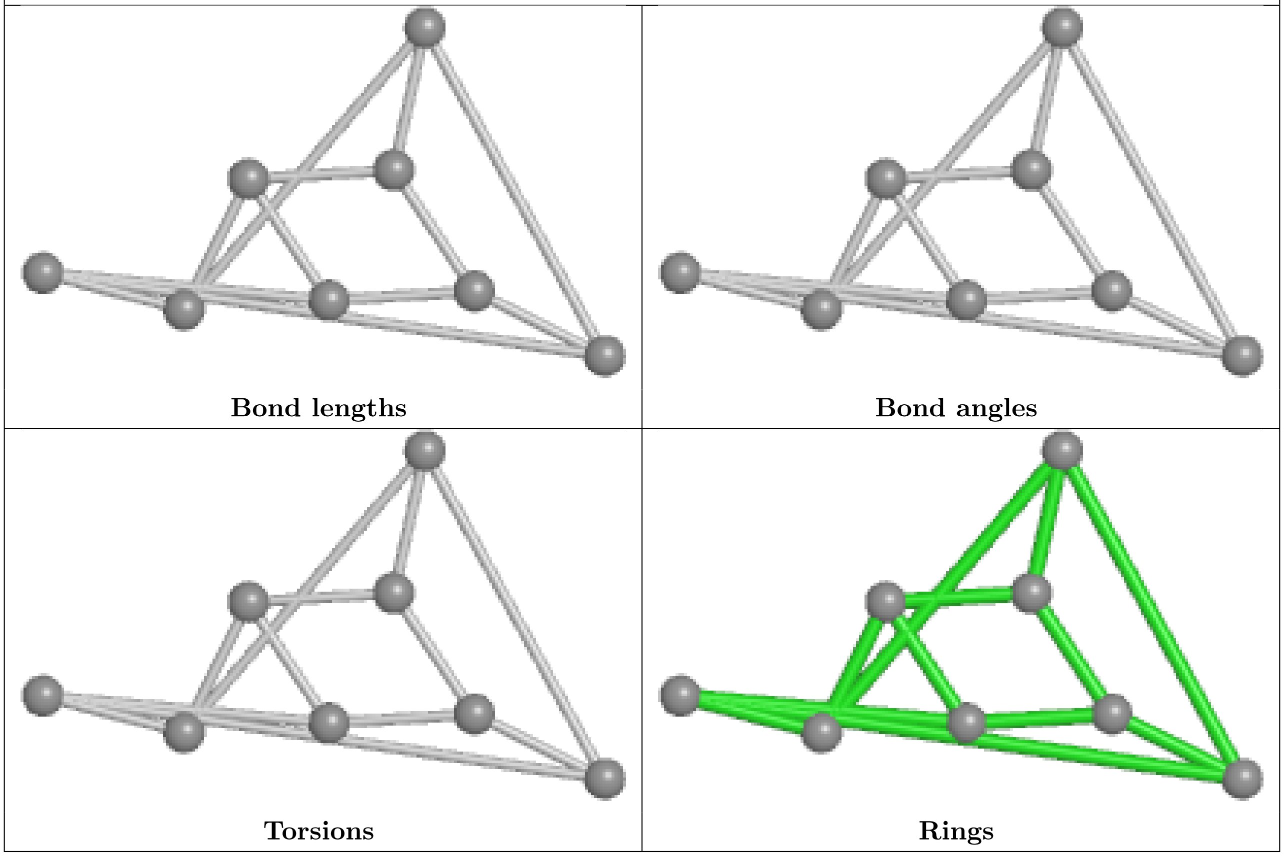
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 F 502



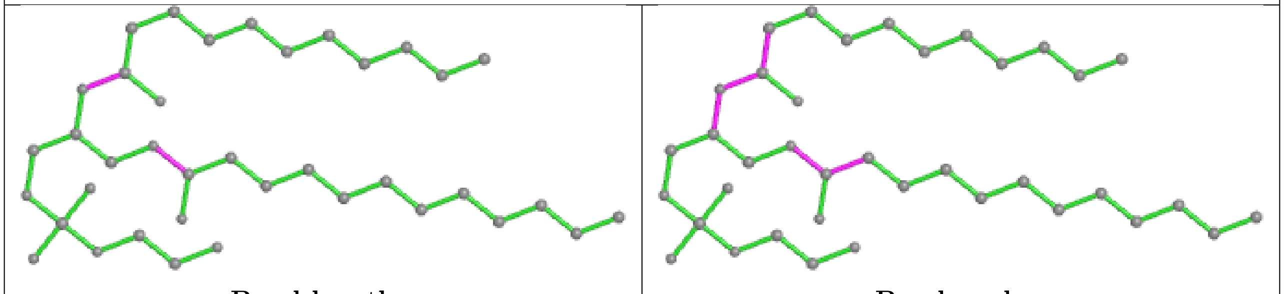
Bond lengths

Bond angles

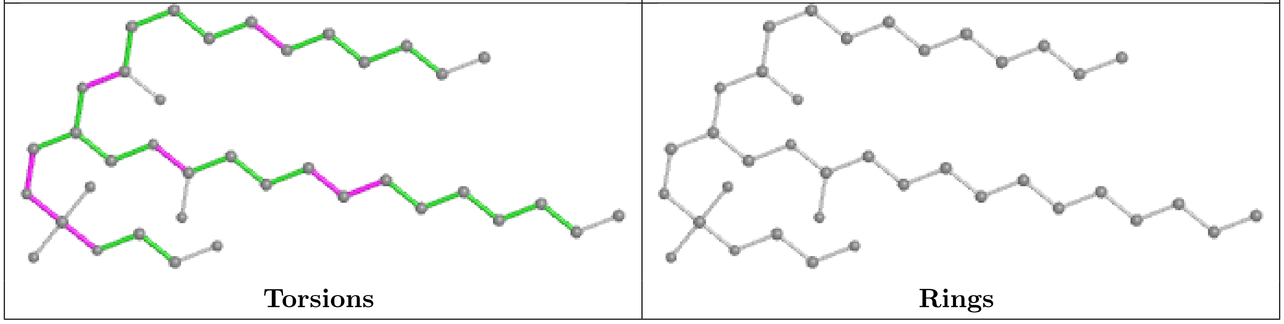
Torsions

Rings

Ligand 3PE L 705

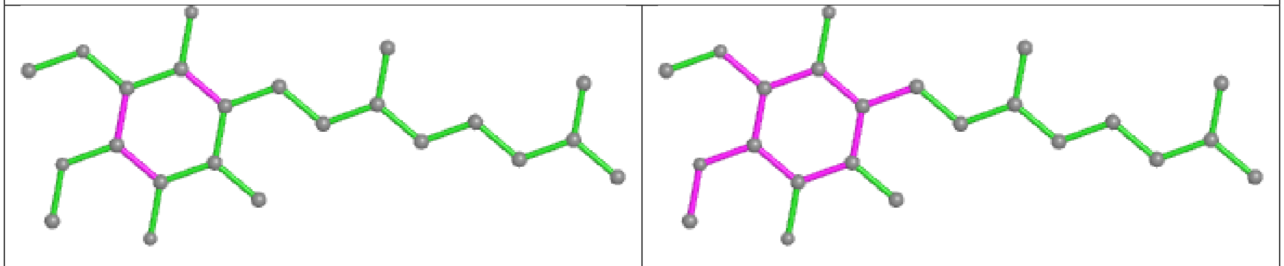


Bond lengths Bond angles

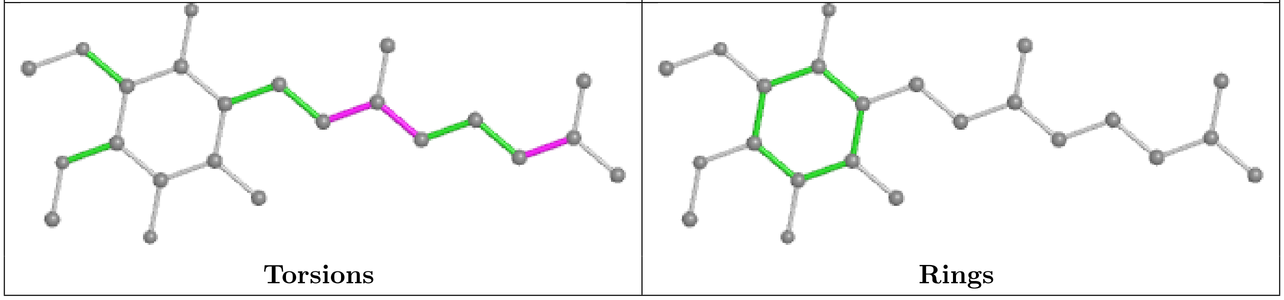


Torsions Rings

Ligand U10 Ac 404

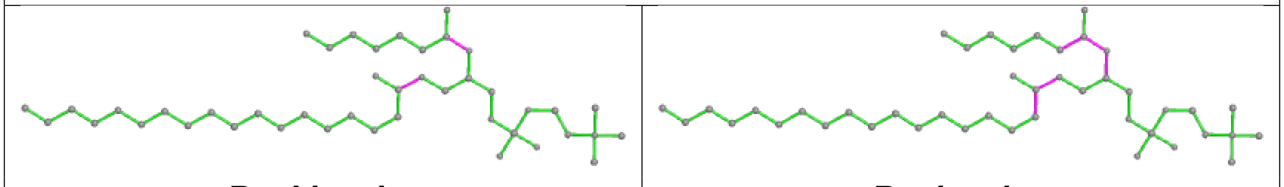


Bond lengths Bond angles

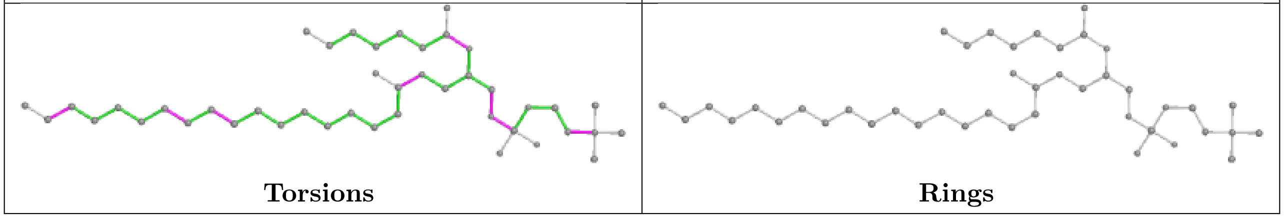


Torsions Rings

Ligand PC1 B 304

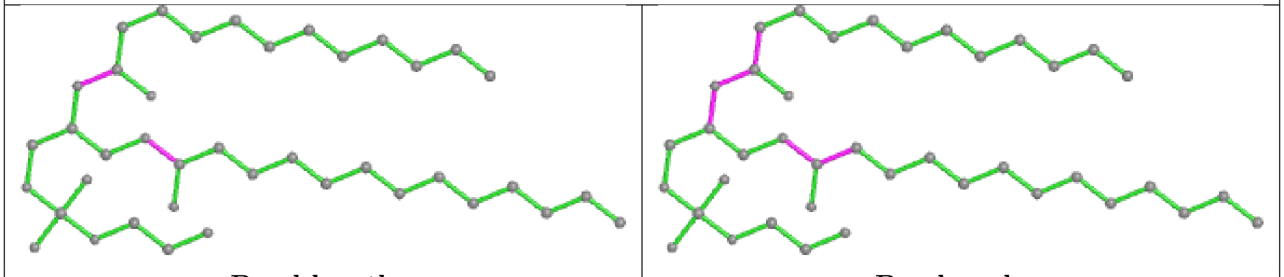


Bond lengths Bond angles

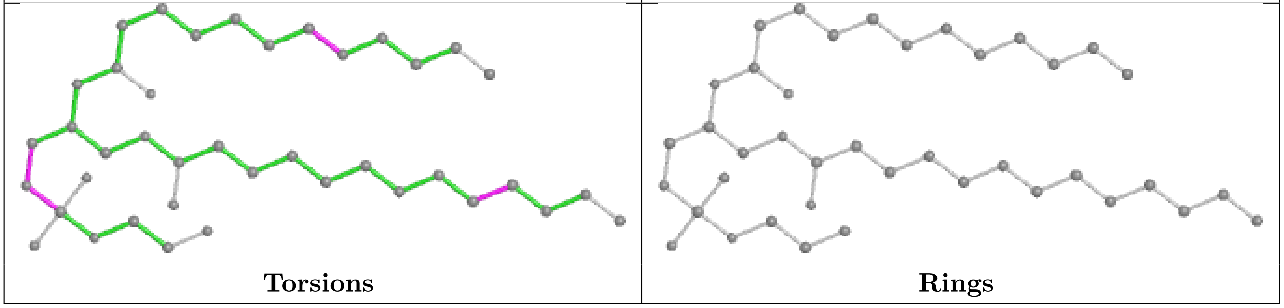


Torsions Rings

Ligand 3PE L 701

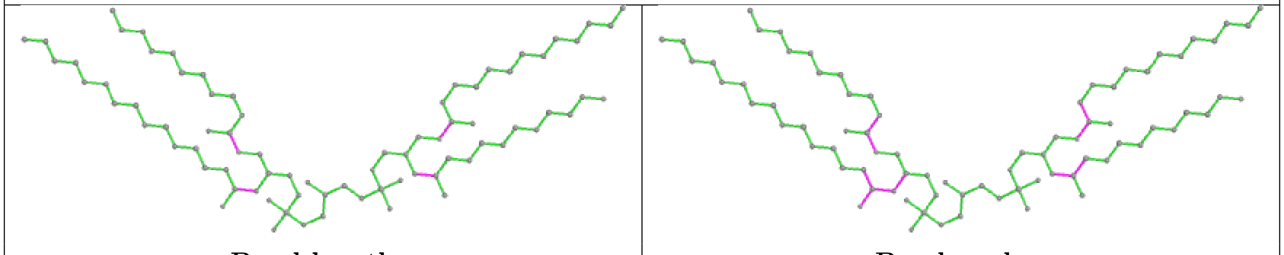


Bond lengths Bond angles

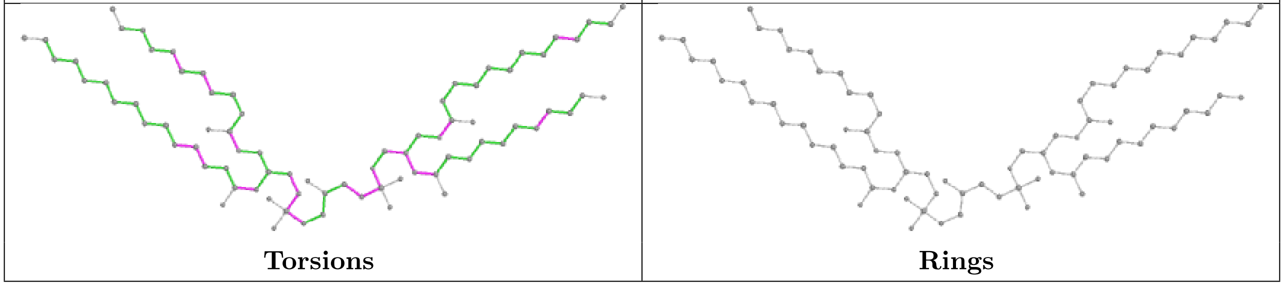


Torsions Rings

Ligand CDL L 704

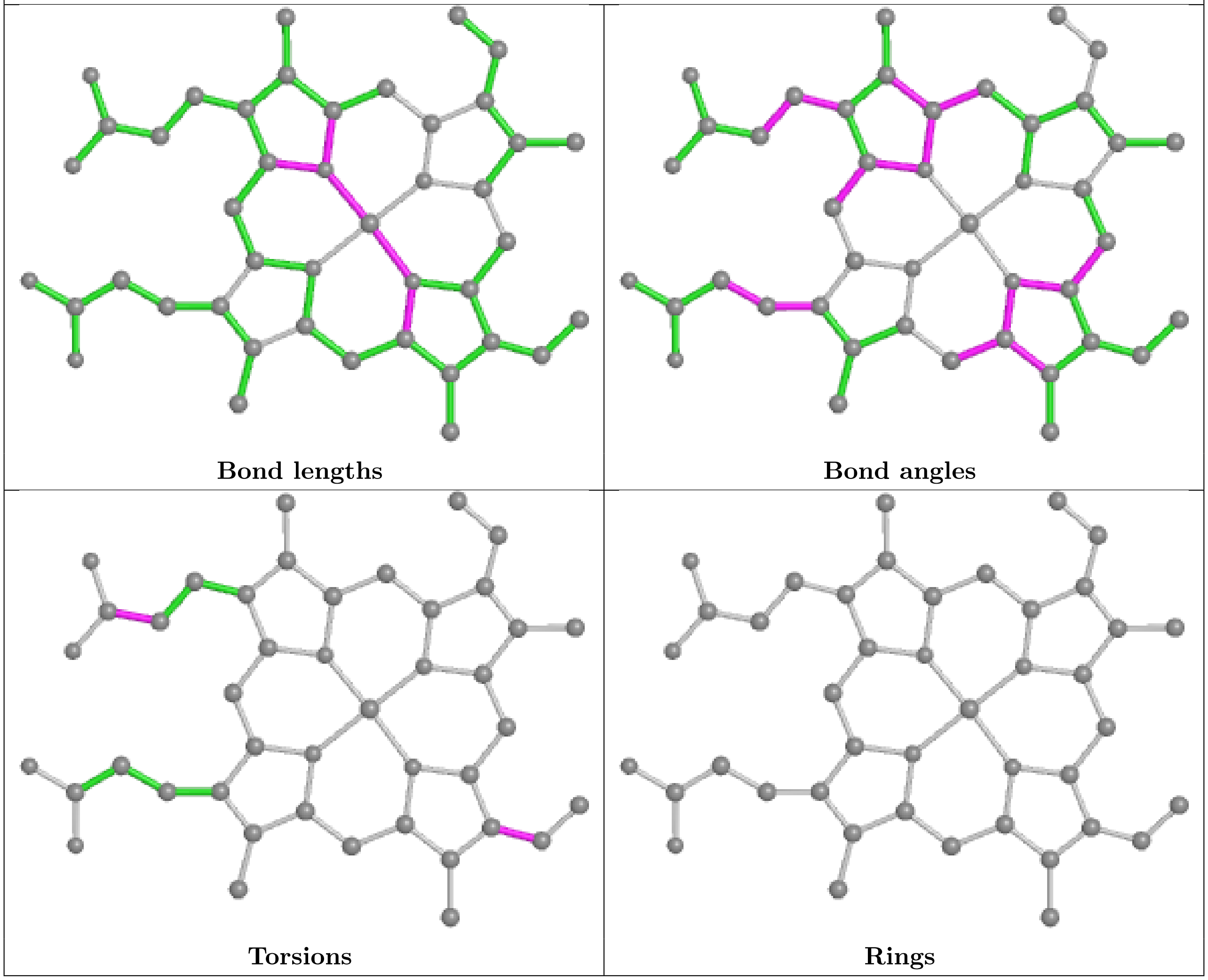


Bond lengths Bond angles



Torsions Rings

Ligand HEM AC 402



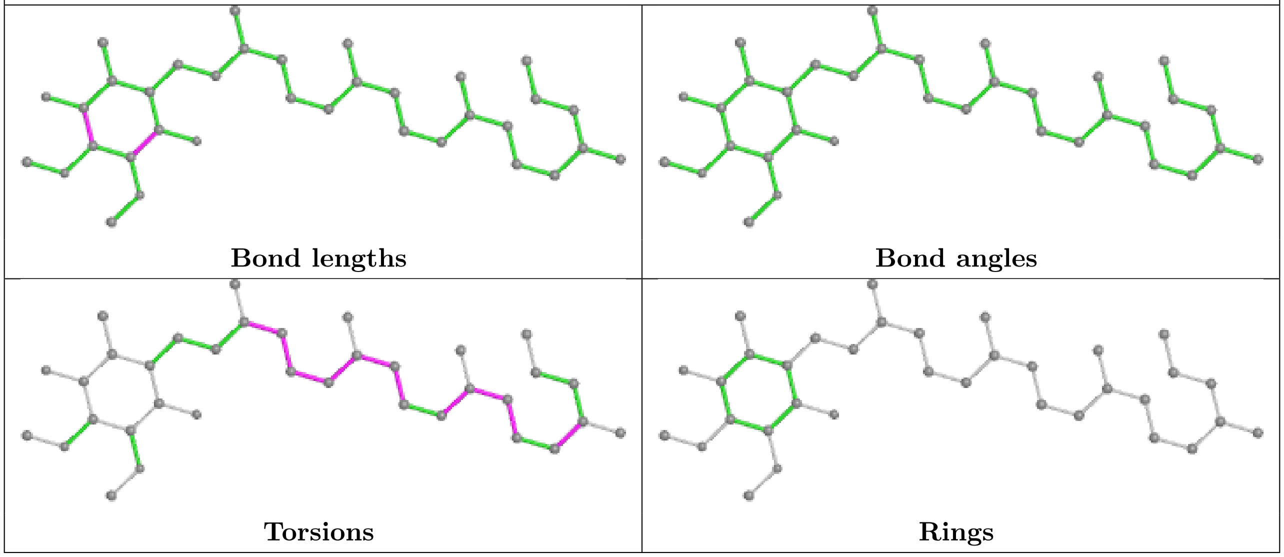
Bond lengths

Bond angles

Torsions

Rings

Ligand UQ9 H 400



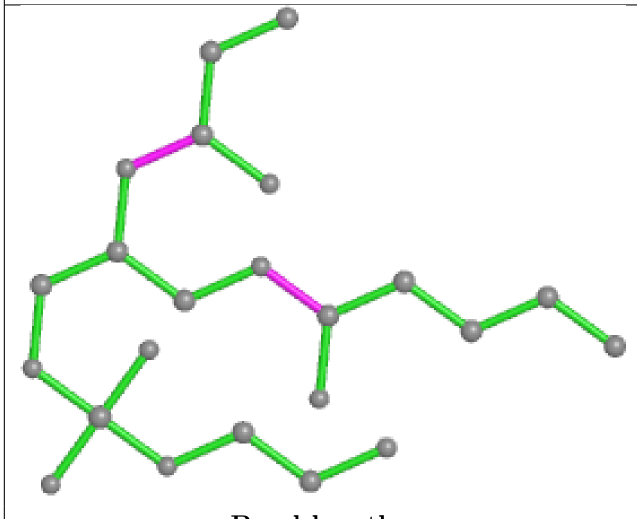
Bond lengths

Bond angles

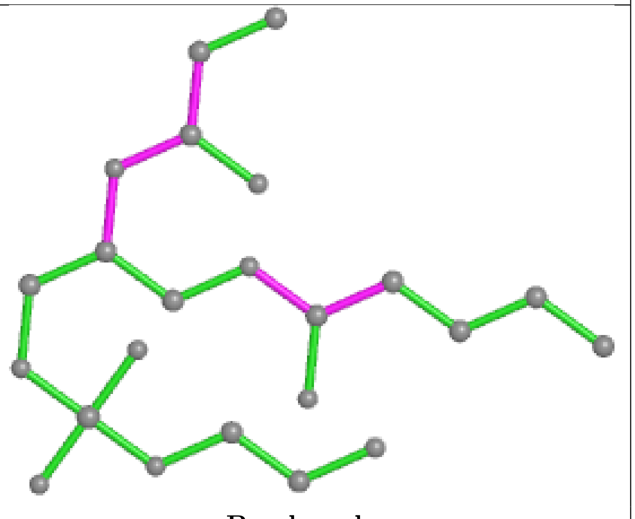
Torsions

Rings

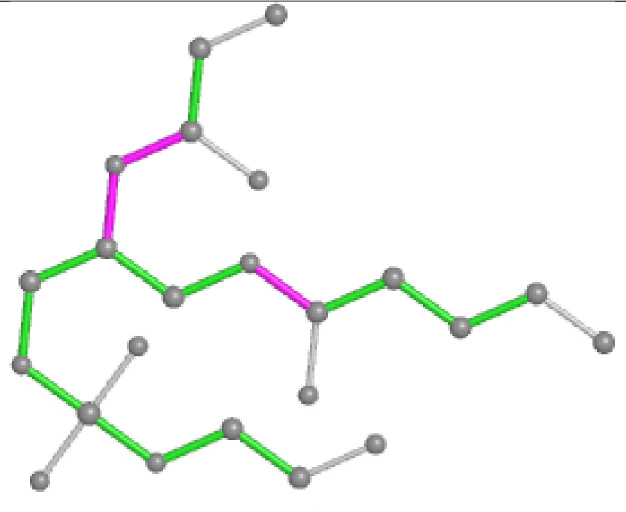
Ligand 3PE Aa 501



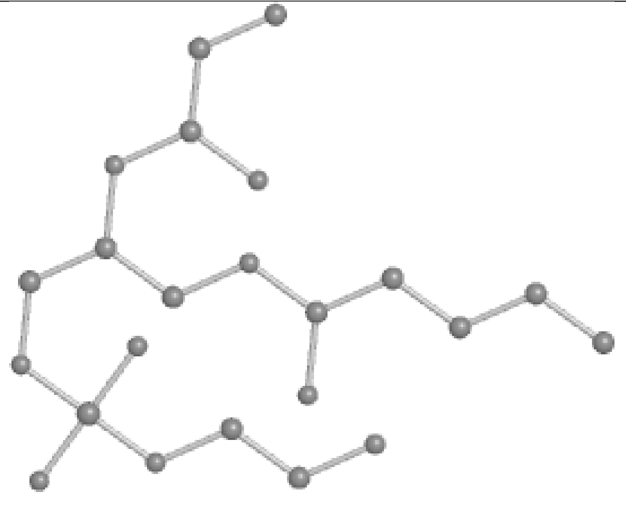
Bond lengths



Bond angles

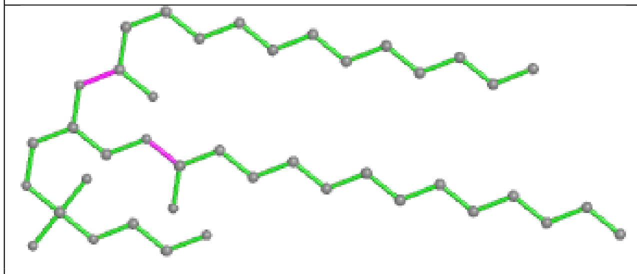


Torsions

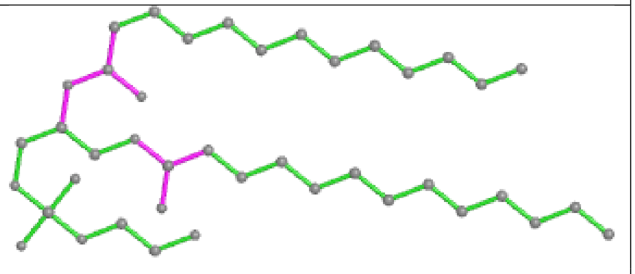


Rings

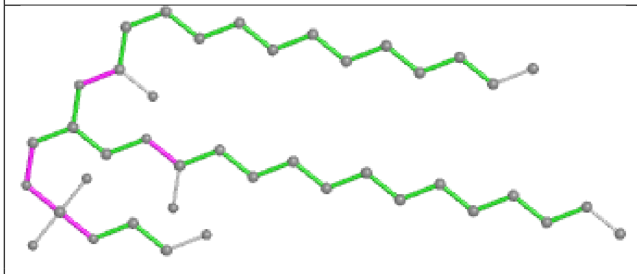
Ligand 3PE Y 201



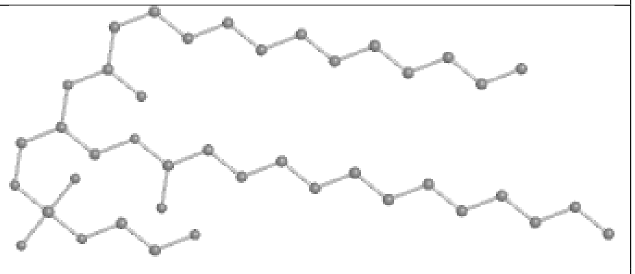
Bond lengths



Bond angles

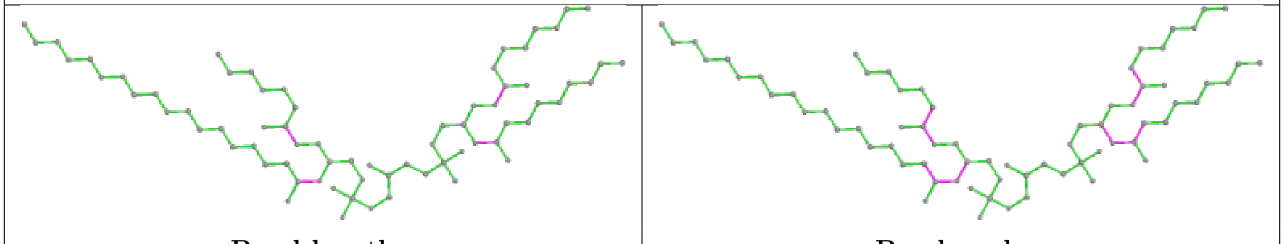


Torsions

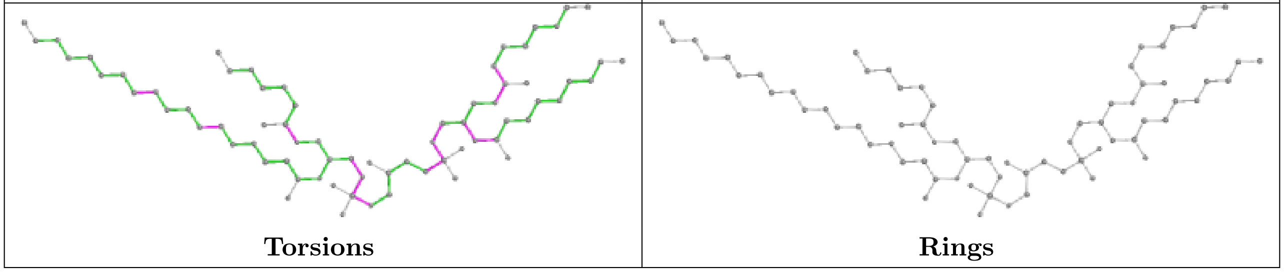


Rings

Ligand CDL h 201

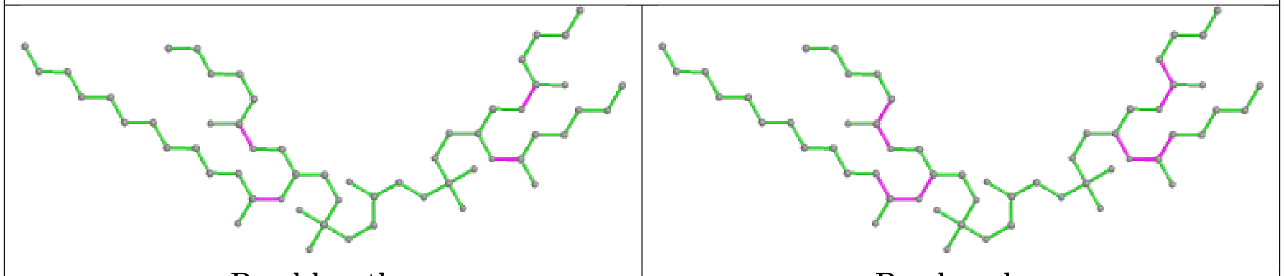


Bond lengths **Bond angles**

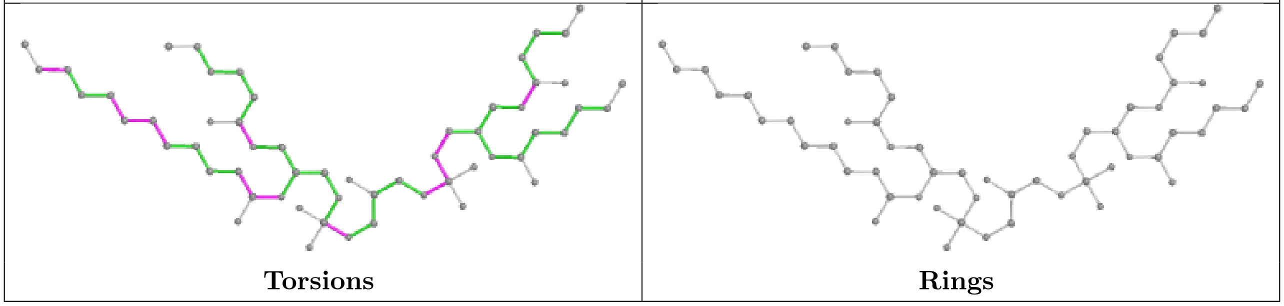


Torsions **Rings**

Ligand CDL a 101

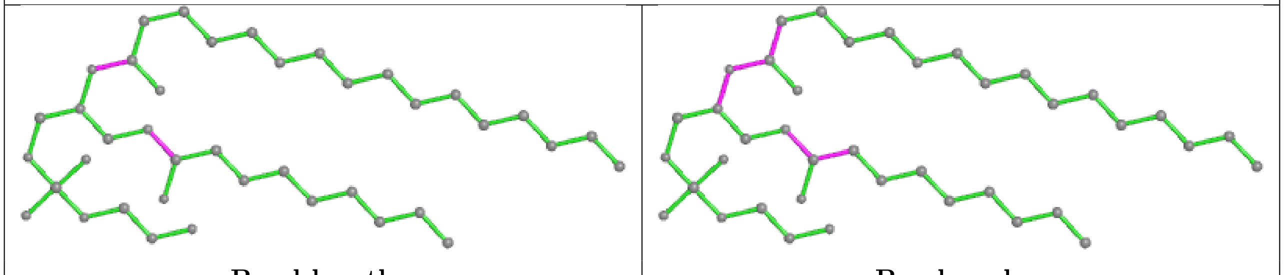


Bond lengths **Bond angles**



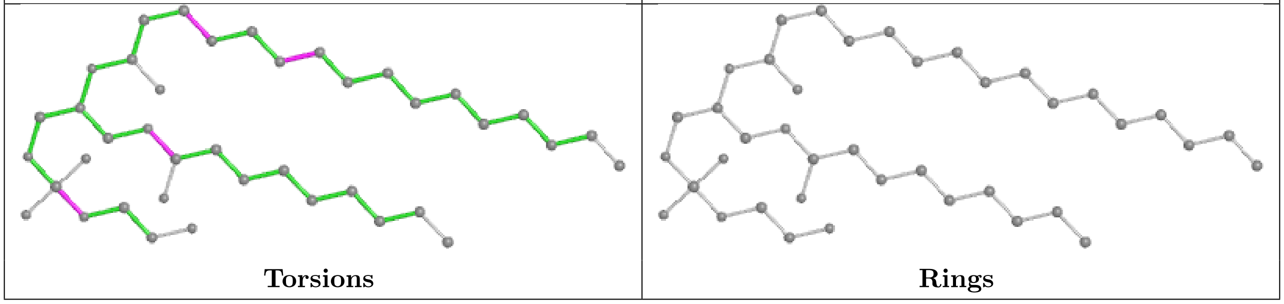
Torsions **Rings**

Ligand 3PE L 703



Bond lengths

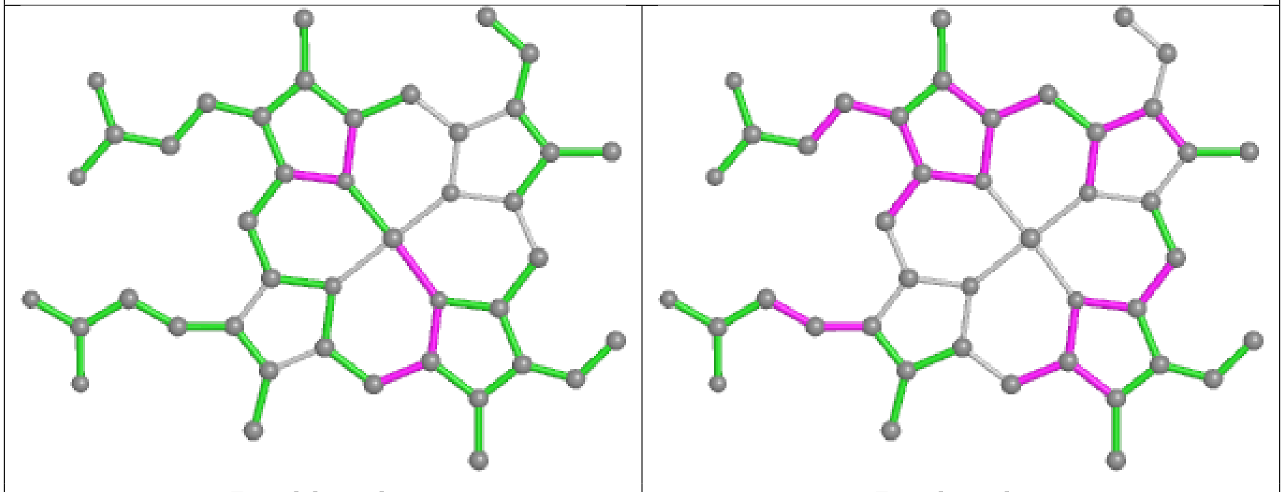
Bond angles



Torsions

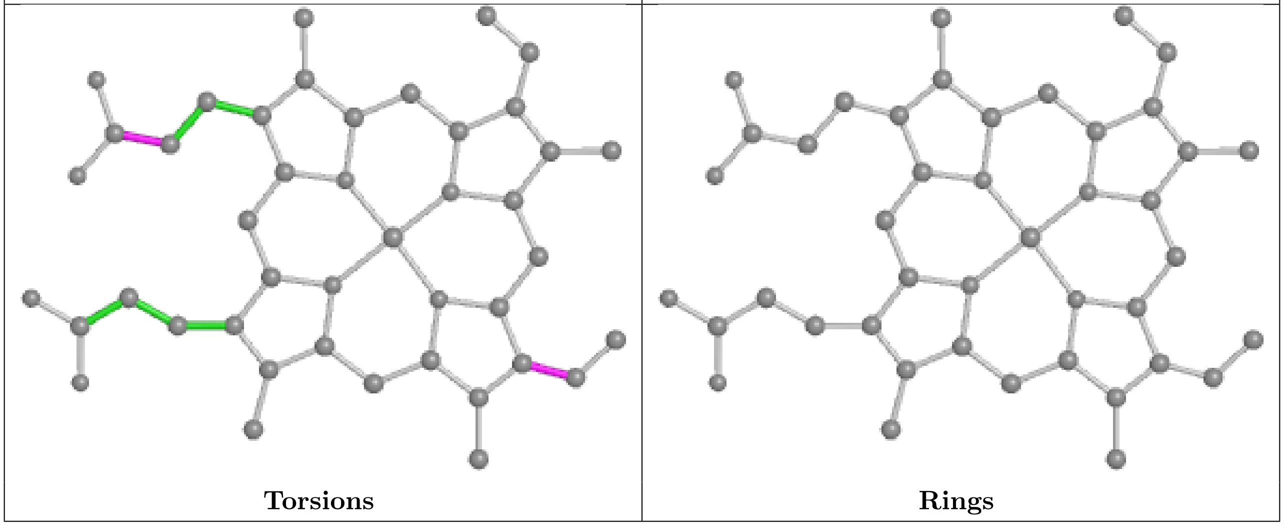
Rings

Ligand HEM Ac 402



Bond lengths

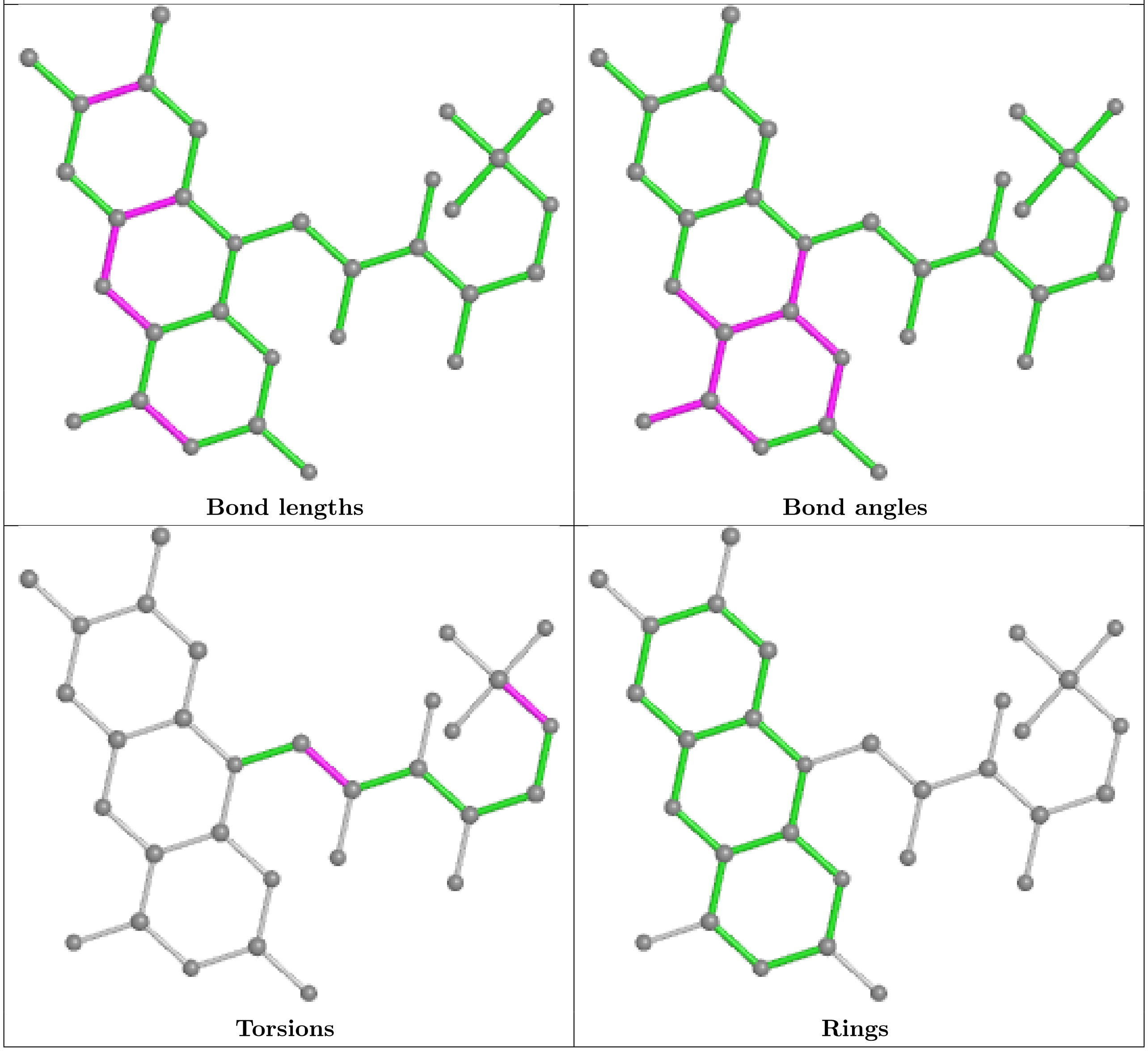
Bond angles



Torsions

Rings

Ligand FMN F 501



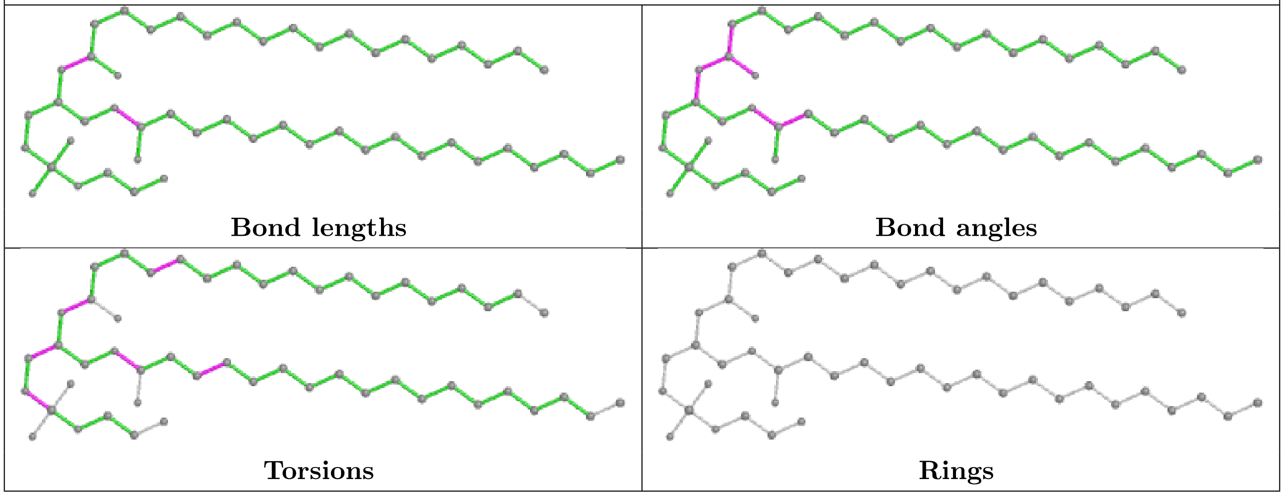
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE m 202



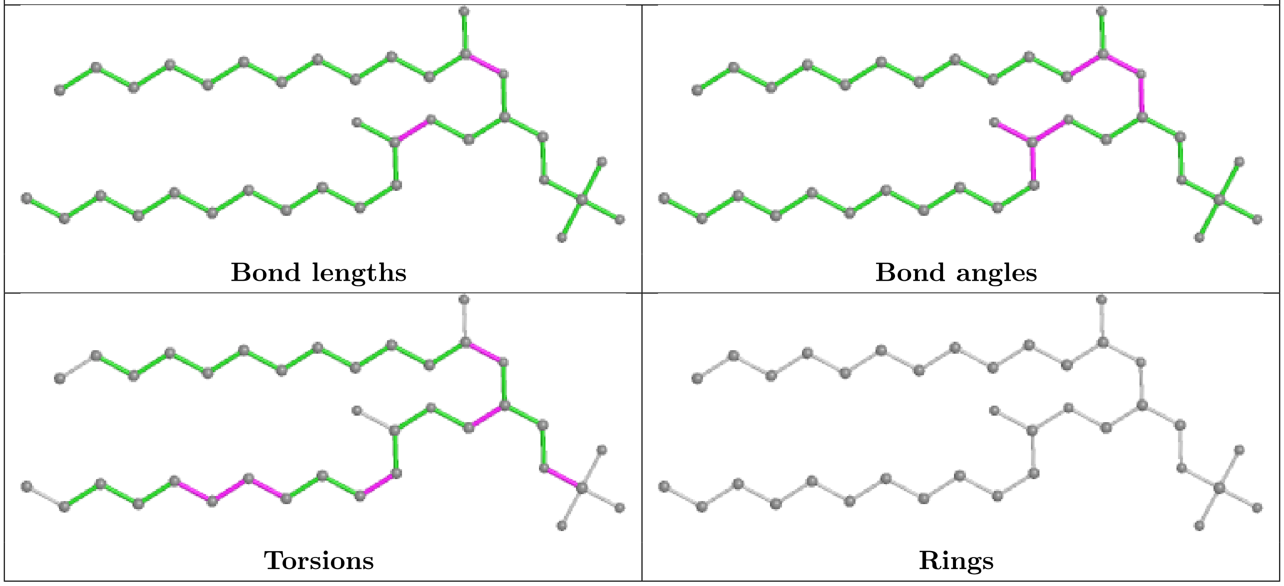
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PH Ad 402



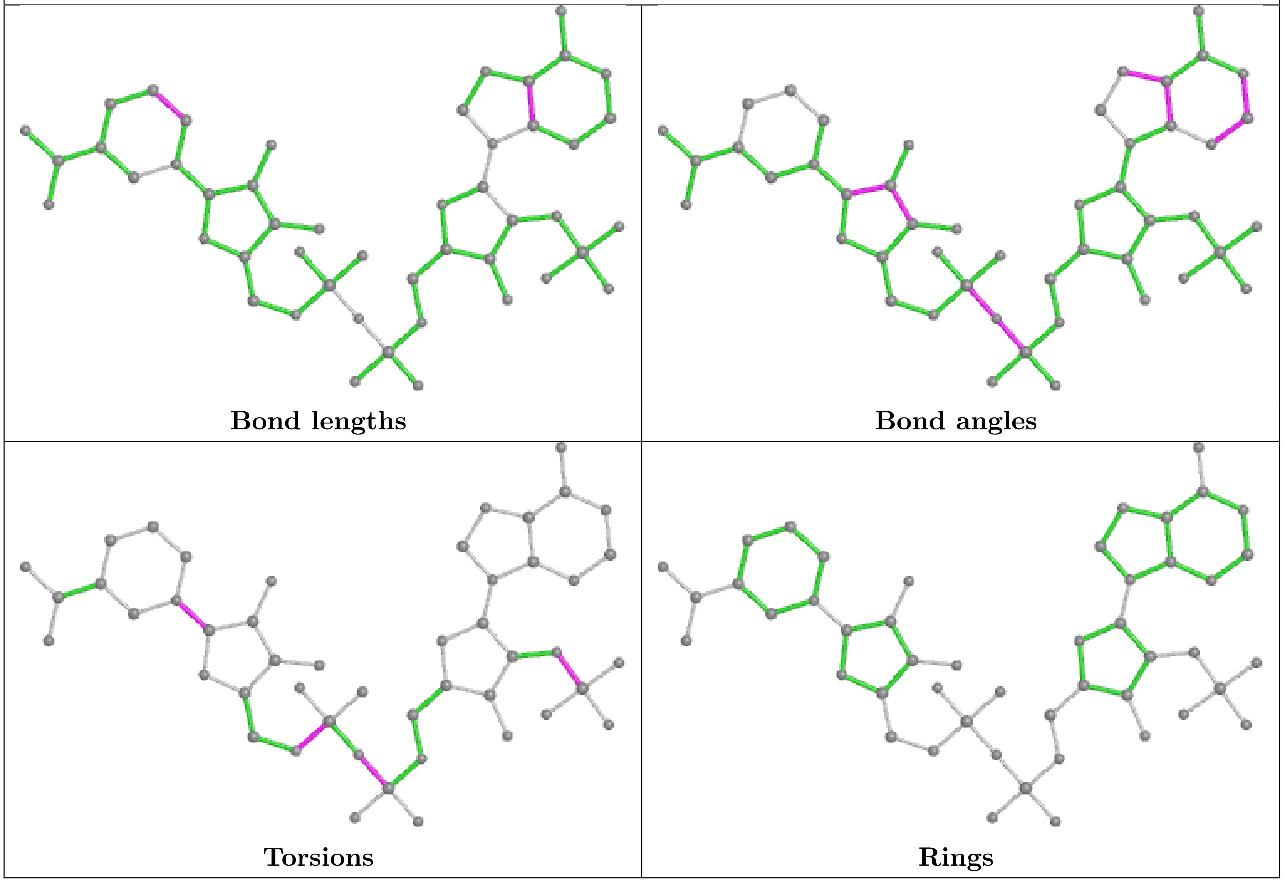
Bond lengths

Bond angles

Torsions

Rings

Ligand NDP P 401



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

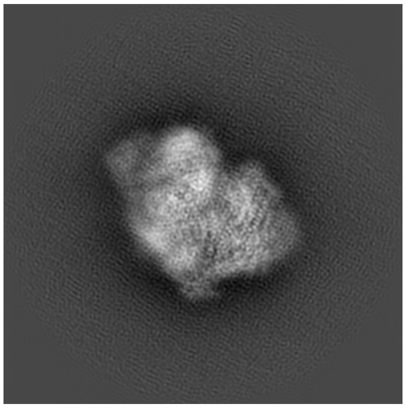
6 Map visualisation

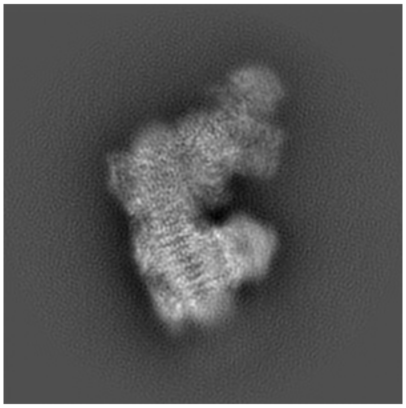
This section contains visualisations of the EMDB entry EMD-35340. These allow visual inspection of the internal detail of the map and identification of artifacts.

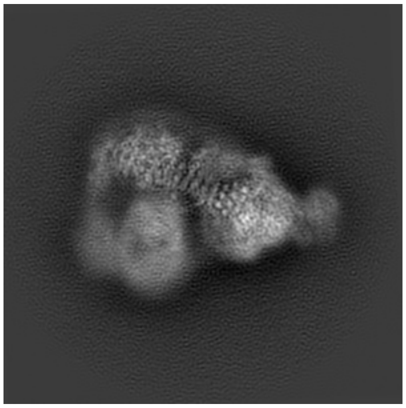
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

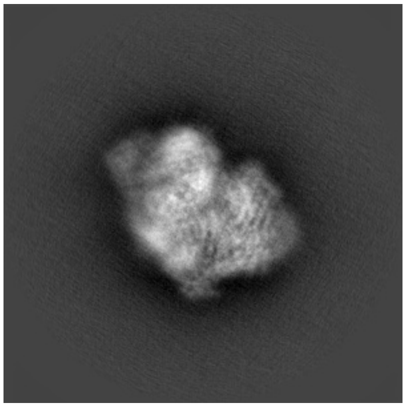
6.1.1 Primary map

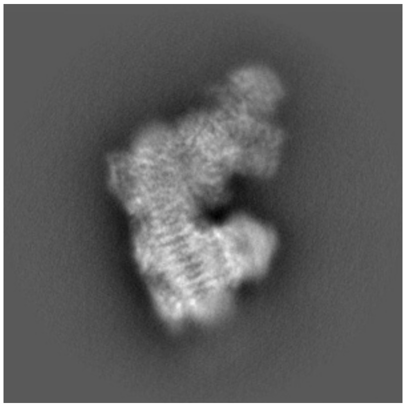

X

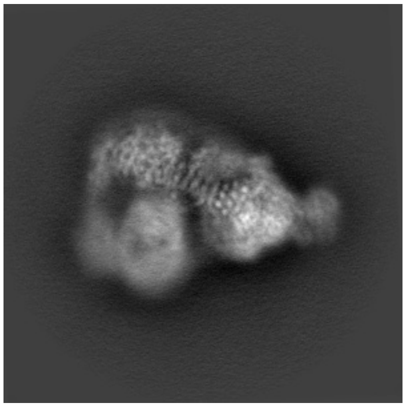

Y


Z

6.1.2 Raw map


X

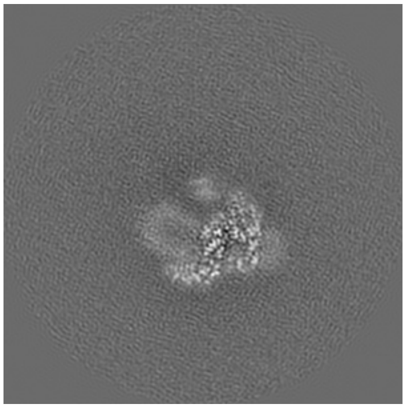

Y


Z

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

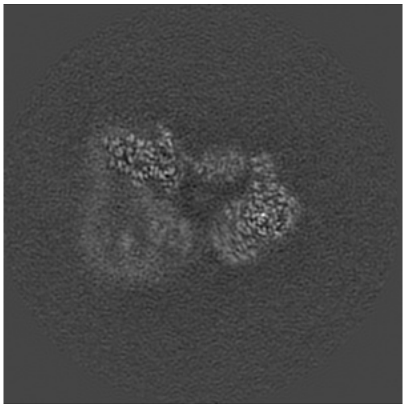
6.2 Central slices

6.2.1 Primary map



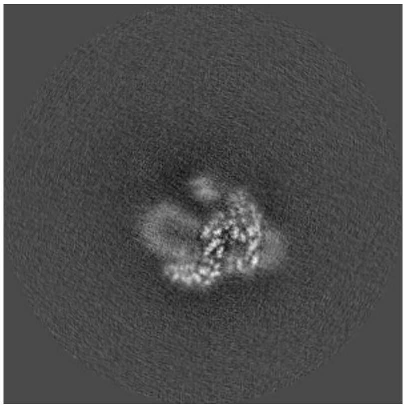
X Index: 192

Y Index: 192

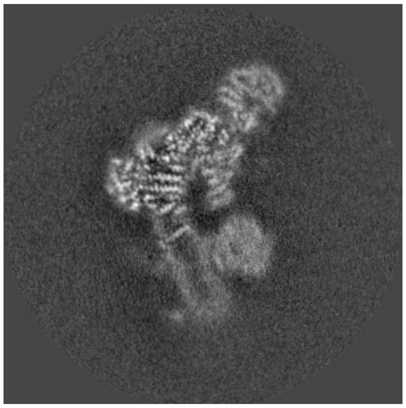


Z Index: 192

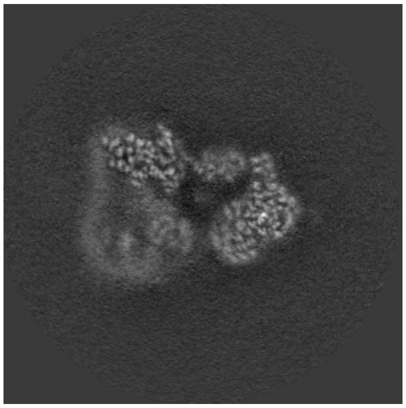
6.2.2 Raw map



X Index: 192



Y Index: 192

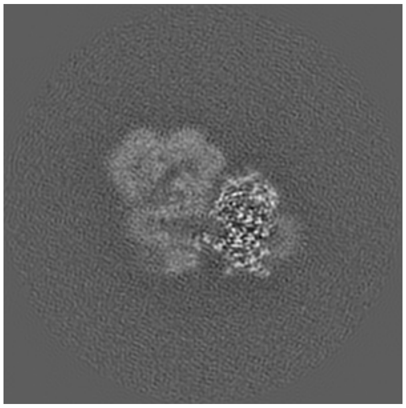


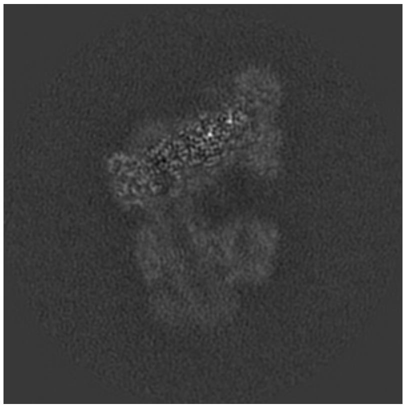
Z Index: 192

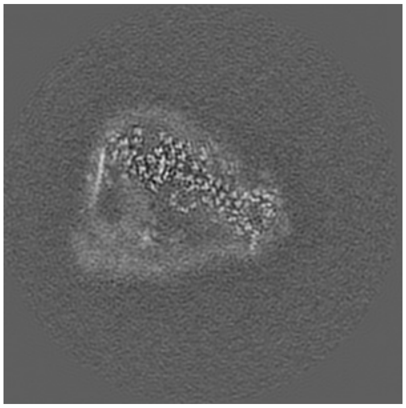
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

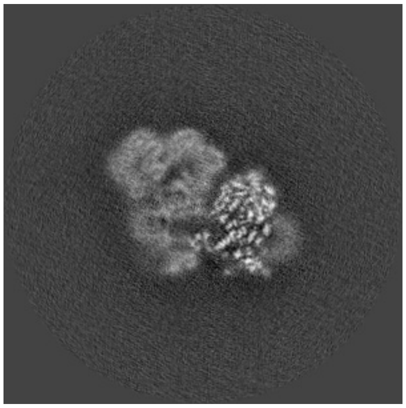
6.3.1 Primary map

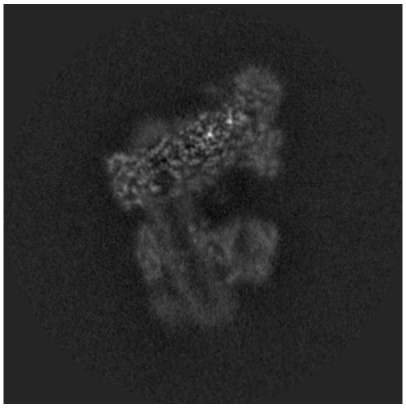

X Index: 157

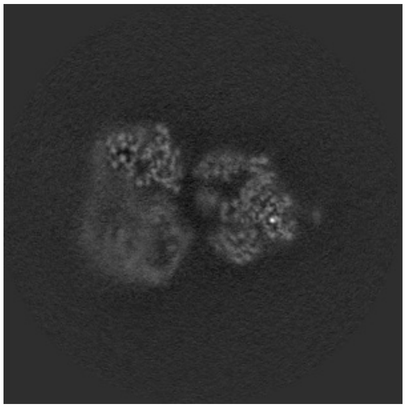

Y Index: 176


Z Index: 167

6.3.2 Raw map


X Index: 159

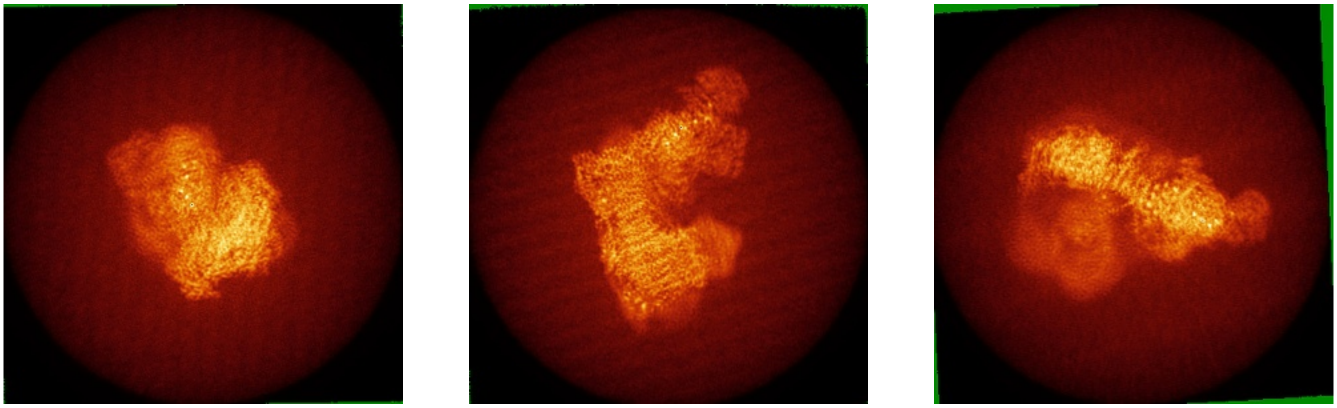

Y Index: 176


Z Index: 198

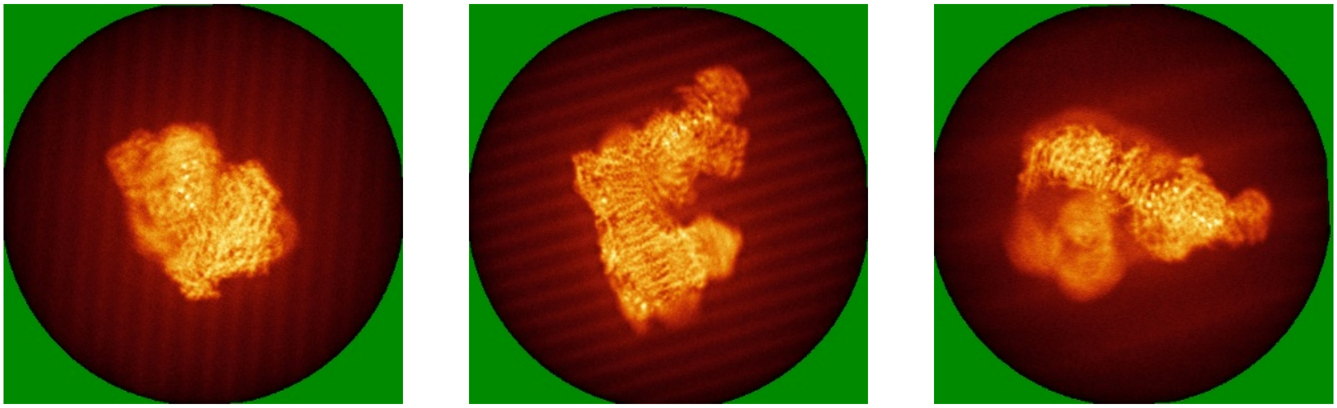
The images above show the largest variance slices of the map in three orthogonal directions.

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

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

6.5.1 Primary map

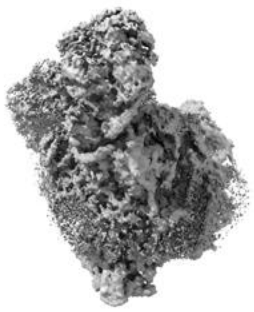
X

Y

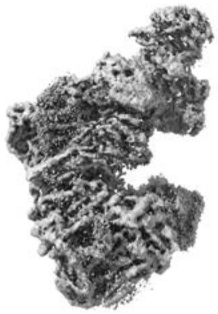
Z

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.

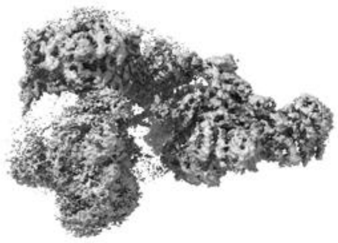
6.5.2 Raw map



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.

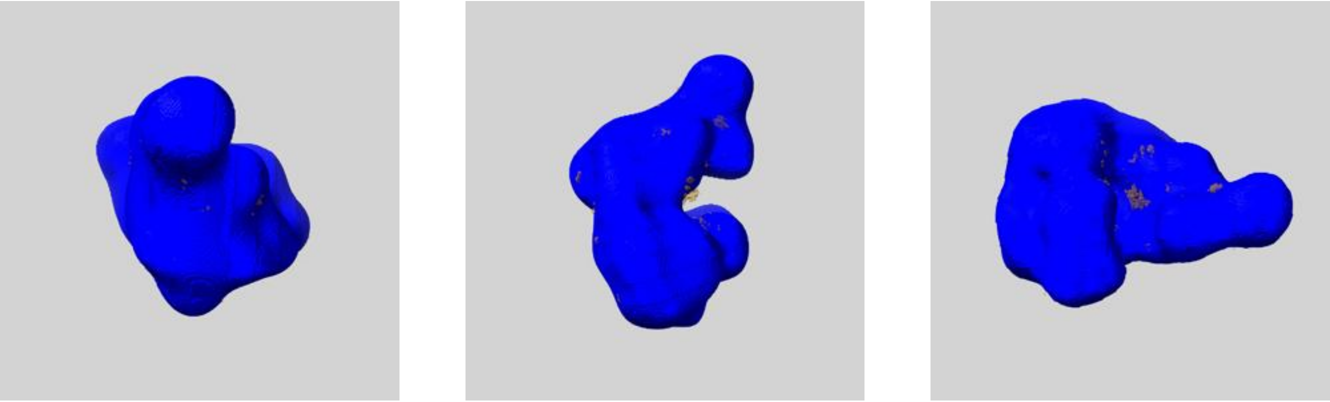
6.6 Mask visualisation ⓘ

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_35340_msk_1.map ⓘ

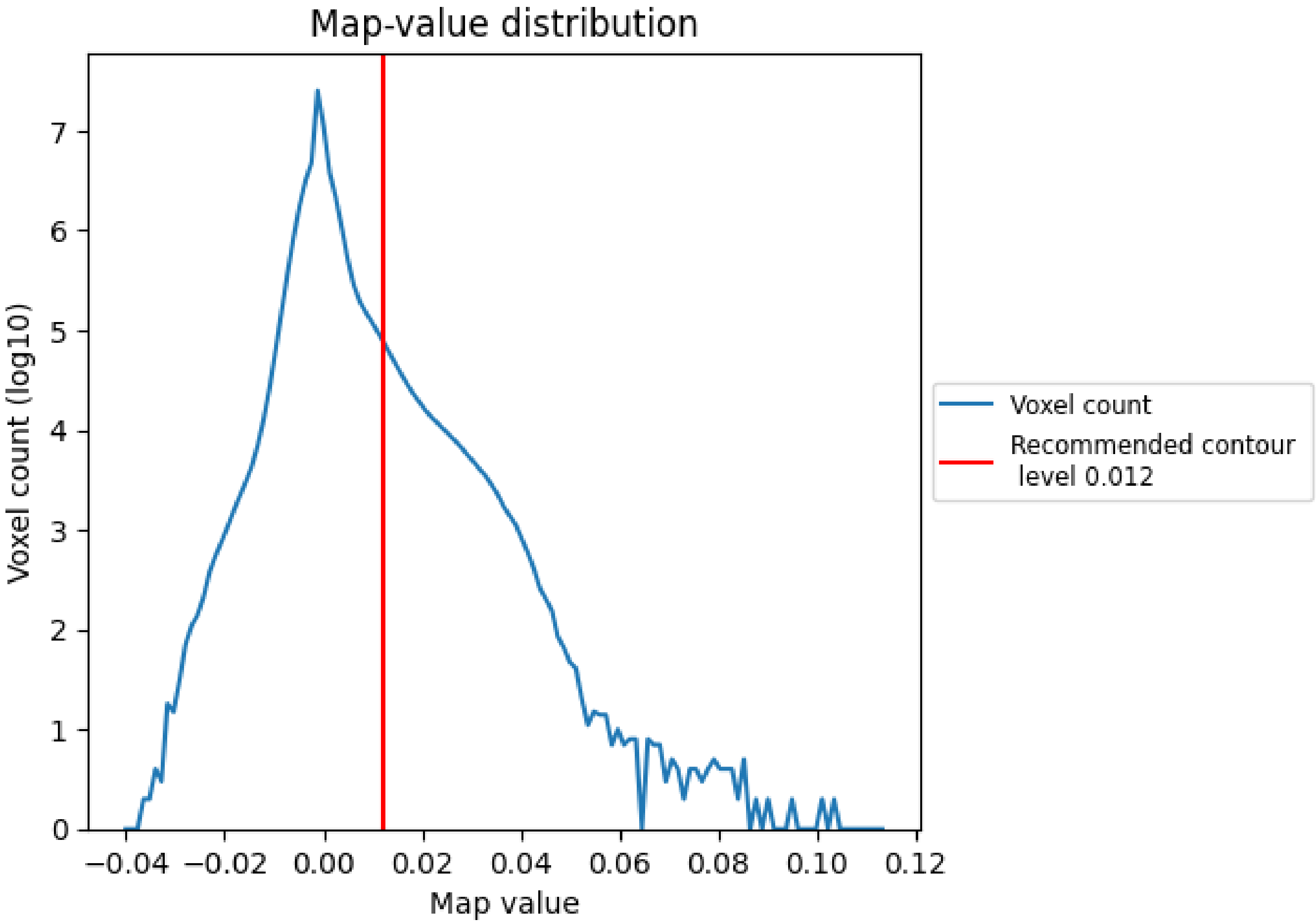


X Y Z

7 Map analysis ⓘ

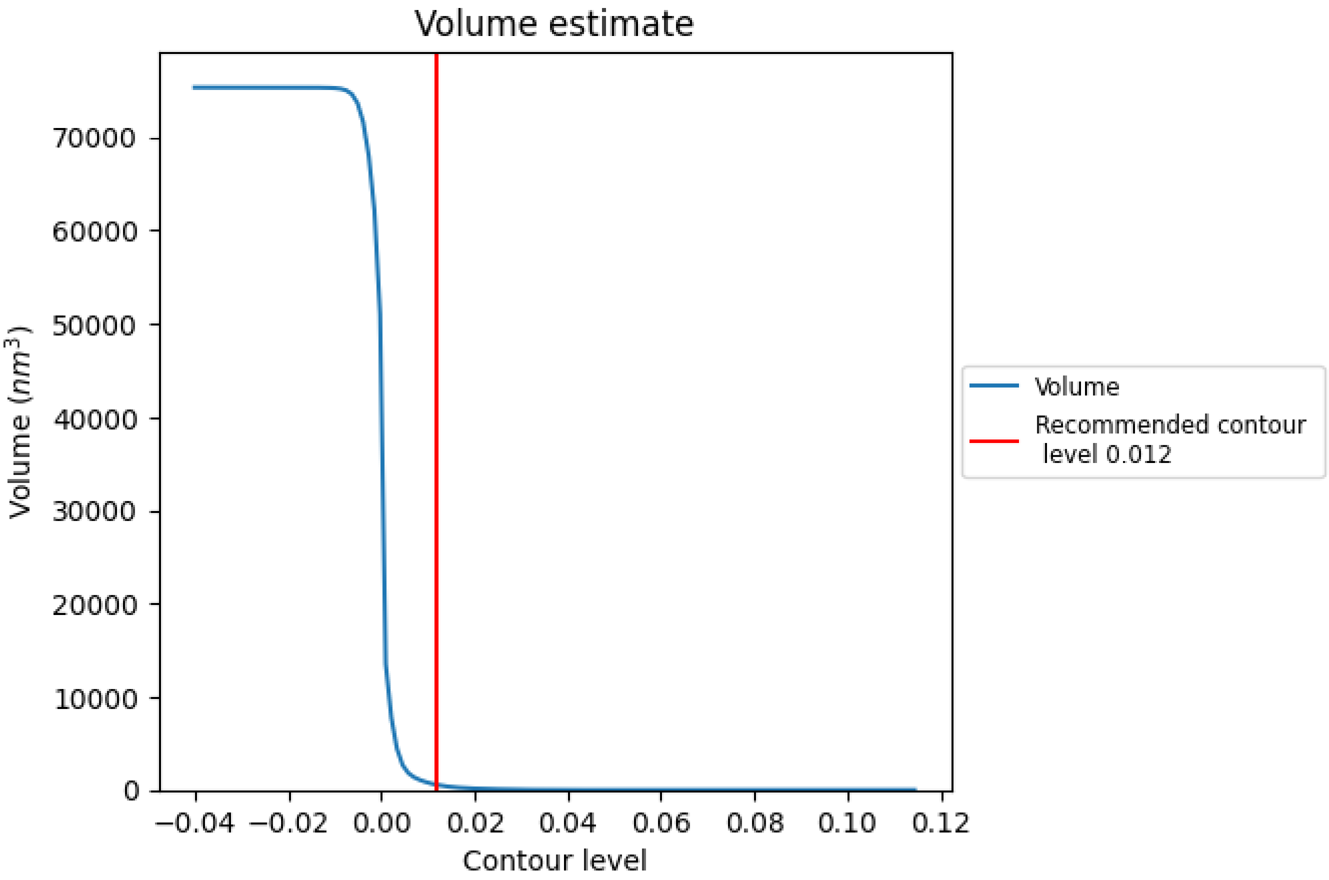
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

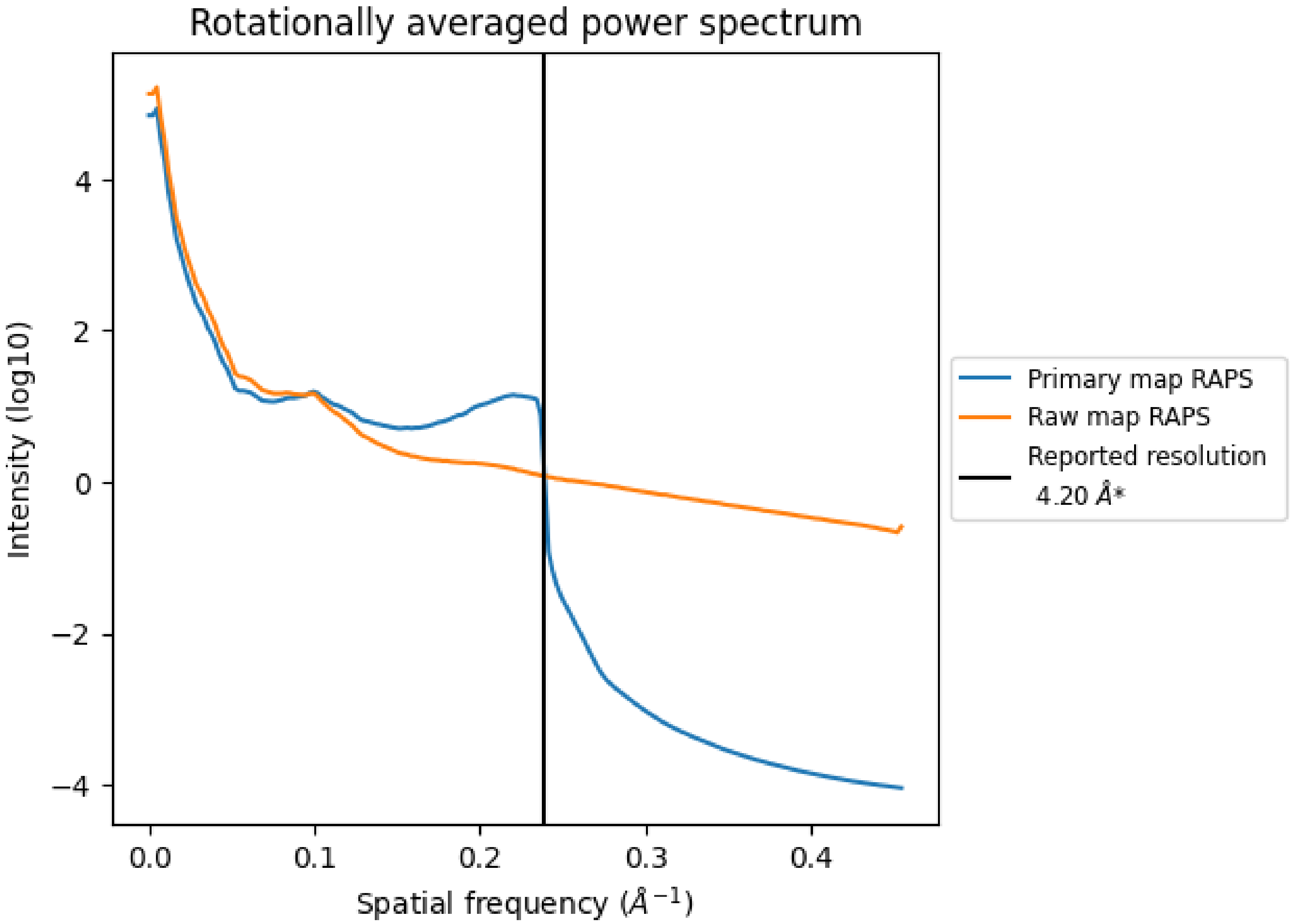
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 542 nm^3; this corresponds to an approximate mass of 490 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

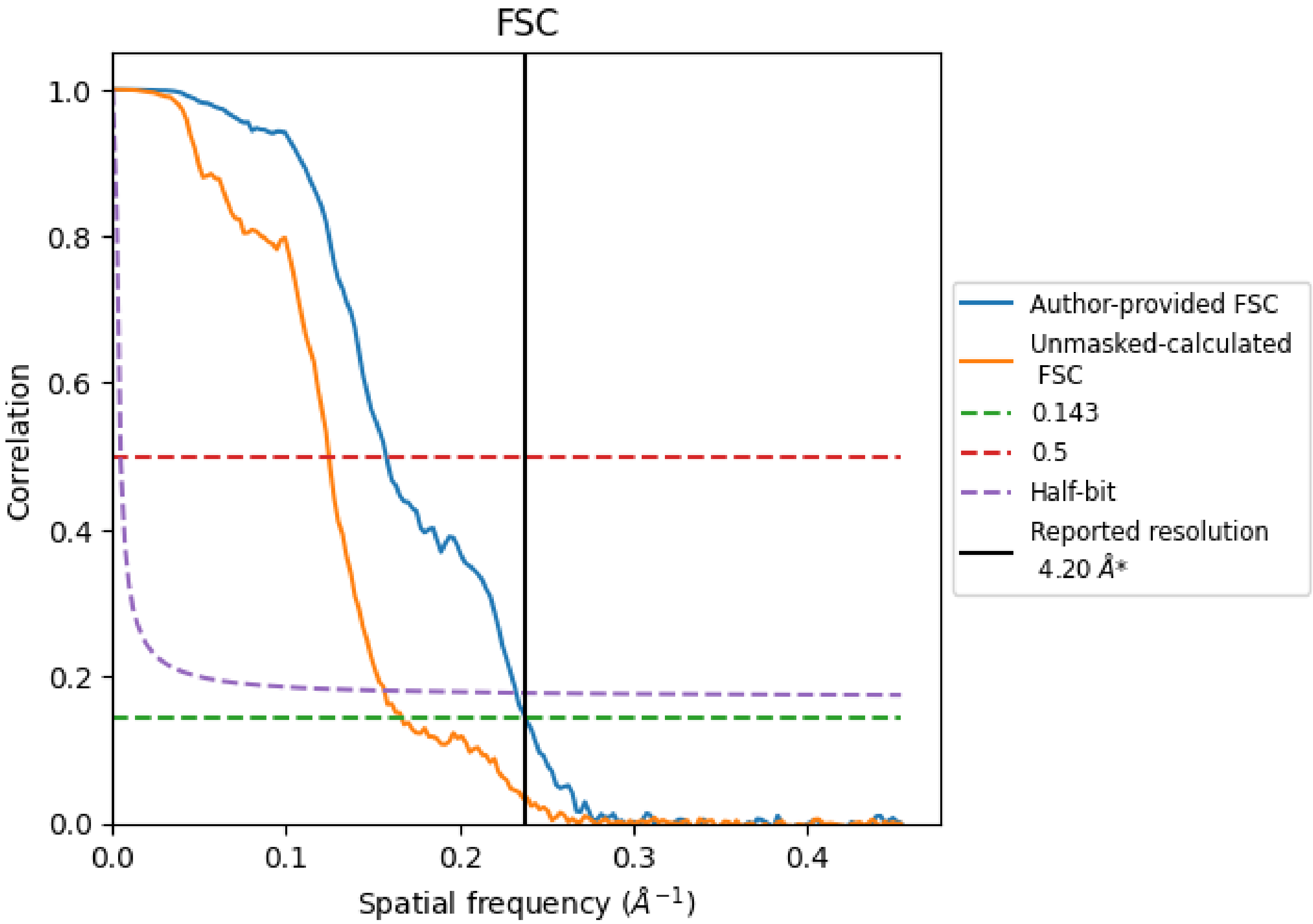


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



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

8.2 Resolution estimates

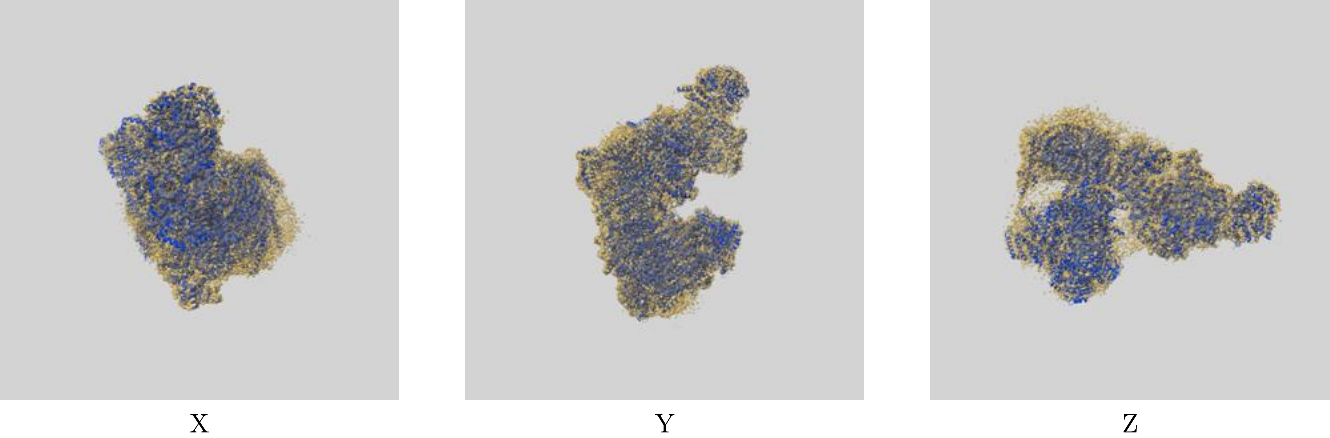
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.34	4.30
Unmasked-calculated*	6.00	8.02	6.38

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-35340 and PDB model 8IBD. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay ⓘ



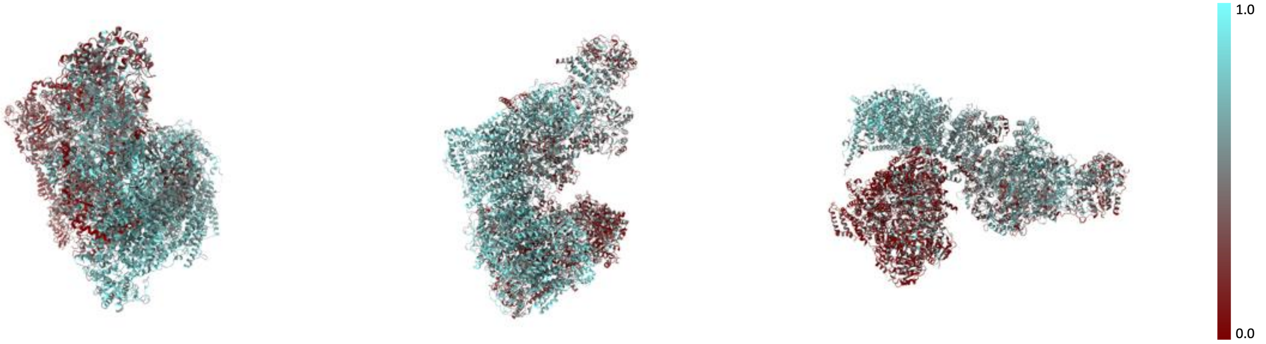
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

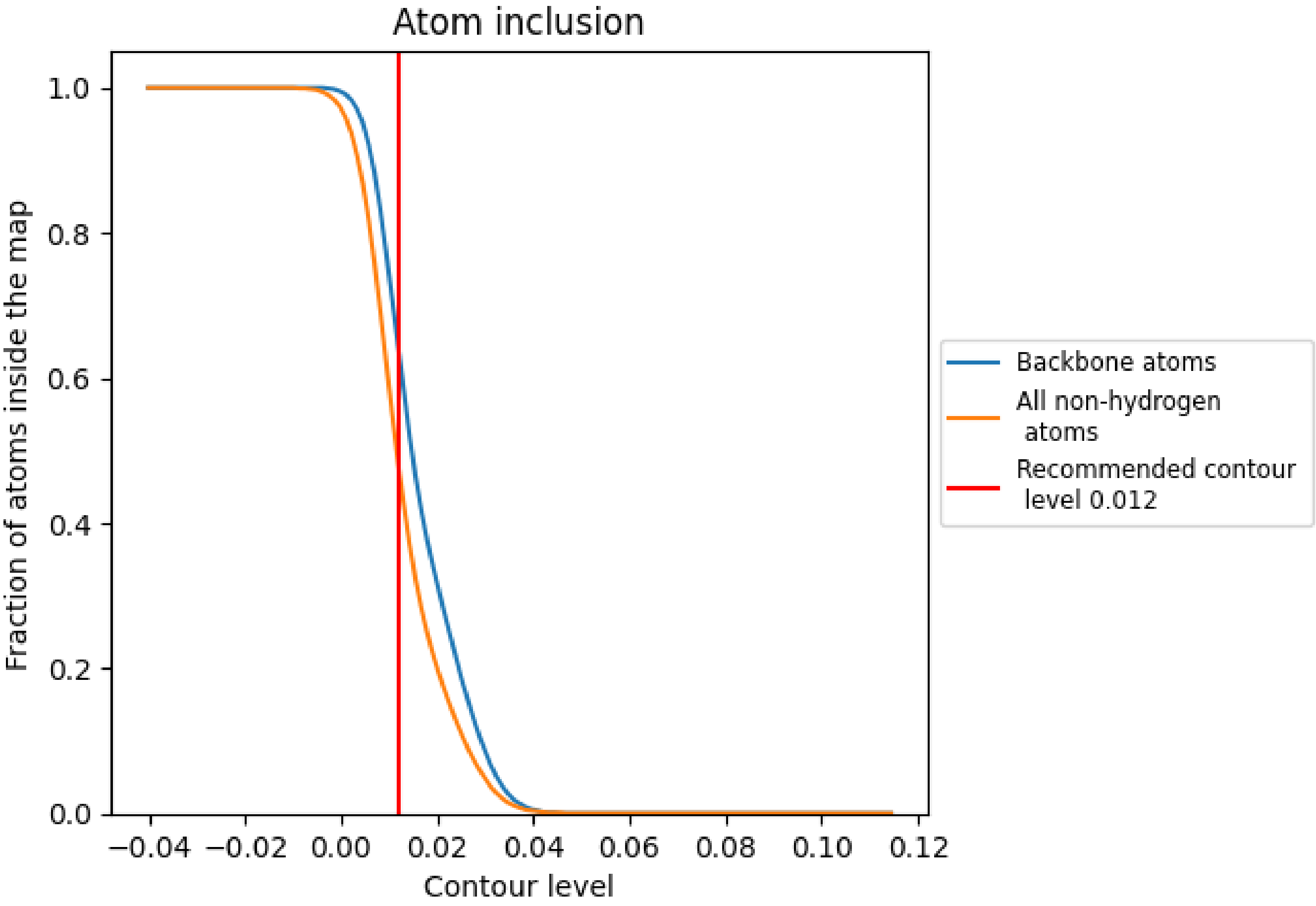
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4760	0.2320
A	0.5720	0.3400
AA	0.2260	0.0500
AB	0.2790	0.0900
AC	0.1360	0.0600
AD	0.1840	0.0400
AE	0.0400	0.0110
AF	0.2120	0.0620
AG	0.1030	0.0200
AH	0.1380	0.0390
AI	0.0610	0.0570
AJ	0.0870	-0.0090
AK	0.0170	-0.0420
Aa	0.2460	0.0880
Ab	0.2610	0.0640
Ac	0.2520	0.1320
Ad	0.3300	0.1260
Ae	0.0650	0.0450
Af	0.2580	0.1320
Ag	0.1940	0.1060
Ah	0.2590	0.0910
Ai	0.0400	0.0720
Aj	0.1070	0.1090
Ak	0.0240	0.0290
B	0.6760	0.3570
C	0.6330	0.2840
D	0.6690	0.3480
E	0.3820	0.1930
F	0.4370	0.1890
G	0.5440	0.2330
H	0.6730	0.3720
I	0.7440	0.3600
J	0.5640	0.3220
K	0.6160	0.3800
L	0.6650	0.3660

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Chain	Atom inclusion	Q-score
M	0.7000	0.3940
N	0.6830	0.3940
O	0.4740	0.2590
P	0.4870	0.2060
Q	0.4780	0.2770
R	0.2910	0.1840
S	0.4200	0.1130
T	0.2970	0.1400
U	0.7030	0.3250
V	0.5450	0.2120
W	0.4600	0.1940
X	0.7290	0.3370
Y	0.5570	0.3280
Z	0.7300	0.3220
a	0.6740	0.3380
b	0.7270	0.3520
c	0.6160	0.2950
d	0.6980	0.3570
e	0.7060	0.3520
f	0.6930	0.3500
g	0.6790	0.3590
h	0.7020	0.3620
i	0.6860	0.3330
j	0.7040	0.3200
k	0.7240	0.3210
l	0.7000	0.3590
m	0.6240	0.3380
n	0.7220	0.3400
o	0.6530	0.2710
p	0.7140	0.3460
q	0.1400	0.1820
r	0.1940	0.1580
s	0.1220	0.1140