Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:21 pm GMT

PDB ID	:	2YBB
EMDB ID	:	EMD-1876
Title	:	Fitted model for bovine mitochondrial supercomplex I1III2IV1 by single particle cryo-EM (EMD-1876)
Authors	:	Althoff, T.; Mills, D.J.; Popot, J.-L.; Kuehlbrandt, W.
Deposited on	:	2011-03-02
Resolution	:	19.00 Å(reported)
Based on initial models	:	3M9C, 1OCC, 1PP9, 2B4Z, 1BGY, 3IAM

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

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

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

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

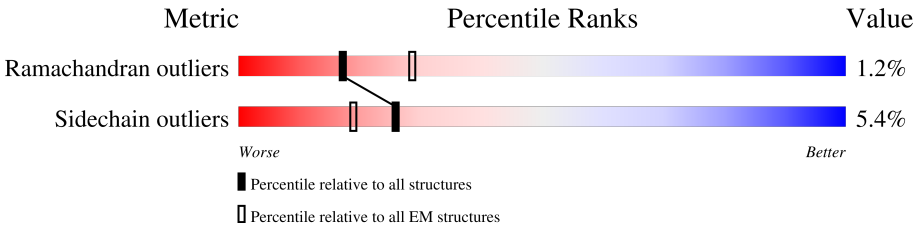
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 19.00 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	154571	4023
Sidechain outliers	154315	3826

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	1	438	9% 90% 9%
2	2	181	23% 88% 10%
3	3	783	15% 88% 8%
4	4	409	17% 83% 10% 8%
5	5	207	13% 87% 8% 5%
6	6	181	7% 72% 6% 20%
7	7	129	36% 91% 7%
8	8	182	76% 9% 15%
9	A	446	9% 98%

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Mol	Chain	Length	Quality of chain
9	a	446	98%
10	B	439	10% 96%
10	b	439	5% 95%
11	C	379	16% 94%
11	c	379	16% 95%
12	D	241	99%
12	d	241	5% 99%
13	E	196	30% 97%
13	e	196	37% 98%
14	F	110	89% 10%
14	f	110	31% 89% 10%
15	G	81	91% 7%
15	g	81	11% 90% 6%
16	H	78	12% 82% 15%
16	h	78	82% 15%
17	I	65	12% 62% 35%
17	i	65	5% 60% 5% 35%
18	J	62	5% 95% 5%
18	j	62	15% 95% 5%
19	K	56	18% 32% 7% 61%
19	k	56	29% 9% 61%
20	L	514	18% 92% 8%
21	M	227	90% 10%
22	N	261	9% 90% 10%
23	O	147	12% 92% 6%

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Mol	Chain	Length	Quality of chain
24	P	109	16% 94% 6%
25	Q	98	53% 92% 7%
26	R	84	11% 74% 25%
27	S	85	36% 76% 12% 12%
28	T	73	93% 7%
29	U	59	14% 85% 8%
30	V	56	20% 84% 12%
31	W	47	11% 96%
32	X	46	30% 87% 7% 7%
33	Y	104	56% 99%
34	m	474	24% 100%
35	n	391	28% 100%
36	o	378	26% 100%
37	p	281	20% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	HEA	L	515	X	-	-	-
49	HEA	L	516	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 72626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	437	3417	2180	595	624	18	0	0

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	179	1410	897	239	266	8	0	0

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	754	5880	3743	1055	1051	31	0	0

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	378	3018	1946	511	550	11	0	0

- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	196	1607	1043	273	288	3	0	0

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	144	1102	700	192	197	13	0	0

- Molecule 7 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	127	Total	C	N	O	S	0	0
			1031	664	183	181	3		

- Molecule 8 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	154	Total	C	N	O	S	0	0
			1193	759	201	222	11		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		
9	a	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	424	Total	C	N	O	S	0	1
			3177	1996	562	612	7		
10	b	424	Total	C	N	O	S	0	0
			3180	1998	562	613	7		

- Molecule 11 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	365	Total	C	N	O	S	0	0
			2892	1940	450	485	17		
11	c	370	Total	C	N	O	S	0	0
			2931	1968	455	490	18		

- Molecule 12 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

- Molecule 13 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		
13	e	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		

- Molecule 14 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	99	Total	C	N	O	S	0	0
			861	545	155	159	2		
14	f	99	Total	C	N	O	S	0	0
			861	545	155	159	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	engineered mutation	UNP P00129
f	56	ASP	ASN	engineered mutation	UNP P00129

- Molecule 15 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	75	Total	C	N	O	S	0	2
			621	406	117	97	1		
15	g	76	Total	C	N	O	S	0	2
			626	409	118	98	1		

- Molecule 16 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	66	Total	C	N	O	S	0	0
			539	327	98	109	5		
16	h	66	Total	C	N	O	S	0	0
			539	327	98	109	5		

- Molecule 17 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	42	Total	C	N	O	S	0	0
			285	174	55	55	1		
17	i	42	Total	C	N	O	S	0	0
			285	174	55	55	1		

- Molecule 18 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	J	62	Total	C	N	O	0	0
			507	333	88	86		
18	j	62	Total	C	N	O	0	0
			507	333	88	86		

- Molecule 19 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	22	Total	C	N	O	0	0
			159	103	29	27		
19	k	22	Total	C	N	O	0	0
			159	103	29	27		

- Molecule 20 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 22 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 23 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1,

MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 24 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 25 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 26 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 27 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 28 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 29 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	57	Total	C	N	O	S	0	1
			442	285	74	80	3		

- Molecule 30 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 31 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 32 is a protein called CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 33 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	104	Total	C	N	O	S	7	0
			875	552	155	163	5		

- Molecule 34 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,.

Mol	Chain	Residues	Atoms			AltConf	Trace
34	m	474	Total	C	N	0	0
			1422	948	474		

- Molecule 35 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,.

Mol	Chain	Residues	Atoms			AltConf	Trace
35	n	391	Total	C	N	0	0
			1173	782	391		

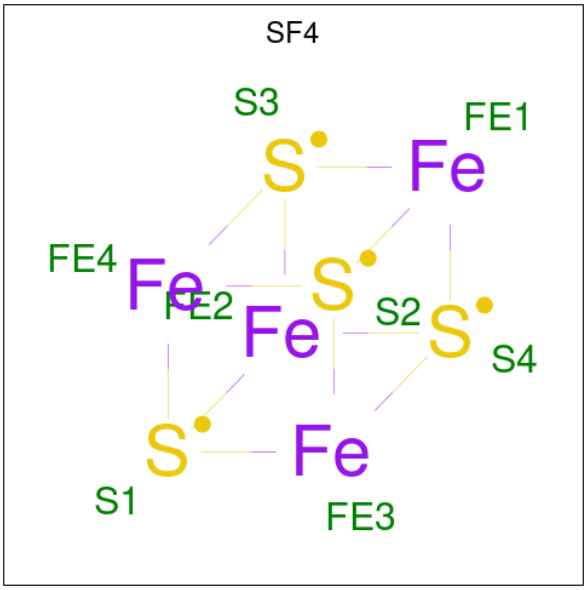
- Molecule 36 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms			AltConf	Trace
36	o	378	Total	C	N	0	0
			1134	756	378		

- Molecule 37 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

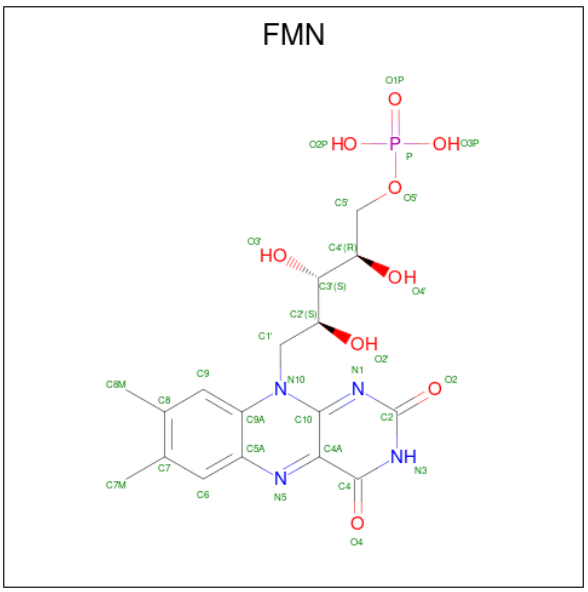
Mol	Chain	Residues	Atoms			AltConf	Trace
37	p	281	Total	C	N	0	0
			843	562	281		

- Molecule 38 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



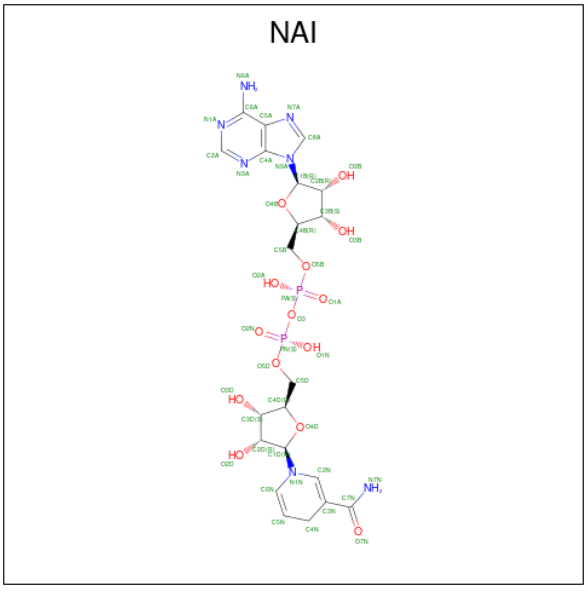
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	Fe	S	0
			8	4	4	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	6	1	Total	Fe	S	0
			8	4	4	
38	8	1	Total	Fe	S	0
			16	8	8	
38	8	1	Total	Fe	S	0
			16	8	8	

- Molecule 39 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 40 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

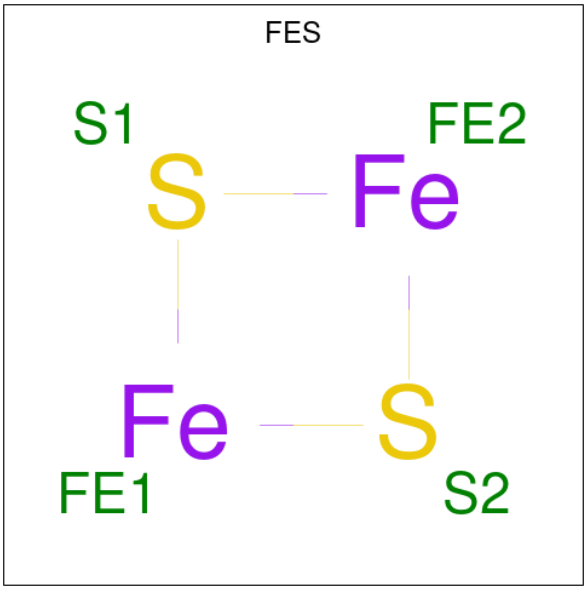


Mol	Chain	Residues	Atoms					AltConf
40	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
41	1	1	Total Mg 1 1	0
41	2	1	Total Mg 1 1	0
41	3	2	Total Mg 2 2	0
41	4	1	Total Mg 1 1	0
41	5	1	Total Mg 1 1	0
41	L	1	Total Mg 1 1	0

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

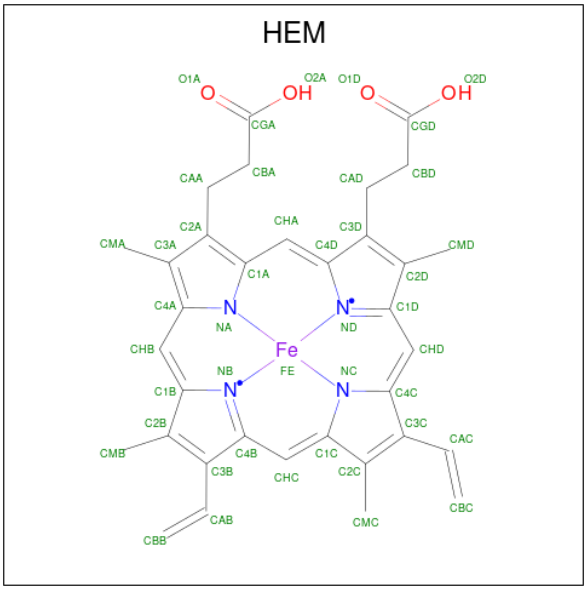


Mol	Chain	Residues	Atoms	AltConf
42	2	1	Total Fe S 4 2 2	0
42	3	1	Total Fe S 4 2 2	0
42	E	1	Total Fe S 4 2 2	0
42	e	1	Total Fe S 4 2 2	0

- Molecule 43 is CALCIUM ION (three-letter code: CA) (formula: Ca).

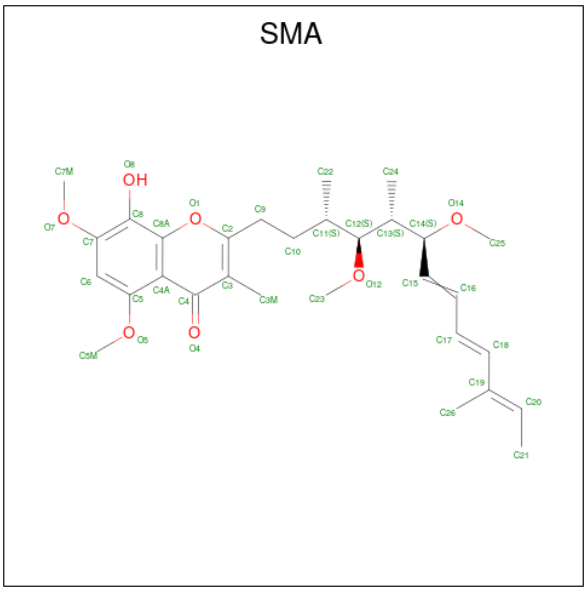
Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total Ca 1 1	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



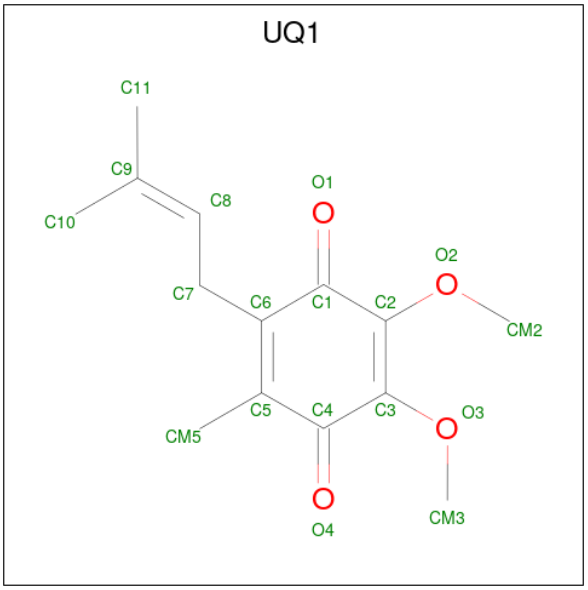
Mol	Chain	Residues	Atoms	AltConf
44	C	1	Total C Fe N O 86 68 2 8 8	0
44	C	1	Total C Fe N O 86 68 2 8 8	0
44	Y	1	Total C Fe N O 43 34 1 4 4	0
44	c	1	Total C Fe N O 86 68 2 8 8	0
44	c	1	Total C Fe N O 86 68 2 8 8	0

- Molecule 45 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



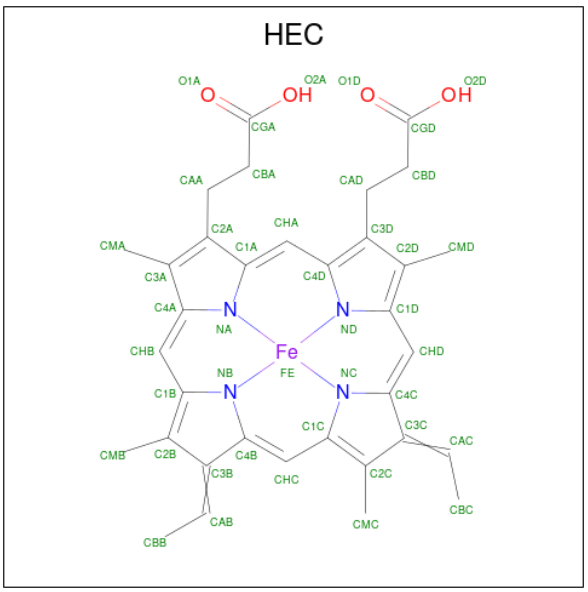
Mol	Chain	Residues	Atoms	AltConf
45	C	1	Total C O 37 30 7	0
45	c	1	Total C O 37 30 7	0

- Molecule 46 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



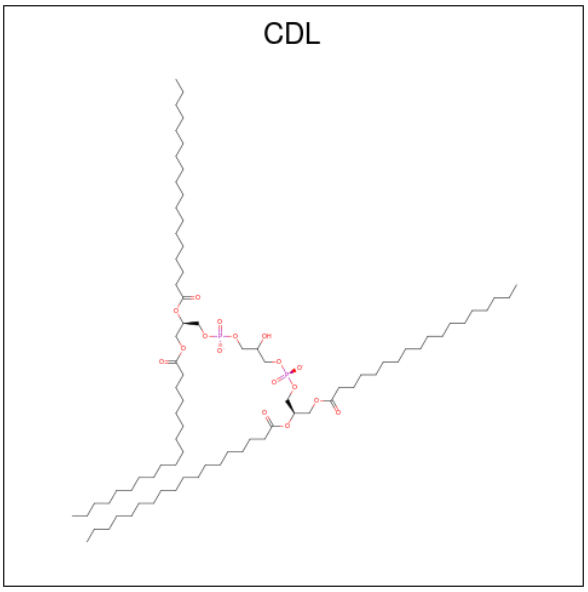
Mol	Chain	Residues	Atoms	AltConf
46	C	1	Total C O 14 10 4	0
46	c	1	Total C O 14 10 4	0

- Molecule 47 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	

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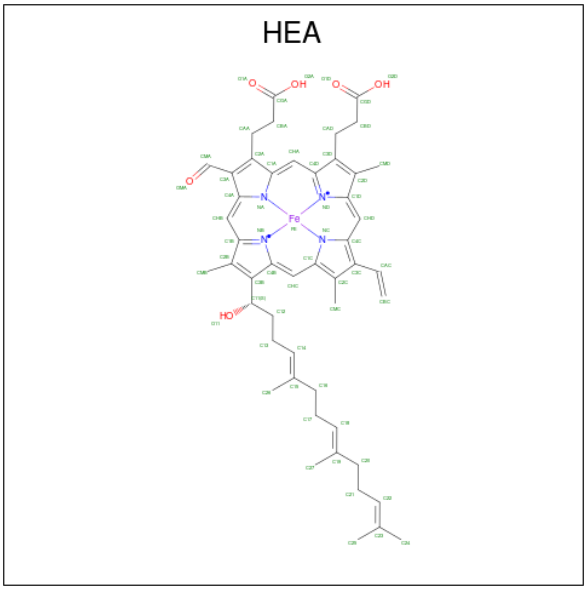
Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	
48	d	1	Total	C	O	P	0
			50	31	17	2	
48	g	1	Total	C	O	P	0
			49	30	17	2	

- Molecule 49 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
49	L	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 50 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
50	L	1	Total	Cu	0
			1	1	
50	M	2	Total	Cu	0
			2	2	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
51	Q	1	Total Zn 1 1	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms	AltConf
52	A	187	Total O 187 187	0
52	B	149	Total O 149 149	0
52	C	125	Total O 125 125	0
52	D	118	Total O 118 118	0
52	E	54	Total O 54 54	0
52	F	57	Total O 57 57	0
52	G	24	Total O 24 24	0
52	H	14	Total O 14 14	0
52	I	16	Total O 16 16	0
52	J	5	Total O 5 5	0
52	Y	161	Total O 161 161	0
52	a	134	Total O 134 134	0
52	b	130	Total O 130 130	0
52	c	122	Total O 122 122	0
52	d	109	Total O 109 109	0
52	e	64	Total O 64 64	0
52	f	73	Total O 73 73	0
52	g	21	Total O 21 21	0
52	h	16	Total O 16 16	0

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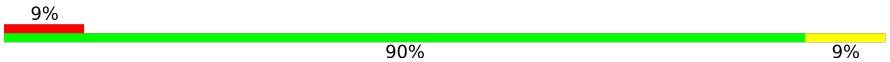
Mol	Chain	Residues	Atoms	AltConf
52	i	10	Total O 10 10	0
52	j	9	Total O 9 9	0

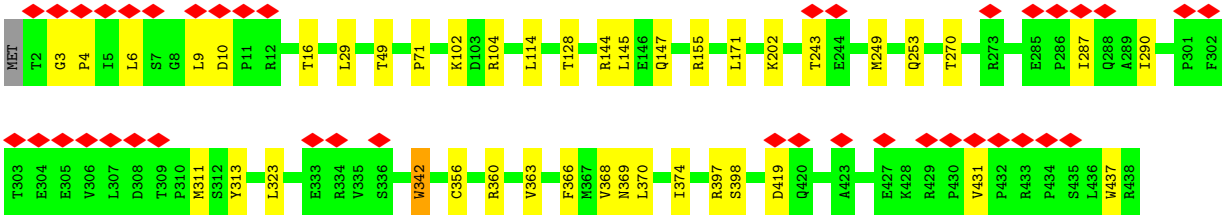
3 Residue-property plots (i)

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

• Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1

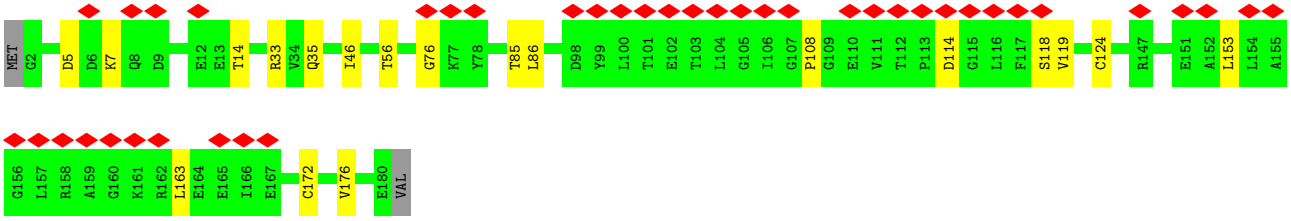
Chain 1:





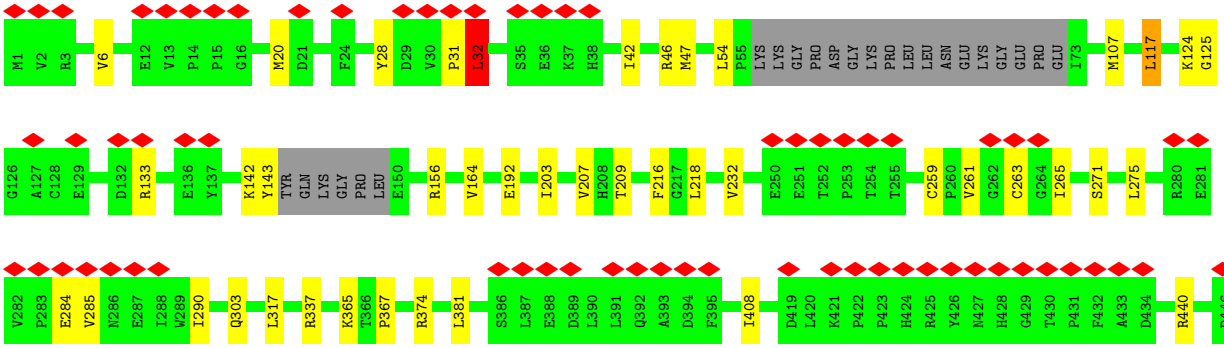
• Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2

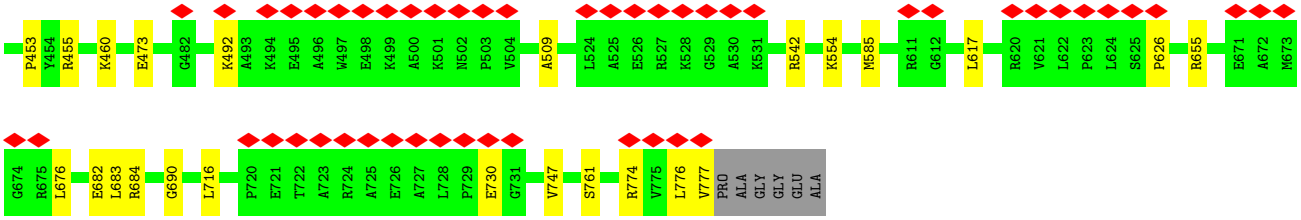
Chain 2:



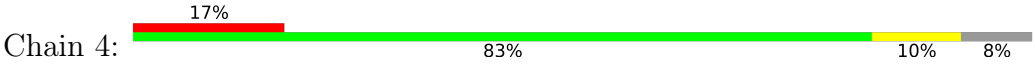
• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3

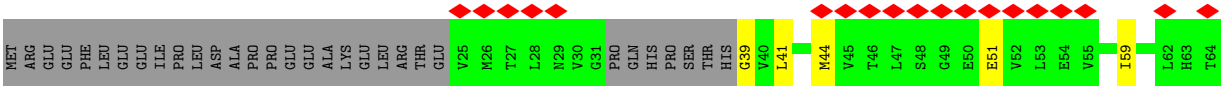
Chain 3:

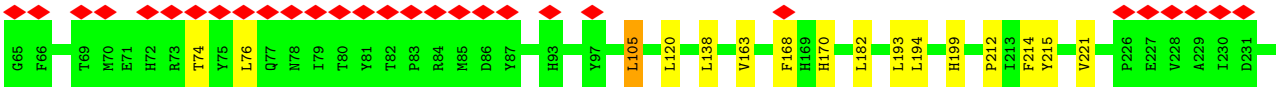


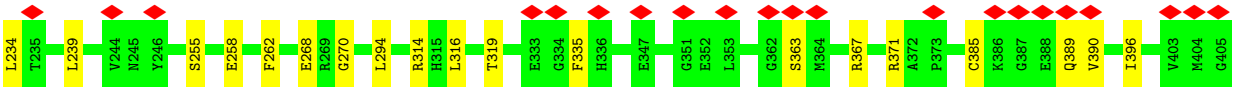


• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4

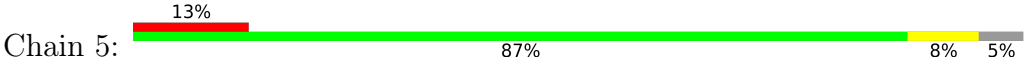


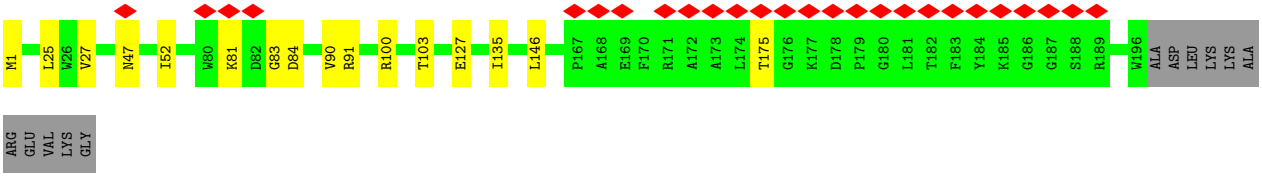




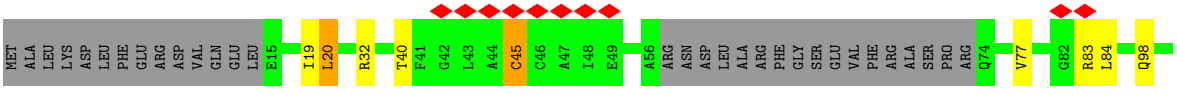


• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5

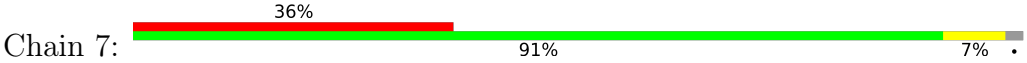


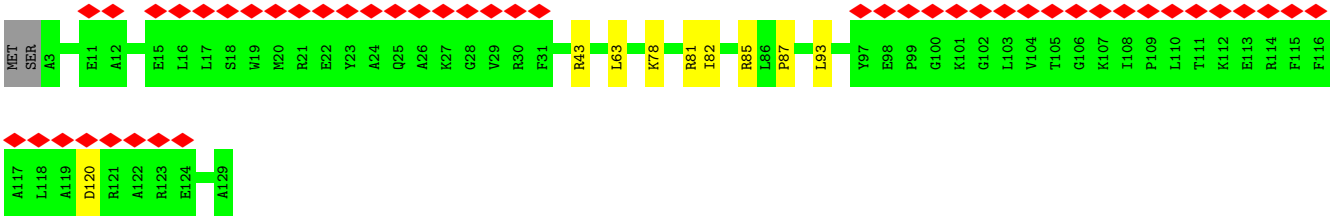


• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6



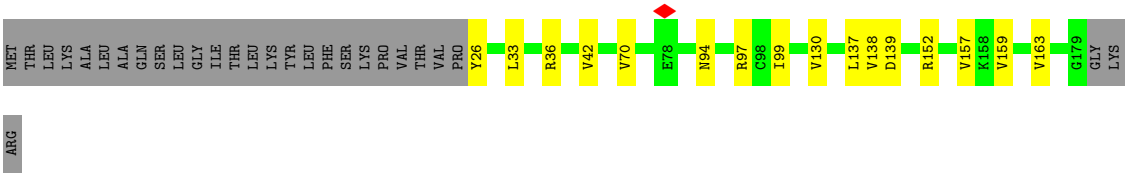
• Molecule 7: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15





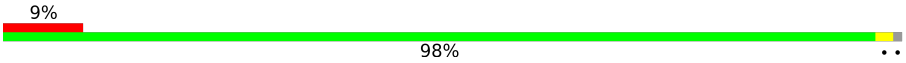
• Molecule 8: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9

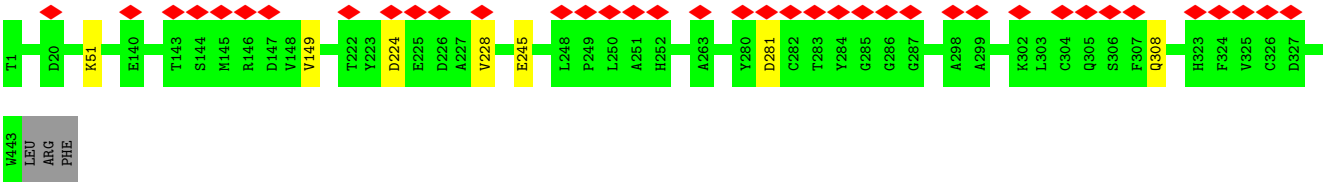
Chain 8:



• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

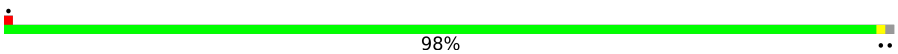
Chain A:

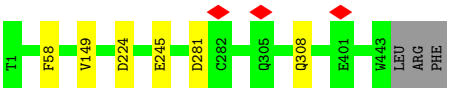




• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

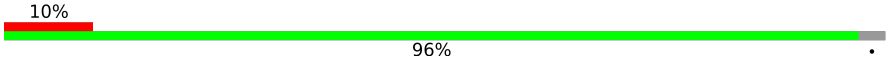
Chain a:

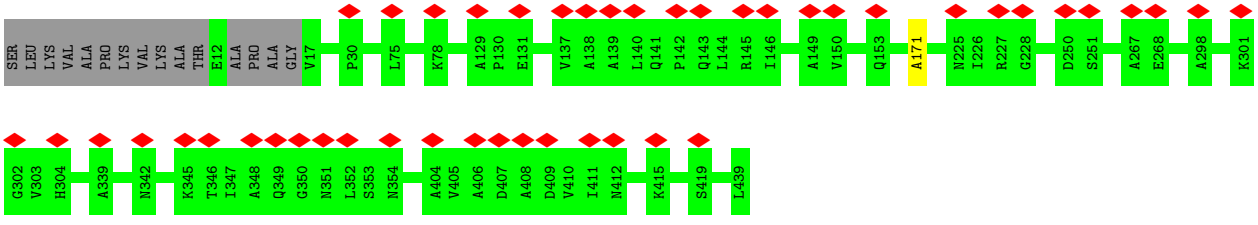




• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

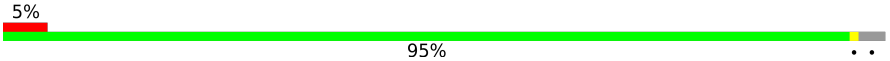
Chain B:

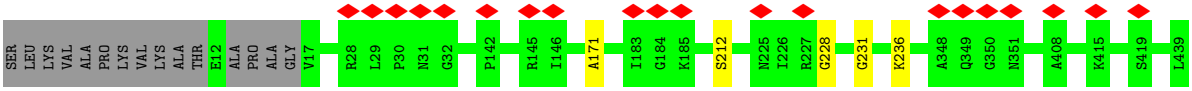




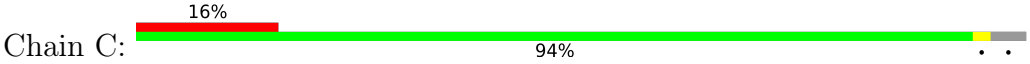
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

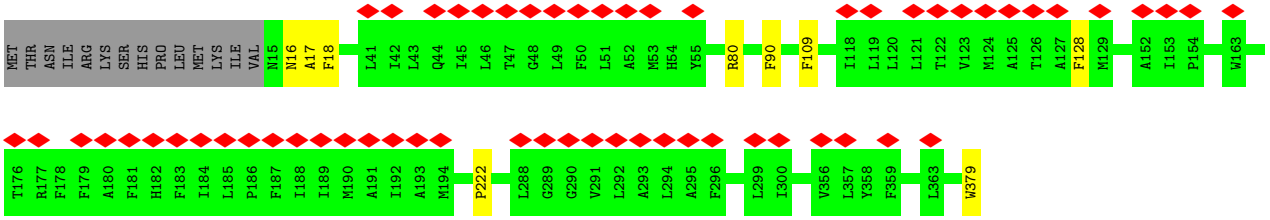
Chain b:



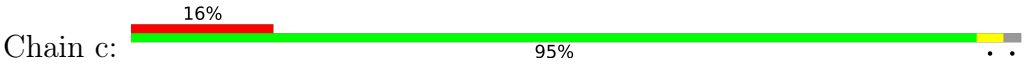


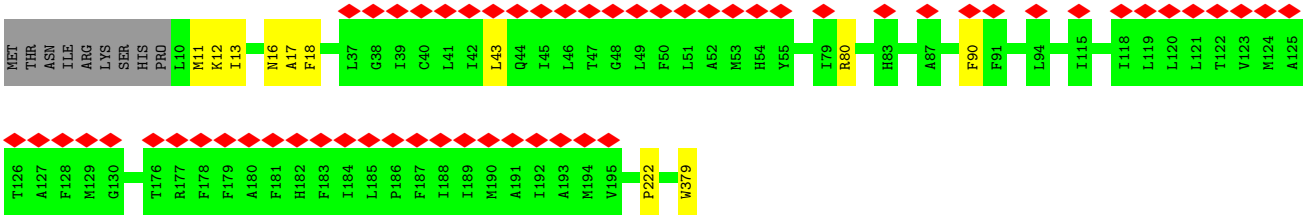
• Molecule 11: CYTOCHROME B



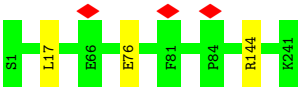


• Molecule 11: CYTOCHROME B

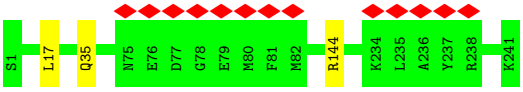




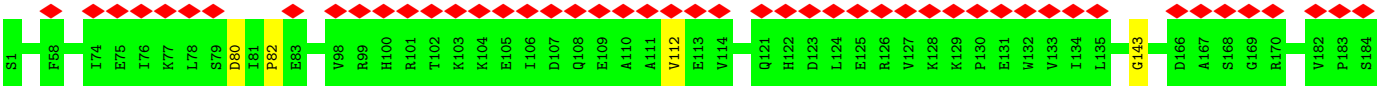
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

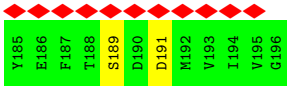


• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



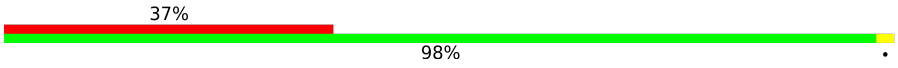
• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

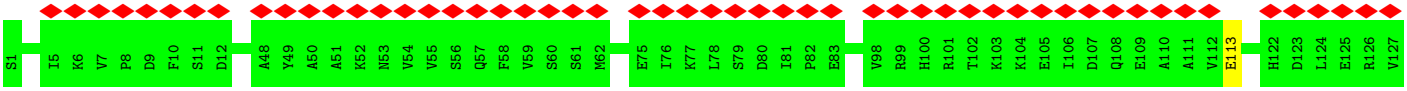


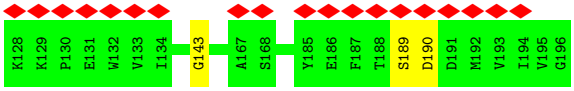


• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain e:





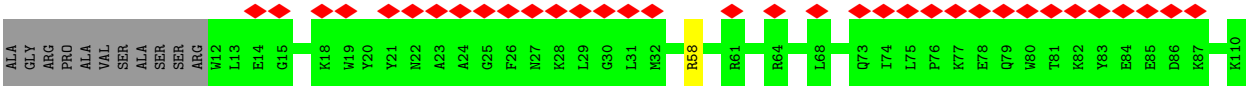


• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F:

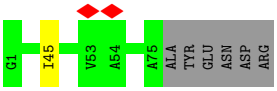
• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain f:



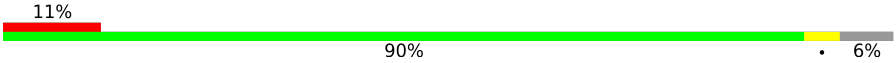
• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

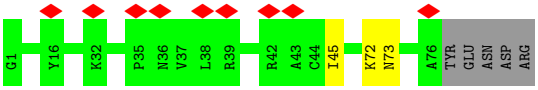
Chain G:



• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

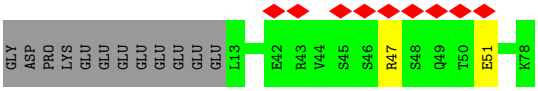
Chain g:





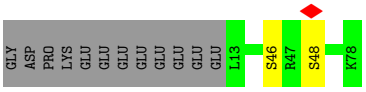
• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain H:



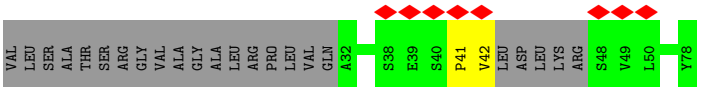
• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain h:



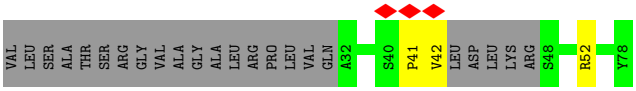
• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:



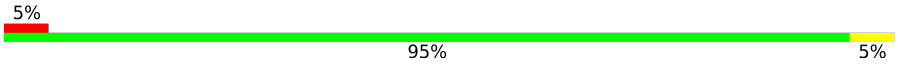
• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

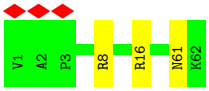
Chain i:



• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

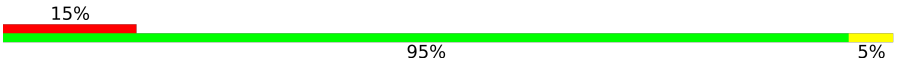
Chain J:

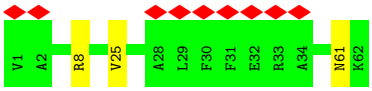




• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

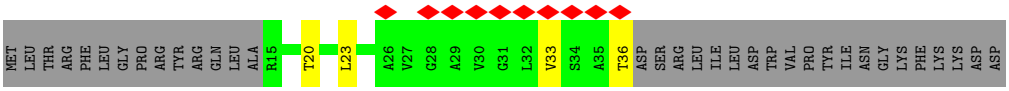
Chain j:





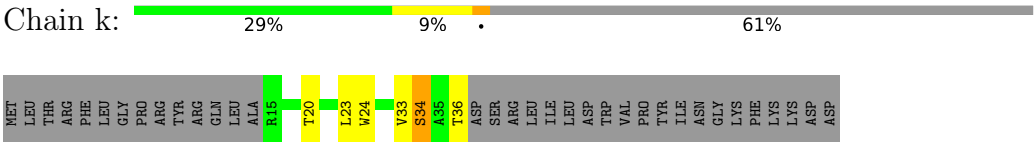
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain K:



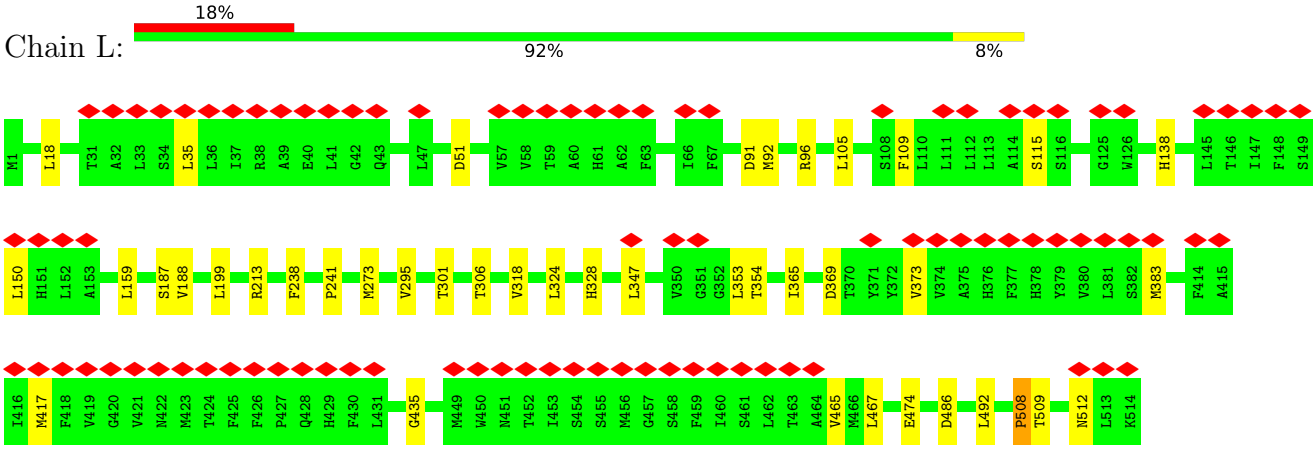
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain k:



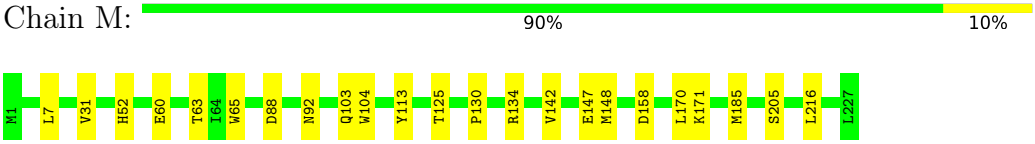
• Molecule 20: CYTOCHROME C OXIDASE SUBUNIT 1

Chain L:



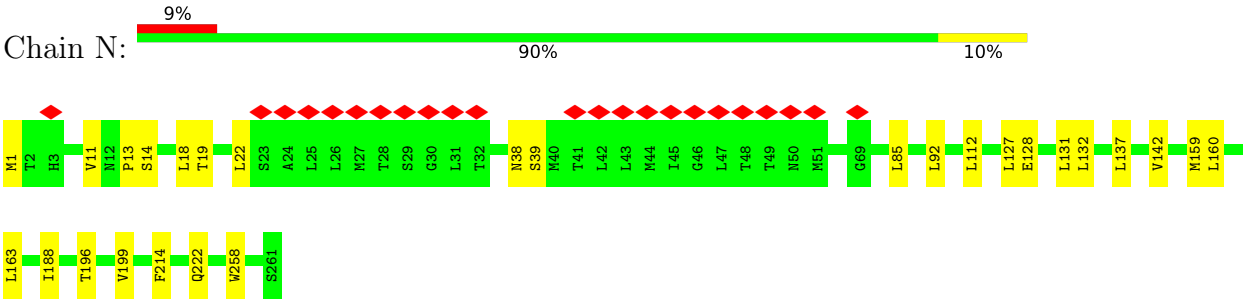
• Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 2

Chain M:



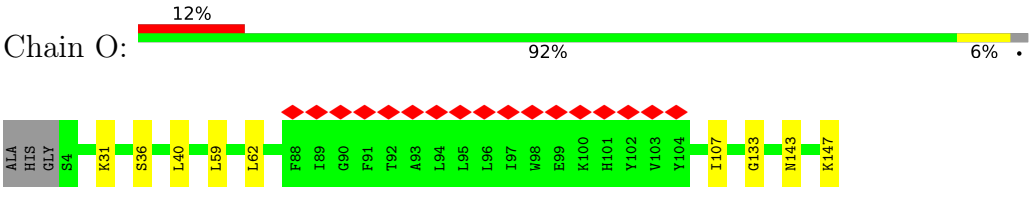
• Molecule 22: CYTOCHROME C OXIDASE SUBUNIT 3

Chain N:



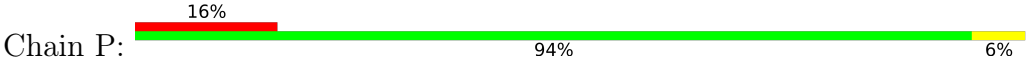
• Molecule 23: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1, MITOCHONDRIAL

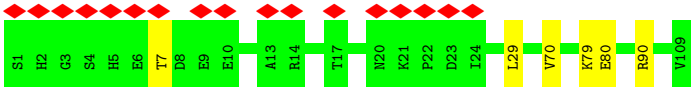
Chain O:



• Molecule 24: CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL

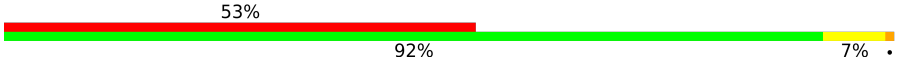
Chain P:

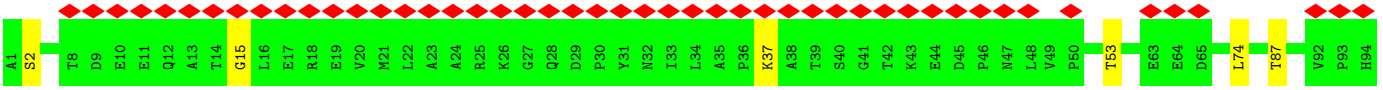


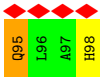


• Molecule 25: CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL

Chain Q:

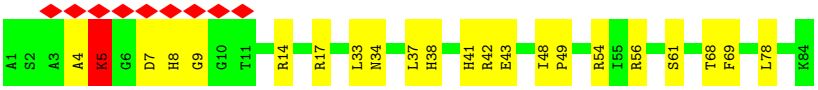






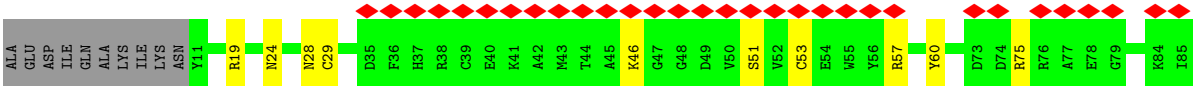
• Molecule 26: CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB

Chain R:



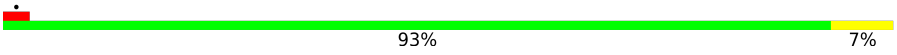
• Molecule 27: CYTOCHROME C OXIDASE SUBUNIT 6B1

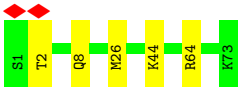
Chain S:



• Molecule 28: CYTOCHROME C OXIDASE SUBUNIT 6C

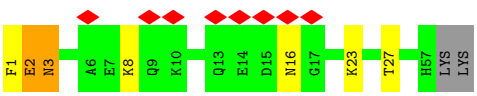
Chain T:





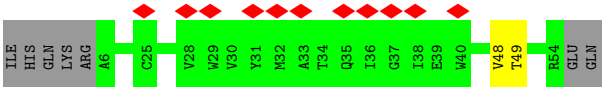
• Molecule 29: CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL

Chain U:



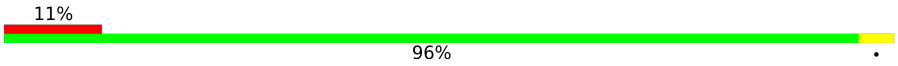
• Molecule 30: CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL

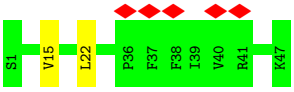
Chain V:



• Molecule 31: CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL

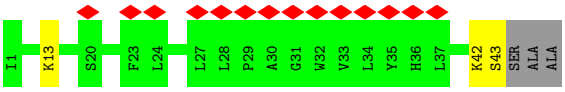
Chain W:





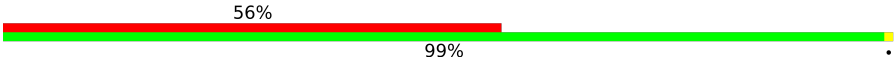
• Molecule 32: CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL

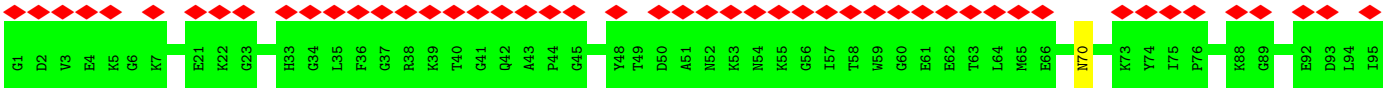
Chain X:

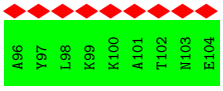


• Molecule 33: CYTOCHROME C

Chain Y:

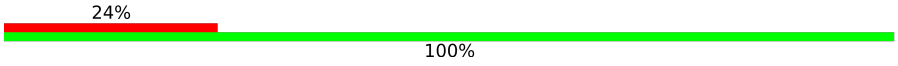


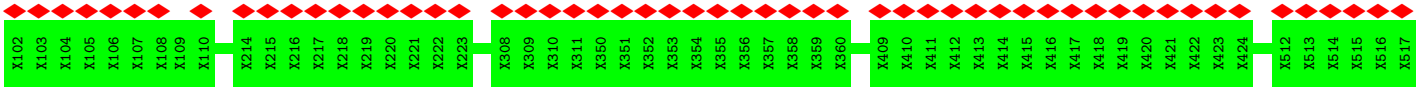


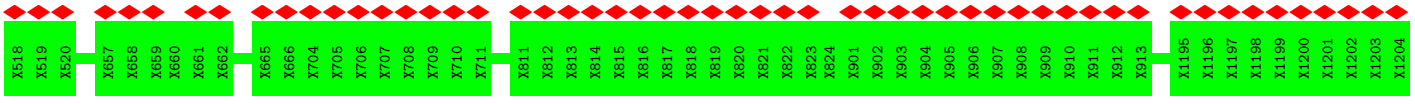


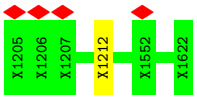
• Molecule 34: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,

Chain m:



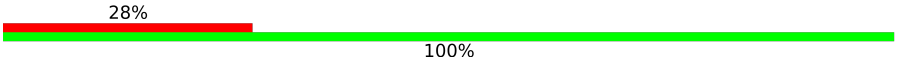


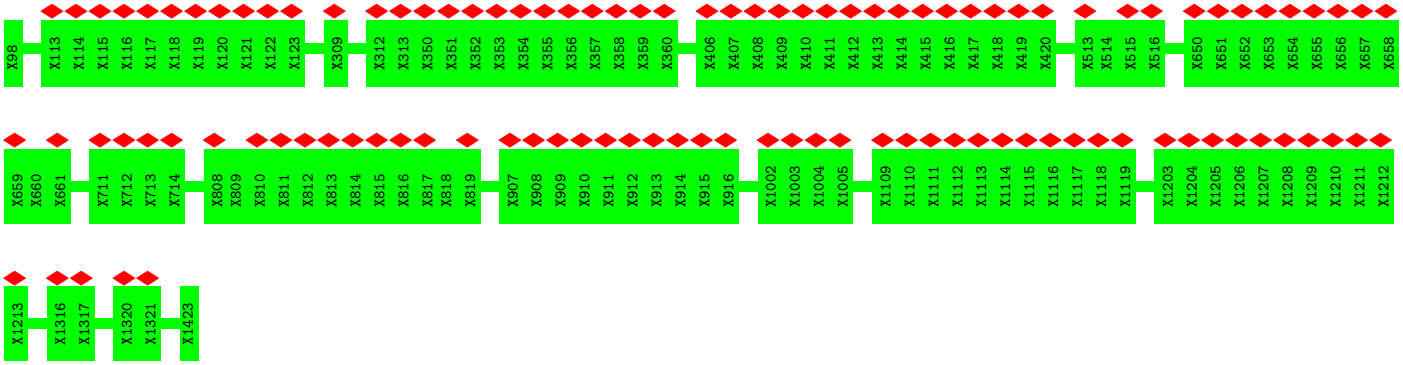




• Molecule 35: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,

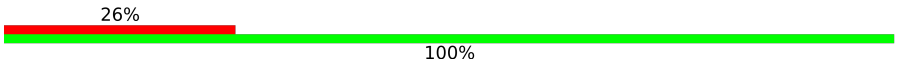
Chain n:

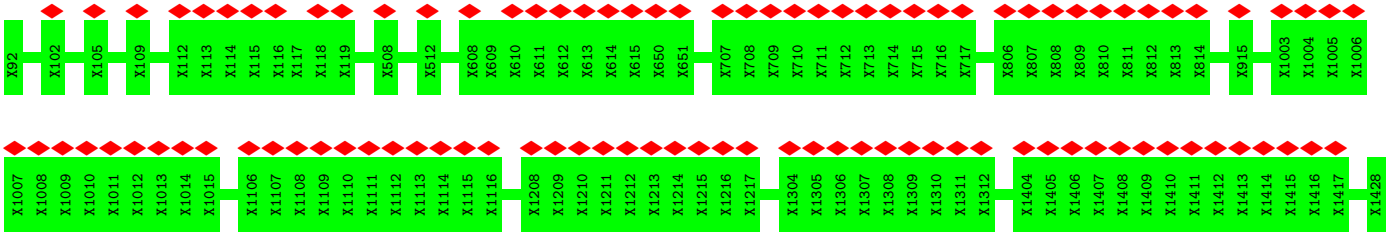




• Molecule 36: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

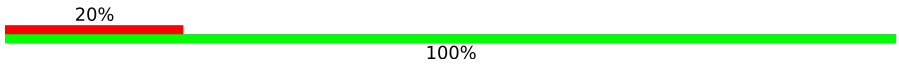
Chain o:

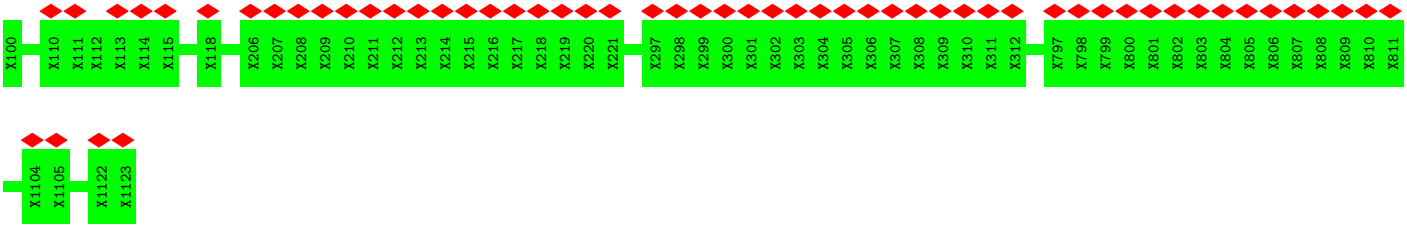




• Molecule 37: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain p:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10684	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPPING ON EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	58829	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	18.839	Depositor
Minimum map value	-8.249	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	533.12, 533.12, 533.12	wwPDB
Map dimensions	112, 112, 112	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	4.76, 4.76, 4.76	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FMN, HEA, NAI, UQ1, FES, SF4, CDL, ZN, CU, MG, SMA, HEM, CA

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	1	0.45	1/3506 (0.0%)	0.63	2/4745 (0.0%)
2	2	0.45	0/1443	0.64	0/1958
3	3	0.43	0/6019	0.61	1/8163 (0.0%)
4	4	0.40	0/3096	0.59	2/4207 (0.0%)
5	5	0.44	0/1656	0.61	0/2246
6	6	0.48	0/1126	0.64	0/1528
7	7	0.43	0/1059	0.60	0/1429
8	8	0.48	0/1224	0.66	0/1663
9	A	0.32	0/3472	0.66	0/4714
9	a	0.33	0/3472	0.67	0/4714
10	B	0.32	0/3235	0.65	0/4387
10	b	0.31	0/3239	0.65	1/4393 (0.0%)
11	C	0.37	0/2986	0.65	1/4089 (0.0%)
11	c	0.35	0/3024	0.64	0/4137
12	D	0.34	0/1978	0.65	0/2684
12	d	0.34	0/1978	0.65	0/2684
13	E	0.32	0/1553	0.67	1/2100 (0.0%)
13	e	0.35	0/1553	0.69	1/2100 (0.0%)
14	F	0.32	0/878	0.64	0/1175
14	f	0.32	0/878	0.65	0/1175
15	G	0.32	0/642	0.65	0/869
15	g	0.34	0/647	0.68	0/876
16	H	0.31	0/544	0.60	0/729
16	h	0.31	0/544	0.56	0/729
17	I	0.32	0/285	0.66	0/384
17	i	0.32	0/285	0.69	0/384
18	J	0.37	0/520	0.65	0/699
18	j	0.36	0/520	0.65	0/699
19	K	0.42	0/163	1.01	0/225
19	k	0.46	0/163	1.17	0/225
20	L	0.60	0/4164	0.76	1/5688 (0.0%)
21	M	0.57	0/1868	0.79	0/2544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	N	0.56	0/2211	0.68	0/3023
23	O	0.57	0/1229	0.64	1/1658 (0.1%)
24	P	0.50	0/898	0.66	0/1218
25	Q	0.56	0/765	0.81	0/1038
26	R	0.54	0/699	0.73	1/950 (0.1%)
27	S	0.55	0/648	0.73	0/877
28	T	0.60	0/611	0.65	0/810
29	U	0.61	0/451	0.72	0/610
30	V	0.57	0/398	0.66	0/546
31	W	0.63	0/399	0.62	0/534
32	X	0.51	0/345	0.65	0/470
33	Y	0.31	0/891	0.60	0/1186
All	All	0.43	1/67265 (0.0%)	0.66	12/91262 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	k	0	1
34	m	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	356	CYS	CB-SG	-5.05	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	39	GLY	N-CA-C	-7.72	93.79	113.10
4	4	105	LEU	CA-CB-CG	7.21	131.89	115.30
10	b	228	GLY	N-CA-C	-6.96	95.71	113.10
23	O	133	GLY	N-CA-C	6.43	129.19	113.10
3	3	32	LEU	CA-CB-CG	5.91	128.89	115.30
13	e	143	GLY	N-CA-C	5.69	127.33	113.10
13	E	143	GLY	N-CA-C	5.38	126.54	113.10
26	R	5	LYS	N-CA-C	5.22	125.09	111.00
11	C	109	PHE	N-CA-C	-5.21	96.93	111.00
20	L	435	GLY	N-CA-C	5.16	125.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	356	CYS	CB-CA-C	-5.16	100.09	110.40
1	1	342	TRP	CA-CB-CG	5.09	123.36	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	k	24	TRP	Mainchain
34	m	1212	UNK	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	9	44
2	2	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	6	34
3	3	748/783 (96%)	624 (83%)	101 (14%)	23 (3%)	4	27
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	6	33
5	5	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	7	36
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	3	25
7	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	19	60
8	8	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	22	63
9	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	29	69
9	a	441/446 (99%)	424 (96%)	16 (4%)	1 (0%)	47	81
10	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	b	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	29 69
11	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	19 60
11	c	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	11 46
12	D	239/241 (99%)	234 (98%)	5 (2%)	0	100 100
12	d	239/241 (99%)	235 (98%)	4 (2%)	0	100 100
13	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	7 36
13	e	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	29 69
14	F	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
14	f	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
15	G	73/81 (90%)	72 (99%)	1 (1%)	0	100 100
15	g	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	11 46
16	H	64/78 (82%)	61 (95%)	3 (5%)	0	100 100
16	h	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	9 44
17	I	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	5 31
17	i	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	5 31
18	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9 42
18	j	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9 42
19	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	2 20
19	k	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0 9
20	L	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19 60
21	M	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12 48
22	N	259/261 (99%)	249 (96%)	10 (4%)	0	100 100
23	O	142/147 (97%)	135 (95%)	7 (5%)	0	100 100
24	P	107/109 (98%)	104 (97%)	3 (3%)	0	100 100
25	Q	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3 22
26	R	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1 17
27	S	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	11 46
28	T	71/73 (97%)	65 (92%)	6 (8%)	0	100 100
29	U	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	3 24
30	V	47/56 (84%)	41 (87%)	6 (13%)	0	100 100
31	W	45/47 (96%)	42 (93%)	3 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	X	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
33	Y	109/104 (105%)	106 (97%)	3 (3%)	0	100	100
All	All	8228/8726 (94%)	7616 (93%)	511 (6%)	101 (1%)	17	50

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE
3	3	367	PRO
3	3	509	ALA
4	4	212	PRO
4	4	255	SER
5	5	81	LYS
7	7	87	PRO
9	A	224	ASP
11	C	16	ASN
11	C	17	ALA
17	I	41	PRO
18	J	61	ASN
20	L	328	HIS
20	L	508	PRO
25	Q	2	SER
25	Q	87	THR
25	Q	95	GLN
26	R	4	ALA
26	R	9	GLY
27	S	46	LYS
29	U	2	GLU
9	a	224	ASP
11	c	17	ALA
15	g	72	LYS
17	i	41	PRO
18	j	61	ASN
1	1	360	ARG
2	2	86	LEU
2	2	124	CYS
3	3	31	PRO

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Mol	Chain	Res	Type
3	3	32	LEU
3	3	125	GLY
3	3	164	VAL
3	3	263	CYS
3	3	453	PRO
3	3	554	LYS
4	4	51	GLU
4	4	258	GLU
5	5	83	GLY
6	6	45	CYS
8	8	152	ARG
10	B	171	ALA
13	E	112	VAL
26	R	5	LYS
10	b	171	ALA
10	b	231	GLY
11	c	16	ASN
16	h	48	SER
1	1	71	PRO
2	2	76	GLY
3	3	28	TYR
3	3	271	SER
3	3	285	VAL
3	3	365	LYS
3	3	374	ARG
3	3	690	GLY
4	4	214	PHE
4	4	389	GLN
6	6	98	GLN
6	6	126	ASN
21	M	104	TRP
26	R	61	SER
13	e	189	SER
19	k	33	VAL
1	1	313	TYR
3	3	682	GLU
3	3	730	GLU
4	4	268	GLU
4	4	270	GLY
6	6	77	VAL
20	L	51	ASP
3	3	203	ILE

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Mol	Chain	Res	Type
3	3	455	ARG
5	5	127	GLU
9	A	228	VAL
11	C	18	PHE
13	E	189	SER
13	E	191	ASP
21	M	103	GLN
29	U	3	ASN
11	c	11	MET
19	k	34	SER
1	1	311	MET
4	4	390	VAL
6	6	20	LEU
20	L	91	ASP
21	M	158	ASP
26	R	49	PRO
11	c	18	PHE
1	1	202	LYS
5	5	52	ILE
13	E	82	PRO
1	1	3	GLY
11	c	13	ILE
25	Q	15	GLY
3	3	626	PRO
19	K	33	VAL

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	1	355/356 (100%)	321 (90%)	34 (10%)	8 27
2	2	150/152 (99%)	135 (90%)	15 (10%)	7 26
3	3	607/628 (97%)	560 (92%)	47 (8%)	13 37
4	4	326/355 (92%)	296 (91%)	30 (9%)	9 29
5	5	167/175 (95%)	155 (93%)	12 (7%)	14 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	6	117/149 (78%)	107 (92%)	10 (8%)	10 33
7	7	104/106 (98%)	96 (92%)	8 (8%)	13 37
8	8	126/150 (84%)	111 (88%)	15 (12%)	5 20
9	A	364/370 (98%)	359 (99%)	5 (1%)	67 80
9	a	364/370 (98%)	359 (99%)	5 (1%)	67 80
10	B	332/343 (97%)	332 (100%)	0	100 100
10	b	332/343 (97%)	330 (99%)	2 (1%)	86 92
11	C	312/327 (95%)	307 (98%)	5 (2%)	62 79
11	c	316/327 (97%)	310 (98%)	6 (2%)	57 75
12	D	206/206 (100%)	203 (98%)	3 (2%)	65 80
12	d	206/206 (100%)	203 (98%)	3 (2%)	65 80
13	E	168/168 (100%)	167 (99%)	1 (1%)	86 92
13	e	168/168 (100%)	166 (99%)	2 (1%)	71 83
14	F	90/98 (92%)	89 (99%)	1 (1%)	73 84
14	f	90/98 (92%)	89 (99%)	1 (1%)	73 84
15	G	66/71 (93%)	65 (98%)	1 (2%)	65 80
15	g	66/71 (93%)	64 (97%)	2 (3%)	41 63
16	H	63/74 (85%)	61 (97%)	2 (3%)	39 61
16	h	63/74 (85%)	62 (98%)	1 (2%)	62 79
17	I	28/51 (55%)	27 (96%)	1 (4%)	35 59
17	i	28/51 (55%)	26 (93%)	2 (7%)	14 39
18	J	51/52 (98%)	49 (96%)	2 (4%)	32 56
18	j	51/52 (98%)	49 (96%)	2 (4%)	32 56
19	K	15/46 (33%)	12 (80%)	3 (20%)	1 7
19	k	15/46 (33%)	11 (73%)	4 (27%)	0 3
20	L	427/427 (100%)	389 (91%)	38 (9%)	9 30
21	M	211/211 (100%)	191 (90%)	20 (10%)	8 27
22	N	226/226 (100%)	199 (88%)	27 (12%)	5 20
23	O	128/129 (99%)	120 (94%)	8 (6%)	18 43
24	P	95/95 (100%)	89 (94%)	6 (6%)	18 43
25	Q	81/81 (100%)	76 (94%)	5 (6%)	18 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	R	68/68 (100%)	50 (74%)	18 (26%)	0 3
27	S	67/75 (89%)	58 (87%)	9 (13%)	4 17
28	T	58/58 (100%)	53 (91%)	5 (9%)	10 32
29	U	47/50 (94%)	40 (85%)	7 (15%)	3 15
30	V	39/46 (85%)	37 (95%)	2 (5%)	24 48
31	W	40/40 (100%)	38 (95%)	2 (5%)	24 49
32	X	37/38 (97%)	34 (92%)	3 (8%)	11 35
33	Y	91/84 (108%)	90 (99%)	1 (1%)	73 84
All	All	6961/7311 (95%)	6585 (95%)	376 (5%)	26 47

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	9	LEU
1	1	10	ASP
1	1	16	THR
1	1	29	LEU
1	1	49	THR
1	1	102	LYS
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	144	ARG
1	1	145	LEU
1	1	147	GLN
1	1	155	ARG
1	1	171	LEU
1	1	243	THR
1	1	249	MET
1	1	253	GLN
1	1	270	THR
1	1	287	ILE
1	1	290	ILE
1	1	323	LEU
1	1	342	TRP
1	1	363	VAL
1	1	366	PHE
1	1	368	VAL

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Mol	Chain	Res	Type
1	1	369	ASN
1	1	370	LEU
1	1	374	ILE
1	1	397	ARG
1	1	398	SER
1	1	419	ASP
1	1	431	VAL
1	1	437	TRP
2	2	5	ASP
2	2	7	LYS
2	2	14	THR
2	2	33	ARG
2	2	35	GLN
2	2	46	ILE
2	2	56	THR
2	2	85	THR
2	2	114	ASP
2	2	118	SER
2	2	119	VAL
2	2	153	LEU
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
3	3	20	MET
3	3	32	LEU
3	3	42	ILE
3	3	46	ARG
3	3	47	MET
3	3	54	LEU
3	3	107	MET
3	3	117	LEU
3	3	124	LYS
3	3	133	ARG
3	3	142	LYS
3	3	143	TYR
3	3	156	ARG
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	218	LEU
3	3	232	VAL
3	3	259	CYS

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Mol	Chain	Res	Type
3	3	261	VAL
3	3	265	ILE
3	3	275	LEU
3	3	284	GLU
3	3	290	ILE
3	3	303	GLN
3	3	317	LEU
3	3	337	ARG
3	3	381	LEU
3	3	408	ILE
3	3	440	ARG
3	3	450	LEU
3	3	460	LYS
3	3	473	GLU
3	3	492	LYS
3	3	542	ARG
3	3	585	MET
3	3	617	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	716	LEU
3	3	747	VAL
3	3	761	SER
3	3	774	ARG
3	3	776	LEU
3	3	777	VAL
4	4	41	LEU
4	4	44	MET
4	4	59	ILE
4	4	74	THR
4	4	76	LEU
4	4	105	LEU
4	4	120	LEU
4	4	138	LEU
4	4	163	VAL
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU
4	4	193	LEU
4	4	194	LEU

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Mol	Chain	Res	Type
4	4	199	HIS
4	4	215	TYR
4	4	221	VAL
4	4	234	LEU
4	4	239	LEU
4	4	262	PHE
4	4	294	LEU
4	4	314	ARG
4	4	316	LEU
4	4	319	THR
4	4	335	PHE
4	4	363	SER
4	4	367	ARG
4	4	371	ARG
4	4	385	CYS
4	4	396	ILE
5	5	1	MET
5	5	25	LEU
5	5	27	VAL
5	5	47	ASN
5	5	84	ASP
5	5	90	VAL
5	5	91	ARG
5	5	100	ARG
5	5	103	THR
5	5	135	ILE
5	5	146	LEU
5	5	175	THR
6	6	19	ILE
6	6	20	LEU
6	6	32	ARG
6	6	40	THR
6	6	45	CYS
6	6	83	ARG
6	6	84	LEU
6	6	121	TYR
6	6	147	LEU
6	6	153	GLN
7	7	43	ARG
7	7	63	LEU
7	7	78	LYS
7	7	81	ARG

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Mol	Chain	Res	Type
7	7	82	ILE
7	7	85	ARG
7	7	93	LEU
7	7	120	ASP
8	8	26	TYR
8	8	33	LEU
8	8	36	ARG
8	8	42	VAL
8	8	70	VAL
8	8	94	ASN
8	8	97	ARG
8	8	99	ILE
8	8	130	VAL
8	8	137	LEU
8	8	138	VAL
8	8	139	ASP
8	8	157	VAL
8	8	159	VAL
8	8	163	VAL
9	A	51	LYS
9	A	149	VAL
9	A	245	GLU
9	A	281	ASP
9	A	308	GLN
11	C	80	ARG
11	C	90	PHE
11	C	128	PHE
11	C	222	PRO
11	C	379	TRP
12	D	17	LEU
12	D	76	GLU
12	D	144	ARG
13	E	80	ASP
14	F	58	ARG
15	G	45	ILE
16	H	47	ARG
16	H	51	GLU
17	I	42	VAL
18	J	8	ARG
18	J	16	ARG
19	K	20	THR
19	K	23	LEU

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Mol	Chain	Res	Type
19	K	36	THR
20	L	18	LEU
20	L	35	LEU
20	L	92	MET
20	L	96	ARG
20	L	105	LEU
20	L	109	PHE
20	L	115	SER
20	L	138	HIS
20	L	150	LEU
20	L	159	LEU
20	L	187	SER
20	L	188	VAL
20	L	199	LEU
20	L	213	ARG
20	L	238	PHE
20	L	241	PRO
20	L	273	MET
20	L	295	VAL
20	L	301	THR
20	L	306	THR
20	L	318	VAL
20	L	324	LEU
20	L	347	LEU
20	L	353	LEU
20	L	354	THR
20	L	365	ILE
20	L	369	ASP
20	L	373	VAL
20	L	383	MET
20	L	417	MET
20	L	465	VAL
20	L	467	LEU
20	L	474	GLU
20	L	486	ASP
20	L	492	LEU
20	L	508	PRO
20	L	509	THR
20	L	512	ASN
21	M	7	LEU
21	M	31	VAL
21	M	52	HIS

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Mol	Chain	Res	Type
21	M	60	GLU
21	M	63	THR
21	M	65	TRP
21	M	88	ASP
21	M	92	ASN
21	M	113	TYR
21	M	125	THR
21	M	130	PRO
21	M	134	ARG
21	M	142	VAL
21	M	147	GLU
21	M	148	MET
21	M	170	LEU
21	M	171	LYS
21	M	185	MET
21	M	205	SER
21	M	216	LEU
22	N	1	MET
22	N	11	VAL
22	N	13	PRO
22	N	14	SER
22	N	18	LEU
22	N	19	THR
22	N	22	LEU
22	N	38	ASN
22	N	39	SER
22	N	85	LEU
22	N	92	LEU
22	N	112	LEU
22	N	127	LEU
22	N	128	GLU
22	N	131	LEU
22	N	132	LEU
22	N	137	LEU
22	N	142	VAL
22	N	159	MET
22	N	160	LEU
22	N	163	LEU
22	N	188	ILE
22	N	196	THR
22	N	199	VAL
22	N	214	PHE

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Mol	Chain	Res	Type
22	N	222	GLN
22	N	258	TRP
23	O	31	LYS
23	O	36	SER
23	O	40	LEU
23	O	59	LEU
23	O	62	LEU
23	O	107	ILE
23	O	143	ASN
23	O	147	LYS
24	P	7	THR
24	P	29	LEU
24	P	70	VAL
24	P	79	LYS
24	P	80	GLU
24	P	90	ARG
25	Q	37	LYS
25	Q	53	THR
25	Q	74	LEU
25	Q	95	GLN
25	Q	98	HIS
26	R	5	LYS
26	R	7	ASP
26	R	8	HIS
26	R	14	ARG
26	R	17	ARG
26	R	33	LEU
26	R	34	ASN
26	R	37	LEU
26	R	38	HIS
26	R	41	HIS
26	R	42	ARG
26	R	43	GLU
26	R	48	ILE
26	R	54	ARG
26	R	56	ARG
26	R	68	THR
26	R	69	PHE
26	R	78	LEU
27	S	19	ARG
27	S	24	ASN
27	S	28	ASN

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Mol	Chain	Res	Type
27	S	29	CYS
27	S	51	SER
27	S	53	CYS
27	S	57	ARG
27	S	60	TYR
27	S	75	ARG
28	T	2	THR
28	T	8	GLN
28	T	26	MET
28	T	44	LYS
28	T	64	ARG
29	U	1	PHE
29	U	2	GLU
29	U	3	ASN
29	U	8	LYS
29	U	16	ASN
29	U	23	LYS
29	U	27	THR
30	V	48	VAL
30	V	49	THR
31	W	15	VAL
31	W	22	LEU
32	X	13	LYS
32	X	42	LYS
32	X	43	SER
33	Y	70	ASN
9	a	58	PHE
9	a	149	VAL
9	a	245	GLU
9	a	281	ASP
9	a	308	GLN
10	b	212	SER
10	b	236	LYS
11	c	12	LYS
11	c	43	LEU
11	c	80	ARG
11	c	90	PHE
11	c	222	PRO
11	c	379	TRP
12	d	17	LEU
12	d	35	GLN
12	d	144	ARG

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Mol	Chain	Res	Type
13	e	113	GLU
13	e	190	ASP
14	f	58	ARG
15	g	45	ILE
15	g	73	ASN
16	h	46	SER
17	i	42	VAL
17	i	52	ARG
18	j	8	ARG
18	j	25	VAL
19	k	20	THR
19	k	23	LEU
19	k	34	SER
19	k	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	87	HIS
1	1	161	ASN
1	1	219	ASN
1	1	369	ASN
2	2	137	ASN
3	3	303	GLN
3	3	757	HIS
4	4	292	GLN
4	4	327	HIS
4	4	330	HIS
5	5	40	HIS
5	5	47	ASN
5	5	112	ASN
7	7	92	HIS
8	8	94	ASN
9	A	15	GLN
9	A	61	HIS
9	A	136	GLN
9	A	213	GLN
9	A	271	GLN
10	B	22	GLN
10	B	104	ASN
10	B	343	GLN
10	B	412	ASN

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Mol	Chain	Res	Type
11	C	68	HIS
11	C	159	ASN
12	D	106	ASN
13	E	57	GLN
13	E	116	GLN
15	G	28	HIS
15	G	73	ASN
20	L	11	ASN
20	L	12	HIS
20	L	43	GLN
20	L	99	ASN
20	L	170	ASN
20	L	256	HIS
20	L	360	ASN
20	L	413	HIS
20	L	512	ASN
21	M	103	GLN
21	M	203	ASN
22	N	6	HIS
22	N	12	ASN
22	N	133	ASN
22	N	148	HIS
22	N	158	HIS
22	N	207	HIS
22	N	222	GLN
22	N	232	HIS
23	O	109	HIS
24	P	34	ASN
25	Q	66	ASN
26	R	52	HIS
27	S	23	GLN
27	S	24	ASN
27	S	25	GLN
27	S	28	ASN
27	S	37	HIS
28	T	8	GLN
29	U	3	ASN
29	U	16	ASN
30	V	10	HIS
30	V	15	ASN
30	V	41	ASN
32	X	39	ASN

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Mol	Chain	Res	Type
33	Y	54	ASN
33	Y	70	ASN
9	a	15	GLN
9	a	61	HIS
9	a	136	GLN
9	a	165	GLN
9	a	213	GLN
9	a	271	GLN
10	b	104	ASN
10	b	240	HIS
10	b	343	GLN
10	b	412	ASN
11	c	68	HIS
11	c	159	ASN
13	e	57	GLN
14	f	73	GLN
15	g	28	HIS
17	i	71	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
46	UQ1	c	3002	-	14,14,18	2.05	8 (57%)	18,20,25	0.40	0
42	FES	3	787	3	0,4,4	-	-	-		
44	HEM	c	502	11	41,50,50	1.87	10 (24%)	45,82,82	1.68	7 (15%)
48	CDL	g	3004	-	48,48,99	1.14	4 (8%)	54,60,111	1.10	2 (3%)
42	FES	2	182	2	0,4,4	-	-	-		
38	SF4	3	786	3	0,12,12	-	-	-		
46	UQ1	C	2002	-	14,14,18	2.25	8 (57%)	18,20,25	0.53	0
38	SF4	8	183	8	0,12,12	-	-	-		
45	SMA	C	2001	-	38,38,38	1.41	7 (18%)	48,52,52	1.09	4 (8%)
44	HEM	C	501	11	41,50,50	1.92	7 (17%)	45,82,82	1.99	12 (26%)
38	SF4	6	182	6	0,12,12	-	-	-		
44	HEM	c	501	11	41,50,50	1.83	7 (17%)	45,82,82	1.49	7 (15%)
40	NAI	1	441	-	42,48,48	3.75	29 (69%)	47,73,73	1.55	6 (12%)
48	CDL	d	3003	-	49,49,99	1.08	5 (10%)	55,61,111	1.14	4 (7%)
49	HEA	L	515	20	57,67,67	1.25	6 (10%)	61,103,103	1.49	11 (18%)
42	FES	E	501	13	0,4,4	-	-	-		
42	FES	e	501	13	0,4,4	-	-	-		
44	HEM	Y	500	33	41,50,50	1.73	10 (24%)	45,82,82	1.87	11 (24%)
45	SMA	c	3001	-	38,38,38	1.55	9 (23%)	48,52,52	1.12	4 (8%)
38	SF4	1	439	1	0,12,12	-	-	-		
48	CDL	G	2004	-	43,43,99	1.12	2 (4%)	49,55,111	1.20	4 (8%)
44	HEM	C	502	11	41,50,50	1.75	7 (17%)	45,82,82	1.97	16 (35%)
38	SF4	8	184	8	0,12,12	-	-	-		
48	CDL	G	2003	-	49,49,99	1.09	3 (6%)	55,61,111	1.07	4 (7%)
49	HEA	L	516	20	57,67,67	1.46	6 (10%)	61,103,103	1.43	11 (18%)
39	FMN	1	440	-	33,33,33	1.24	2 (6%)	48,50,50	1.84	12 (25%)
47	HEC	d	501	12	32,50,50	1.89	5 (15%)	24,82,82	1.23	3 (12%)
47	HEC	D	501	12	32,50,50	1.90	6 (18%)	24,82,82	1.40	4 (16%)
38	SF4	3	785	3	0,12,12	-	-	-		
38	SF4	3	784	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	UQ1	c	3002	-	-	2/4/28/33	0/1/1/1
42	FES	3	787	3	-	-	0/1/1/1
44	HEM	c	502	11	-	4/12/54/54	-
48	CDL	g	3004	-	-	21/57/57/110	-
42	FES	2	182	2	-	-	0/1/1/1
38	SF4	3	786	3	-	-	0/6/5/5
46	UQ1	C	2002	-	-	0/4/28/33	0/1/1/1
45	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
38	SF4	8	183	8	-	-	0/6/5/5
44	HEM	C	501	11	-	4/12/54/54	-
38	SF4	6	182	6	-	-	0/6/5/5
49	HEA	L	515	20	3/3/7/16	6/32/76/76	-
40	NAI	1	441	-	-	7/25/72/72	0/5/5/5
44	HEM	c	501	11	-	4/12/54/54	-
48	CDL	d	3003	-	-	37/58/58/110	-
42	FES	E	501	13	-	-	0/1/1/1
42	FES	e	501	13	-	-	0/1/1/1
44	HEM	Y	500	33	-	4/12/54/54	-
45	SMA	c	3001	-	-	2/34/34/34	0/2/2/2
48	CDL	G	2004	-	-	34/52/52/110	-
38	SF4	1	439	1	-	-	0/6/5/5
44	HEM	C	502	11	-	4/12/54/54	-
48	CDL	G	2003	-	-	26/58/58/110	-
38	SF4	8	184	8	-	-	0/6/5/5
49	HEA	L	516	20	3/3/7/16	5/32/76/76	-
39	FMN	1	440	-	-	6/18/18/18	0/3/3/3
47	HEC	d	501	12	-	4/10/54/54	-
47	HEC	D	501	12	-	4/10/54/54	-
38	SF4	3	785	3	-	-	0/6/5/5
38	SF4	3	784	3	-	-	0/6/5/5

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C2A-N1A	11.40	1.55	1.33
40	1	441	NAI	C2B-C1B	-9.84	1.38	1.53
49	L	516	HEA	C3A-C2A	-6.47	1.31	1.40
47	d	501	HEC	C3C-C2C	-6.11	1.34	1.40
47	D	501	HEC	C2B-C3B	-5.90	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C3D-C4D	-5.77	1.38	1.53
44	C	501	HEM	C3C-CAC	-5.62	1.36	1.47
40	1	441	NAI	C2B-C3B	-5.61	1.38	1.53
44	c	502	HEM	CBB-CAB	5.40	1.57	1.30
44	c	501	HEM	CBB-CAB	5.30	1.56	1.30
40	1	441	NAI	C3B-C4B	-5.26	1.39	1.53
44	c	501	HEM	C3C-CAC	-5.13	1.37	1.47
44	C	502	HEM	C3C-CAC	-5.11	1.37	1.47
44	Y	500	HEM	C3C-CAC	-5.11	1.37	1.47
40	1	441	NAI	C2D-C1D	-5.08	1.37	1.53
44	c	502	HEM	C3C-CAC	-5.01	1.37	1.47
44	C	501	HEM	CBB-CAB	4.89	1.54	1.30
47	D	501	HEC	C3C-C2C	-4.86	1.35	1.40
44	C	502	HEM	CBB-CAB	4.74	1.53	1.30
47	d	501	HEC	C4B-C3B	4.56	1.51	1.43
40	1	441	NAI	C7N-N7N	4.47	1.45	1.33
39	1	440	FMN	C4A-N5	4.19	1.38	1.30
40	1	441	NAI	PA-O1A	4.16	1.65	1.50
44	c	501	HEM	CAB-C3B	-4.10	1.36	1.47
40	1	441	NAI	PN-O2N	4.05	1.65	1.50
40	1	441	NAI	C7N-C3N	3.94	1.57	1.48
49	L	516	HEA	C3A-CMA	-3.89	1.37	1.46
44	Y	500	HEM	C3B-C2B	3.83	1.45	1.37
44	C	501	HEM	CBC-CAC	3.73	1.54	1.29
40	1	441	NAI	C6A-N6A	3.68	1.47	1.34
44	c	502	HEM	CAB-C3B	-3.66	1.37	1.47
44	C	502	HEM	CBC-CAC	3.64	1.53	1.29
45	c	3001	SMA	C6-C5	3.64	1.45	1.38
40	1	441	NAI	C4N-C5N	3.60	1.58	1.48
40	1	441	NAI	C5A-N7A	3.56	1.52	1.39
44	Y	500	HEM	C1B-NB	-3.52	1.34	1.40
44	c	502	HEM	CBC-CAC	3.50	1.52	1.29
47	d	501	HEC	C2B-C3B	-3.47	1.37	1.40
44	C	501	HEM	CAB-C3B	-3.42	1.38	1.47
44	c	501	HEM	CBC-CAC	3.42	1.52	1.29
40	1	441	NAI	O4B-C1B	-3.40	1.36	1.41
44	C	501	HEM	C4D-C3D	3.34	1.50	1.45
49	L	515	HEA	C3C-C2C	-3.29	1.35	1.40
45	C	2001	SMA	C4A-C5	3.28	1.46	1.40
47	D	501	HEC	C3C-C4C	3.27	1.49	1.43
45	c	3001	SMA	O1-C2	3.27	1.40	1.36
40	1	441	NAI	C2D-C3D	-3.25	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	O4D-C4D	-3.23	1.37	1.45
44	c	502	HEM	C1A-NA	3.21	1.42	1.36
46	C	2002	UQ1	O3-C3	3.20	1.44	1.36
44	Y	500	HEM	C3B-C4B	-3.17	1.38	1.44
40	1	441	NAI	C6A-C5A	3.15	1.55	1.43
45	c	3001	SMA	C6-C7	3.13	1.44	1.38
44	C	501	HEM	C2C-C1C	3.06	1.49	1.42
40	1	441	NAI	C6A-N1A	-3.06	1.23	1.37
46	C	2002	UQ1	C3-C4	3.03	1.57	1.48
40	1	441	NAI	O4B-C4B	-3.02	1.38	1.45
46	C	2002	UQ1	C2-C1	3.01	1.57	1.48
45	C	2001	SMA	C6-C7	3.01	1.44	1.38
49	L	515	HEA	C3A-CMA	-2.99	1.39	1.46
46	C	2002	UQ1	C7-C6	2.98	1.57	1.50
46	c	3002	UQ1	C7-C6	2.98	1.57	1.50
45	C	2001	SMA	C7-C8	2.95	1.44	1.40
46	C	2002	UQ1	O2-C2	2.91	1.44	1.36
45	c	3001	SMA	C4A-C5	2.90	1.45	1.40
45	C	2001	SMA	C6-C5	2.89	1.44	1.38
47	d	501	HEC	C3C-C4C	2.89	1.48	1.43
46	C	2002	UQ1	CM5-C5	2.86	1.56	1.50
39	1	440	FMN	C9A-N10	-2.82	1.36	1.41
46	c	3002	UQ1	CM5-C5	2.80	1.56	1.50
44	Y	500	HEM	C4A-CHB	-2.76	1.33	1.41
47	D	501	HEC	C2A-C1A	2.74	1.48	1.42
49	L	515	HEA	C4C-NC	2.72	1.41	1.36
44	c	501	HEM	C4A-NA	2.68	1.41	1.36
45	c	3001	SMA	C20-C19	2.68	1.35	1.33
45	c	3001	SMA	C7-C8	2.67	1.43	1.40
44	c	501	HEM	C4D-C3D	2.66	1.49	1.45
49	L	516	HEA	C1D-C2D	2.65	1.49	1.44
49	L	516	HEA	C1D-ND	-2.65	1.35	1.40
40	1	441	NAI	C1D-N1N	-2.64	1.38	1.46
48	G	2004	CDL	O1-C1	2.61	1.51	1.43
46	c	3002	UQ1	C2-C1	2.60	1.56	1.48
49	L	516	HEA	C3C-C2C	-2.59	1.36	1.40
40	1	441	NAI	O3B-C3B	-2.57	1.36	1.43
46	c	3002	UQ1	O2-C2	2.55	1.43	1.36
44	c	502	HEM	C1B-C2B	2.53	1.49	1.44
46	c	3002	UQ1	O3-C3	2.53	1.43	1.36
44	C	502	HEM	C2C-C1C	2.53	1.48	1.42
40	1	441	NAI	O4D-C1D	-2.52	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	502	HEM	C3B-C4B	2.48	1.49	1.44
45	c	3001	SMA	C3-C2	2.48	1.39	1.34
46	c	3002	UQ1	C6-C1	2.48	1.56	1.47
47	D	501	HEC	C4B-C3B	2.47	1.47	1.43
40	1	441	NAI	PN-O1N	-2.47	1.43	1.55
48	g	3004	CDL	O1-C1	2.47	1.50	1.43
47	d	501	HEC	C4D-ND	2.45	1.41	1.36
48	g	3004	CDL	OA8-CA6	-2.44	1.39	1.45
44	C	502	HEM	C1D-C2D	2.43	1.49	1.44
40	1	441	NAI	PN-O5D	2.42	1.69	1.59
46	C	2002	UQ1	C6-C1	2.40	1.55	1.47
46	c	3002	UQ1	C3-C4	2.37	1.55	1.48
46	c	3002	UQ1	C5-C4	2.36	1.55	1.47
40	1	441	NAI	C4A-N3A	2.35	1.38	1.35
44	Y	500	HEM	CHB-C1B	2.35	1.41	1.35
49	L	516	HEA	CMD-C2D	2.34	1.55	1.50
48	g	3004	CDL	OB8-CB6	-2.33	1.39	1.45
45	C	2001	SMA	C3-C2	2.32	1.39	1.34
46	C	2002	UQ1	C5-C4	2.32	1.55	1.47
48	g	3004	CDL	CA3-CA4	2.31	1.57	1.50
44	C	502	HEM	C4D-C3D	2.30	1.49	1.45
44	Y	500	HEM	C1D-C2D	2.30	1.49	1.44
45	C	2001	SMA	C20-C19	2.29	1.35	1.33
44	c	502	HEM	C1D-C2D	2.28	1.49	1.44
48	d	3003	CDL	O1-C1	2.27	1.50	1.43
48	G	2003	CDL	O1-C1	2.25	1.50	1.43
40	1	441	NAI	O2B-C2B	-2.25	1.37	1.43
40	1	441	NAI	C2A-N3A	2.23	1.35	1.32
49	L	515	HEA	C3A-C2A	-2.21	1.37	1.40
40	1	441	NAI	PA-O2A	-2.20	1.45	1.55
44	Y	500	HEM	C1A-NA	2.19	1.40	1.36
47	D	501	HEC	C4D-ND	2.19	1.40	1.36
44	c	502	HEM	CMC-C2C	2.17	1.56	1.51
45	C	2001	SMA	O1-C2	2.15	1.39	1.36
49	L	515	HEA	C1C-NC	2.15	1.40	1.36
44	c	501	HEM	C2C-C1C	2.14	1.47	1.42
45	c	3001	SMA	C4A-C4	2.14	1.52	1.46
44	C	501	HEM	CHD-C1D	-2.14	1.34	1.41
40	1	441	NAI	C4N-C3N	2.13	1.54	1.49
49	L	515	HEA	CHD-C1D	2.11	1.40	1.35
45	c	3001	SMA	C8-C8A	2.10	1.42	1.39
48	G	2003	CDL	CA3-CA4	2.07	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	G	2004	CDL	OA8-CA6	-2.06	1.40	1.45
44	c	502	HEM	CHB-C1B	2.05	1.40	1.35
48	d	3003	CDL	CB3-CB4	2.05	1.57	1.50
48	d	3003	CDL	OA8-CA6	-2.05	1.40	1.45
48	d	3003	CDL	OB8-CB6	-2.05	1.40	1.45
44	Y	500	HEM	C4D-C3D	2.02	1.48	1.45
44	Y	500	HEM	C2C-C1C	2.01	1.47	1.42
48	d	3003	CDL	OB2-CB2	-2.01	1.37	1.44
44	c	502	HEM	CHA-C4D	2.00	1.40	1.35
48	G	2003	CDL	OB8-CB6	-2.00	1.40	1.45

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C	501	HEM	C4A-C3A-C2A	-5.90	102.89	107.00
44	c	502	HEM	C4C-CHD-C1D	5.58	129.93	122.56
44	Y	500	HEM	C2C-C3C-C4C	-5.48	103.07	106.90
39	1	440	FMN	C5'-C4'-C3'	-5.12	102.31	112.20
39	1	440	FMN	O2'-C2'-C3'	5.10	121.51	109.10
44	C	501	HEM	C4C-CHD-C1D	4.92	129.05	122.56
40	1	441	NAI	N3A-C2A-N1A	-4.79	121.19	128.68
45	c	3001	SMA	C9-C10-C11	-4.72	105.90	114.52
44	C	502	HEM	C4B-C3B-C2B	-4.69	103.39	107.11
44	c	502	HEM	CMA-C3A-C4A	-4.55	121.47	128.46
48	G	2004	CDL	CB4-OB6-CB5	-4.32	109.85	117.90
44	C	501	HEM	C2D-C1D-ND	4.29	115.02	109.88
45	C	2001	SMA	C9-C10-C11	-4.26	106.74	114.52
44	Y	500	HEM	C3B-C2B-C1B	-4.25	103.33	106.49
49	L	515	HEA	C17-C18-C19	-3.98	118.07	127.66
44	c	501	HEM	C4C-CHD-C1D	3.93	127.74	122.56
44	C	502	HEM	CHD-C1D-ND	-3.90	120.19	124.43
40	1	441	NAI	C4D-O4D-C1D	-3.85	100.98	109.47
48	d	3003	CDL	CB4-OB6-CB5	-3.83	110.77	117.90
48	g	3004	CDL	CA4-OA6-CA5	-3.79	110.84	117.90
44	C	502	HEM	C4C-CHD-C1D	3.70	127.44	122.56
44	C	502	HEM	CHC-C4B-NB	-3.66	120.45	124.43
44	c	502	HEM	CMC-C2C-C3C	3.65	131.51	124.68
49	L	516	HEA	C4A-CHB-C1B	3.62	127.34	122.56
44	c	501	HEM	C4A-C3A-C2A	-3.62	104.48	107.00
44	C	501	HEM	CHD-C1D-ND	-3.61	120.51	124.43
48	G	2003	CDL	CA4-OA6-CA5	-3.56	111.26	117.90
39	1	440	FMN	C1'-C2'-C3'	-3.45	100.13	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	c	501	HEM	C4B-CHC-C1C	3.38	127.01	122.56
47	D	501	HEC	CMD-C2D-C1D	-3.36	123.29	128.46
44	C	502	HEM	C1B-NB-C4B	-3.36	101.60	105.07
44	C	501	HEM	C4B-CHC-C1C	3.26	126.86	122.56
44	C	501	HEM	CBA-CAA-C2A	-3.25	107.07	112.62
49	L	515	HEA	C13-C14-C15	-3.19	119.98	127.66
39	1	440	FMN	C4'-C3'-C2'	3.17	119.96	113.36
44	C	501	HEM	C4D-ND-C1D	-3.17	101.80	105.07
44	Y	500	HEM	CMA-C3A-C4A	-3.15	123.62	128.46
44	C	502	HEM	C4B-CHC-C1C	3.14	126.70	122.56
39	1	440	FMN	O4-C4-C4A	-3.14	118.28	126.60
44	Y	500	HEM	CAD-CBD-CGD	3.13	120.33	113.60
44	C	502	HEM	CMC-C2C-C3C	3.12	130.52	124.68
44	Y	500	HEM	C2B-C1B-NB	3.12	113.54	109.84
44	Y	500	HEM	C4A-C3A-C2A	3.10	109.16	107.00
44	Y	500	HEM	CBD-CAD-C3D	-3.07	104.11	112.63
40	1	441	NAI	O4D-C1D-N1N	3.05	114.02	108.06
44	C	502	HEM	CBD-CAD-C3D	-3.01	104.26	112.63
48	g	3004	CDL	CB4-OB6-CB5	-3.00	110.42	117.79
44	c	501	HEM	CMC-C2C-C3C	2.99	130.26	124.68
44	c	502	HEM	CMA-C3A-C2A	2.96	130.53	124.94
39	1	440	FMN	C4-N3-C2	-2.92	120.24	125.64
44	C	501	HEM	C4B-C3B-C2B	-2.91	104.81	107.11
48	d	3003	CDL	CA6-CA4-CA3	-2.91	104.92	111.79
49	L	516	HEA	CBA-CAA-C2A	2.88	117.45	112.60
44	C	501	HEM	C1D-C2D-C3D	-2.85	103.96	106.96
40	1	441	NAI	O5B-C5B-C4B	2.85	118.80	108.99
40	1	441	NAI	C3N-C7N-N7N	2.83	122.70	117.67
45	c	3001	SMA	C4A-C4-C3	-2.83	114.62	118.79
49	L	515	HEA	C1B-C2B-C3B	2.80	110.16	106.80
44	C	502	HEM	CMA-C3A-C2A	2.74	130.11	124.94
48	G	2004	CDL	CA6-CA4-CA3	-2.72	105.34	111.79
48	G	2003	CDL	CB4-OB6-CB5	-2.70	111.14	117.79
44	C	502	HEM	CMA-C3A-C4A	-2.68	124.35	128.46
45	C	2001	SMA	C4A-C4-C3	-2.65	114.89	118.79
44	C	502	HEM	C4D-ND-C1D	-2.65	102.34	105.07
44	c	502	HEM	C4B-CHC-C1C	2.64	126.05	122.56
47	D	501	HEC	CMA-C3A-C2A	2.60	129.85	124.94
48	d	3003	CDL	CA4-OA6-CA5	-2.58	111.43	117.79
44	C	502	HEM	CHB-C1B-NB	-2.58	121.20	124.38
44	C	502	HEM	C2D-C1D-ND	2.57	112.97	109.88
44	c	502	HEM	CMD-C2D-C1D	2.57	128.96	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	L	516	HEA	CMD-C2D-C1D	2.56	128.94	125.04
49	L	516	HEA	C4D-CHA-C1A	2.54	125.92	122.56
44	Y	500	HEM	C4C-CHD-C1D	2.49	125.84	122.56
49	L	516	HEA	CMC-C2C-C3C	2.46	129.28	124.68
39	1	440	FMN	O2-C2-N1	-2.45	117.77	121.83
39	1	440	FMN	C10-C4A-N5	-2.44	119.68	124.86
47	d	501	HEC	CMC-C2C-C1C	-2.42	124.74	128.46
49	L	515	HEA	C17-C16-C15	-2.41	105.06	112.98
49	L	516	HEA	C1D-C2D-C3D	-2.40	104.44	106.96
44	C	502	HEM	C2B-C1B-NB	2.39	112.68	109.84
44	c	501	HEM	CMA-C3A-C2A	2.38	129.43	124.94
48	G	2003	CDL	CB6-CB4-CB3	-2.37	106.19	111.79
49	L	515	HEA	C20-C19-C18	2.36	125.89	121.12
49	L	515	HEA	C16-C17-C18	-2.34	104.19	111.88
47	D	501	HEC	C2B-C3B-C4B	2.33	108.87	106.35
49	L	515	HEA	CAD-C3D-C4D	2.33	128.73	124.66
49	L	516	HEA	C25-C23-C24	2.32	119.73	114.60
47	D	501	HEC	CMD-C2D-C3D	2.30	129.27	124.94
39	1	440	FMN	C4A-C4-N3	2.30	119.02	113.19
49	L	516	HEA	CMB-C2B-C3B	-2.29	125.98	130.34
49	L	516	HEA	C13-C14-C15	-2.28	122.17	127.66
44	C	501	HEM	CHA-C4D-ND	-2.27	121.57	124.38
45	c	3001	SMA	O1-C2-C9	-2.26	105.80	110.58
39	1	440	FMN	C1'-N10-C9A	-2.25	116.77	120.51
44	c	501	HEM	CMD-C2D-C1D	2.24	128.45	125.04
44	c	501	HEM	CAD-C3D-C4D	2.22	128.53	124.66
48	d	3003	CDL	CB6-OB8-CB7	-2.20	111.57	117.10
48	G	2004	CDL	CA4-OA6-CA5	-2.20	112.38	117.79
49	L	516	HEA	C26-C15-C16	2.20	118.97	115.27
44	C	502	HEM	CHA-C4D-ND	-2.19	121.68	124.38
47	d	501	HEC	C1D-C2D-C3D	2.17	108.51	107.00
49	L	515	HEA	C12-C13-C14	-2.16	106.54	112.23
44	C	501	HEM	C3B-C2B-C1B	2.14	108.08	106.49
49	L	515	HEA	C4B-C3B-C2B	-2.13	103.78	107.41
49	L	515	HEA	C4A-CHB-C1B	2.12	125.36	122.56
39	1	440	FMN	C4A-C10-N10	2.12	119.58	116.48
47	d	501	HEC	CBA-CAA-C2A	-2.10	109.06	112.60
44	C	502	HEM	C4A-C3A-C2A	-2.10	105.53	107.00
44	Y	500	HEM	C1D-C2D-C3D	-2.10	104.75	106.96
39	1	440	FMN	O5'-C5'-C4'	2.10	114.96	109.36
48	G	2003	CDL	CA6-OA8-CA7	-2.09	111.85	117.10
44	c	502	HEM	CAD-C3D-C4D	2.09	128.31	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	2004	CDL	CB6-CB4-CB3	-2.09	106.85	111.79
45	c	3001	SMA	C9-C2-C3	2.07	130.11	127.07
49	L	515	HEA	C27-C19-C18	-2.06	118.39	123.68
45	C	2001	SMA	C9-C2-C3	2.05	130.08	127.07
45	C	2001	SMA	O1-C2-C9	-2.05	106.23	110.58
49	L	516	HEA	CBD-CAD-C3D	2.05	118.32	112.63
44	Y	500	HEM	O2A-CGA-CBA	2.04	120.57	114.03
44	Y	500	HEM	C4B-CHC-C1C	2.03	125.24	122.56
40	1	441	NAI	O7N-C7N-N7N	-2.03	118.13	122.88
44	C	501	HEM	CHC-C4B-NB	-2.02	122.24	124.43

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
49	L	515	HEA	NA
49	L	515	HEA	ND
49	L	515	HEA	NB
49	L	516	HEA	NA
49	L	516	HEA	ND
49	L	516	HEA	NB

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	1	440	FMN	N10-C1'-C2'-O2'
39	1	440	FMN	N10-C1'-C2'-C3'
39	1	440	FMN	C1'-C2'-C3'-O3'
39	1	440	FMN	C1'-C2'-C3'-C4'
40	1	441	NAI	O4B-C4B-C5B-O5B
40	1	441	NAI	C3B-C4B-C5B-O5B
40	1	441	NAI	C5D-O5D-PN-O3
45	C	2001	SMA	C3-C2-C9-C10
45	C	2001	SMA	O1-C2-C9-C10
45	c	3001	SMA	C3-C2-C9-C10
45	c	3001	SMA	O1-C2-C9-C10
48	G	2003	CDL	OA7-CA5-OA6-CA4
48	G	2003	CDL	C11-CA5-OA6-CA4
48	G	2003	CDL	CB2-OB2-PB2-OB3
48	G	2003	CDL	OB5-CB3-CB4-OB6
48	G	2004	CDL	CA2-C1-CB2-OB2
48	G	2004	CDL	CA2-OA2-PA1-OA3
48	G	2004	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
48	G	2004	CDL	CA3-OA5-PA1-OA3
48	G	2004	CDL	CA3-OA5-PA1-OA4
48	G	2004	CDL	OA7-CA5-OA6-CA4
48	G	2004	CDL	CB3-OB5-PB2-OB3
48	G	2004	CDL	CB3-OB5-PB2-OB4
48	G	2004	CDL	C51-CB5-OB6-CB4
48	d	3003	CDL	CA2-OA2-PA1-OA3
48	d	3003	CDL	CA2-OA2-PA1-OA4
48	d	3003	CDL	CA2-OA2-PA1-OA5
48	d	3003	CDL	CA3-OA5-PA1-OA2
48	d	3003	CDL	CA3-OA5-PA1-OA3
48	d	3003	CDL	CA3-OA5-PA1-OA4
48	d	3003	CDL	OA6-CA4-CA6-OA8
48	d	3003	CDL	CB2-OB2-PB2-OB3
48	d	3003	CDL	CB2-OB2-PB2-OB4
48	d	3003	CDL	CB2-OB2-PB2-OB5
48	d	3003	CDL	CB3-OB5-PB2-OB3
48	g	3004	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	CA2-OA2-PA1-OA3
48	g	3004	CDL	CA2-OA2-PA1-OA4
49	L	515	HEA	C12-C11-C3B-C2B
48	d	3003	CDL	C51-CB5-OB6-CB4
48	g	3004	CDL	C11-CA5-OA6-CA4
48	G	2003	CDL	C31-CA7-OA8-CA6
48	d	3003	CDL	C71-CB7-OB8-CB6
48	d	3003	CDL	OB7-CB5-OB6-CB4
48	g	3004	CDL	OA7-CA5-OA6-CA4
48	G	2004	CDL	OB7-CB5-OB6-CB4
48	g	3004	CDL	C71-CB7-OB8-CB6
48	G	2004	CDL	C11-CA5-OA6-CA4
48	G	2003	CDL	OA9-CA7-OA8-CA6
48	G	2003	CDL	C71-CB7-OB8-CB6
48	d	3003	CDL	OB9-CB7-OB8-CB6
48	g	3004	CDL	OB9-CB7-OB8-CB6
48	G	2004	CDL	O1-C1-CB2-OB2
48	g	3004	CDL	O1-C1-CA2-OA2
48	G	2003	CDL	OB9-CB7-OB8-CB6
39	1	440	FMN	O2'-C2'-C3'-C4'
49	L	515	HEA	C15-C16-C17-C18
48	d	3003	CDL	CA2-C1-CB2-OB2
48	d	3003	CDL	O1-C1-CB2-OB2
48	g	3004	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
39	1	440	FMN	O2'-C2'-C3'-O3'
48	d	3003	CDL	CA7-C31-C32-C33
48	d	3003	CDL	CA5-C11-C12-C13
48	G	2003	CDL	O1-C1-CA2-OA2
48	G	2003	CDL	CB2-OB2-PB2-OB5
48	G	2004	CDL	CA2-OA2-PA1-OA5
48	G	2004	CDL	CA3-OA5-PA1-OA2
48	G	2004	CDL	CB2-OB2-PB2-OB5
48	G	2004	CDL	CB3-OB5-PB2-OB2
48	g	3004	CDL	CA2-OA2-PA1-OA5
48	G	2003	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	OB7-CB5-OB6-CB4
48	g	3004	CDL	C71-C72-C73-C74
48	g	3004	CDL	CB7-C71-C72-C73
48	d	3003	CDL	C37-C38-C39-C40
48	G	2003	CDL	C51-CB5-OB6-CB4
48	G	2004	CDL	C33-C34-C35-C36
48	d	3003	CDL	C31-C32-C33-C34
48	d	3003	CDL	C38-C39-C40-C41
48	G	2004	CDL	O1-C1-CA2-OA2
48	d	3003	CDL	C36-C37-C38-C39
48	G	2003	CDL	OB7-CB5-OB6-CB4
48	d	3003	CDL	C33-C34-C35-C36
48	g	3004	CDL	C53-C54-C55-C56
44	Y	500	HEM	C2B-C3B-CAB-CBB
48	G	2004	CDL	C31-C32-C33-C34
48	d	3003	CDL	CB3-OB5-PB2-OB2
48	G	2004	CDL	OA5-CA3-CA4-CA6
48	G	2004	CDL	C31-CA7-OA8-CA6
48	G	2003	CDL	CB3-CB4-CB6-OB8
48	d	3003	CDL	CA3-CA4-CA6-OA8
48	g	3004	CDL	CB3-CB4-CB6-OB8
48	G	2003	CDL	C73-C74-C75-C76
48	d	3003	CDL	C32-C33-C34-C35
48	G	2004	CDL	OA6-CA4-CA6-OA8
48	G	2004	CDL	OA9-CA7-OA8-CA6
48	g	3004	CDL	C54-C55-C56-C57
48	d	3003	CDL	C39-C40-C41-C42
48	G	2003	CDL	OB5-CB3-CB4-CB6
48	d	3003	CDL	OA5-CA3-CA4-CA6
48	d	3003	CDL	C35-C36-C37-C38
48	G	2004	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
48	g	3004	CDL	OA5-CA3-CA4-OA6
48	G	2004	CDL	CB2-C1-CA2-OA2
48	g	3004	CDL	OA5-CA3-CA4-CA6
48	G	2004	CDL	C71-CB7-OB8-CB6
48	G	2004	CDL	CB3-CB4-CB6-OB8
48	G	2004	CDL	OA5-CA3-CA4-OA6
48	d	3003	CDL	OA5-CA3-CA4-OA6
44	Y	500	HEM	C4B-C3B-CAB-CBB
48	G	2003	CDL	OB6-CB4-CB6-OB8
48	G	2003	CDL	C72-C73-C74-C75
48	d	3003	CDL	C34-C35-C36-C37
40	1	441	NAI	C5D-O5D-PN-O1N
48	G	2003	CDL	CB2-OB2-PB2-OB4
48	G	2004	CDL	CB2-OB2-PB2-OB3
48	G	2003	CDL	C71-C72-C73-C74
48	G	2003	CDL	CB7-C71-C72-C73
48	g	3004	CDL	OB6-CB4-CB6-OB8
48	G	2004	CDL	OB5-CB3-CB4-CB6
40	1	441	NAI	O4D-C1D-N1N-C2N
44	C	501	HEM	CAD-CBD-CGD-O1D
44	c	502	HEM	CAA-CBA-CGA-O1A
44	c	501	HEM	CAD-CBD-CGD-O1D
44	C	502	HEM	CAA-CBA-CGA-O2A
44	c	502	HEM	CAA-CBA-CGA-O2A
48	g	3004	CDL	C52-C53-C54-C55
44	C	502	HEM	CAA-CBA-CGA-O1A
49	L	516	HEA	CAD-CBD-CGD-O2D
48	d	3003	CDL	C11-C12-C13-C14
44	c	501	HEM	CAD-CBD-CGD-O2D
49	L	516	HEA	CAD-CBD-CGD-O1D
48	G	2003	CDL	OA5-CA3-CA4-OA6
44	C	501	HEM	CAA-CBA-CGA-O1A
44	C	501	HEM	CAD-CBD-CGD-O2D
46	c	3002	UQ1	C4-C3-O3-CM3
48	G	2003	CDL	C78-C79-C80-C81
48	G	2004	CDL	OB9-CB7-OB8-CB6
44	C	501	HEM	CAA-CBA-CGA-O2A
44	Y	500	HEM	CAA-CBA-CGA-O2A
48	G	2003	CDL	C76-C77-C78-C79
48	G	2004	CDL	C12-C11-CA5-OA6
44	Y	500	HEM	CAA-CBA-CGA-O1A
47	D	501	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
49	L	515	HEA	CAD-CBD-CGD-O2D
44	c	502	HEM	CAD-CBD-CGD-O2D
47	D	501	HEC	CAA-CBA-CGA-O2A
48	d	3003	CDL	C32-C31-CA7-OA8
44	c	501	HEM	CAA-CBA-CGA-O2A
47	d	501	HEC	CAD-CBD-CGD-O1D
44	c	501	HEM	CAA-CBA-CGA-O1A
44	c	502	HEM	CAD-CBD-CGD-O1D
49	L	516	HEA	CAA-CBA-CGA-O2A
47	d	501	HEC	CAA-CBA-CGA-O2A
48	G	2003	CDL	OA5-CA3-CA4-CA6
47	D	501	HEC	CAA-CBA-CGA-O1A
49	L	515	HEA	CAD-CBD-CGD-O1D
48	G	2003	CDL	C51-C52-C53-C54
47	d	501	HEC	CAD-CBD-CGD-O2D
49	L	516	HEA	CAA-CBA-CGA-O1A
48	G	2004	CDL	C32-C31-CA7-OA8
46	c	3002	UQ1	C2-C3-O3-CM3
44	C	502	HEM	CAD-CBD-CGD-O2D
47	D	501	HEC	CAD-CBD-CGD-O2D
40	1	441	NAI	C5B-O5B-PA-O1A
40	1	441	NAI	C2N-C3N-C7N-N7N
48	g	3004	CDL	CB2-OB2-PB2-OB3
48	d	3003	CDL	C12-C11-CA5-OA6
47	d	501	HEC	CAA-CBA-CGA-O1A
48	G	2004	CDL	C32-C31-CA7-OA9
48	d	3003	CDL	C32-C31-CA7-OA9
49	L	515	HEA	CAA-CBA-CGA-O2A
44	C	502	HEM	CAD-CBD-CGD-O1D
48	d	3003	CDL	OA9-CA7-OA8-CA6
49	L	516	HEA	C26-C15-C16-C17
49	L	515	HEA	O11-C11-C3B-C2B

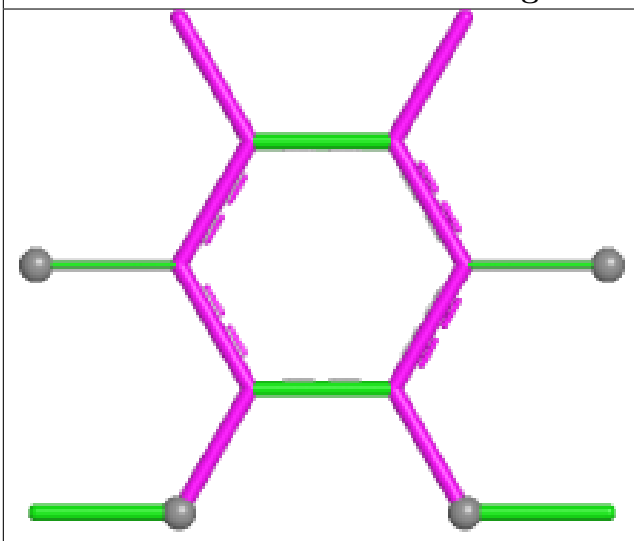
There are no ring outliers.

No monomer is involved in short contacts.

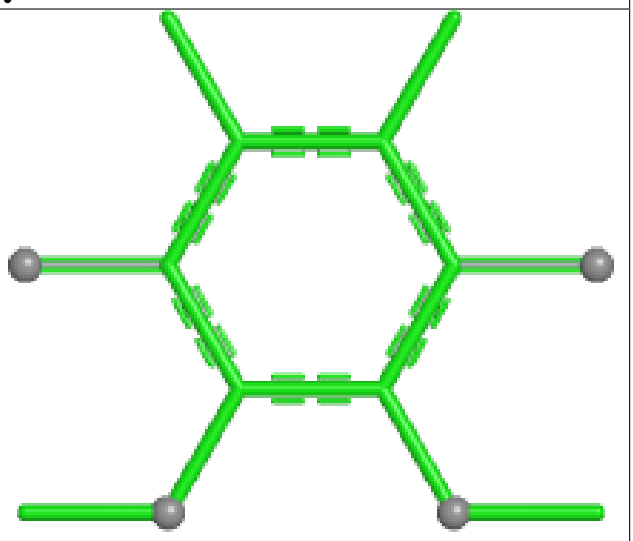
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

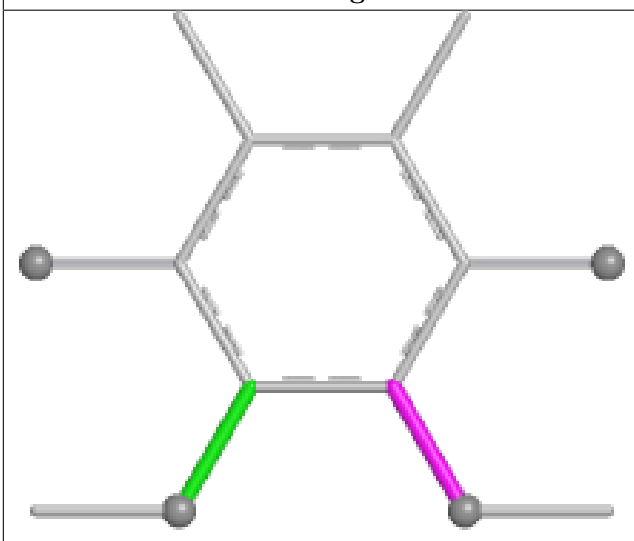
Ligand UQ1 c 3002



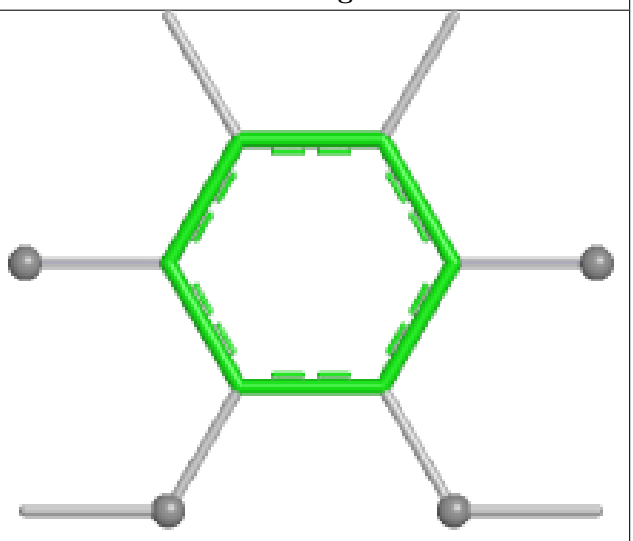
Bond lengths



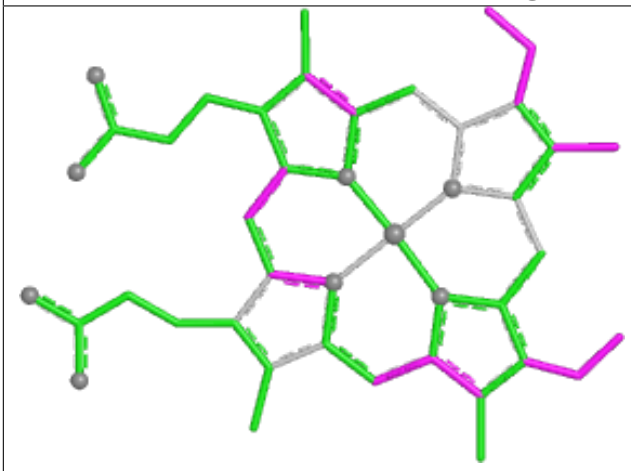
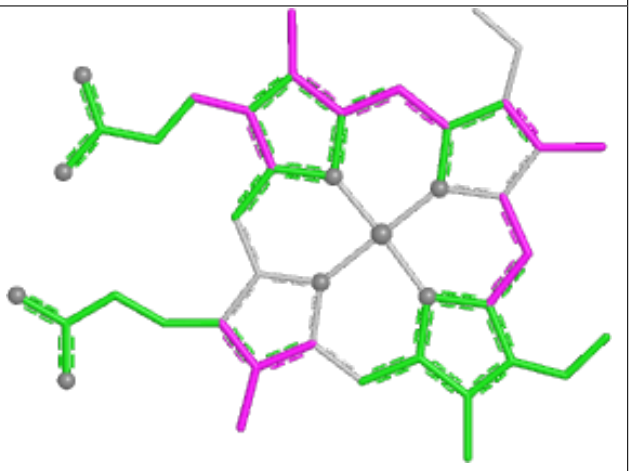
Bond angles



Torsions



Rings

Ligand HEM c 502	
	
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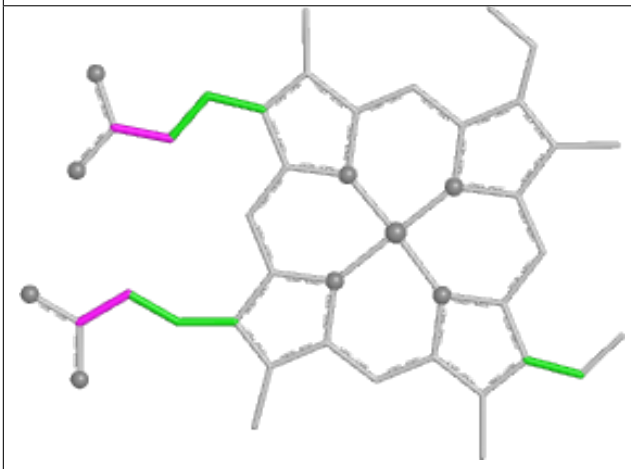
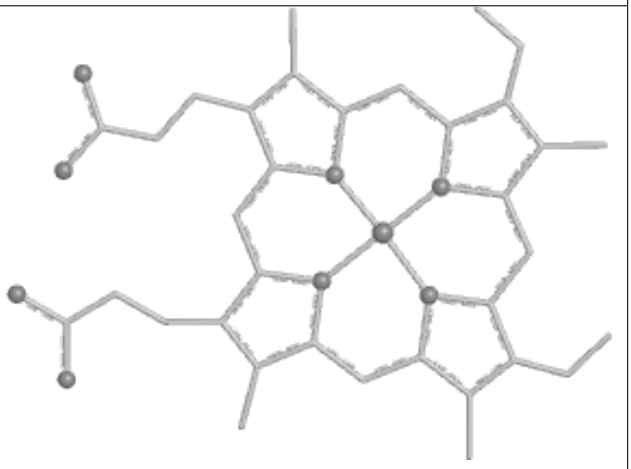
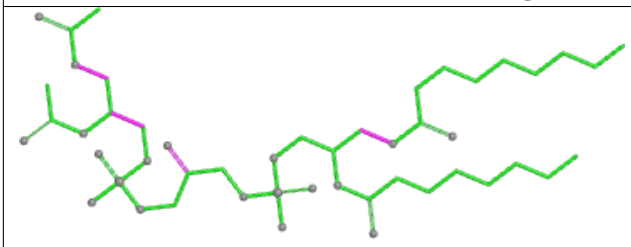
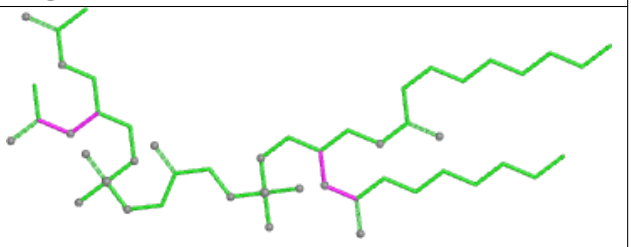
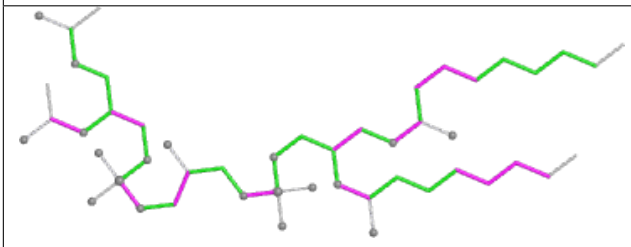
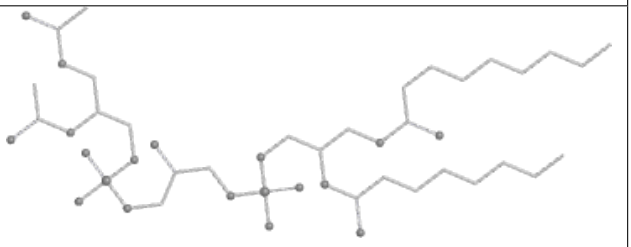
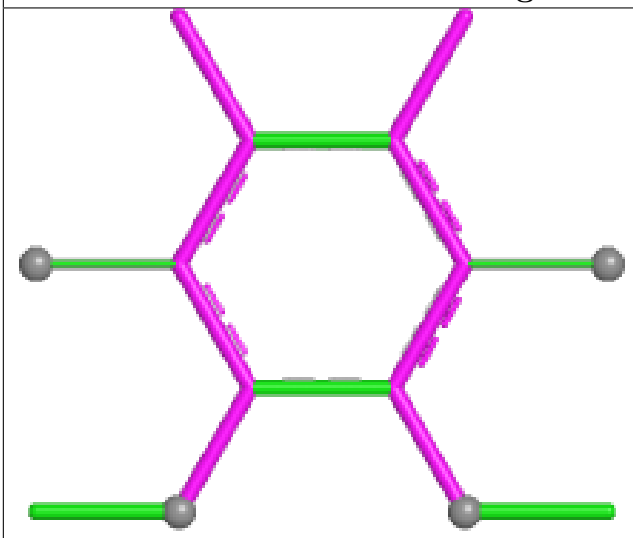
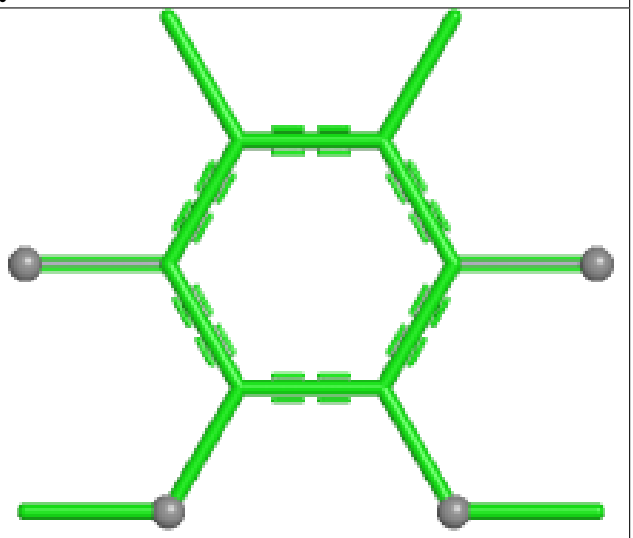
	
Torsions	Rings

Ligand CDL g 3004	
	
Bond lengths	Bond angles
	
Torsions	Rings

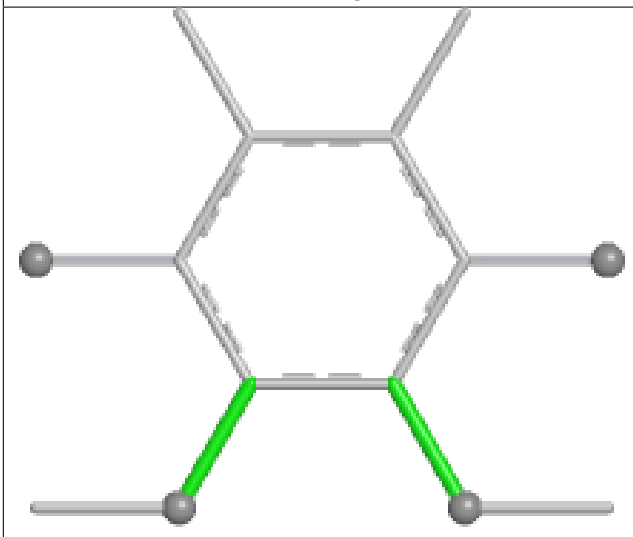
Ligand UQ1 C 2002



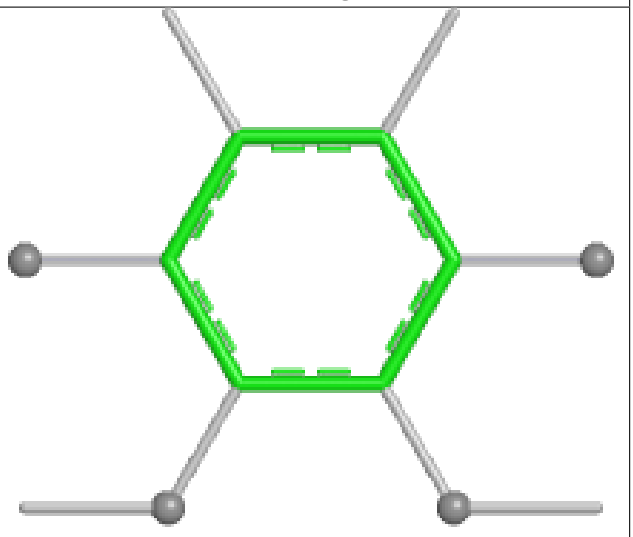
Bond lengths



Bond angles

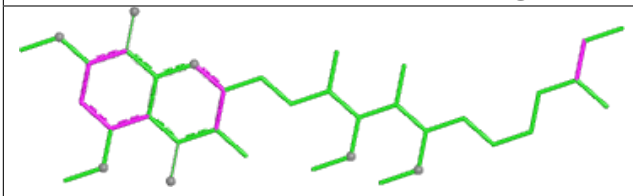


Torsions

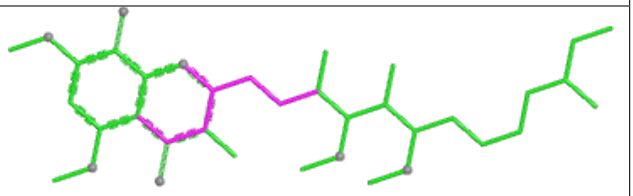


Rings

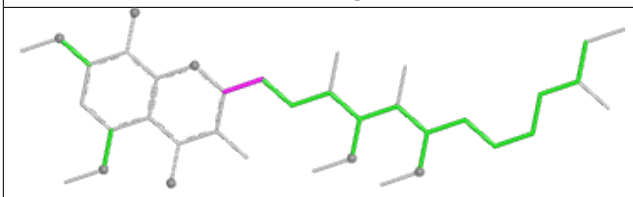
Ligand SMA C 2001



Bond lengths



Bond angles



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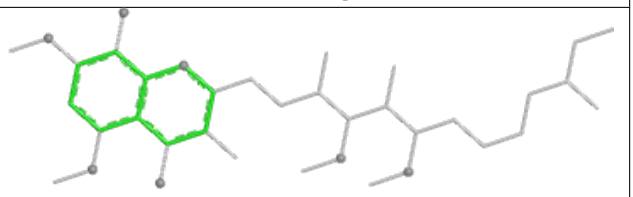
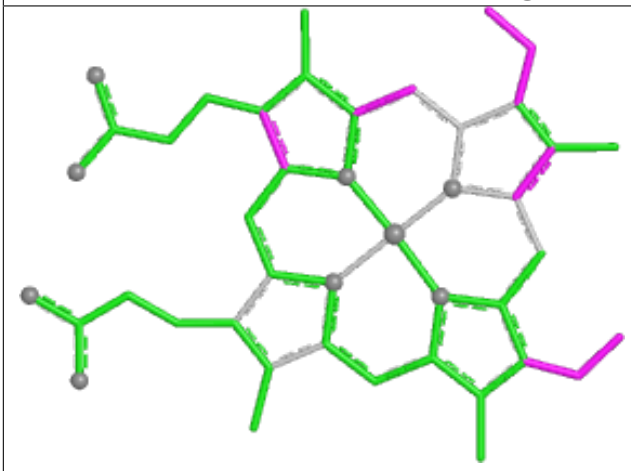
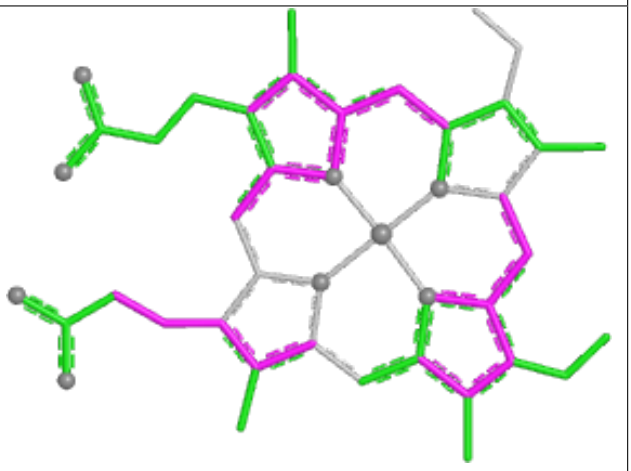
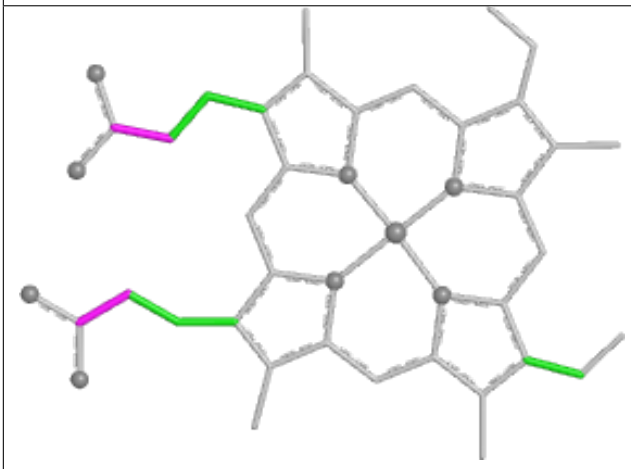
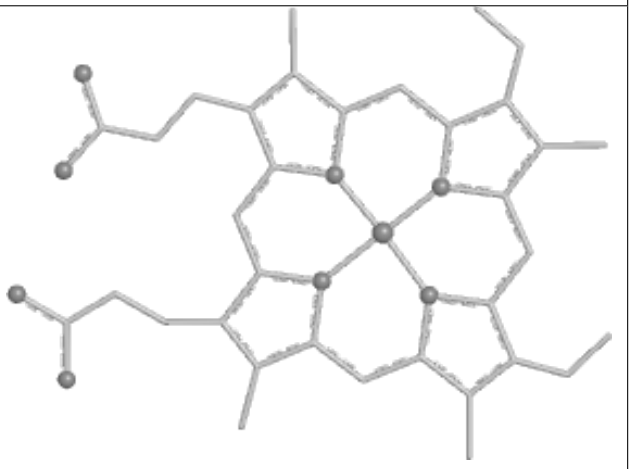
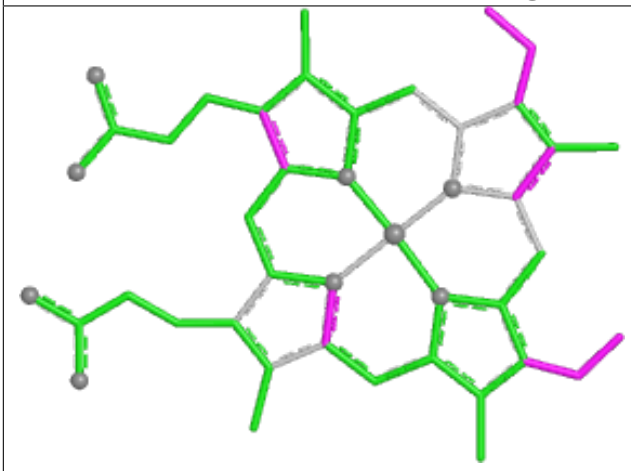
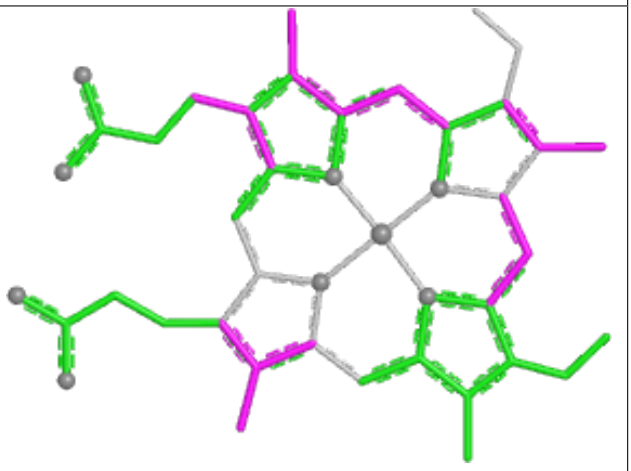
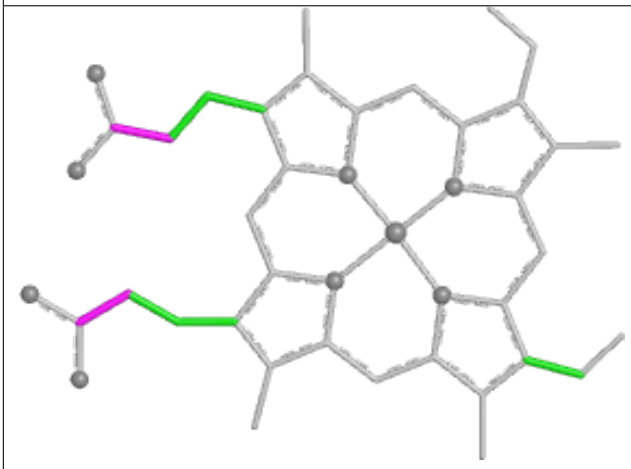
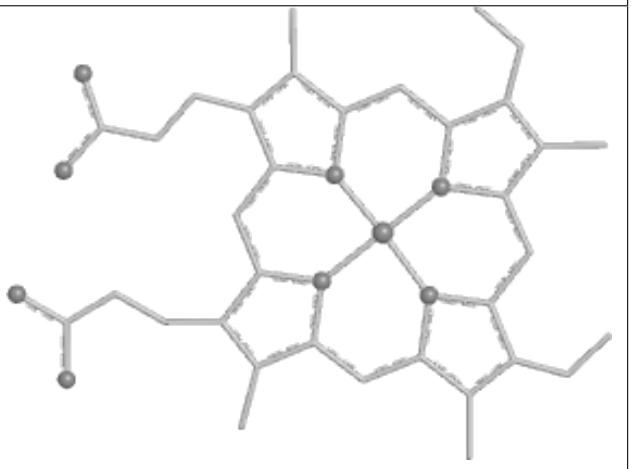
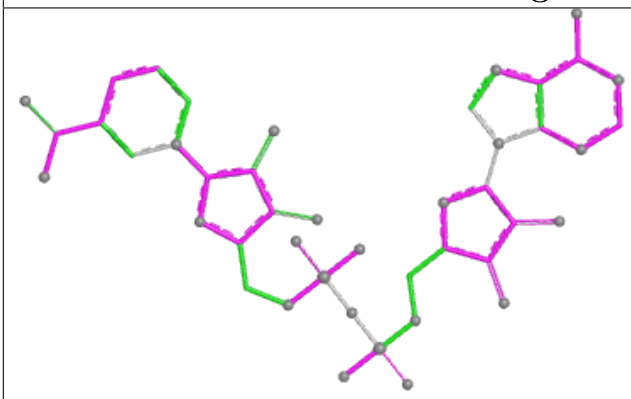


Rings

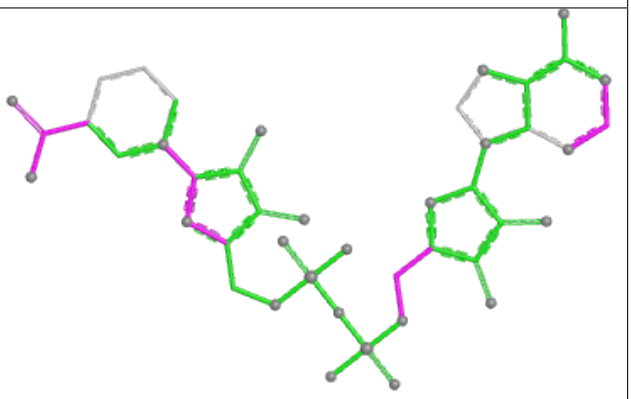
Ligand HEM C 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HEM c 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

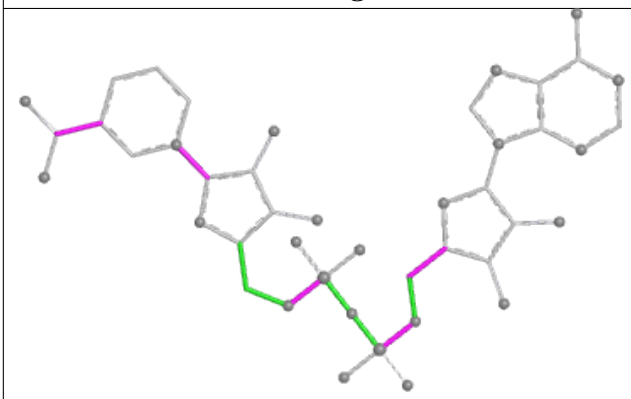
Ligand NAI 1 441



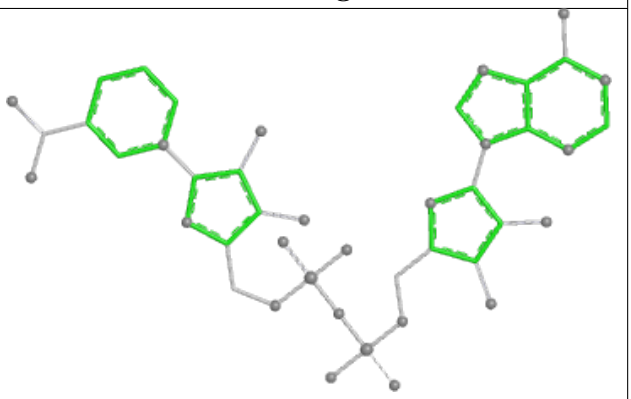
Bond lengths



Bond angles

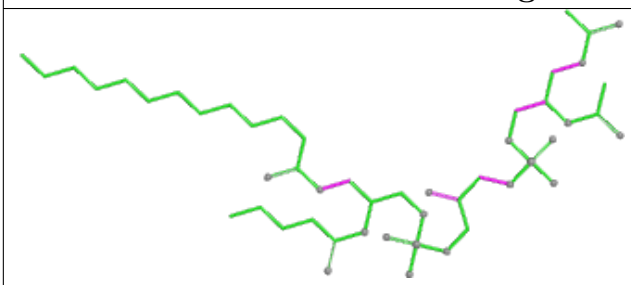


Torsions

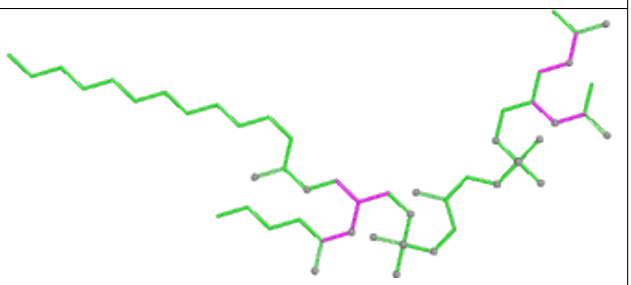


Rings

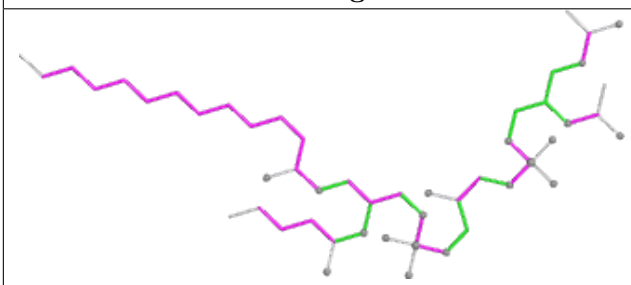
Ligand CDL d 3003



Bond lengths



Bond angles



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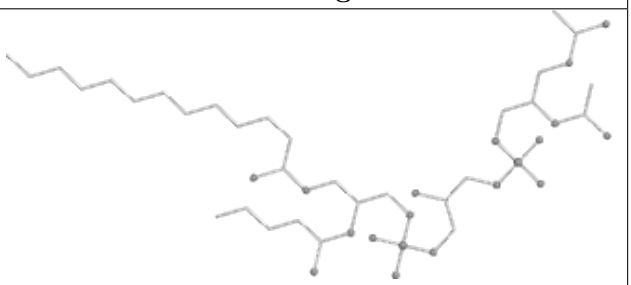
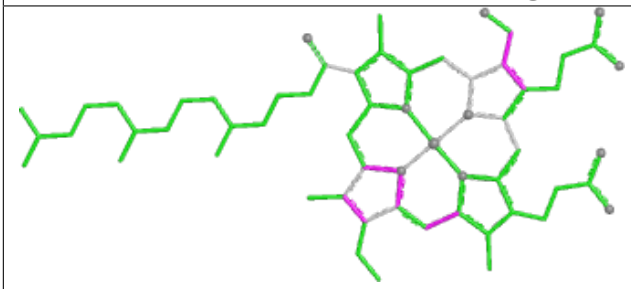
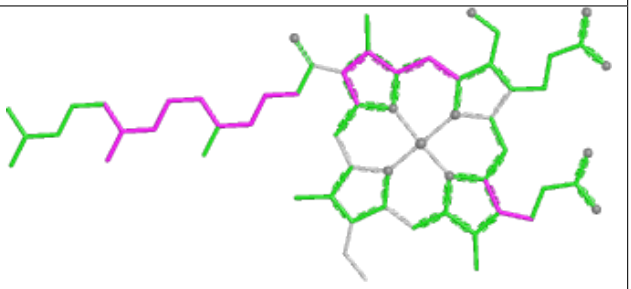


Rings

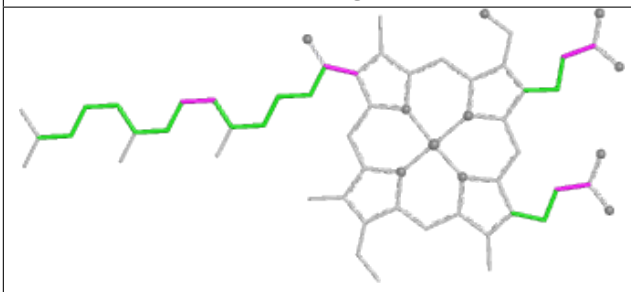
Ligand HEA L 515



Bond lengths



Bond angles



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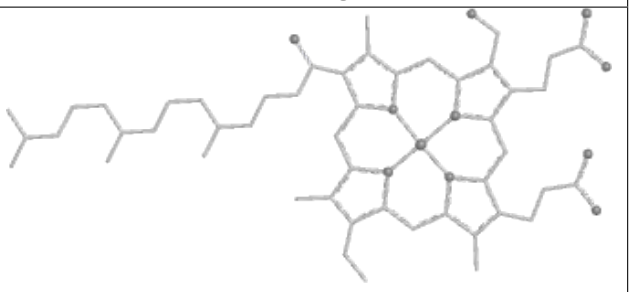
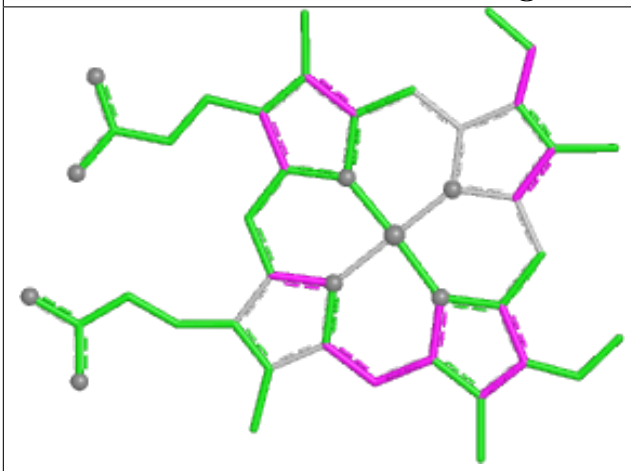
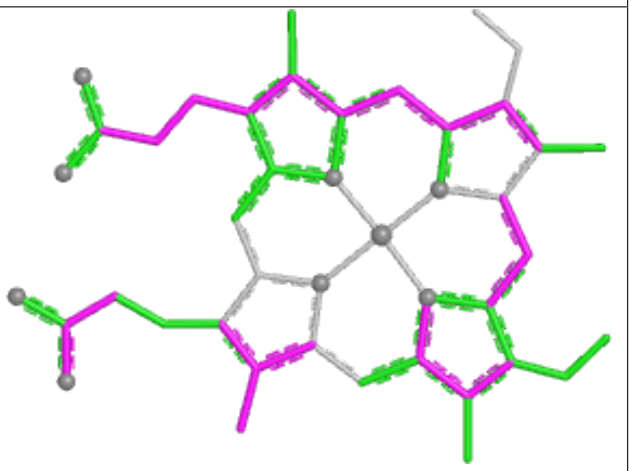


Rings

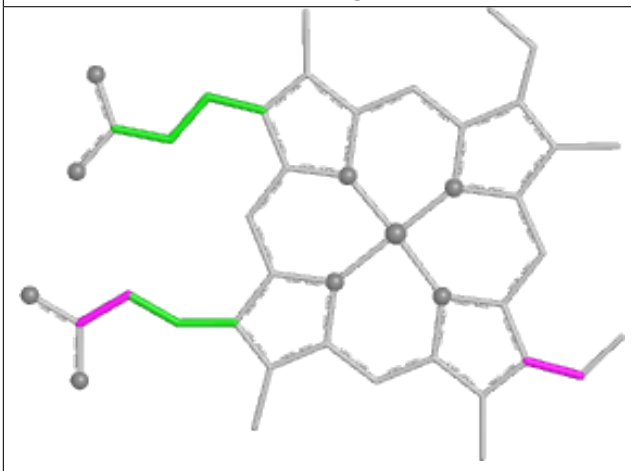
Ligand HEM Y 500



Bond lengths



Bond angles



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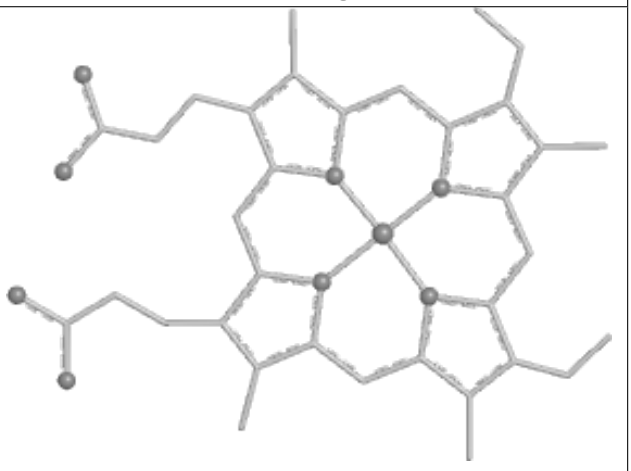
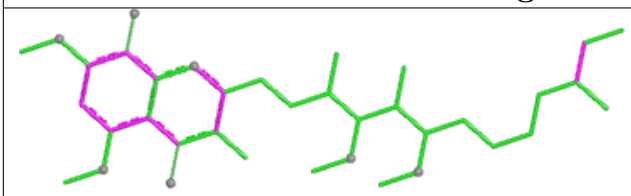
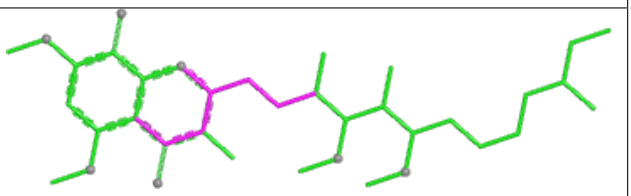
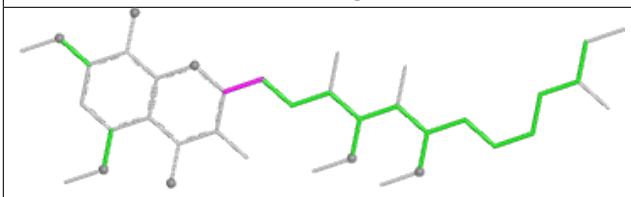
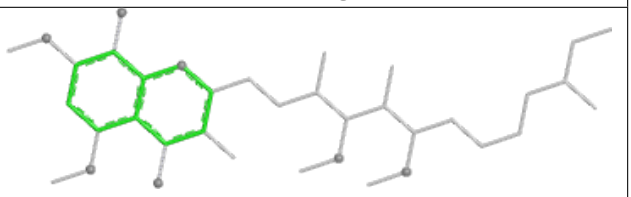
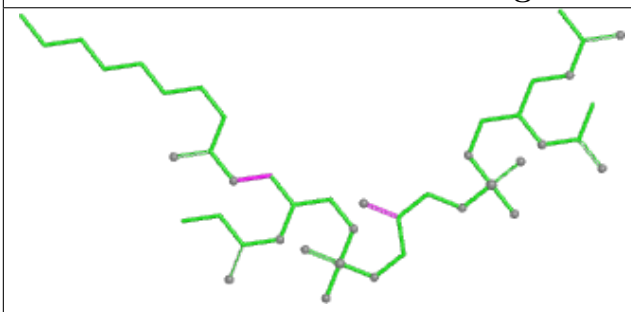
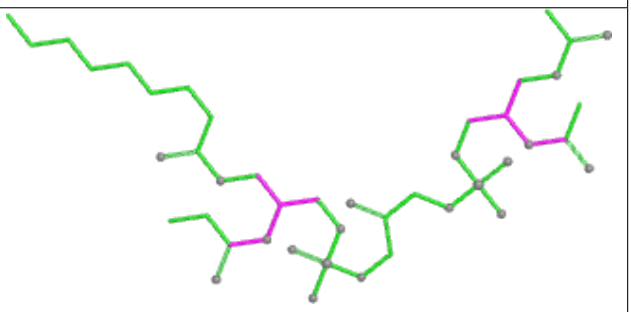
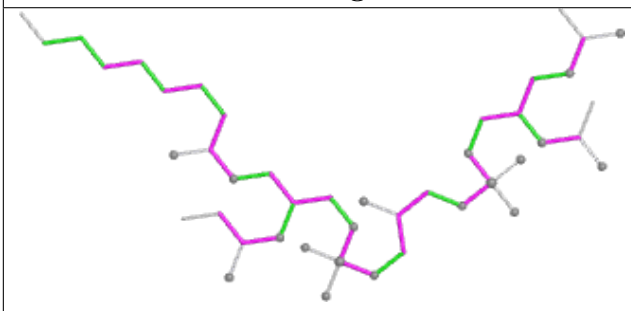
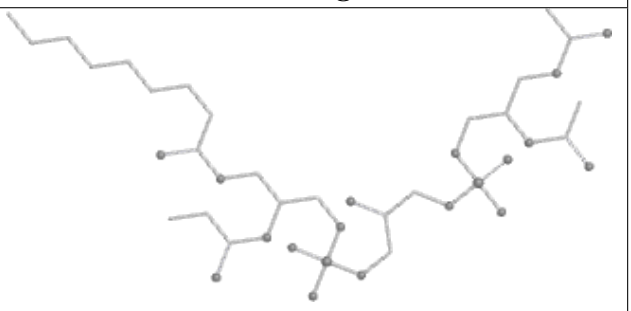
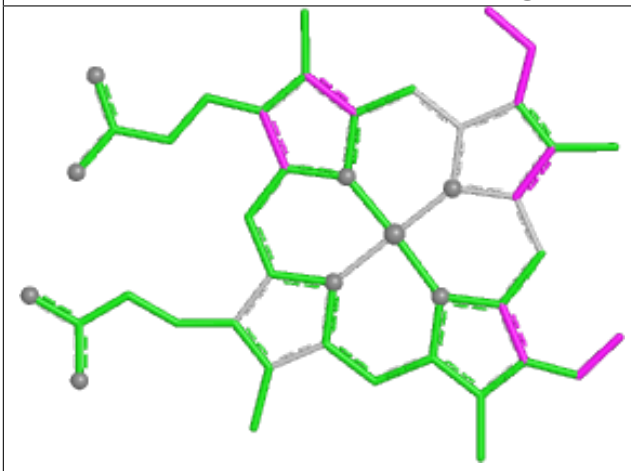


Rings

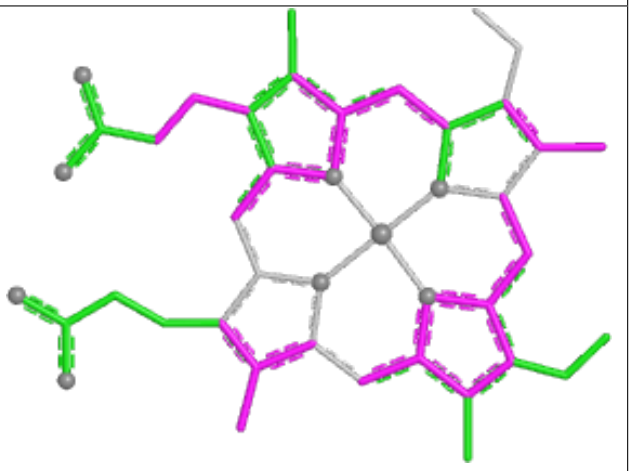
Ligand SMA c 3001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL G 2004	
 Bond lengths	 Bond angles
 Torsions	 Rings

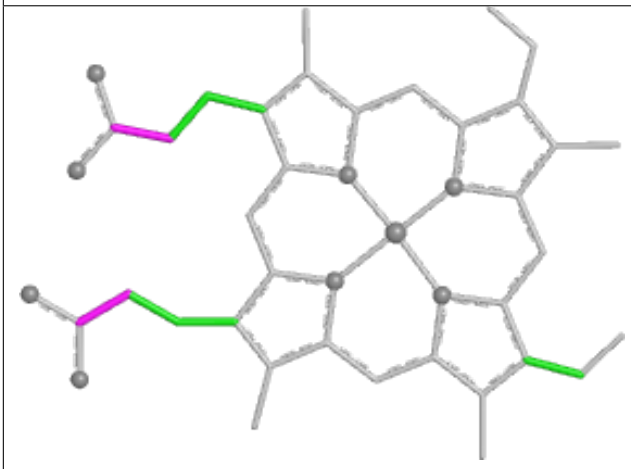
Ligand HEM C 502



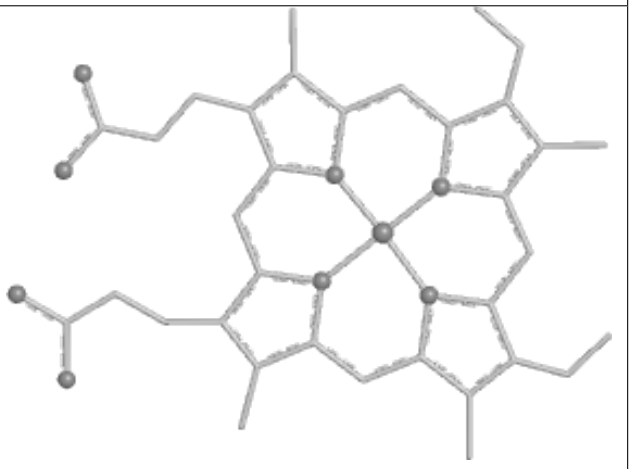
Bond lengths



Bond angles

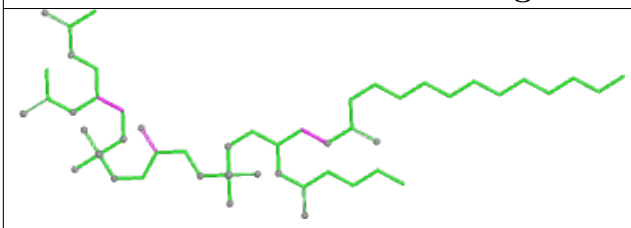


Torsions

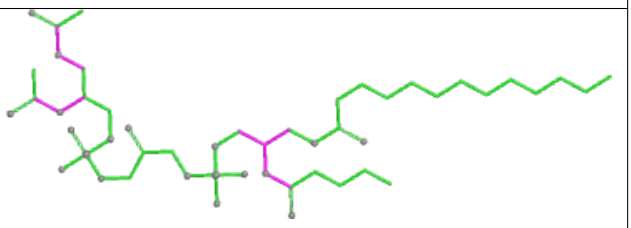


Rings

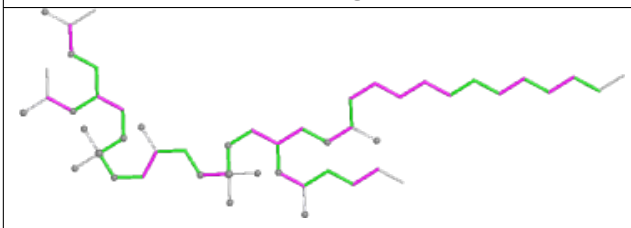
Ligand CDL G 2003



Bond lengths



Bond angles



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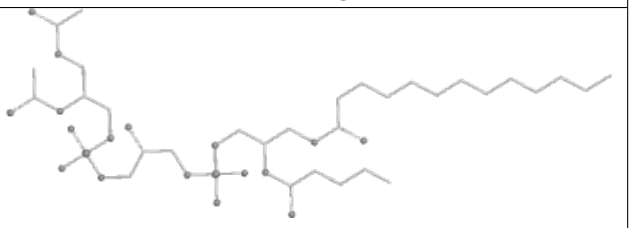
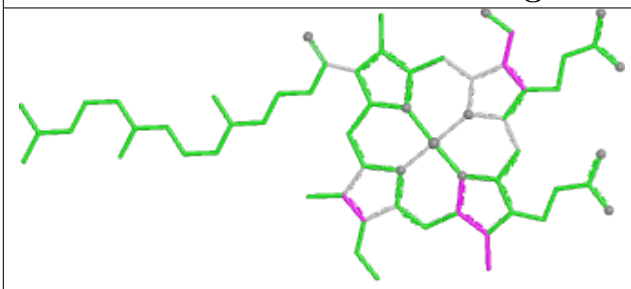
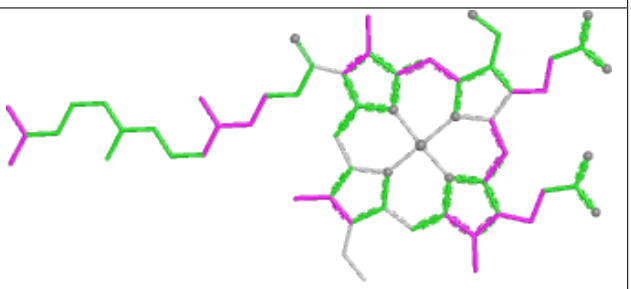
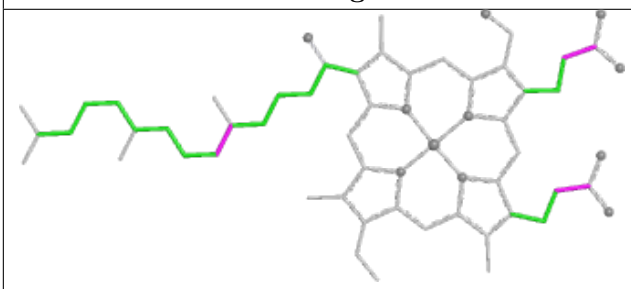
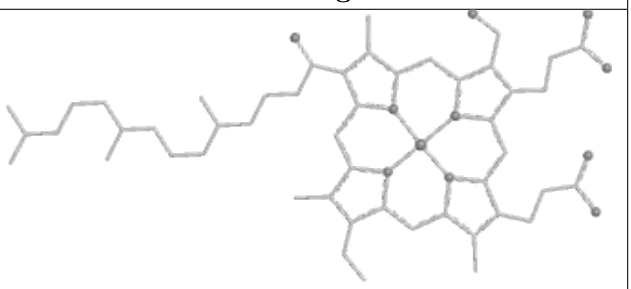
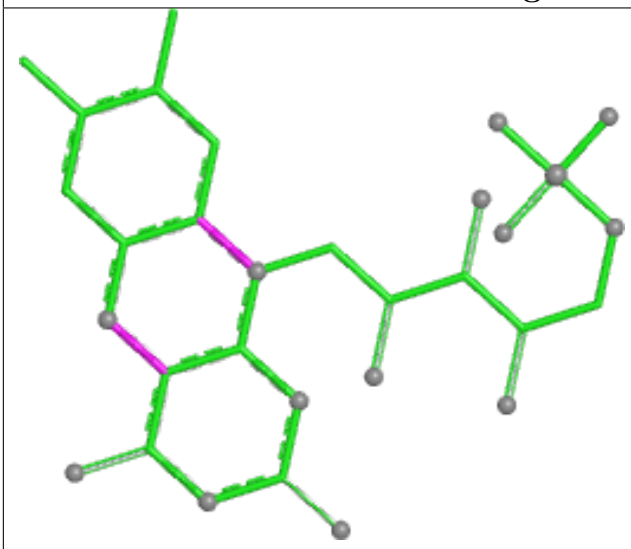


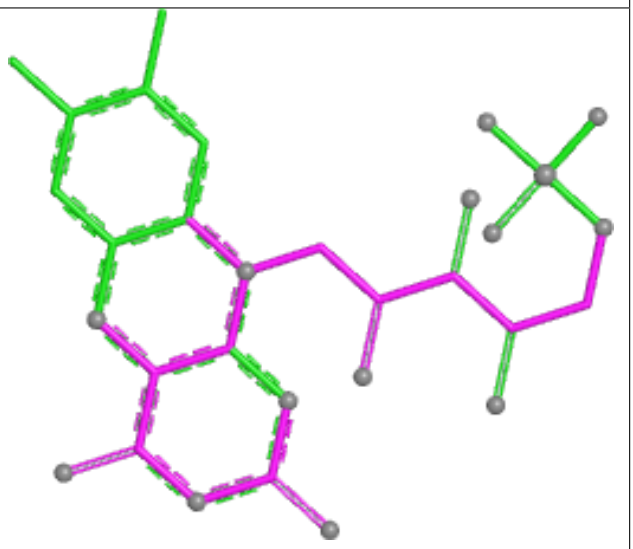
Rings

Ligand HEA L 516	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

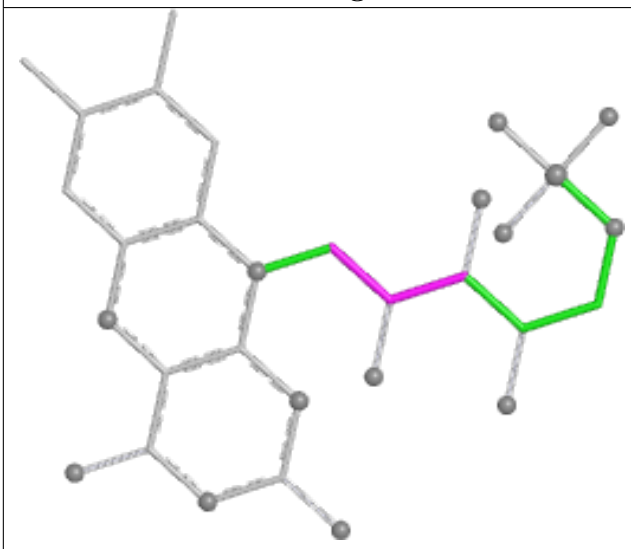
Ligand FMN 1 440



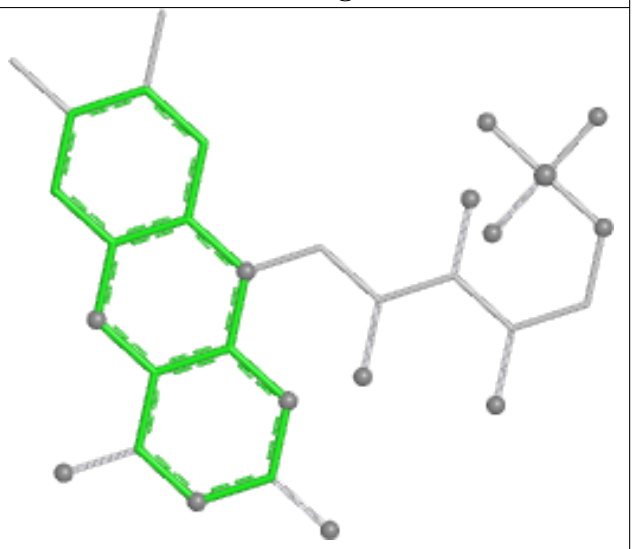
Bond lengths



Bond angles

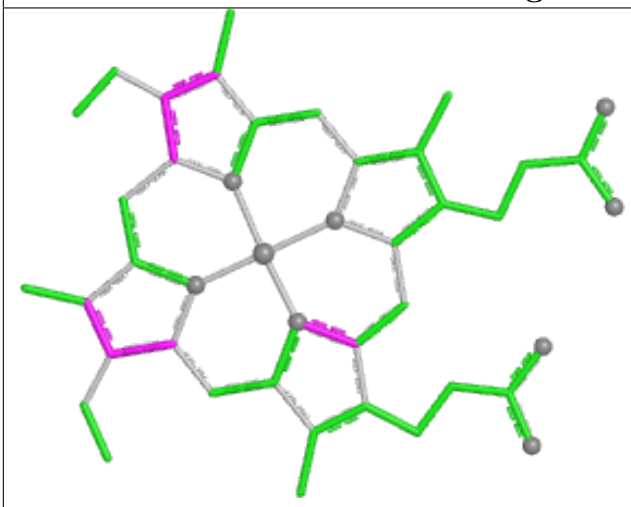


Torsions

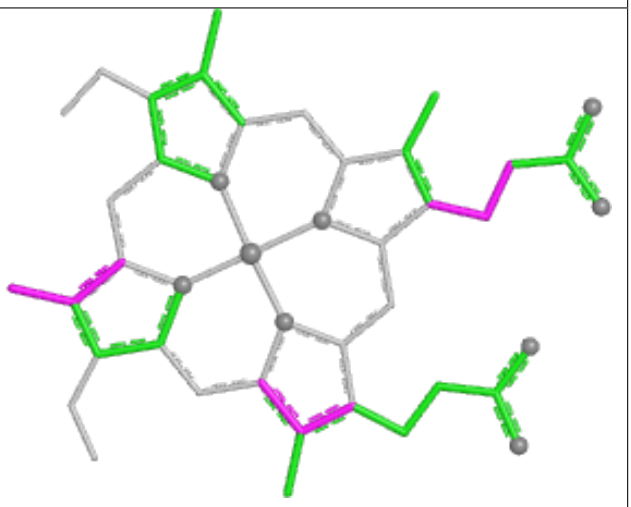


Rings

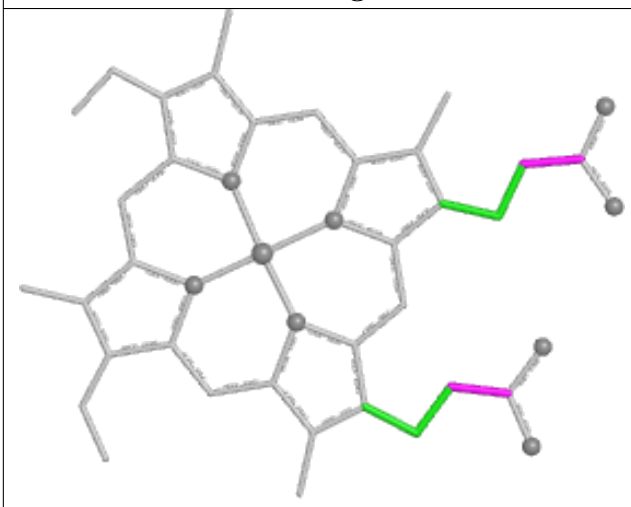
Ligand HEC d 501



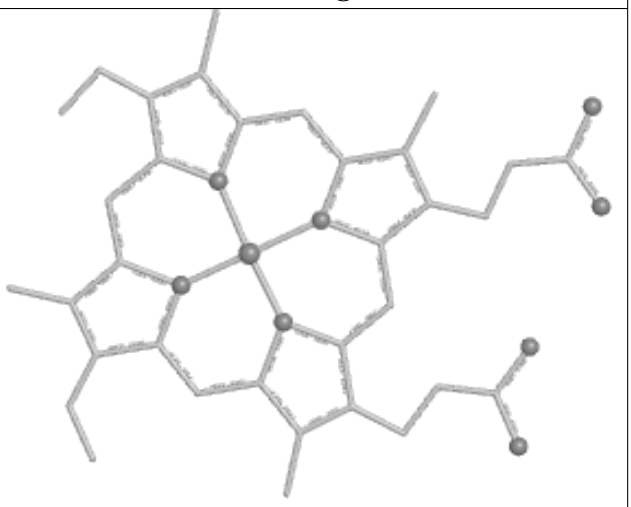
Bond lengths



Bond angles

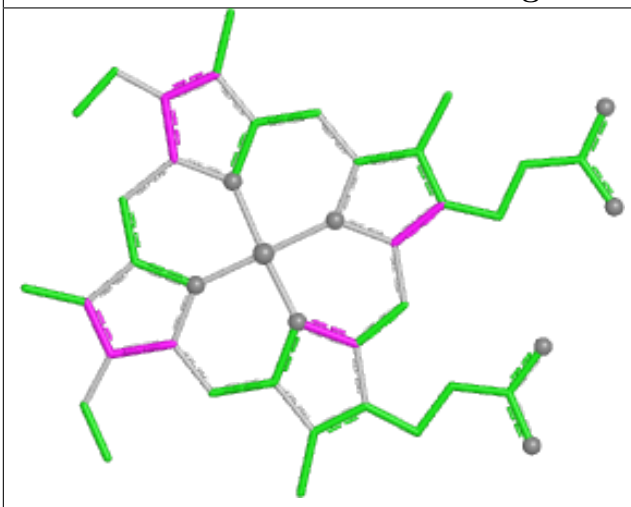


Torsions

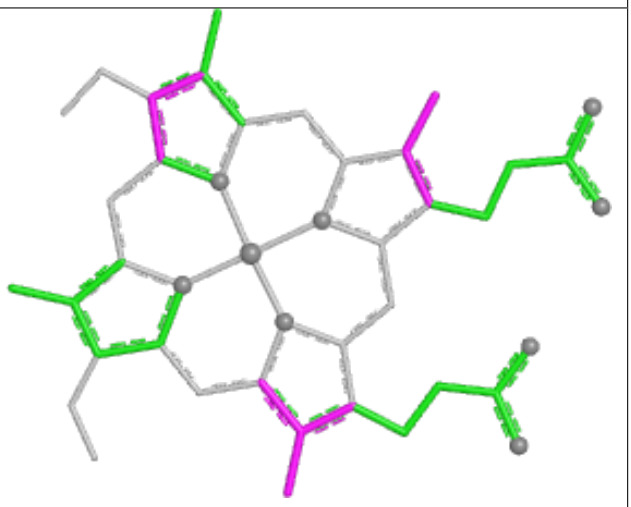


Rings

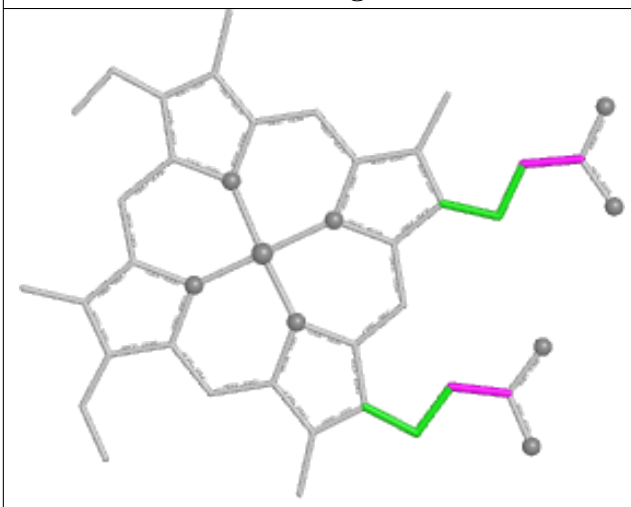
Ligand HEC D 501



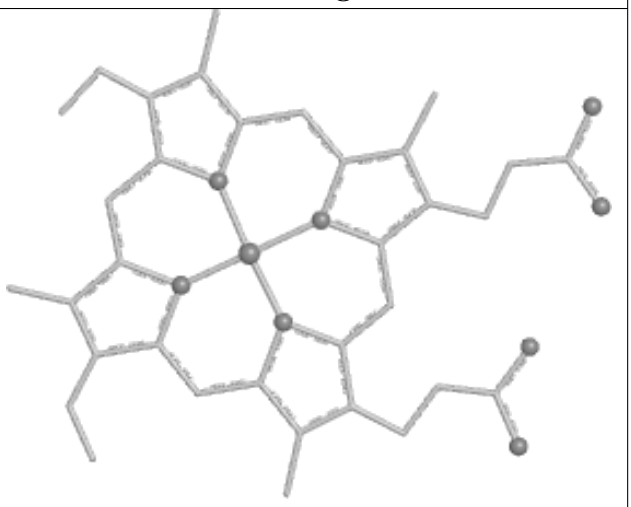
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	m	20
35	n	16
36	o	16
37	p	10
29	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m	428:UNK	C	495:UNK	N	56.90
1	n	1024:UNK	C	1050:UNK	N	55.04
1	o	366:UNK	C	395:UNK	N	50.88
1	m	1417:UNK	C	1501:UNK	N	47.70
1	o	665:UNK	C	700:UNK	N	47.65
1	o	524:UNK	C	601:UNK	N	47.16
1	m	1326:UNK	C	1401:UNK	N	46.61
1	o	428:UNK	C	501:UNK	N	46.47
1	p	725:UNK	C	797:UNK	N	45.46
1	n	1328:UNK	C	1399:UNK	N	43.88
1	n	829:UNK	C	899:UNK	N	43.18
1	o	1222:UNK	C	1295:UNK	N	42.97
1	n	520:UNK	C	601:UNK	N	42.94
1	p	824:UNK	C	900:UNK	N	41.53
1	o	923:UNK	C	1001:UNK	N	41.07
1	p	524:UNK	C	603:UNK	N	40.88
1	m	1022:UNK	C	1050:UNK	N	40.59
1	m	520:UNK	C	601:UNK	N	40.17
1	n	228:UNK	C	301:UNK	N	39.55
1	m	922:UNK	C	1003:UNK	N	39.30
1	o	1059:UNK	C	1096:UNK	N	38.87
1	p	624:UNK	C	702:UNK	N	37.28
1	o	226:UNK	C	301:UNK	N	37.24
1	m	229:UNK	C	301:UNK	N	36.09
1	o	1022:UNK	C	1050:UNK	N	35.98
1	n	923:UNK	C	1002:UNK	N	34.04
1	m	360:UNK	C	401:UNK	N	33.91
1	o	723:UNK	C	801:UNK	N	33.47
1	n	1065:UNK	C	1100:UNK	N	30.93
1	o	121:UNK	C	202:UNK	N	29.63
1	n	123:UNK	C	201:UNK	N	28.64
1	m	1061:UNK	C	1101:UNK	N	28.15
1	n	424:UNK	C	495:UNK	N	16.18
1	m	824:UNK	C	901:UNK	N	15.99
1	n	367:UNK	C	398:UNK	N	15.97
1	m	666:UNK	C	704:UNK	N	15.22
1	n	1121:UNK	C	1200:UNK	N	14.33
1	m	732:UNK	C	802:UNK	N	14.14
1	o	823:UNK	C	903:UNK	N	13.62
1	n	734:UNK	C	800:UNK	N	12.90
1	p	919:UNK	C	997:UNK	N	12.22
1	p	125:UNK	C	202:UNK	N	11.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	n	1222:UNK	C	1300:UNK	N	11.26
1	m	613:UNK	C	650:UNK	N	11.20
1	o	1122:UNK	C	1200:UNK	N	11.16
1	o	1320:UNK	C	1401:UNK	N	11.09
1	p	423:UNK	C	494:UNK	N	10.86
1	n	663:UNK	C	704:UNK	N	10.34
1	o	615:UNK	C	650:UNK	N	10.27
1	m	1123:UNK	C	1195:UNK	N	9.82
1	m	127:UNK	C	201:UNK	N	9.74
1	p	324:UNK	C	397:UNK	N	9.72
1	n	615:UNK	C	650:UNK	N	9.60
1	m	1218:UNK	C	1298:UNK	N	9.44
1	p	223:UNK	C	295:UNK	N	8.96
1	m	311:UNK	C	350:UNK	N	6.99
1	o	313:UNK	C	350:UNK	N	6.87
1	p	1021:UNK	C	1098:UNK	N	6.64
1	n	313:UNK	C	350:UNK	N	5.71
1	m	1597:UNK	C	1601:UNK	N	4.80
1	m	1543:UNK	C	1545:UNK	N	4.39
1	U	56:PRO	C	57:HIS	N	3.69
1	m	1564:UNK	C	1566:UNK	N	3.11

6 Map visualisation

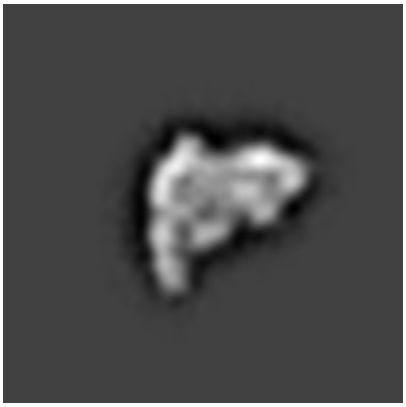
This section contains visualisations of the EMDB entry EMD-1876. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X



Y

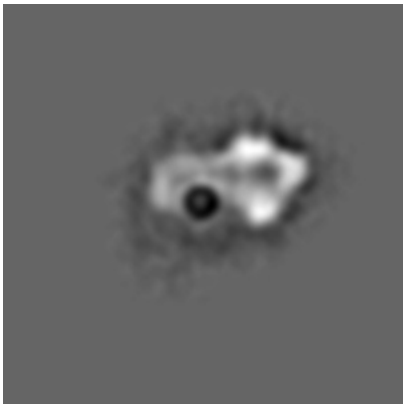
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 56



Y Index: 56

Z Index: 56

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 67

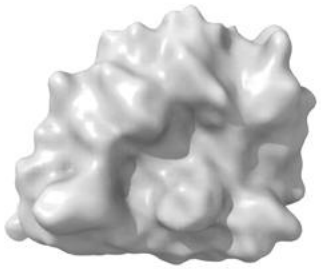
Y Index: 37

Z Index: 45

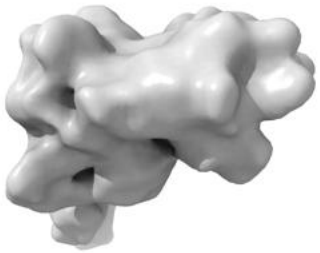
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

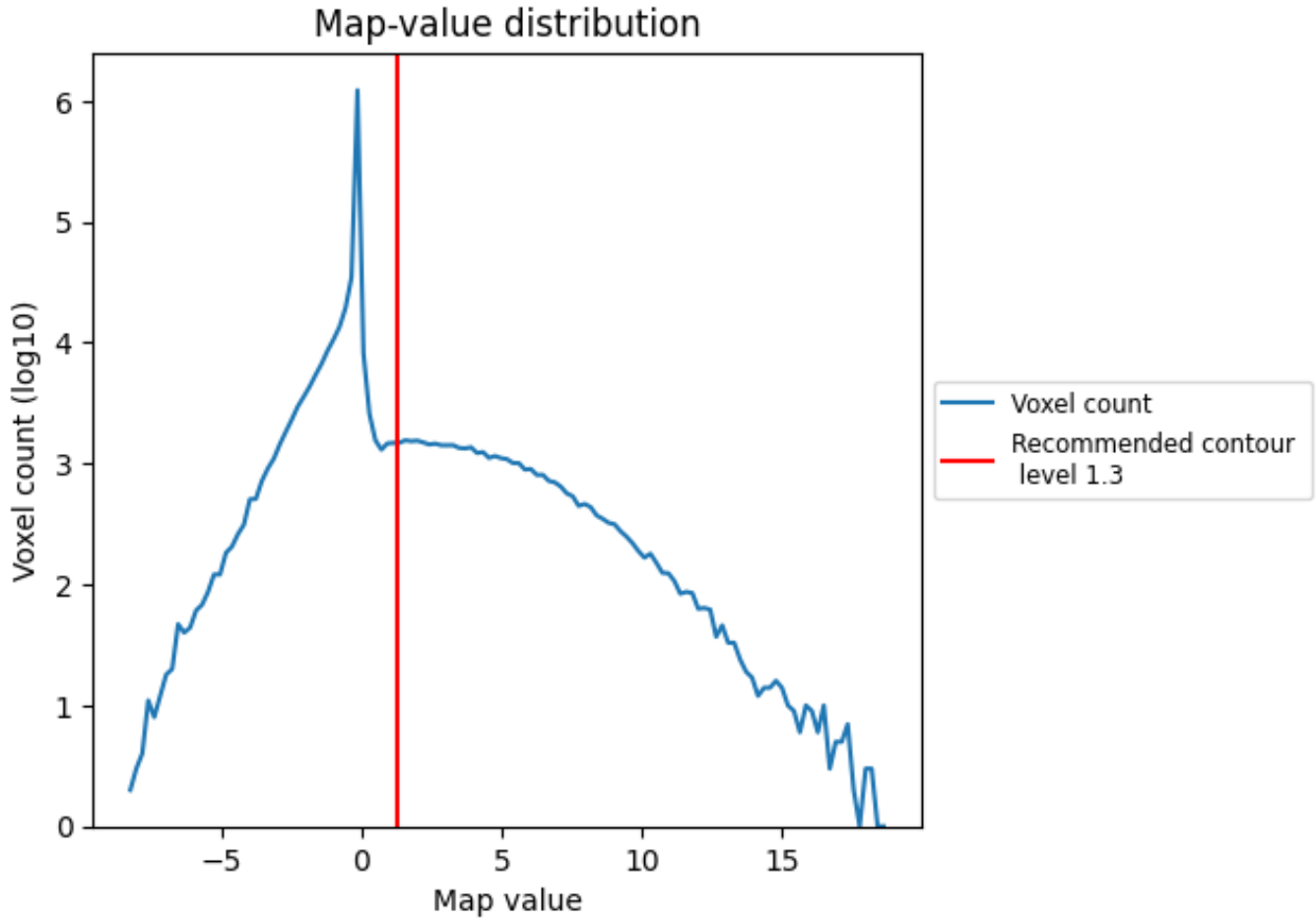
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

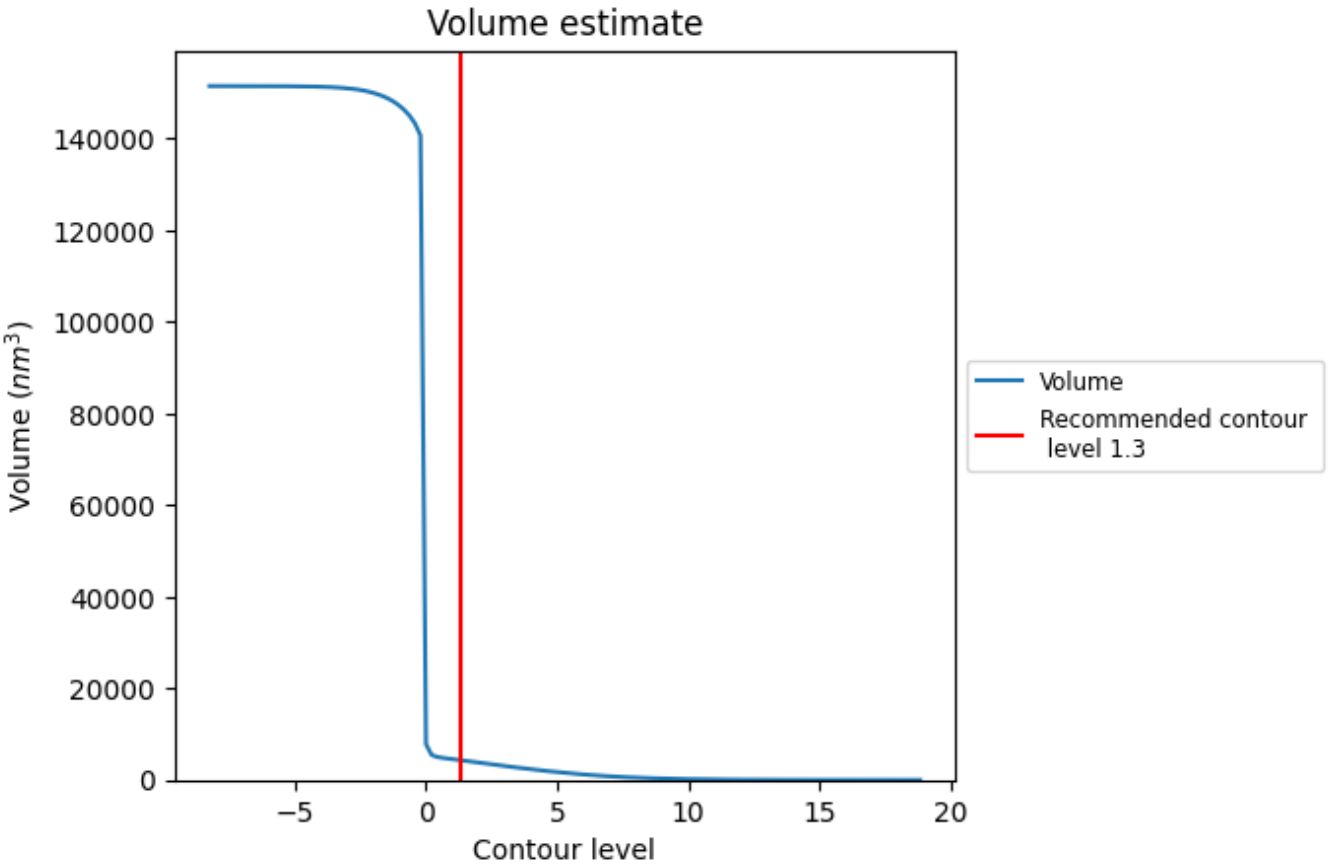
This section contains the results of statistical analysis of the map.

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.

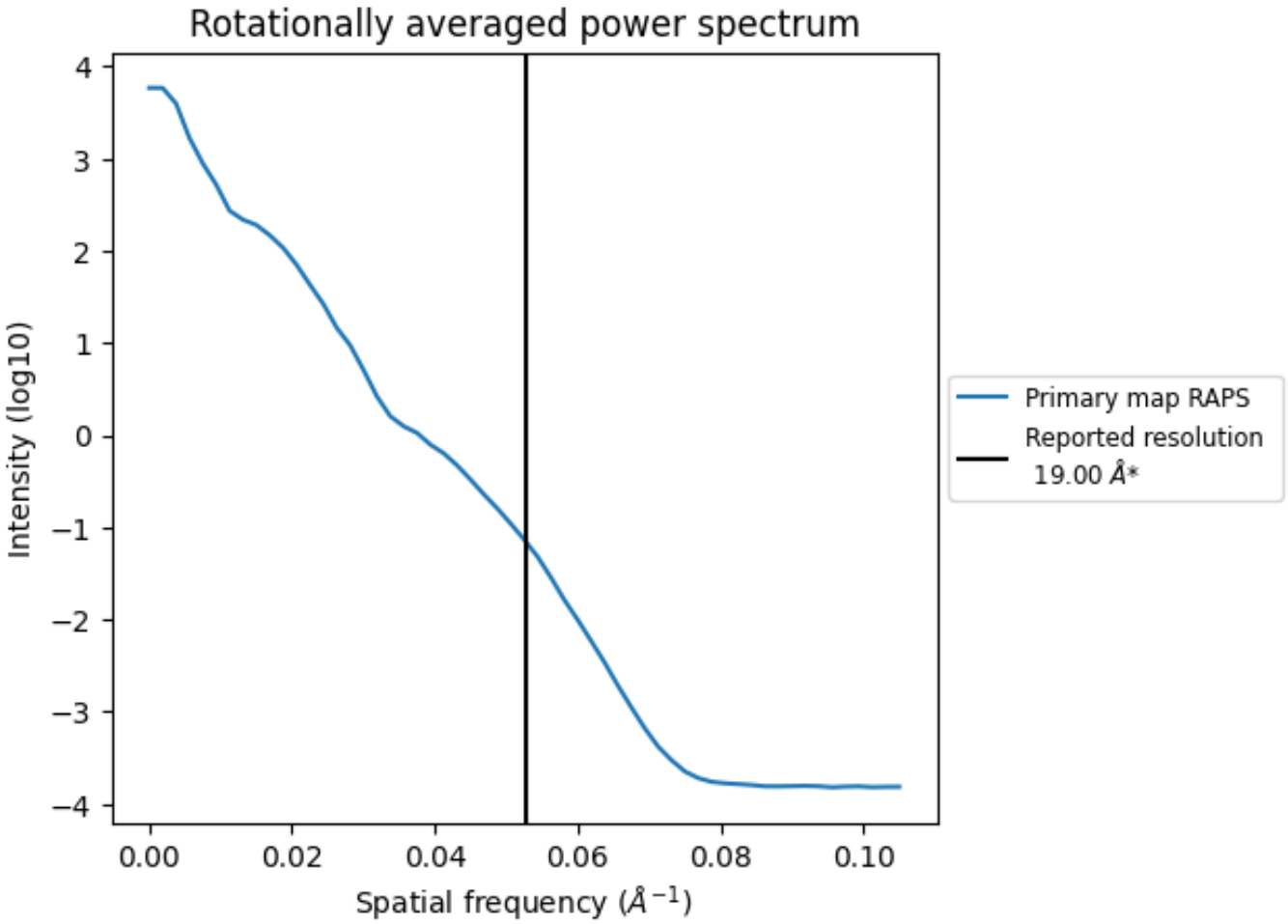
7.2 Volume estimate



The volume at the recommended contour level is 4344 nm^3; this corresponds to an approximate mass of 3924 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.053 Å^{-1}

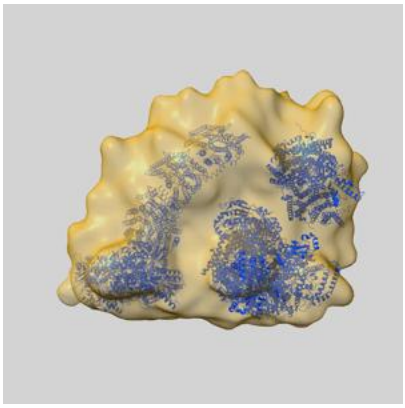
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

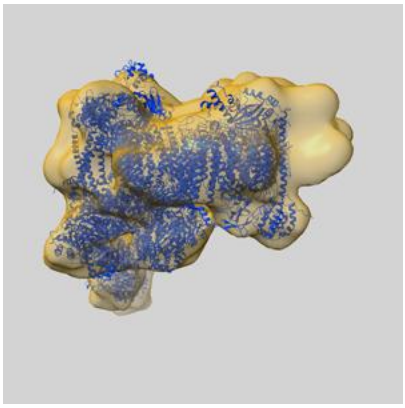
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1876 and PDB model 2YBB. Per-residue inclusion information can be found in section 3 on page 20.

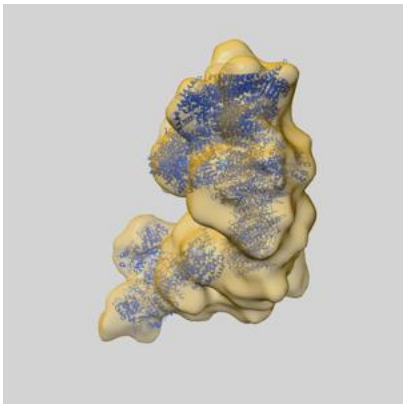
9.1 Map-model overlay



X



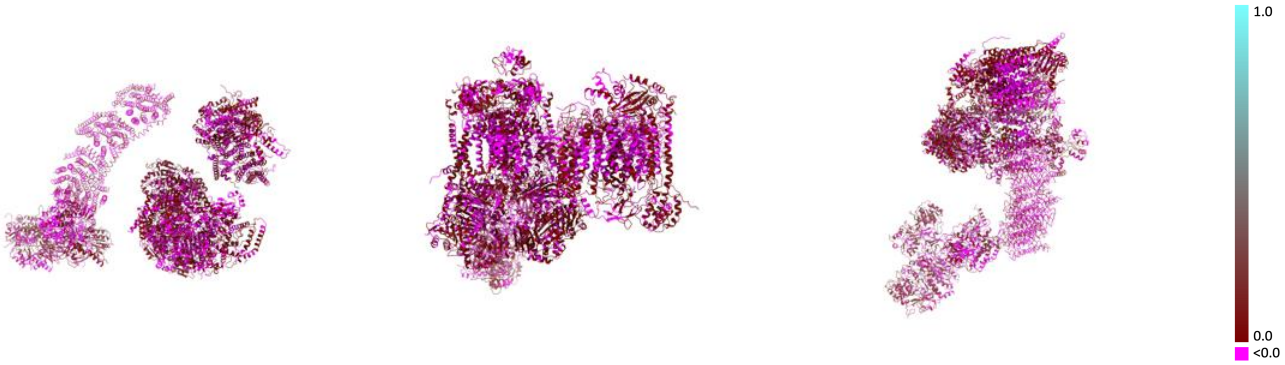
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

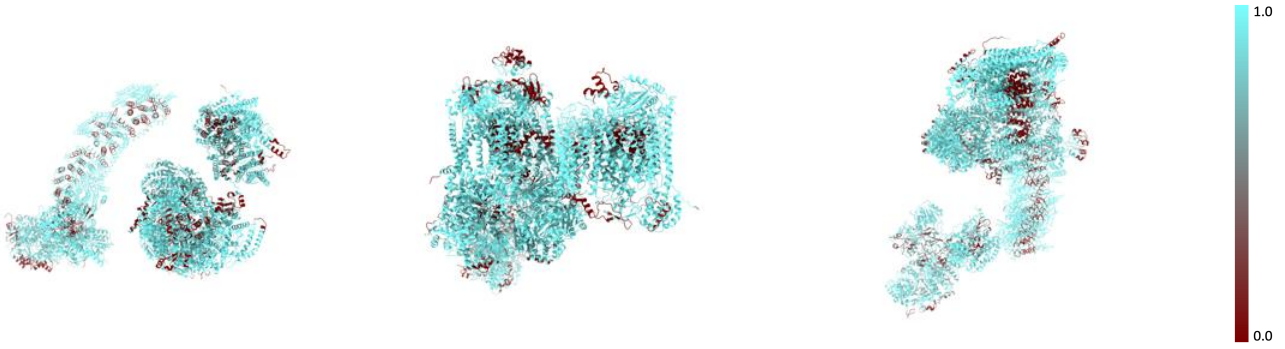
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

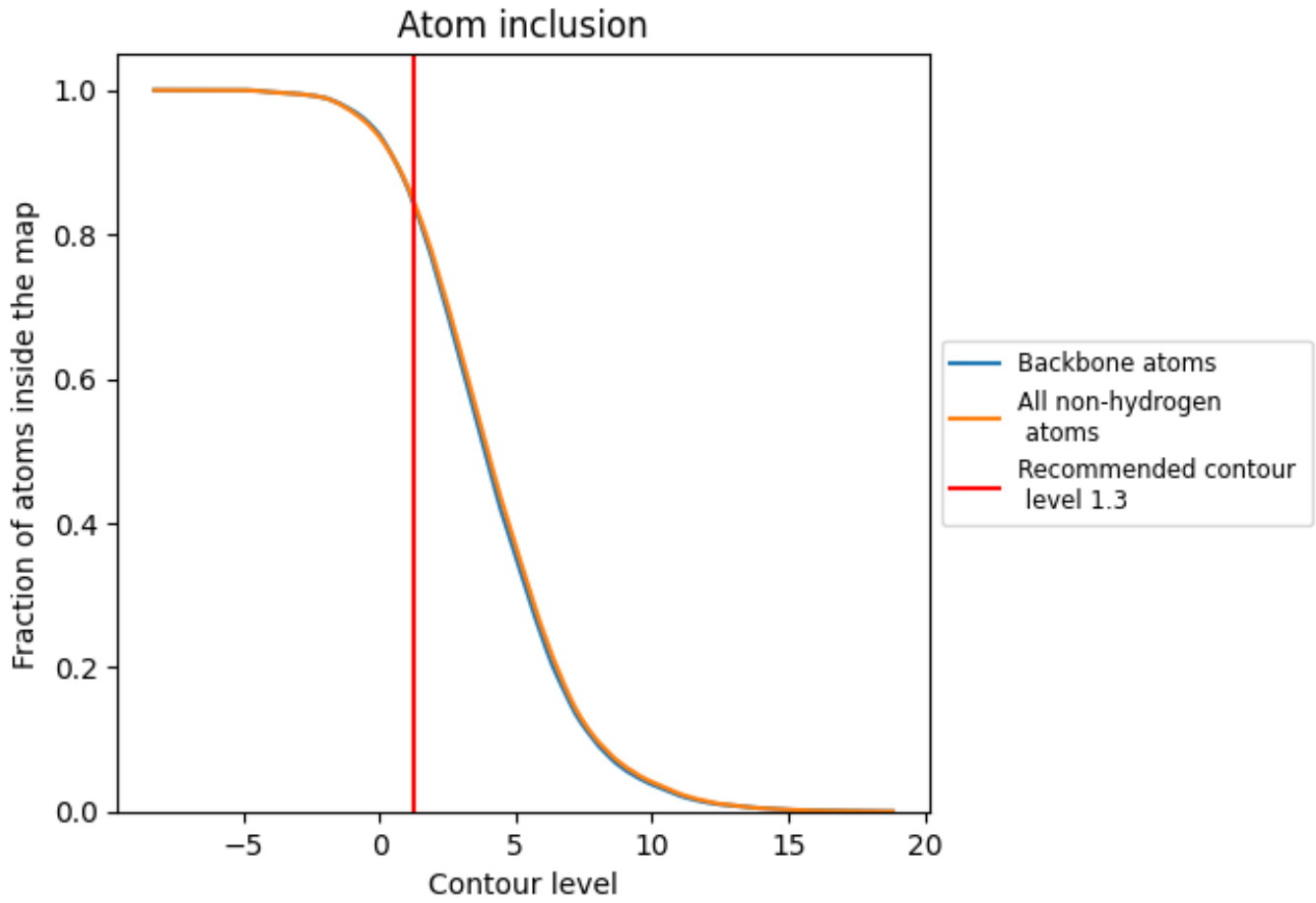
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.3).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.0170
1	0.8931	0.0350
2	0.7616	0.0130
3	0.8339	0.0270
4	0.7927	-0.0220
5	0.8619	-0.0010
6	0.9050	0.0170
7	0.6074	-0.0040
8	0.9856	0.0240
A	0.9031	0.0290
B	0.8766	0.0320
C	0.8103	0.0030
D	0.9785	0.0410
E	0.6419	-0.0200
F	0.9988	0.0630
G	0.9841	0.0320
H	0.8672	0.0440
I	0.8375	0.0050
J	0.9434	0.0100
K	0.6000	-0.0350
L	0.7930	-0.0120
M	1.0000	0.0490
N	0.9201	0.0280
O	0.8660	0.0450
P	0.8333	0.0410
Q	0.4722	-0.0070
R	0.8913	0.0240
S	0.5924	-0.0160
T	0.9810	0.0360
U	0.8387	0.0360
V	0.7333	0.0010
W	0.8632	0.0270
X	0.6386	-0.0240
Y	0.4550	0.0100
a	0.9853	0.0300

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Chain	Atom inclusion	Q-score
b	0.9428	0.0450
c	0.8194	-0.0010
d	0.9332	0.0440
e	0.6118	-0.0070
f	0.6277	0.0300
g	0.8819	0.0310
h	0.9715	0.0510
i	0.9350	-0.0200
j	0.8404	0.0400
k	1.0000	0.1370
m	0.7616	-0.0190
n	0.7306	-0.0200
o	0.7372	-0.0140
p	0.8055	0.0010