Full wwPDB EM Validation Report ⓘ

May 3, 2023 – 06:50 pm BST

PDB ID	:	8BQ6
EMDB ID	:	EMD-16172
Title	:	Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (Complete conformation 2 composition)
Authors	:	Klusch, N.; Kuehlbrandt, W.
Deposited on	:	2022-11-18
Resolution	:	2.80 Å(reported)

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

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

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

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

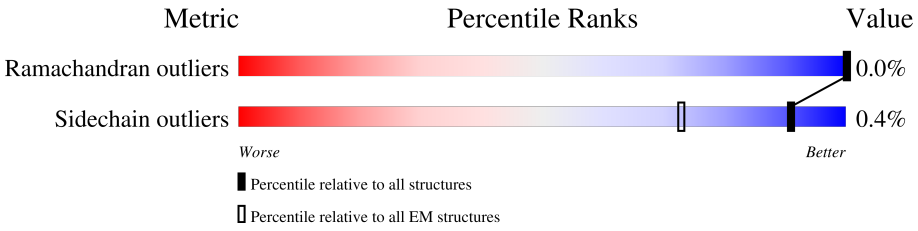
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 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	A	119	77% · 21%
2	B	218	71% · 28%
3	C	190	94% · 5%
4	D	394	97%
5	E	255	24% 75% · 25%
6	F	486	13% 89% 11%
7	G	748	14% 92% 8%
8	H	325	100%
9	I	222	74% 26%

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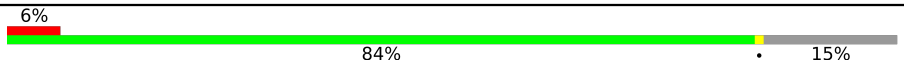
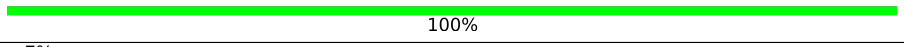
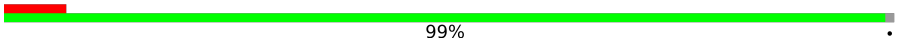
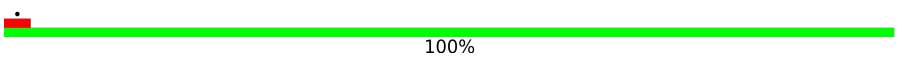
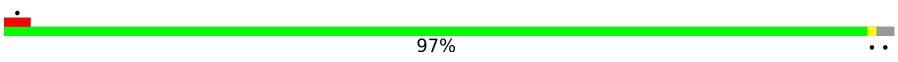
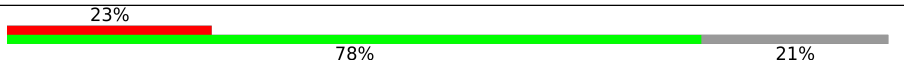
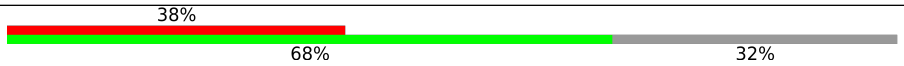
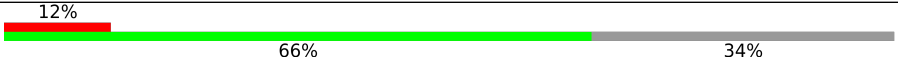
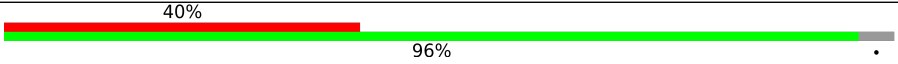
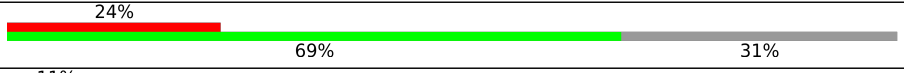
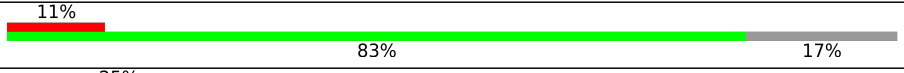
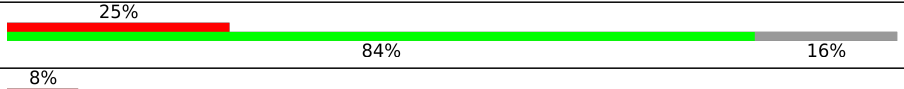
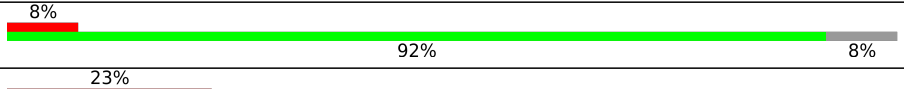
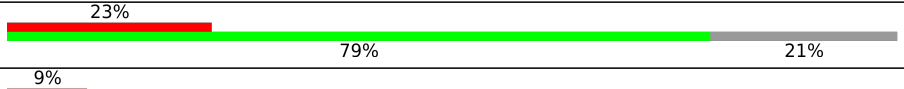
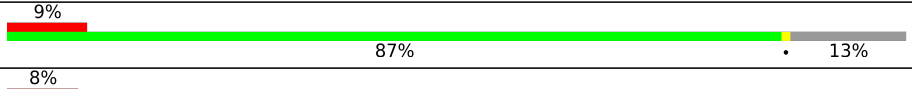
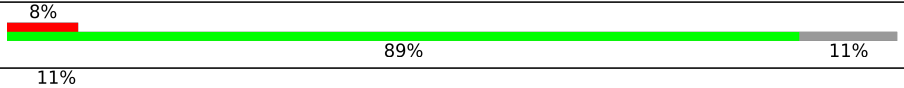
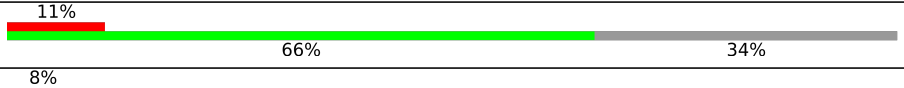
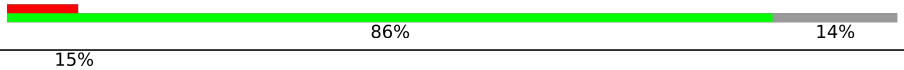
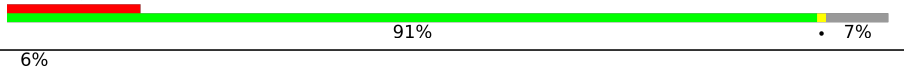
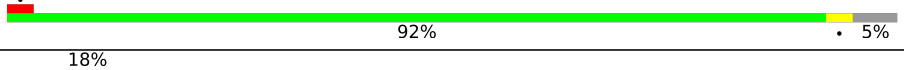
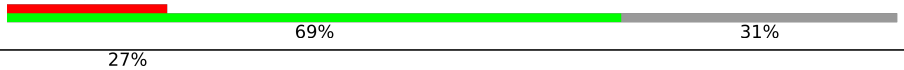
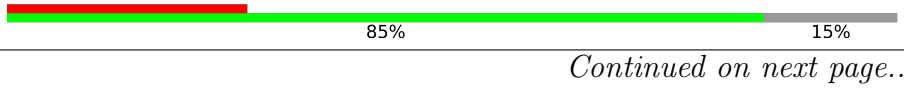
Mol	Chain	Length	Quality of chain
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Y	159	
26	Z	143	
27	a	65	
28	b	65	
29	c	88	
30	d	81	
31	e	83	
32	f	106	
33	g	114	
34	i	98	

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Mol	Chain	Length	Quality of chain
35	j	69	29% 74% 26%
36	k	72	38% 67% 33%
37	l	125	15% 59% 41%
38	m	71	18% 97%
39	n	117	9% 92% 7%
40	o	103	23% 78% 22%
41	p	106	16% 85% 15%
42	q	159	50% 50%
43	u	63	8% 87% 13%
44	v	113	26% 74%
45	x	256	81% 18%
46	y	278	95% 5%
47	z	275	84% 15%
48	AA	503	26% 83% 17%
48	BA	503	24% 83% 17%
49	AB	531	6% 92% 8%
49	BB	531	7% 92% 8%
50	AC	393	97%
50	BC	393	97%
51	AD	272	41% 72% 28%
51	BD	272	37% 72% 28%
52	AE	307	79% 21%
52	BE	307	7% 79% 21%
53	AF	122	95% 5%
53	BF	122	5% 95% 5%

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Mol	Chain	Length	Quality of chain
54	AG	72	96%
54	BG	72	11% 94% 6%
55	AH	69	17% 93% 7%
55	BH	69	43% 91% 9%
56	AI	72	6% 79% 21%
56	BI	72	15% 79% 21%
57	AJ	57	40% 49% 51%
57	BJ	57	19% 49% 51%

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
66	COO	y	301	X	-	-	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 96522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	94	802	565	110	123	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1244	797	218	215	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	181	1545	997	266	276	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	385	3079	1957	542	556	24	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5243	3285	919	1000	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1349	849	229	261	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1399	949	213	228	9		

- Molecule 11 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			784	525	121	131	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	665	Total	C	N	O	S	0	0
			5222	3474	808	901	39		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	494	Total	C	N	O	S	0	0
			3946	2664	610	647	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	1	0
			3832	2582	578	644	28		

- Molecule 15 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			963	603	170	186	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	316	Total	C	N	O	S	0	0
			2453	1580	414	444	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	105	Total	C	N	O	S	0	0
			837	536	144	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	73	Total	C	N	O	S	0	0
			571	359	101	105	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			659	417	104	135	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	87	Total	C	N	O	S	0	0
			677	427	110	139	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	98	Total 776	C 486	N 134	O 144	S 12	0	0

- Molecule 25 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	125	Total 928	C 596	N 162	O 167	S 3	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	125	Total 997	C 640	N 175	O 177	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	58	Total 469	C 302	N 84	O 78	S 5	0	0

- Molecule 28 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	43	Total 315	C 206	N 51	O 55	S 3	0	0

- Molecule 29 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	76	Total 617	C 396	N 115	O 100	S 6	0	0

- Molecule 30 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	65	Total	C	N	O	S	0	0
			554	343	103	100	8		

- Molecule 32 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 33 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	79	Total	C	N	O	S	0	0
			641	412	111	115	3		

- Molecule 34 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	48	Total	C	N	O	S	0	0
			382	244	72	63	3		

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

8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	74	Total	C	N	O	S	0	0
			562	367	91	103	1		

- Molecule 38 is a protein called B15 – 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	90	Total	C	N	O	S	0	0
			757	479	141	133	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	80	Total	C	N	O	S	1	0
			669	427	120	120	2		

- Molecule 43 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	55	Total	C	N	O	S	0	0
			463	298	84	78	3		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	v	29	Total	C	N	O	0	0
			219	142	38	39		

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	210	Total	C	N	O	S	0	0
			1629	1043	280	301	5		

- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	265	Total	C	N	O	S	0	0
			2013	1258	359	388	8		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 48 is a protein called Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	420	Total	C	N	O	S	0	0
			3201	2034	530	621	16		
48	BA	420	Total	C	N	O	S	0	0
			3202	2035	530	621	16		

- Molecule 49 is a protein called Probable mitochondrial-processing peptidase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	BB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

- Molecule 50 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
50	BC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AD	196	Total	C	N	O	S	0	0
			1528	978	264	281	5		
51	BD	195	Total	C	N	O	S	0	0
			1519	973	263	278	5		

- Molecule 52 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
52	BE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		
53	BF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	69	Total	C	N	O	S	0	0
			581	387	95	98	1		
54	BG	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AH	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
55	BH	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

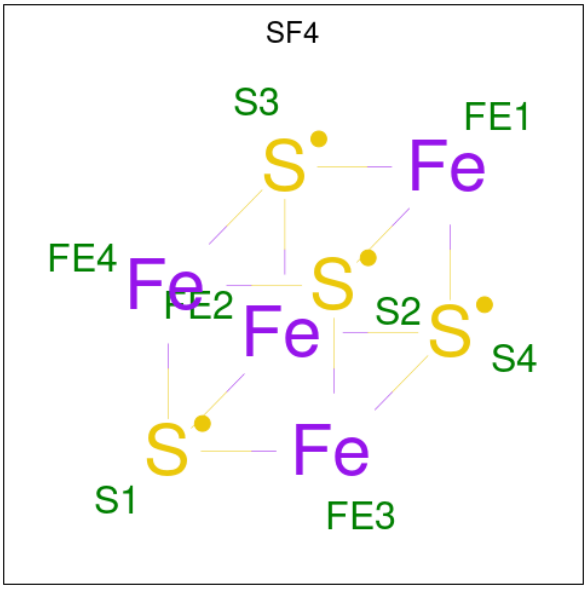
- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
56	BI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

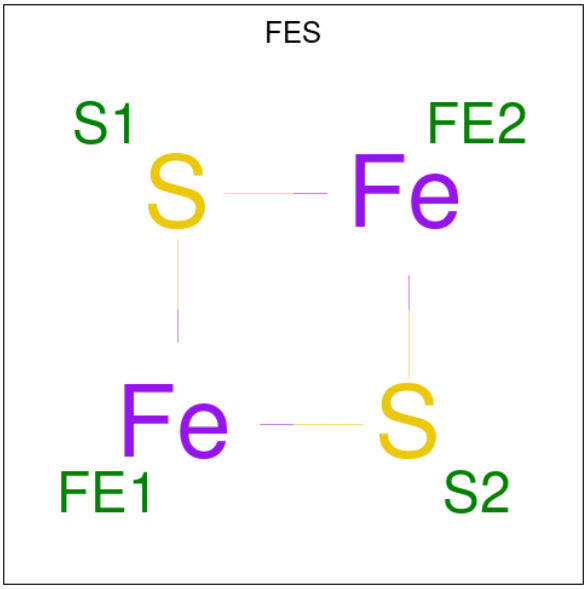
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		
57	BJ	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



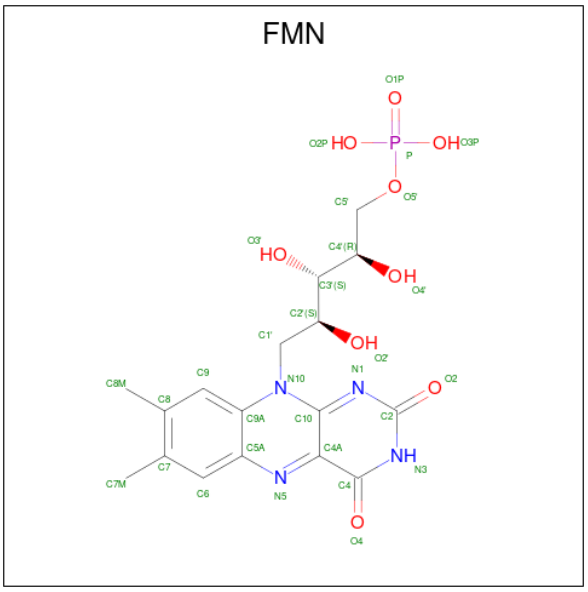
Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total Fe S 8 4 4	0
58	F	1	Total Fe S 8 4 4	0
58	G	1	Total Fe S 8 4 4	0
58	G	1	Total Fe S 8 4 4	0
58	I	1	Total Fe S 8 4 4	0
58	I	1	Total Fe S 8 4 4	0

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



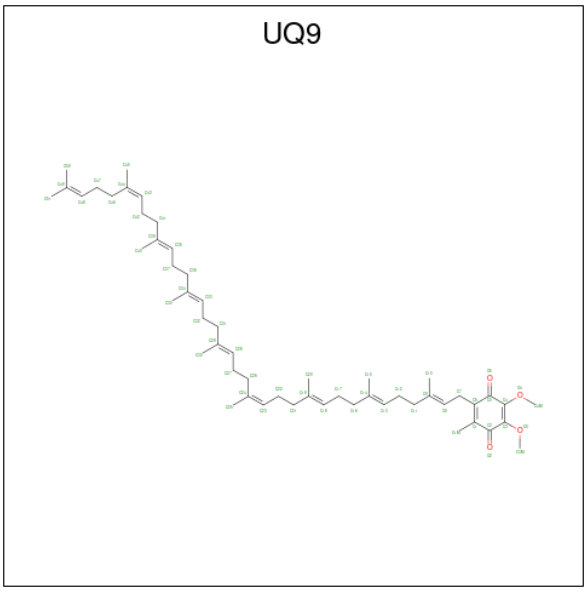
Mol	Chain	Residues	Atoms	AltConf
59	E	1	Total Fe S 4 2 2	0
59	G	1	Total Fe S 4 2 2	0
59	AD	1	Total Fe S 4 2 2	0
59	BD	1	Total Fe S 4 2 2	0

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



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

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

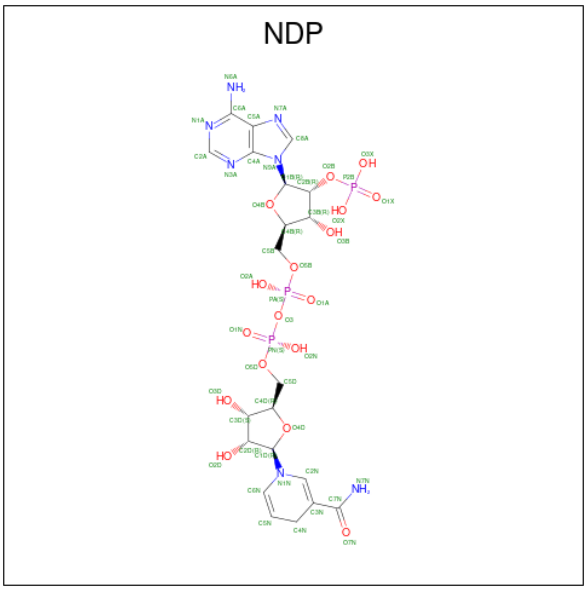


Mol	Chain	Residues	Atoms				AltConf
61	H	1	Total	C	O		0
			35	31	4		

- Molecule 62 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
62	O	1	Total Fe 1 1	0

- Molecule 63 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

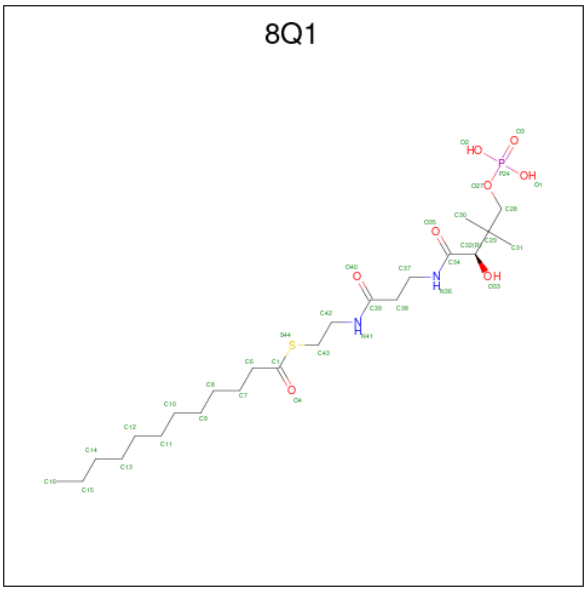


Mol	Chain	Residues	Atoms	AltConf
63	P	1	Total C N O P 48 21 7 17 3	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

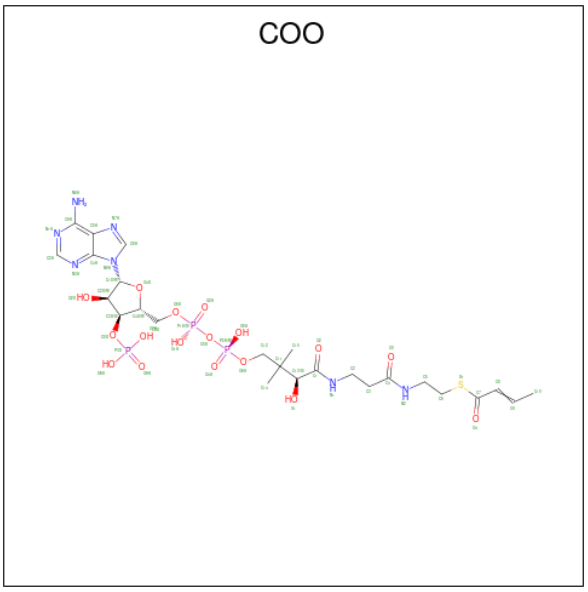
Mol	Chain	Residues	Atoms	AltConf
64	R	1	Total Zn 1 1	0
64	y	1	Total Zn 1 1	0
64	AB	1	Total Zn 1 1	0
64	BB	1	Total Zn 1 1	0

- Molecule 65 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



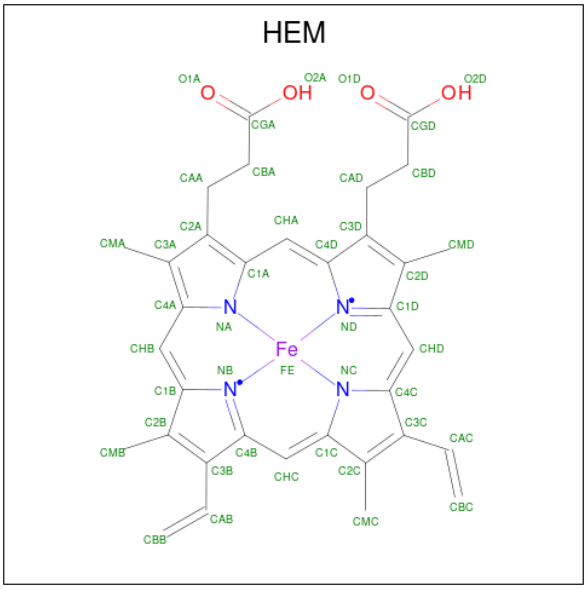
Mol	Chain	Residues	Atoms						AltConf
65	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
65	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 66 is CROTONYL COENZYME A (three-letter code: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



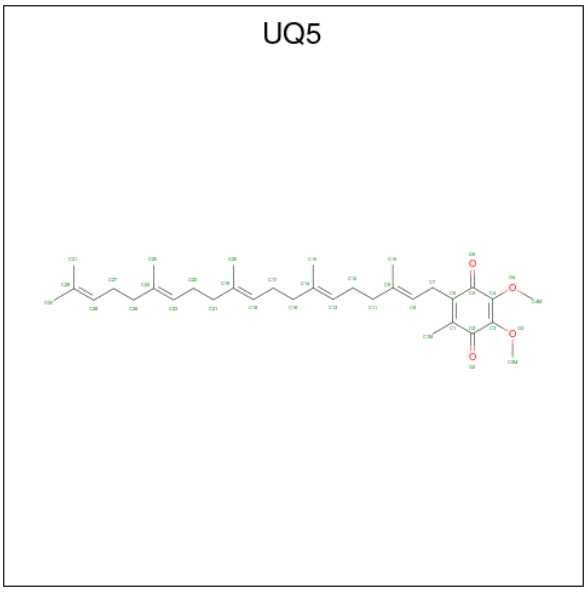
Mol	Chain	Residues	Atoms						AltConf
66	y	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

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



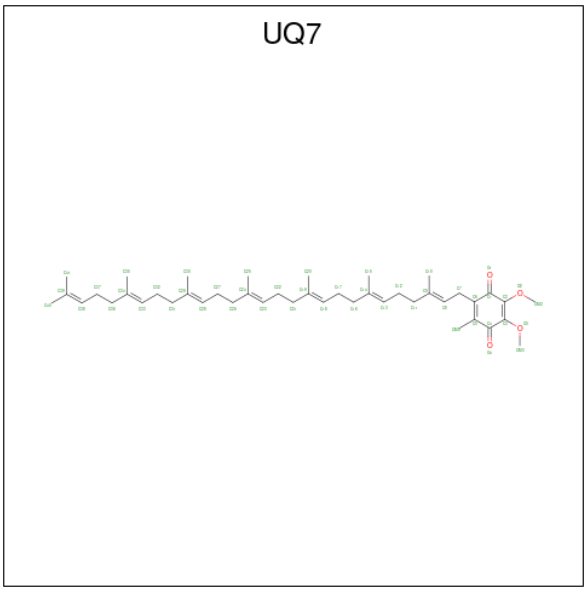
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 68 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: $C_{34}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			38	34	4	
68	AC	1	Total	C	O	0
			38	34	4	
68	BC	1	Total	C	O	0
			38	34	4	

- Molecule 69 is UBIQUINONE-7 (three-letter code: UQ7) (formula: $C_{44}H_{66}O_4$) (labeled as "Ligand of Interest" by depositor).



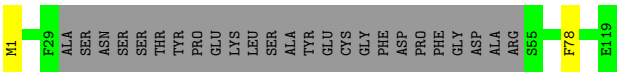
Mol	Chain	Residues	Atoms			AltConf
69	BC	1	Total 48	C 44	O 4	0

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.

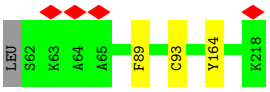
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



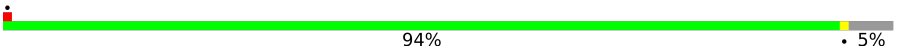
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

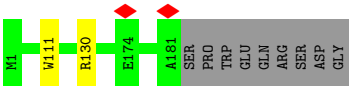
Chain B:



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

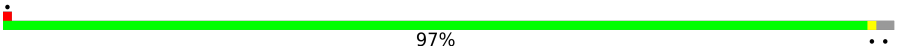
Chain C:

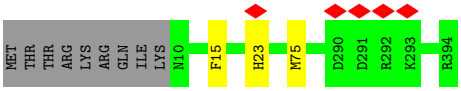




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

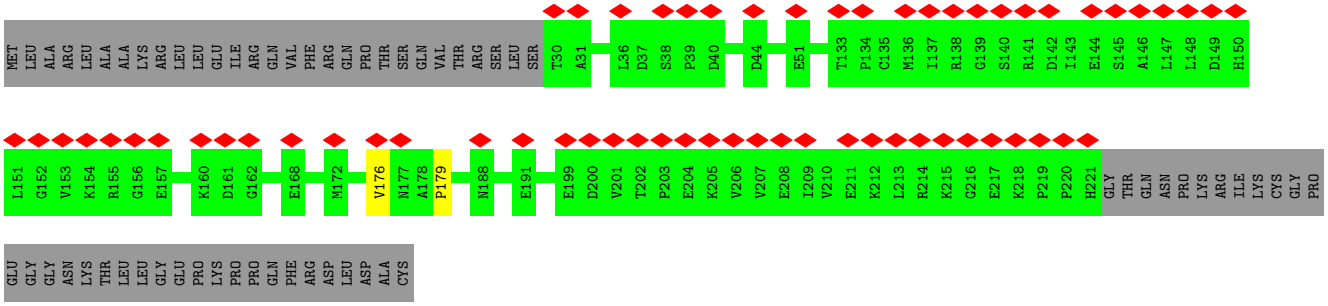
Chain D:



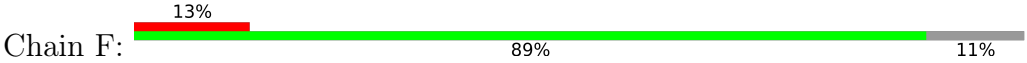


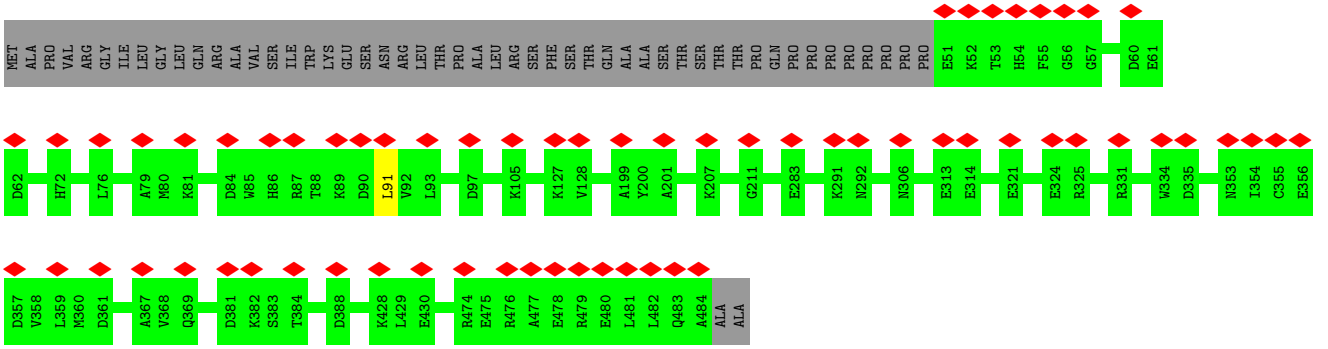
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

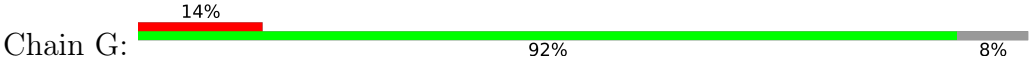


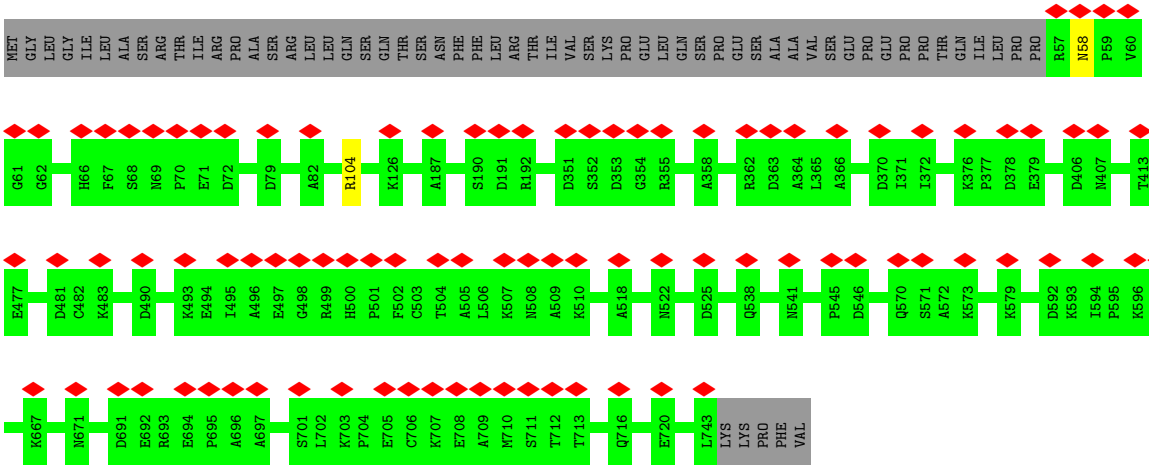
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



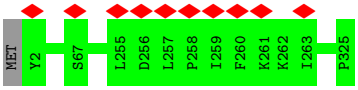


• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial



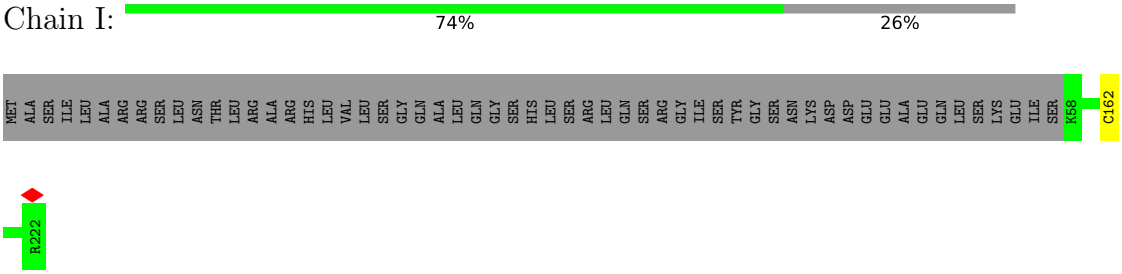


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



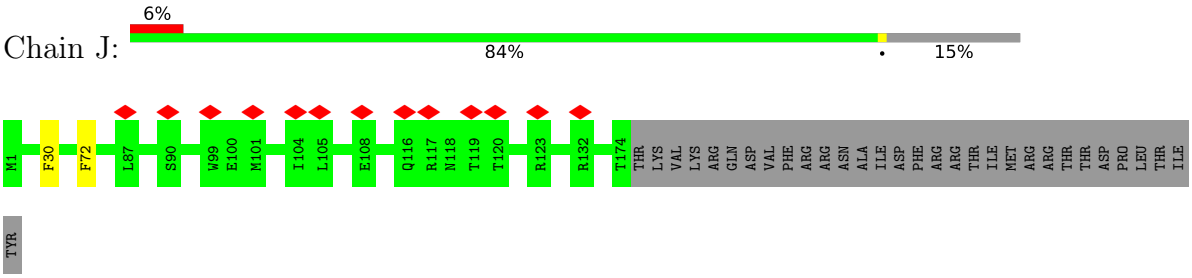
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I:



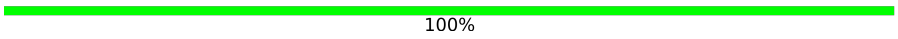
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



• Molecule 11: NADH dehydrogenase subunit 4L

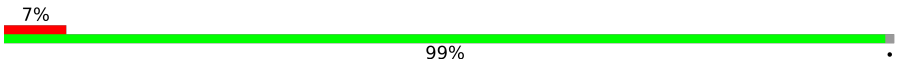
Chain K:

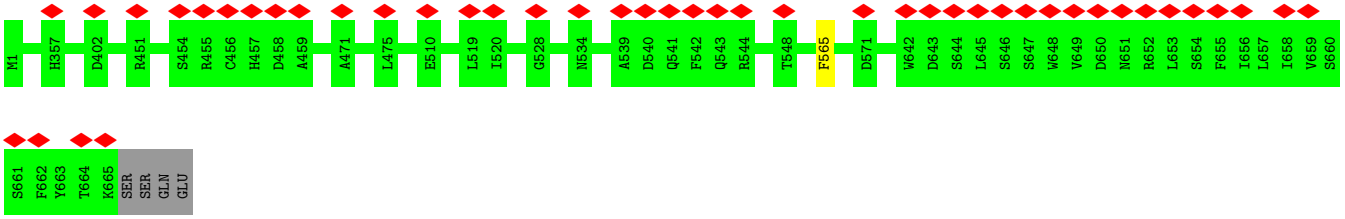


There are no outlier residues recorded for this chain.

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

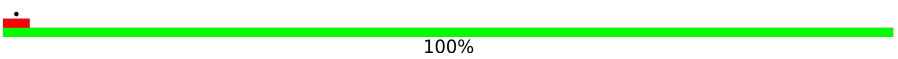
Chain L:

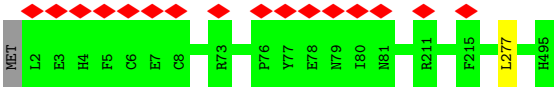




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

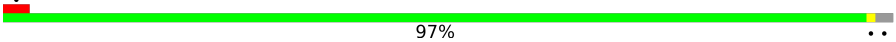
Chain M:

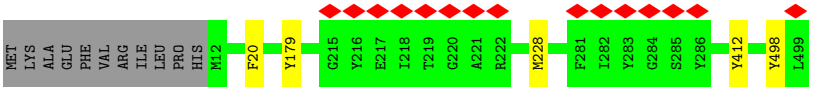




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

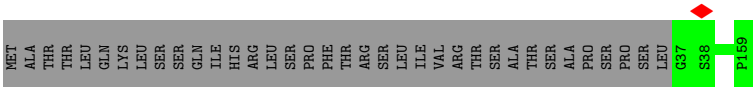
Chain N:





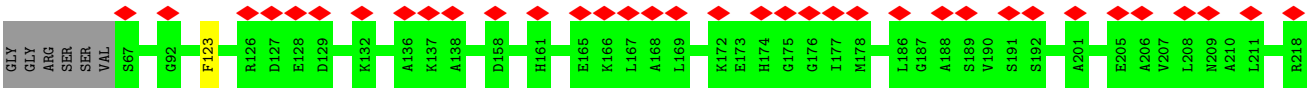
• Molecule 15: AT3G07480.1

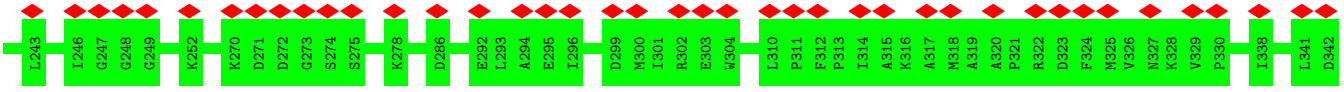
Chain O:

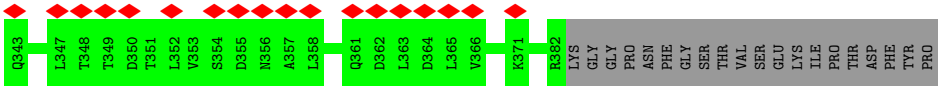


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

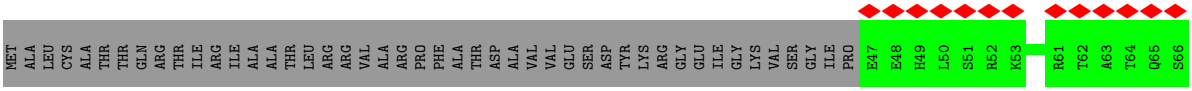


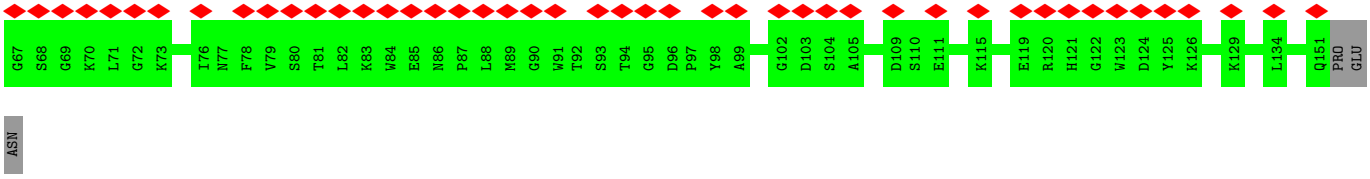




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

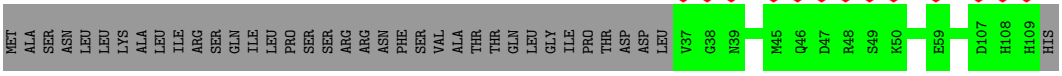
Chain Q:





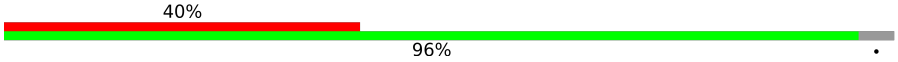
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

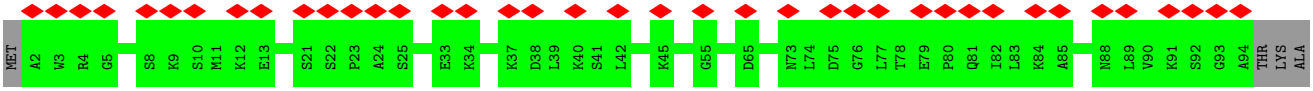
Chain R:



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

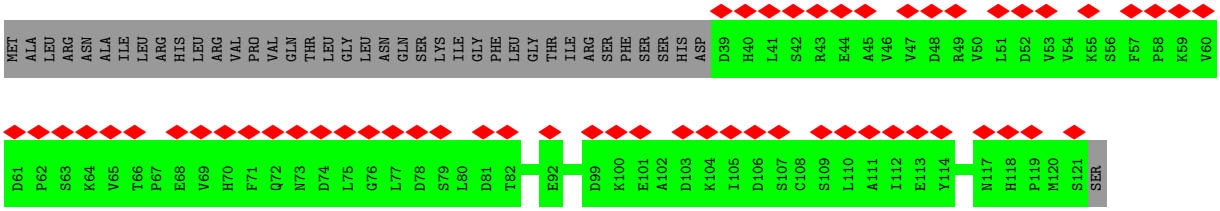
Chain S:





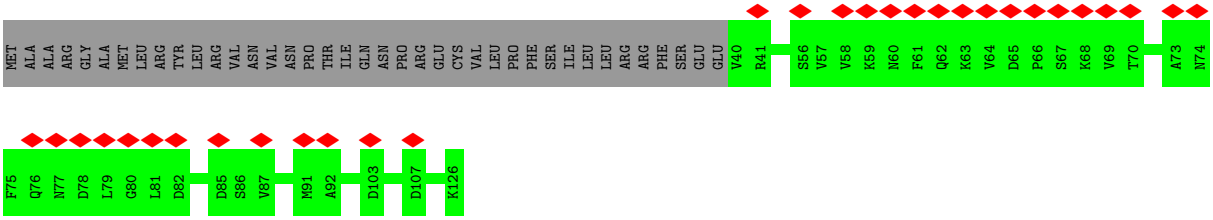
• Molecule 20: Acyl carrier protein 1, mitochondrial

Chain T:



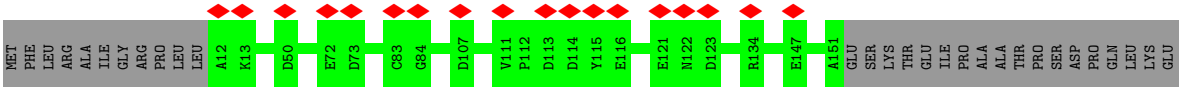
• Molecule 21: Acyl carrier protein 2, mitochondrial

Chain U:



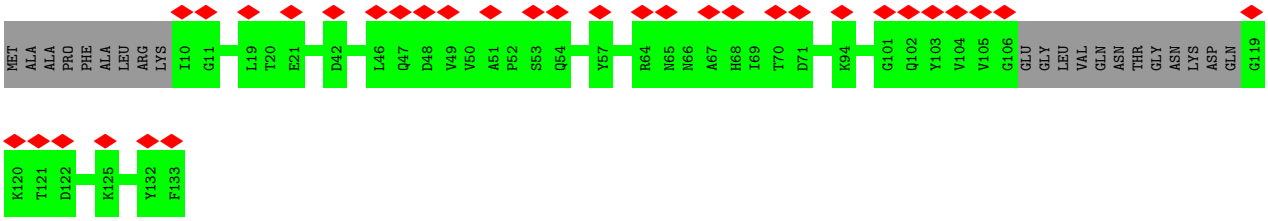
• Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

Chain V:



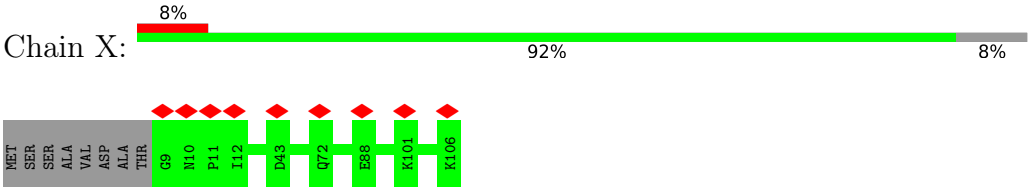
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



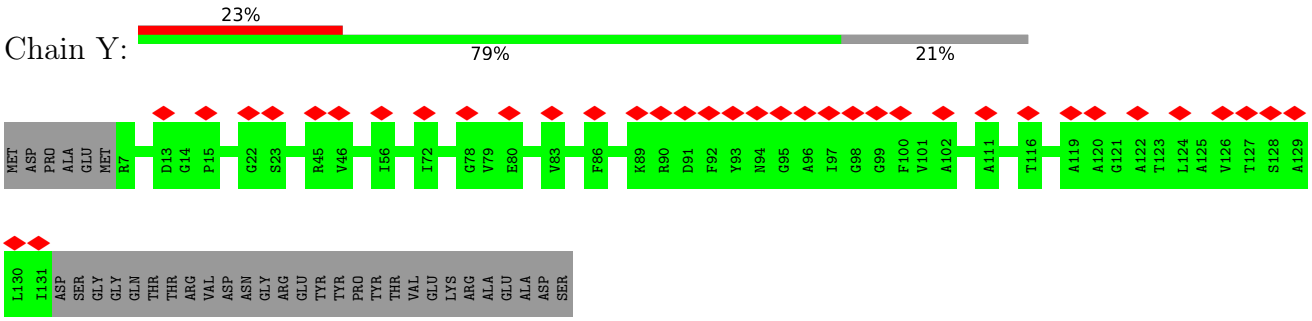
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

Chain X:



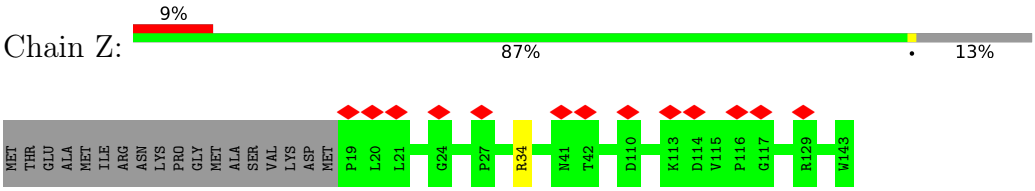
• Molecule 25: Outer envelope pore protein 16-3, chloroplastic/mitochondrial

Chain Y:



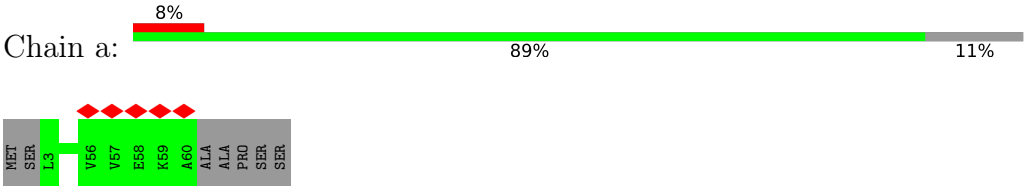
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A

Chain Z:



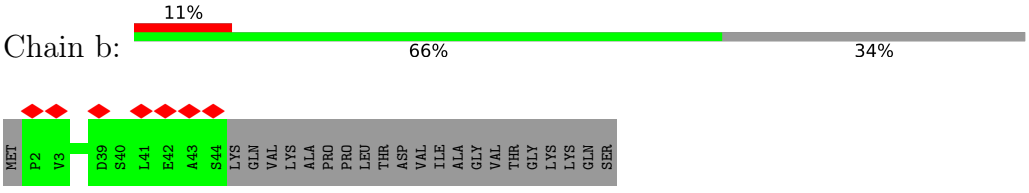
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



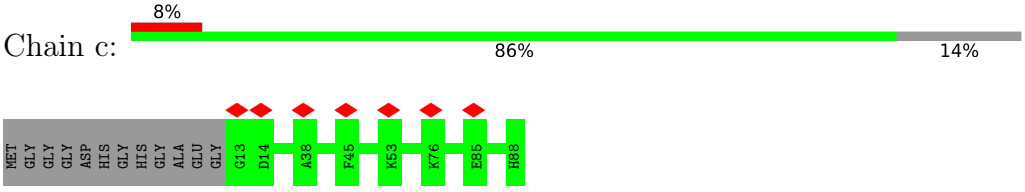
• Molecule 28: At2g46540/F11C10.23

Chain b:



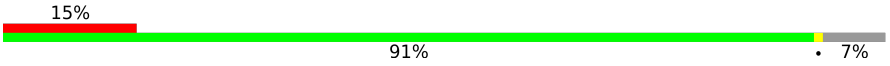
• Molecule 29: Transmembrane protein

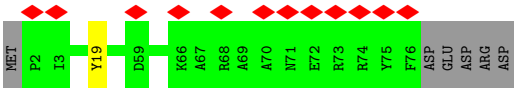
Chain c:



• Molecule 30: Excitatory amino acid transporter

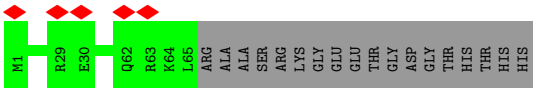
Chain d:





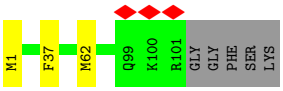
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B

Chain e:



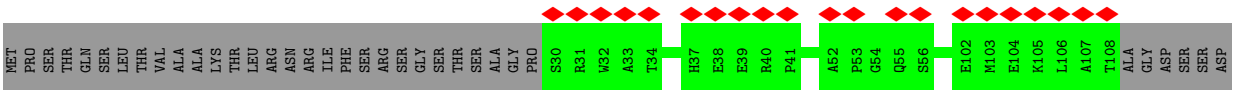
• Molecule 32: At4g16450

Chain f:



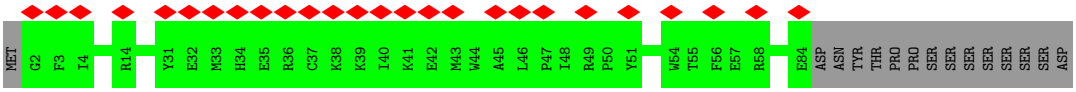
• Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

Chain g:



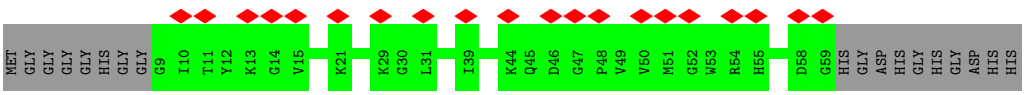
• Molecule 34: P1

Chain i:



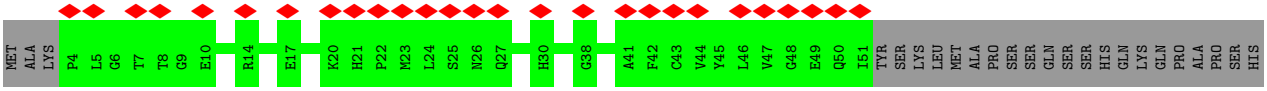
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

Chain j:



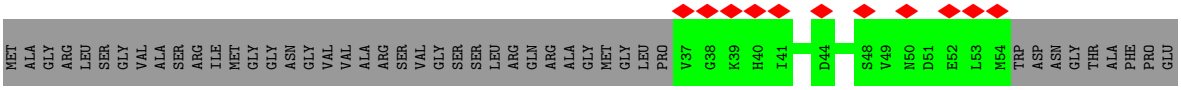
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A

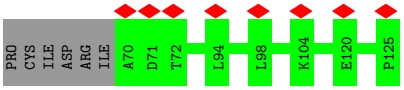
Chain k:



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

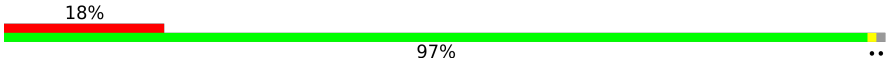
Chain l:

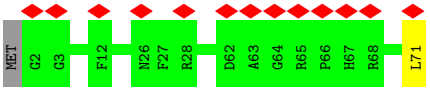




• Molecule 38: B15 – 1 beta subcomplex subunit 4

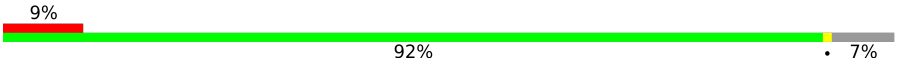
Chain m:

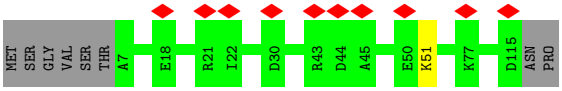




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

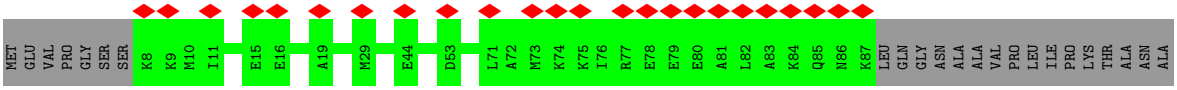
Chain n:





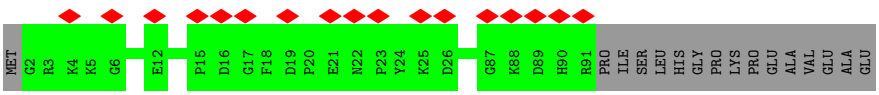
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



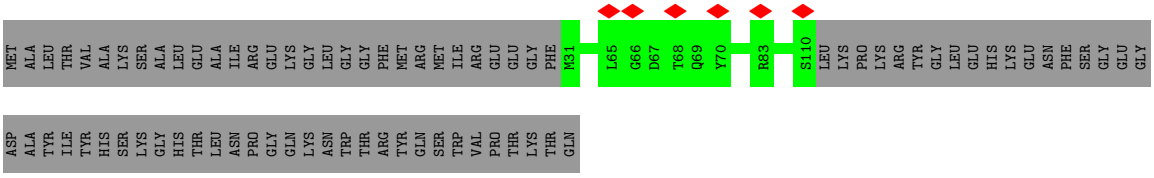
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

Chain p:

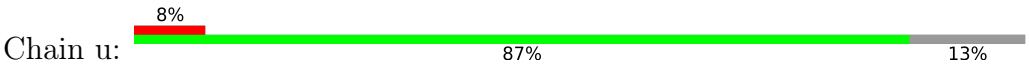


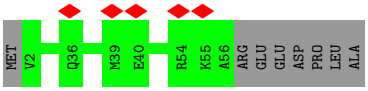
• Molecule 42: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

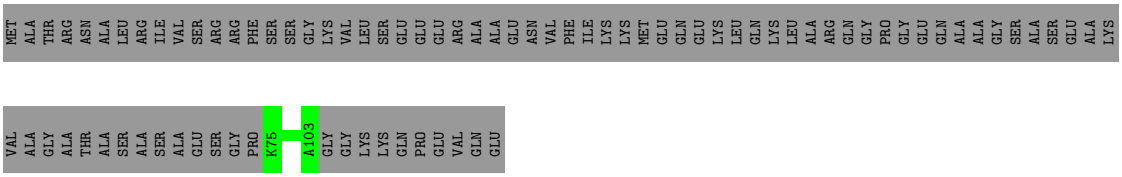


• Molecule 43: Uncharacterized protein At1g67785

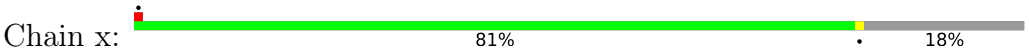


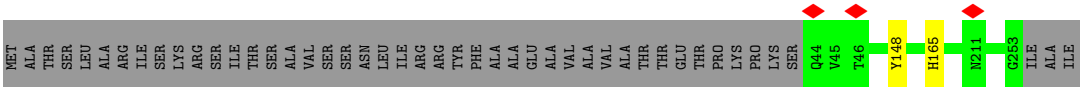


• Molecule 44: Uncharacterized protein At2g27730, mitochondrial

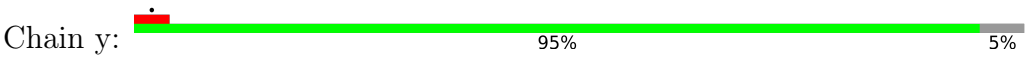


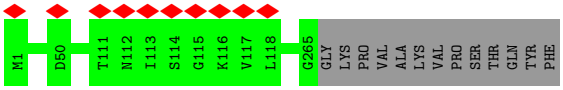
• Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial



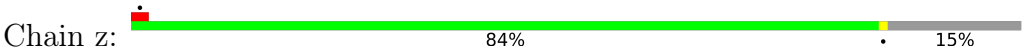


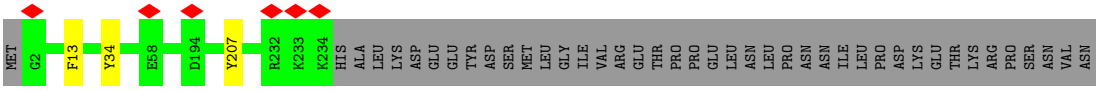
• Molecule 46: Gamma carbonic anhydrase 2, mitochondrial



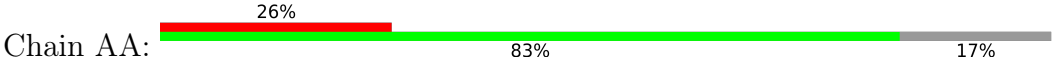


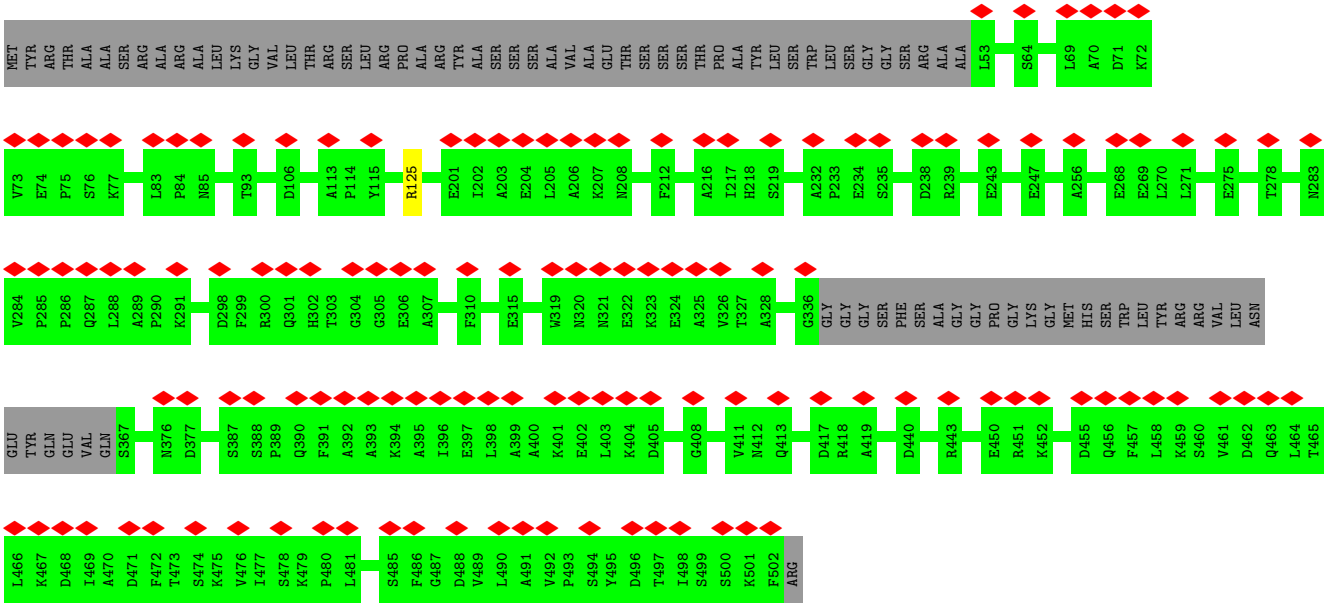
• Molecule 47: Gamma carbonic anhydrase 1, mitochondrial





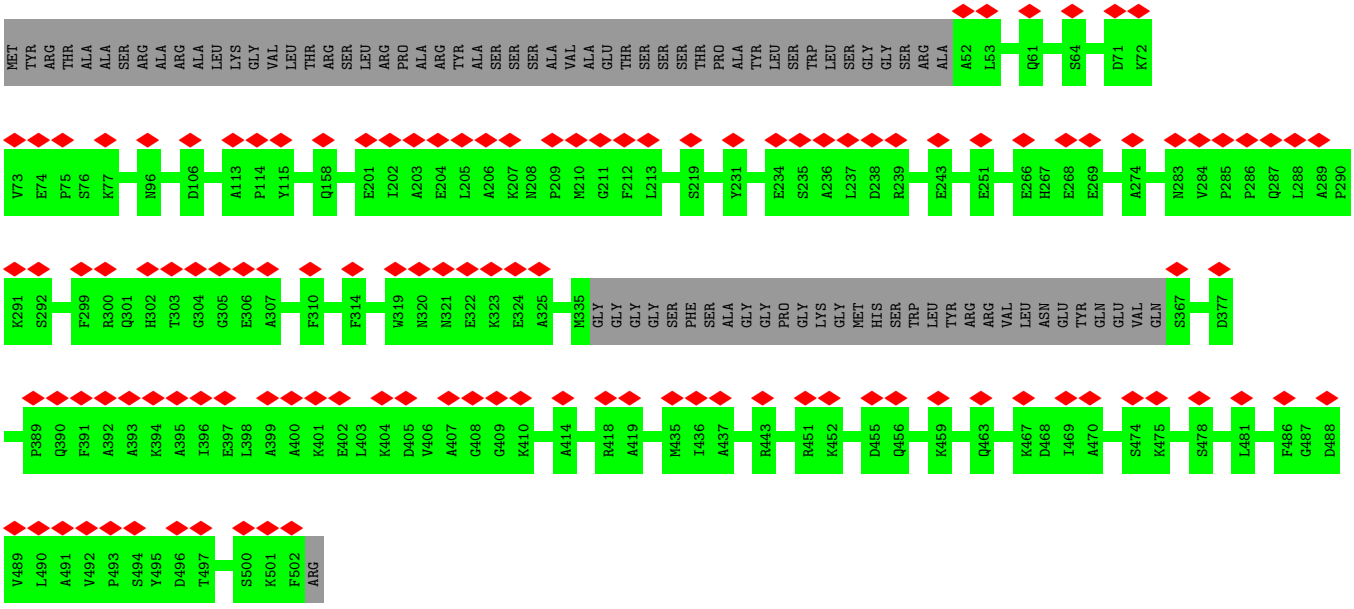
• Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial





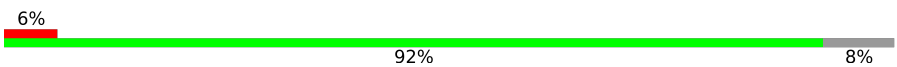
• Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

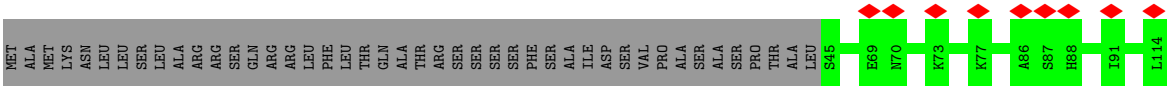
Chain BA:

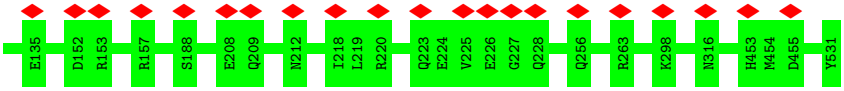


• Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain AB:

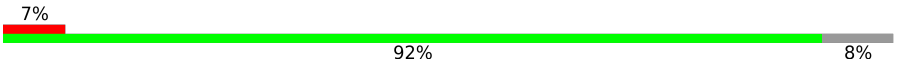


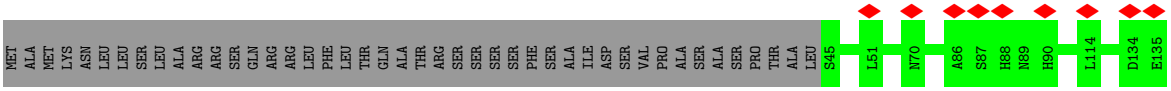


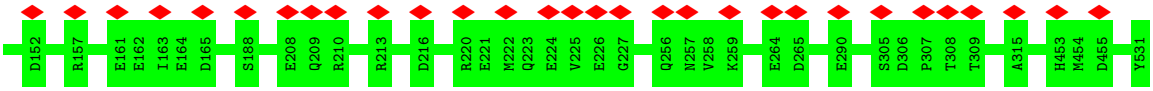


• Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain BB:

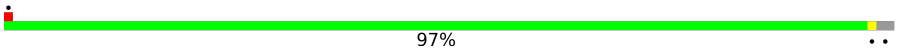


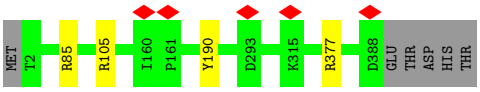




• Molecule 50: Cytochrome b

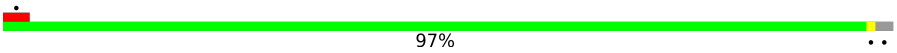
Chain AC:

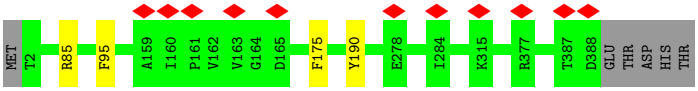




• Molecule 50: Cytochrome b

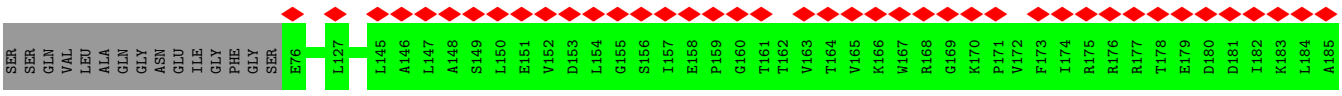
Chain BC:

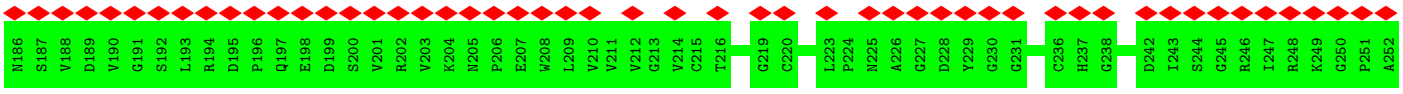


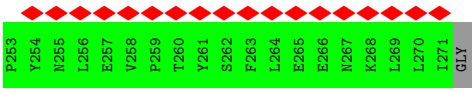


• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

Chain AD:

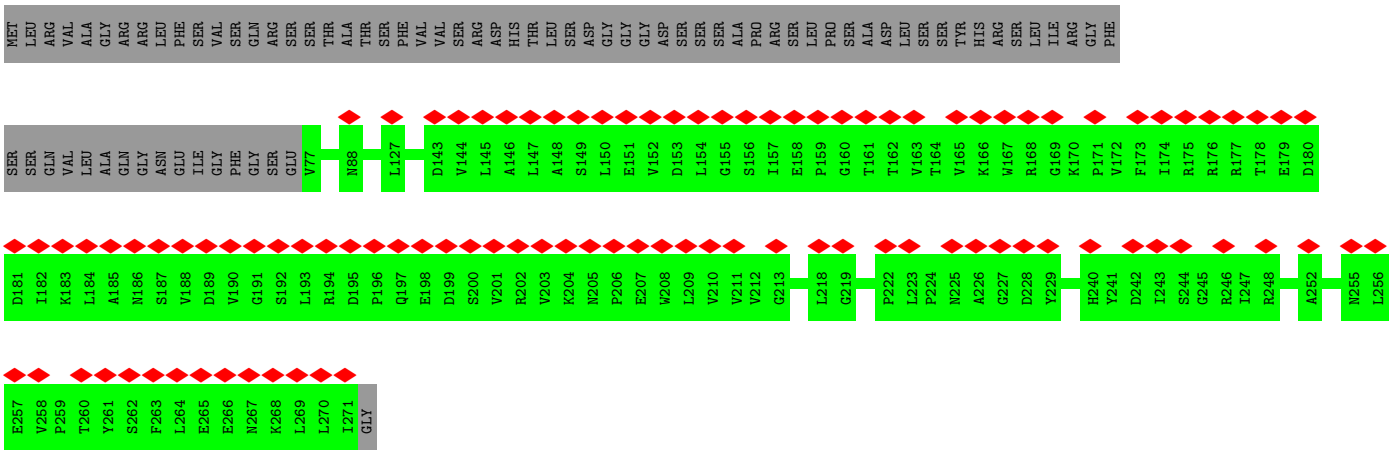






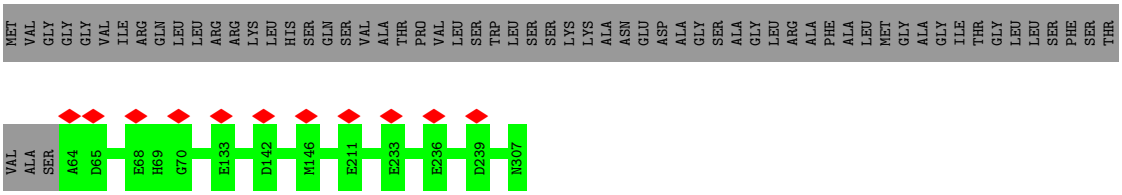
• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

Chain BD:



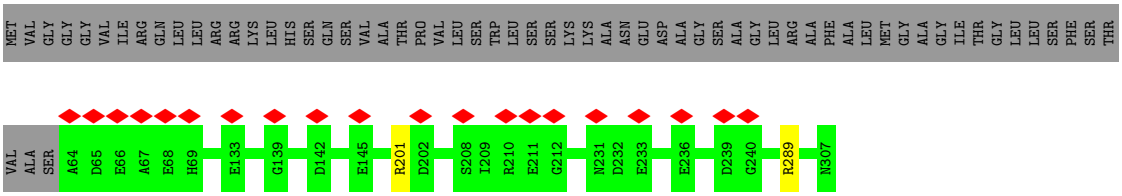
• Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

Chain AE:



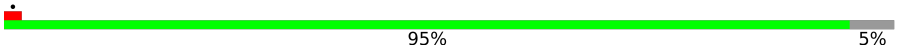
• Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

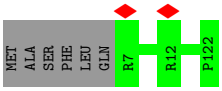
Chain BE:



• Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

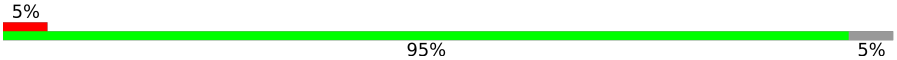
Chain AF:

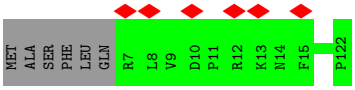




• Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

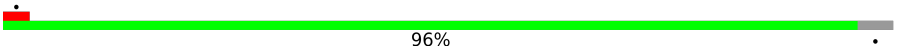
Chain BF:

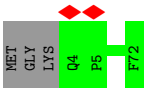




• Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

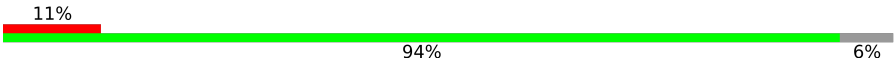
Chain AG:

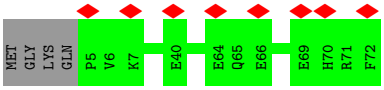




• Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

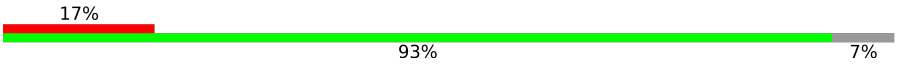
Chain BG:

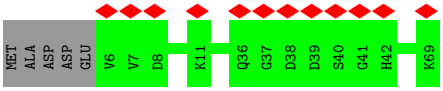




• Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial

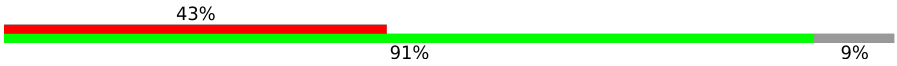
Chain AH:

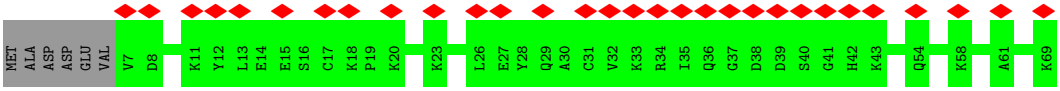




• Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial

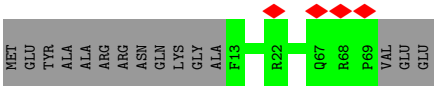
Chain BH:





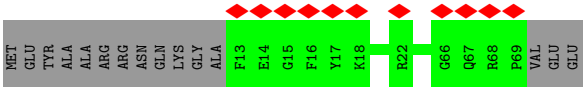
• Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain AI:



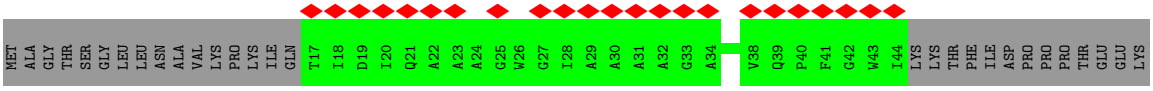
• Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain BI:



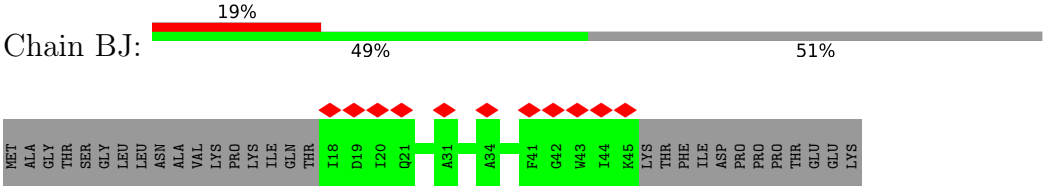
• Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain AJ:



• Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain BJ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	429.75, 429.75, 429.75	wwPDB
Map dimensions	750, 750, 750	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FE, FME, HEM, ZN, UQ5, UQ7, UQ9, COO, NDP, 8Q1, FMN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/820	0.60	0/1113
2	B	0.36	0/1279	0.56	0/1734
3	C	0.38	0/1590	0.55	0/2152
4	D	0.39	0/3149	0.60	0/4259
5	E	0.34	0/1535	0.54	1/2084 (0.0%)
6	F	0.31	0/3441	0.52	1/4641 (0.0%)
7	G	0.36	0/5338	0.56	0/7231
8	H	0.45	0/2609	0.58	0/3553
9	I	0.33	0/1378	0.56	0/1862
10	J	0.37	0/1435	0.55	0/1957
11	K	0.39	0/785	0.56	0/1062
12	L	0.37	0/5368	0.52	0/7291
13	M	0.40	0/4057	0.55	0/5513
14	N	0.41	0/3937	0.59	2/5345 (0.0%)
15	O	0.34	0/979	0.56	0/1326
16	P	0.39	0/2509	0.55	0/3401
17	Q	0.29	0/862	0.48	0/1166
18	R	0.28	0/585	0.46	0/793
19	S	0.33	0/739	0.52	0/996
20	T	0.51	0/671	0.62	0/911
21	U	0.61	0/687	0.70	0/929
22	V	0.30	0/1146	0.50	0/1555
23	W	0.42	0/923	0.52	0/1249
24	X	0.41	0/790	0.53	0/1060
25	Y	0.32	0/944	0.59	0/1277
26	Z	0.35	0/1027	0.55	0/1392
27	a	0.32	0/481	0.49	0/646
28	b	0.32	0/320	0.57	0/434
29	c	0.35	0/637	0.54	0/860
30	d	0.43	0/605	0.58	0/815
31	e	0.34	0/567	0.55	0/755
32	f	0.34	0/771	0.50	0/1042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	g	0.32	0/661	0.53	0/899
34	i	0.34	0/741	0.59	0/997
35	j	0.40	0/433	0.53	0/592
36	k	0.35	0/392	0.54	0/526
37	l	0.37	0/575	0.53	0/781
38	m	0.36	0/592	0.55	0/793
39	n	0.43	0/938	0.60	1/1273 (0.1%)
40	o	0.35	0/666	0.52	0/886
41	p	0.38	0/777	0.59	0/1043
42	q	0.31	0/690	0.55	0/936
43	u	0.40	0/472	0.55	0/632
44	v	0.32	0/222	0.49	0/300
45	x	0.33	0/1669	0.56	0/2279
46	y	0.33	0/2046	0.53	0/2772
47	z	0.36	0/1804	0.59	0/2441
48	AA	0.35	0/3265	0.54	0/4431
48	BA	0.32	0/3266	0.53	0/4433
49	AB	0.32	0/3908	0.54	0/5305
49	BB	0.31	0/3908	0.53	0/5305
50	AC	0.35	0/3208	0.48	0/4395
50	BC	0.34	0/3208	0.50	0/4395
51	AD	0.32	0/1567	0.54	0/2135
51	BD	0.31	0/1558	0.54	0/2123
52	AE	0.36	0/1968	0.52	0/2672
52	BE	0.33	0/1968	0.49	0/2672
53	AF	0.33	0/993	0.60	0/1336
53	BF	0.32	0/993	0.56	0/1336
54	AG	0.30	0/600	0.47	0/815
54	BG	0.28	0/591	0.47	0/802
55	AH	0.42	0/531	0.54	0/713
55	BH	0.29	0/524	0.44	0/703
56	AI	0.42	0/488	0.59	0/655
56	BI	0.35	0/488	0.55	0/655
57	AJ	0.27	0/210	0.41	0/290
57	BJ	0.25	0/212	0.36	0/291
All	All	0.36	0/98096	0.54	5/133016 (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
14	N	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	179	PRO	N-CA-C	-7.09	93.65	112.10
39	n	51	LYS	CD-CE-NZ	6.48	126.61	111.70
14	N	228	MET	CG-SD-CE	-5.95	90.68	100.20
14	N	228	MET	CA-CB-CG	-5.41	104.10	113.30
6	F	91	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	412[B]	TYR	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	90/119 (76%)	88 (98%)	2 (2%)	0	100 100
2	B	155/218 (71%)	149 (96%)	6 (4%)	0	100 100
3	C	179/190 (94%)	177 (99%)	2 (1%)	0	100 100
4	D	383/394 (97%)	367 (96%)	15 (4%)	1 (0%)	41 72
5	E	190/255 (74%)	181 (95%)	9 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	432/486 (89%)	420 (97%)	12 (3%)	0	100	100
7	G	685/748 (92%)	665 (97%)	20 (3%)	0	100	100
8	H	322/325 (99%)	316 (98%)	6 (2%)	0	100	100
9	I	163/222 (73%)	162 (99%)	1 (1%)	0	100	100
10	J	172/205 (84%)	170 (99%)	2 (1%)	0	100	100
11	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
12	L	663/669 (99%)	638 (96%)	25 (4%)	0	100	100
13	M	492/495 (99%)	484 (98%)	8 (2%)	0	100	100
14	N	487/499 (98%)	475 (98%)	12 (2%)	0	100	100
15	O	121/159 (76%)	118 (98%)	3 (2%)	0	100	100
16	P	314/402 (78%)	303 (96%)	11 (4%)	0	100	100
17	Q	103/154 (67%)	99 (96%)	4 (4%)	0	100	100
18	R	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
19	S	91/97 (94%)	90 (99%)	1 (1%)	0	100	100
20	T	81/122 (66%)	78 (96%)	3 (4%)	0	100	100
21	U	85/126 (68%)	78 (92%)	7 (8%)	0	100	100
22	V	138/169 (82%)	132 (96%)	6 (4%)	0	100	100
23	W	108/133 (81%)	103 (95%)	5 (5%)	0	100	100
24	X	96/106 (91%)	94 (98%)	2 (2%)	0	100	100
25	Y	123/159 (77%)	119 (97%)	4 (3%)	0	100	100
26	Z	123/143 (86%)	119 (97%)	4 (3%)	0	100	100
27	a	56/65 (86%)	56 (100%)	0	0	100	100
28	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
29	c	74/88 (84%)	71 (96%)	3 (4%)	0	100	100
30	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
31	e	63/83 (76%)	62 (98%)	1 (2%)	0	100	100
32	f	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
33	g	77/114 (68%)	76 (99%)	1 (1%)	0	100	100
34	i	81/98 (83%)	79 (98%)	2 (2%)	0	100	100
35	j	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
36	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	l	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
38	m	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
39	n	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
40	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
41	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
42	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
43	u	53/63 (84%)	50 (94%)	3 (6%)	0	100	100
44	v	27/113 (24%)	26 (96%)	1 (4%)	0	100	100
45	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
46	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
47	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
48	AA	416/503 (83%)	399 (96%)	17 (4%)	0	100	100
48	BA	416/503 (83%)	402 (97%)	14 (3%)	0	100	100
49	AB	485/531 (91%)	473 (98%)	12 (2%)	0	100	100
49	BB	485/531 (91%)	478 (99%)	7 (1%)	0	100	100
50	AC	385/393 (98%)	378 (98%)	7 (2%)	0	100	100
50	BC	385/393 (98%)	377 (98%)	8 (2%)	0	100	100
51	AD	194/272 (71%)	181 (93%)	13 (7%)	0	100	100
51	BD	193/272 (71%)	182 (94%)	11 (6%)	0	100	100
52	AE	242/307 (79%)	239 (99%)	3 (1%)	0	100	100
52	BE	242/307 (79%)	240 (99%)	2 (1%)	0	100	100
53	AF	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
53	BF	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
54	AG	67/72 (93%)	67 (100%)	0	0	100	100
54	BG	66/72 (92%)	66 (100%)	0	0	100	100
55	AH	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
55	BH	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
56	AI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
56	BI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
57	AJ	26/57 (46%)	26 (100%)	0	0	100	100
57	BJ	26/57 (46%)	24 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11985/14108 (85%)	11664 (97%)	320 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	23	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	85/105 (81%)	84 (99%)	1 (1%)	71 92
2	B	132/184 (72%)	129 (98%)	3 (2%)	50 82
3	C	171/179 (96%)	169 (99%)	2 (1%)	71 92
4	D	331/340 (97%)	329 (99%)	2 (1%)	86 96
5	E	166/220 (76%)	165 (99%)	1 (1%)	86 96
6	F	353/396 (89%)	353 (100%)	0	100 100
7	G	570/625 (91%)	568 (100%)	2 (0%)	91 97
8	H	271/272 (100%)	271 (100%)	0	100 100
9	I	147/195 (75%)	146 (99%)	1 (1%)	84 95
10	J	156/186 (84%)	154 (99%)	2 (1%)	69 91
11	K	85/85 (100%)	85 (100%)	0	100 100
12	L	564/568 (99%)	563 (100%)	1 (0%)	93 98
13	M	433/434 (100%)	432 (100%)	1 (0%)	93 98
14	N	407/416 (98%)	404 (99%)	3 (1%)	84 95
15	O	108/141 (77%)	108 (100%)	0	100 100
16	P	263/334 (79%)	262 (100%)	1 (0%)	91 97
17	Q	89/128 (70%)	89 (100%)	0	100 100
18	R	64/97 (66%)	64 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	82/85 (96%)	82 (100%)	0	100 100
20	T	78/112 (70%)	78 (100%)	0	100 100
21	U	78/113 (69%)	78 (100%)	0	100 100
22	V	123/148 (83%)	123 (100%)	0	100 100
23	W	98/114 (86%)	98 (100%)	0	100 100
24	X	88/94 (94%)	88 (100%)	0	100 100
25	Y	92/120 (77%)	92 (100%)	0	100 100
26	Z	100/115 (87%)	99 (99%)	1 (1%)	76 93
27	a	48/53 (91%)	48 (100%)	0	100 100
28	b	35/53 (66%)	35 (100%)	0	100 100
29	c	66/71 (93%)	66 (100%)	0	100 100
30	d	60/66 (91%)	59 (98%)	1 (2%)	60 87
31	e	60/73 (82%)	60 (100%)	0	100 100
32	f	80/83 (96%)	78 (98%)	2 (2%)	47 80
33	g	68/96 (71%)	68 (100%)	0	100 100
34	i	75/90 (83%)	75 (100%)	0	100 100
35	j	42/51 (82%)	42 (100%)	0	100 100
36	k	39/60 (65%)	39 (100%)	0	100 100
37	l	60/97 (62%)	60 (100%)	0	100 100
38	m	58/59 (98%)	57 (98%)	1 (2%)	60 87
39	n	92/99 (93%)	92 (100%)	0	100 100
40	o	70/87 (80%)	70 (100%)	0	100 100
41	p	80/93 (86%)	80 (100%)	0	100 100
42	q	69/133 (52%)	69 (100%)	0	100 100
43	u	47/54 (87%)	47 (100%)	0	100 100
44	v	22/84 (26%)	22 (100%)	0	100 100
45	x	179/216 (83%)	177 (99%)	2 (1%)	73 92
46	y	221/232 (95%)	221 (100%)	0	100 100
47	z	188/228 (82%)	185 (98%)	3 (2%)	62 88
48	AA	347/408 (85%)	346 (100%)	1 (0%)	92 98
48	BA	347/408 (85%)	347 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	AB	415/452 (92%)	415 (100%)	0	100	100
49	BB	415/452 (92%)	415 (100%)	0	100	100
50	AC	330/336 (98%)	326 (99%)	4 (1%)	71	92
50	BC	330/336 (98%)	326 (99%)	4 (1%)	71	92
51	AD	170/232 (73%)	170 (100%)	0	100	100
51	BD	169/232 (73%)	169 (100%)	0	100	100
52	AE	200/247 (81%)	200 (100%)	0	100	100
52	BE	200/247 (81%)	198 (99%)	2 (1%)	76	93
53	AF	105/110 (96%)	105 (100%)	0	100	100
53	BF	105/110 (96%)	105 (100%)	0	100	100
54	AG	63/65 (97%)	63 (100%)	0	100	100
54	BG	62/65 (95%)	62 (100%)	0	100	100
55	AH	58/62 (94%)	58 (100%)	0	100	100
55	BH	57/62 (92%)	57 (100%)	0	100	100
56	AI	48/59 (81%)	48 (100%)	0	100	100
56	BI	48/59 (81%)	48 (100%)	0	100	100
57	AJ	16/41 (39%)	16 (100%)	0	100	100
57	BJ	16/41 (39%)	16 (100%)	0	100	100
All	All	10294/11908 (86%)	10253 (100%)	41 (0%)	91	97

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	PHE
2	B	89	PHE
2	B	93	CYS
2	B	164	TYR
3	C	111	TRP
3	C	130	ARG
4	D	15	PHE
4	D	75	MET
5	E	176	VAL
7	G	58	ASN
7	G	104	ARG
9	I	162	CYS
10	J	30	PHE

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Mol	Chain	Res	Type
10	J	72	PHE
12	L	565	PHE
13	M	277	LEU
14	N	20	PHE
14	N	179	TYR
14	N	498	TYR
16	P	123	PHE
26	Z	34	ARG
30	d	19	TYR
32	f	37	PHE
32	f	62	MET
38	m	71	LEU
45	x	148	TYR
45	x	165	HIS
47	z	13	PHE
47	z	34	TYR
47	z	207	TYR
48	AA	125	ARG
50	AC	85	ARG
50	AC	105	ARG
50	AC	190	TYR
50	AC	377	ARG
50	BC	85	ARG
50	BC	95	PHE
50	BC	175	PHE
50	BC	190	TYR
52	BE	201	ARG
52	BE	289	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	GLN
2	B	203	GLN
4	D	311	HIS
6	F	404	GLN
7	G	184	GLN
7	G	302	ASN
8	H	176	GLN
10	J	80	HIS
13	M	341	HIS
13	M	411	ASN

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Mol	Chain	Res	Type
13	M	434	ASN
13	M	487	ASN
14	N	491	HIS
16	P	343	GLN
17	Q	65	GLN
20	T	118	HIS
23	W	102	GLN
24	X	87	ASN
25	Y	84	GLN
25	Y	94	ASN
29	c	32	HIS
35	j	18	HIS
41	p	22	ASN
42	q	45	HIS
44	v	83	ASN
45	x	61	GLN
46	y	42	HIS
46	y	72	GLN
47	z	223	ASN
48	AA	415	HIS
50	AC	6	GLN
50	AC	20	ASN
50	AC	183	ASN
52	AE	101	GLN
48	BA	463	GLN
49	BB	337	GLN
49	BB	453	HIS
54	BG	19	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.70	1 (12%)	7,9,11	2.10	3 (42%)
32	FME	f	1	32	8,9,10	0.75	1 (12%)	7,9,11	1.73	1 (14%)
11	FME	K	1	11	8,9,10	0.95	0	7,9,11	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/7/9/11	-
32	FME	f	1	32	-	5/7/9/11	-
11	FME	K	1	11	-	6/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	FME	O-C	4.15	1.36	1.19
32	f	1	FME	O-C	2.04	1.28	1.19

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	1	FME	O-C-CA	-4.27	113.59	124.78
1	A	1	FME	O-C-CA	-4.08	114.07	124.78
1	A	1	FME	C-CA-N	2.67	114.56	109.73
1	A	1	FME	CA-N-CN	2.23	126.25	122.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	O-C-CA-CB
32	f	1	FME	O1-CN-N-CA
32	f	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
32	f	1	FME	N-CA-CB-CG
32	f	1	FME	C-CA-CB-CG
32	f	1	FME	CA-CB-CG-SD
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
11	K	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 5 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
66	COO	y	301	-	45,55,55	3.96	16 (35%)	55,81,81	2.70	12 (21%)
68	UQ5	AC	502	-	38,38,38	0.52	0	46,49,49	0.69	0
58	SF4	G	803	7	0,12,12	-	-	-		
58	SF4	F	501	6	0,12,12	-	-	-		
60	FMN	F	500	-	33,33,33	1.06	2 (6%)	48,50,50	1.24	6 (12%)
67	HEM	BC	500	50	41,50,50	1.41	3 (7%)	45,82,82	1.36	7 (15%)
61	UQ9	H	500	-	35,35,58	0.79	2 (5%)	42,45,73	0.95	5 (11%)
68	UQ5	AC	503	-	38,38,38	0.47	0	46,49,49	0.89	1 (2%)
59	FES	AD	301	51	0,4,4	-	-	-		
63	NDP	P	500	-	45,52,52	0.63	1 (2%)	53,80,80	0.68	1 (1%)
59	FES	BD	301	51	0,4,4	-	-	-		
67	HEM	AC	500	50	41,50,50	1.43	3 (7%)	45,82,82	1.36	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
65	8Q1	W	200	-	31,34,34	0.32	0	40,43,43	0.49	0
58	SF4	I	500	9	0,12,12	-	-	-		
58	SF4	B	500	2	0,12,12	-	-	-		
67	HEM	BE	400	52	41,50,50	1.41	3 (7%)	45,82,82	1.39	6 (13%)
59	FES	G	801	7	0,4,4	-	-	-		
59	FES	E	500	5	0,4,4	-	-	-		
68	UQ5	BC	502	-	38,38,38	0.46	0	46,49,49	0.70	0
67	HEM	BC	501	50	41,50,50	1.38	5 (12%)	45,82,82	1.83	11 (24%)
69	UQ7	BC	503	-	48,48,48	0.44	0	58,61,61	0.59	0
58	SF4	I	501	9	0,12,12	-	-	-		
67	HEM	AC	501	50	41,50,50	1.38	6 (14%)	45,82,82	1.80	10 (22%)
65	8Q1	n	200	-	31,34,34	0.30	0	40,43,43	0.62	1 (2%)
58	SF4	G	802	7	0,12,12	-	-	-		
67	HEM	AE	400	52	41,50,50	1.40	3 (7%)	45,82,82	1.38	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	COO	y	301	-	1/1/12/16	21/50/70/70	0/3/3/3
68	UQ5	AC	502	-	-	7/33/57/57	0/1/1/1
58	SF4	G	803	7	-	-	0/6/5/5
58	SF4	F	501	6	-	-	0/6/5/5
60	FMN	F	500	-	-	5/18/18/18	0/3/3/3
67	HEM	BC	500	50	-	2/12/54/54	-
61	UQ9	H	500	-	-	19/30/54/81	0/1/1/1
68	UQ5	AC	503	-	-	12/33/57/57	0/1/1/1
63	NDP	P	500	-	-	6/30/77/77	0/5/5/5
59	FES	AD	301	51	-	-	0/1/1/1
59	FES	BD	301	51	-	-	0/1/1/1
67	HEM	AC	500	50	-	4/12/54/54	-
65	8Q1	W	200	-	-	22/41/41/41	-
58	SF4	I	500	9	-	-	0/6/5/5
58	SF4	B	500	2	-	-	0/6/5/5
67	HEM	BE	400	52	-	2/12/54/54	-
59	FES	G	801	7	-	-	0/1/1/1
59	FES	E	500	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	UQ5	BC	502	-	-	8/33/57/57	0/1/1/1
67	HEM	BC	501	50	-	7/12/54/54	-
69	UQ7	BC	503	-	-	8/45/69/69	0/1/1/1
58	SF4	I	501	9	-	-	0/6/5/5
67	HEM	AC	501	50	-	7/12/54/54	-
65	8Q1	n	200	-	-	19/41/41/41	-
58	SF4	G	802	7	-	-	0/6/5/5
67	HEM	AE	400	52	-	2/12/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	y	301	COO	C2A-N1A	-15.84	1.04	1.33
66	y	301	COO	C2A-N3A	-8.97	1.17	1.32
66	y	301	COO	C5A-C4A	8.01	1.62	1.40
66	y	301	COO	C1-N1	7.63	1.50	1.33
66	y	301	COO	C4-N2	6.55	1.48	1.33
66	y	301	COO	O4X-C1X	6.09	1.49	1.41
66	y	301	COO	C6A-N1A	-5.59	1.12	1.37
66	y	301	COO	C4A-N3A	5.53	1.43	1.35
67	AE	400	HEM	C3C-C2C	-4.07	1.34	1.40
66	y	301	COO	C5A-N7A	-4.03	1.25	1.39
67	BE	400	HEM	C3C-C2C	-3.98	1.34	1.40
67	BC	500	HEM	C3C-C2C	-3.98	1.34	1.40
66	y	301	COO	C2X-C1X	-3.92	1.47	1.53
67	AC	500	HEM	C3C-C2C	-3.84	1.35	1.40
67	AC	501	HEM	C1B-NB	-3.82	1.33	1.40
67	BC	501	HEM	C1B-NB	-3.80	1.33	1.40
60	F	500	FMN	C4A-N5	3.71	1.38	1.30
67	BE	400	HEM	C3C-CAC	3.70	1.55	1.47
67	AC	500	HEM	C3C-CAC	3.63	1.55	1.47
67	BC	500	HEM	C3C-CAC	3.54	1.55	1.47
67	AE	400	HEM	C3C-CAC	3.48	1.54	1.47
67	BC	501	HEM	C4D-ND	-3.44	1.34	1.40
67	AC	501	HEM	C4D-ND	-3.38	1.34	1.40
66	y	301	COO	P3X-O3X	3.34	1.65	1.59
67	AC	501	HEM	FE-NB	3.10	2.12	1.96
66	y	301	COO	C6A-N6A	3.04	1.45	1.34
67	BC	501	HEM	FE-NB	2.98	2.11	1.96
67	BC	500	HEM	CAB-C3B	2.84	1.55	1.47
67	AC	500	HEM	CAB-C3B	2.82	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	y	301	COO	C3-C4	2.71	1.56	1.51
61	H	500	UQ9	C4-C5	-2.69	1.41	1.48
67	BE	400	HEM	CAB-C3B	2.67	1.54	1.47
67	AE	400	HEM	CAB-C3B	2.63	1.54	1.47
66	y	301	COO	C2X-C3X	-2.38	1.47	1.52
66	y	301	COO	O3-C4	-2.32	1.18	1.23
66	y	301	COO	P1A-O5X	2.29	1.68	1.59
67	BC	501	HEM	C1D-ND	-2.21	1.34	1.38
60	F	500	FMN	C10-N1	2.19	1.37	1.33
61	H	500	UQ9	C3-C2	-2.18	1.42	1.48
67	BC	501	HEM	C4B-NB	-2.10	1.34	1.38
67	AC	501	HEM	C4B-NB	-2.06	1.34	1.38
67	AC	501	HEM	C1D-ND	-2.06	1.34	1.38
67	AC	501	HEM	CHB-C1B	2.01	1.40	1.35
63	P	500	NDP	C8A-N7A	-2.01	1.31	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	y	301	COO	C4A-C5A-N7A	-14.04	94.77	109.40
66	y	301	COO	C6-S1-C7	7.42	109.12	99.80
66	y	301	COO	C1X-N9A-C4A	-6.80	114.70	126.64
68	AC	503	UQ5	C7-C6-C5	-4.38	113.21	118.48
67	BC	501	HEM	CHD-C1D-ND	4.38	129.19	124.43
67	AC	501	HEM	CHD-C1D-ND	4.34	129.15	124.43
67	AC	501	HEM	CHC-C4B-NB	4.29	129.09	124.43
66	y	301	COO	C2A-N1A-C6A	4.27	126.06	118.75
67	BC	501	HEM	CHC-C4B-NB	4.26	129.06	124.43
67	AC	501	HEM	C1B-NB-C4B	4.23	109.44	105.07
67	BC	501	HEM	C1B-NB-C4B	3.99	109.19	105.07
67	BC	501	HEM	CHA-C4D-ND	3.82	129.10	124.38
67	AC	501	HEM	CHA-C4D-ND	3.74	129.00	124.38
67	BC	501	HEM	CHB-C1B-NB	3.66	128.91	124.38
67	AC	501	HEM	CHB-C1B-NB	3.62	128.86	124.38
66	y	301	COO	C5A-C6A-N1A	3.34	127.92	120.35
60	F	500	FMN	C4-N3-C2	-3.24	119.66	125.64
67	BE	400	HEM	CMC-C2C-C3C	3.07	130.42	124.68
67	AE	400	HEM	CMC-C2C-C3C	3.02	130.33	124.68
60	F	500	FMN	C4A-C10-N10	3.02	120.89	116.48
67	BC	501	HEM	C4D-ND-C1D	2.98	108.15	105.07
66	y	301	COO	C5A-C6A-N6A	-2.96	115.85	120.35
67	AE	400	HEM	C4D-ND-C1D	2.93	108.09	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AC	500	HEM	C4B-CHC-C1C	2.83	126.30	122.56
67	AE	400	HEM	CAA-CBA-CGA	-2.78	105.96	113.76
61	H	500	UQ9	C7-C6-C5	2.77	121.81	118.48
66	y	301	COO	C3X-C2X-C1X	2.76	106.00	99.89
67	AC	500	HEM	C1B-NB-C4B	2.75	107.91	105.07
61	H	500	UQ9	C1-C6-C5	-2.73	117.01	119.58
66	y	301	COO	C2-C3-C4	-2.72	107.83	112.36
67	AC	501	HEM	C4D-ND-C1D	2.68	107.84	105.07
60	F	500	FMN	C4A-C4-N3	2.67	119.96	113.19
67	BC	500	HEM	C4D-ND-C1D	2.65	107.81	105.07
66	y	301	COO	P1A-O3A-P2A	-2.63	123.81	132.83
67	AC	500	HEM	C4D-ND-C1D	2.61	107.77	105.07
67	BE	400	HEM	CAA-CBA-CGA	-2.60	106.47	113.76
67	BE	400	HEM	C4D-ND-C1D	2.59	107.75	105.07
67	BC	500	HEM	CBD-CAD-C3D	-2.58	105.47	112.63
67	BC	500	HEM	C1B-NB-C4B	2.55	107.71	105.07
66	y	301	COO	C10-C9-C8	-2.50	120.41	125.34
67	BC	500	HEM	CMC-C2C-C3C	2.47	129.30	124.68
67	AC	501	HEM	CHD-C1D-C2D	-2.46	121.13	124.98
67	BE	400	HEM	CAD-CBD-CGD	-2.45	108.33	113.60
60	F	500	FMN	C10-C4A-N5	-2.43	119.70	124.86
67	BC	501	HEM	C4B-C3B-C2B	-2.40	105.21	107.11
67	AC	500	HEM	CMC-C2C-C3C	2.40	129.17	124.68
66	y	301	COO	C3-C4-N2	2.40	120.45	116.42
61	H	500	UQ9	C4-C3-C2	-2.37	116.02	120.68
60	F	500	FMN	O4-C4-C4A	-2.35	120.38	126.60
67	BE	400	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
67	BC	501	HEM	CHD-C1D-C2D	-2.29	121.41	124.98
67	BC	500	HEM	C4C-CHD-C1D	2.27	125.55	122.56
67	AC	501	HEM	C4B-C3B-C2B	-2.26	105.32	107.11
67	AE	400	HEM	C4B-CHC-C1C	2.21	125.48	122.56
60	F	500	FMN	C4A-C10-N1	-2.18	119.66	124.73
67	AC	500	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
67	BC	500	HEM	C3D-C4D-ND	-2.14	107.78	110.17
66	y	301	COO	C6-C5-N2	-2.13	107.94	112.42
67	AC	501	HEM	CHA-C4D-C3D	-2.12	121.36	125.33
67	BC	501	HEM	CHB-C1B-C2B	-2.11	120.88	126.72
67	AC	500	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
67	BC	501	HEM	CHA-C4D-C3D	-2.10	121.38	125.33
61	H	500	UQ9	C6-C1-C2	-2.10	117.53	119.18
67	BC	500	HEM	C4B-CHC-C1C	2.09	125.32	122.56
67	BE	400	HEM	C3D-C4D-ND	-2.07	107.86	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	AE	400	HEM	C3D-C4D-ND	-2.05	107.88	110.17
67	AE	400	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
63	P	500	NDP	C5A-C6A-N6A	2.04	123.45	120.35
67	AC	501	HEM	CHB-C1B-C2B	-2.03	121.11	126.72
65	n	200	8Q1	C37-C38-C39	2.03	115.73	112.36
67	BC	501	HEM	O2A-CGA-CBA	2.03	120.54	114.03
61	H	500	UQ9	C3-C4-C5	-2.02	116.71	120.68
67	AE	400	HEM	C1B-NB-C4B	2.02	107.16	105.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
66	y	301	COO	C13

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	F	500	FMN	N10-C1'-C2'-O2'
60	F	500	FMN	N10-C1'-C2'-C3'
60	F	500	FMN	C5'-O5'-P-O2P
60	F	500	FMN	C5'-O5'-P-O3P
61	H	500	UQ9	C17-C18-C19-C21
61	H	500	UQ9	C17-C18-C19-C20
61	H	500	UQ9	C12-C11-C9-C10
61	H	500	UQ9	C12-C11-C9-C8
61	H	500	UQ9	C7-C8-C9-C11
61	H	500	UQ9	C7-C8-C9-C10
65	W	200	8Q1	O27-C28-C29-C31
65	W	200	8Q1	O27-C28-C29-C32
65	W	200	8Q1	C29-C28-O27-P24
65	W	200	8Q1	C28-C29-C32-C34
65	W	200	8Q1	C28-C29-C32-O33
65	W	200	8Q1	C30-C29-C32-C34
65	W	200	8Q1	C30-C29-C32-O33
65	W	200	8Q1	C31-C29-C32-C34
65	W	200	8Q1	C31-C29-C32-O33
65	W	200	8Q1	C28-O27-P24-O2
65	W	200	8Q1	C28-O27-P24-O1
65	n	200	8Q1	O4-C1-S44-C43
65	n	200	8Q1	C6-C1-S44-C43
65	n	200	8Q1	C29-C32-C34-N36
65	n	200	8Q1	C29-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
65	n	200	8Q1	O33-C32-C34-N36
65	n	200	8Q1	O33-C32-C34-O35
65	n	200	8Q1	C32-C34-N36-C37
65	n	200	8Q1	N36-C37-C38-C39
66	y	301	COO	C13-C11-C12-O6A
66	y	301	COO	C14-C11-C12-O6A
66	y	301	COO	C15-C11-C12-O6A
66	y	301	COO	C5X-O5X-P1A-O2A
66	y	301	COO	C5X-O5X-P1A-O1A
66	y	301	COO	O4X-C4X-C5X-O5X
66	y	301	COO	C3X-O3X-P3X-O7A
66	y	301	COO	O4-C7-S1-C6
66	y	301	COO	C8-C7-S1-C6
66	y	301	COO	S1-C7-C8-C9
69	BC	503	UQ7	C14-C16-C17-C18
69	BC	503	UQ7	C23-C24-C26-C27
69	BC	503	UQ7	C25-C24-C26-C27
68	BC	502	UQ5	C12-C11-C9-C10
68	BC	502	UQ5	C12-C11-C9-C8
65	n	200	8Q1	O35-C34-N36-C37
61	H	500	UQ9	C22-C23-C24-C25
61	H	500	UQ9	C12-C13-C14-C15
61	H	500	UQ9	C22-C23-C24-C26
61	H	500	UQ9	C12-C13-C14-C16
66	y	301	COO	C3X-C4X-C5X-O5X
61	H	500	UQ9	C24-C26-C27-C28
68	AC	502	UQ5	C12-C11-C9-C10
68	BC	502	UQ5	C25-C24-C26-C27
68	AC	502	UQ5	C12-C11-C9-C8
68	BC	502	UQ5	C23-C24-C26-C27
61	H	500	UQ9	C19-C21-C22-C23
61	H	500	UQ9	C14-C16-C17-C18
68	AC	502	UQ5	C9-C11-C12-C13
68	AC	503	UQ5	C14-C16-C17-C18
68	AC	503	UQ5	C19-C21-C22-C23
68	BC	502	UQ5	C19-C21-C22-C23
69	BC	503	UQ7	C9-C11-C12-C13
69	BC	503	UQ7	C19-C21-C22-C23
69	BC	503	UQ7	C29-C31-C32-C33
66	y	301	COO	C2X-C3X-O3X-P3X
65	W	200	8Q1	O40-C39-N41-C42
65	W	200	8Q1	C38-C39-N41-C42

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Mol	Chain	Res	Type	Atoms
63	P	500	NDP	C2D-C1D-N1N-C2N
63	P	500	NDP	C2D-C1D-N1N-C6N
67	BC	501	HEM	C2A-CAA-CBA-CGA
68	AC	503	UQ5	C24-C26-C27-C28
68	BC	502	UQ5	C9-C11-C12-C13
66	y	301	COO	C4X-C3X-O3X-P3X
61	H	500	UQ9	C16-C17-C18-C19
68	AC	503	UQ5	C15-C14-C16-C17
65	W	200	8Q1	C6-C7-C8-C9
65	W	200	8Q1	O27-C28-C29-C30
65	W	200	8Q1	C11-C12-C13-C14
65	n	200	8Q1	C7-C8-C9-C10
65	n	200	8Q1	C9-C10-C11-C12
67	AC	501	HEM	C2A-CAA-CBA-CGA
61	H	500	UQ9	C15-C14-C16-C17
61	H	500	UQ9	C13-C14-C16-C17
65	n	200	8Q1	C10-C11-C12-C13
68	AC	503	UQ5	C18-C19-C21-C22
66	y	301	COO	O4-C7-C8-C9
68	AC	503	UQ5	C20-C19-C21-C22
68	AC	503	UQ5	C13-C14-C16-C17
68	AC	502	UQ5	C6-C7-C8-C9
65	W	200	8Q1	C13-C14-C15-C16
60	F	500	FMN	C5'-O5'-P-O1P
68	BC	502	UQ5	C24-C26-C27-C28
68	AC	503	UQ5	C12-C11-C9-C10
65	W	200	8Q1	O4-C1-S44-C43
65	W	200	8Q1	C1-C6-C7-C8
65	W	200	8Q1	C7-C8-C9-C10
65	n	200	8Q1	O27-C28-C29-C31
65	W	200	8Q1	C6-C1-S44-C43
67	AC	501	HEM	C2B-C3B-CAB-CBB
67	BC	501	HEM	C2B-C3B-CAB-CBB
68	AC	503	UQ5	C12-C11-C9-C8
68	AC	503	UQ5	C2-C3-O3-C3M
63	P	500	NDP	O4D-C1D-N1N-C2N
66	y	301	COO	C12-O6A-P2A-O3A
66	y	301	COO	P1A-O3A-P2A-O5A
66	y	301	COO	C12-O6A-P2A-O4A
65	n	200	8Q1	O27-C28-C29-C32
63	P	500	NDP	O4D-C1D-N1N-C6N
63	P	500	NDP	O4B-C4B-C5B-O5B

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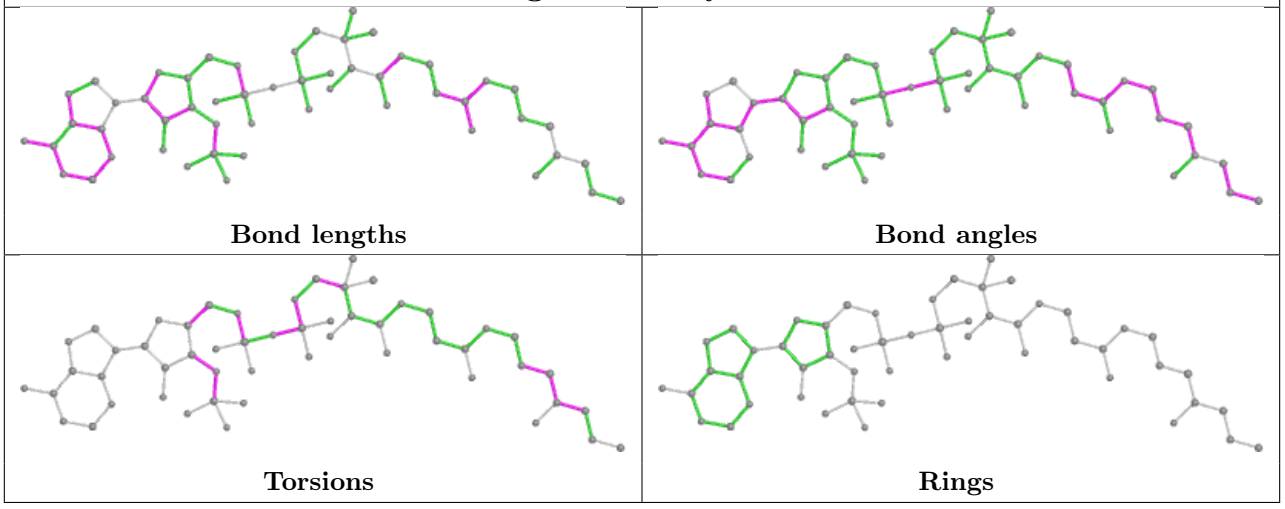
Mol	Chain	Res	Type	Atoms
61	H	500	UQ9	C20-C19-C21-C22
65	n	200	8Q1	O27-C28-C29-C30
65	n	200	8Q1	C11-C10-C9-C8
68	BC	502	UQ5	C14-C16-C17-C18
67	BC	501	HEM	C4B-C3B-CAB-CBB
69	BC	503	UQ7	C28-C29-C31-C32
67	AE	400	HEM	CAA-CBA-CGA-O1A
65	W	200	8Q1	C11-C10-C9-C8
69	BC	503	UQ7	C30-C29-C31-C32
67	BE	400	HEM	CAA-CBA-CGA-O2A
68	AC	503	UQ5	C4-C3-O3-C3M
67	BE	400	HEM	CAA-CBA-CGA-O1A
67	AE	400	HEM	CAA-CBA-CGA-O2A
68	AC	502	UQ5	C15-C14-C16-C17
68	AC	502	UQ5	C2-C3-O3-C3M
66	y	301	COO	C5-C6-S1-C7
61	H	500	UQ9	C18-C19-C21-C22
67	AC	500	HEM	CAA-CBA-CGA-O2A
67	AC	501	HEM	CAD-CBD-CGD-O2D
67	AC	501	HEM	CAD-CBD-CGD-O1D
65	n	200	8Q1	C28-O27-P24-O2
66	y	301	COO	C3X-O3X-P3X-O9A
68	AC	502	UQ5	C13-C14-C16-C17
68	AC	503	UQ5	C5-C6-C7-C8
67	BC	500	HEM	CAA-CBA-CGA-O2A
67	BC	501	HEM	CAA-CBA-CGA-O2A
61	H	500	UQ9	C2-C3-O3-C3M
67	BC	501	HEM	CAD-CBD-CGD-O2D
67	AC	500	HEM	CAA-CBA-CGA-O1A
67	BC	500	HEM	CAA-CBA-CGA-O1A
67	AC	501	HEM	C4B-C3B-CAB-CBB
67	BC	501	HEM	CAA-CBA-CGA-O1A
65	n	200	8Q1	C31-C29-C32-C34
67	AC	501	HEM	CAA-CBA-CGA-O2A
67	BC	501	HEM	CAD-CBD-CGD-O1D
66	y	301	COO	C5X-O5X-P1A-O3A
66	y	301	COO	P1A-O3A-P2A-O4A
67	AC	500	HEM	CAD-CBD-CGD-O2D
63	P	500	NDP	C2N-C3N-C7N-N7N
67	AC	501	HEM	CAA-CBA-CGA-O1A
67	AC	500	HEM	CAD-CBD-CGD-O1D
65	n	200	8Q1	C28-C29-C32-C34

There are no ring outliers.

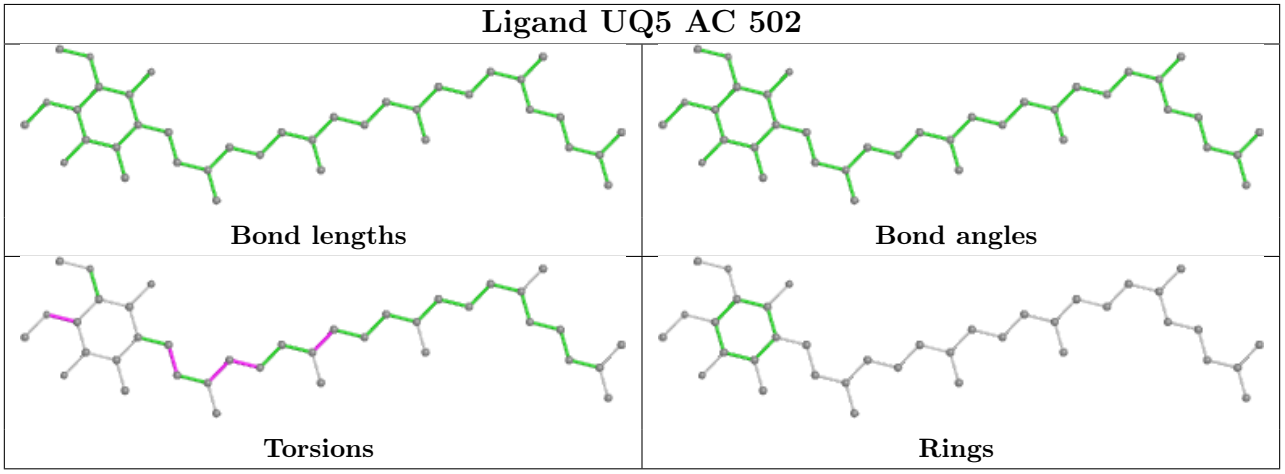
No monomer is involved in short contacts.

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.

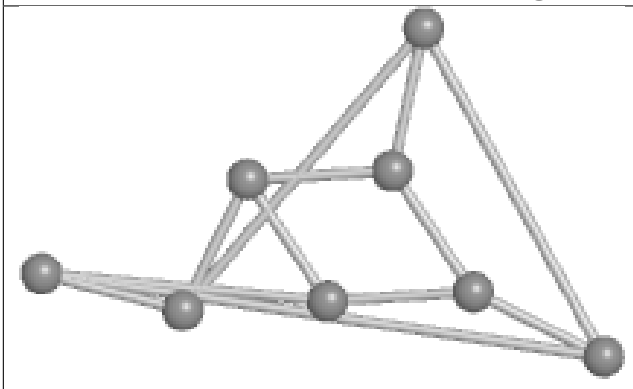
Ligand COO y 301



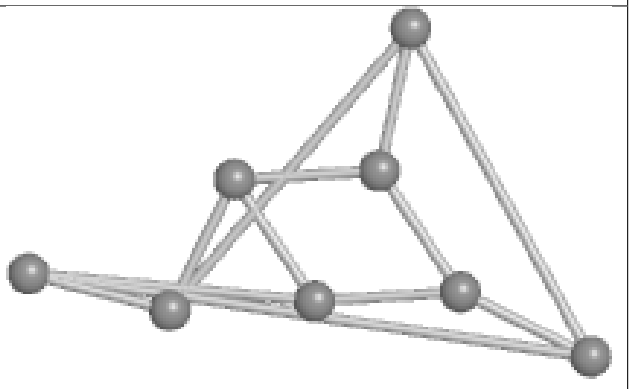
Ligand UQ5 AC 502



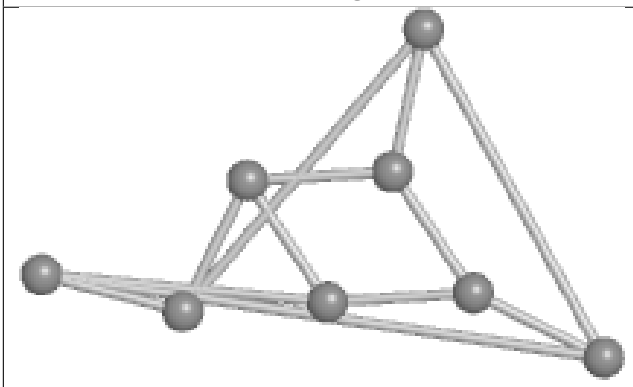
Ligand SF4 G 803



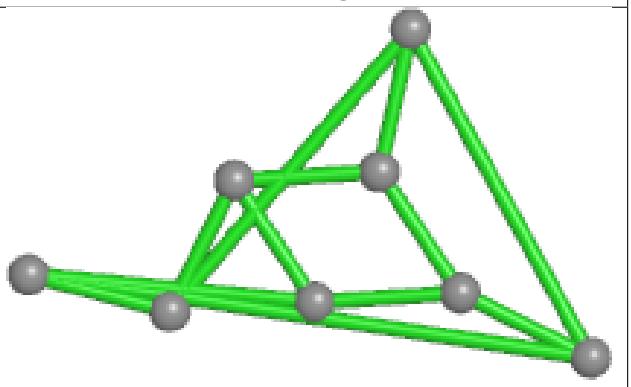
Bond lengths



Bond angles

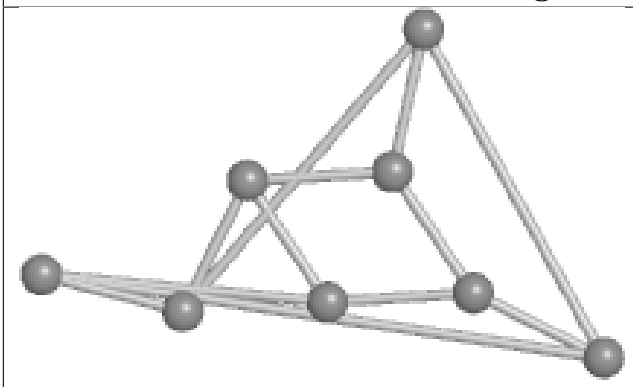


Torsions

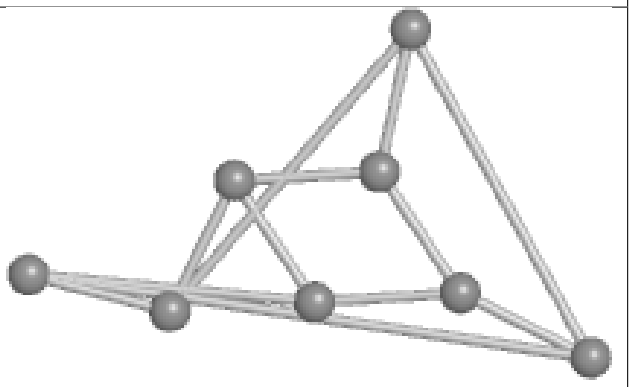


Rings

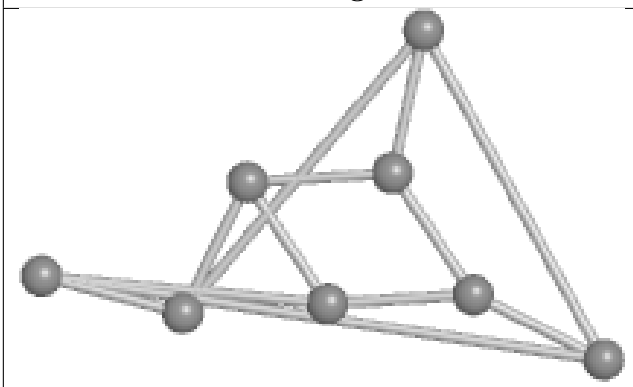
Ligand SF4 F 501



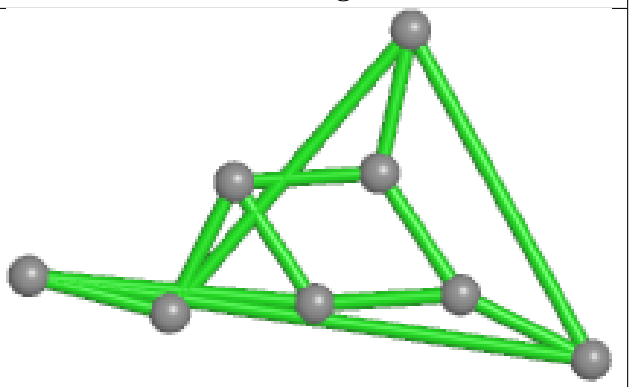
Bond lengths



Bond angles

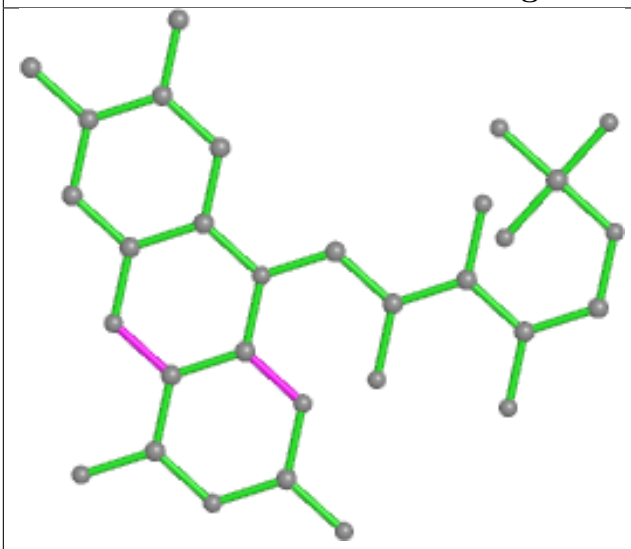


Torsions



Rings

Ligand FMN F 500



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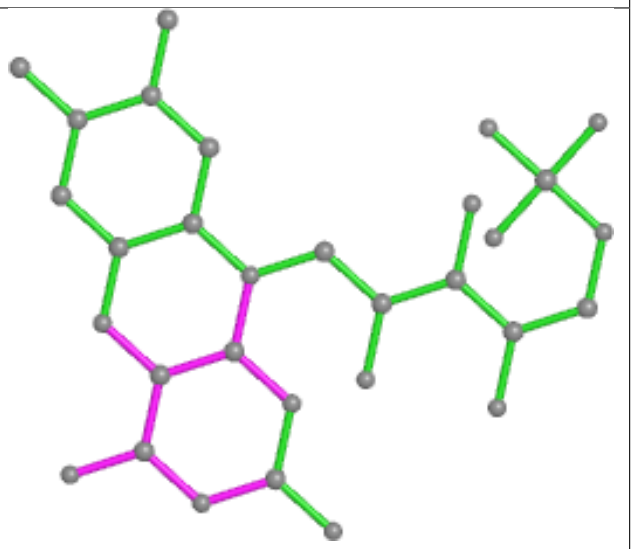

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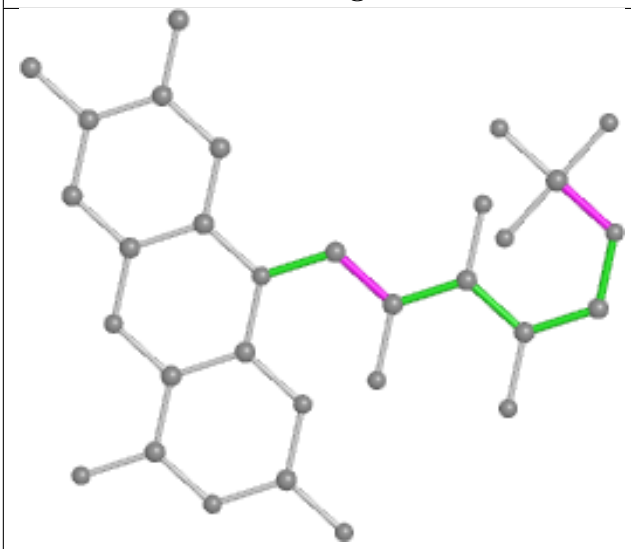

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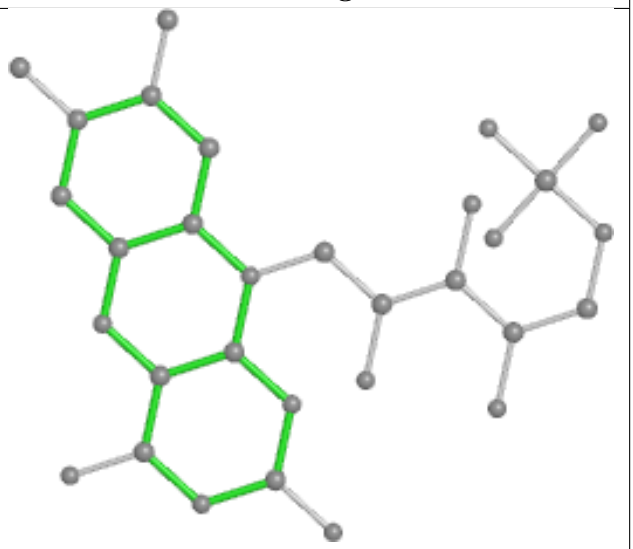
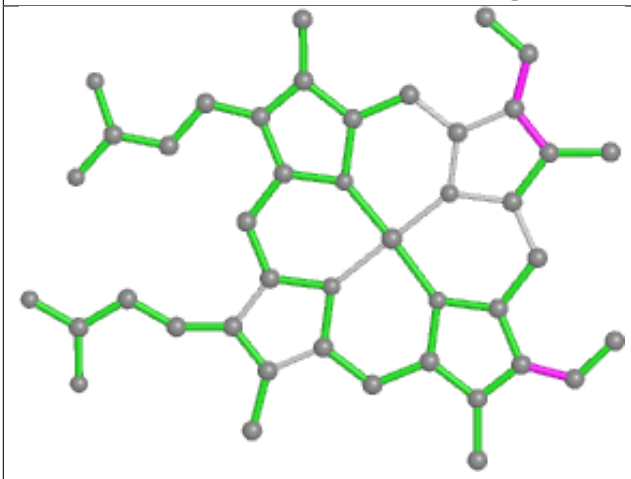


Rings

Ligand HEM BC 500



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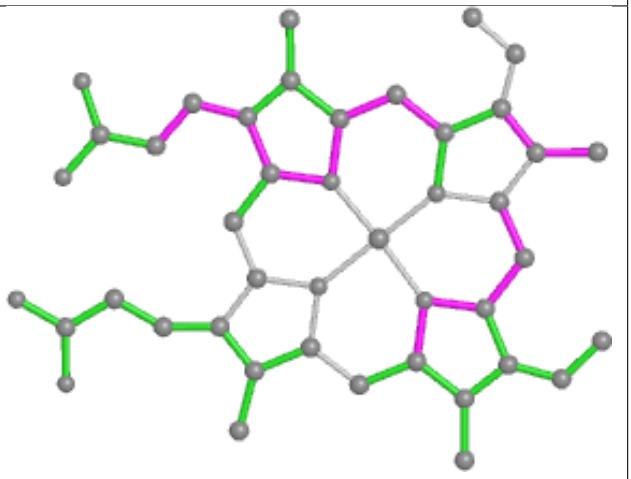

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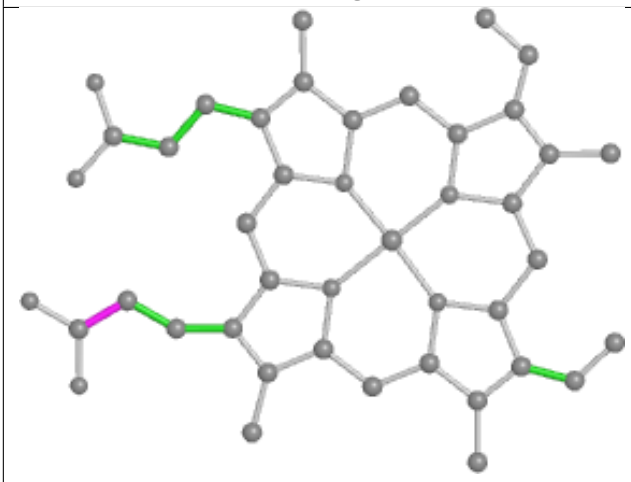

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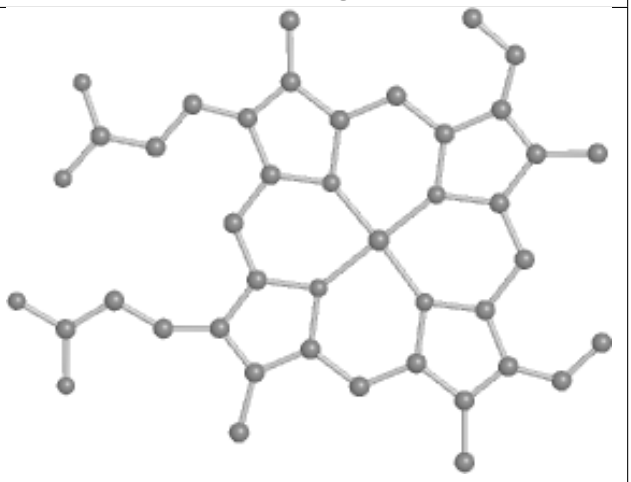
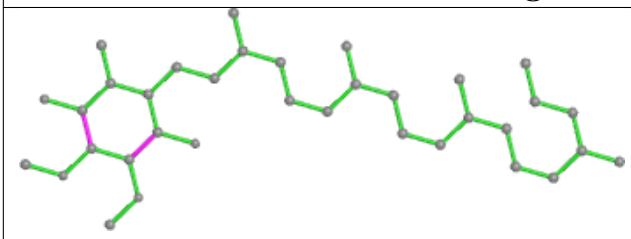


Rings

Ligand UQ9 H 500



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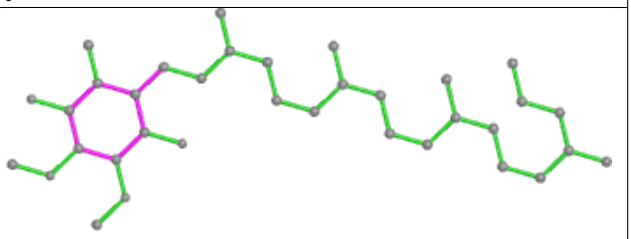
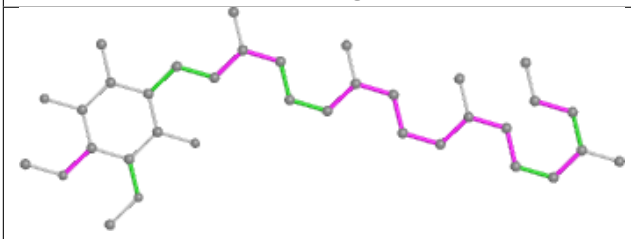


Bond angles



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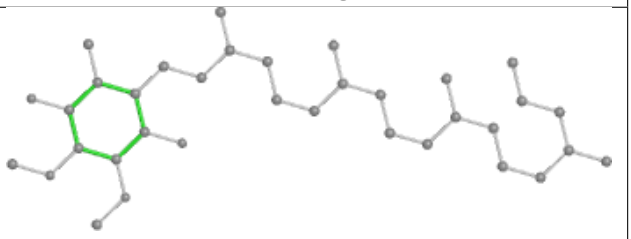
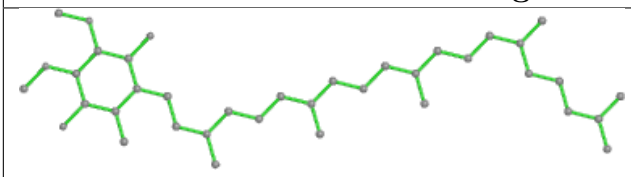


Rings

Ligand UQ5 AC 503



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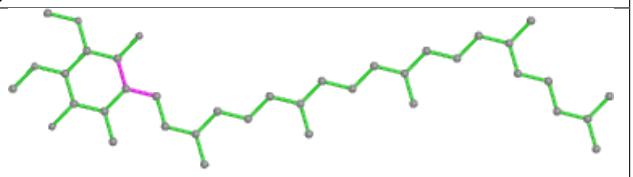
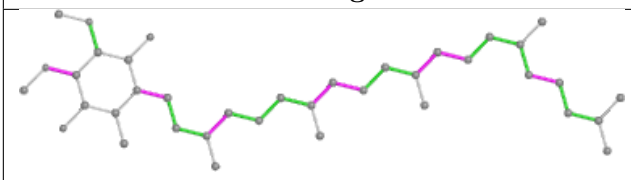


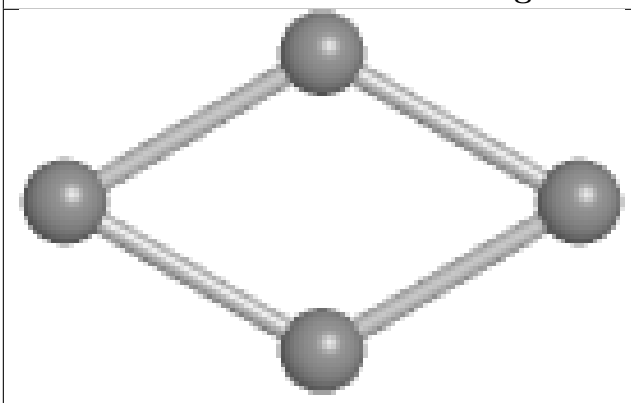
Bond angles



Torsions

Rings

Ligand FES AD 301



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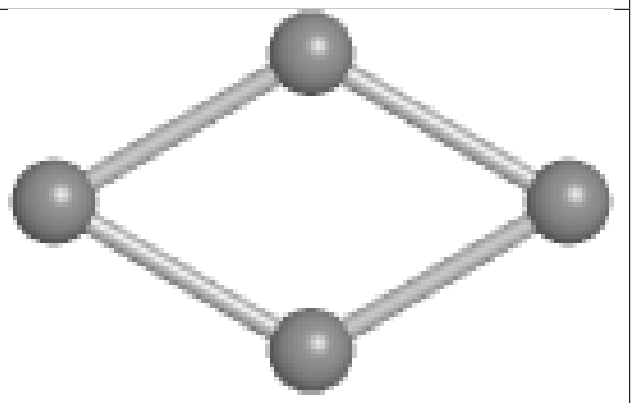

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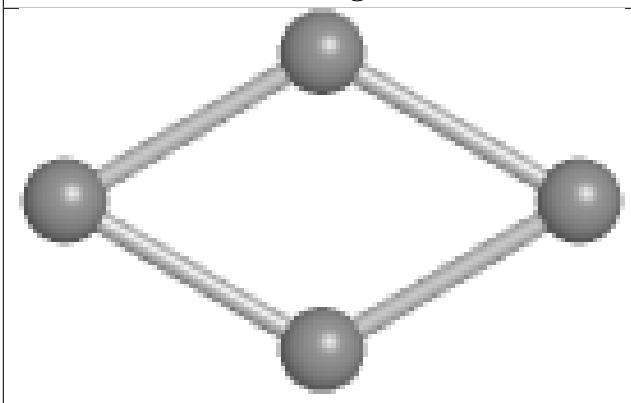

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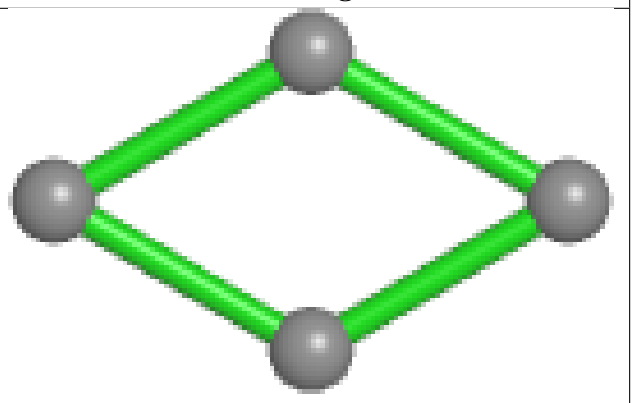
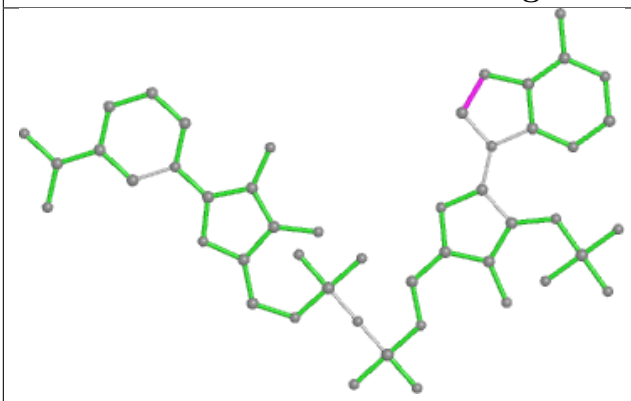


Rings

Ligand NDP P 500



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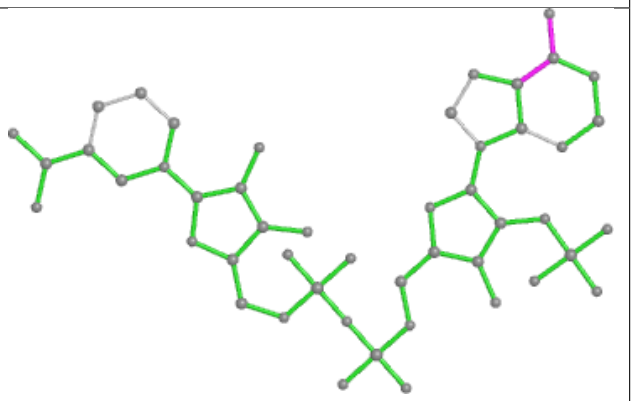
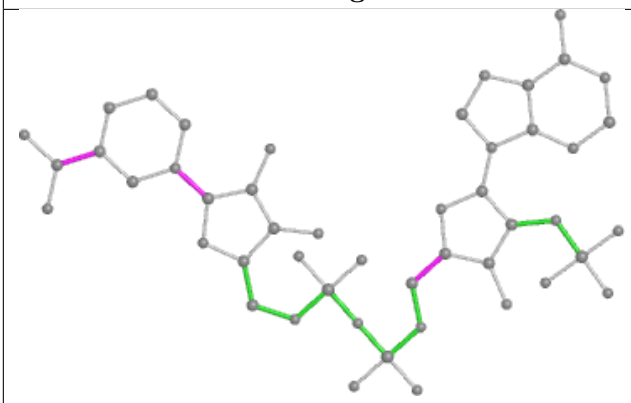


Bond angles



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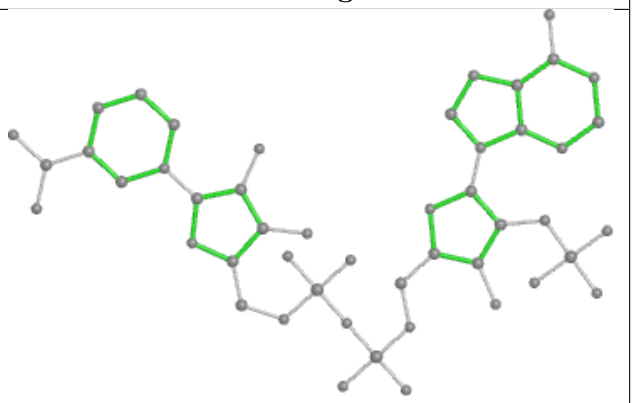
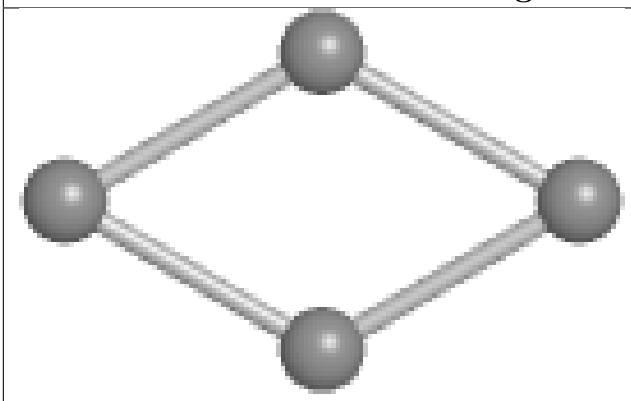


Rings

Ligand FES BD 301



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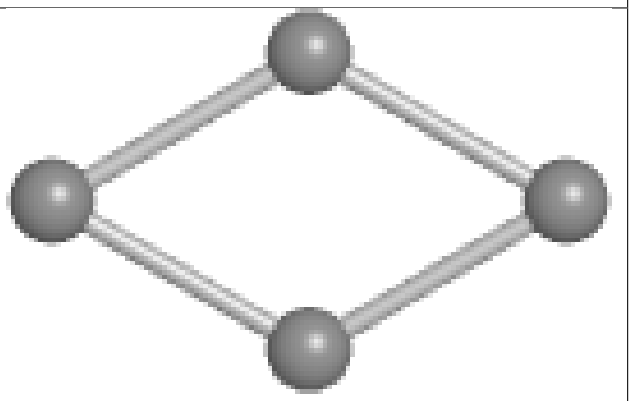
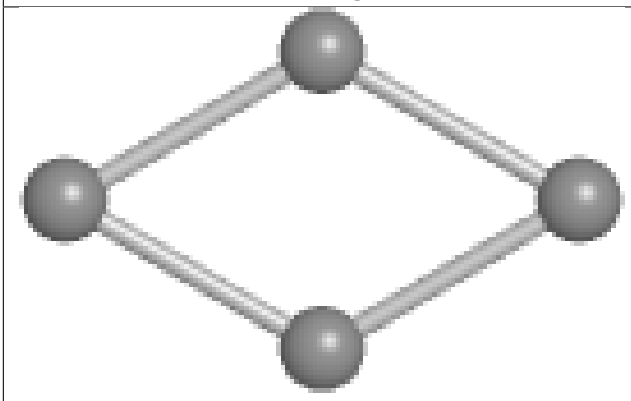


Bond angles



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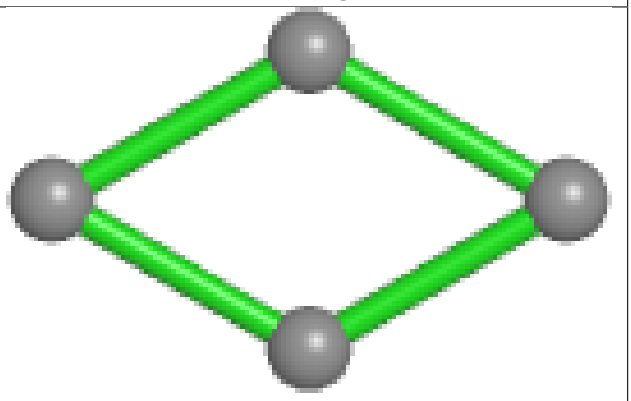
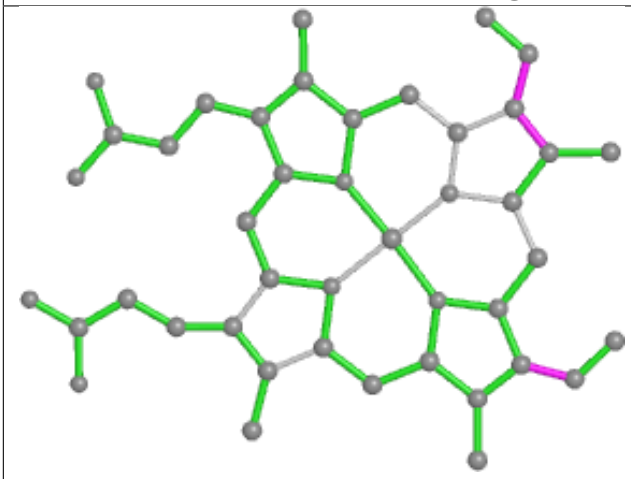


Rings

Ligand HEM AC 500



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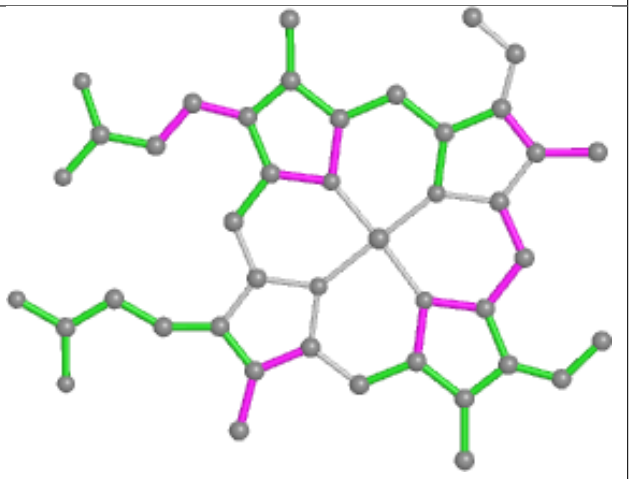
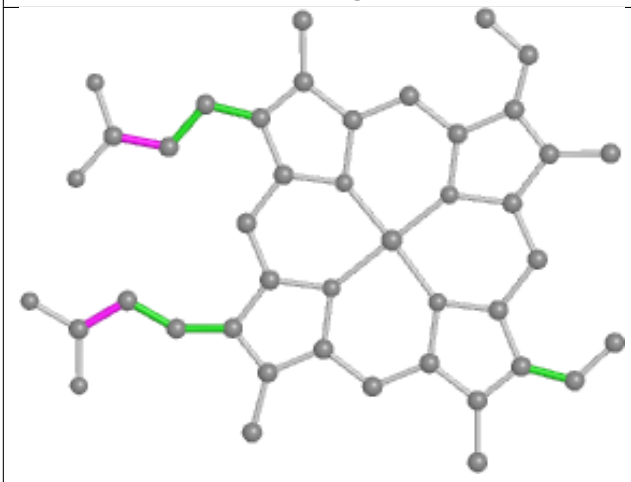
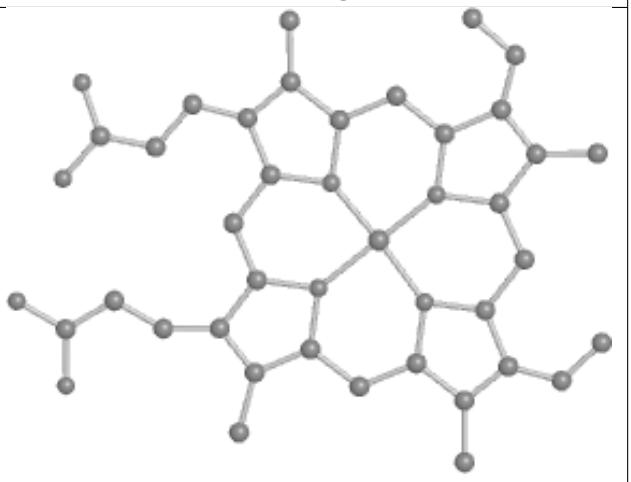


Bond angles

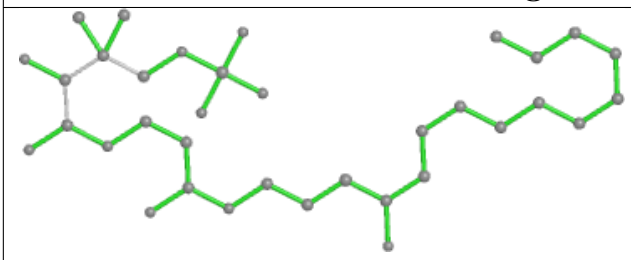


Torsions



Rings

Ligand 8Q1 W 200



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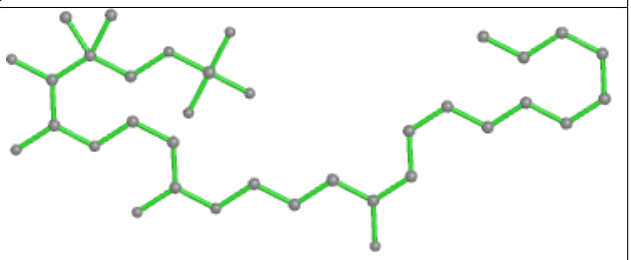
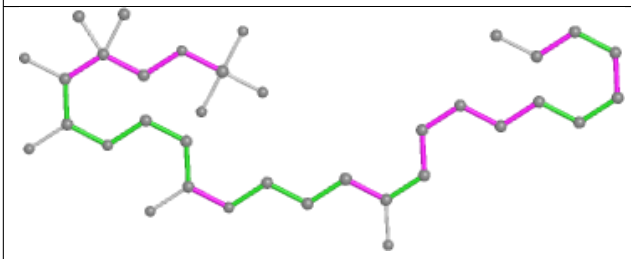


Bond angles



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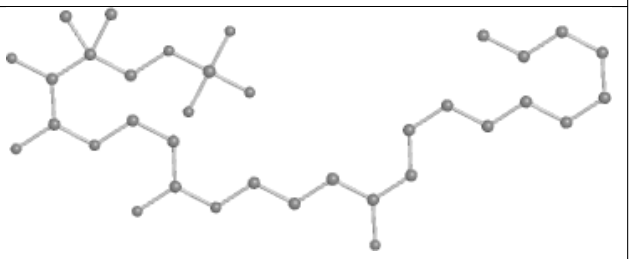
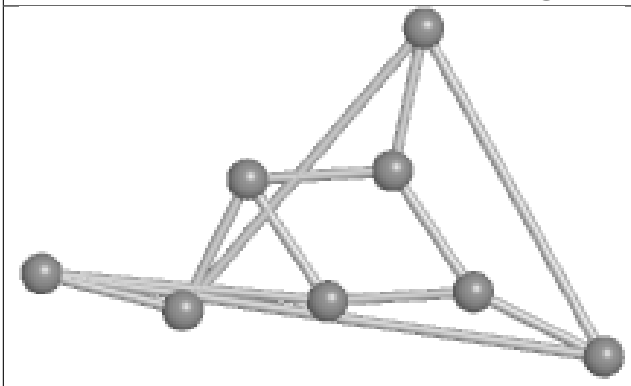


Rings

Ligand SF4 I 500



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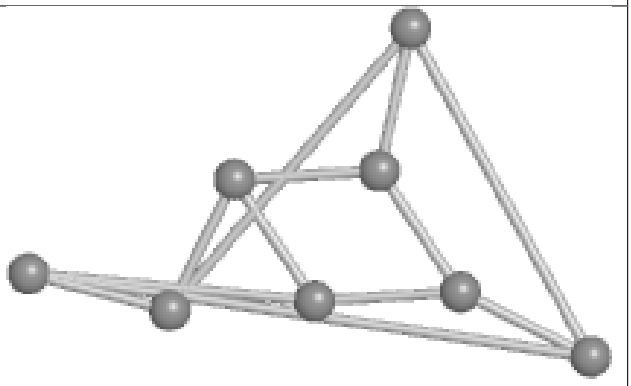

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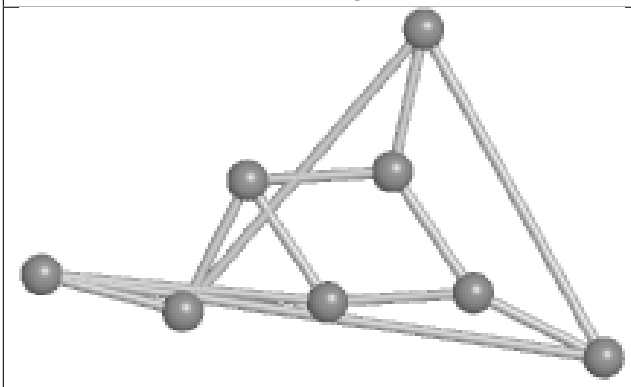

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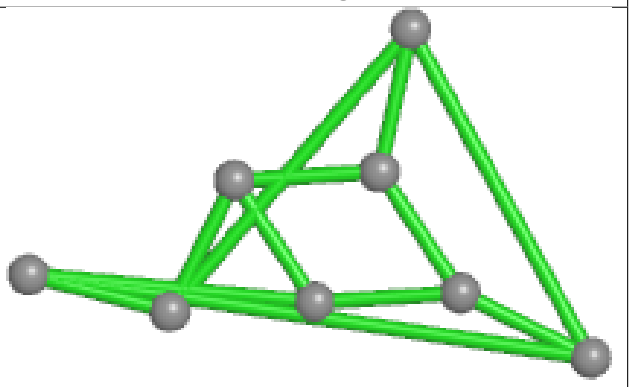
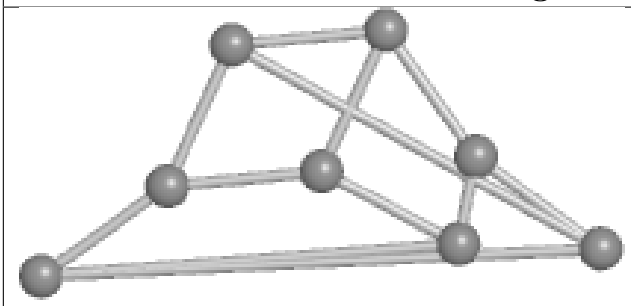


Rings

Ligand SF4 B 500



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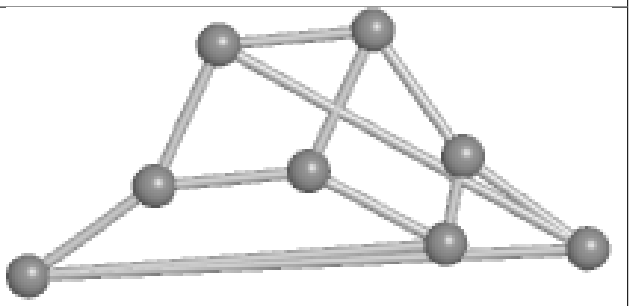
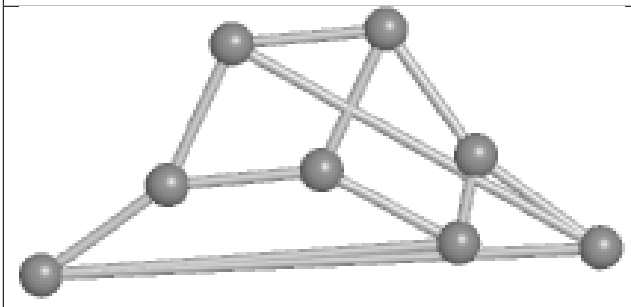


Bond angles



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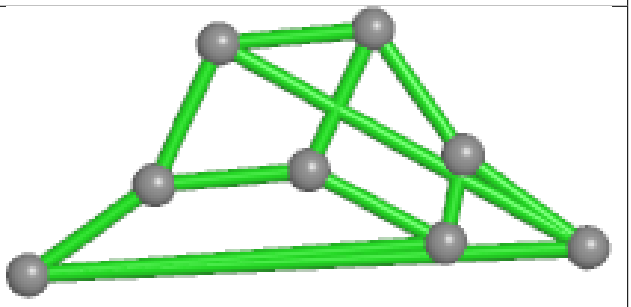
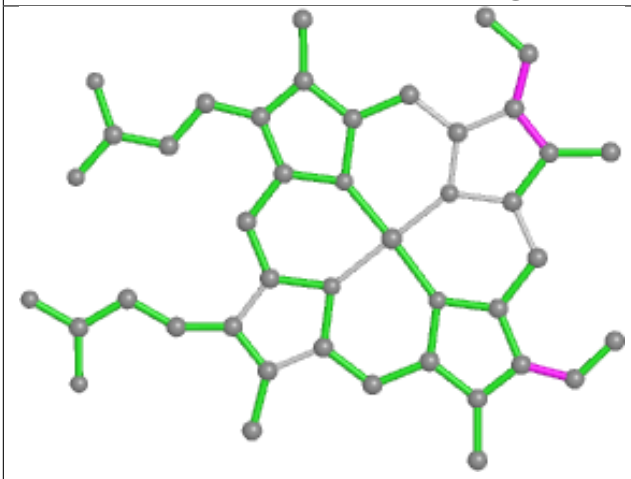


Rings

Ligand HEM BE 400



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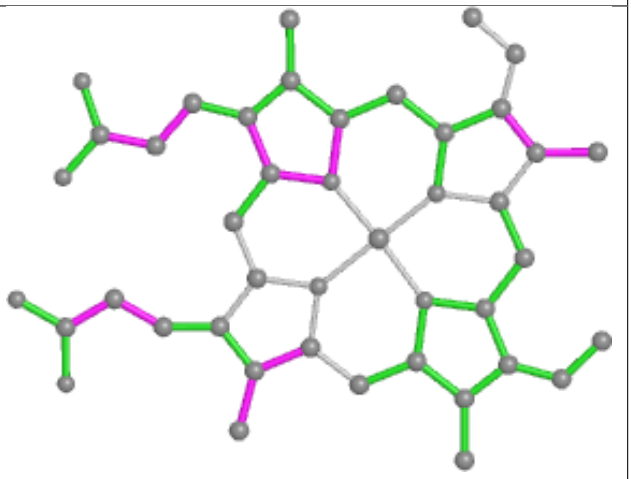
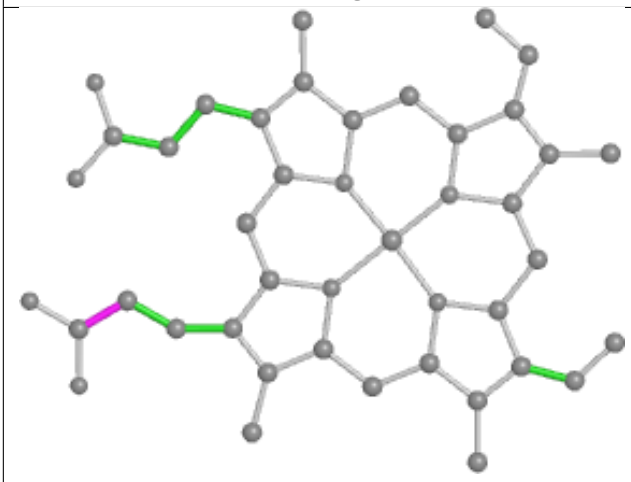


Bond angles



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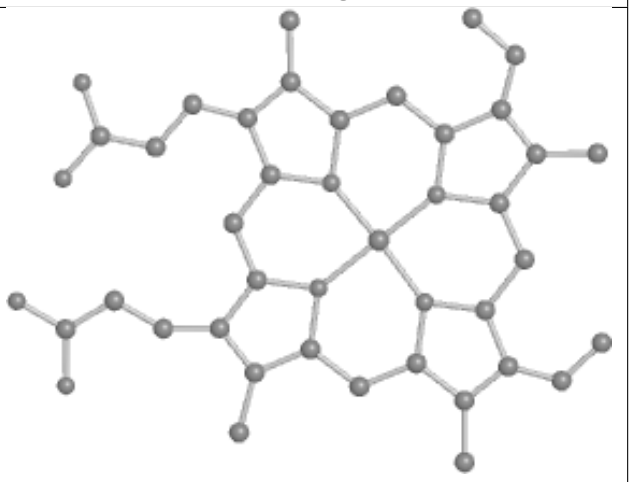
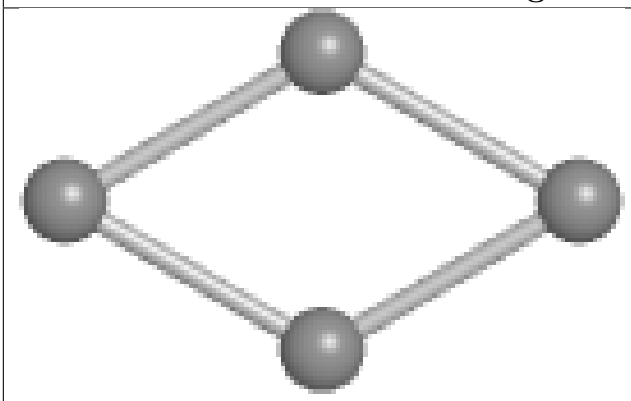
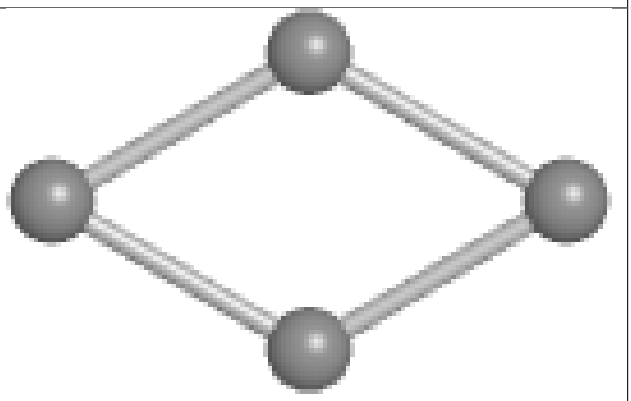


Rings

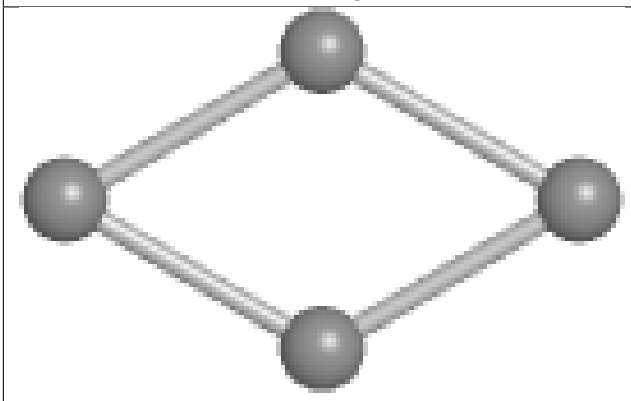
Ligand FES G 801



Bond lengths



Bond angles



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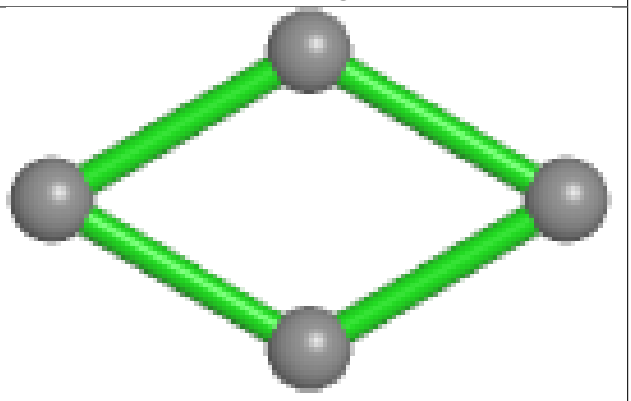
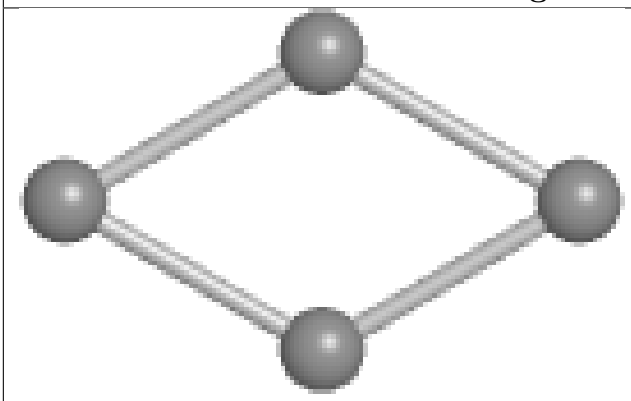
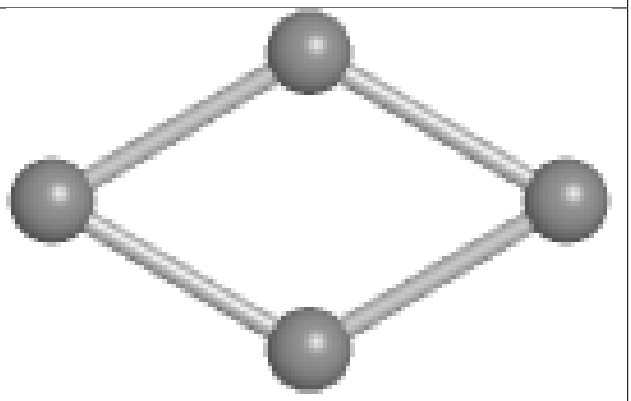


Rings

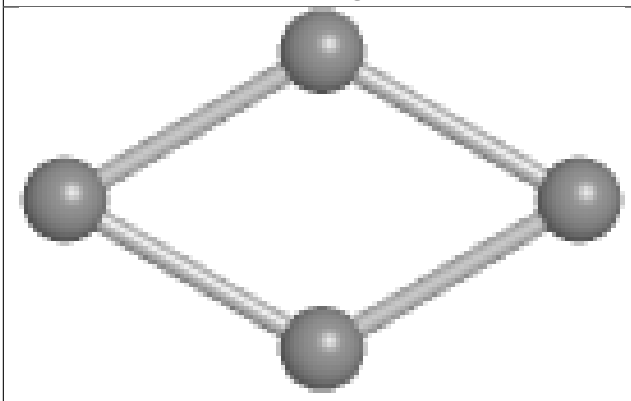
Ligand FES E 500



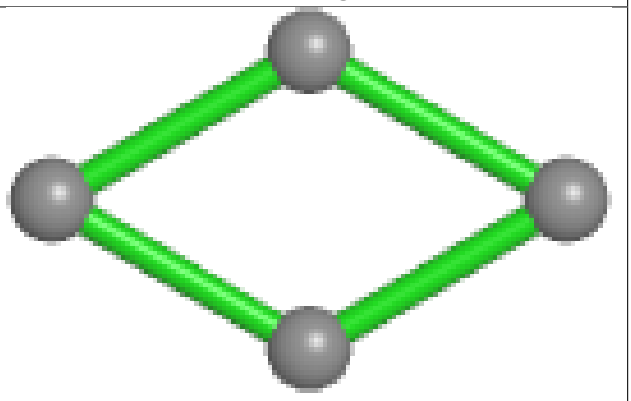
Bond lengths



Bond angles

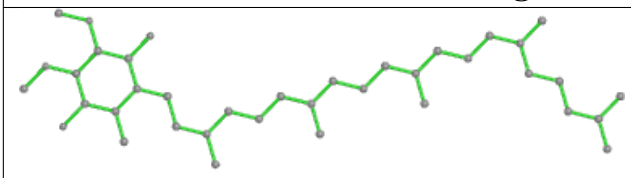


Torsions

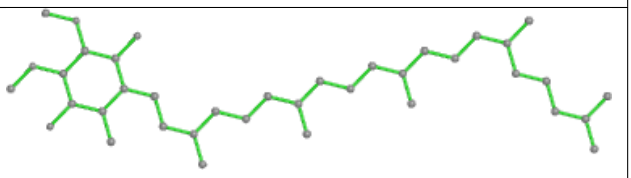


Rings

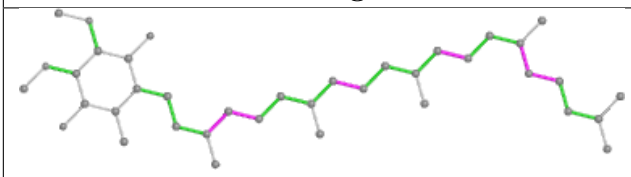
Ligand UQ5 BC 502



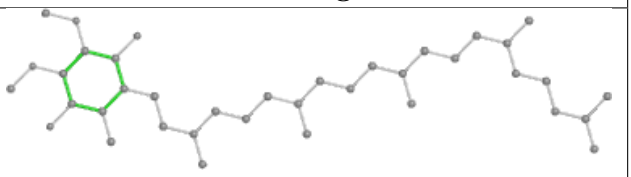
Bond lengths



Bond angles

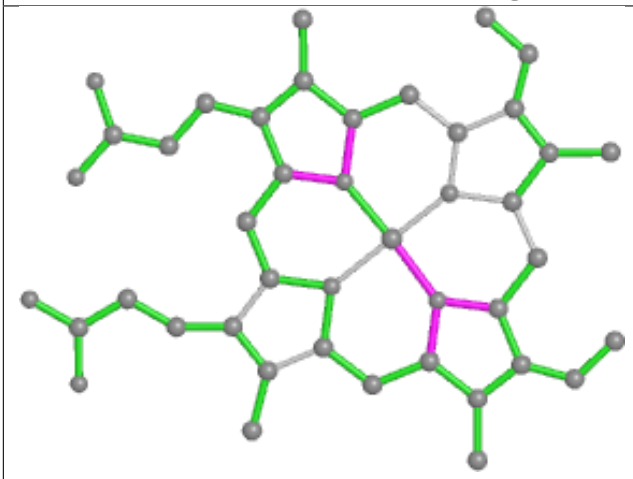


Torsions

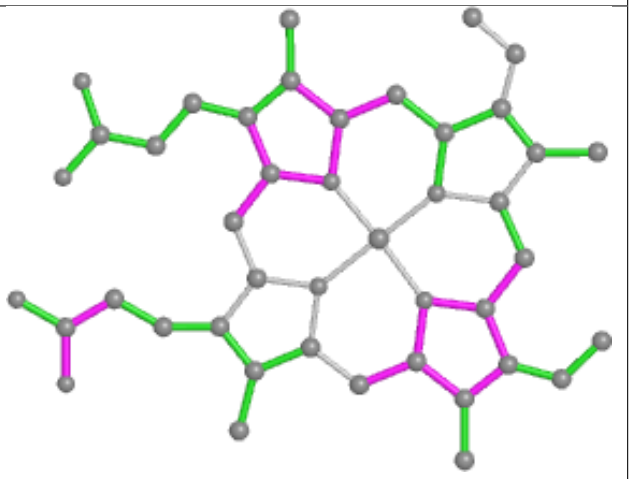


Rings

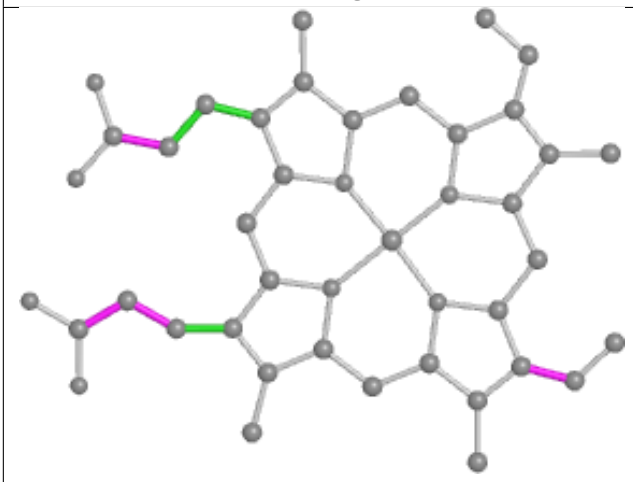
Ligand HEM BC 501



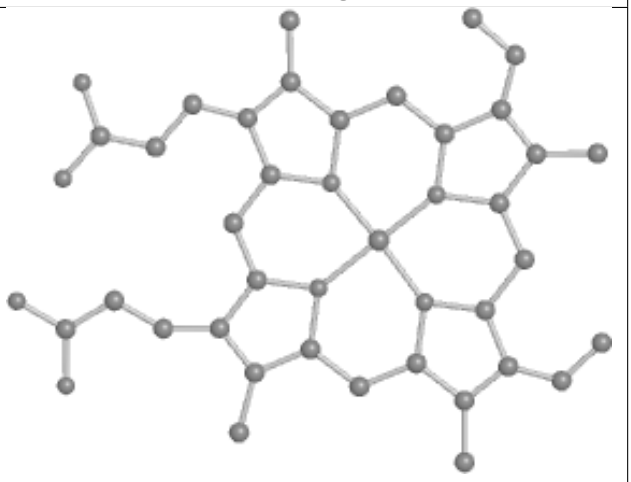
Bond lengths



Bond angles

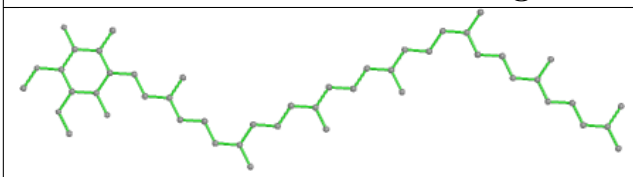


Torsions

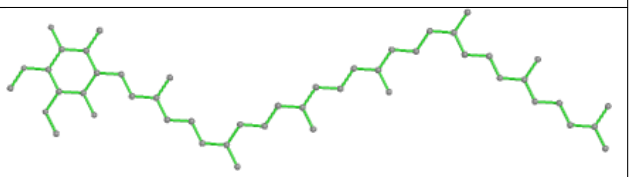


Rings

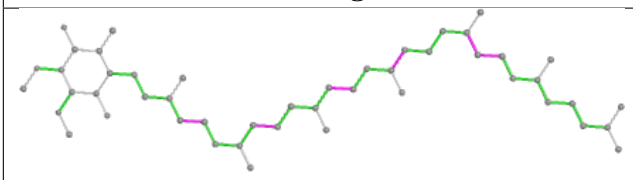
Ligand UQ7 BC 503



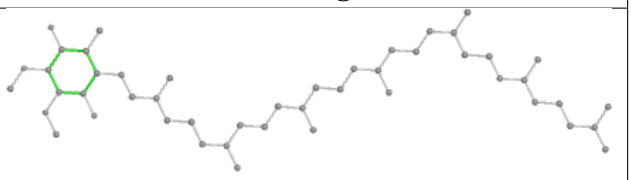
Bond lengths



Bond angles

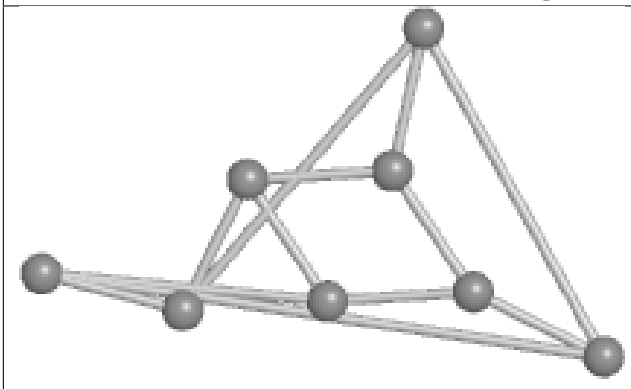


Torsions

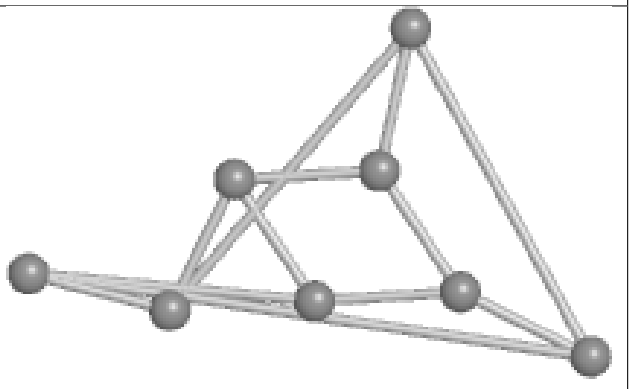


Rings

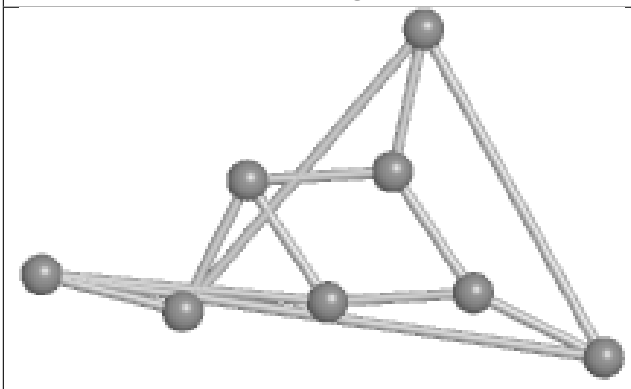
Ligand SF4 I 501



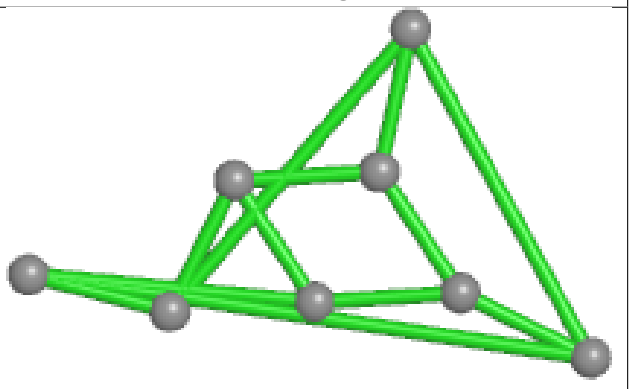
Bond lengths



Bond angles

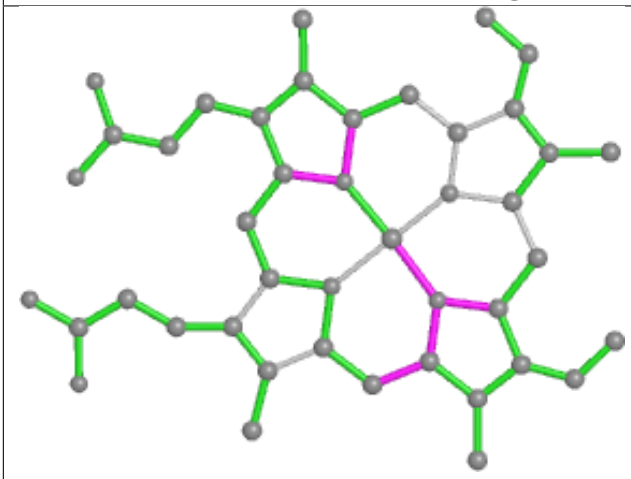


Torsions

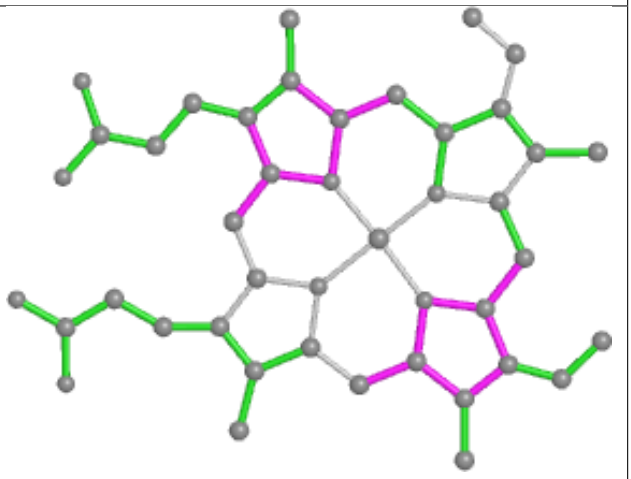


Rings

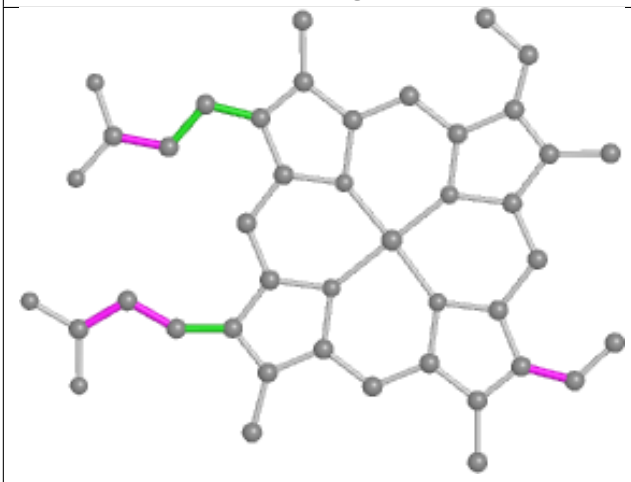
Ligand HEM AC 501



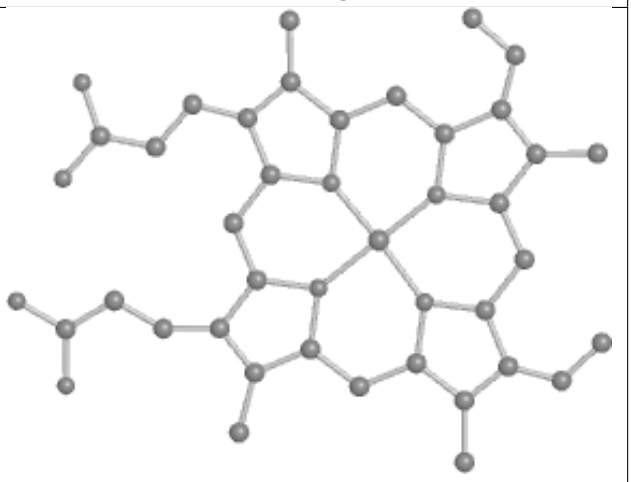
Bond lengths



Bond angles

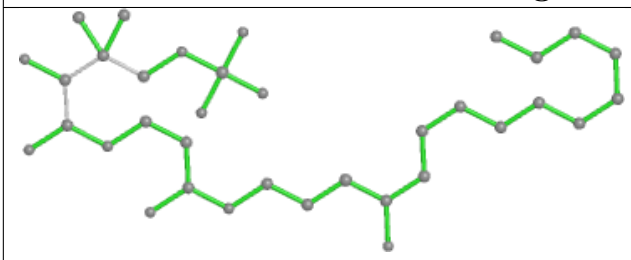


Torsions

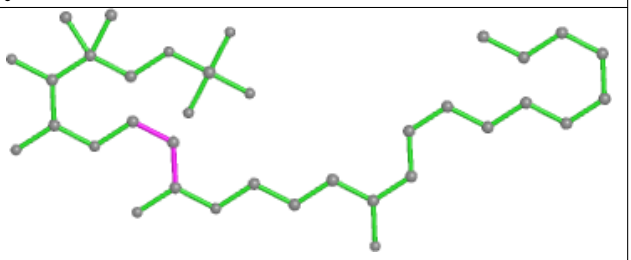


Rings

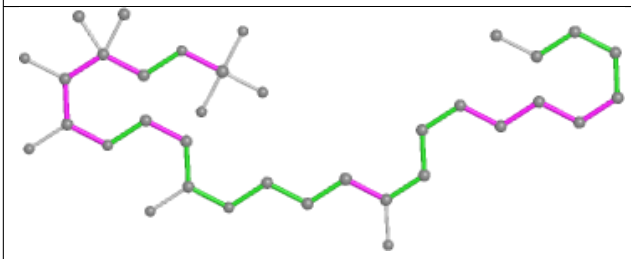
Ligand 8Q1 n 200



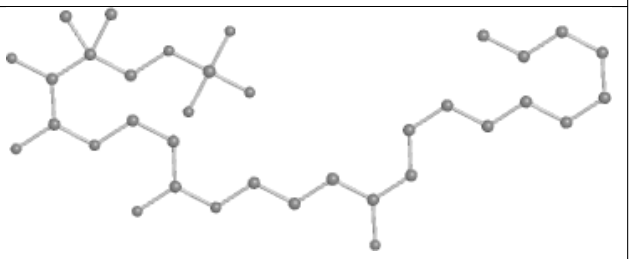
Bond lengths



Bond angles

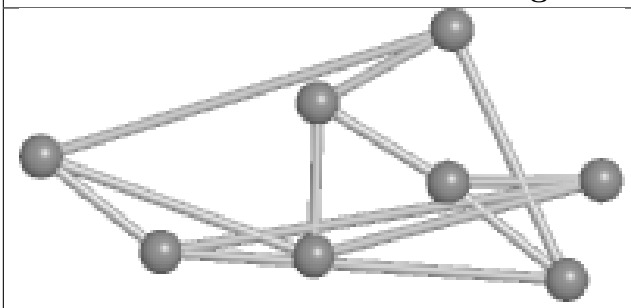


Torsions

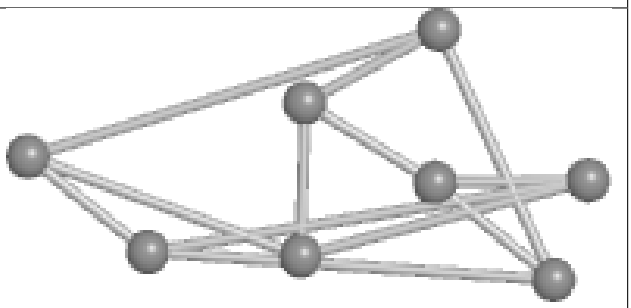


Rings

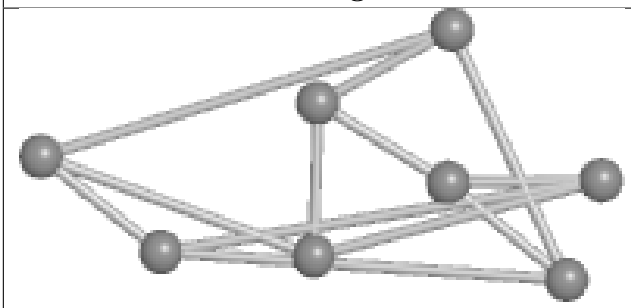
Ligand SF4 G 802



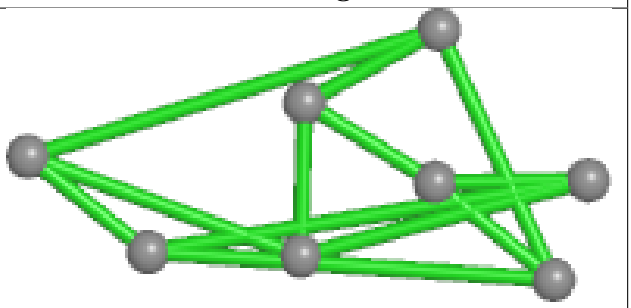
Bond lengths



Bond angles

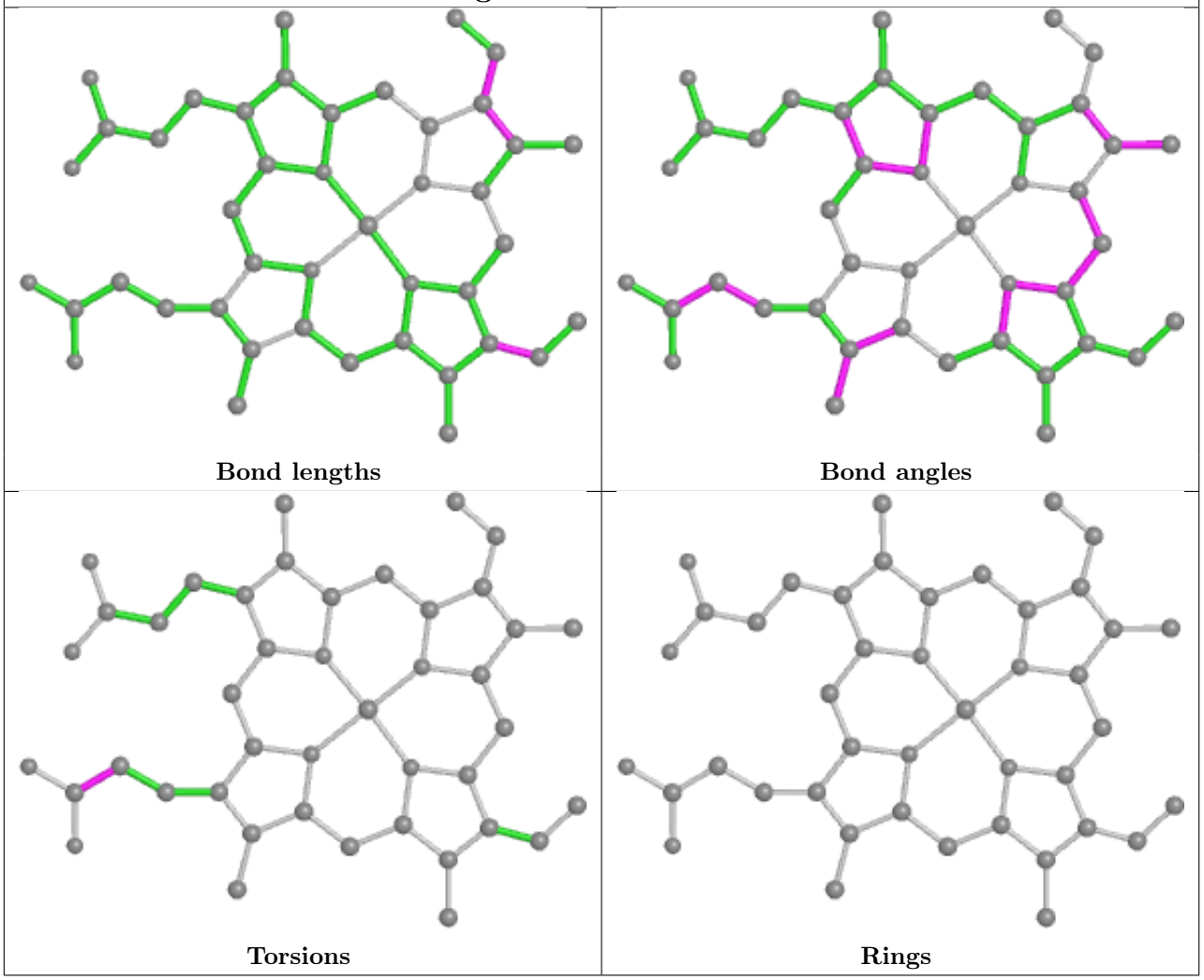


Torsions



Rings

Ligand HEM AE 400



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

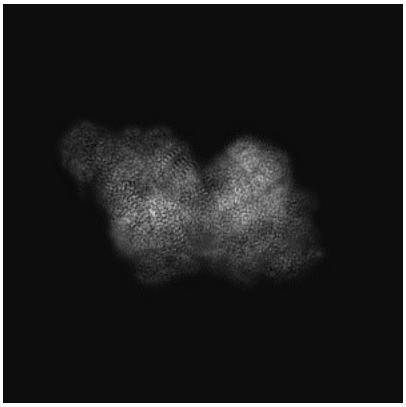
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16172. These allow visual inspection of the internal detail of the map and identification of artifacts.

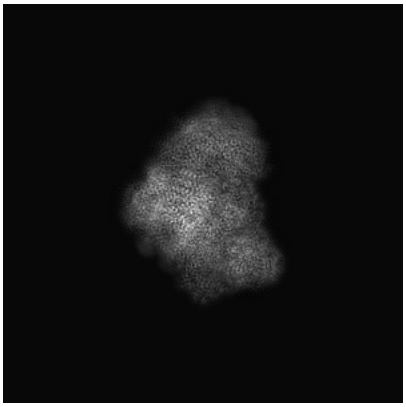
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

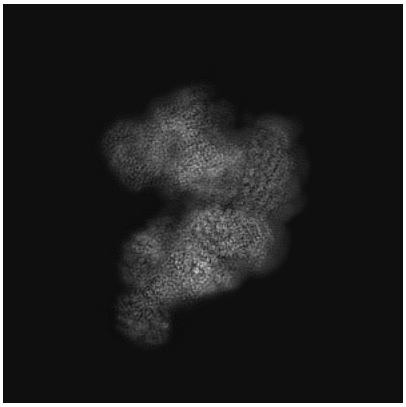
6.1.1 Primary map



X



Y

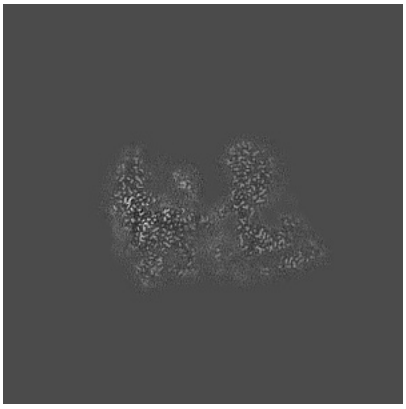


Z

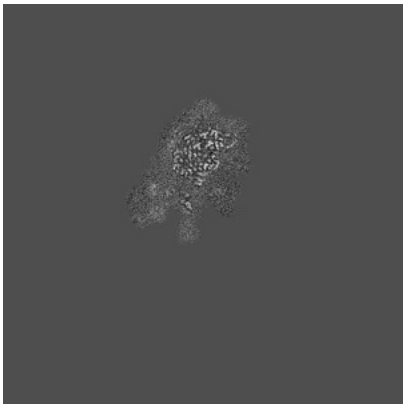
The images above show the map projected in three orthogonal directions.

6.2 Central slices

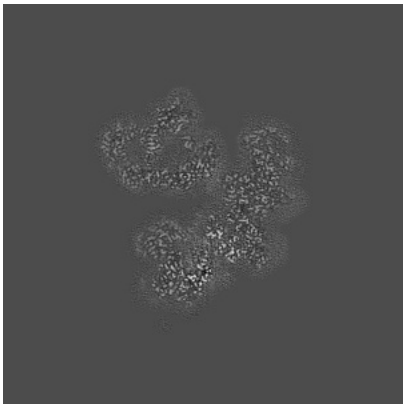
6.2.1 Primary map



X Index: 375



Y Index: 375

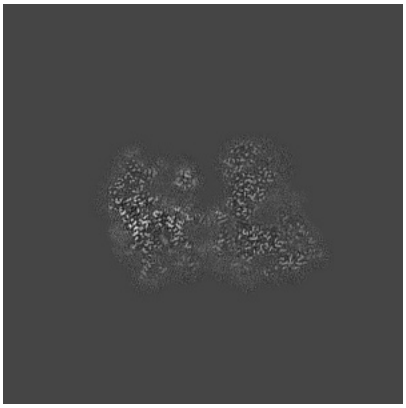


Z Index: 375

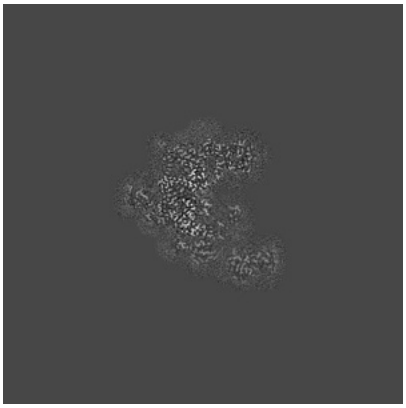
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

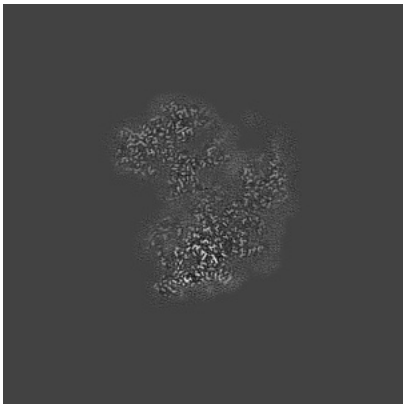
6.3.1 Primary map



X Index: 366



Y Index: 283

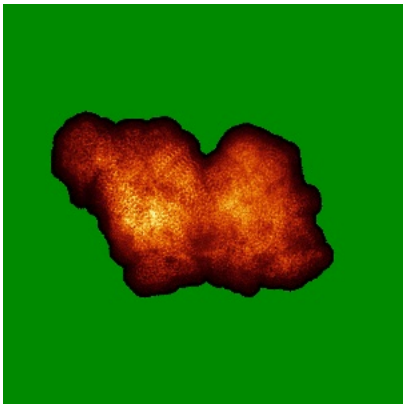


Z Index: 345

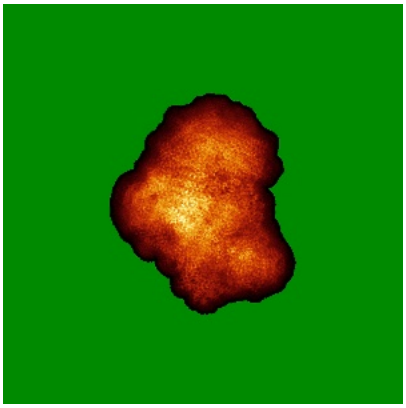
The images above show the largest variance slices of the map in three orthogonal directions.

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

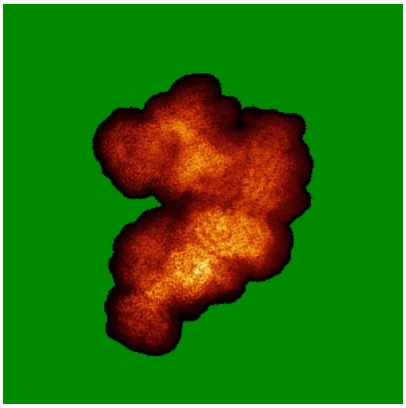
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

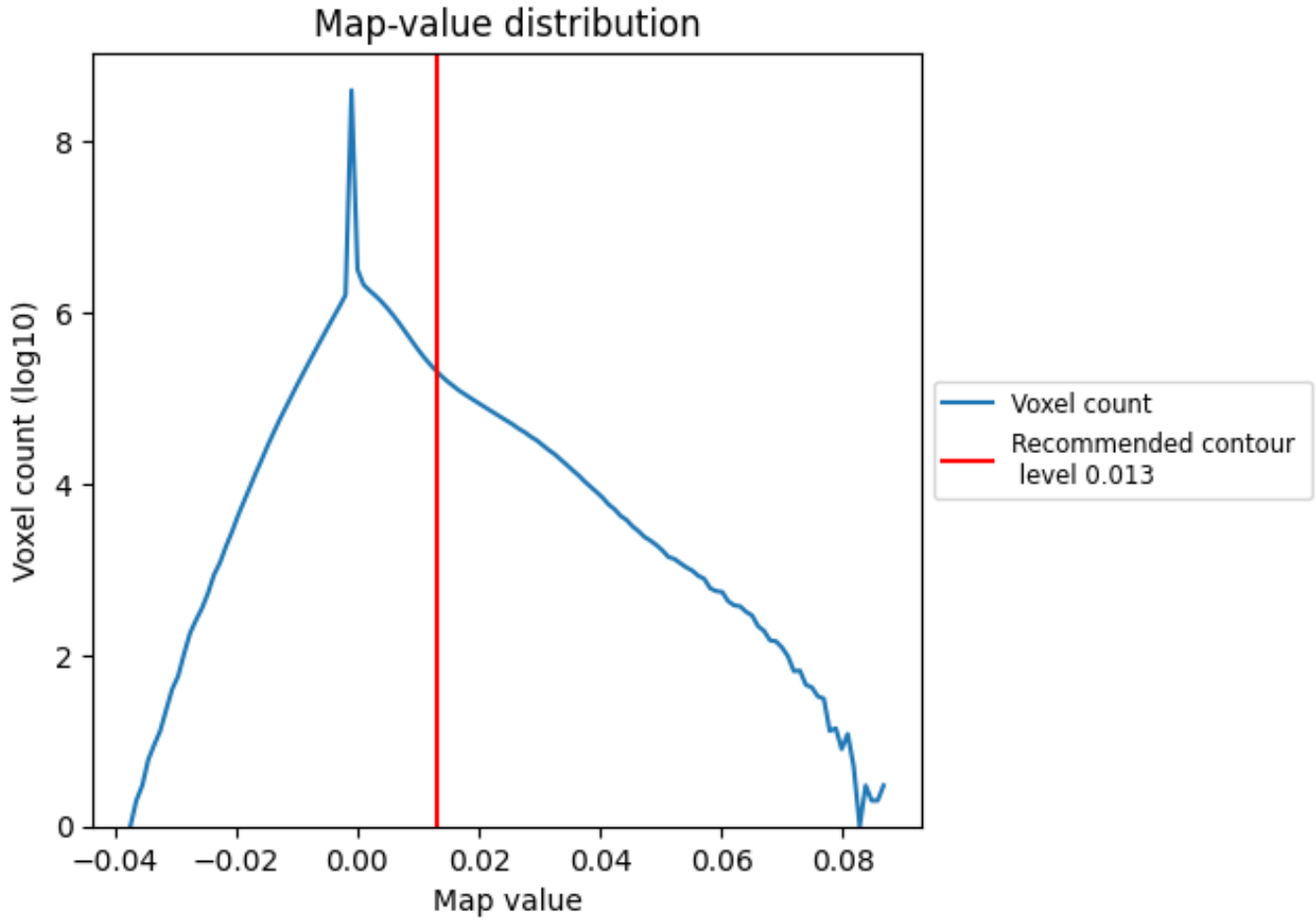
6.6 Mask visualisation (i)

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

7 Map analysis

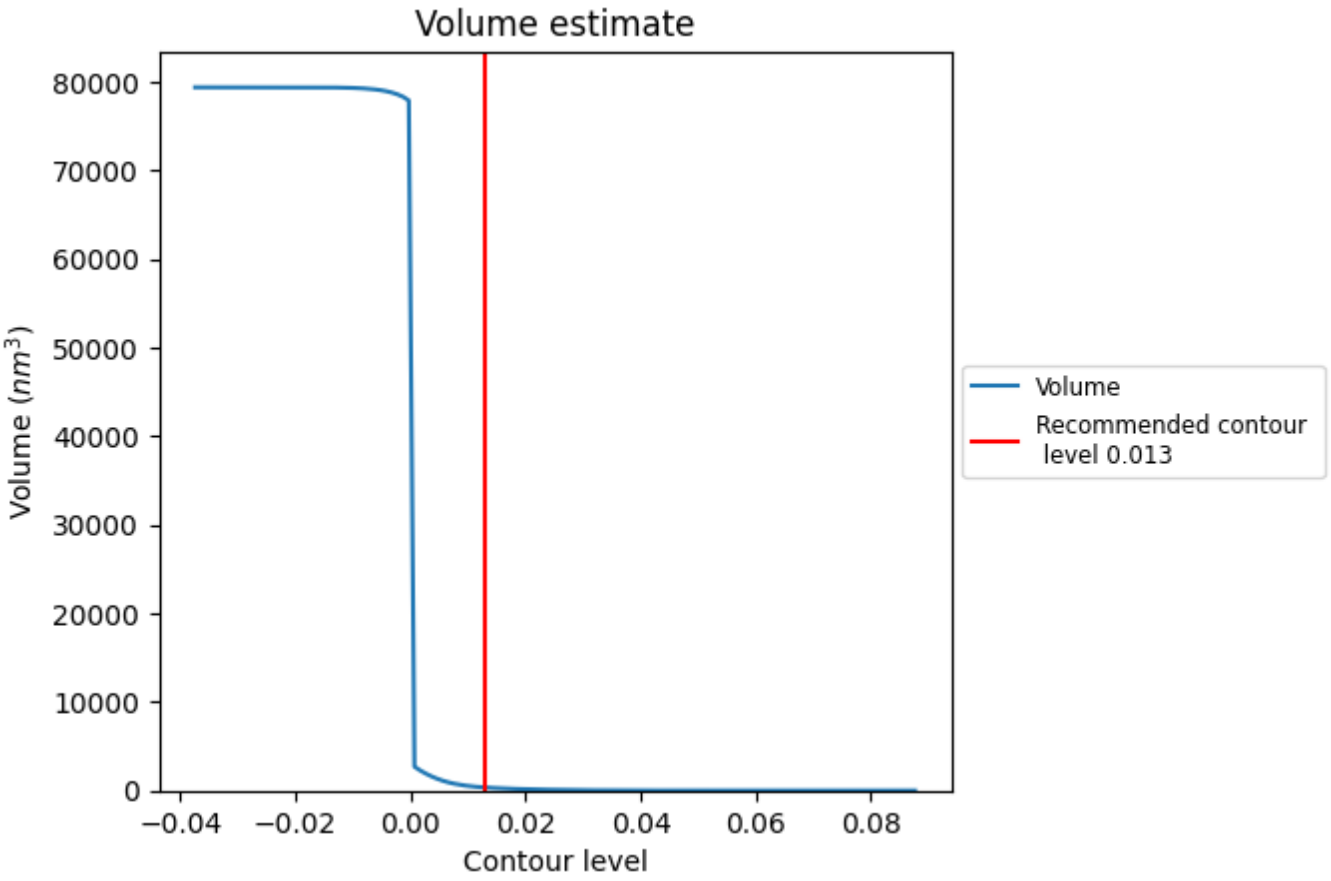
This section contains the results of statistical analysis of the map.

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.

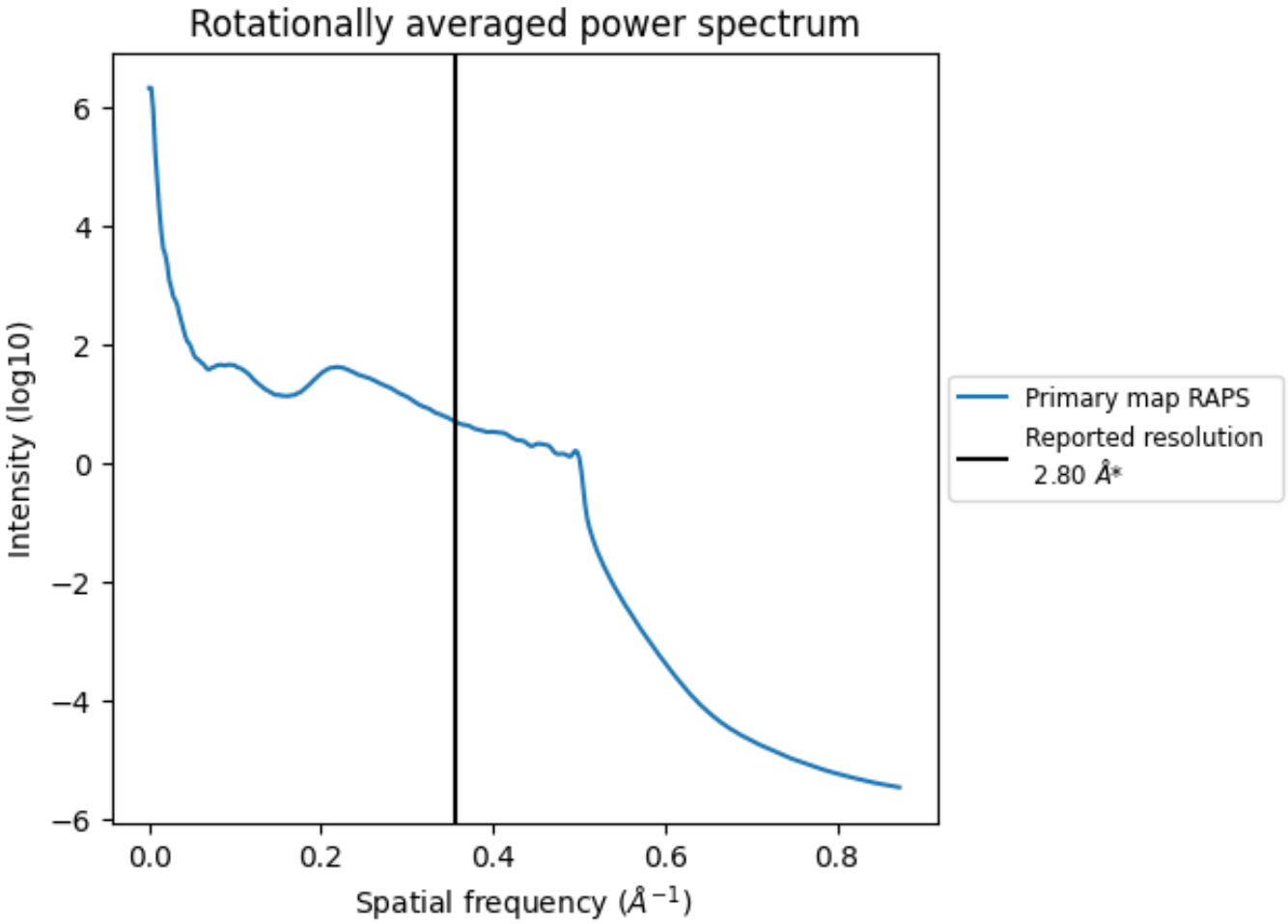
7.2 Volume estimate



The volume at the recommended contour level is 348 nm^3; this corresponds to an approximate mass of 314 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)

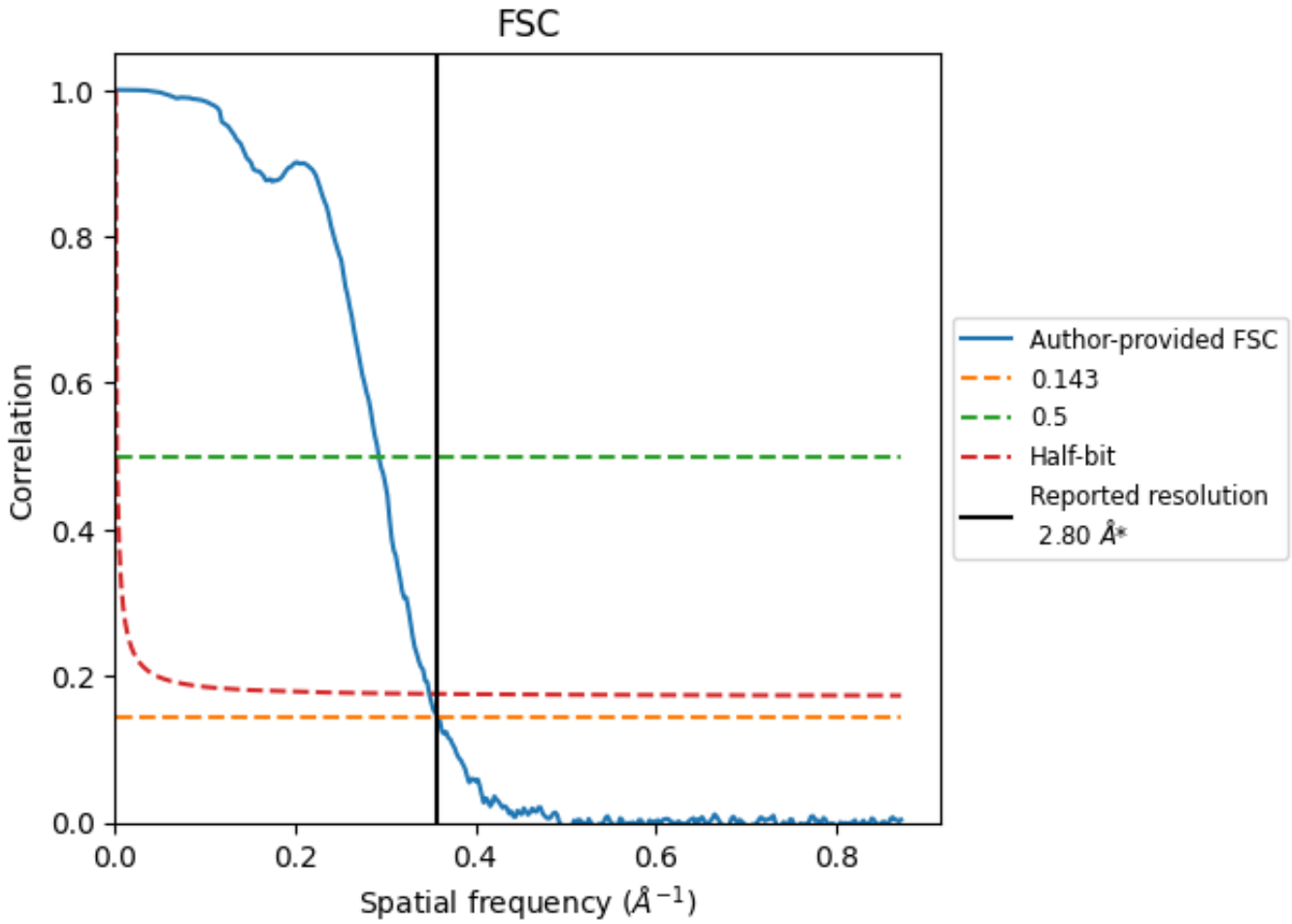


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

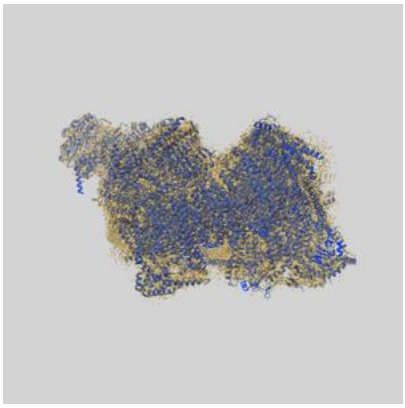
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.42	2.87
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

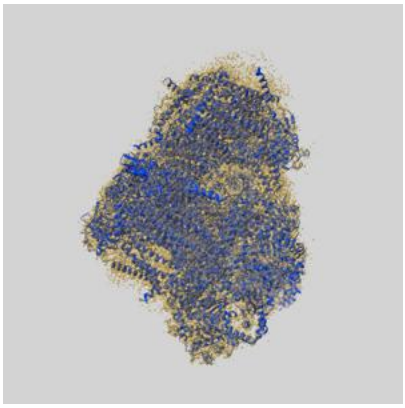
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16172 and PDB model 8BQ6. Per-residue inclusion information can be found in section 3 on page 23.

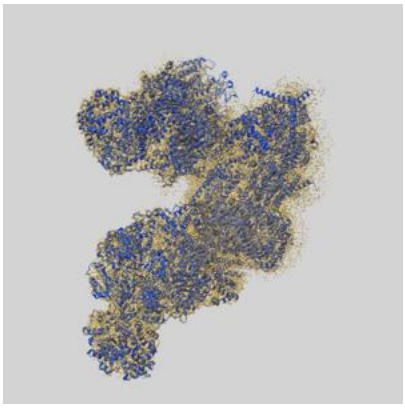
9.1 Map-model overlay



X



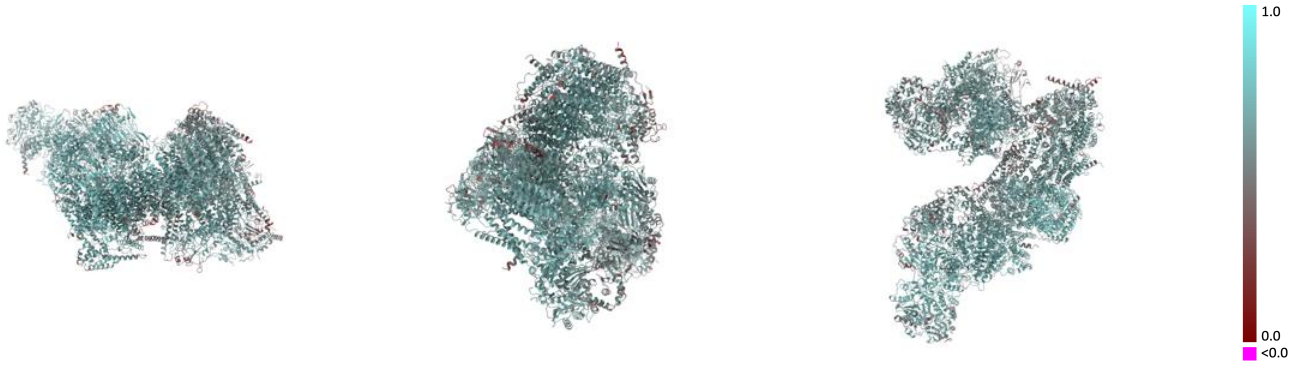
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

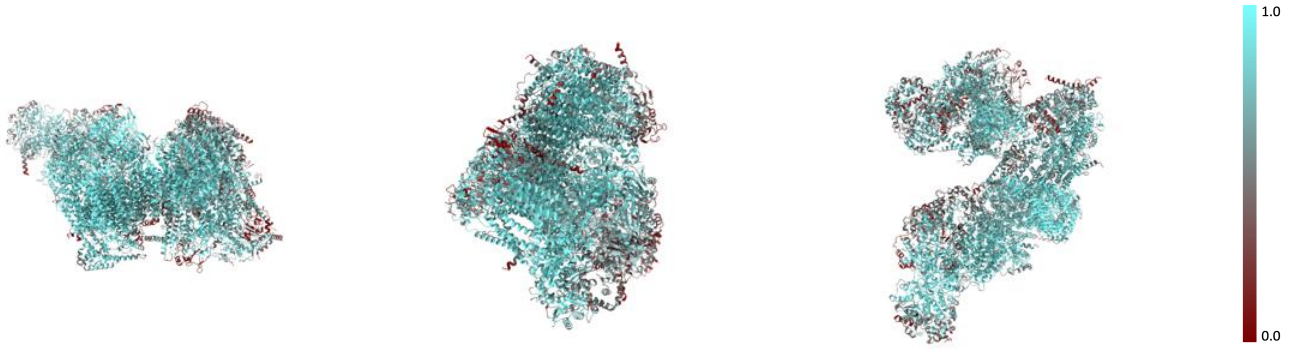
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

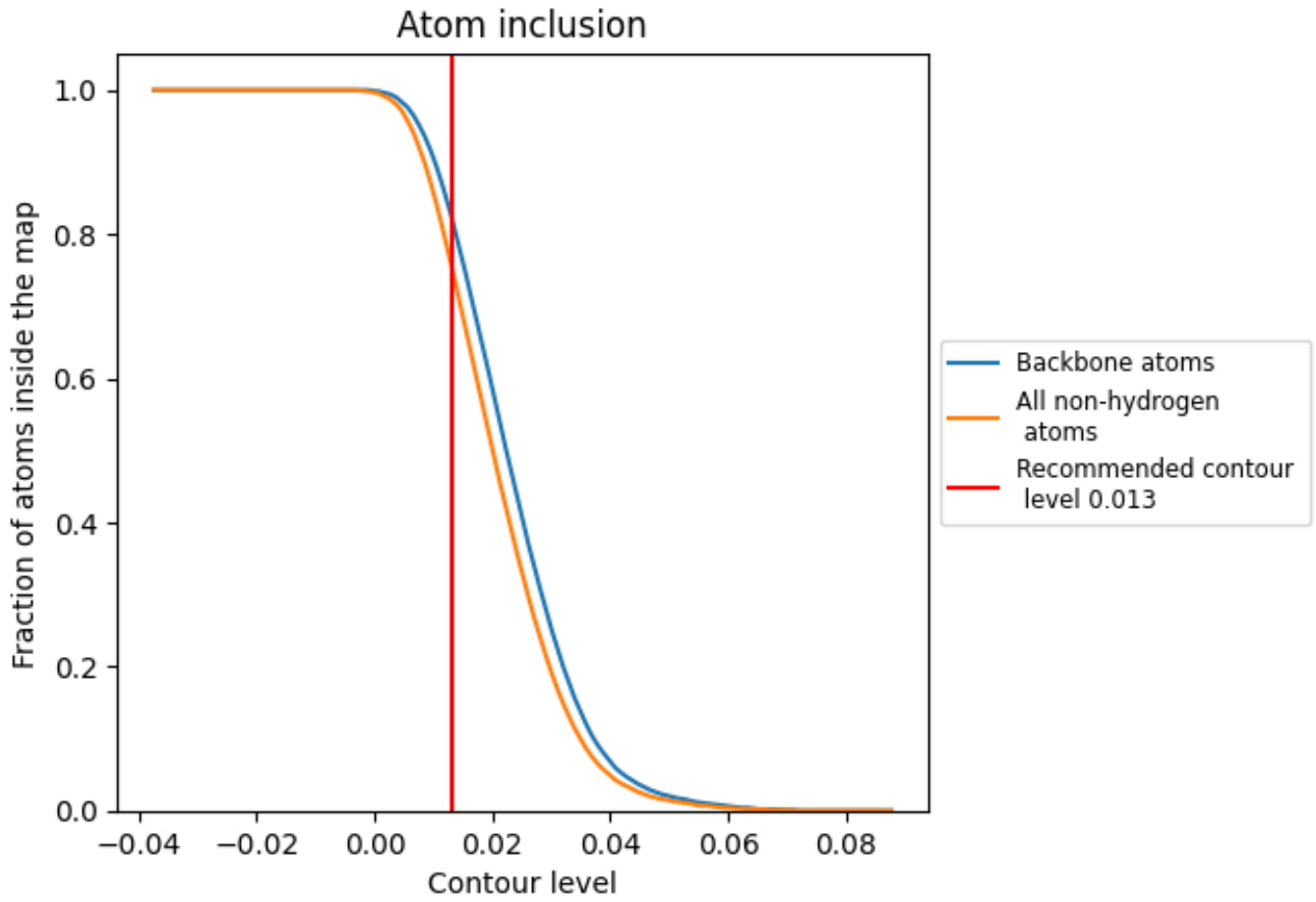
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.6280
A	0.9520	0.6900
AA	0.5340	0.5470
AB	0.7810	0.6360
AC	0.8840	0.6700
AD	0.4040	0.5070
AE	0.8620	0.6630
AF	0.8600	0.6720
AG	0.8150	0.6300
AH	0.7460	0.5890
AI	0.7580	0.6320
AJ	0.3000	0.4920
B	0.9500	0.7180
BA	0.5760	0.5650
BB	0.7830	0.6290
BC	0.8420	0.6490
BD	0.4270	0.5060
BE	0.7980	0.6330
BF	0.8160	0.6390
BG	0.6800	0.6010
BH	0.4760	0.5230
BI	0.6510	0.5710
BJ	0.5450	0.5330
C	0.8700	0.7030
D	0.9430	0.7160
E	0.6000	0.5770
F	0.6970	0.6260
G	0.7340	0.6390
H	0.9370	0.6930
I	0.9470	0.7170
J	0.8790	0.6680
K	0.9390	0.7030
L	0.8040	0.6340
M	0.8840	0.6630
N	0.9120	0.6930

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Chain	Atom inclusion	Q-score
O	0.9420	0.6630
P	0.5970	0.5790
Q	0.4090	0.5980
R	0.7530	0.6680
S	0.4770	0.5330
T	0.3030	0.4250
U	0.5600	0.4830
V	0.6930	0.6390
W	0.5540	0.5930
X	0.7130	0.5920
Y	0.5750	0.4950
Z	0.7760	0.6180
a	0.8520	0.6460
b	0.7680	0.5950
c	0.6990	0.5860
d	0.7310	0.5990
e	0.8340	0.6500
f	0.8870	0.6750
g	0.6300	0.5600
i	0.5660	0.5190
j	0.4430	0.4690
k	0.3950	0.4610
l	0.5870	0.5510
m	0.7310	0.6100
n	0.7370	0.5620
o	0.5320	0.5230
p	0.6880	0.5690
q	0.8280	0.6690
u	0.7270	0.5670
v	0.8550	0.6630
x	0.9380	0.7090
y	0.8800	0.6720
z	0.8710	0.6690