wwPDB EM Validation Summary Report (i)

Sep 20, 2026 – 09:48 pm BST

PDB ID	:	8BQ5 / pdb_00008bq5
EMDB ID	:	EMD-16171
Title	:	Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (Complete conformation 1 composition)
Authors	:	Klusch, N.; Kuehlbrandt, W.
Deposited on	:	2022-11-18
Resolution	:	2.73 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

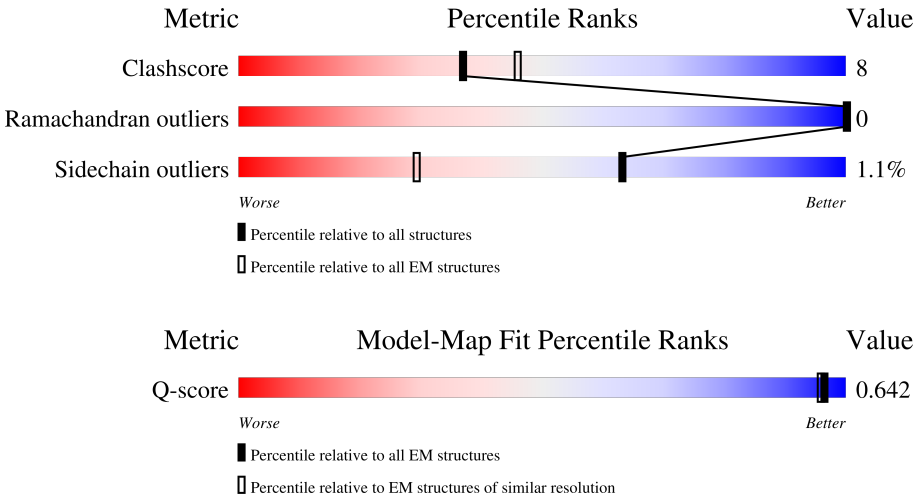
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.73 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	64% 14% • 21%
2	B	218	61% 11% 28%
3	C	190	85% 11% 5%
4	D	394	84% 14% •

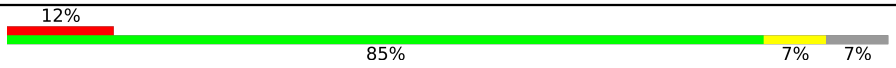
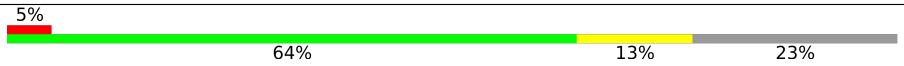
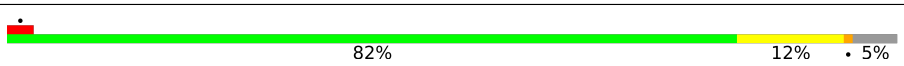
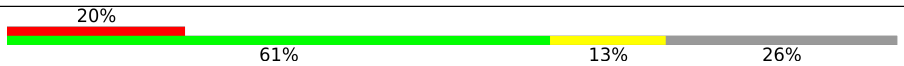
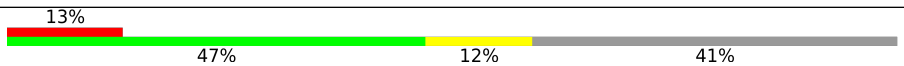
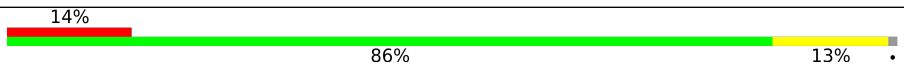
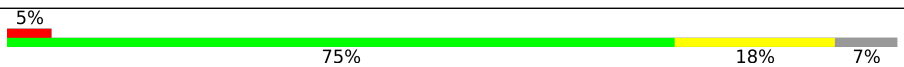
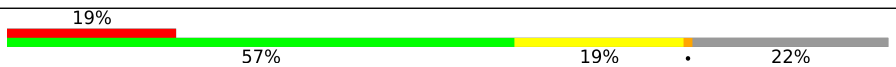
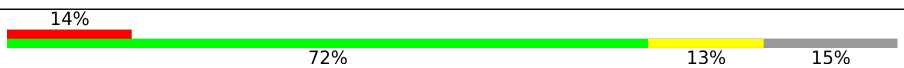
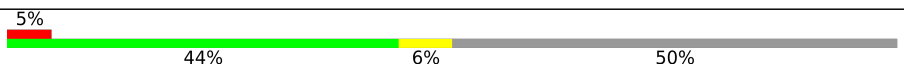
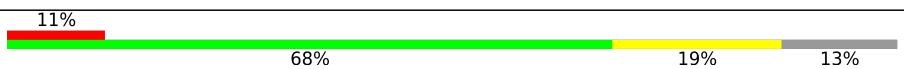
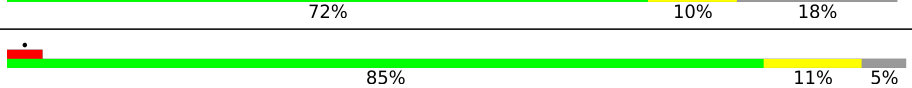
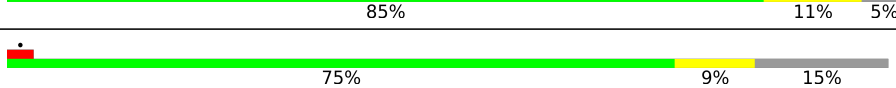
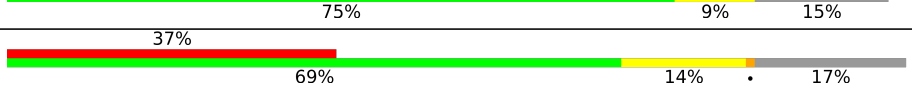
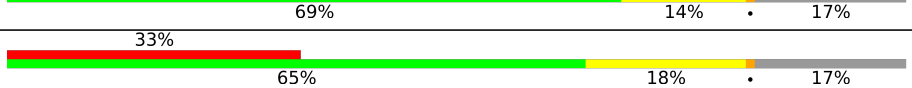
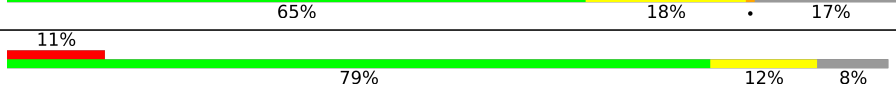
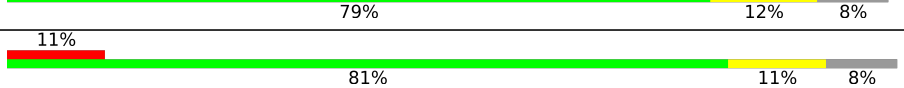
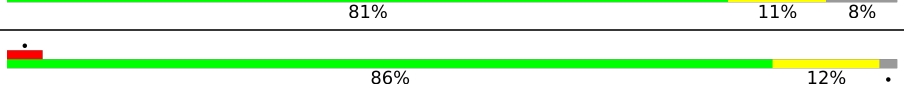
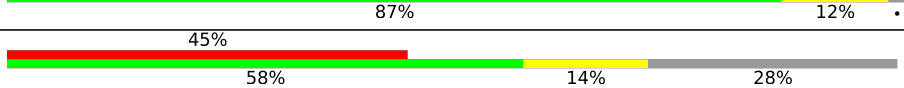
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Mol	Chain	Length	Quality of chain
5	E	255	21% 61% 14% 25%
6	F	486	12% 77% 12% 11%
7	G	748	10% 78% 13% 8%
8	H	325	84% 15%
9	I	222	67% 7% 26%
10	J	205	67% 18% 15%
11	K	100	77% 21%
12	L	669	5% 81% 18%
13	M	495	80% 20%
14	N	499	82% 15%
15	O	159	67% 10% 23%
16	P	402	16% 65% 14% 21%
17	Q	154	24% 59% 9% 32%
18	R	110	13% 62% 5% 34%
19	S	97	18% 77% 19%
20	T	122	37% 48% 20% 32%
21	U	126	17% 54% 15% 31%
22	V	169	9% 70% 13% 17%
23	W	133	19% 75% 9% 16%
24	X	106	8% 76% 16% 8%
25	Y	159	23% 62% 16% 21%
26	Z	143	10% 69% 18% 13%
27	a	65	8% 75% 14% 11%
28	b	65	9% 63% 34%
29	c	88	9% 67% 19% 14%

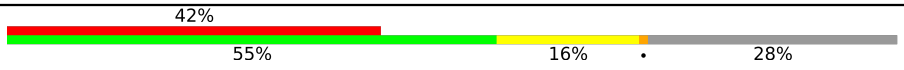
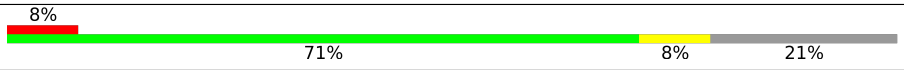
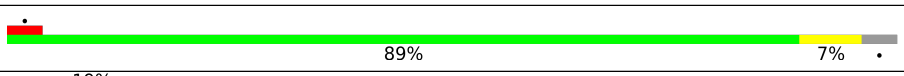
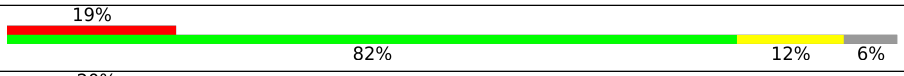
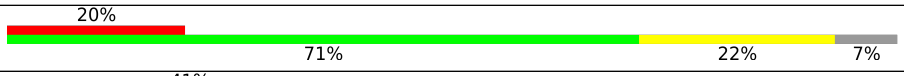
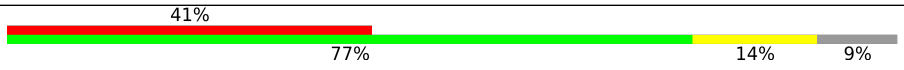
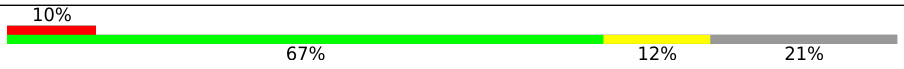
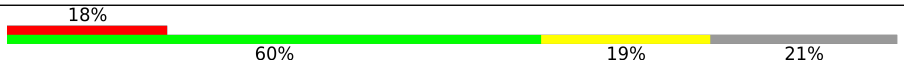
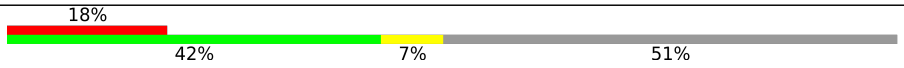
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Mol	Chain	Length	Quality of chain
30	d	81	
31	e	83	
32	f	106	
33	g	114	
34	i	98	
35	j	69	
36	k	72	
37	l	125	
38	m	71	
39	n	117	
40	o	103	
41	p	106	
42	q	159	
43	u	63	
44	v	113	
45	x	256	
46	y	278	
47	z	275	
48	AA	503	
48	BA	503	
49	AB	531	
49	BB	531	
50	AC	393	
50	BC	393	
51	AD	272	

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Mol	Chain	Length	Quality of chain
51	BD	272	
52	AE	307	
52	BE	307	
53	AF	122	
53	BF	122	
54	AG	72	
54	BG	72	
55	AH	69	
55	BH	69	
56	AI	72	
56	BI	72	
57	AJ	57	
57	BJ	57	

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
58	SF4	F	501	-	-	X	-
59	FES	E	500	-	-	X	-
66	COO	x	301	X	-	-	-

2 Entry composition (i)

There are 69 unique types of molecules in this entry. The entry contains 96290 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	C	N	O	S	0	0
			776	486	134	144	12		

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

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

- 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	C	N	O	S	0	0
			997	640	175	177	5		

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

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

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

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

- Molecule 29 is a protein called Transmembrane protein.

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

- 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	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- 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	69	Total	C	N	O	S	0	0
			559	362	95	99	3		

- Molecule 34 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	68	Total	C	N	O	S	0	0
			591	370	110	108	3		

- 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	418	Total	C	N	O	S	0	0
			3190	2029	528	618	15		

- 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		

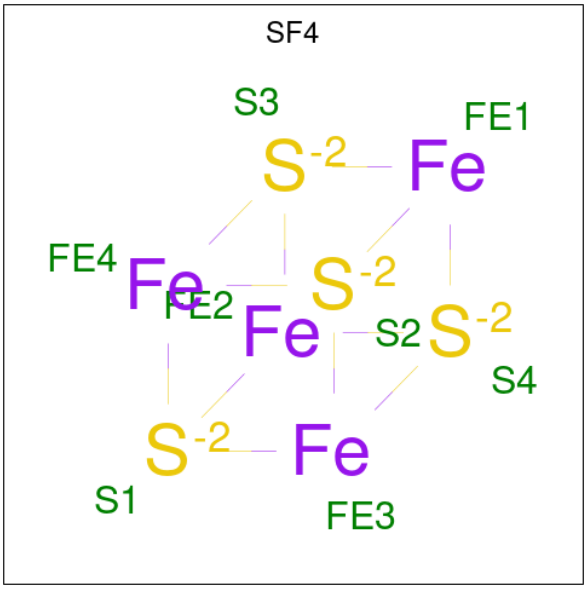
- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

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.

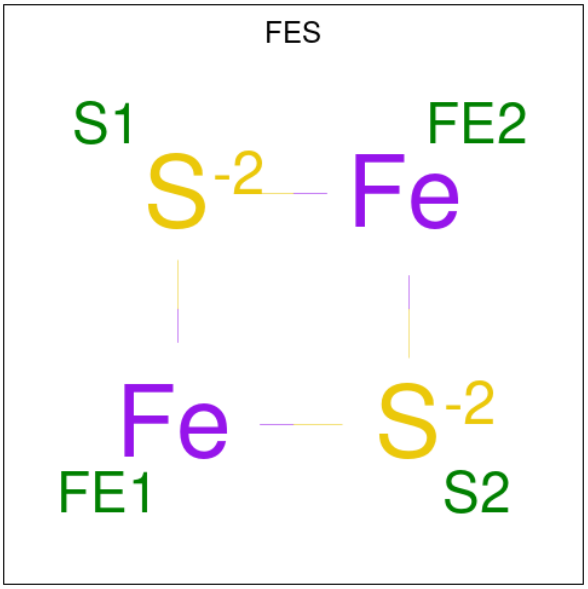
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		
57	BJ	28	Total	C	N	O	0	0
			205	139	34	32		

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



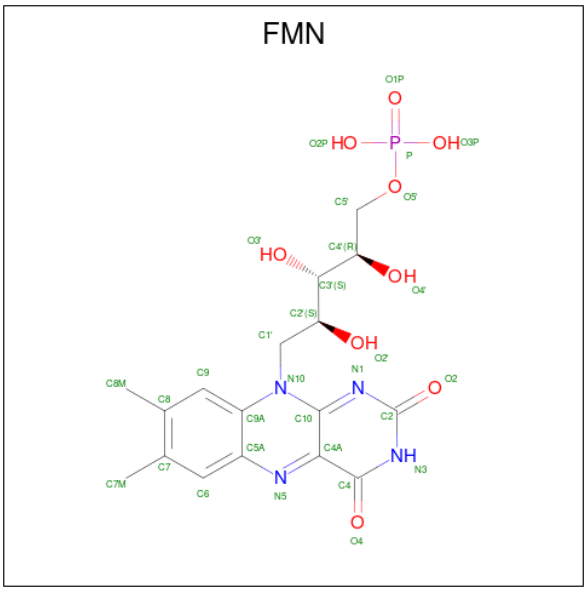
Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total Fe S 8 4 4	0
58	F	1	Total Fe S 8 4 4	0
58	G	1	Total Fe S 8 4 4	0
58	G	1	Total Fe S 8 4 4	0
58	I	1	Total Fe S 8 4 4	0
58	I	1	Total Fe S 8 4 4	0

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



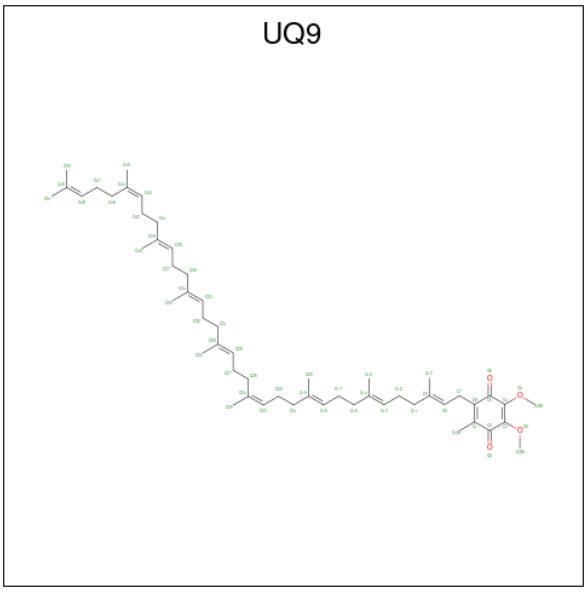
Mol	Chain	Residues	Atoms	AltConf
59	E	1	Total Fe S 4 2 2	0
59	G	1	Total Fe S 4 2 2	0
59	AD	1	Total Fe S 4 2 2	0
59	BD	1	Total Fe S 4 2 2	0

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: 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 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).

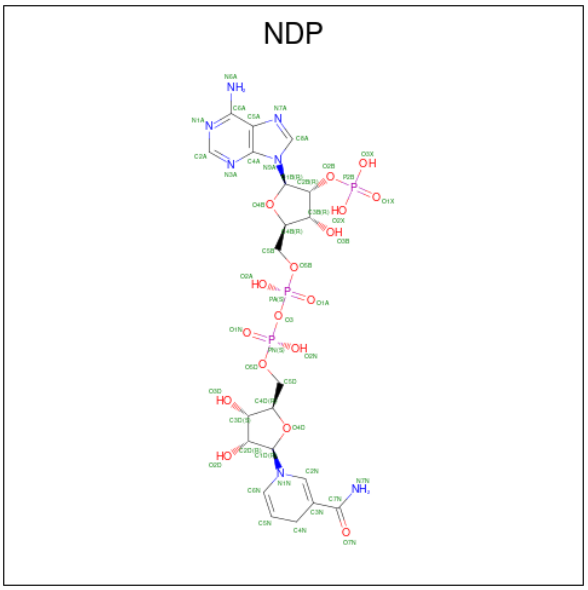


Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is FE (III) ION (CCD ID: 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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

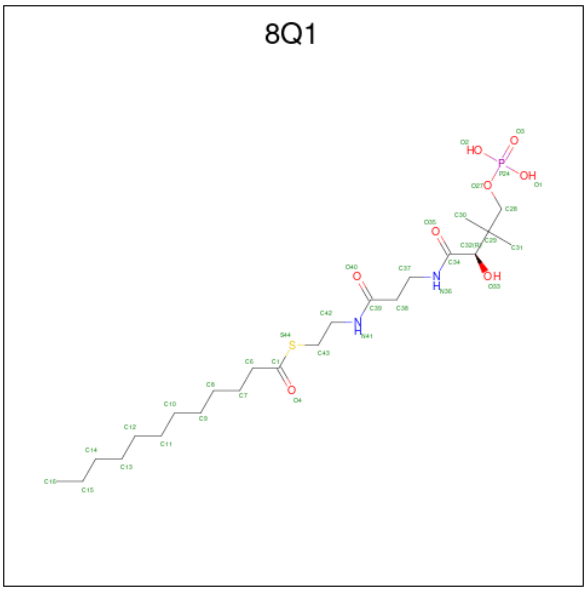


Mol	Chain	Residues	Atoms	AltConf
63	P	1	Total C N O P 48 21 7 17 3	0

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

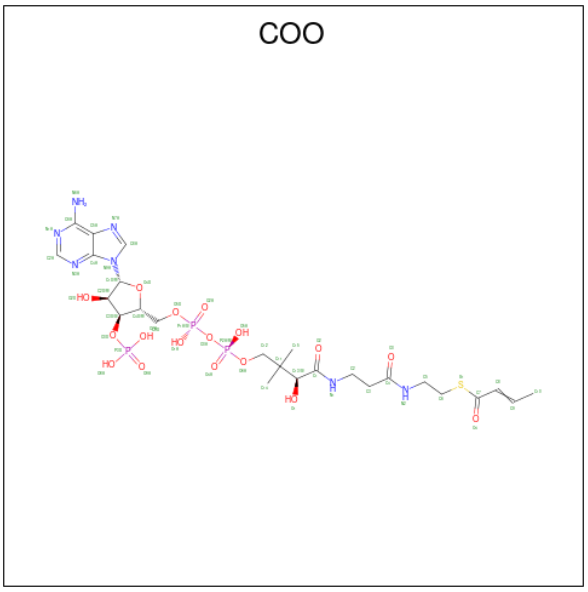
Mol	Chain	Residues	Atoms	AltConf
64	R	1	Total Zn 1 1	0
64	y	1	Total Zn 1 1	0
64	AB	1	Total Zn 1 1	0
64	BB	1	Total Zn 1 1	0

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



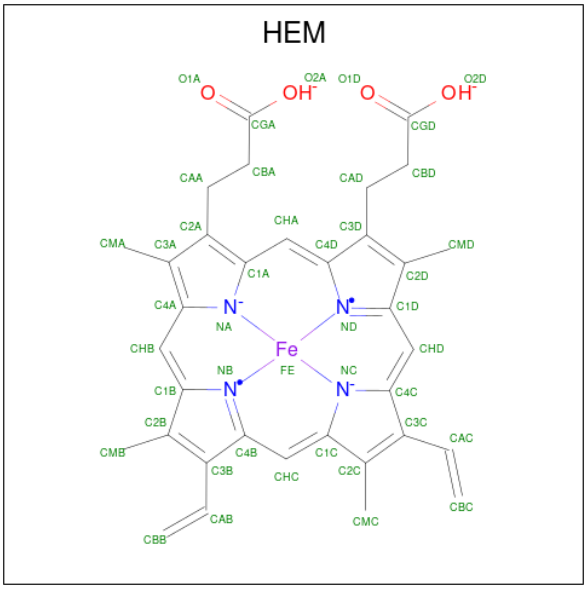
Mol	Chain	Residues	Atoms						AltConf
65	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
65	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



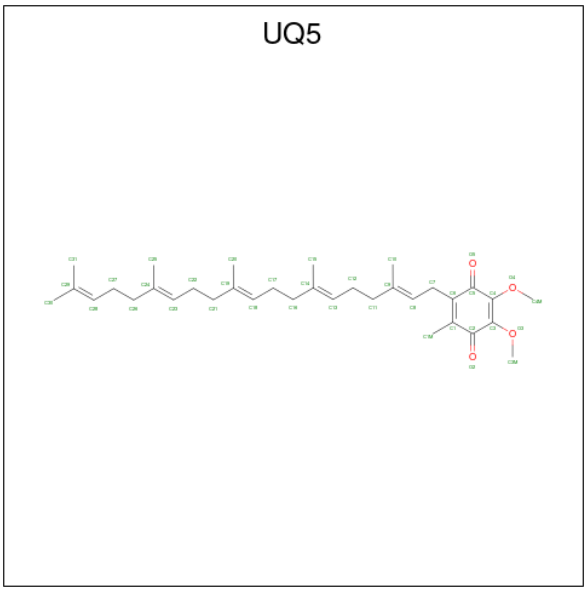
Mol	Chain	Residues	Atoms						AltConf
66	x	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

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



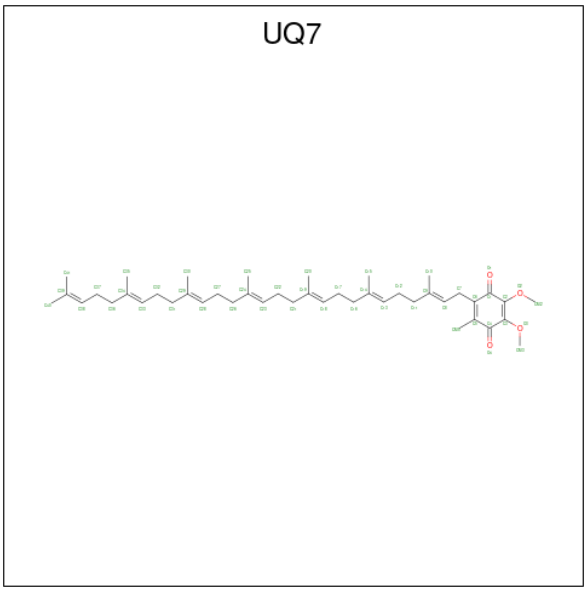
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	BE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



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

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



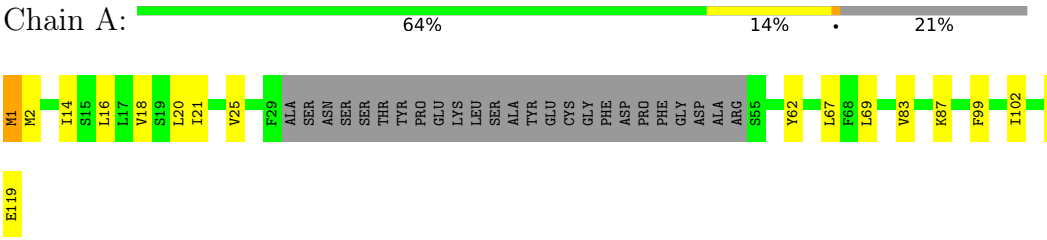
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
69	BC	1	48	44	4	0

3 Residue-property plots

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

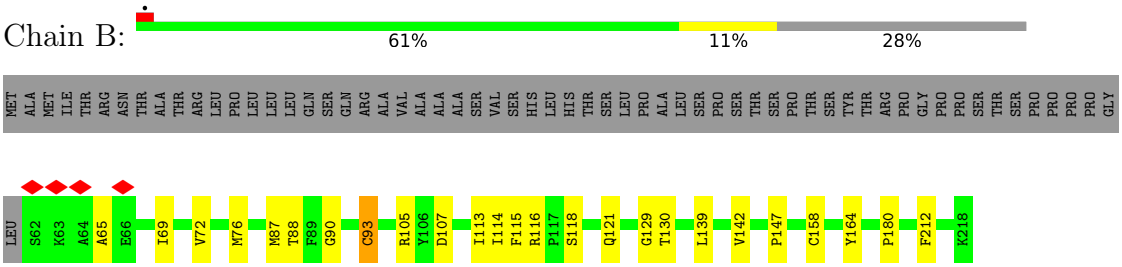
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



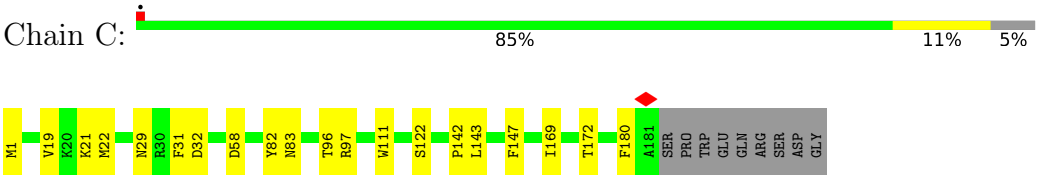
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



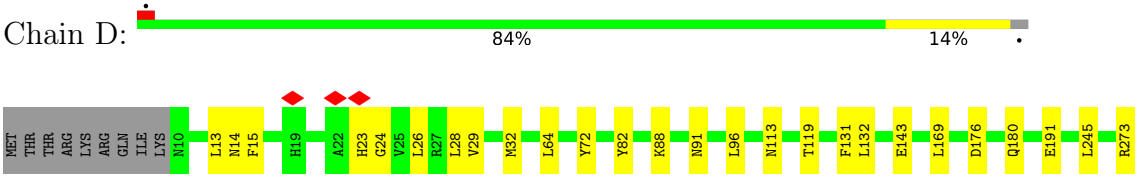
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

Chain C:



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

Chain D:

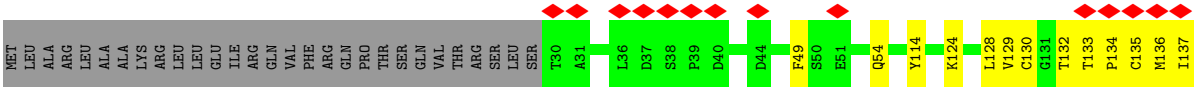


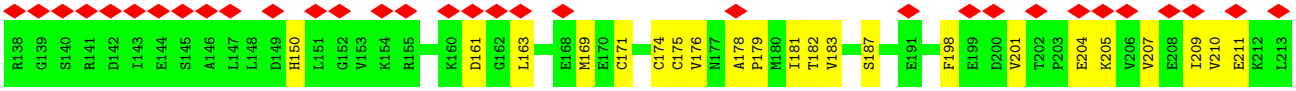


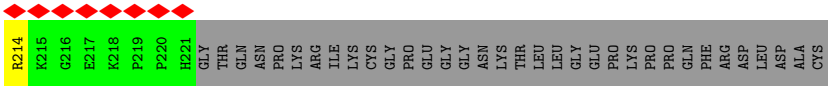
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:





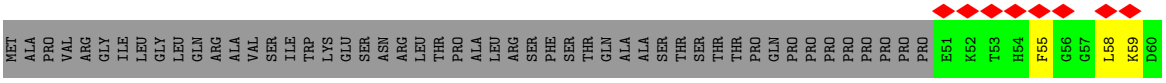


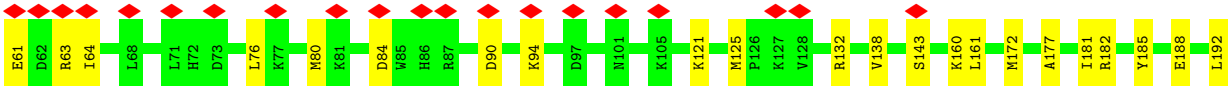


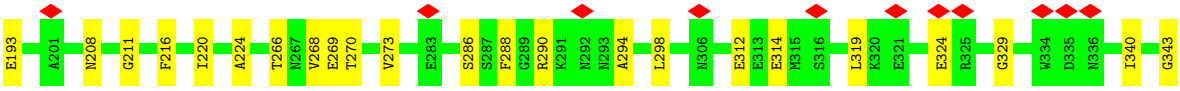
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:







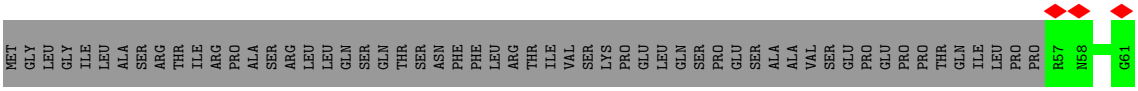




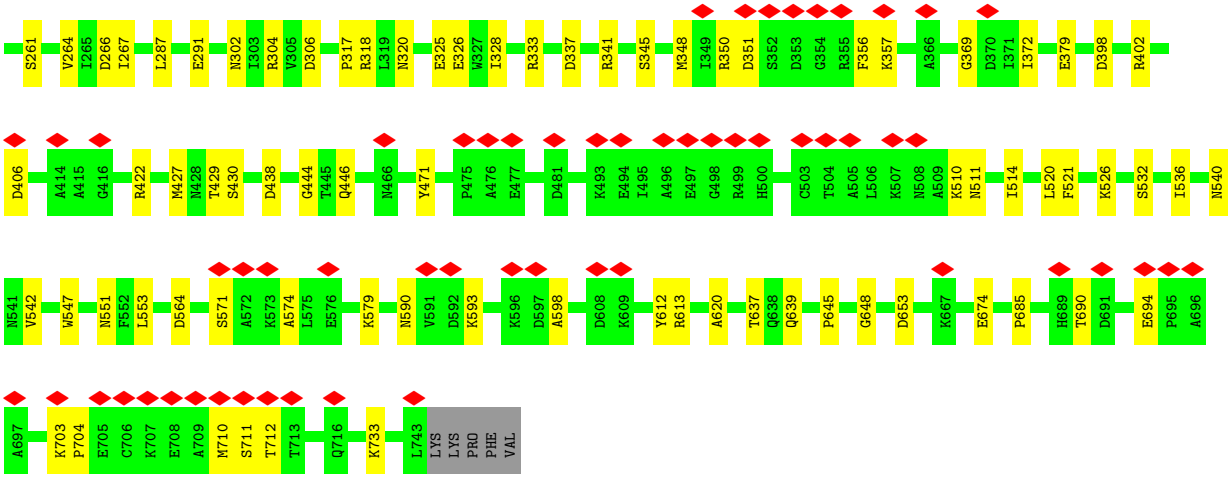
• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

Chain G:

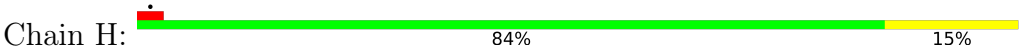


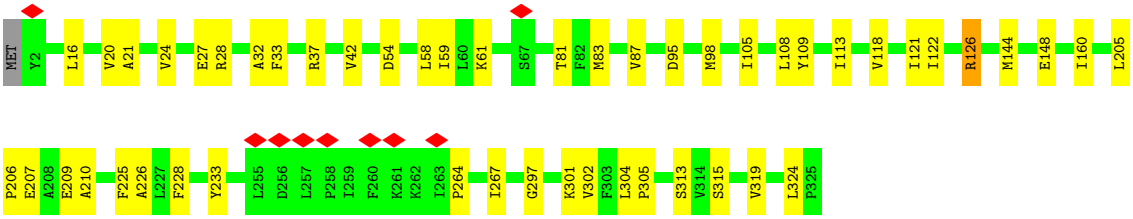






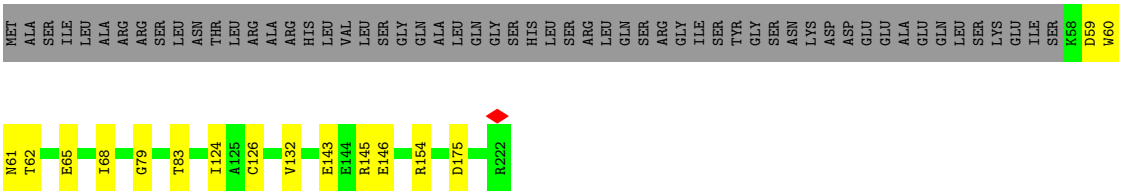
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1





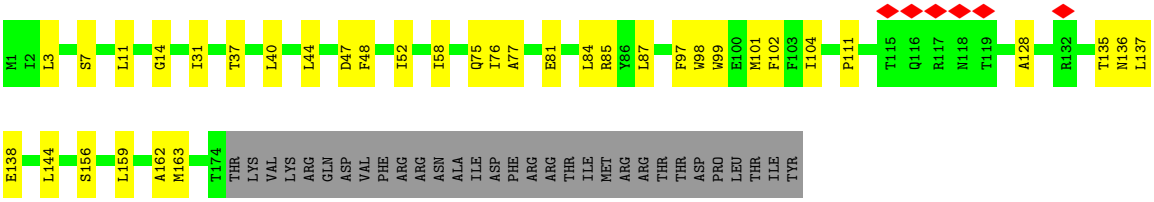
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial



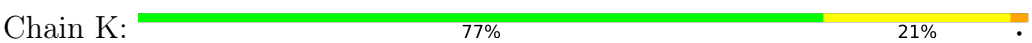


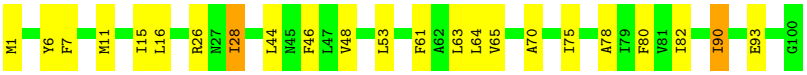
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



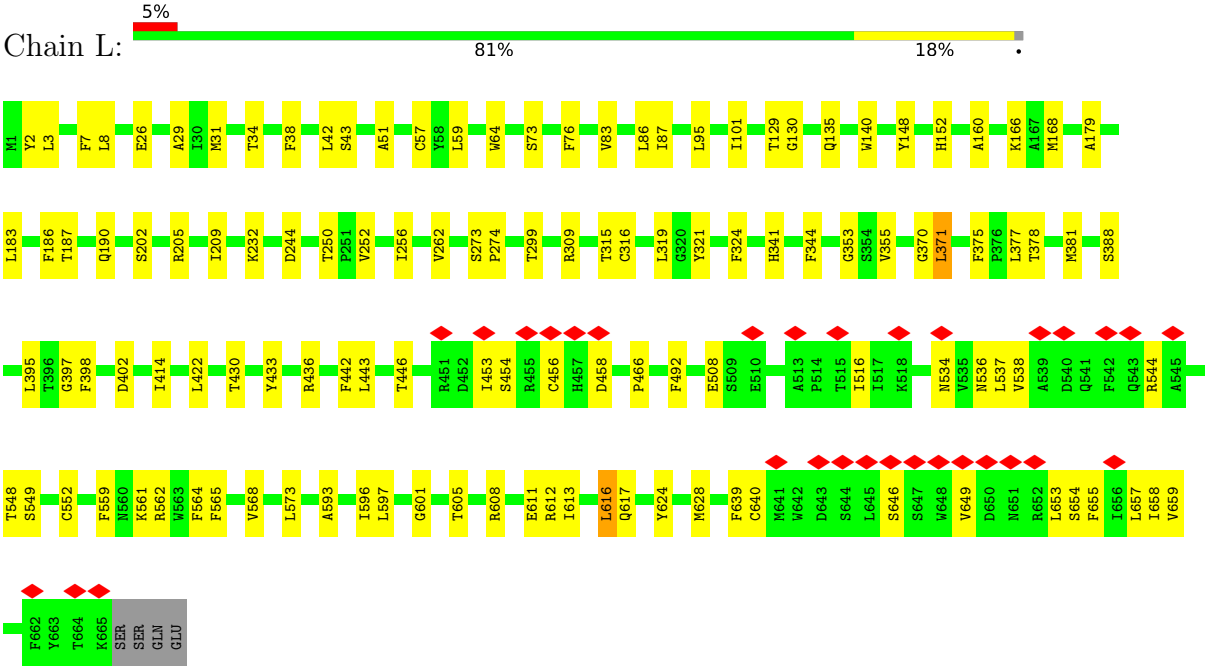


• Molecule 11: NADH dehydrogenase subunit 4L

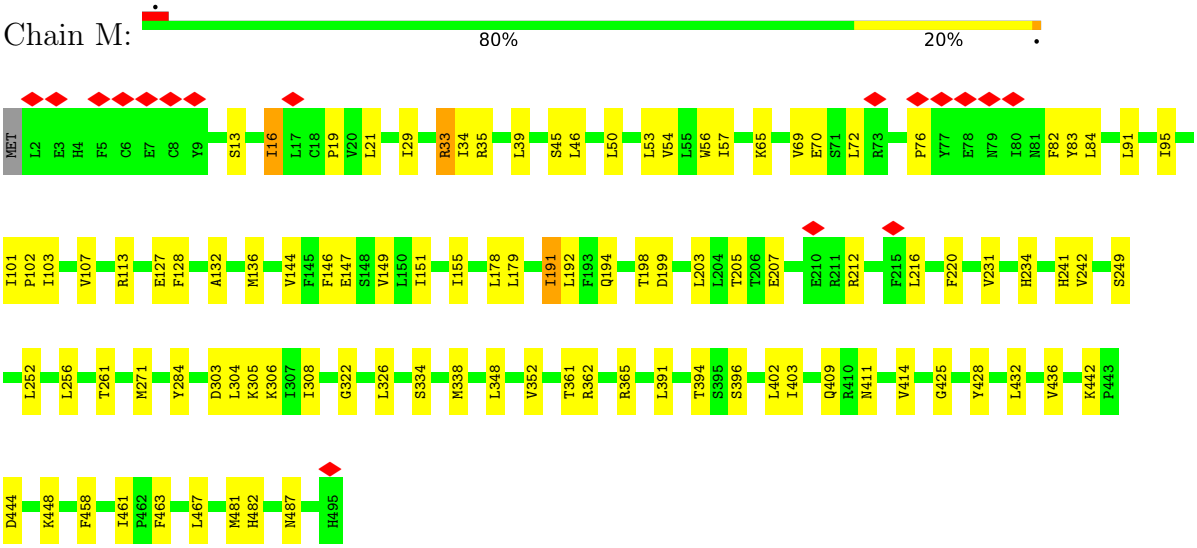




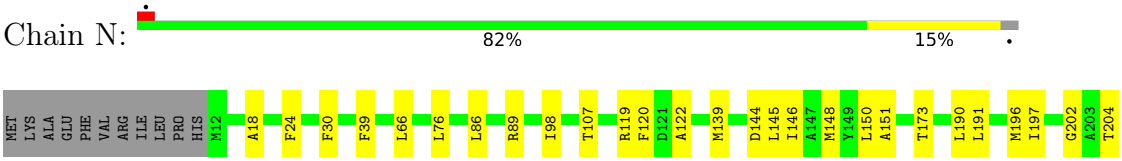
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

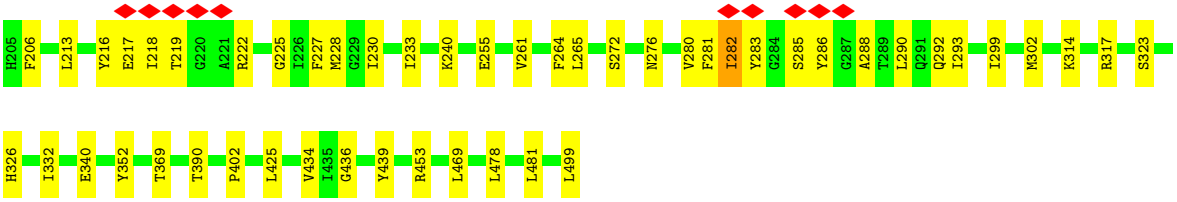


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



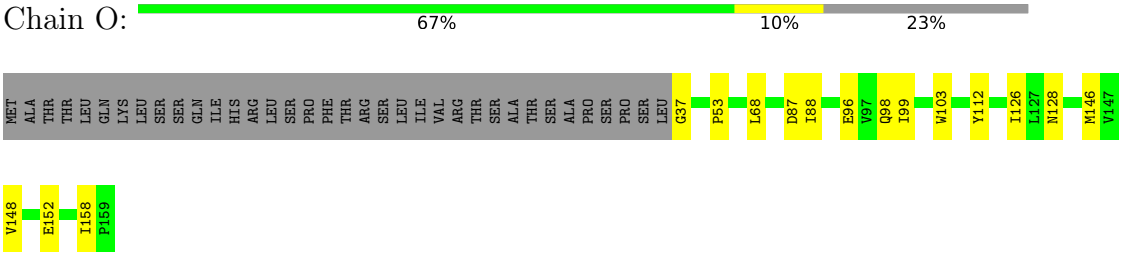
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2





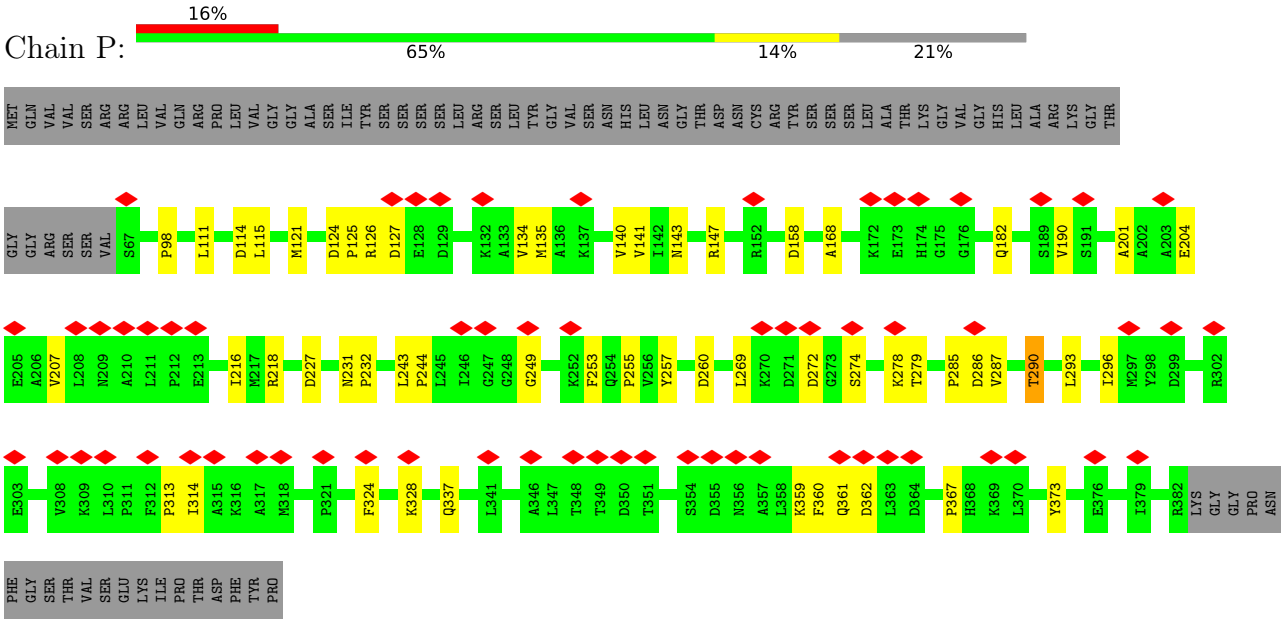
• Molecule 15: AT3G07480.1

Chain O:



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

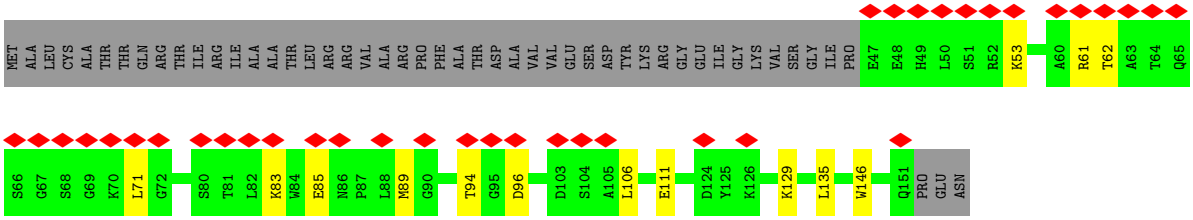
Chain P:



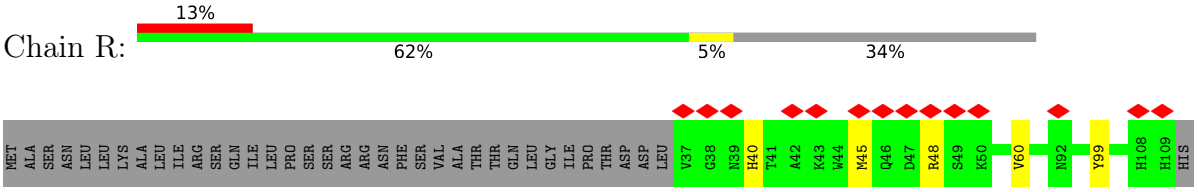
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

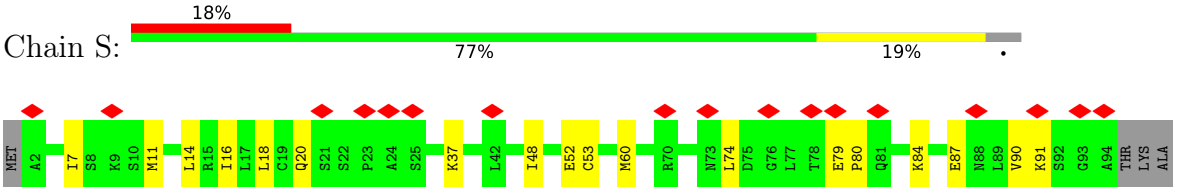




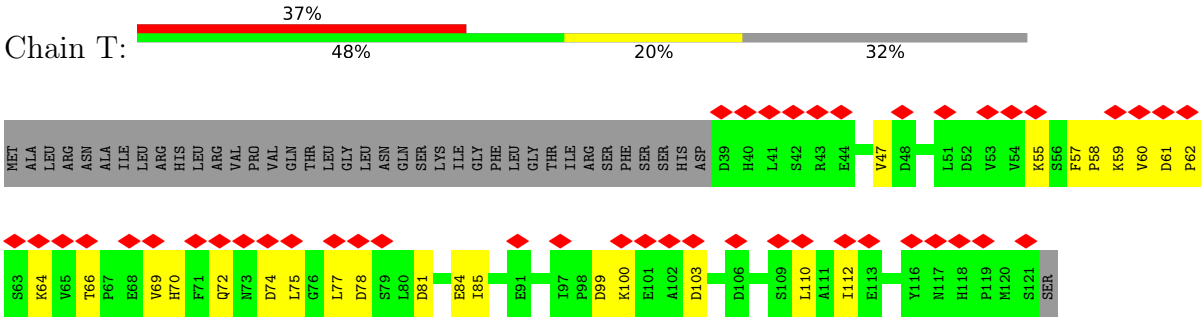
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



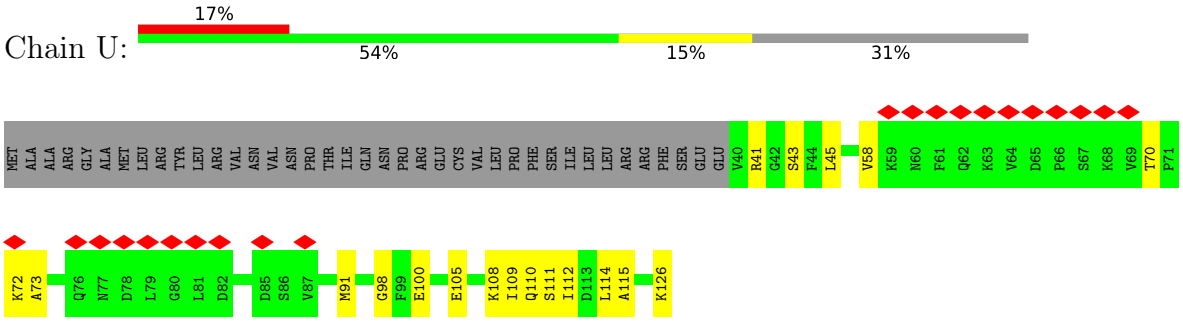
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



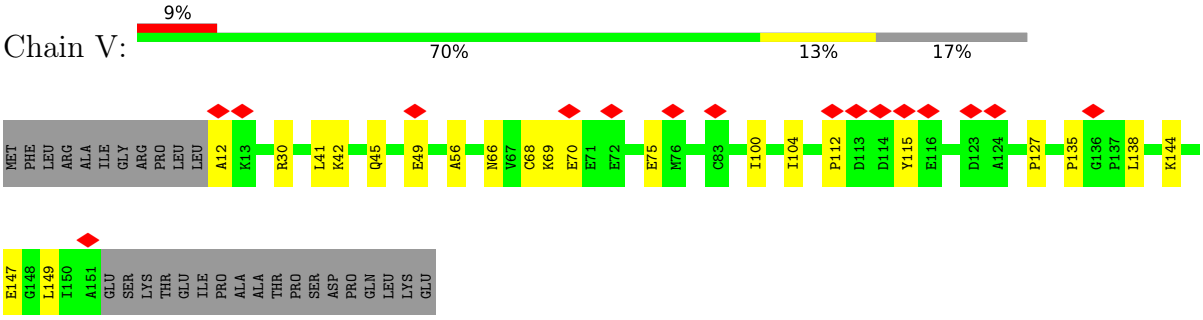
• Molecule 20: Acyl carrier protein 1, mitochondrial



• Molecule 21: Acyl carrier protein 2, mitochondrial

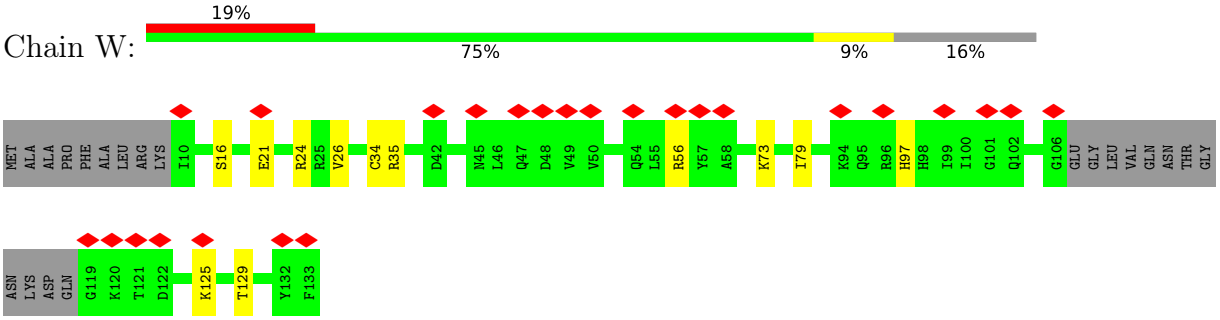


• Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



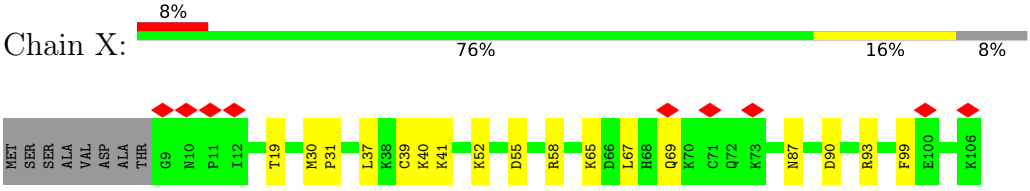
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



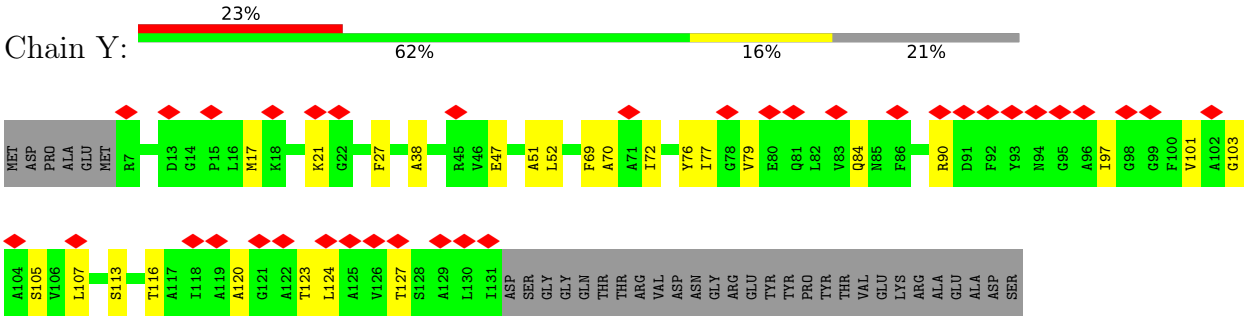
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

Chain X:



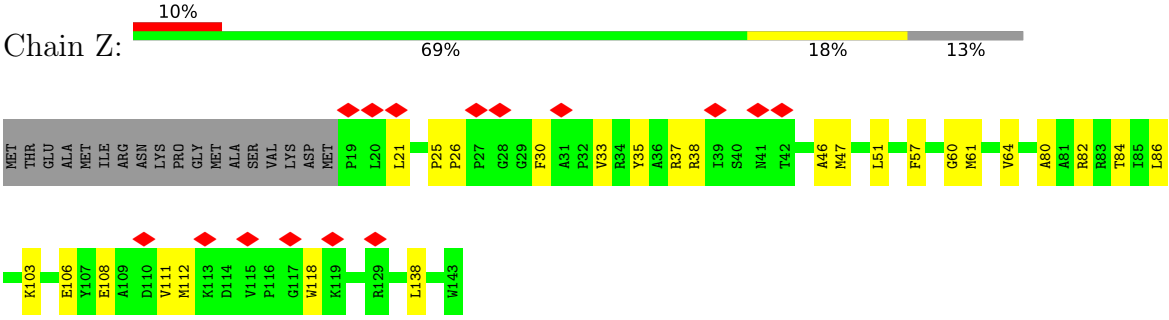
• Molecule 25: Outer envelope pore protein 16-3, chloroplastic/mitochondrial

Chain Y:



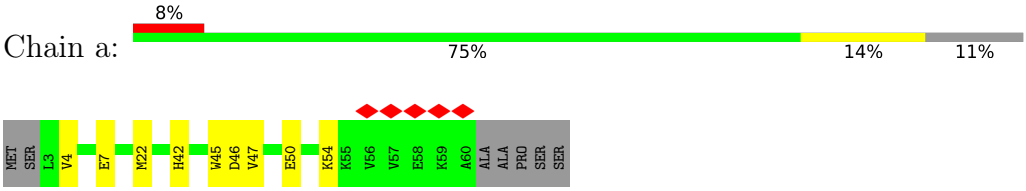
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A

Chain Z:



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

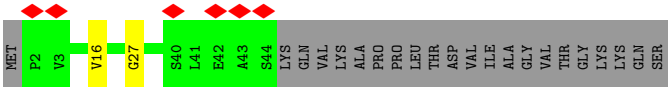
Chain a:



• Molecule 28: At2g46540/F11C10.23

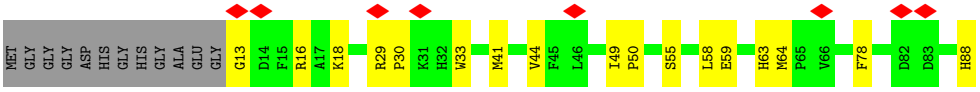
Chain b:



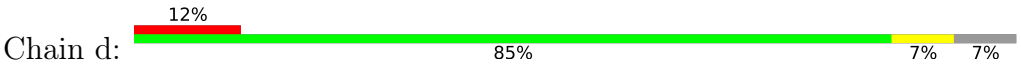


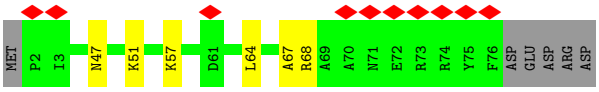
• Molecule 29: Transmembrane protein





• Molecule 30: Excitatory amino acid transporter



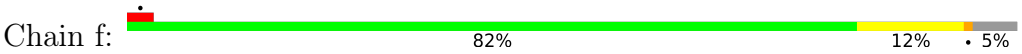


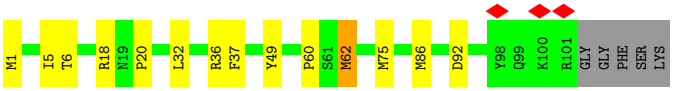
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B





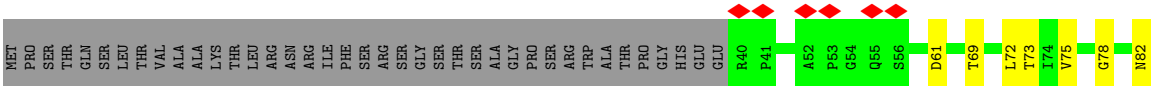
• Molecule 32: At4g16450

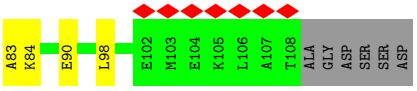




• Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

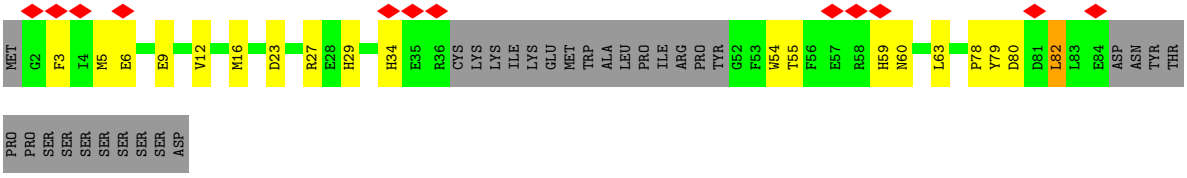






• Molecule 34: P1

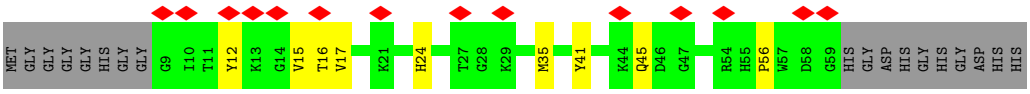




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

Chain j:

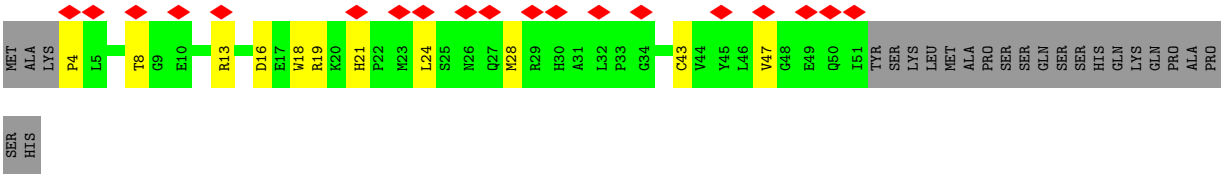




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A

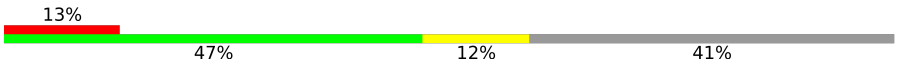
Chain k:

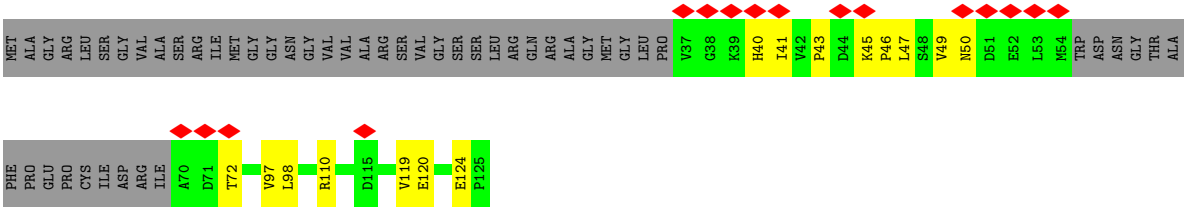




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:

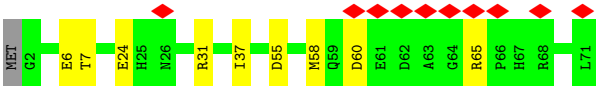




• Molecule 38: B15 – 1 beta subcomplex subunit 4

Chain m:

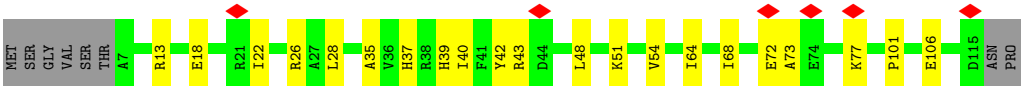




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

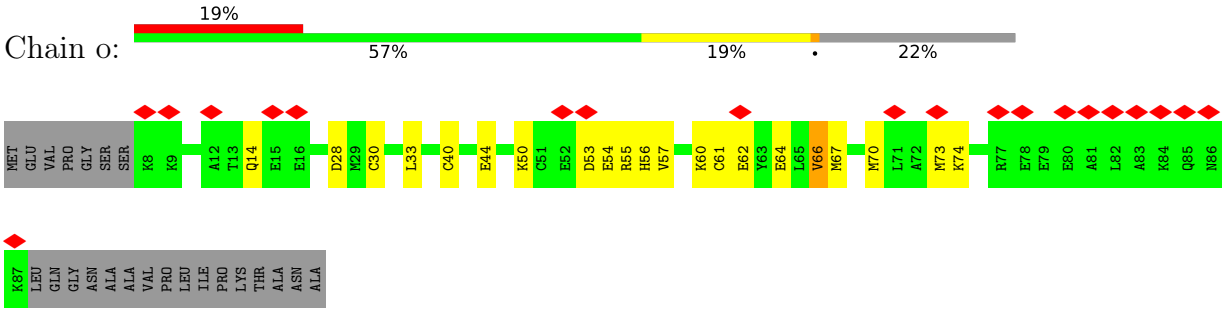
Chain n:





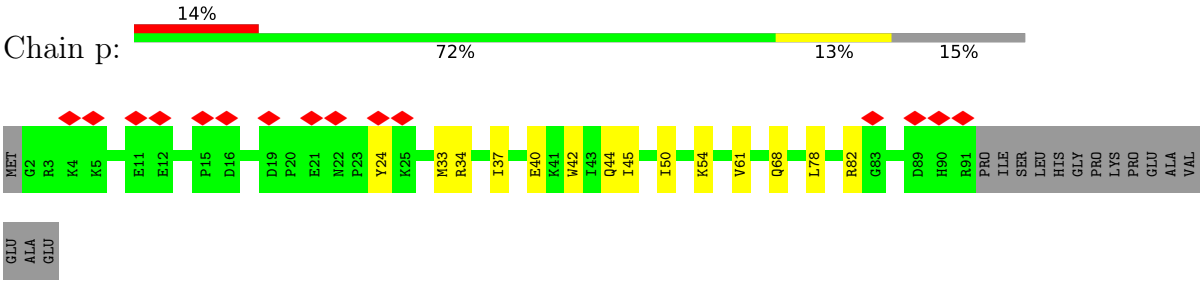
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



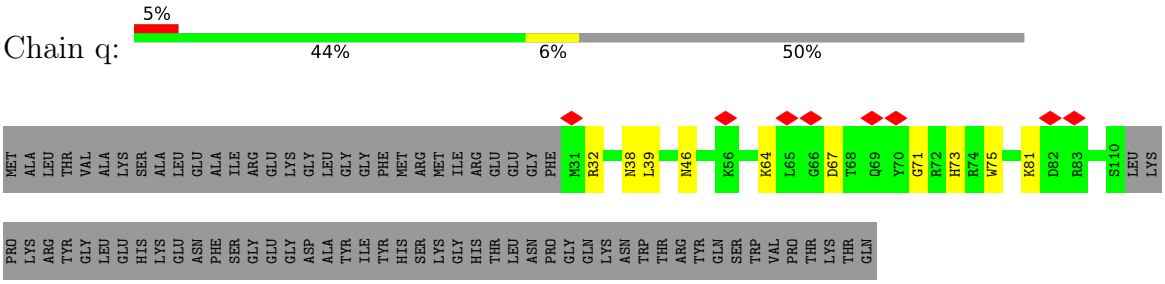
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

Chain p:



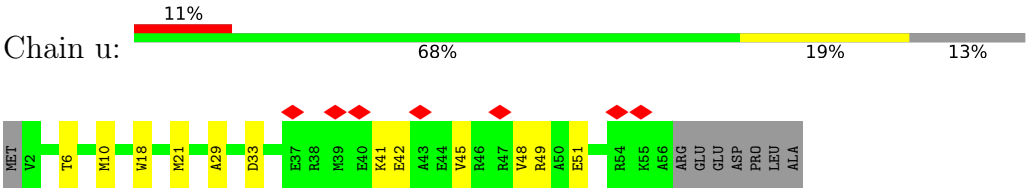
• Molecule 42: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



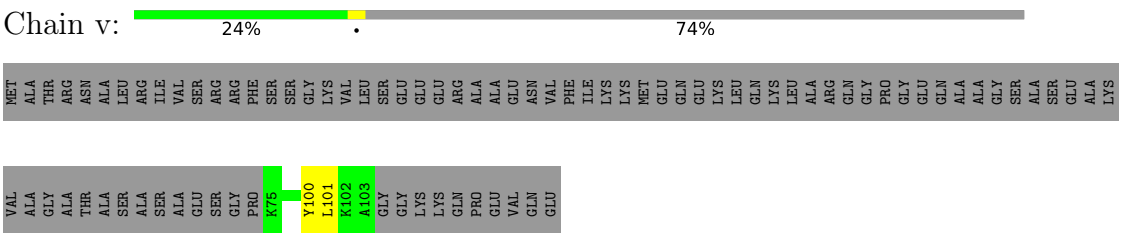
• Molecule 43: Uncharacterized protein At1g67785

Chain u:



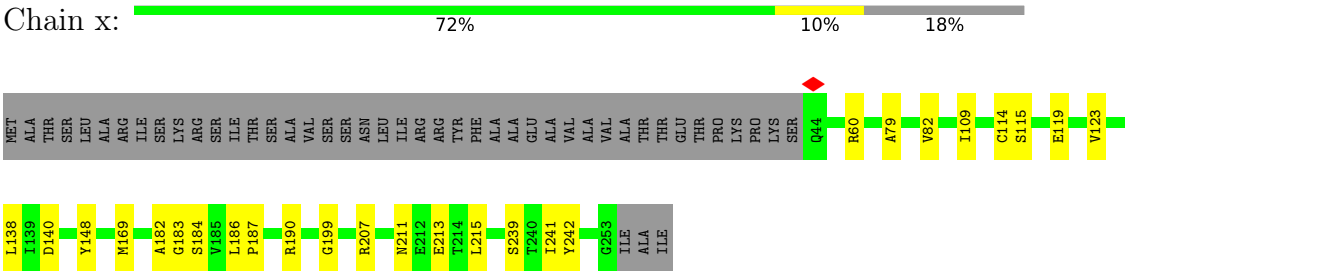
• Molecule 44: Uncharacterized protein At2g27730, mitochondrial

Chain v:



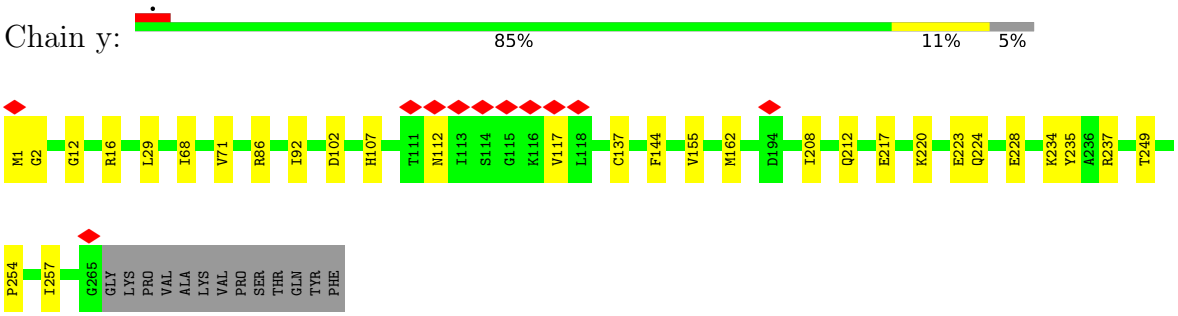
• Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial

Chain x:



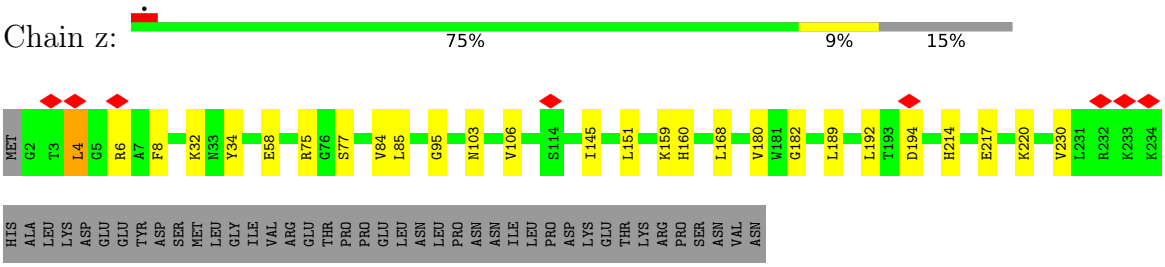
• Molecule 46: Gamma carbonic anhydrase 2, mitochondrial

Chain y:



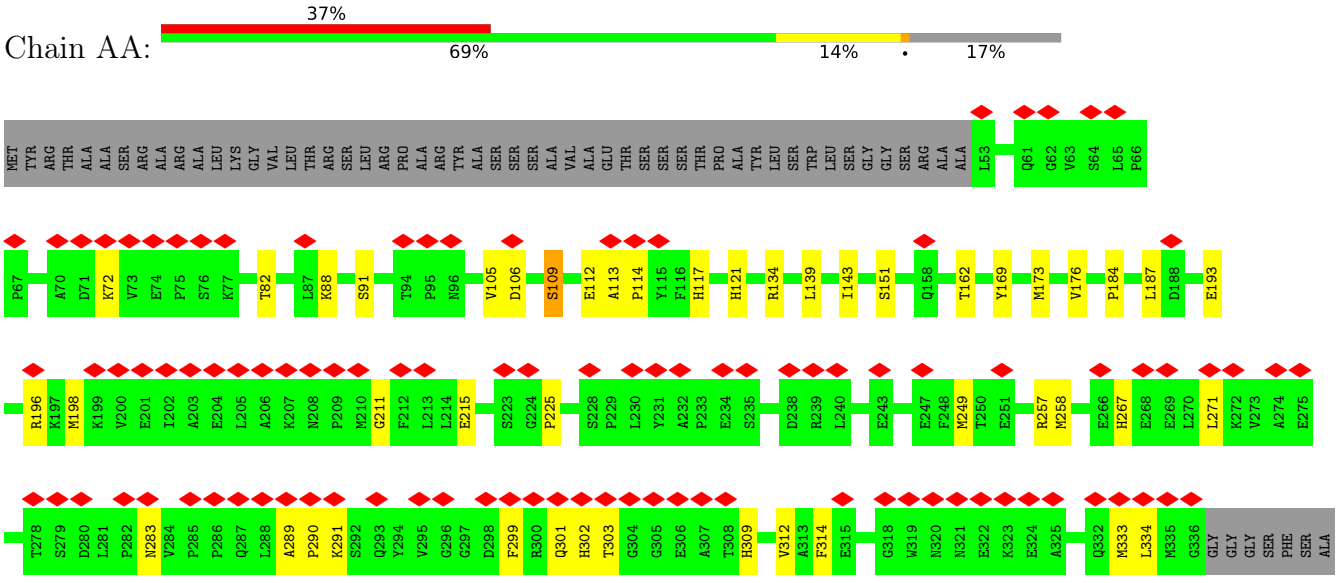
• Molecule 47: Gamma carbonic anhydrase 1, mitochondrial

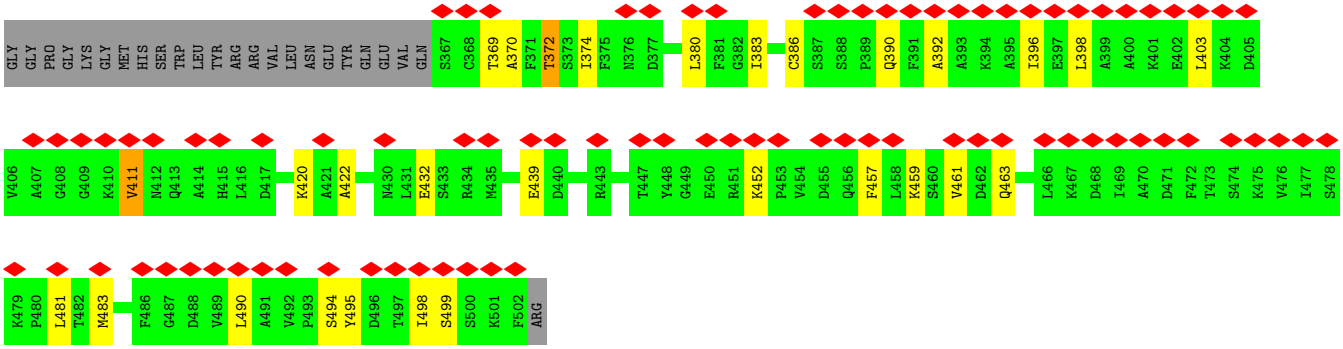
Chain z:



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

Chain AA:

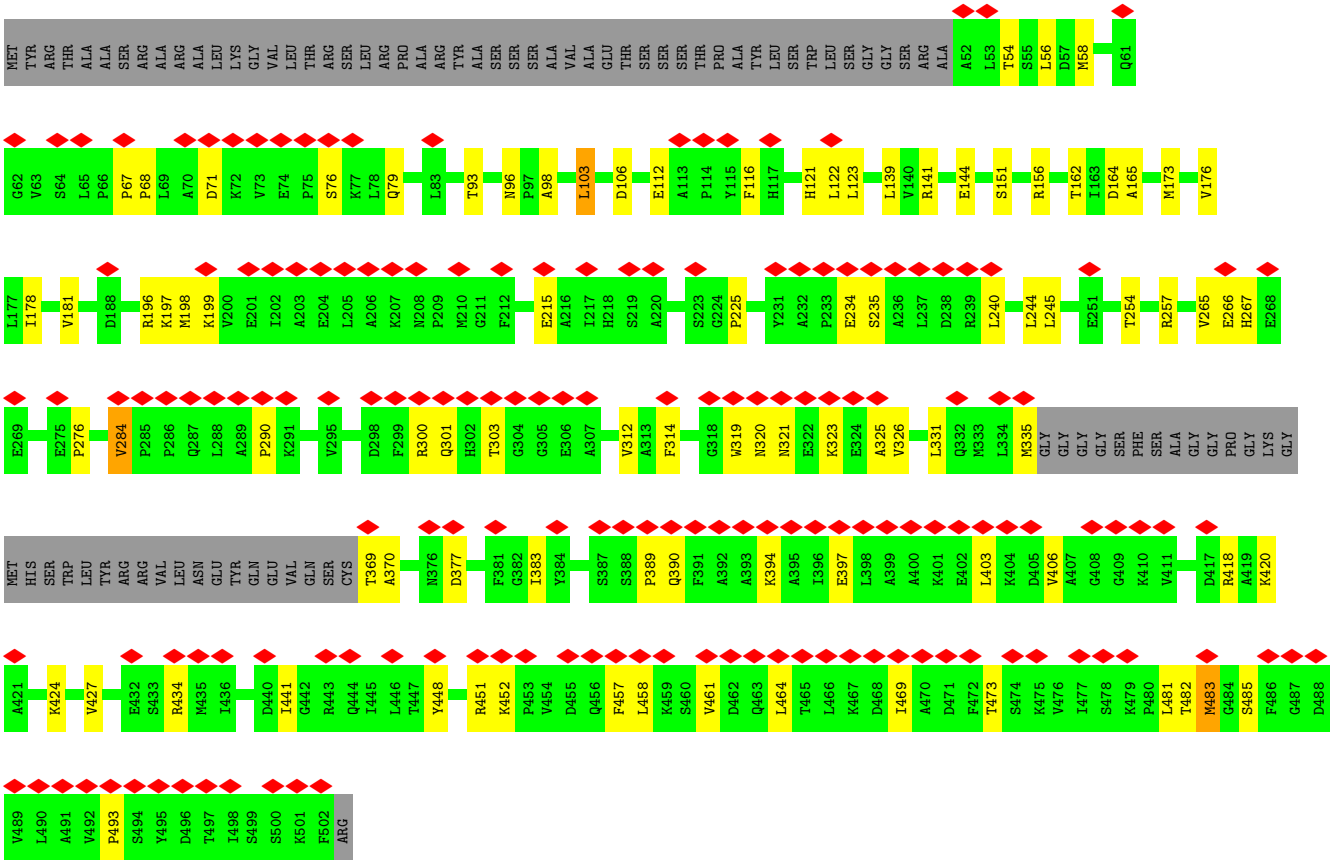




• Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

Chain BA:

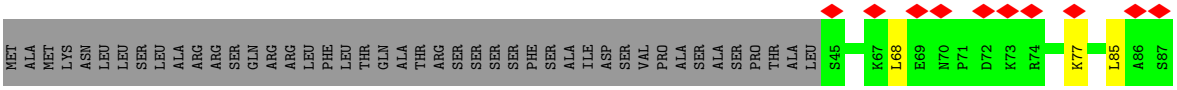


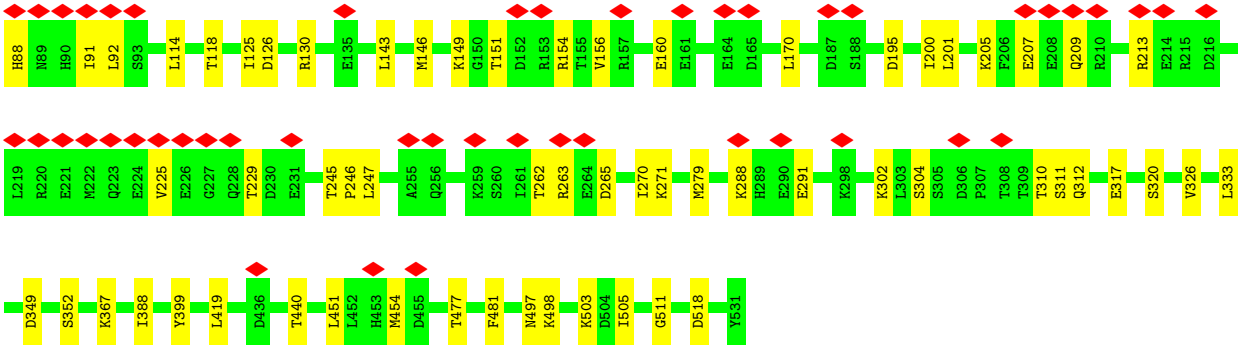


• Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain AB:



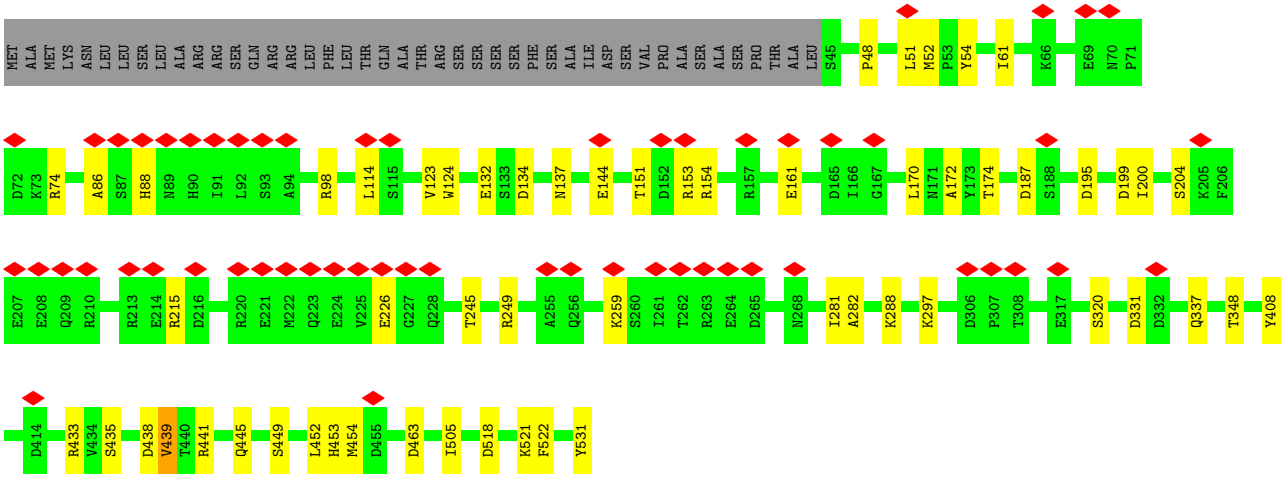




• Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain BB:

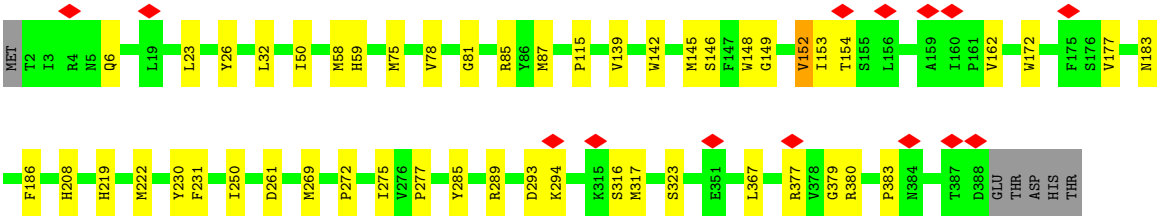




• Molecule 50: Cytochrome b

Chain AC:



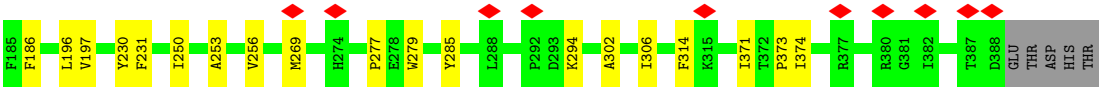


• Molecule 50: Cytochrome b

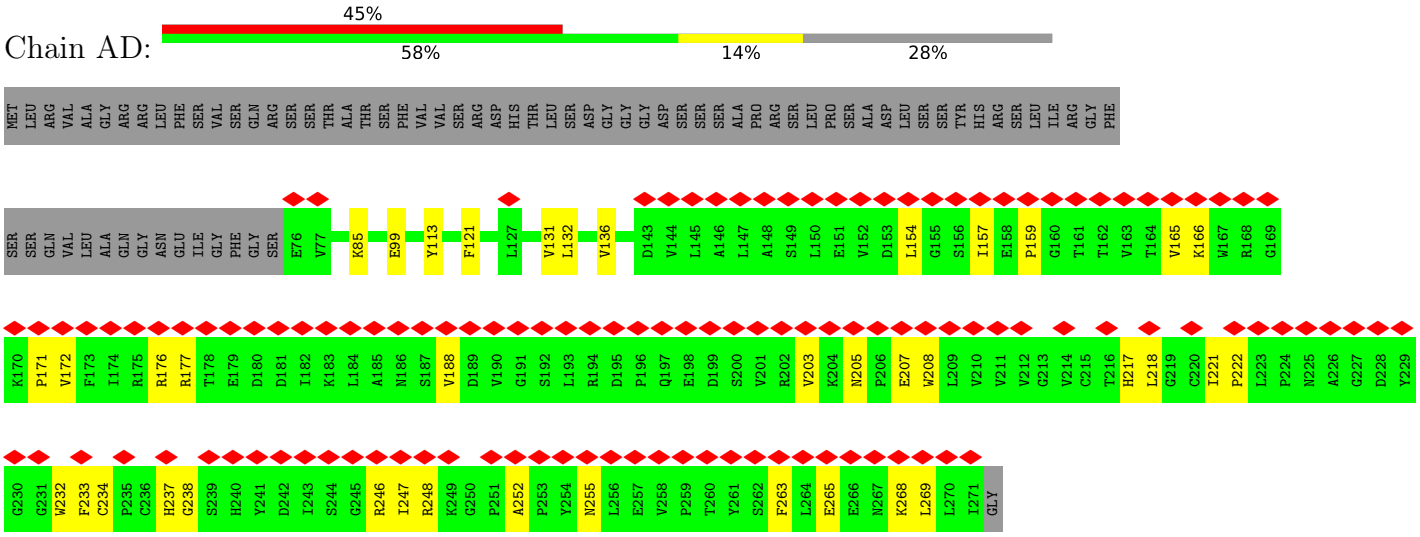
Chain BC:



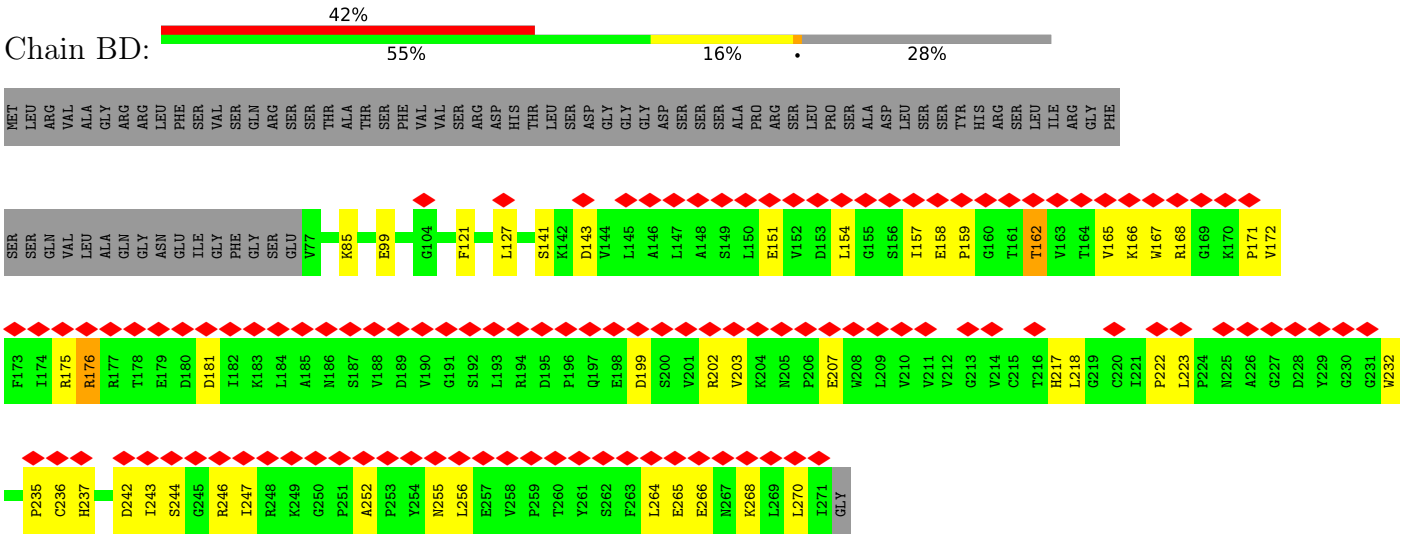




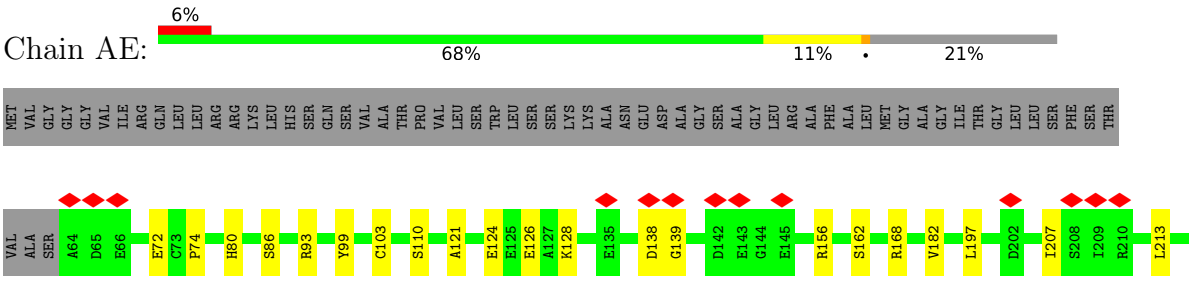
• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

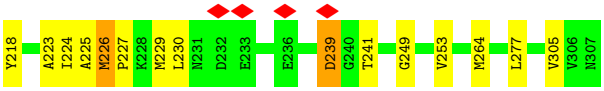


• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

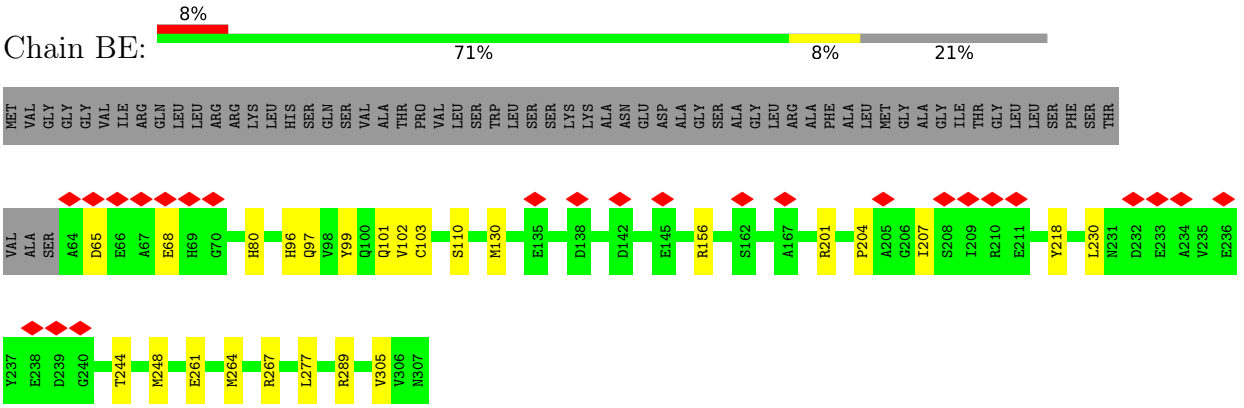


• Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

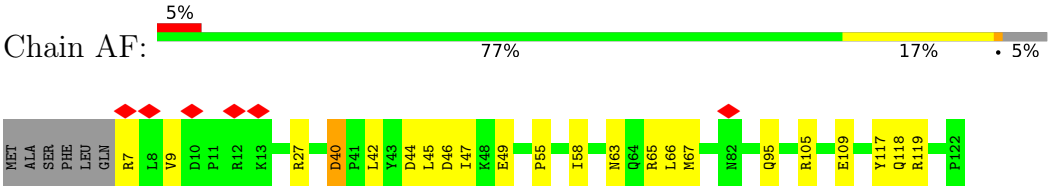




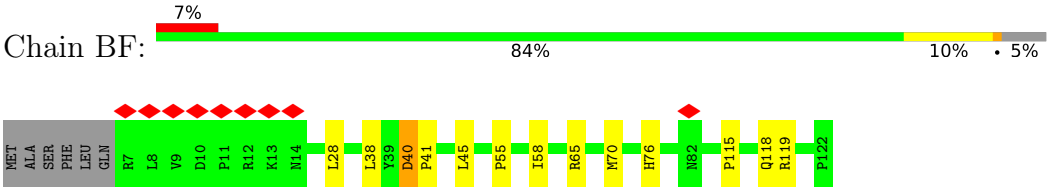
• Molecule 52: Cytochrome c1 2, heme protein, mitochondrial



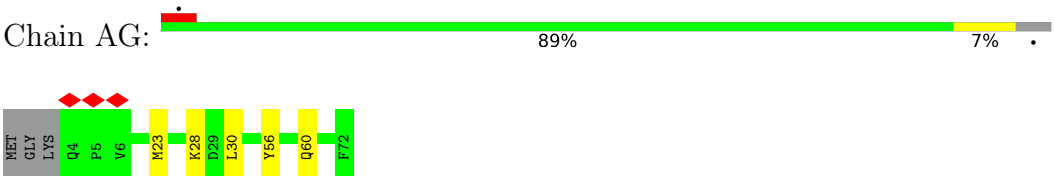
• Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial



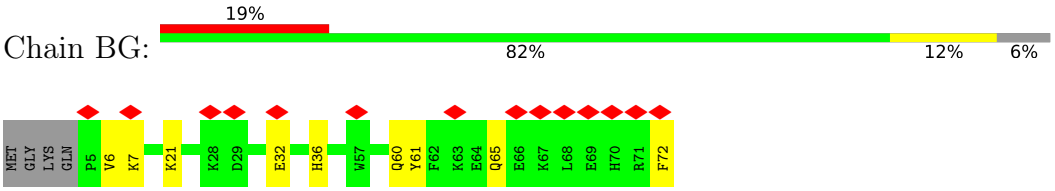
• Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial



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

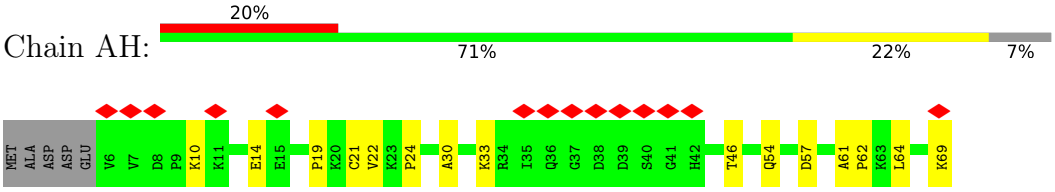


• Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial



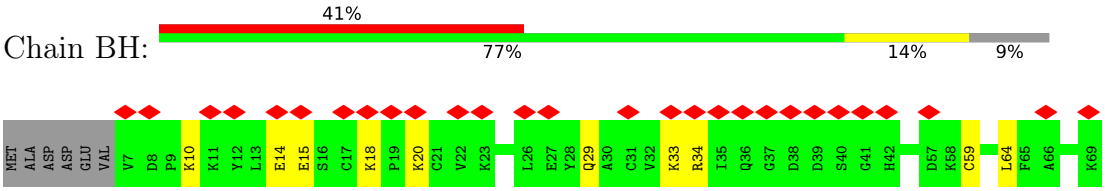
• Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial

Chain AH:



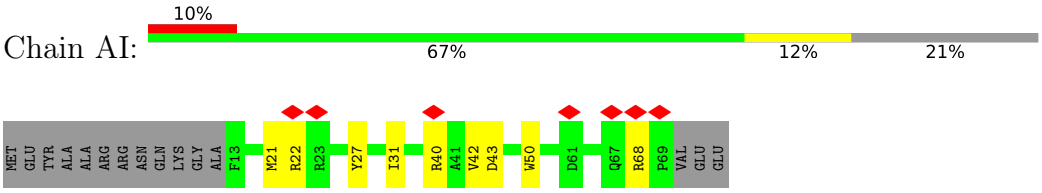
• Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial

Chain BH:



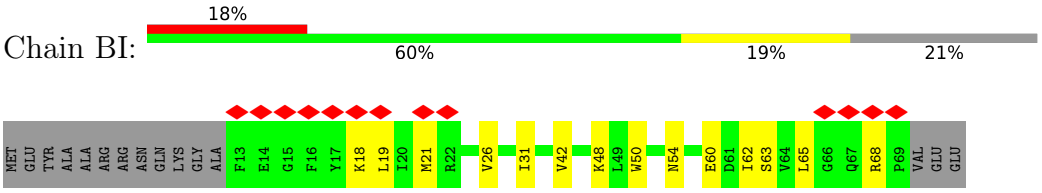
• Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain AI:



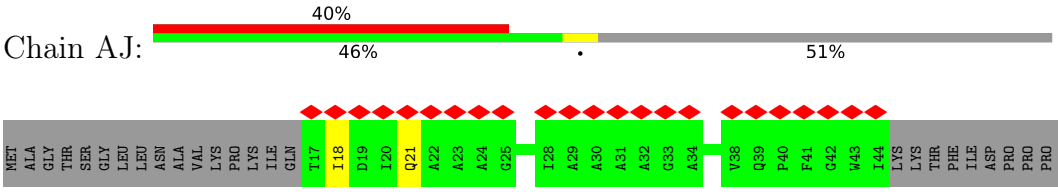
• Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain BI:



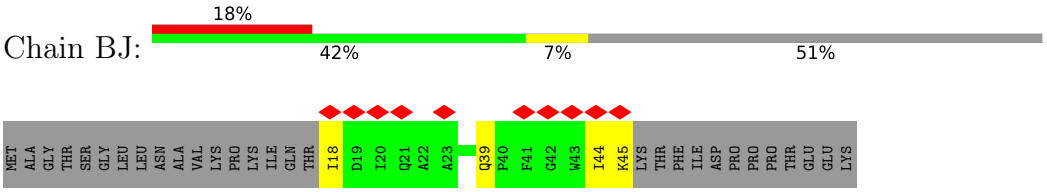
• Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial

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	61200	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	0.099	Depositor
Minimum map value	-0.040	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 (i)

5.1 Standard geometry (i)

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

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	0.41	0/820	0.61	0/1113
2	B	0.47	0/1279	0.64	0/1734
3	C	0.30	0/1590	0.47	0/2152
4	D	0.39	0/3149	0.58	0/4259
5	E	0.40	0/1535	0.61	1/2084 (0.0%)
6	F	0.28	0/3441	0.45	0/4641
7	G	0.32	0/5338	0.50	0/7231
8	H	0.45	0/2609	0.65	0/3553
9	I	0.31	0/1378	0.51	0/1862
10	J	0.40	0/1435	0.59	0/1957
11	K	0.43	0/785	0.66	0/1062
12	L	0.43	0/5368	0.63	1/7291 (0.0%)
13	M	0.40	1/4057 (0.0%)	0.59	0/5513
14	N	0.38	0/3937	0.58	0/5345
15	O	0.32	0/979	0.43	0/1326
16	P	0.44	0/2509	0.65	1/3401 (0.0%)
17	Q	0.53	0/862	0.68	0/1166
18	R	0.17	0/585	0.30	0/793
19	S	0.28	0/739	0.45	0/996
20	T	0.54	0/671	0.74	0/911
21	U	0.63	0/687	0.88	0/929
22	V	0.35	0/1146	0.54	0/1555
23	W	0.45	0/923	0.65	0/1249
24	X	0.50	0/790	0.76	0/1060
25	Y	0.17	0/944	0.39	0/1277
26	Z	0.43	0/1027	0.65	0/1392
27	a	0.38	0/481	0.62	0/646
28	b	0.15	0/320	0.39	0/434
29	c	0.39	0/637	0.49	0/860
30	d	0.35	0/605	0.55	0/815
31	e	0.24	0/559	0.40	0/745
32	f	0.55	0/771	0.81	1/1042 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.12	0/575	0.31	0/781
34	i	0.52	0/605	0.71	0/812
35	j	0.47	0/433	0.69	0/592
36	k	0.58	0/392	0.85	0/526
37	l	0.39	0/575	0.57	0/781
38	m	0.31	0/592	0.52	0/793
39	n	0.30	0/938	0.44	0/1273
40	o	0.49	0/666	0.64	0/886
41	p	0.52	0/777	0.74	0/1043
42	q	0.11	0/690	0.30	0/936
43	u	0.15	0/472	0.27	0/632
44	v	0.14	0/222	0.29	0/300
45	x	0.32	0/1669	0.53	0/2279
46	y	0.34	0/2046	0.54	1/2772 (0.0%)
47	z	0.54	0/1804	0.78	0/2441
48	AA	0.50	0/3265	0.66	0/4431
48	BA	0.31	0/3254	0.50	2/4417 (0.0%)
49	AB	0.28	0/3908	0.42	0/5305
49	BB	0.29	0/3908	0.46	0/5305
50	AC	0.36	0/3208	0.52	0/4395
50	BC	0.40	0/3208	0.58	0/4395
51	AD	0.39	0/1567	0.55	0/2135
51	BD	0.29	0/1558	0.48	1/2123 (0.0%)
52	AE	0.34	1/1968 (0.1%)	0.41	0/2672
52	BE	0.22	0/1968	0.36	0/2672
53	AF	0.35	0/993	0.53	1/1336 (0.1%)
53	BF	0.43	0/993	0.62	1/1336 (0.1%)
54	AG	0.38	0/600	0.56	0/815
54	BG	0.28	0/591	0.41	0/802
55	AH	0.14	0/531	0.34	0/713
55	BH	0.14	0/524	0.35	0/703
56	AI	0.11	0/488	0.31	0/655
56	BI	0.14	0/488	0.31	0/655
57	AJ	0.09	0/210	0.28	0/290
57	BJ	0.48	0/212	0.57	0/291
All	All	0.38	2/97854 (0.0%)	0.56	10/132687 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AE	226	MET	SD-CE	-9.55	1.55	1.79
13	M	29	ILE	N-CA	5.14	1.50	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	313	PRO	CA-N-CD	-9.72	98.39	112.00
48	BA	389	PRO	CA-N-CD	-8.29	100.40	112.00
48	BA	389	PRO	N-CD-CG	-6.21	93.89	103.20
12	L	344	PHE	CA-CB-CG	5.83	119.64	113.80
53	AF	40	ASP	CB-CA-C	5.53	116.36	108.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	817	15	0
2	B	1244	0	1231	27	0
3	C	1545	0	1501	12	0
4	D	3079	0	3049	42	0
5	E	1500	0	1475	33	0
6	F	3368	0	3354	42	0
7	G	5243	0	5228	96	0
8	H	2536	0	2641	40	0
9	I	1349	0	1293	16	0
10	J	1399	0	1472	38	0
11	K	784	0	843	41	0
12	L	5222	0	5253	114	0
13	M	3946	0	4086	99	0
14	N	3832	0	3933	91	0
15	O	963	0	975	13	0
16	P	2453	0	2493	35	0
17	Q	837	0	818	13	0
18	R	571	0	559	4	0
19	S	727	0	759	17	0
20	T	659	0	644	21	0
21	U	677	0	665	13	0
22	V	1123	0	1112	15	0
23	W	904	0	901	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	776	0	775	16	0
25	Y	928	0	960	29	0
26	Z	997	0	979	22	0
27	a	469	0	472	6	0
28	b	315	0	338	2	0
29	c	617	0	619	19	0
30	d	592	0	610	8	0
31	e	546	0	510	12	0
32	f	765	0	766	9	0
33	g	559	0	563	9	0
34	i	591	0	551	22	0
35	j	415	0	406	10	0
36	k	382	0	380	18	0
37	l	562	0	567	18	0
38	m	577	0	564	7	0
39	n	911	0	879	16	0
40	o	657	0	669	15	0
41	p	757	0	743	14	0
42	q	669	0	630	7	0
43	u	463	0	471	10	0
44	v	219	0	227	2	0
45	x	1629	0	1636	22	0
46	y	2013	0	2024	17	0
47	z	1772	0	1771	34	0
48	AA	3201	0	3201	56	0
48	BA	3190	0	3193	64	0
49	AB	3834	0	3797	48	0
49	BB	3834	0	3797	54	0
50	AC	3093	0	3074	70	0
50	BC	3093	0	3074	41	0
51	AD	1528	0	1529	28	0
51	BD	1519	0	1523	44	0
52	AE	1917	0	1844	35	0
52	BE	1917	0	1844	16	0
53	AF	976	0	1001	36	0
53	BF	976	0	1001	13	0
54	AG	581	0	589	3	0
54	BG	572	0	582	6	0
55	AH	518	0	518	13	0
55	BH	511	0	511	6	0
56	AI	476	0	469	18	0
56	BI	476	0	469	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AJ	203	0	197	1	0
57	BJ	205	0	203	2	0
58	B	8	0	0	1	0
58	F	8	0	0	2	0
58	G	16	0	0	0	0
58	I	16	0	0	0	0
59	AD	4	0	0	1	0
59	BD	4	0	0	0	0
59	E	4	0	0	4	0
59	G	4	0	0	1	0
60	F	31	0	19	2	0
61	H	35	0	43	13	0
62	O	1	0	0	0	0
63	P	48	0	26	2	0
64	AB	1	0	0	0	0
64	BB	1	0	0	0	0
64	R	1	0	0	0	0
64	y	1	0	0	0	0
65	W	35	0	0	0	0
65	n	35	0	0	0	0
66	x	53	0	37	2	0
67	AC	86	0	60	1	0
67	AE	43	0	30	9	0
67	BC	86	0	60	4	0
67	BE	43	0	30	3	0
68	AC	76	0	100	15	0
68	BC	38	0	50	5	0
69	BC	48	0	66	8	0
All	All	96290	0	96149	1460	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1460 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:33:ARG:NH1	47:z:6:ARG:HH22	1.08	1.49
50:AC:222:MET:HE1	53:AF:66:LEU:CB	1.57	1.32
7:G:427:MET:HE2	7:G:553:LEU:CA	1.58	1.31
7:G:302:ASN:ND2	7:G:320:ASN:HD22	1.26	1.30
52:AE:72:GLU:OE2	55:AH:54:GLN:NE2	1.64	1.27

There are no symmetry-related clashes.

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%)	148 (96%)	7 (4%)	0	100	100
3	C	179/190 (94%)	178 (99%)	1 (1%)	0	100	100
4	D	383/394 (97%)	367 (96%)	16 (4%)	0	100	100
5	E	190/255 (74%)	184 (97%)	6 (3%)	0	100	100
6	F	432/486 (89%)	423 (98%)	9 (2%)	0	100	100
7	G	685/748 (92%)	668 (98%)	17 (2%)	0	100	100
8	H	322/325 (99%)	314 (98%)	8 (2%)	0	100	100
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
11	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
12	L	663/669 (99%)	641 (97%)	22 (3%)	0	100	100
13	M	492/495 (99%)	486 (99%)	6 (1%)	0	100	100
14	N	487/499 (98%)	472 (97%)	15 (3%)	0	100	100
15	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
16	P	314/402 (78%)	302 (96%)	12 (4%)	0	100	100
17	Q	103/154 (67%)	98 (95%)	5 (5%)	0	100	100
18	R	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
19	S	91/97 (94%)	89 (98%)	2 (2%)	0	100	100
20	T	81/122 (66%)	77 (95%)	4 (5%)	0	100	100
21	U	85/126 (68%)	82 (96%)	3 (4%)	0	100	100
22	V	138/169 (82%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	108/133 (81%)	105 (97%)	3 (3%)	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%)	120 (98%)	3 (2%)	0	100	100
27	a	56/65 (86%)	53 (95%)	3 (5%)	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%)	72 (99%)	1 (1%)	0	100	100
31	e	62/83 (75%)	60 (97%)	2 (3%)	0	100	100
32	f	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
33	g	67/114 (59%)	67 (100%)	0	0	100	100
34	i	64/98 (65%)	64 (100%)	0	0	100	100
35	j	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
36	k	46/72 (64%)	43 (94%)	3 (6%)	0	100	100
37	l	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
38	m	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
39	n	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
40	o	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
41	p	88/106 (83%)	85 (97%)	3 (3%)	0	100	100
42	q	79/159 (50%)	74 (94%)	5 (6%)	0	100	100
43	u	53/63 (84%)	53 (100%)	0	0	100	100
44	v	27/113 (24%)	27 (100%)	0	0	100	100
45	x	208/256 (81%)	204 (98%)	4 (2%)	0	100	100
46	y	263/278 (95%)	258 (98%)	5 (2%)	0	100	100
47	z	231/275 (84%)	226 (98%)	5 (2%)	0	100	100
48	AA	416/503 (83%)	404 (97%)	12 (3%)	0	100	100
48	BA	414/503 (82%)	401 (97%)	13 (3%)	0	100	100
49	AB	485/531 (91%)	476 (98%)	9 (2%)	0	100	100
49	BB	485/531 (91%)	477 (98%)	8 (2%)	0	100	100
50	AC	385/393 (98%)	375 (97%)	10 (3%)	0	100	100
50	BC	385/393 (98%)	379 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	AD	194/272 (71%)	185 (95%)	9 (5%)	0	100	100
51	BD	193/272 (71%)	181 (94%)	12 (6%)	0	100	100
52	AE	242/307 (79%)	239 (99%)	3 (1%)	0	100	100
52	BE	242/307 (79%)	241 (100%)	1 (0%)	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%)	65 (98%)	1 (2%)	0	100	100
55	AH	62/69 (90%)	62 (100%)	0	0	100	100
55	BH	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
56	AI	55/72 (76%)	54 (98%)	1 (2%)	0	100	100
56	BI	55/72 (76%)	55 (100%)	0	0	100	100
57	AJ	26/57 (46%)	24 (92%)	2 (8%)	0	100	100
57	BJ	26/57 (46%)	24 (92%)	2 (8%)	0	100	100
All	All	11955/14108 (85%)	11657 (98%)	298 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	63	77
2	B	132/184 (72%)	128 (97%)	4 (3%)	36	58
3	C	171/179 (96%)	168 (98%)	3 (2%)	51	69
4	D	331/340 (97%)	329 (99%)	2 (1%)	78	87
5	E	166/220 (76%)	165 (99%)	1 (1%)	78	87
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	570/625 (91%)	567 (100%)	3 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	271/272 (100%)	270 (100%)	1 (0%)	84 90
9	I	147/195 (75%)	147 (100%)	0	100 100
10	J	156/186 (84%)	151 (97%)	5 (3%)	34 56
11	K	85/85 (100%)	83 (98%)	2 (2%)	43 63
12	L	564/568 (99%)	560 (99%)	4 (1%)	76 85
13	M	433/434 (100%)	426 (98%)	7 (2%)	55 72
14	N	407/416 (98%)	404 (99%)	3 (1%)	76 85
15	O	108/141 (77%)	108 (100%)	0	100 100
16	P	263/334 (79%)	258 (98%)	5 (2%)	50 68
17	Q	89/128 (70%)	89 (100%)	0	100 100
18	R	64/97 (66%)	63 (98%)	1 (2%)	55 72
19	S	82/85 (96%)	82 (100%)	0	100 100
20	T	78/112 (70%)	77 (99%)	1 (1%)	61 75
21	U	78/113 (69%)	76 (97%)	2 (3%)	40 62
22	V	123/148 (83%)	123 (100%)	0	100 100
23	W	98/114 (86%)	97 (99%)	1 (1%)	68 80
24	X	88/94 (94%)	88 (100%)	0	100 100
25	Y	92/120 (77%)	89 (97%)	3 (3%)	33 55
26	Z	100/115 (87%)	99 (99%)	1 (1%)	68 80
27	a	48/53 (91%)	47 (98%)	1 (2%)	47 66
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%)	60 (100%)	0	100 100
31	e	59/73 (81%)	59 (100%)	0	100 100
32	f	80/83 (96%)	78 (98%)	2 (2%)	42 63
33	g	60/96 (62%)	60 (100%)	0	100 100
34	i	61/90 (68%)	60 (98%)	1 (2%)	55 72
35	j	42/51 (82%)	41 (98%)	1 (2%)	43 63
36	k	39/60 (65%)	39 (100%)	0	100 100
37	l	60/97 (62%)	58 (97%)	2 (3%)	33 55
38	m	58/59 (98%)	57 (98%)	1 (2%)	53 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	n	92/99 (93%)	91 (99%)	1 (1%)	65 79
40	o	70/87 (80%)	69 (99%)	1 (1%)	59 74
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%)	178 (99%)	1 (1%)	78 87
46	y	221/232 (95%)	220 (100%)	1 (0%)	81 88
47	z	188/228 (82%)	186 (99%)	2 (1%)	65 79
48	AA	347/408 (85%)	341 (98%)	6 (2%)	53 71
48	BA	345/408 (85%)	339 (98%)	6 (2%)	53 71
49	AB	415/452 (92%)	410 (99%)	5 (1%)	63 77
49	BB	415/452 (92%)	413 (100%)	2 (0%)	81 88
50	AC	330/336 (98%)	328 (99%)	2 (1%)	78 87
50	BC	330/336 (98%)	328 (99%)	2 (1%)	78 87
51	AD	170/232 (73%)	166 (98%)	4 (2%)	43 63
51	BD	169/232 (73%)	166 (98%)	3 (2%)	51 69
52	AE	200/247 (81%)	198 (99%)	2 (1%)	68 80
52	BE	200/247 (81%)	198 (99%)	2 (1%)	68 80
53	AF	105/110 (96%)	105 (100%)	0	100 100
53	BF	105/110 (96%)	104 (99%)	1 (1%)	68 80
54	AG	63/65 (97%)	62 (98%)	1 (2%)	55 72
54	BG	62/65 (95%)	60 (97%)	2 (3%)	34 56
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%)	45 (94%)	3 (6%)	16 29
57	AJ	16/41 (39%)	16 (100%)	0	100 100
57	BJ	16/41 (39%)	13 (81%)	3 (19%)	1 2
All	All	10269/11908 (86%)	10161 (99%)	108 (1%)	63 79

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	m	31	ARG
49	AB	229	THR
53	BF	70	MET
40	o	66	VAL
48	AA	283	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
41	p	36	HIS
49	AB	202	GLN
54	BG	70	HIS
42	q	45	HIS
48	AA	252	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
32	FME	f	1	32	8,9,10	0.69	0	7,9,11	1.61	1 (14%)
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	1.17	1 (14%)
1	FME	A	1	1	8,9,10	1.72	1 (12%)	7,9,11	1.49	1 (14%)

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
32	FME	f	1	32	-	2/7/9/11	-
11	FME	K	1	11	-	5/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	FME	O-C	4.16	1.36	1.19

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	O-C-CA	-3.47	115.69	124.78
32	f	1	FME	O-C-CA	-3.41	115.85	124.78
11	K	1	FME	C-CA-N	2.32	113.93	109.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
58	SF4	F	501	6	0,12,12	-	-	-		
67	HEM	BE	400	52	50,50,50	1.32	6 (12%)	66,82,82	1.21	6 (9%)
67	HEM	BC	501	50	50,50,50	1.61	9 (18%)	66,82,82	1.69	13 (19%)
58	SF4	B	500	2	0,12,12	-	-	-		
65	8Q1	n	200	-	31,34,34	1.74	6 (19%)	40,43,43	1.82	8 (20%)
63	NDP	P	500	-	49,52,52	0.49	0	66,80,80	0.46	0
59	FES	E	500	5	0,4,4	-	-	-		
60	FMN	F	500	-	33,33,33	1.07	2 (6%)	48,50,50	1.19	6 (12%)
67	HEM	AC	501	50	50,50,50	1.61	7 (14%)	66,82,82	1.68	14 (21%)
59	FES	AD	301	51	0,4,4	-	-	-		
68	UQ5	BC	502	-	38,38,38	0.45	0	46,49,49	0.57	0
61	UQ9	H	500	-	35,35,58	2.51	13 (37%)	42,45,73	2.08	12 (28%)
66	COO	x	301	-	48,55,55	4.17	15 (31%)	68,81,81	4.30	21 (30%)
65	8Q1	W	200	-	31,34,34	0.35	0	40,43,43	0.48	0
69	UQ7	BC	503	-	48,48,48	0.43	0	58,61,61	0.53	1 (1%)
58	SF4	I	500	9	0,12,12	-	-	-		
67	HEM	BC	500	50	50,50,50	1.37	7 (14%)	66,82,82	1.16	6 (9%)
58	SF4	I	501	9	0,12,12	-	-	-		
68	UQ5	AC	502	-	38,38,38	0.49	0	46,49,49	0.64	1 (2%)
67	HEM	AC	500	50	50,50,50	1.61	8 (16%)	66,82,82	1.65	11 (16%)
58	SF4	G	802	7	0,12,12	-	-	-		
59	FES	BD	301	51	0,4,4	-	-	-		
68	UQ5	AC	503	-	38,38,38	0.50	0	46,49,49	0.83	1 (2%)
59	FES	G	801	7	0,4,4	-	-	-		
67	HEM	AE	400	-	50,50,50	2.22	6 (12%)	66,82,82	1.76	11 (16%)
58	SF4	G	803	7	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	HEM	BE	400	52	-	1/14/54/54	-
58	SF4	F	501	6	-	-	0/6/5/5
67	HEM	BC	501	50	-	9/14/54/54	-
58	SF4	B	500	2	-	-	0/6/5/5
65	8Q1	n	200	-	-	22/41/41/41	-
63	NDP	P	500	-	-	7/34/77/77	0/5/5/5
60	FMN	F	500	-	-	2/18/18/18	0/3/3/3
58	SF4	G	803	7	-	-	0/6/5/5
59	FES	E	500	5	-	-	0/1/1/1
67	HEM	AC	501	50	-	7/14/54/54	-
59	FES	AD	301	51	-	-	0/1/1/1
61	UQ9	H	500	-	-	7/30/54/81	0/1/1/1
66	COO	x	301	-	1/1/12/16	11/54/70/70	0/3/3/3
65	8Q1	W	200	-	-	18/41/41/41	-
67	HEM	BC	500	50	-	2/14/54/54	-
58	SF4	I	500	9	-	-	0/6/5/5
58	SF4	I	501	9	-	-	0/6/5/5
59	FES	G	801	7	-	-	0/1/1/1
68	UQ5	AC	502	-	-	11/33/57/57	0/1/1/1
67	HEM	AC	500	50	-	8/14/54/54	-
58	SF4	G	802	7	-	-	0/6/5/5
59	FES	BD	301	51	-	-	0/1/1/1
68	UQ5	AC	503	-	-	11/33/57/57	0/1/1/1
68	UQ5	BC	502	-	-	8/33/57/57	0/1/1/1
67	HEM	AE	400	-	-	2/14/54/54	-
69	UQ7	BC	503	-	-	8/45/69/69	0/1/1/1

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	x	301	COO	C2A-N1A	-15.86	1.04	1.33
66	x	301	COO	C5A-C4A	12.51	1.62	1.39
67	AE	400	HEM	FE-NB	10.51	2.27	1.94
61	H	500	UQ9	C6-C1	9.65	1.52	1.35
66	x	301	COO	C2A-N3A	-8.84	1.17	1.33

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	x	301	COO	C5A-C4A-N3A	-16.00	105.88	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	x	301	COO	C6A-C5A-N7A	14.58	159.21	132.02
66	x	301	COO	C4A-C5A-N7A	-12.78	95.05	110.62
66	x	301	COO	C4A-N9A-C8A	-11.78	92.96	105.73
66	x	301	COO	C6A-C5A-C4A	-8.52	105.73	117.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
66	x	301	COO	C13

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	H	500	UQ9	C1-C6-C7-C8
61	H	500	UQ9	C5-C6-C7-C8
65	W	200	8Q1	O27-C28-C29-C31
65	W	200	8Q1	O27-C28-C29-C32
65	W	200	8Q1	C28-C29-C32-C34

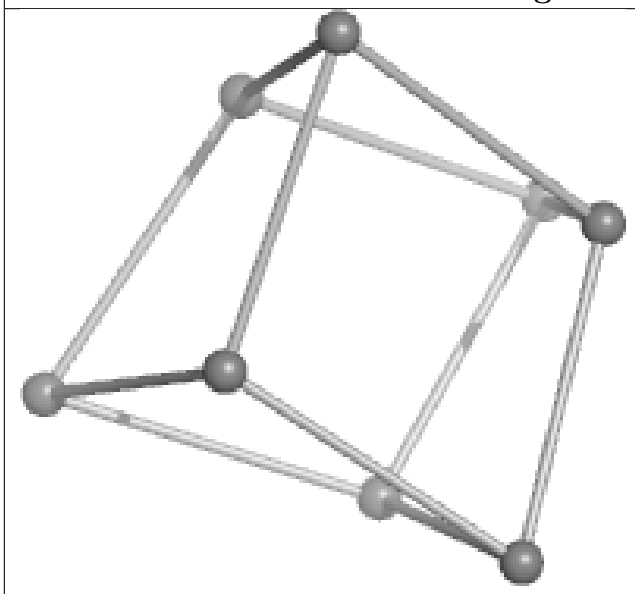
There are no ring outliers.

18 monomers are involved in 73 short contacts:

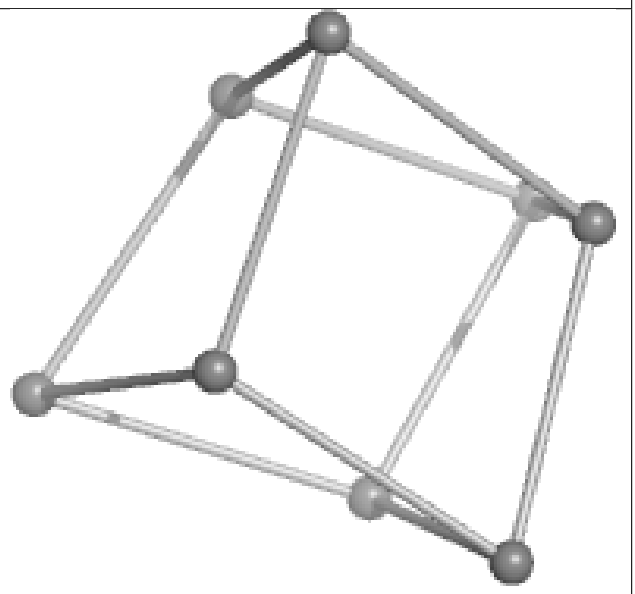
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	F	501	SF4	2	0
67	BE	400	HEM	3	0
67	BC	501	HEM	1	0
58	B	500	SF4	1	0
63	P	500	NDP	2	0
59	E	500	FES	4	0
60	F	500	FMN	2	0
67	AC	501	HEM	1	0
59	AD	301	FES	1	0
68	BC	502	UQ5	5	0
61	H	500	UQ9	13	0
66	x	301	COO	2	0
69	BC	503	UQ7	8	0
67	BC	500	HEM	3	0
68	AC	502	UQ5	5	0
68	AC	503	UQ5	10	0
59	G	801	FES	1	0
67	AE	400	HEM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

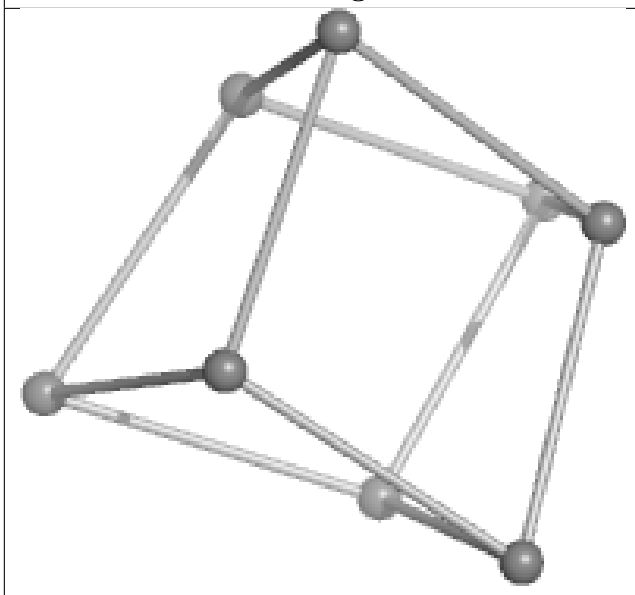
Ligand SF4 F 501



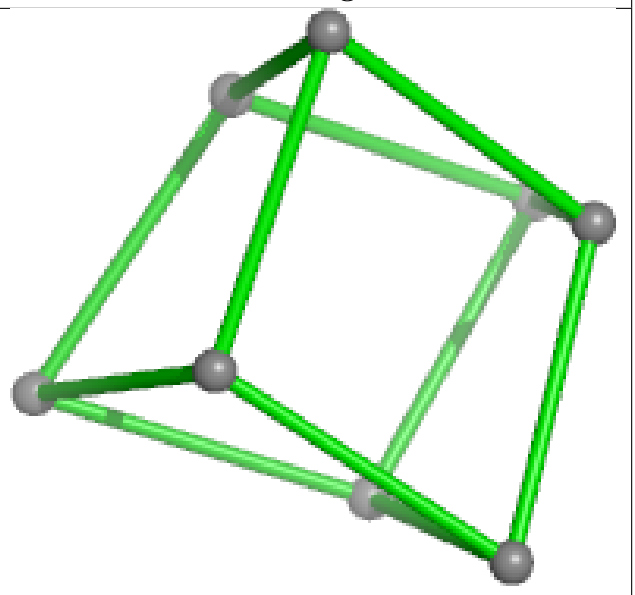
Bond lengths



Bond angles

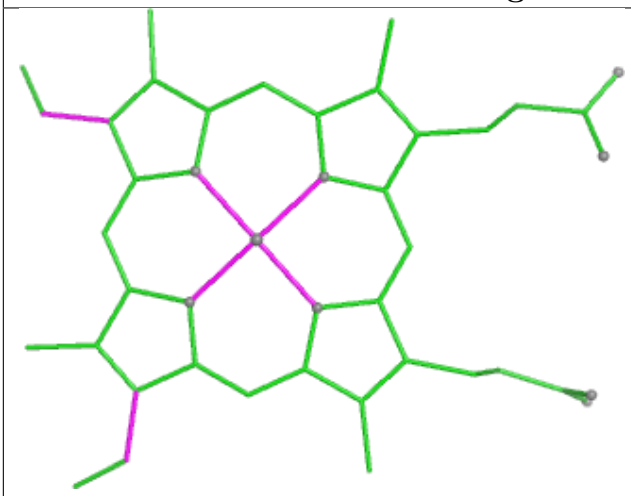


Torsions

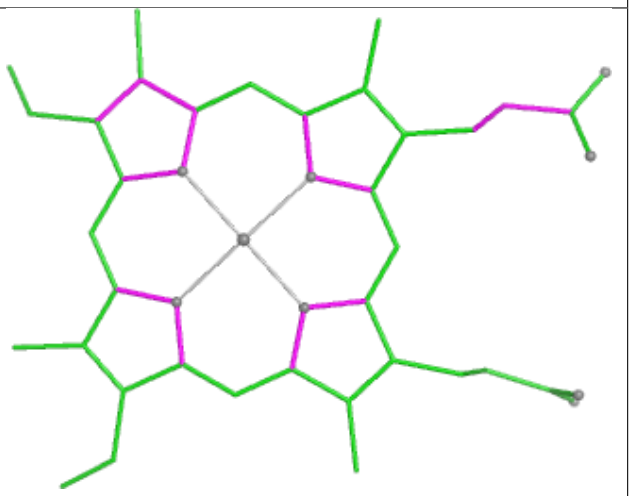


Rings

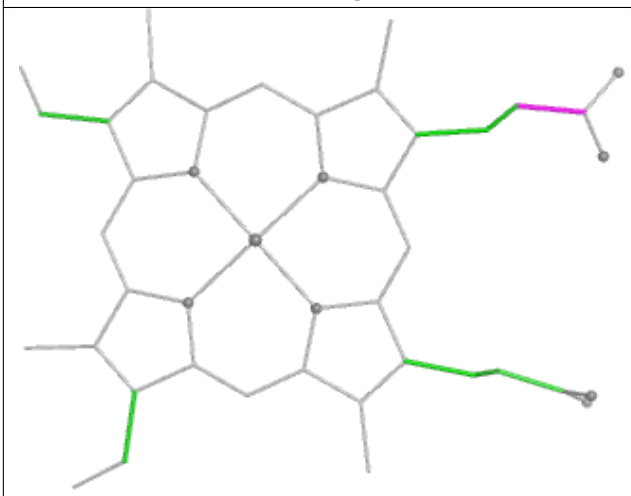
Ligand HEM BE 400



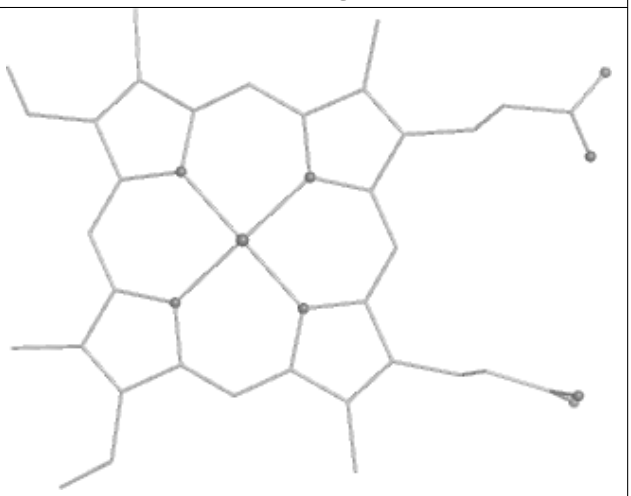
Bond lengths



Bond angles

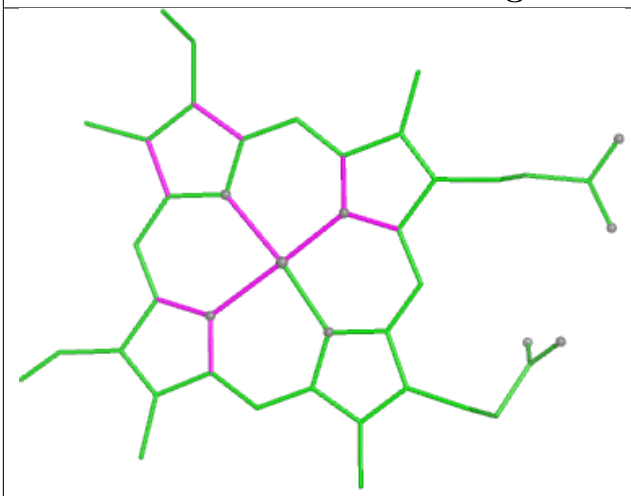


Torsions

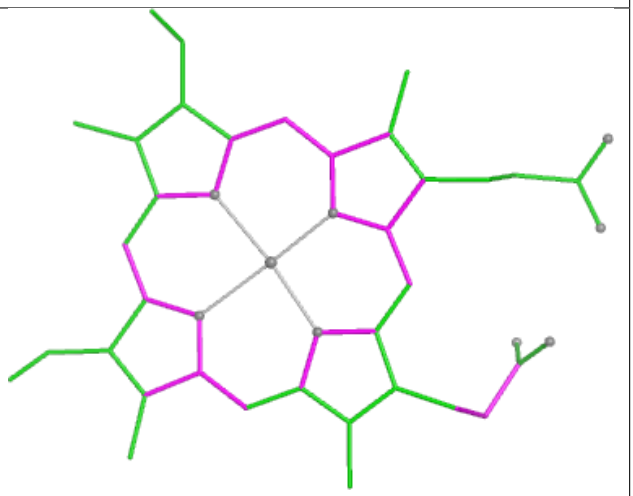


Rings

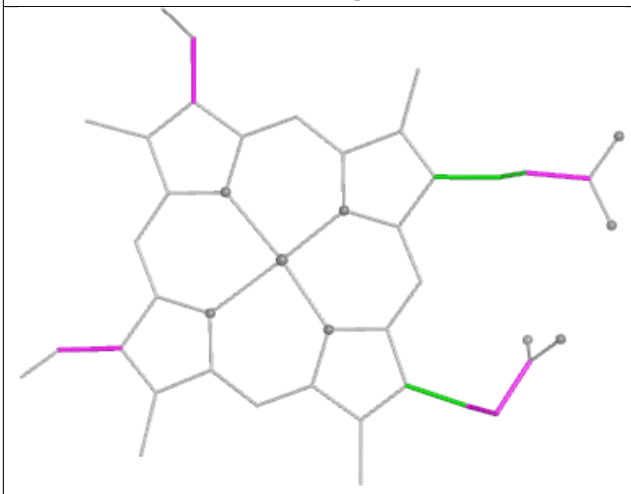
Ligand HEM BC 501



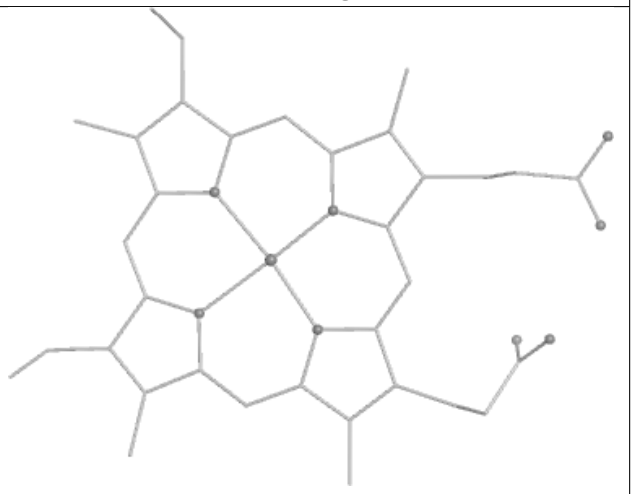
Bond lengths



Bond angles

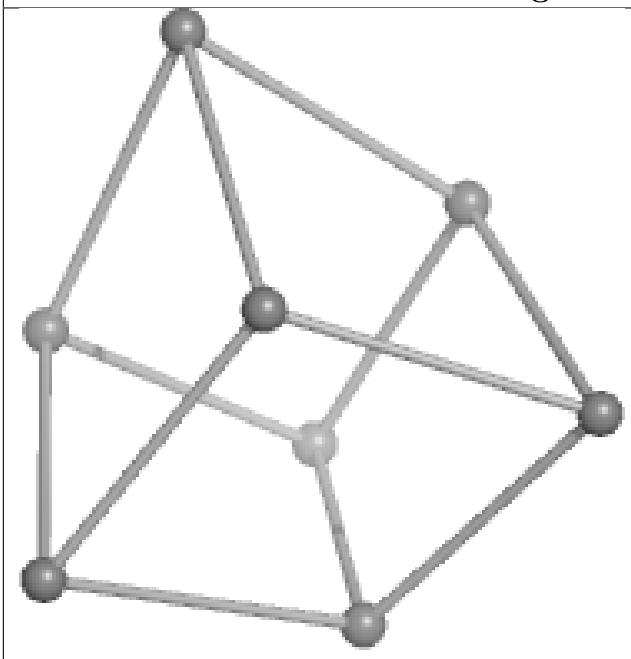


Torsions

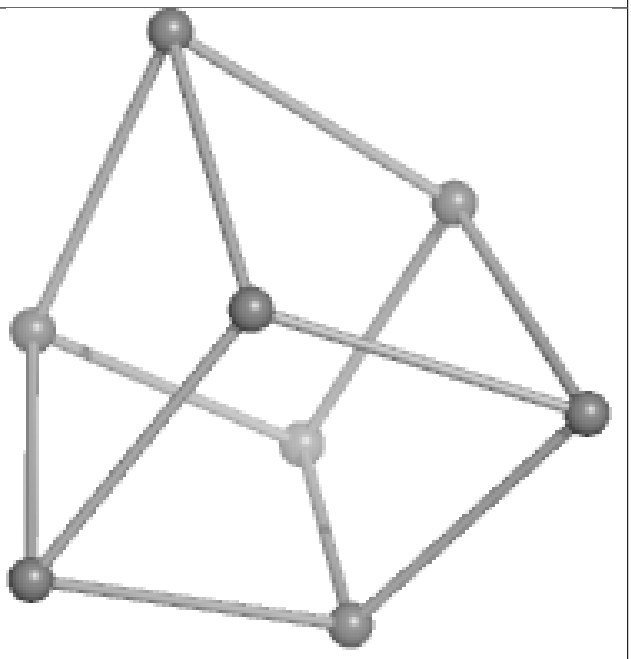


Rings

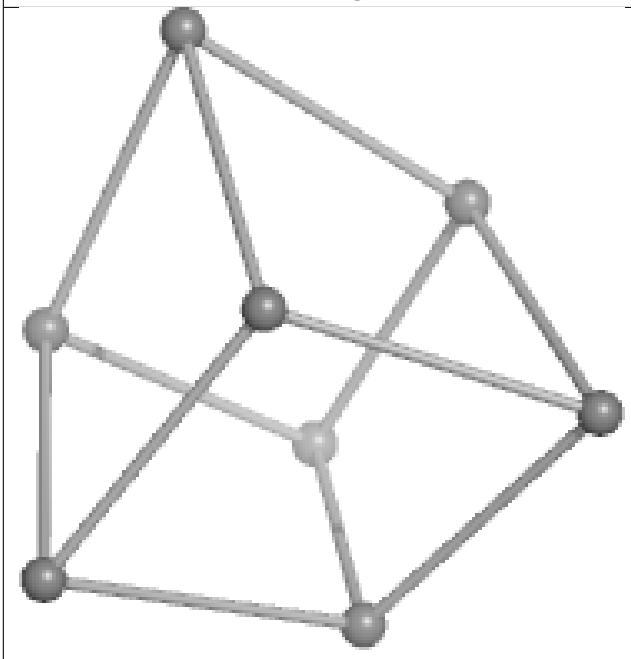
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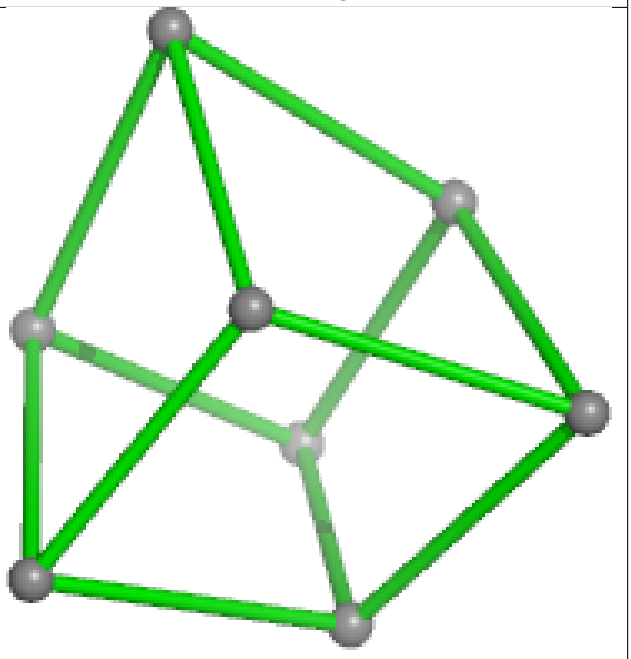
Bond lengths



Bond angles

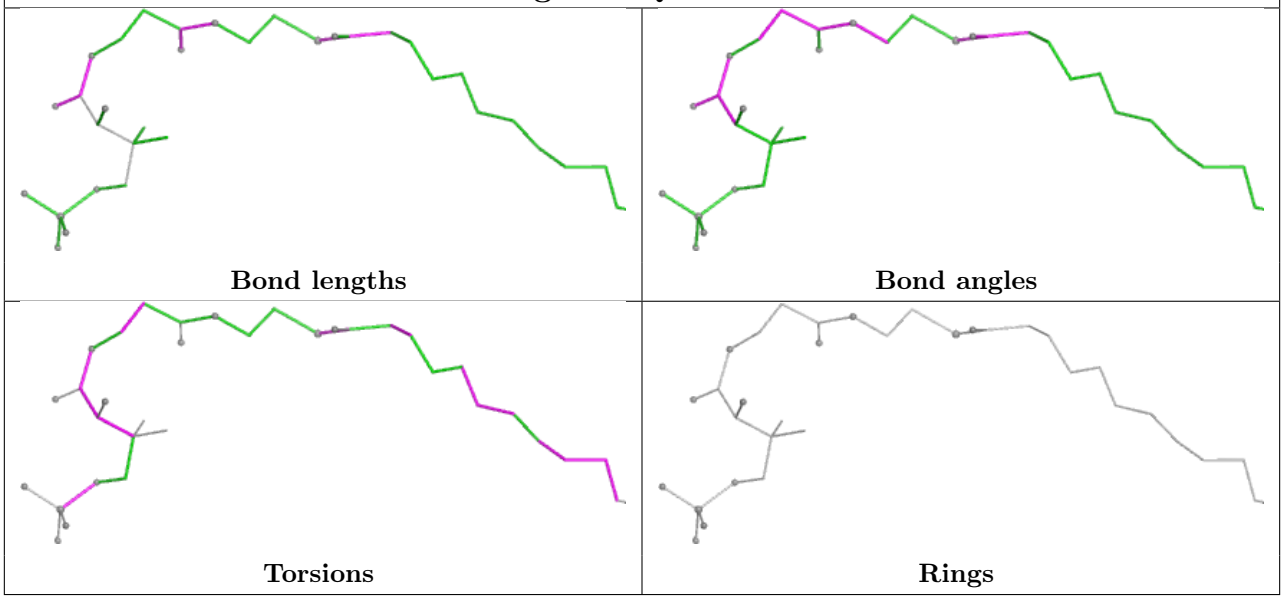


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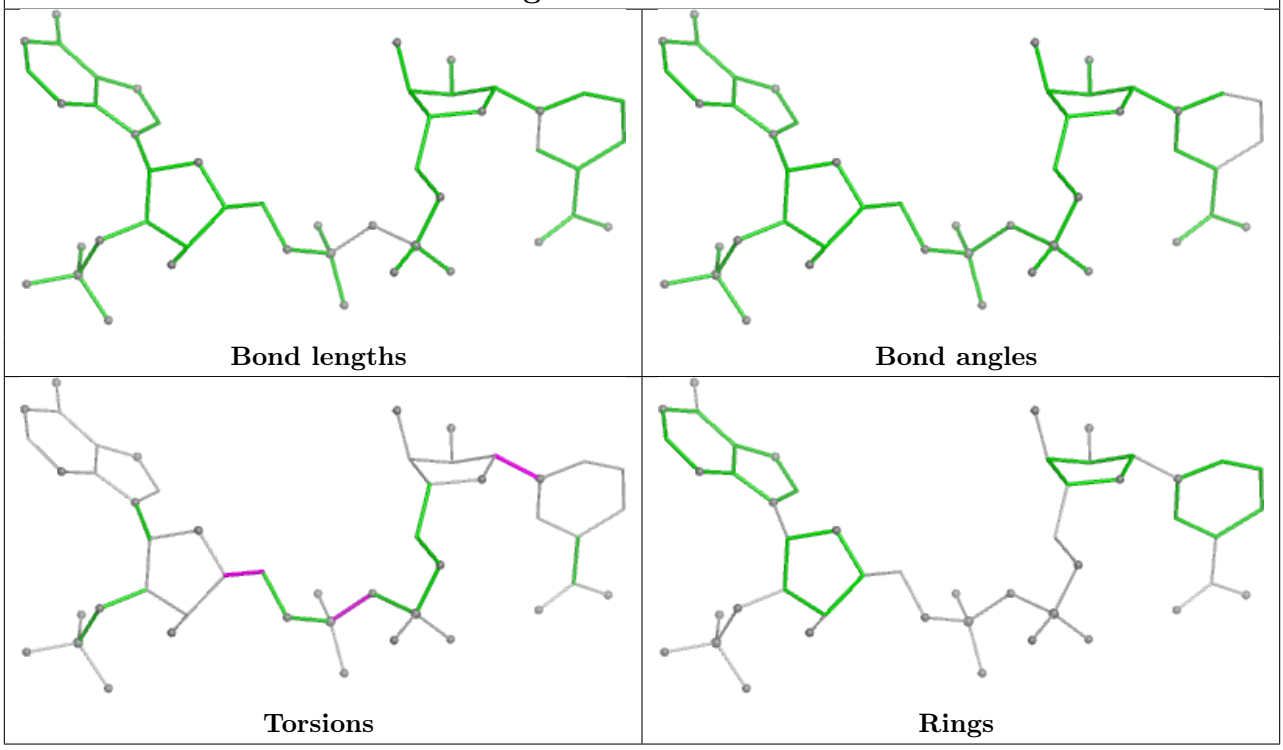


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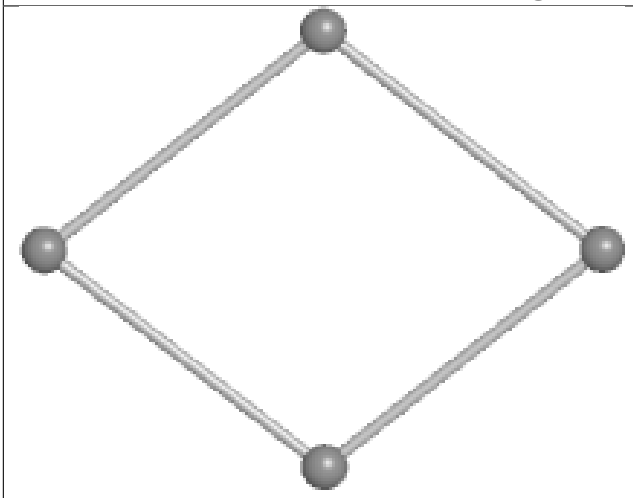
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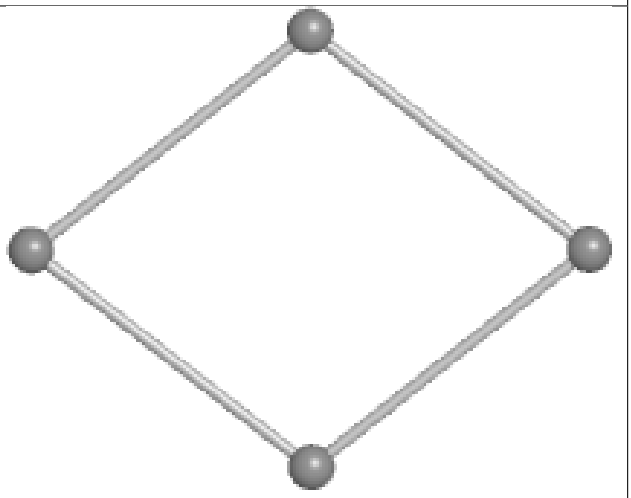
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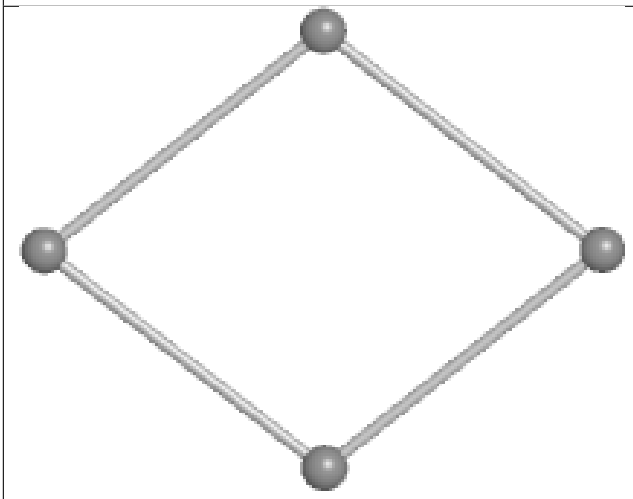
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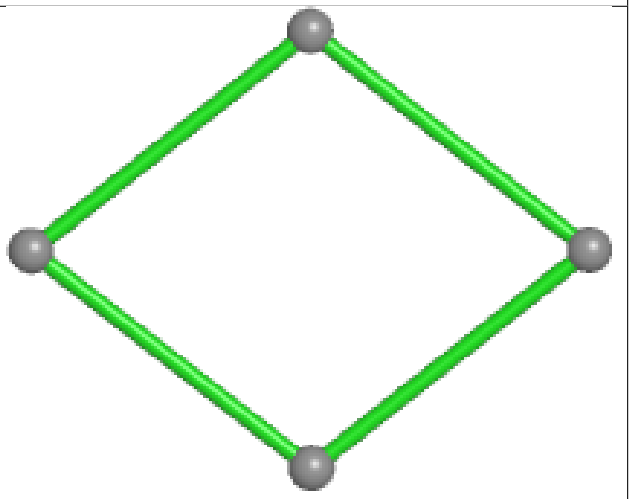
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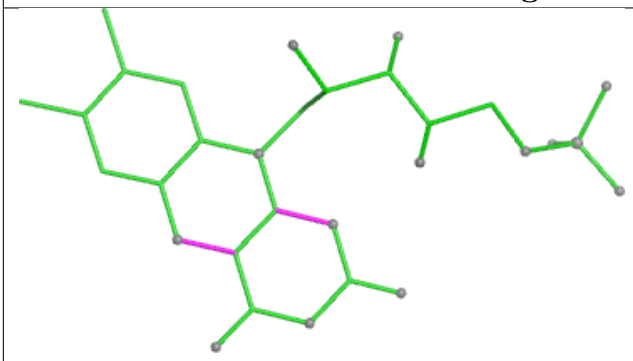


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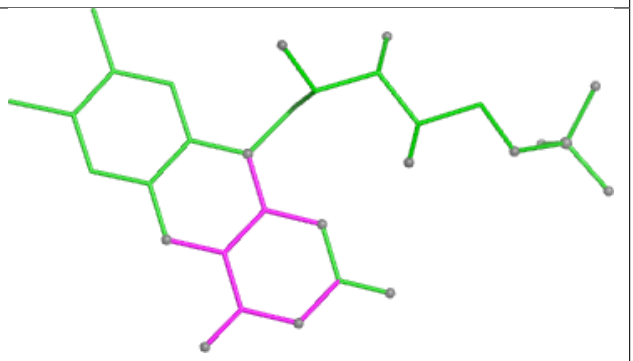


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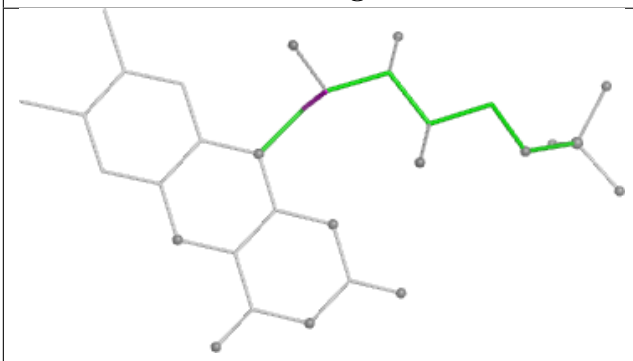
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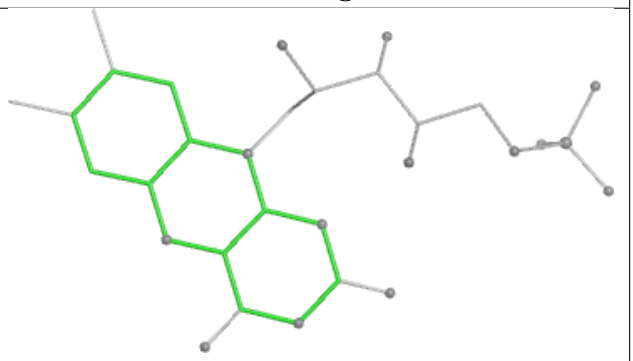
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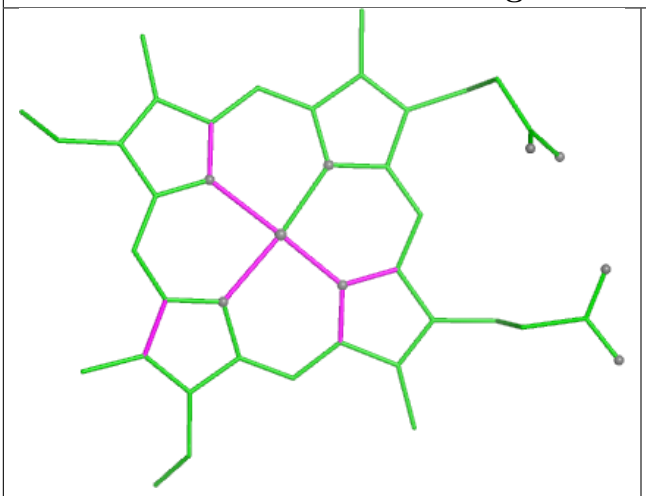


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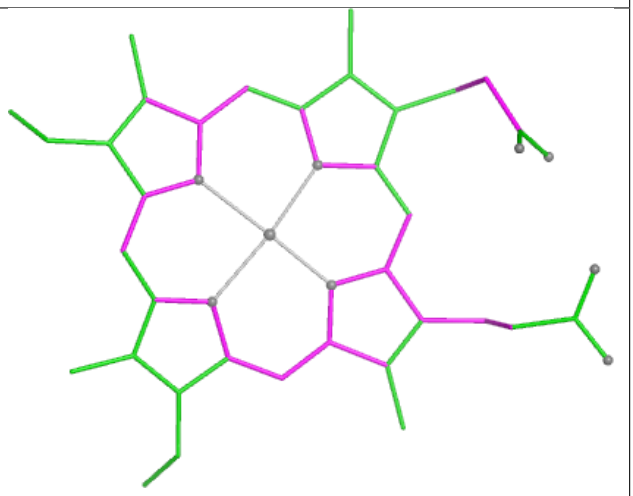


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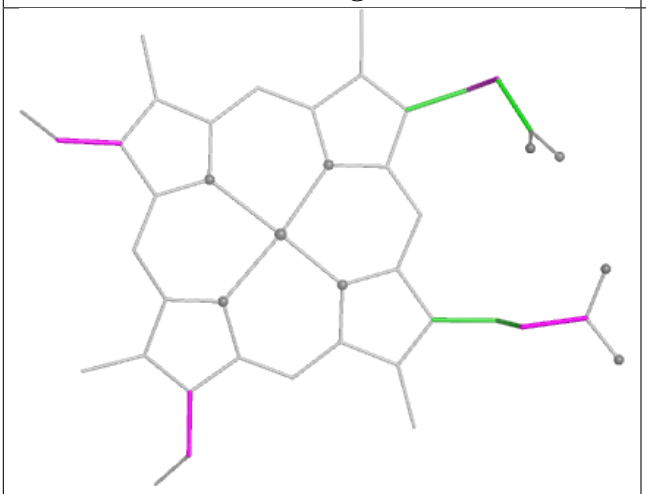
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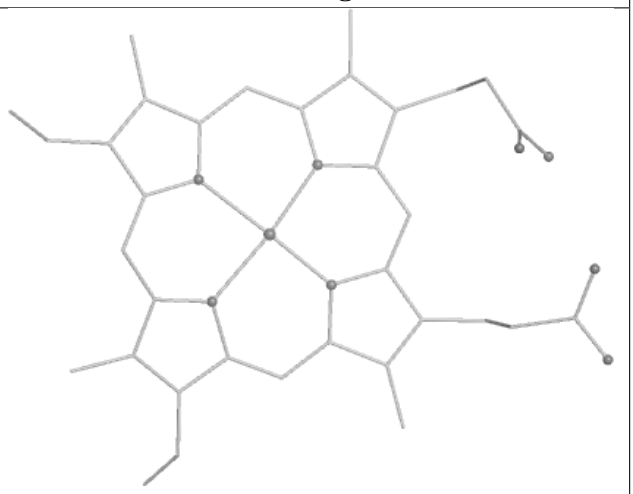
Bond lengths



Bond angles

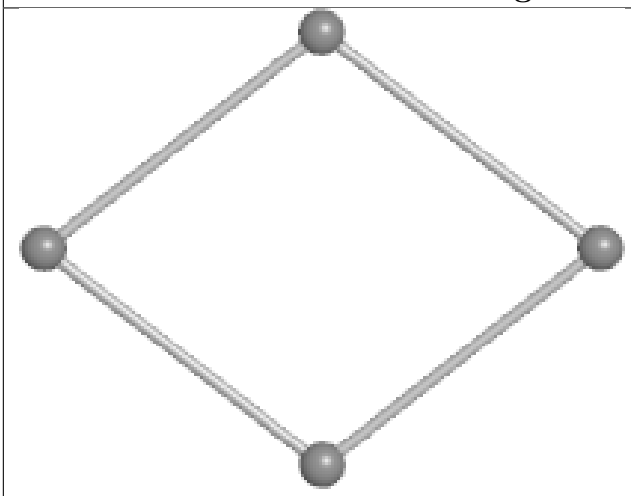


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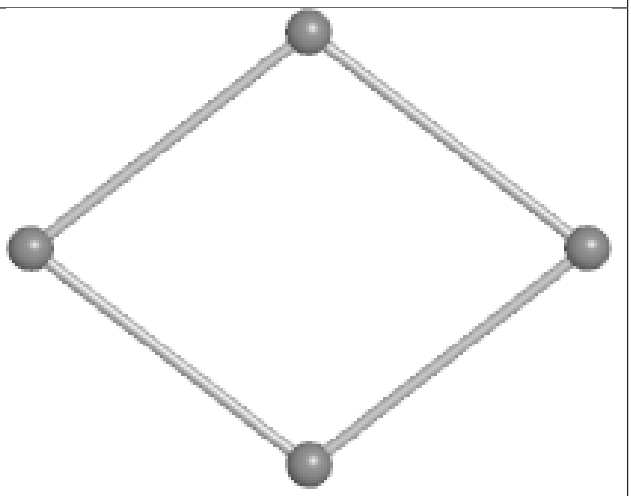


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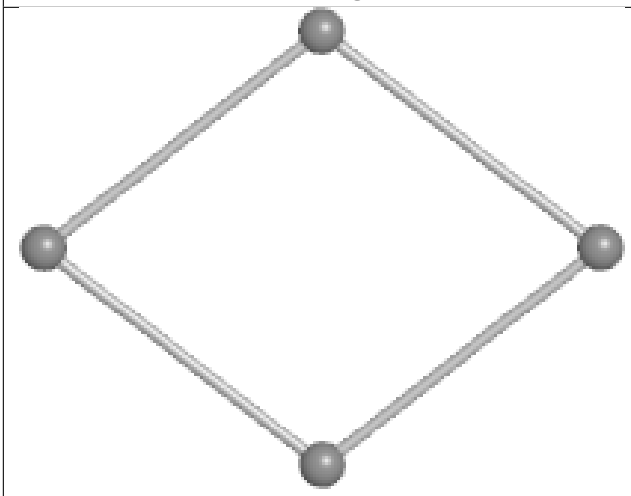
Ligand FES AD 301



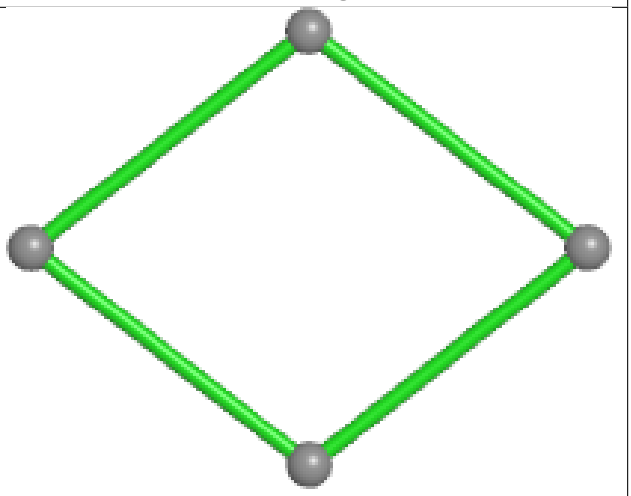
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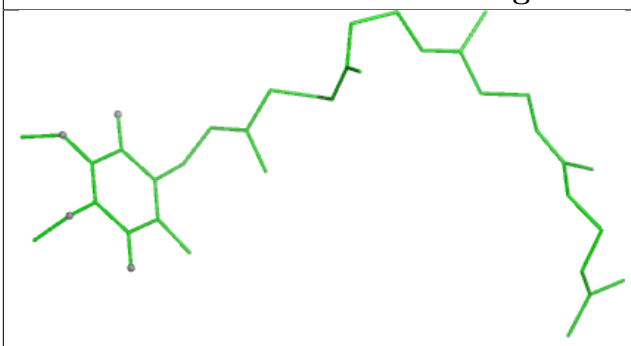


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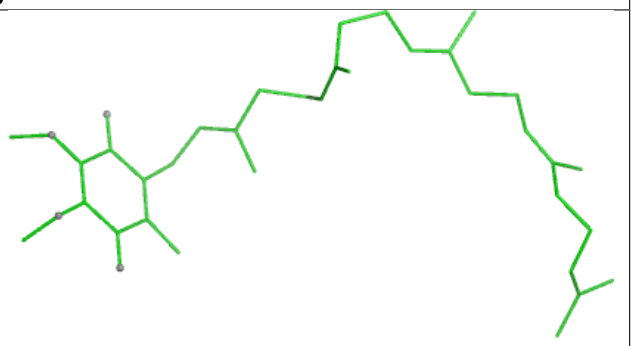


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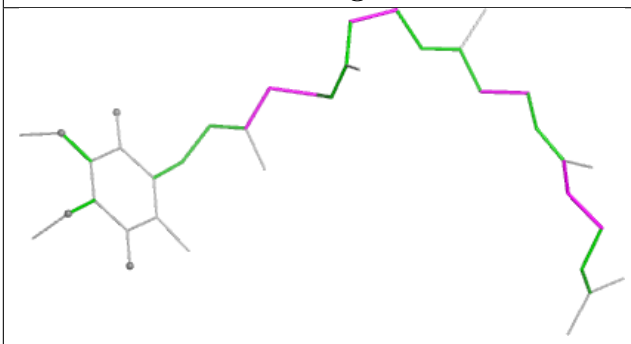
Ligand UQ5 BC 502



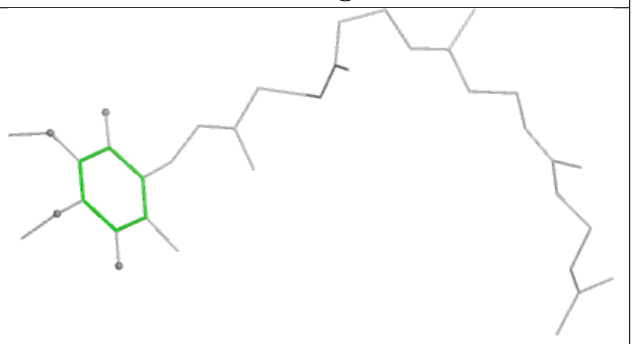
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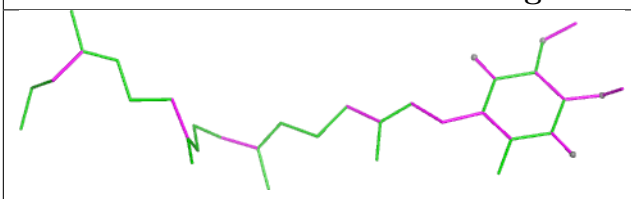


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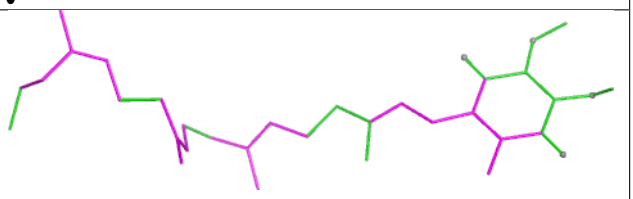


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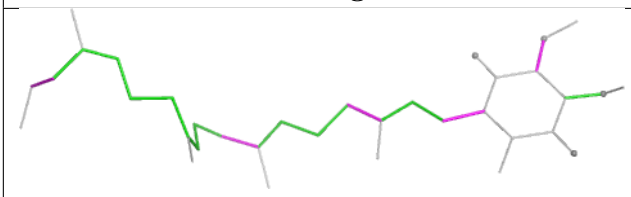
Ligand UQ9 H 500



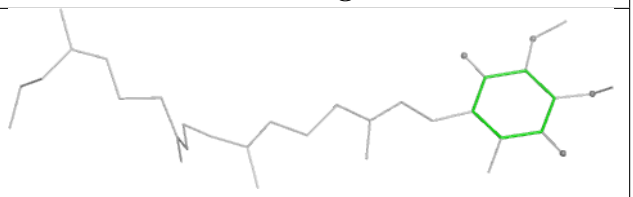
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Bond angles

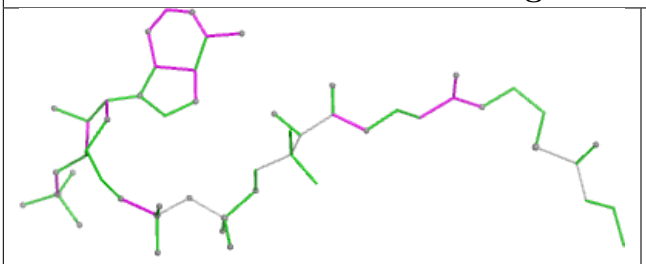


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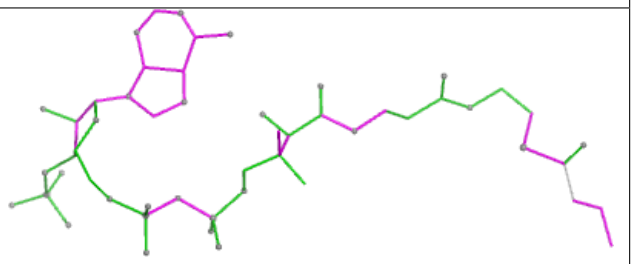


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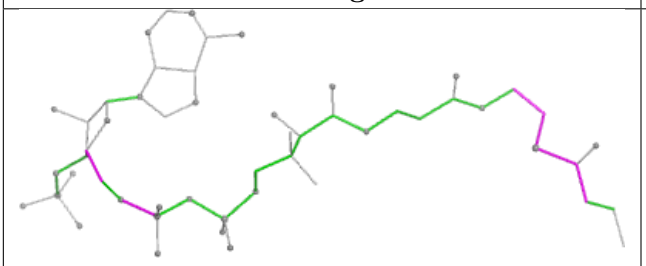
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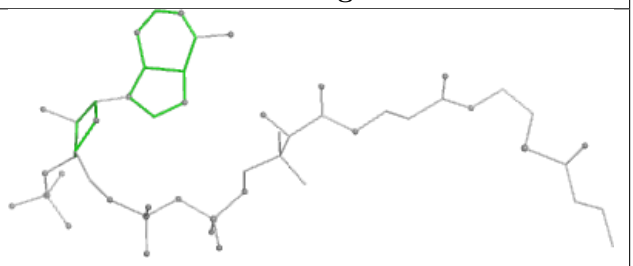
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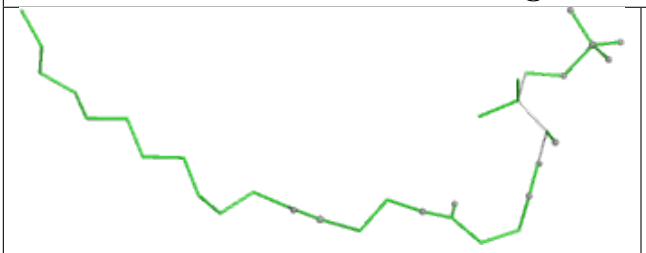


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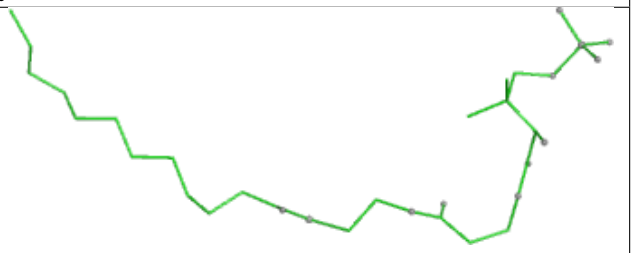


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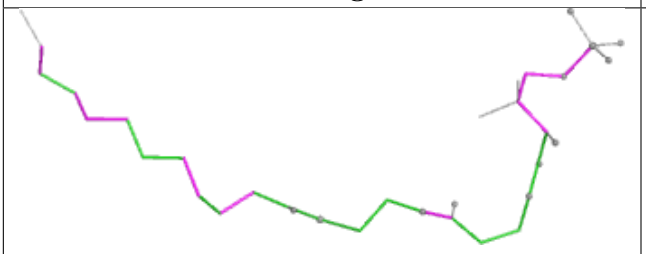
Ligand 8Q1 W 200



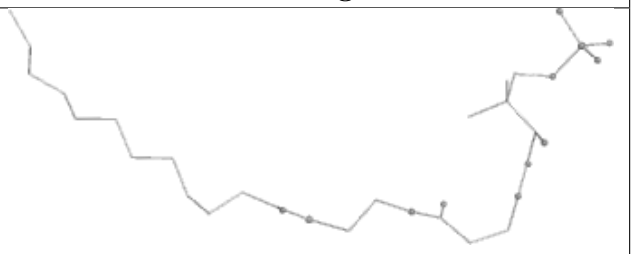
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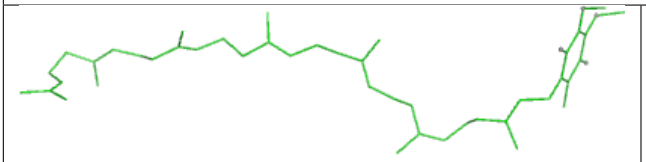


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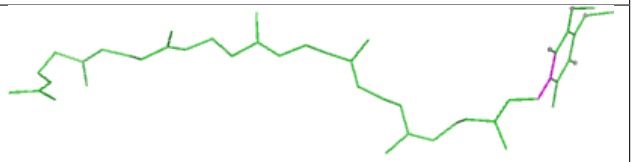


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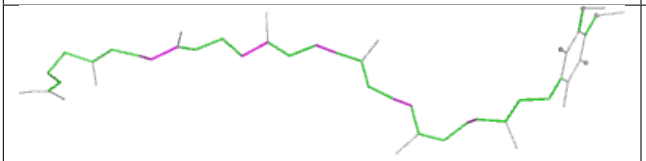
Ligand UQ7 BC 503



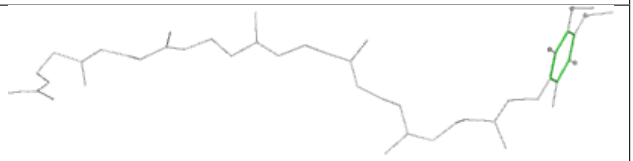
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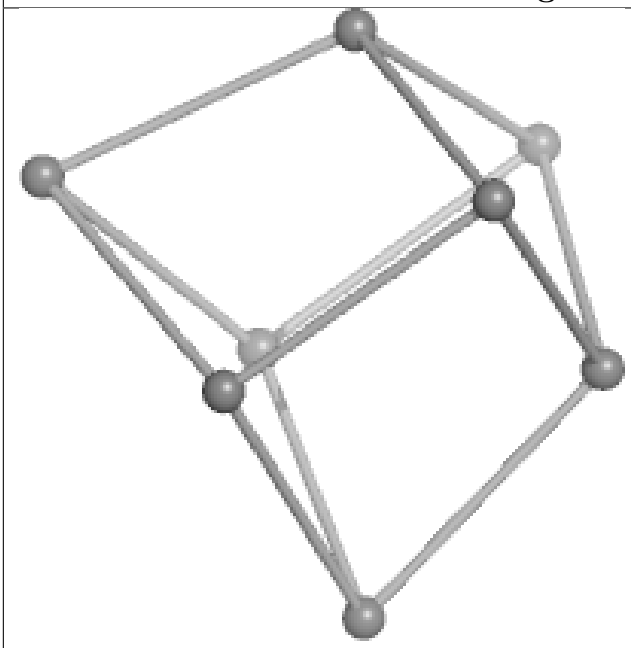


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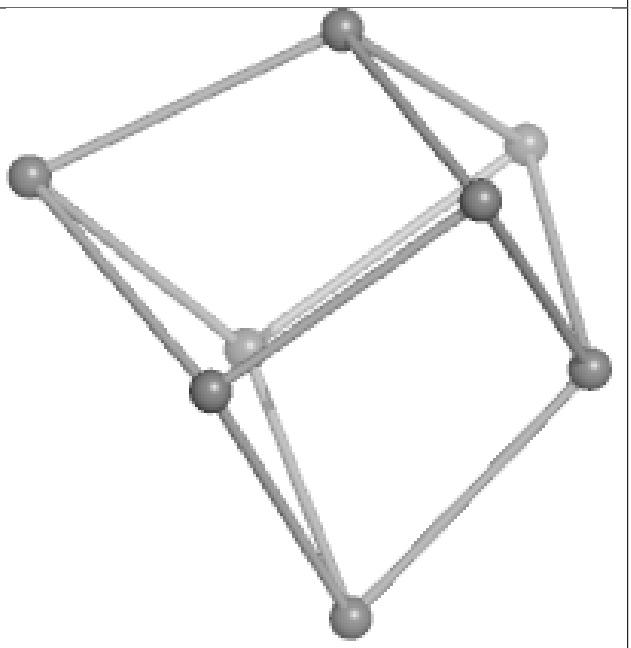


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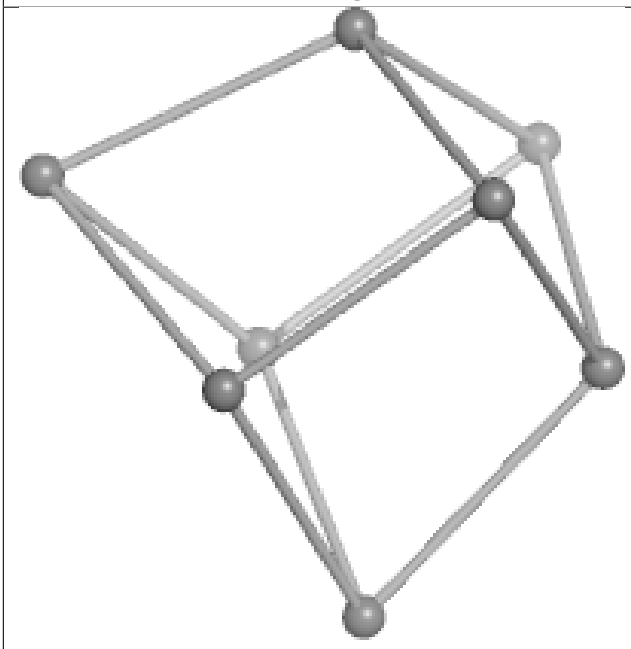
Ligand SF4 I 500



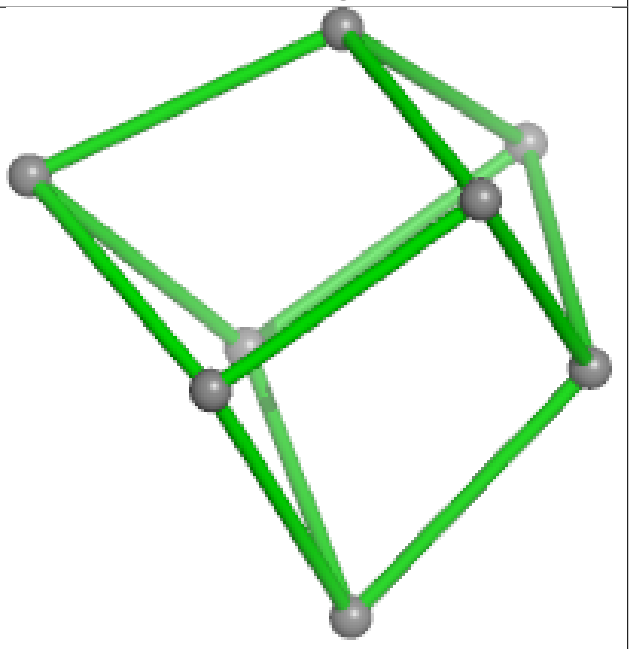
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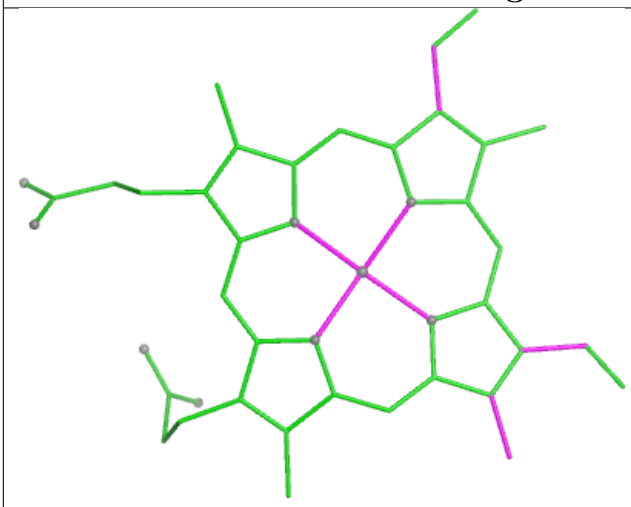


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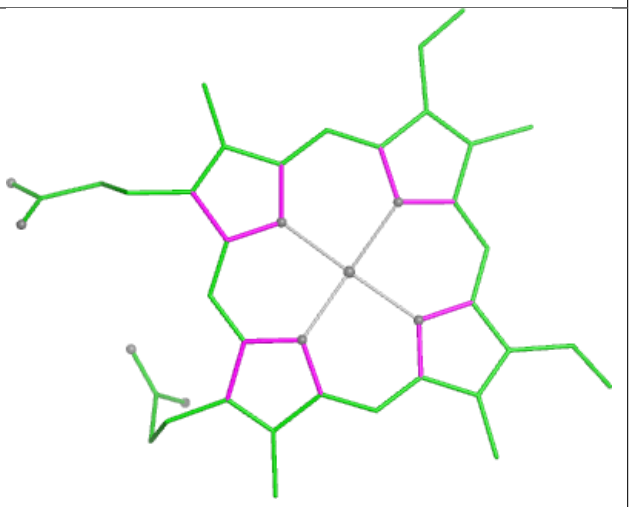


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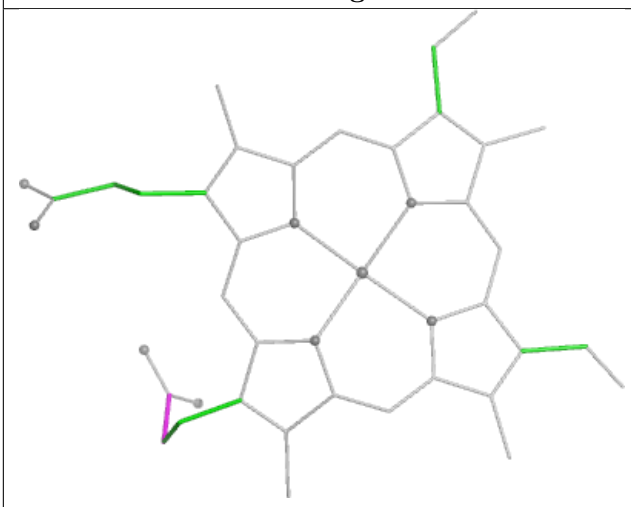
Ligand HEM BC 500



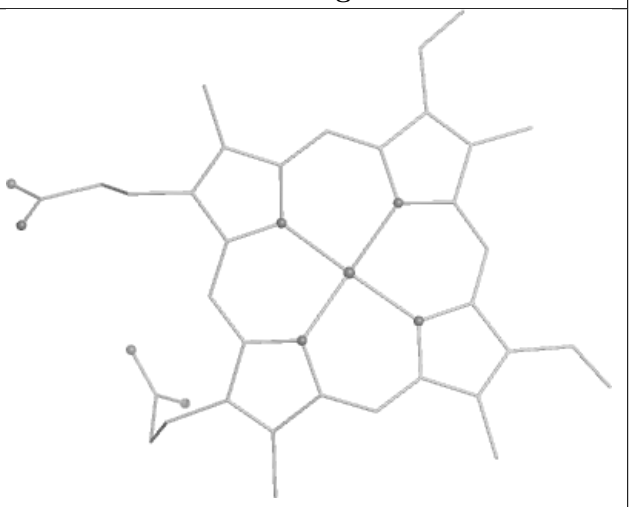
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Bond angles

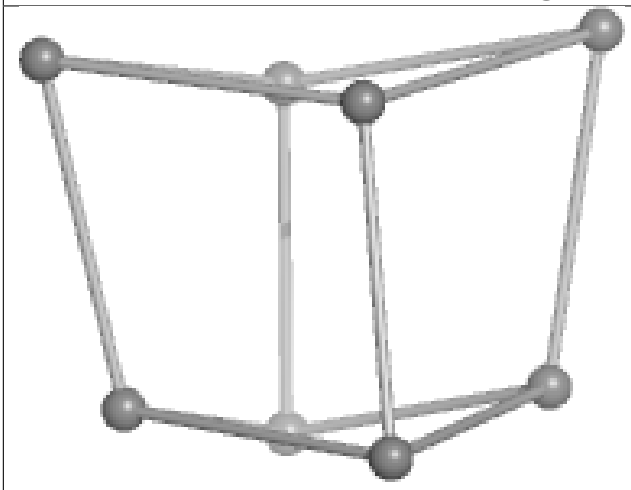


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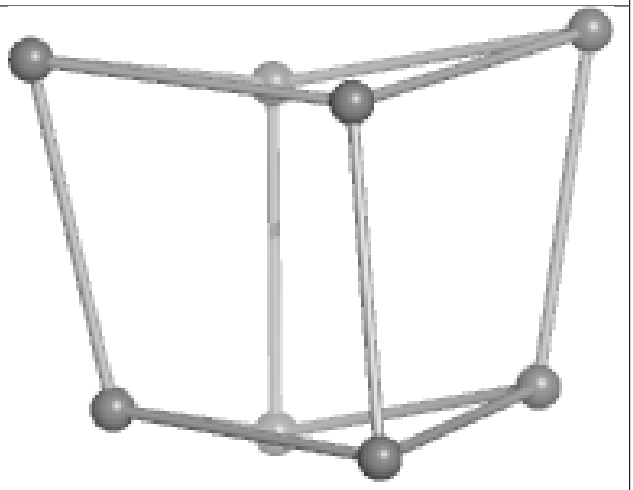


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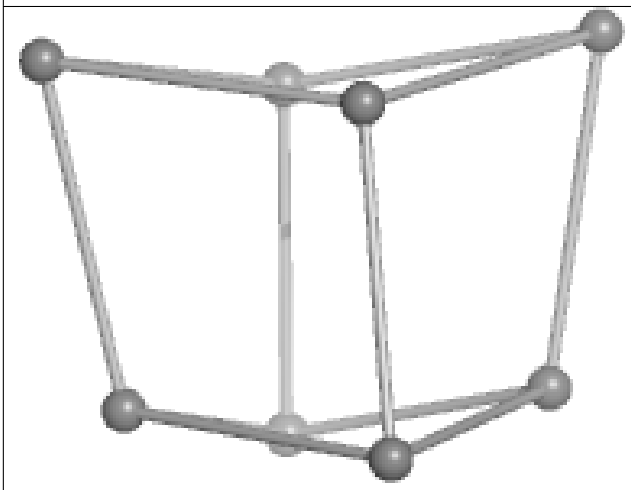
Ligand SF4 I 501



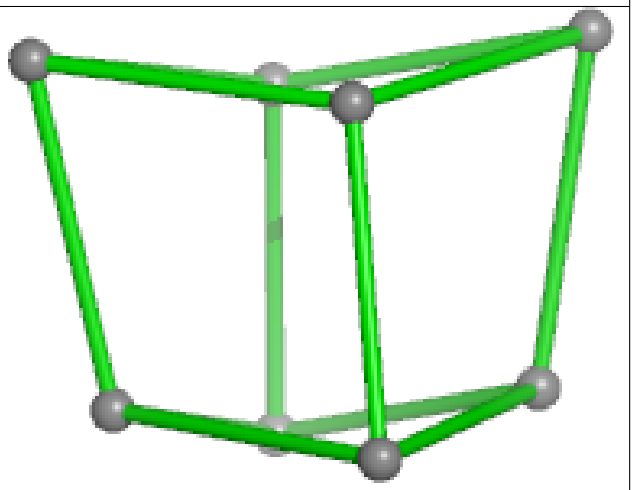
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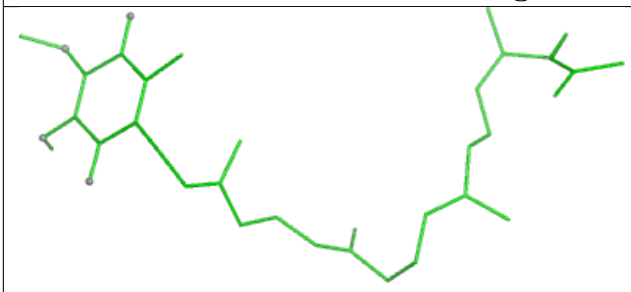


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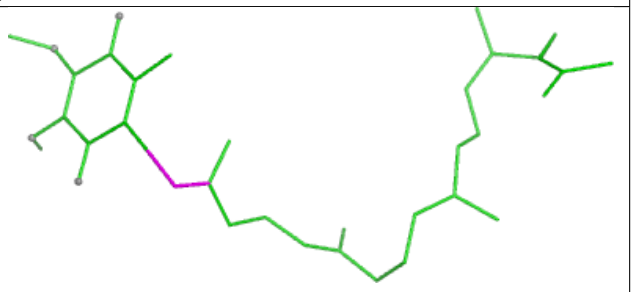


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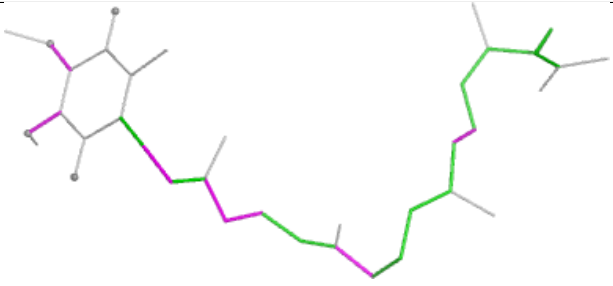
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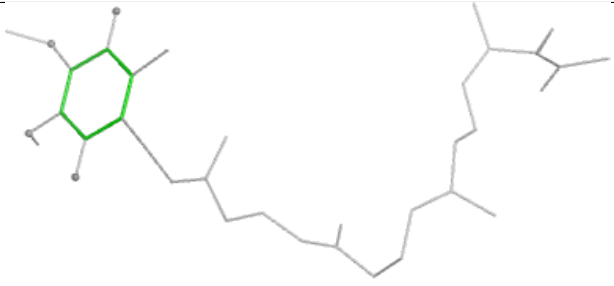
Bond lengths



Bond angles

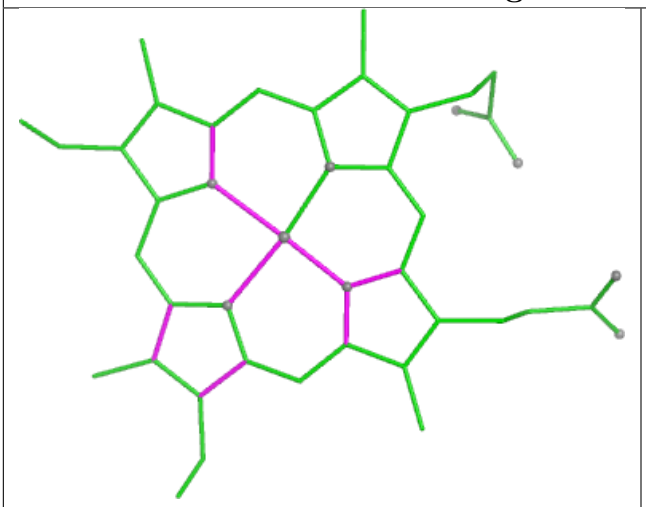


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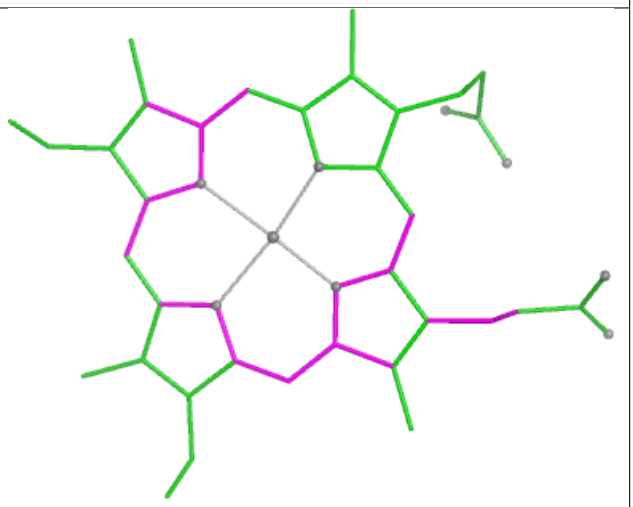


Rings

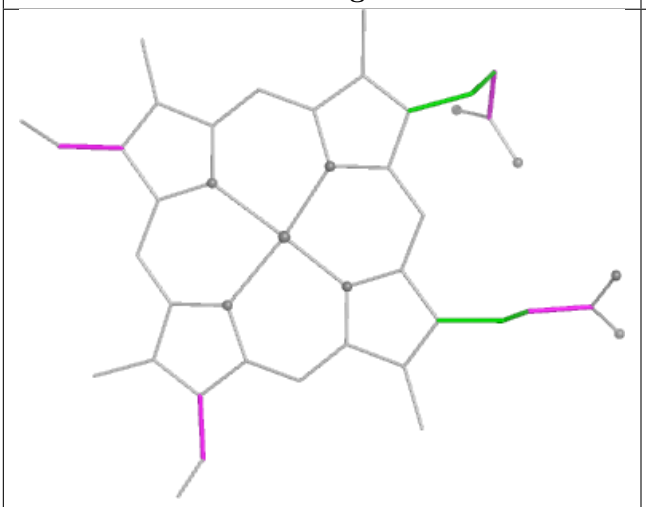
Ligand HEM AC 500



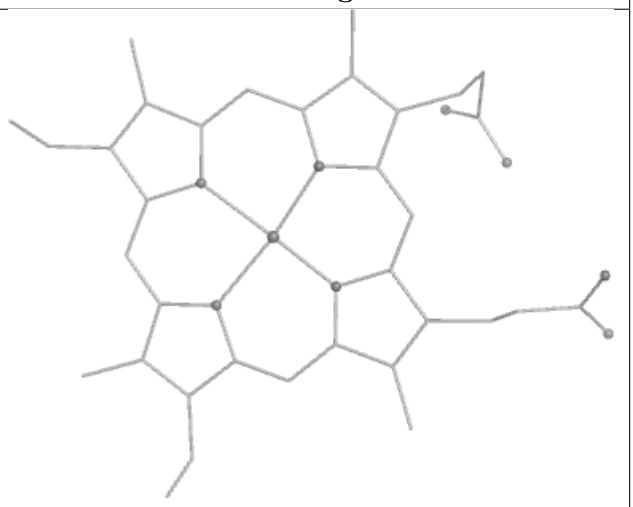
Bond lengths



Bond angles

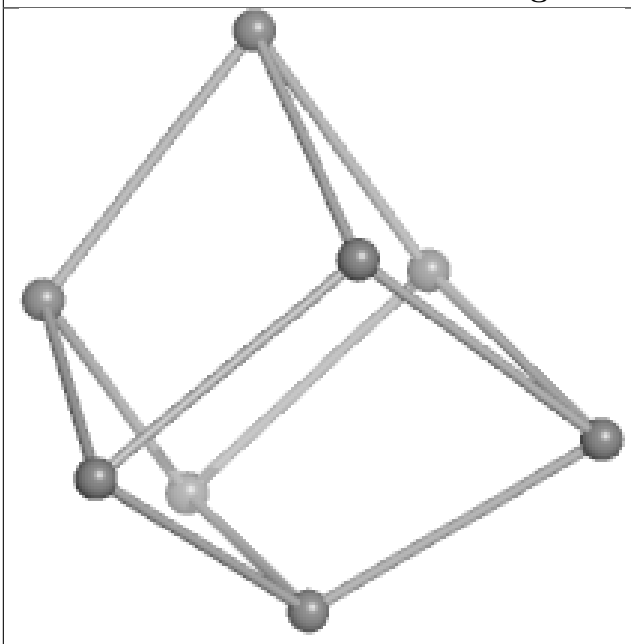


Torsions

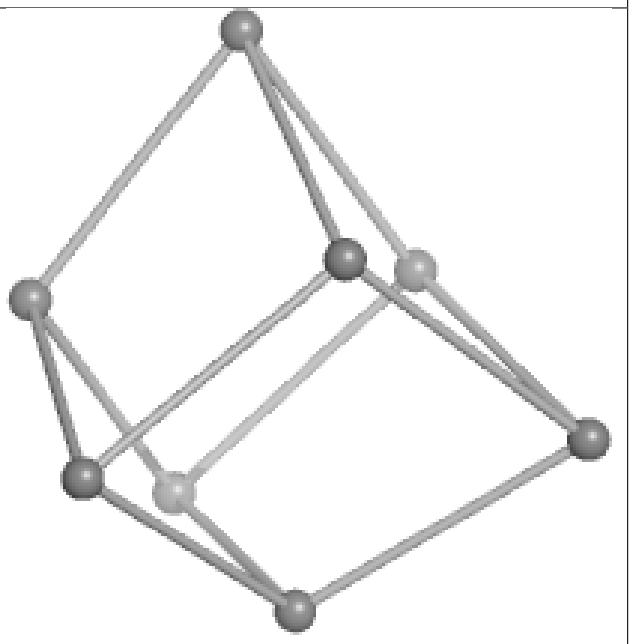


Rings

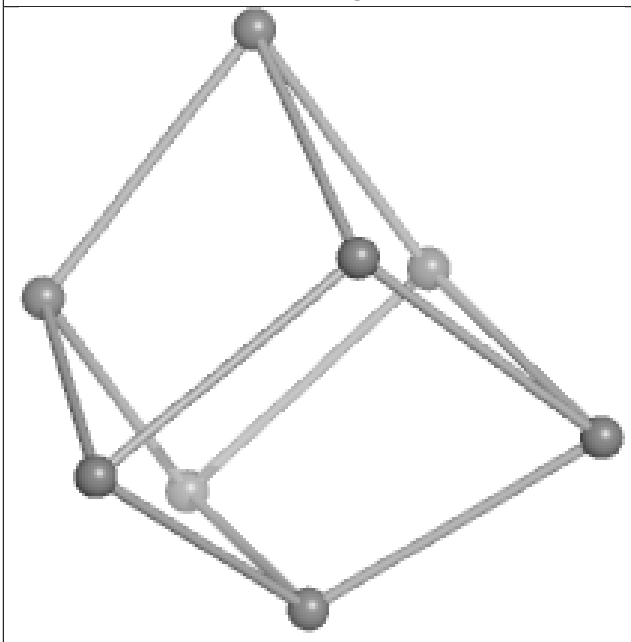
Ligand SF4 G 802



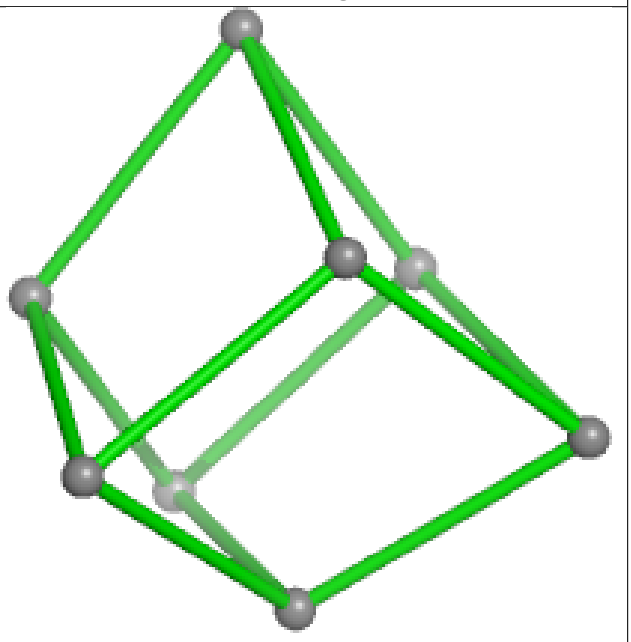
Bond lengths



Bond angles

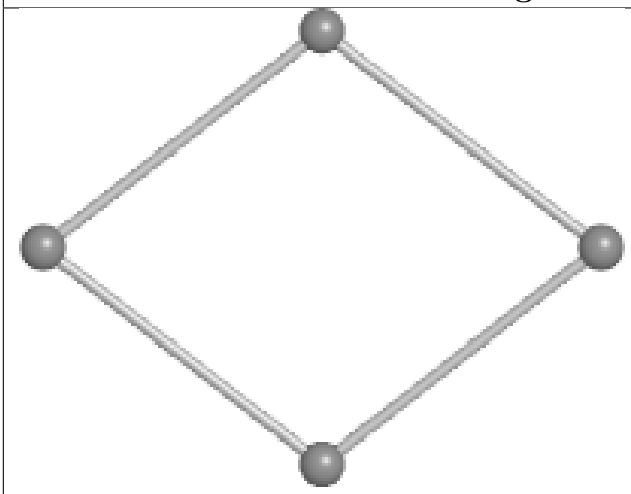


Torsions

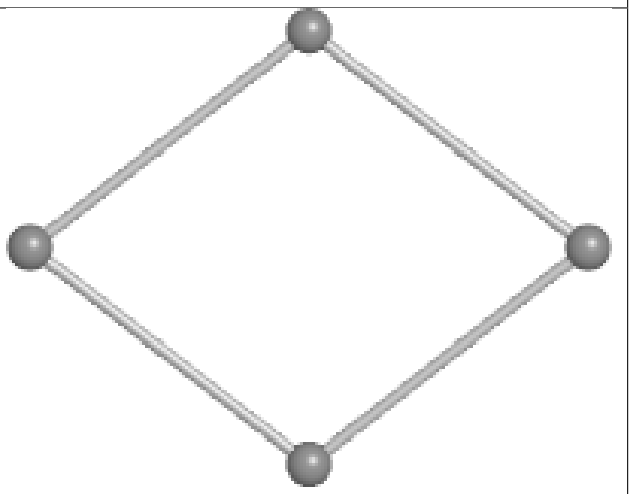


Rings

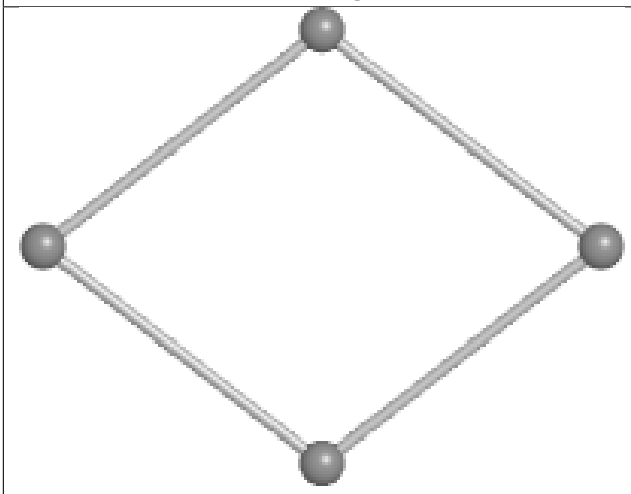
Ligand FES BD 301



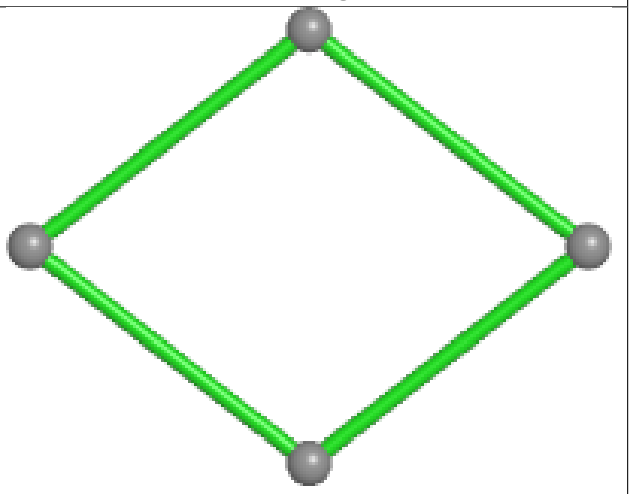
Bond lengths



Bond angles

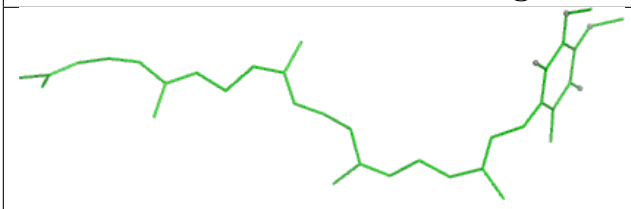


Torsions

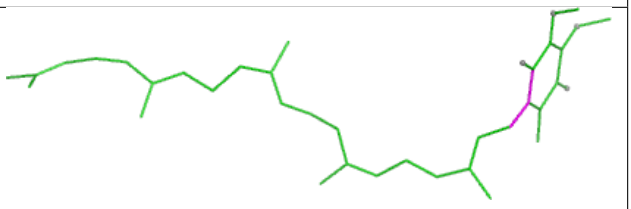


Rings

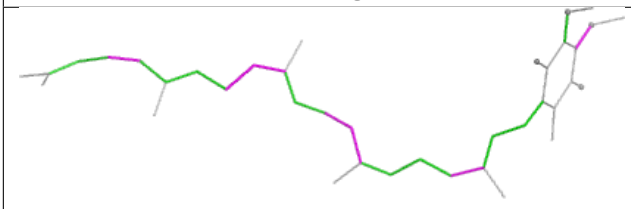
Ligand UQ5 AC 503



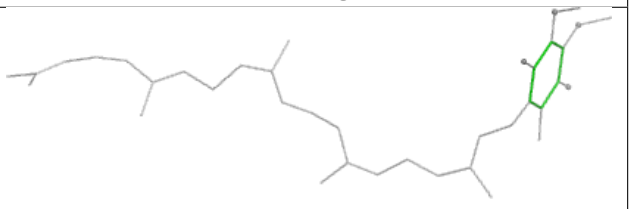
Bond lengths



Bond angles

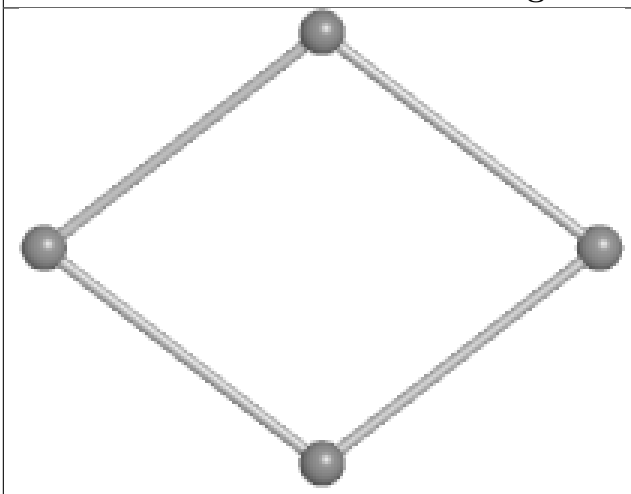


Torsions

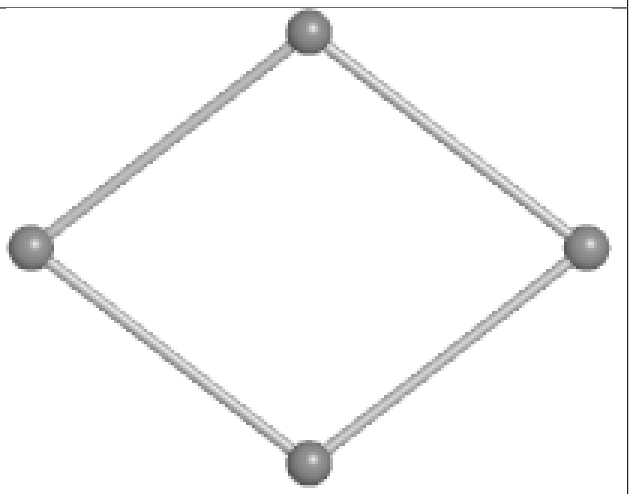


Rings

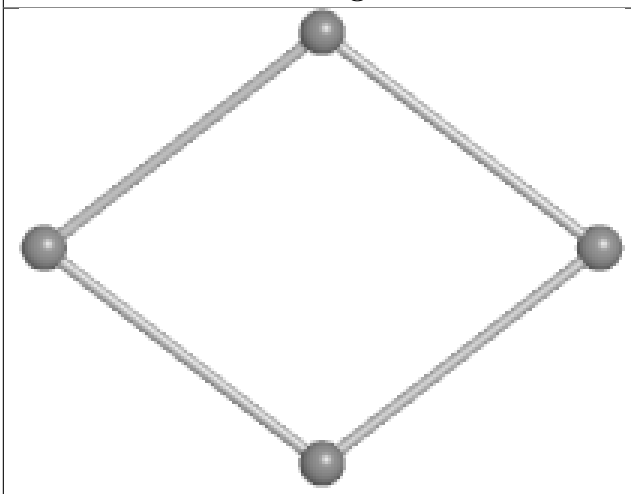
Ligand FES G 801



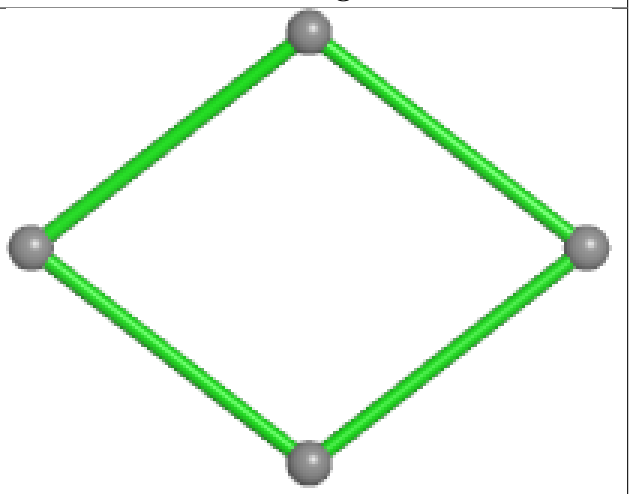
Bond lengths



Bond angles

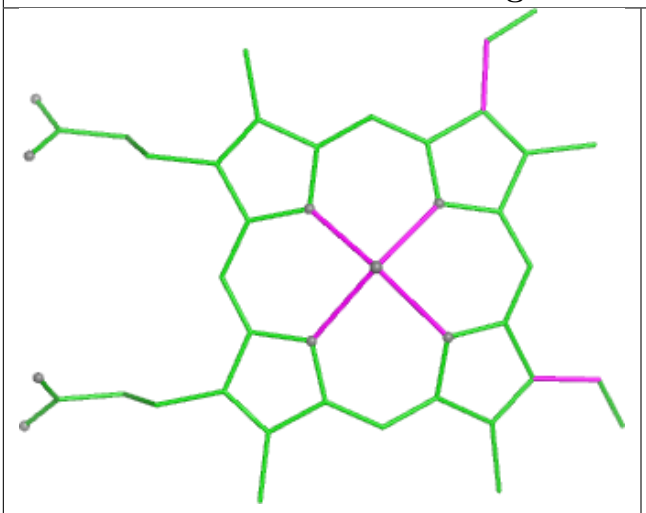


Torsions

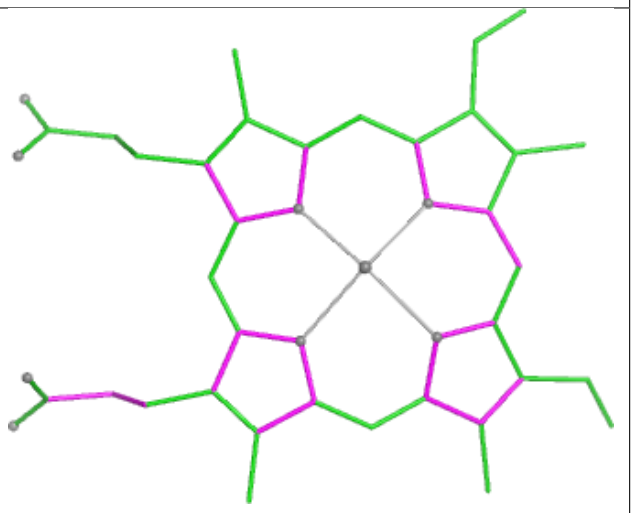


Rings

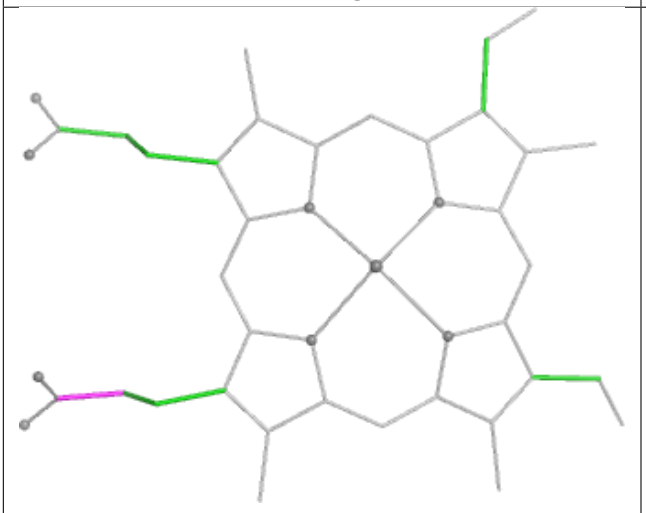
Ligand HEM AE 400



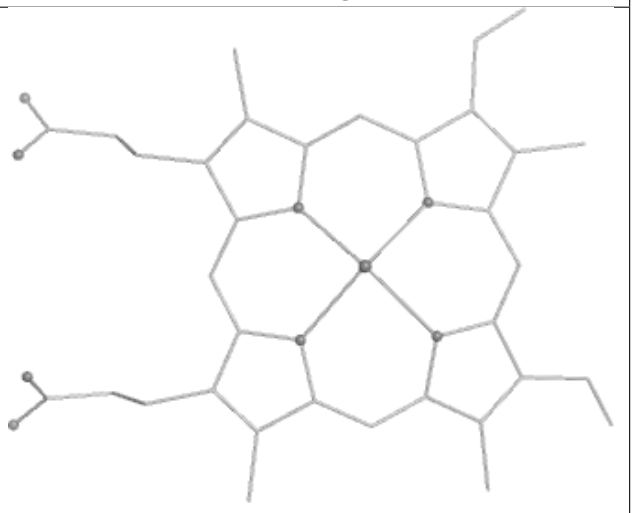
Bond lengths



Bond angles

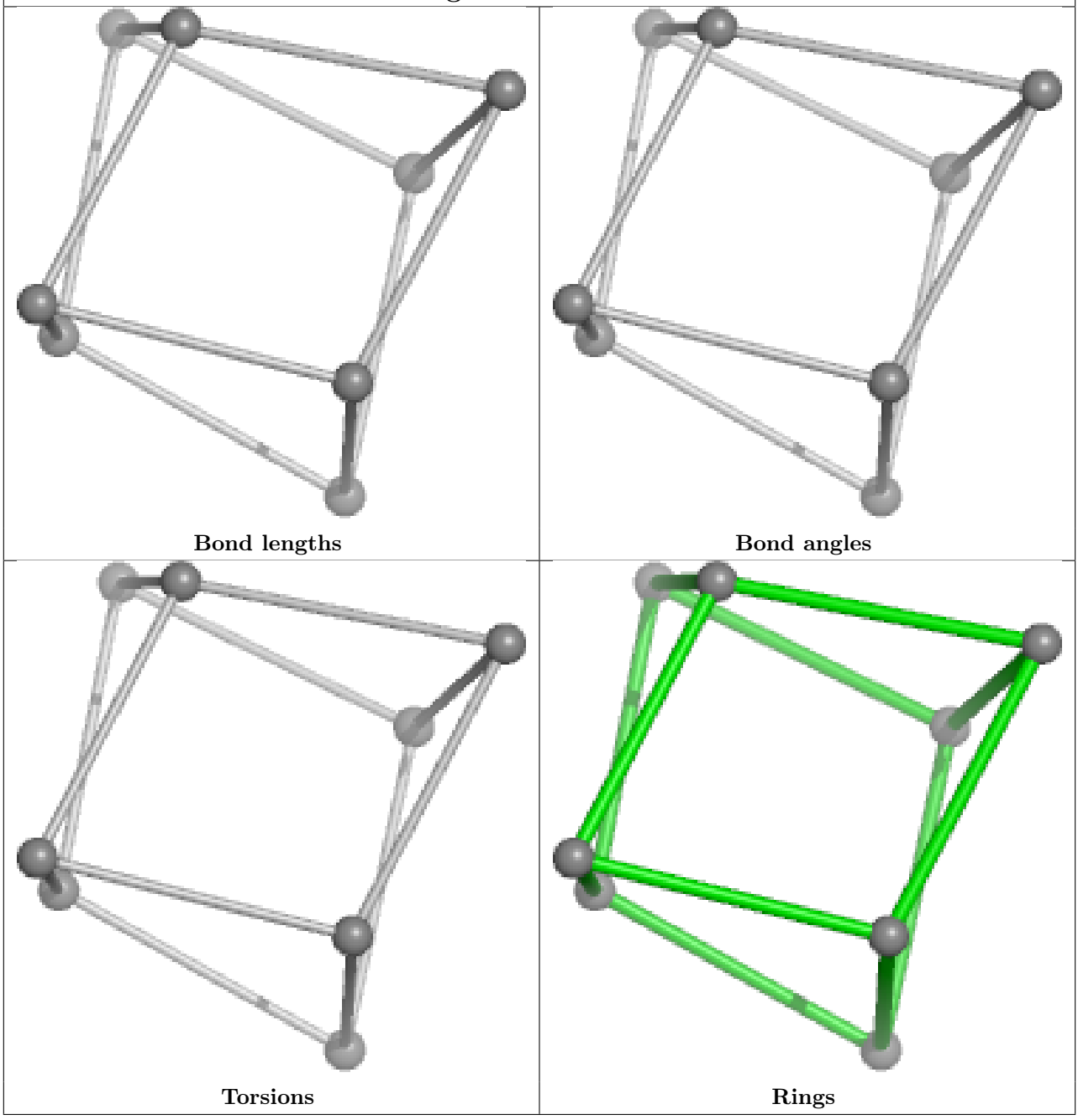


Torsions



Rings

Ligand SF4 G 803



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.

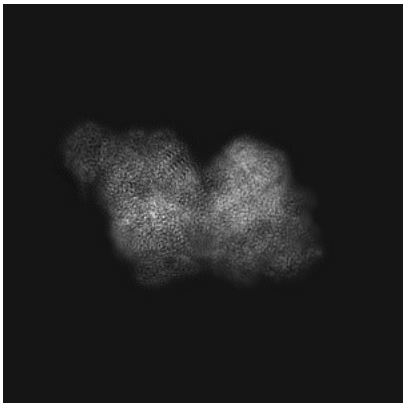
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16171. These allow visual inspection of the internal detail of the map and identification of artifacts.

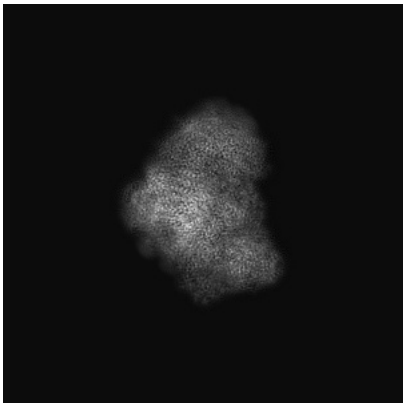
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

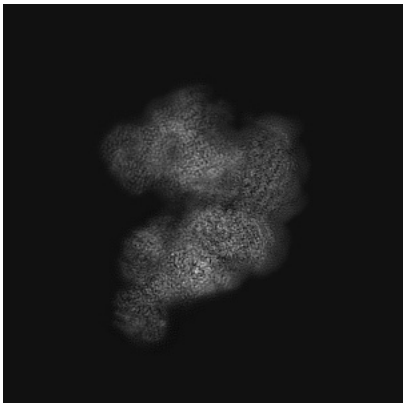
6.1.1 Primary map



X



Y

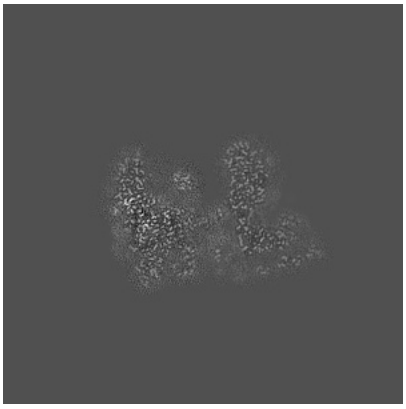


Z

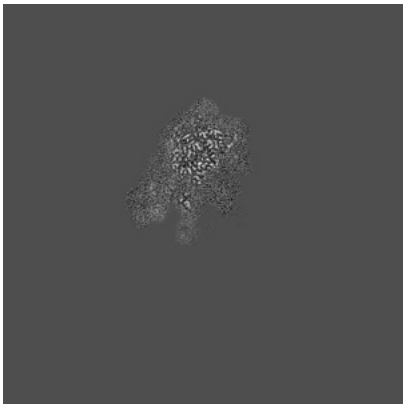
The images above show the map projected in three orthogonal directions.

6.2 Central slices

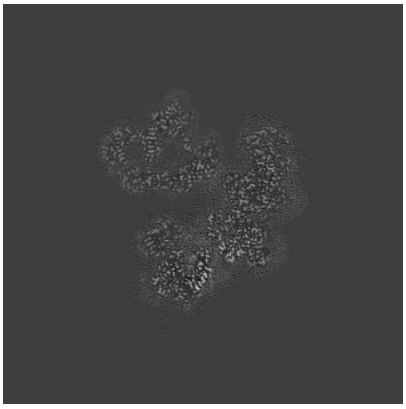
6.2.1 Primary map



X Index: 375



Y Index: 375

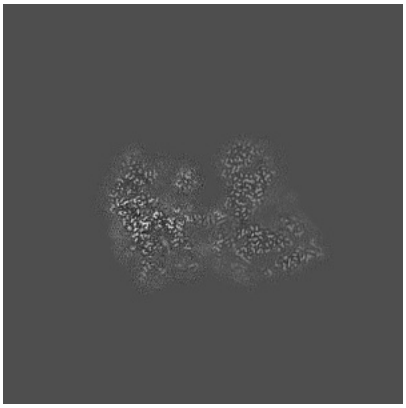


Z Index: 375

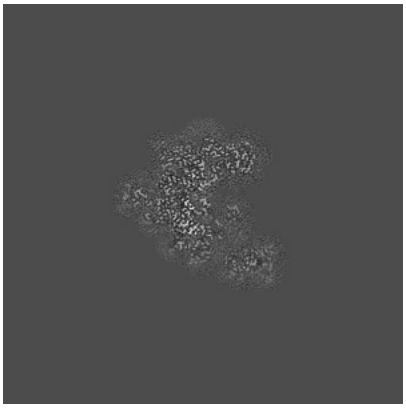
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

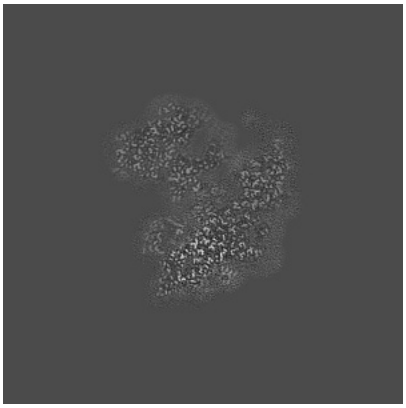
6.3.1 Primary map



X Index: 367



Y Index: 284

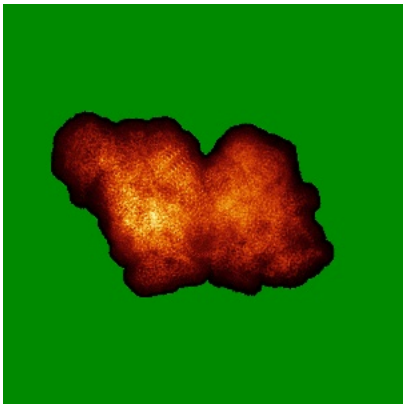


Z Index: 350

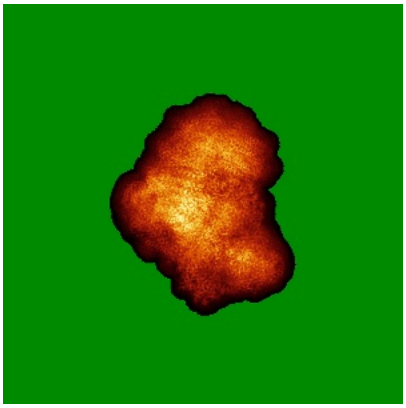
The images above show the largest variance slices of the map in three orthogonal directions.

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

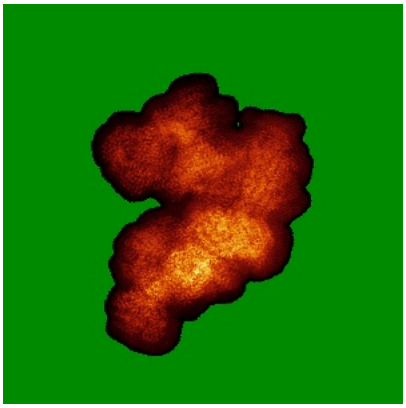
6.4.1 Primary map



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.

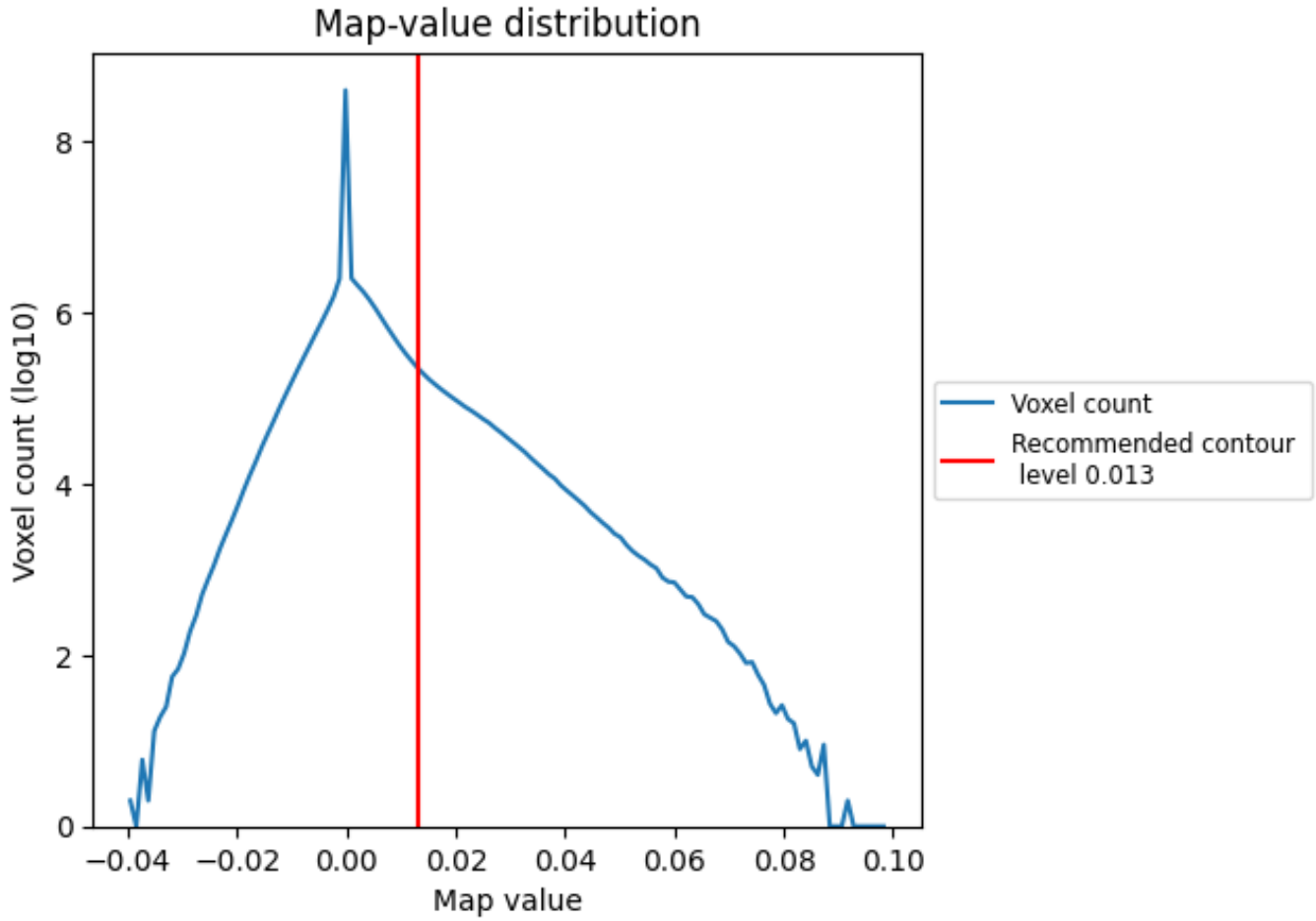
6.6 Mask visualisation (i)

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

7 Map analysis

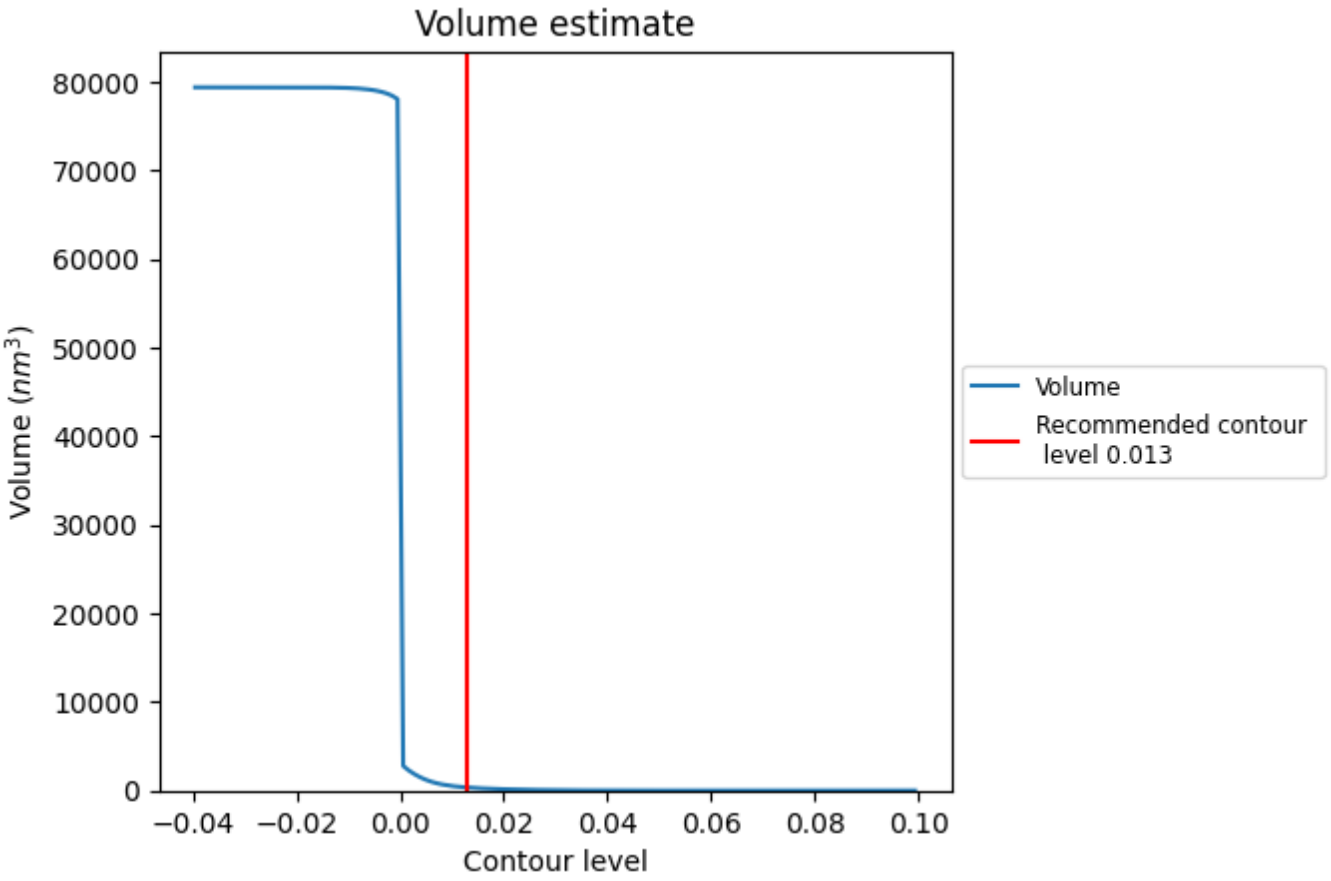
This section contains the results of statistical analysis of the map.

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.

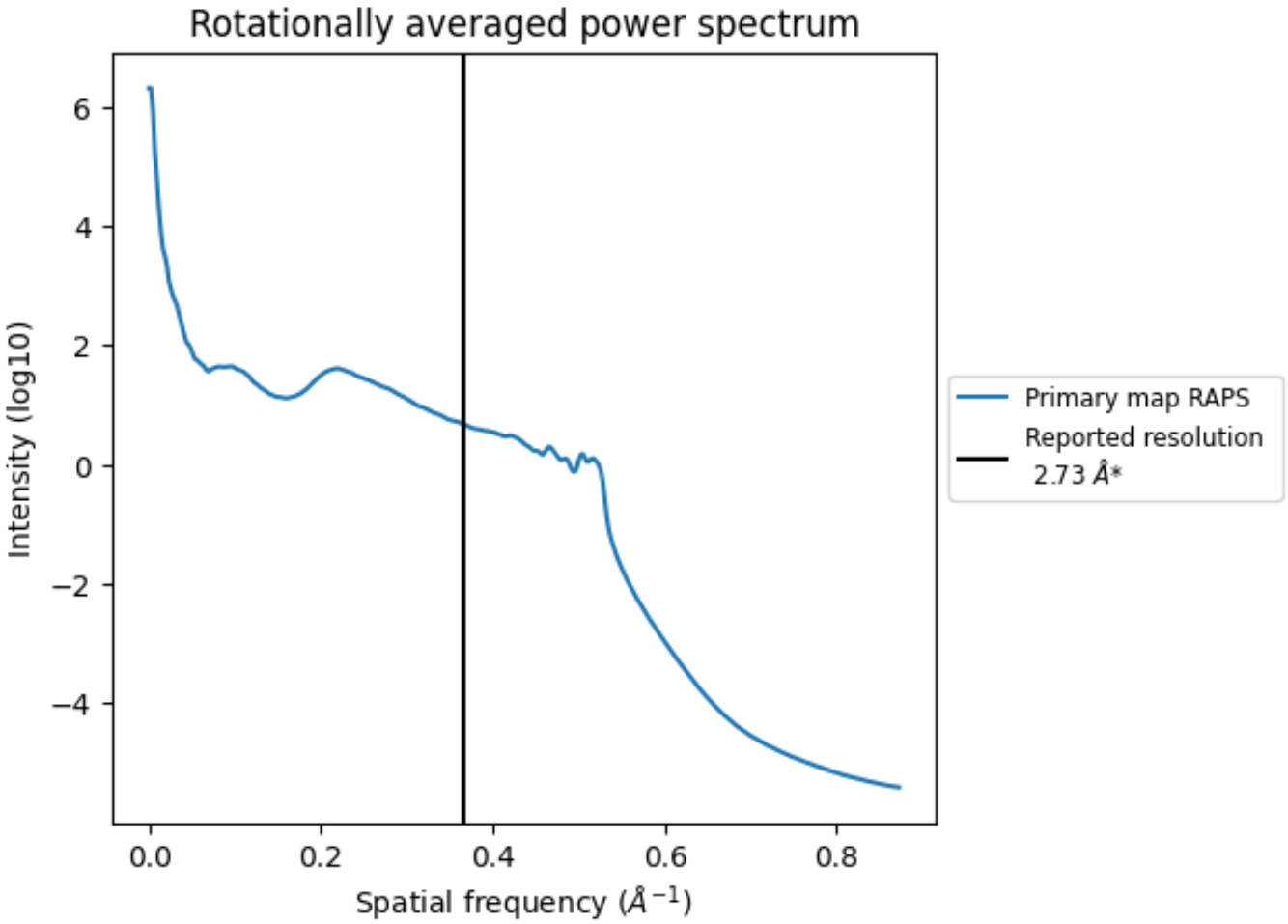
7.2 Volume estimate (i)



The volume at the recommended contour level is 345 nm^3; this corresponds to an approximate mass of 312 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)

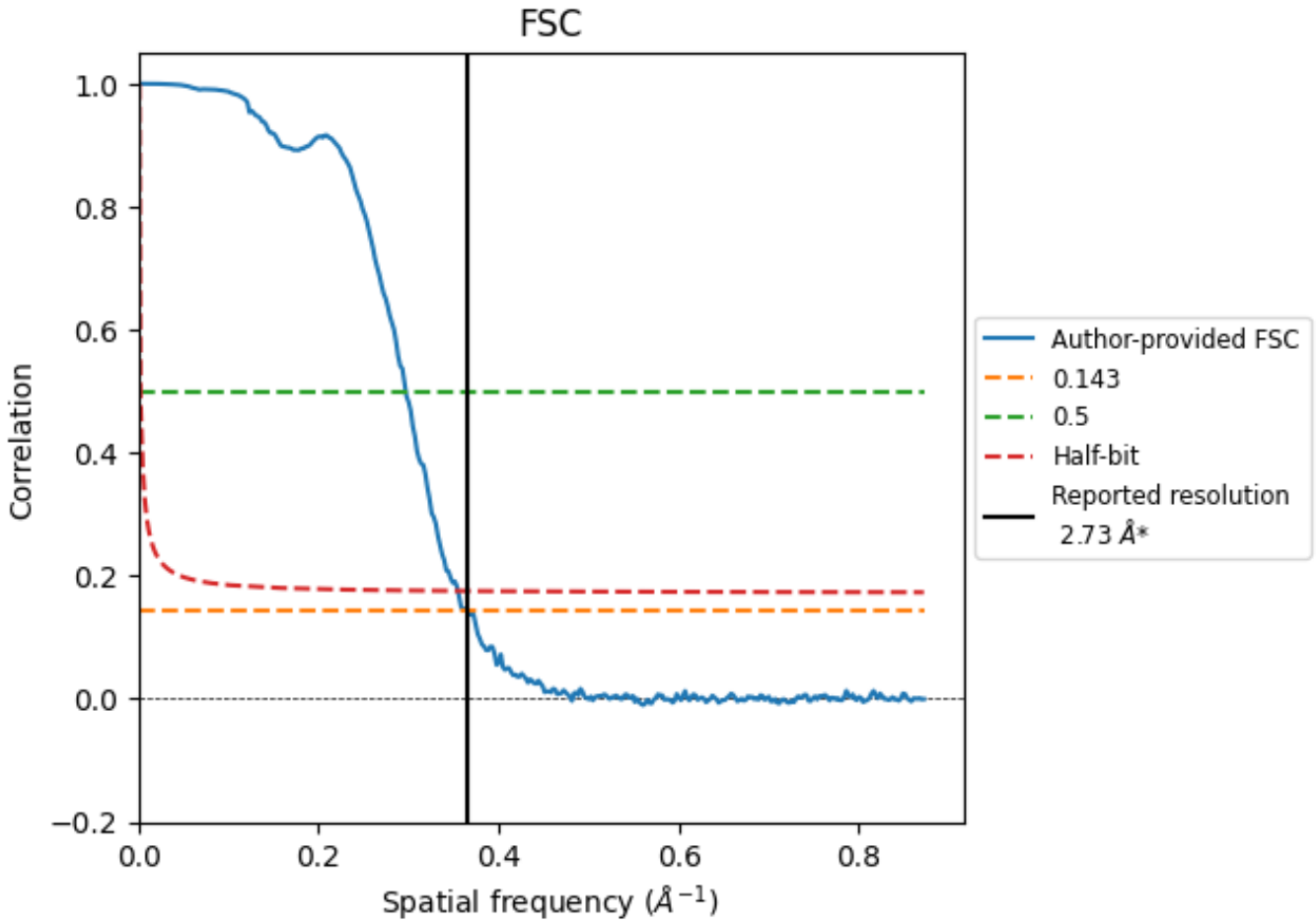


*Reported resolution corresponds to spatial frequency of 0.366 $Å^{-1}$

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 0.366 Å^{-1}

8.2 Resolution estimates (i)

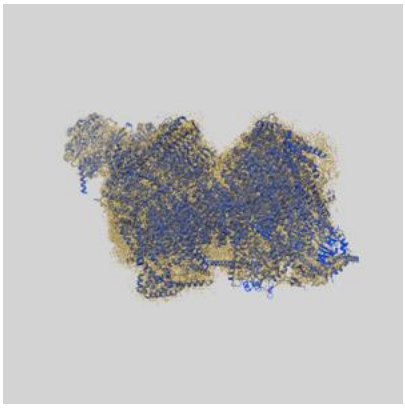
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.37	2.82
Unmasked-calculated*	-	-	-

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

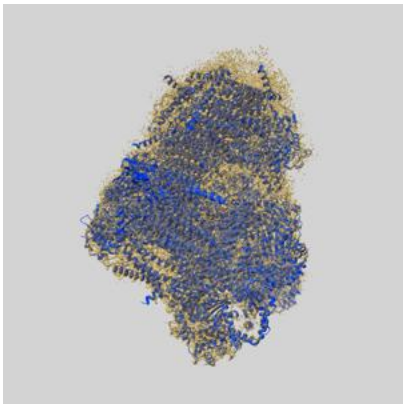
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16171 and PDB model 8BQ5. Per-residue inclusion information can be found in section 3 on page 23.

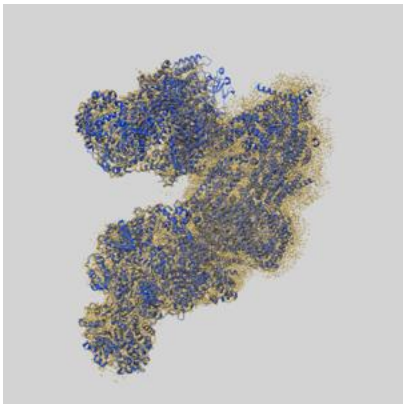
9.1 Map-model overlay



X



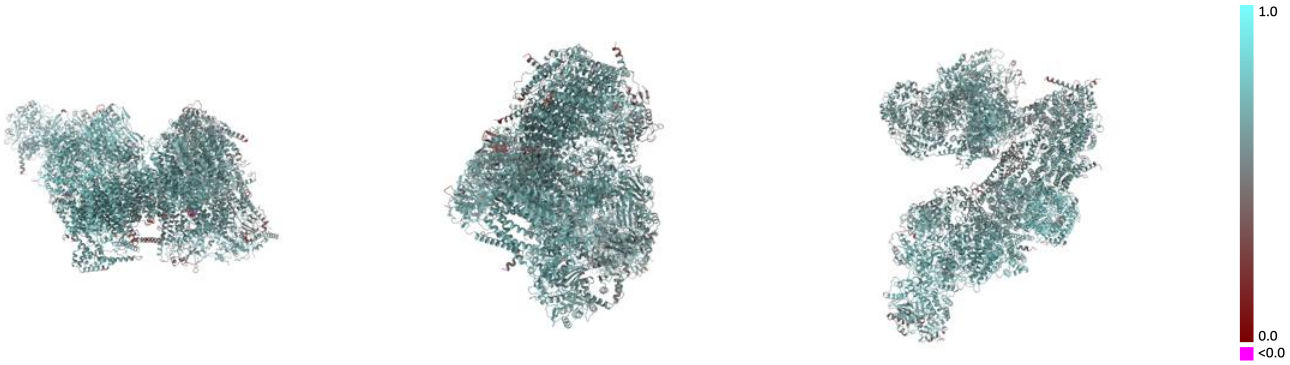
Y



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.

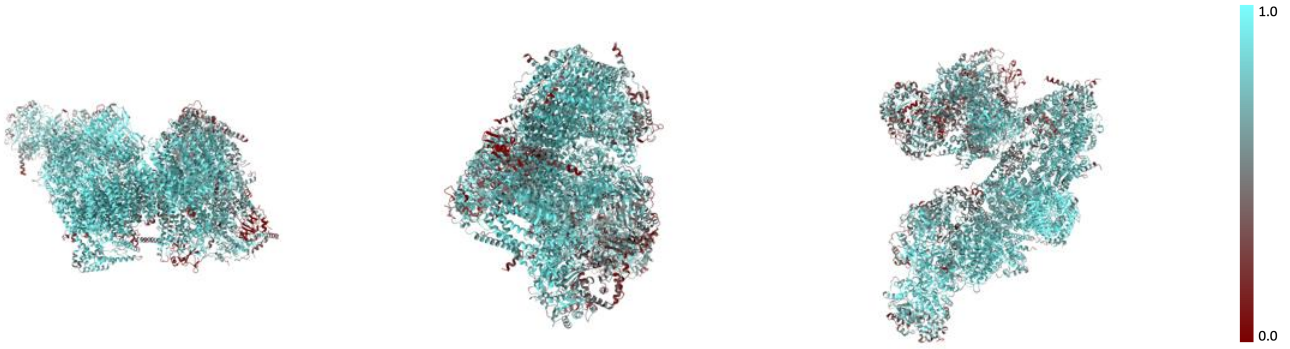
9.2 Q-score mapped to coordinate model (i)



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.

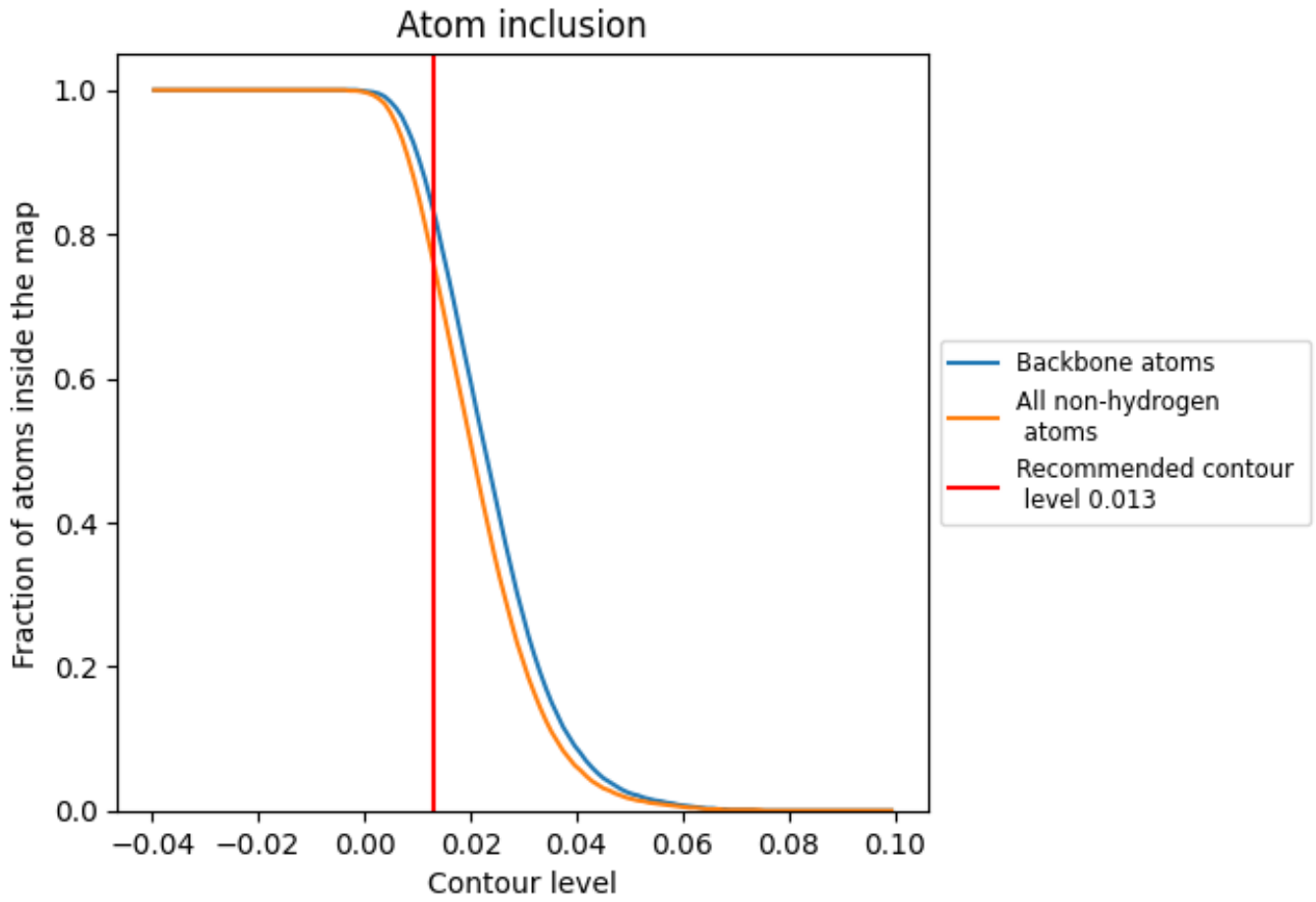
9.3 Atom inclusion mapped to coordinate model (i)



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	0.7620	0.6420
A	0.9440	0.7030
AA	0.4630	0.5720
AB	0.7400	0.6440
AC	0.8500	0.6750
AD	0.3440	0.5320
AE	0.8260	0.6630
AF	0.8320	0.6700
AG	0.8200	0.6390
AH	0.6850	0.5870
AI	0.6970	0.6380
AJ	0.2300	0.5310
B	0.9550	0.7280
BA	0.4840	0.5810
BB	0.7440	0.6430
BC	0.8170	0.6610
BD	0.3730	0.5390
BE	0.7700	0.6500
BF	0.7680	0.6440
BG	0.6390	0.6190
BH	0.4600	0.5750
BI	0.5990	0.5890
BJ	0.4850	0.5590
C	0.8950	0.7170
D	0.9460	0.7240
E	0.6460	0.5950
F	0.7230	0.6360
G	0.7820	0.6650
H	0.9400	0.6990
I	0.9520	0.7250
J	0.9000	0.6860
K	0.9560	0.7090
L	0.8430	0.6460
M	0.8950	0.6710
N	0.9290	0.7030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	0.9400	0.6760
P	0.6510	0.6050
Q	0.5290	0.6230
R	0.7530	0.6760
S	0.6370	0.5910
T	0.3910	0.4860
U	0.6340	0.5230
V	0.7200	0.6410
W	0.6220	0.6120
X	0.7530	0.6160
Y	0.5830	0.4920
Z	0.7870	0.6240
a	0.8670	0.6600
b	0.7780	0.5950
c	0.7040	0.5920
d	0.7750	0.6170
e	0.8410	0.6450
f	0.9080	0.6930
g	0.7110	0.5760
i	0.6660	0.5550
j	0.5300	0.5110
k	0.4490	0.4800
l	0.6050	0.5550
m	0.7780	0.6320
n	0.7700	0.5780
o	0.5740	0.5280
p	0.7300	0.5910
q	0.8230	0.6780
u	0.7580	0.5500
v	0.8650	0.6560
x	0.9420	0.7140
y	0.8950	0.6870
z	0.8790	0.6770