



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:02 AM JST

PDB ID : 7DKF / pdb_00007dkf
EMDB ID : EMD-30706
Title : Activity optimized supercomplex state4
Authors : Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on : 2020-11-24
Resolution : 8.30 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

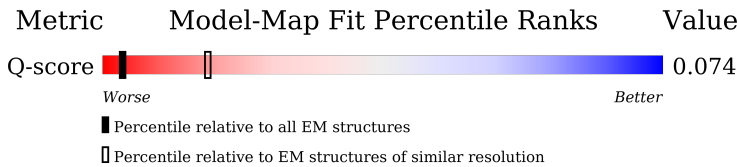
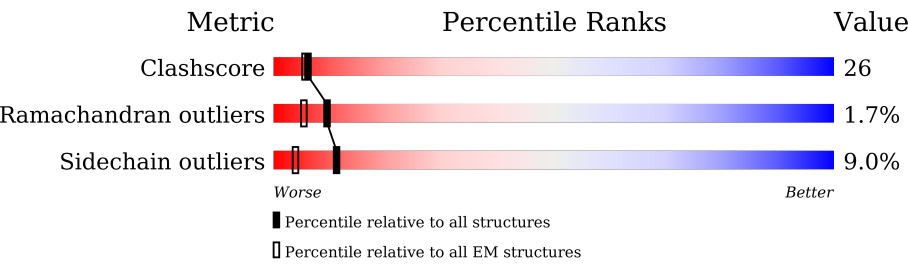
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 8.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	280 (7.82 - 8.80)

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 $\leq 5\%$. 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	A1	480	9% 15% 46% 24% 5% 10%
1	M1	480	23% 16% 48% 23% • 10%
2	B1	453	10% 20% 50% 20% • 8%
2	N1	453	14% 21% 49% 20% • 8%

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Mol	Chain	Length	Quality of chain
3	C1	379	
3	O1	379	
4	D1	325	
4	P1	325	
5	E1	196	
5	Q1	196	
6	F1	111	
6	R1	111	
7	G1	82	
7	S1	82	
8	H1	91	
8	T1	91	
9	I1	78	
9	U1	78	
10	J1	64	
10	V1	64	
11	K1	56	
11	W1	56	
12	22	347	
13	32	115	
14	42	459	
15	52	98	
16	72	175	
17	82	444	
18	92	217	

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Mol	Chain	Length	Quality of chain
19	A2	704	
20	B2	430	
21	C2	228	
22	D2	179	
23	E2	176	
24	F2	75	
25	G2	133	
26	H2	105	
27	I2	96	
28	J2	70	
29	K2	98	
30	L2	83	
31	N2	115	
32	O2	127	
33	P2	112	
34	Q2	171	
35	R2	345	
36	S2	320	
37	T2	140	
38	U2	145	
39	V2	143	
40	M2	88	
40	W2	88	
41	X2	57	
42	Y2	72	

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Mol	Chain	Length	Quality of chain
43	Z2	97	
44	a2	128	
45	b2	143	
46	c2	127	
47	d2	136	
48	f2	178	
49	h2	125	
50	i2	49	
51	j2	120	
52	12	318	
53	62	606	
54	g2	176	
55	e2	158	
56	A3	514	
57	B3	227	
58	C3	261	
59	D3	169	
60	E3	152	
61	F3	129	
62	G3	97	
63	H3	86	
64	I3	74	
65	J3	80	
66	K3	80	
67	L3	63	

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Mol	Chain	Length	Quality of chain
68	M3	70	24% 43% 17% 39%

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
75	SF4	A2	801	-	-	X	-
75	SF4	A2	802	-	-	X	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 105456 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	432	Total	C	N	O	S	0	0
			3356	2098	595	643	20		
1	M1	432	Total	C	N	O	S	0	0
			3356	2098	595	643	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		
2	N1	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
3	O1	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
4	P1	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	75	Total	C	N	O	S	0	0
			566	352	94	118	2		
5	Q1	196	Total	C	N	O	S	0	0
			1518	956	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
6	R1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
7	S1	81	Total	C	N	O	S	0	0
			682	441	128	112	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	64	Total	C	N	O	S	0	0
			524	316	96	107	5		
8	T1	64	Total	C	N	O	S	0	0
			524	316	96	107	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	33	Total	C	N	O	S	0	0
			248	152	51	44	1		
9	U1	33	Total	C	N	O	S	0	0
			248	152	51	44	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J1	62	Total	C	N	O	0	0
			511	335	89	87		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	V1	62	Total	C	N	O	0	0
			511	335	89	87		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K1	22	Total	C	N	O	0	0
			164	109	29	26		
11	W1	22	Total	C	N	O	0	0
			164	109	29	26		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	344	Total	C	N	O	S	0	0
			2582	1707	404	437	34		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	32	93	Total	C	N	O	S	0	0
			719	492	104	120	3		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	42	458	Total	C	N	O	S	1	0
			3447	2293	548	574	32		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	52	96	Total	C	N	O	S	0	0
			697	454	109	124	10		

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	72	172	Total	C	N	O	S	0	0
			1186	798	179	202	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	82	427	Total	C	N	O	S	0	0
			2965	1864	552	534	15		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	92	207	Total	C	N	O	S	0	0
			1535	978	261	286	10		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A2	688	Total	C	N	O	S	0	0
			5183	3254	915	978	36		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B2	385	Total	C	N	O	S	0	0
			3076	1963	530	559	24		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C2	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D2	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E2	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F2	28	Total	C	N	O	S	0	0
			183	116	32	35			

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G2	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H2	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I2	71	Total	C	N	O	S	0	0
			532	332	99	98	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J2	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K2	84	Total	C	N	O	S	0	0
			652	409	125	118			

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L2	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N2	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	O2	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	P2	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Q2	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R2	306	Total	C	N	O	S	0	0
			2334	1505	417	409	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S2	319	Total	C	N	O	S	0	0
			2299	1457	395	438	9		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	T2	138	Total	C	N	O	S	0	0
			942	599	165	172	6		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	U2	91	Total	C	N	O	S	0	0
			734	480	123	128	3		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V2	138	Total	C	N	O	S	0	0
			1093	702	189	193	9		

- Molecule 40 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W2	83	Total	C	N	O	S	0	0
			596	386	95	111	4		
40	M2	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X2	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y2	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z2	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	a2	114	Total	C	N	O	S	0	0
			857	550	159	148			

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	b2	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c2	90	Total	C	N	O	S	0	0
			617	391	119	107			

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	d2	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f2	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	h2	91	Total	C	N	O	S	0	0
			721	461	123	135	2		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	i2	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j2	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

- Molecule 52 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	12	309	Total	C	N	O	S	0	0
			2442	1642	376	401	23		

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	62	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	g2	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	e2	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A3	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B3	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C3	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	D3	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	E3	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	F3	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	G3	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	H3	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	I3	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	J3	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	K3	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

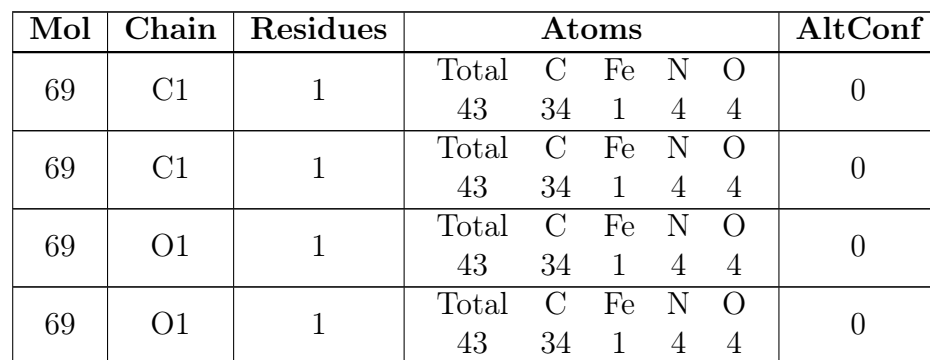
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	L3	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	M3	43	Total	C	N	O	0	0
			335	223	53	59		

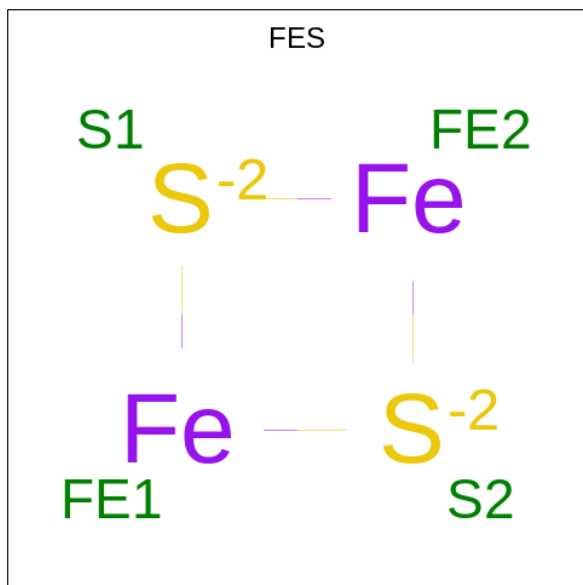
- Molecule 69 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- # HEC
-
- The chemical structure of HEC (Hexaethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains: CMC, CBC, CAC, C2C, C3C, C4C, CHC, C3B, C4B, CMB, C2B, C1B, CHB, C4A, C3A, CMA, C2A, C1A, CBA, CAA, CGA, CBA, CBA, CAA, CGA, CBA, CBA, CAA, CGA. Two carboxylic acid groups are attached to the ring, labeled O2D, O1D, O2A, and O1A.

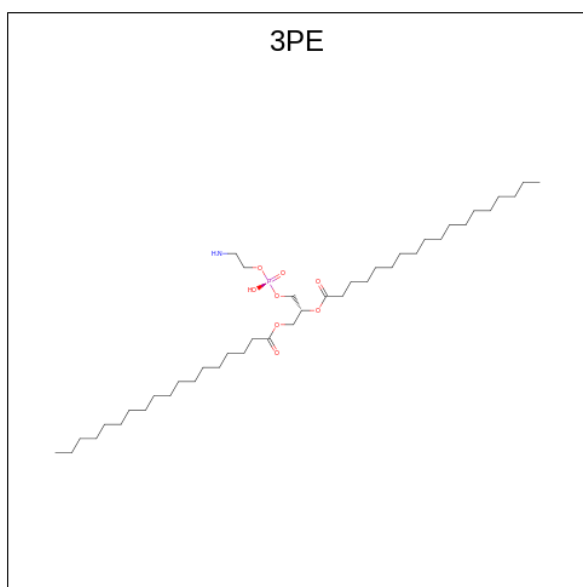
Mol	Chain	Residues	Atoms					AltConf
70	D1	1	Total 43	C 34	Fe 1	N 4	O 4	0
70	P1	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



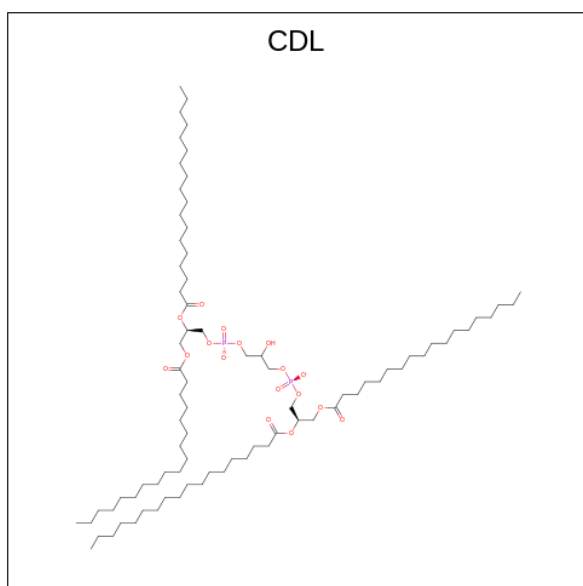
Mol	Chain	Residues	Atoms			AltConf
71	Q1	1	Total	Fe	S	0
			4	2	2	
71	92	1	Total	Fe	S	0
			4	2	2	
71	A2	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



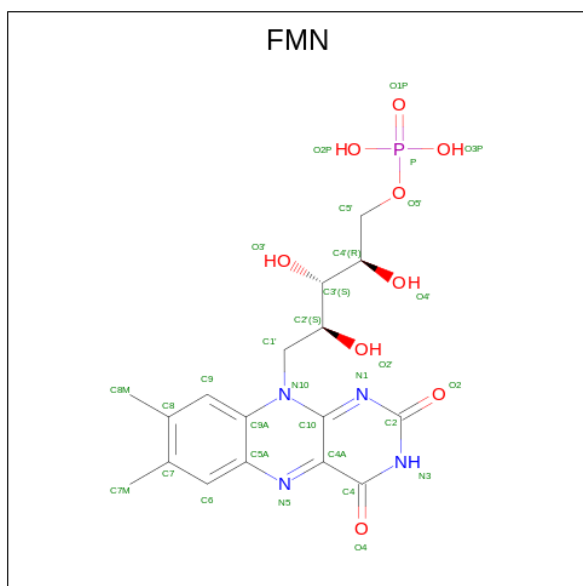
Mol	Chain	Residues	Atoms					AltConf
72	22	1	Total	C	N	O	P	0
			41	31	1	8	1	
72	42	1	Total	C	N	O	P	0
			41	31	1	8	1	
72	B2	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 73 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



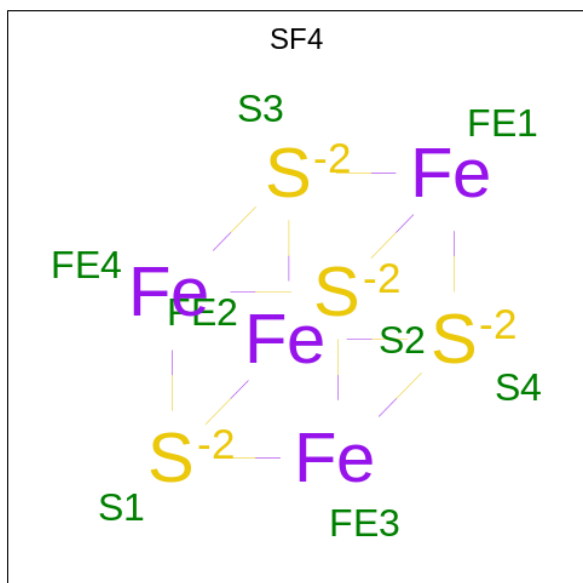
Mol	Chain	Residues	Atoms				AltConf
73	42	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 74 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
74	82	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 75 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

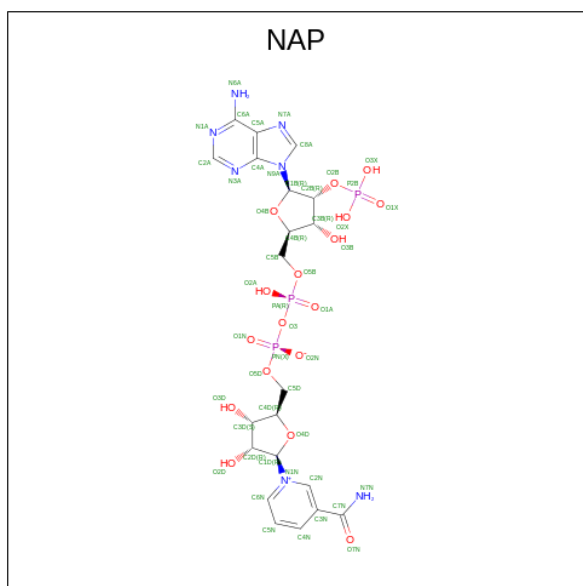


Mol	Chain	Residues	Atoms			AltConf
75	82	1	Total 8	Fe 4	S 4	0
75	A2	1	Total 8	Fe 4	S 4	0
75	A2	1	Total 8	Fe 4	S 4	0
75	D2	1	Total 8	Fe 4	S 4	0
75	E2	1	Total 8	Fe 4	S 4	0
75	E2	1	Total 8	Fe 4	S 4	0

- Molecule 76 is ZINC ION (CCD ID: ZN) (formula: Zn).

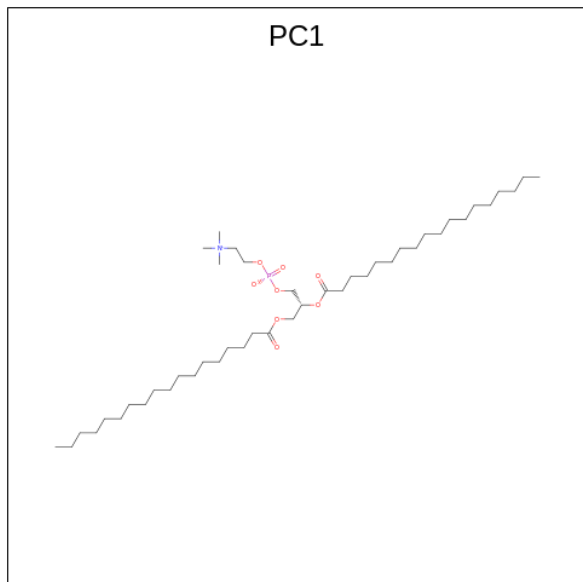
Mol	Chain	Residues	Atoms	AltConf
76	I2	1	Total Zn 1 1	0
76	F3	1	Total Zn 1 1	0

- Molecule 77 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



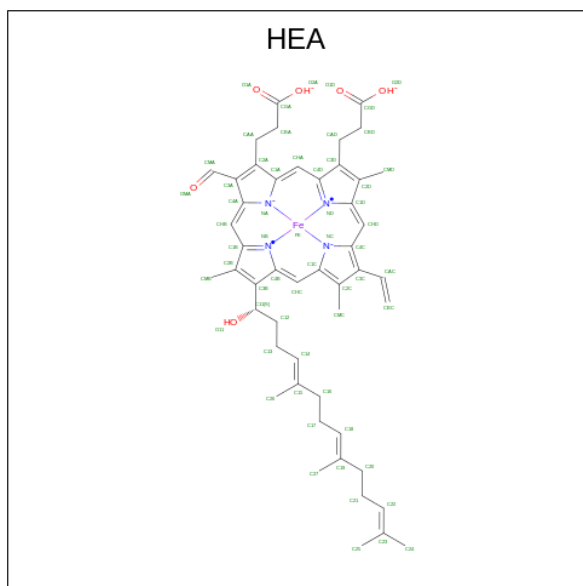
Mol	Chain	Residues	Atoms					AltConf
77	R2	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 78 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
78	S2	1	Total	C	N	O	P	0
			47	37	1	8	1	
78	j2	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
79	A3	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
79	A3	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	A3	1	Total	Cu	0
			1	1	
80	B3	2	Total	Cu	0
			2	2	

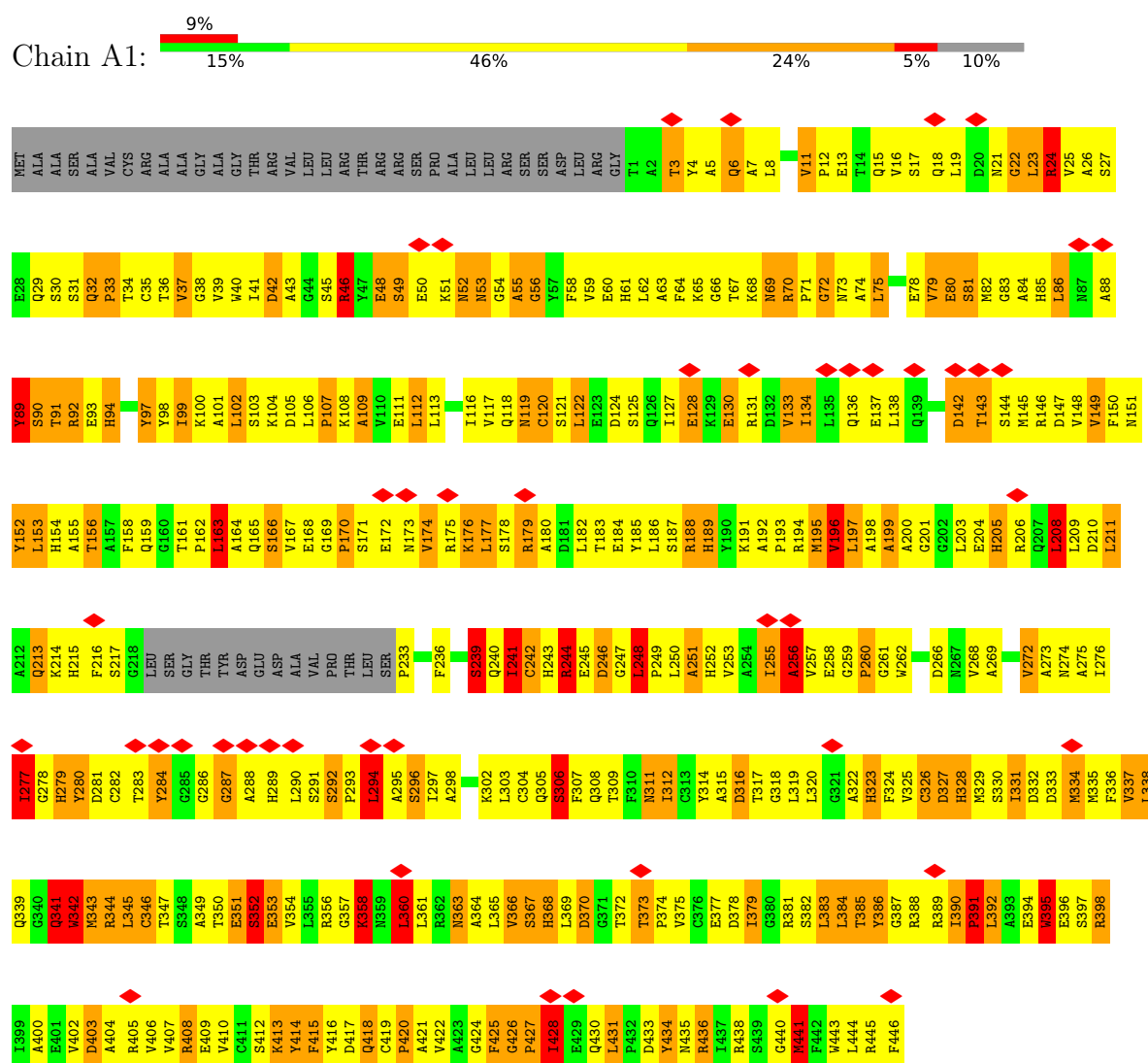
- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	A3	1	Total	Mg	0
			1	1	

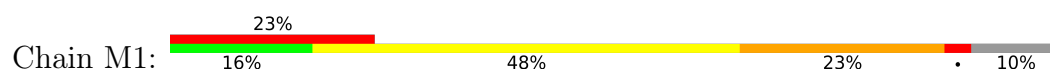
3 Residue-property plots

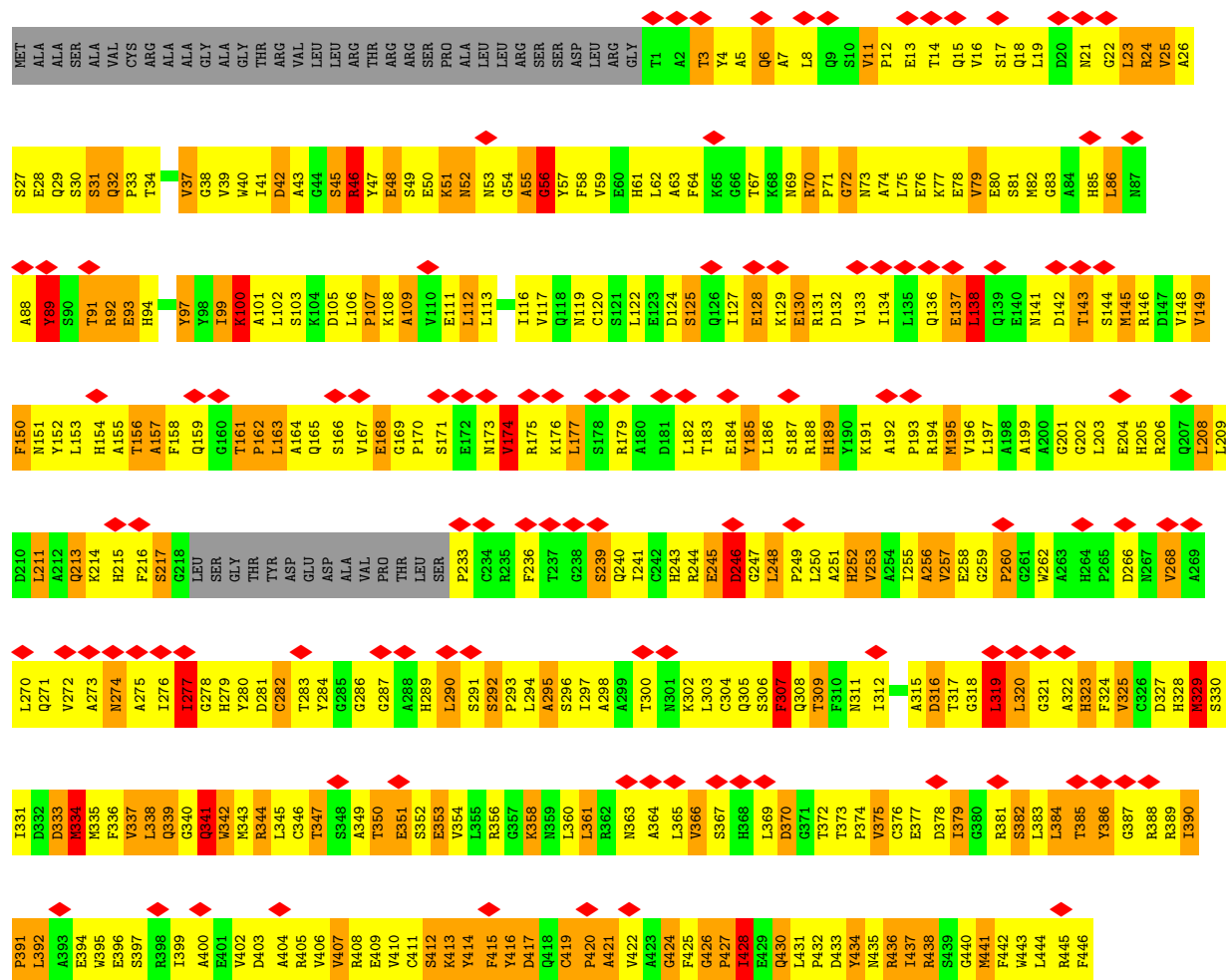
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytochrome b-c1 complex subunit 1, mitochondrial

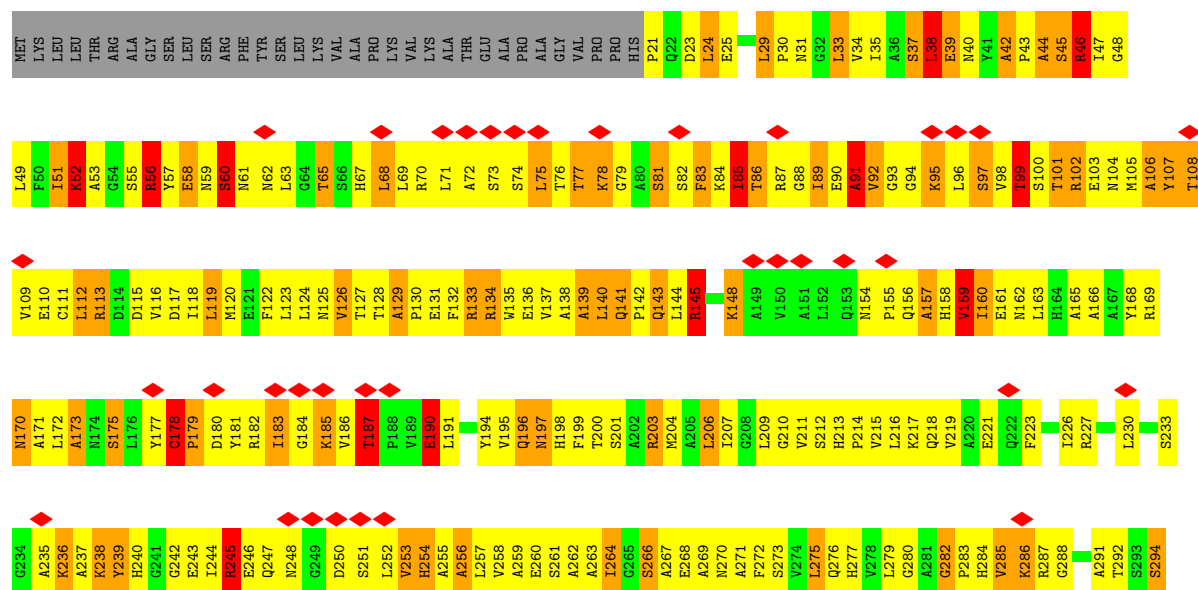
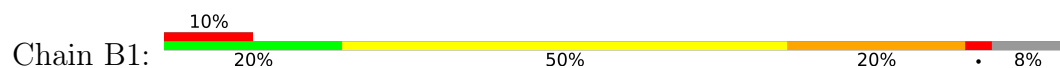


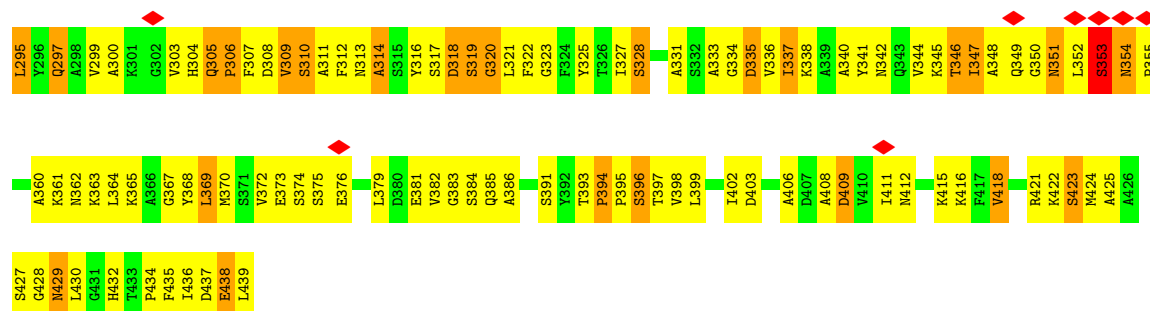
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



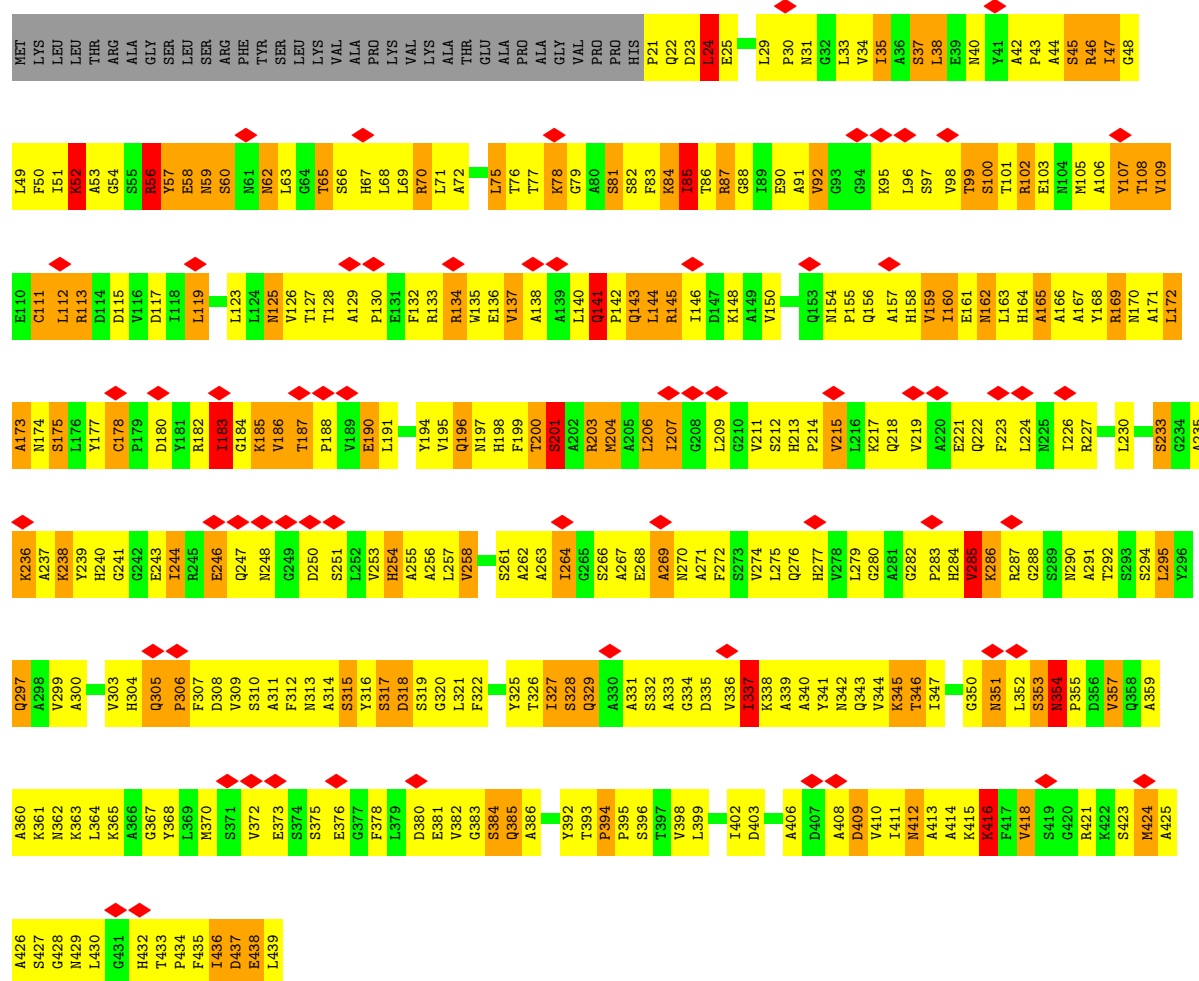
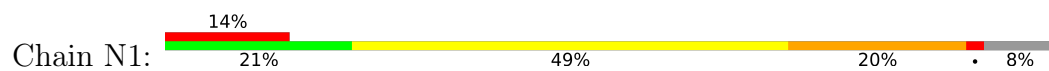


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

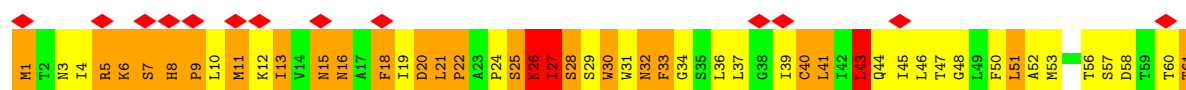
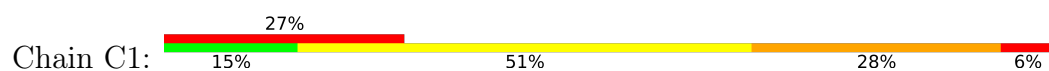


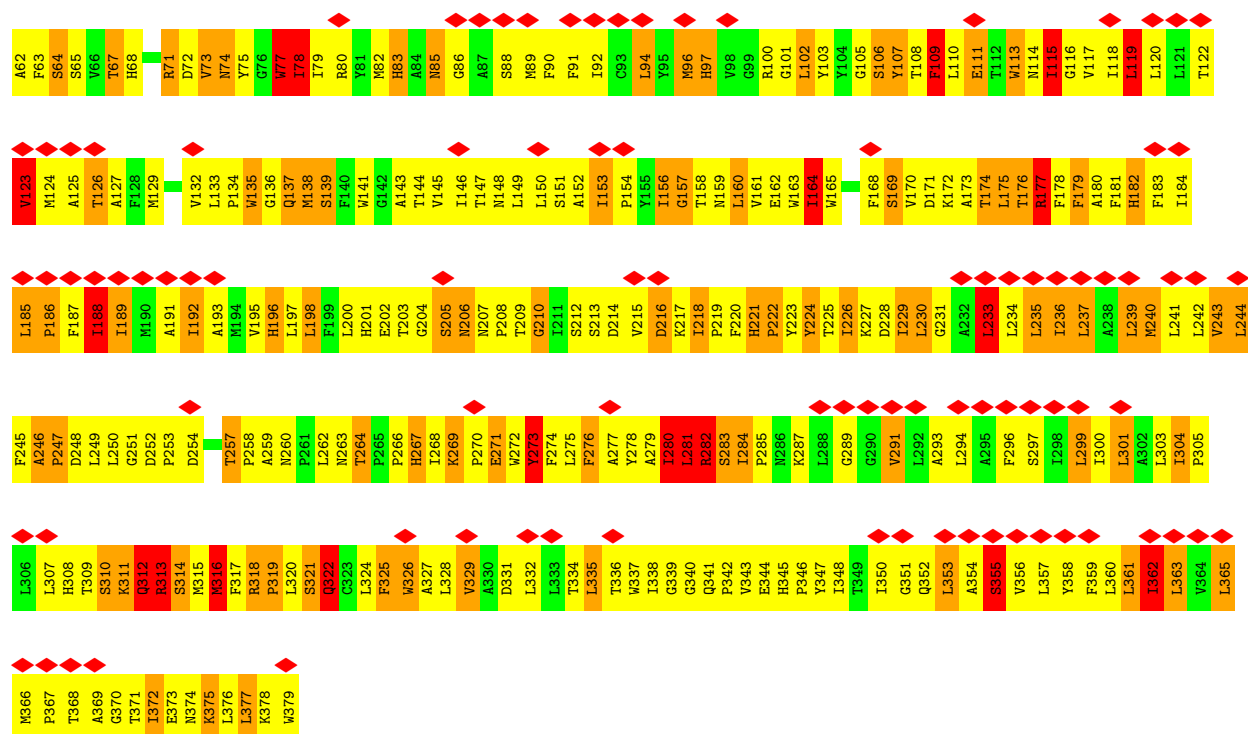


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

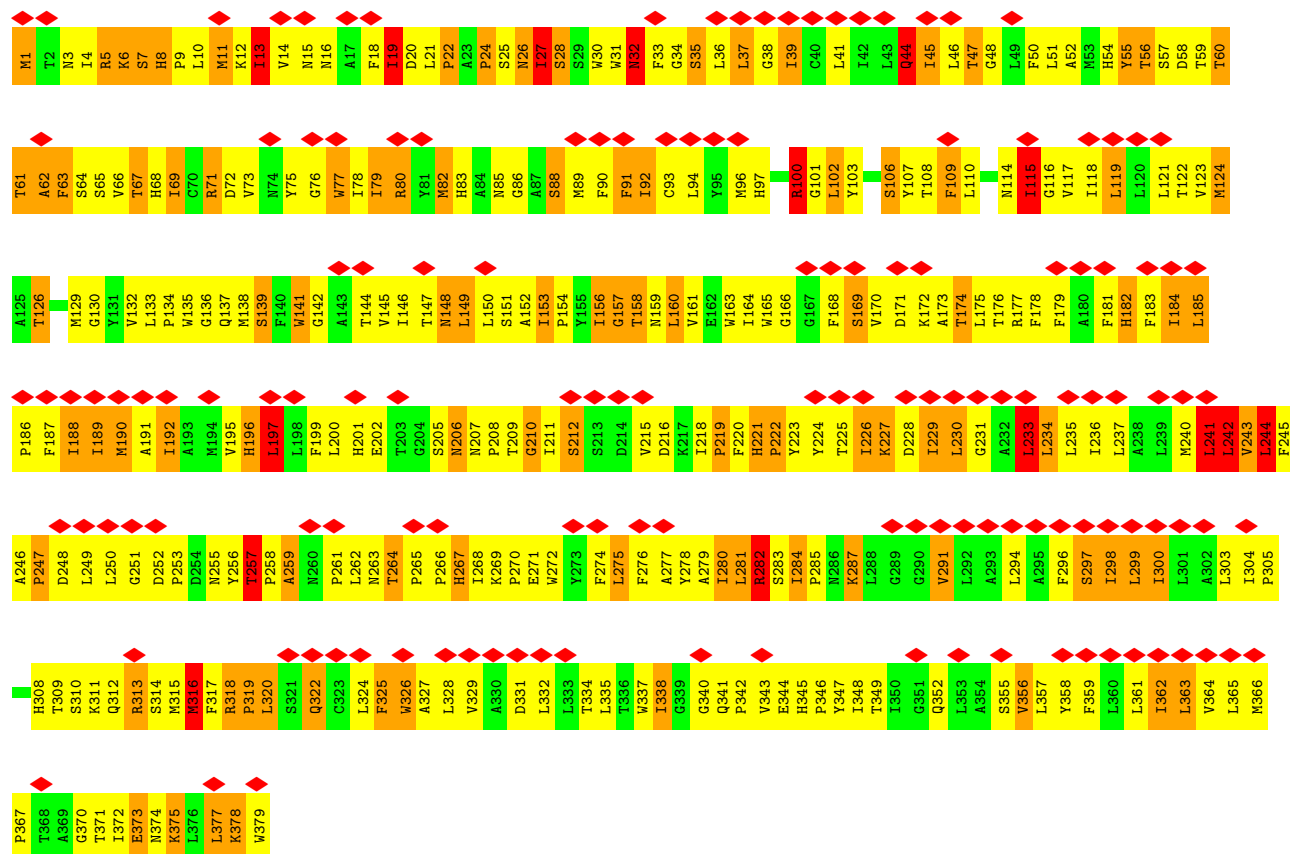
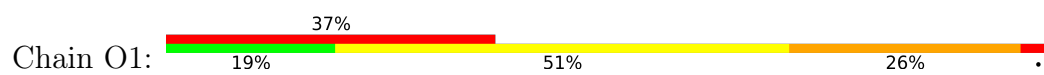


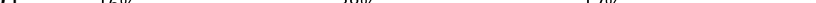
• Molecule 3: Cytochrome b

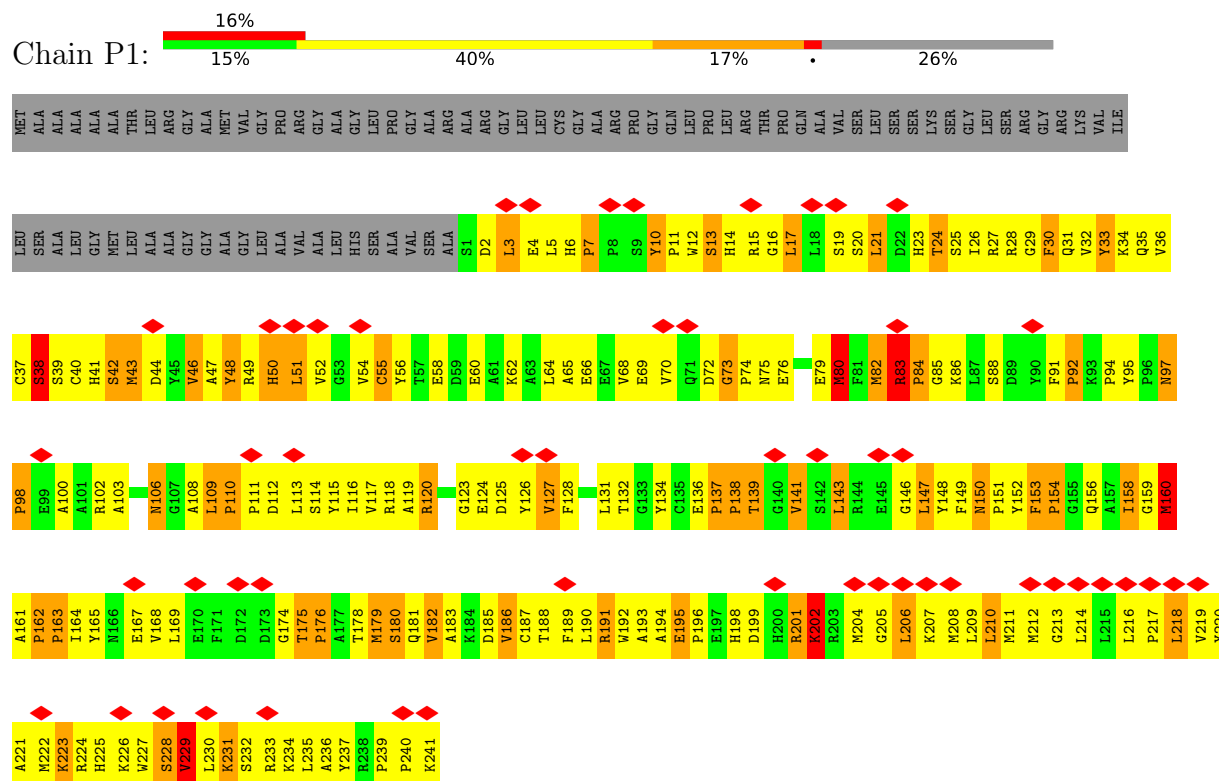
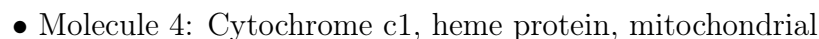




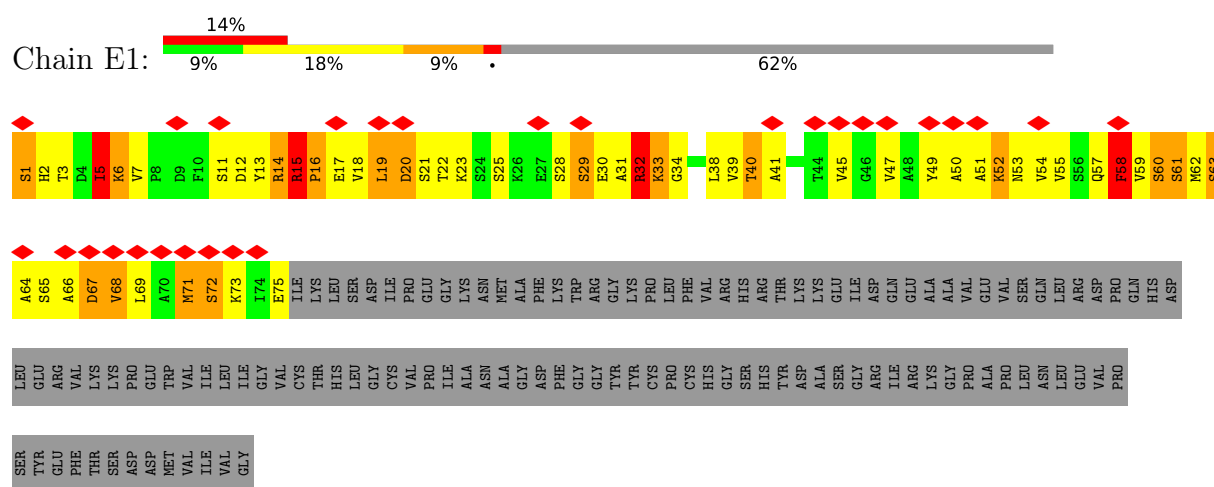
• Molecule 3: Cytochrome b



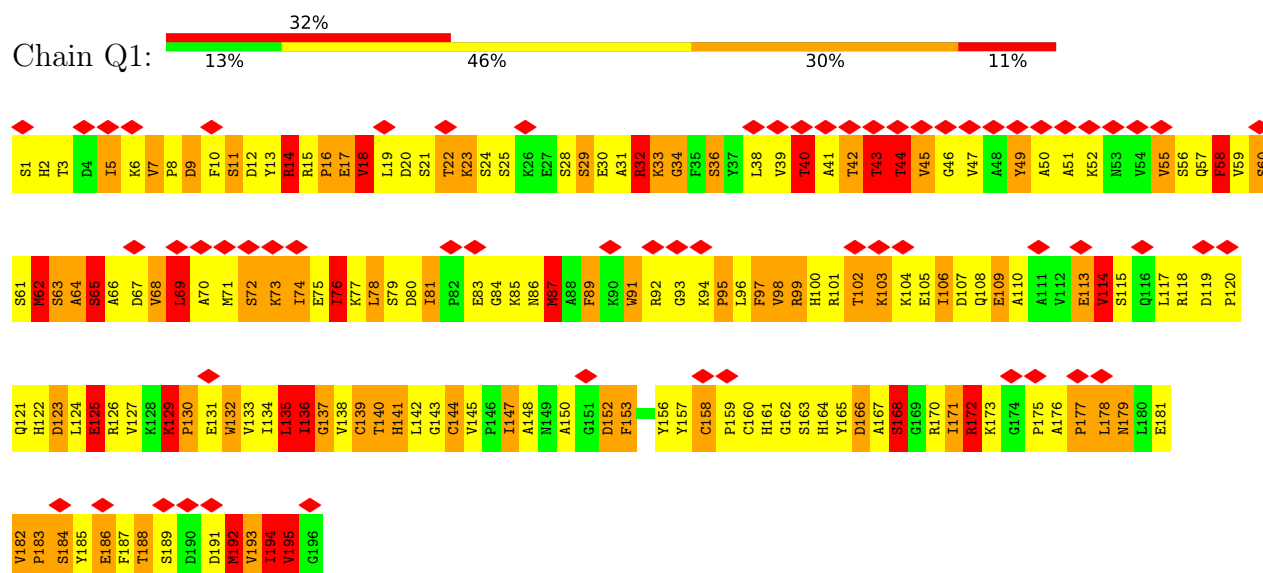
- Chain D1: 



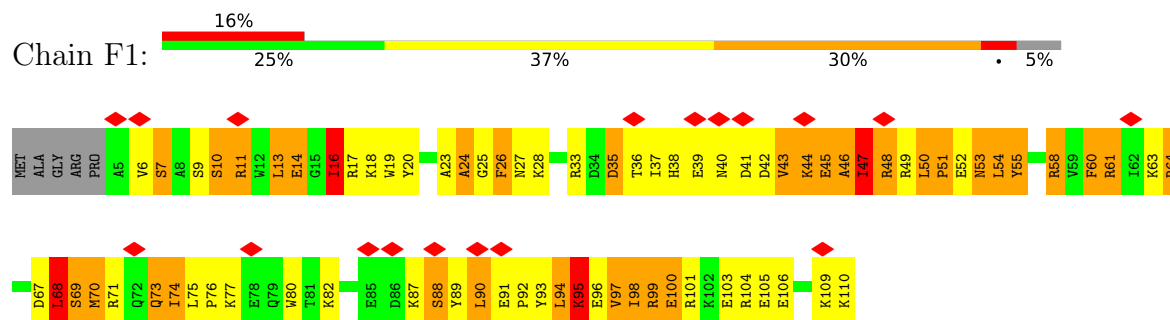
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



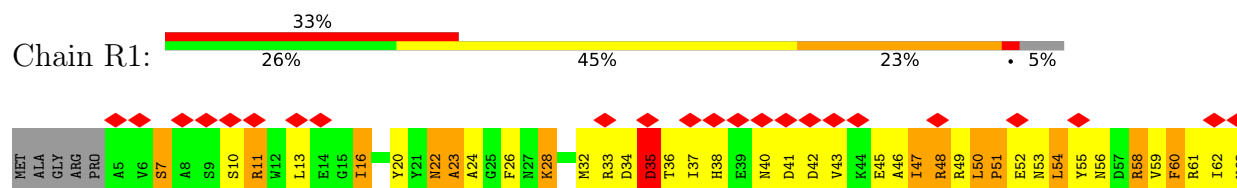
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

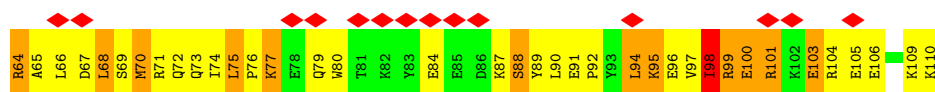


• Molecule 6: Cytochrome b-c1 complex subunit 7

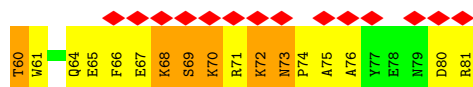
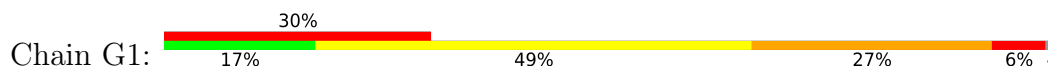


• Molecule 6: Cytochrome b-c1 complex subunit 7

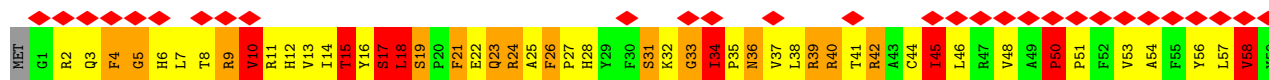
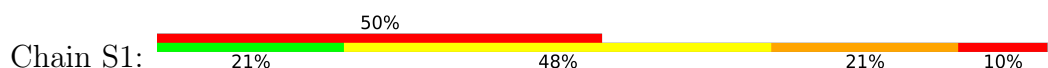




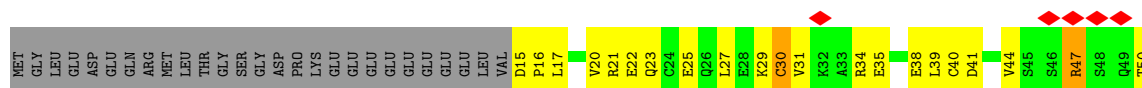
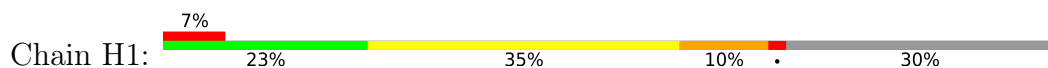
• Molecule 7: Cytochrome b-c1 complex subunit 8



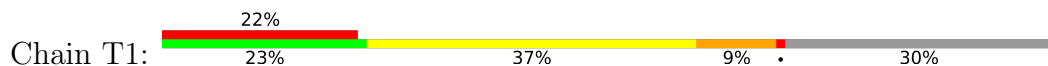
• Molecule 7: Cytochrome b-c1 complex subunit 8



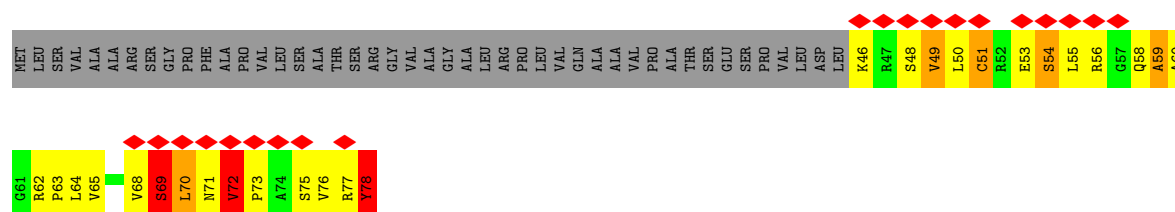
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



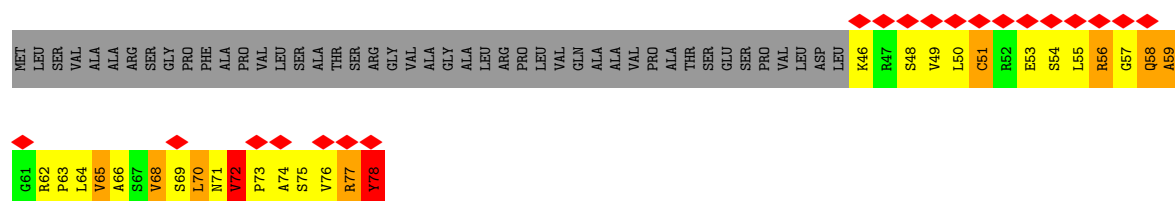
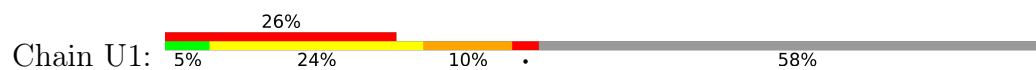
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



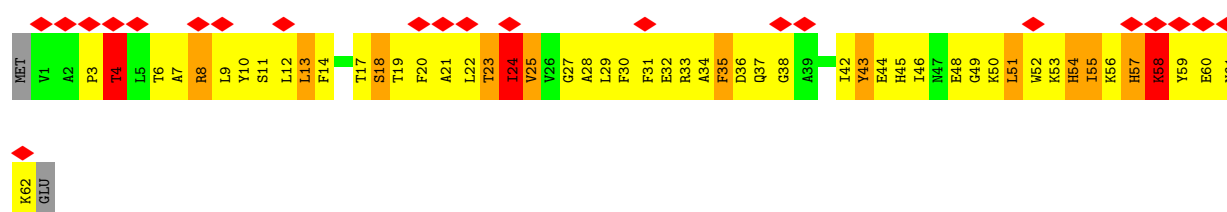
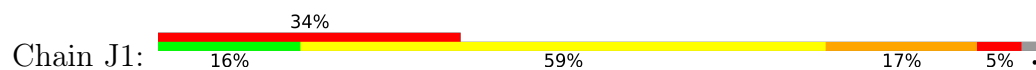
• Molecule 9: Cytochrome b-c1 complex subunit 9



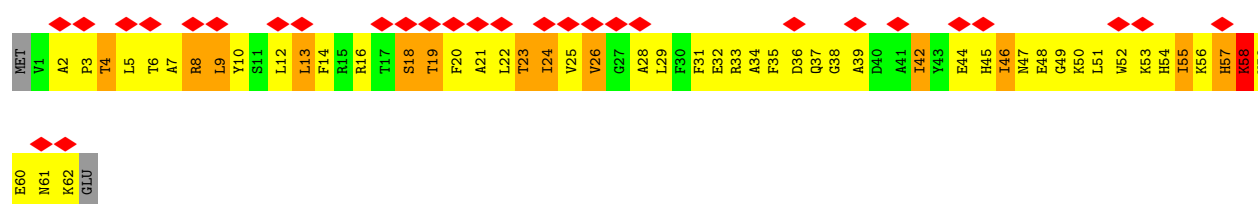
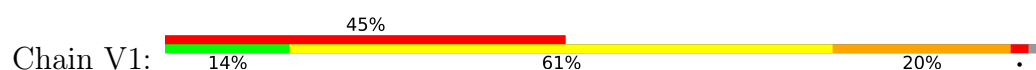
- Molecule 9: Cytochrome b-c1 complex subunit 9



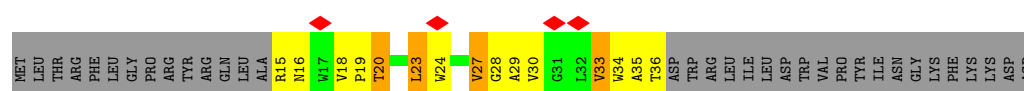
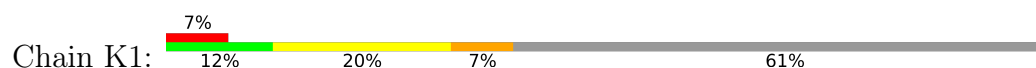
- Molecule 10: Cytochrome b-c1 complex subunit 9



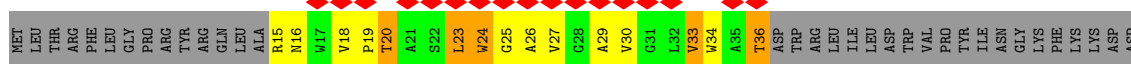
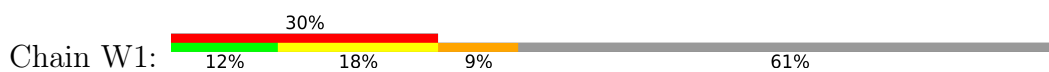
- Molecule 10: Cytochrome b-c1 complex subunit 9



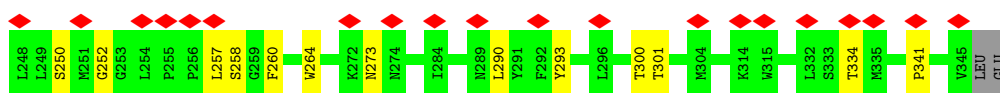
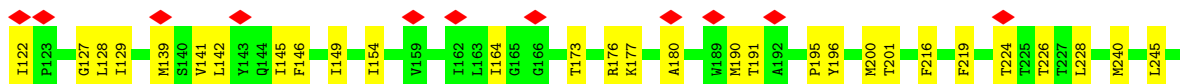
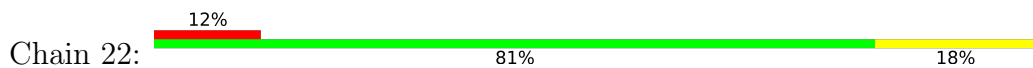
- Molecule 11: Cytochrome b-c1 complex subunit 10



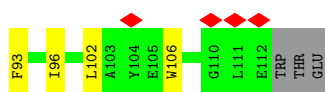
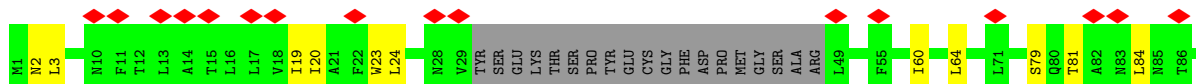
- Molecule 11: Cytochrome b-c1 complex subunit 10



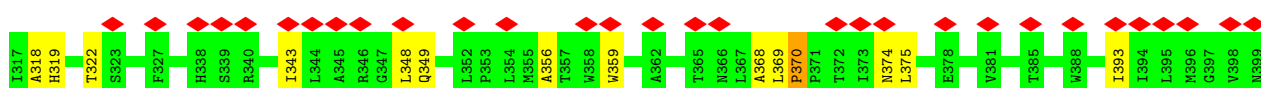
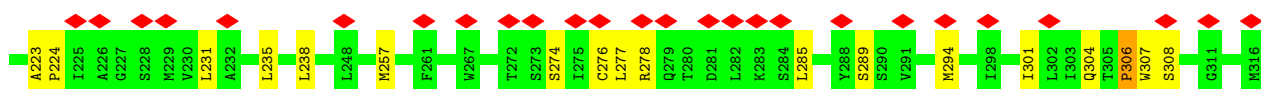
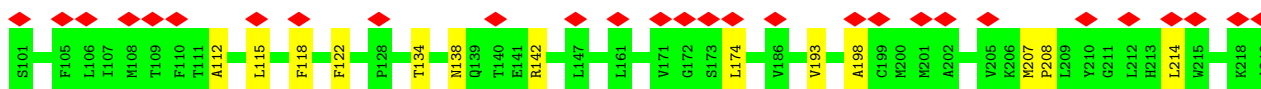
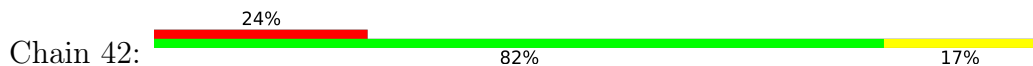
• Molecule 12: NADH-ubiquinone oxidoreductase chain 2

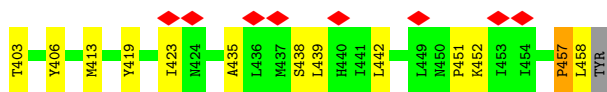


• Molecule 13: NADH-ubiquinone oxidoreductase chain 3

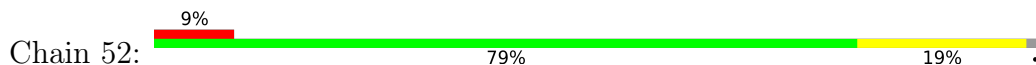


• Molecule 14: NADH-ubiquinone oxidoreductase chain 4

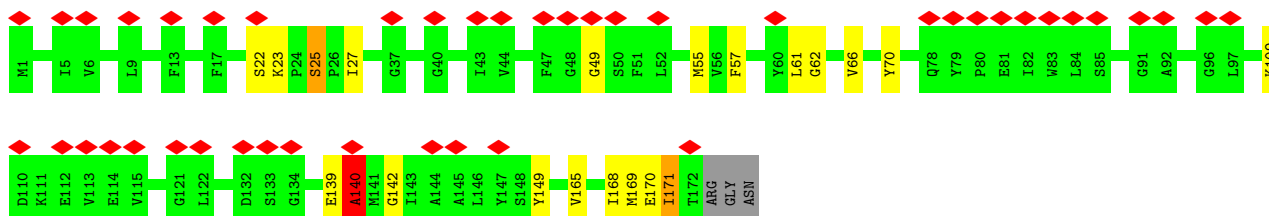
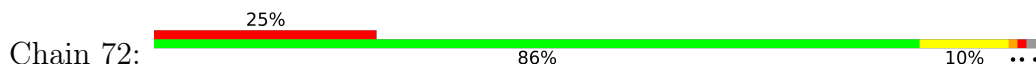




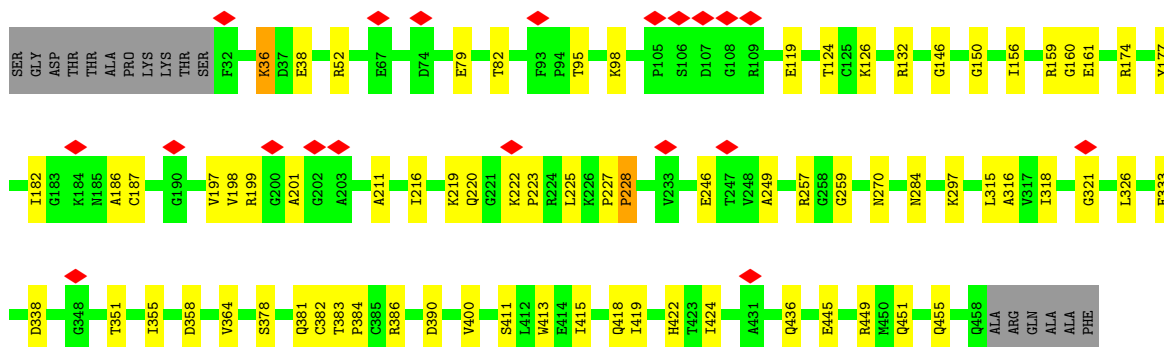
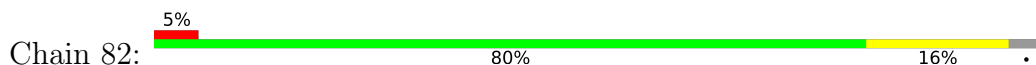
- Molecule 15: NADH-ubiquinone oxidoreductase chain 4L



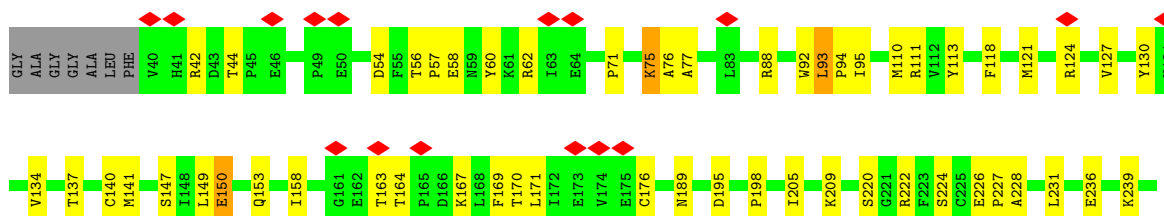
- Molecule 16: NADH-ubiquinone oxidoreductase chain 6

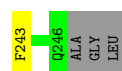


- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

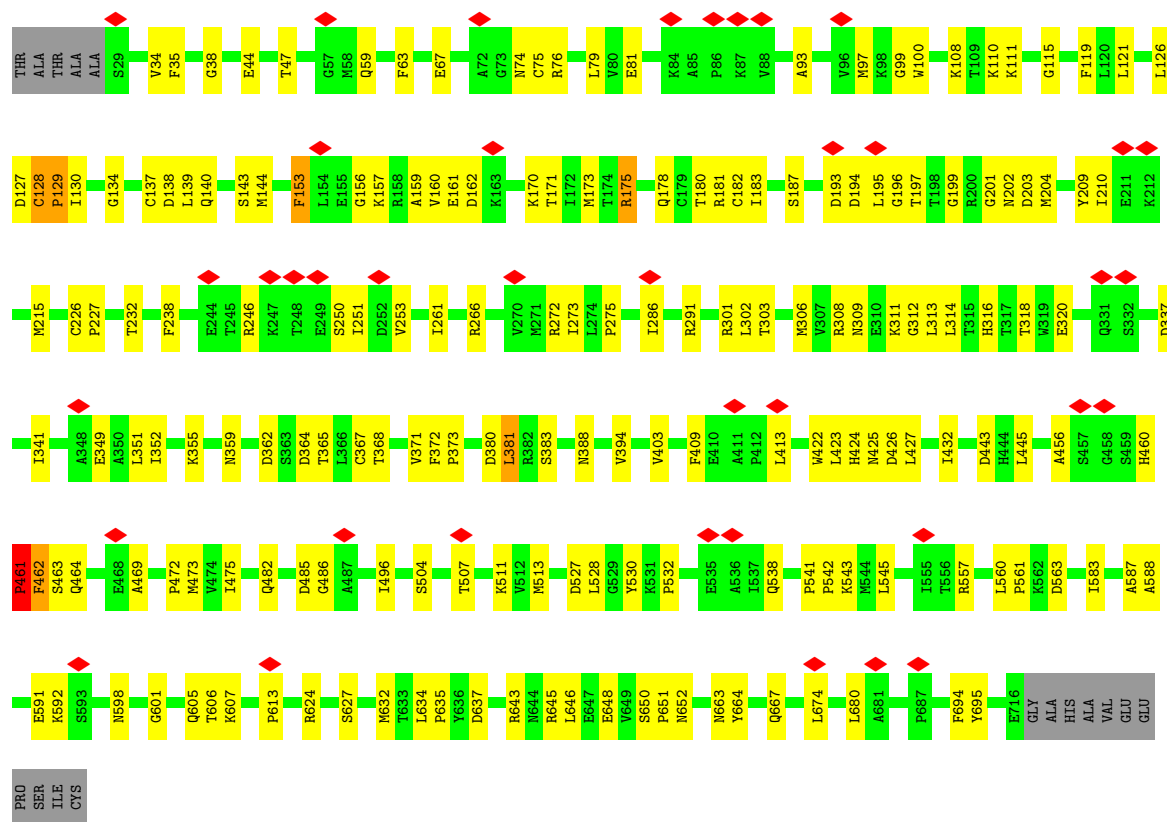
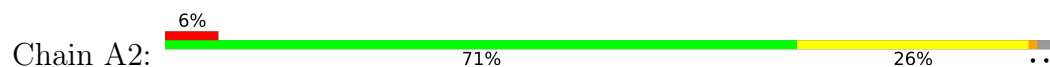


- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

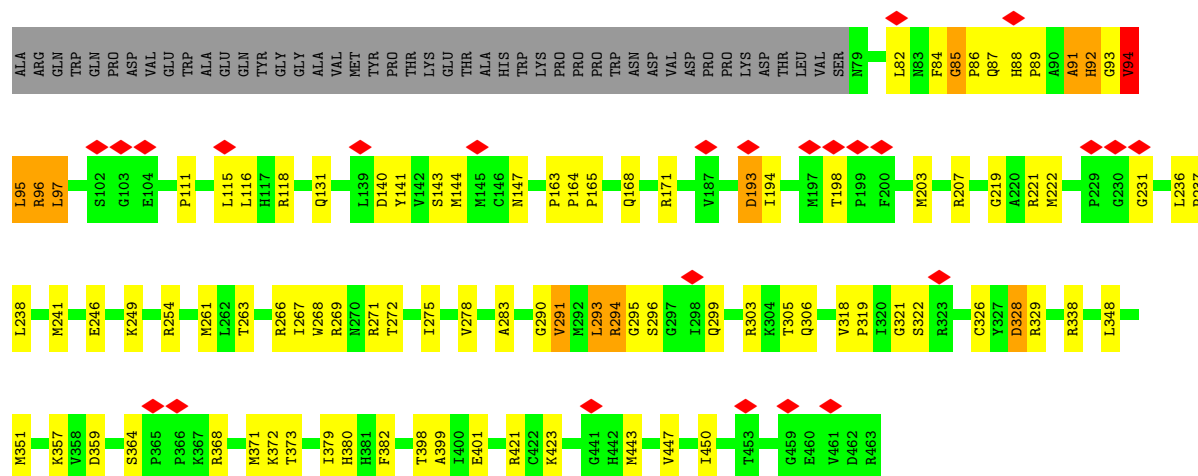




- Molecule 19: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

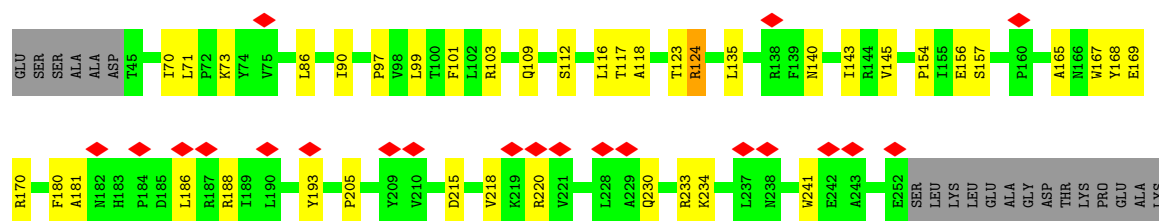


- Molecule 20: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



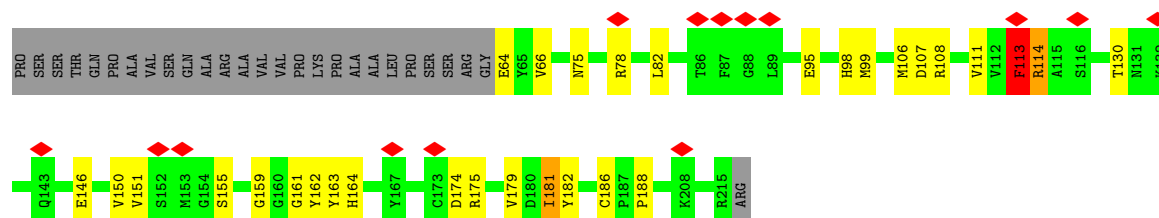
- Molecule 21: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C2: 



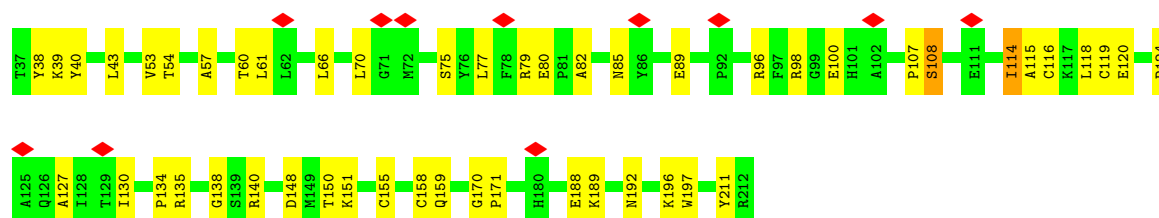
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D2: 



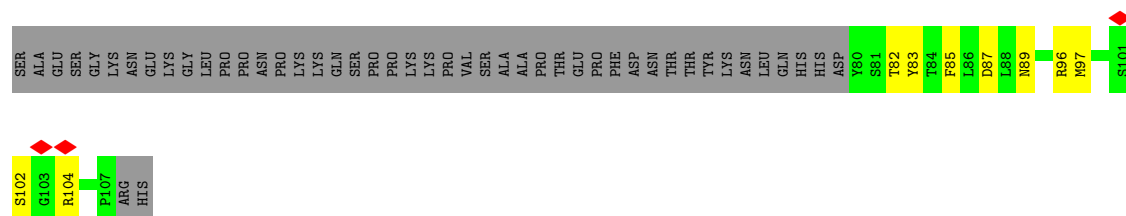
- Molecule 23: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E2: 



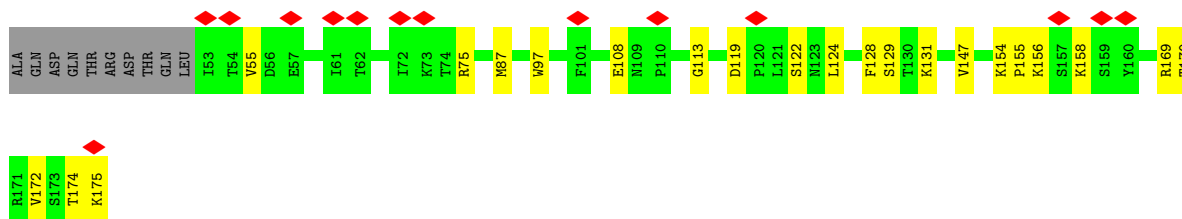
- Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F2: 

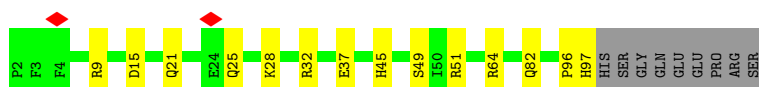
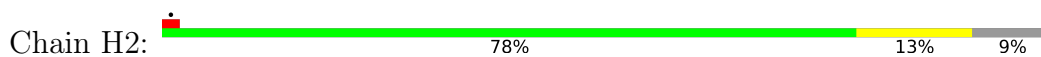


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

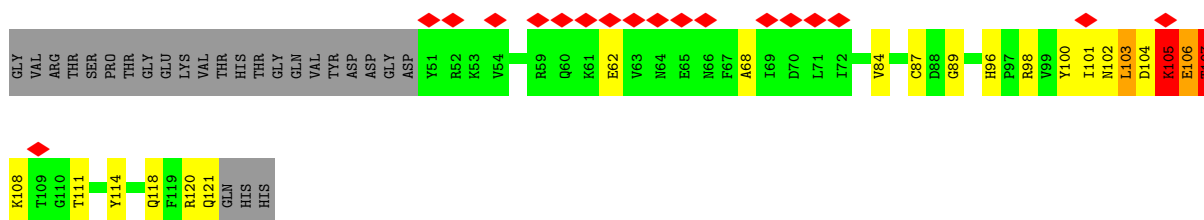
Chain G2: 



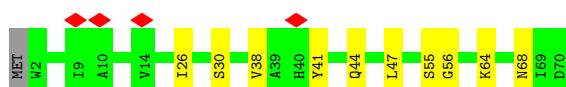
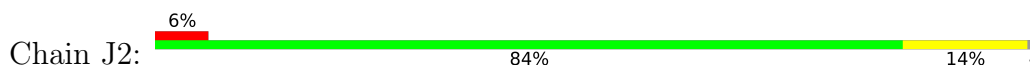
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



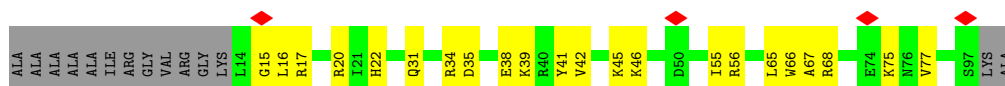
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



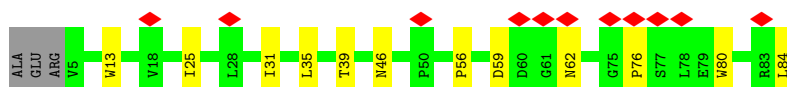
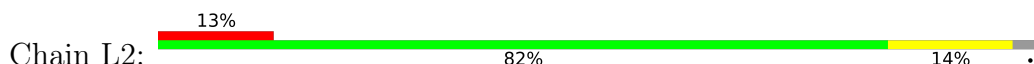
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



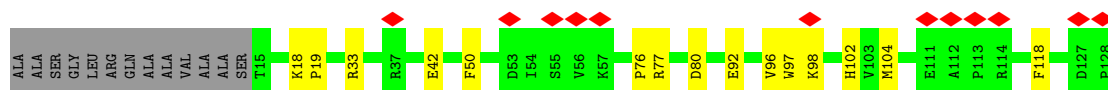
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N2:  83% 14%



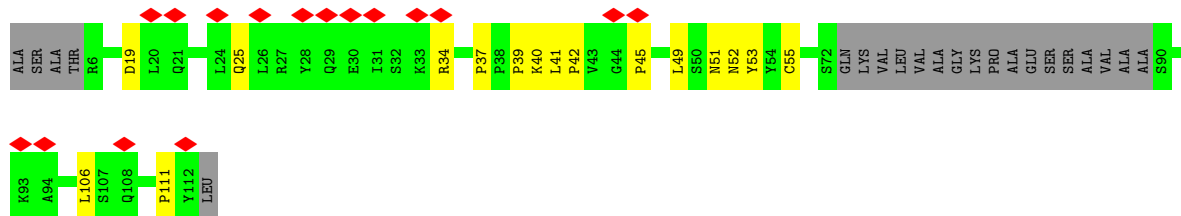
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O2:  9% 78% 12% 10%



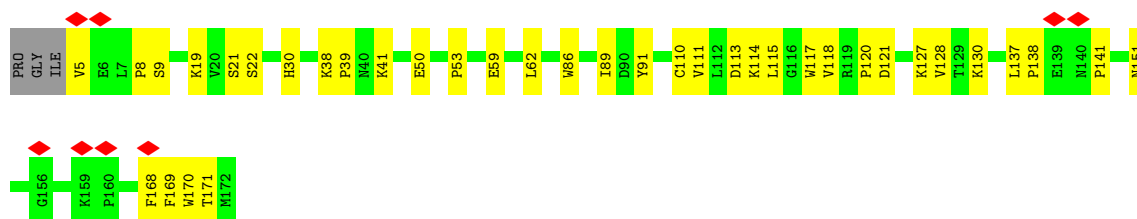
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P2:  14% 66% 14% 20%



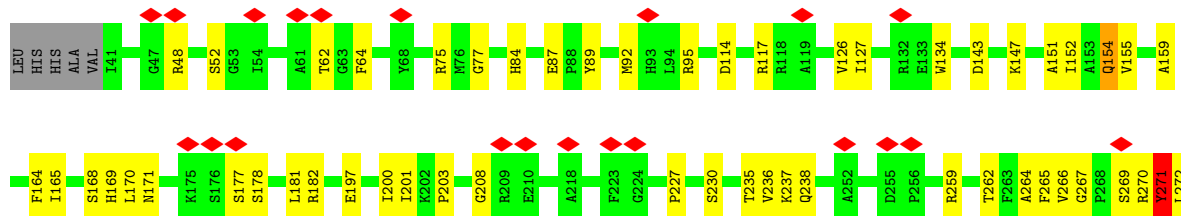
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

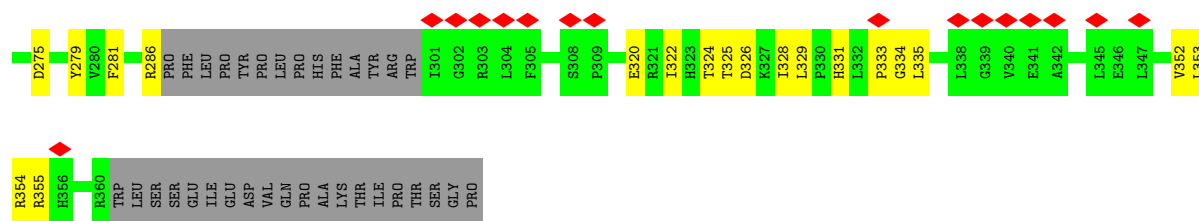
Chain Q2:  5% 77% 22%



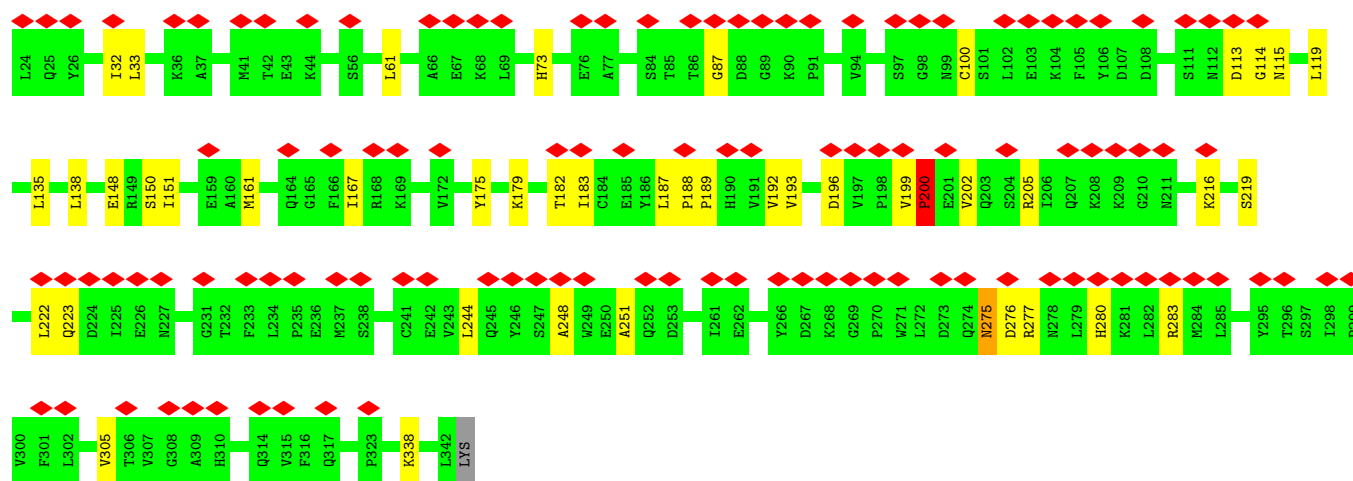
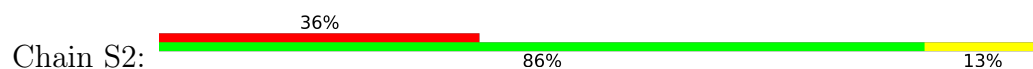
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R2:  11% 68% 21% 11%

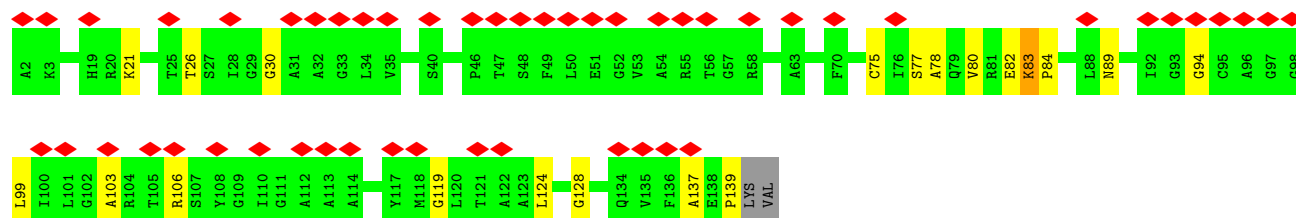
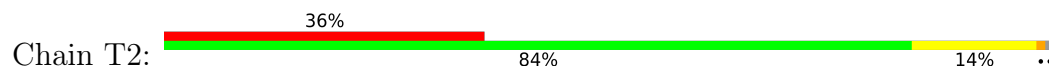




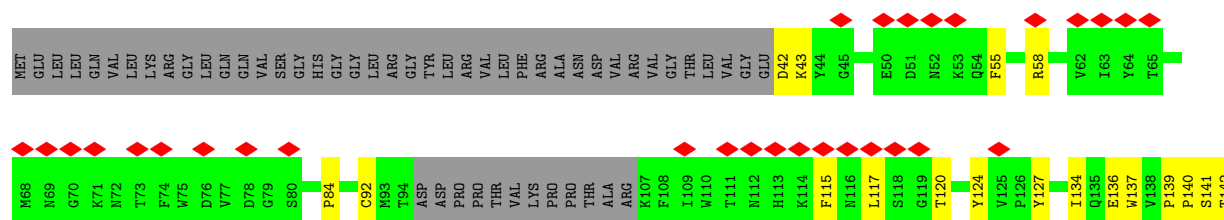
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

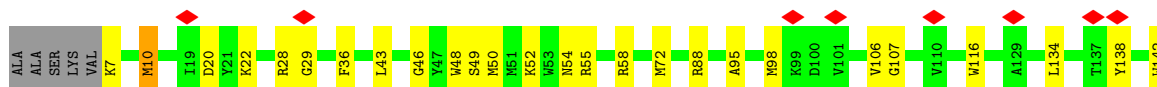
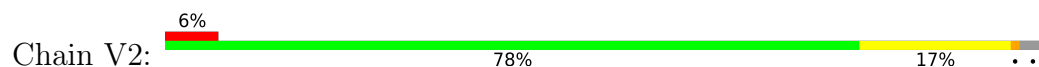


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

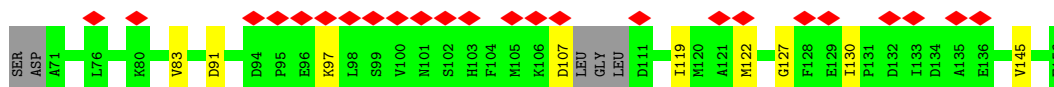
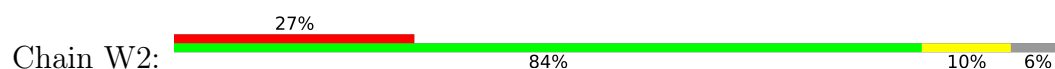




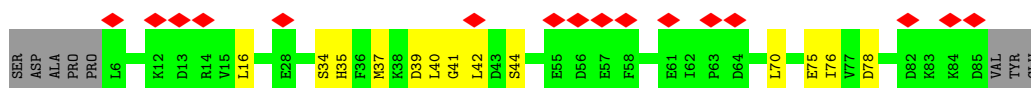
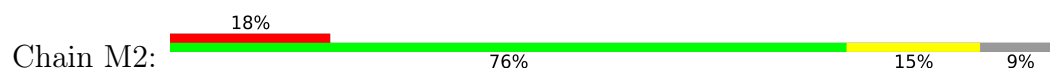
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



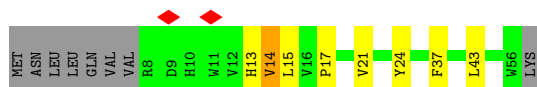
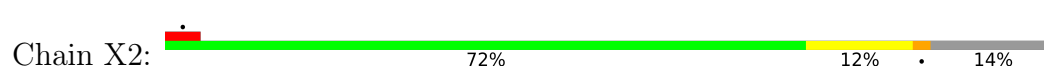
- Molecule 40: Acyl carrier protein, mitochondrial



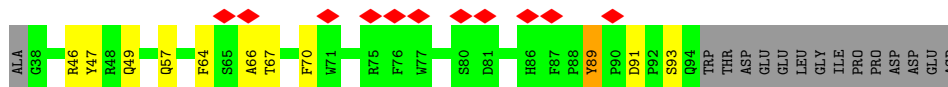
- Molecule 40: Acyl carrier protein, mitochondrial



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

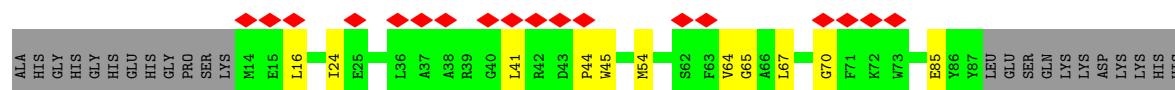


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

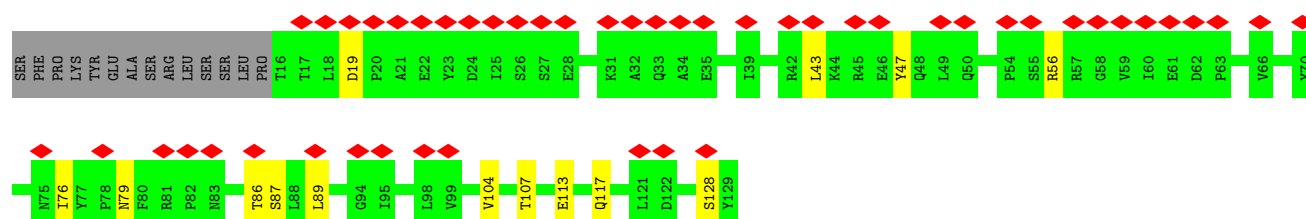
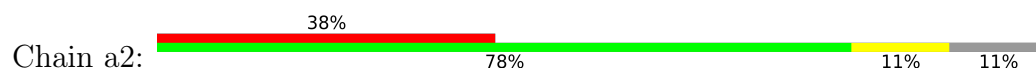


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

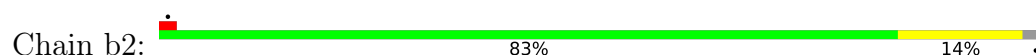




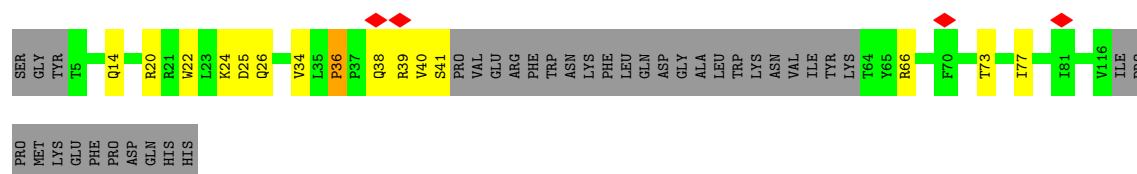
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



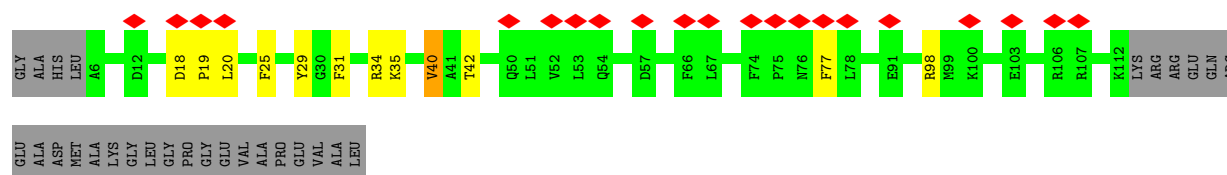
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



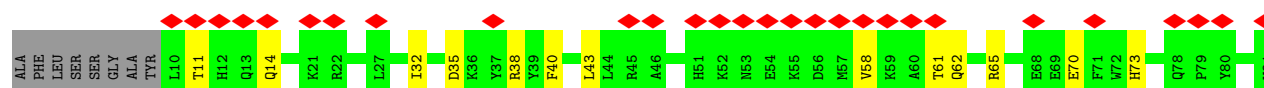
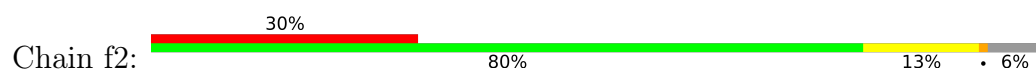
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

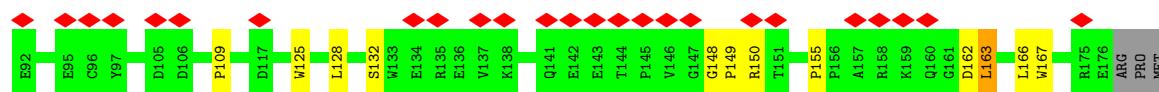


- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

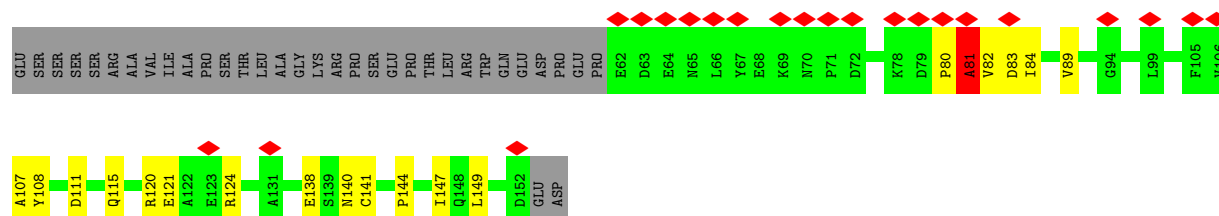


- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

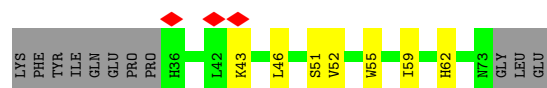




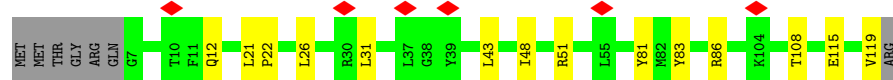
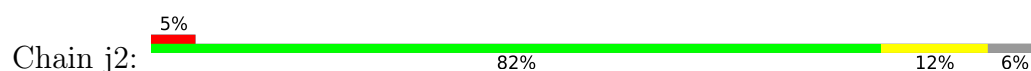
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



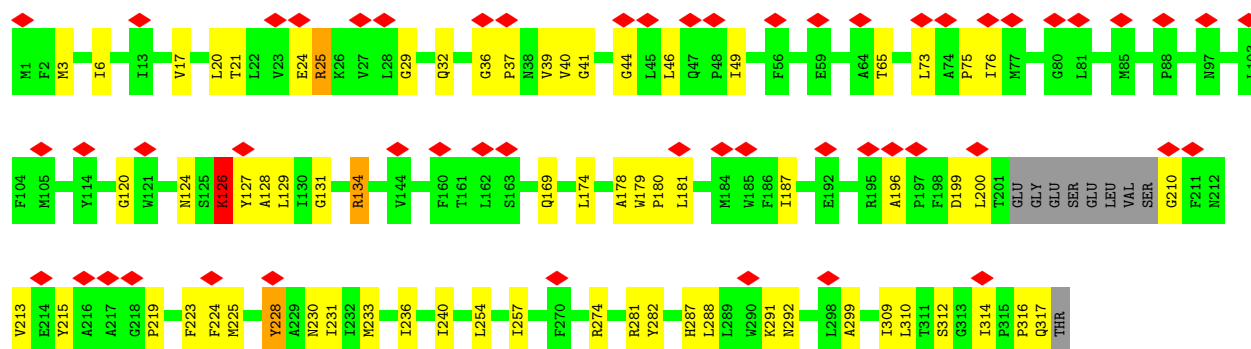
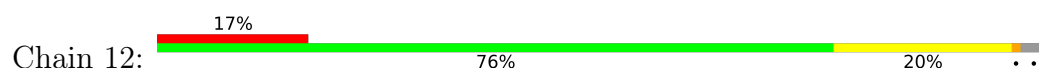
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



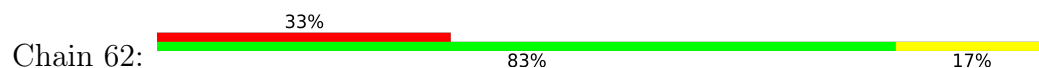
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 subunit C2

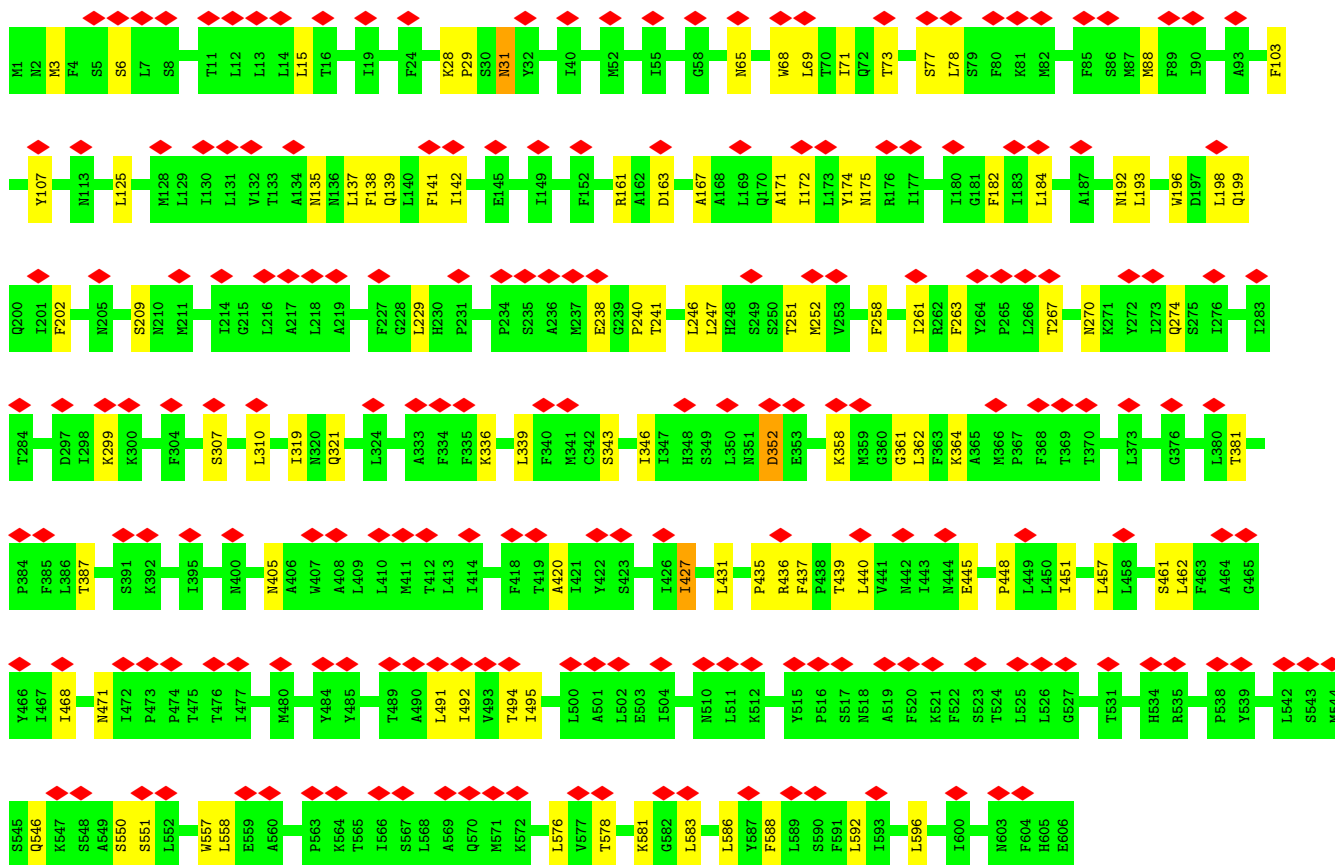


- Molecule 52: NADH-ubiquinone oxidoreductase chain 1

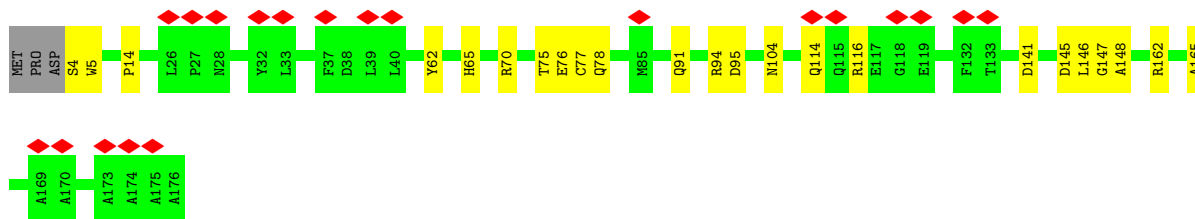
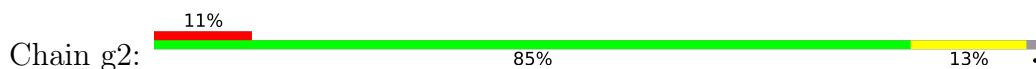


- Molecule 53: NADH-ubiquinone oxidoreductase chain 5

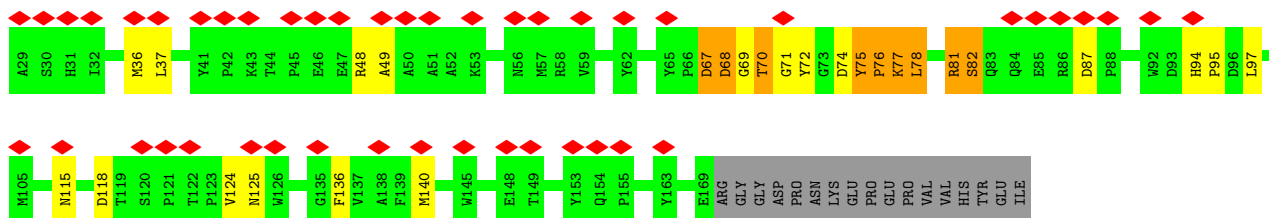
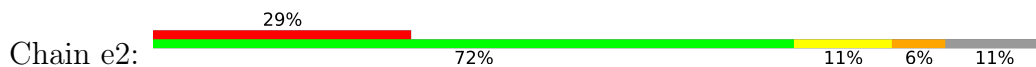




• Molecule 54: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

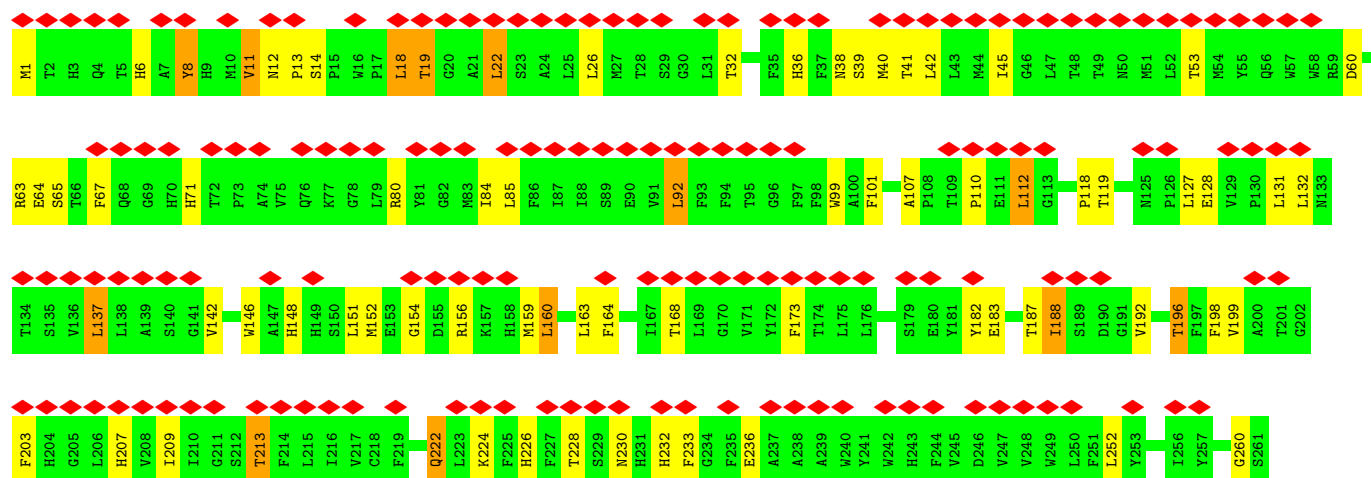


• Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

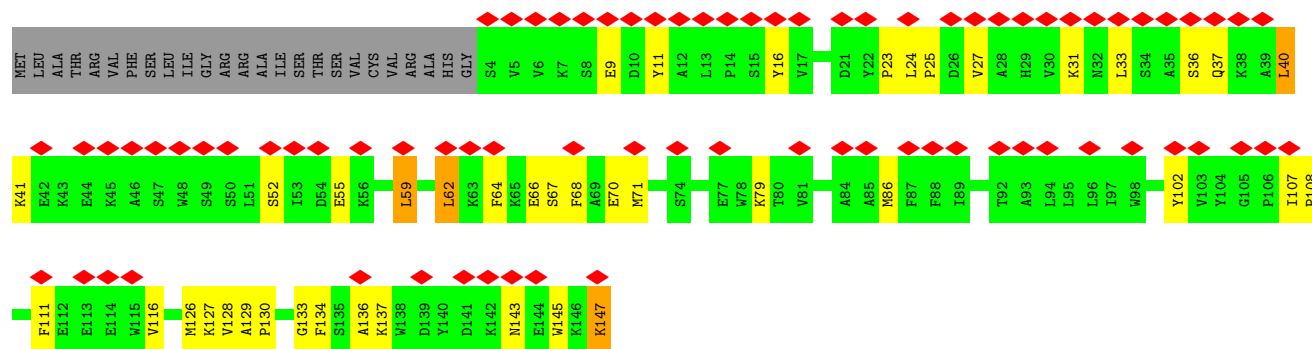


• Molecule 56: Cytochrome c oxidase subunit 1

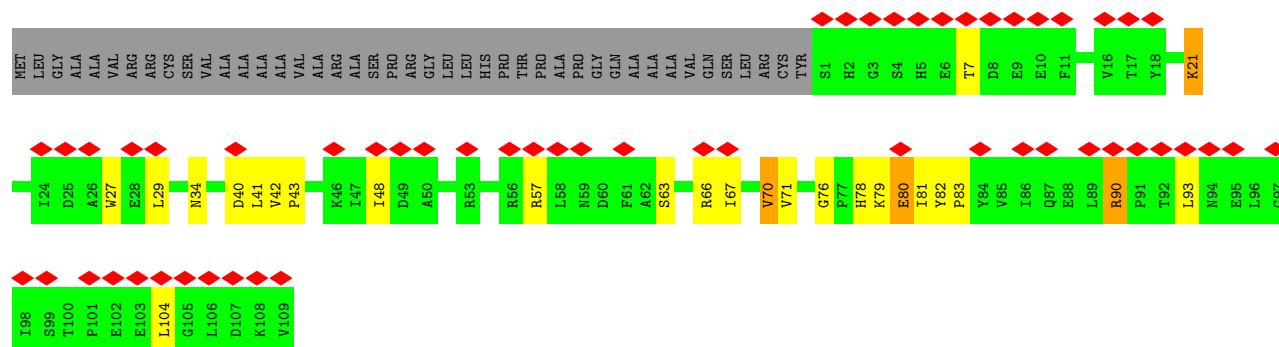




- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

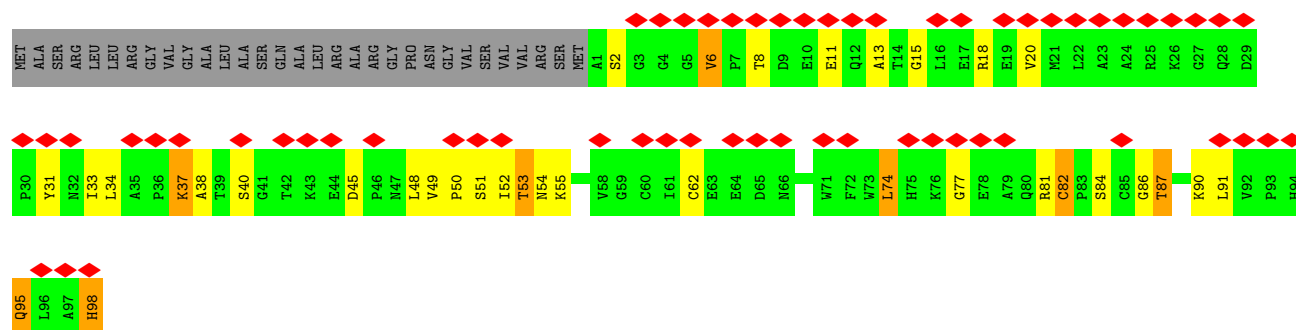


- Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

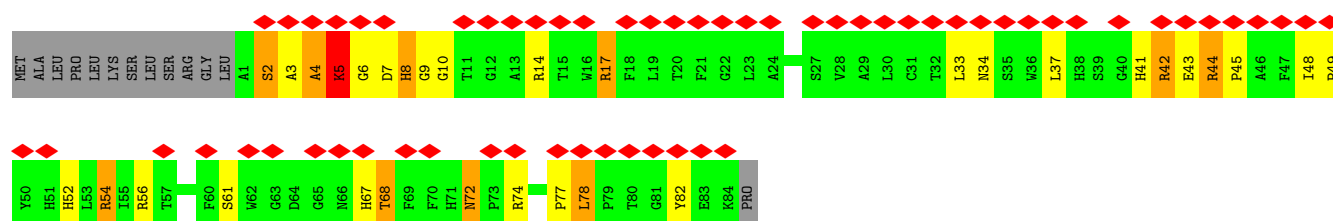


- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial

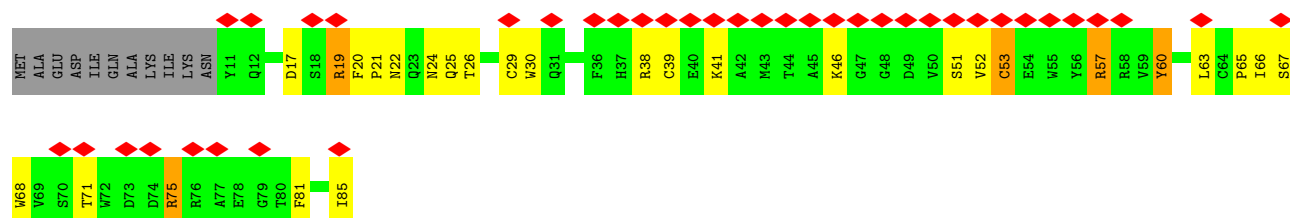




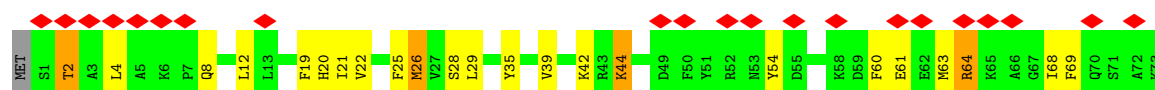
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 63: Cytochrome c oxidase subunit 6B1

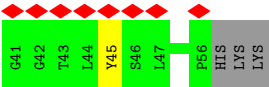


- Molecule 64: Cytochrome c oxidase subunit 6C

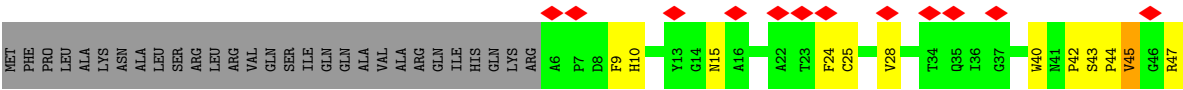


- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial

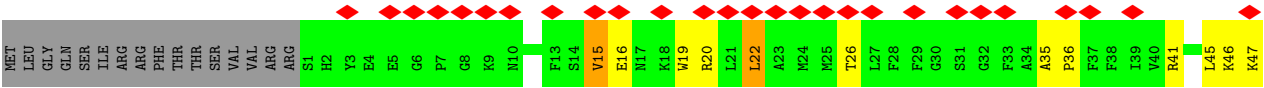




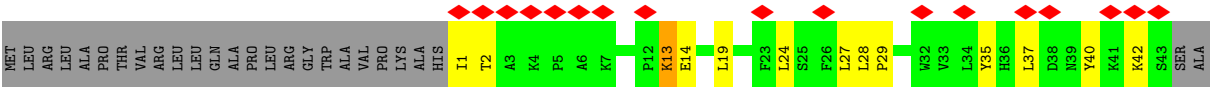
• Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.334	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, FMN, MG, SF4, PC1, FES, CU, HEC, HEA, ZN, NAP, HEM

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	A1	0.78	3/3426 (0.1%)	2.03	135/4644 (2.9%)
1	M1	0.83	4/3426 (0.1%)	2.04	113/4644 (2.4%)
2	B1	0.67	2/3198 (0.1%)	1.89	85/4336 (2.0%)
2	N1	0.65	0/3198	1.81	69/4336 (1.6%)
3	C1	0.92	2/3108 (0.1%)	2.20	137/4252 (3.2%)
3	O1	0.93	6/3108 (0.2%)	2.07	110/4252 (2.6%)
4	D1	0.68	0/1978	1.88	55/2684 (2.0%)
4	P1	0.70	2/1978 (0.1%)	1.83	54/2684 (2.0%)
5	E1	0.76	0/574	2.03	15/775 (1.9%)
5	Q1	0.80	1/1551 (0.1%)	2.16	63/2097 (3.0%)
6	F1	0.74	1/935 (0.1%)	1.83	22/1253 (1.8%)
6	R1	0.73	0/935	1.94	23/1253 (1.8%)
7	G1	0.73	0/704	1.89	25/951 (2.6%)
7	S1	0.74	0/704	1.77	23/951 (2.4%)
8	H1	0.57	0/529	1.61	10/708 (1.4%)
8	T1	0.50	0/529	1.51	4/708 (0.6%)
9	I1	0.61	0/250	1.87	5/335 (1.5%)
9	U1	0.63	0/250	1.85	7/335 (2.1%)
10	J1	0.61	0/524	1.61	8/707 (1.1%)
10	V1	0.63	0/524	1.71	7/707 (1.0%)
11	K1	0.53	0/170	1.37	1/236 (0.4%)
11	W1	0.58	0/170	1.48	1/236 (0.4%)
12	22	0.35	0/2646	0.77	8/3618 (0.2%)
13	32	0.33	0/736	0.91	3/1011 (0.3%)
14	42	0.31	0/3538	0.75	4/4845 (0.1%)
15	52	0.33	0/706	0.75	0/960
16	72	0.29	0/1213	0.75	5/1659 (0.3%)
17	82	0.28	0/3035	0.73	6/4130 (0.1%)
18	92	0.27	0/1572	0.69	0/2150
19	A2	0.33	0/5269	0.71	10/7152 (0.1%)
20	B2	0.40	0/3150	0.77	3/4260 (0.1%)
21	C2	0.33	0/1756	0.69	2/2394 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	D2	0.37	0/1231	0.67	0/1669
23	E2	0.37	0/1418	0.76	3/1922 (0.2%)
24	F2	0.36	0/188	1.31	5/259 (1.9%)
25	G2	0.33	0/1004	0.78	4/1359 (0.3%)
26	H2	0.30	0/800	0.69	0/1076
27	I2	0.27	0/540	0.84	2/725 (0.3%)
28	J2	0.25	0/545	0.54	0/740
29	K2	0.27	0/663	0.67	0/896
30	L2	0.30	0/623	0.80	4/862 (0.5%)
31	N2	0.27	0/882	0.71	0/1203
32	O2	0.26	0/948	0.66	4/1279 (0.3%)
33	P2	0.29	0/719	0.79	1/981 (0.1%)
34	Q2	0.28	0/1381	0.78	2/1869 (0.1%)
35	R2	0.28	0/2392	0.78	5/3248 (0.2%)
36	S2	0.28	0/2348	0.78	6/3198 (0.2%)
37	T2	0.26	0/959	0.70	1/1305 (0.1%)
38	U2	0.29	0/765	0.82	3/1050 (0.3%)
39	V2	0.29	0/1121	0.66	0/1515
40	M2	0.24	0/651	0.79	0/876
40	W2	0.24	0/603	0.73	0/817
41	X2	0.27	0/383	0.86	2/523 (0.4%)
42	Y2	0.27	0/428	0.64	0/592
43	Z2	0.30	0/506	0.90	4/688 (0.6%)
44	a2	0.25	0/878	0.72	4/1195 (0.3%)
45	b2	0.29	0/1058	0.71	0/1434
46	c2	0.32	0/632	0.94	5/871 (0.6%)
47	d2	0.33	0/724	0.69	2/989 (0.2%)
48	f2	0.24	0/1191	0.71	2/1639 (0.1%)
49	h2	0.29	0/743	0.78	0/1013
50	i2	0.20	0/286	0.44	0/392
51	j2	0.28	0/922	0.78	5/1254 (0.4%)
52	l2	0.35	0/2513	0.78	1/3432 (0.0%)
53	62	0.25	0/4892	0.65	2/6660 (0.0%)
54	g2	0.25	0/1380	0.65	0/1872
55	e2	0.40	0/888	1.05	6/1234 (0.5%)
56	A3	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
57	B3	0.77	0/1868	1.12	10/2544 (0.4%)
58	C3	0.74	0/2211	1.01	7/3023 (0.2%)
59	D3	0.67	0/1229	0.96	3/1658 (0.2%)
60	E3	0.64	0/898	1.03	6/1218 (0.5%)
61	F3	0.72	0/765	1.13	4/1038 (0.4%)
62	G3	0.69	0/698	1.09	6/950 (0.6%)
63	H3	0.68	0/648	1.18	5/877 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
64	I3	0.71	0/611	0.94	2/810 (0.2%)
65	J3	0.70	0/451	1.04	3/610 (0.5%)
66	K3	0.75	0/398	1.01	0/546
67	L3	0.77	0/399	0.98	2/534 (0.4%)
68	M3	0.69	0/345	0.98	1/470 (0.2%)
All	All	0.55	28/107280 (0.0%)	1.27	1171/145866 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	13
1	M1	0	3
2	B1	0	9
2	N1	0	6
3	C1	0	14
3	O1	0	6
4	D1	0	5
4	P1	0	4
5	E1	0	1
5	Q1	0	9
6	F1	0	2
7	G1	0	2
7	S1	0	3
8	T1	0	1
9	I1	0	1
9	U1	0	1
10	J1	0	1
11	W1	0	1
12	22	0	2
14	42	0	3
15	52	0	1
16	72	0	3
17	82	0	1
18	92	0	3
19	A2	0	6
20	B2	0	3
22	D2	0	4
23	E2	0	2
33	P2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	Q2	0	2
35	R2	0	2
36	S2	0	1
37	T2	0	1
39	V2	0	3
40	M2	0	1
42	Y2	0	1
45	b2	0	1
48	f2	0	1
49	h2	0	2
52	l2	0	1
53	62	0	2
55	e2	0	4
All	All	0	133

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M1	253	VAL	C-O	11.17	1.36	1.24
3	O1	37	LEU	C-N	-8.10	1.24	1.33
56	A3	61	HIS	CG-CD2	7.61	1.44	1.35
56	A3	378	HIS	ND1-CE1	7.16	1.39	1.32
3	O1	221	HIS	CD2-NE2	-7.09	1.30	1.37

The worst 5 of 1171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	253	VAL	O-C-N	-23.38	98.86	123.18
1	M1	253	VAL	CA-C-O	16.98	137.42	120.27
3	C1	196	HIS	CA-CB-CG	16.18	129.98	113.80
3	O1	196	HIS	CA-CB-CG	15.64	129.44	113.80
3	O1	44	GLN	CA-C-N	15.24	139.75	120.70

There are no chirality outliers.

5 of 133 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	118	GLN	Mainchain
1	A1	122	LEU	Mainchain
1	A1	196	VAL	Mainchain
1	A1	210	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A1	53	ASN	Mainchain

5.2 Too-close contacts

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	A1	3356	0	3263	486	0
1	M1	3356	0	3263	470	0
2	B1	3141	0	3123	417	0
2	N1	3141	0	3123	423	0
3	C1	3011	0	3077	463	0
3	O1	3011	0	3077	430	0
4	D1	1919	0	1868	309	0
4	P1	1919	0	1868	295	0
5	E1	566	0	564	67	0
5	Q1	1518	0	1499	266	0
6	F1	916	0	911	96	0
6	R1	916	0	911	95	0
7	G1	682	0	679	108	0
7	S1	682	0	679	99	0
8	H1	524	0	504	69	0
8	T1	524	0	504	76	0
9	I1	248	0	265	53	0
9	U1	248	0	265	64	0
10	J1	511	0	518	73	0
10	V1	511	0	518	78	0
11	K1	164	0	161	29	0
11	W1	164	0	161	28	0
12	22	2582	0	2612	35	0
13	32	719	0	741	9	0
14	42	3447	0	3442	48	0
15	52	697	0	708	14	0
16	72	1186	0	1123	13	0
17	82	2965	0	2595	73	0
18	92	1535	0	1491	62	0
19	A2	5183	0	5174	337	0
20	B2	3076	0	3041	95	0
21	C2	1705	0	1645	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D2	1200	0	1195	27	0
23	E2	1388	0	1340	43	0
24	F2	183	0	132	6	0
25	G2	981	0	965	35	0
26	H2	780	0	753	12	0
27	I2	532	0	513	48	0
28	J2	530	0	503	7	0
29	K2	652	0	636	32	0
30	L2	602	0	592	9	0
31	N2	862	0	868	10	0
32	O2	925	0	907	9	0
33	P2	698	0	659	23	0
34	Q2	1345	0	1282	26	0
35	R2	2334	0	2258	51	0
36	S2	2299	0	2028	23	0
37	T2	942	0	890	11	0
38	U2	734	0	628	91	0
39	V2	1093	0	1048	22	0
40	M2	642	0	642	7	0
40	W2	596	0	553	6	0
41	X2	372	0	314	4	0
42	Y2	409	0	318	7	0
43	Z2	493	0	395	6	0
44	a2	857	0	765	11	0
45	b2	1032	0	954	14	0
46	c2	617	0	492	8	0
47	d2	708	0	514	9	0
48	f2	1156	0	892	14	0
49	h2	721	0	632	13	0
50	i2	277	0	240	4	0
51	j2	892	0	835	10	0
52	12	2442	0	2563	72	0
53	62	4765	0	4894	62	0
54	g2	1351	0	1262	18	0
55	e2	864	0	567	26	0
56	A3	4025	0	4003	91	0
57	B3	1822	0	1834	73	0
58	C3	2124	0	2042	51	0
59	D3	1195	0	1183	33	0
60	E3	878	0	868	21	0
61	F3	748	0	728	22	0
62	G3	671	0	645	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	H3	628	0	582	21	0
64	I3	598	0	612	16	0
65	J3	441	0	439	14	0
66	K3	384	0	366	12	0
67	L3	386	0	388	9	0
68	M3	335	0	352	12	0
69	C1	86	0	60	18	0
69	O1	86	0	60	25	0
70	D1	43	0	30	5	0
70	P1	43	0	30	5	0
71	92	4	0	0	0	0
71	A2	4	0	0	0	0
71	Q1	4	0	0	0	0
72	22	41	0	59	3	0
72	42	41	0	59	1	0
72	B2	51	0	82	1	0
73	42	82	0	114	2	0
74	82	31	0	19	2	0
75	82	8	0	0	0	0
75	A2	16	0	0	12	0
75	D2	8	0	0	0	0
75	E2	16	0	0	0	0
76	F3	1	0	0	0	0
76	I2	1	0	0	1	0
77	R2	48	0	23	3	0
78	S2	47	0	71	0	0
78	j2	39	0	55	1	0
79	A3	120	0	108	4	0
80	A3	1	0	0	0	0
80	B3	2	0	0	0	0
81	A3	1	0	0	0	0
All	All	105456	0	102214	5423	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 26.

The worst 5 of 5423 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)
18:92:42:ARG:NH1	19:A2:199:GLY:HA2	1.33	1.42
19:A2:306:MET:SD	38:U2:139:PRO:HG3	1.60	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:12:126:LYS:HD3	52:12:127:TYR:N	1.31	1.38
19:A2:227:PRO:HD2	75:A2:802:SF4:S1	1.63	1.37
35:R2:170:LEU:O	35:R2:328:ILE:HD11	1.21	1.36

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	A1	428/480 (89%)	348 (81%)	57 (13%)	23 (5%)	1	15
1	M1	428/480 (89%)	360 (84%)	50 (12%)	18 (4%)	2	17
2	B1	417/453 (92%)	341 (82%)	67 (16%)	9 (2%)	5	29
2	N1	417/453 (92%)	344 (82%)	62 (15%)	11 (3%)	4	25
3	C1	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	2	20
3	O1	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3	23
4	D1	239/325 (74%)	188 (79%)	36 (15%)	15 (6%)	1	13
4	P1	239/325 (74%)	195 (82%)	32 (13%)	12 (5%)	1	16
5	E1	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	4	25
5	Q1	194/196 (99%)	149 (77%)	34 (18%)	11 (6%)	1	14
6	F1	104/111 (94%)	89 (86%)	12 (12%)	3 (3%)	3	23
6	R1	104/111 (94%)	86 (83%)	16 (15%)	2 (2%)	6	32
7	G1	79/82 (96%)	63 (80%)	13 (16%)	3 (4%)	2	19
7	S1	79/82 (96%)	60 (76%)	16 (20%)	3 (4%)	2	19
8	H1	62/91 (68%)	52 (84%)	10 (16%)	0	100	100
8	T1	62/91 (68%)	51 (82%)	10 (16%)	1 (2%)	7	38
9	I1	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U1	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	7
10	J1	60/64 (94%)	41 (68%)	13 (22%)	6 (10%)	0	7
10	V1	60/64 (94%)	45 (75%)	11 (18%)	4 (7%)	1	12
11	K1	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
11	W1	20/56 (36%)	17 (85%)	3 (15%)	0	100	100
12	22	342/347 (99%)	295 (86%)	47 (14%)	0	100	100
13	32	89/115 (77%)	74 (83%)	14 (16%)	1 (1%)	11	46
14	42	457/459 (100%)	383 (84%)	70 (15%)	4 (1%)	14	51
15	52	94/98 (96%)	82 (87%)	12 (13%)	0	100	100
16	72	170/175 (97%)	140 (82%)	28 (16%)	2 (1%)	10	44
17	82	425/444 (96%)	346 (81%)	78 (18%)	1 (0%)	43	78
18	92	205/217 (94%)	169 (82%)	35 (17%)	1 (0%)	24	63
19	A2	686/704 (97%)	572 (83%)	107 (16%)	7 (1%)	12	49
20	B2	383/430 (89%)	334 (87%)	40 (10%)	9 (2%)	5	28
21	C2	206/228 (90%)	177 (86%)	29 (14%)	0	100	100
22	D2	150/179 (84%)	130 (87%)	19 (13%)	1 (1%)	18	56
23	E2	174/176 (99%)	158 (91%)	15 (9%)	1 (1%)	21	59
24	F2	26/75 (35%)	19 (73%)	7 (27%)	0	100	100
25	G2	121/133 (91%)	100 (83%)	20 (16%)	1 (1%)	16	54
26	H2	94/105 (90%)	73 (78%)	21 (22%)	0	100	100
27	I2	69/96 (72%)	53 (77%)	14 (20%)	2 (3%)	3	23
28	J2	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
29	K2	82/98 (84%)	63 (77%)	19 (23%)	0	100	100
30	L2	78/83 (94%)	66 (85%)	12 (15%)	0	100	100
31	N2	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
32	O2	112/127 (88%)	97 (87%)	15 (13%)	0	100	100
33	P2	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
34	Q2	166/171 (97%)	126 (76%)	40 (24%)	0	100	100
35	R2	302/345 (88%)	241 (80%)	59 (20%)	2 (1%)	18	56
36	S2	317/320 (99%)	246 (78%)	69 (22%)	2 (1%)	21	59
37	T2	136/140 (97%)	116 (85%)	20 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	U2	87/145 (60%)	63 (72%)	24 (28%)	0	100	100
39	V2	136/143 (95%)	121 (89%)	14 (10%)	1 (1%)	18	56
40	M2	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
40	W2	79/88 (90%)	68 (86%)	11 (14%)	0	100	100
41	X2	47/57 (82%)	38 (81%)	8 (17%)	1 (2%)	5	30
42	Y2	55/72 (76%)	46 (84%)	9 (16%)	0	100	100
43	Z2	72/97 (74%)	57 (79%)	15 (21%)	0	100	100
44	a2	112/128 (88%)	95 (85%)	17 (15%)	0	100	100
45	b2	137/143 (96%)	113 (82%)	24 (18%)	0	100	100
46	c2	86/127 (68%)	68 (79%)	18 (21%)	0	100	100
47	d2	105/136 (77%)	82 (78%)	21 (20%)	2 (2%)	6	32
48	f2	165/178 (93%)	135 (82%)	30 (18%)	0	100	100
49	h2	89/125 (71%)	62 (70%)	25 (28%)	2 (2%)	5	29
50	i2	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
51	j2	111/120 (92%)	92 (83%)	19 (17%)	0	100	100
52	12	305/318 (96%)	269 (88%)	34 (11%)	2 (1%)	18	56
53	62	604/606 (100%)	536 (89%)	67 (11%)	1 (0%)	43	78
54	g2	171/176 (97%)	139 (81%)	32 (19%)	0	100	100
55	e2	139/158 (88%)	82 (59%)	50 (36%)	7 (5%)	1	16
56	A3	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
57	B3	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
58	C3	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	D3	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	E3	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	F3	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
62	G3	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	13
63	H3	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	40
64	I3	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	J3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	20
66	K3	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	L3	45/63 (71%)	42 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	M3	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13415/15148 (89%)	11221 (84%)	1971 (15%)	223 (2%)	9	36

5 of 223 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	327	ASP
1	A1	426	GLY
1	A1	427	PRO
2	B1	141	GLN
2	B1	183	ILE

5.3.2 Protein sidechains ⓘ

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	A1	358/394 (91%)	269 (75%)	89 (25%)	0	4
1	M1	358/394 (91%)	276 (77%)	82 (23%)	1	6
2	B1	328/355 (92%)	254 (77%)	74 (23%)	1	6
2	N1	328/355 (92%)	254 (77%)	74 (23%)	1	6
3	C1	327/327 (100%)	251 (77%)	76 (23%)	1	5
3	O1	327/327 (100%)	259 (79%)	68 (21%)	1	6
4	D1	206/257 (80%)	172 (84%)	34 (16%)	2	10
4	P1	206/257 (80%)	170 (82%)	36 (18%)	2	9
5	E1	65/168 (39%)	47 (72%)	18 (28%)	0	3
5	Q1	167/168 (99%)	110 (66%)	57 (34%)	0	1
6	F1	96/99 (97%)	68 (71%)	28 (29%)	0	2
6	R1	96/99 (97%)	76 (79%)	20 (21%)	1	6
7	G1	71/72 (99%)	53 (75%)	18 (25%)	0	3
7	S1	71/72 (99%)	51 (72%)	20 (28%)	0	3
8	H1	61/85 (72%)	50 (82%)	11 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	T1	61/85 (72%)	50 (82%)	11 (18%)	2	9
9	I1	27/60 (45%)	18 (67%)	9 (33%)	0	2
9	U1	27/60 (45%)	19 (70%)	8 (30%)	0	2
10	J1	52/54 (96%)	43 (83%)	9 (17%)	2	9
10	V1	52/54 (96%)	42 (81%)	10 (19%)	1	8
11	K1	15/46 (33%)	11 (73%)	4 (27%)	0	3
11	W1	15/46 (33%)	10 (67%)	5 (33%)	0	2
12	22	274/316 (87%)	274 (100%)	0	100	100
13	32	75/101 (74%)	75 (100%)	0	100	100
14	42	351/413 (85%)	351 (100%)	0	100	100
15	52	75/86 (87%)	75 (100%)	0	100	100
16	72	104/142 (73%)	104 (100%)	0	100	100
17	82	236/353 (67%)	236 (100%)	0	100	100
18	92	160/183 (87%)	159 (99%)	1 (1%)	78	83
19	A2	551/588 (94%)	548 (100%)	3 (0%)	81	83
20	B2	330/371 (89%)	324 (98%)	6 (2%)	51	68
21	C2	183/204 (90%)	182 (100%)	1 (0%)	81	83
22	D2	126/150 (84%)	123 (98%)	3 (2%)	43	64
23	E2	145/151 (96%)	144 (99%)	1 (1%)	76	81
24	F2	13/69 (19%)	13 (100%)	0	100	100
25	G2	105/119 (88%)	105 (100%)	0	100	100
26	H2	80/95 (84%)	80 (100%)	0	100	100
27	I2	53/79 (67%)	49 (92%)	4 (8%)	12	33
28	J2	50/59 (85%)	50 (100%)	0	100	100
29	K2	66/81 (82%)	66 (100%)	0	100	100
30	L2	63/71 (89%)	63 (100%)	0	100	100
31	N2	88/101 (87%)	88 (100%)	0	100	100
32	O2	95/113 (84%)	95 (100%)	0	100	100
33	P2	72/96 (75%)	72 (100%)	0	100	100
34	Q2	142/154 (92%)	140 (99%)	2 (1%)	59	72
35	R2	230/298 (77%)	229 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	S2	205/283 (72%)	203 (99%)	2 (1%)	68	78
37	T2	79/101 (78%)	79 (100%)	0	100	100
38	U2	71/131 (54%)	71 (100%)	0	100	100
39	V2	107/120 (89%)	107 (100%)	0	100	100
40	M2	73/81 (90%)	73 (100%)	0	100	100
40	W2	55/81 (68%)	55 (100%)	0	100	100
41	X2	32/54 (59%)	32 (100%)	0	100	100
42	Y2	29/62 (47%)	29 (100%)	0	100	100
43	Z2	28/75 (37%)	28 (100%)	0	100	100
44	a2	70/114 (61%)	69 (99%)	1 (1%)	59	72
45	b2	85/124 (68%)	85 (100%)	0	100	100
46	c2	45/121 (37%)	45 (100%)	0	100	100
47	d2	42/119 (35%)	42 (100%)	0	100	100
48	f2	80/160 (50%)	80 (100%)	0	100	100
49	h2	70/112 (62%)	70 (100%)	0	100	100
50	i2	23/45 (51%)	23 (100%)	0	100	100
51	j2	88/106 (83%)	88 (100%)	0	100	100
52	l2	267/275 (97%)	259 (97%)	8 (3%)	36	57
53	62	523/534 (98%)	522 (100%)	1 (0%)	87	87
54	g2	130/157 (83%)	130 (100%)	0	100	100
55	e2	44/141 (31%)	43 (98%)	1 (2%)	44	64
56	A3	427/427 (100%)	387 (91%)	40 (9%)	8	26
57	B3	211/211 (100%)	191 (90%)	20 (10%)	8	25
58	C3	226/226 (100%)	199 (88%)	27 (12%)	5	18
59	D3	128/148 (86%)	117 (91%)	11 (9%)	10	29
60	E3	95/123 (77%)	89 (94%)	6 (6%)	16	37
61	F3	81/103 (79%)	73 (90%)	8 (10%)	7	24
62	G3	68/79 (86%)	52 (76%)	16 (24%)	1	5
63	H3	67/76 (88%)	58 (87%)	9 (13%)	4	14
64	I3	58/59 (98%)	51 (88%)	7 (12%)	5	17
65	J3	47/68 (69%)	41 (87%)	6 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	K3	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	L3	40/55 (73%)	37 (92%)	3 (8%)	12	33
68	M3	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10651/12921 (82%)	9696 (91%)	955 (9%)	11	27

5 of 955 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N1	65	THR
59	D3	36	SER
3	O1	262	LEU
58	C3	188	ILE
66	K3	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
21	C2	140	ASN
44	a2	79	ASN
61	F3	66	ASN
26	H2	45	HIS
35	R2	169	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 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
78	PC1	S2	401	-	46,46,53	0.99	4 (8%)	52,54,61	1.03	2 (3%)
72	3PE	42	502	-	40,40,50	0.94	3 (7%)	43,45,55	1.20	2 (4%)
75	SF4	D2	301	-	0,12,12	-	-	-	-	-
75	SF4	E2	302	23	0,12,12	-	-	-	-	-
77	NAP	R2	601	-	49,52,52	4.40	22 (44%)	69,80,80	1.87	18 (26%)
70	HEC	D1	301	4	50,50,50	1.28	3 (6%)	68,82,82	1.14	5 (7%)
75	SF4	82	502	-	0,12,12	-	-	-	-	-
78	PC1	j2	201	-	38,38,53	1.08	4 (10%)	44,46,61	1.03	2 (4%)
75	SF4	A2	801	19	0,12,12	-	-	-	-	-
75	SF4	E2	301	23	0,12,12	-	-	-	-	-
79	HEA	A3	601	56	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
69	HEM	O1	402	3	50,50,50	1.35	7 (14%)	66,82,82	1.76	15 (22%)
69	HEM	C1	402	3	50,50,50	1.26	6 (12%)	66,82,82	1.85	18 (27%)
69	HEM	C1	401	3	50,50,50	1.30	6 (12%)	66,82,82	1.54	10 (15%)
74	FMN	82	501	-	33,33,33	1.05	2 (6%)	48,50,50	1.42	10 (20%)
71	FES	92	301	18	0,4,4	-	-	-	-	-
70	HEC	P1	301	4	50,50,50	1.31	5 (10%)	68,82,82	1.04	4 (5%)
75	SF4	A2	802	19	0,12,12	-	-	-	-	-
79	HEA	A3	602	56	66,67,67	1.22	7 (10%)	78,103,103	1.37	12 (15%)
72	3PE	22	401	-	40,40,50	0.94	3 (7%)	43,45,55	1.13	2 (4%)
69	HEM	O1	401	3	50,50,50	1.40	7 (14%)	66,82,82	1.92	18 (27%)
71	FES	A2	803	19	0,4,4	-	-	-	-	-
72	3PE	B2	501	20	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
73	CDL	42	501	-	81,81,99	0.96	6 (7%)	87,93,111	1.10	5 (5%)
71	FES	Q1	201	5	0,4,4	-	-	-	-	-

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
78	PC1	S2	401	-	-	20/50/50/57	-
72	3PE	42	502	-	-	25/44/44/54	-
75	SF4	D2	301	-	-	-	0/6/5/5
75	SF4	E2	302	23	-	-	0/6/5/5
77	NAP	R2	601	-	-	17/35/67/67	0/5/5/5
70	HEC	D1	301	4	-	8/14/54/54	-
75	SF4	82	502	-	-	-	0/6/5/5
78	PC1	j2	201	-	-	21/42/42/57	-
75	SF4	A2	801	19	-	-	0/6/5/5
75	SF4	E2	301	23	-	-	0/6/5/5
79	HEA	A3	601	56	-	9/36/76/76	-
69	HEM	O1	402	3	-	4/14/54/54	-
69	HEM	C1	402	3	-	6/14/54/54	-
69	HEM	C1	401	3	-	4/14/54/54	-
74	FMN	82	501	-	-	7/18/18/18	0/3/3/3
71	FES	92	301	18	-	-	0/1/1/1
70	HEC	P1	301	4	-	8/14/54/54	-
75	SF4	A2	802	19	-	-	0/6/5/5
79	HEA	A3	602	56	-	7/36/76/76	-
72	3PE	22	401	-	-	20/44/44/54	-
69	HEM	O1	401	3	-	6/14/54/54	-
71	FES	A2	803	19	-	-	0/1/1/1
72	3PE	B2	501	20	-	26/54/54/54	-
73	CDL	42	501	-	-	42/92/92/110	-
71	FES	Q1	201	5	-	-	0/1/1/1

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	R2	601	NAP	O4D-C1D	16.06	1.63	1.41
77	R2	601	NAP	C2D-C1D	-14.73	1.31	1.53
77	R2	601	NAP	C2B-C1B	-9.08	1.29	1.53
77	R2	601	NAP	O4B-C1B	8.42	1.62	1.42
77	R2	601	NAP	C7N-N7N	7.23	1.46	1.33

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	R2	601	NAP	N3A-C2A-N1A	-5.76	119.60	128.60
69	O1	401	HEM	C3B-C2B-C1B	-5.51	102.40	106.49
77	R2	601	NAP	C5A-C4A-N3A	-4.97	120.26	126.75
69	O1	402	HEM	C3B-C2B-C1B	4.94	110.15	106.49
69	O1	401	HEM	CMA-C3A-C4A	-4.91	117.90	125.37

There are no chirality outliers.

5 of 230 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	O1	401	HEM	C2B-C3B-CAB-CBB
72	22	401	3PE	C1-O11-P-O14
72	22	401	3PE	C22-C21-O21-C2
72	42	502	3PE	C11-O13-P-O12
72	42	502	3PE	C11-O13-P-O14

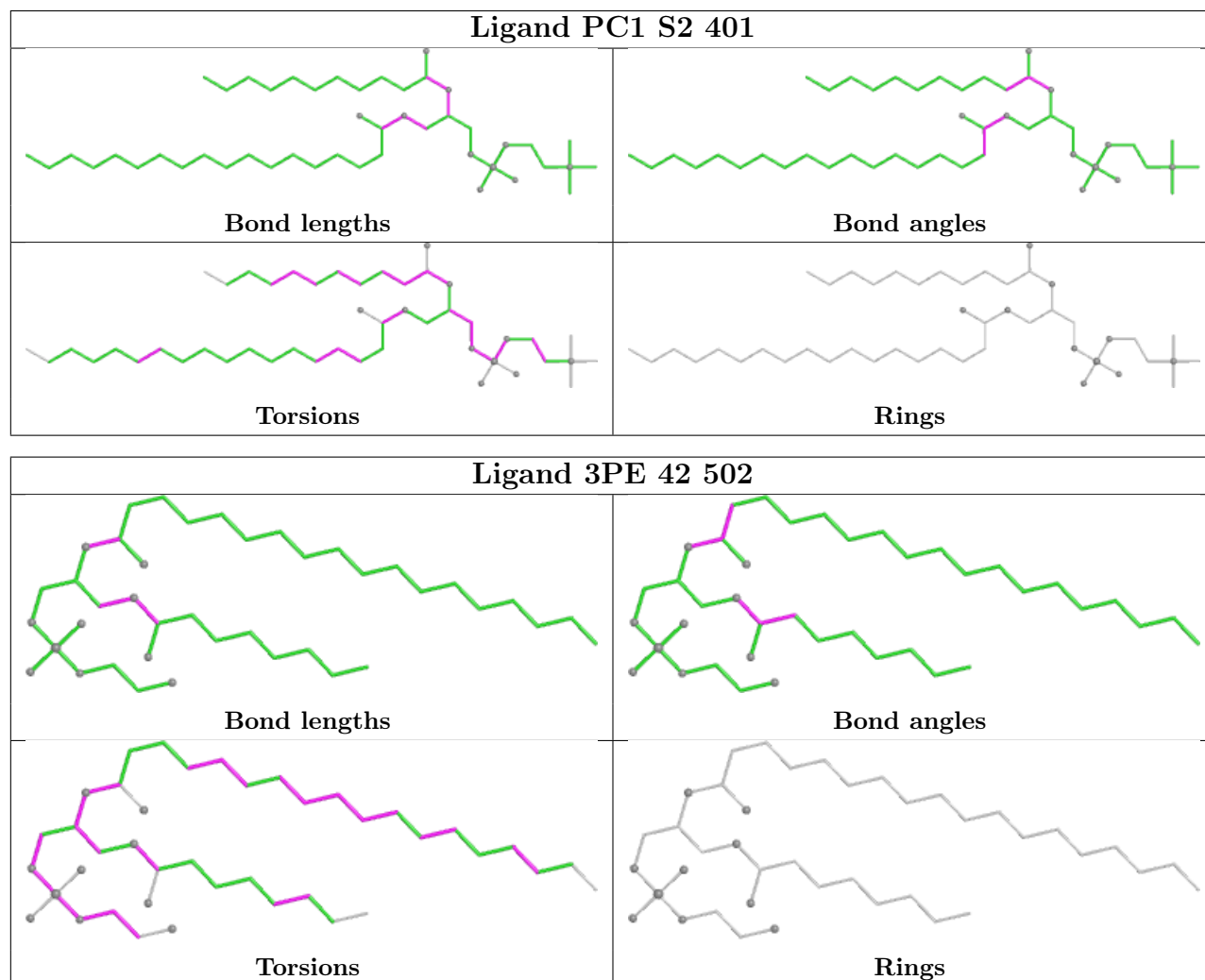
There are no ring outliers.

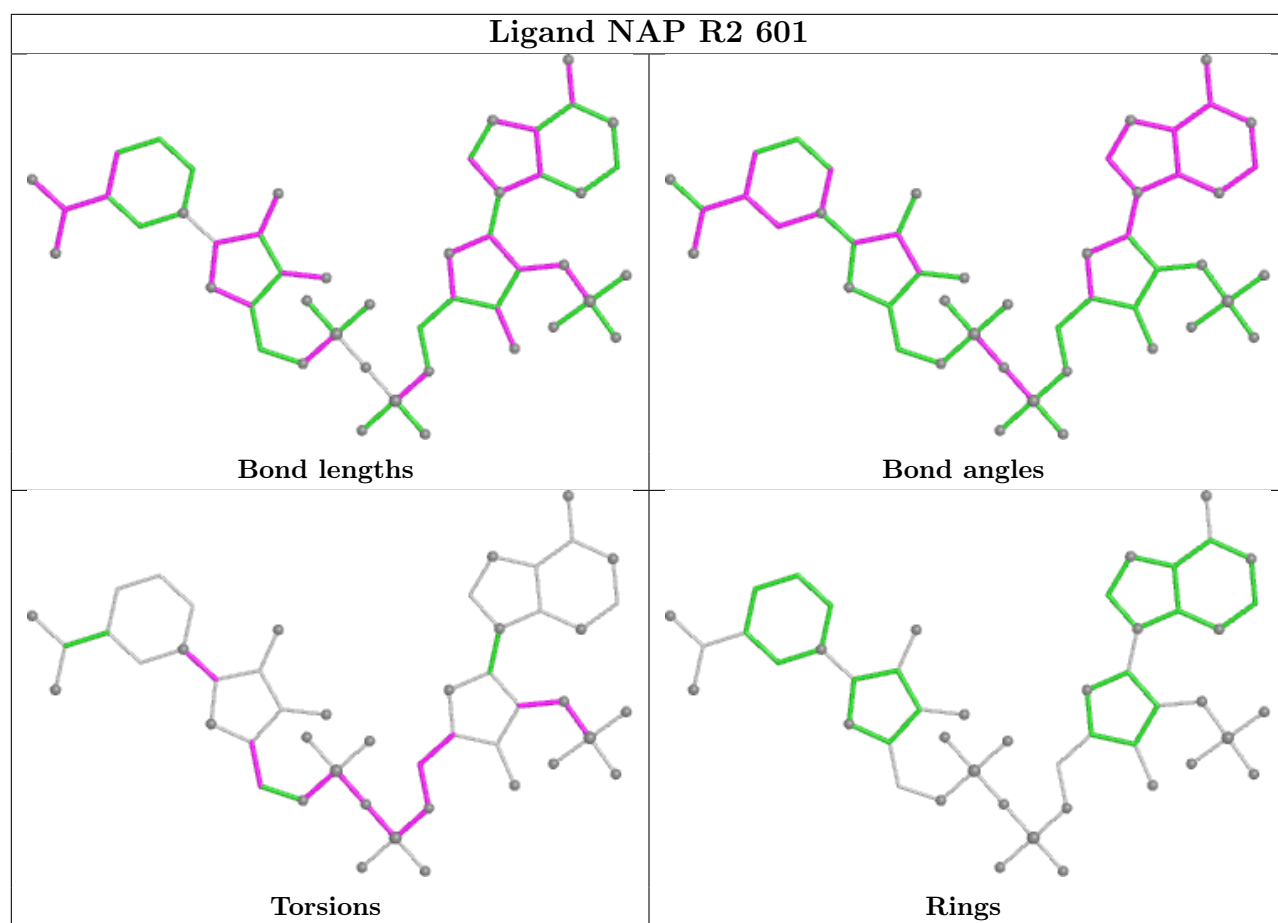
17 monomers are involved in 82 short contacts:

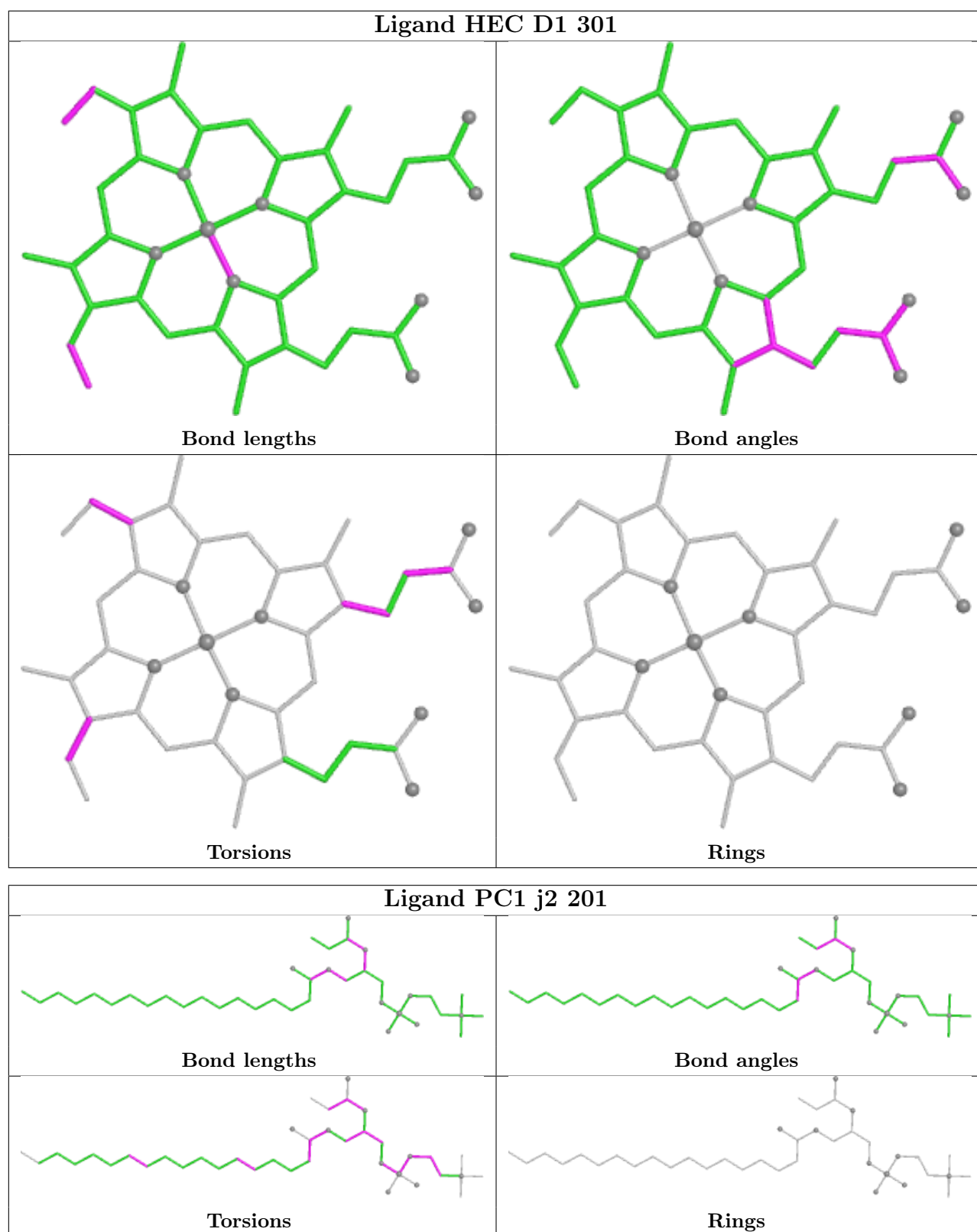
Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	42	502	3PE	1	0
77	R2	601	NAP	3	0
70	D1	301	HEC	5	0
78	j2	201	PC1	1	0
75	A2	801	SF4	4	0
79	A3	601	HEA	1	0
69	O1	402	HEM	14	0
69	C1	402	HEM	13	0
69	C1	401	HEM	5	0
74	82	501	FMN	2	0
70	P1	301	HEC	5	0
75	A2	802	SF4	8	0
79	A3	602	HEA	3	0
72	22	401	3PE	3	0
69	O1	401	HEM	11	0
72	B2	501	3PE	1	0
73	42	501	CDL	2	0

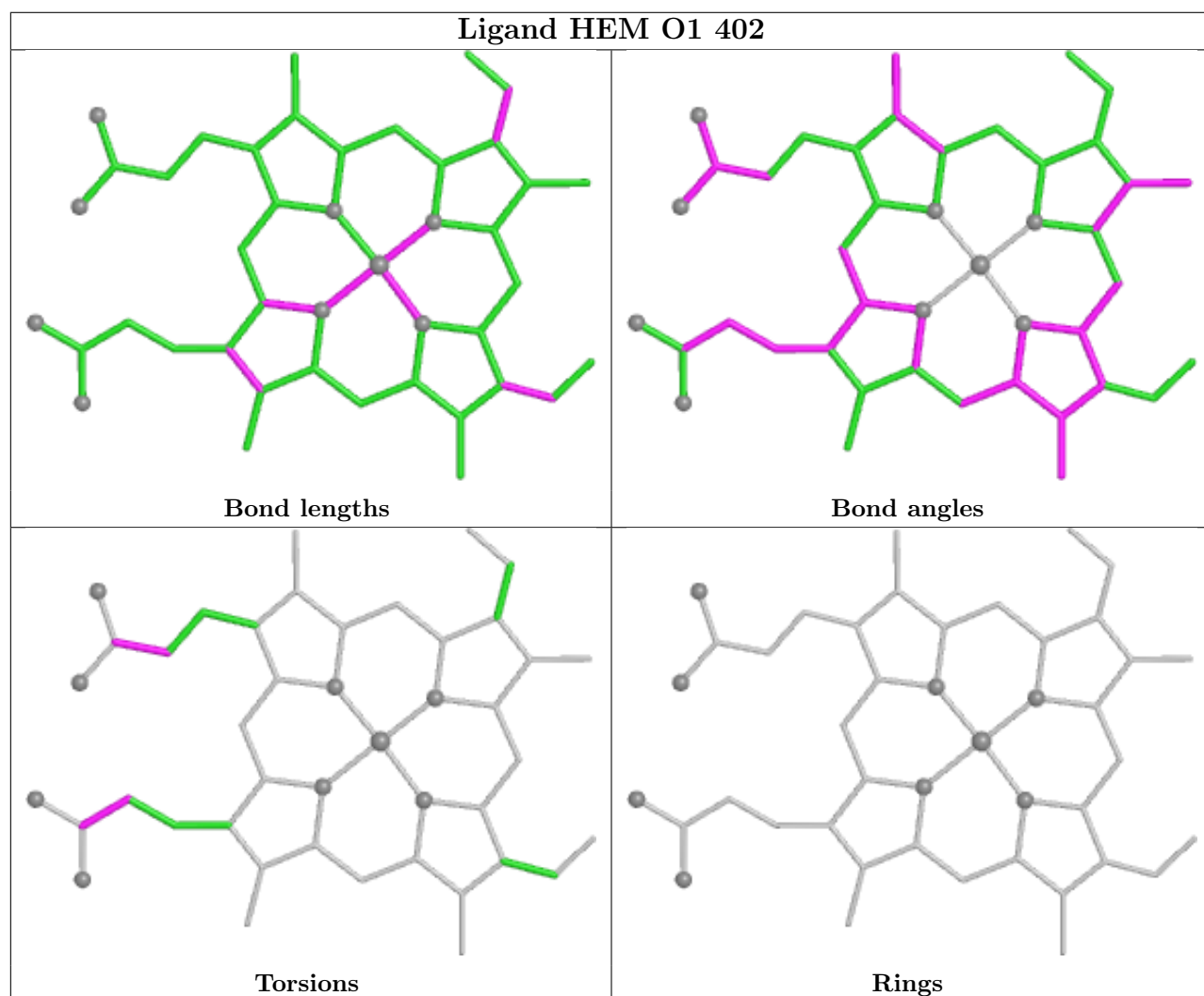
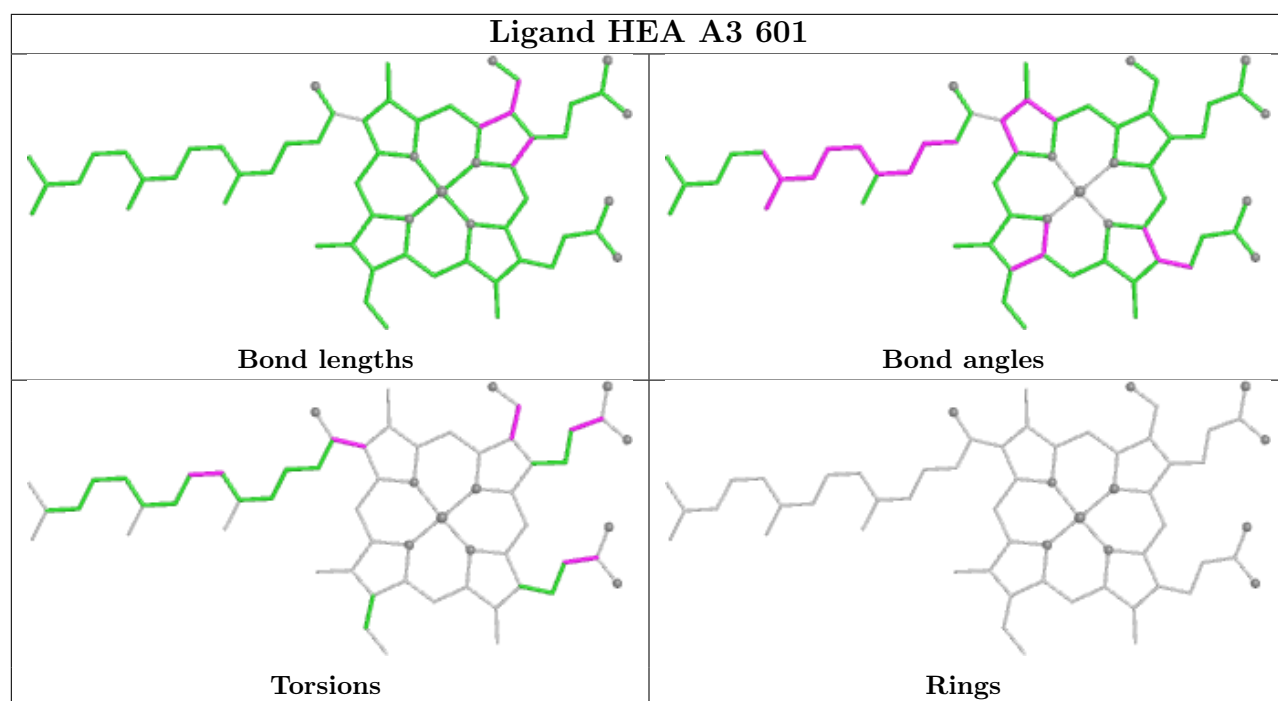
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

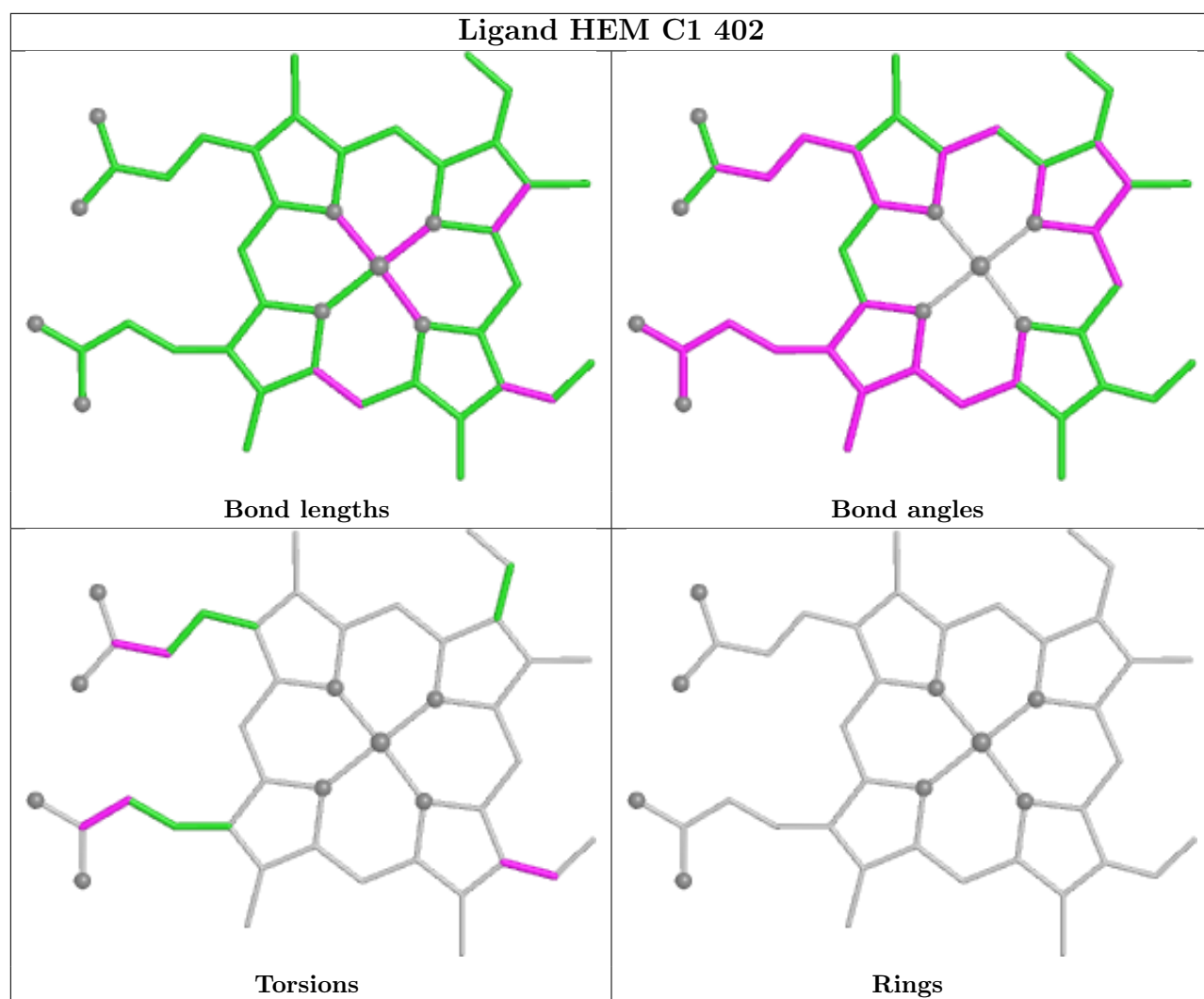
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



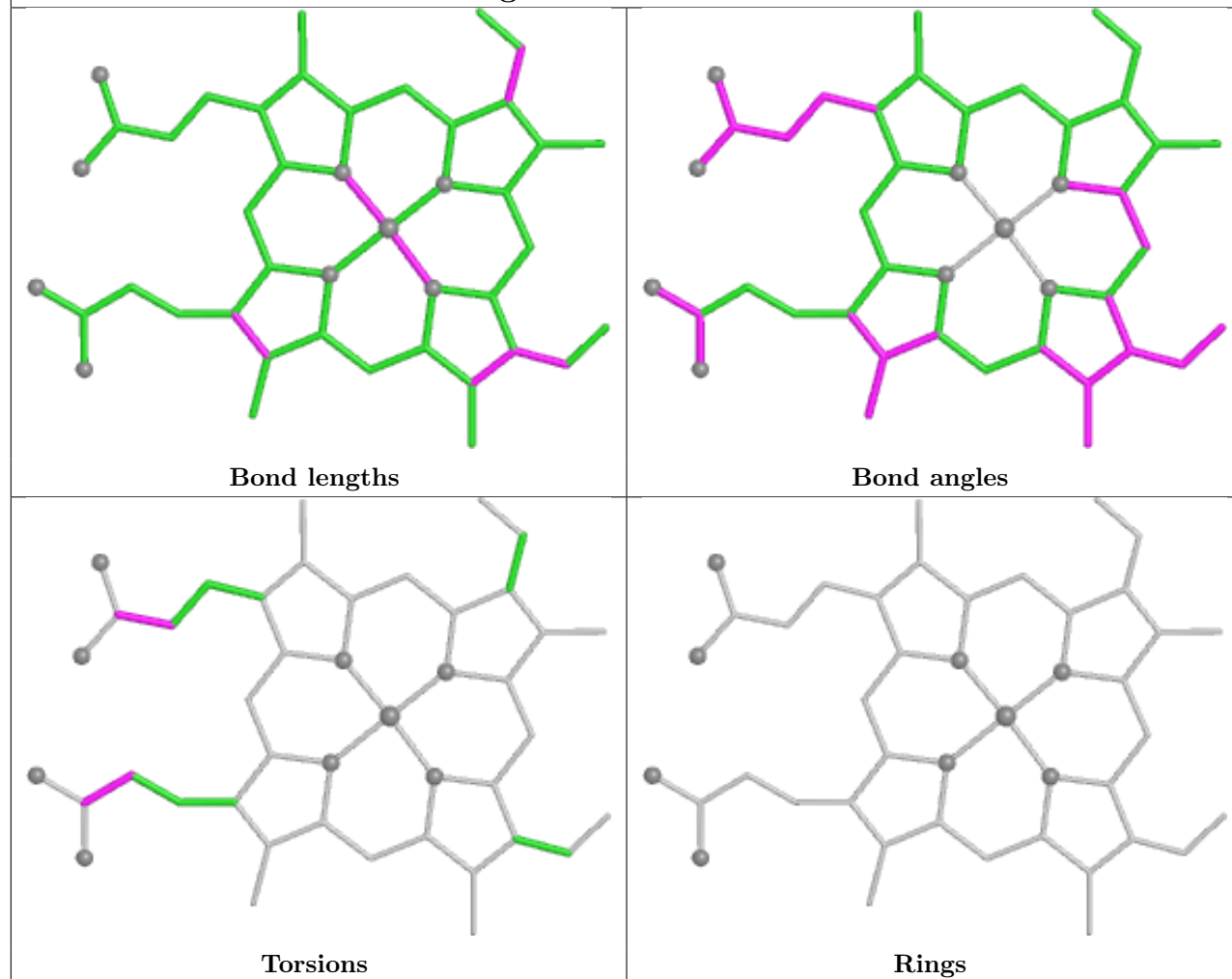




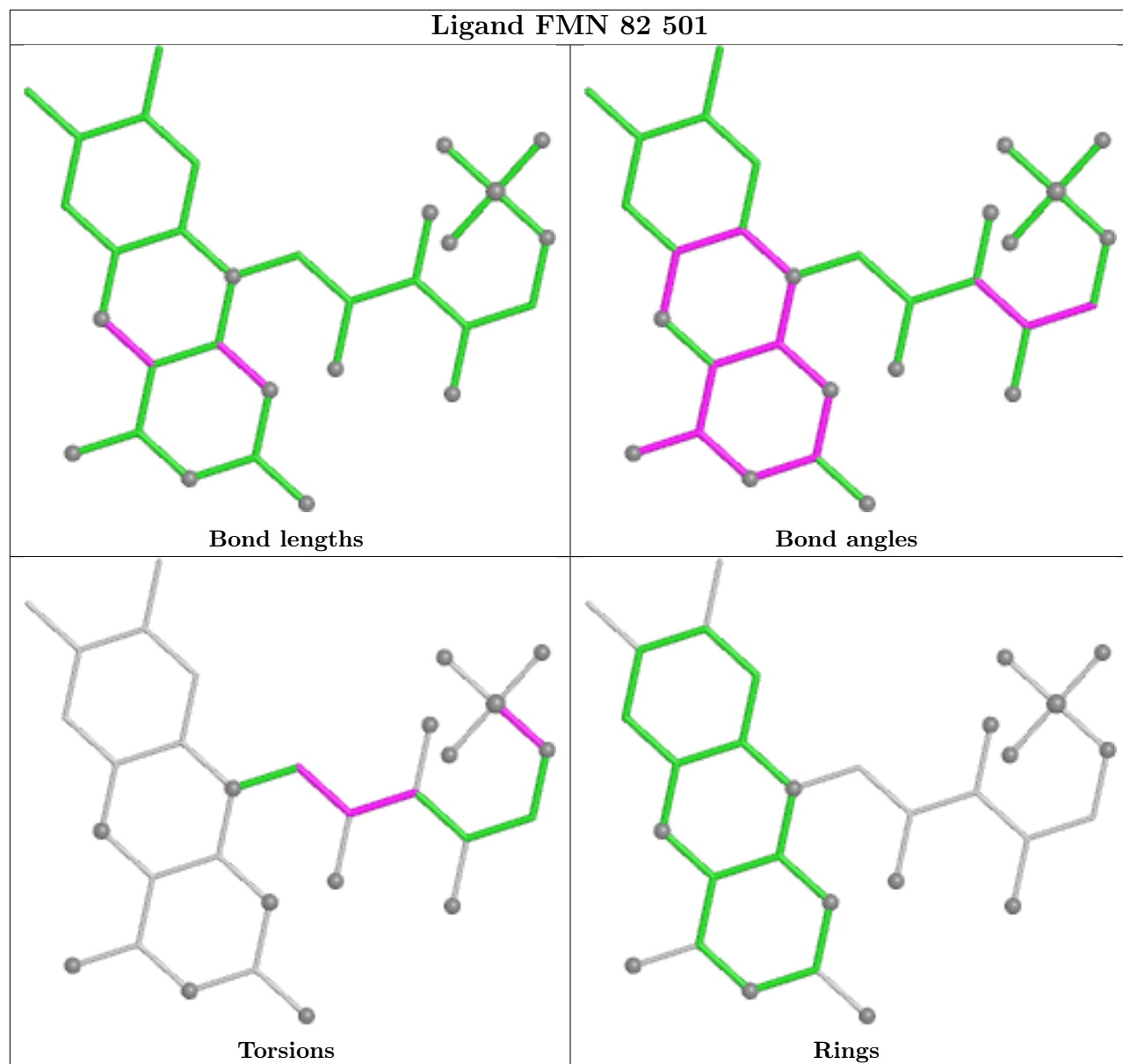




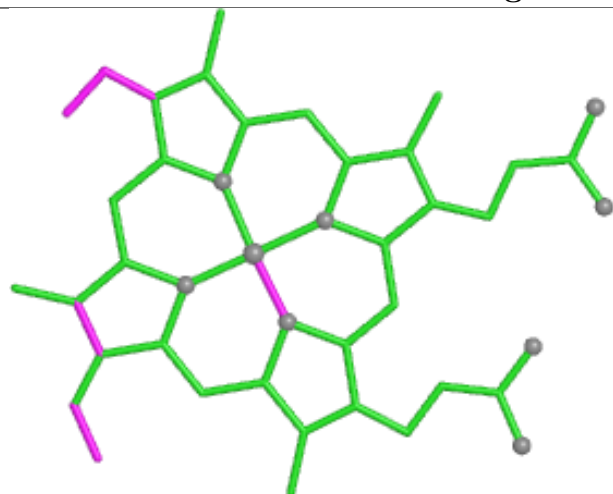
Ligand HEM C1 401



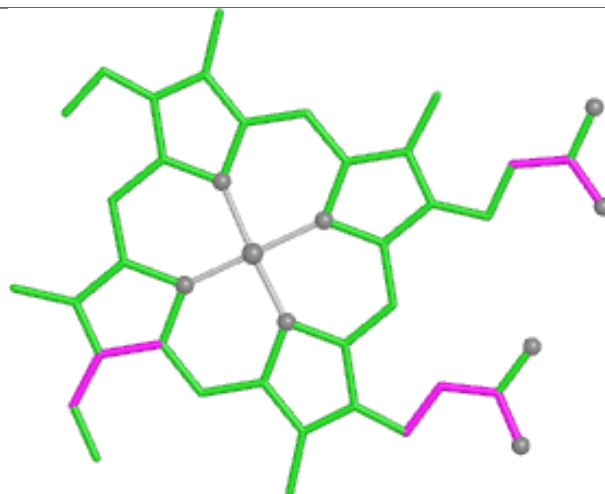
Ligand FMN 82 501



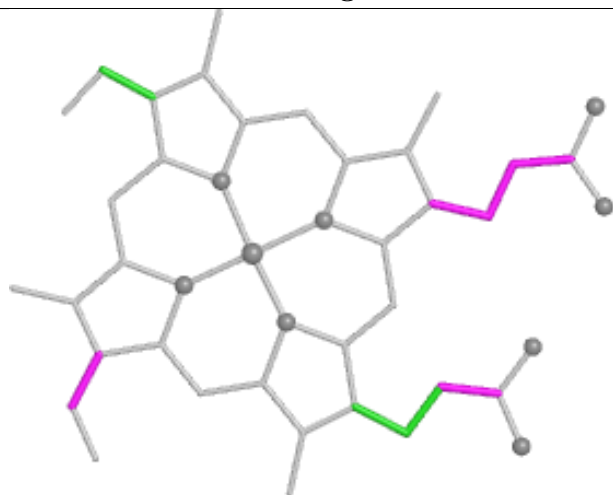
Ligand HEC P1 301



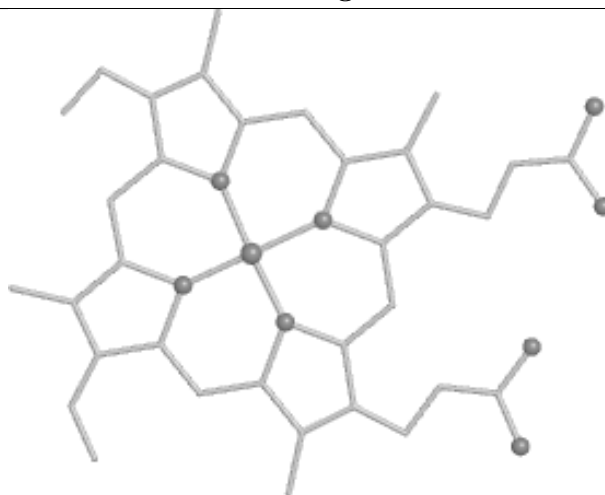
Bond lengths



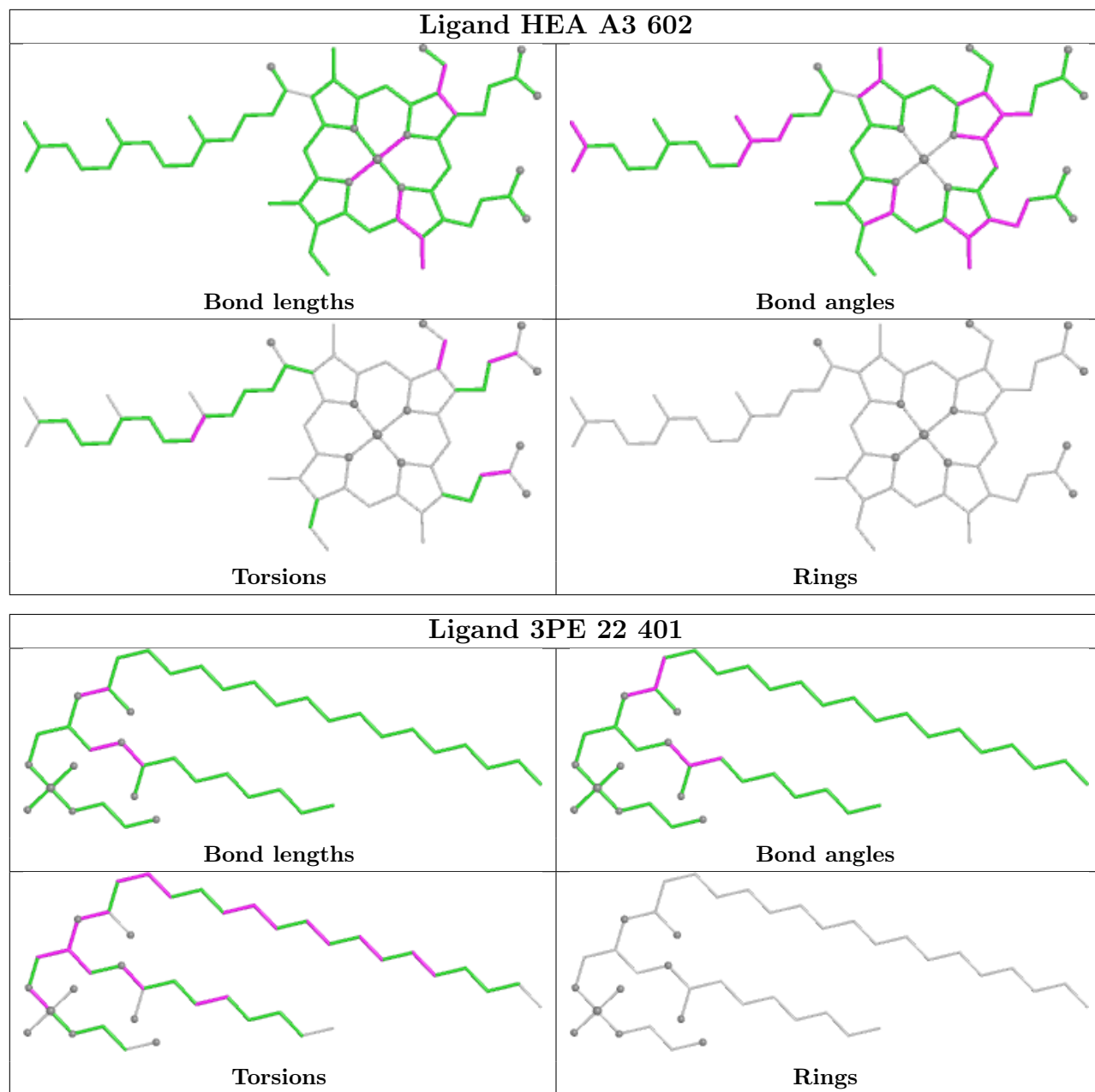
Bond angles



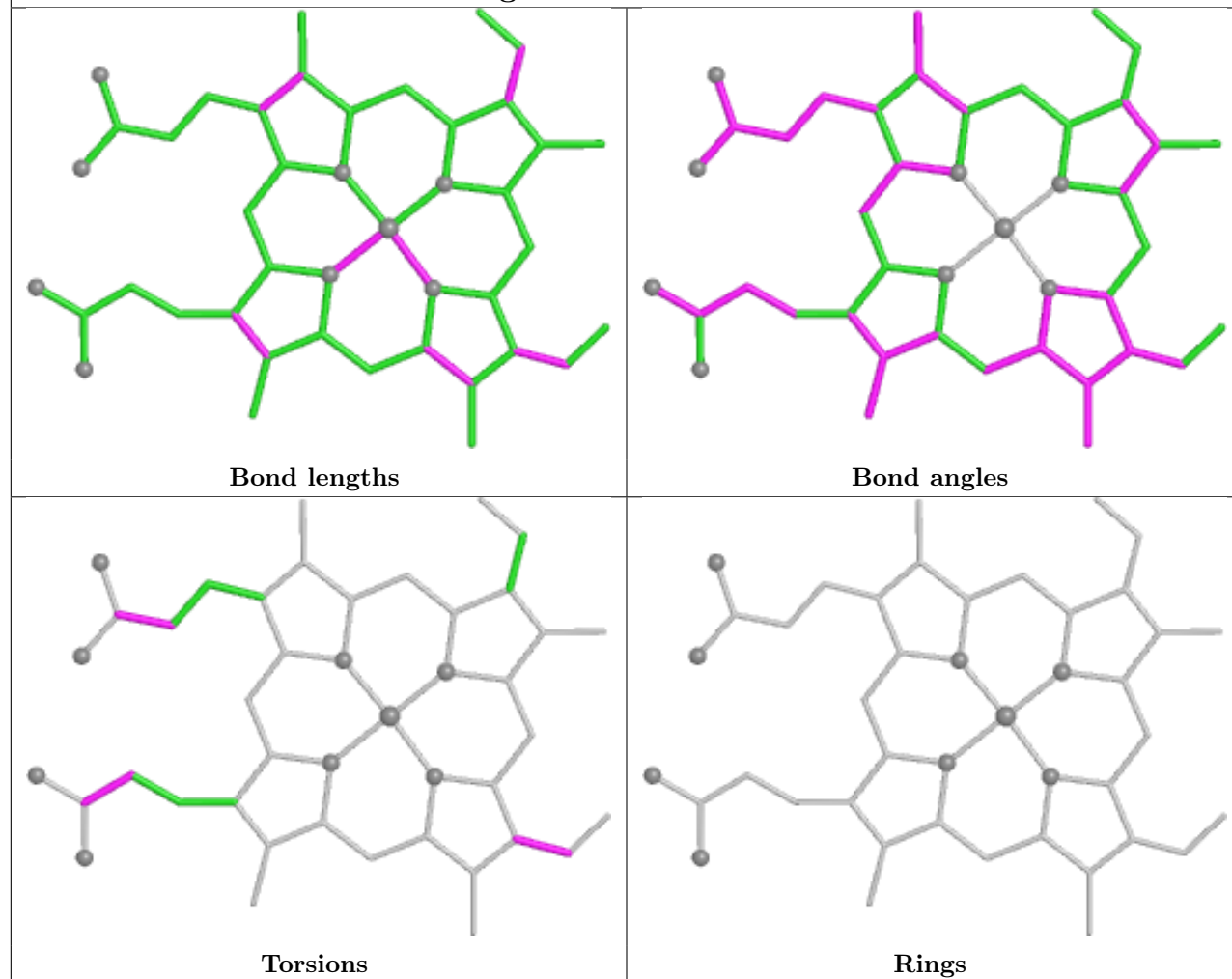
Torsions



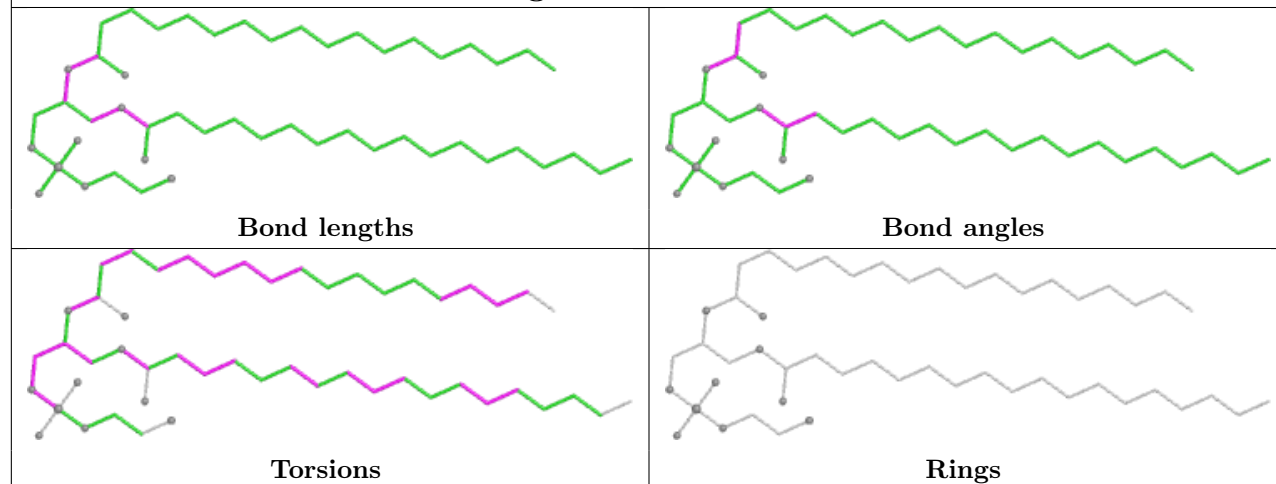
Rings

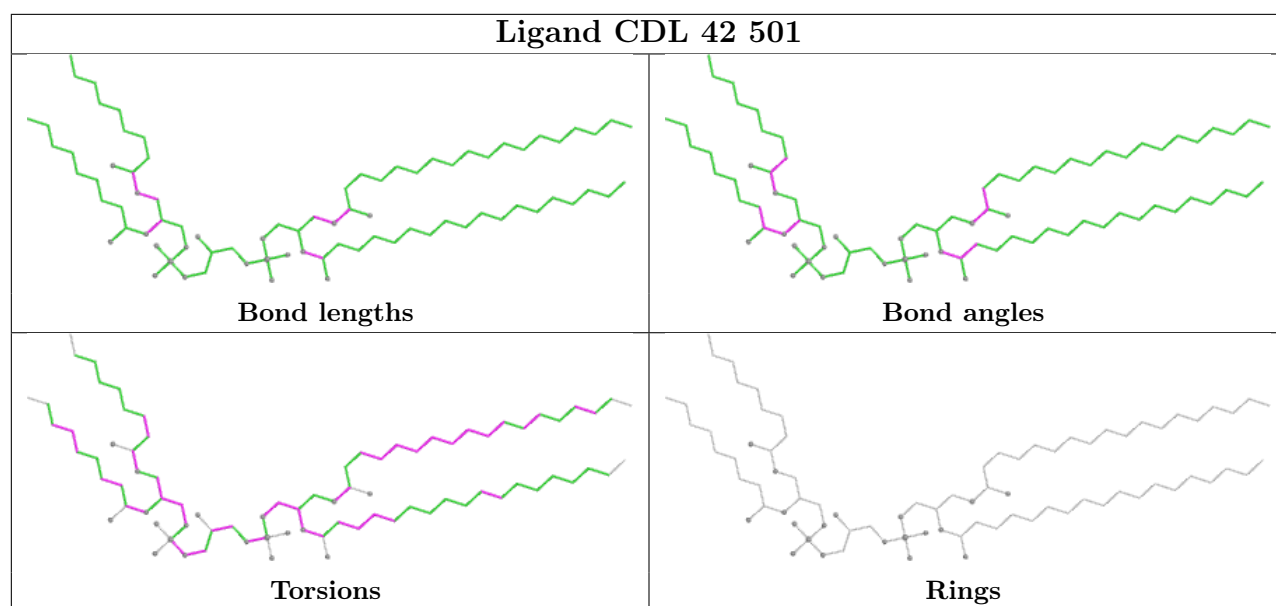


Ligand HEM O1 401



Ligand 3PE B2 501





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.

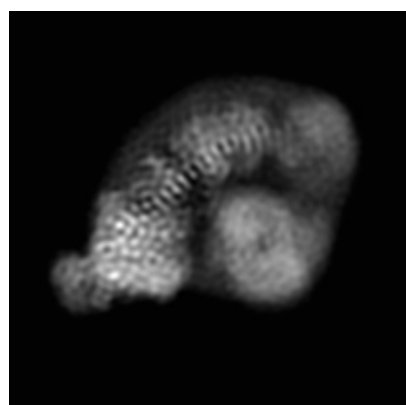
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30706. These allow visual inspection of the internal detail of the map and identification of artifacts.

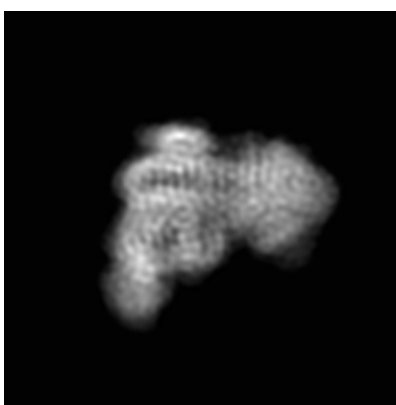
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

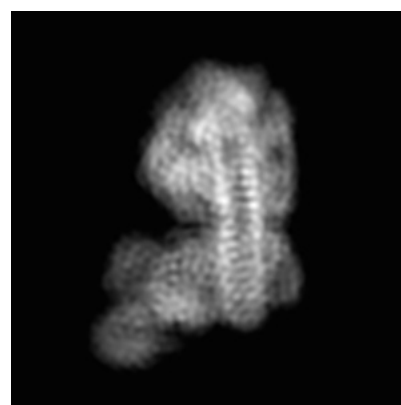
6.1.1 Primary map



X



Y

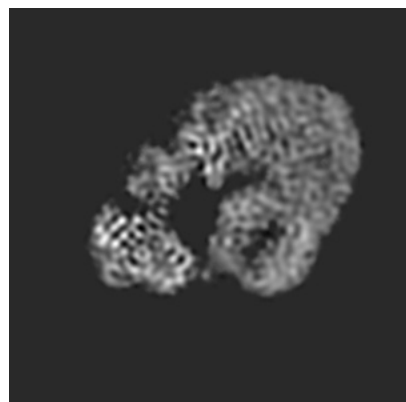


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

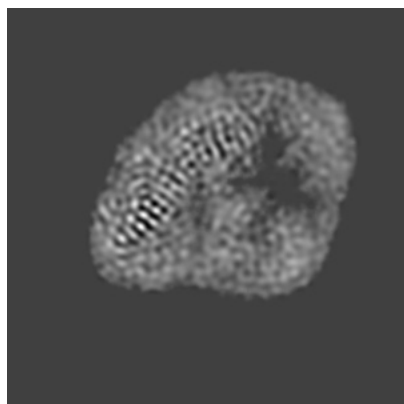


Z Index: 140

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

6.3 Largest variance slices [i](#)

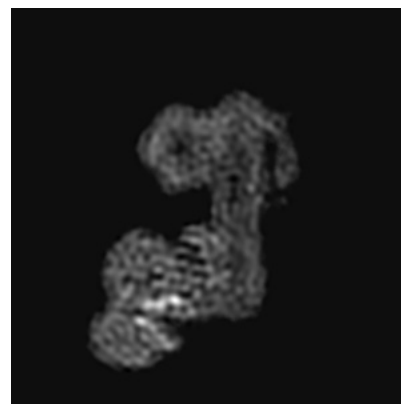
6.3.1 Primary map



X Index: 149



Y Index: 79



Z Index: 95

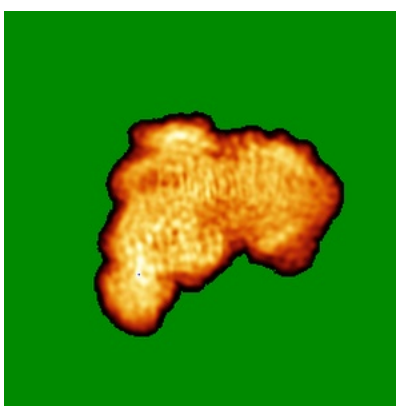
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

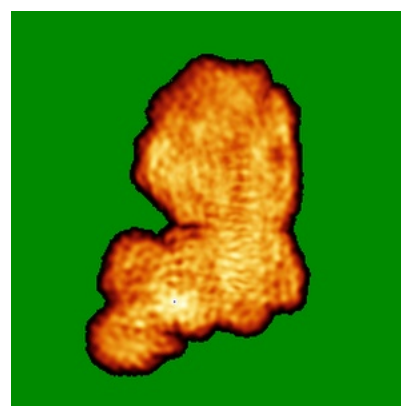
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

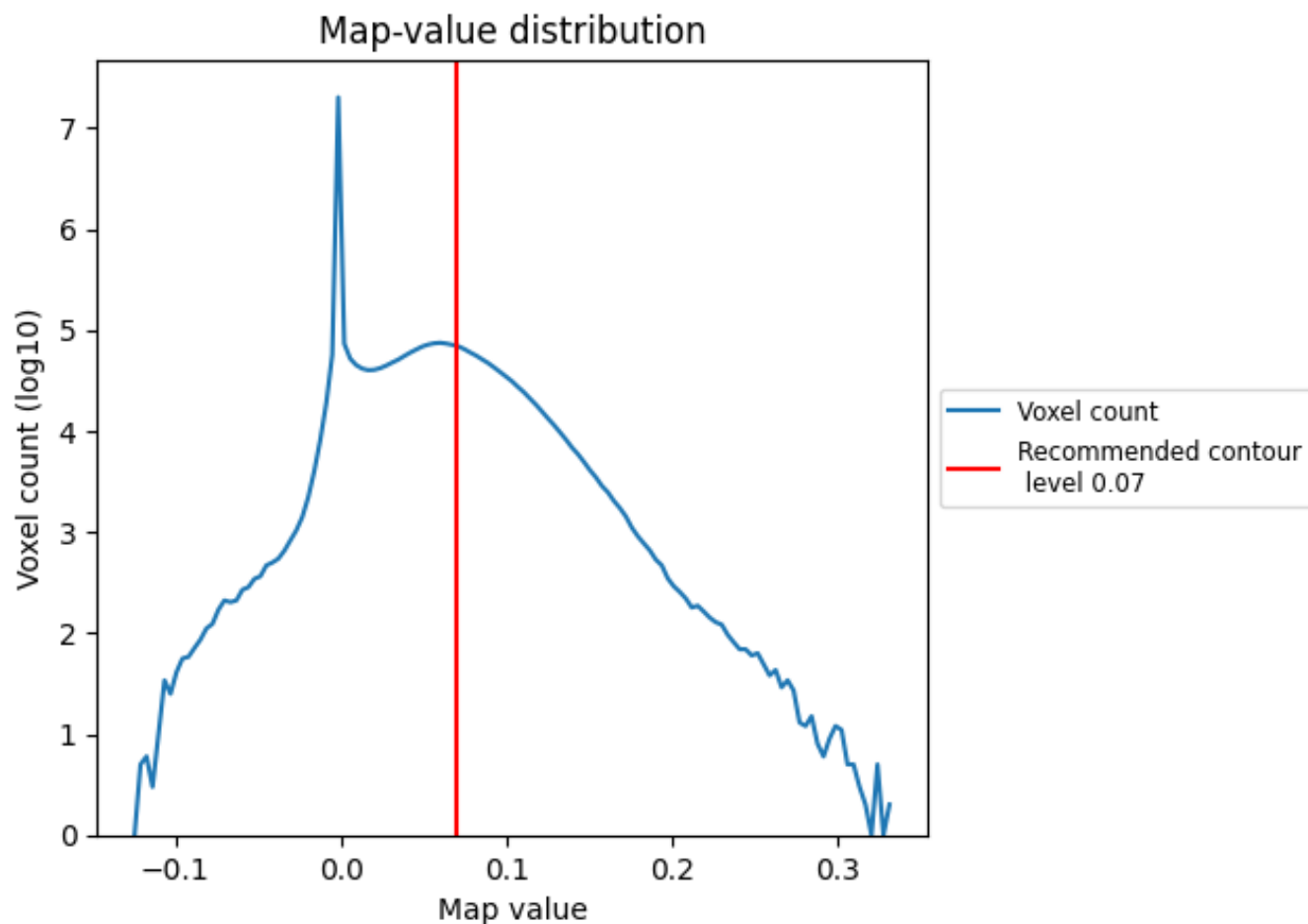
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

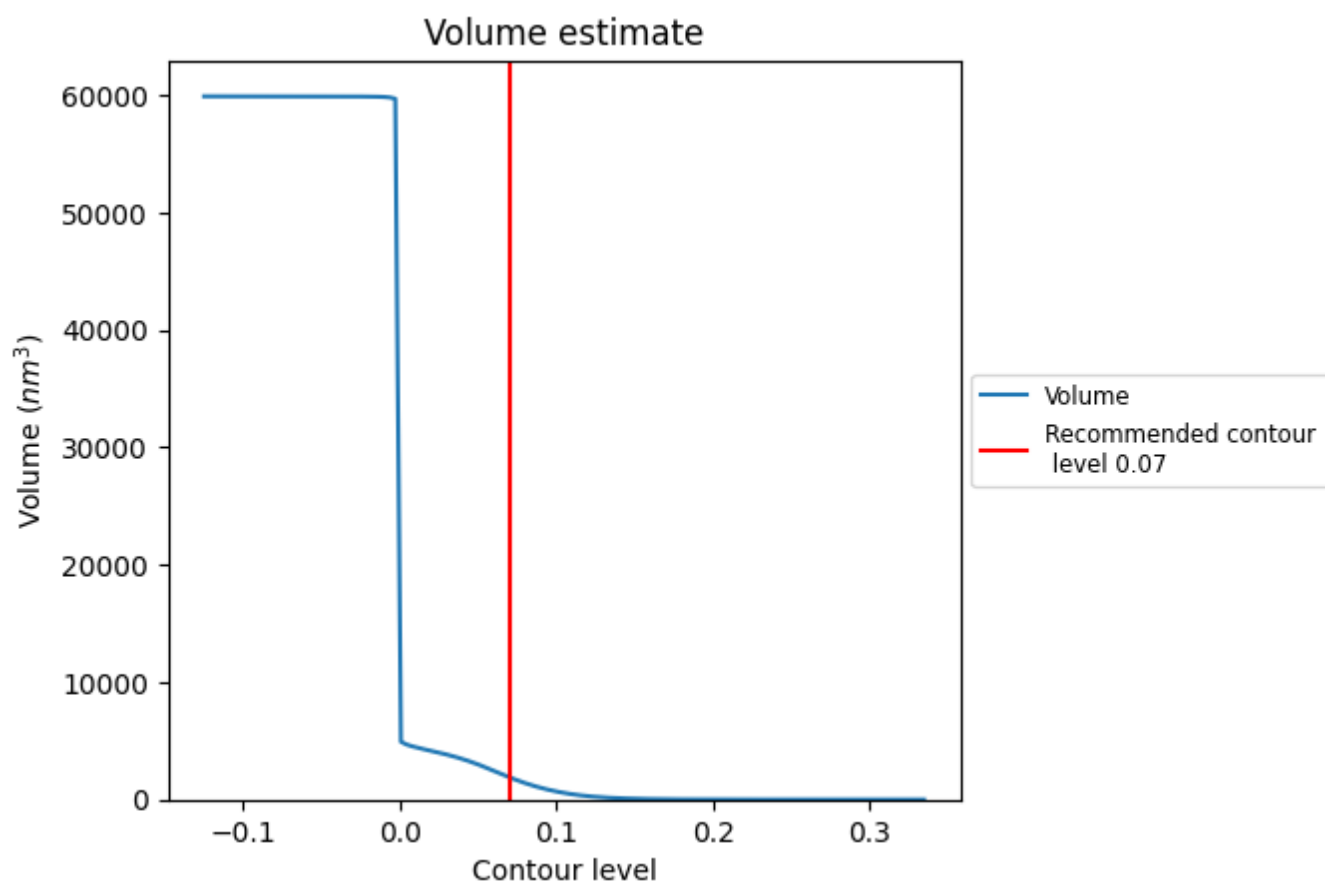
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

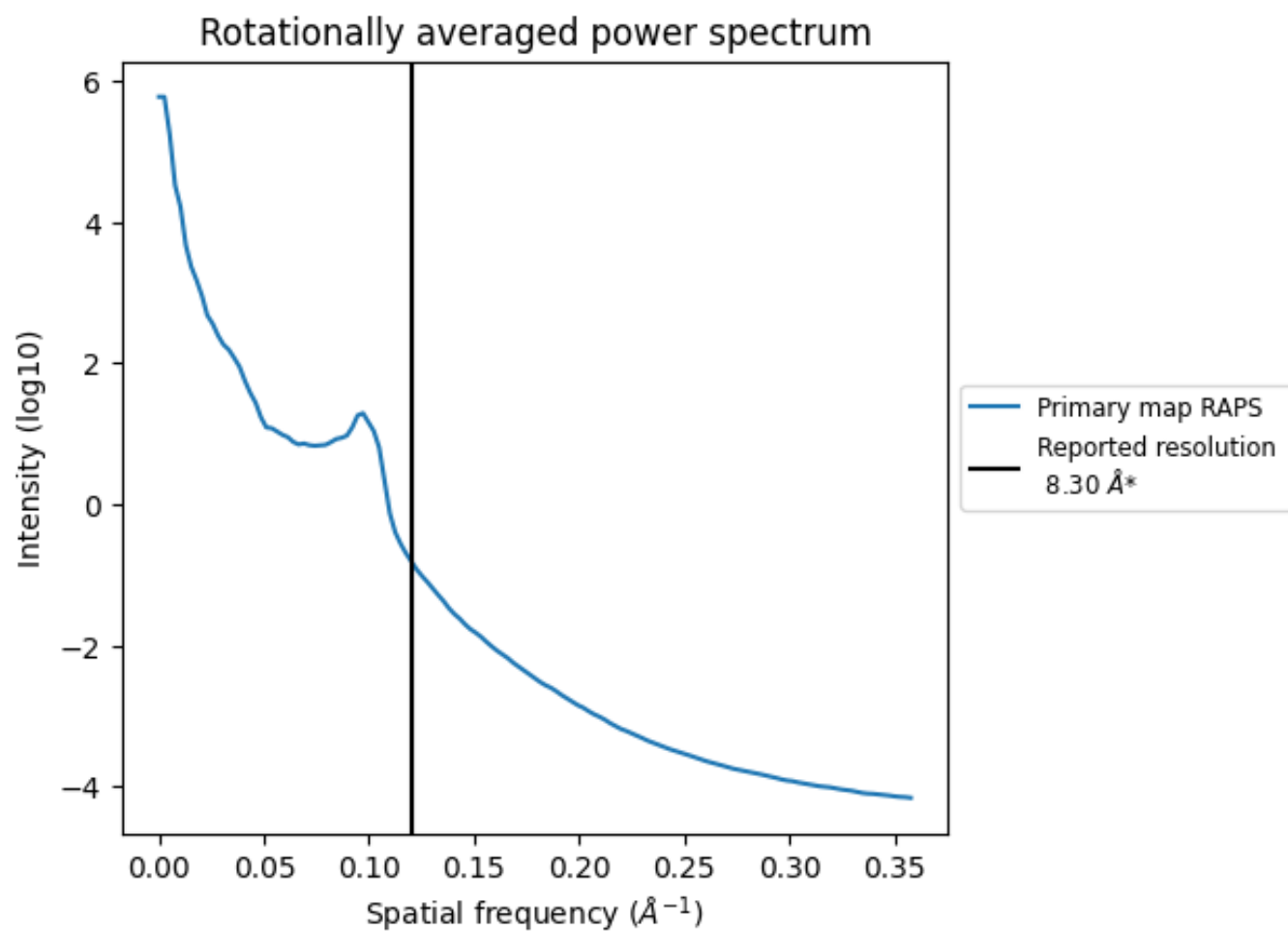
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1904 nm³; this corresponds to an approximate mass of 1720 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.120 Å⁻¹

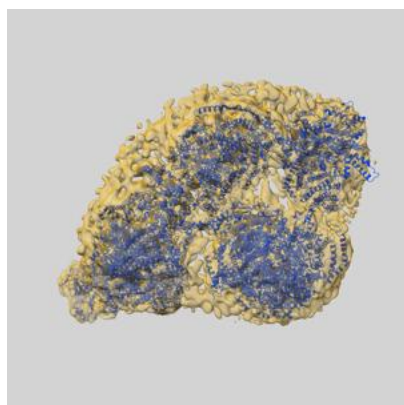
8 Fourier-Shell correlation ⓘ

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

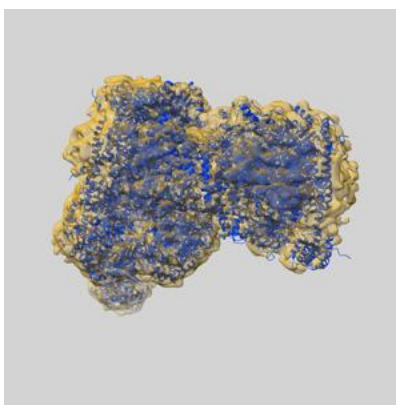
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30706 and PDB model 7DKF. Per-residue inclusion information can be found in section [3](#) on page [25](#).

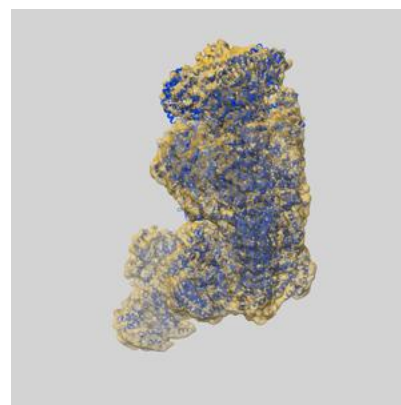
9.1 Map-model overlay [i](#)



X



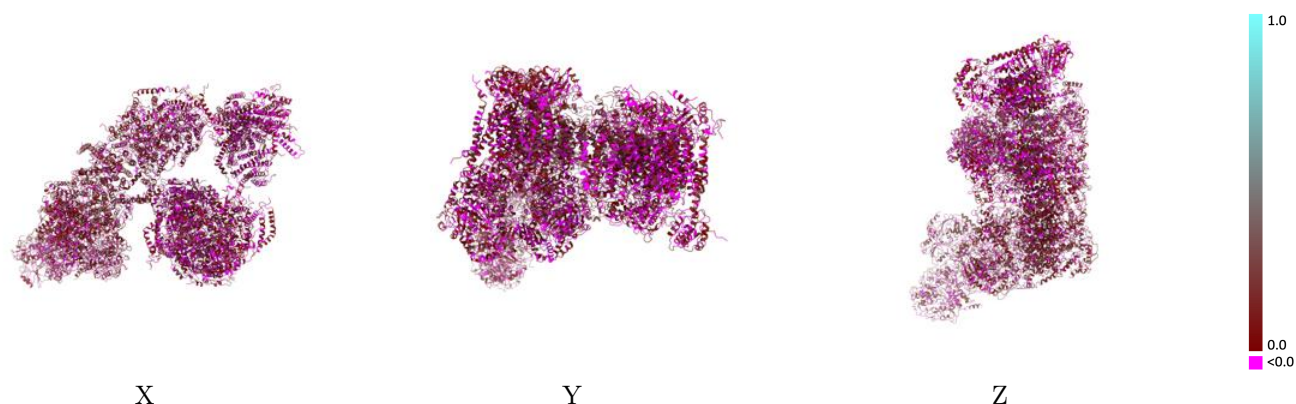
Y



Z

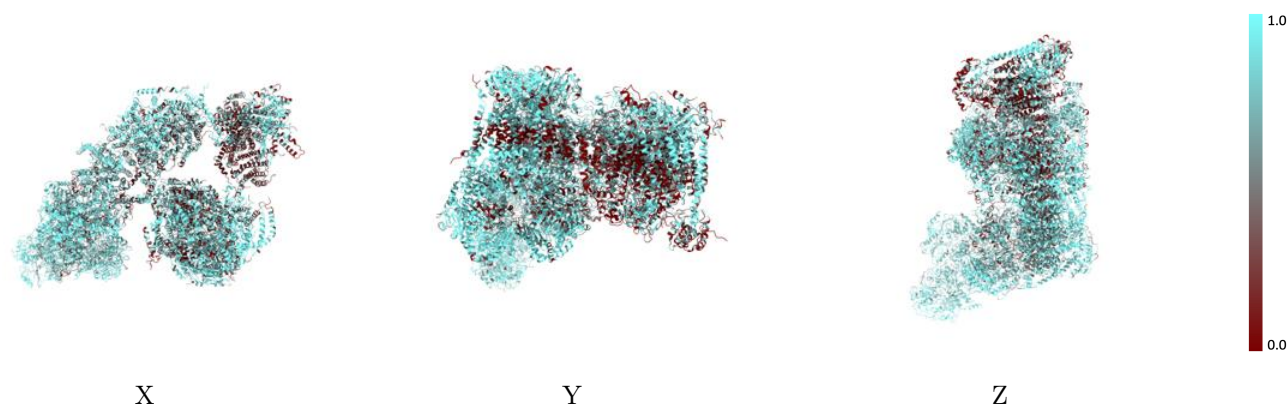
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



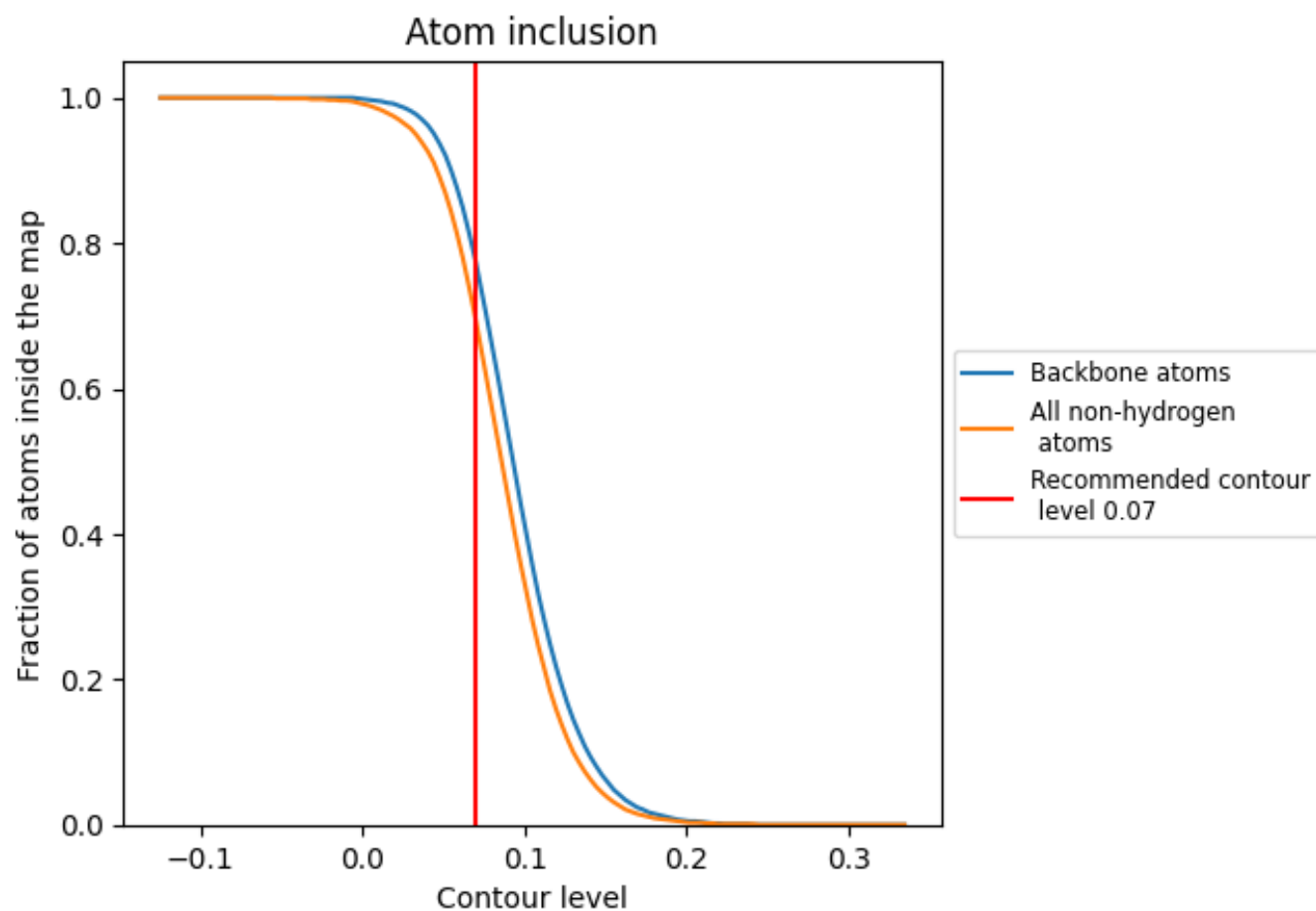
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 69% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.0740
12	 0.6860	 0.0940
22	 0.6830	 0.1120
32	 0.6530	 0.1220
42	 0.6360	 0.0960
52	 0.7230	 0.1370
62	 0.5780	 0.0660
72	 0.6180	 0.1000
82	 0.9020	 0.0870
92	 0.8570	 0.0660
A1	 0.8310	 0.0620
A2	 0.8730	 0.0890
A3	 0.4940	 0.0340
B1	 0.8390	 0.0590
B2	 0.7920	 0.0930
B3	 0.6750	 0.0240
C1	 0.6440	 0.0780
C2	 0.7840	 0.0880
C3	 0.3640	 0.0330
D1	 0.8390	 0.0660
D2	 0.7750	 0.0850
D3	 0.4080	 0.0180
E1	 0.6030	 0.0280
E2	 0.8570	 0.0840
E3	 0.4270	 0.0480
F1	 0.7560	 0.0750
F2	 0.8600	 0.1250
F3	 0.3470	 0.0430
G1	 0.6280	 0.0510
G2	 0.7500	 0.0850
G3	 0.2610	 0.0210
H1	 0.8150	 0.0760
H2	 0.8520	 0.1200
H3	 0.4570	 0.0170
I1	 0.3710	 -0.0560



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Chain	Atom inclusion	Q-score
I2	 0.6500	 0.0530
I3	 0.6620	 0.0800
J1	 0.6190	 0.0260
J2	 0.8410	 0.1030
J3	 0.2490	 0.0540
K1	 0.6160	 0.0770
K2	 0.9020	 0.1150
K3	 0.5650	 0.0470
L2	 0.7600	 0.1050
L3	 0.4180	 0.0440
M1	 0.6890	 0.0380
M2	 0.6580	 0.1210
M3	 0.4820	 0.1140
N1	 0.7870	 0.0460
N2	 0.8970	 0.1390
O1	 0.5690	 0.0530
O2	 0.7560	 0.1220
P1	 0.7400	 0.0410
P2	 0.7500	 0.1080
Q1	 0.6350	 0.0400
Q2	 0.8640	 0.1250
R1	 0.5960	 0.0680
R2	 0.7930	 0.0950
S1	 0.4540	 0.0610
S2	 0.5560	 0.1020
T1	 0.6370	 0.0660
T2	 0.5780	 0.1090
U1	 0.3420	 -0.0100
U2	 0.5780	 0.0750
V1	 0.4770	 0.0600
V2	 0.8740	 0.1340
W1	 0.3020	 0.0720
W2	 0.6500	 0.0430
X2	 0.8470	 0.1100
Y2	 0.7370	 0.0930
Z2	 0.6530	 0.0540
a2	 0.5460	 0.0940
b2	 0.8980	 0.1150
c2	 0.8810	 0.1120
d2	 0.7520	 0.0280
e2	 0.6240	 0.0750
f2	 0.6410	 0.0690

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Chain	Atom inclusion	Q-score
g2	 0.8340	 0.0960
h2	 0.7420	 0.1060
i2	 0.8430	 0.1620
j2	 0.8470	 0.1310