



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:38 AM UTC

PDB ID : 7DGQ / pdb_00007dgq
EMDB ID : EMD-30673
Title : Activity optimized supercomplex state1
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 : 2020-11-12
Resolution : 5.00 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

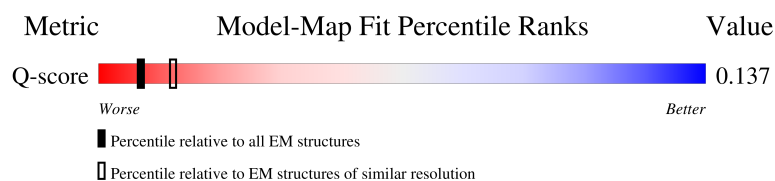
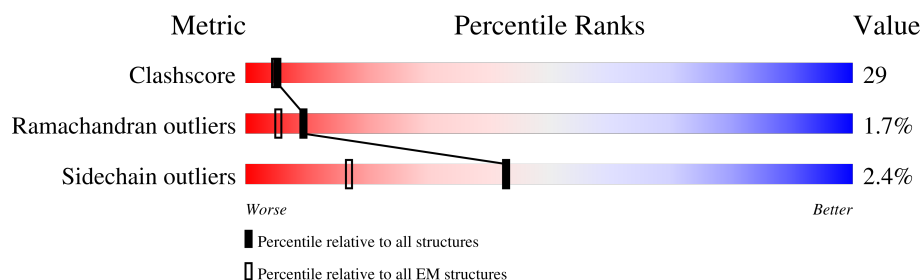
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	3	115	23% 51% 44% ..
2	1	318	7% 42% 48% 8% .
3	9	217	50% 42% .. 5%
4	7	175	11% 45% 45% 7% ..

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Mol	Chain	Length	Quality of chain
5	4	459	
6	5	98	
7	6	606	
8	2	347	
9	8	444	
10	C3	514	
11	C1	227	
12	A9	261	
13	A7	169	
14	B4	152	
15	A5	129	
16	A6	97	
17	C0	86	
18	C2	74	
19	B2	80	
20	B3	80	
21	A0	63	
22	A8	70	
23	A	704	
24	B	430	
25	C	228	
26	D	179	
27	E	176	
28	F	75	
29	G	133	

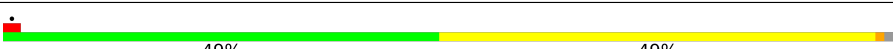
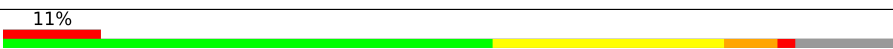
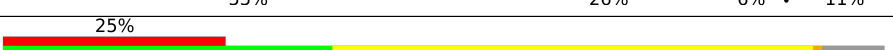
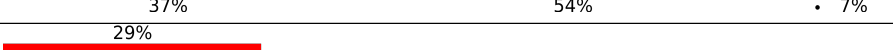
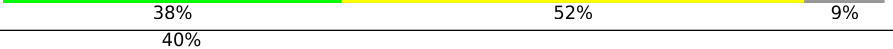
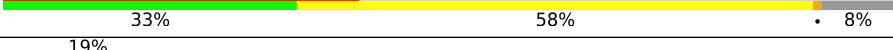
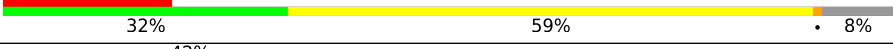
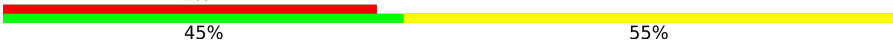
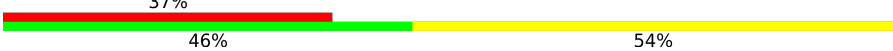
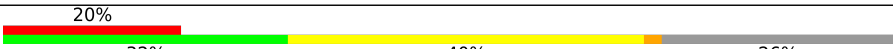
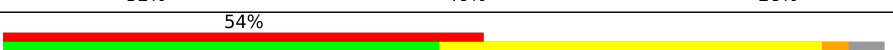
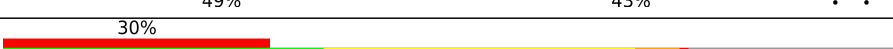
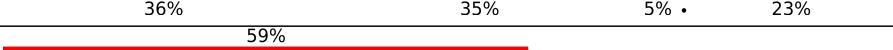
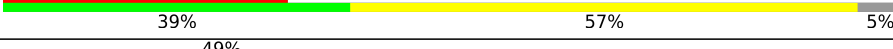
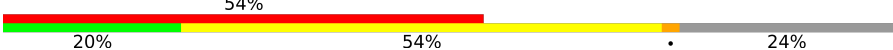
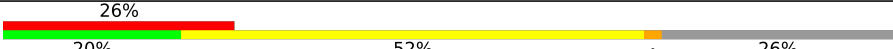
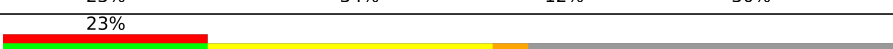
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Mol	Chain	Length	Quality of chain
30	H	105	
31	I	96	
32	J	70	
33	K	98	
34	L	83	
35	N	115	
36	O	127	
37	P	112	
38	Q	171	
39	R	345	
40	S	320	
41	T	140	
42	U	145	
43	V	143	
44	M	86	
44	W	86	
45	X	57	
46	Y	72	
47	Z	98	
48	a	128	
49	b	143	
50	c	128	
51	d	117	
52	f	178	
53	h	125	

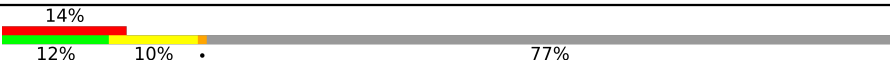
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Mol	Chain	Length	Quality of chain
54	i	49	
55	j	120	
56	g	176	
57	e	158	
58	k	480	
58	w	480	
59	l	453	
59	x	453	
60	m	379	
60	y	379	
61	o	325	
61	z	325	
62	A1	196	
62	p	196	
63	A2	111	
63	q	111	
64	A3	82	
64	r	82	
65	B7	91	
65	s	91	
66	A4	56	
66	t	56	
67	B6	64	
67	u	64	
68	B5	78	

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Mol	Chain	Length	Quality of chain
68	v	78	

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
71	FES	A	803	-	-	X	-
73	FMN	8	501	-	-	X	-
74	SF4	A	801	-	-	X	-
74	SF4	A	802	-	-	X	-
82	UQ2	A2	201	-	-	X	-

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 107321 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
1	3	112	Total	C	N	O	S	0	0
			882	596	128	151	7		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	318	Total	C	N	O	S	0	0
			2503	1678	385	417	23		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	207	Total	C	N	O	S	0	0
			1579	1006	269	294	10		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	172	Total	C	N	O	S	0	0
			1235	835	181	211	8		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	458	Total	C	N	O	S	1	0
			3577	2382	561	599	35		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	96	Total	C	N	O	S	0	0
			712	464	110	125	13		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	606	Total	C	N	O	S	0	0
			4766	3172	732	820	42		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	344	Total	C	N	O	S	0	0
			2681	1779	413	449	40		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	427	Total	C	N	O	S	0	0
			3065	1927	563	559	16		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C3	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C1	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A9	261	Total	C	N	O	S	0	0
			2125	1421	338	353	13		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A7	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B4	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A5	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C0	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C2	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B2	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B3	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A0	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A8	43	Total	C	N	O		0	0
			335	223	53	59			

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	688	Total	C	N	O	S	0	0
			5218	3273	920	988	37		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	430	Total	C	N	O	S	0	0
			3422	2185	588	624	25		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	C	208	Total	C	N	O	S	0	0
			1726	1114	297	312	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	152	Total	C	N	O	S	0	0
			1206	772	212	208	14		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	176	Total	C	N	O	S	0	0
			1401	880	243	267	11		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	28	Total	C	N	O	S	0	0
			186	118	32	35	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	123	Total	C	N	O	S	0	0
			985	622	178	182	3		

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

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	71	Total	C	N	O	S	0	0
			535	333	99	100	3		

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

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	84	Total	C	N	O		0	0
			656	412	126	118			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	90	Total	C	N	O	S	0	0
			702	445	129	126	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	309	Total	C	N	O	S	0	0
			2349	1514	420	412	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	138	Total	C	N	O	S	0	0
			923	584	162	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	138	Total	C	N	O	S	0	0
			1087	699	186	193	9		

- Molecule 44 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	86	Total	C	N	O	S	0	0
			616	400	98	114	4		
44	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

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

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d	107	Total	C	N	O	S	0	0
			710	447	134	125	4		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	h	84	Total	C	N	O	S	0	0
			658	423	115	118	2		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	i	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	k	446	Total	C	N	O	S	0	0
			3454	2159	608	667	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	436	Total	C	N	O	S	0	0
			3385	2117	599	649	20		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	l	419	Total	C	N	O	S	0	0
			3135	1969	553	606	7		
59	x	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 60 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	m	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
60	y	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 61 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	o	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
61	z	241	Total	C	N	O	S	0	0
			1906	1216	329	347	14		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	p	151	Total	C	N	O	S	0	0
			938	572	170	194	2		
62	A1	188	Total	C	N	O	S	0	0
			1117	679	207	229	2		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	q	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
63	A2	106	Total	C	N	O	S	0	0
			907	574	166	165	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	r	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
64	A3	81	Total	C	N	O	S	0	0
			676	438	125	112	1		

- Molecule 65 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	s	67	Total	C	N	O	S	0	0
			548	332	99	112	5		
65	B7	69	Total	C	N	O	S	0	0
			566	342	101	118	5		

- Molecule 66 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	t	33	Total	C	N	O	0	0
			262	174	46	42		
66	A4	39	Total	C	N	O	0	0
			318	212	56	50		

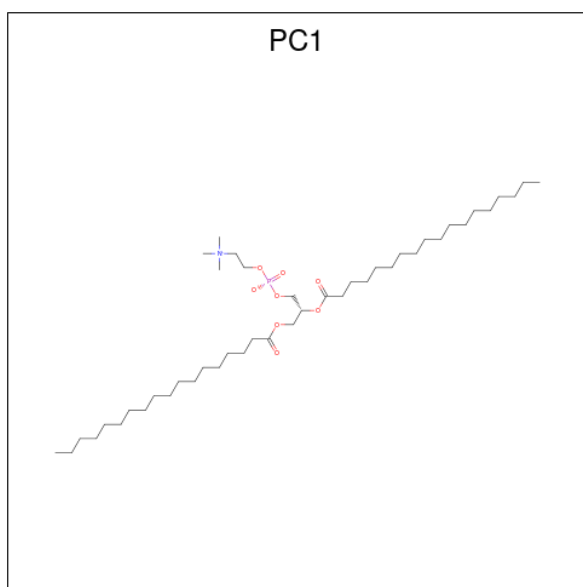
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	u	62	Total	C	N	O	0	0
			511	335	89	87		
67	B6	62	Total	C	N	O	0	0
			511	335	89	87		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

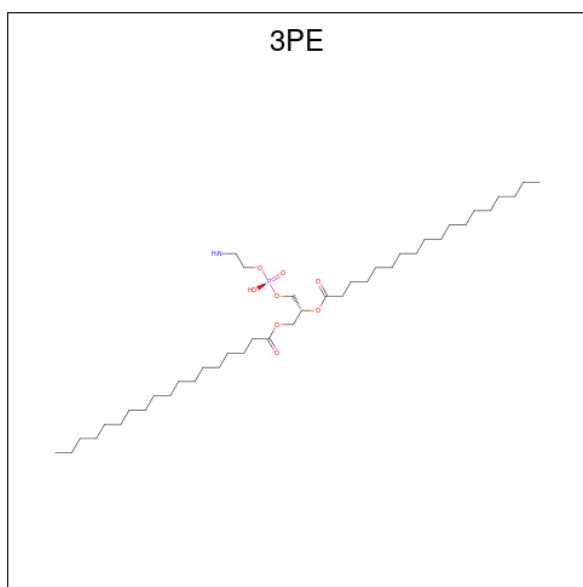
Mol	Chain	Residues	Atoms				AltConf	Trace
68	v	18	Total	C	N	O	0	0
			114	70	22	22		
68	B5	22	Total	C	N	O	0	0
			148	91	30	27		

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



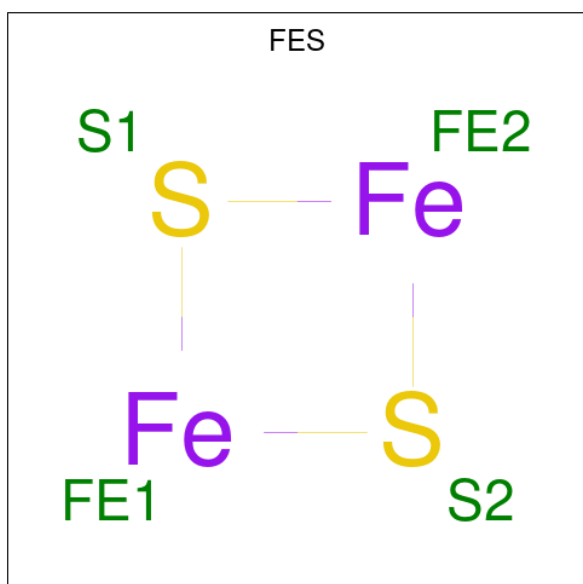
Mol	Chain	Residues	Atoms					AltConf
69	3	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 70 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



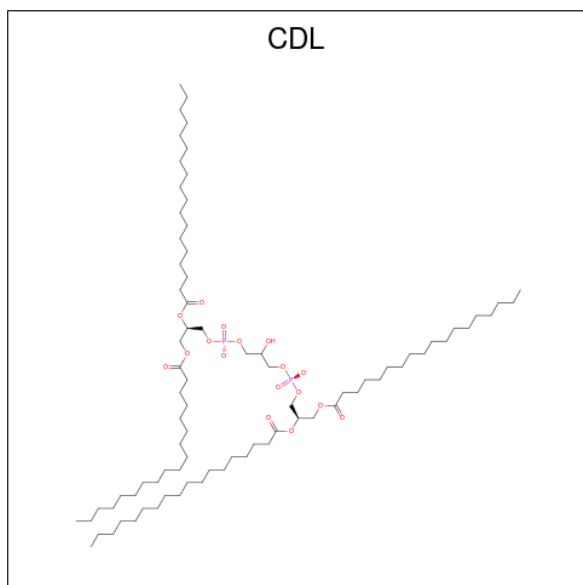
Mol	Chain	Residues	Atoms					AltConf
70	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	j	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



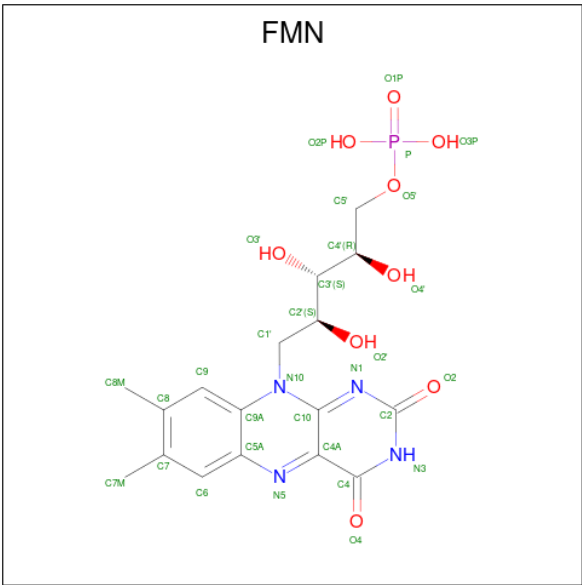
Mol	Chain	Residues	Atoms			AltConf
71	9	1	Total	Fe	S	0
			4	2	2	
71	A	1	Total	Fe	S	0
			4	2	2	
71	m	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



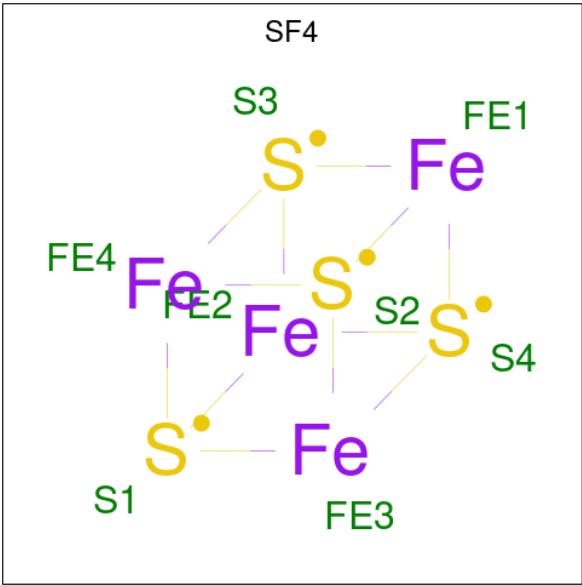
Mol	Chain	Residues	Atoms				AltConf
72	6	1	Total	C	O	P	0
			64	45	17	2	
72	J	1	Total	C	O	P	0
			58	39	17	2	
72	b	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 73 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
73	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
74	8	1	Total	Fe	S	0
			8	4	4	
74	A	1	Total	Fe	S	0
			8	4	4	
74	A	1	Total	Fe	S	0
			8	4	4	

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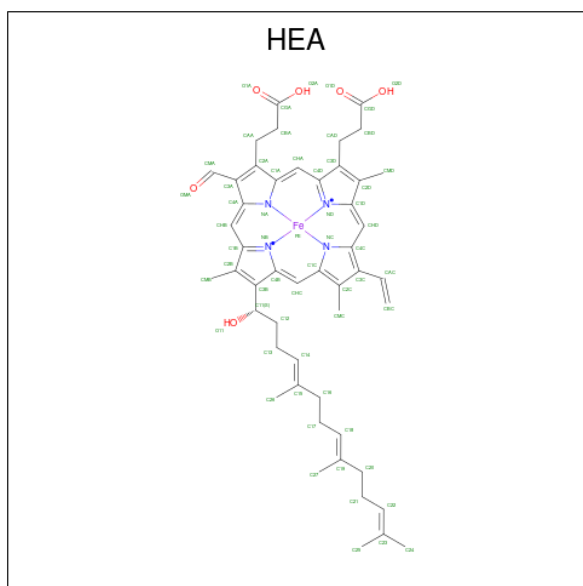
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Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 75 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	C3	1	Total	Cu	0
			1	1	
75	C1	2	Total	Cu	0
			2	2	

- Molecule 76 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
76	C3	1	Total 60	C 49	Fe 1	N 4	O 6	0
76	C3	1	Total 60	C 49	Fe 1	N 4	O 6	0

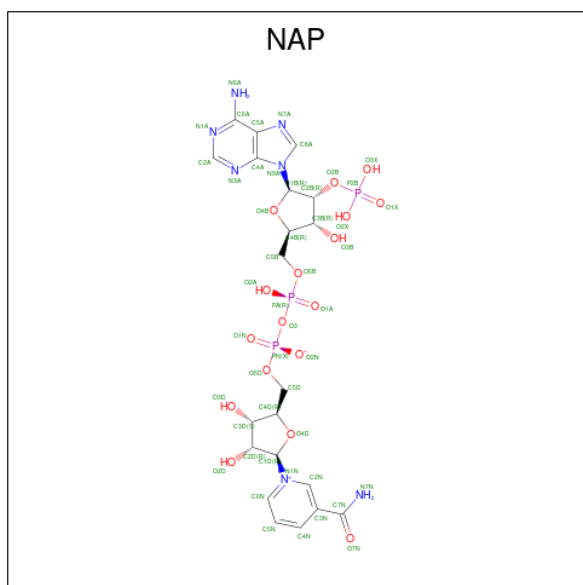
- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	C1	1	Total	Mg	0
			1	1	

- Molecule 78 is ZINC ION (CCD ID: ZN) (formula: Zn).

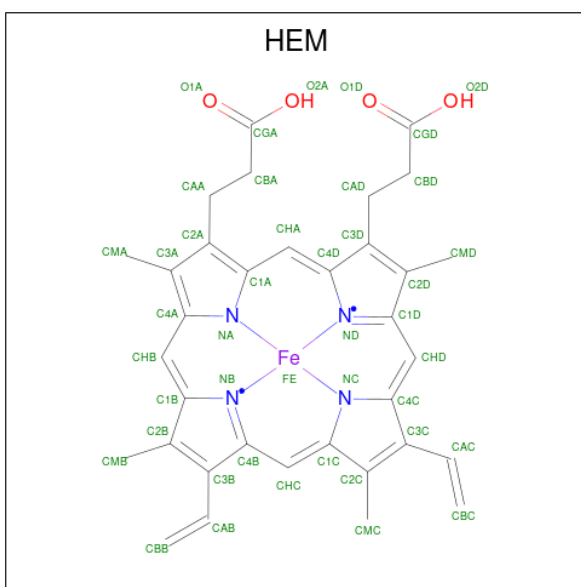
Mol	Chain	Residues	Atoms		AltConf
78	A5	1	Total	Zn	0
			1	1	
78	I	1	Total	Zn	0
			1	1	

- Molecule 79 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



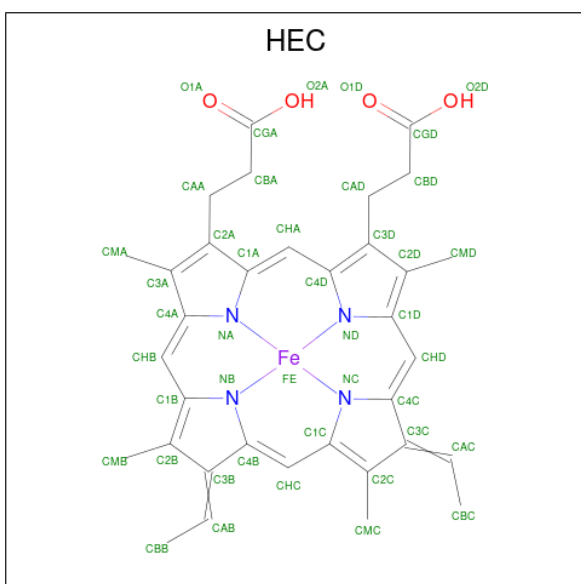
Mol	Chain	Residues	Atoms					AltConf
79	R	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



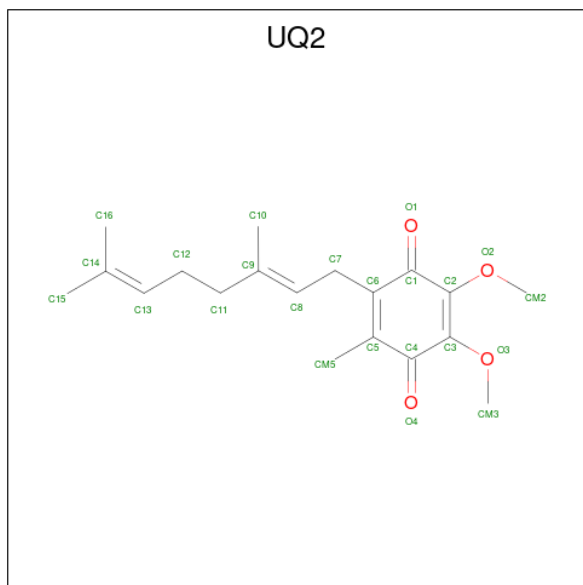
Mol	Chain	Residues	Atoms					AltConf
80	m	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	m	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
81	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	z	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).

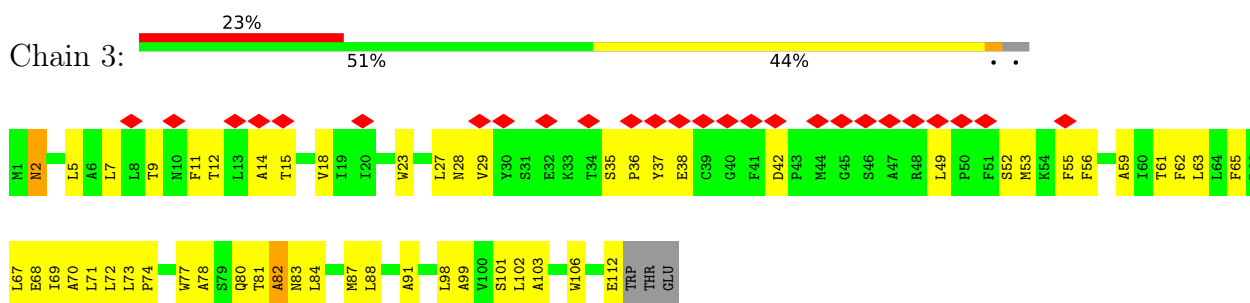


Mol	Chain	Residues	Atoms				AltConf
82	A2	1	Total	C	O		0
			23	19	4		

3 Residue-property plots

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

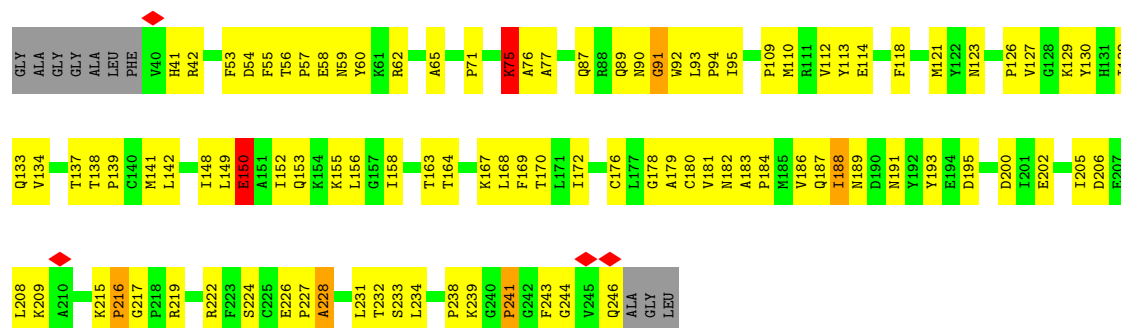


- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

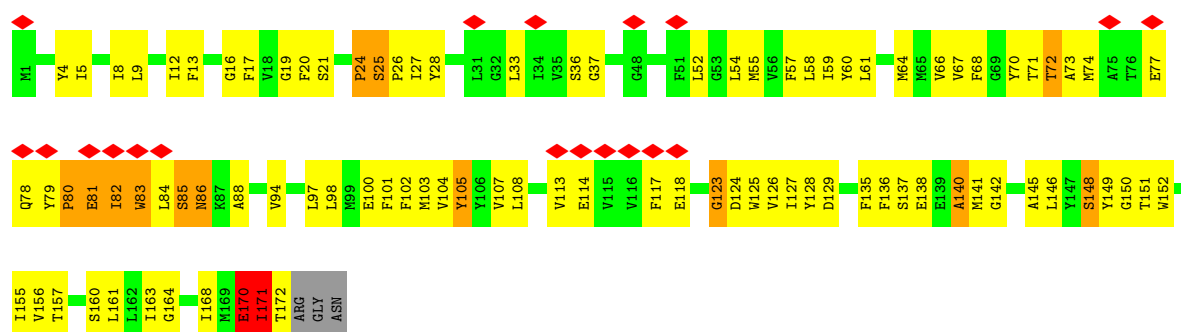
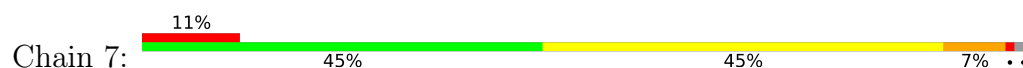


- Molecule 3: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

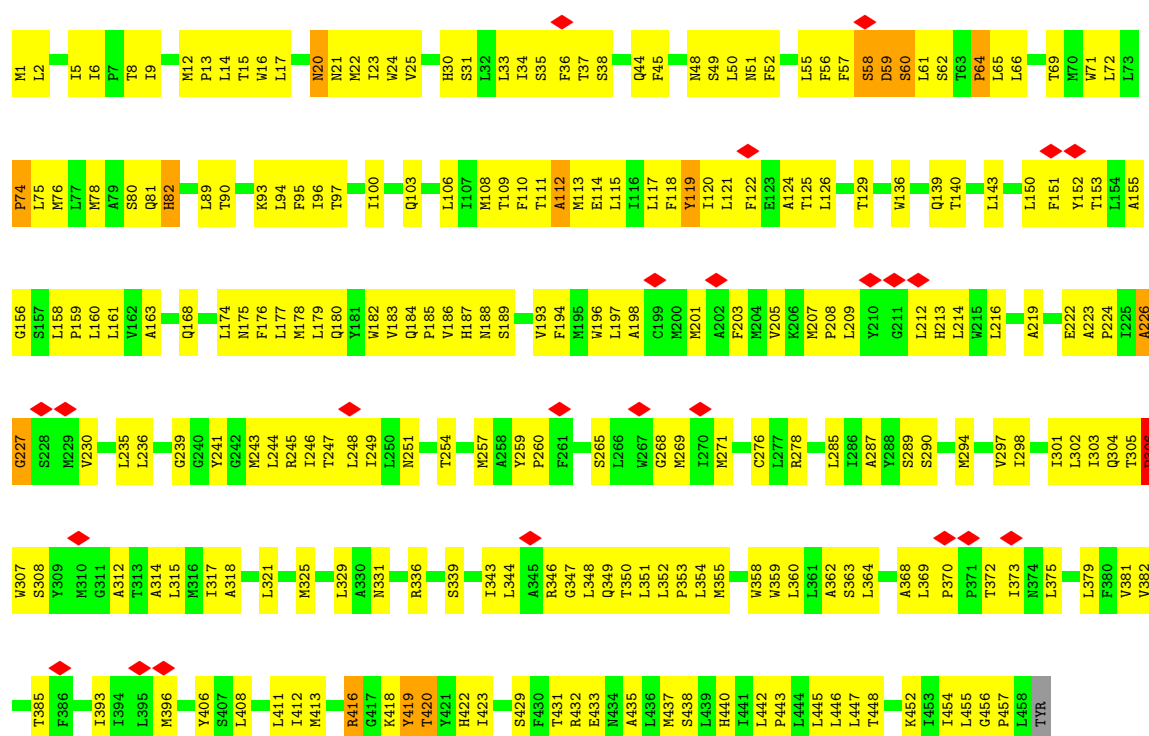




• Molecule 4: NADH-ubiquinone oxidoreductase chain 6



• Molecule 5: NADH-ubiquinone oxidoreductase chain 4



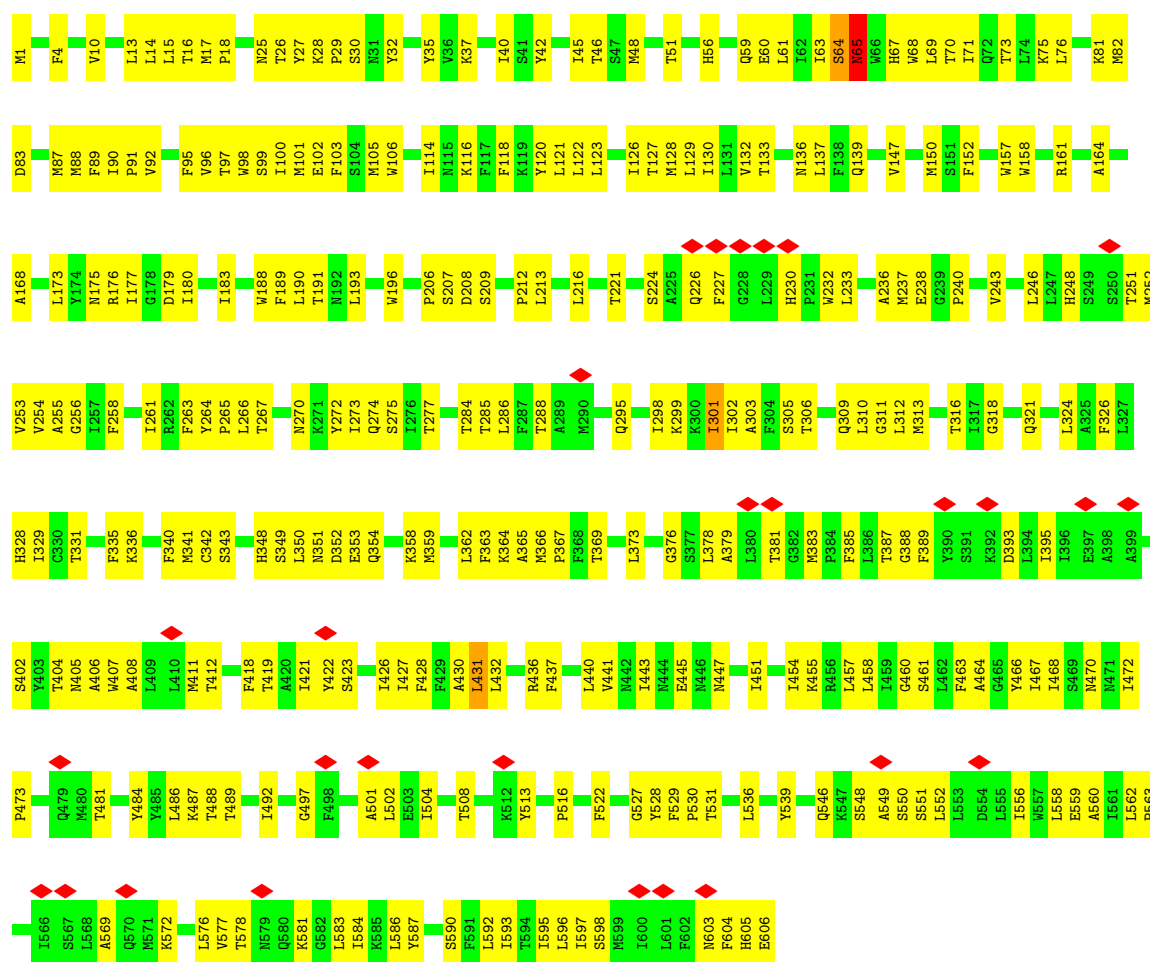
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5:  46% 45% 7%



• Molecule 7: NADH-ubiquinone oxidoreductase chain 5

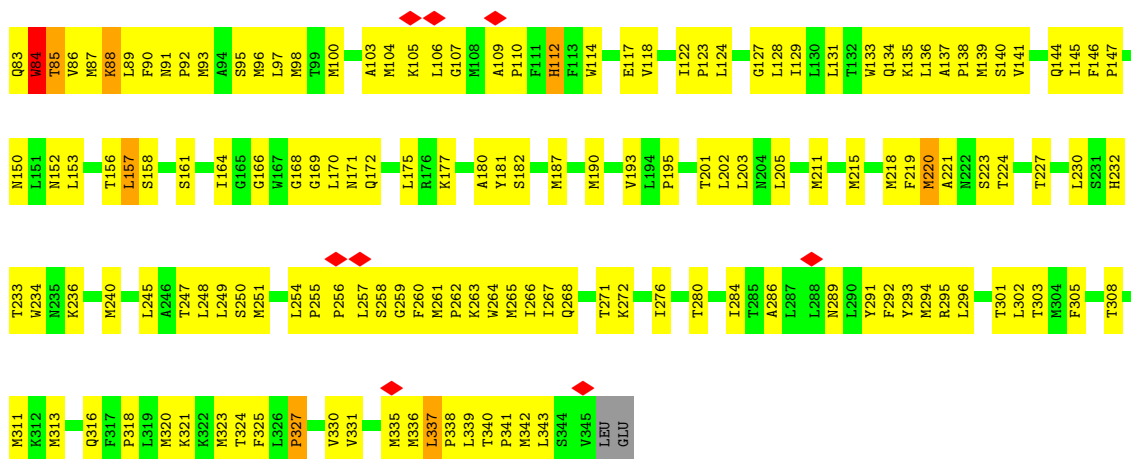
Chain 6:  5% 52% 48%



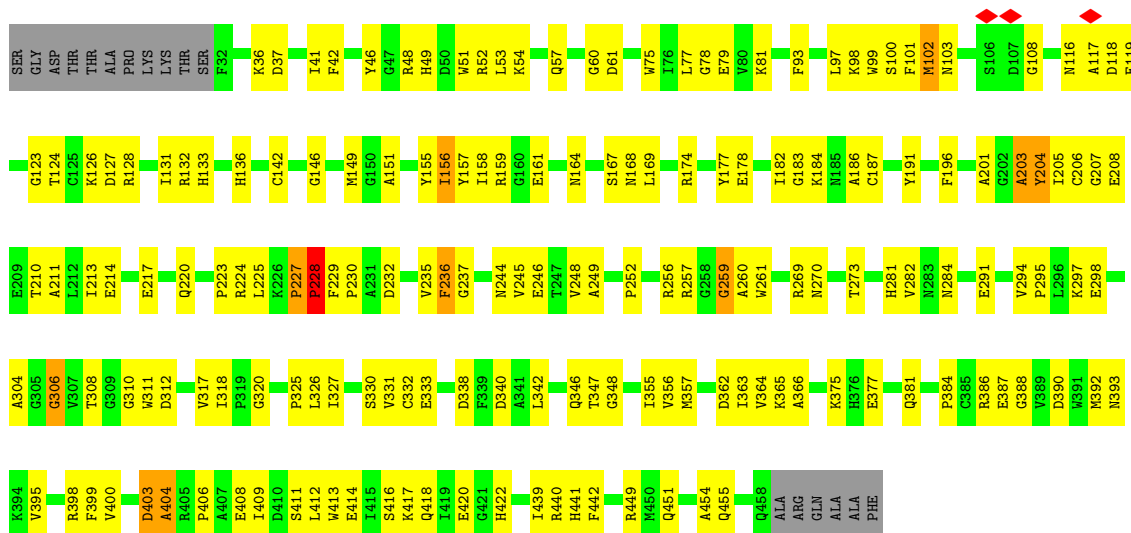
• Molecule 8: NADH-ubiquinone oxidoreductase chain 2

Chain 2:  45% 51% 2%

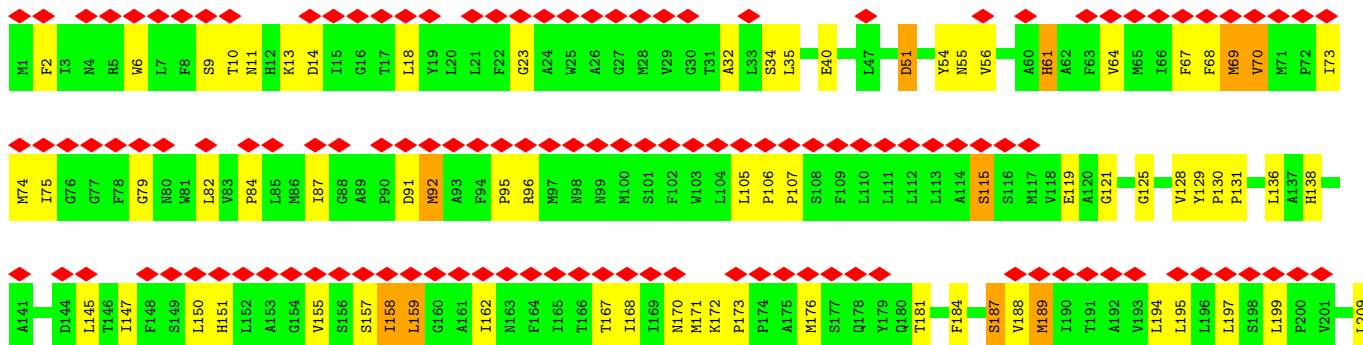
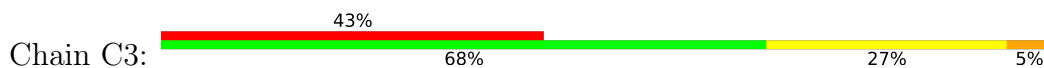


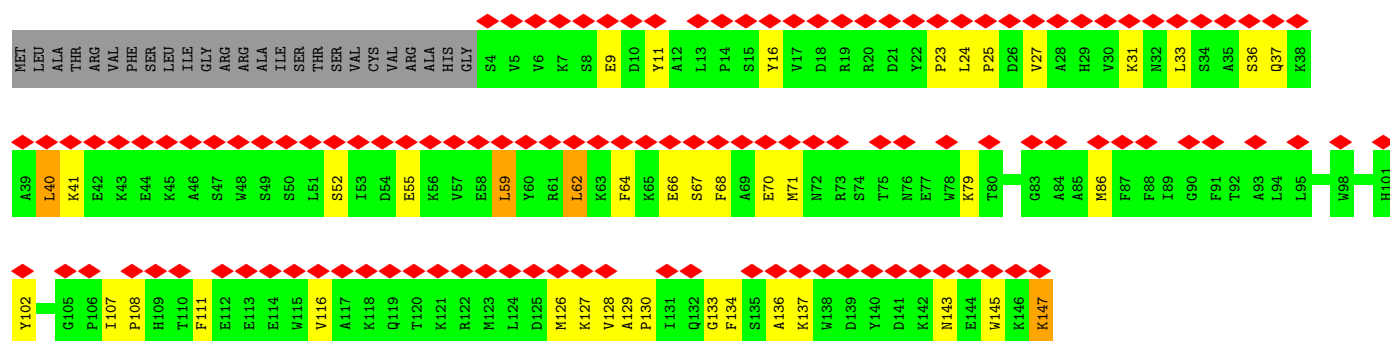
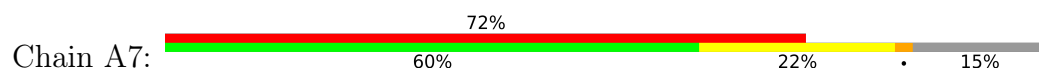


• Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

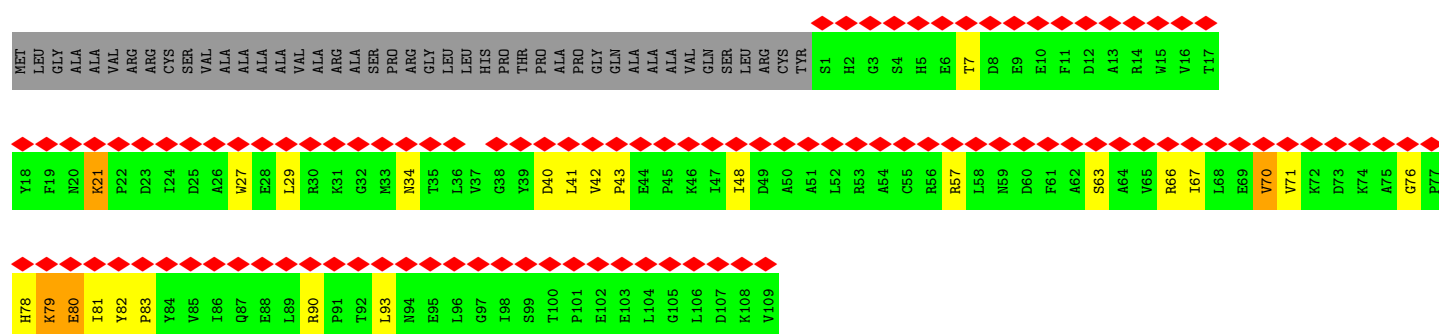
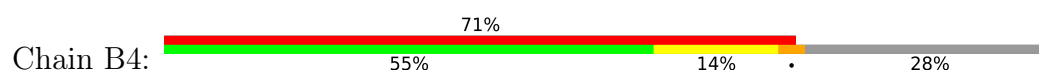


• Molecule 10: Cytochrome c oxidase subunit 1

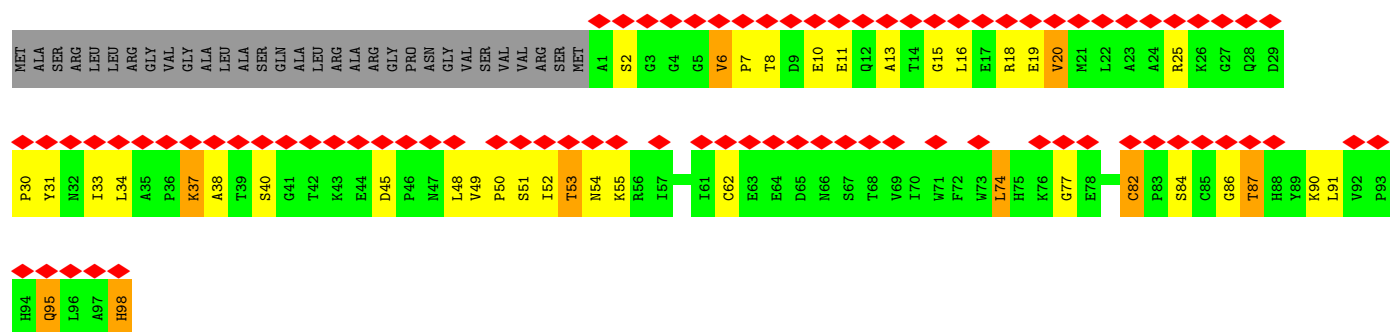




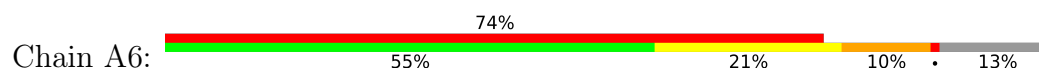
• Molecule 14: Cytochrome c oxidase subunit 5A, mitochondrial

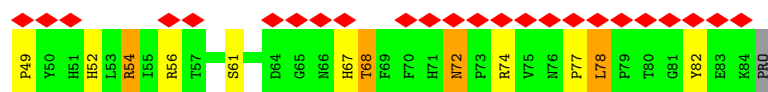


• Molecule 15: Cytochrome c oxidase subunit 5B, mitochondrial

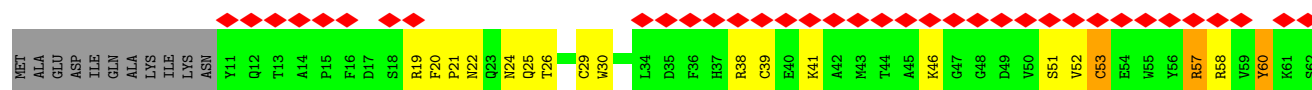


• Molecule 16: Cytochrome c oxidase subunit 6A2, mitochondrial

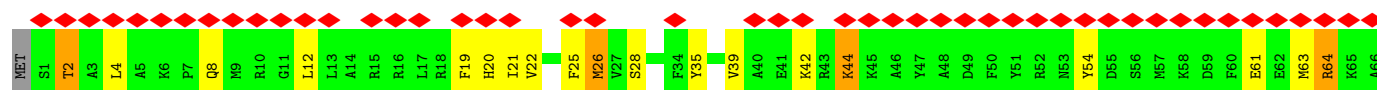
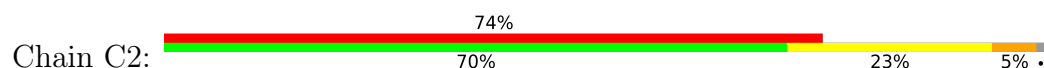




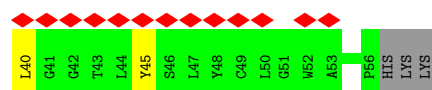
• Molecule 17: Cytochrome c oxidase subunit 6B1



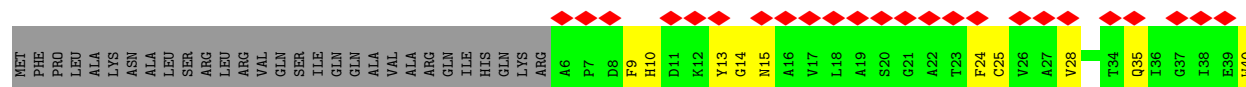
• Molecule 18: Cytochrome c oxidase subunit 6C



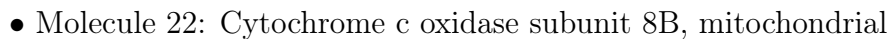
• Molecule 19: Cytochrome c oxidase subunit 7A1, mitochondrial



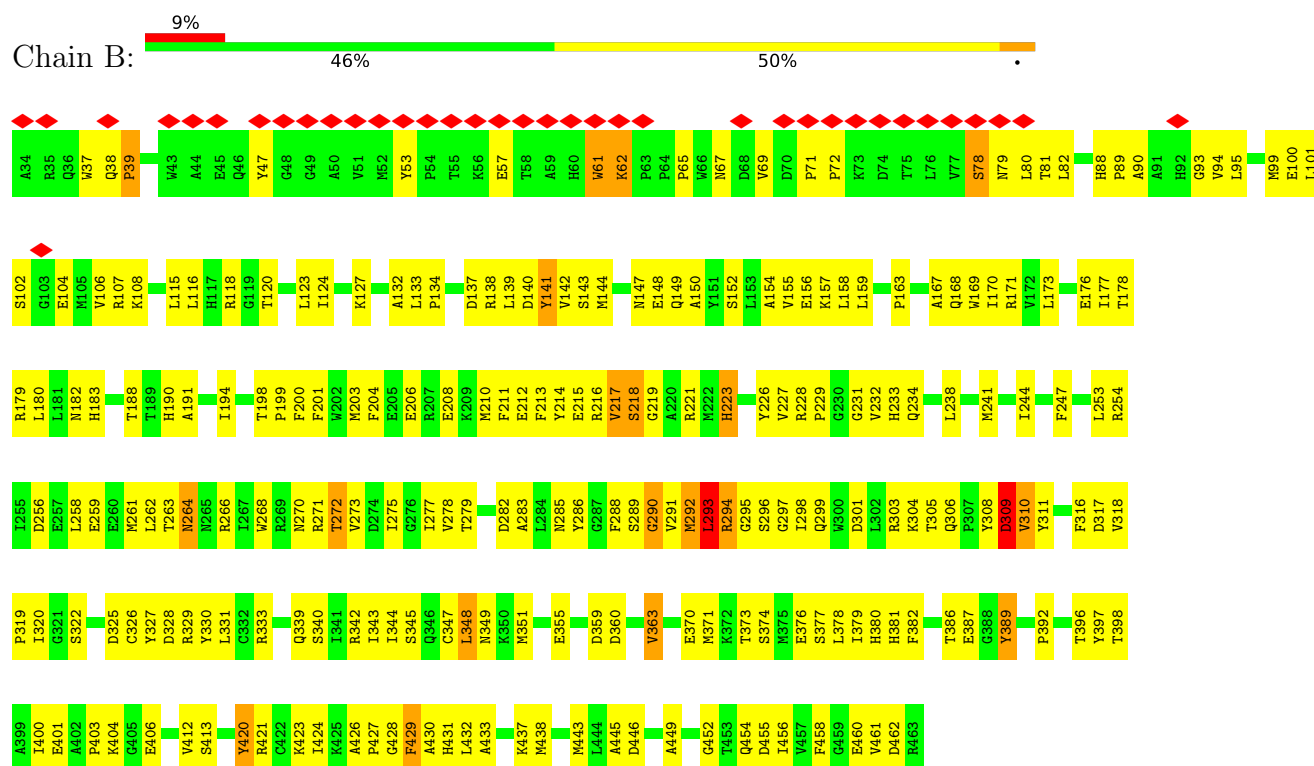
• Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial



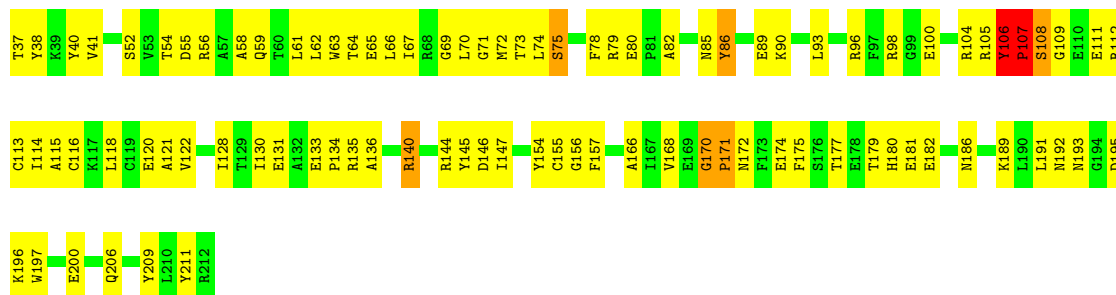
• Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





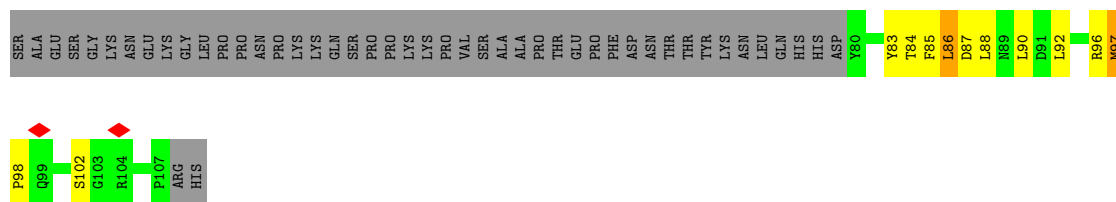
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E: 48% 48%



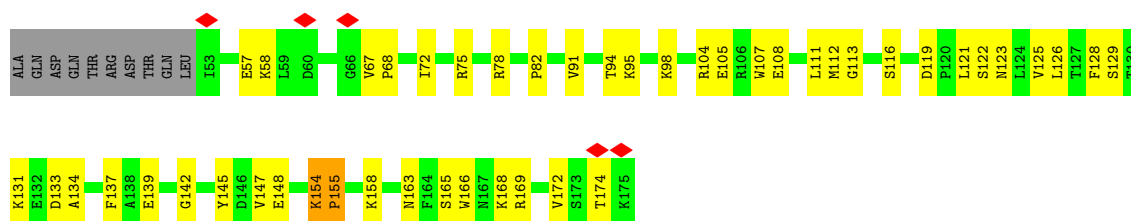
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F: 21% 13% 63%



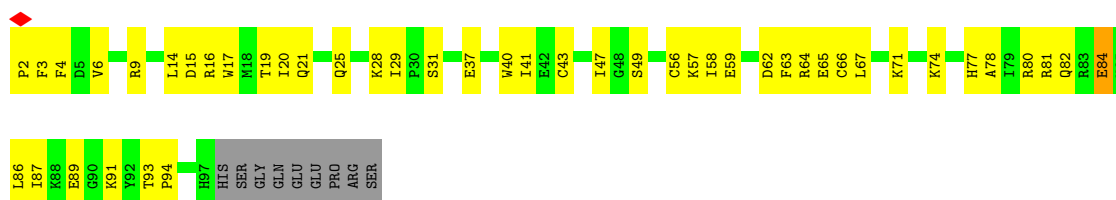
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G: 57% 34% 8%



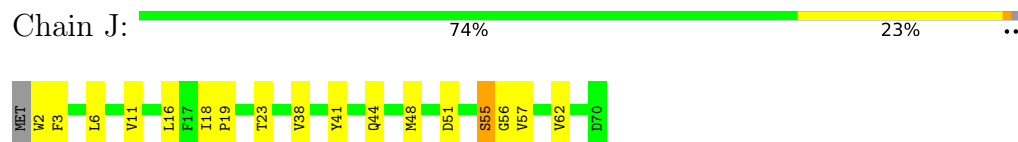
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain H: 48% 43% 9%

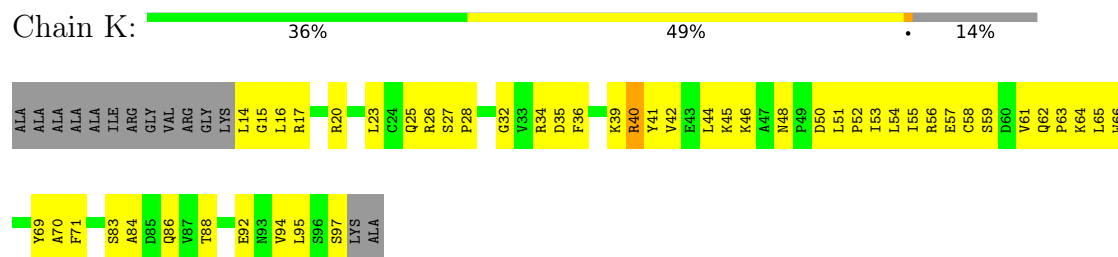


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

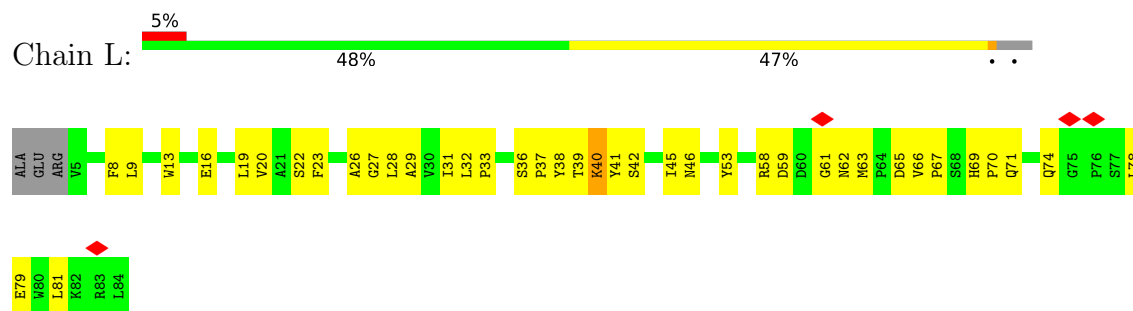
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



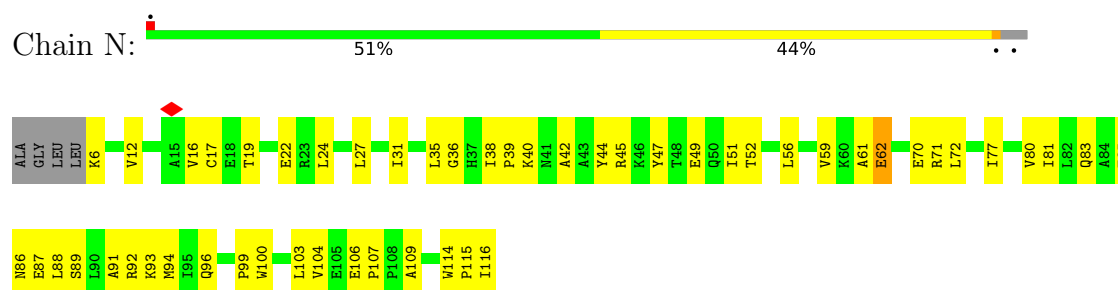
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

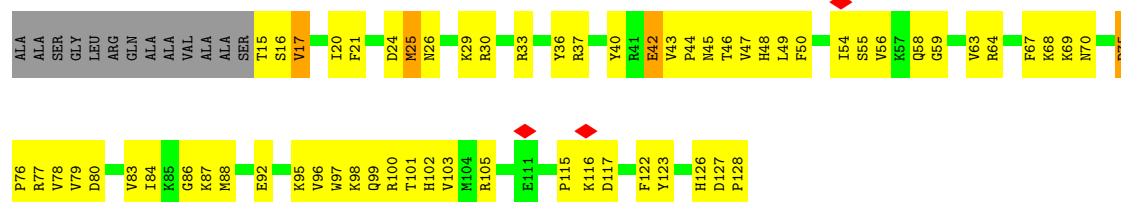


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



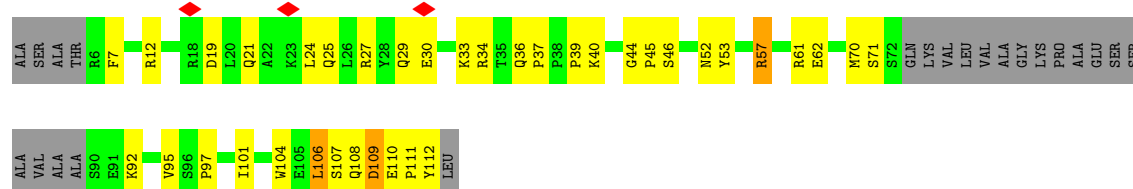
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O: 



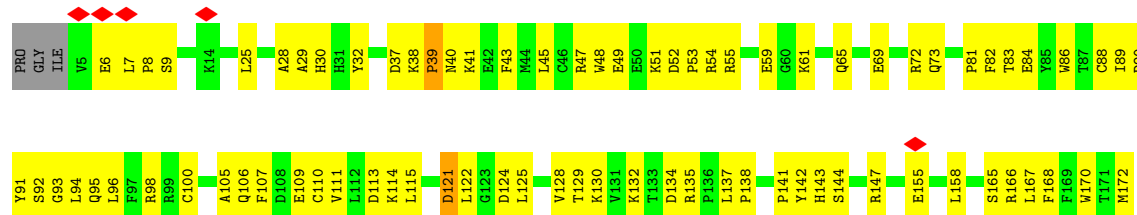
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P: 



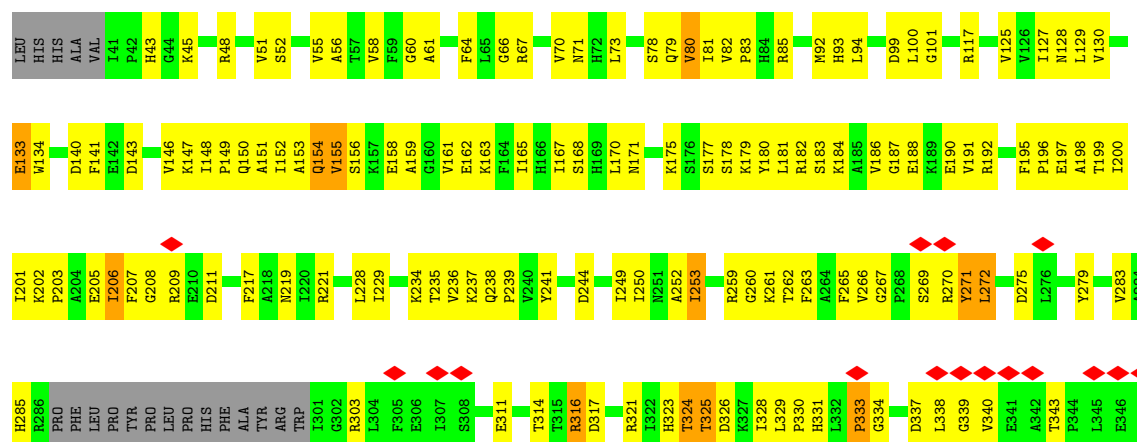
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Q: 



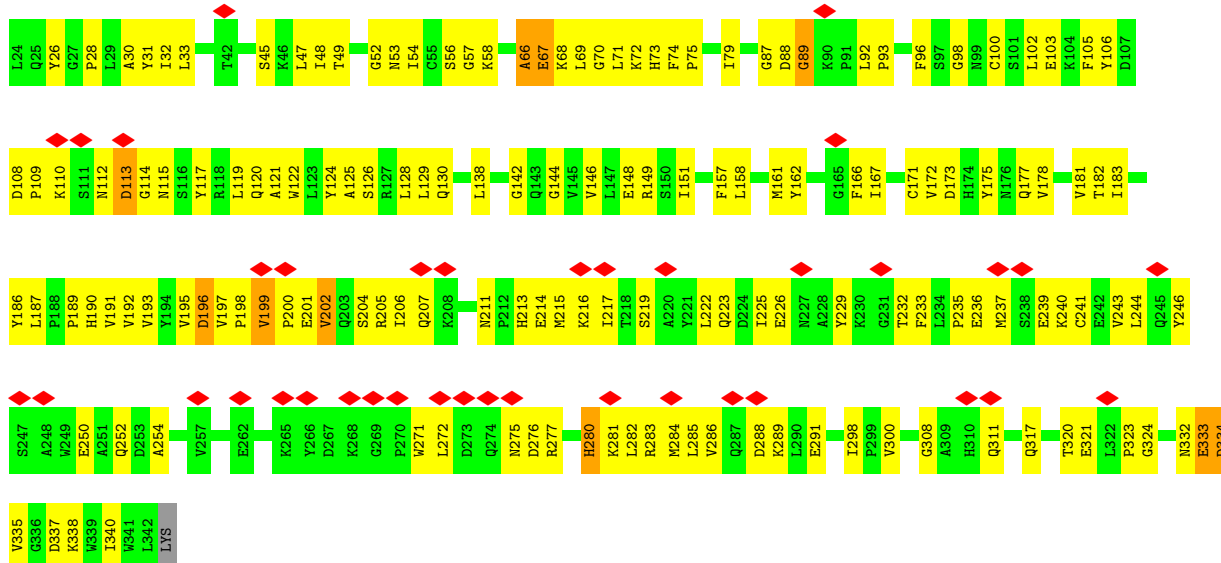
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R: 

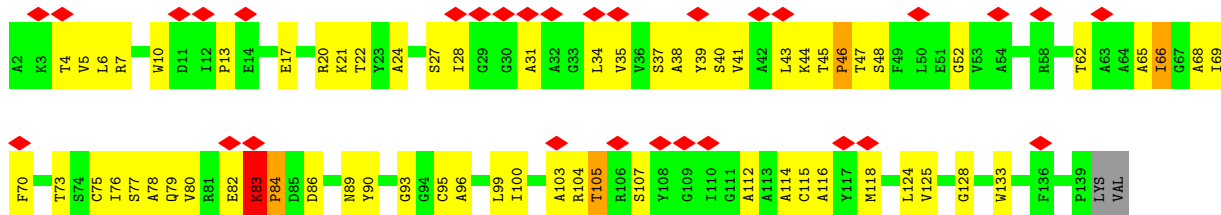




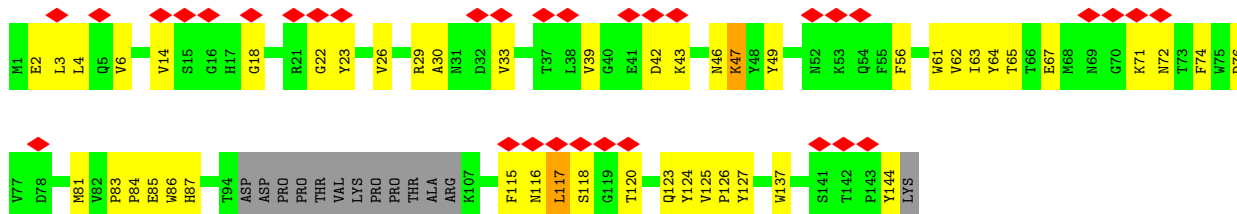
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



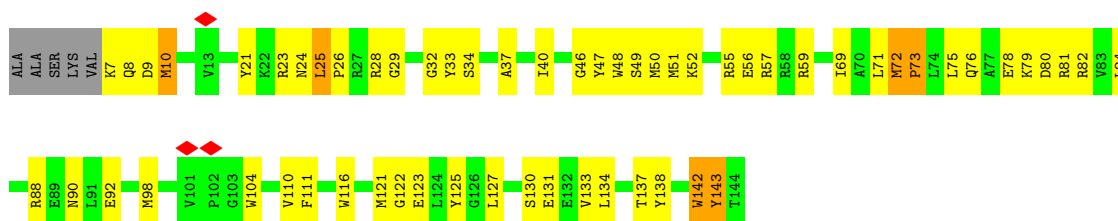
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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



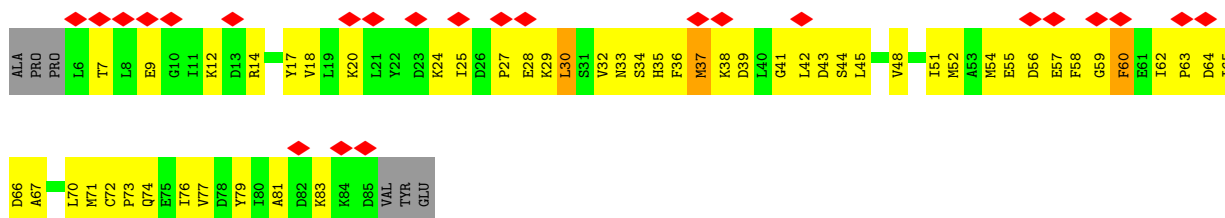
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 44: Acyl carrier protein, mitochondrial



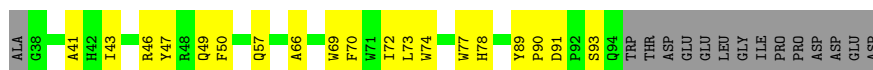
- Molecule 44: Acyl carrier protein, mitochondrial



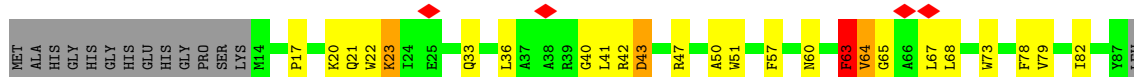
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



GLU
SER
PHE
GLN
LYS
LYS
ASP
LYS
LYS
HIS

- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain a: 9% 61% 28% 11%

SER PHE PRO LYS TYR GLU ALA SER ARG LEU SER LEU PRO T16 E22 I25 S26 S27 E28 T29 R30 L37 R40 L43 E46 Y47 Q50 Y51 Y52 D53 P54 S55 R56 R57 G58 V59 A64 W68 T69 Y70 N75 I76 N79 F80 T84 K85 T86

G90 A91 L92 F93 G94 I95 L98 F105 D108 R109 D110 L121 D122 N126 I127 S128 Y129

- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain b: 57% 40% 3%

SER GLY ASP HIS K52 K53 G61 K65 R66 F67 L68 K69 L70 L76 G79 A83 T87 V91 F92 I93 A96 E97 E100 I101 W110 E111 Y112 R119 W120 I121 A122 G128 P129 E130 K131 N132 Y133 E134 R135 T136 M137 A138 I139 E143 A144 E145

K146 L149 R150 L151 K152 E153 R157 R158 L159 M160 R161 A162 R163 G164 D165 G166 P167 W168 I174 K184 A185 T186 P187 D188 N189

- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain c: 38% 31% 30%

NET SER GLY TYR T5 P6 E7 R11 L12 Q13 Q14 L15 R16 E17 L18 R19 R20 R21 K24 L28 S29 P30 R31 E32 P33 V34 L35 L36 P37 Q38 R39 V40 S41 PRO VAL GLU ARG PHE TRP ASN LYS PHE LEU GLN ASP GLY ALA LEU TRP LYS ASN VAL ILE TYR T64

Y65 R66 H67 S68 A71 V75 L76 P78 H83 R87 Y88 H89 T92 K93 P94 R94 K95 T96 R103 I104 F105 P106 G107 V116 ILE PRO PRO MET LYS GLU PHE PRO ASP GLN HIS HIS

- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

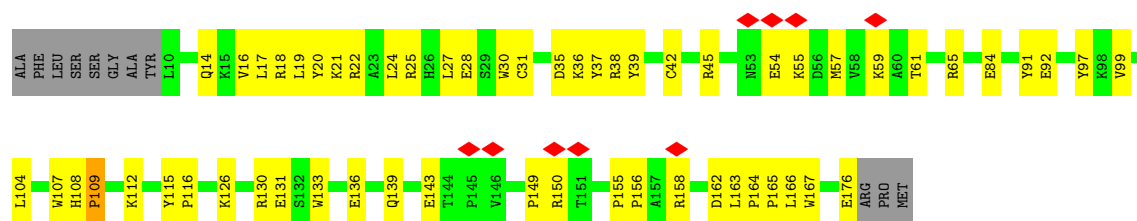
Chain d: 65% 24% 9%

GLY ALA HIS LEU A6 Y9 L10 A13 D18 P19 L20 F25 F31 P32 E33 R34 K35 E36 K39 V40 A41 T42 Q43 K46 Q50 R56 L63 F66 K70 F74 P75 N76 F77 L78 H82 E83 D86 W87 D88 H92 Y96 R104

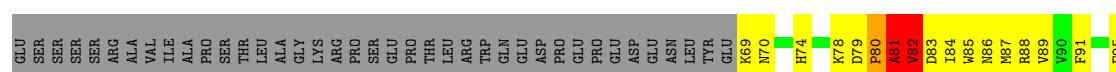
K112 LYS ARG ARG GLU GLN ARG

- Molecule 52: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

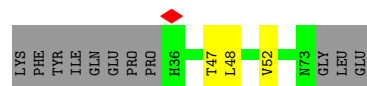
Chain f: 5% 61% 32% 6%



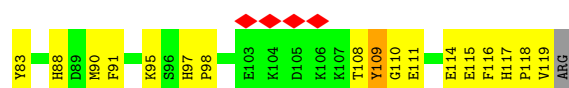
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2

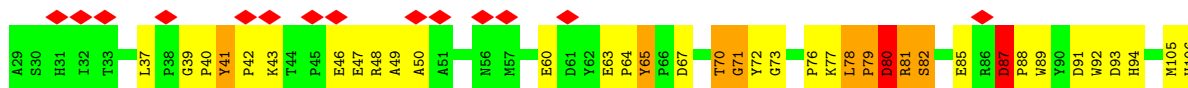


- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

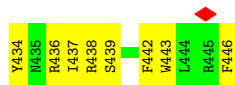
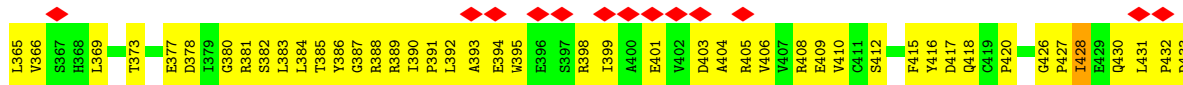
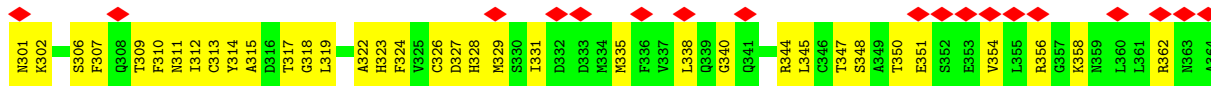
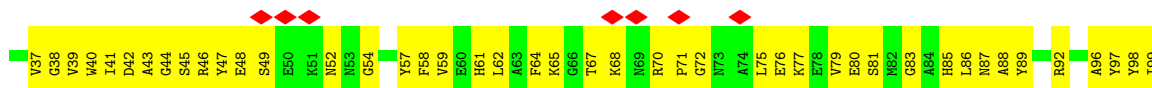
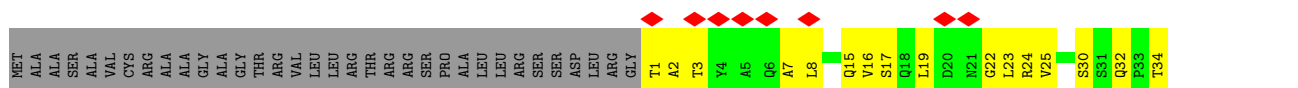




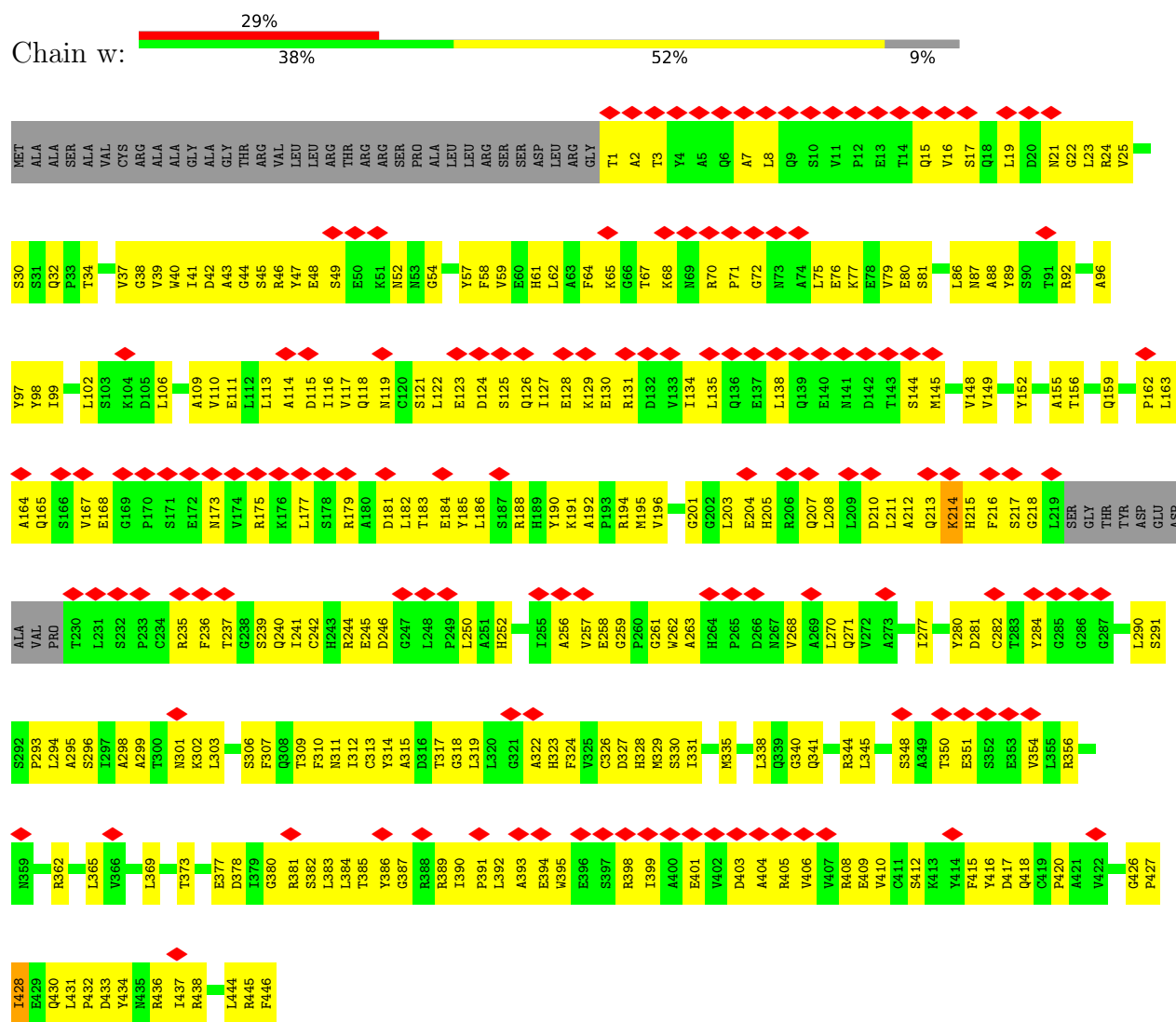
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



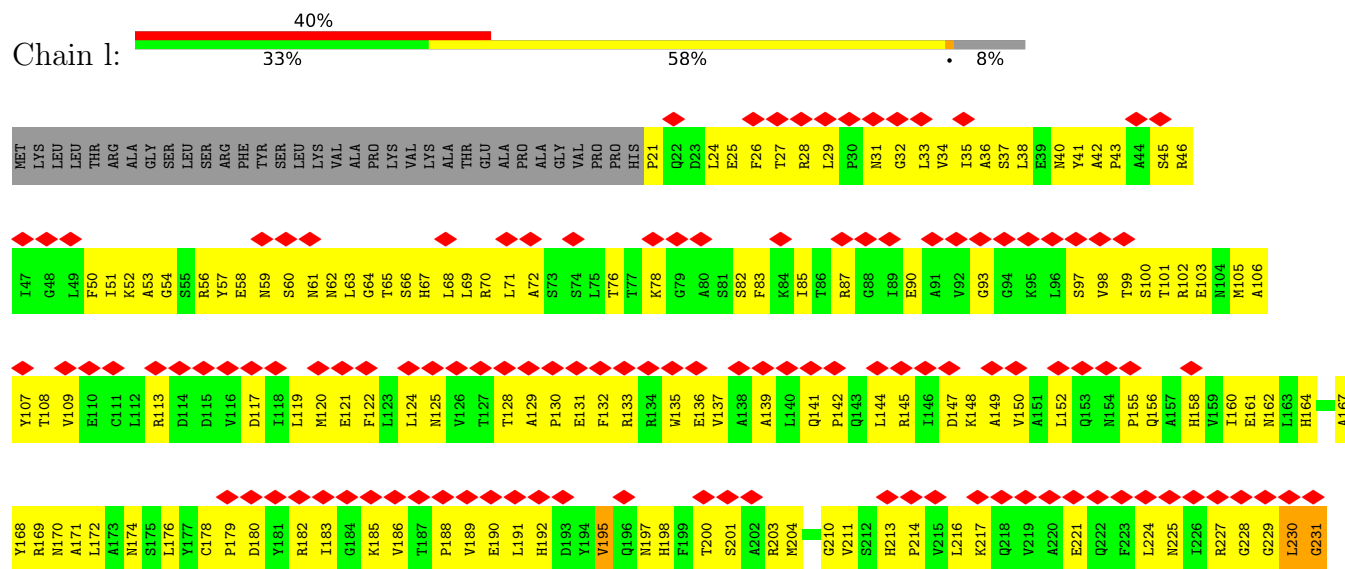
- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial

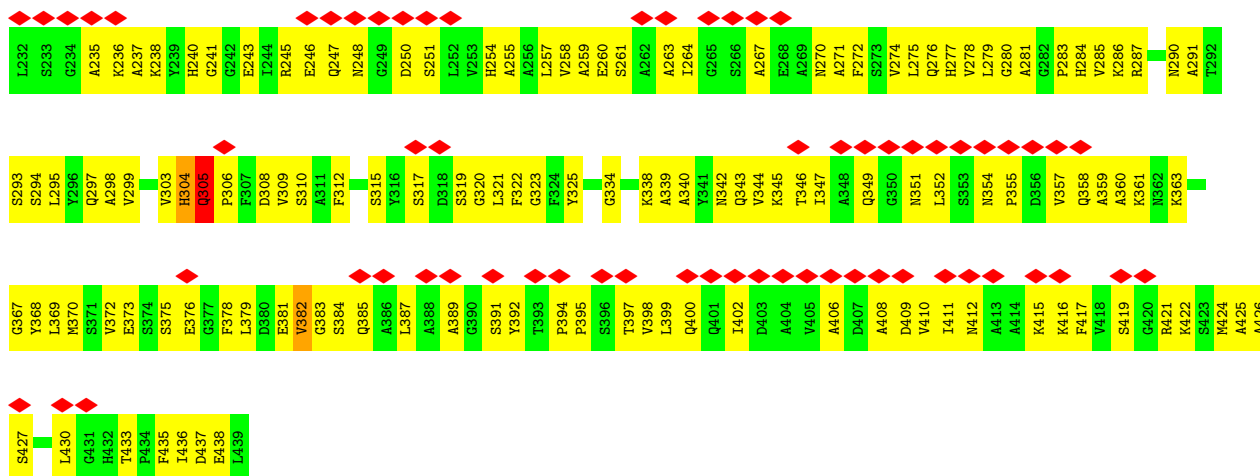


- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial

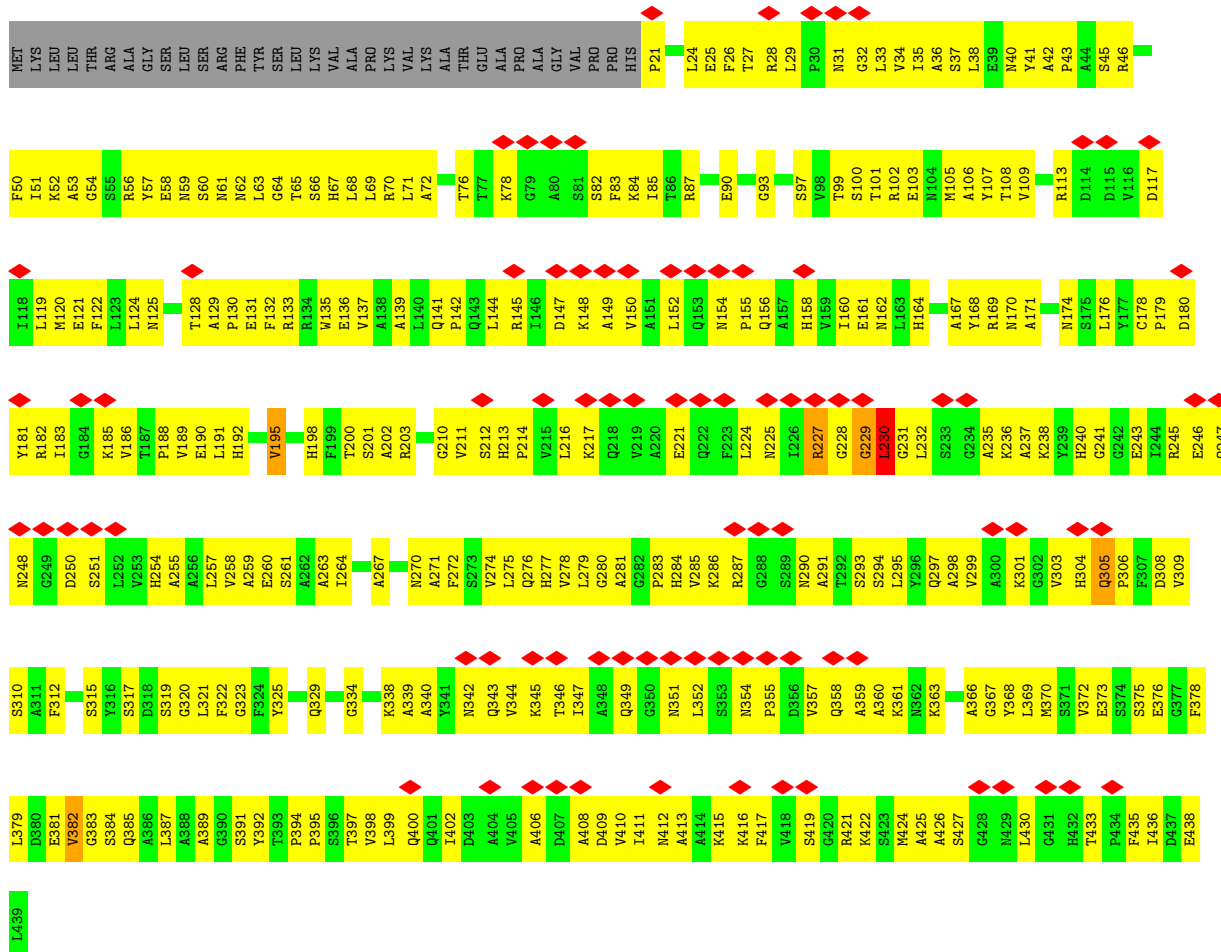


- Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

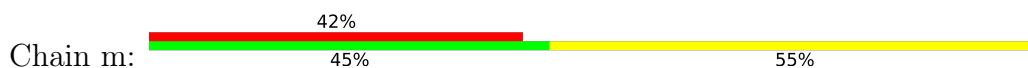


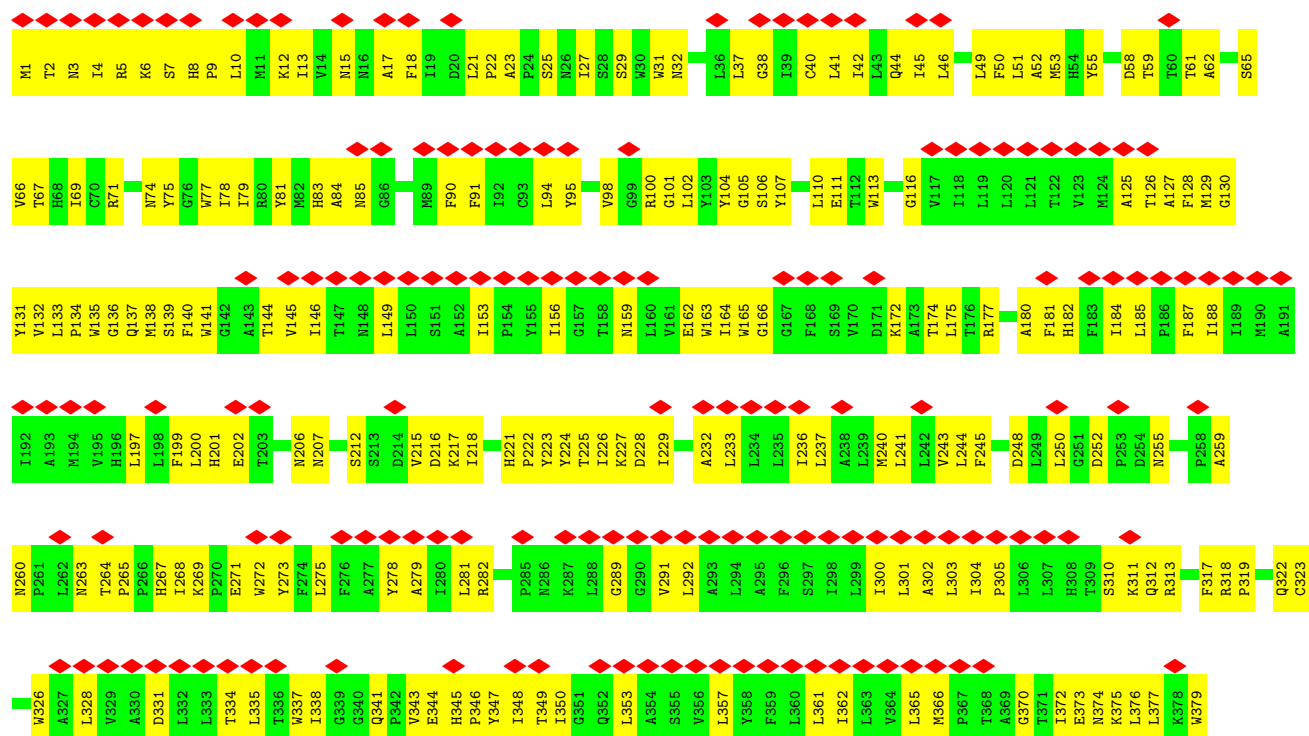


• Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

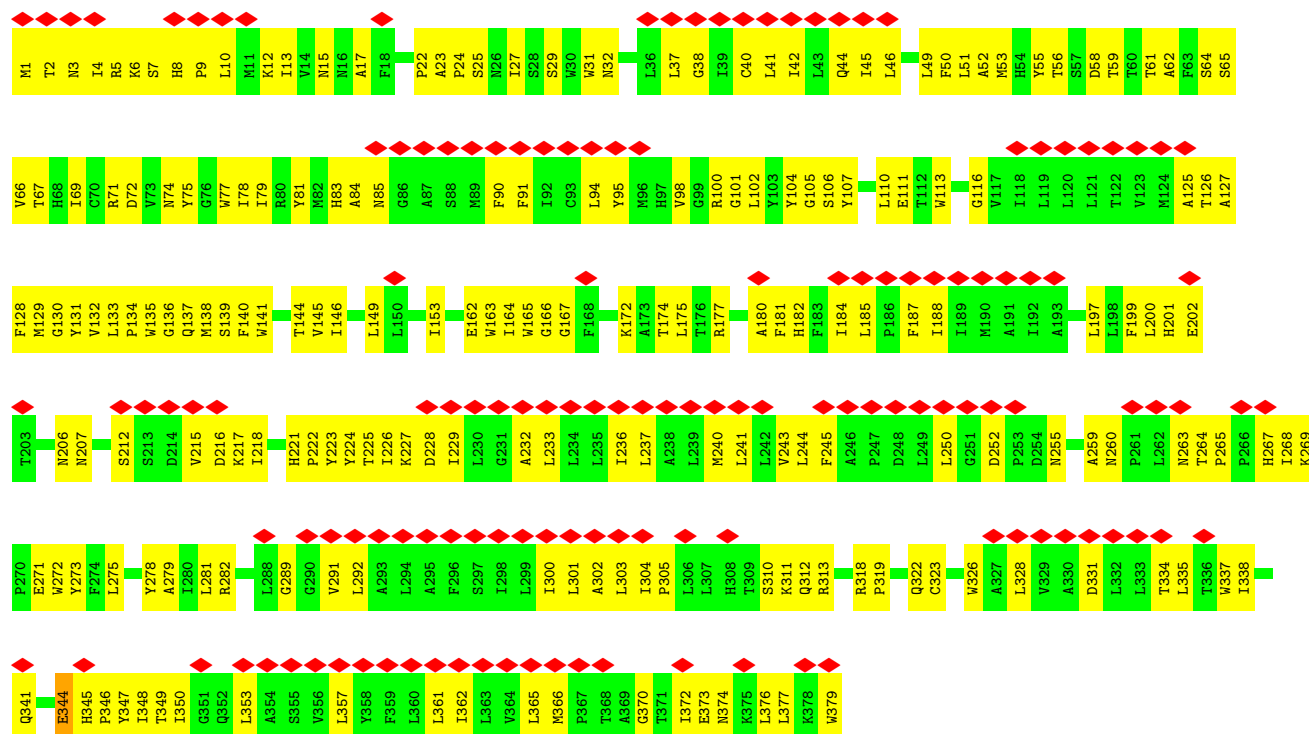


• Molecule 60: Cytochrome b

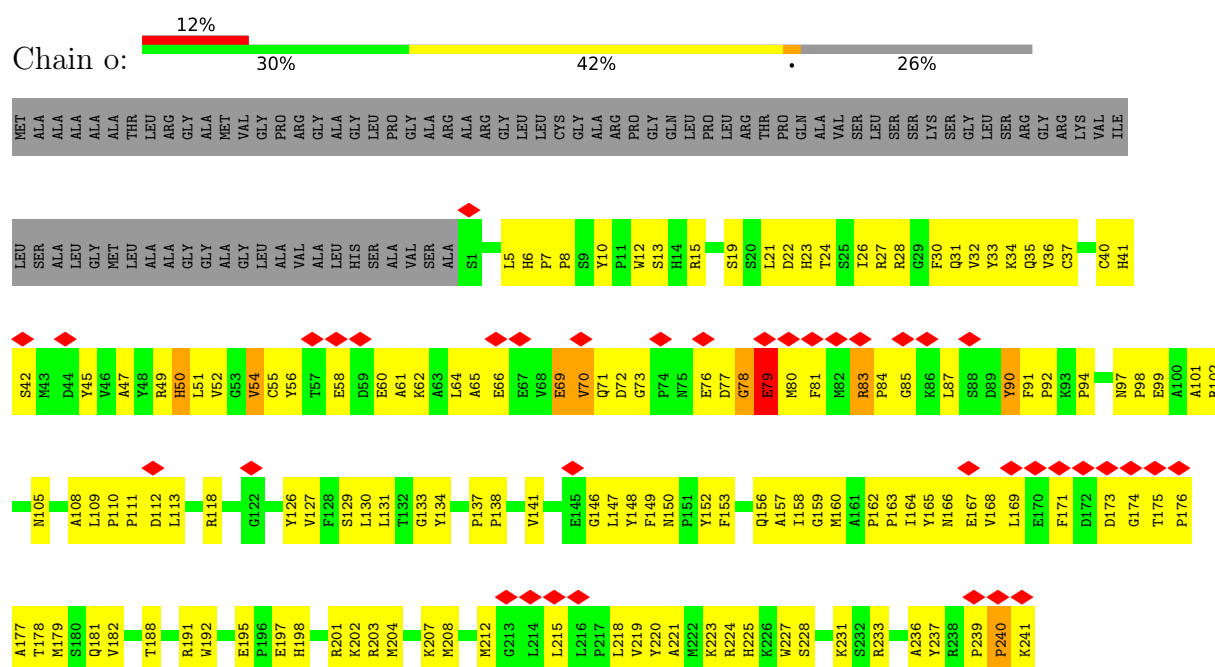




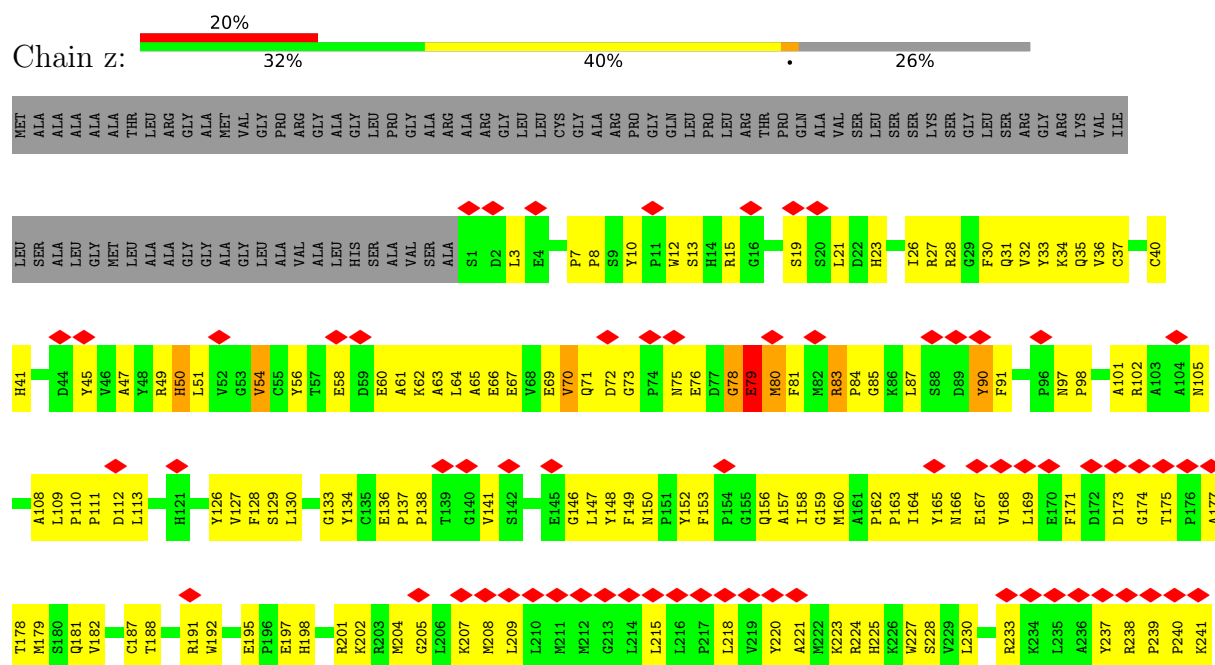
• Molecule 60: Cytochrome b



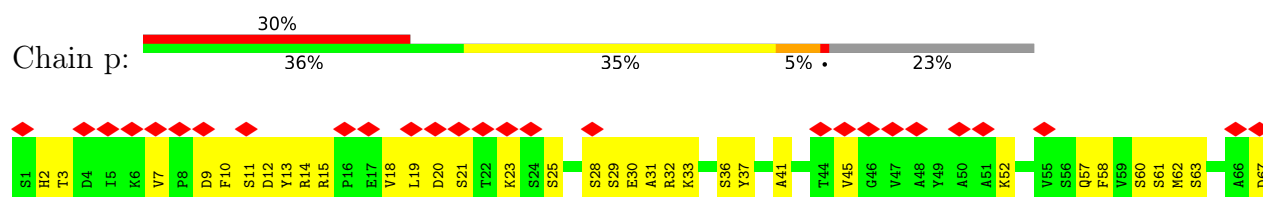
• Molecule 61: Cytochrome c1, heme protein, mitochondrial

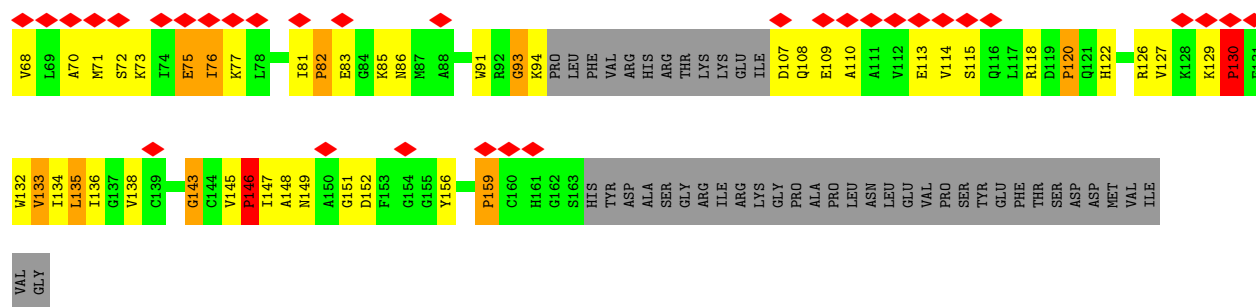


- Molecule 61: Cytochrome c1, heme protein, mitochondrial

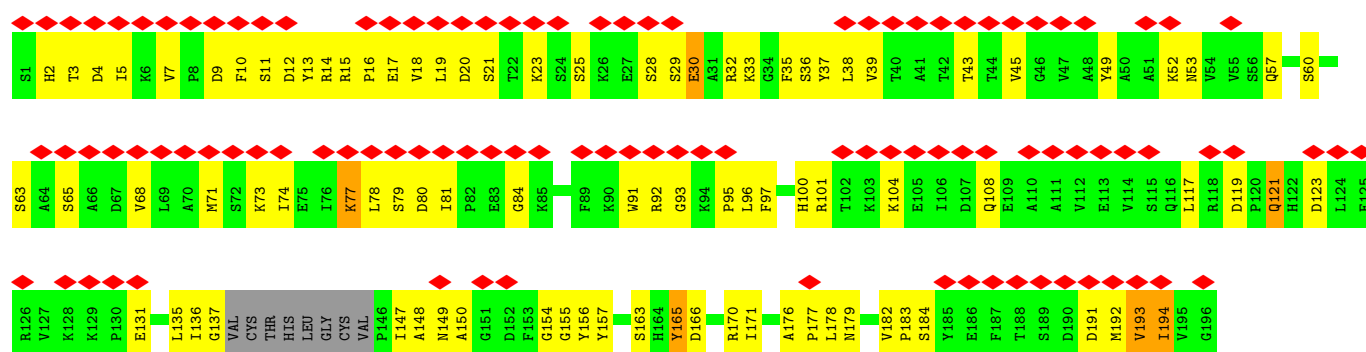


- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial

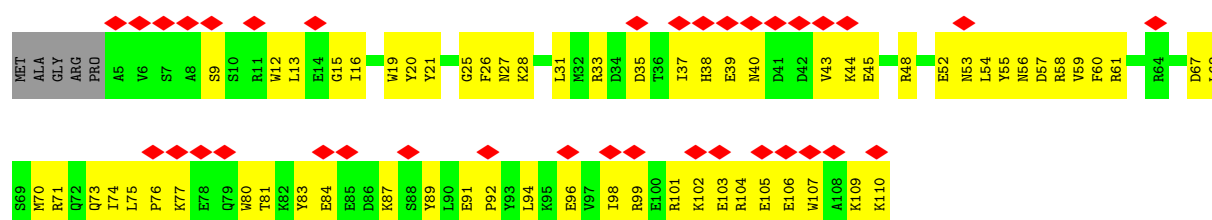




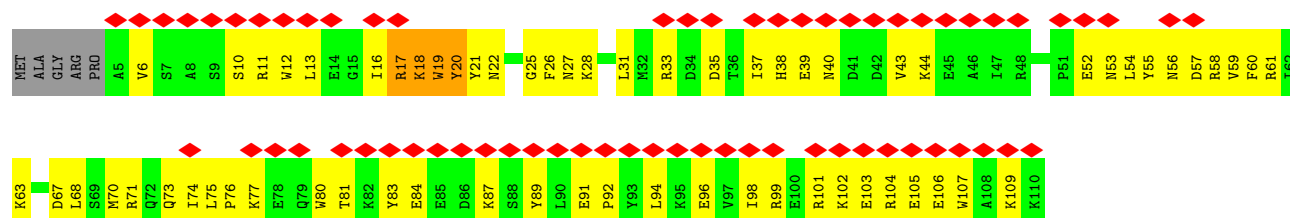
- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 63: Cytochrome b-c1 complex subunit 7

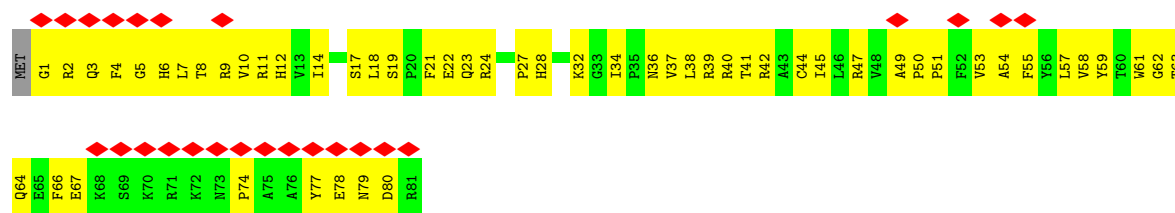


- Molecule 63: Cytochrome b-c1 complex subunit 7

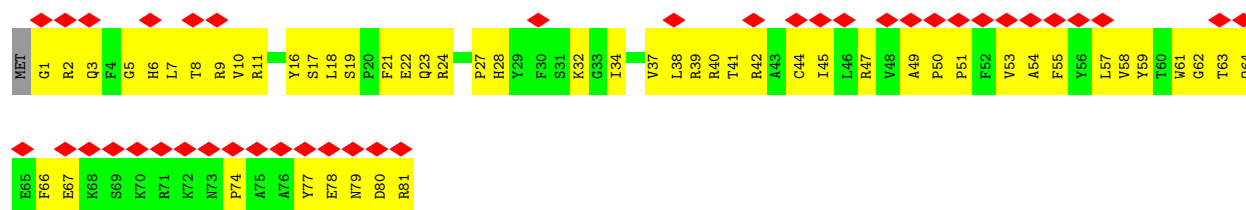


- Molecule 64: Cytochrome b-c1 complex subunit 8

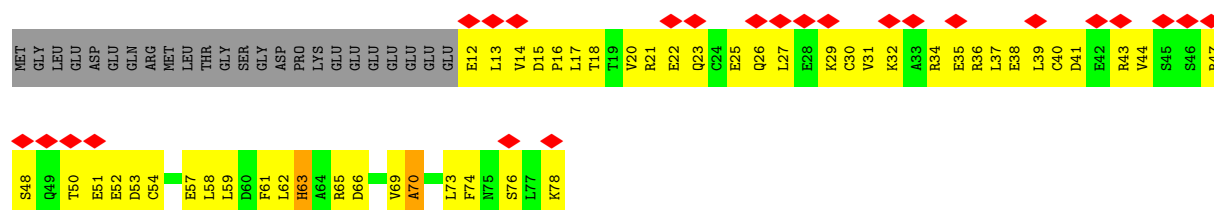
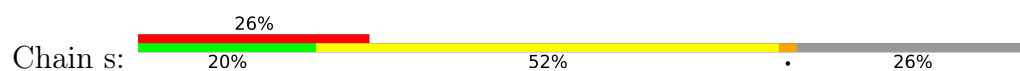




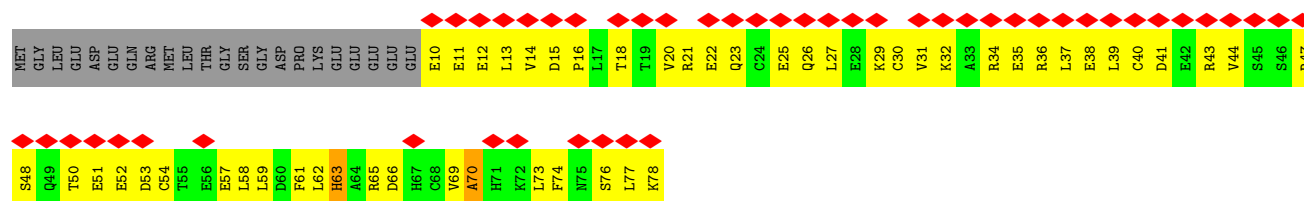
• Molecule 64: Cytochrome b-c1 complex subunit 8



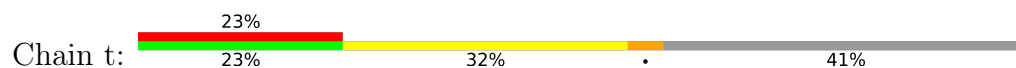
• Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial



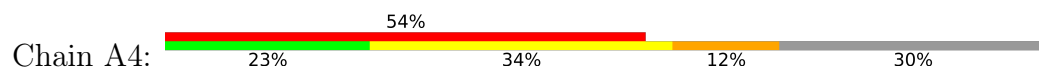
• Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial

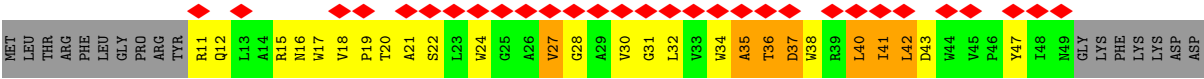


• Molecule 66: Cytochrome b-c1 complex subunit 10

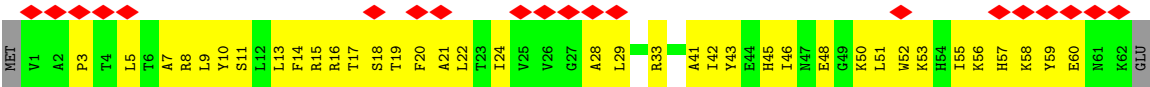


• Molecule 66: Cytochrome b-c1 complex subunit 10

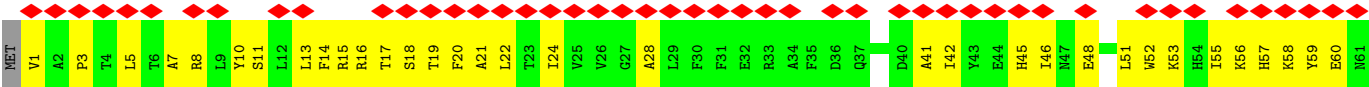
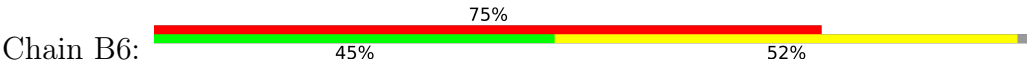




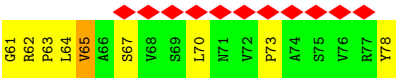
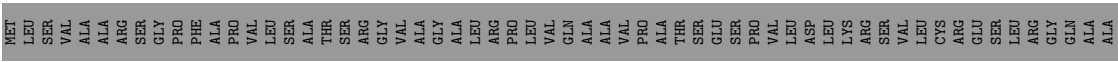
• Molecule 67: Cytochrome b-c1 complex subunit 9



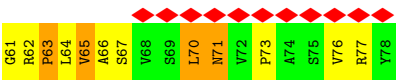
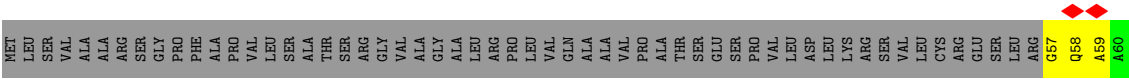
• Molecule 67: Cytochrome b-c1 complex subunit 9



• Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48729	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	0.398	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.019	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: MG, NAP, 3PE, SF4, CDL, ZN, HEA, CU, HEM, HEC, UQ2, PC1, FMN, FES

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	3	0.54	0/905	0.82	2/1237 (0.2%)
2	1	0.71	1/2575 (0.0%)	1.05	15/3518 (0.4%)
3	9	0.43	0/1618	0.69	0/2207
4	7	0.56	0/1267	0.88	2/1731 (0.1%)
5	4	0.65	1/3674 (0.0%)	0.88	6/5020 (0.1%)
6	5	0.67	0/721	1.04	5/977 (0.5%)
7	6	0.44	0/4893	0.74	2/6661 (0.0%)
8	2	0.74	1/2749 (0.0%)	0.97	5/3744 (0.1%)
9	8	0.46	0/3136	0.80	12/4258 (0.3%)
10	C3	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
11	C1	0.77	0/1868	1.12	10/2544 (0.4%)
12	A9	0.74	0/2212	1.02	7/3025 (0.2%)
13	A7	0.67	0/1229	0.96	3/1658 (0.2%)
14	B4	0.64	0/898	1.02	6/1218 (0.5%)
15	A5	0.72	0/765	1.13	3/1038 (0.3%)
16	A6	0.69	0/698	1.10	6/950 (0.6%)
17	C0	0.68	0/648	1.17	5/877 (0.6%)
18	C2	0.71	0/611	0.94	2/810 (0.2%)
19	B2	0.70	0/451	1.04	3/610 (0.5%)
20	B3	0.75	0/398	1.01	1/546 (0.2%)
21	A0	0.77	0/399	0.98	2/534 (0.4%)
22	A8	0.68	0/345	0.99	1/470 (0.2%)
23	A	0.69	2/5304 (0.0%)	0.95	8/7193 (0.1%)
24	B	0.85	0/3512	1.06	12/4763 (0.3%)
25	C	0.74	0/1777	0.95	3/2420 (0.1%)
26	D	0.93	2/1237 (0.2%)	1.06	1/1676 (0.1%)
27	E	0.88	0/1431	1.11	8/1938 (0.4%)
28	F	0.40	0/191	1.08	2/262 (0.8%)
29	G	0.72	0/1008	0.97	3/1363 (0.2%)
30	H	0.54	0/800	0.80	0/1076
31	I	0.53	0/543	0.99	3/729 (0.4%)
32	J	0.56	0/545	0.68	0/740

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.42	0/667	0.70	0/900
34	L	0.43	0/623	0.75	0/862
35	N	0.48	0/882	0.88	2/1203 (0.2%)
36	O	0.50	0/948	0.83	3/1279 (0.2%)
37	P	0.49	0/723	0.81	1/985 (0.1%)
38	Q	0.44	0/1381	0.82	2/1869 (0.1%)
39	R	0.51	0/2407	0.86	6/3269 (0.2%)
40	S	0.35	0/2348	0.79	5/3198 (0.2%)
41	T	0.45	0/938	0.75	0/1278
42	U	0.39	0/1053	0.85	3/1439 (0.2%)
43	V	0.53	1/1115 (0.1%)	0.79	1/1508 (0.1%)
44	M	0.42	0/651	0.77	0/876
44	W	0.32	0/624	0.73	1/847 (0.1%)
45	X	0.36	0/383	0.71	0/523
46	Y	0.35	0/428	0.72	0/592
47	Z	0.35	0/506	0.85	2/688 (0.3%)
48	a	0.44	0/878	0.71	0/1195
49	b	0.51	0/1058	0.78	0/1434
50	c	0.38	0/632	1.01	3/871 (0.3%)
51	d	0.44	1/726 (0.1%)	0.70	2/992 (0.2%)
52	f	0.32	0/1191	0.73	2/1639 (0.1%)
53	h	0.44	0/679	0.82	1/926 (0.1%)
54	i	0.34	0/286	0.56	0/392
55	j	0.50	0/922	0.85	4/1254 (0.3%)
56	g	0.43	1/1380 (0.1%)	0.77	3/1872 (0.2%)
57	e	0.47	0/888	1.03	9/1234 (0.7%)
58	k	0.44	0/3527	0.67	4/4787 (0.1%)
58	w	0.43	0/3455	0.63	0/4685
59	l	0.41	0/3192	0.62	5/4329 (0.1%)
59	x	0.40	0/3198	0.64	3/4336 (0.1%)
60	m	0.53	0/3108	0.61	0/4252
60	y	0.53	0/3108	0.62	0/4252
61	o	0.49	1/1978 (0.1%)	0.71	4/2684 (0.1%)
61	z	0.51	2/1965 (0.1%)	0.71	5/2669 (0.2%)
62	A1	0.38	0/1124	0.82	2/1538 (0.1%)
62	p	0.44	0/945	1.09	10/1288 (0.8%)
63	A2	0.46	0/926	0.65	0/1243
63	q	0.47	0/935	0.61	0/1253
64	A3	0.43	0/698	0.69	0/944
64	r	0.43	0/704	0.69	0/951
65	B7	0.38	0/571	0.71	0/765
65	s	0.38	0/553	0.67	0/741
66	A4	0.43	0/330	0.81	1/457 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
66	t	0.33	0/272	0.59	1/377 (0.3%)
67	B6	0.36	0/524	0.55	0/707
67	u	0.36	0/524	0.54	0/707
68	B5	0.51	0/149	1.27	0/203
68	v	0.43	0/114	1.43	2/156 (1.3%)
All	All	0.58	20/108789 (0.0%)	0.86	261/147930 (0.2%)

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	3	0	2
2	1	0	3
3	9	0	6
4	7	0	6
5	4	0	9
6	5	0	4
7	6	0	5
8	2	0	10
9	8	0	8
23	A	0	16
24	B	0	4
26	D	0	6
27	E	0	5
30	H	0	2
31	I	0	1
33	K	0	1
34	L	0	1
35	N	0	1
36	O	0	1
37	P	0	3
38	Q	0	2
39	R	0	8
40	S	0	4
41	T	0	2
42	U	0	3
43	V	0	3
44	M	0	3
44	W	0	2
47	Z	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	a	0	1
49	b	0	4
51	d	0	1
52	f	0	3
53	h	0	3
55	j	0	4
56	g	0	2
57	e	0	7
58	k	0	6
58	w	0	2
59	l	0	4
59	x	0	3
60	y	0	1
61	o	0	6
61	z	0	6
62	A1	0	8
62	p	0	5
68	B5	0	4
All	All	0	193

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	161	LEU	CA-C	-9.73	1.38	1.52
51	d	74	PHE	C-N	8.08	1.52	1.33
10	C3	61	HIS	CG-CD2	7.56	1.44	1.35
10	C3	378	HIS	ND1-CE1	7.07	1.39	1.32
23	A	240	ALA	C-N	6.90	1.52	1.33

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	128	CYS	CA-C-N	-13.74	102.66	119.84
23	A	128	CYS	C-N-CA	-13.74	102.66	119.84
59	x	230	LEU	N-CA-C	12.23	128.22	110.24
9	8	227	PRO	CA-C-N	-10.53	108.02	118.97
9	8	227	PRO	C-N-CA	-10.53	108.02	118.97

There are no chirality outliers.

5 of 193 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	125	SER	Peptide
2	1	195	ARG	Peptide
2	1	66	SER	Mainchain
1	3	42	ASP	Peptide
1	3	69	ILE	Peptide

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	3	882	0	915	69	0
2	1	2503	0	2617	290	0
3	9	1579	0	1558	103	0
4	7	1235	0	1182	109	0
5	4	3577	0	3674	238	0
6	5	712	0	742	64	0
7	6	4766	0	4897	231	0
8	2	2681	0	2823	191	0
9	8	3065	0	2801	167	0
10	C3	4025	0	4003	89	0
11	C1	1822	0	1834	74	0
12	A9	2125	0	2046	52	0
13	A7	1195	0	1183	34	0
14	B4	878	0	868	20	0
15	A5	748	0	728	26	0
16	A6	671	0	645	28	0
17	C0	628	0	582	22	0
18	C2	598	0	612	15	0
19	B2	441	0	439	15	0
20	B3	384	0	366	13	0
21	A0	386	0	388	8	0
22	A8	335	0	352	13	0
23	A	5218	0	5232	308	0
24	B	3422	0	3345	252	0
25	C	1726	0	1677	108	0
26	D	1206	0	1204	86	0
27	E	1401	0	1353	108	0
28	F	186	0	139	15	0
29	G	985	0	976	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	780	0	753	65	0
31	I	535	0	514	41	0
32	J	530	0	503	13	0
33	K	656	0	647	34	0
34	L	602	0	592	43	0
35	N	862	0	868	41	0
36	O	925	0	907	53	0
37	P	702	0	670	42	0
38	Q	1345	0	1282	78	0
39	R	2349	0	2264	135	0
40	S	2299	0	2027	135	0
41	T	923	0	865	50	0
42	U	1019	0	900	50	0
43	V	1087	0	1037	69	0
44	M	642	0	642	54	0
44	W	616	0	579	27	0
45	X	372	0	314	14	0
46	Y	409	0	318	17	0
47	Z	493	0	395	27	0
48	a	857	0	765	34	0
49	b	1032	0	954	55	0
50	c	617	0	492	34	0
51	d	710	0	521	24	0
52	f	1156	0	892	49	0
53	h	658	0	584	43	0
54	i	277	0	240	2	0
55	j	892	0	835	50	0
56	g	1351	0	1262	79	0
57	e	864	0	567	39	0
58	k	3454	0	3350	279	0
58	w	3385	0	3296	253	0
59	l	3135	0	3112	263	0
59	x	3141	0	3123	282	0
60	m	3011	0	3077	217	0
60	y	3011	0	3077	204	0
61	o	1919	0	1870	180	0
61	z	1906	0	1841	153	0
62	A1	1117	0	808	75	0
62	p	938	0	733	74	0
63	A2	907	0	893	114	0
63	q	916	0	911	70	0
64	A3	676	0	668	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	r	682	0	679	64	0
65	B7	566	0	542	55	0
65	s	548	0	530	54	0
66	A4	318	0	314	54	0
66	t	262	0	250	38	0
67	B6	511	0	518	38	0
67	u	511	0	518	52	0
68	B5	148	0	154	22	0
68	v	114	0	107	10	0
69	2	46	0	66	8	0
69	3	47	0	71	8	0
69	Q	46	0	66	4	0
69	S	47	0	71	5	0
69	j	39	0	55	3	0
70	1	51	0	82	5	0
70	2	41	0	59	5	0
70	4	41	0	59	1	0
70	B	51	0	82	9	0
70	j	46	0	69	3	0
71	9	4	0	0	0	0
71	A	4	0	0	2	0
71	m	4	0	0	0	0
72	6	64	0	72	12	0
72	J	58	0	60	6	0
72	b	82	0	114	4	0
73	8	31	0	19	10	0
74	8	8	0	0	0	0
74	A	16	0	0	6	0
74	D	8	0	0	1	0
74	E	16	0	0	1	0
75	C1	2	0	0	0	0
75	C3	1	0	0	0	0
76	C3	120	0	108	4	0
77	C1	1	0	0	0	0
78	A5	1	0	0	0	0
78	I	1	0	0	0	0
79	R	48	0	23	4	0
80	m	86	0	60	20	0
80	y	86	0	60	19	0
81	o	43	0	32	9	0
81	z	43	0	32	9	0
82	A2	23	0	26	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	107321	0	104027	6050	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 29.

The worst 5 of 6050 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)
1:3:84:LEU:HD21	2:1:309:ILE:CD1	1.22	1.60
2:1:172:MET:HE1	2:1:176:LEU:CD1	0.98	1.45
2:1:172:MET:CE	2:1:176:LEU:HD12	0.89	1.35
23:A:355:LYS:HD2	23:A:530:TYR:CE1	1.61	1.35
2:1:79:LEU:CD1	2:1:222:LEU:HD22	1.55	1.34

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	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	14	50
2	1	316/318 (99%)	254 (80%)	49 (16%)	13 (4%)	2	17
3	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	20
4	7	170/175 (97%)	133 (78%)	27 (16%)	10 (6%)	1	13
5	4	457/459 (100%)	392 (86%)	57 (12%)	8 (2%)	6	32
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	6	604/606 (100%)	519 (86%)	82 (14%)	3 (0%)	24	63
8	2	342/347 (99%)	284 (83%)	56 (16%)	2 (1%)	21	58
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	C3	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
11	C1	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	40
12	A9	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
13	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
14	B4	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
15	A5	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
16	A6	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	12
17	C0	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	38
18	C2	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
19	B2	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	19
20	B3	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
21	A0	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
22	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
23	A	686/704 (97%)	560 (82%)	112 (16%)	14 (2%)	6	30
24	B	428/430 (100%)	344 (80%)	77 (18%)	7 (2%)	7	36
25	C	206/228 (90%)	172 (84%)	32 (16%)	2 (1%)	12	47
26	D	150/179 (84%)	122 (81%)	24 (16%)	4 (3%)	4	24
27	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	7	34
28	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	2	18
29	G	121/133 (91%)	102 (84%)	18 (15%)	1 (1%)	16	53
30	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	3	20
31	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	17
32	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	3	22
33	K	82/98 (84%)	66 (80%)	15 (18%)	1 (1%)	10	42
34	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
35	N	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
36	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	4	24
37	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
38	Q	166/171 (97%)	115 (69%)	48 (29%)	3 (2%)	6	32
39	R	305/345 (88%)	240 (79%)	60 (20%)	5 (2%)	7	36
40	S	317/320 (99%)	239 (75%)	67 (21%)	11 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	T	136/140 (97%)	115 (85%)	12 (9%)	9 (7%)	1	11
42	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
43	V	136/143 (95%)	111 (82%)	22 (16%)	3 (2%)	5	28
44	M	78/86 (91%)	56 (72%)	19 (24%)	3 (4%)	2	18
44	W	84/86 (98%)	68 (81%)	15 (18%)	1 (1%)	10	42
45	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
46	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	6	32
47	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	4	24
48	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
49	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	18	55
50	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
51	d	105/117 (90%)	89 (85%)	13 (12%)	3 (3%)	3	23
52	f	165/178 (93%)	129 (78%)	34 (21%)	2 (1%)	10	42
53	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	2	19
54	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
55	j	111/120 (92%)	96 (86%)	15 (14%)	0	100	100
56	g	171/176 (97%)	142 (83%)	27 (16%)	2 (1%)	10	42
57	e	139/158 (88%)	80 (58%)	47 (34%)	12 (9%)	0	8
58	k	444/480 (92%)	405 (91%)	35 (8%)	4 (1%)	14	50
58	w	432/480 (90%)	400 (93%)	29 (7%)	3 (1%)	18	55
59	l	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	12	47
59	x	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	12	47
60	m	377/379 (100%)	341 (90%)	35 (9%)	1 (0%)	36	72
60	y	377/379 (100%)	341 (90%)	36 (10%)	0	100	100
61	o	239/325 (74%)	204 (85%)	34 (14%)	1 (0%)	30	67
61	z	239/325 (74%)	205 (86%)	32 (13%)	2 (1%)	16	53
62	A1	184/196 (94%)	137 (74%)	41 (22%)	6 (3%)	3	20
62	p	147/196 (75%)	100 (68%)	35 (24%)	12 (8%)	0	9
63	A2	104/111 (94%)	91 (88%)	8 (8%)	5 (5%)	2	16
63	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
64	A3	79/82 (96%)	72 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	r	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
65	B7	67/91 (74%)	57 (85%)	7 (10%)	3 (4%)	2	16
65	s	65/91 (71%)	55 (85%)	7 (11%)	3 (5%)	2	16
66	A4	37/56 (66%)	23 (62%)	8 (22%)	6 (16%)	0	3
66	t	31/56 (55%)	24 (77%)	7 (23%)	0	100	100
67	B6	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
67	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
68	B5	20/78 (26%)	10 (50%)	8 (40%)	2 (10%)	0	7
68	v	16/78 (20%)	8 (50%)	7 (44%)	1 (6%)	1	12
All	All	13628/15127 (90%)	11521 (84%)	1873 (14%)	234 (2%)	9	34

5 of 234 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	170	GLU
2	1	174	LEU
2	1	268	MET
4	7	79	TYR
4	7	82	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	3	96/101 (95%)	96 (100%)	0	100	100
2	1	274/275 (100%)	257 (94%)	17 (6%)	16	38
3	9	170/183 (93%)	168 (99%)	2 (1%)	63	74
4	7	115/142 (81%)	112 (97%)	3 (3%)	40	61
5	4	389/413 (94%)	389 (100%)	0	100	100
6	5	80/86 (93%)	80 (100%)	0	100	100
7	6	524/534 (98%)	522 (100%)	2 (0%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2	304/316 (96%)	302 (99%)	2 (1%)	76	80
9	8	270/353 (76%)	269 (100%)	1 (0%)	84	83
10	C3	427/427 (100%)	387 (91%)	40 (9%)	8	26
11	C1	211/211 (100%)	191 (90%)	20 (10%)	8	26
12	A9	226/226 (100%)	199 (88%)	27 (12%)	5	19
13	A7	128/148 (86%)	117 (91%)	11 (9%)	10	29
14	B4	95/123 (77%)	89 (94%)	6 (6%)	16	38
15	A5	81/103 (79%)	73 (90%)	8 (10%)	7	24
16	A6	68/79 (86%)	52 (76%)	16 (24%)	1	5
17	C0	67/76 (88%)	58 (87%)	9 (13%)	4	15
18	C2	58/59 (98%)	51 (88%)	7 (12%)	5	18
19	B2	47/68 (69%)	41 (87%)	6 (13%)	4	17
20	B3	39/66 (59%)	36 (92%)	3 (8%)	12	32
21	A0	40/55 (73%)	37 (92%)	3 (8%)	12	33
22	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
23	A	560/588 (95%)	538 (96%)	22 (4%)	28	50
24	B	363/371 (98%)	350 (96%)	13 (4%)	31	52
25	C	188/204 (92%)	175 (93%)	13 (7%)	14	36
26	D	127/150 (85%)	124 (98%)	3 (2%)	43	63
27	E	148/151 (98%)	146 (99%)	2 (1%)	59	72
28	F	14/69 (20%)	14 (100%)	0	100	100
29	G	106/119 (89%)	106 (100%)	0	100	100
30	H	80/95 (84%)	80 (100%)	0	100	100
31	I	54/79 (68%)	50 (93%)	4 (7%)	13	34
32	J	50/59 (85%)	49 (98%)	1 (2%)	48	66
33	K	67/81 (83%)	67 (100%)	0	100	100
34	L	63/71 (89%)	63 (100%)	0	100	100
35	N	88/101 (87%)	88 (100%)	0	100	100
36	O	95/113 (84%)	95 (100%)	0	100	100
37	P	73/96 (76%)	72 (99%)	1 (1%)	59	72
38	Q	142/154 (92%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	R	230/298 (77%)	228 (99%)	2 (1%)	70	77
40	S	205/283 (72%)	205 (100%)	0	100	100
41	T	76/101 (75%)	76 (100%)	0	100	100
42	U	95/131 (72%)	95 (100%)	0	100	100
43	V	106/120 (88%)	106 (100%)	0	100	100
44	M	73/79 (92%)	73 (100%)	0	100	100
44	W	57/79 (72%)	55 (96%)	2 (4%)	32	53
45	X	32/54 (59%)	32 (100%)	0	100	100
46	Y	29/62 (47%)	29 (100%)	0	100	100
47	Z	28/76 (37%)	28 (100%)	0	100	100
48	a	70/114 (61%)	70 (100%)	0	100	100
49	b	85/124 (68%)	85 (100%)	0	100	100
50	c	45/122 (37%)	45 (100%)	0	100	100
51	d	43/107 (40%)	43 (100%)	0	100	100
52	f	80/160 (50%)	80 (100%)	0	100	100
53	h	63/112 (56%)	63 (100%)	0	100	100
54	i	23/45 (51%)	23 (100%)	0	100	100
55	j	88/106 (83%)	88 (100%)	0	100	100
56	g	130/157 (83%)	130 (100%)	0	100	100
57	e	44/141 (31%)	41 (93%)	3 (7%)	14	36
58	k	369/394 (94%)	369 (100%)	0	100	100
58	w	362/394 (92%)	362 (100%)	0	100	100
59	l	327/355 (92%)	327 (100%)	0	100	100
59	x	328/355 (92%)	328 (100%)	0	100	100
60	m	327/327 (100%)	326 (100%)	1 (0%)	86	84
60	y	327/327 (100%)	326 (100%)	1 (0%)	86	84
61	o	206/257 (80%)	206 (100%)	0	100	100
61	z	202/257 (79%)	202 (100%)	0	100	100
62	A1	64/168 (38%)	64 (100%)	0	100	100
62	p	65/168 (39%)	65 (100%)	0	100	100
63	A2	93/99 (94%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	q	96/99 (97%)	96 (100%)	0	100	100
64	A3	70/72 (97%)	69 (99%)	1 (1%)	59	72
64	r	71/72 (99%)	71 (100%)	0	100	100
65	B7	66/85 (78%)	66 (100%)	0	100	100
65	s	64/85 (75%)	64 (100%)	0	100	100
66	A4	31/46 (67%)	31 (100%)	0	100	100
66	t	24/46 (52%)	22 (92%)	2 (8%)	10	30
67	B6	52/54 (96%)	51 (98%)	1 (2%)	50	66
67	u	52/54 (96%)	52 (100%)	0	100	100
68	B5	15/60 (25%)	14 (93%)	1 (7%)	15	37
68	v	11/60 (18%)	11 (100%)	0	100	100
All	All	10788/12907 (84%)	10529 (98%)	259 (2%)	43	63

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	C	222	VAL
27	E	67	ILE
12	A9	85	LEU
12	A9	26	LEU
32	J	18	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
30	H	82	GLN
53	h	86	ASN
64	A3	79	ASN
59	x	174	ASN
34	L	46	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\# Z > 2$
74	SF4	8	502	-	0,12,12	-	-	-		
74	SF4	E	302	27	0,12,12	-	-	-		
71	FES	9	301	-	0,4,4	-	-	-		
74	SF4	E	301	27	0,12,12	-	-	-		
71	FES	m	403	-	0,4,4	-	-	-		
70	3PE	1	401	-	50,50,50	0.88	3 (6%)	53,55,55	1.14	2 (3%)
70	3PE	2	401	-	40,40,50	0.95	3 (7%)	43,45,55	1.09	2 (4%)
74	SF4	A	802	-	0,12,12	-	-	-		
70	3PE	4	501	-	40,40,50	0.91	3 (7%)	43,45,55	1.38	3 (6%)
81	HEC	z	301	61	46,50,50	1.96	6 (13%)	58,82,82	2.38	11 (18%)
72	CDL	b	201	-	81,81,99	0.98	8 (9%)	87,93,111	1.16	4 (4%)
76	HEA	C3	602	10	67,67,67	1.21	4 (5%)	81,103,103	1.34	10 (12%)
80	HEM	m	401	60	50,50,50	1.83	16 (32%)	67,82,82	1.36	8 (11%)
82	UQ2	A2	201	-	23,23,23	1.86	2 (8%)	30,31,31	1.48	6 (20%)
73	FMN	8	501	-	33,33,33	1.20	2 (6%)	48,50,50	1.68	13 (27%)
71	FES	A	803	23	0,4,4	-	-	-		
80	HEM	m	402	60	50,50,50	1.77	17 (34%)	67,82,82	1.27	8 (11%)
69	PC1	3	200	-	46,46,53	1.00	3 (6%)	52,54,61	1.09	2 (3%)
69	PC1	j	201	-	38,38,53	1.17	6 (15%)	44,46,61	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	PC1	2	402	-	45,45,53	1.03	4 (8%)	51,53,61	1.00	2 (3%)
72	CDL	J	101	-	57,57,99	1.18	7 (12%)	63,69,111	1.20	5 (7%)
81	HEC	o	301	61	46,50,50	1.95	6 (13%)	58,82,82	2.38	11 (18%)
70	3PE	j	202	-	45,45,50	0.91	3 (6%)	48,50,55	1.08	2 (4%)
80	HEM	y	401	60	50,50,50	1.83	16 (32%)	67,82,82	1.36	8 (11%)
80	HEM	y	402	60	50,50,50	1.77	18 (36%)	67,82,82	1.27	8 (11%)
74	SF4	D	301	26	0,12,12	-	-	-		
74	SF4	A	801	23	0,12,12	-	-	-		
70	3PE	B	501	-	50,50,50	0.88	2 (4%)	53,55,55	1.34	4 (7%)
72	CDL	6	701	-	63,63,99	1.09	8 (12%)	69,75,111	1.27	4 (5%)
76	HEA	C3	603	10	67,67,67	1.19	7 (10%)	81,103,103	1.34	12 (14%)
69	PC1	S	401	-	46,46,53	1.04	5 (10%)	52,54,61	1.09	2 (3%)
69	PC1	Q	201	-	45,45,53	1.08	3 (6%)	51,53,61	1.14	2 (3%)
79	NAP	R	601	-	50,52,52	4.21	22 (44%)	71,80,80	1.97	18 (25%)

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
74	SF4	8	502	-	-	-	0/6/5/5
74	SF4	E	302	27	-	-	0/6/5/5
71	FES	9	301	-	-	-	0/1/1/1
74	SF4	E	301	27	-	-	0/6/5/5
71	FES	m	403	-	-	-	0/1/1/1
70	3PE	1	401	-	-	14/54/54/54	-
70	3PE	2	401	-	-	24/44/44/54	-
74	SF4	A	802	-	-	-	0/6/5/5
70	3PE	4	501	-	-	23/44/44/54	-
81	HEC	z	301	61	-	5/14/54/54	-
72	CDL	b	201	-	-	39/92/92/110	-
76	HEA	C3	602	10	-	7/36/76/76	-
80	HEM	m	401	60	-	3/14/54/54	-
82	UQ2	A2	201	-	-	7/15/39/39	0/1/1/1
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
71	FES	A	803	23	-	-	0/1/1/1
80	HEM	m	402	60	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	PC1	3	200	-	-	23/50/50/57	-
69	PC1	j	201	-	-	21/42/42/57	-
69	PC1	2	402	-	-	29/49/49/57	-
72	CDL	J	101	-	-	23/68/68/110	-
81	HEC	o	301	61	-	5/14/54/54	-
70	3PE	j	202	-	-	21/49/49/54	-
80	HEM	y	401	60	-	3/14/54/54	-
80	HEM	y	402	60	-	1/14/54/54	-
74	SF4	D	301	26	-	-	0/6/5/5
74	SF4	A	801	23	-	-	0/6/5/5
70	3PE	B	501	-	-	28/54/54/54	-
72	CDL	6	701	-	-	33/74/74/110	-
76	HEA	C3	603	10	-	7/36/76/76	-
69	PC1	S	401	-	-	26/50/50/57	-
69	PC1	Q	201	-	-	23/49/49/57	-
79	NAP	R	601	-	-	16/35/67/67	0/5/5/5

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	R	601	NAP	O4D-C1D	16.46	1.62	1.40
79	R	601	NAP	C2B-C1B	-10.09	1.28	1.53
79	R	601	NAP	O4B-C1B	8.64	1.62	1.42
79	R	601	NAP	PN-O3	8.41	1.68	1.59
82	A2	201	UQ2	C6-C5	7.78	1.49	1.35

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	z	301	HEC	CBC-CAC-C3C	-10.95	105.55	127.43
81	o	301	HEC	CBC-CAC-C3C	-10.93	105.58	127.43
81	z	301	HEC	CBB-CAB-C3B	-10.54	106.38	127.43
81	o	301	HEC	CBB-CAB-C3B	-10.52	106.41	127.43
79	R	601	NAP	N3A-C2A-N1A	-6.56	118.65	128.58

There are no chirality outliers.

5 of 391 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	3	200	PC1	C22-C21-O21-C2
69	2	402	PC1	C11-O13-P-O12
69	2	402	PC1	C1-O11-P-O12
69	2	402	PC1	C1-O11-P-O14
69	2	402	PC1	C1-O11-P-O13

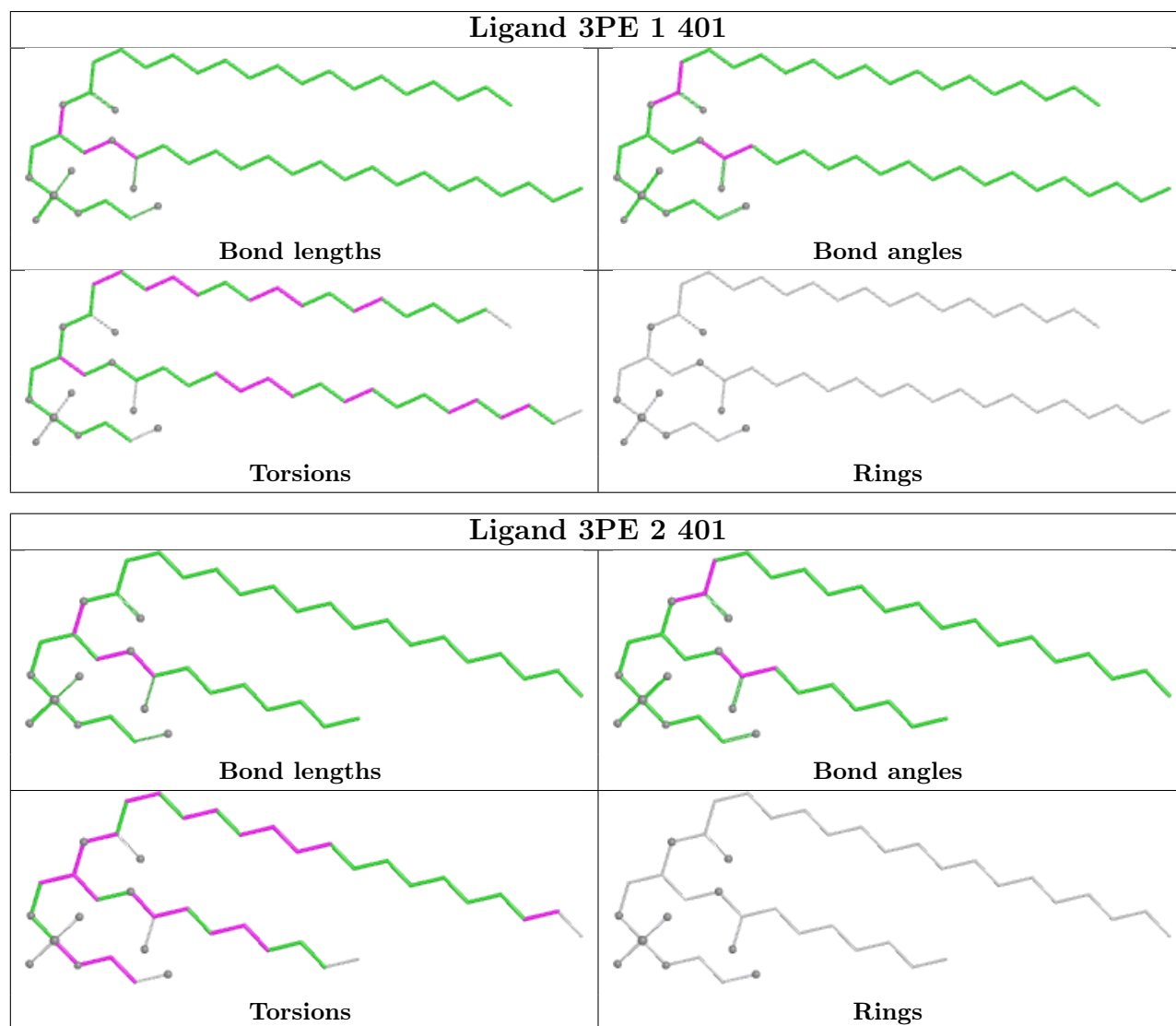
There are no ring outliers.

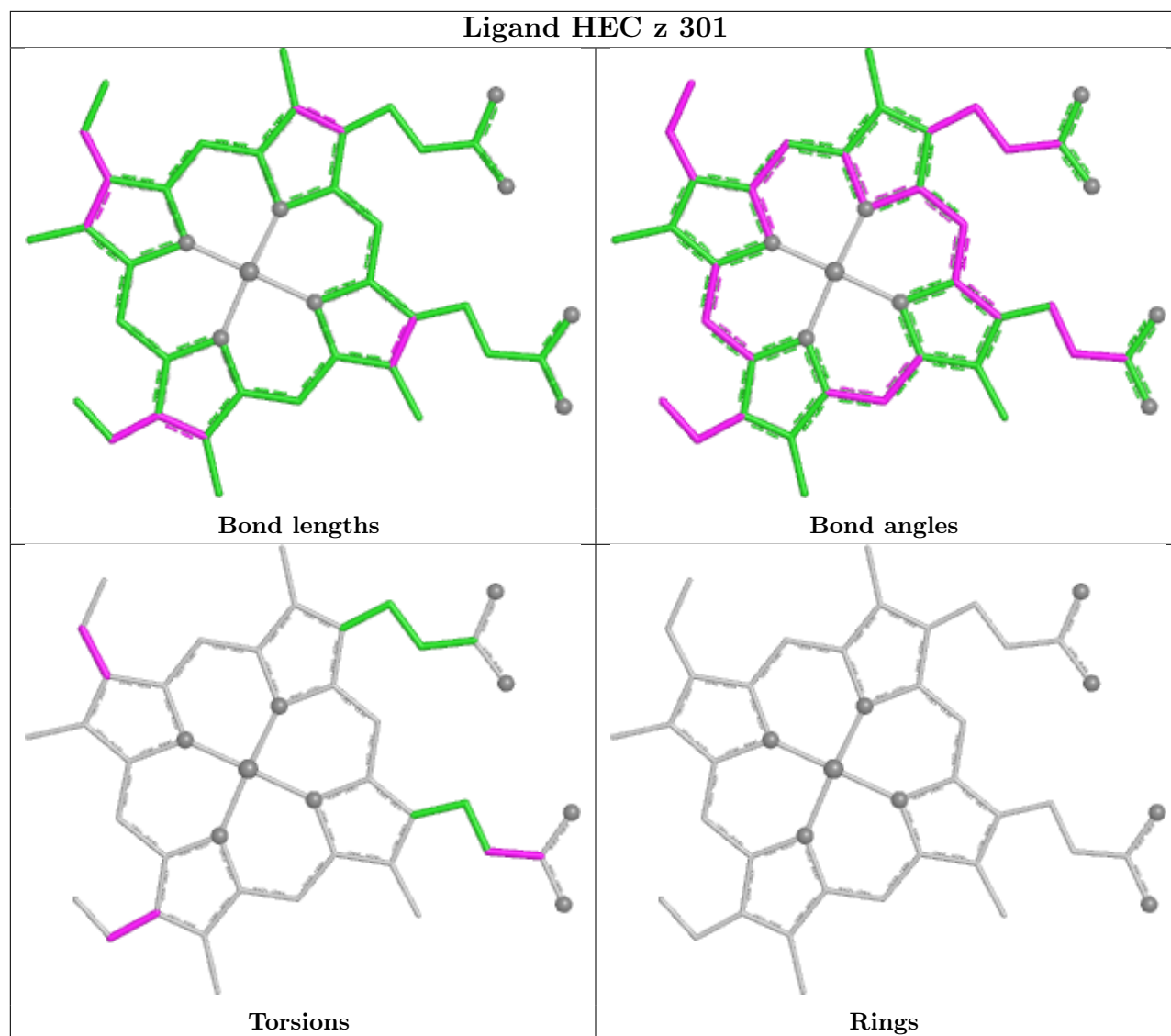
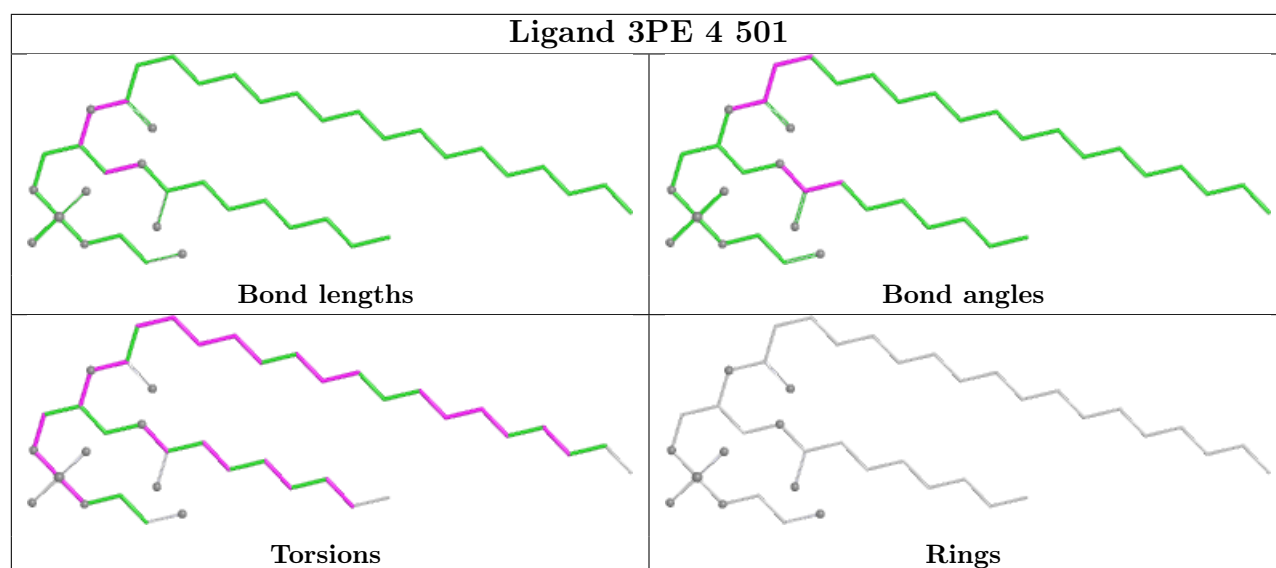
29 monomers are involved in 182 short contacts:

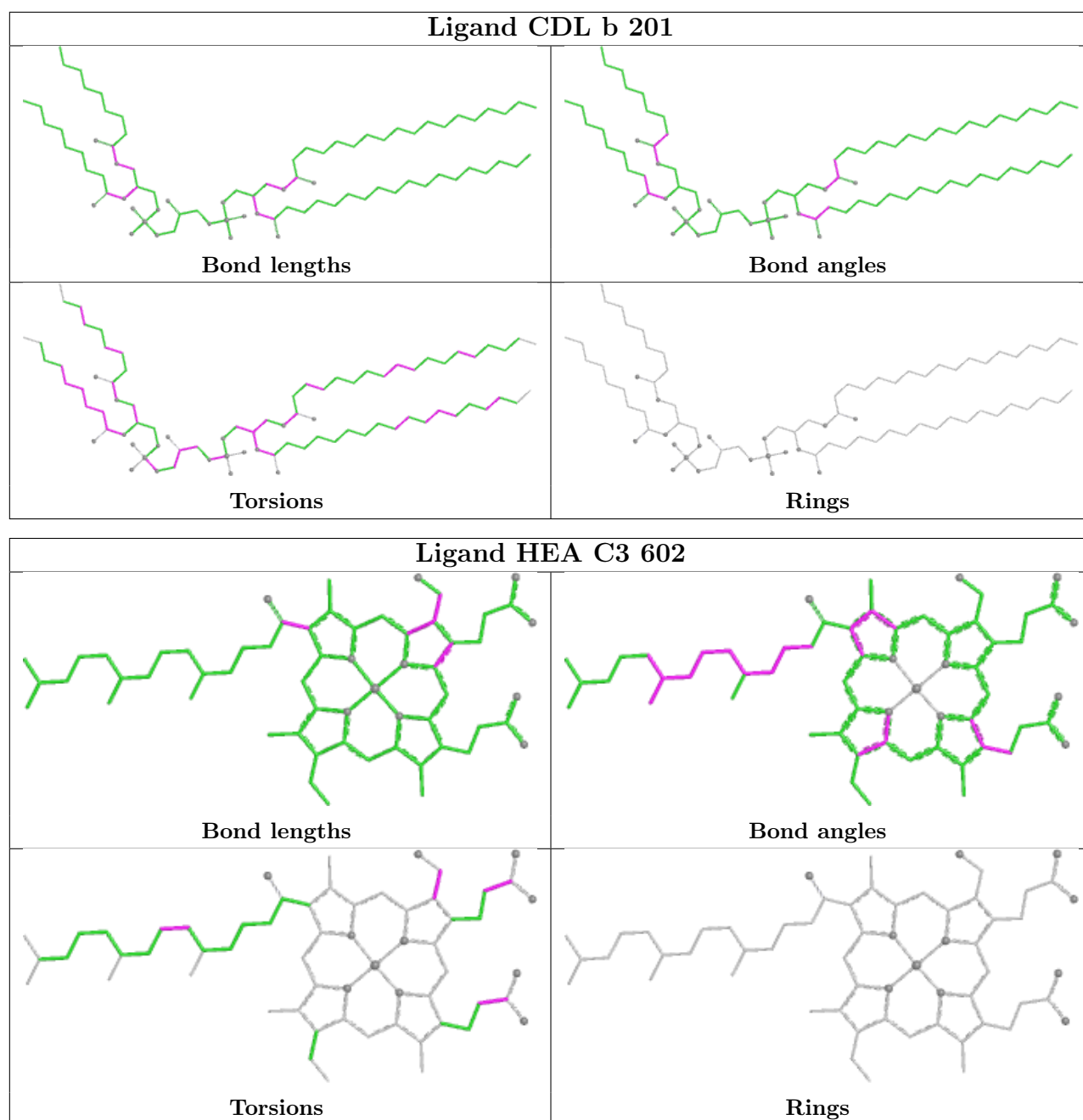
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	E	302	SF4	1	0
70	1	401	3PE	5	0
70	2	401	3PE	5	0
74	A	802	SF4	3	0
70	4	501	3PE	1	0
81	z	301	HEC	9	0
72	b	201	CDL	4	0
76	C3	602	HEA	1	0
80	m	401	HEM	14	0
82	A2	201	UQ2	24	0
73	8	501	FMN	10	0
71	A	803	FES	2	0
80	m	402	HEM	6	0
69	3	200	PC1	8	0
69	j	201	PC1	3	0
69	2	402	PC1	8	0
72	J	101	CDL	6	0
81	o	301	HEC	9	0
70	j	202	3PE	3	0
80	y	401	HEM	13	0
80	y	402	HEM	6	0
74	D	301	SF4	1	0
74	A	801	SF4	3	0
70	B	501	3PE	9	0
72	6	701	CDL	12	0
76	C3	603	HEA	3	0
69	S	401	PC1	5	0
69	Q	201	PC1	4	0
79	R	601	NAP	4	0

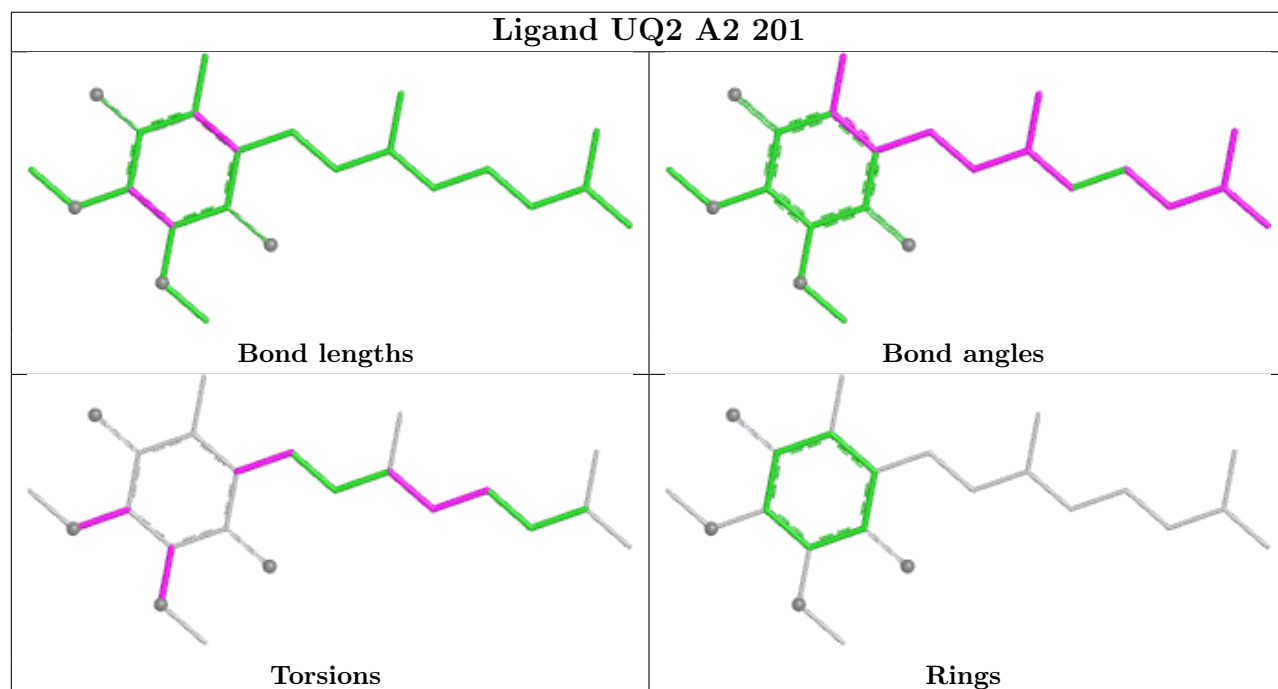
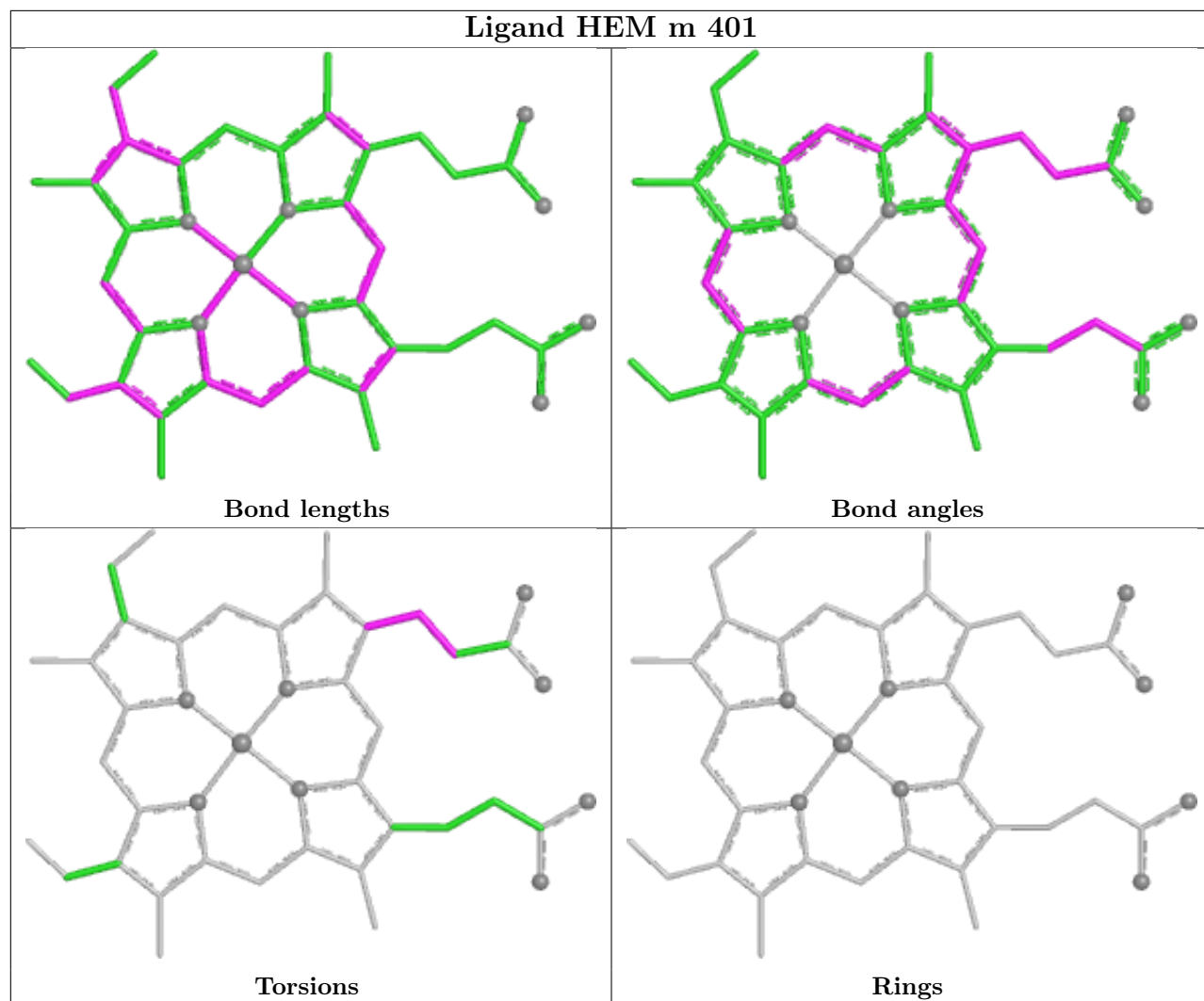
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

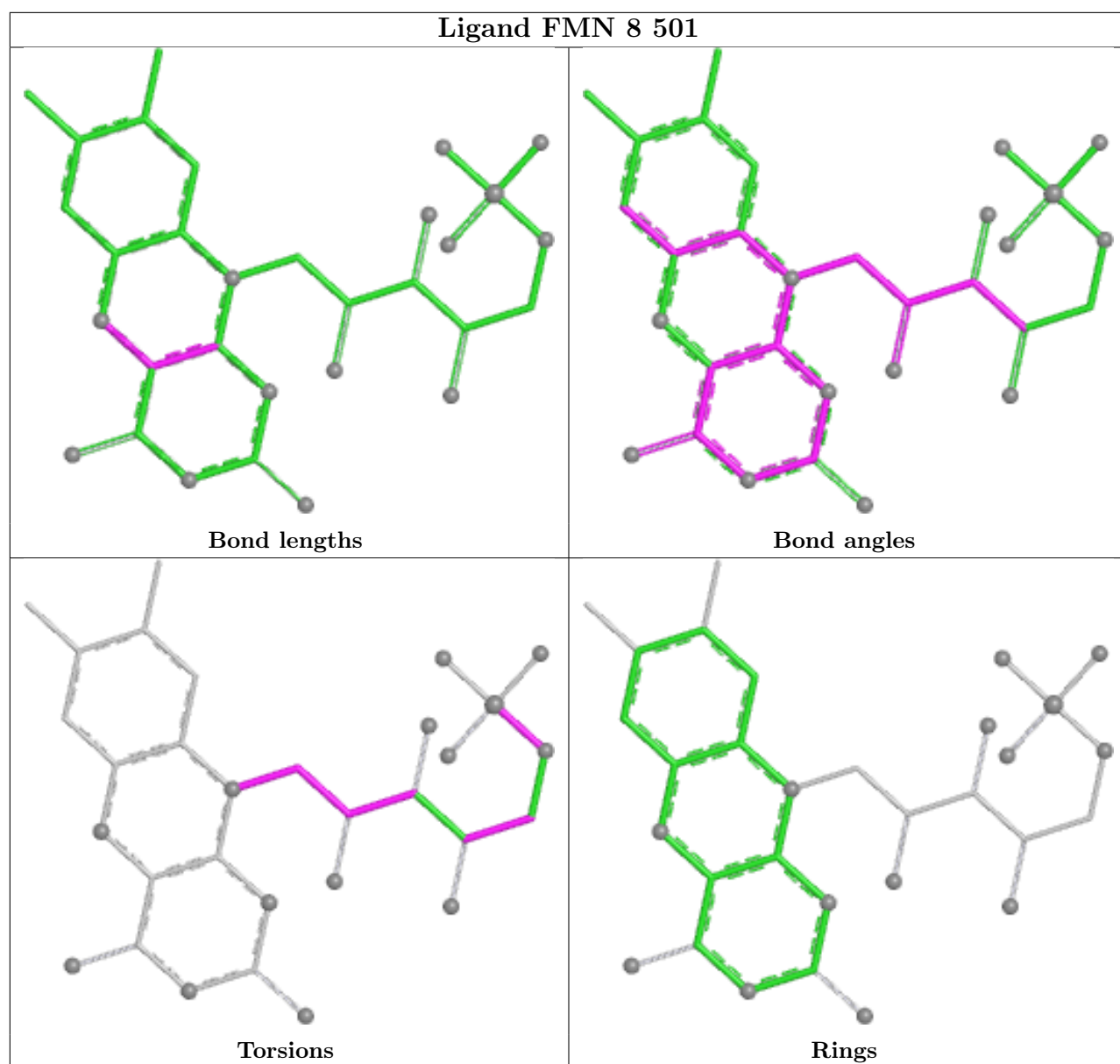
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

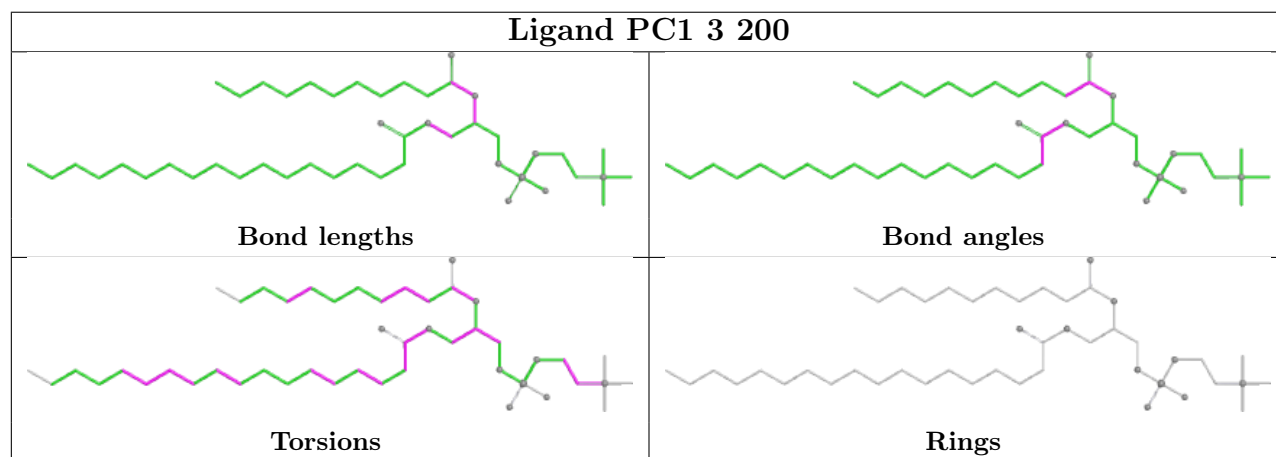
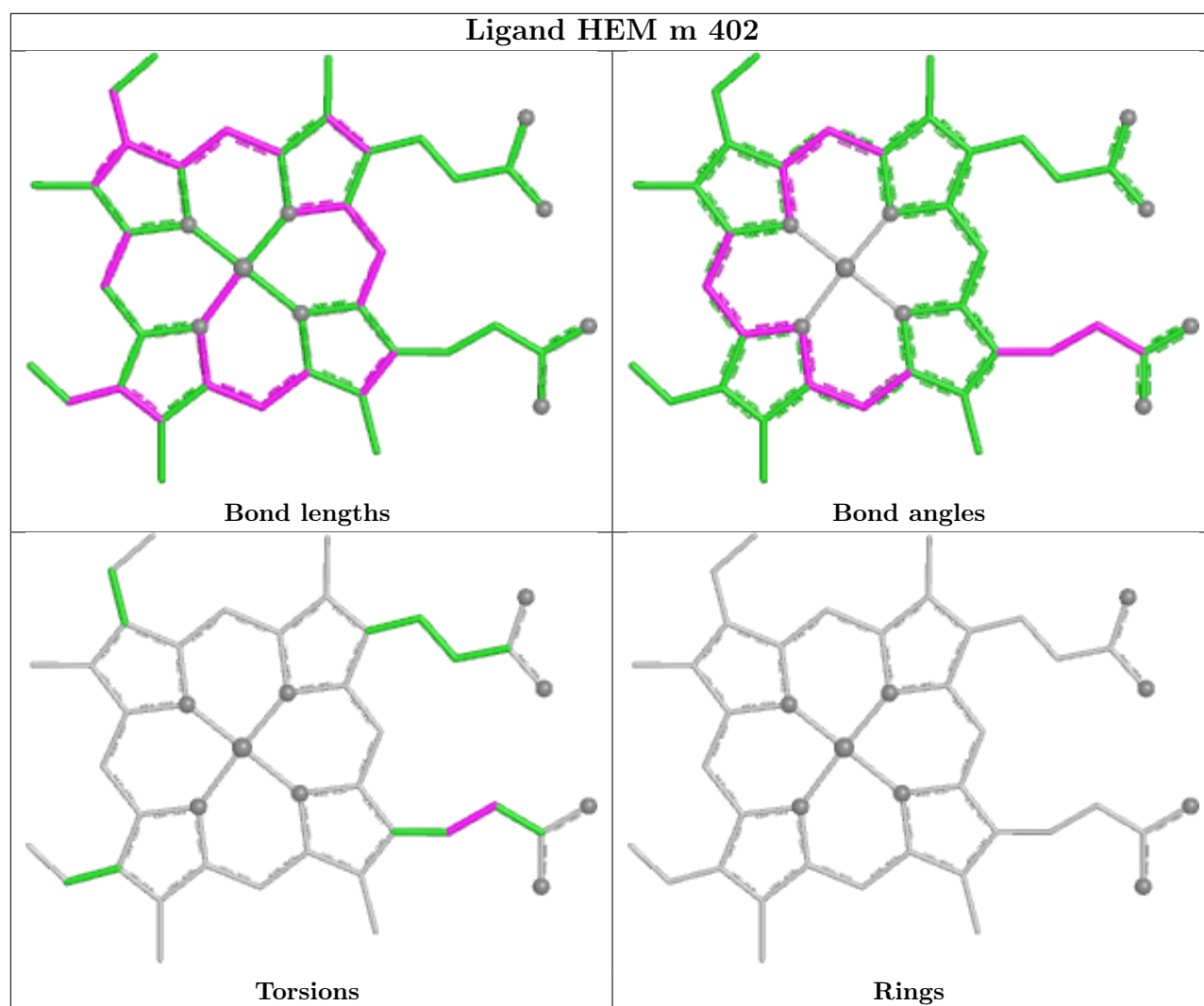


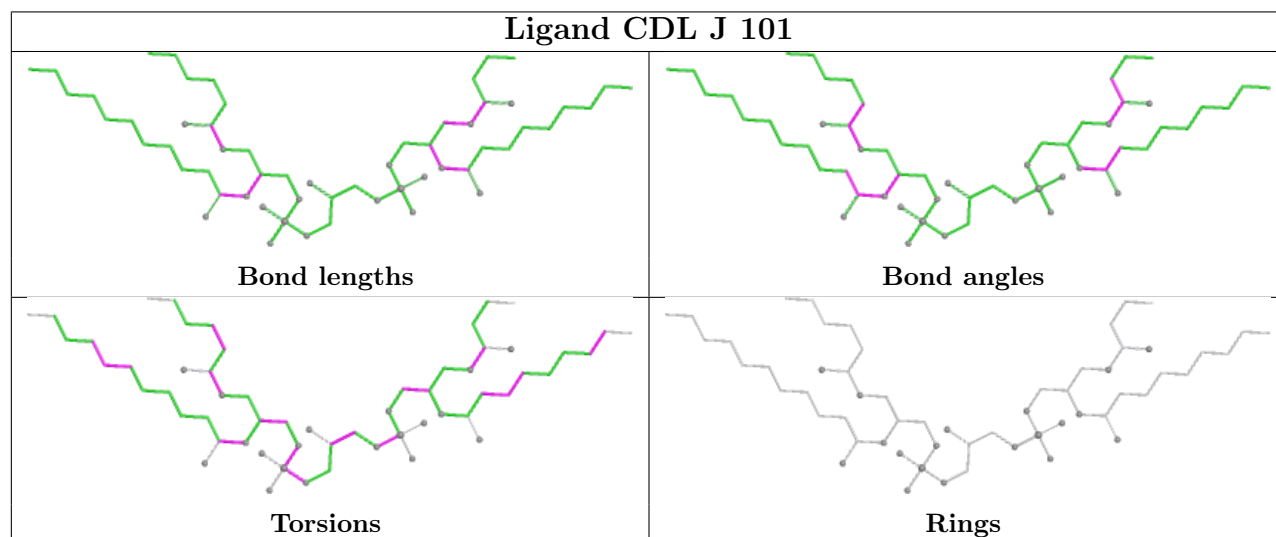
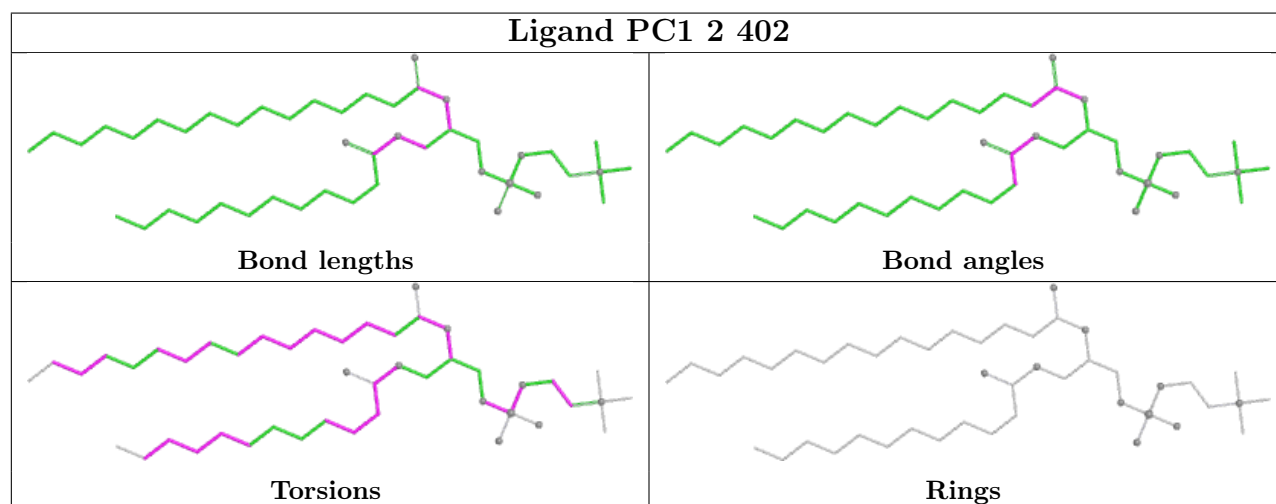
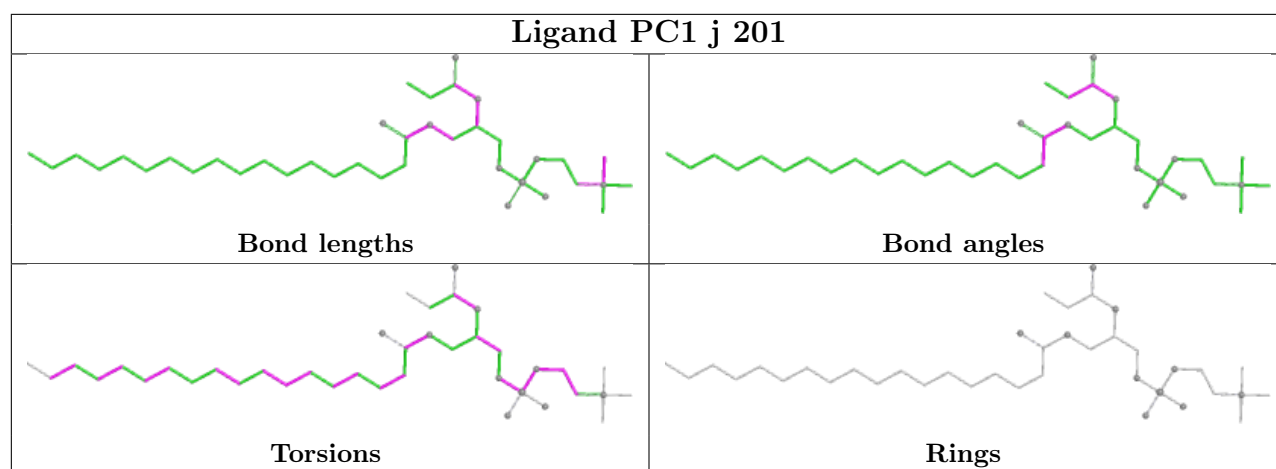




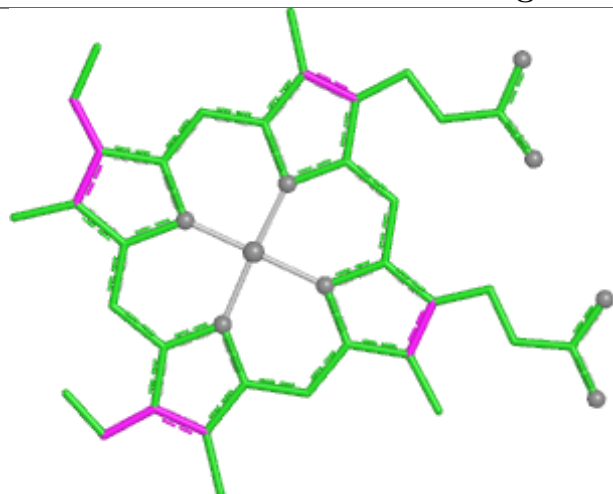




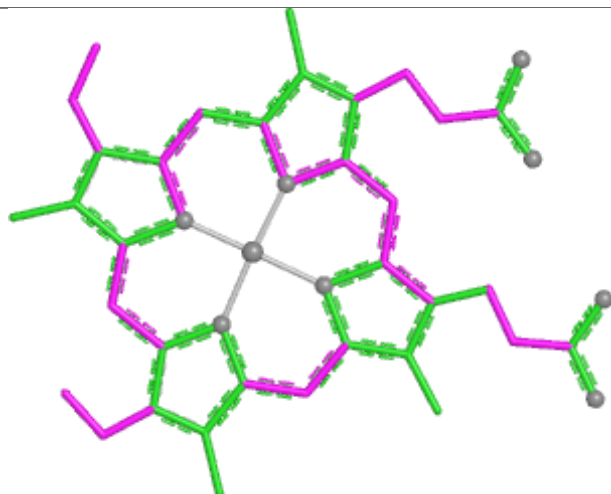




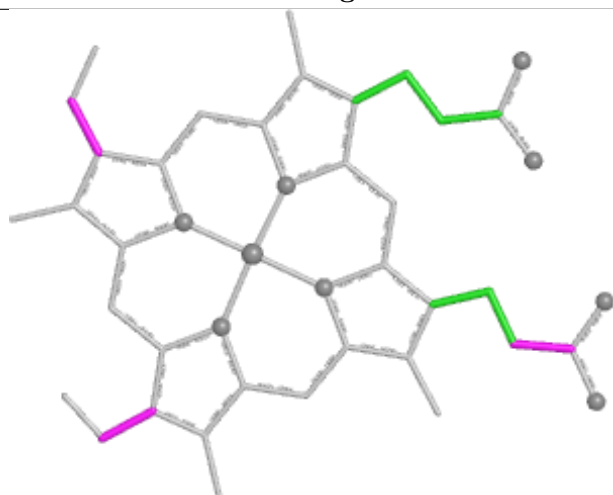
Ligand HEC o 301



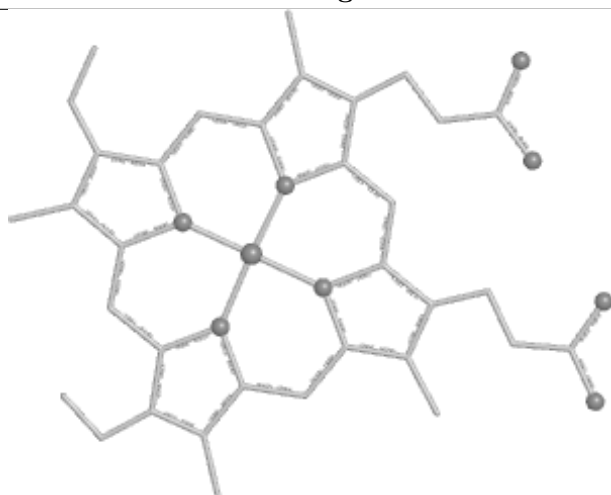
Bond lengths



Bond angles

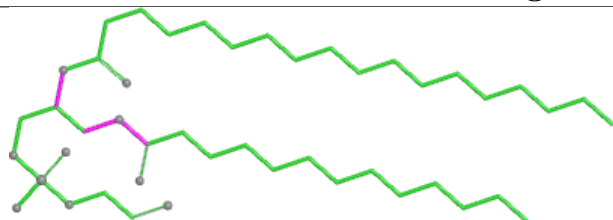


Torsions

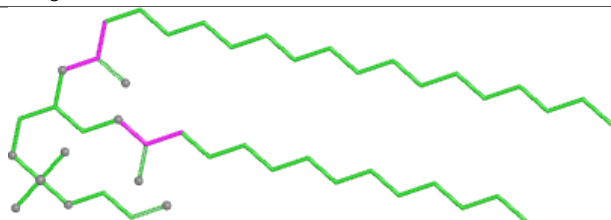


Rings

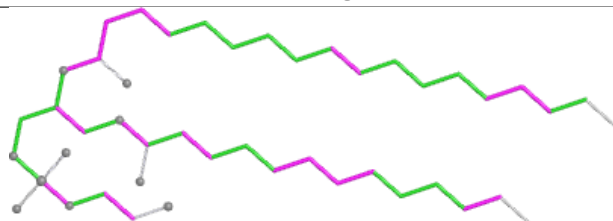
Ligand 3PE j 202



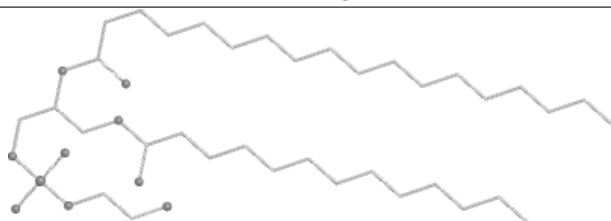
Bond lengths



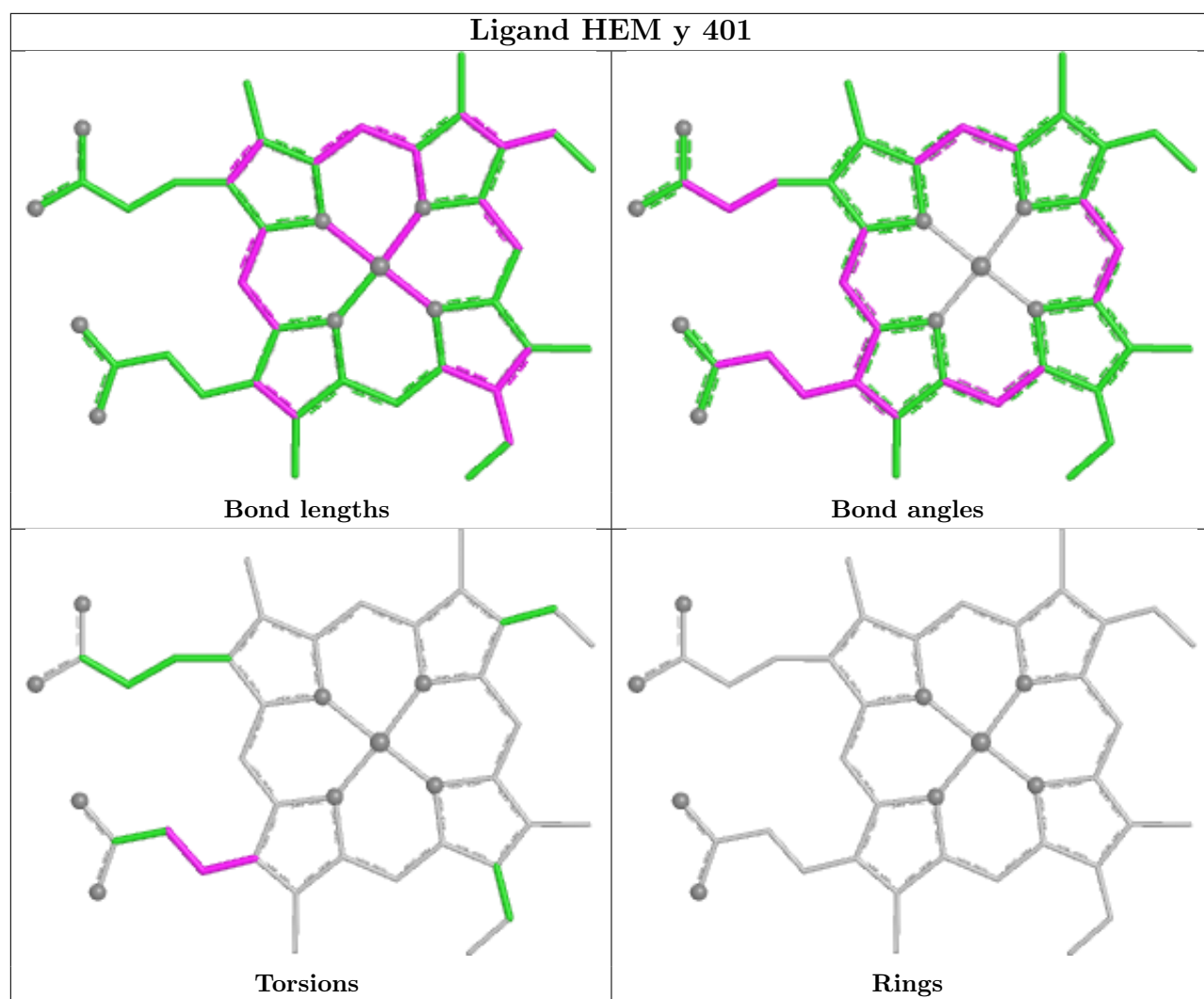
Bond angles

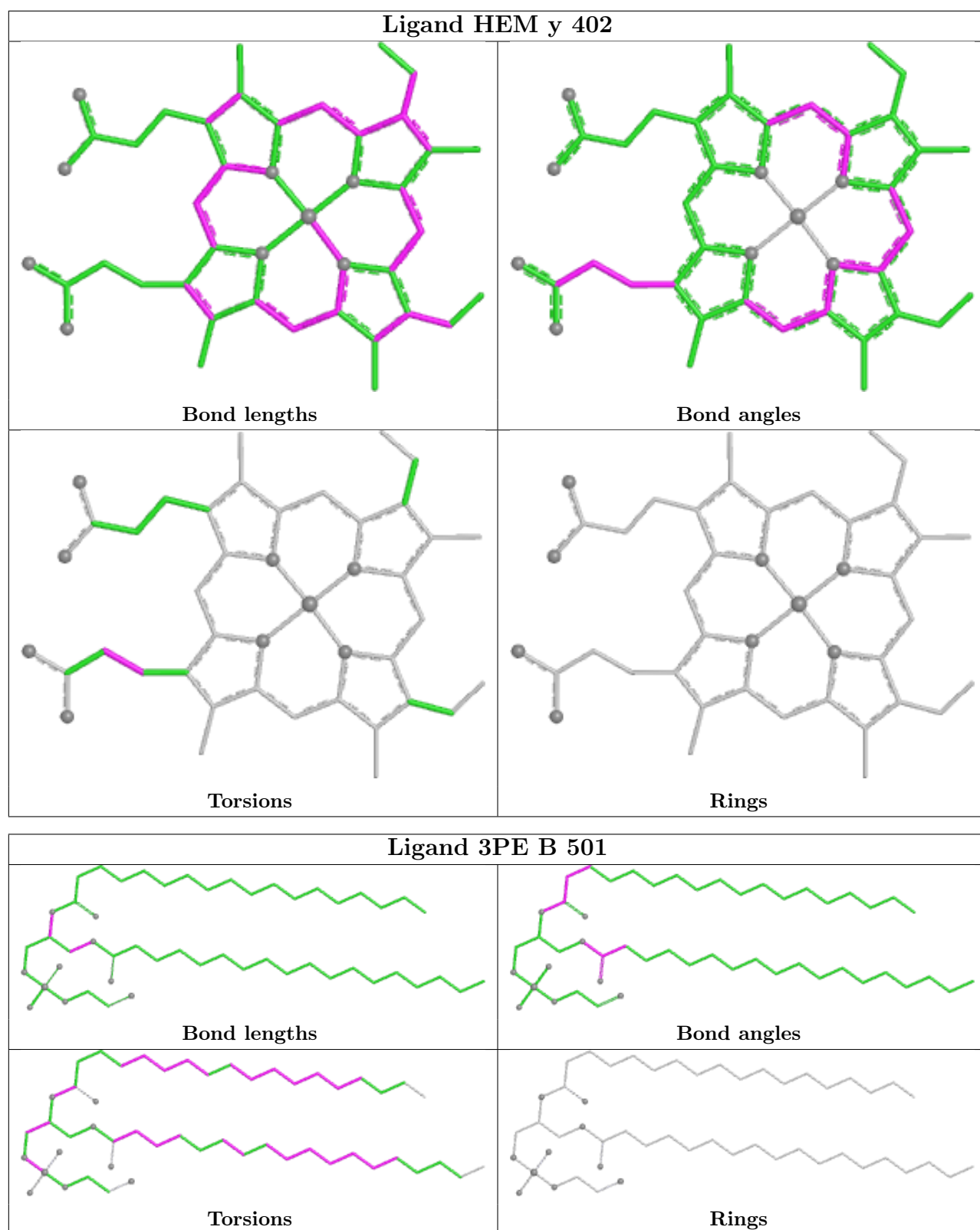


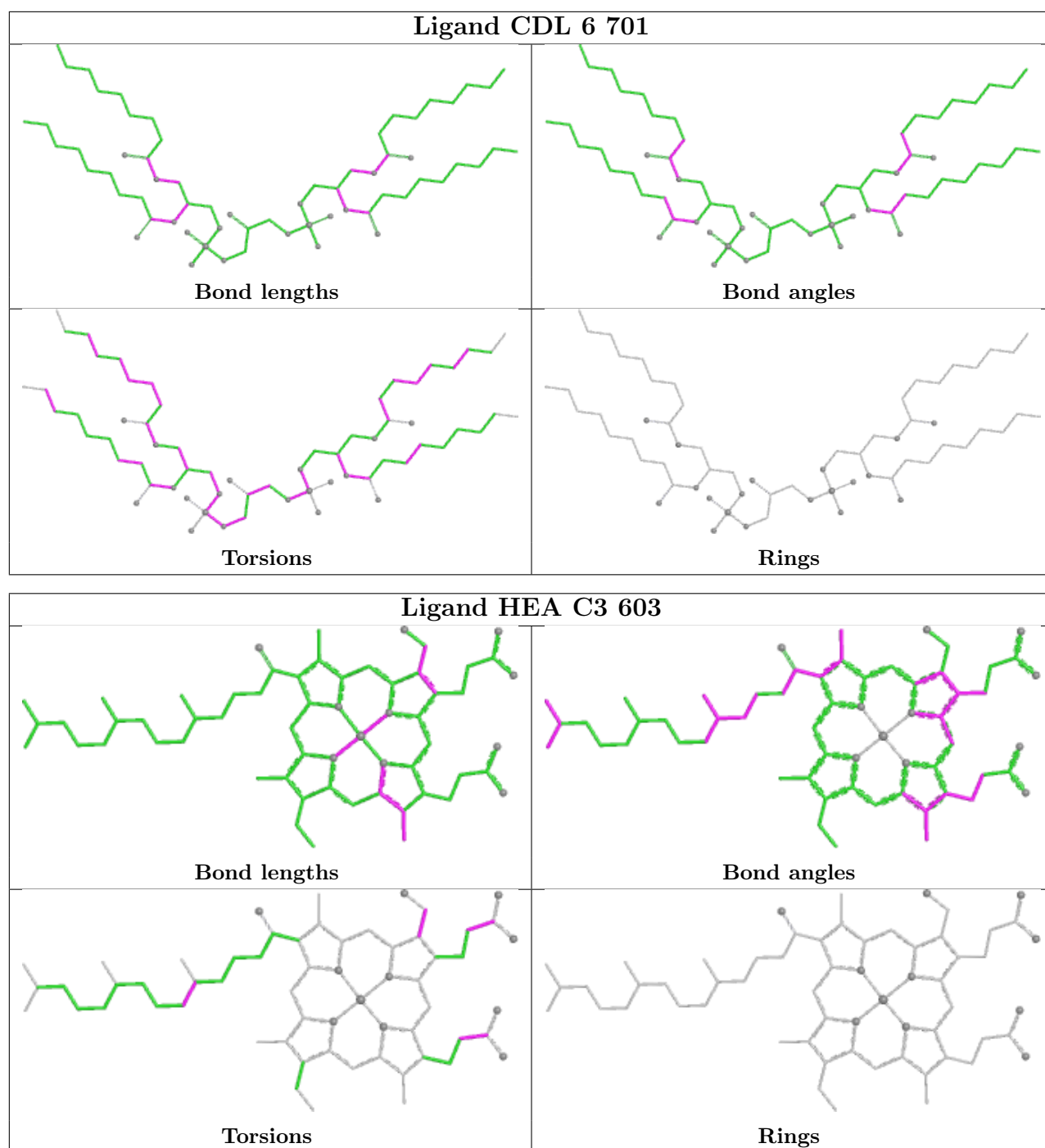
Torsions

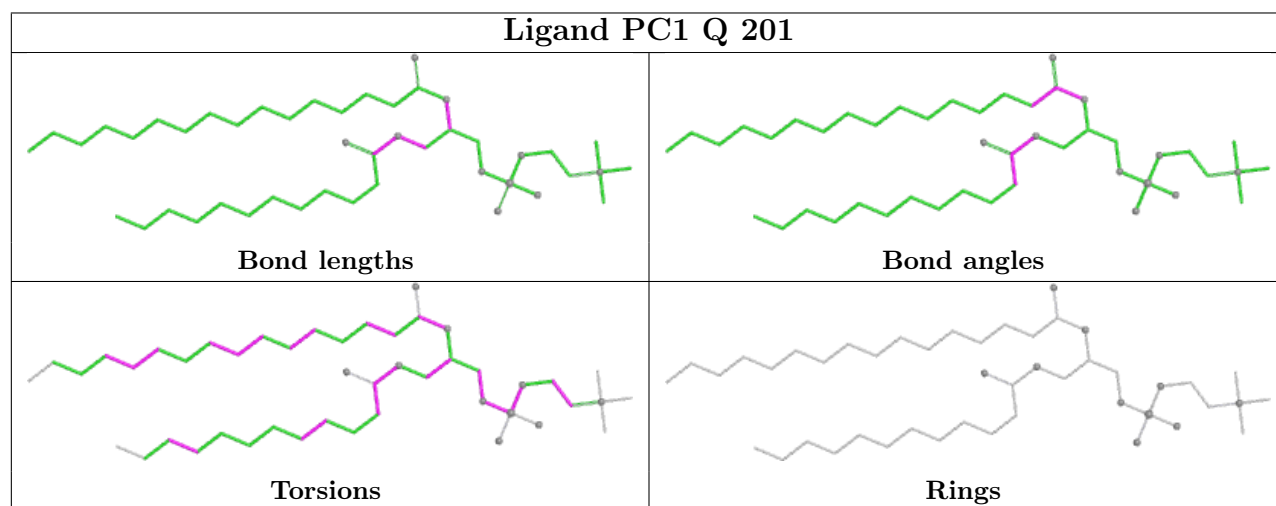
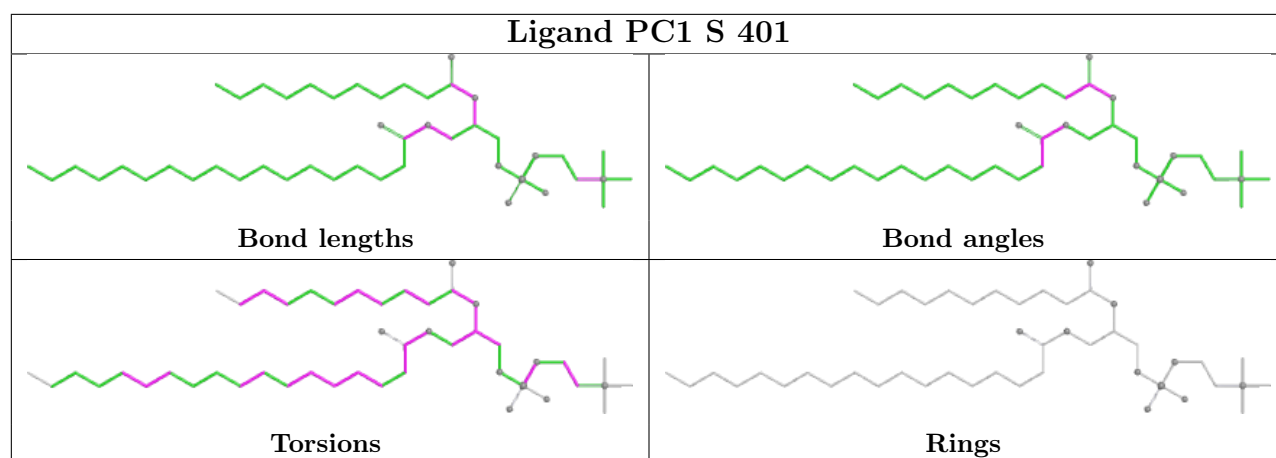


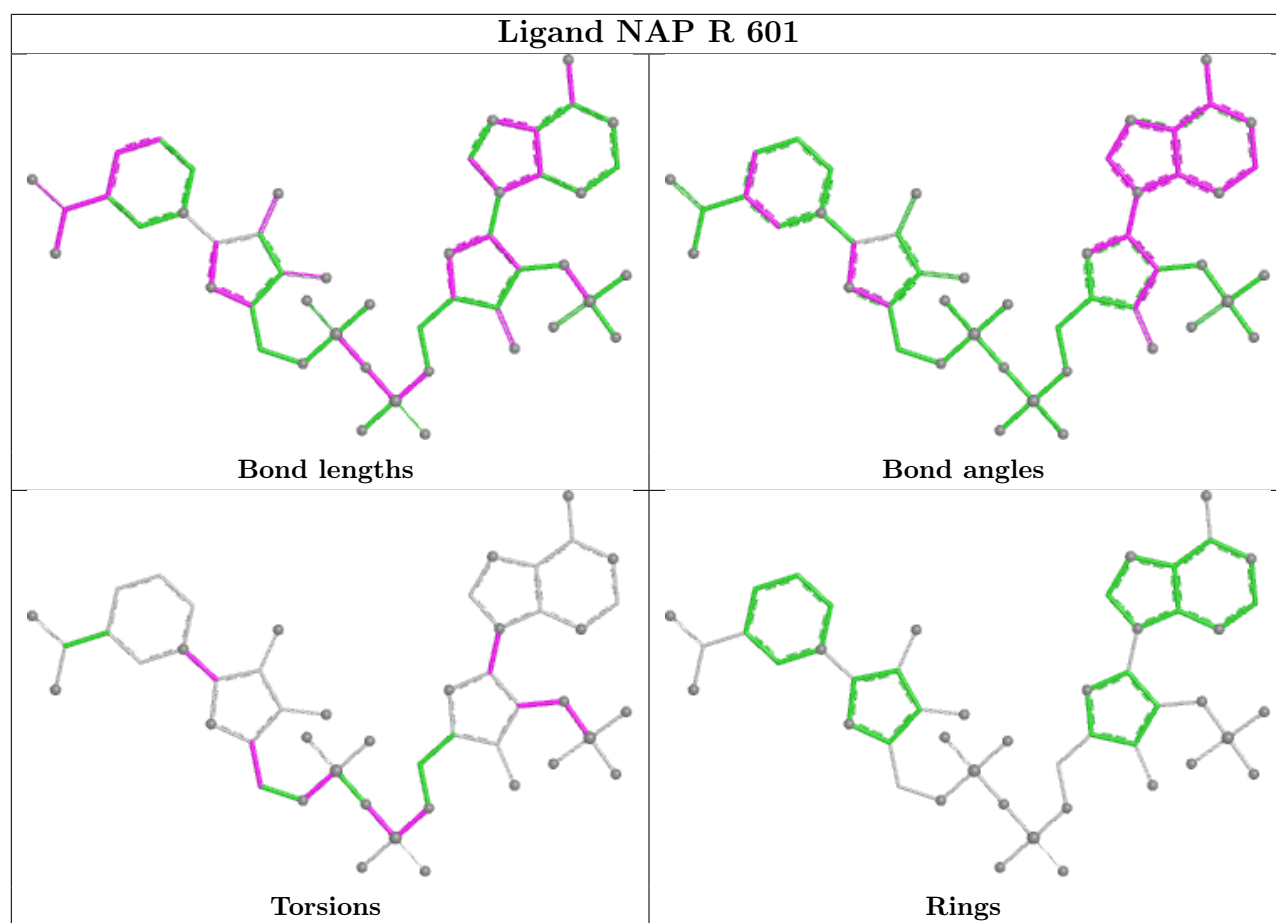
Rings











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.

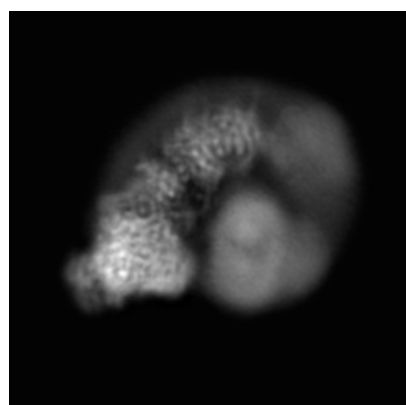
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30673. These allow visual inspection of the internal detail of the map and identification of artifacts.

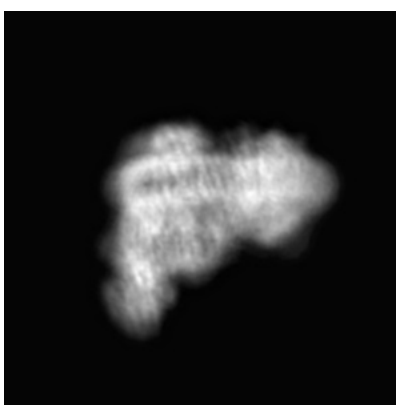
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

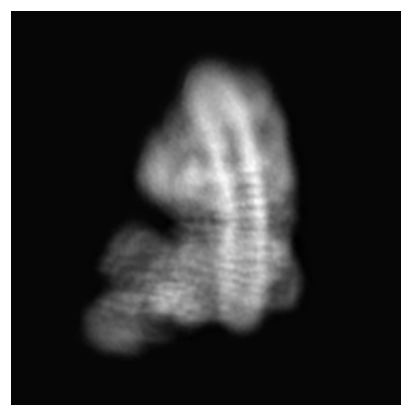
6.1.1 Primary map



X



Y

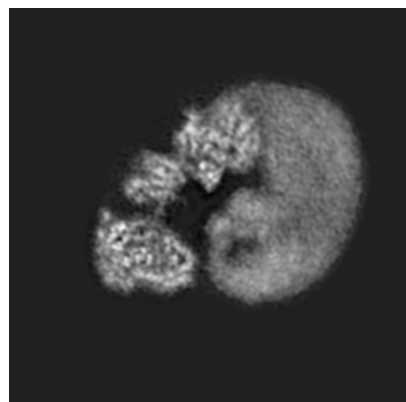


Z

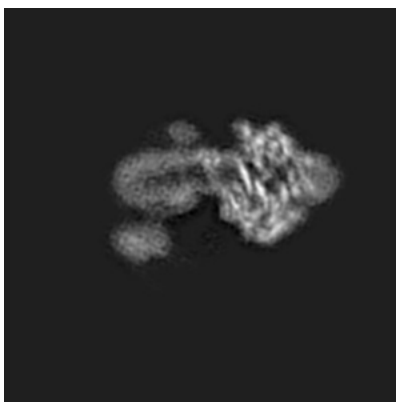
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

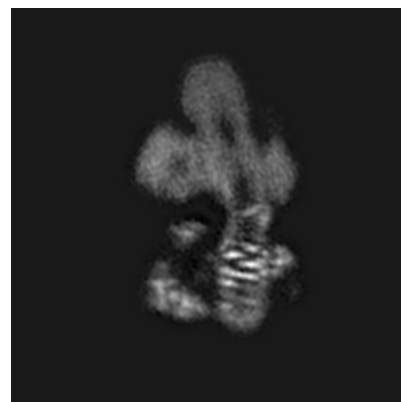
6.2.1 Primary map



X Index: 140



Y Index: 140

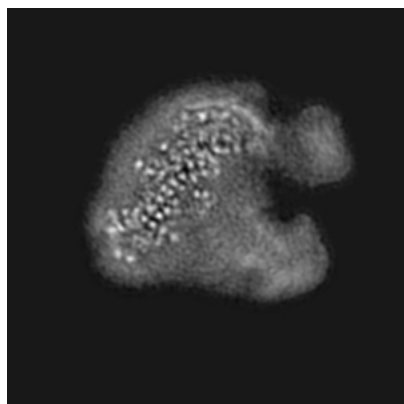


Z Index: 140

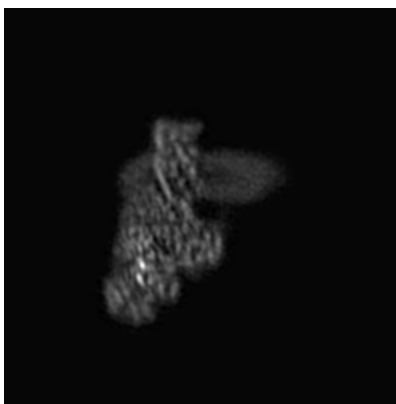
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

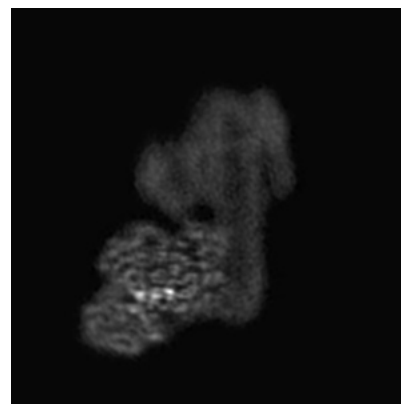
6.3.1 Primary map



X Index: 173



Y Index: 78

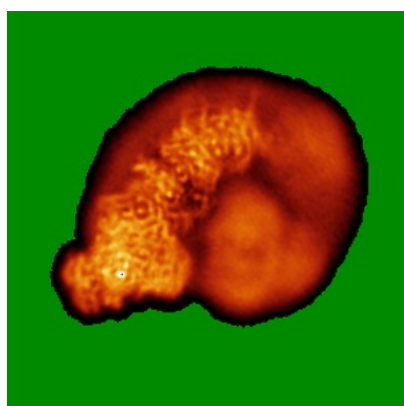


Z Index: 95

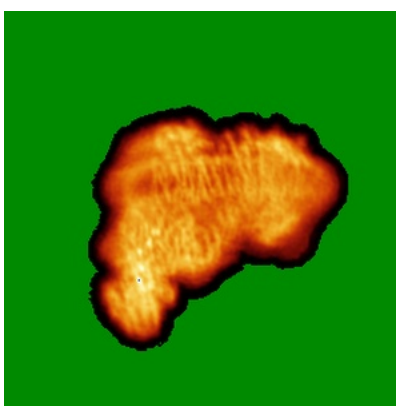
The images above show the largest variance slices of the map in three orthogonal directions.

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.

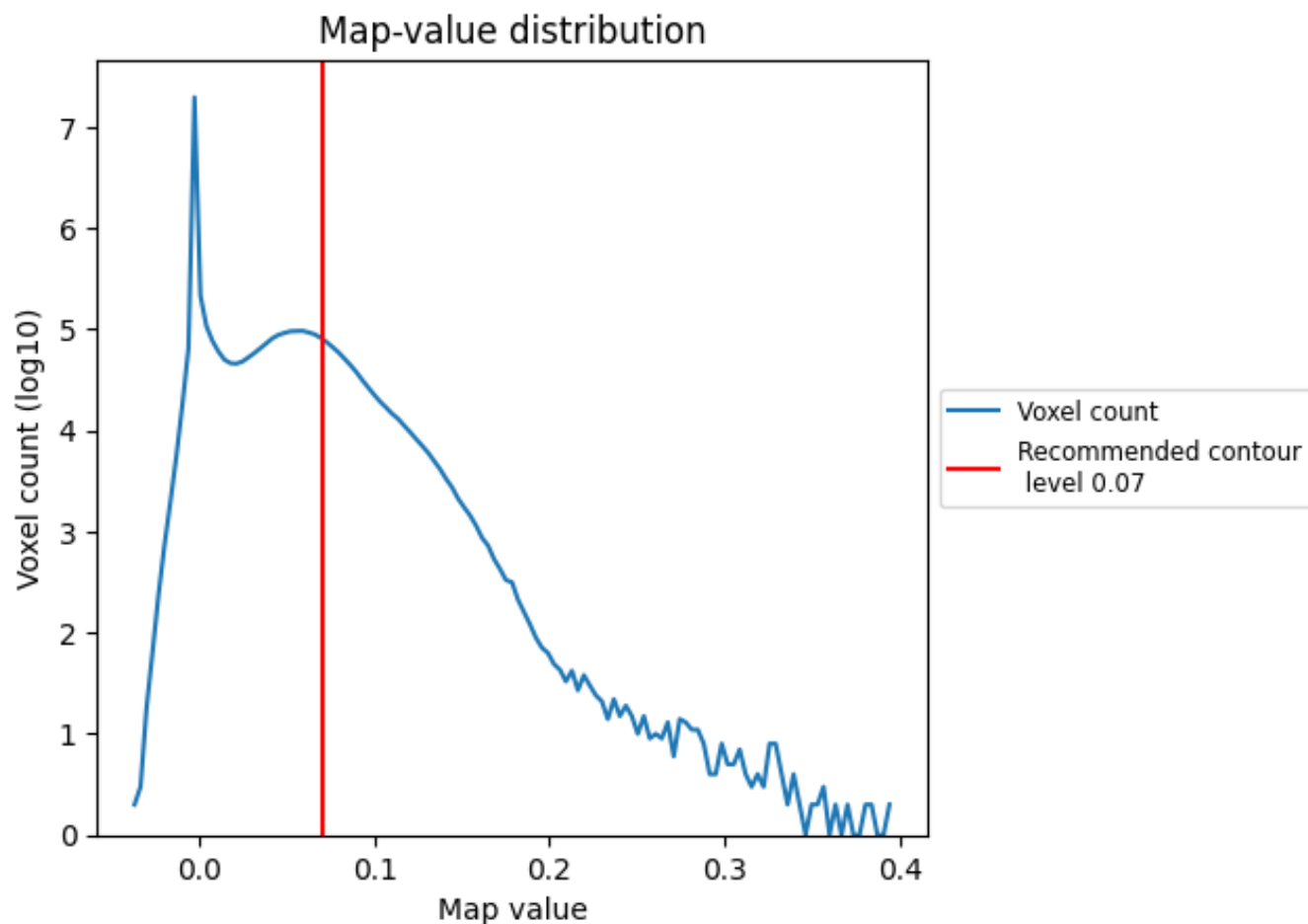
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

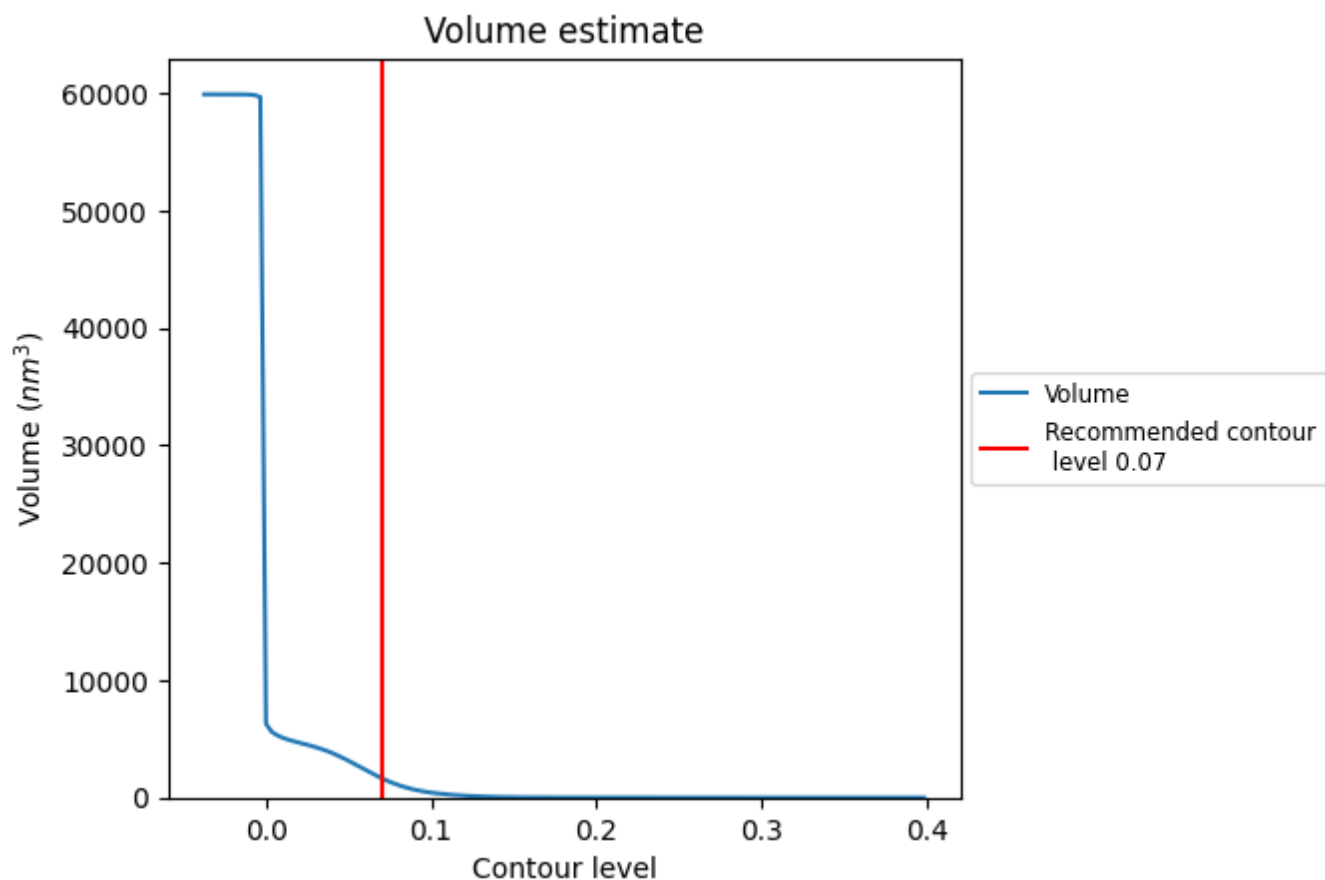
This section contains the results of statistical analysis of the map.

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.

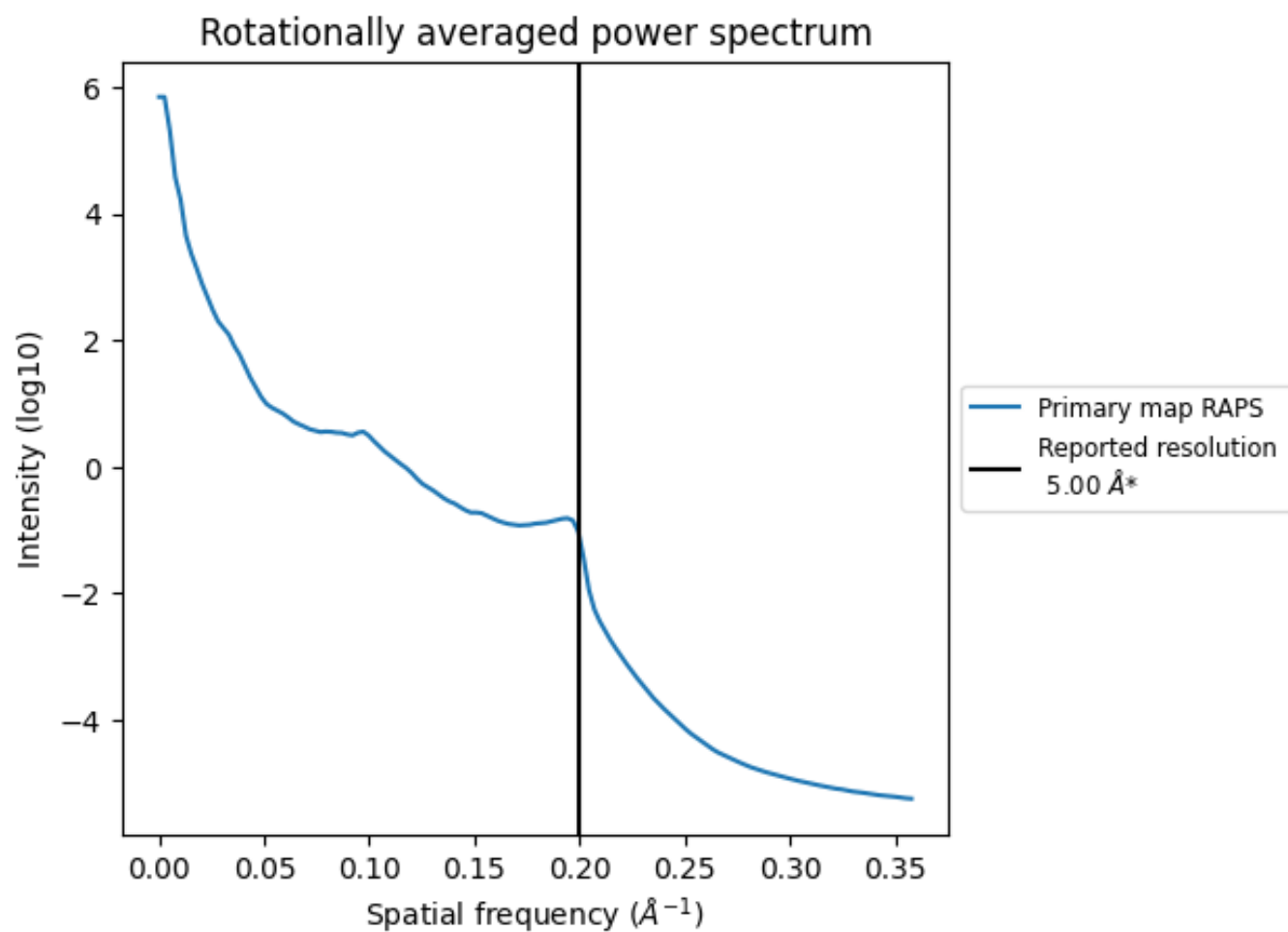
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1648 nm³; this corresponds to an approximate mass of 1489 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 0.200 Å⁻¹

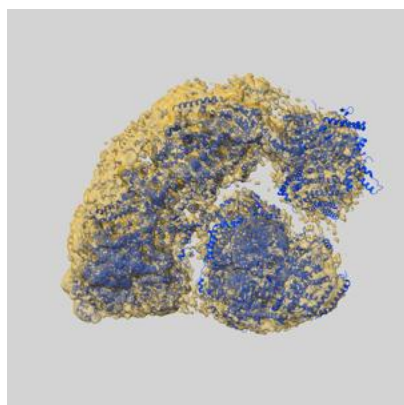
8 Fourier-Shell correlation

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

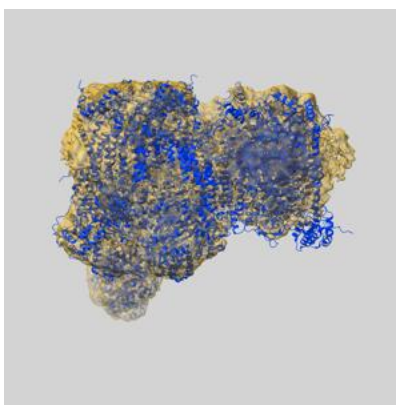
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30673 and PDB model 7DGQ. Per-residue inclusion information can be found in section [3](#) on page [26](#).

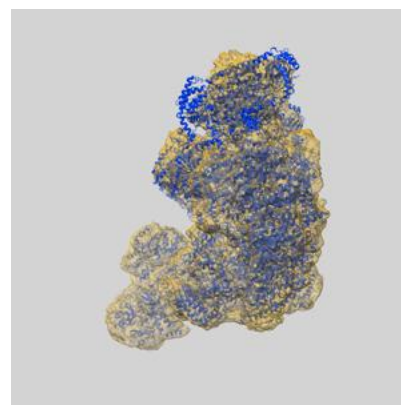
9.1 Map-model overlay [i](#)



X



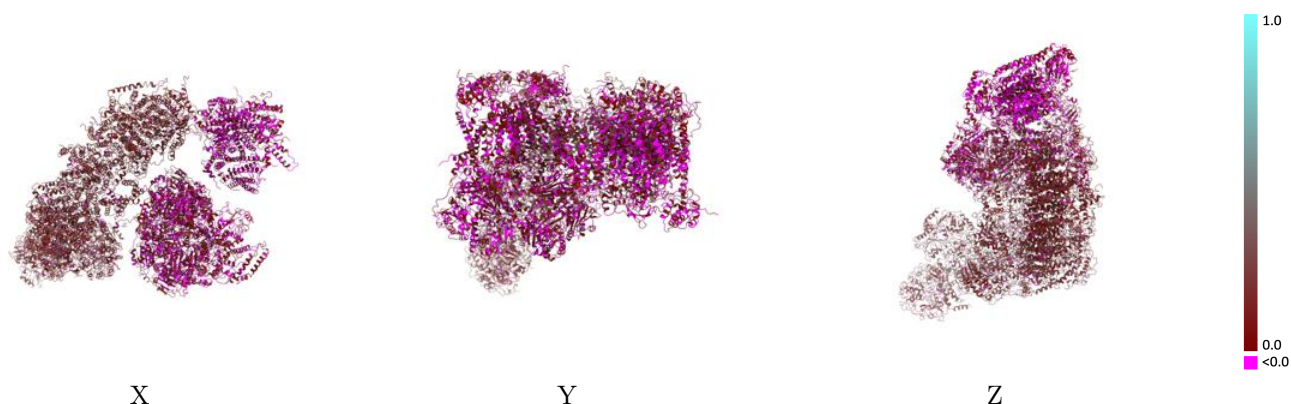
Y



Z

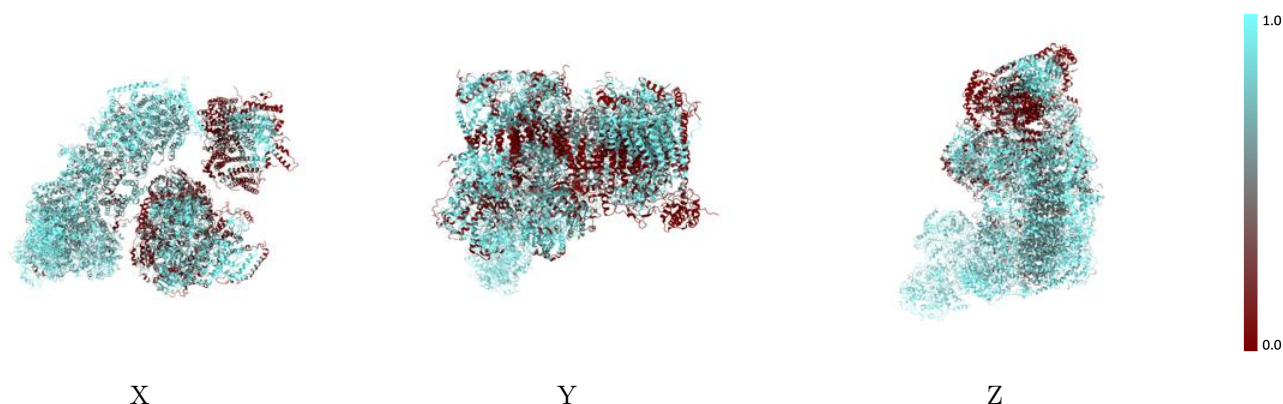
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



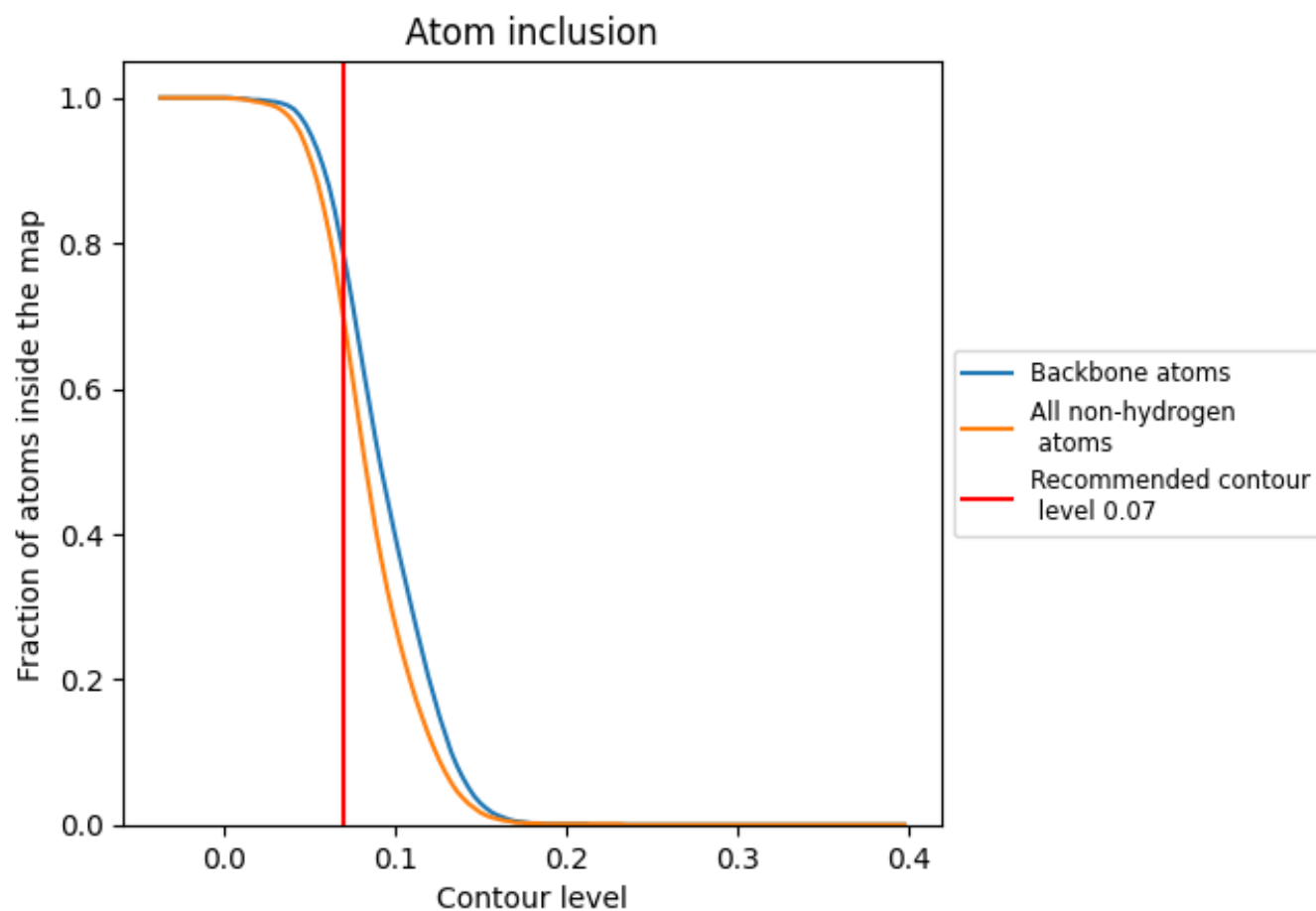
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% 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	 0.1370
1	 0.7230	 0.1890
2	 0.7400	 0.2030
3	 0.5620	 0.1640
4	 0.7340	 0.1990
5	 0.7100	 0.1980
6	 0.7260	 0.1730
7	 0.6960	 0.2000
8	 0.9590	 0.1910
9	 0.9320	 0.1940
A	 0.9350	 0.2080
A0	 0.2080	 0.0080
A1	 0.4260	 0.0540
A2	 0.3530	 0.1290
A3	 0.4260	 0.1100
A4	 0.2550	 0.0880
A5	 0.1520	 0.0210
A6	 0.1560	 -0.0070
A7	 0.1290	 0.0360
A8	 0.2350	 0.0120
A9	 0.2670	 0.0190
B	 0.8150	 0.2060
B2	 0.1040	 0.0280
B3	 0.2530	 0.0350
B4	 0.0250	 0.0460
B5	 0.3060	 0.0850
B6	 0.1840	 0.0610
B7	 0.2870	 0.0630
C	 0.9060	 0.2300
C0	 0.3150	 0.0330
C1	 0.6680	 0.0290
C2	 0.2380	 0.0360
C3	 0.5320	 0.0100
D	 0.8570	 0.2290
E	 0.9310	 0.2160



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Chain	Atom inclusion	Q-score
F	 0.9010	 0.1820
G	 0.8670	 0.2370
H	 0.8870	 0.2380
I	 0.7860	 0.1900
J	 0.8710	 0.1910
K	 0.9180	 0.1800
L	 0.8310	 0.2070
M	 0.5950	 0.1790
N	 0.9200	 0.2110
O	 0.8260	 0.2030
P	 0.8650	 0.2350
Q	 0.8940	 0.2120
R	 0.8110	 0.1950
S	 0.8080	 0.1830
T	 0.6510	 0.2090
U	 0.7060	 0.2000
V	 0.8730	 0.2090
W	 0.9360	 0.1850
X	 0.8610	 0.2150
Y	 0.9550	 0.2070
Z	 0.8570	 0.1800
a	 0.7880	 0.2130
b	 0.8670	 0.2180
c	 0.9450	 0.2240
d	 0.9700	 0.1850
e	 0.8140	 0.2280
f	 0.8950	 0.2100
g	 0.9180	 0.2010
h	 0.8660	 0.2000
i	 0.8940	 0.2010
j	 0.8150	 0.1980
k	 0.6740	 0.0470
l	 0.5390	 0.0510
m	 0.5360	 0.0590
o	 0.7830	 0.0660
p	 0.5510	 0.0480
q	 0.6250	 0.0590
r	 0.6620	 0.0710
s	 0.5900	 0.0660
t	 0.5810	 0.1060
u	 0.6010	 0.0350
v	 0.3040	 -0.0110

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Chain	Atom inclusion	Q-score
w	 0.5850	 0.0780
x	 0.7490	 0.0720
y	 0.5750	 0.0820
z	 0.6910	 0.0590