



## Full wwPDB EM Validation Report ⓘ

Feb 8, 2025 – 07:37 PM EST

PDB ID : 8UCA  
EMDB ID : EMD-42122  
Title : Formation of I2+III2 supercomplex rescues respiratory chain defects  
Authors : Letts, J.A.; Padavannil, A.  
Deposited on : 2023-09-26  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

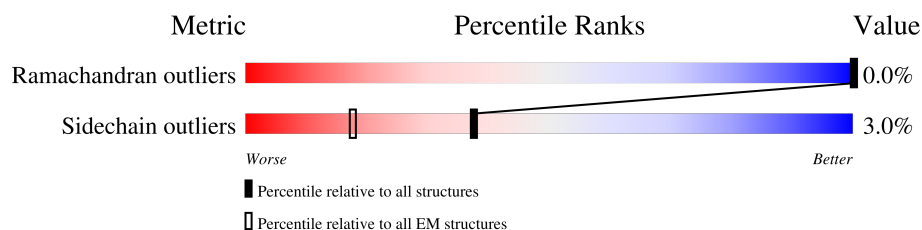
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
1	3a	115	
2	S3	263	
2	s3	263	
3	S2	463	
3	s2	463	
4	1	318	
4	1a	318	
5	6	172	

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Mol	Chain	Length	Quality of chain
5	6a	172	
6	4L	98	
6	4l	98	
7	5	607	
7	5a	607	
8	4	459	
8	4a	459	
9	2	345	
9	2a	345	
10	AL	355	
10	al	355	
11	A9	377	
11	a9	377	
12	S4	175	
12	s4	175	
13	S6	116	
13	s6	116	
14	A2	99	
14	a2	99	
15	AB	156	
15	AC	156	
15	ab	156	
15	ac	156	
16	A5	116	
16	a5	116	

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Mol	Chain	Length	Quality of chain
17	A6	131	<div> <div>24%</div> <div>83%</div> <div>15%</div> </div>
17	a6	131	<div> <div>27%</div> <div>82%</div> <div>15%</div> </div>
18	A8	172	<div> <div>21%</div> <div>94%</div> <div>••</div> </div>
18	a8	172	<div> <div>44%</div> <div>93%</div> <div>6% •</div> </div>
19	AM	142	<div> <div>44%</div> <div>94%</div> <div>5% •</div> </div>
19	am	142	<div> <div>52%</div> <div>96%</div> <div>••</div> </div>
20	AO	144	<div> <div>23%</div> <div>94%</div> <div>••</div> </div>
20	ao	144	<div> <div>42%</div> <div>94%</div> <div>••</div> </div>
21	A1	70	<div> <div>23%</div> <div>96%</div> <div>••</div> </div>
21	a1	70	<div> <div>49%</div> <div>94%</div> <div>••</div> </div>
22	A3	84	<div> <div>46%</div> <div>94%</div> <div>5% •</div> </div>
22	a3	84	<div> <div>68%</div> <div>94%</div> <div>5% •</div> </div>
23	C1	76	<div> <div>29%</div> <div>63%</div> <div>• 36%</div> </div>
23	c1	76	<div> <div>34%</div> <div>58%</div> <div>• 41%</div> </div>
24	C2	120	<div> <div>18%</div> <div>95%</div> <div>5%</div> </div>
24	c2	120	<div> <div>32%</div> <div>95%</div> <div>5%</div> </div>
25	S5	106	<div> <div>29%</div> <div>95%</div> <div>••</div> </div>
25	s5	106	<div> <div>40%</div> <div>95%</div> <div>••</div> </div>
26	B1	57	<div> <div>37%</div> <div>96%</div> <div>••</div> </div>
26	b1	57	<div> <div>54%</div> <div>91%</div> <div>7% •</div> </div>
27	BM	151	<div> <div>15%</div> <div>62%</div> <div>• 35%</div> </div>
27	bm	151	<div> <div>20%</div> <div>64%</div> <div>• 34%</div> </div>
28	B5	189	<div> <div>9%</div> <div>71%</div> <div>• 26%</div> </div>
28	b5	189	<div> <div>16%</div> <div>72%</div> <div>• 27%</div> </div>
29	B6	127	<div> <div>16%</div> <div>73%</div> <div>• 26%</div> </div>

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Mol	Chain	Length	Quality of chain
29	b6	127	
30	B2	105	
30	b2	105	
31	B3	104	
31	b3	104	
32	B8	186	
32	b8	186	
33	B4	129	
33	b4	129	
34	B9	179	
34	b9	179	
35	B7	136	
35	b7	136	
36	BL	176	
36	bl	176	
37	AN	145	
37	an	145	
38	A7	112	
38	a7	112	
39	V3	104	
39	v3	104	
40	3A	446	
40	3L	446	
41	3B	439	
41	3M	439	

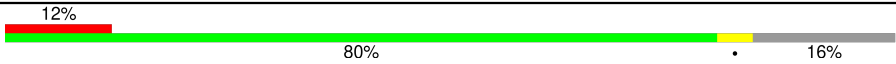

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Mol	Chain	Length	Quality of chain
42	3C	380	
42	3N	380	
43	3D	241	
43	3O	241	
44	3E	196	
44	3P	196	
45	3F	110	
45	3Q	110	
46	3G	81	
46	3R	81	
47	3H	76	
47	3S	76	
48	3J	63	
48	3U	63	
49	3K	56	
49	3V	56	
50	3T	78	
51	V1	457	
51	v1	457	
52	V2	244	
52	v2	244	
53	S1	716	
53	s1	716	
54	S7	224	
54	s7	224	

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Mol	Chain	Length	Quality of chain
55	S8	212	
55	s8	212	

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 162102 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	113	Total	C	N	O	S	0	0
			914	622	131	155	6		
1	3a	111	Total	C	N	O	S	0	0
			893	607	128	152	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S3	206	Total	C	N	O	S	0	0
			1712	1105	294	310	3		
2	s3	205	Total	C	N	O	S	0	0
			1701	1099	290	309	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	423	Total	C	N	O	S	0	0
			3410	2180	586	620	24		
3	s2	421	Total	C	N	O	S	0	0
			3386	2165	581	616	24		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	317	Total	C	N	O	S	0	0
			2530	1700	383	426	21		
4	1a	316	Total	C	N	O	S	0	0
			2522	1695	382	425	20		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	170	Total	C	N	O	S	0	0
			1290	868	184	224	14		
5	6a	171	Total	C	N	O	S	0	0
			1298	873	185	225	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4L	97	Total	C	N	O	S	0	0
			729	473	111	135	10		
6	4l	97	Total	C	N	O	S	0	0
			727	471	111	135	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		
7	5a	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		
8	4a	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		
9	2a	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	al	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		
11	a9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		
12	s4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		
13	s6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		
14	a2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AB	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	AC	88	Total	C	N	O	S	0	0
			706	453	104	144	5		
15	ab	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	ac	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A5	114	Total	C	N	O	S	0	0
			927	604	154	166	3		
16	a5	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A6	112	Total	C	N	O	S	0	0
			957	612	178	161	6		
17	a6	111	Total	C	N	O	S	0	0
			950	607	177	160	6		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A8	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		
18	a8	170	Total	C	N	O	S	0	0
			1389	884	249	246	10		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		
19	am	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AO	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		
20	ao	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		
21	a1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		
22	a3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C1	49	Total	C	N	O	S	0	0
			407	266	70	70	1		
23	c1	45	Total	C	N	O	S	0	0
			377	247	65	64	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		
24	c2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		
25	s5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		
26	b1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BM	98	Total	C	N	O	S	0	0
			826	536	133	153	4		
27	bm	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		
28	b5	138	Total	C	N	O	S	0	0
			1158	760	193	202	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	94	Total	C	N	O	S	0	0
			783	511	137	132	3		
29	b6	90	Total	C	N	O	S	0	0
			761	495	133	130	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	64	Total	C	N	O	S	0	0
			555	365	92	97	1		
30	b2	63	Total	C	N	O	S	0	0
			545	359	89	96	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B3	70	Total	C	N	O	S	0	0
			569	376	99	92	2		
31	b3	71	Total	C	N	O	S	0	0
			573	378	100	93	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		
32	b8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B4	125	Total	C	N	O		0	0
			1044	673	188	183			
33	b4	125	Total	C	N	O		0	0
			1044	673	188	183			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B9	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		
34	b9	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	114	Total	C	N	O	S	0	0
			984	620	185	171	8		
35	b7	117	Total	C	N	O	S	0	0
			1005	634	189	174	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	167	Total	C	N	O	S	0	0
			1410	888	251	263	8		
36	bl	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AN	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		
37	an	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A7	92	Total	C	N	O	S	0	0
			741	469	139	130	3		
38	a7	70	Total	C	N	O	S	0	0
			560	350	108	100	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	V3	40	Total	C	N	O	0	0
			339	213	62	64		
39	v3	36	Total	C	N	O	0	0
			303	190	56	57		

- Molecule 40 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
40	3L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 41 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
41	3M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 42 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
42	3N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 43 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
43	3O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 44 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3E	80	Total	C	N	O	S	0	0
			602	374	100	126	2		
44	3P	81	Total	C	N	O	S	0	0
			610	380	101	127	2		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	3Q	99	Total	C	N	O	S	0	0
			879	563	156	157	3		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3G	79	Total	C	N	O	S	0	0
			670	432	123	114	1		
46	3R	71	Total	C	N	O		0	0
			600	389	112	99			

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
47	3S	66	Total	C	N	O	S	0	0
			545	333	101	106	5		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	3J	56	Total	C	N	O	0	0
			460	302	81	77		
48	3U	59	Total	C	N	O	0	0
			489	320	85	84		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3K	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
49	3V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3T	56	Total	C	N	O	S	0	0
			397	250	76	69	2		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochond-

drial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V1	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		
51	v1	422	Total	C	N	O	S	0	0
			3259	2053	584	600	22		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	209	Total	C	N	O	S	0	0
			1630	1038	273	308	11		
52	v2	192	Total	C	N	O	S	0	0
			1517	965	255	286	11		

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		
53	s1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		
54	s7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

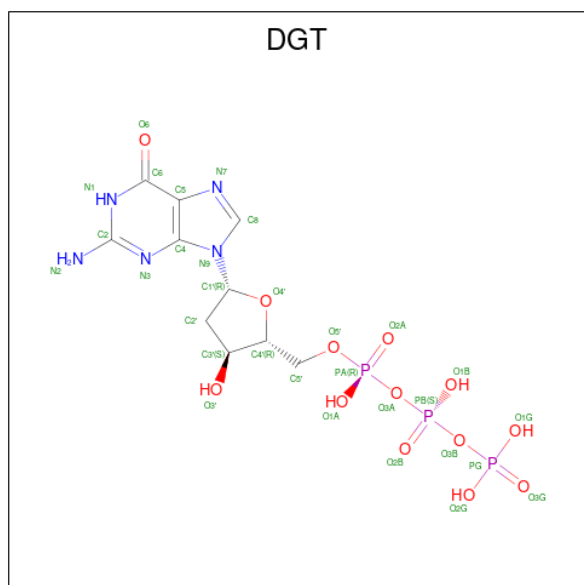
- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S8	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		
55	s8	164	Total	C	N	O	S	0	0
			1309	821	226	250	12		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

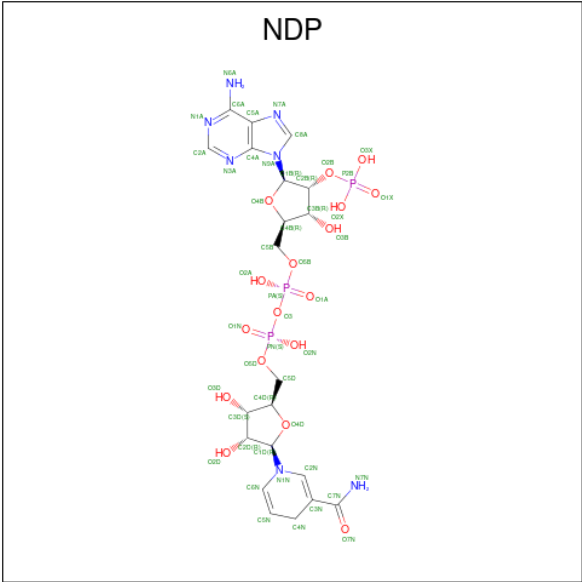
Mol	Chain	Residues	Atoms		AltConf
56	AL	1	Total	Mg	0
			1	1	
56	al	1	Total	Mg	0
			1	1	

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
57	AL	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	al	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
58	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	
58	a9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	S6	1	Total	Zn	0
			1	1	
59	s6	1	Total	Zn	0
			1	1	

- Molecule 60 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

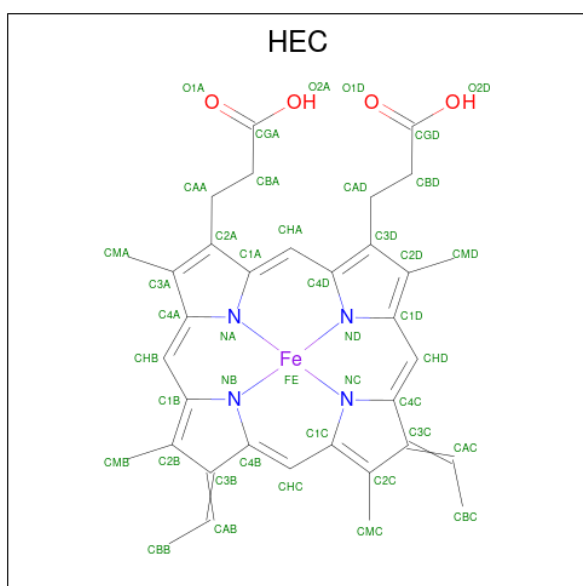


- Molecule 61 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



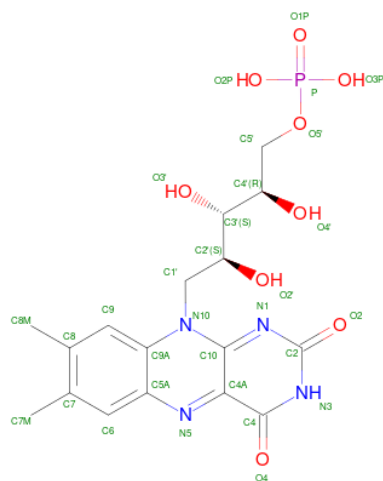
Mol	Chain	Residues	Atoms					AltConf
61	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 62 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



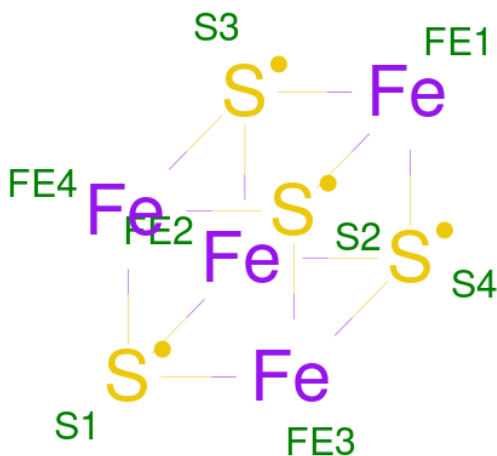
Mol	Chain	Residues	Atoms					AltConf
62	3D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	3O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 63 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					AltConf
63	V1	1	Total 31	C 17	N 4	O 9	P 1	0
63	v1	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 64 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



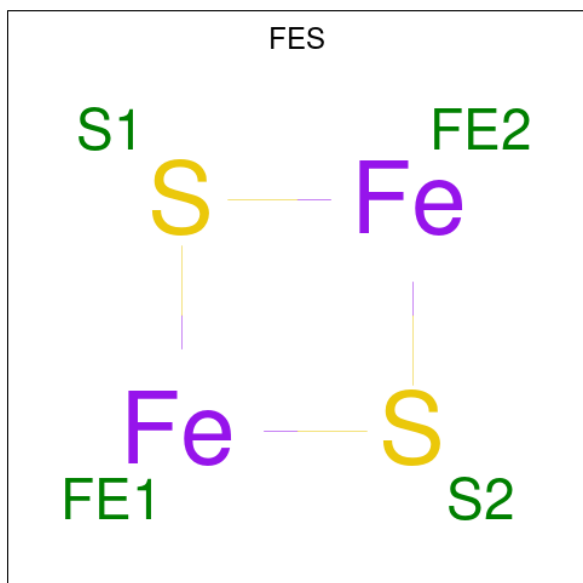
Mol	Chain	Residues	Atoms			AltConf
64	V1	1	Total 8	Fe 4	S 4	0
64	S1	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
64	S1	1	Total	Fe	S	0
			8	4	4	
64	S7	1	Total	Fe	S	0
			8	4	4	
64	S8	1	Total	Fe	S	0
			8	4	4	
64	S8	1	Total	Fe	S	0
			8	4	4	
64	v1	1	Total	Fe	S	0
			8	4	4	
64	s1	1	Total	Fe	S	0
			8	4	4	
64	s1	1	Total	Fe	S	0
			8	4	4	
64	s7	1	Total	Fe	S	0
			8	4	4	
64	s8	1	Total	Fe	S	0
			8	4	4	
64	s8	1	Total	Fe	S	0
			8	4	4	

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
65	V2	1	Total	Fe	S	0
			4	2	2	

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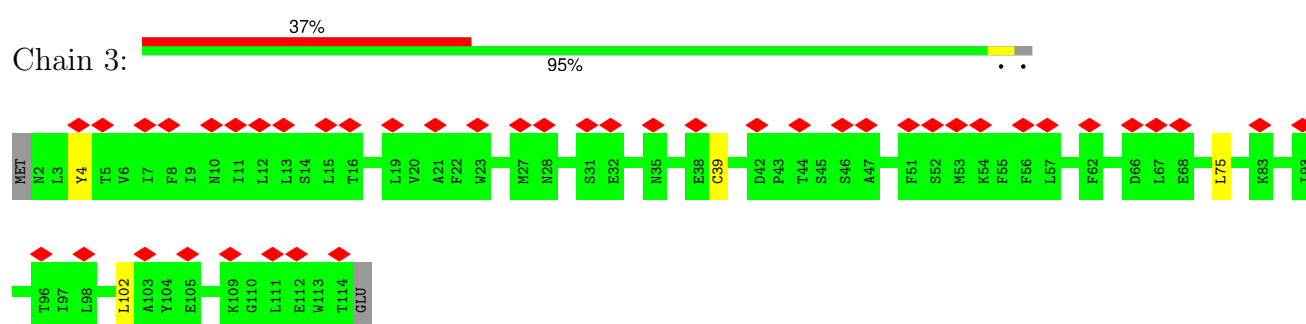
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Mol	Chain	Residues	Atoms			AltConf
65	S1	1	Total 4	Fe 2	S 2	0
65	v2	1	Total 4	Fe 2	S 2	0
65	s1	1	Total 4	Fe 2	S 2	0

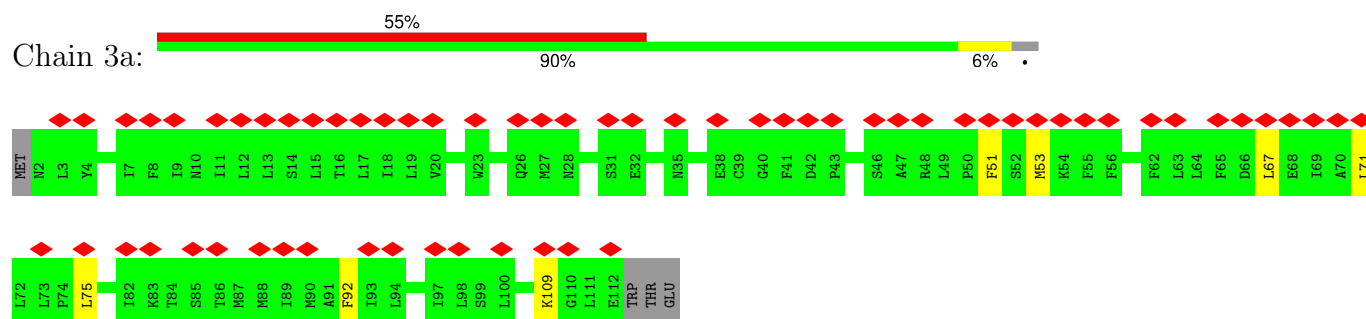
### 3 Residue-property plots [i](#)

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

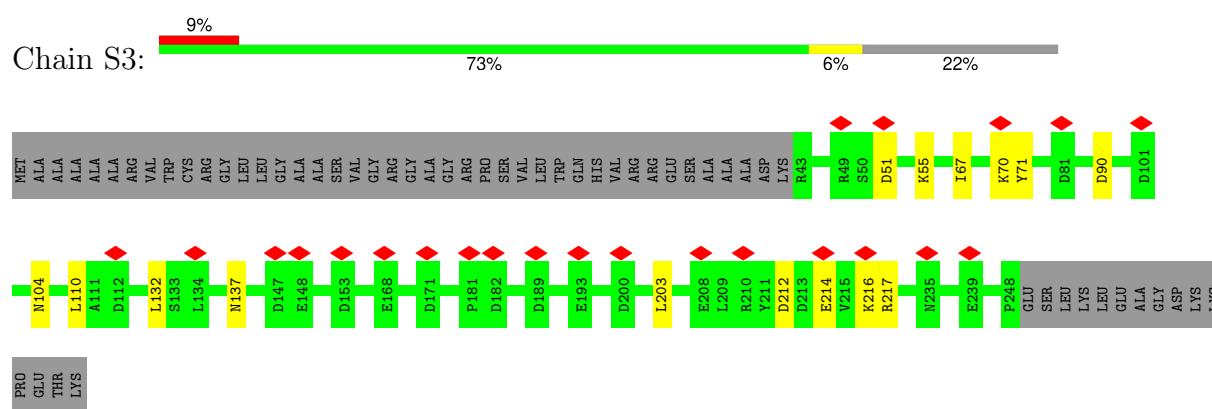
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



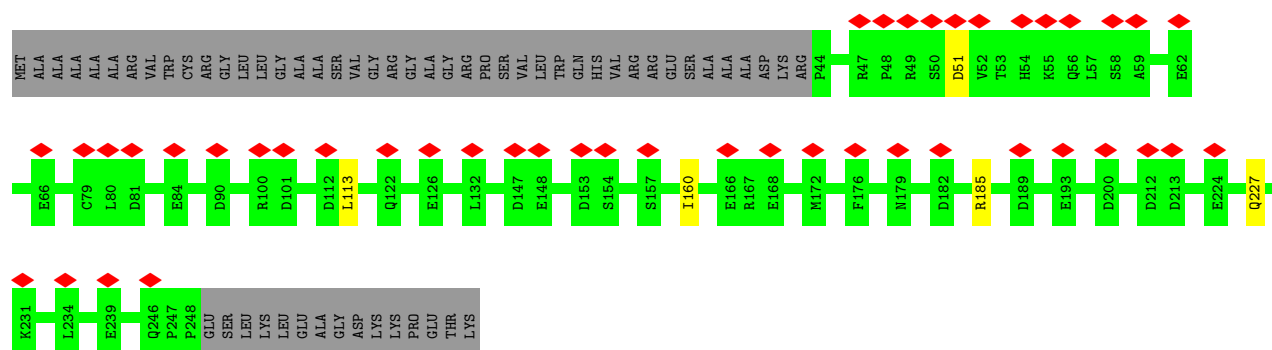
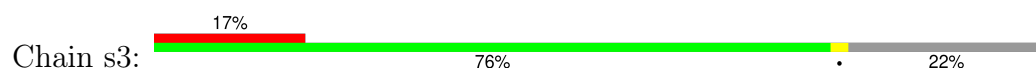
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



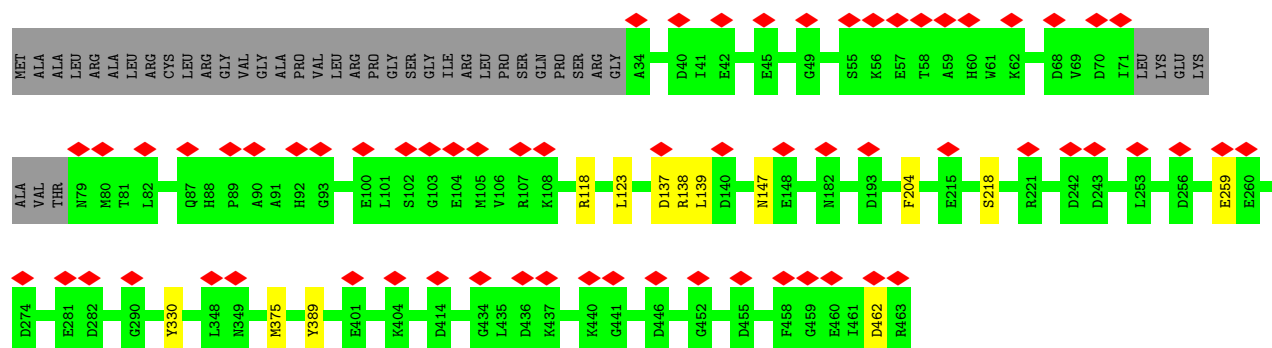
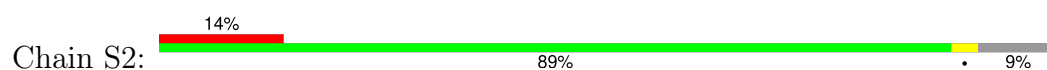
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



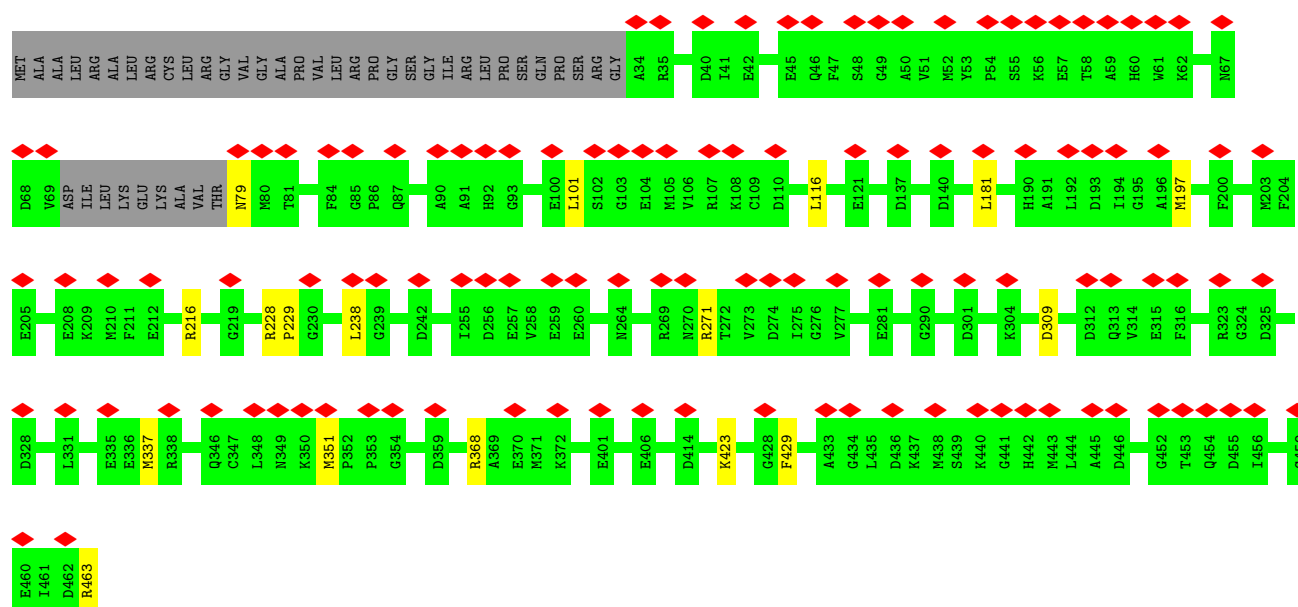
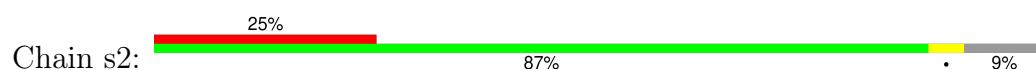
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



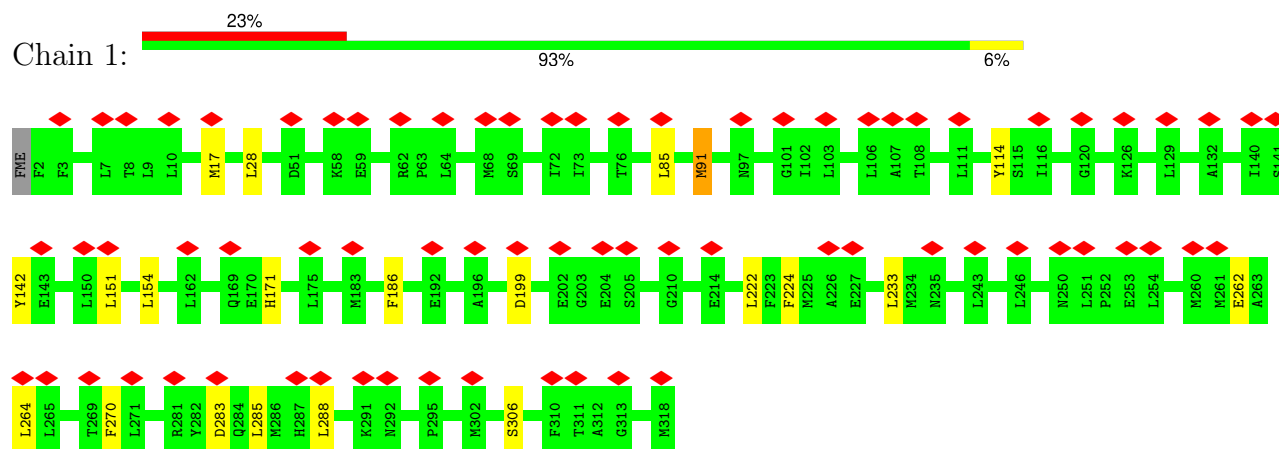
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



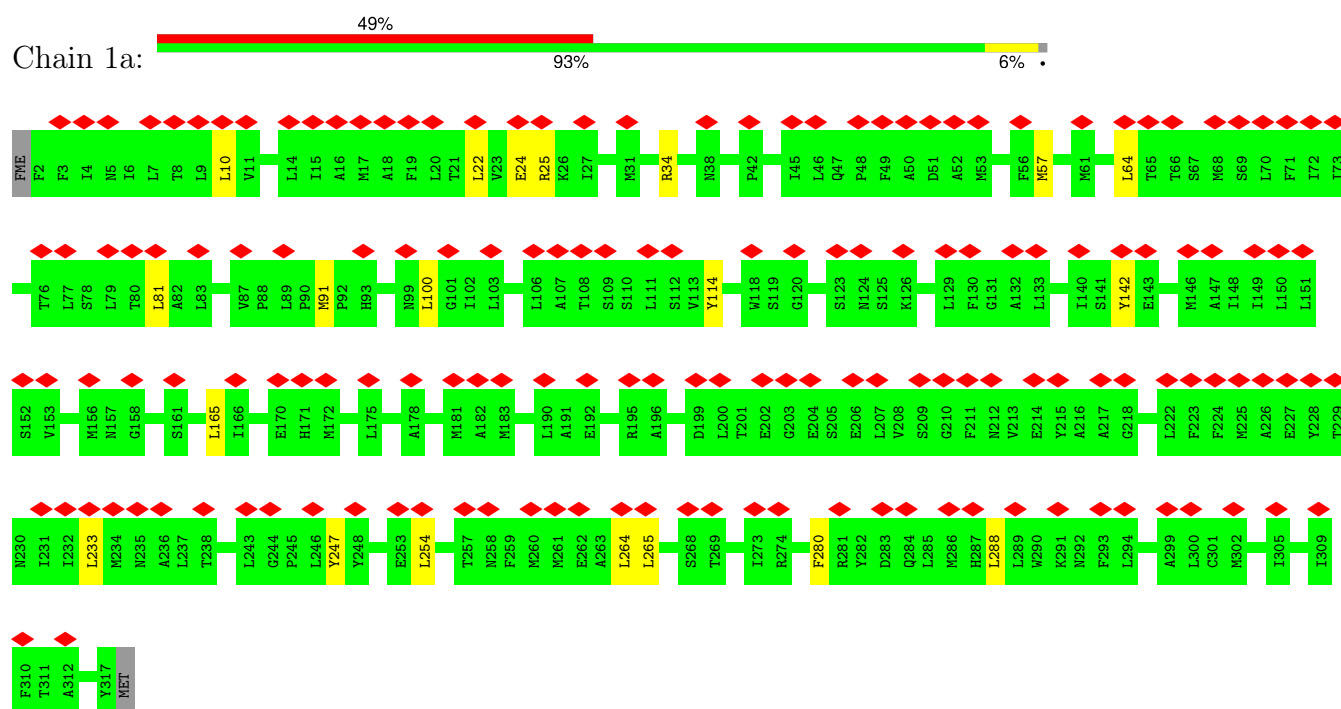
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



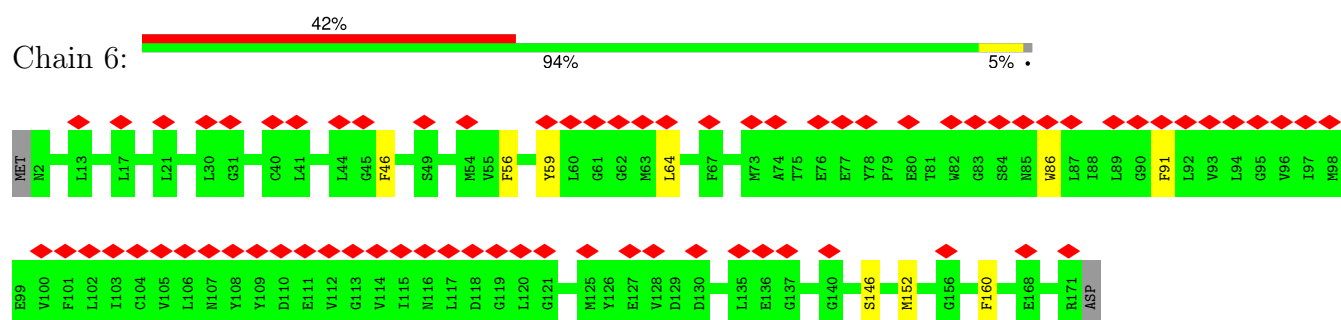
- Molecule 4: NADH-ubiquinone oxidoreductase chain 1



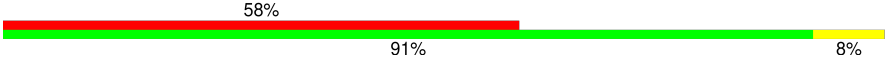
- Molecule 4: NADH-ubiquinone oxidoreductase chain 1

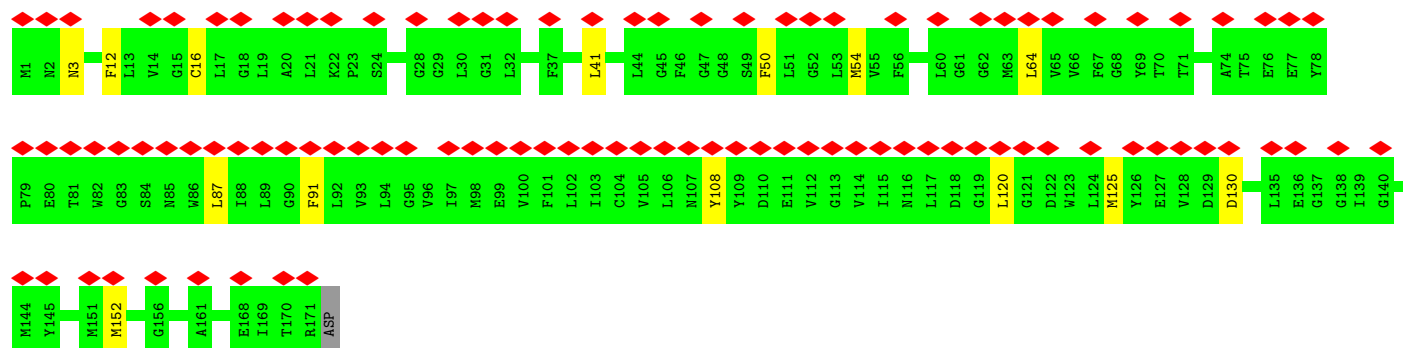


- Molecule 5: NADH-ubiquinone oxidoreductase chain 6



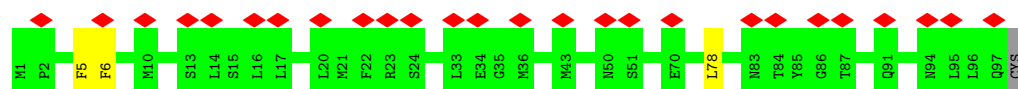
- Molecule 5: NADH-ubiquinone oxidoreductase chain 6

Chain 6a: 



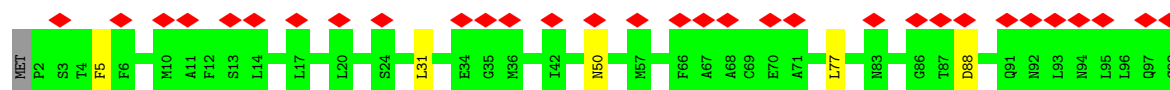
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 



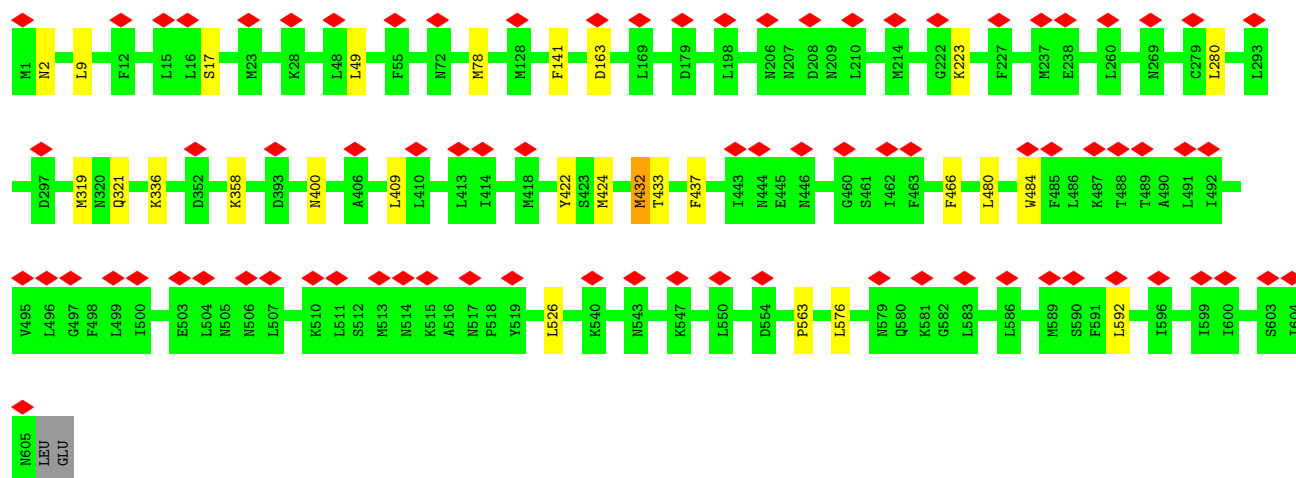
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 



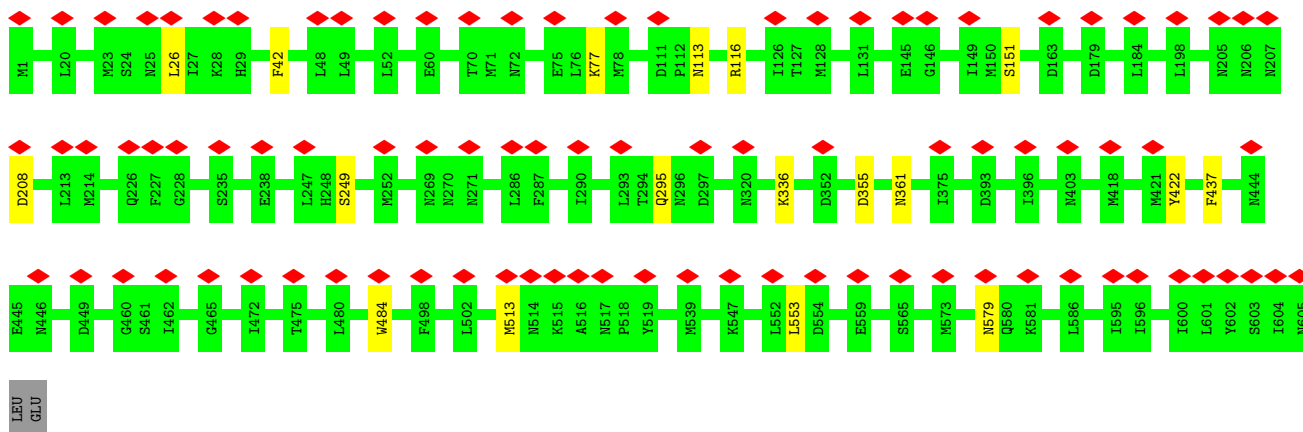
- Molecule 7: NADH-ubiquinone oxidoreductase chain 5

Chain 5: 

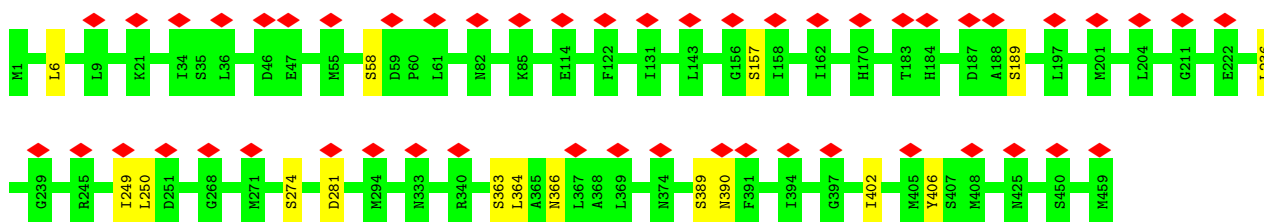


- Molecule 7: NADH-ubiquinone oxidoreductase chain 5

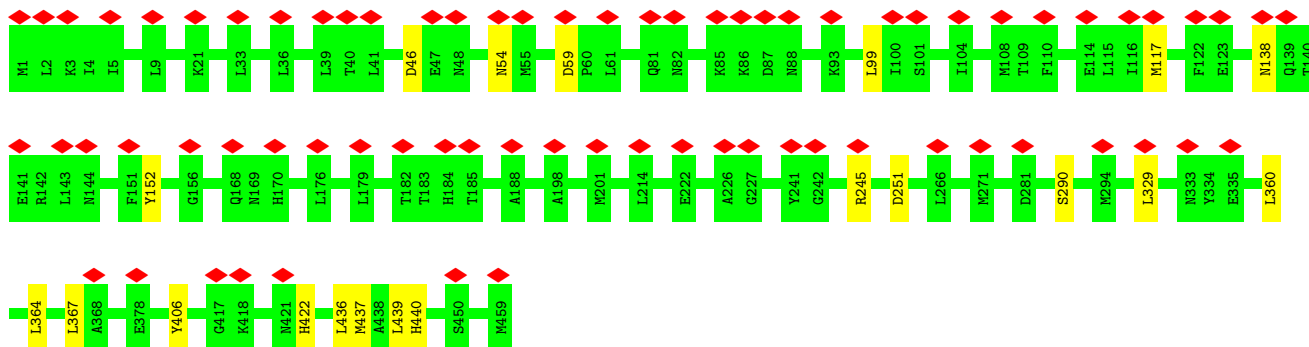
Chain 5a: 



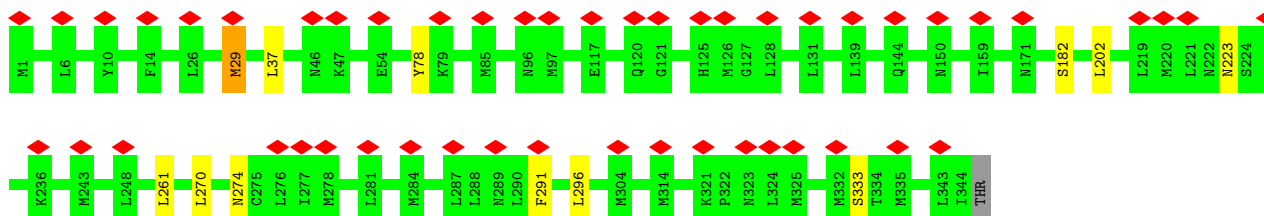
• Molecule 8: NADH-ubiquinone oxidoreductase chain 4



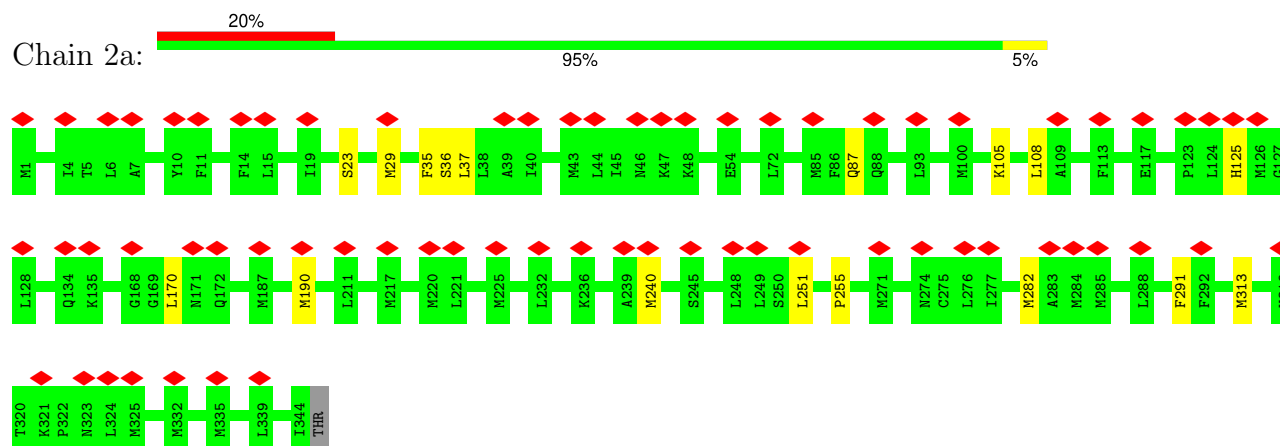
• Molecule 8: NADH-ubiquinone oxidoreductase chain 4



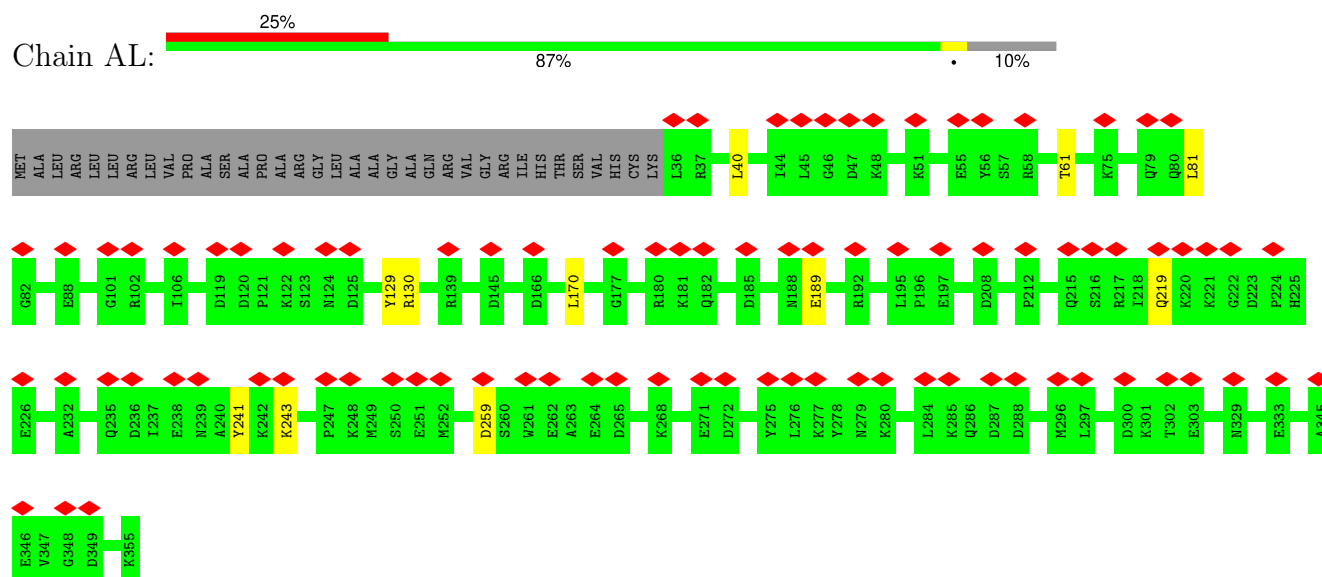
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2



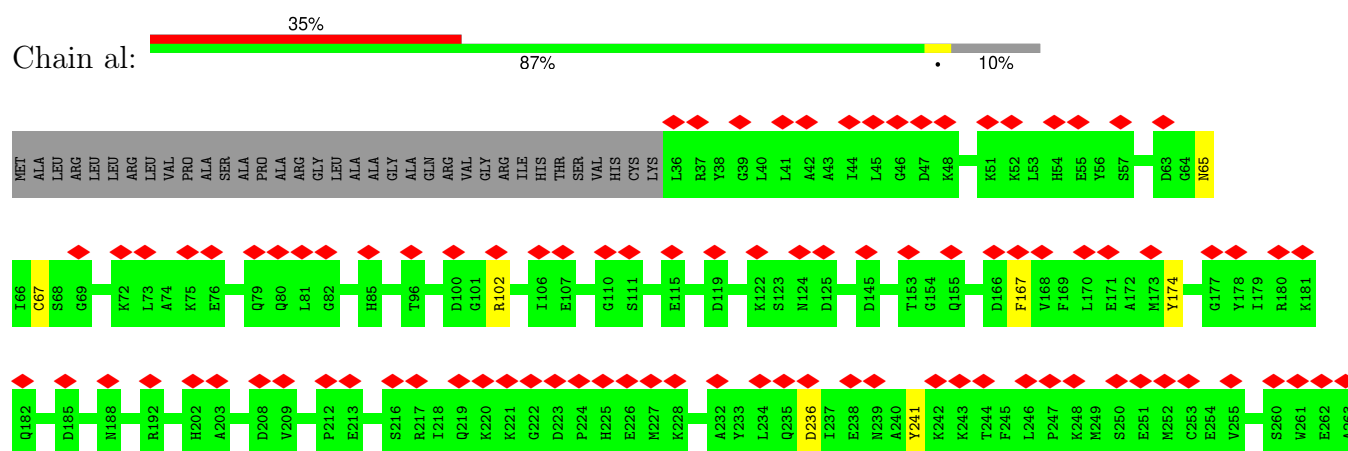
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

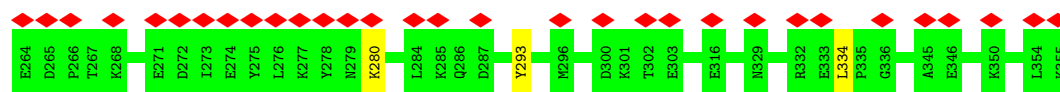


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

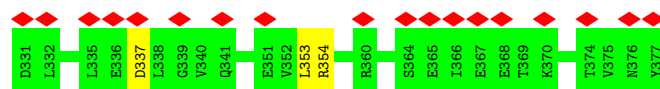
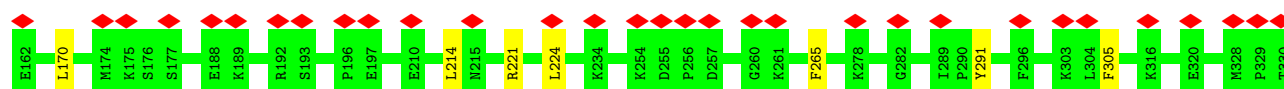
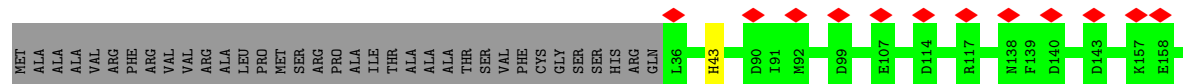


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

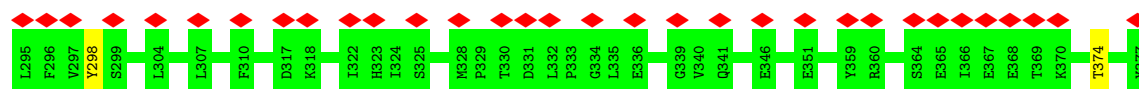
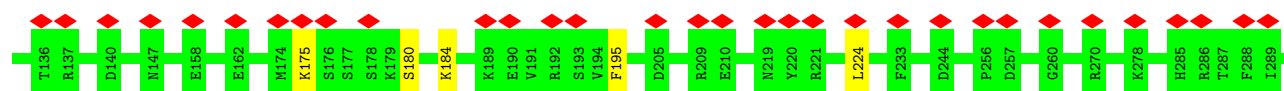
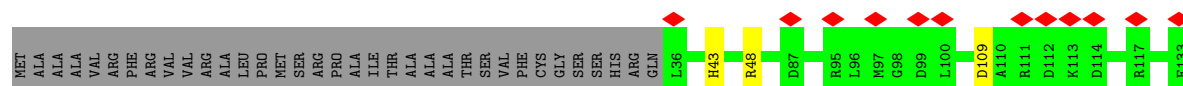
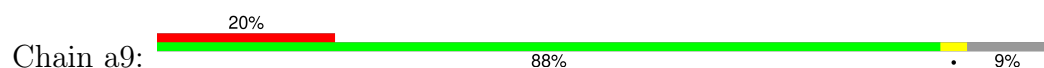




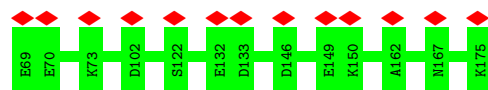
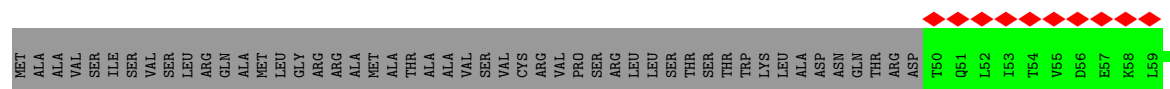
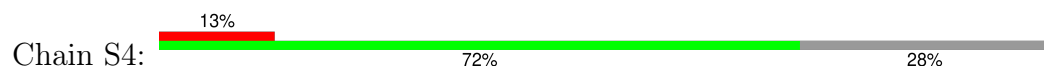
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



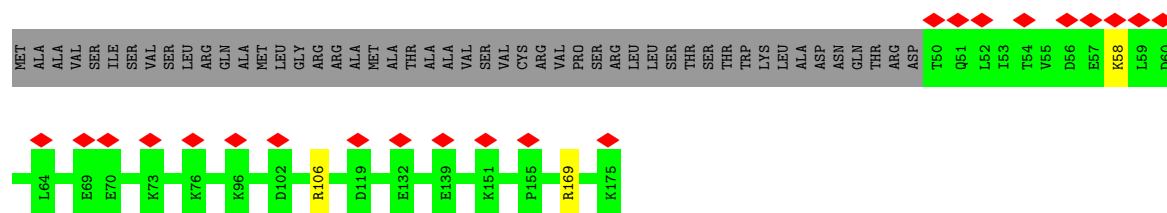
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



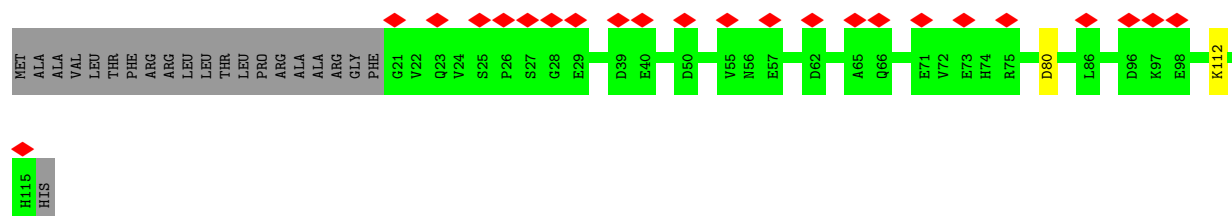
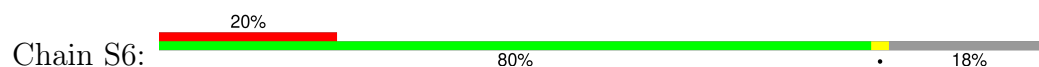
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



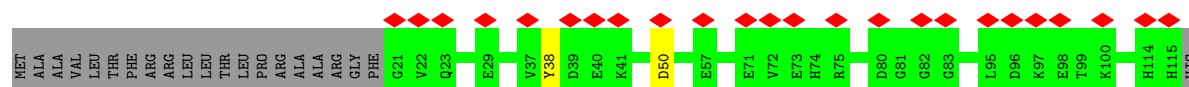
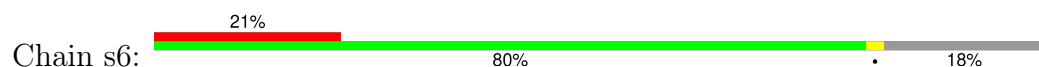




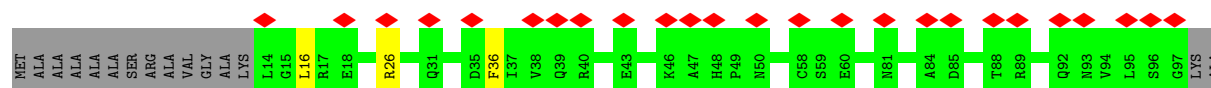
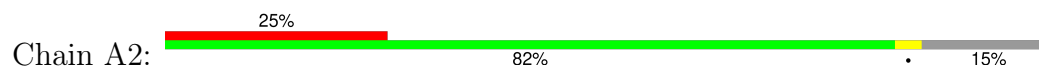
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



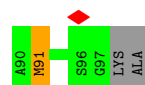
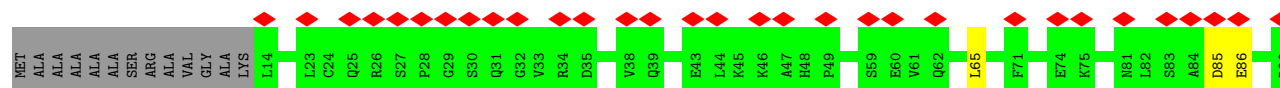
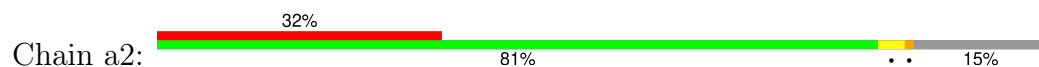
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

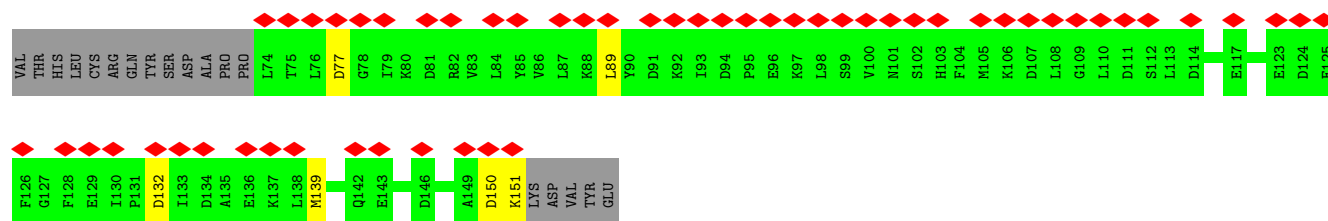


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

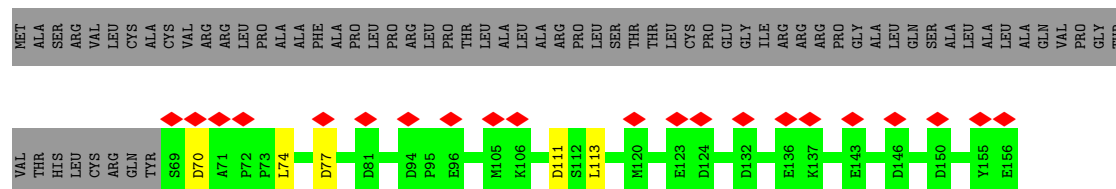


- Molecule 15: Acyl carrier protein, mitochondrial

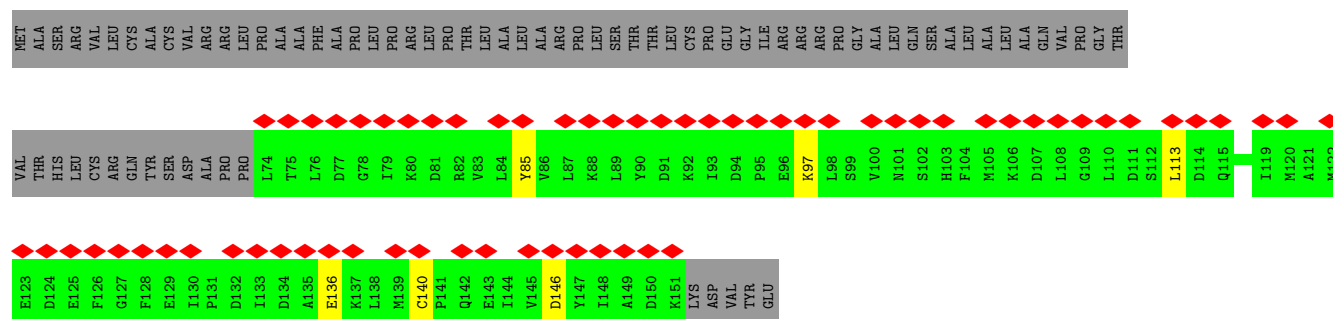
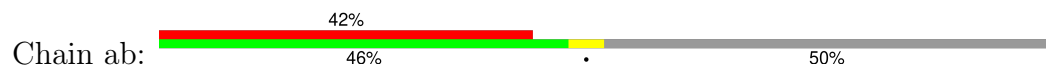




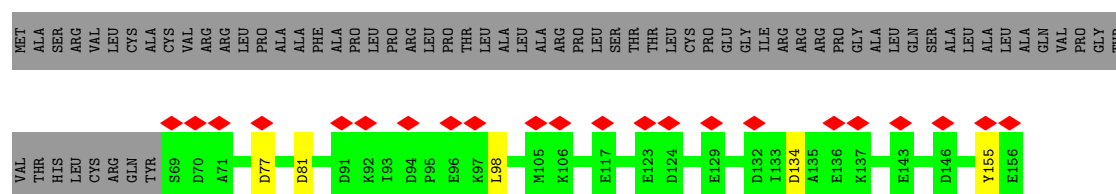
- Molecule 15: Acyl carrier protein, mitochondrial



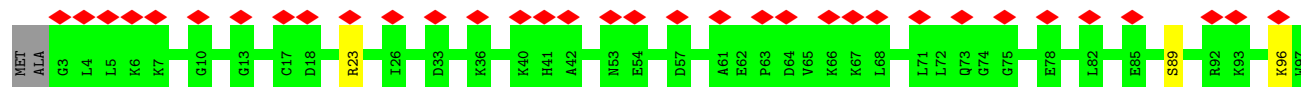
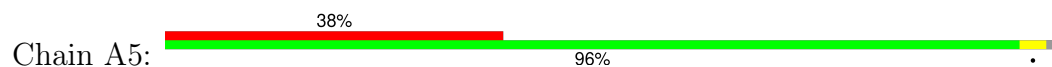
- Molecule 15: Acyl carrier protein, mitochondrial

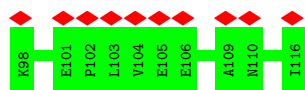


- Molecule 15: Acyl carrier protein, mitochondrial

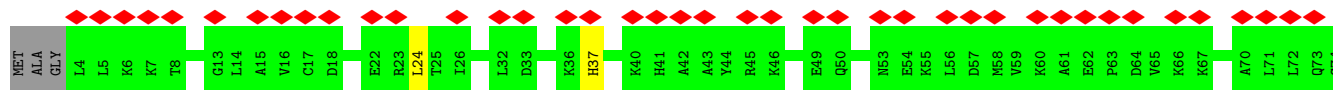


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

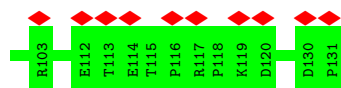
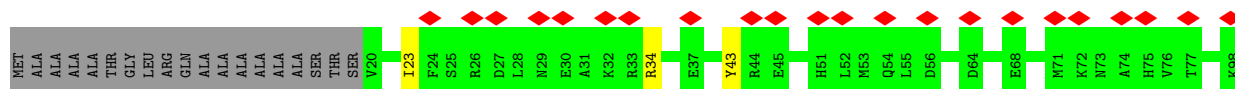
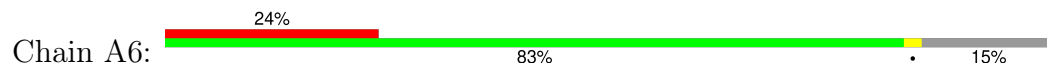




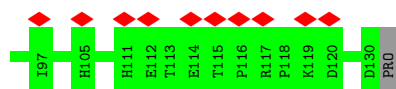
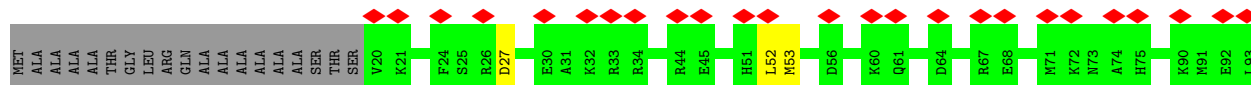
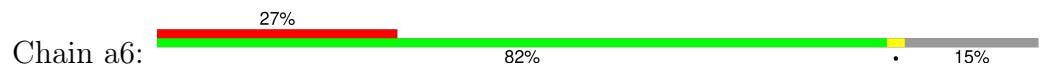
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



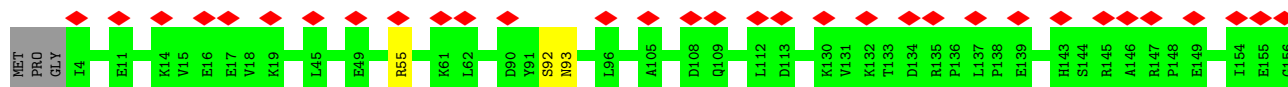
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



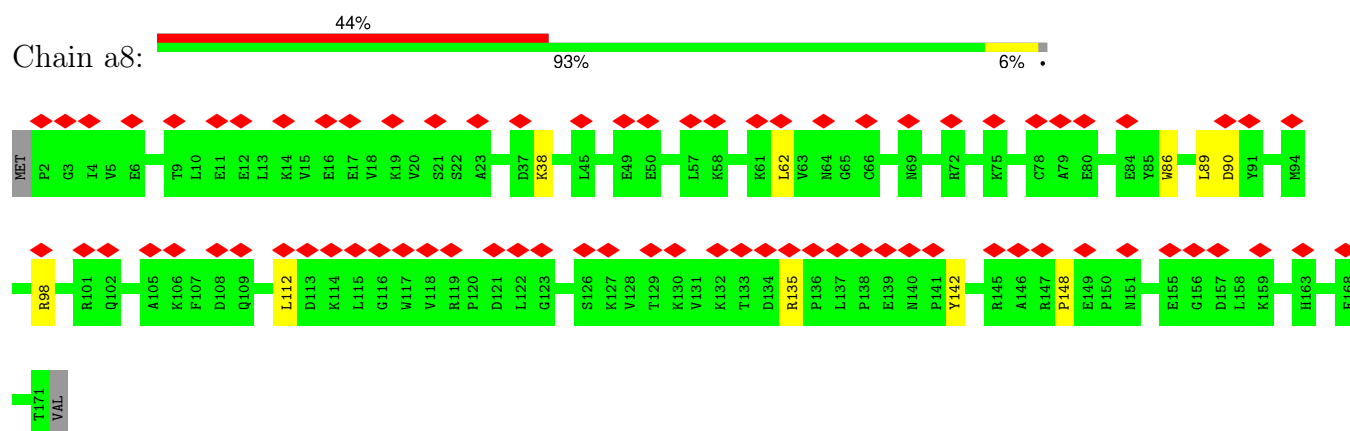
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



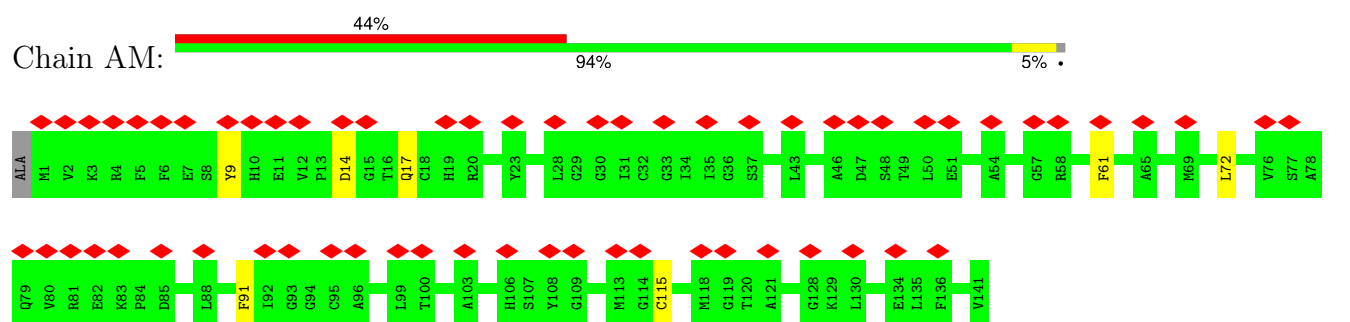
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



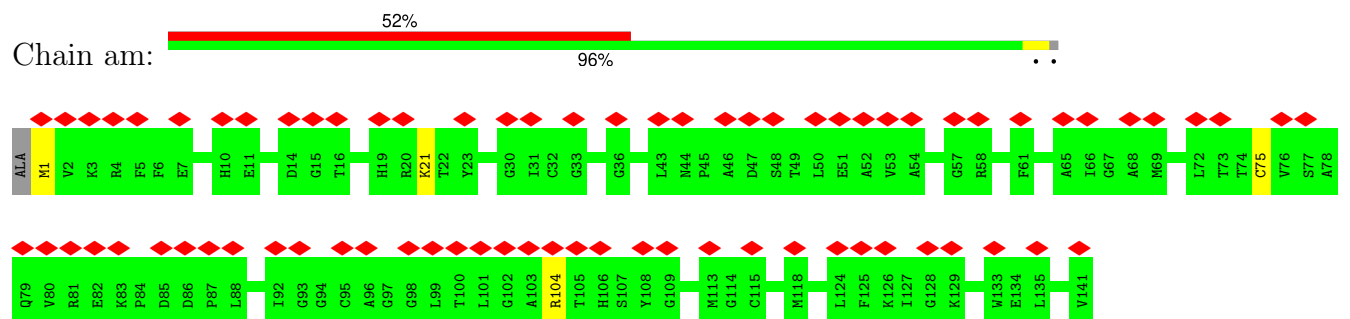
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



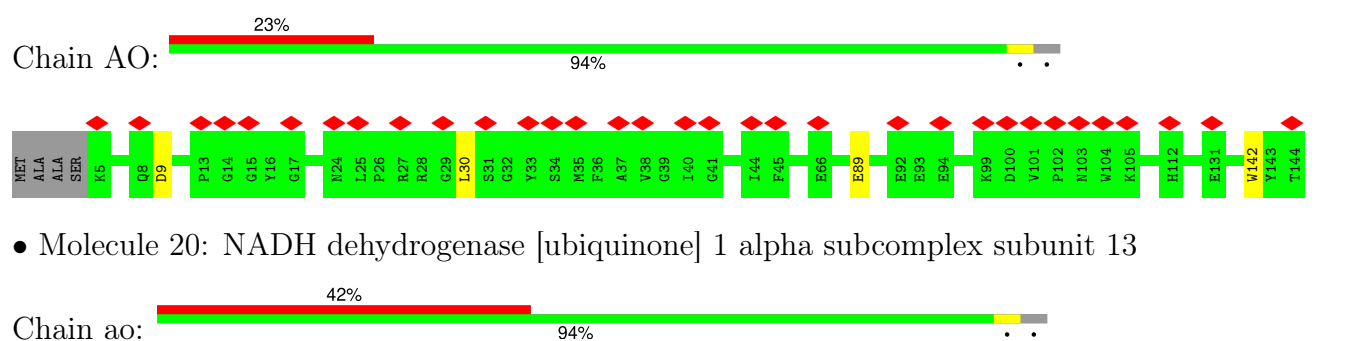
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



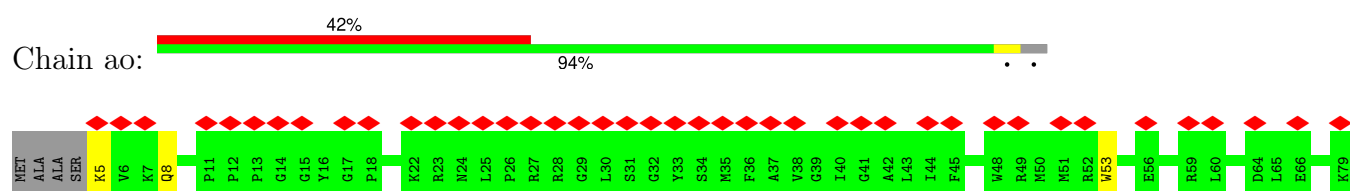
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

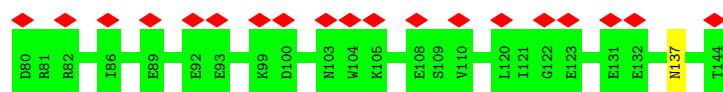


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13





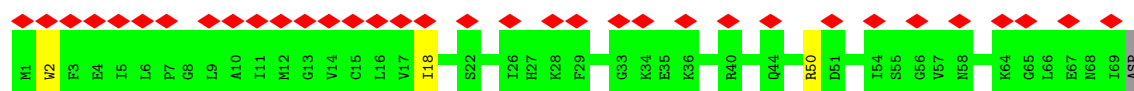
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain A1: 



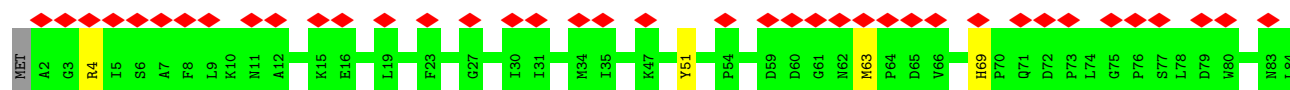
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1: 



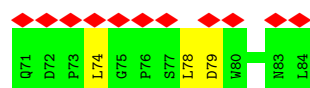
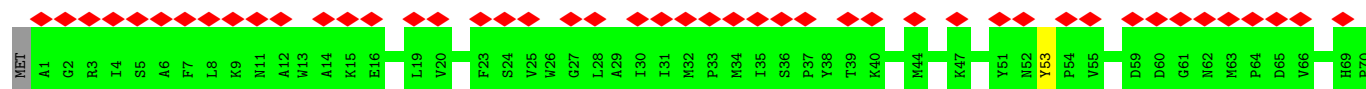
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3: 



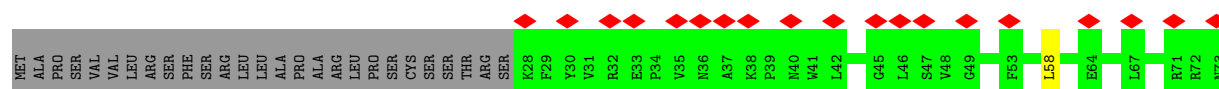
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain a3: 

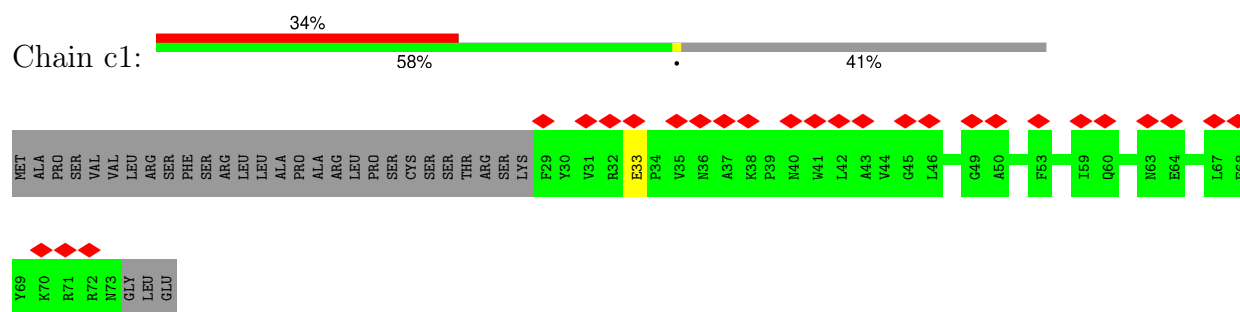


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

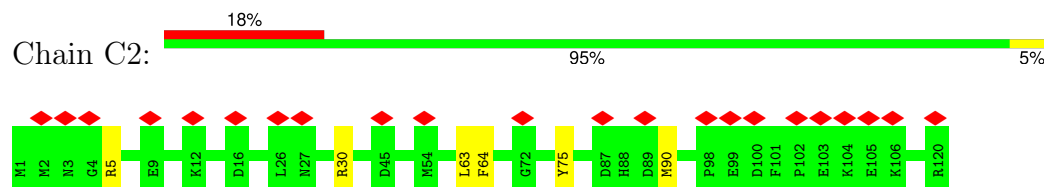
Chain C1: 



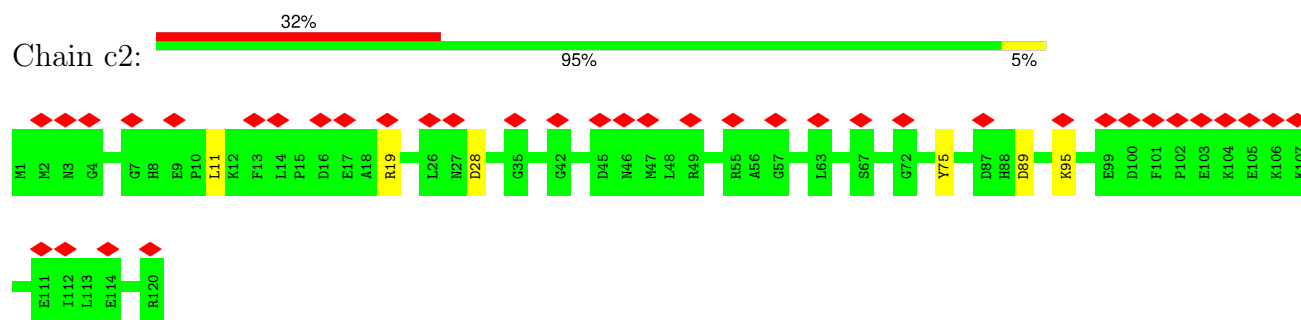
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



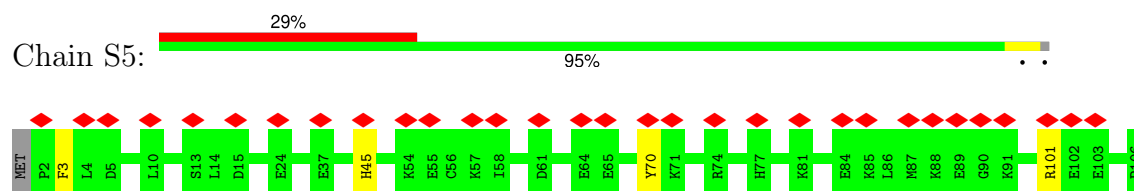
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



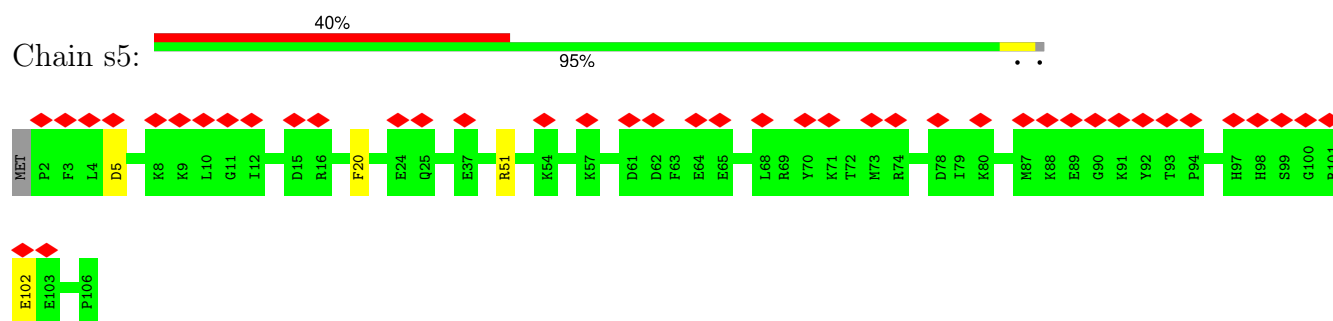
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



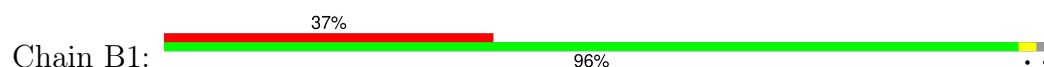
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

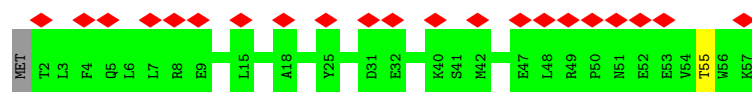


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

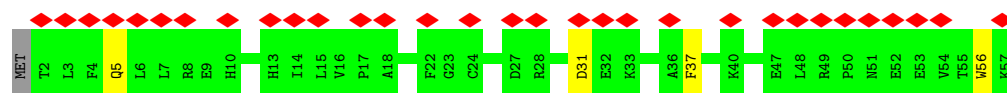
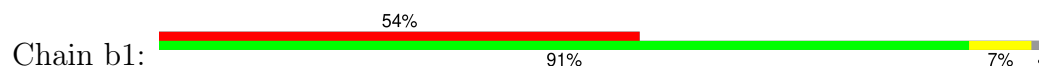


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

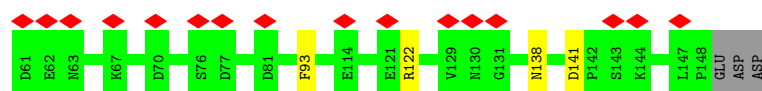
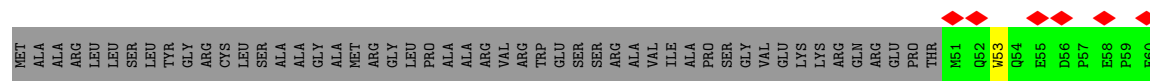




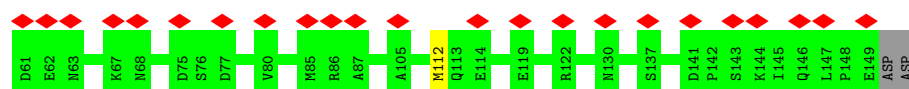
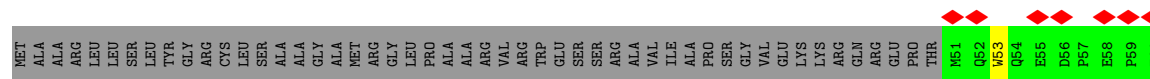
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



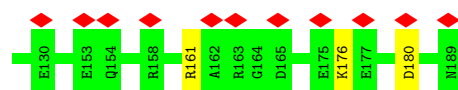
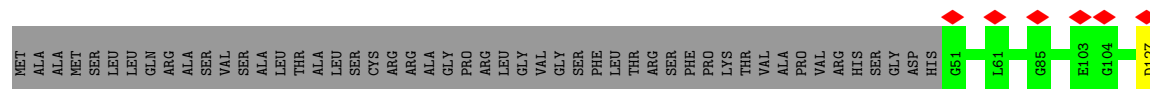
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



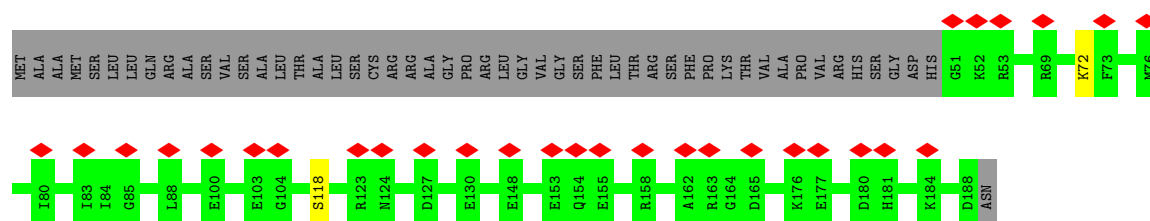
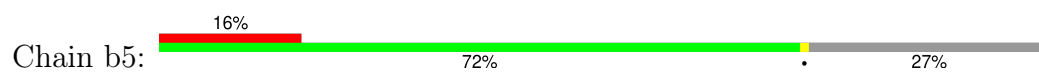
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



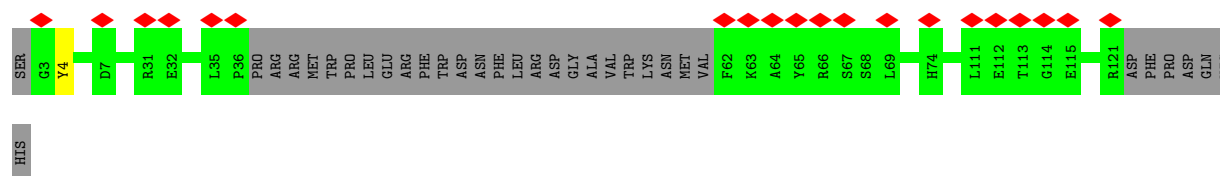
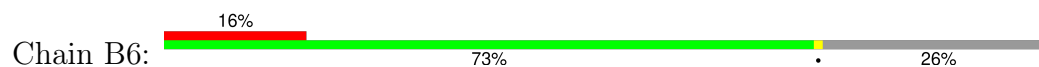
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



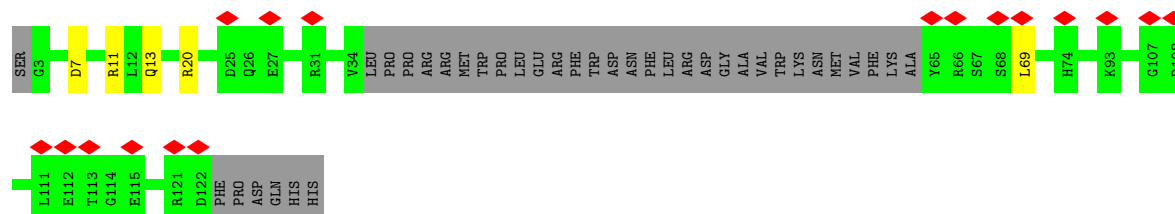
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



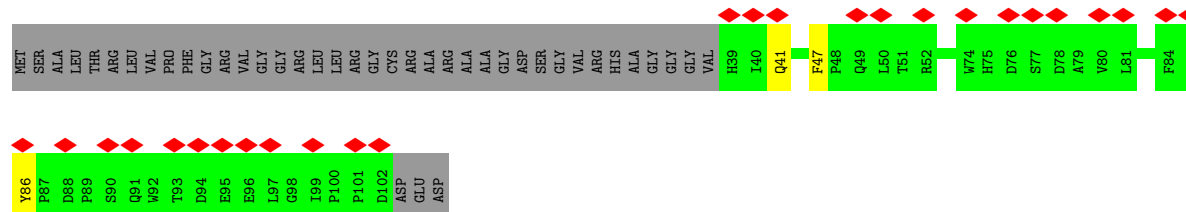
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



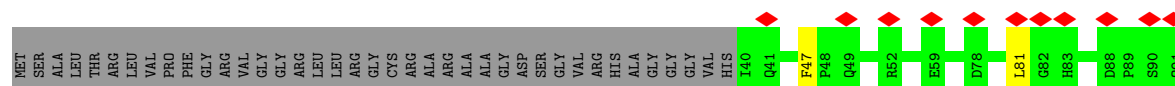
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

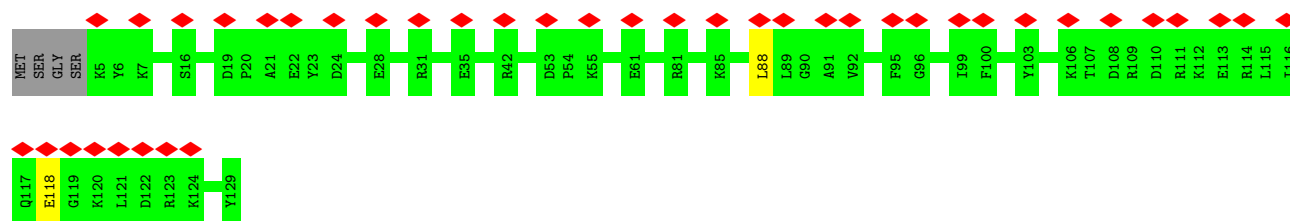


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

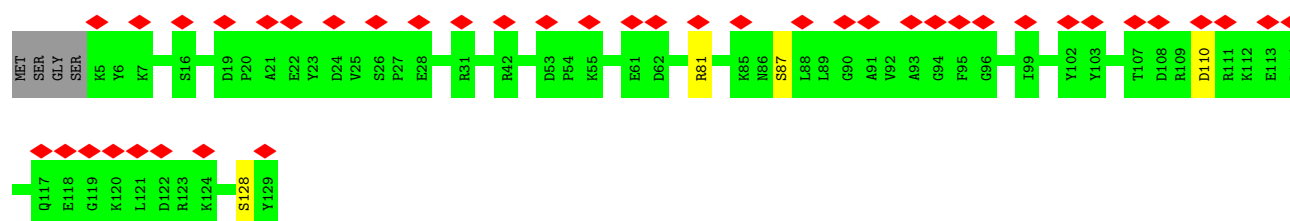




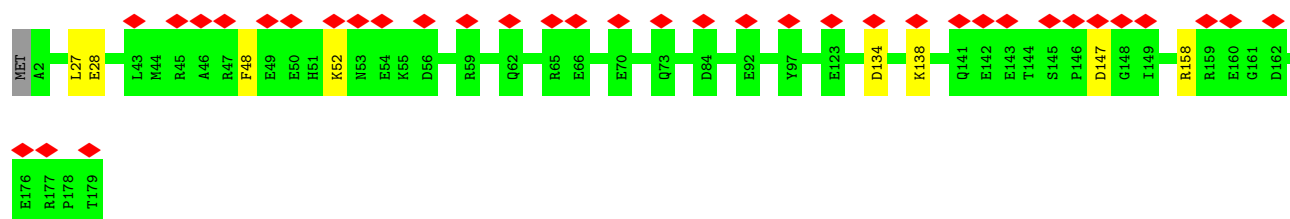




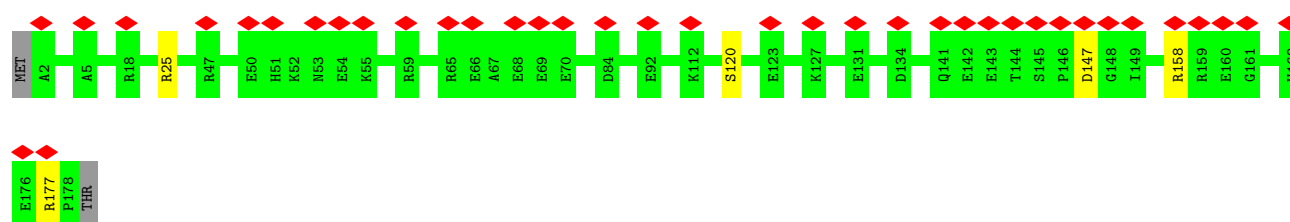
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



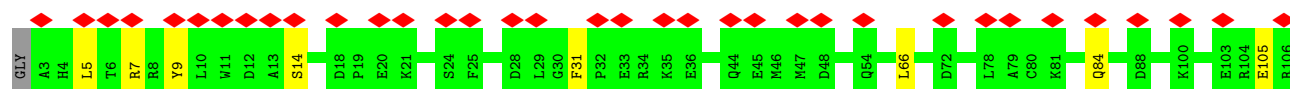
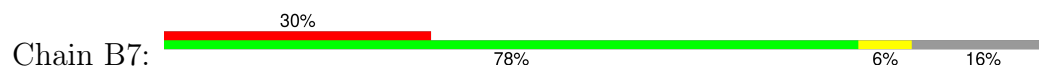
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

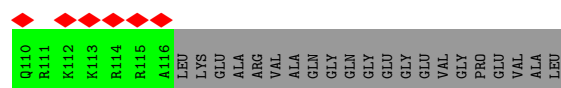


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

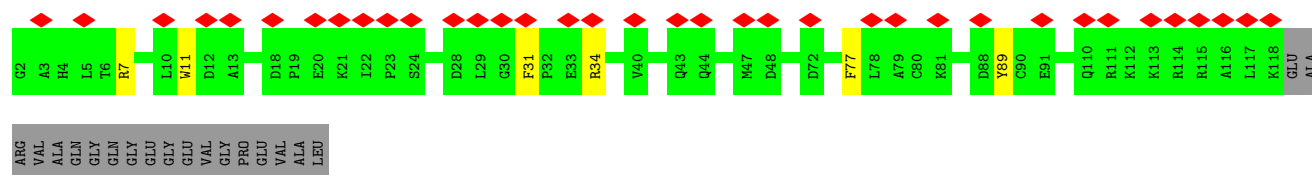
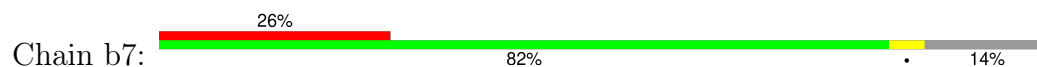


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

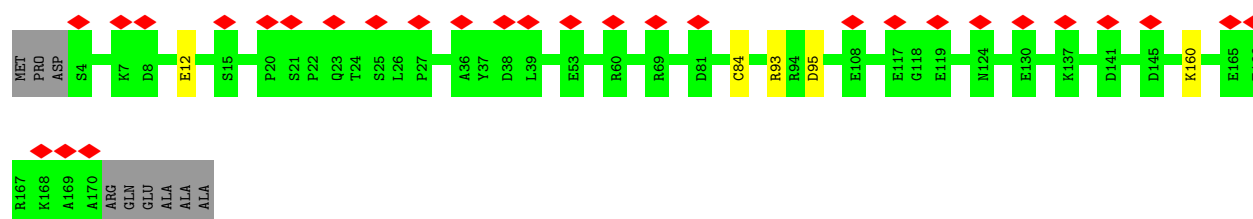




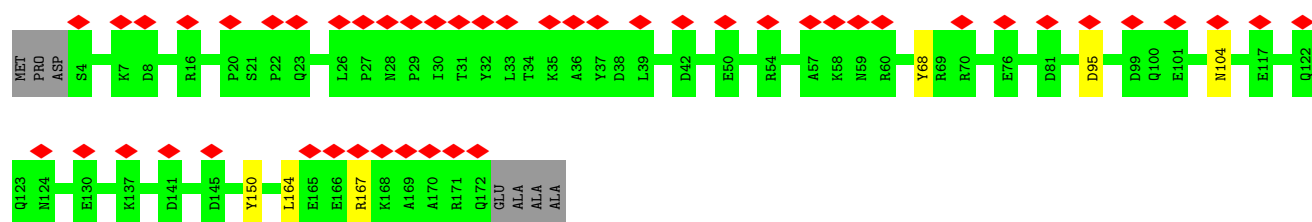
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



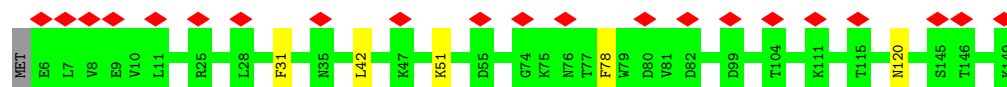
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

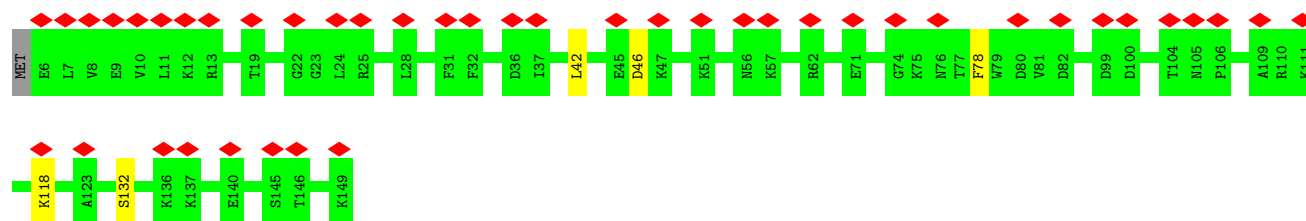


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

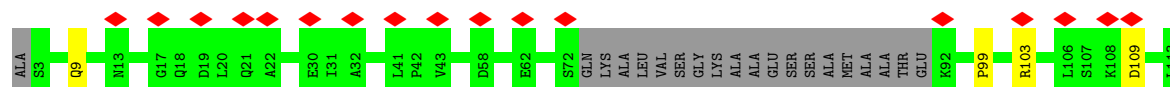
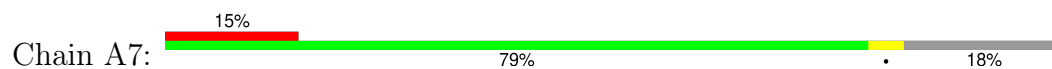


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

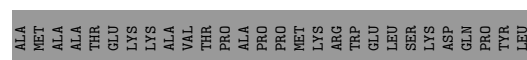
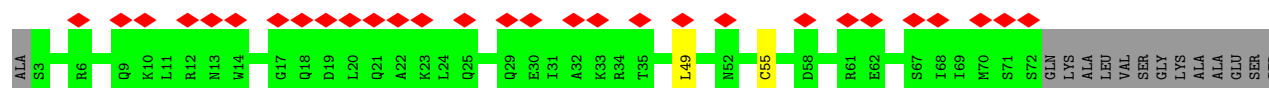




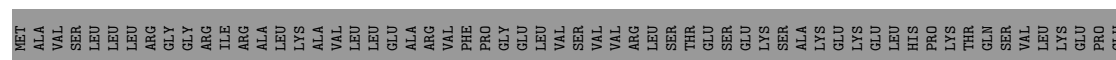
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



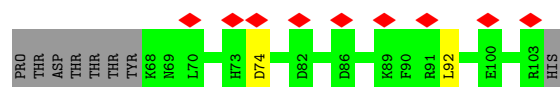
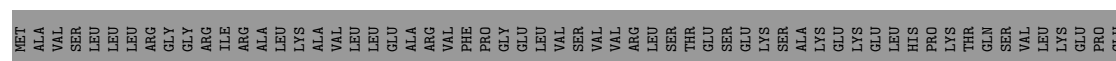
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

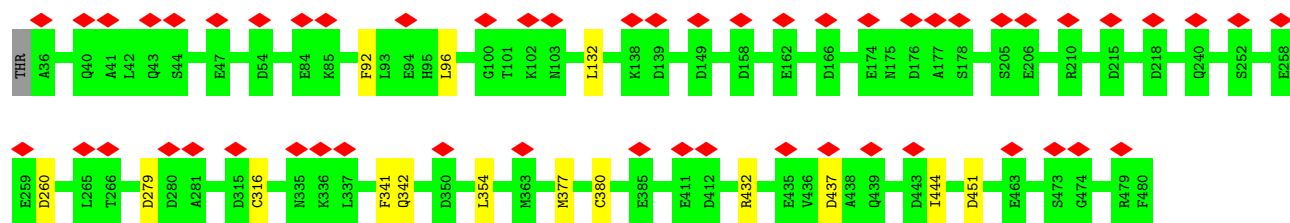


- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

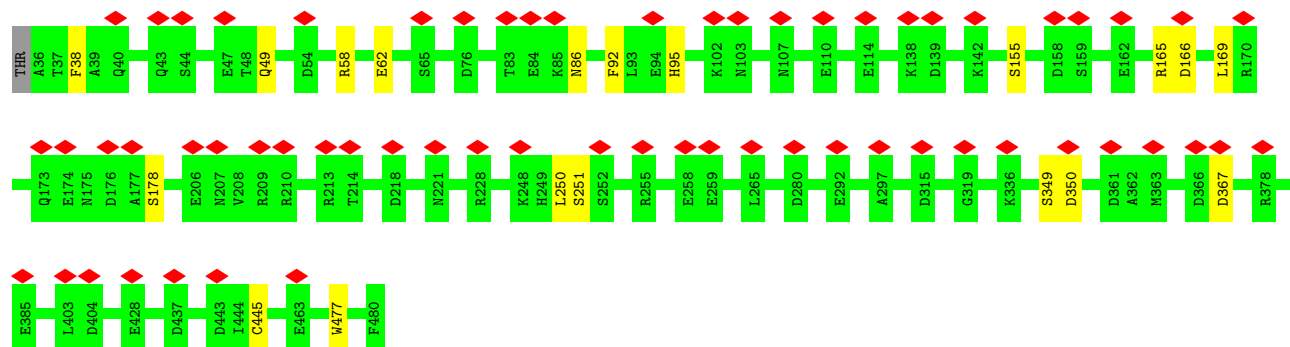


- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial

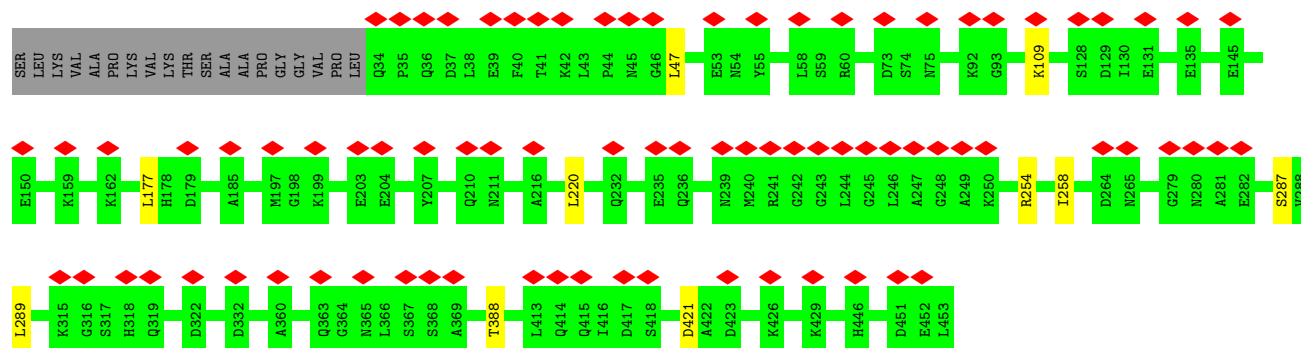




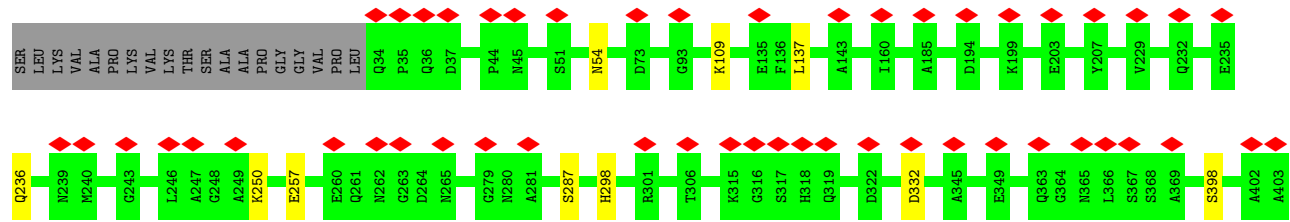
- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial

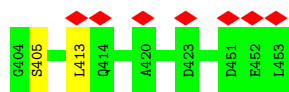


- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial

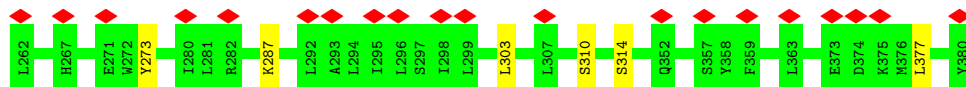


- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial

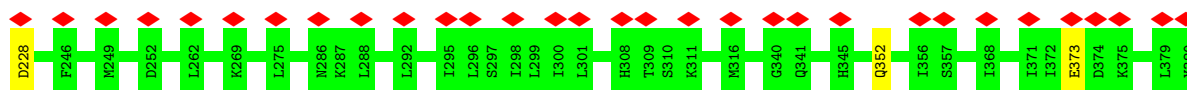
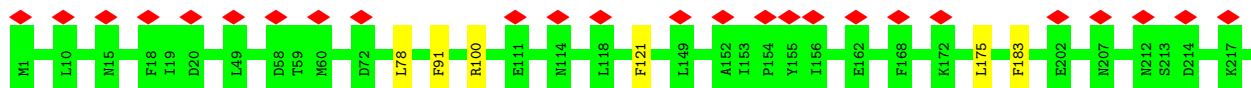




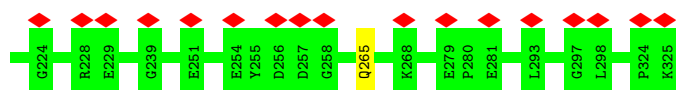
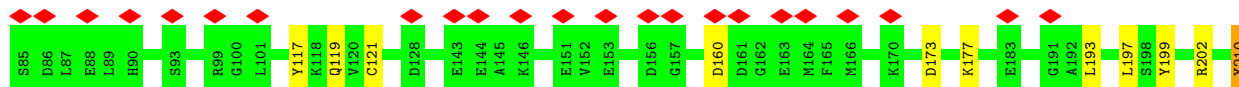
- Molecule 42: Cytochrome b



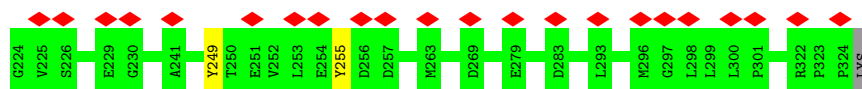
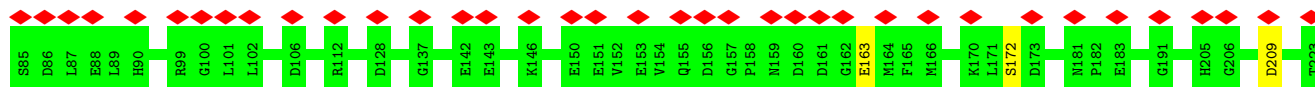
- Molecule 42: Cytochrome b



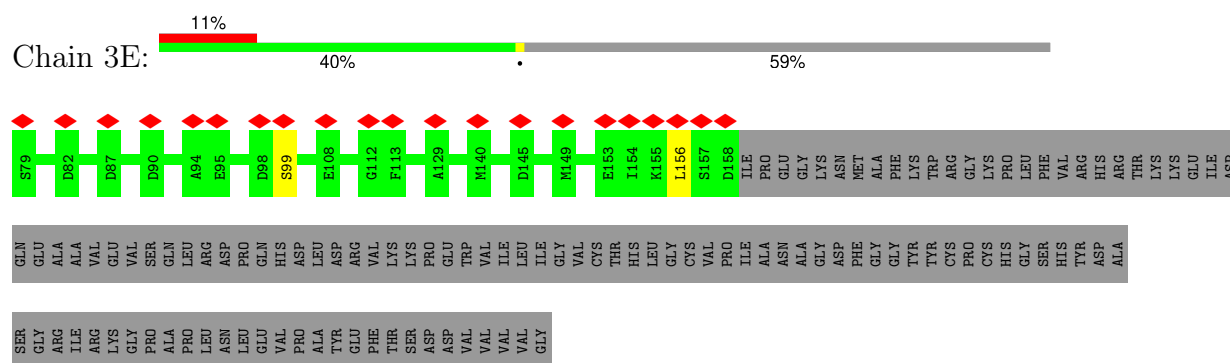
- Molecule 43: Cytochrome c1, heme protein, mitochondrial



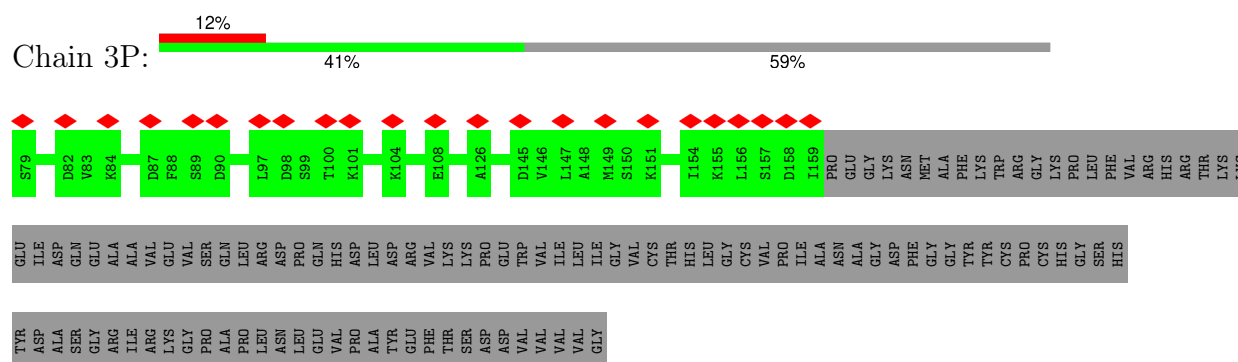
- Molecule 43: Cytochrome c1, heme protein, mitochondrial



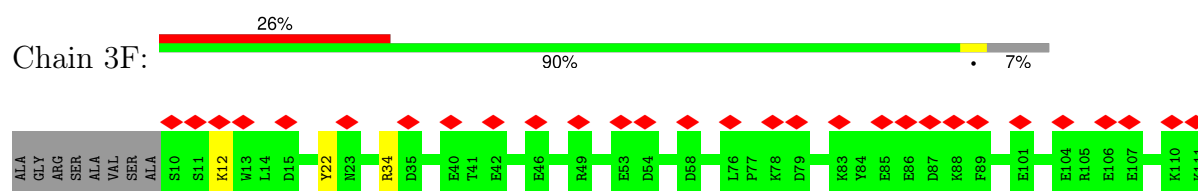
- Molecule 44: Cytochrome b-c1 complex subunit 9



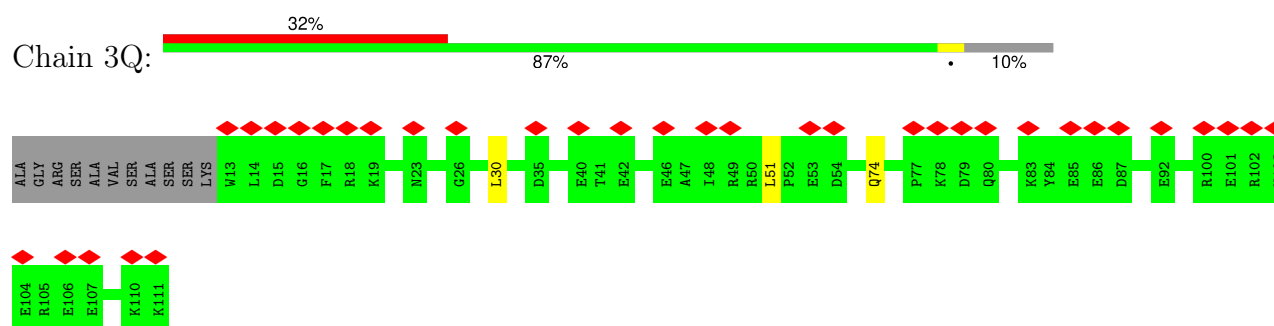
- Molecule 44: Cytochrome b-c1 complex subunit 9



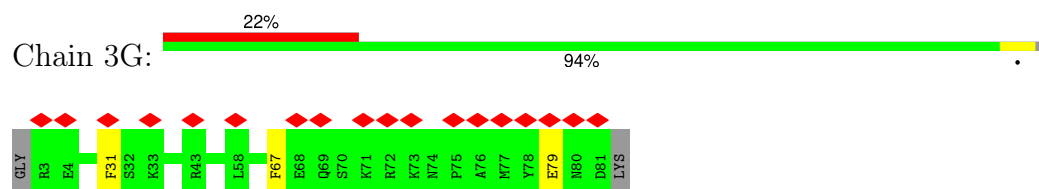
- Molecule 45: Cytochrome b-c1 complex subunit 7



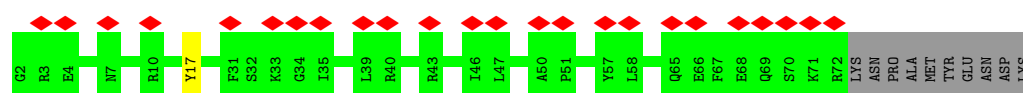
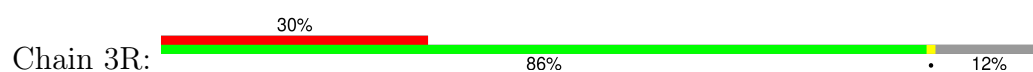
- Molecule 45: Cytochrome b-c1 complex subunit 7



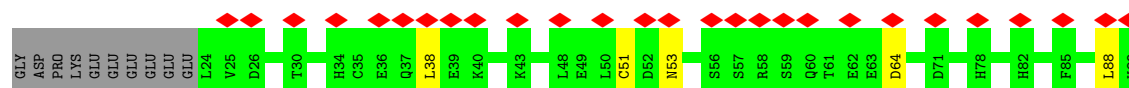
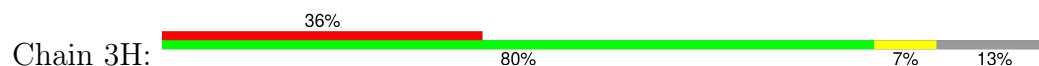
- Molecule 46: Cytochrome b-c1 complex subunit 8



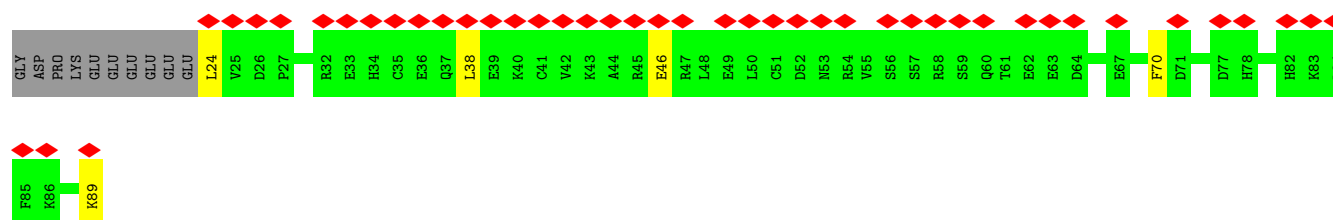
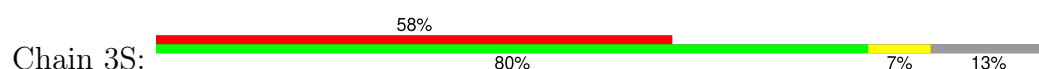
- Molecule 46: Cytochrome b-c1 complex subunit 8



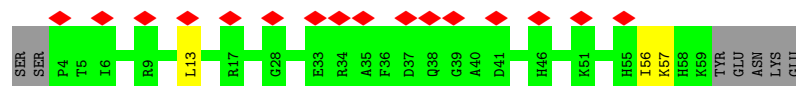
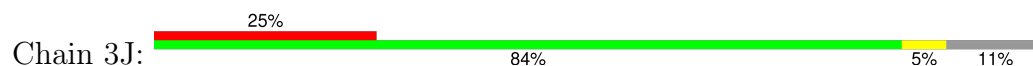
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



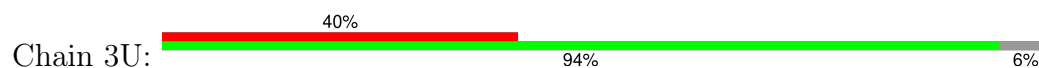
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



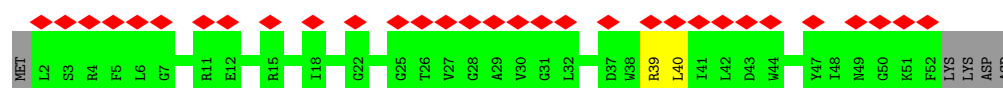
- Molecule 48: Cytochrome b-c1 complex subunit 9



- Molecule 48: Cytochrome b-c1 complex subunit 9



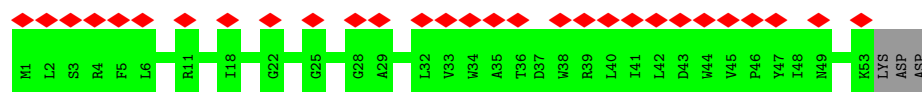
- Molecule 49: Cytochrome b-c1 complex subunit 10



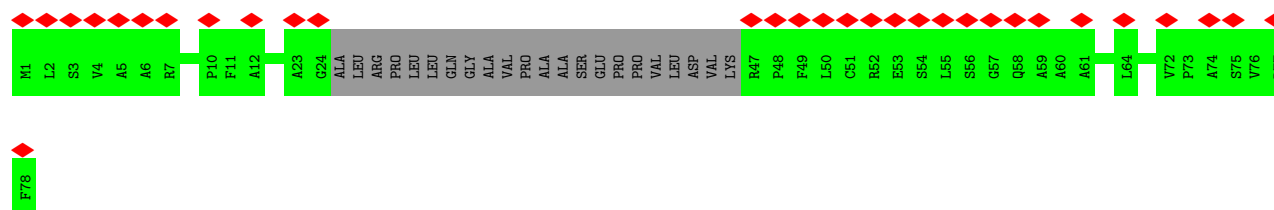
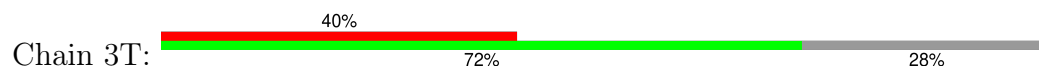
- Molecule 49: Cytochrome b-c1 complex subunit 10



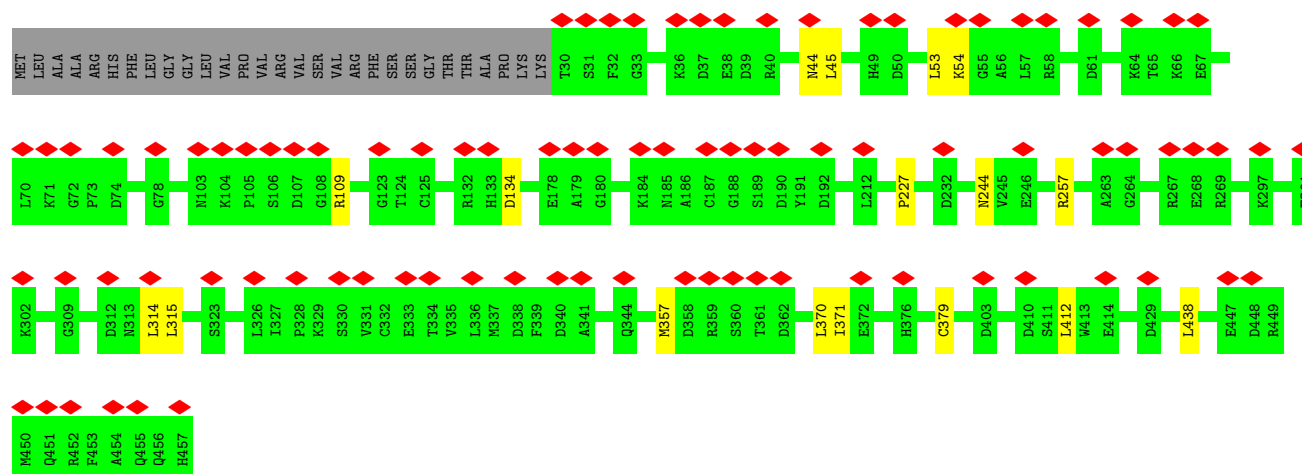
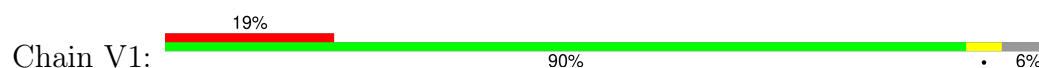




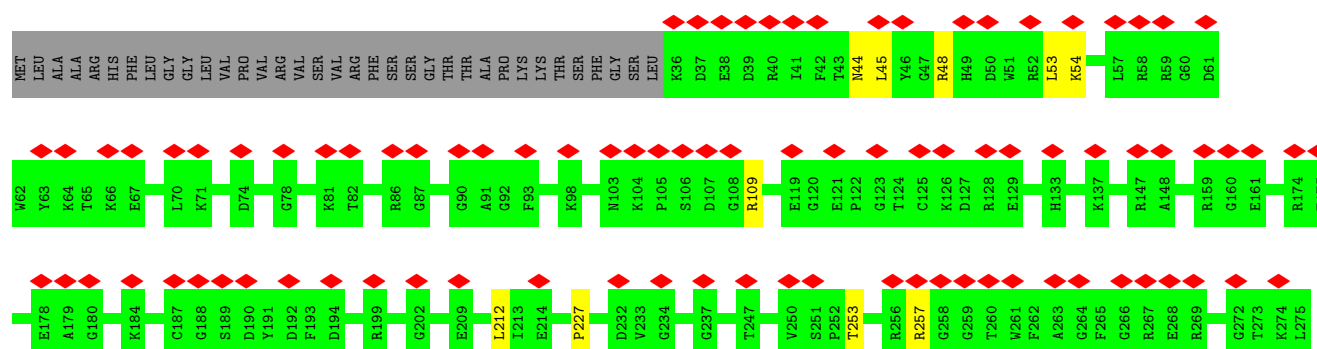
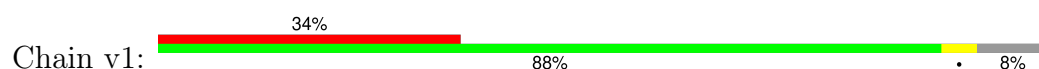
- Molecule 50: Cytochrome b-c1 complex subunit Rieske, mitochondrial

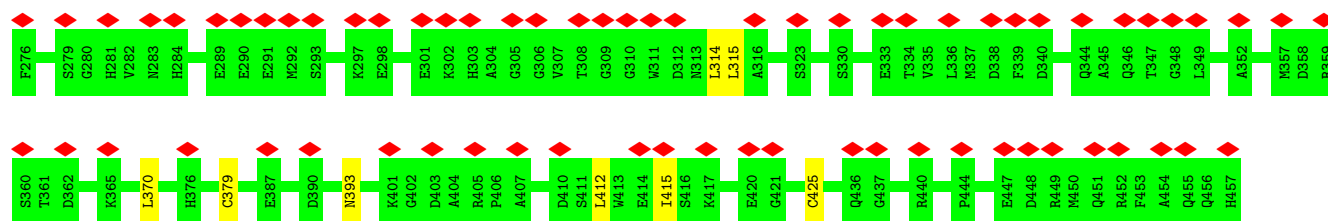


- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

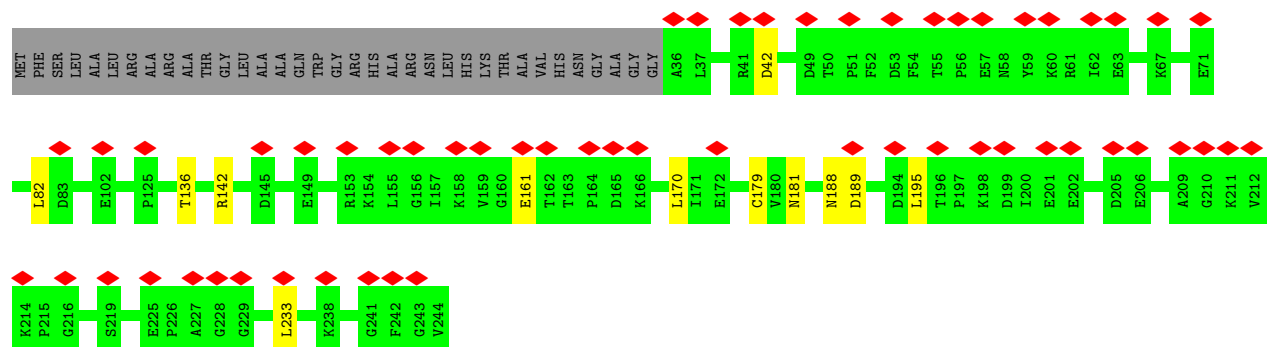
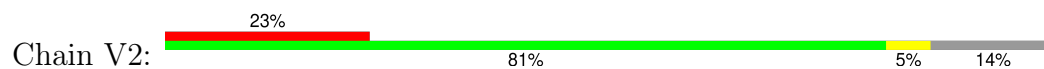


- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

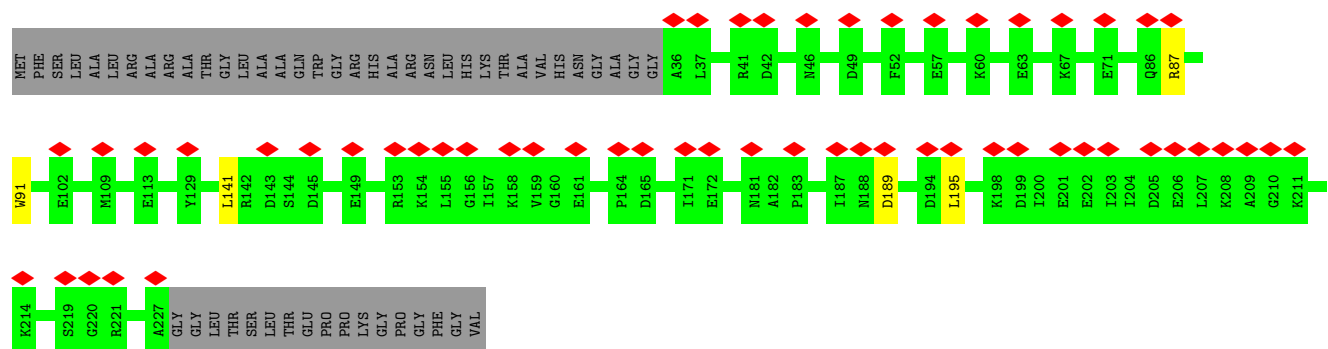
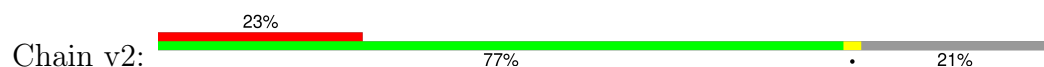




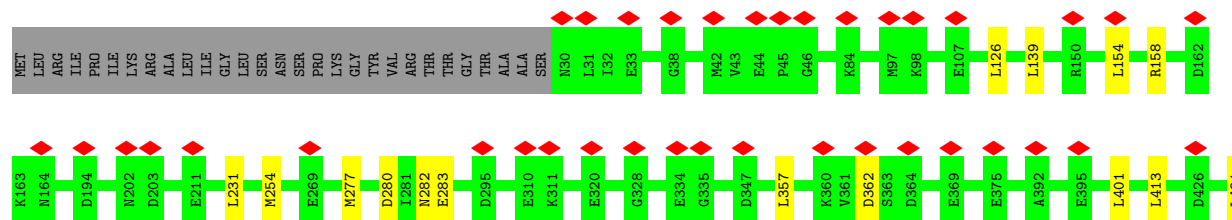
- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

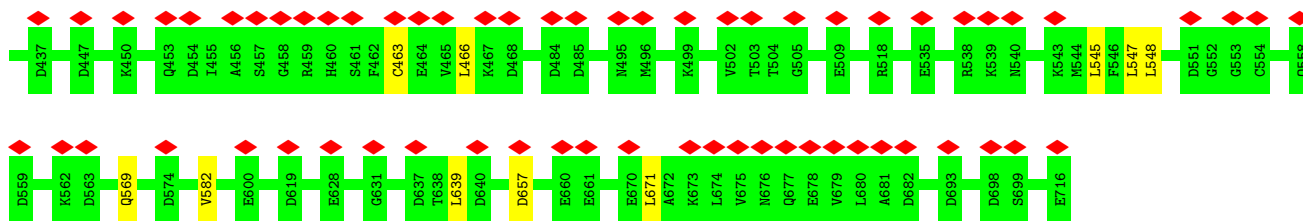


- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

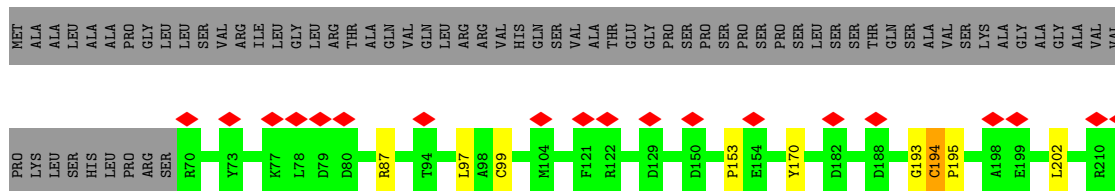




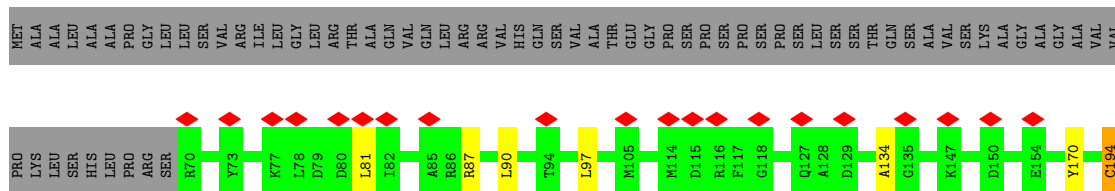
- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

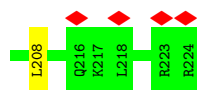


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

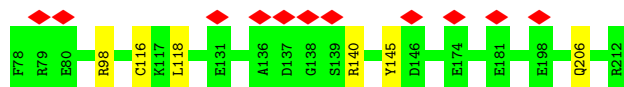
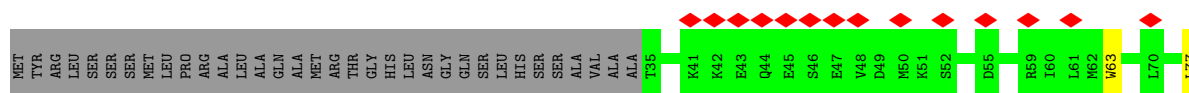
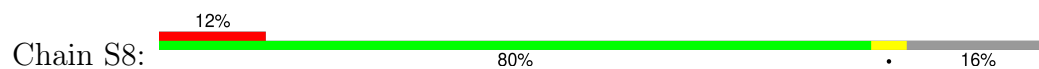


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

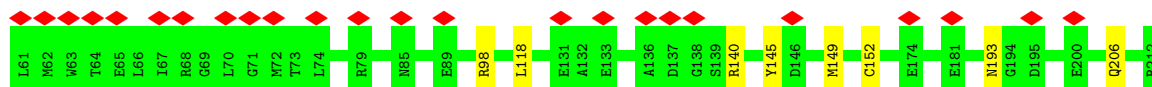
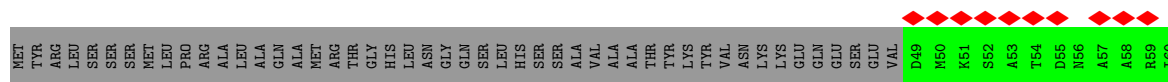
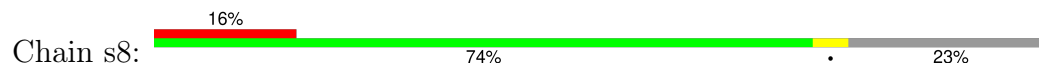




- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.227	Depositor
Minimum map value	-9.364	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.291	Depositor
Recommended contour level	3.4	Depositor
Map size ( $\text{\AA}$ )	249.92, 338.8, 238.48	wwPDB
Map dimensions	271, 385, 284	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.88, 0.88, 0.88	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EHZ, SF4, HEM, HEC, FES, DGT, ZN, 2MR, NDP, FMN, MG

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	0.42	0/940	0.83	1/1285 (0.1%)
1	3a	0.41	0/917	0.78	3/1252 (0.2%)
2	S3	0.38	0/1762	0.74	2/2401 (0.1%)
2	s3	0.37	0/1751	0.73	2/2386 (0.1%)
3	S2	0.38	0/3485	0.71	5/4720 (0.1%)
3	s2	0.38	0/3469	0.71	5/4698 (0.1%)
4	1	0.43	0/2607	0.87	12/3564 (0.3%)
4	1a	0.41	0/2599	0.87	11/3554 (0.3%)
5	6	0.40	0/1322	0.67	1/1799 (0.1%)
5	6a	0.37	0/1330	0.71	3/1809 (0.2%)
6	4L	0.39	0/740	0.72	0/1005
6	4l	0.37	0/738	0.72	1/1002 (0.1%)
7	5	0.39	0/4913	0.77	11/6685 (0.2%)
7	5a	0.39	0/4913	0.71	2/6685 (0.0%)
8	4	0.41	0/3717	0.82	7/5062 (0.1%)
8	4a	0.37	0/3717	0.80	10/5062 (0.2%)
9	2	0.39	0/2756	0.80	5/3751 (0.1%)
9	2a	0.49	3/2756 (0.1%)	0.94	10/3751 (0.3%)
10	AL	0.32	0/2674	0.59	0/3626
10	al	0.32	0/2674	0.63	3/3626 (0.1%)
11	A9	0.36	0/2823	0.68	3/3828 (0.1%)
11	a9	0.33	0/2823	0.66	1/3828 (0.0%)
12	S4	0.30	0/1044	0.61	0/1409
12	s4	0.30	0/1044	0.60	0/1409
13	S6	0.31	0/762	0.59	0/1026
13	s6	0.31	0/762	0.66	1/1026 (0.1%)
14	A2	0.33	0/682	0.75	1/920 (0.1%)
14	a2	0.31	0/682	0.75	2/920 (0.2%)
15	AB	0.33	0/637	0.66	0/858
15	AC	0.33	0/718	0.73	1/970 (0.1%)
15	ab	0.30	0/637	0.62	1/858 (0.1%)
15	ac	0.30	0/718	0.59	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	A5	0.29	0/949	0.64	0/1286
16	a5	0.32	0/945	0.67	2/1281 (0.2%)
17	A6	0.34	0/980	0.71	1/1317 (0.1%)
17	a6	0.34	0/972	0.69	1/1305 (0.1%)
18	A8	0.37	0/1422	0.70	1/1921 (0.1%)
18	a8	0.34	0/1427	0.66	3/1927 (0.2%)
19	AM	0.36	0/1069	0.65	1/1449 (0.1%)
19	am	0.35	0/1069	0.61	0/1449
20	AO	0.33	0/1192	0.62	0/1608
20	ao	0.33	0/1192	0.64	0/1608
21	A1	0.40	0/577	0.71	0/777
21	a1	0.42	1/577 (0.2%)	0.71	0/777
22	A3	0.31	0/671	0.54	0/921
22	a3	0.31	0/671	0.66	2/921 (0.2%)
23	C1	0.31	0/418	0.58	0/567
23	c1	0.32	0/388	0.56	0/528
24	C2	0.34	0/1028	0.63	1/1387 (0.1%)
24	c2	0.34	0/1028	0.64	1/1387 (0.1%)
25	S5	0.33	0/900	0.61	0/1199
25	s5	0.33	0/900	0.61	0/1199
26	B1	0.34	0/495	0.63	0/667
26	b1	0.36	0/495	0.69	1/667 (0.1%)
27	BM	0.35	0/854	0.58	0/1163
27	bm	0.36	0/863	0.69	1/1175 (0.1%)
28	B5	0.34	0/1201	0.64	0/1626
28	b5	0.34	0/1193	0.64	0/1615
29	B6	0.37	0/807	0.70	0/1096
29	b6	0.31	0/784	0.68	1/1063 (0.1%)
30	B2	0.34	0/580	0.65	0/794
30	b2	0.32	0/569	0.59	1/779 (0.1%)
31	B3	0.34	0/587	0.65	0/793
31	b3	0.35	0/591	0.62	0/798
32	B8	0.32	0/1356	0.58	0/1851
32	b8	0.32	0/1356	0.60	0/1851
33	B4	0.34	0/1073	0.64	0/1455
33	b4	0.34	0/1073	0.64	1/1455 (0.1%)
34	B9	0.34	0/1596	0.67	3/2162 (0.1%)
34	b9	0.32	0/1589	0.62	0/2152
35	B7	0.31	0/1009	0.68	2/1355 (0.1%)
35	b7	0.35	0/1030	0.66	0/1382
36	BL	0.32	0/1443	0.60	0/1951
36	bl	0.32	0/1463	0.60	0/1977
37	AN	0.34	0/1243	0.67	1/1692 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	an	0.32	0/1243	0.63	0/1692
38	A7	0.28	0/759	0.60	0/1027
38	a7	0.31	0/572	0.64	0/774
39	V3	0.31	0/349	0.75	1/473 (0.2%)
39	v3	0.34	0/311	0.72	1/420 (0.2%)
40	3A	0.35	1/3529 (0.0%)	0.72	5/4793 (0.1%)
40	3L	0.37	0/3530	0.77	4/4793 (0.1%)
41	3B	0.33	0/3205	0.68	5/4332 (0.1%)
41	3M	0.33	0/3205	0.64	2/4332 (0.0%)
42	3C	0.35	0/3147	0.66	3/4297 (0.1%)
42	3N	0.37	0/3147	0.65	1/4297 (0.0%)
43	3D	0.35	0/1978	0.68	5/2685 (0.2%)
43	3O	0.31	0/1968	0.62	0/2674
44	3E	0.32	0/609	0.62	1/821 (0.1%)
44	3P	0.33	0/617	0.61	0/832
45	3F	0.30	0/922	0.65	0/1234
45	3Q	0.31	0/901	0.69	2/1207 (0.2%)
46	3G	0.39	0/689	0.78	0/931
46	3R	0.39	0/617	0.72	0/833
47	3H	0.36	0/552	0.77	2/739 (0.3%)
47	3S	0.30	0/552	0.69	2/739 (0.3%)
48	3J	0.45	0/473	0.85	2/637 (0.3%)
48	3U	0.36	0/503	0.60	0/678
49	3K	0.36	0/437	0.69	0/598
49	3V	0.36	0/454	0.64	0/619
50	3T	0.33	0/403	0.67	0/546
51	V1	0.38	0/3376	0.78	7/4561 (0.2%)
51	v1	0.39	0/3333	0.77	7/4503 (0.2%)
52	V2	0.43	0/1670	0.81	7/2276 (0.3%)
52	v2	0.40	0/1553	0.80	1/2116 (0.0%)
53	S1	0.35	0/5377	0.77	18/7285 (0.2%)
53	s1	0.35	0/5377	0.74	12/7285 (0.2%)
54	S7	0.47	1/1272 (0.1%)	0.87	3/1722 (0.2%)
54	s7	0.40	0/1272	0.86	6/1722 (0.3%)
55	S8	0.43	1/1438 (0.1%)	0.78	2/1946 (0.1%)
55	s8	0.42	0/1337	0.77	1/1808 (0.1%)
All	All	0.36	7/165414 (0.0%)	0.71	229/224305 (0.1%)

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
2	S3	0	1
4	1	0	2
7	5a	0	1
8	4	0	2
18	A8	0	1
37	AN	0	1
41	3B	0	1
42	3C	0	1
51	V1	0	1
51	v1	0	2
52	V2	0	4
52	v2	0	1
54	S7	0	4
54	s7	0	3
All	All	0	25

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2a	255	PRO	CB-CG	-11.26	0.93	1.50
9	2a	255	PRO	CG-CD	-8.09	1.24	1.50
54	S7	194	CYS	CB-SG	-7.07	1.70	1.82
9	2a	255	PRO	N-CA	6.87	1.58	1.47
55	S8	116	CYS	CB-SG	-6.02	1.72	1.82
21	a1	18	ILE	C-N	5.62	1.45	1.34
40	3A	380	CYS	CB-SG	-5.40	1.73	1.81

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2a	255	PRO	N-CD-CG	-17.40	77.11	103.20
9	2a	255	PRO	CA-CB-CG	-16.51	72.64	104.00
9	2a	255	PRO	CB-CG-CD	14.85	164.40	106.50
7	5	526	LEU	CA-CB-CG	10.95	140.48	115.30
52	V2	189	ASP	CB-CG-OD1	10.38	127.64	118.30
40	3L	250	LEU	CA-CB-CG	10.21	138.79	115.30
51	v1	314	LEU	CA-CB-CG	9.88	138.02	115.30
51	v1	370	LEU	CA-CB-CG	9.19	136.43	115.30
40	3A	444	ILE	CG1-CB-CG2	-9.10	91.39	111.40
3	S2	139	LEU	CB-CG-CD1	-9.01	95.68	111.00
4	1	233	LEU	CB-CG-CD2	-8.95	95.78	111.00
13	s6	50	ASP	CB-CG-OD2	8.87	126.28	118.30
8	4	364	LEU	CA-CB-CG	8.64	135.18	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	S1	126	LEU	CA-CB-CG	8.57	135.01	115.30
8	4a	59	ASP	CB-CG-OD2	8.52	125.97	118.30
8	4	236	LEU	CA-CB-CG	8.40	134.61	115.30
9	2a	37	LEU	CA-CB-CG	8.29	134.37	115.30
8	4a	329	LEU	CA-CB-CG	8.28	134.35	115.30
8	4	236	LEU	CB-CG-CD2	-8.27	96.93	111.00
53	s1	126	LEU	CA-CB-CG	8.27	134.32	115.30
51	V1	438	LEU	CA-CB-CG	8.03	133.78	115.30
27	bm	112	MET	CA-CB-CG	7.99	126.88	113.30
11	A9	224	LEU	CA-CB-CG	7.97	133.63	115.30
9	2a	255	PRO	CA-N-CD	-7.92	100.41	111.50
43	3D	210	TYR	CB-CG-CD2	-7.87	116.28	121.00
8	4a	364	LEU	CA-CB-CG	7.84	133.33	115.30
5	6a	64	LEU	CA-CB-CG	7.80	133.25	115.30
7	5	49	LEU	CA-CB-CG	7.75	133.13	115.30
4	1a	81	LEU	CA-CB-CG	7.75	133.13	115.30
42	3C	119	LEU	CA-CB-CG	7.73	133.08	115.30
4	1a	64	LEU	CA-CB-CG	7.62	132.83	115.30
53	s1	548	LEU	CA-CB-CG	7.60	132.78	115.30
51	V1	314	LEU	CA-CB-CG	7.51	132.58	115.30
4	1a	100	LEU	CA-CB-CG	7.49	132.52	115.30
44	3E	156	LEU	CA-CB-CG	7.45	132.44	115.30
8	4a	436	LEU	CA-CB-CG	7.43	132.38	115.30
48	3J	56	ILE	CG1-CB-CG2	-7.41	95.10	111.40
53	s1	431	LEU	CA-CB-CG	7.36	132.22	115.30
2	s3	160	ILE	CG1-CB-CG2	-7.28	95.38	111.40
54	s7	97	LEU	CA-CB-CG	7.26	131.99	115.30
47	3H	38	LEU	CA-CB-CG	7.25	131.98	115.30
4	1	288	LEU	CA-CB-CG	7.23	131.94	115.30
40	3L	445	CYS	CA-CB-SG	7.20	126.95	114.00
4	1a	233	LEU	CA-CB-CG	7.17	131.79	115.30
51	v1	415	ILE	CG1-CB-CG2	-7.10	95.77	111.40
22	a3	78	LEU	CA-CB-CG	7.07	131.55	115.30
3	S2	139	LEU	CA-CB-CG	7.05	131.52	115.30
51	v1	412	LEU	CA-CB-CG	7.01	131.43	115.30
53	S1	582	VAL	CG1-CB-CG2	-6.97	99.75	110.90
9	2a	190	MET	CA-CB-CG	6.97	125.14	113.30
55	S8	118	LEU	CA-CB-CG	6.94	131.26	115.30
40	3A	96	LEU	CA-CB-CG	6.92	131.22	115.30
8	4	6	LEU	CA-CB-CG	6.87	131.11	115.30
48	3J	13	LEU	CA-CB-CG	6.84	131.03	115.30
53	S1	139	LEU	CA-CB-CG	6.80	130.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a5	24	LEU	CB-CG-CD2	-6.78	99.47	111.00
4	1	85	LEU	CA-CB-CG	6.75	130.82	115.30
11	a9	224	LEU	CA-CB-CG	6.73	130.77	115.30
18	a8	62	LEU	CA-CB-CG	6.72	130.76	115.30
2	S3	67	ILE	CG1-CB-CG2	-6.69	96.69	111.40
5	6a	41	LEU	CA-CB-CG	6.68	130.68	115.30
9	2a	251	LEU	CA-CB-CG	6.67	130.64	115.30
9	2	202	LEU	CA-CB-CG	6.67	130.63	115.30
7	5	319	MET	CA-CB-CG	6.66	124.62	113.30
42	3C	377	LEU	CA-CB-CG	6.65	130.60	115.30
54	s7	201	LEU	CB-CG-CD2	-6.63	99.73	111.00
26	b1	31	ASP	CB-CG-OD1	6.61	124.25	118.30
30	b2	81	LEU	CA-CB-CG	6.61	130.51	115.30
9	2a	108	LEU	CA-CB-CG	6.61	130.49	115.30
4	1a	264	LEU	CA-CB-CG	6.58	130.43	115.30
53	s1	231	LEU	CA-CB-CG	6.58	130.43	115.30
8	4a	367	LEU	CA-CB-CG	6.56	130.39	115.30
16	a5	24	LEU	CA-CB-CG	6.48	130.21	115.30
8	4	250	LEU	CB-CG-CD1	6.48	122.02	111.00
51	V1	412	LEU	CA-CB-CG	6.46	130.17	115.30
53	s1	547	LEU	CA-CB-CG	6.45	130.14	115.30
39	v3	92	LEU	CA-CB-CG	6.43	130.10	115.30
53	s1	254	MET	CA-CB-CG	6.41	124.20	113.30
45	3Q	51	LEU	CA-CB-CG	6.39	130.01	115.30
4	1a	22	LEU	CA-CB-CG	6.38	129.98	115.30
4	1a	10	LEU	CA-CB-CG	6.35	129.90	115.30
40	3A	354	LEU	CA-CB-CG	6.35	129.90	115.30
53	s1	639	LEU	CA-CB-CG	6.34	129.89	115.30
3	s2	181	LEU	CA-CB-CG	6.34	129.87	115.30
4	1a	288	LEU	CA-CB-CG	6.34	129.88	115.30
1	3a	75	LEU	CB-CG-CD2	-6.33	100.24	111.00
34	B9	48	PHE	CB-CG-CD1	6.31	125.22	120.80
39	V3	83	LEU	CA-CB-CG	6.30	129.79	115.30
47	3H	88	LEU	CA-CB-CG	6.27	129.73	115.30
11	A9	214	LEU	CB-CG-CD1	-6.26	100.36	111.00
53	S1	362	ASP	CB-CG-OD1	6.24	123.92	118.30
53	S1	545	LEU	CA-CB-CG	6.23	129.63	115.30
14	a2	65	LEU	CA-CB-CG	6.23	129.62	115.30
41	3M	413	LEU	CA-CB-CG	6.22	129.60	115.30
17	a6	52	LEU	CA-CB-CG	6.18	129.52	115.30
1	3a	71	LEU	CA-CB-CG	6.18	129.51	115.30
35	B7	5	LEU	CA-CB-CG	6.17	129.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	3D	193	LEU	CA-CB-CG	6.17	129.49	115.30
53	S1	283	GLU	CA-CB-CG	6.17	126.97	113.40
52	V2	189	ASP	CB-CG-OD2	-6.15	112.77	118.30
7	5	9	LEU	CA-CB-CG	6.14	129.42	115.30
10	al	334	LEU	CA-CB-CG	6.12	129.37	115.30
55	s8	118	LEU	CA-CB-CG	6.11	129.36	115.30
9	2	37	LEU	CA-CB-CG	6.11	129.34	115.30
19	AM	17	GLN	CA-CB-CG	6.09	126.81	113.40
53	s1	545	LEU	CA-CB-CG	6.09	129.30	115.30
52	V2	42	ASP	CB-CG-OD1	6.08	123.78	118.30
43	3D	210	TYR	CA-CB-CG	6.08	124.94	113.40
41	3M	137	LEU	CA-CB-CG	6.06	129.25	115.30
53	S1	466	LEU	CA-CB-CG	6.05	129.22	115.30
53	s1	362	ASP	CB-CG-OD1	6.05	123.74	118.30
24	C2	63	LEU	CA-CB-CG	6.04	129.20	115.30
4	1	222	LEU	CB-CG-CD1	-6.02	100.77	111.00
7	5	576	LEU	CA-CB-CG	6.00	129.09	115.30
3	s2	197	MET	CA-CB-CG	5.99	123.49	113.30
18	A8	168	PHE	CB-CG-CD1	5.99	124.99	120.80
4	1	233	LEU	CA-CB-CG	5.98	129.05	115.30
5	6	64	LEU	CA-CB-CG	5.97	129.04	115.30
4	1	114	TYR	CB-CG-CD2	-5.96	117.42	121.00
3	S2	375	MET	CB-CG-SD	5.95	130.24	112.40
33	b4	110	ASP	CB-CG-OD1	5.93	123.64	118.30
53	s1	357	LEU	CA-CB-CG	5.93	128.93	115.30
22	a3	74	LEU	CA-CB-CG	5.91	128.90	115.30
53	S1	671	LEU	CA-CB-CG	5.91	128.89	115.30
42	3N	373	GLU	CA-CB-CG	5.90	126.38	113.40
51	v1	315	LEU	CA-CB-CG	5.90	128.86	115.30
29	b6	69	LEU	CA-CB-CG	5.86	128.78	115.30
11	A9	170	LEU	CA-CB-CG	5.83	128.71	115.30
14	a2	91	MET	CA-CB-CG	5.83	123.21	113.30
8	4	406	TYR	CA-CB-CG	5.83	124.47	113.40
53	S1	357	LEU	CA-CB-CG	5.82	128.68	115.30
8	4a	439	LEU	CA-CB-CG	5.81	128.67	115.30
53	S1	401	LEU	CA-CB-CG	5.81	128.66	115.30
7	5	409	LEU	CA-CB-CG	5.81	128.66	115.30
43	3D	197	LEU	CA-CB-CG	5.80	128.64	115.30
43	3D	210	TYR	CB-CG-CD1	5.80	124.48	121.00
8	4a	406	TYR	CA-CB-CG	5.79	124.40	113.40
53	S1	283	GLU	CB-CA-C	5.79	121.98	110.40
53	S1	547	LEU	CA-CB-CG	5.78	128.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	al	67	CYS	CA-CB-SG	5.78	124.40	114.00
53	S1	639	LEU	CA-CB-CG	5.78	128.59	115.30
41	3B	220	LEU	CB-CG-CD2	-5.77	101.20	111.00
51	V1	370	LEU	CA-CB-CG	5.75	128.52	115.30
51	V1	315	LEU	CA-CB-CG	5.74	128.51	115.30
53	S1	431	LEU	CA-CB-CG	5.74	128.51	115.30
7	5a	422	TYR	CA-CB-CG	5.74	124.30	113.40
8	4a	117	MET	CA-CB-CG	5.73	123.04	113.30
54	s7	90	LEU	CA-CB-CG	5.72	128.47	115.30
4	1	222	LEU	CA-CB-CG	5.71	128.43	115.30
41	3B	220	LEU	CA-CB-CG	5.69	128.39	115.30
5	6a	64	LEU	CB-CG-CD2	-5.65	101.39	111.00
40	3A	132	LEU	CA-CB-CG	5.64	128.27	115.30
7	5	280	LEU	CA-CB-CG	5.63	128.24	115.30
3	s2	116	LEU	CB-CG-CD1	-5.62	101.44	111.00
7	5	432	MET	C-N-CA	5.62	135.75	121.70
8	4	402	ILE	CG1-CB-CG2	-5.62	99.04	111.40
53	s1	476	LEU	CA-CB-CG	5.61	128.21	115.30
41	3B	177	LEU	CA-CB-CG	5.59	128.16	115.30
42	3C	49	LEU	CA-CB-CG	5.59	128.15	115.30
41	3B	289	LEU	CA-CB-CG	5.58	128.13	115.30
53	S1	413	LEU	CA-CB-CG	-5.58	102.48	115.30
1	3	75	LEU	CA-CB-CG	5.57	128.12	115.30
34	B9	27	LEU	C-N-CA	5.57	135.62	121.70
52	V2	195	LEU	CA-CB-CG	5.57	128.10	115.30
6	4l	77	LEU	CB-CG-CD2	-5.56	101.54	111.00
4	1	28	LEU	CA-CB-CG	5.56	128.09	115.30
24	c2	11	LEU	CA-CB-CG	5.55	128.07	115.30
2	S3	132	LEU	CA-CB-CG	5.55	128.07	115.30
52	V2	170	LEU	CA-CB-CG	5.55	128.07	115.30
53	S1	231	LEU	CA-CB-CG	5.55	128.06	115.30
51	v1	212	LEU	CA-CB-CG	5.55	128.06	115.30
47	3S	38	LEU	CA-CB-CG	5.54	128.04	115.30
54	s7	208	LEU	CA-CB-CG	5.53	128.01	115.30
7	5	592	LEU	CA-CB-CG	5.52	128.00	115.30
3	s2	101	LEU	CA-CB-CG	5.52	128.00	115.30
54	S7	97	LEU	CA-CB-CG	5.51	127.98	115.30
3	S2	123	LEU	CA-CB-CG	5.50	127.96	115.30
4	1	151	LEU	CB-CG-CD2	-5.49	101.67	111.00
41	3B	47	LEU	CA-CB-CG	5.48	127.91	115.30
7	5	480	LEU	CA-CB-CG	5.47	127.88	115.30
54	s7	194	CYS	CA-CB-SG	-5.47	104.16	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	ab	113	LEU	CA-CB-CG	5.45	127.84	115.30
14	A2	16	LEU	CA-CB-CG	5.45	127.83	115.30
55	S8	77	LEU	CA-CB-CG	5.45	127.83	115.30
9	2a	29	MET	CA-CB-CG	5.40	122.47	113.30
54	S7	202	LEU	CA-CB-CG	5.38	127.68	115.30
15	AC	113	LEU	CB-CG-CD1	-5.38	101.85	111.00
9	2	261	LEU	CA-CB-CG	5.37	127.64	115.30
7	5	422	TYR	CA-CB-CG	5.35	123.57	113.40
52	v2	141	LEU	CA-CB-CG	5.34	127.59	115.30
51	V1	53	LEU	C-N-CA	5.33	135.03	121.70
4	1	142	TYR	CA-CB-CG	5.31	123.49	113.40
18	a8	112	LEU	CA-CB-CG	5.29	127.46	115.30
52	V2	233	LEU	CA-CB-CG	5.28	127.44	115.30
17	A6	23	ILE	CG1-CB-CG2	-5.28	99.79	111.40
18	a8	89	LEU	CA-CB-CG	5.27	127.42	115.30
53	S1	548	LEU	CA-CB-CG	5.26	127.39	115.30
8	4a	437	MET	CA-CB-CG	-5.25	104.37	113.30
54	s7	81	LEU	CA-CB-CG	5.25	127.38	115.30
40	3L	349	SER	C-N-CA	5.25	134.82	121.70
45	3Q	30	LEU	CA-CB-CG	5.24	127.35	115.30
9	2a	170	LEU	CA-CB-CG	5.24	127.34	115.30
54	S7	99	CYS	CA-CB-SG	5.23	123.42	114.00
15	ac	98	LEU	CA-CB-CG	5.22	127.31	115.30
47	3S	24	LEU	CA-CB-CG	5.20	127.25	115.30
53	S1	254	MET	CA-CB-CG	5.19	122.13	113.30
51	v1	53	LEU	C-N-CA	5.19	134.68	121.70
52	V2	233	LEU	CB-CG-CD2	5.18	119.81	111.00
9	2	29	MET	CA-CB-CG	5.18	122.10	113.30
37	AN	42	LEU	CA-CB-CG	5.17	127.19	115.30
4	1a	233	LEU	CB-CG-CD1	-5.17	102.21	111.00
3	S2	139	LEU	CB-CG-CD2	5.15	119.76	111.00
4	1	285	LEU	CA-CB-CG	5.14	127.13	115.30
40	3L	169	LEU	CA-CB-CG	5.14	127.13	115.30
1	3a	67	LEU	CB-CG-CD2	-5.11	102.31	111.00
4	1	264	LEU	CA-CB-CG	5.10	127.03	115.30
9	2	296	LEU	CA-CB-CG	5.09	127.00	115.30
34	B9	28	GLU	CA-CB-CG	5.08	124.59	113.40
53	s1	466	LEU	CA-CB-CG	5.08	126.97	115.30
7	5a	513	MET	CA-CB-CG	5.07	121.92	113.30
2	s3	113	LEU	CA-CB-CG	5.07	126.95	115.30
3	s2	337	MET	CA-CB-CG	5.06	121.90	113.30
8	4a	99	LEU	CB-CG-CD2	5.06	119.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	3A	377	MET	CA-CB-CG	-5.05	104.71	113.30
35	B7	66	LEU	CA-CB-CG	5.05	126.91	115.30
51	V1	371	ILE	CG1-CB-CG2	-5.04	100.32	111.40
4	1a	22	LEU	CB-CG-CD1	-5.03	102.45	111.00
4	1a	265	LEU	CA-CB-CG	5.02	126.84	115.30
10	al	236	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1	154	LEU	Peptide
4	1	199	ASP	Peptide
41	3B	258	ILE	Peptide
42	3C	26	ASN	Peptide
8	4	249	ILE	Peptide
8	4	366	ASN	Peptide
7	5a	437	PHE	Peptide
18	A8	166	ARG	Sidechain
37	AN	120	ASN	Peptide
2	S3	70	LYS	Peptide
54	S7	153	PRO	Peptide
54	S7	193	GLY	Peptide
54	S7	194	CYS	Peptide
54	S7	195	PRO	Peptide
51	V1	227	PRO	Peptide
52	V2	136	THR	Peptide
52	V2	142	ARG	Peptide
52	V2	179	CYS	Peptide
52	V2	181	ASN	Peptide
54	s7	134	ALA	Peptide
54	s7	194	CYS	Peptide
54	s7	195	PRO	Peptide
51	v1	227	PRO	Peptide
51	v1	253	THR	Peptide
52	v2	87	ARG	Sidechain

## 5.2 Too-close contacts

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



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
1	3a	109/115 (95%)	102 (94%)	7 (6%)	0	100	100
2	S3	204/263 (78%)	197 (97%)	7 (3%)	0	100	100
2	s3	203/263 (77%)	188 (93%)	15 (7%)	0	100	100
3	S2	418/463 (90%)	401 (96%)	17 (4%)	0	100	100
3	s2	416/463 (90%)	400 (96%)	16 (4%)	0	100	100
4	1	315/318 (99%)	294 (93%)	20 (6%)	1 (0%)	37	67
4	1a	314/318 (99%)	293 (93%)	20 (6%)	1 (0%)	37	67
5	6	168/172 (98%)	160 (95%)	8 (5%)	0	100	100
5	6a	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
6	4L	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
6	4l	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	5	603/607 (99%)	573 (95%)	28 (5%)	2 (0%)	37	67
7	5a	603/607 (99%)	562 (93%)	41 (7%)	0	100	100
8	4	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
8	4a	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
9	2	342/345 (99%)	331 (97%)	11 (3%)	0	100	100
9	2a	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
10	AL	318/355 (90%)	299 (94%)	19 (6%)	0	100	100
10	al	318/355 (90%)	304 (96%)	14 (4%)	0	100	100
11	A9	340/377 (90%)	321 (94%)	19 (6%)	0	100	100
11	a9	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
12	S4	124/175 (71%)	118 (95%)	6 (5%)	0	100	100
12	s4	124/175 (71%)	122 (98%)	2 (2%)	0	100	100
13	S6	93/116 (80%)	93 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	s6	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
14	A2	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
14	a2	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
15	AB	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	AC	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
15	ab	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	ac	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
16	A5	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
16	a5	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
17	A6	110/131 (84%)	105 (96%)	5 (4%)	0	100	100
17	a6	109/131 (83%)	103 (94%)	6 (6%)	0	100	100
18	A8	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
18	a8	168/172 (98%)	162 (96%)	6 (4%)	0	100	100
19	AM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
19	am	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
20	AO	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
20	ao	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
21	A1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
21	a1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
22	A3	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
22	a3	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
23	C1	47/76 (62%)	47 (100%)	0	0	100	100
23	c1	43/76 (57%)	42 (98%)	1 (2%)	0	100	100
24	C2	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
24	c2	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
25	S5	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
25	s5	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
26	B1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
26	b1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	BM	96/151 (64%)	93 (97%)	3 (3%)	0	100	100
27	bm	97/151 (64%)	93 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	B5	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
28	b5	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
29	B6	90/127 (71%)	89 (99%)	1 (1%)	0	100	100
29	b6	86/127 (68%)	83 (96%)	3 (4%)	0	100	100
30	B2	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
30	b2	61/105 (58%)	61 (100%)	0	0	100	100
31	B3	68/104 (65%)	65 (96%)	3 (4%)	0	100	100
31	b3	69/104 (66%)	66 (96%)	3 (4%)	0	100	100
32	B8	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
32	b8	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
33	B4	123/129 (95%)	121 (98%)	2 (2%)	0	100	100
33	b4	123/129 (95%)	118 (96%)	5 (4%)	0	100	100
34	B9	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
34	b9	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	B7	112/136 (82%)	110 (98%)	2 (2%)	0	100	100
35	b7	115/136 (85%)	109 (95%)	6 (5%)	0	100	100
36	BL	165/176 (94%)	159 (96%)	6 (4%)	0	100	100
36	bl	167/176 (95%)	159 (95%)	8 (5%)	0	100	100
37	AN	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
37	an	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
38	A7	88/112 (79%)	84 (96%)	4 (4%)	0	100	100
38	a7	68/112 (61%)	63 (93%)	5 (7%)	0	100	100
39	V3	38/104 (36%)	38 (100%)	0	0	100	100
39	v3	34/104 (33%)	34 (100%)	0	0	100	100
40	3A	443/446 (99%)	427 (96%)	16 (4%)	0	100	100
40	3L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
41	3B	418/439 (95%)	405 (97%)	13 (3%)	0	100	100
41	3M	418/439 (95%)	396 (95%)	22 (5%)	0	100	100
42	3C	378/380 (100%)	366 (97%)	12 (3%)	0	100	100
42	3N	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
43	3D	239/241 (99%)	230 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	3O	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
44	3E	78/196 (40%)	76 (97%)	2 (3%)	0	100	100
44	3P	79/196 (40%)	73 (92%)	6 (8%)	0	100	100
45	3F	100/110 (91%)	97 (97%)	3 (3%)	0	100	100
45	3Q	97/110 (88%)	94 (97%)	3 (3%)	0	100	100
46	3G	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
46	3R	69/81 (85%)	63 (91%)	6 (9%)	0	100	100
47	3H	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
47	3S	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
48	3J	54/63 (86%)	52 (96%)	1 (2%)	1 (2%)	6	35
48	3U	57/63 (90%)	56 (98%)	1 (2%)	0	100	100
49	3K	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
49	3V	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
50	3T	52/78 (67%)	50 (96%)	2 (4%)	0	100	100
51	V1	426/457 (93%)	371 (87%)	55 (13%)	0	100	100
51	v1	420/457 (92%)	375 (89%)	45 (11%)	0	100	100
52	V2	207/244 (85%)	178 (86%)	28 (14%)	1 (0%)	25	57
52	v2	190/244 (78%)	176 (93%)	14 (7%)	0	100	100
53	S1	685/716 (96%)	620 (90%)	65 (10%)	0	100	100
53	s1	685/716 (96%)	619 (90%)	66 (10%)	0	100	100
54	S7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
54	s7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
55	S8	176/212 (83%)	158 (90%)	18 (10%)	0	100	100
55	s8	162/212 (76%)	145 (90%)	16 (10%)	1 (1%)	22	54
All	All	19905/22630 (88%)	18869 (95%)	1029 (5%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1	91	MET
7	5	433	THR
4	1a	91	MET
48	3J	57	LYS
55	s8	152	CYS

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Mol	Chain	Res	Type
52	V2	188	ASN
7	5	563	PRO

### 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	102/104 (98%)	99 (97%)	3 (3%)	37	59
1	3a	100/104 (96%)	96 (96%)	4 (4%)	27	52
2	S3	188/227 (83%)	176 (94%)	12 (6%)	14	42
2	s3	187/227 (82%)	184 (98%)	3 (2%)	58	74
3	S2	364/394 (92%)	355 (98%)	9 (2%)	42	62
3	s2	362/394 (92%)	350 (97%)	12 (3%)	33	57
4	1	279/279 (100%)	270 (97%)	9 (3%)	34	57
4	1a	278/279 (100%)	268 (96%)	10 (4%)	30	55
5	6	136/138 (99%)	128 (94%)	8 (6%)	16	44
5	6a	137/138 (99%)	125 (91%)	12 (9%)	8	32
6	4L	87/88 (99%)	84 (97%)	3 (3%)	32	56
6	4l	87/88 (99%)	83 (95%)	4 (5%)	23	49
7	5	548/550 (100%)	533 (97%)	15 (3%)	40	61
7	5a	548/550 (100%)	533 (97%)	15 (3%)	40	61
8	4	415/415 (100%)	407 (98%)	8 (2%)	52	70
8	4a	415/415 (100%)	405 (98%)	10 (2%)	44	63
9	2	307/308 (100%)	299 (97%)	8 (3%)	41	61
9	2a	307/308 (100%)	297 (97%)	10 (3%)	33	57
10	AL	284/309 (92%)	273 (96%)	11 (4%)	27	53
10	al	284/309 (92%)	277 (98%)	7 (2%)	42	62
11	A9	299/325 (92%)	291 (97%)	8 (3%)	40	61
11	a9	299/325 (92%)	290 (97%)	9 (3%)	36	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	S4	112/153 (73%)	112 (100%)	0	100	100
12	s4	112/153 (73%)	109 (97%)	3 (3%)	40	61
13	S6	80/96 (83%)	78 (98%)	2 (2%)	42	62
13	s6	80/96 (83%)	79 (99%)	1 (1%)	65	77
14	A2	74/80 (92%)	72 (97%)	2 (3%)	40	61
14	a2	74/80 (92%)	71 (96%)	3 (4%)	26	52
15	AB	72/135 (53%)	66 (92%)	6 (8%)	9	34
15	AC	81/135 (60%)	77 (95%)	4 (5%)	21	47
15	ab	72/135 (53%)	67 (93%)	5 (7%)	13	39
15	ac	81/135 (60%)	77 (95%)	4 (5%)	21	47
16	A5	101/102 (99%)	98 (97%)	3 (3%)	36	58
16	a5	101/102 (99%)	100 (99%)	1 (1%)	73	82
17	A6	106/114 (93%)	104 (98%)	2 (2%)	52	70
17	a6	105/114 (92%)	103 (98%)	2 (2%)	52	70
18	A8	152/154 (99%)	147 (97%)	5 (3%)	33	57
18	a8	152/154 (99%)	145 (95%)	7 (5%)	23	49
19	AM	106/106 (100%)	100 (94%)	6 (6%)	17	45
19	am	106/106 (100%)	102 (96%)	4 (4%)	28	53
20	AO	121/123 (98%)	117 (97%)	4 (3%)	33	57
20	ao	121/123 (98%)	117 (97%)	4 (3%)	33	57
21	A1	59/60 (98%)	57 (97%)	2 (3%)	32	56
21	a1	59/60 (98%)	57 (97%)	2 (3%)	32	56
22	A3	72/73 (99%)	68 (94%)	4 (6%)	17	45
22	a3	72/73 (99%)	70 (97%)	2 (3%)	38	60
23	C1	43/67 (64%)	42 (98%)	1 (2%)	45	64
23	c1	40/67 (60%)	39 (98%)	1 (2%)	42	62
24	C2	107/107 (100%)	102 (95%)	5 (5%)	22	48
24	c2	107/107 (100%)	102 (95%)	5 (5%)	22	48
25	S5	93/94 (99%)	89 (96%)	4 (4%)	25	50
25	s5	93/94 (99%)	89 (96%)	4 (4%)	25	50
26	B1	52/53 (98%)	51 (98%)	1 (2%)	52	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	b1	52/53 (98%)	49 (94%)	3 (6%)	17	44
27	BM	89/129 (69%)	84 (94%)	5 (6%)	17	45
27	bm	90/129 (70%)	89 (99%)	1 (1%)	70	80
28	B5	123/162 (76%)	119 (97%)	4 (3%)	33	57
28	b5	122/162 (75%)	120 (98%)	2 (2%)	58	74
29	B6	86/119 (72%)	85 (99%)	1 (1%)	67	79
29	b6	85/119 (71%)	81 (95%)	4 (5%)	22	48
30	B2	60/87 (69%)	57 (95%)	3 (5%)	20	47
30	b2	59/87 (68%)	58 (98%)	1 (2%)	56	73
31	B3	55/78 (70%)	54 (98%)	1 (2%)	54	71
31	b3	55/78 (70%)	55 (100%)	0	100	100
32	B8	140/161 (87%)	137 (98%)	3 (2%)	48	67
32	b8	140/161 (87%)	137 (98%)	3 (2%)	48	67
33	B4	111/114 (97%)	109 (98%)	2 (2%)	54	71
33	b4	111/114 (97%)	108 (97%)	3 (3%)	40	61
34	B9	163/164 (99%)	158 (97%)	5 (3%)	35	57
34	b9	162/164 (99%)	157 (97%)	5 (3%)	35	57
35	B7	106/120 (88%)	100 (94%)	6 (6%)	17	45
35	b7	108/120 (90%)	102 (94%)	6 (6%)	17	45
36	BL	152/158 (96%)	147 (97%)	5 (3%)	33	57
36	bl	154/158 (98%)	148 (96%)	6 (4%)	27	53
37	AN	130/131 (99%)	127 (98%)	3 (2%)	45	64
37	an	130/131 (99%)	125 (96%)	5 (4%)	28	53
38	A7	83/95 (87%)	79 (95%)	4 (5%)	21	48
38	a7	63/95 (66%)	61 (97%)	2 (3%)	34	57
39	V3	39/95 (41%)	34 (87%)	5 (13%)	3	19
39	v3	35/95 (37%)	34 (97%)	1 (3%)	37	59
40	3A	372/373 (100%)	363 (98%)	9 (2%)	44	63
40	3L	372/373 (100%)	357 (96%)	15 (4%)	27	52
41	3B	330/344 (96%)	325 (98%)	5 (2%)	60	75
41	3M	330/344 (96%)	320 (97%)	10 (3%)	36	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	3C	332/332 (100%)	321 (97%)	11 (3%)	33	57
42	3N	332/332 (100%)	324 (98%)	8 (2%)	44	63
43	3D	206/206 (100%)	196 (95%)	10 (5%)	21	47
43	3O	205/206 (100%)	200 (98%)	5 (2%)	44	63
44	3E	69/166 (42%)	68 (99%)	1 (1%)	62	76
44	3P	70/166 (42%)	70 (100%)	0	100	100
45	3F	94/98 (96%)	91 (97%)	3 (3%)	34	57
45	3Q	91/98 (93%)	90 (99%)	1 (1%)	70	80
46	3G	72/73 (99%)	69 (96%)	3 (4%)	25	51
46	3R	64/73 (88%)	63 (98%)	1 (2%)	58	74
47	3H	63/72 (88%)	60 (95%)	3 (5%)	21	48
47	3S	63/72 (88%)	60 (95%)	3 (5%)	21	48
48	3J	47/54 (87%)	47 (100%)	0	100	100
48	3U	50/54 (93%)	50 (100%)	0	100	100
49	3K	41/46 (89%)	39 (95%)	2 (5%)	21	47
49	3V	43/46 (94%)	43 (100%)	0	100	100
50	3T	41/58 (71%)	41 (100%)	0	100	100
51	V1	343/366 (94%)	334 (97%)	9 (3%)	41	61
51	v1	338/366 (92%)	329 (97%)	9 (3%)	40	61
52	V2	182/204 (89%)	180 (99%)	2 (1%)	70	80
52	v2	170/204 (83%)	167 (98%)	3 (2%)	54	71
53	S1	579/602 (96%)	571 (99%)	8 (1%)	62	76
53	s1	579/602 (96%)	574 (99%)	5 (1%)	75	84
54	S7	131/185 (71%)	129 (98%)	2 (2%)	60	75
54	s7	131/185 (71%)	129 (98%)	2 (2%)	60	75
55	S8	145/178 (82%)	140 (97%)	5 (3%)	32	56
55	s8	138/178 (78%)	132 (96%)	6 (4%)	25	50
All	All	17545/19460 (90%)	17026 (97%)	519 (3%)	37	58

All (519) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	4	TYR

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Mol	Chain	Res	Type
1	3	39	CYS
1	3	102	LEU
2	S3	51	ASP
2	S3	55	LYS
2	S3	71	TYR
2	S3	90	ASP
2	S3	104	ASN
2	S3	110	LEU
2	S3	137	ASN
2	S3	203	LEU
2	S3	212	ASP
2	S3	214	GLU
2	S3	216	LYS
2	S3	217	ARG
3	S2	137	ASP
3	S2	138	ARG
3	S2	147	ASN
3	S2	204	PHE
3	S2	218	SER
3	S2	259	GLU
3	S2	330	TYR
3	S2	389	TYR
3	S2	462	ASP
4	1	17	MET
4	1	91	MET
4	1	171	HIS
4	1	186	PHE
4	1	224	PHE
4	1	262	GLU
4	1	270	PHE
4	1	283	ASP
4	1	306	SER
5	6	46	PHE
5	6	56	PHE
5	6	59	TYR
5	6	86	TRP
5	6	91	PHE
5	6	146	SER
5	6	152	MET
5	6	160	PHE
6	4L	5	PHE
6	4L	6	PHE

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Mol	Chain	Res	Type
6	4L	78	LEU
7	5	2	ASN
7	5	17	SER
7	5	78	MET
7	5	141	PHE
7	5	163	ASP
7	5	223	LYS
7	5	321	GLN
7	5	336	LYS
7	5	358	LYS
7	5	400	ASN
7	5	424	MET
7	5	432	MET
7	5	437	PHE
7	5	466	PHE
7	5	484	TRP
8	4	58	SER
8	4	157	SER
8	4	189	SER
8	4	274	SER
8	4	281	ASP
8	4	363	SER
8	4	389	SER
8	4	390	ASN
9	2	29	MET
9	2	78	TYR
9	2	182	SER
9	2	223	ASN
9	2	270	LEU
9	2	274	ASN
9	2	291	PHE
9	2	333	SER
10	AL	40	LEU
10	AL	61	THR
10	AL	81	LEU
10	AL	129	TYR
10	AL	130	ARG
10	AL	170	LEU
10	AL	189	GLU
10	AL	219	GLN
10	AL	241	TYR
10	AL	243	LYS

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Mol	Chain	Res	Type
10	AL	259	ASP
11	A9	43	HIS
11	A9	221	ARG
11	A9	265	PHE
11	A9	291	TYR
11	A9	305	PHE
11	A9	337	ASP
11	A9	353	LEU
11	A9	354	ARG
13	S6	80	ASP
13	S6	112	LYS
14	A2	26	ARG
14	A2	36	PHE
15	AB	77	ASP
15	AB	89	LEU
15	AB	132	ASP
15	AB	139	MET
15	AB	150	ASP
15	AB	151	LYS
15	AC	70	ASP
15	AC	74	LEU
15	AC	77	ASP
15	AC	111	ASP
16	A5	23	ARG
16	A5	89	SER
16	A5	96	LYS
17	A6	34	ARG
17	A6	43	TYR
18	A8	55	ARG
18	A8	92	SER
18	A8	93	ASN
18	A8	167	PHE
18	A8	170	TRP
19	AM	9	TYR
19	AM	14	ASP
19	AM	61	PHE
19	AM	72	LEU
19	AM	91	PHE
19	AM	115	CYS
20	AO	9	ASP
20	AO	30	LEU
20	AO	89	GLU

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Mol	Chain	Res	Type
20	AO	142	TRP
21	A1	51	ASP
21	A1	60	TYR
22	A3	4	ARG
22	A3	51	TYR
22	A3	63	MET
22	A3	69	HIS
23	C1	58	LEU
24	C2	5	ARG
24	C2	30	ARG
24	C2	64	PHE
24	C2	75	TYR
24	C2	90	MET
25	S5	3	PHE
25	S5	45	HIS
25	S5	70	TYR
25	S5	101	ARG
26	B1	55	THR
27	BM	53	TRP
27	BM	93	PHE
27	BM	122	ARG
27	BM	138	ASN
27	BM	141	ASP
28	B5	127	ASP
28	B5	161	ARG
28	B5	176	LYS
28	B5	180	ASP
29	B6	4	TYR
30	B2	41	GLN
30	B2	47	PHE
30	B2	86	TYR
31	B3	19	LYS
32	B8	125	SER
32	B8	160	GLN
32	B8	167	TYR
33	B4	88	LEU
33	B4	118	GLU
34	B9	52	LYS
34	B9	134	ASP
34	B9	138	LYS
34	B9	147	ASP
34	B9	158	ARG

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Mol	Chain	Res	Type
35	B7	7	ARG
35	B7	9	TYR
35	B7	14	SER
35	B7	31	PHE
35	B7	84	GLN
35	B7	105	GLU
36	BL	12	GLU
36	BL	84	CYS
36	BL	93	ARG
36	BL	95	ASP
36	BL	160	LYS
37	AN	31	PHE
37	AN	51	LYS
37	AN	78	PHE
38	A7	9	GLN
38	A7	99	PRO
38	A7	103	ARG
38	A7	109	ASP
39	V3	74	ASP
39	V3	88	SER
39	V3	89	LYS
39	V3	91	ARG
39	V3	104	HIS
1	3a	51	PHE
1	3a	53	MET
1	3a	92	PHE
1	3a	109	LYS
2	s3	51	ASP
2	s3	185	ARG
2	s3	227	GLN
3	s2	79	ASN
3	s2	216	ARG
3	s2	228	ARG
3	s2	229	PRO
3	s2	238	LEU
3	s2	271	ARG
3	s2	309	ASP
3	s2	351	MET
3	s2	368	ARG
3	s2	423	LYS
3	s2	429	PHE
3	s2	463	ARG

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Mol	Chain	Res	Type
4	1a	24	GLU
4	1a	25	ARG
4	1a	34	ARG
4	1a	57	MET
4	1a	114	TYR
4	1a	142	TYR
4	1a	165	LEU
4	1a	247	TYR
4	1a	254	LEU
4	1a	280	PHE
5	6a	3	ASN
5	6a	12	PHE
5	6a	16	CYS
5	6a	50	PHE
5	6a	54	MET
5	6a	87	LEU
5	6a	91	PHE
5	6a	108	TYR
5	6a	120	LEU
5	6a	125	MET
5	6a	130	ASP
5	6a	152	MET
6	4l	5	PHE
6	4l	31	LEU
6	4l	50	ASN
6	4l	88	ASP
7	5a	26	LEU
7	5a	42	PHE
7	5a	77	LYS
7	5a	113	ASN
7	5a	116	ARG
7	5a	151	SER
7	5a	208	ASP
7	5a	249	SER
7	5a	295	GLN
7	5a	336	LYS
7	5a	355	ASP
7	5a	361	ASN
7	5a	484	TRP
7	5a	553	LEU
7	5a	579	ASN
8	4a	46	ASP

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Mol	Chain	Res	Type
8	4a	54	ASN
8	4a	138	ASN
8	4a	152	TYR
8	4a	245	ARG
8	4a	251	ASP
8	4a	290	SER
8	4a	360	LEU
8	4a	422	HIS
8	4a	440	HIS
9	2a	23	SER
9	2a	35	PHE
9	2a	36	SER
9	2a	87	GLN
9	2a	105	LYS
9	2a	125	HIS
9	2a	240	MET
9	2a	282	MET
9	2a	291	PHE
9	2a	313	MET
10	al	65	ASN
10	al	102	ARG
10	al	167	PHE
10	al	174	TYR
10	al	241	TYR
10	al	280	LYS
10	al	293	TYR
11	a9	43	HIS
11	a9	48	ARG
11	a9	109	ASP
11	a9	175	LYS
11	a9	180	SER
11	a9	184	LYS
11	a9	195	PHE
11	a9	298	TYR
11	a9	374	THR
12	s4	58	LYS
12	s4	106	ARG
12	s4	169	ARG
13	s6	38	TYR
14	a2	85	ASP
14	a2	86	GLU
14	a2	91	MET

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Mol	Chain	Res	Type
15	ab	85	TYR
15	ab	97	LYS
15	ab	136	GLU
15	ab	140	CYS
15	ab	146	ASP
15	ac	77	ASP
15	ac	81	ASP
15	ac	134	ASP
15	ac	155	TYR
16	a5	37	HIS
17	a6	27	ASP
17	a6	53	MET
18	a8	38	LYS
18	a8	86	TRP
18	a8	90	ASP
18	a8	98	ARG
18	a8	135	ARG
18	a8	142	TYR
18	a8	148	PRO
19	am	1	MET
19	am	21	LYS
19	am	75	CYS
19	am	104	ARG
20	ao	5	LYS
20	ao	8	GLN
20	ao	53	TRP
20	ao	137	ASN
21	a1	2	TRP
21	a1	50	ARG
22	a3	53	TYR
22	a3	79	ASP
23	c1	33	GLU
24	c2	19	ARG
24	c2	28	ASP
24	c2	75	TYR
24	c2	89	ASP
24	c2	95	LYS
25	s5	5	ASP
25	s5	20	PHE
25	s5	51	ARG
25	s5	102	GLU
26	b1	5	GLN

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Mol	Chain	Res	Type
26	b1	37	PHE
26	b1	56	TRP
27	bm	53	TRP
28	b5	72	LYS
28	b5	118	SER
29	b6	7	ASP
29	b6	11	ARG
29	b6	13	GLN
29	b6	20	ARG
30	b2	47	PHE
32	b8	98	ARG
32	b8	99	MET
32	b8	159	LYS
33	b4	81	ARG
33	b4	87	SER
33	b4	128	SER
34	b9	25	ARG
34	b9	120	SER
34	b9	147	ASP
34	b9	158	ARG
34	b9	177	ARG
35	b7	7	ARG
35	b7	11	TRP
35	b7	31	PHE
35	b7	34	ARG
35	b7	77	PHE
35	b7	89	TYR
36	bl	68	TYR
36	bl	95	ASP
36	bl	104	ASN
36	bl	150	TYR
36	bl	164	LEU
36	bl	167	ARG
37	an	42	LEU
37	an	46	ASP
37	an	78	PHE
37	an	118	LYS
37	an	132	SER
38	a7	49	LEU
38	a7	55	CYS
39	v3	74	ASP
40	3A	92	PHE

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Mol	Chain	Res	Type
40	3A	260	ASP
40	3A	279	ASP
40	3A	316	CYS
40	3A	341	PHE
40	3A	342	GLN
40	3A	432	ARG
40	3A	437	ASP
40	3A	451	ASP
41	3B	109	LYS
41	3B	254	ARG
41	3B	287	SER
41	3B	388	THR
41	3B	421	ASP
42	3C	12	LYS
42	3C	103	TYR
42	3C	107	TYR
42	3C	171	ASP
42	3C	183	PHE
42	3C	200	LEU
42	3C	273	TYR
42	3C	287	LYS
42	3C	303	LEU
42	3C	310	SER
42	3C	314	SER
43	3D	117	TYR
43	3D	119	GLN
43	3D	121	CYS
43	3D	160	ASP
43	3D	173	ASP
43	3D	177	LYS
43	3D	199	TYR
43	3D	202	ARG
43	3D	210	TYR
43	3D	265	GLN
44	3E	99	SER
45	3F	12	LYS
45	3F	22	TYR
45	3F	34	ARG
46	3G	31	PHE
46	3G	67	PHE
46	3G	79	GLU
47	3H	51	CYS

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Mol	Chain	Res	Type
47	3H	53	ASN
47	3H	64	ASP
49	3K	39	ARG
49	3K	40	LEU
40	3L	38	PHE
40	3L	49	GLN
40	3L	58	ARG
40	3L	62	GLU
40	3L	86	ASN
40	3L	92	PHE
40	3L	95	HIS
40	3L	155	SER
40	3L	165	ARG
40	3L	166	ASP
40	3L	178	SER
40	3L	251	SER
40	3L	350	ASP
40	3L	367	ASP
40	3L	477	TRP
41	3M	54	ASN
41	3M	109	LYS
41	3M	236	GLN
41	3M	250	LYS
41	3M	257	GLU
41	3M	287	SER
41	3M	298	HIS
41	3M	332	ASP
41	3M	398	SER
41	3M	405	SER
42	3N	78	LEU
42	3N	91	PHE
42	3N	100	ARG
42	3N	121	PHE
42	3N	175	LEU
42	3N	183	PHE
42	3N	228	ASP
42	3N	352	GLN
43	3O	163	GLU
43	3O	172	SER
43	3O	209	ASP
43	3O	249	TYR
43	3O	255	TYR

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Mol	Chain	Res	Type
45	3Q	74	GLN
46	3R	17	TYR
47	3S	46	GLU
47	3S	70	PHE
47	3S	89	LYS
51	V1	44	ASN
51	V1	45	LEU
51	V1	54	LYS
51	V1	109	ARG
51	V1	134	ASP
51	V1	244	ASN
51	V1	257	ARG
51	V1	357	MET
51	V1	379	CYS
52	V2	82	LEU
52	V2	161	GLU
53	S1	154	LEU
53	S1	158	ARG
53	S1	277	MET
53	S1	280	ASP
53	S1	282	ASN
53	S1	463	CYS
53	S1	569	GLN
53	S1	657	ASP
54	S7	87	ARG
54	S7	170	TYR
55	S8	63	TRP
55	S8	98	ARG
55	S8	140	ARG
55	S8	145	TYR
55	S8	206	GLN
51	v1	44	ASN
51	v1	45	LEU
51	v1	48	ARG
51	v1	54	LYS
51	v1	109	ARG
51	v1	257	ARG
51	v1	379	CYS
51	v1	393	ASN
51	v1	425	CYS
52	v2	91	TRP
52	v2	189	ASP

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Mol	Chain	Res	Type
52	v2	195	LEU
53	s1	139	LEU
53	s1	158	ARG
53	s1	419	ARG
53	s1	514	ASN
53	s1	621	LYS
54	s7	87	ARG
54	s7	170	TYR
55	s8	98	ARG
55	s8	140	ARG
55	s8	145	TYR
55	s8	149	MET
55	s8	193	ASN
55	s8	206	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
8	4	304	GLN
15	AB	115	GLN
18	A8	151	ASN
22	A3	52	ASN
7	5a	446	ASN
14	a2	80	ASN
37	an	73	ASN
38	a7	21	GLN
47	3H	74	HIS
47	3H	78	HIS
40	3L	199	GLN
52	V2	190	ASN
53	s1	514	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2MR	s2	118	3	3,4,13	0.83	0	2,4,15	1.27	0
3	2MR	S2	118	3	10,12,13	2.72	3 (30%)	5,13,15	7.36	4 (80%)

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
3	2MR	s2	118	3	-	1/1/2/15	-
3	2MR	S2	118	3	-	4/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S2	118	2MR	CZ-NE	5.73	1.46	1.34
3	S2	118	2MR	CZ-NH2	5.42	1.44	1.33
3	S2	118	2MR	CQ1-NH1	-2.49	1.41	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S2	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
3	S2	118	2MR	CD-NE-CZ	10.13	142.39	123.36
3	S2	118	2MR	CQ2-NH2-CZ	3.05	130.19	123.65
3	S2	118	2MR	CG-CD-NE	-2.38	105.52	112.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	s2	118	2MR	O-C-CA-CB
3	S2	118	2MR	CA-CB-CG-CD
3	S2	118	2MR	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	S2	118	2MR	N-CA-CB-CG
3	S2	118	2MR	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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$
63	FMN	v1	501	-	33,33,33	0.27	0	48,50,50	0.54	1 (2%)
64	SF4	s1	802	53	0,12,12	-	-	-		
64	SF4	s1	801	53	0,12,12	-	-	-		
57	DGT	AL	502	56	29,33,33	0.98	2 (6%)	37,52,52	0.77	0
58	NDP	a9	501	-	47,52,52	0.54	0	61,80,80	0.58	1 (1%)
65	FES	S1	803	53	0,4,4	-	-	-		
62	HEC	3O	401	43	32,50,50	1.76	5 (15%)	30,82,82	3.15	15 (50%)
65	FES	v2	301	52	0,4,4	-	-	-		
64	SF4	s8	301	55	0,12,12	-	-	-		
62	HEC	3D	401	43	32,50,50	1.98	7 (21%)	30,82,82	3.42	17 (56%)
63	FMN	V1	501	-	33,33,33	0.30	0	48,50,50	0.48	0
64	SF4	S7	301	54,3	0,12,12	-	-	-		
64	SF4	s8	302	55	0,12,12	-	-	-		
65	FES	V2	301	52	0,4,4	-	-	-		
61	HEM	3N	402	42	42,50,50	1.30	6 (14%)	46,82,82	1.69	10 (21%)
58	NDP	A9	501	-	47,52,52	0.53	0	61,80,80	0.60	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	HEM	3C	402	42	42,50,50	1.29	6 (14%)	46,82,82	1.71	11 (23%)
61	HEM	3C	401	42	42,50,50	1.25	5 (11%)	46,82,82	1.75	10 (21%)
64	SF4	S1	802	53	0,12,12	-	-	-	-	-
60	EHZ	A6	201	-	31,36,37	0.20	0	36,44,47	1.26	1 (2%)
64	SF4	S8	301	55	0,12,12	-	-	-	-	-
65	FES	s1	803	53	0,4,4	-	-	-	-	-
61	HEM	3N	401	42	42,50,50	1.26	4 (9%)	46,82,82	1.72	9 (19%)
64	SF4	S8	302	55	0,12,12	-	-	-	-	-
60	EHZ	B9	201	-	31,36,37	0.20	0	36,44,47	1.04	1 (2%)
60	EHZ	5a	701	-	31,36,37	0.25	0	36,44,47	1.14	1 (2%)
64	SF4	s7	301	54	0,12,12	-	-	-	-	-
64	SF4	V1	502	51	0,12,12	-	-	-	-	-
60	EHZ	a6	201	-	31,36,37	0.19	0	36,44,47	1.25	1 (2%)
57	DGT	al	502	-	29,33,33	0.98	2 (6%)	37,52,52	0.77	0
64	SF4	v1	502	51	0,12,12	-	-	-	-	-
64	SF4	S1	801	53	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	FMN	v1	501	-	-	4/18/18/18	0/3/3/3
64	SF4	s1	802	53	-	-	0/6/5/5
64	SF4	s1	801	53	-	-	0/6/5/5
57	DGT	AL	502	56	-	1/18/34/34	0/3/3/3
58	NDP	a9	501	-	-	10/30/77/77	0/5/5/5
65	FES	S1	803	53	-	-	0/1/1/1
62	HEC	3O	401	43	-	5/10/54/54	-
65	FES	v2	301	52	-	-	0/1/1/1
64	SF4	s8	301	55	-	-	0/6/5/5
62	HEC	3D	401	43	-	7/10/54/54	-
63	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
64	SF4	S7	301	54,3	-	-	0/6/5/5
64	SF4	s8	302	55	-	-	0/6/5/5
65	FES	V2	301	52	-	-	0/1/1/1
61	HEM	3N	402	42	-	5/12/54/54	-
58	NDP	A9	501	-	-	9/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	HEM	3C	402	42	-	5/12/54/54	-
61	HEM	3C	401	42	-	7/12/54/54	-
64	SF4	S1	802	53	-	-	0/6/5/5
60	EHZ	A6	201	-	-	3/42/44/45	-
64	SF4	S8	301	55	-	-	0/6/5/5
65	FES	s1	803	53	-	-	0/1/1/1
61	HEM	3N	401	42	-	7/12/54/54	-
64	SF4	S8	302	55	-	-	0/6/5/5
60	EHZ	B9	201	-	-	8/42/44/45	-
60	EHZ	5a	701	-	-	4/42/44/45	-
64	SF4	s7	301	54	-	-	0/6/5/5
64	SF4	V1	502	51	-	-	0/6/5/5
60	EHZ	a6	201	-	-	10/42/44/45	-
57	DGT	al	502	-	-	2/18/34/34	0/3/3/3
64	SF4	v1	502	51	-	-	0/6/5/5
64	SF4	S1	801	53	-	-	0/6/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	3D	401	HEC	C3C-C2C	-5.58	1.34	1.40
62	3D	401	HEC	C2B-C3B	-5.02	1.35	1.40
62	3O	401	HEC	C3C-C2C	-5.01	1.35	1.40
62	3O	401	HEC	C2B-C3B	-4.87	1.35	1.40
61	3C	402	HEM	C4D-ND	-3.81	1.33	1.40
61	3N	402	HEM	C4D-ND	-3.62	1.34	1.40
61	3N	401	HEM	C4D-ND	-3.58	1.34	1.40
61	3C	401	HEM	C4D-ND	-3.43	1.34	1.40
61	3C	401	HEM	C1B-NB	-3.43	1.34	1.40
62	3O	401	HEC	CBC-CAC	-3.37	1.37	1.49
62	3D	401	HEC	CBC-CAC	-3.37	1.37	1.49
61	3N	401	HEM	C1B-NB	-3.32	1.34	1.40
61	3N	402	HEM	C1B-NB	-3.30	1.34	1.40
61	3C	402	HEM	C1D-ND	-3.10	1.32	1.38
61	3C	402	HEM	C1B-NB	-2.98	1.35	1.40
62	3D	401	HEC	CAA-C2A	2.95	1.57	1.52
61	3C	401	HEM	C1D-ND	-2.85	1.33	1.38
61	3N	401	HEM	C1D-ND	-2.84	1.33	1.38
61	3N	402	HEM	C1D-ND	-2.80	1.33	1.38
62	3D	401	HEC	O1A-CGA	2.74	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AL	502	DGT	C5-C6	-2.69	1.42	1.47
57	al	502	DGT	C5-C6	-2.66	1.42	1.47
61	3N	402	HEM	C3B-C4B	2.54	1.49	1.44
61	3N	401	HEM	CHB-C1B	2.43	1.40	1.34
62	3O	401	HEC	CBB-CAB	-2.37	1.40	1.49
62	3D	401	HEC	CBB-CAB	-2.28	1.41	1.49
61	3C	401	HEM	CHB-C1B	2.26	1.40	1.34
61	3C	402	HEM	CHB-C1B	2.25	1.40	1.34
62	3D	401	HEC	C2A-C1A	2.22	1.47	1.42
61	3N	402	HEM	CHA-C4D	2.13	1.39	1.34
61	3C	402	HEM	C4B-NB	-2.12	1.34	1.38
61	3N	402	HEM	CHB-C1B	2.12	1.39	1.34
57	al	502	DGT	C8-N7	-2.12	1.31	1.34
57	AL	502	DGT	C8-N7	-2.09	1.31	1.34
61	3C	402	HEM	CHA-C4D	2.07	1.39	1.34
62	3O	401	HEC	CMD-C2D	2.05	1.55	1.51
61	3C	401	HEM	C4B-NB	-2.03	1.34	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	3D	401	HEC	CBB-CAB-C3B	-7.38	110.23	127.49
60	a6	201	EHZ	C10-S1-C9	7.12	122.89	101.84
60	A6	201	EHZ	C10-S1-C9	6.83	122.02	101.84
62	3O	401	HEC	CBD-CAD-C3D	6.62	123.67	112.54
62	3O	401	HEC	CBB-CAB-C3B	-6.34	112.65	127.49
60	5a	701	EHZ	C10-S1-C9	6.03	119.67	101.84
60	B9	201	EHZ	C10-S1-C9	5.84	119.11	101.84
62	3D	401	HEC	CBD-CAD-C3D	5.81	122.31	112.54
62	3O	401	HEC	CMD-C2D-C1D	-5.76	120.02	128.46
62	3D	401	HEC	CBA-CAA-C2A	5.71	121.96	112.55
62	3O	401	HEC	CBC-CAC-C3C	-5.67	114.23	127.49
62	3D	401	HEC	CBC-CAC-C3C	-5.61	114.37	127.49
62	3D	401	HEC	CMB-C2B-C3B	5.55	132.34	125.82
62	3D	401	HEC	CMA-C3A-C2A	5.23	134.80	124.94
62	3D	401	HEC	CMB-C2B-C1B	-4.89	121.29	128.46
62	3D	401	HEC	CMD-C2D-C1D	-4.88	121.31	128.46
62	3O	401	HEC	CMB-C2B-C3B	4.69	131.33	125.82
61	3N	401	HEM	CHC-C4B-NB	4.68	129.47	124.44
61	3C	401	HEM	CHB-C1B-NB	4.64	130.12	124.37
61	3C	401	HEM	CHC-C4B-NB	4.61	129.40	124.44
61	3C	402	HEM	CHC-C4B-NB	4.60	129.39	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	3O	401	HEC	CMB-C2B-C1B	-4.59	121.73	128.46
61	3N	402	HEM	CHB-C1B-NB	4.46	129.90	124.37
61	3N	401	HEM	CHB-C1B-NB	4.44	129.87	124.37
62	3O	401	HEC	CMC-C2C-C3C	3.67	130.14	125.82
61	3C	402	HEM	CHB-C1B-NB	3.66	128.91	124.37
62	3D	401	HEC	CMC-C2C-C3C	3.55	129.99	125.82
62	3O	401	HEC	CMD-C2D-C3D	3.54	131.61	124.94
61	3N	402	HEM	C4D-ND-C1D	3.48	109.33	105.21
62	3D	401	HEC	CAA-CBA-CGA	3.40	123.00	113.83
61	3C	401	HEM	C1B-NB-C4B	3.23	109.03	105.21
62	3O	401	HEC	CMC-C2C-C1C	-3.21	123.75	128.46
61	3C	402	HEM	C4D-ND-C1D	3.14	108.92	105.21
62	3D	401	HEC	CMC-C2C-C1C	-3.07	123.95	128.46
61	3C	401	HEM	CHA-C4D-ND	3.07	128.18	124.37
61	3C	402	HEM	CHD-C1D-ND	3.07	127.74	124.44
62	3O	401	HEC	CBA-CAA-C2A	3.04	117.56	112.55
61	3C	402	HEM	C1B-NB-C4B	2.99	108.75	105.21
62	3O	401	HEC	C4C-C3C-C2C	2.96	109.55	106.35
62	3O	401	HEC	O1D-CGD-CBD	-2.96	113.71	123.09
62	3D	401	HEC	C4C-C3C-C2C	2.91	109.50	106.35
61	3N	402	HEM	C1B-NB-C4B	2.89	108.62	105.21
62	3D	401	HEC	C1D-C2D-C3D	2.87	108.99	107.00
61	3N	401	HEM	CHA-C4D-ND	2.84	127.89	124.37
61	3N	401	HEM	C4B-C3B-C2B	-2.76	104.74	107.28
62	3D	401	HEC	O1D-CGD-CBD	-2.76	114.34	123.09
61	3N	401	HEM	C1B-NB-C4B	2.75	108.46	105.21
61	3C	401	HEM	CHD-C1D-ND	2.73	127.38	124.44
61	3N	401	HEM	C4D-ND-C1D	2.73	108.44	105.21
63	v1	501	FMN	C4'-C3'-C2'	-2.71	109.06	113.57
61	3C	401	HEM	C4D-ND-C1D	2.71	108.41	105.21
61	3N	401	HEM	CHD-C1D-ND	2.70	127.34	124.44
61	3N	402	HEM	CHC-C4B-NB	2.69	127.33	124.44
61	3C	402	HEM	C3B-C4B-NB	-2.67	107.55	109.47
61	3N	401	HEM	C3B-C2B-C1B	2.67	108.42	106.41
62	3O	401	HEC	CMA-C3A-C2A	2.55	129.75	124.94
61	3N	402	HEM	CHB-C1B-C2B	-2.55	119.73	126.94
62	3D	401	HEC	CMD-C2D-C3D	2.52	129.70	124.94
61	3N	402	HEM	C3B-C4B-NB	-2.49	107.68	109.47
61	3C	401	HEM	CHB-C1B-C2B	-2.48	119.92	126.94
61	3C	402	HEM	CBB-CAB-C3B	-2.48	115.16	127.53
61	3N	402	HEM	CHD-C1D-ND	2.39	127.00	124.44
58	A9	501	NDP	C5A-C6A-N6A	2.37	123.92	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	3N	402	HEM	C3B-C2B-C1B	2.36	108.19	106.41
61	3N	402	HEM	C4B-C3B-C2B	-2.32	105.14	107.28
61	3C	401	HEM	C3B-C4B-NB	-2.31	107.81	109.47
61	3C	401	HEM	CMA-C3A-C4A	-2.31	125.07	128.46
61	3N	401	HEM	CHB-C1B-C2B	-2.30	120.42	126.94
58	a9	501	NDP	C5A-C6A-N6A	2.28	123.79	120.31
62	3D	401	HEC	C2B-C3B-C4B	2.27	108.80	106.35
62	3O	401	HEC	O1A-CGA-CBA	-2.25	115.96	123.09
61	3C	402	HEM	CHB-C1B-C2B	-2.21	120.68	126.94
61	3N	402	HEM	CHA-C4D-ND	2.21	127.11	124.37
61	3C	402	HEM	CBD-CAD-C3D	2.19	118.58	112.53
62	3D	401	HEC	O2A-CGA-O1A	2.15	128.87	123.33
61	3C	401	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
61	3C	402	HEM	CMA-C3A-C4A	-2.07	125.42	128.46
62	3O	401	HEC	C2B-C3B-C4B	2.05	108.56	106.35
61	3C	402	HEM	CAA-CBA-CGA	-2.05	108.32	113.83

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	al	502	DGT	PB-O3A-PA-O5'
58	A9	501	NDP	C5B-O5B-PA-O3
58	A9	501	NDP	C2N-C3N-C7N-O7N
58	A9	501	NDP	C2N-C3N-C7N-N7N
58	a9	501	NDP	C5D-O5D-PN-O3
58	a9	501	NDP	C5D-O5D-PN-O1N
58	a9	501	NDP	C5D-O5D-PN-O2N
58	a9	501	NDP	C2D-C1D-N1N-C2N
58	a9	501	NDP	C2N-C3N-C7N-N7N
60	A6	201	EHZ	O2-C9-S1-C10
60	A6	201	EHZ	C8-C9-S1-C10
60	B9	201	EHZ	O1-C7-C8-C9
60	B9	201	EHZ	O5-C16-C17-C19
60	B9	201	EHZ	O5-C16-C17-C20
60	a6	201	EHZ	O1-C7-C8-C9
60	a6	201	EHZ	O4-C15-C16-O5
60	a6	201	EHZ	C15-C16-C17-C18
60	a6	201	EHZ	C15-C16-C17-C19
60	a6	201	EHZ	C15-C16-C17-C20
61	3C	401	HEM	C2B-C3B-CAB-CBB
61	3C	401	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
61	3C	402	HEM	C2B-C3B-CAB-CBB
61	3C	402	HEM	C4B-C3B-CAB-CBB
61	3N	401	HEM	C2B-C3B-CAB-CBB
61	3N	402	HEM	C2A-CAA-CBA-CGA
62	3D	401	HEC	C1A-C2A-CAA-CBA
62	3D	401	HEC	C3A-C2A-CAA-CBA
62	3O	401	HEC	C2D-C3D-CAD-CBD
62	3O	401	HEC	C4D-C3D-CAD-CBD
63	V1	501	FMN	C1'-C2'-C3'-O3'
63	V1	501	FMN	C1'-C2'-C3'-C4'
63	v1	501	FMN	C5'-O5'-P-O2P
63	v1	501	FMN	C5'-O5'-P-O3P
60	5a	701	EHZ	C13-C12-N1-C11
63	V1	501	FMN	O2'-C2'-C3'-C4'
60	5a	701	EHZ	O3-C12-N1-C11
63	V1	501	FMN	O2'-C2'-C3'-O3'
58	a9	501	NDP	C2D-C1D-N1N-C6N
61	3C	401	HEM	C2A-CAA-CBA-CGA
61	3N	401	HEM	C2A-CAA-CBA-CGA
61	3N	401	HEM	C4B-C3B-CAB-CBB
58	a9	501	NDP	O4D-C1D-N1N-C2N
63	v1	501	FMN	C5'-O5'-P-O1P
60	B9	201	EHZ	O5-C16-C17-C18
58	A9	501	NDP	O4D-C1D-N1N-C6N
60	B9	201	EHZ	C15-C16-C17-C19
60	a6	201	EHZ	C19-C17-C20-O6
58	A9	501	NDP	C2B-O2B-P2B-O1X
57	AL	502	DGT	C5'-O5'-PA-O2A
57	al	502	DGT	C5'-O5'-PA-O2A
60	a6	201	EHZ	O5-C16-C17-C20
61	3C	402	HEM	C2A-CAA-CBA-CGA
62	3D	401	HEC	C2A-CAA-CBA-CGA
63	V1	501	FMN	C4'-C5'-O5'-P
58	A9	501	NDP	O4D-C4D-C5D-O5D
58	a9	501	NDP	O4B-C4B-C5B-O5B
60	5a	701	EHZ	O5-C16-C17-C19
58	A9	501	NDP	PN-O3-PA-O2A
60	A6	201	EHZ	C10-C11-N1-C12
60	a6	201	EHZ	N2-C15-C16-O5
60	B9	201	EHZ	C21-C1-C2-C3
61	3N	401	HEM	CAA-CBA-CGA-O1A
61	3N	402	HEM	CAD-CBD-CGD-O1D

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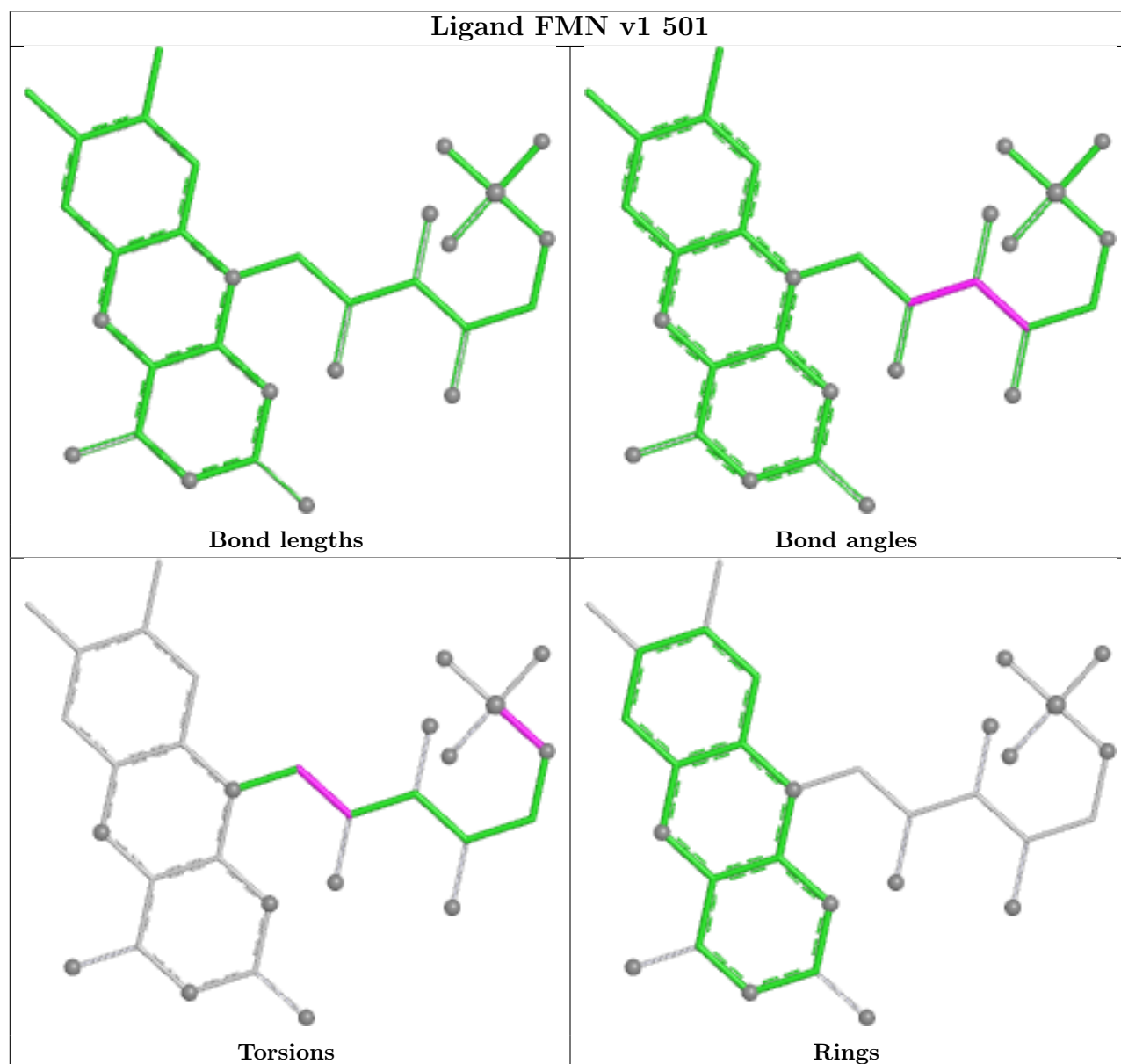
Mol	Chain	Res	Type	Atoms
61	3C	401	HEM	CAD-CBD-CGD-O1D
61	3N	401	HEM	CAA-CBA-CGA-O2A
61	3C	402	HEM	CAA-CBA-CGA-O1A
62	3O	401	HEC	CAD-CBD-CGD-O2D
58	a9	501	NDP	PA-O3-PN-O1N
61	3C	401	HEM	CAD-CBD-CGD-O2D
61	3N	402	HEM	CAD-CBD-CGD-O2D
60	B9	201	EHZ	C6-C7-C8-C9
61	3C	402	HEM	CAA-CBA-CGA-O2A
61	3N	401	HEM	CAD-CBD-CGD-O2D
62	3D	401	HEC	CAD-CBD-CGD-O1D
62	3D	401	HEC	CAA-CBA-CGA-O2A
62	3O	401	HEC	CAD-CBD-CGD-O1D
61	3C	401	HEM	CAA-CBA-CGA-O2A
61	3C	401	HEM	CAA-CBA-CGA-O1A
61	3N	401	HEM	CAD-CBD-CGD-O1D
60	a6	201	EHZ	O5-C16-C17-C18
58	A9	501	NDP	PN-O3-PA-O1A
62	3D	401	HEC	CAD-CBD-CGD-O2D
58	A9	501	NDP	C3D-C4D-C5D-O5D
61	3N	402	HEM	CAA-CBA-CGA-O1A
60	5a	701	EHZ	C22-C23-C24-C25
60	B9	201	EHZ	C15-C16-C17-C20
60	a6	201	EHZ	C18-C17-C20-O6
63	v1	501	FMN	N10-C1'-C2'-O2'
61	3N	402	HEM	CAA-CBA-CGA-O2A
62	3D	401	HEC	CAA-CBA-CGA-O1A
58	a9	501	NDP	O4D-C4D-C5D-O5D
62	3O	401	HEC	CAA-CBA-CGA-O2A

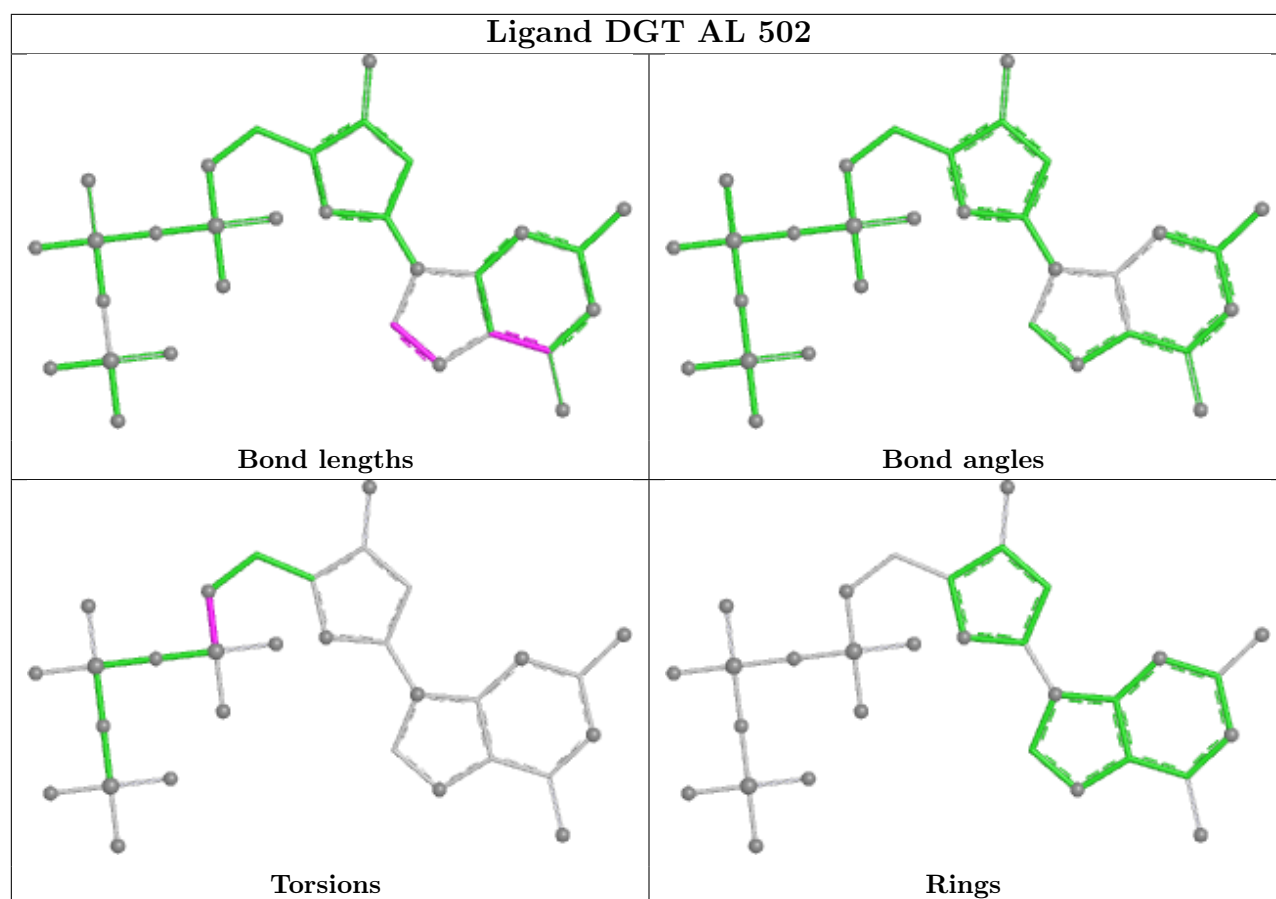
There are no ring outliers.

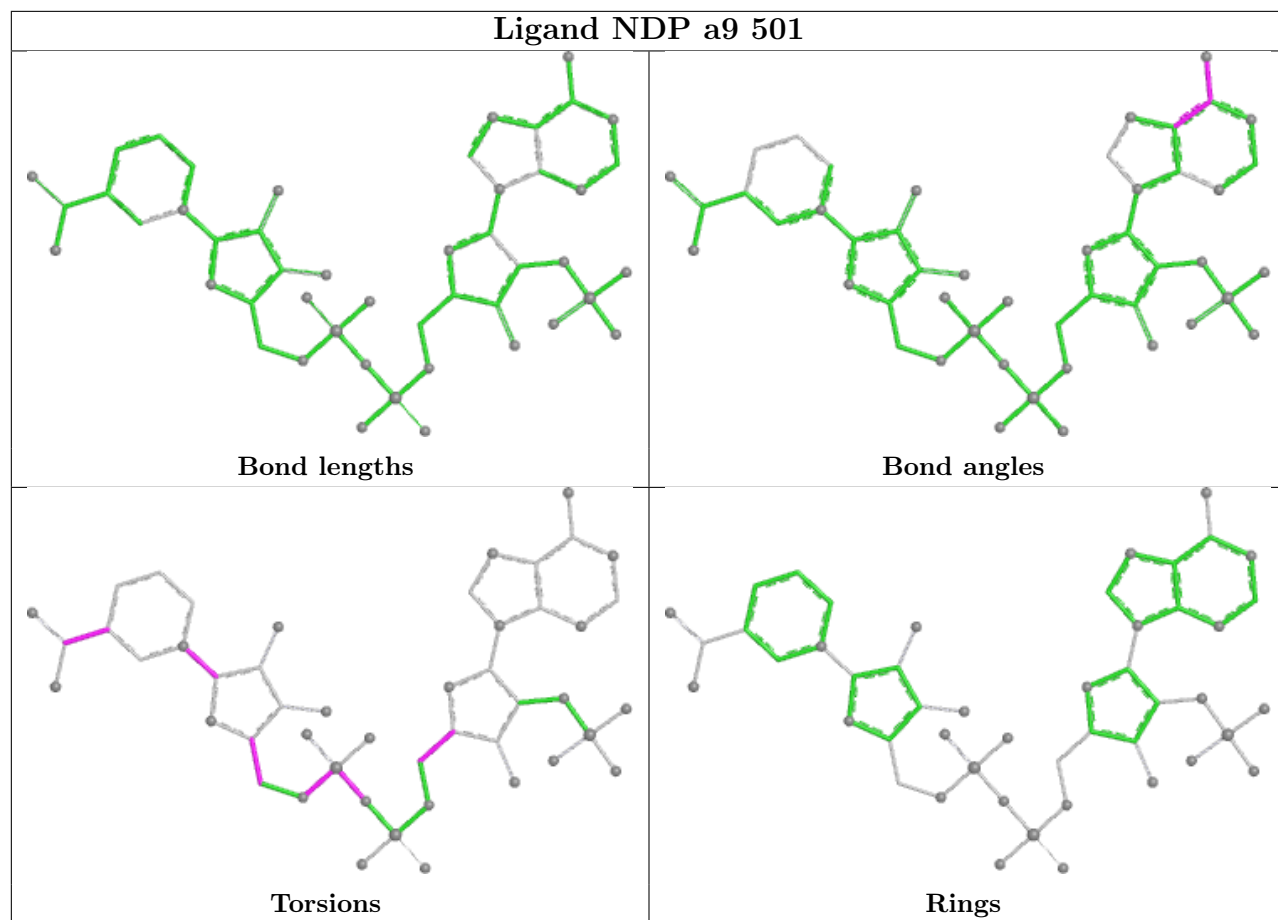
No monomer is involved in short contacts.

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

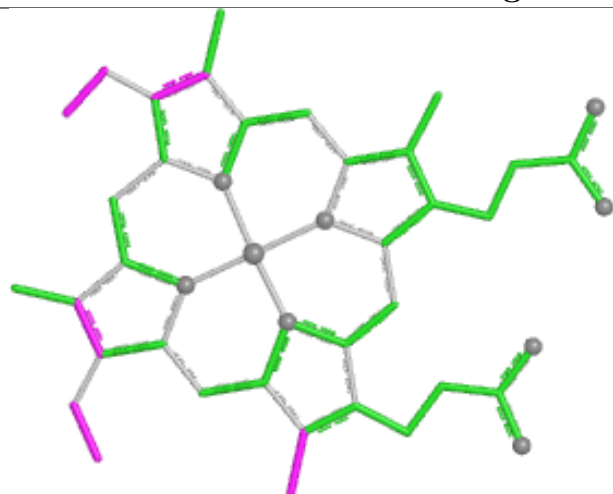




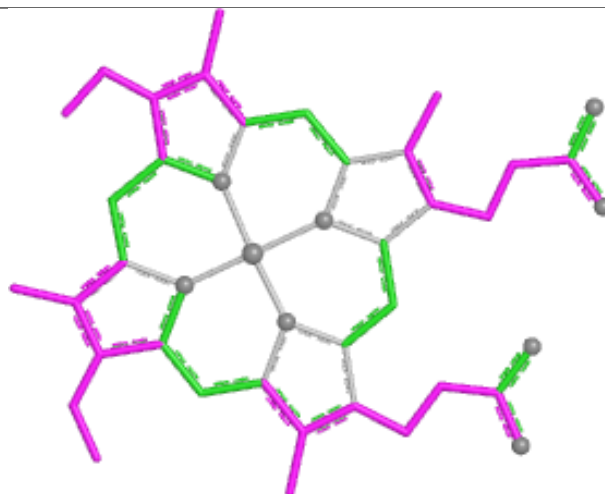




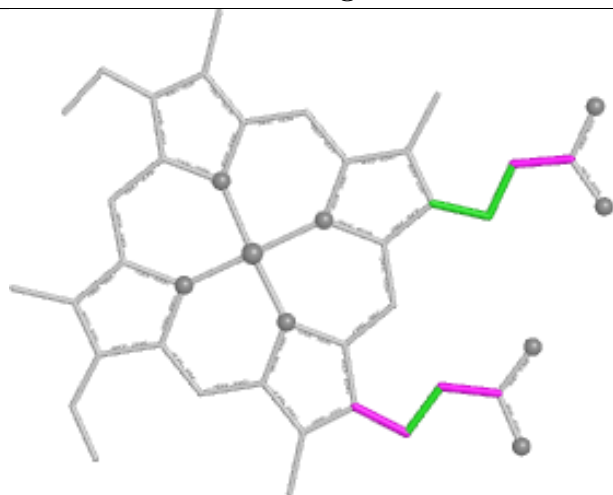
## Ligand HEC 3O 401



Bond lengths



Bond angles

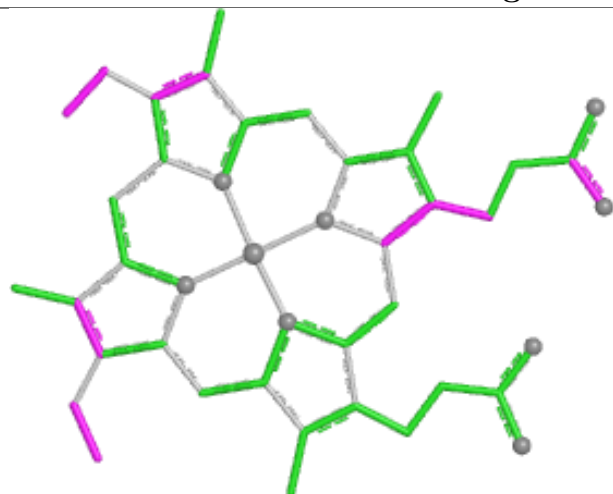


Torsions

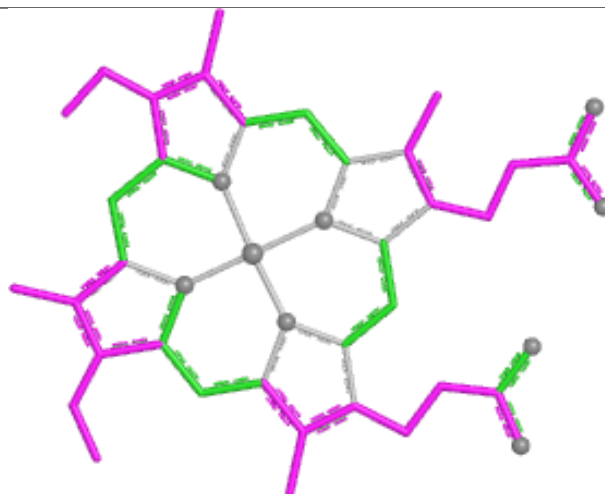


Rings

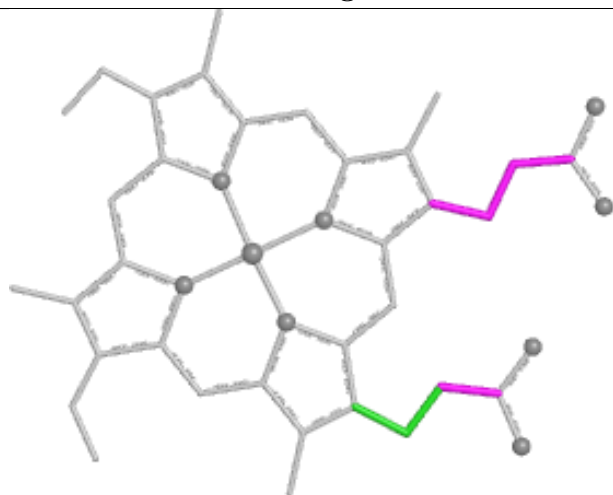
## Ligand HEC 3D 401



Bond lengths



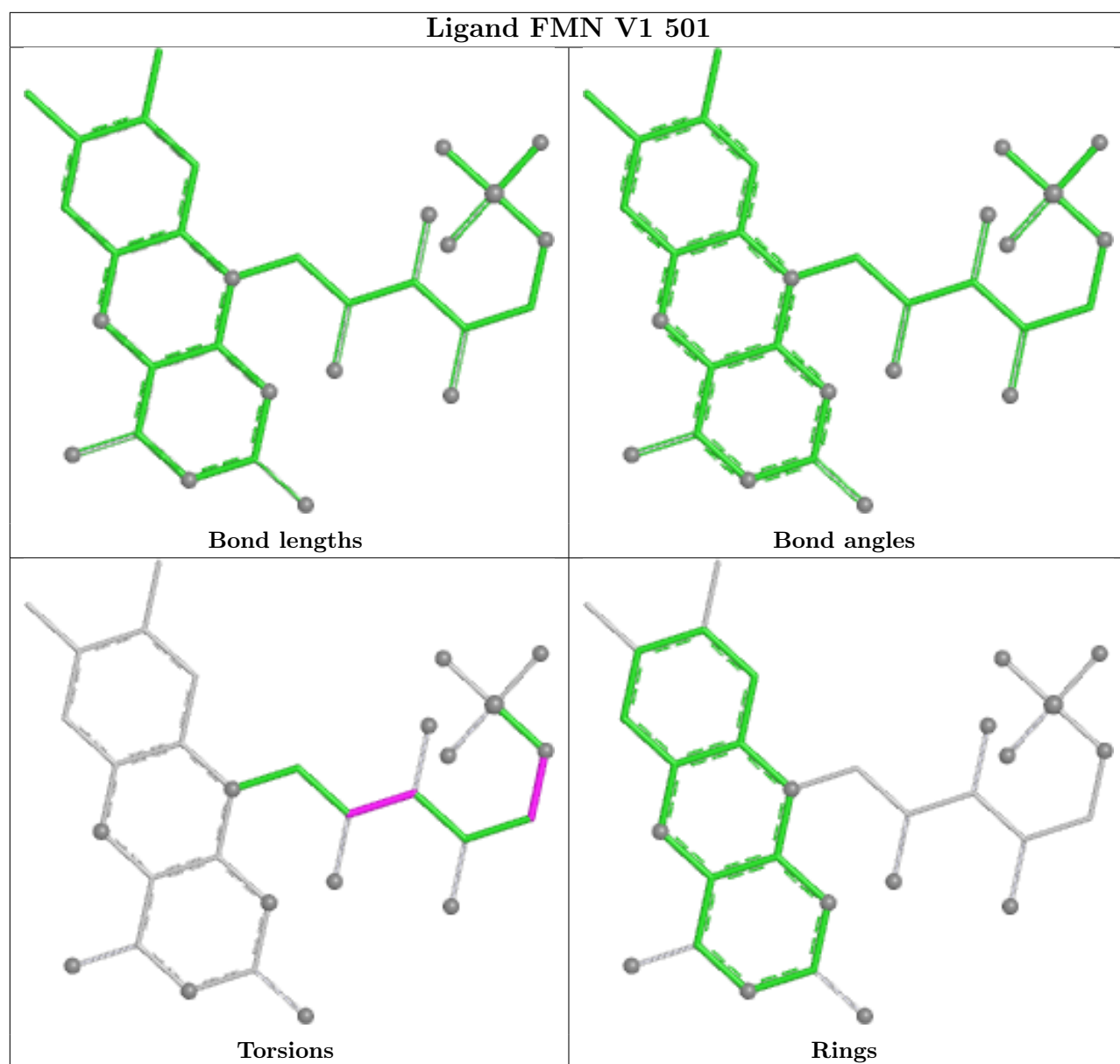
Bond angles



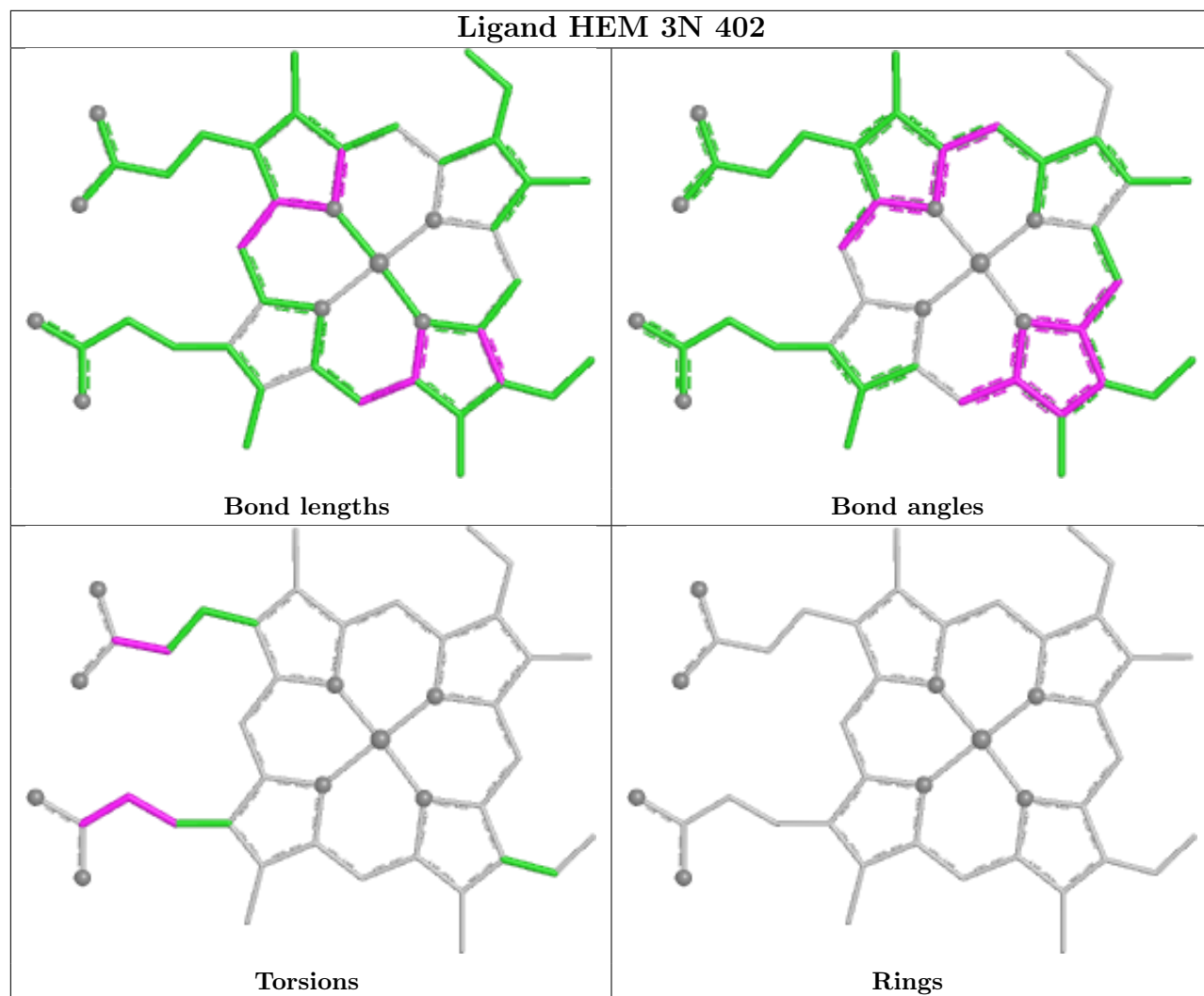
Torsions

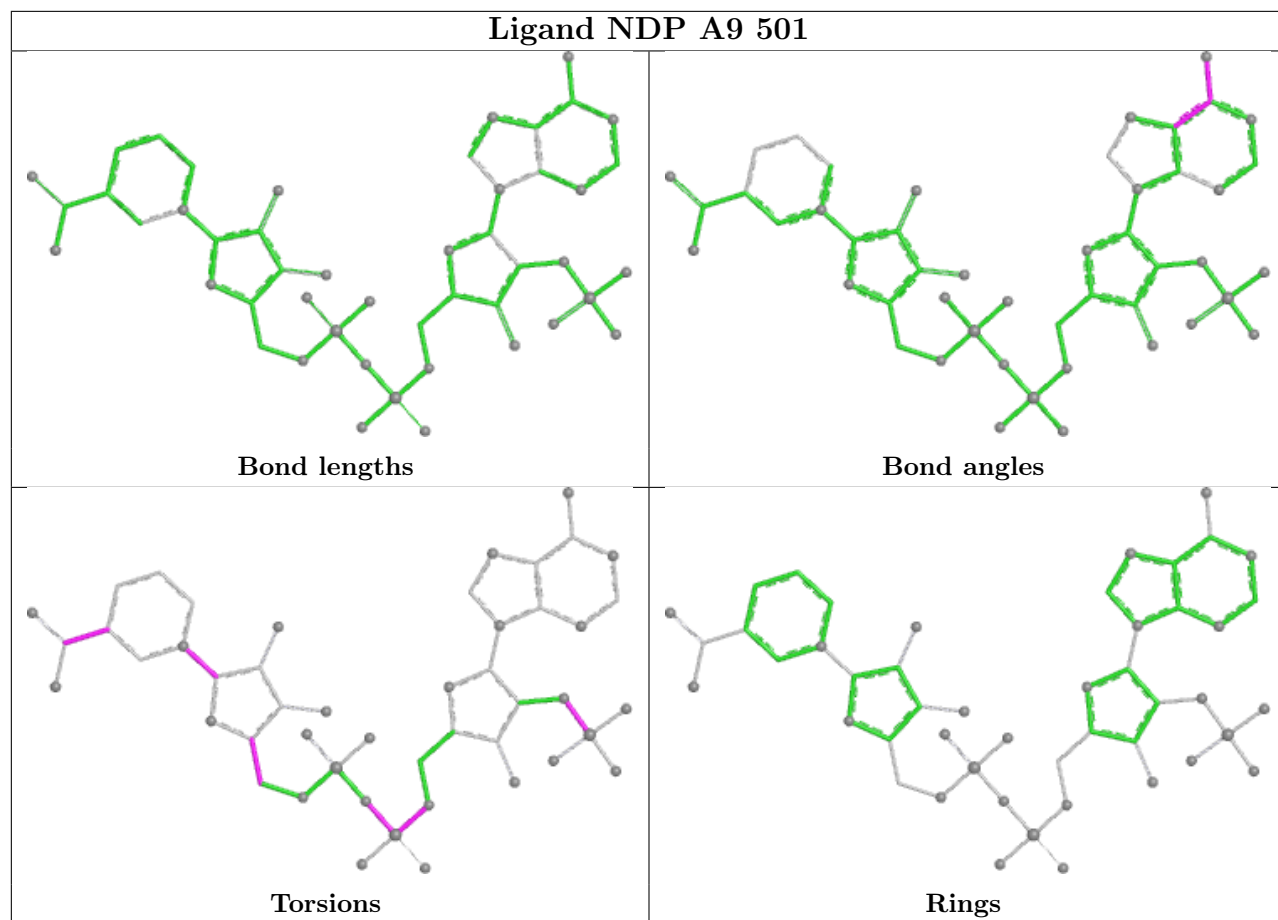


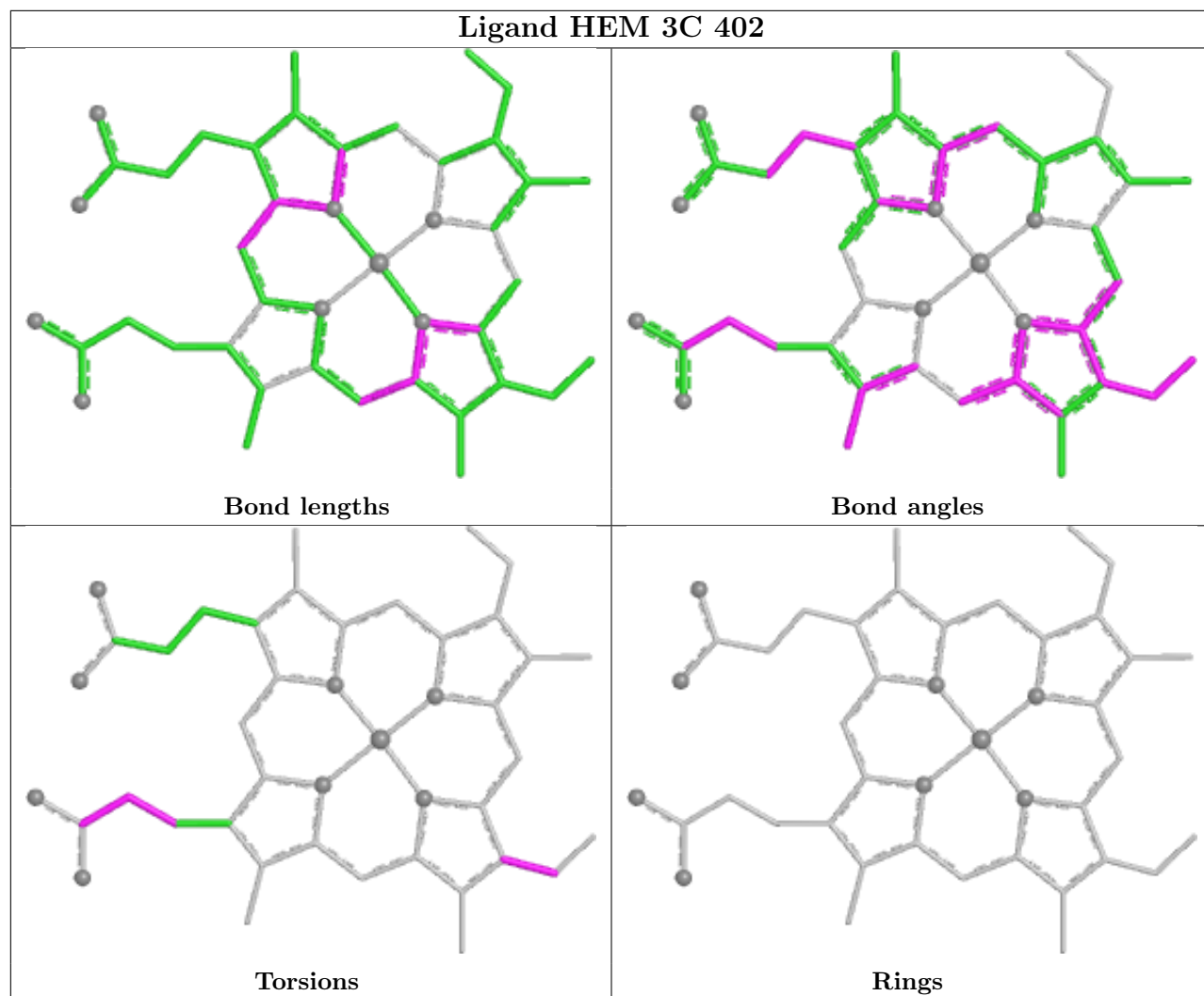
Rings



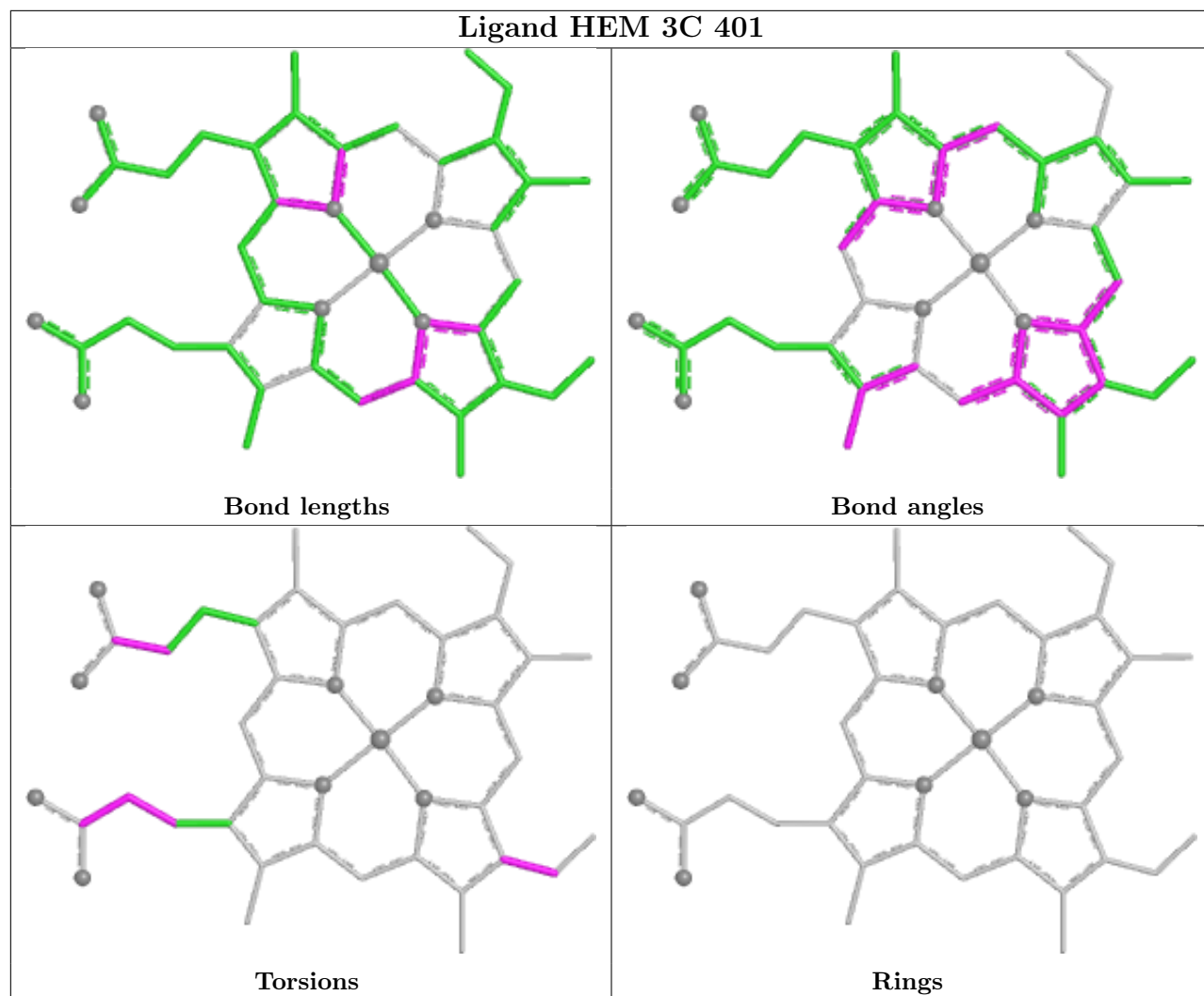
## Ligand HEM 3N 402

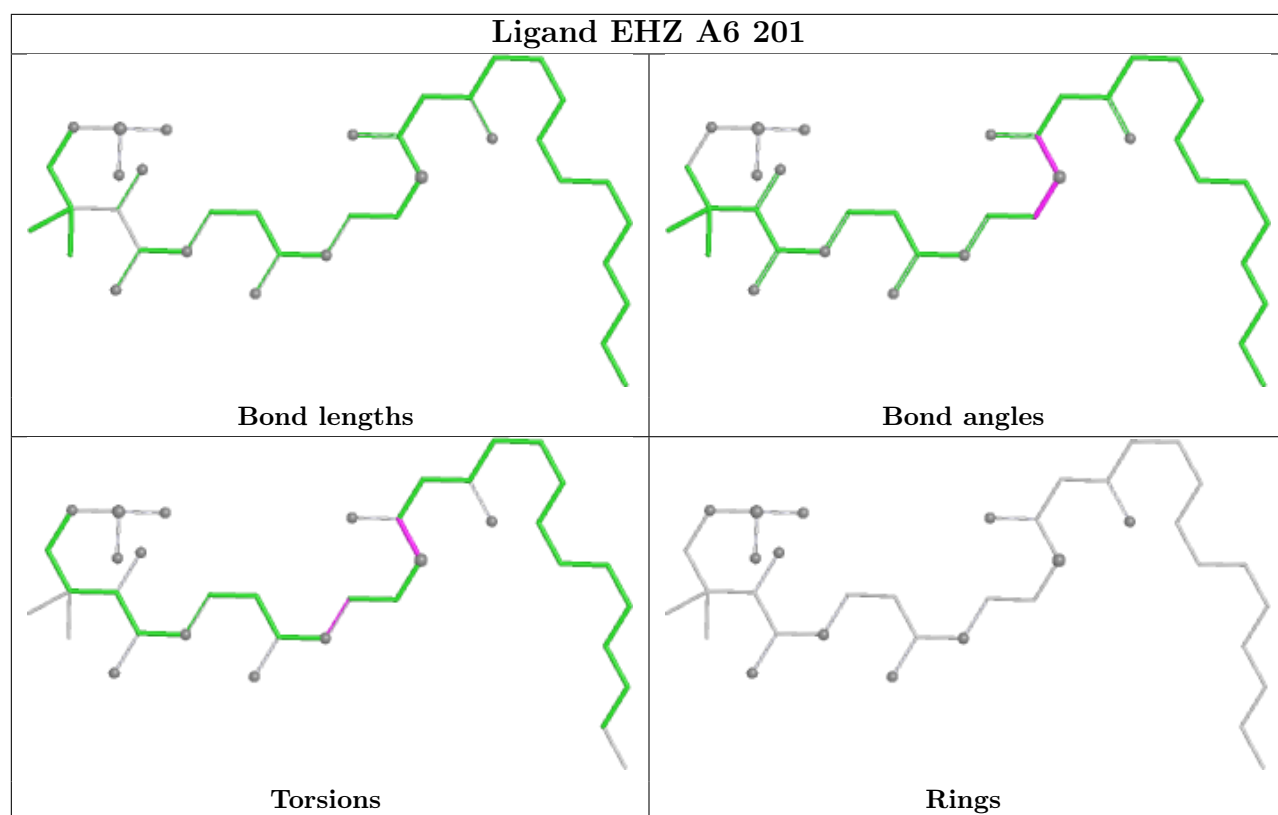






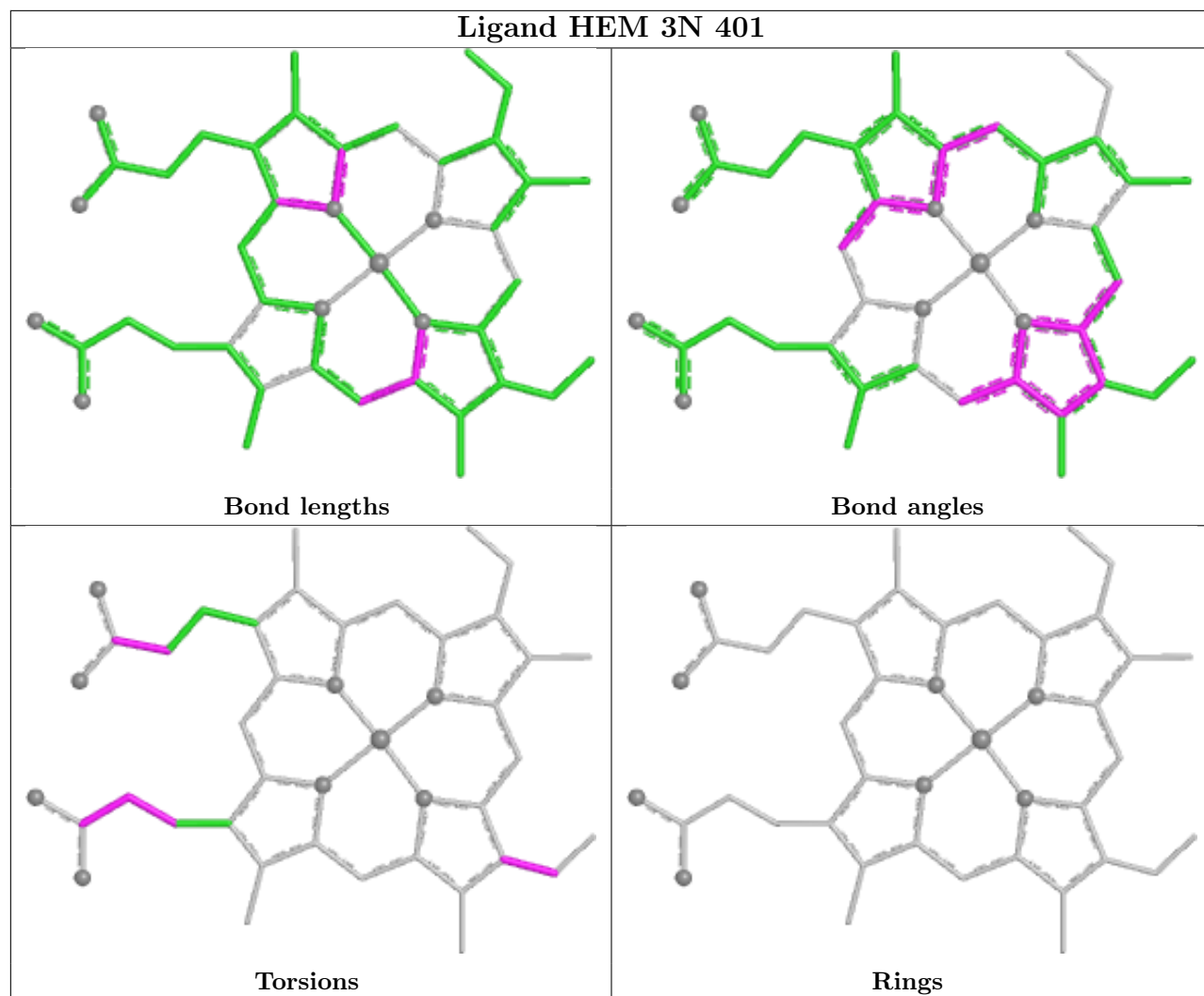
## Ligand HEM 3C 401

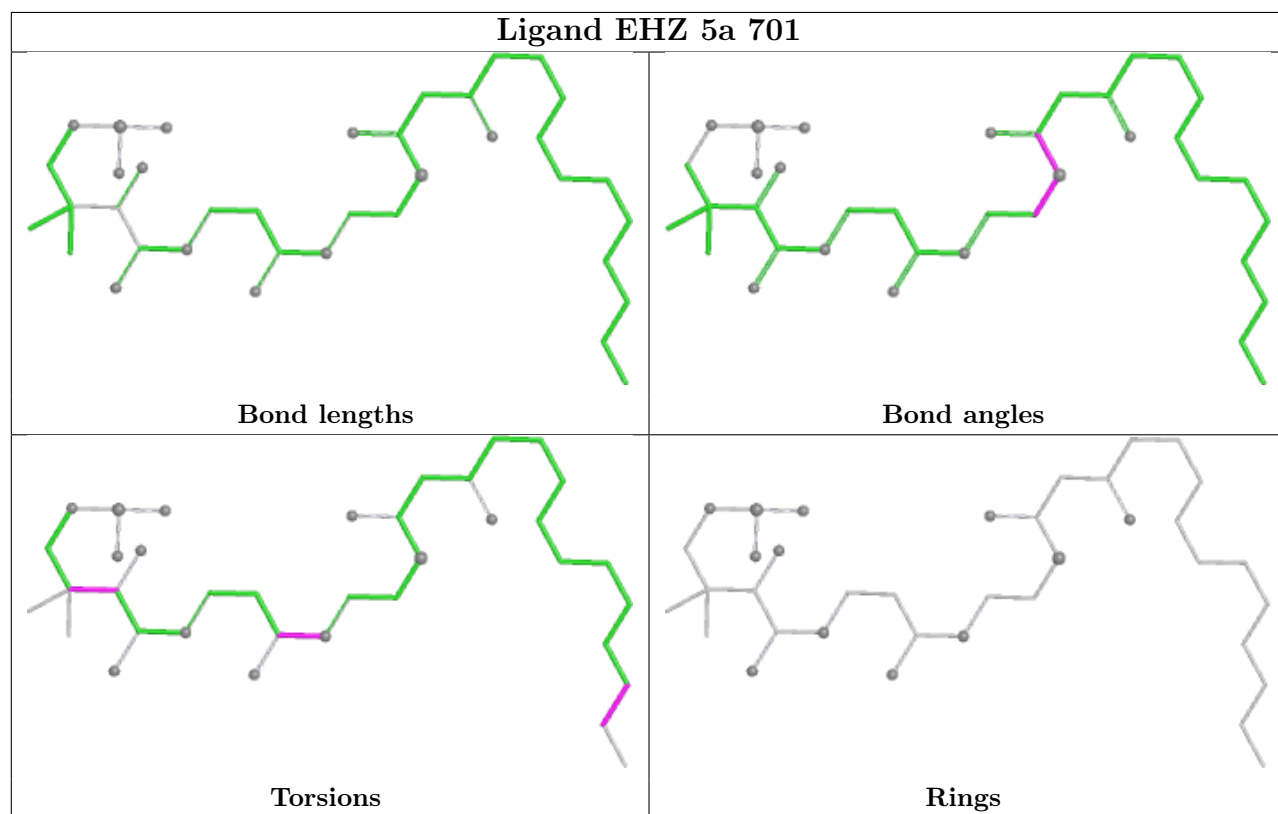
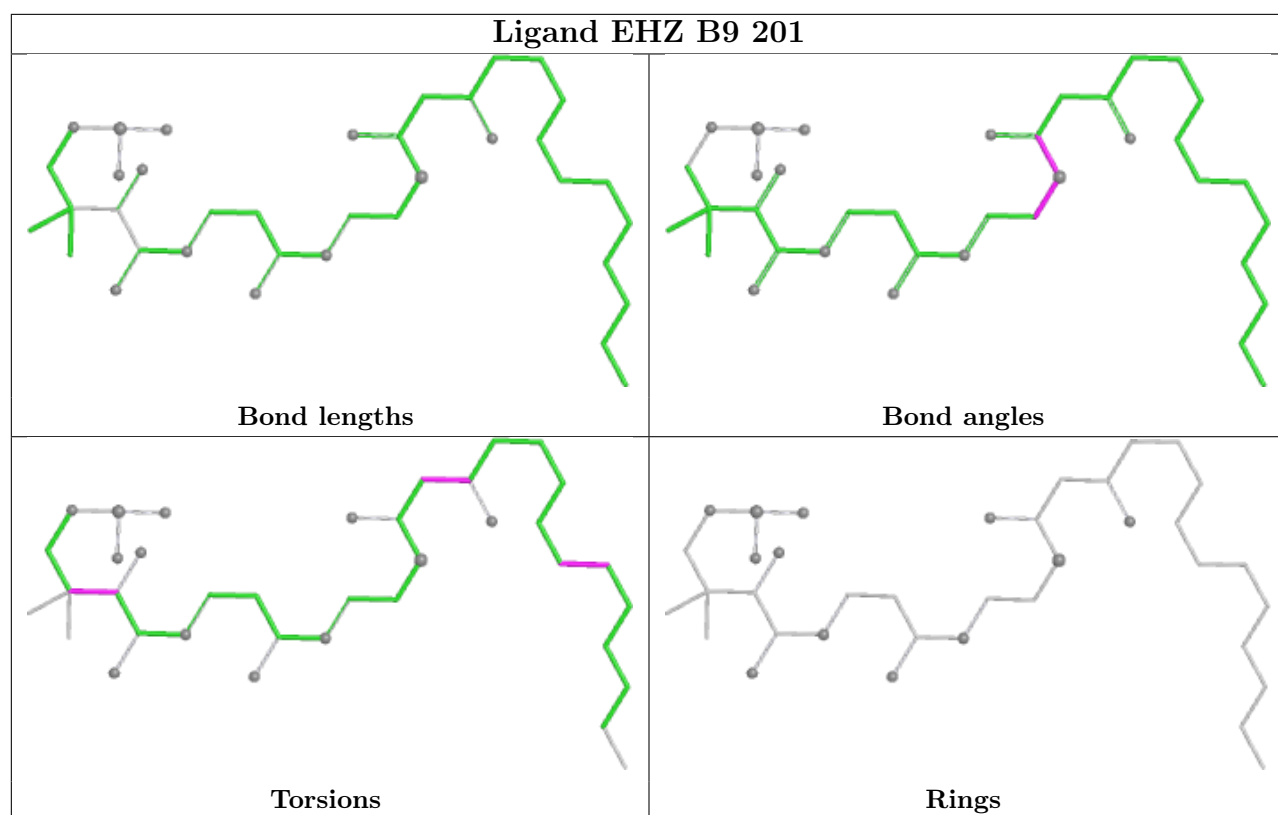


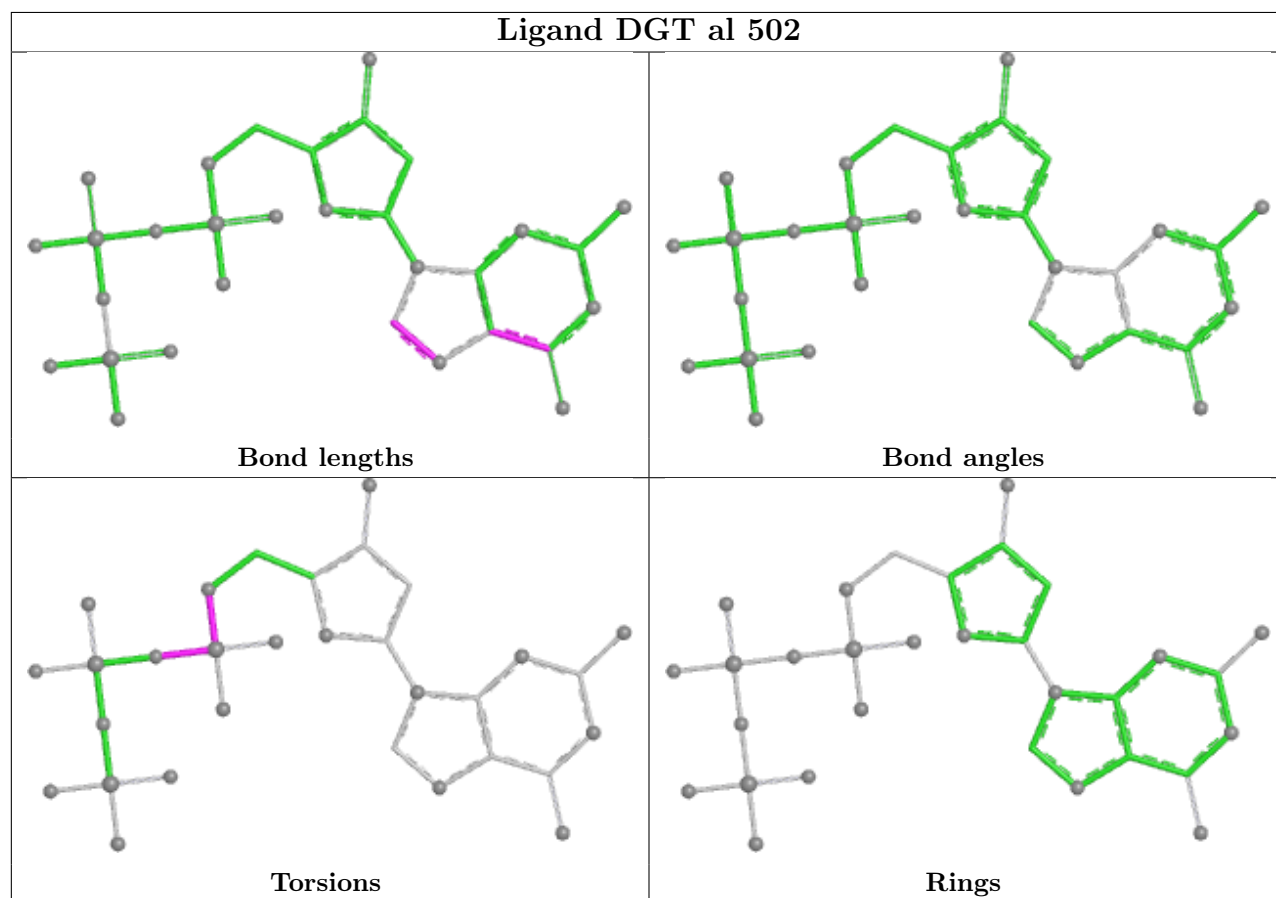
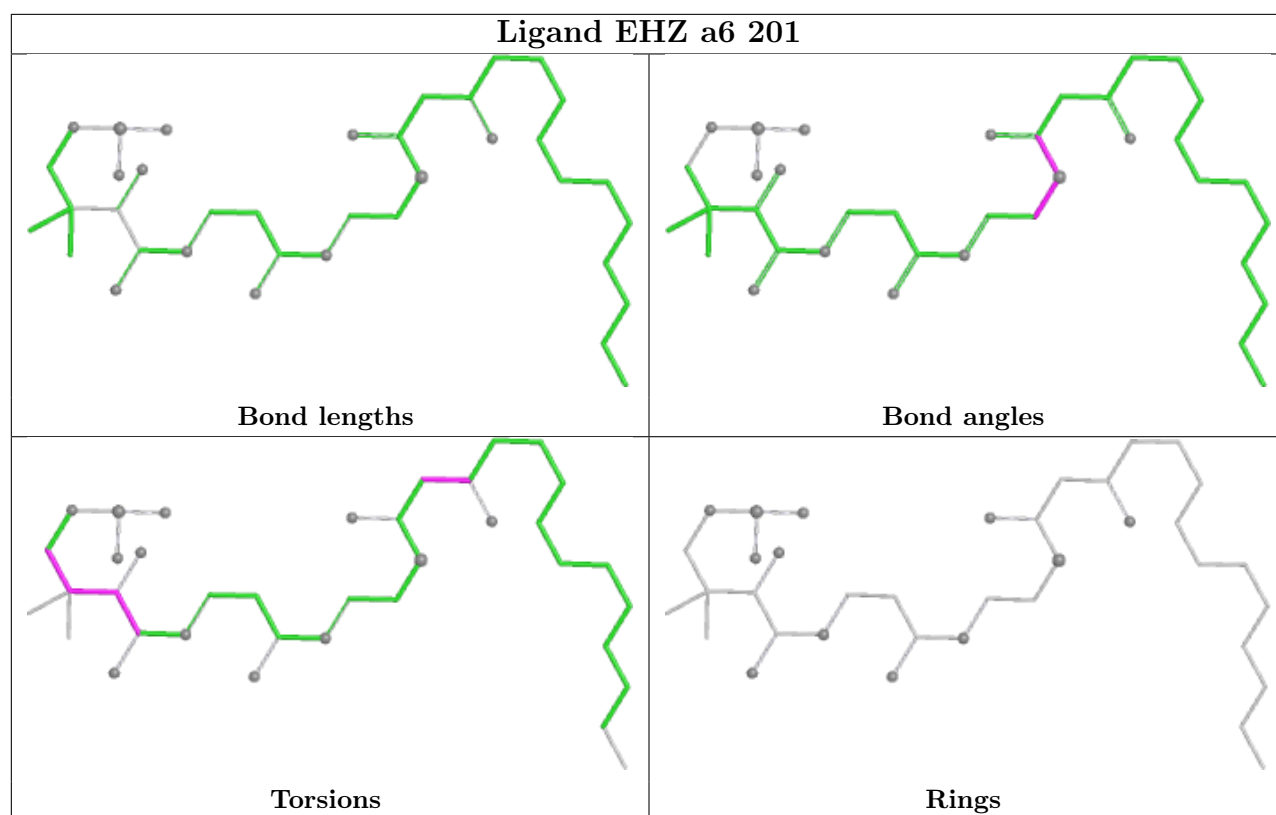




## Ligand HEM 3N 401







## 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.

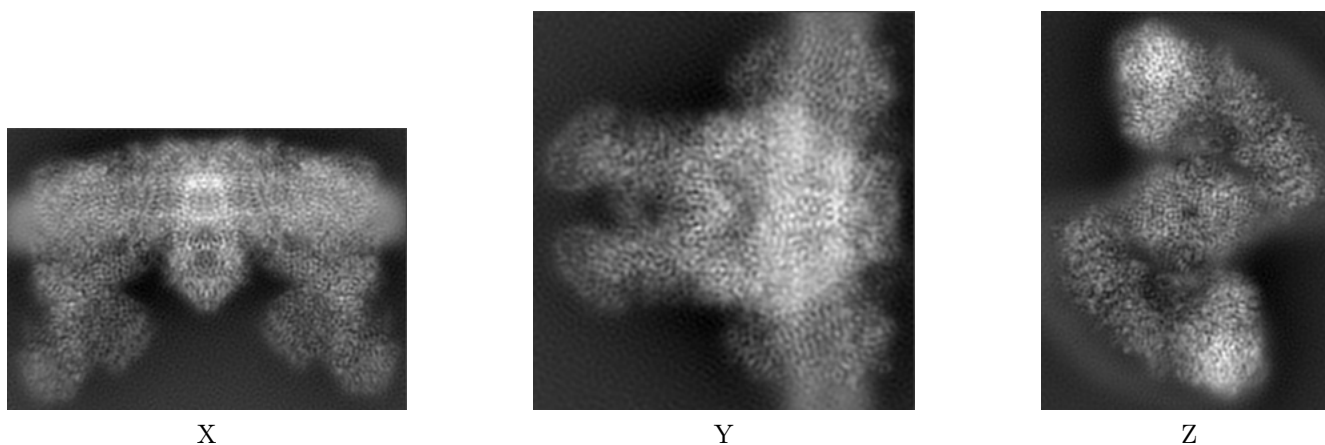
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42122. 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](#)

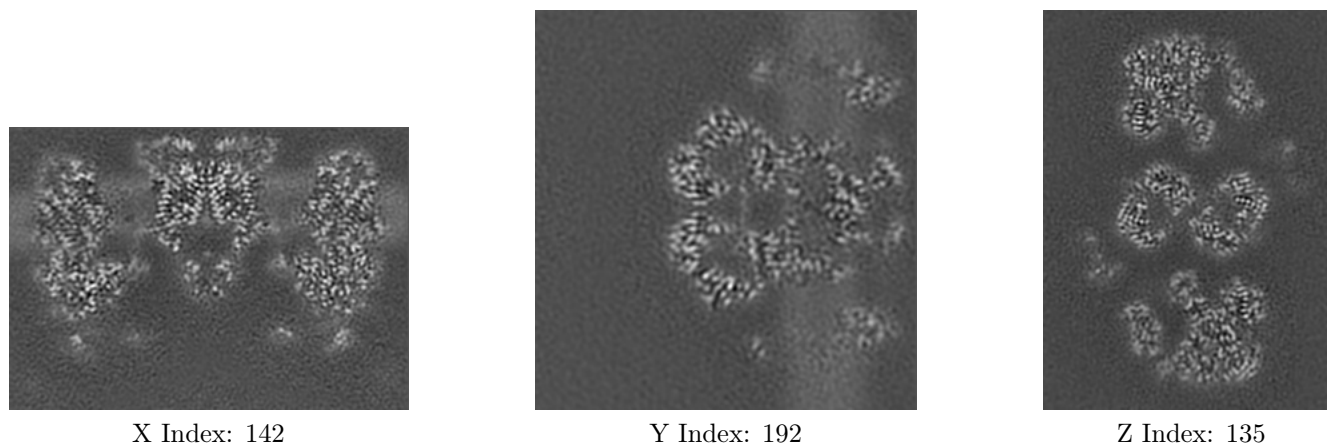
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

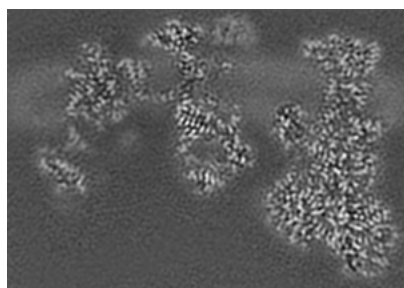
#### 6.2.1 Primary map



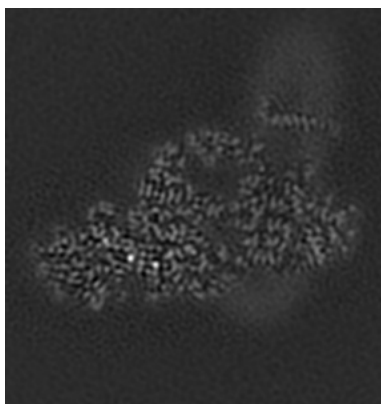
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

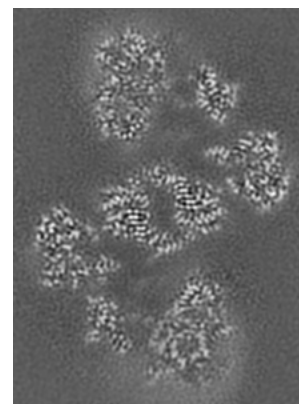
### 6.3.1 Primary map



X Index: 114



Y Index: 323

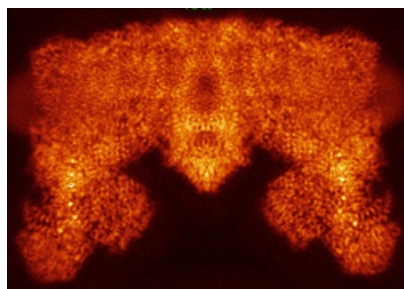


Z Index: 159

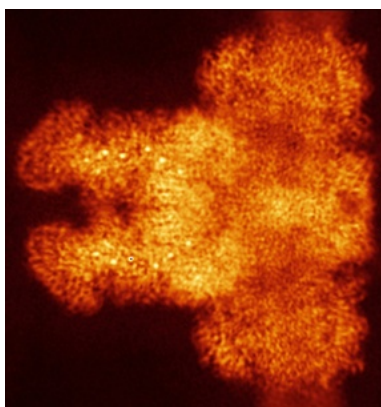
The images above show the largest variance slices of the map in three orthogonal directions.

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

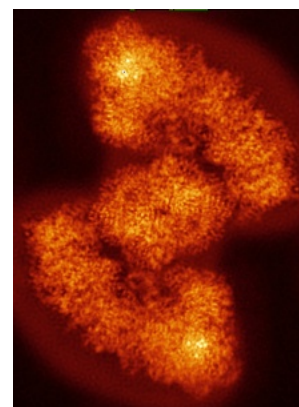
### 6.4.1 Primary map



X



Y

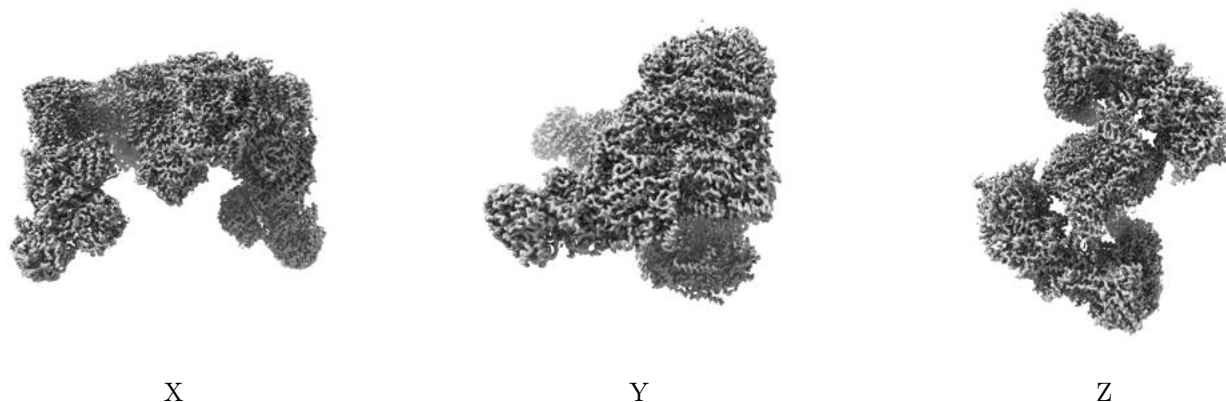


Z

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 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

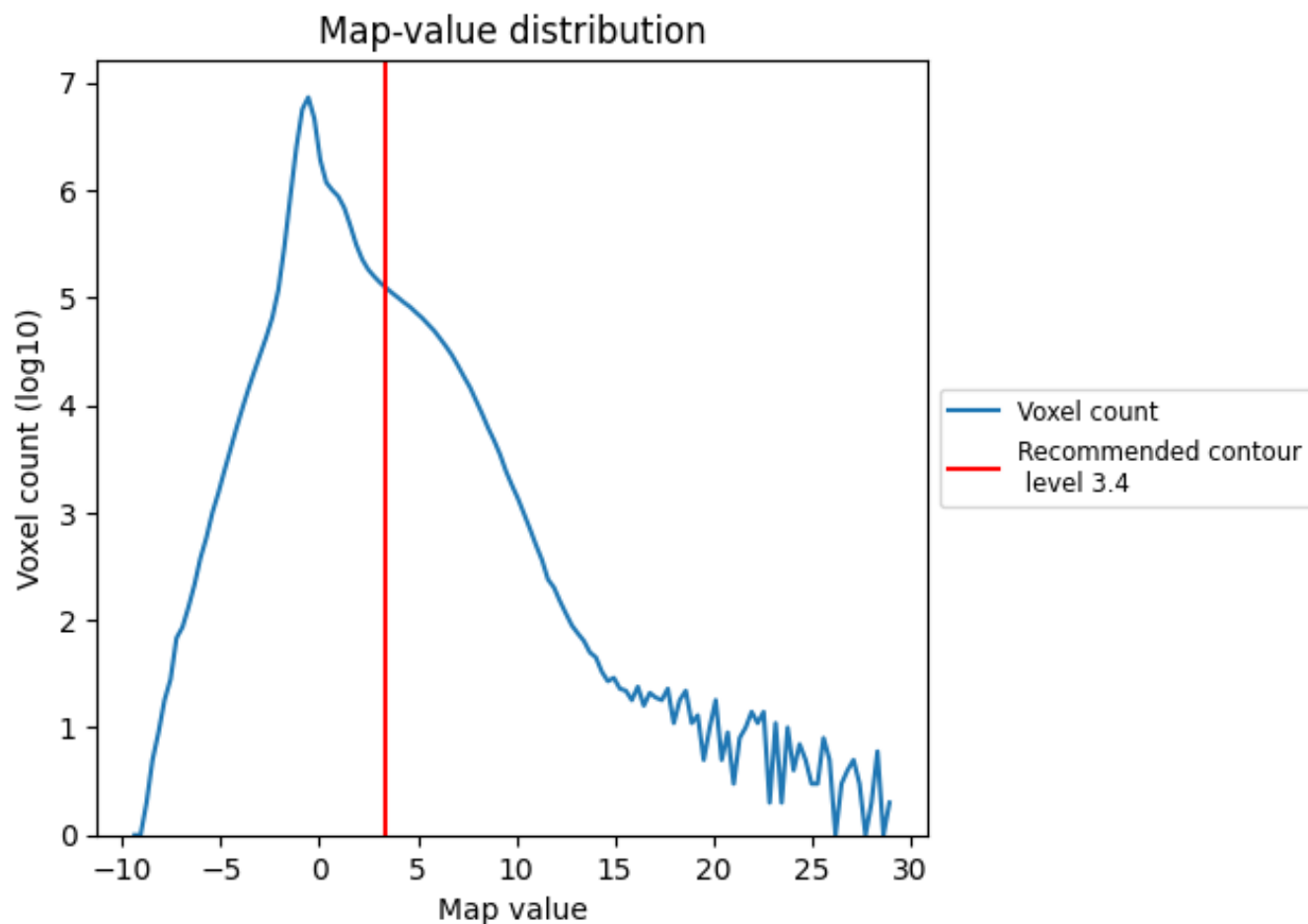
## 6.6 Mask visualisation [i](#)

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.

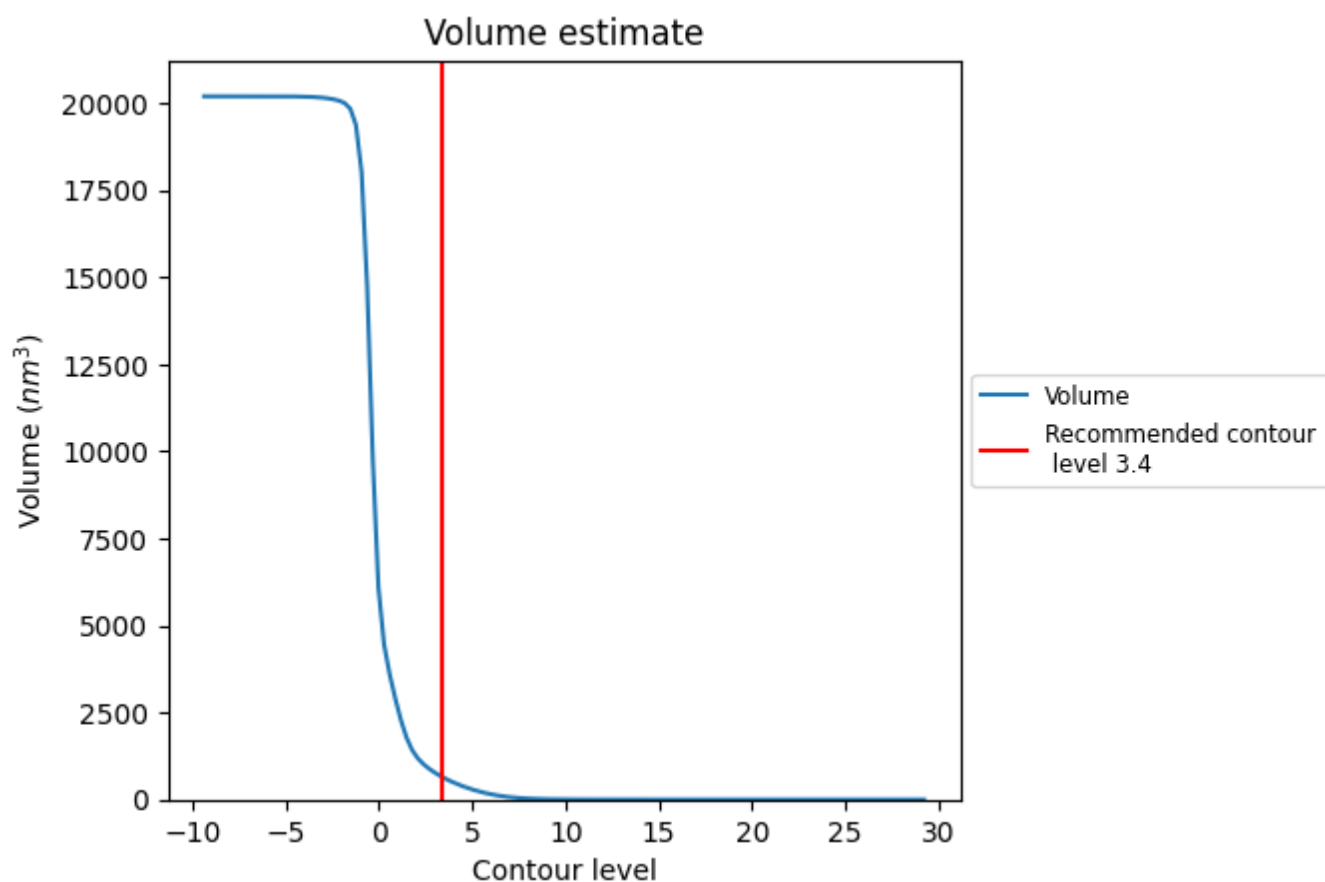
### 7.1 Map-value distribution [i](#)



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 650 nm<sup>3</sup>; this corresponds to an approximate mass of 587 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

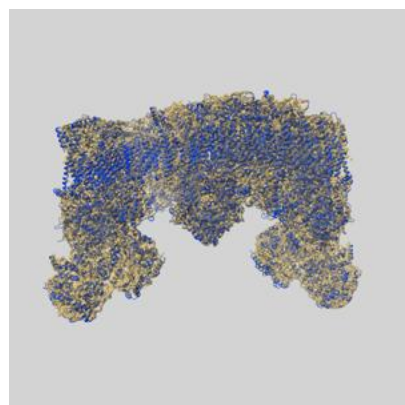
## 8 Fourier-Shell correlation ⓘ

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

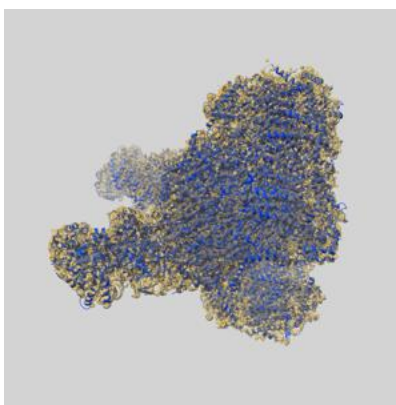
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42122 and PDB model 8UCA. Per-residue inclusion information can be found in section [3](#) on page [26](#).

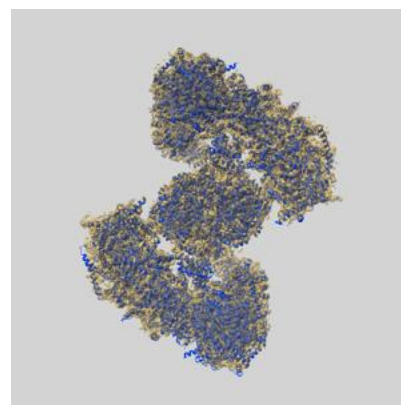
### 9.1 Map-model overlay [i](#)



X



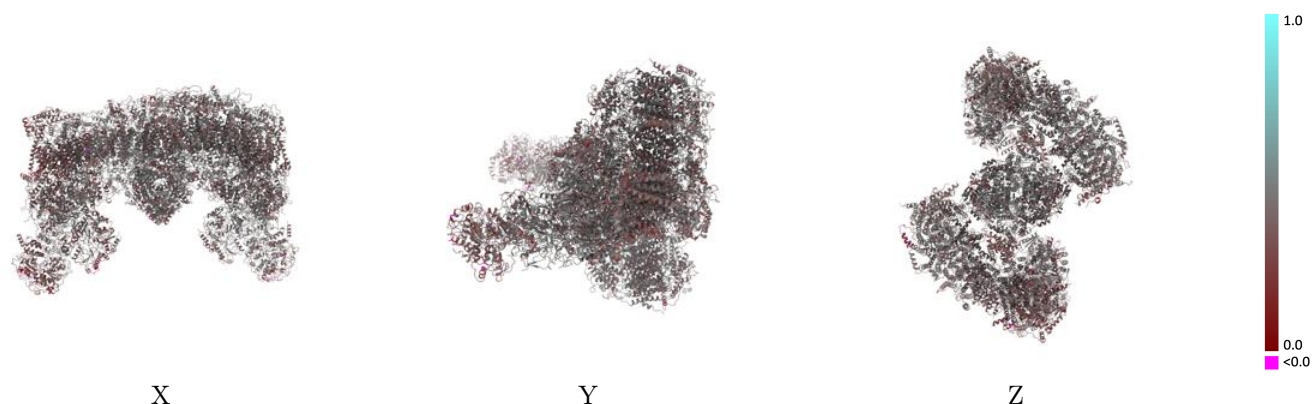
Y



Z

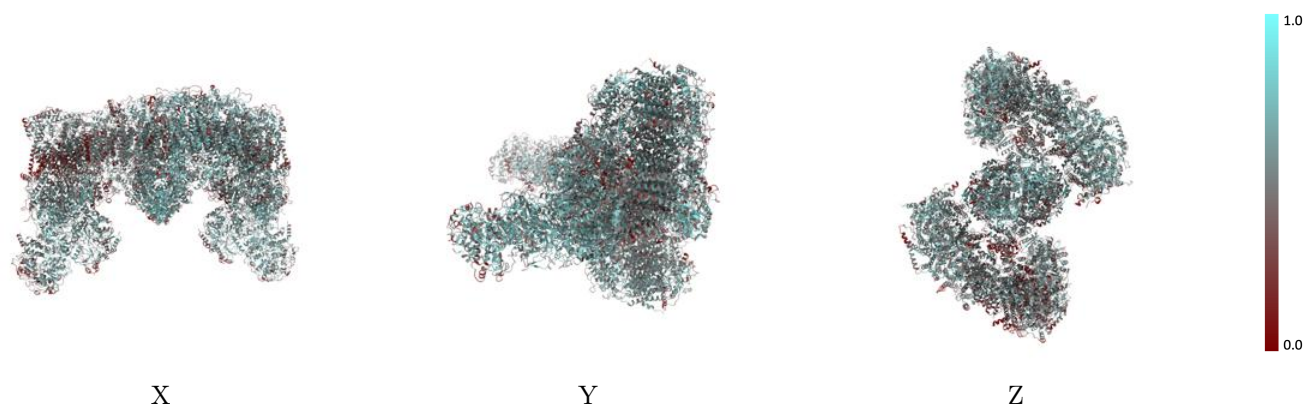
The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



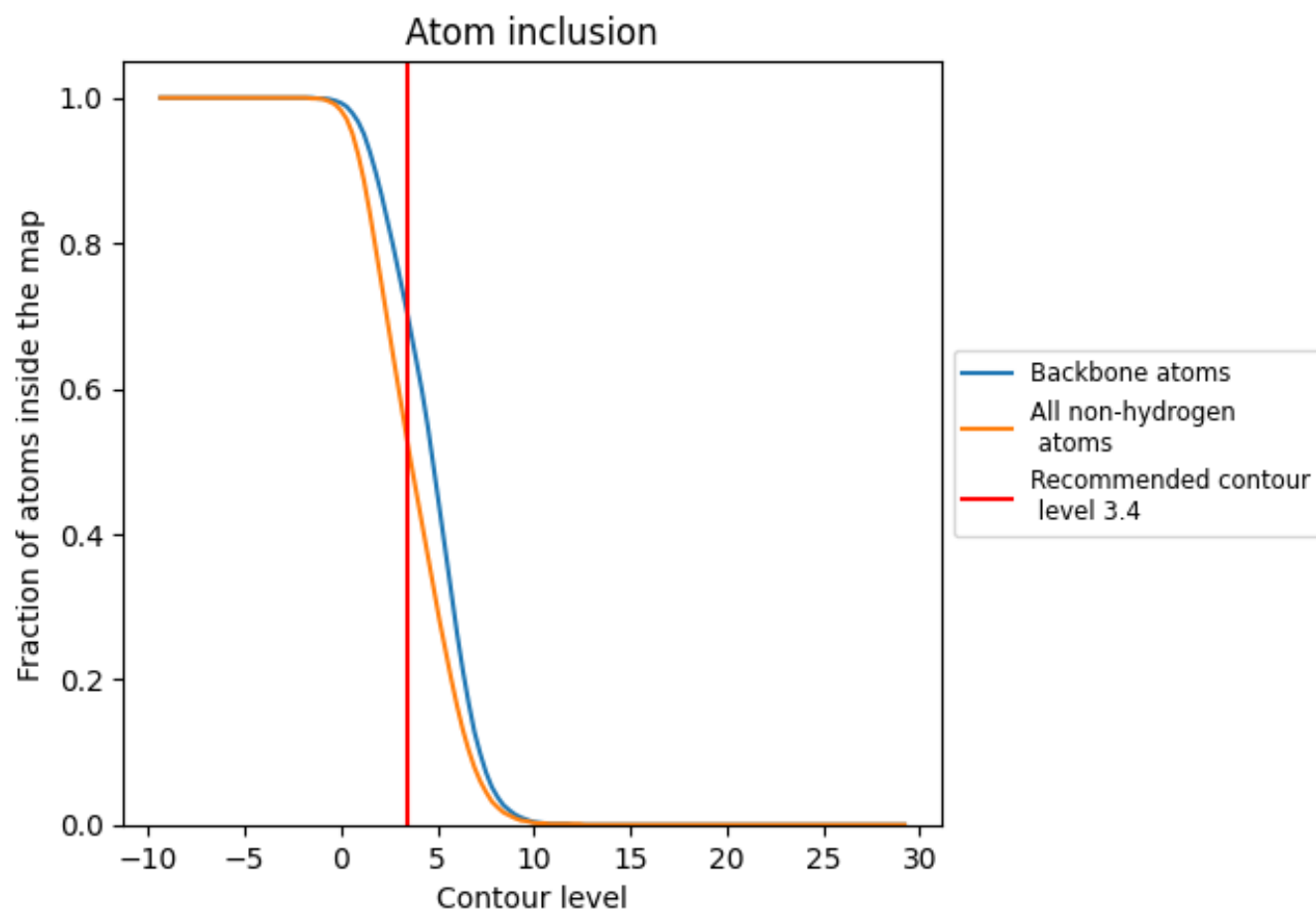
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.4).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.4110
1	 0.5210	 0.4050
1a	 0.3980	 0.3640
2	 0.5480	 0.4290
2a	 0.5150	 0.4220
3	 0.4490	 0.3920
3A	 0.6140	 0.4350
3B	 0.5740	 0.4260
3C	 0.5920	 0.4440
3D	 0.6190	 0.4400
3E	 0.5060	 0.4320
3F	 0.5480	 0.4460
3G	 0.5250	 0.4390
3H	 0.4370	 0.3540
3J	 0.5230	 0.4200
3K	 0.3370	 0.4010
3L	 0.6100	 0.4420
3M	 0.6080	 0.4430
3N	 0.5740	 0.4400
3O	 0.6000	 0.4380
3P	 0.4920	 0.4320
3Q	 0.4910	 0.4430
3R	 0.4900	 0.4270
3S	 0.2980	 0.3010
3T	 0.3250	 0.3810
3U	 0.4510	 0.3890
3V	 0.3610	 0.3500
3a	 0.3660	 0.3720
4	 0.5710	 0.4400
4L	 0.4940	 0.3990
4a	 0.5440	 0.4360
4l	 0.4650	 0.4130
5	 0.5710	 0.4280
5a	 0.5540	 0.4230
6	 0.4030	 0.3940









































































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Chain	Atom inclusion	Q-score
6a	 0.3330	 0.3610
A1	 0.5710	 0.3930
A2	 0.5350	 0.3830
A3	 0.4360	 0.3900
A5	 0.4740	 0.4070
A6	 0.5330	 0.4290
A7	 0.5730	 0.4530
A8	 0.5680	 0.4150
A9	 0.5830	 0.4350
AB	 0.2790	 0.3290
AC	 0.5610	 0.4100
AL	 0.5300	 0.4090
AM	 0.4050	 0.3950
AN	 0.6070	 0.4500
AO	 0.5450	 0.4120
B1	 0.4540	 0.4070
B2	 0.4670	 0.3660
B3	 0.5120	 0.4090
B4	 0.5100	 0.4150
B5	 0.5930	 0.4440
B6	 0.5750	 0.4330
B7	 0.4950	 0.3860
B8	 0.5450	 0.4300
B9	 0.5830	 0.4230
BL	 0.5800	 0.4180
BM	 0.5440	 0.4290
C1	 0.4070	 0.4080
C2	 0.5450	 0.4330
S1	 0.6080	 0.4110
S2	 0.5980	 0.4350
S3	 0.6310	 0.4510
S4	 0.5670	 0.4530
S5	 0.5270	 0.4110
S6	 0.5800	 0.4490
S7	 0.6000	 0.4040
S8	 0.6340	 0.4100
V1	 0.5730	 0.3660
V2	 0.5350	 0.3580
V3	 0.5210	 0.3920
a1	 0.4350	 0.3780
a2	 0.4740	 0.3900
a3	 0.2510	 0.3150

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Chain	Atom inclusion	Q-score
a5	 0.4020	 0.3610
a6	 0.4820	 0.4280
a7	 0.4450	 0.3780
a8	 0.4440	 0.3740
a9	 0.5320	 0.4220
ab	 0.1850	 0.2990
ac	 0.5540	 0.4370
al	 0.4470	 0.3890
am	 0.3710	 0.3860
an	 0.5170	 0.4170
ao	 0.4310	 0.3790
b1	 0.3650	 0.3860
b2	 0.5240	 0.4110
b3	 0.5820	 0.4150
b4	 0.5010	 0.4210
b5	 0.5430	 0.4240
b6	 0.5630	 0.4360
b7	 0.5070	 0.3960
b8	 0.5220	 0.4340
b9	 0.5740	 0.4340
bl	 0.5090	 0.3970
bm	 0.5130	 0.4180
c1	 0.3390	 0.3770
c2	 0.4940	 0.4180
s1	 0.5610	 0.3800
s2	 0.5210	 0.4040
s3	 0.5670	 0.4270
s4	 0.5520	 0.4300
s5	 0.4720	 0.4000
s6	 0.5510	 0.4290
s7	 0.5790	 0.3810
s8	 0.5730	 0.3740
v1	 0.4820	 0.3250
v2	 0.5020	 0.3540
v3	 0.5320	 0.3610