



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 08:57 AM UTC

PDB ID : 7DGR / pdb_00007dgr
EMDB ID : EMD-30674
Title : Activity optimized supercomplex state2
Authors : Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on : 2020-11-12
Resolution : 4.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

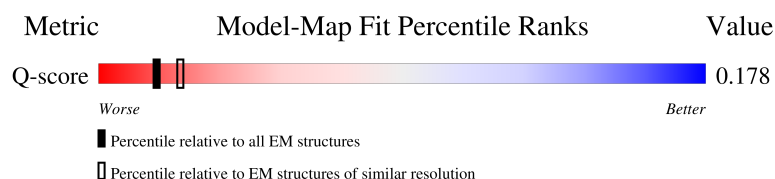
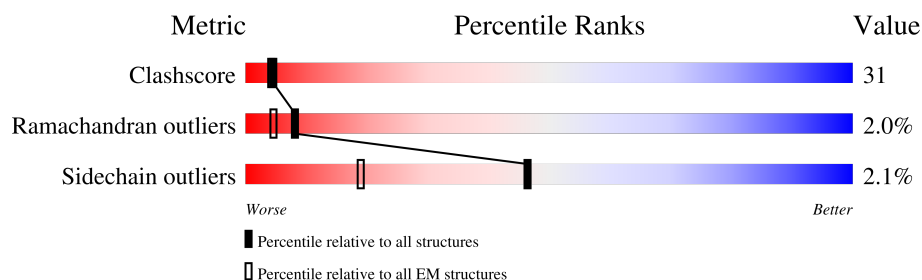
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



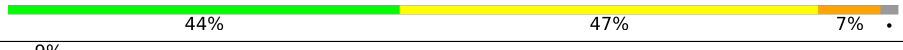
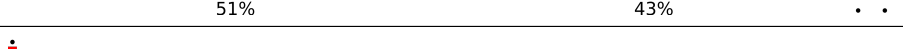
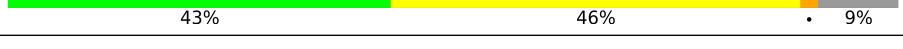
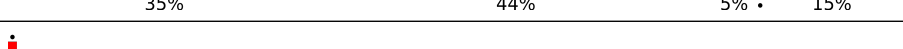
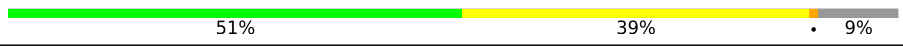
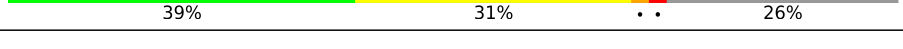
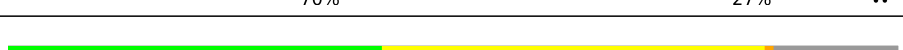
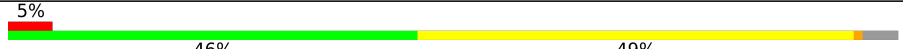
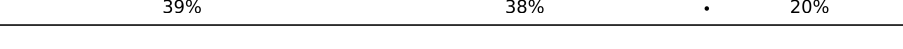
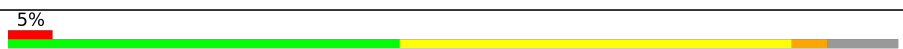
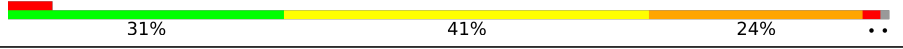
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	9	217	
2	4	459	
3	2	347	
4	7	175	

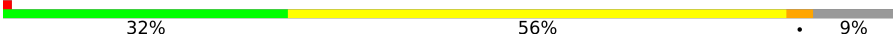
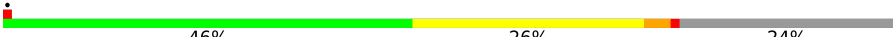
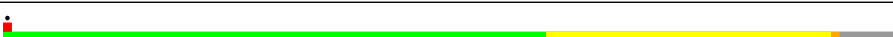
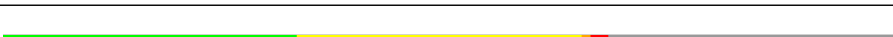
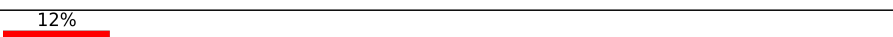
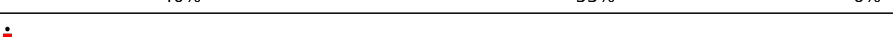
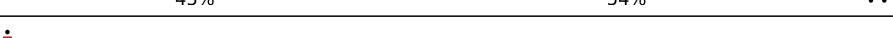
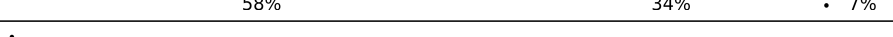
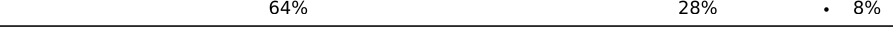
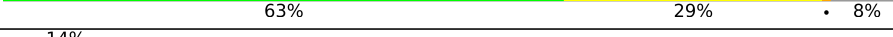
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Mol	Chain	Length	Quality of chain
5	6	606	
6	5	98	
7	3	115	
8	1	318	
9	8	444	
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	

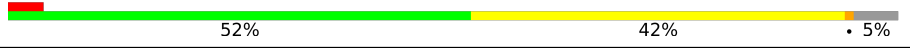
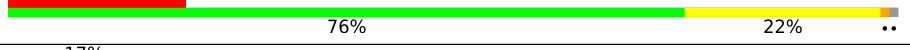
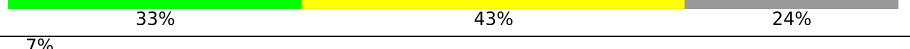
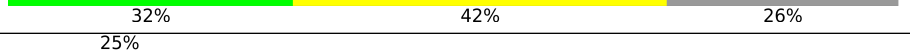
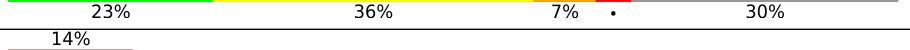
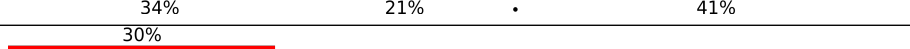
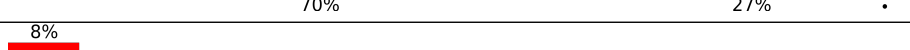
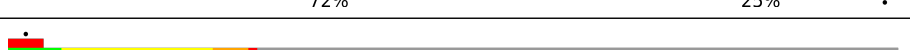
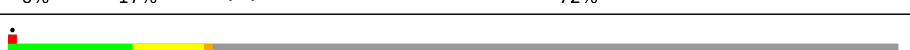
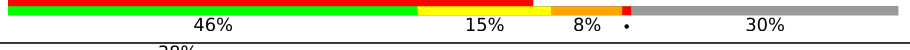
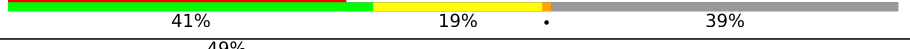
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Mol	Chain	Length	Quality of chain
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	
34	Z	98	
35	a	128	
36	b	143	
37	c	128	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	241	
48	z	241	
49	A0	196	

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Mol	Chain	Length	Quality of chain
49	p	196	
50	A1	111	
50	q	111	
51	A2	82	
51	r	82	
52	B3	91	
52	s	91	
53	A3	56	
53	t	56	
54	B2	64	
54	u	64	
55	B1	78	
55	v	78	
56	A9	514	
57	C4	227	
58	C2	261	
59	A7	169	
60	C0	152	
61	A6	129	
62	A4	97	
63	A5	86	
64	B4	74	
65	C3	80	
66	B0	80	
67	C1	63	

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Mol	Chain	Length	Quality of chain
68	A8	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	FES	A	803	-	-	X	-
70	3PE	4	501	-	-	X	-
70	3PE	4	503	-	-	X	-
70	3PE	B	501	-	-	X	-
71	CDL	4	502	-	-	X	-
71	CDL	6	701	-	-	X	-
72	PC1	2	402	-	-	X	-
72	PC1	L	200	-	-	X	-
73	FMN	8	501	-	-	X	-
74	SF4	8	502	-	-	X	-
74	SF4	A	801	-	-	X	-
74	SF4	A	802	-	-	X	-
74	SF4	D	301	-	-	X	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 107305 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 dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	9	207	Total	C	N	O	S	0	0
			1578	1006	269	293	10		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	458	Total	C	N	O	S	1	0
			3577	2382	561	599	35		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	344	Total	C	N	O	S	0	0
			2681	1779	413	449	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	172	Total	C	N	O	S	0	0
			1239	838	182	211	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	606	Total	C	N	O	S	0	0
			4766	3172	732	820	42		

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

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

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3	112	Total	C	N	O	S	0	0
			879	593	128	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	318	Total	C	N	O	S	0	0
			2503	1678	385	417	23		

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

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

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	71	Total	C	N	O	S	0	0
			533	332	99	99	3		

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

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

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

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

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 7.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	319	Total	C	N	O	S	0	0
			2407	1548	431	425	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	138	Total	C	N	O	S	0	0
			923	586	163	168	6		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 31 is a protein called Acyl carrier protein, mitochondrial.

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

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

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

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

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	107	Total	C	N	O	S	0	0
			713	448	134	127	4		

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

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	113	Total	C	N	O	S	0	0
			883	580	149	151	3		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	446	Total	C	N	O	S	0	0
			3454	2159	608	667	20		
45	w	436	Total	C	N	O	S	0	0
			3385	2117	599	649	20		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

- Molecule 47 is a protein called Cytochrome b.

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

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	151	Total	C	N	O	S	0	0
			938	572	170	194	2		
49	A0	188	Total	C	N	O	S	0	0
			1117	679	207	229	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
50	A1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
51	A2	81	Total	C	N	O	S	0	0
			676	438	125	112	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	67	Total	C	N	O	S	0	0
			548	332	99	112	5		
52	B3	69	Total	C	N	O	S	0	0
			566	342	101	118	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	33	Total	C	N	O	0	0
			262	174	46	42		
53	A3	39	Total	C	N	O	0	0
			318	212	56	50		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	u	62	Total	C	N	O	0	0
			511	335	89	87		
54	B2	62	Total	C	N	O	0	0
			511	335	89	87		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
55	v	18	Total	C	N	O	0	0
			114	70	22	22		

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Mol	Chain	Residues	Atoms				AltConf	Trace
55	B1	22	Total	C	N	O	0	0
			148	91	30	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A9	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	C4	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C2	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	C0	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	A6	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	A4	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	A5	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	B4	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	C3	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	B0	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

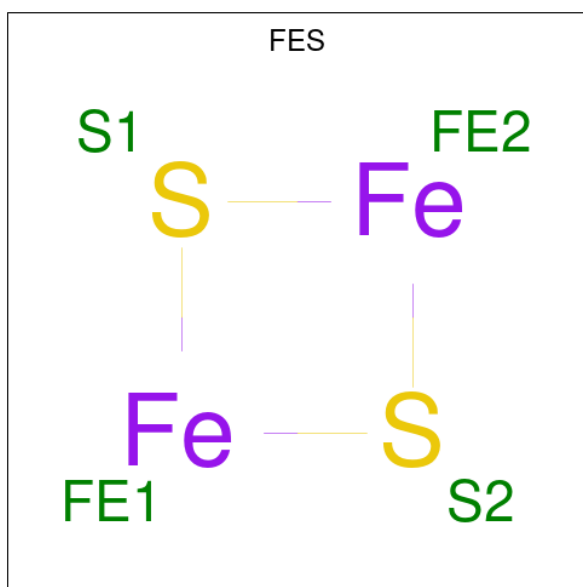
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	C1	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

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

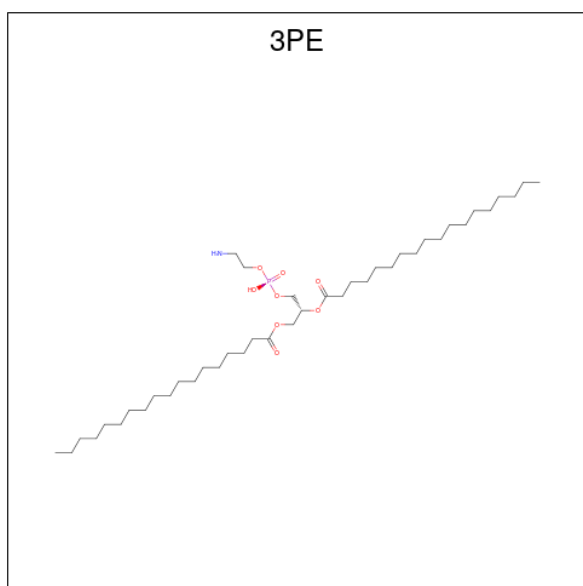
Mol	Chain	Residues	Atoms				AltConf	Trace
68	A8	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



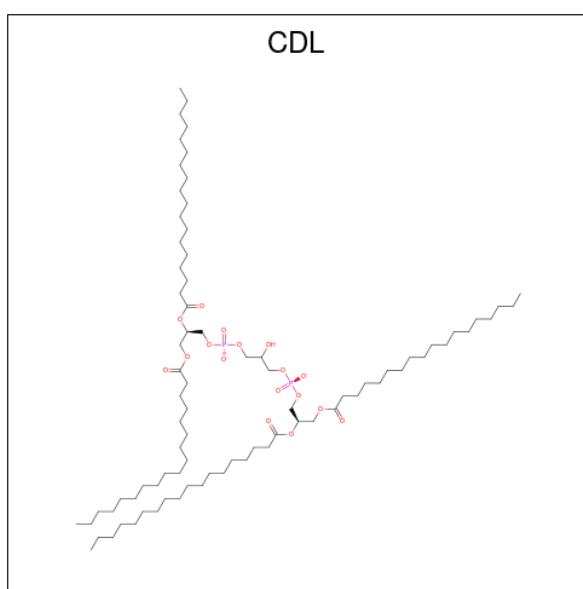
Mol	Chain	Residues	Atoms			AltConf
69	9	1	Total	Fe	S	0
			4	2	2	
69	A	1	Total	Fe	S	0
			4	2	2	
69	m	1	Total	Fe	S	0
			4	2	2	

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



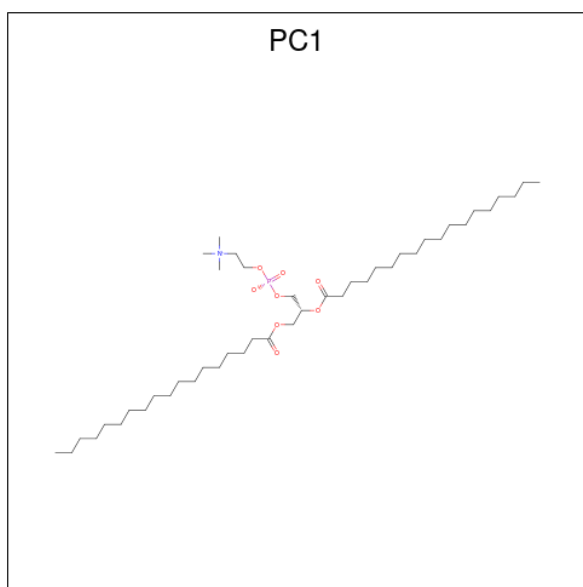
Mol	Chain	Residues	Atoms					AltConf
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 71 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



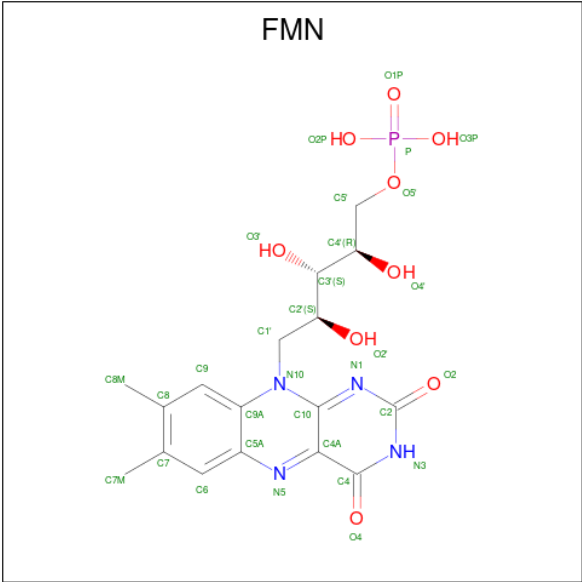
Mol	Chain	Residues	Atoms				AltConf
71	4	1	Total	C	O	P	0
			82	63	17	2	
71	6	1	Total	C	O	P	0
			64	45	17	2	
71	J	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 72 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
72	4	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



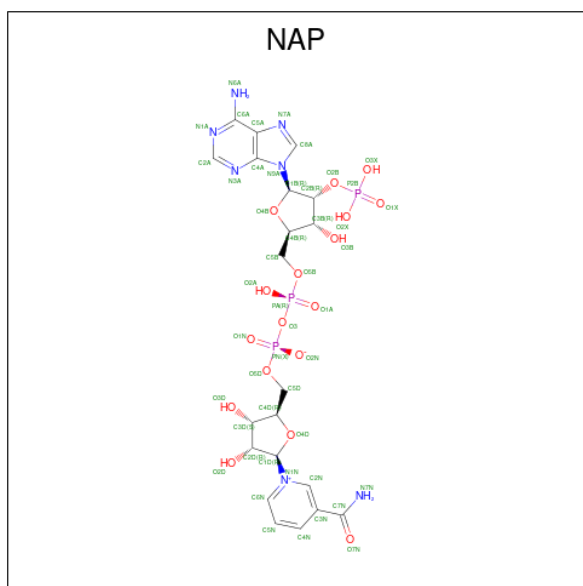
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Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 75 is ZINC ION (CCD ID: ZN) (formula: Zn).

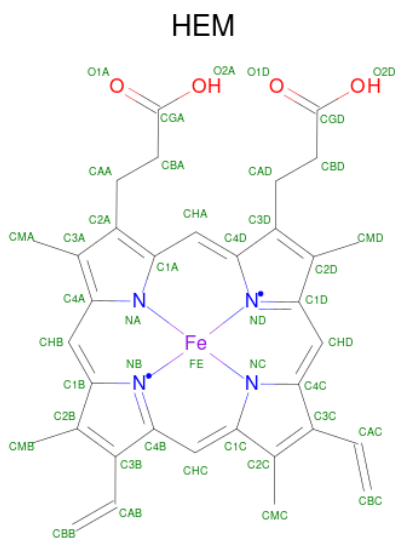
Mol	Chain	Residues	Atoms		AltConf
75	I	1	Total	Zn	0
			1	1	
75	A6	1	Total	Zn	0
			1	1	

- Molecule 76 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



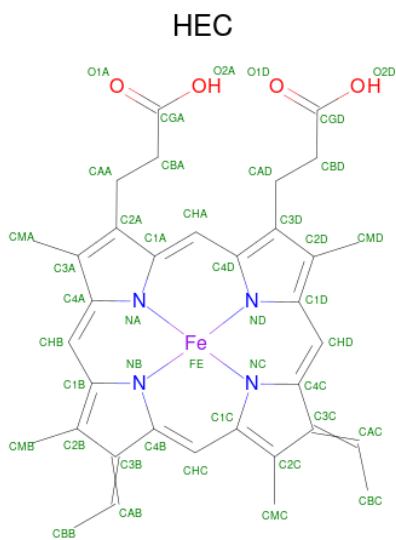
Mol	Chain	Residues	Atoms					AltConf
76	R	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



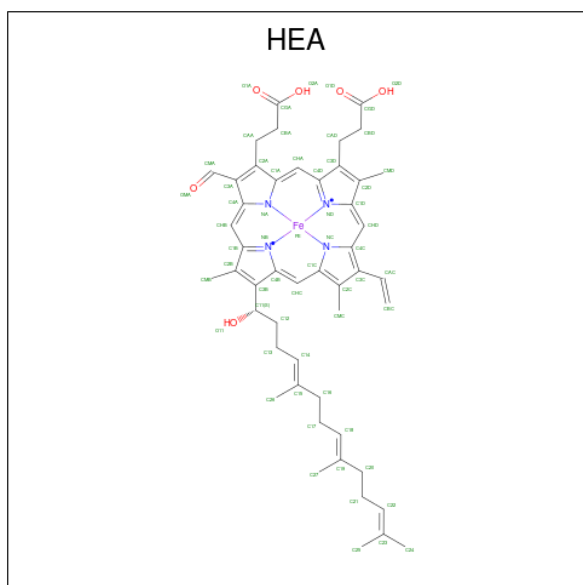
Mol	Chain	Residues	Atoms					AltConf
77	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	y	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	y	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 78 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms					AltConf
79	A9	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
79	A9	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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

Mol	Chain	Residues	Atoms		AltConf
80	A9	1	Total	Cu	0
			1	1	
80	C4	2	Total	Cu	0
			2	2	

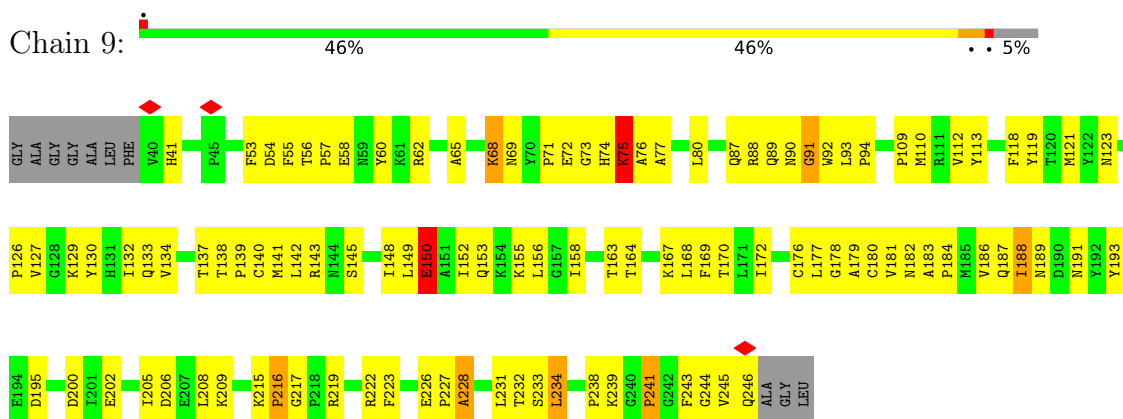
- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	A9	1	Total	Mg	0
			1	1	

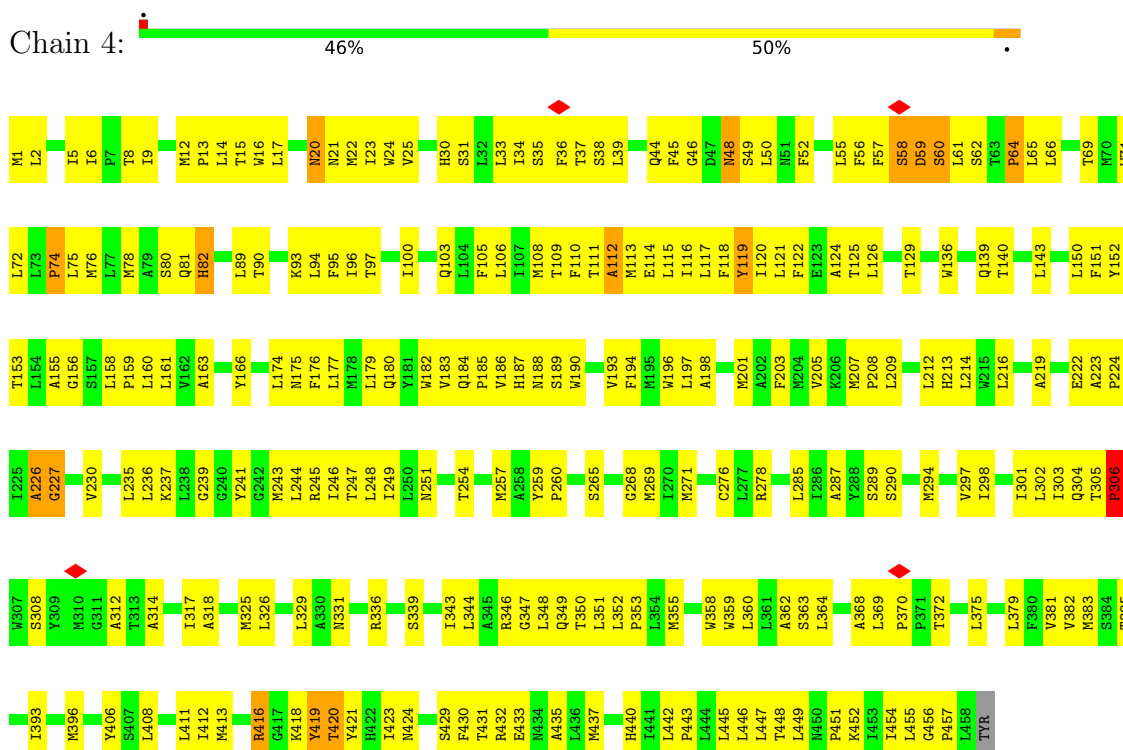
3 Residue-property plots

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

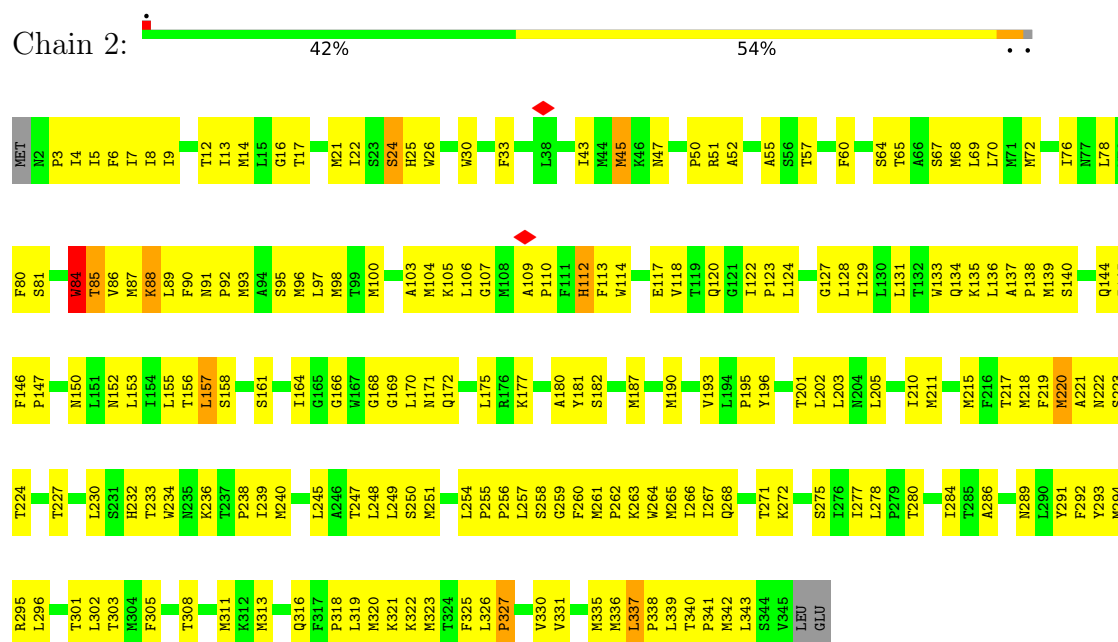
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



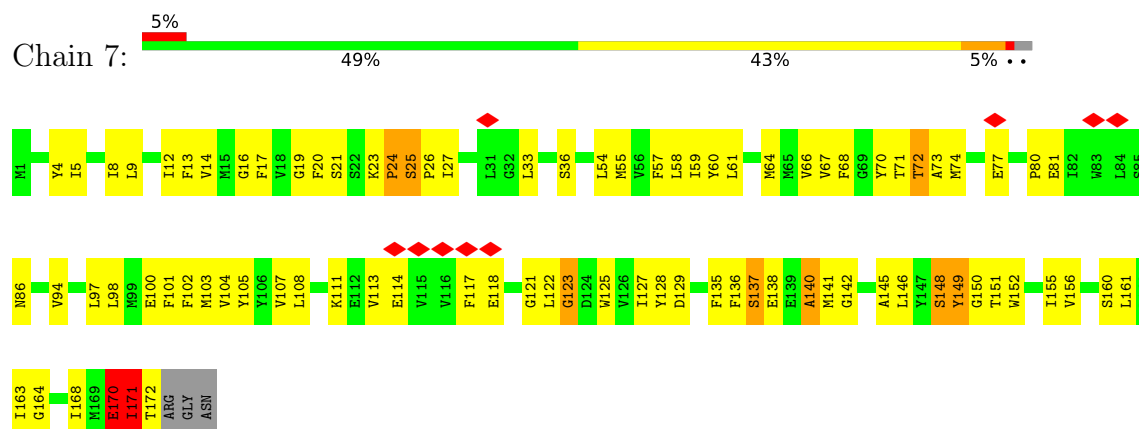
- Molecule 2: NADH-ubiquinone oxidoreductase chain 4



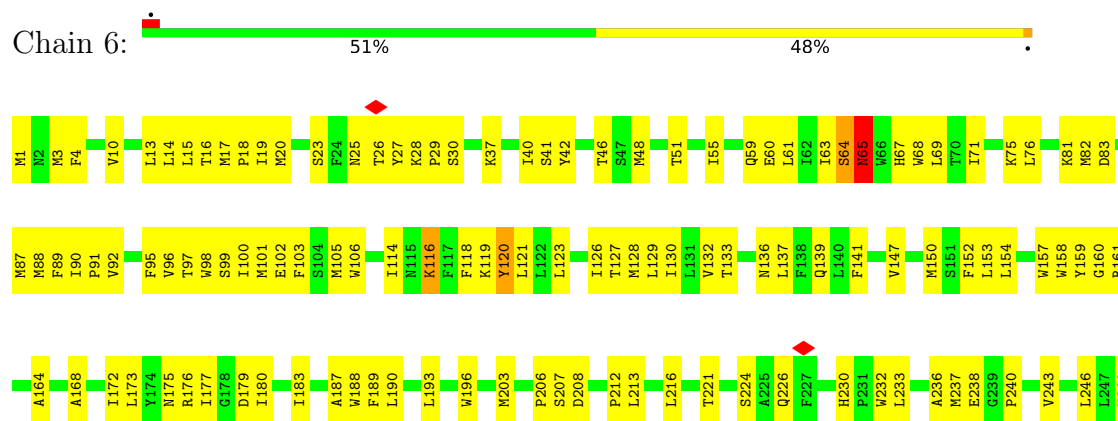
• Molecule 3: NADH-ubiquinone oxidoreductase chain 2

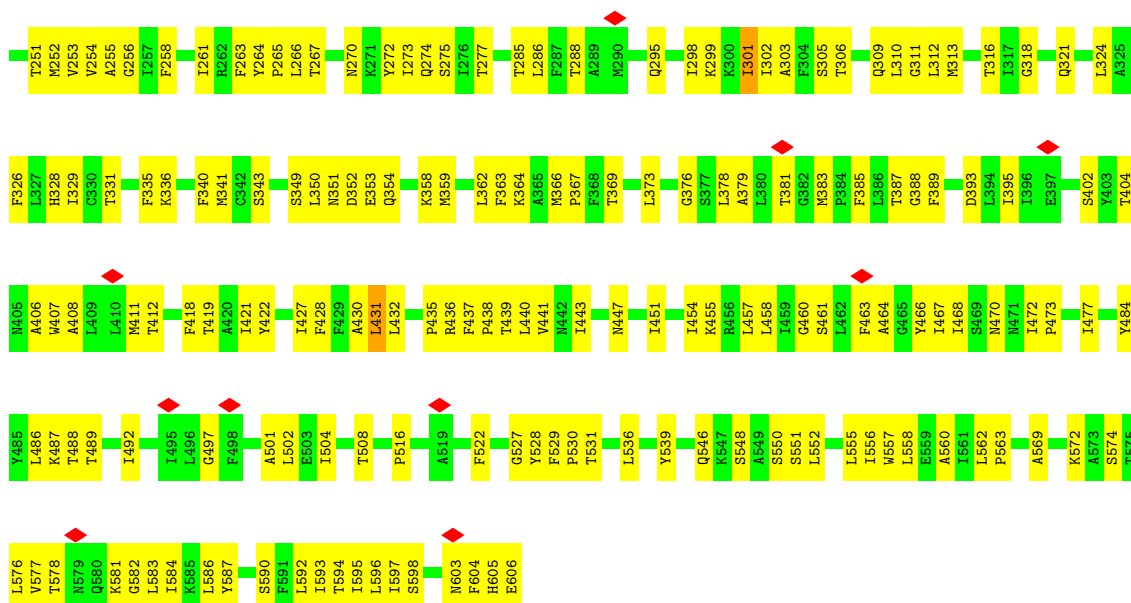


• Molecule 4: NADH-ubiquinone oxidoreductase chain 6



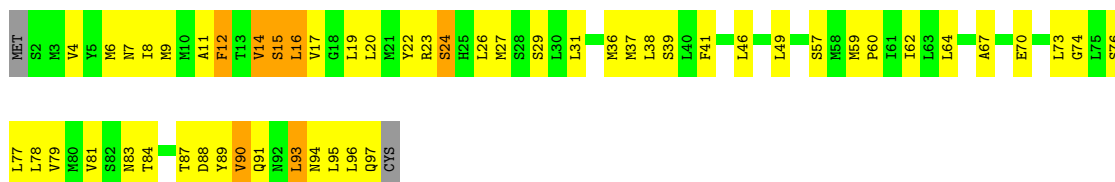
• Molecule 5: NADH-ubiquinone oxidoreductase chain 5





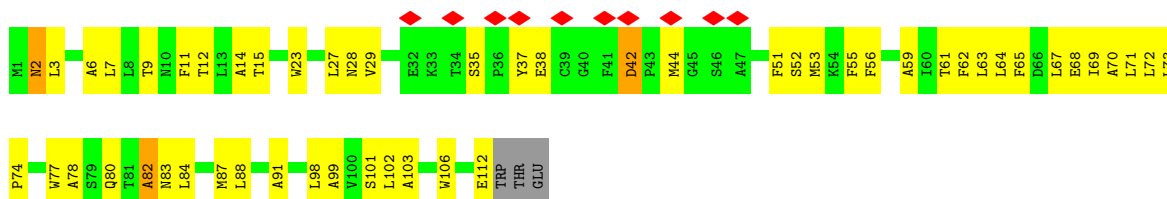
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5: 44% 47% 7% .



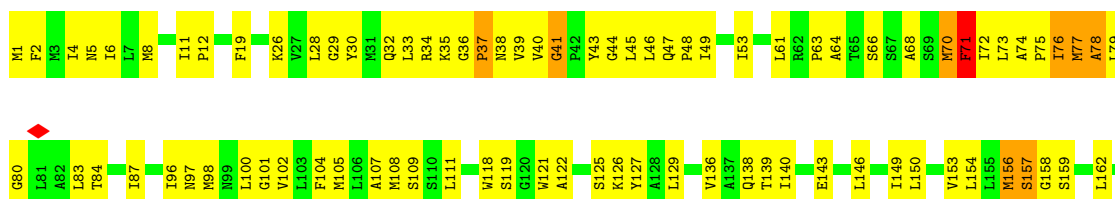
• Molecule 7: NADH-ubiquinone oxidoreductase chain 3

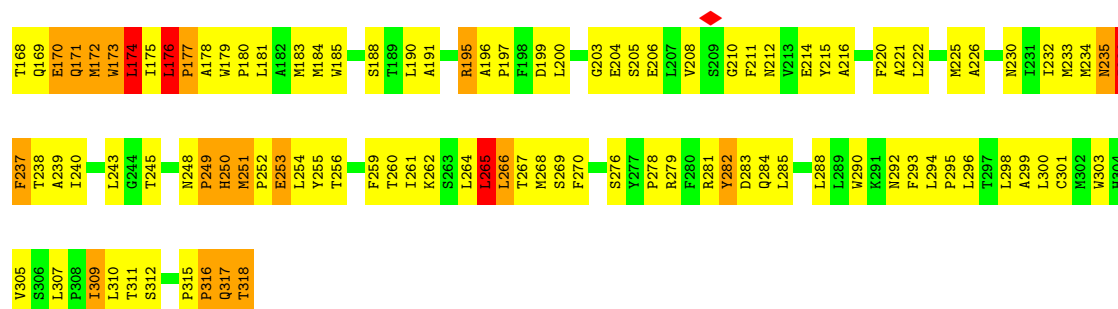
Chain 3: 9% 51% 43% . .



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

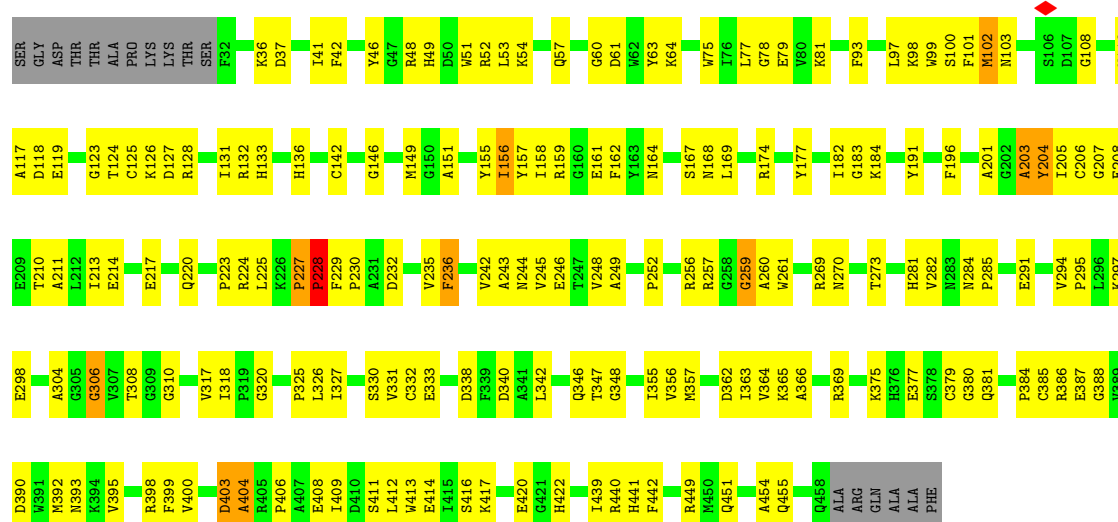
Chain 1: 41% 49% 8% .





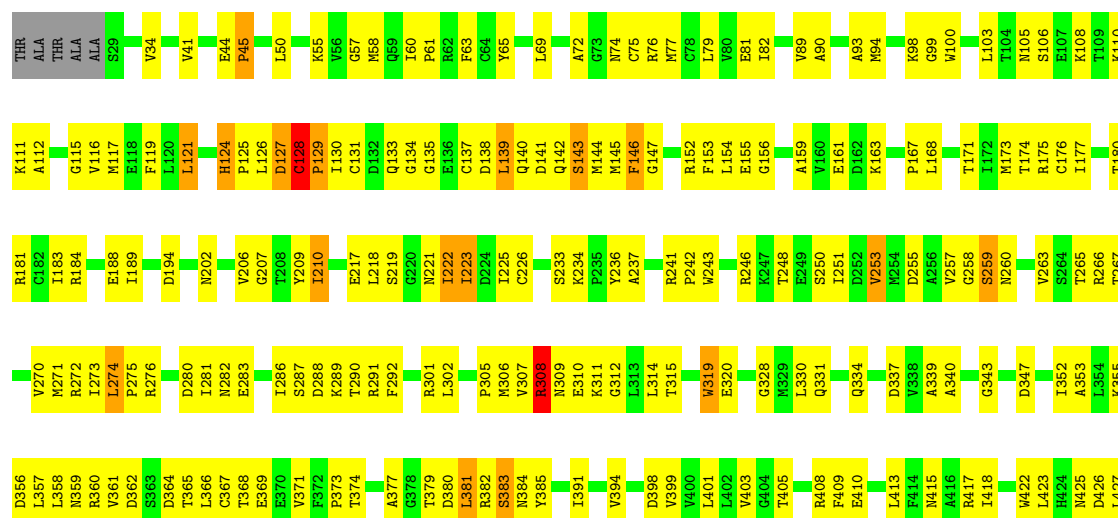
- Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

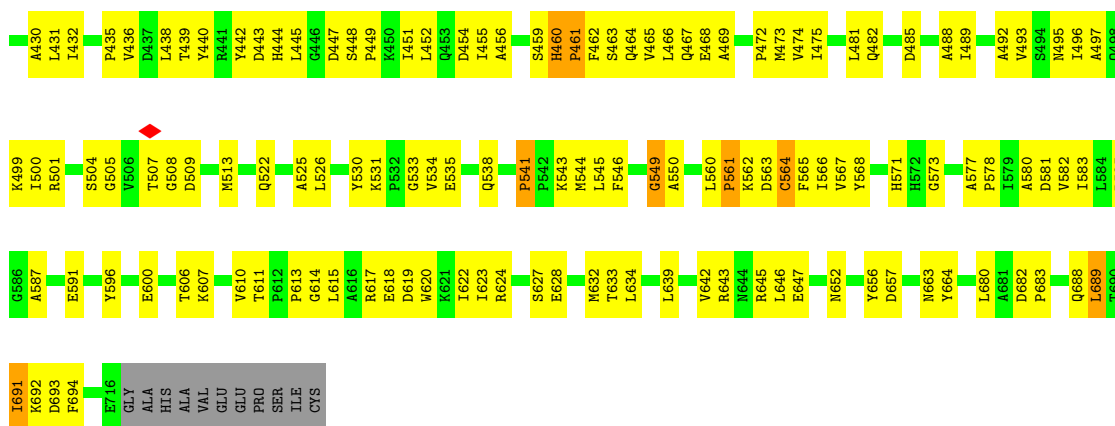
Chain 8: 55% 38%



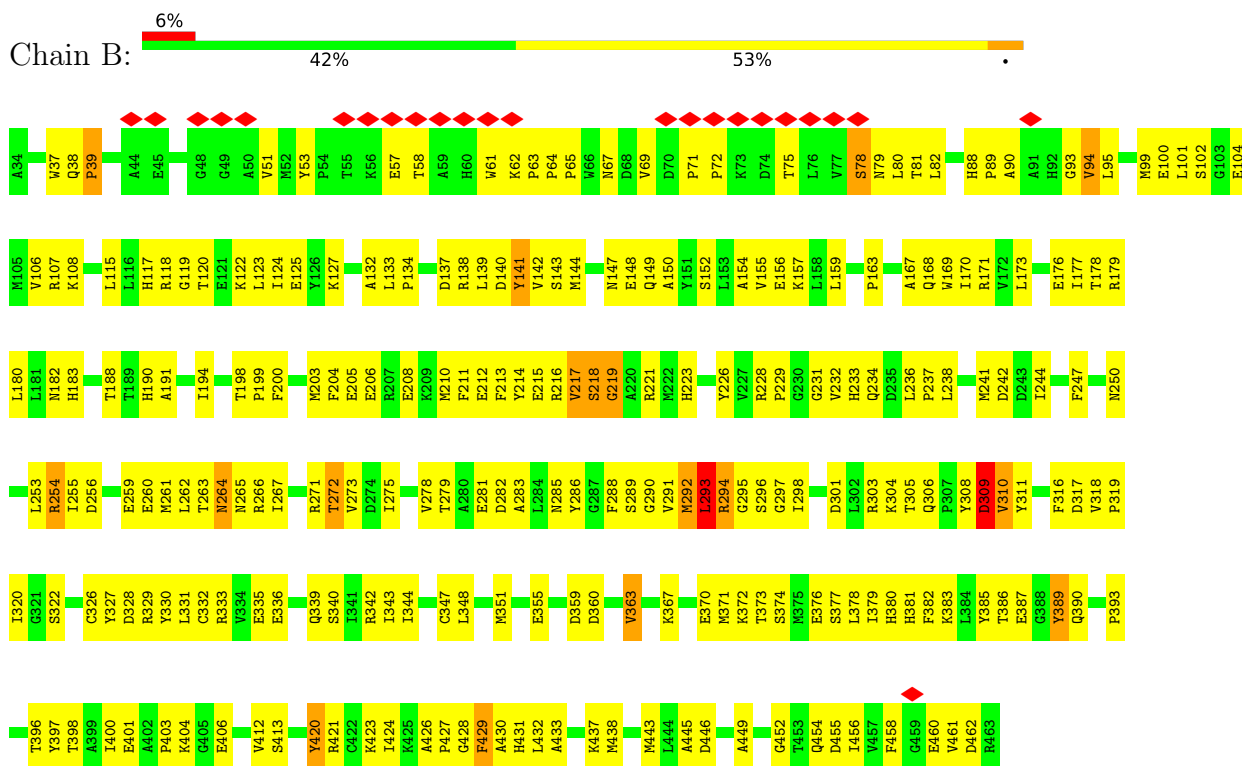
- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A: 50% 44%





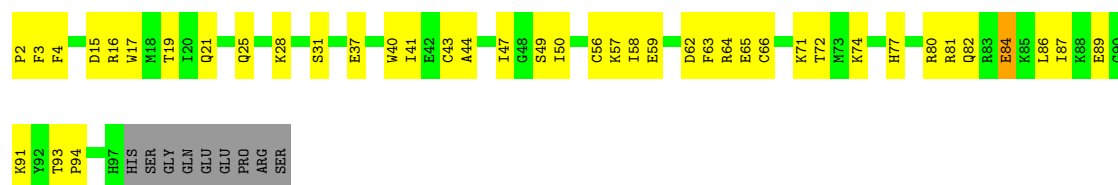
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



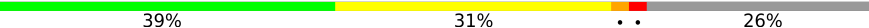
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

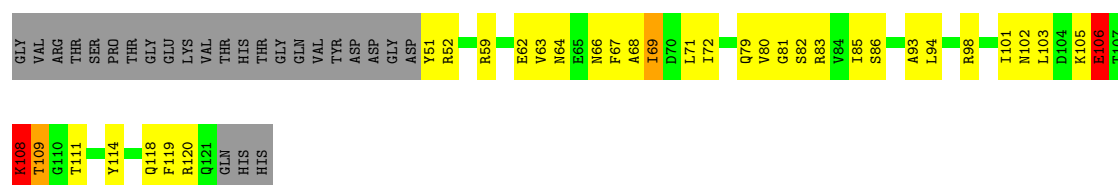


Chain H: 



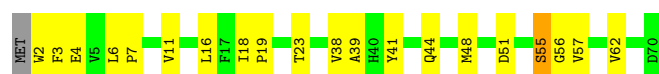
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain I: 



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

Chain J: 



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain K: 



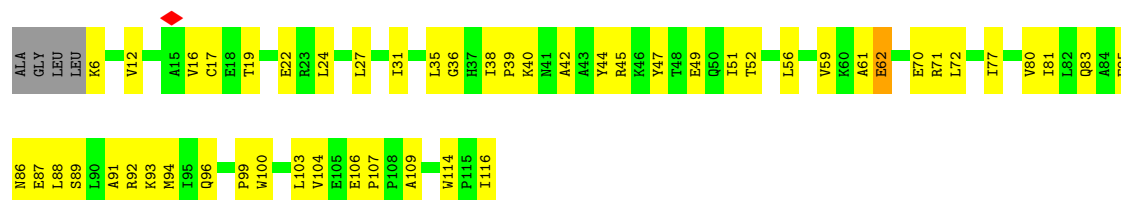
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain L: 

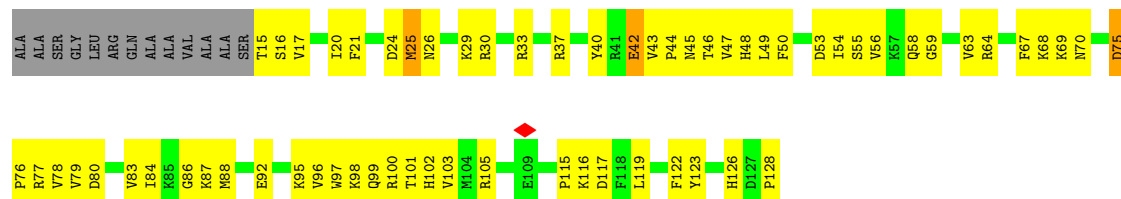


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

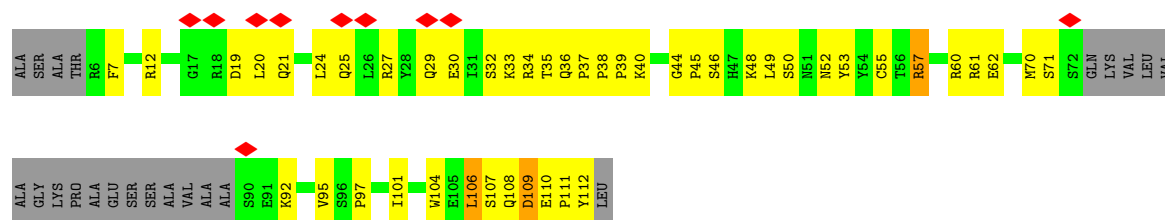
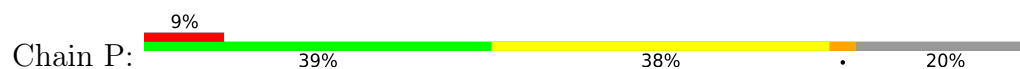
Chain N: 



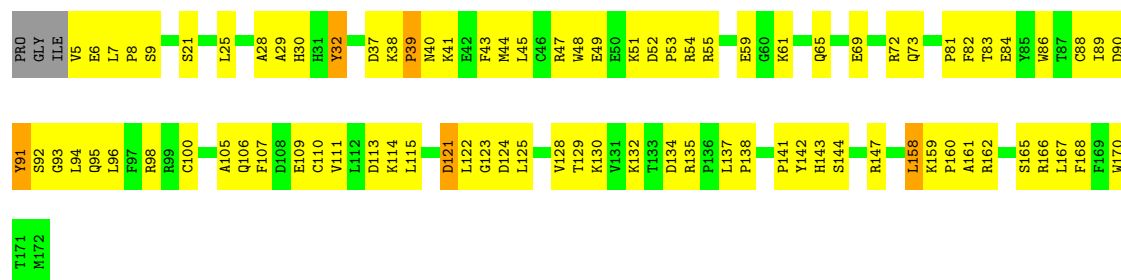
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



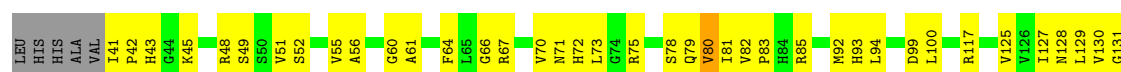
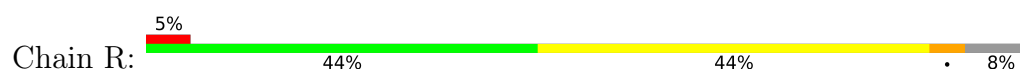
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

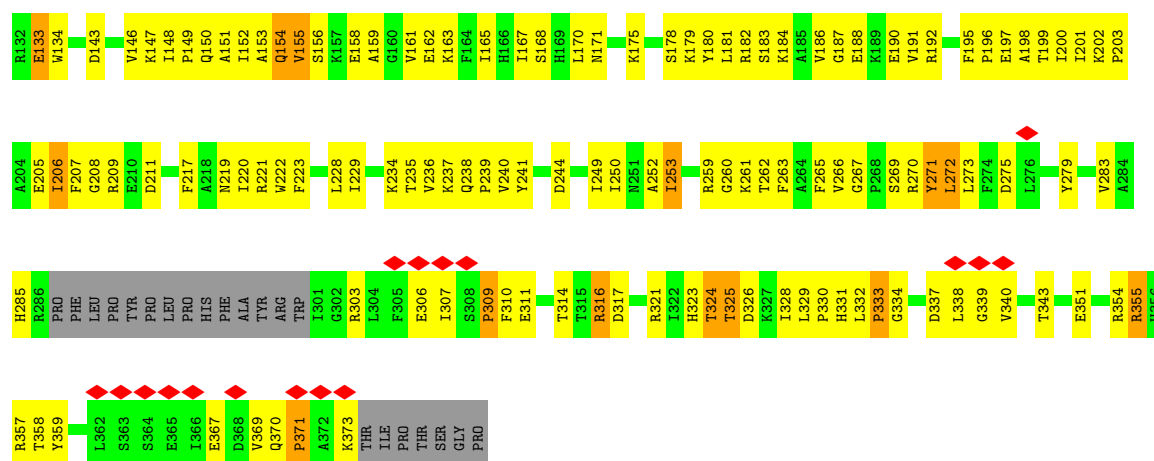


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



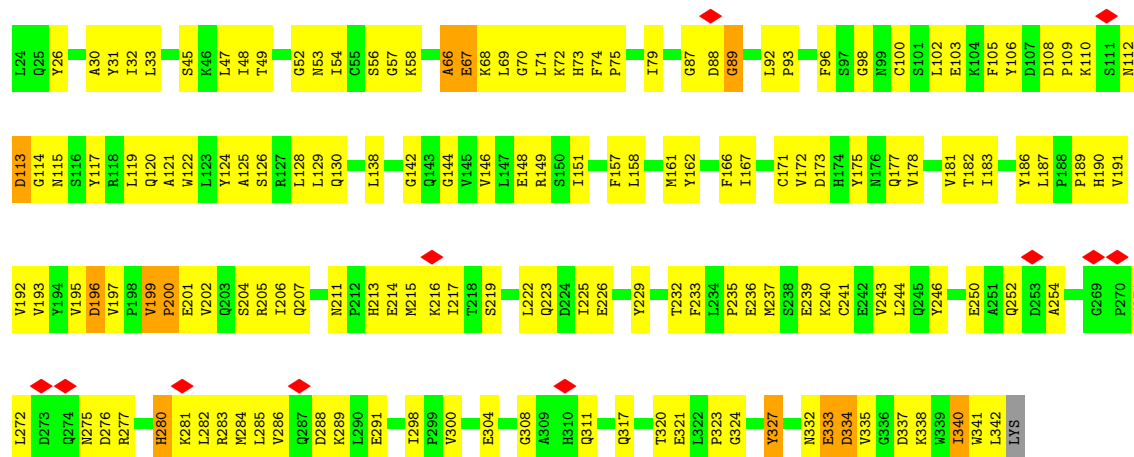
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial





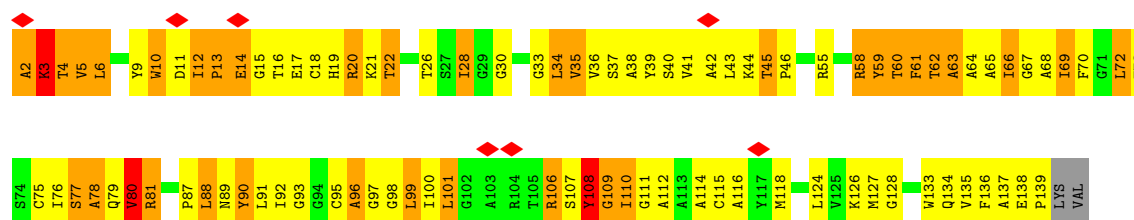
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain S: 51% 45%



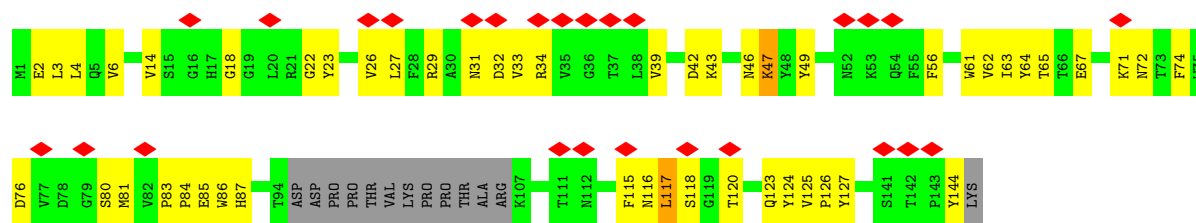
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T: 5% 31% 41% 24%



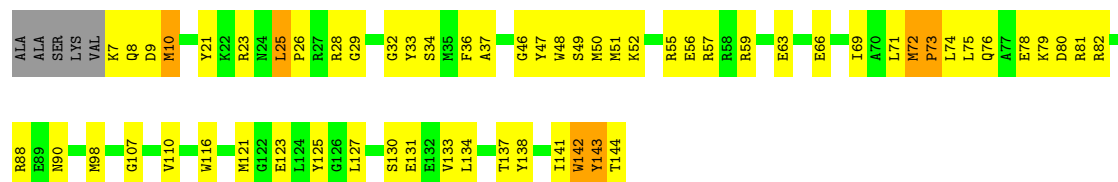
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain U: 18% 57% 33% 9%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain V: 55% 38%



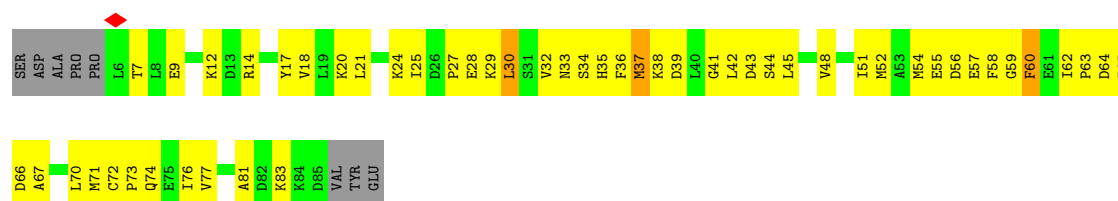
- Molecule 31: Acyl carrier protein, mitochondrial

Chain W: 53% 41%



- Molecule 31: Acyl carrier protein, mitochondrial

Chain M: 32% 56% 9%



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

Chain X: 51% 32% 14%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 54% 25% 21%

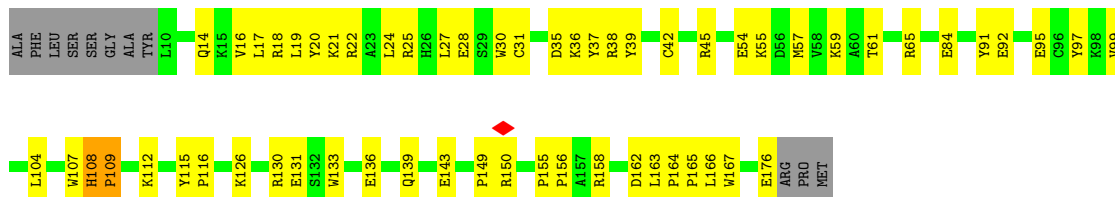


- | | | | | | | | | |
|-----|--|--|--|----|------|------|------|-----|
| GLY | | | | A6 | D18 | P19 | L20 | F75 | F31 | P32 | E33 | R34 | K35 | E36 | M39 | V40 | A41 | T42 | Q43 | M46 | R56 | L63 | I64 | R65 | F66 | K70 | F74 | P75 | N76 | F77 | L78 | H82 | E83 | D86 | W87 | D88 | H92 | V96 | E105 | L108 | K112 | L15 |
|-----|--|--|--|----|------|------|------|-----|

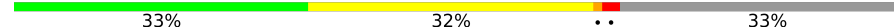
ARG
GLU
GLN
ARG

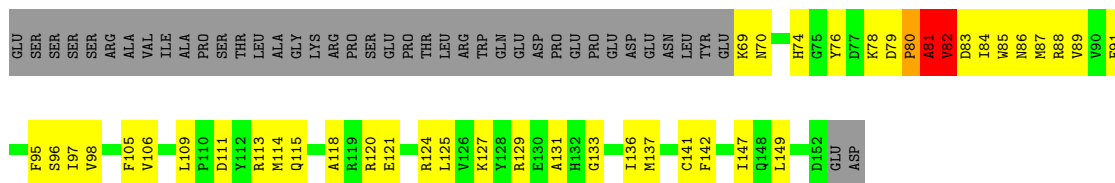
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain f:  61% 32% 6%



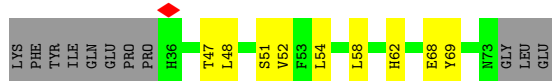
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain h:  33% 32% 33%



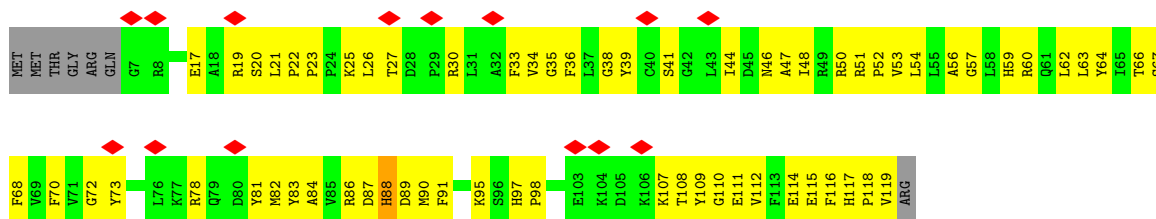
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain i:  59% 18% 22%



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C2

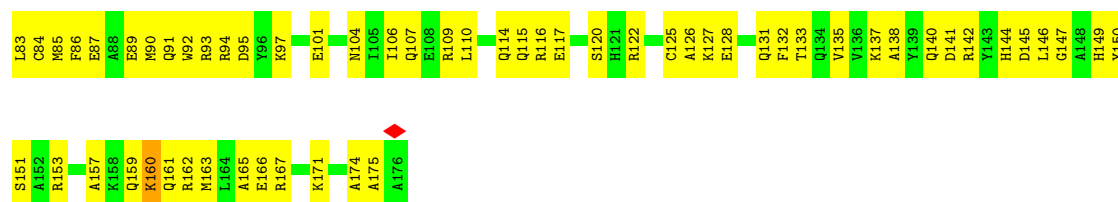
Chain j:  12% 40% 53% 6%



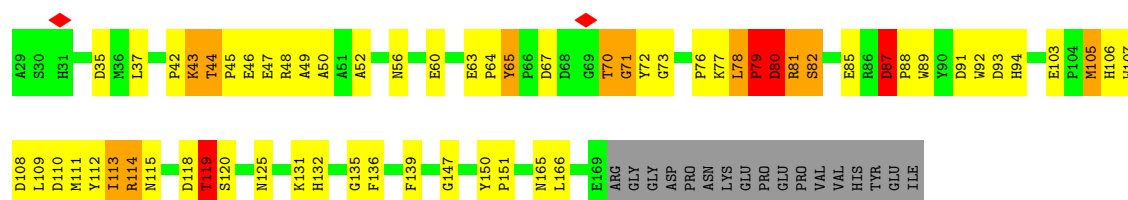
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain g:  43% 54%

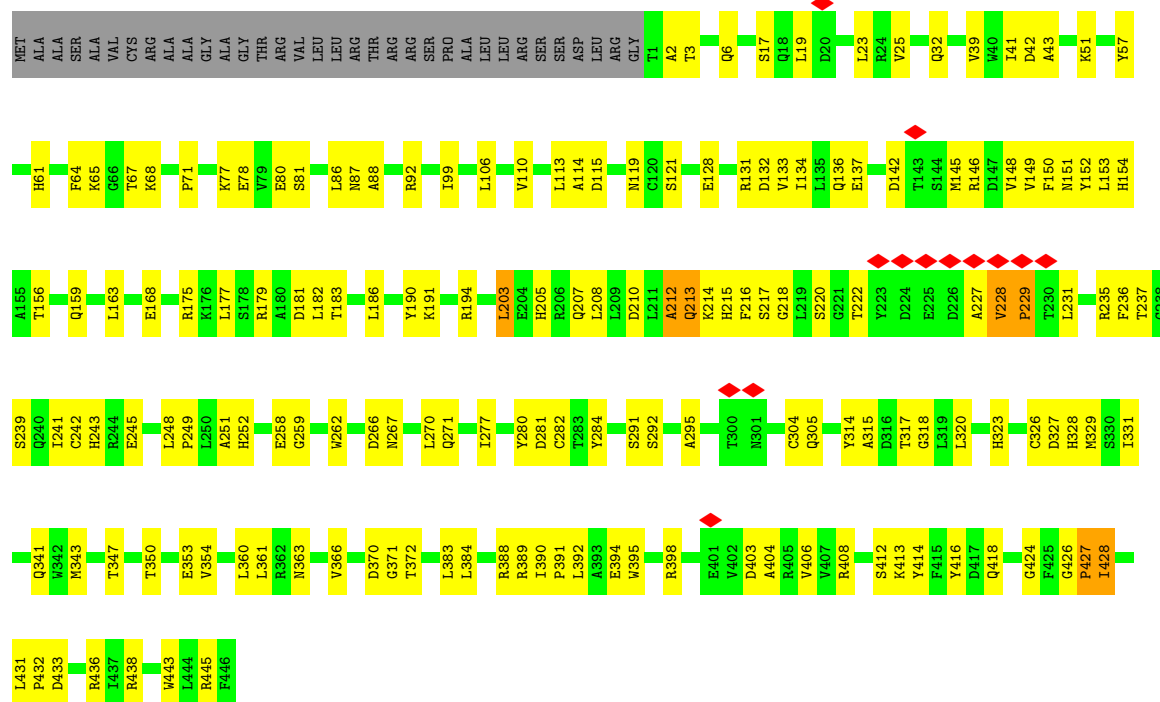




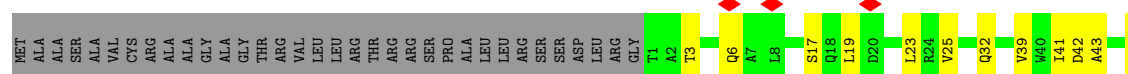
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

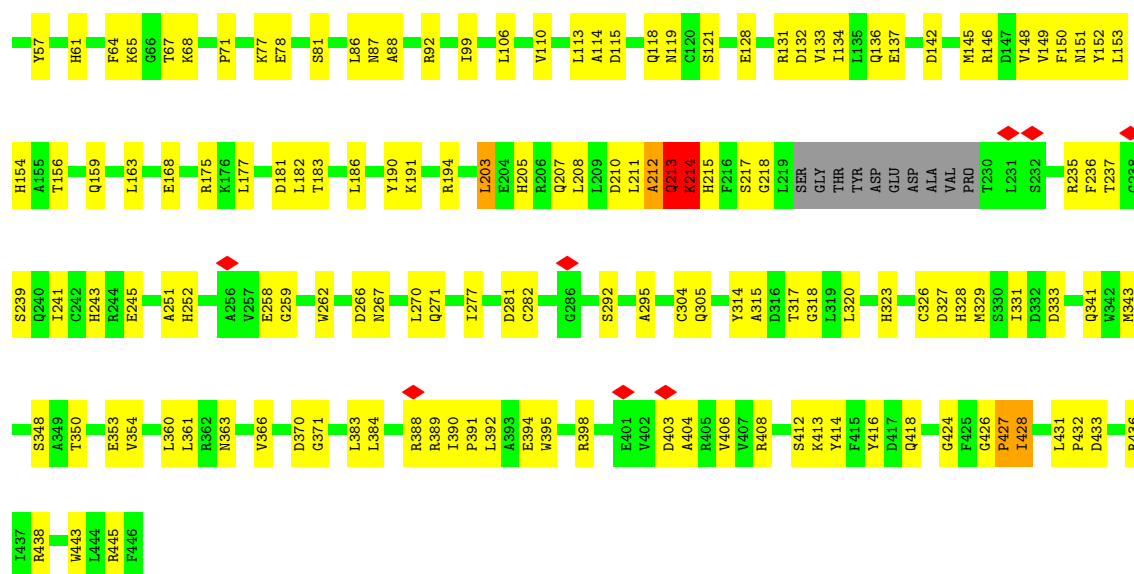


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



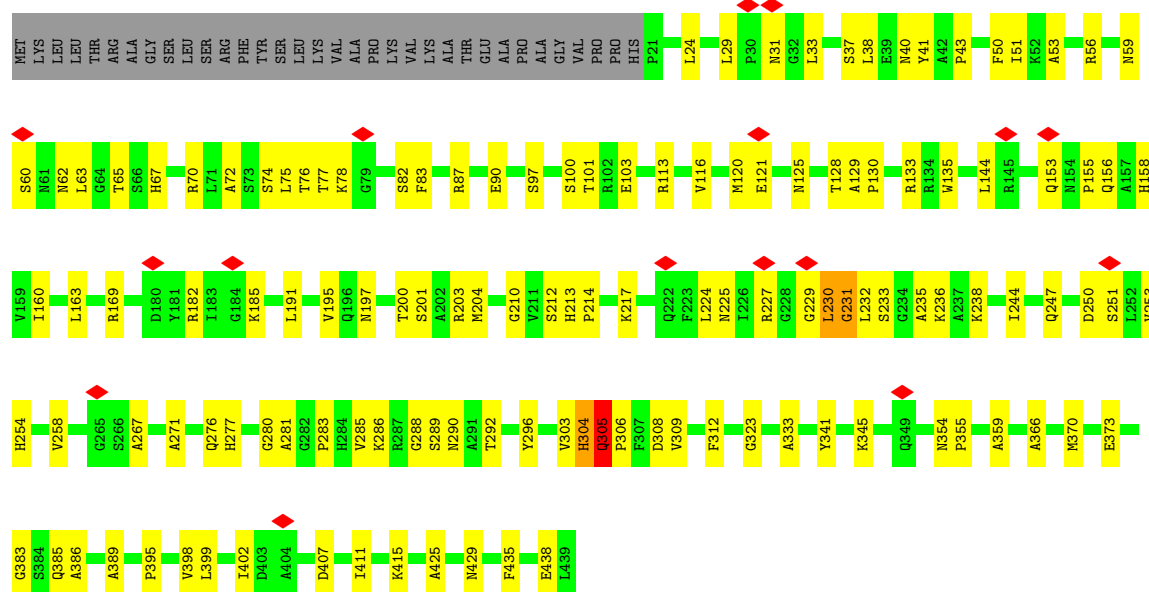
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial





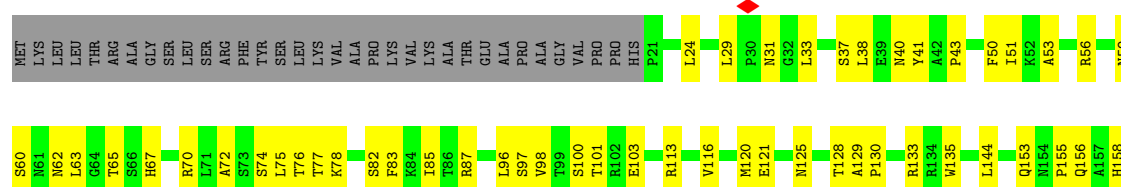
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

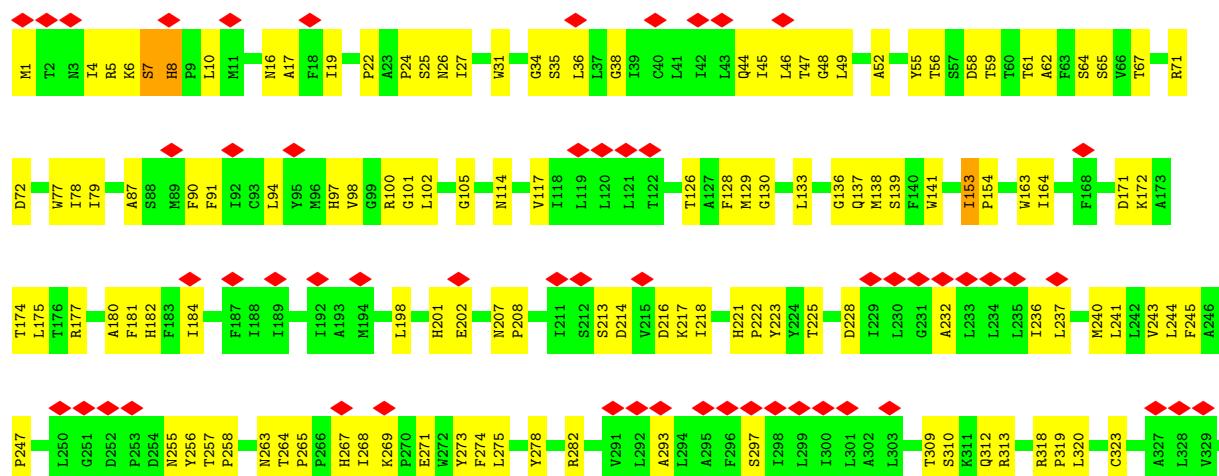
Chain 1: 64% 28% 8%

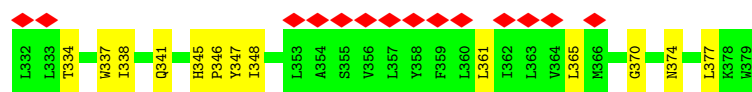


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

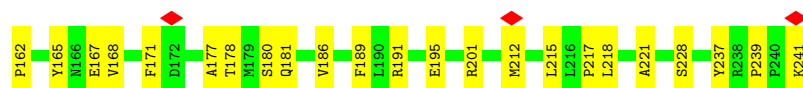
Chain x: 63% 29% 8%



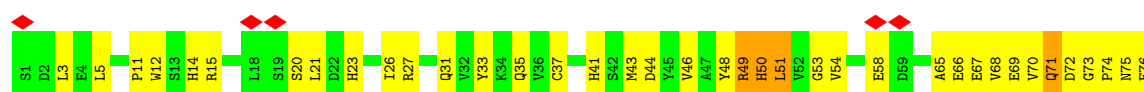




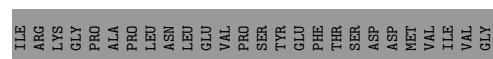
- Molecule 48: Cytochrome c1, heme protein, mitochondrial



- Molecule 48: Cytochrome c1, heme protein, mitochondrial

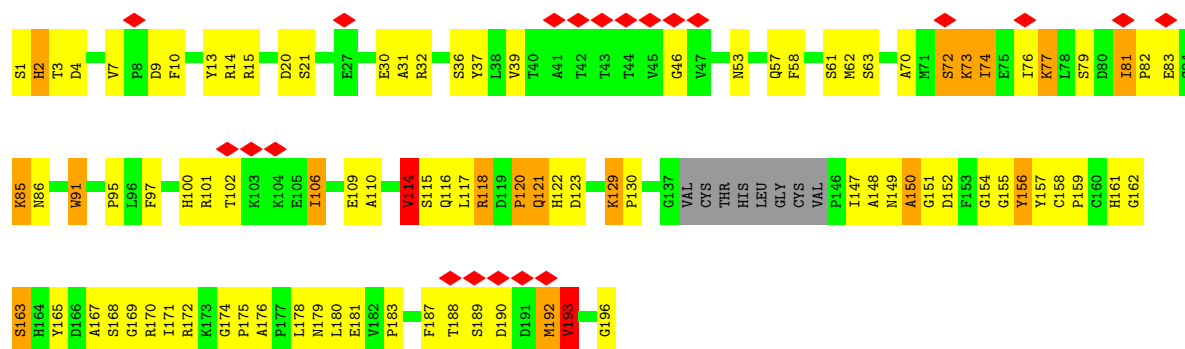


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



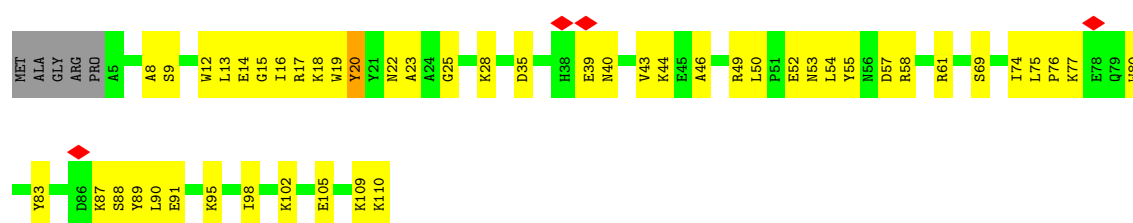
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial





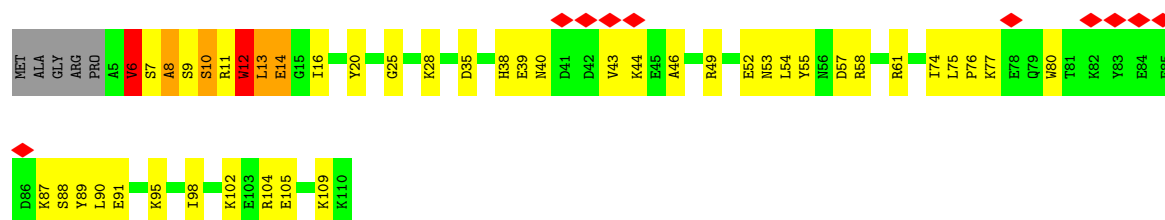
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain q: 52% 42% 5%



- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain A1: 9% 56% 34% 5%



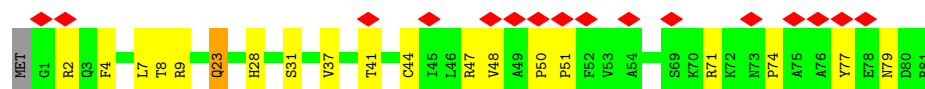
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain r: 17% 71% 28%

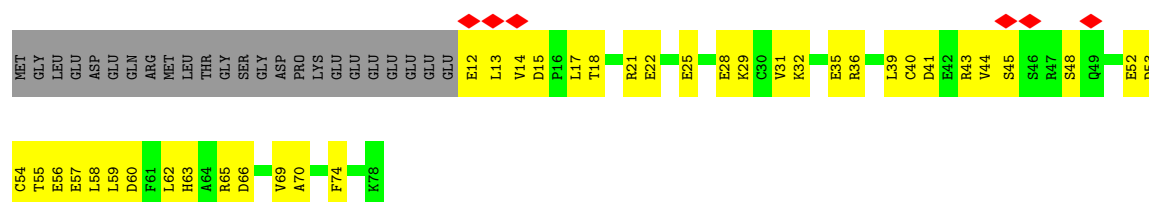


- Molecule 51: Cytochrome b-c1 complex subunit 8

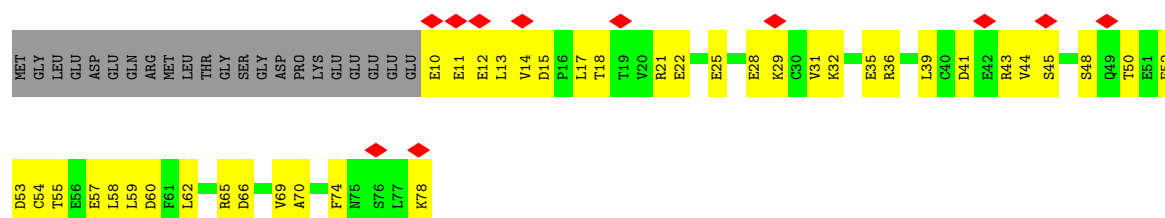
Chain A2: 20% 76% 22%



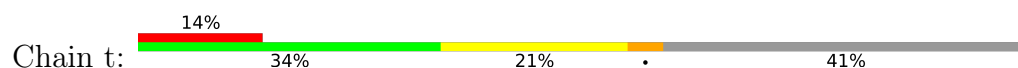
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



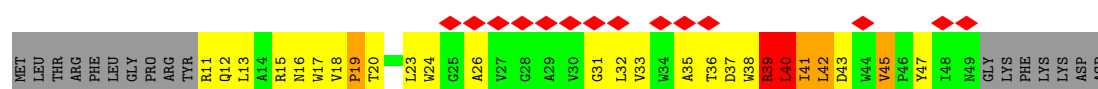
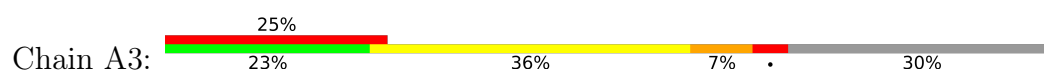
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



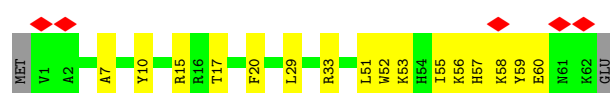
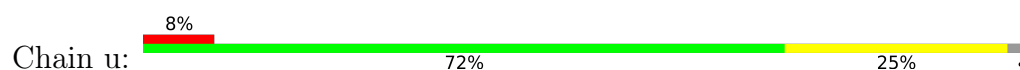
- Molecule 53: Cytochrome b-c1 complex subunit 10



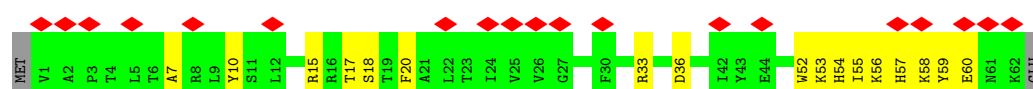
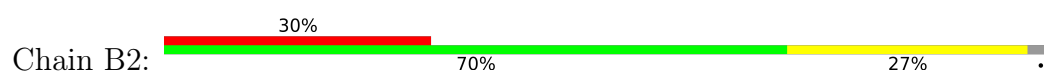
- Molecule 53: Cytochrome b-c1 complex subunit 10



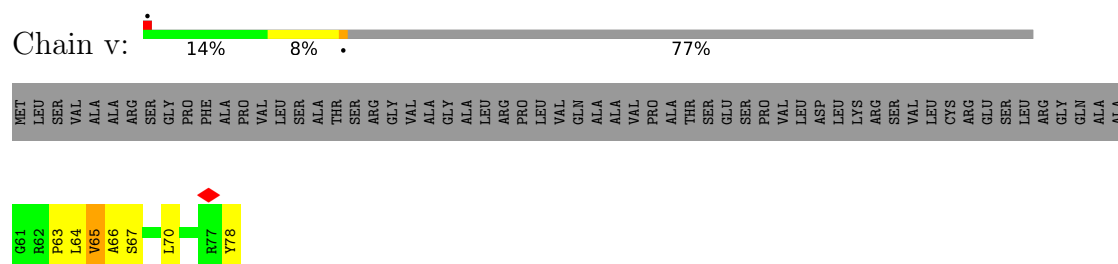
- Molecule 54: Cytochrome b-c1 complex subunit 9



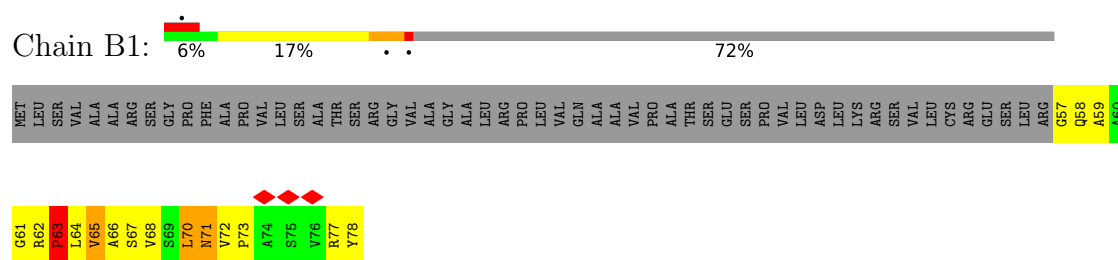
- Molecule 54: Cytochrome b-c1 complex subunit 9



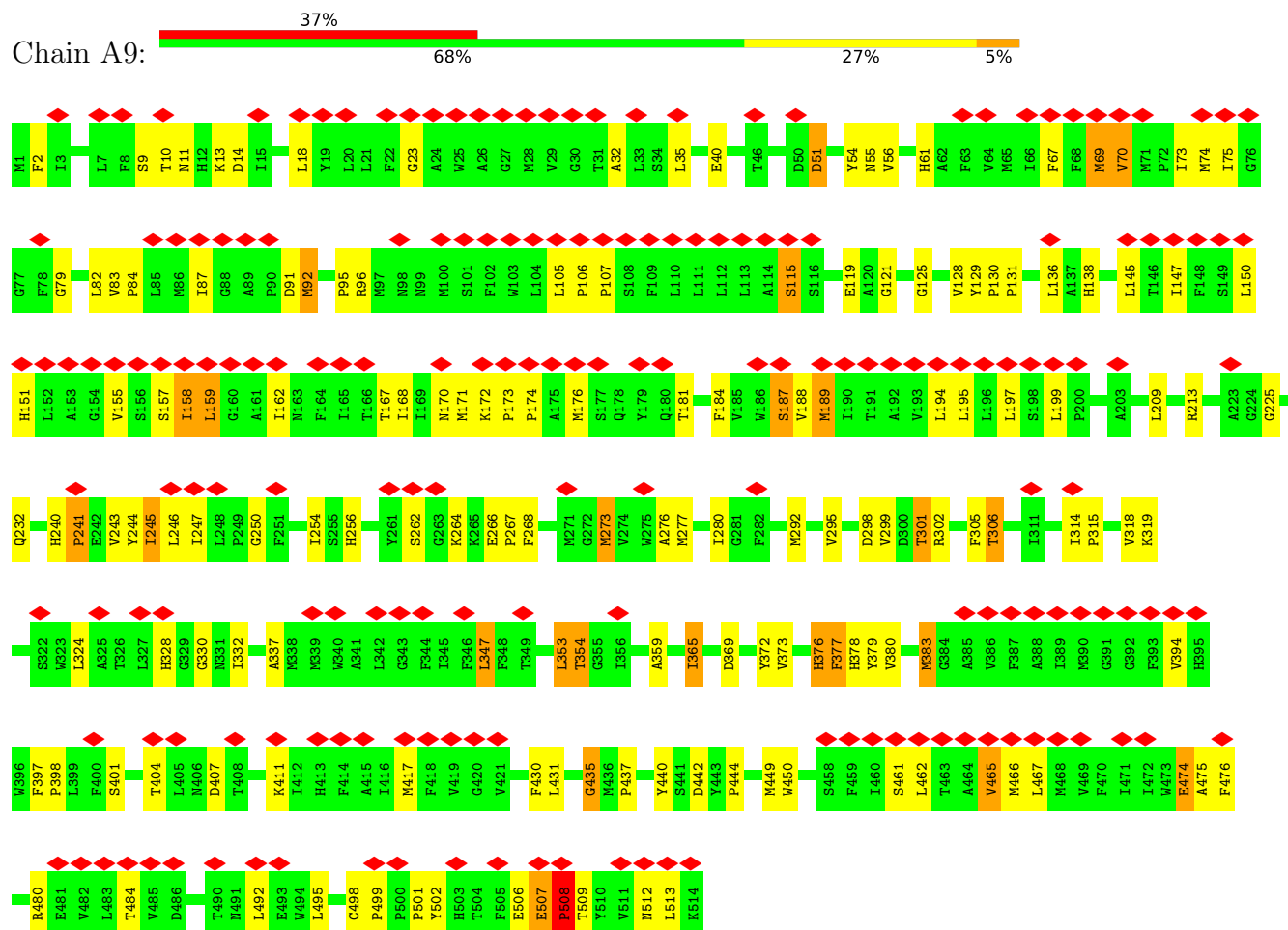
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 56: Cytochrome c oxidase subunit 1



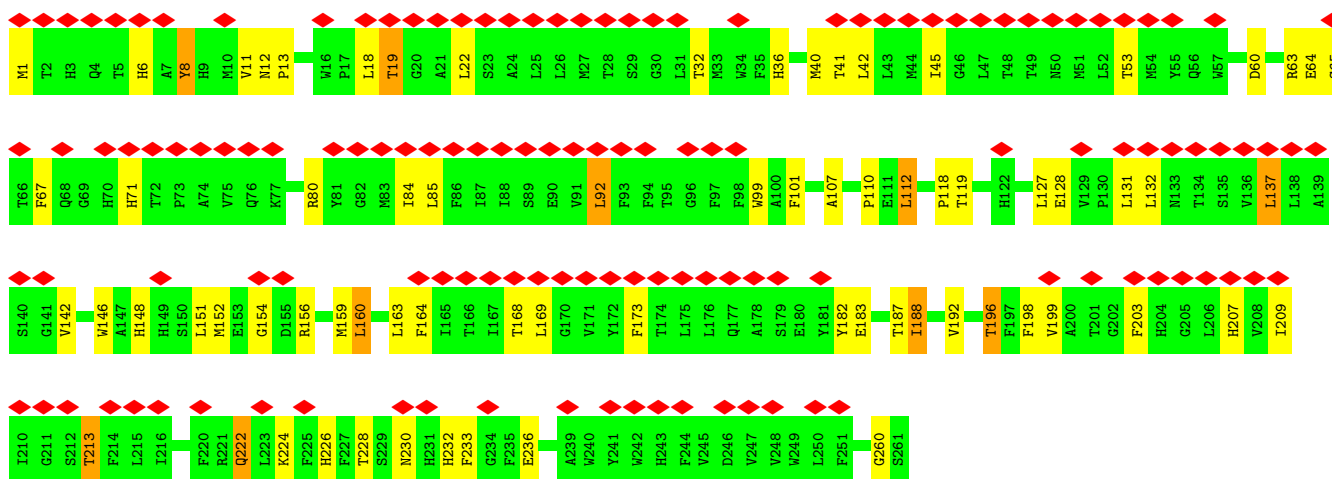
- Molecule 57: Cytochrome c oxidase subunit 2

Chain C4: 17% 61% 33% 5%



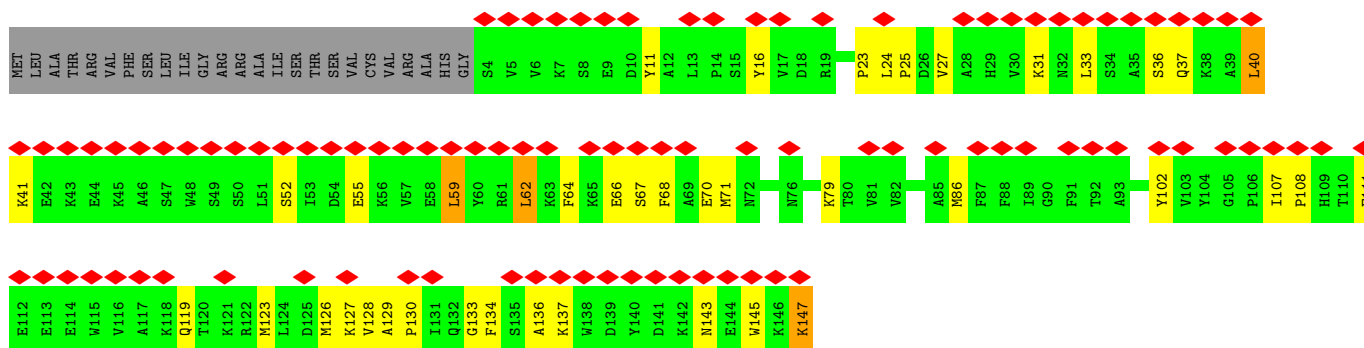
• Molecule 58: Cytochrome c oxidase subunit 3

Chain C2: 51% 72% 24%



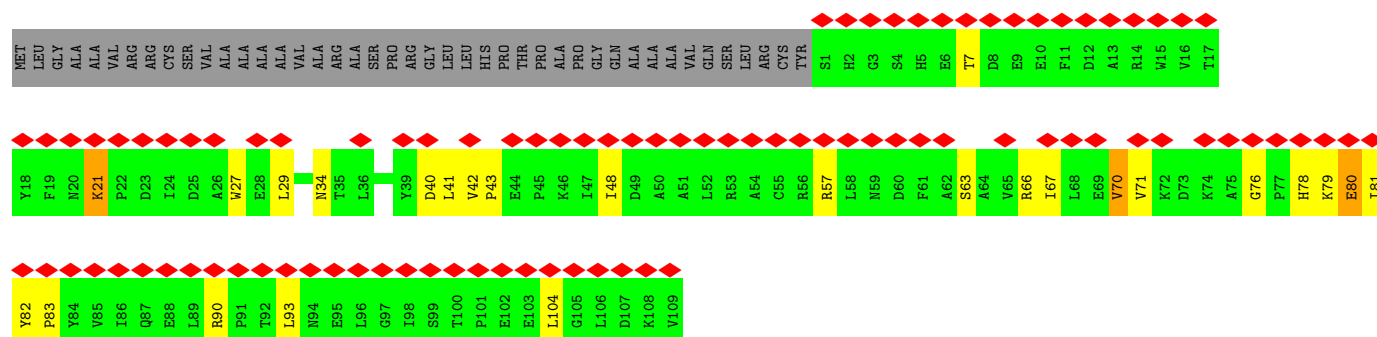
• Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain A7: 58% 60% 22% 15%

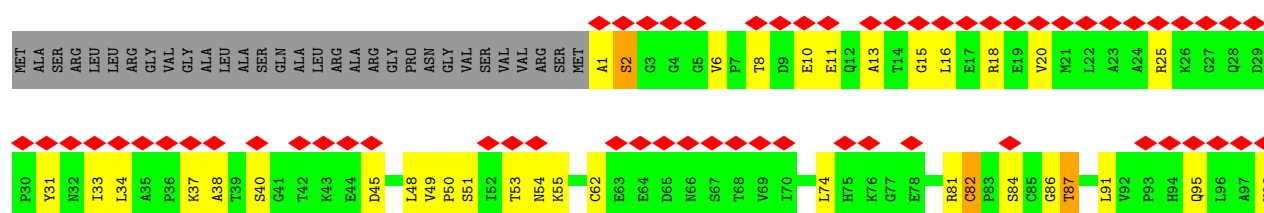


• Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

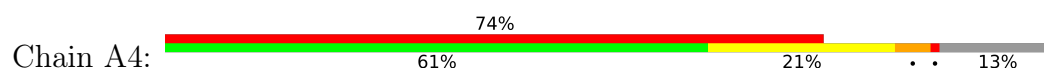
Chain C0: 61% 55% 15% 28%



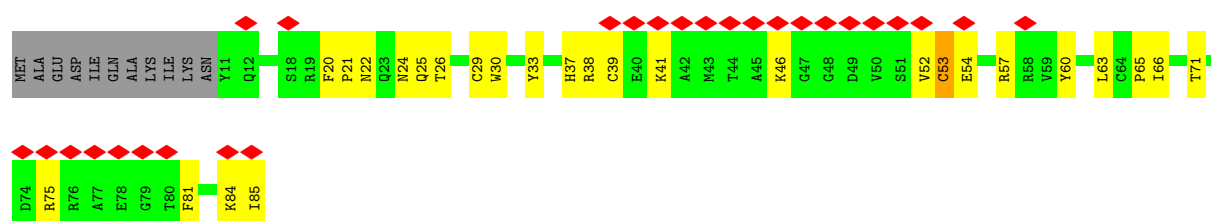
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial



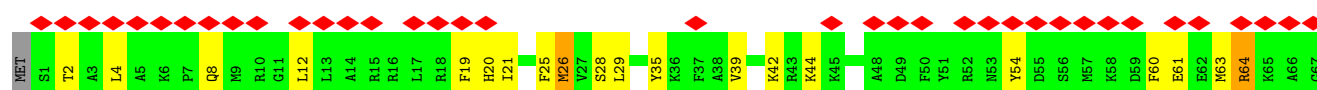
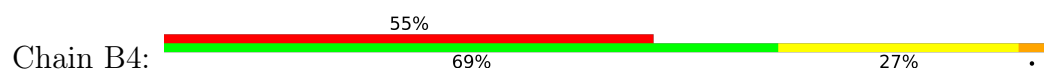
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial

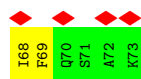


- Molecule 63: Cytochrome c oxidase subunit 6B1

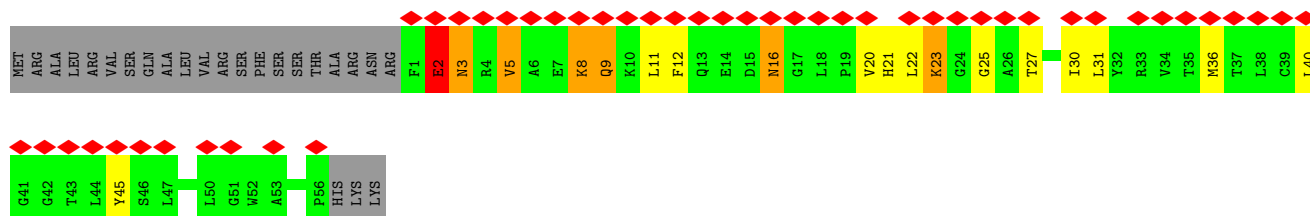


- Molecule 64: Cytochrome c oxidase subunit 6C

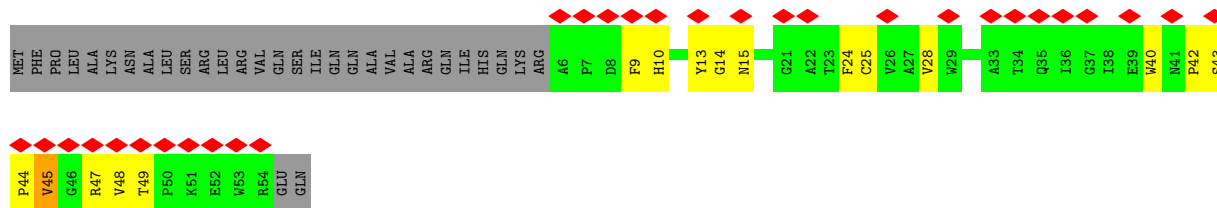
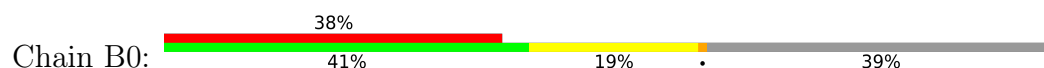




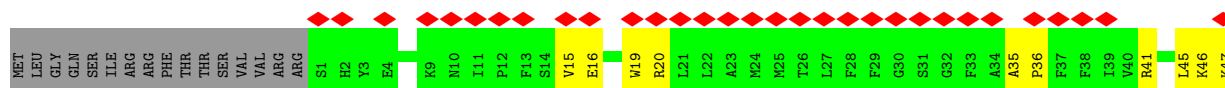
- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial



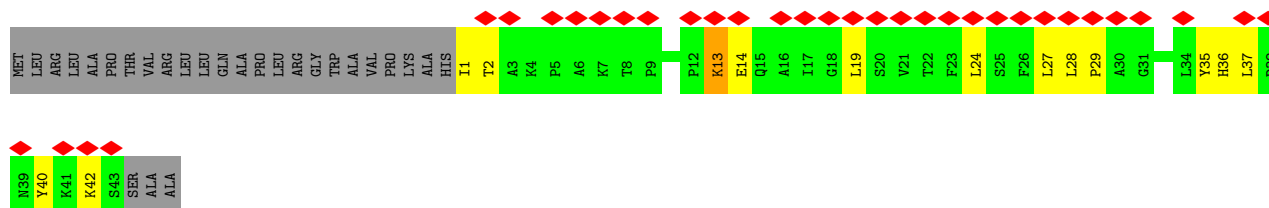
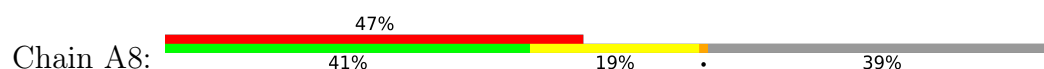
- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.509	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	9	0.43	0/1617	0.69	0/2206
2	4	0.65	1/3674 (0.0%)	0.88	6/5020 (0.1%)
3	2	0.75	1/2749 (0.0%)	0.97	5/3744 (0.1%)
4	7	0.55	0/1271	0.85	1/1735 (0.1%)
5	6	0.44	0/4893	0.74	2/6661 (0.0%)
6	5	0.68	0/721	1.04	5/977 (0.5%)
7	3	0.54	0/902	0.82	2/1233 (0.2%)
8	1	0.70	1/2575 (0.0%)	1.05	15/3518 (0.4%)
9	8	0.46	0/3136	0.80	12/4258 (0.3%)
10	A	0.68	1/5304 (0.0%)	0.95	9/7193 (0.1%)
11	B	0.85	0/3512	1.06	13/4763 (0.3%)
12	C	0.74	0/1777	0.94	3/2420 (0.1%)
13	D	0.91	2/1237 (0.2%)	1.05	1/1676 (0.1%)
14	E	0.88	0/1431	1.11	7/1938 (0.4%)
15	F	0.40	0/191	1.08	2/262 (0.8%)
16	G	0.72	0/1008	0.97	3/1363 (0.2%)
17	H	0.54	0/800	0.80	0/1076
18	I	0.53	0/541	0.99	3/726 (0.4%)
19	J	0.56	0/545	0.68	0/740
20	K	0.42	0/667	0.68	0/900
21	L	0.44	0/623	0.75	0/862
22	N	0.48	0/882	0.88	2/1203 (0.2%)
23	O	0.50	0/948	0.83	3/1279 (0.2%)
24	P	0.49	0/723	0.81	1/985 (0.1%)
25	Q	0.45	0/1381	0.82	2/1869 (0.1%)
26	R	0.49	0/2465	0.86	8/3349 (0.2%)
27	S	0.35	0/2348	0.82	6/3198 (0.2%)
28	T	0.48	0/938	0.99	3/1278 (0.2%)
29	U	0.40	0/1053	0.85	3/1439 (0.2%)
30	V	0.50	0/1115	0.79	1/1508 (0.1%)
31	M	0.43	0/651	0.77	0/876
31	W	0.32	0/624	0.73	1/847 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X	0.36	0/383	0.71	0/523
33	Y	0.35	0/428	0.72	0/592
34	Z	0.35	0/506	0.85	2/688 (0.3%)
35	a	0.43	0/878	0.71	0/1195
36	b	0.51	0/1058	0.78	0/1434
37	c	0.39	0/632	1.01	3/871 (0.3%)
38	d	0.31	0/729	0.70	2/996 (0.2%)
39	f	0.32	0/1191	0.74	2/1639 (0.1%)
40	h	0.44	0/679	0.82	1/926 (0.1%)
41	i	0.34	0/286	0.56	0/392
42	j	0.50	0/912	0.84	4/1240 (0.3%)
43	g	0.43	1/1380 (0.1%)	0.74	2/1872 (0.1%)
44	e	0.47	0/888	1.08	9/1234 (0.7%)
45	k	0.46	0/3527	0.66	3/4787 (0.1%)
45	w	0.46	1/3455 (0.0%)	0.64	2/4685 (0.0%)
46	l	0.41	0/3192	0.58	3/4329 (0.1%)
46	x	0.41	0/3198	0.61	5/4336 (0.1%)
47	m	0.55	0/3108	0.62	0/4252
47	y	0.55	0/3108	0.62	0/4252
48	o	0.46	0/1978	0.65	1/2684 (0.0%)
48	z	0.47	0/1965	0.66	0/2669
49	A0	0.46	0/1124	0.95	5/1538 (0.3%)
49	p	0.47	0/945	1.15	10/1288 (0.8%)
50	A1	0.46	0/935	0.61	0/1253
50	q	0.45	0/935	0.65	1/1253 (0.1%)
51	A2	0.41	0/698	0.62	0/944
51	r	0.41	0/704	0.63	0/951
52	B3	0.31	0/571	0.60	0/765
52	s	0.32	0/553	0.57	0/741
53	A3	0.44	0/330	0.73	0/457
53	t	0.33	0/272	0.52	0/377
54	B2	0.34	0/524	0.50	0/707
54	u	0.34	0/524	0.50	0/707
55	B1	0.57	0/149	1.24	0/203
55	v	0.52	0/114	1.13	0/156
56	A9	0.86	7/4164 (0.2%)	1.16	35/5688 (0.6%)
57	C4	0.77	0/1868	1.12	10/2544 (0.4%)
58	C2	0.74	0/2211	1.02	7/3023 (0.2%)
59	A7	0.67	0/1229	0.96	3/1658 (0.2%)
60	C0	0.64	0/898	1.02	6/1218 (0.5%)
61	A6	0.72	0/765	1.13	4/1038 (0.4%)
62	A4	0.69	0/698	1.10	6/950 (0.6%)
63	A5	0.68	0/648	1.17	5/877 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
64	B4	0.71	0/611	0.94	2/810 (0.2%)
65	C3	0.70	0/451	1.04	3/610 (0.5%)
66	B0	0.74	0/398	1.01	0/546
67	C1	0.77	0/399	0.97	2/534 (0.4%)
68	A8	0.68	0/345	0.99	1/470 (0.2%)
All	All	0.58	15/108846 (0.0%)	0.86	258/148004 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9	0	6
2	4	0	9
3	2	0	10
4	7	0	6
5	6	0	5
6	5	0	4
7	3	0	2
8	1	0	3
9	8	0	8
10	A	0	16
11	B	0	4
13	D	0	6
14	E	0	5
17	H	0	2
18	I	0	1
20	K	0	1
21	L	0	1
22	N	0	1
23	O	0	1
24	P	0	3
25	Q	0	2
26	R	0	9
27	S	0	4
29	U	0	3
30	V	0	2
31	M	0	3
31	W	0	2
34	Z	0	2
35	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	b	0	4
38	d	0	1
39	f	0	3
40	h	0	3
42	j	0	2
43	g	0	1
44	e	0	7
45	k	0	3
45	w	0	4
46	l	0	5
46	x	0	3
47	m	0	4
47	y	0	3
48	o	0	7
48	z	0	7
49	A0	0	3
49	p	0	6
53	A3	0	1
55	B1	0	5
All	All	0	194

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	161	LEU	CA-C	-9.68	1.38	1.52
56	A9	61	HIS	CG-CD2	7.59	1.44	1.35
56	A9	378	HIS	ND1-CE1	7.10	1.39	1.32
56	A9	378	HIS	CE1-NE2	-6.54	1.26	1.32
56	A9	69	MET	SD-CE	-6.26	1.64	1.79

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	128	CYS	CA-C-N	-13.67	102.76	119.84
10	A	128	CYS	C-N-CA	-13.67	102.76	119.84
46	x	230	LEU	N-CA-C	11.27	126.80	110.24
9	8	227	PRO	CA-C-N	-10.59	107.96	118.97
9	8	227	PRO	C-N-CA	-10.59	107.96	118.97

There are no chirality outliers.

5 of 194 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	9	109	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	75	LYS	Peptide
1	9	91	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	1578	0	1553	167	0
2	4	3577	0	3674	398	0
3	2	2681	0	2823	257	0
4	7	1239	0	1193	83	0
5	6	4766	0	4897	363	0
6	5	712	0	742	82	0
7	3	879	0	906	60	0
8	1	2503	0	2617	293	0
9	8	3065	0	2801	239	0
10	A	5218	0	5232	376	0
11	B	3422	0	3345	397	0
12	C	1726	0	1676	219	0
13	D	1206	0	1203	204	0
14	E	1401	0	1353	281	0
15	F	186	0	139	29	0
16	G	985	0	976	78	0
17	H	780	0	753	45	0
18	I	533	0	511	63	0
19	J	530	0	503	30	0
20	K	656	0	647	37	0
21	L	602	0	591	102	0
22	N	862	0	868	40	0
23	O	925	0	907	122	0
24	P	702	0	670	90	0
25	Q	1345	0	1281	161	0
26	R	2407	0	2296	182	0
27	S	2299	0	2028	201	0
28	T	923	0	851	286	0
29	U	1019	0	900	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	1087	0	1037	110	0
31	M	642	0	642	79	0
31	W	616	0	579	44	0
32	X	372	0	314	19	0
33	Y	409	0	318	16	0
34	Z	493	0	395	58	0
35	a	857	0	765	155	0
36	b	1032	0	954	82	0
37	c	617	0	492	36	0
38	d	713	0	522	62	0
39	f	1156	0	892	56	0
40	h	658	0	584	71	0
41	i	277	0	240	54	0
42	j	883	0	823	259	0
43	g	1351	0	1262	190	0
44	e	864	0	567	122	0
45	k	3454	0	3350	137	0
45	w	3385	0	3296	134	0
46	l	3135	0	3112	101	0
46	x	3141	0	3123	114	0
47	m	3011	0	3077	132	0
47	y	3011	0	3077	110	0
48	o	1919	0	1870	90	0
48	z	1906	0	1841	76	0
49	A0	1117	0	807	123	0
49	p	938	0	733	52	0
50	A1	916	0	911	42	0
50	q	916	0	911	78	0
51	A2	676	0	668	20	0
51	r	682	0	679	19	0
52	B3	566	0	542	35	0
52	s	548	0	530	35	0
53	A3	318	0	314	66	0
53	t	262	0	250	13	0
54	B2	511	0	518	23	0
54	u	511	0	518	23	0
55	B1	148	0	154	23	0
55	v	114	0	107	4	0
56	A9	4025	0	4003	88	0
57	C4	1822	0	1834	73	0
58	C2	2124	0	2042	52	0
59	A7	1195	0	1183	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	C0	878	0	868	20	0
61	A6	748	0	728	25	0
62	A4	671	0	645	30	0
63	A5	628	0	582	21	0
64	B4	598	0	612	14	0
65	C3	441	0	439	17	0
66	B0	384	0	366	12	0
67	C1	386	0	388	8	0
68	A8	335	0	352	13	0
69	9	4	0	0	0	0
69	A	4	0	0	2	0
69	m	4	0	0	0	0
70	2	46	0	69	18	0
70	4	82	0	118	52	0
70	B	51	0	82	27	0
71	4	82	0	114	44	0
71	6	64	0	72	66	0
71	J	58	0	60	14	0
72	2	46	0	66	32	0
72	4	46	0	66	13	0
72	L	47	0	71	34	0
72	S	47	0	69	15	0
72	j	39	0	55	1	0
73	8	31	0	19	39	0
74	8	8	0	0	3	0
74	A	16	0	0	11	0
74	D	8	0	0	7	0
74	E	16	0	0	1	0
75	A6	1	0	0	0	0
75	I	1	0	0	0	0
76	R	48	0	23	10	0
77	m	86	0	60	10	0
77	y	86	0	60	10	0
78	o	43	0	32	1	0
78	z	43	0	32	1	0
79	A9	120	0	108	3	0
80	A9	1	0	0	0	0
80	C4	2	0	0	0	0
81	A9	1	0	0	0	0
All	All	107305	0	103928	6529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 6529 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:449:LEU:CB	71:4:502:CDL:H311	1.22	1.66
5:6:55:ILE:HD11	38:d:74:PHE:CZ	1.31	1.66
14:E:62:LEU:HD13	30:V:36:PHE:CZ	1.22	1.66
27:S:284:MET:CB	72:S:401:PC1:C12	1.76	1.61
49:A0:106:ILE:C	49:A0:167:ALA:HB1	1.27	1.60

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	20
2	4	457/459 (100%)	393 (86%)	56 (12%)	8 (2%)	6	33
3	2	342/347 (99%)	283 (83%)	57 (17%)	2 (1%)	21	58
4	7	170/175 (97%)	138 (81%)	25 (15%)	7 (4%)	2	18
5	6	604/606 (100%)	517 (86%)	84 (14%)	3 (0%)	24	63
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	14	49
8	1	316/318 (99%)	255 (81%)	48 (15%)	13 (4%)	2	18
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	7	37
10	A	686/704 (97%)	559 (82%)	112 (16%)	15 (2%)	5	29
11	B	428/430 (100%)	343 (80%)	79 (18%)	6 (1%)	9	39
12	C	206/228 (90%)	173 (84%)	30 (15%)	3 (2%)	8	38
13	D	150/179 (84%)	121 (81%)	25 (17%)	4 (3%)	4	25
14	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	2	19
16	G	121/133 (91%)	101 (84%)	19 (16%)	1 (1%)	16	53
17	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	3	21
18	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	17
19	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	3	22
20	K	82/98 (84%)	65 (79%)	16 (20%)	1 (1%)	10	42
21	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
22	N	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
23	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	4	25
24	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
25	Q	166/171 (97%)	112 (68%)	51 (31%)	3 (2%)	6	33
26	R	315/345 (91%)	243 (77%)	65 (21%)	7 (2%)	5	29
27	S	317/320 (99%)	240 (76%)	67 (21%)	10 (3%)	3	21
28	T	136/140 (97%)	102 (75%)	15 (11%)	19 (14%)	0	3
29	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
30	V	136/143 (95%)	110 (81%)	22 (16%)	4 (3%)	3	23
31	M	78/88 (89%)	56 (72%)	19 (24%)	3 (4%)	2	19
31	W	84/88 (96%)	68 (81%)	15 (18%)	1 (1%)	10	42
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
33	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	6	33
34	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	4	24
35	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
36	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	18	55
37	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
38	d	105/117 (90%)	87 (83%)	15 (14%)	3 (3%)	3	23
39	f	165/178 (93%)	130 (79%)	33 (20%)	2 (1%)	10	42
40	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	2	19
41	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
42	j	111/120 (92%)	94 (85%)	17 (15%)	0	100	100
43	g	171/176 (97%)	141 (82%)	29 (17%)	1 (1%)	21	58
44	e	139/158 (88%)	81 (58%)	45 (32%)	13 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	k	444/480 (92%)	407 (92%)	34 (8%)	3 (1%)	18	55
45	w	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	18	55
46	l	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	43	77
46	x	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	43	77
47	m	377/379 (100%)	348 (92%)	29 (8%)	0	100	100
47	y	377/379 (100%)	349 (93%)	28 (7%)	0	100	100
48	o	239/241 (99%)	213 (89%)	21 (9%)	5 (2%)	5	30
48	z	239/241 (99%)	213 (89%)	20 (8%)	6 (2%)	4	26
49	A0	184/196 (94%)	105 (57%)	48 (26%)	31 (17%)	0	2
49	p	147/196 (75%)	101 (69%)	33 (22%)	13 (9%)	0	9
50	A1	104/111 (94%)	91 (88%)	7 (7%)	6 (6%)	1	14
50	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
51	A2	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
51	r	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
52	B3	67/91 (74%)	59 (88%)	6 (9%)	2 (3%)	3	22
52	s	65/91 (71%)	58 (89%)	5 (8%)	2 (3%)	3	22
53	A3	37/56 (66%)	23 (62%)	10 (27%)	4 (11%)	0	6
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	3	21
54	B2	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
54	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
55	B1	20/78 (26%)	10 (50%)	7 (35%)	3 (15%)	0	3
55	v	16/78 (20%)	8 (50%)	6 (38%)	2 (12%)	0	4
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
57	C4	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	41
58	C2	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	C0	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	A6	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
62	A4	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	13
63	A5	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	39
64	B4	71/74 (96%)	65 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	C3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	19
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	C1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13638/14963 (91%)	11529 (84%)	1839 (14%)	270 (2%)	8	31

5 of 270 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	84	TRP
4	7	141	MET
4	7	171	ILE
8	1	170	GLU
8	1	174	LEU

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	9	169/183 (92%)	166 (98%)	3 (2%)	51	67
2	4	389/413 (94%)	389 (100%)	0	100	100
3	2	304/316 (96%)	302 (99%)	2 (1%)	76	79
4	7	116/142 (82%)	115 (99%)	1 (1%)	70	76
5	6	524/534 (98%)	520 (99%)	4 (1%)	73	77
6	5	80/86 (93%)	80 (100%)	0	100	100
7	3	95/101 (94%)	95 (100%)	0	100	100
8	1	274/275 (100%)	257 (94%)	17 (6%)	16	38
9	8	270/353 (76%)	269 (100%)	1 (0%)	84	82
10	A	560/588 (95%)	556 (99%)	4 (1%)	76	79
11	B	363/371 (98%)	356 (98%)	7 (2%)	50	66
12	C	188/204 (92%)	186 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	D	127/150 (85%)	122 (96%)	5 (4%)	28	49
14	E	148/151 (98%)	145 (98%)	3 (2%)	48	65
15	F	14/69 (20%)	14 (100%)	0	100	100
16	G	106/119 (89%)	106 (100%)	0	100	100
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	53/79 (67%)	49 (92%)	4 (8%)	12	33
19	J	50/59 (85%)	49 (98%)	1 (2%)	48	65
20	K	67/81 (83%)	67 (100%)	0	100	100
21	L	63/71 (89%)	63 (100%)	0	100	100
22	N	88/101 (87%)	88 (100%)	0	100	100
23	O	95/113 (84%)	95 (100%)	0	100	100
24	P	73/96 (76%)	72 (99%)	1 (1%)	59	71
25	Q	142/154 (92%)	141 (99%)	1 (1%)	76	79
26	R	232/298 (78%)	230 (99%)	2 (1%)	70	76
27	S	205/283 (72%)	204 (100%)	1 (0%)	81	81
28	T	73/101 (72%)	48 (66%)	25 (34%)	0	2
29	U	95/131 (72%)	95 (100%)	0	100	100
30	V	106/120 (88%)	106 (100%)	0	100	100
31	M	73/81 (90%)	73 (100%)	0	100	100
31	W	57/81 (70%)	55 (96%)	2 (4%)	32	53
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/76 (37%)	28 (100%)	0	100	100
35	a	70/114 (61%)	70 (100%)	0	100	100
36	b	85/124 (68%)	85 (100%)	0	100	100
37	c	45/122 (37%)	45 (100%)	0	100	100
38	d	44/107 (41%)	44 (100%)	0	100	100
39	f	80/160 (50%)	80 (100%)	0	100	100
40	h	63/112 (56%)	63 (100%)	0	100	100
41	i	23/45 (51%)	23 (100%)	0	100	100
42	j	86/106 (81%)	85 (99%)	1 (1%)	63	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	g	130/157 (83%)	129 (99%)	1 (1%)	73	77
44	e	44/141 (31%)	41 (93%)	3 (7%)	14	36
45	k	369/394 (94%)	369 (100%)	0	100	100
45	w	362/394 (92%)	362 (100%)	0	100	100
46	l	327/355 (92%)	327 (100%)	0	100	100
46	x	328/355 (92%)	328 (100%)	0	100	100
47	m	327/327 (100%)	326 (100%)	1 (0%)	86	84
47	y	327/327 (100%)	326 (100%)	1 (0%)	86	84
48	o	206/206 (100%)	206 (100%)	0	100	100
48	z	202/206 (98%)	202 (100%)	0	100	100
49	A0	64/168 (38%)	61 (95%)	3 (5%)	23	45
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	92 (96%)	4 (4%)	26	48
50	q	96/99 (97%)	96 (100%)	0	100	100
51	A2	70/72 (97%)	69 (99%)	1 (1%)	59	71
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B3	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	31/46 (67%)	28 (90%)	3 (10%)	8	25
53	t	24/46 (52%)	23 (96%)	1 (4%)	26	48
54	B2	52/54 (96%)	50 (96%)	2 (4%)	29	51
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B1	15/60 (25%)	15 (100%)	0	100	100
55	v	11/60 (18%)	11 (100%)	0	100	100
56	A9	427/427 (100%)	387 (91%)	40 (9%)	8	26
57	C4	211/211 (100%)	192 (91%)	19 (9%)	9	28
58	C2	226/226 (100%)	207 (92%)	19 (8%)	10	30
59	A7	128/148 (86%)	119 (93%)	9 (7%)	14	36
60	C0	95/123 (77%)	89 (94%)	6 (6%)	16	38
61	A6	81/103 (79%)	81 (100%)	0	100	100
62	A4	68/79 (86%)	66 (97%)	2 (3%)	37	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	A5	67/76 (88%)	64 (96%)	3 (4%)	24	46
64	B4	58/59 (98%)	53 (91%)	5 (9%)	10	29
65	C3	47/68 (69%)	41 (87%)	6 (13%)	4	17
66	B0	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	C1	40/55 (73%)	40 (100%)	0	100	100
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10787/12809 (84%)	10565 (98%)	222 (2%)	46	65

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	A9	150	LEU
68	A8	42	LYS
56	A9	492	LEU
68	A8	13	LYS
60	C0	90	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 212 such sidechains are listed below:

Mol	Chain	Res	Type
46	l	290	ASN
46	x	198	HIS
63	A5	24	ASN
47	m	8	HIS
48	o	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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
77	HEM	m	401	47	50,50,50	1.70	14 (28%)	67,82,82	1.28	6 (8%)
74	SF4	E	301	14	0,12,12	-	-	-		
74	SF4	E	302	14	0,12,12	-	-	-		
71	CDL	4	502	-	81,81,99	0.99	8 (9%)	87,93,111	1.16	4 (4%)
69	FES	9	301	1	0,4,4	-	-	-		
72	PC1	4	504	-	45,45,53	1.07	3 (6%)	51,53,61	1.14	2 (3%)
71	CDL	J	101	-	57,57,99	1.18	7 (12%)	63,69,111	1.20	5 (7%)
72	PC1	L	200	-	46,46,53	1.00	3 (6%)	52,54,61	1.09	2 (3%)
79	HEA	A9	602	56	67,67,67	1.20	7 (10%)	81,103,103	1.35	12 (14%)
77	HEM	y	401	47	50,50,50	1.70	15 (30%)	67,82,82	1.27	6 (8%)
79	HEA	A9	601	56	67,67,67	1.20	4 (5%)	81,103,103	1.33	10 (12%)
69	FES	A	803	10	0,4,4	-	-	-		
70	3PE	4	503	-	40,40,50	0.91	3 (7%)	43,45,55	1.38	3 (6%)
73	FMN	8	501	-	33,33,33	1.19	2 (6%)	48,50,50	1.68	13 (27%)
69	FES	m	403	-	0,4,4	-	-	-		
70	3PE	B	501	-	50,50,50	0.89	2 (4%)	53,55,55	1.34	4 (7%)
71	CDL	6	701	-	63,63,99	1.09	7 (11%)	69,75,111	1.27	4 (5%)
78	HEC	z	301	48	46,50,50	1.95	7 (15%)	58,82,82	2.03	5 (8%)
70	3PE	2	401	-	45,45,50	0.91	3 (6%)	48,50,55	1.08	2 (4%)
72	PC1	S	401	-	46,46,53	1.05	5 (10%)	52,54,61	1.09	2 (3%)
74	SF4	8	502	-	0,12,12	-	-	-		
76	NAP	R	601	-	50,52,52	4.22	22 (44%)	71,80,80	1.97	18 (25%)
74	SF4	A	802	-	0,12,12	-	-	-		
77	HEM	m	402	47	50,50,50	1.60	13 (26%)	67,82,82	1.13	5 (7%)
77	HEM	y	402	47	50,50,50	1.59	12 (24%)	67,82,82	1.13	5 (7%)
72	PC1	2	402	-	45,45,53	1.03	4 (8%)	51,53,61	1.00	2 (3%)
74	SF4	A	801	10	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PC1	j	201	-	38,38,53	1.17	6 (15%)	44,46,61	1.02	2 (4%)
74	SF4	D	301	13	0,12,12	-	-	-	-	-
70	3PE	4	501	-	40,40,50	1.03	2 (5%)	43,45,55	1.11	3 (6%)
78	HEC	o	301	48	46,50,50	1.95	7 (15%)	58,82,82	2.03	5 (8%)

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
77	HEM	m	401	47	-	4/14/54/54	-
74	SF4	E	301	14	-	-	0/6/5/5
74	SF4	E	302	14	-	-	0/6/5/5
71	CDL	4	502	-	-	39/92/92/110	-
69	FES	9	301	1	-	-	0/1/1/1
72	PC1	4	504	-	-	23/49/49/57	-
71	CDL	J	101	-	-	23/68/68/110	-
72	PC1	L	200	-	-	23/50/50/57	-
79	HEA	A9	602	56	-	7/36/76/76	-
77	HEM	y	401	47	-	4/14/54/54	-
79	HEA	A9	601	56	-	7/36/76/76	-
70	3PE	4	503	-	-	23/44/44/54	-
69	FES	A	803	10	-	-	0/1/1/1
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
69	FES	m	403	-	-	-	0/1/1/1
70	3PE	B	501	-	-	28/54/54/54	-
71	CDL	6	701	-	-	33/74/74/110	-
78	HEC	z	301	48	-	9/14/54/54	-
70	3PE	2	401	-	-	22/49/49/54	-
72	PC1	S	401	-	-	26/50/50/57	-
74	SF4	8	502	-	-	-	0/6/5/5
76	NAP	R	601	-	-	16/35/67/67	0/5/5/5
74	SF4	A	802	-	-	-	0/6/5/5
77	HEM	m	402	47	-	2/14/54/54	-
77	HEM	y	402	47	-	2/14/54/54	-
72	PC1	2	402	-	-	29/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	SF4	A	801	10	-	-	0/6/5/5
72	PC1	j	201	-	-	21/42/42/57	-
74	SF4	D	301	13	-	-	0/6/5/5
70	3PE	4	501	-	-	29/44/44/54	-
78	HEC	o	301	48	-	9/14/54/54	-

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	O4D-C1D	16.50	1.62	1.40
76	R	601	NAP	C2B-C1B	-10.09	1.28	1.53
76	R	601	NAP	O4B-C1B	8.67	1.62	1.42
76	R	601	NAP	PN-O3	8.60	1.68	1.59
76	R	601	NAP	C7N-N7N	7.16	1.46	1.33

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	z	301	HEC	CBC-CAC-C3C	-9.52	108.40	127.43
78	o	301	HEC	CBC-CAC-C3C	-9.49	108.46	127.43
78	o	301	HEC	CBB-CAB-C3B	-9.26	108.93	127.43
78	z	301	HEC	CBB-CAB-C3B	-9.25	108.94	127.43
76	R	601	NAP	N3A-C2A-N1A	-6.58	118.62	128.58

There are no chirality outliers.

5 of 388 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	4	501	3PE	C11-O13-P-O11
70	4	501	3PE	C11-O13-P-O12
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	O13-C11-C12-N
70	4	501	3PE	C22-C21-O21-C2

There are no ring outliers.

27 monomers are involved in 414 short contacts:

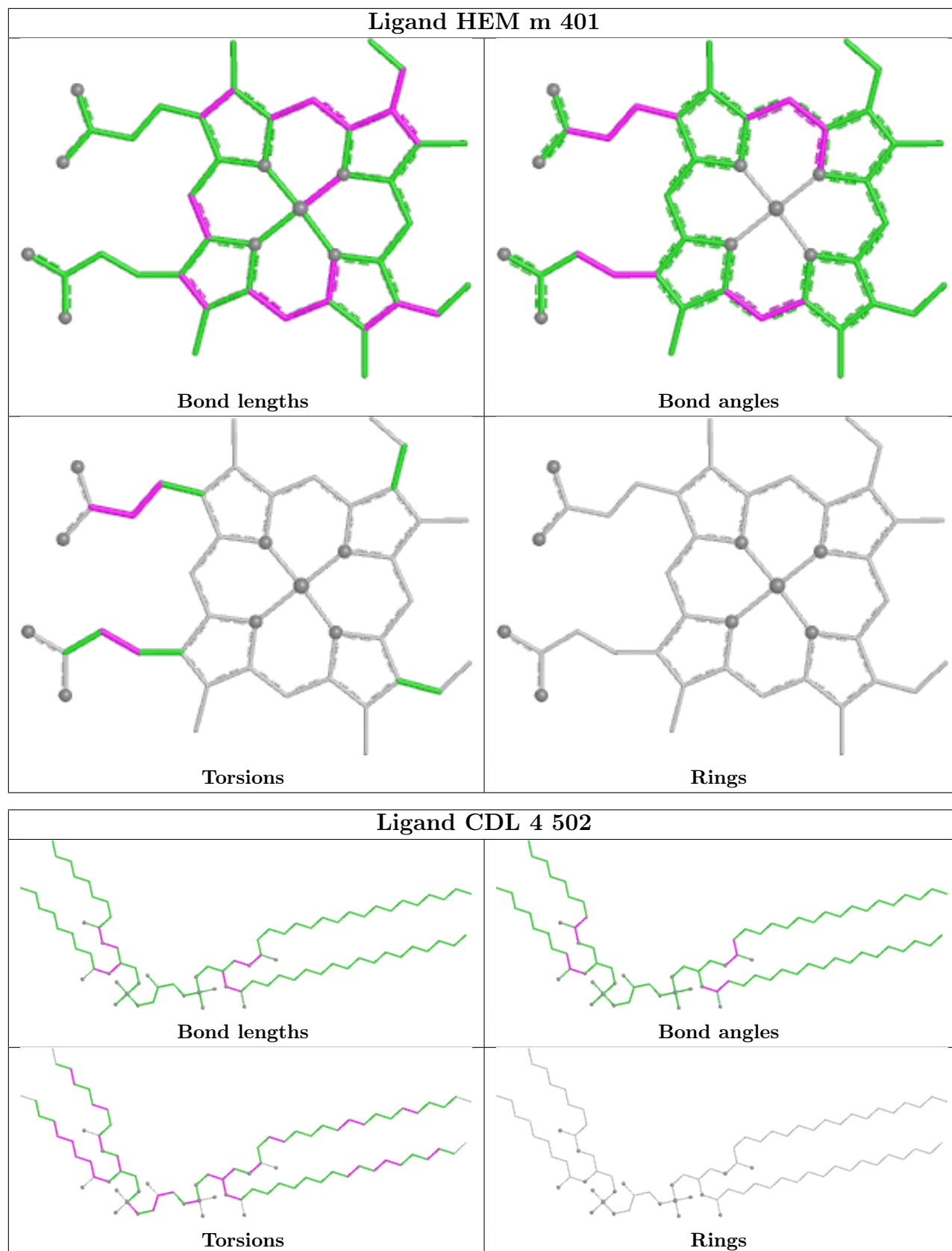
Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	m	401	HEM	4	0
74	E	302	SF4	1	0

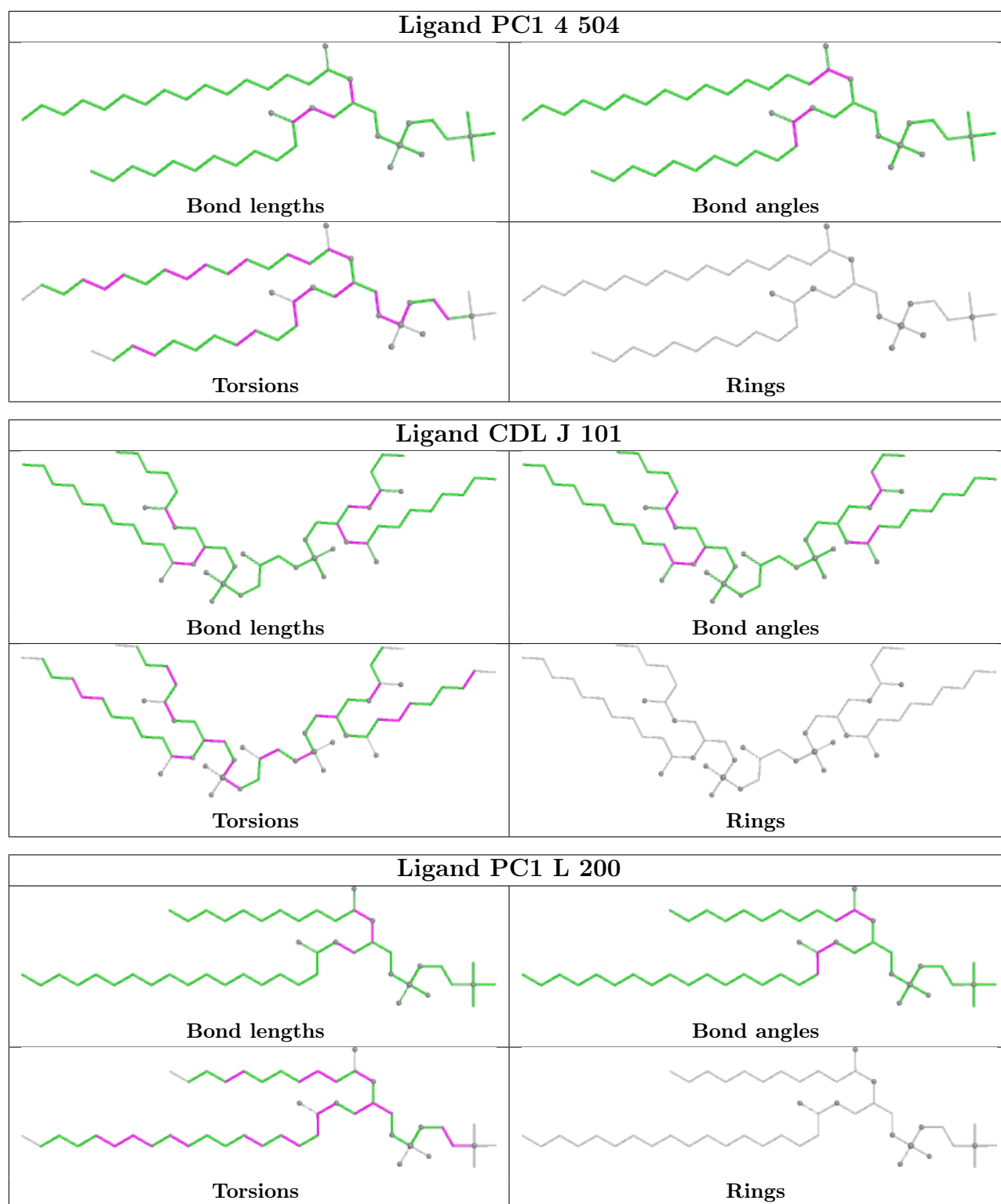
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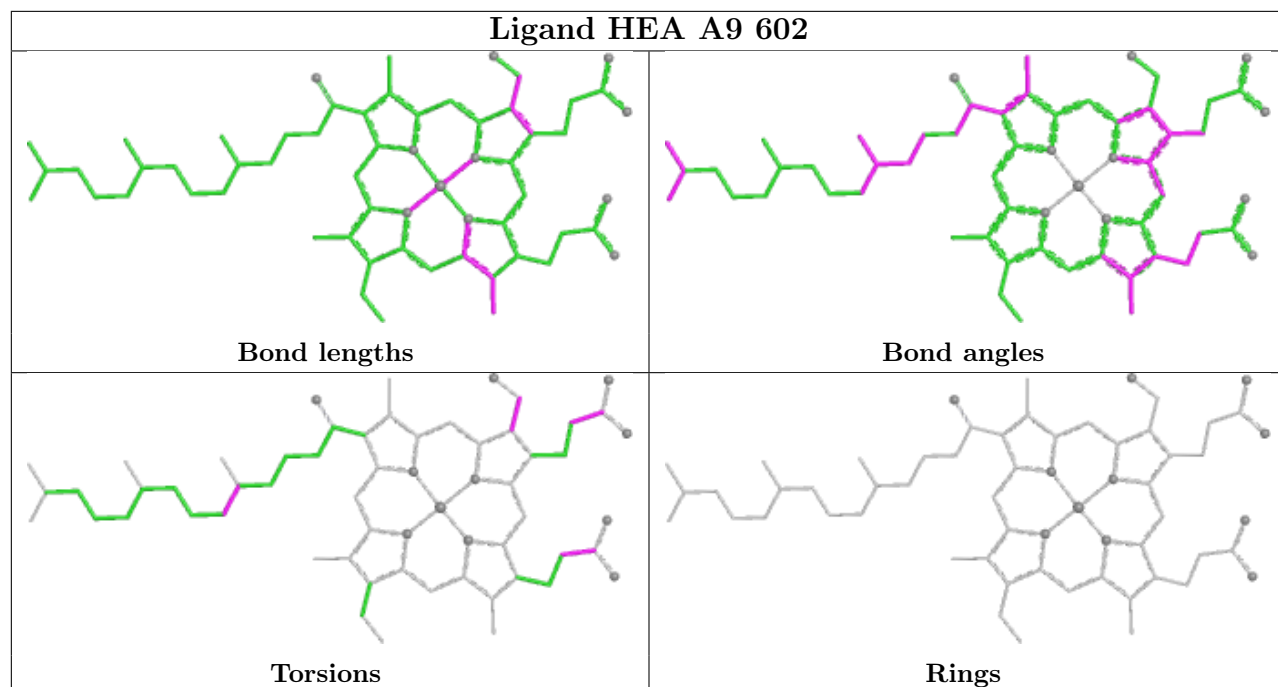
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	4	502	CDL	44	0
72	4	504	PC1	13	0
71	J	101	CDL	14	0
72	L	200	PC1	34	0
79	A9	602	HEA	3	0
77	y	401	HEM	4	0
69	A	803	FES	2	0
70	4	503	3PE	25	0
73	8	501	FMN	39	0
70	B	501	3PE	27	0
71	6	701	CDL	66	0
78	z	301	HEC	1	0
70	2	401	3PE	18	0
72	S	401	PC1	15	0
74	8	502	SF4	3	0
76	R	601	NAP	10	0
74	A	802	SF4	5	0
77	m	402	HEM	6	0
77	y	402	HEM	6	0
72	2	402	PC1	32	0
74	A	801	SF4	6	0
72	j	201	PC1	1	0
74	D	301	SF4	7	0
70	4	501	3PE	27	0
78	o	301	HEC	1	0

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

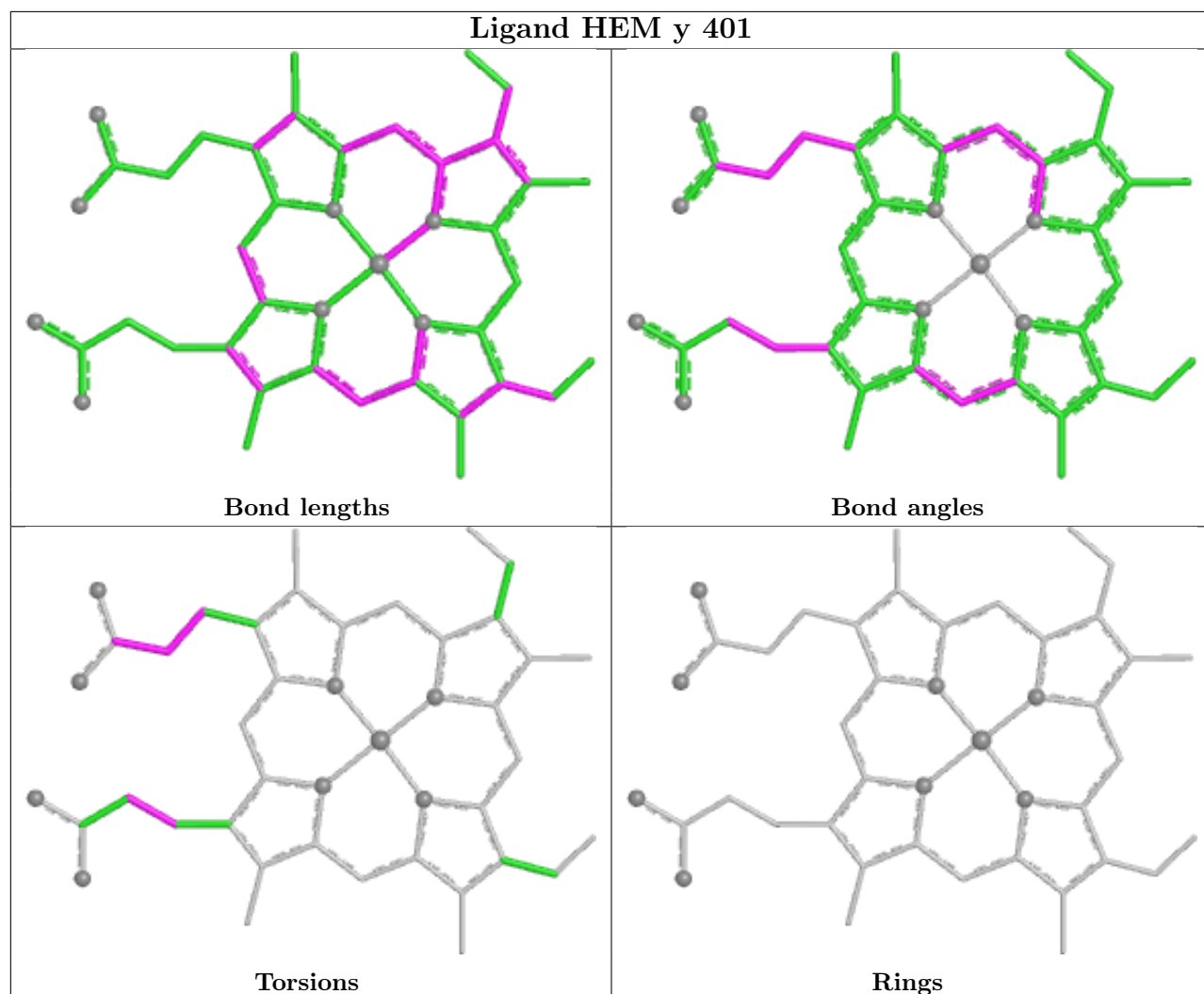


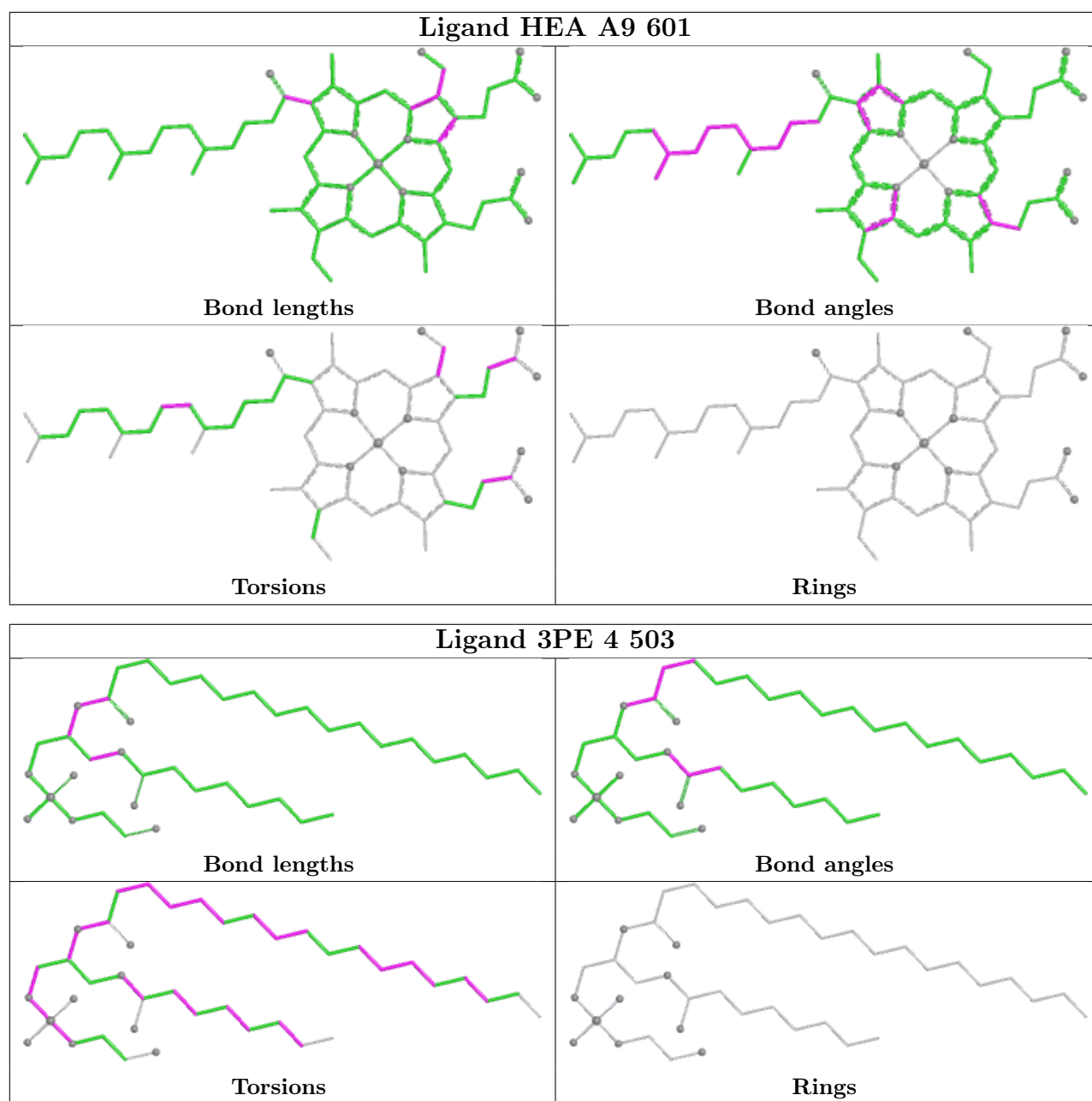


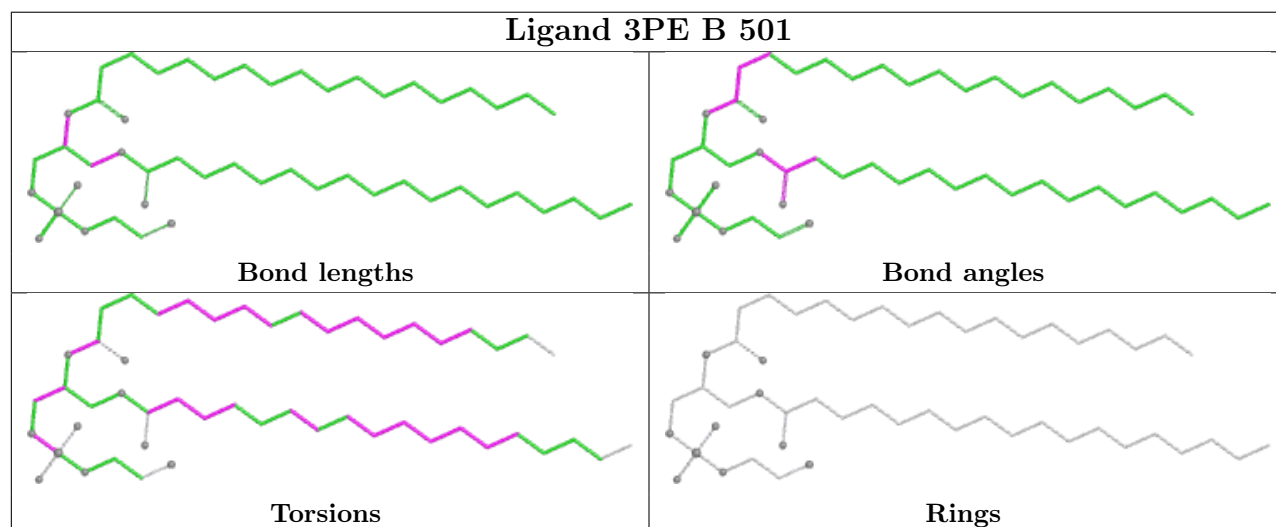
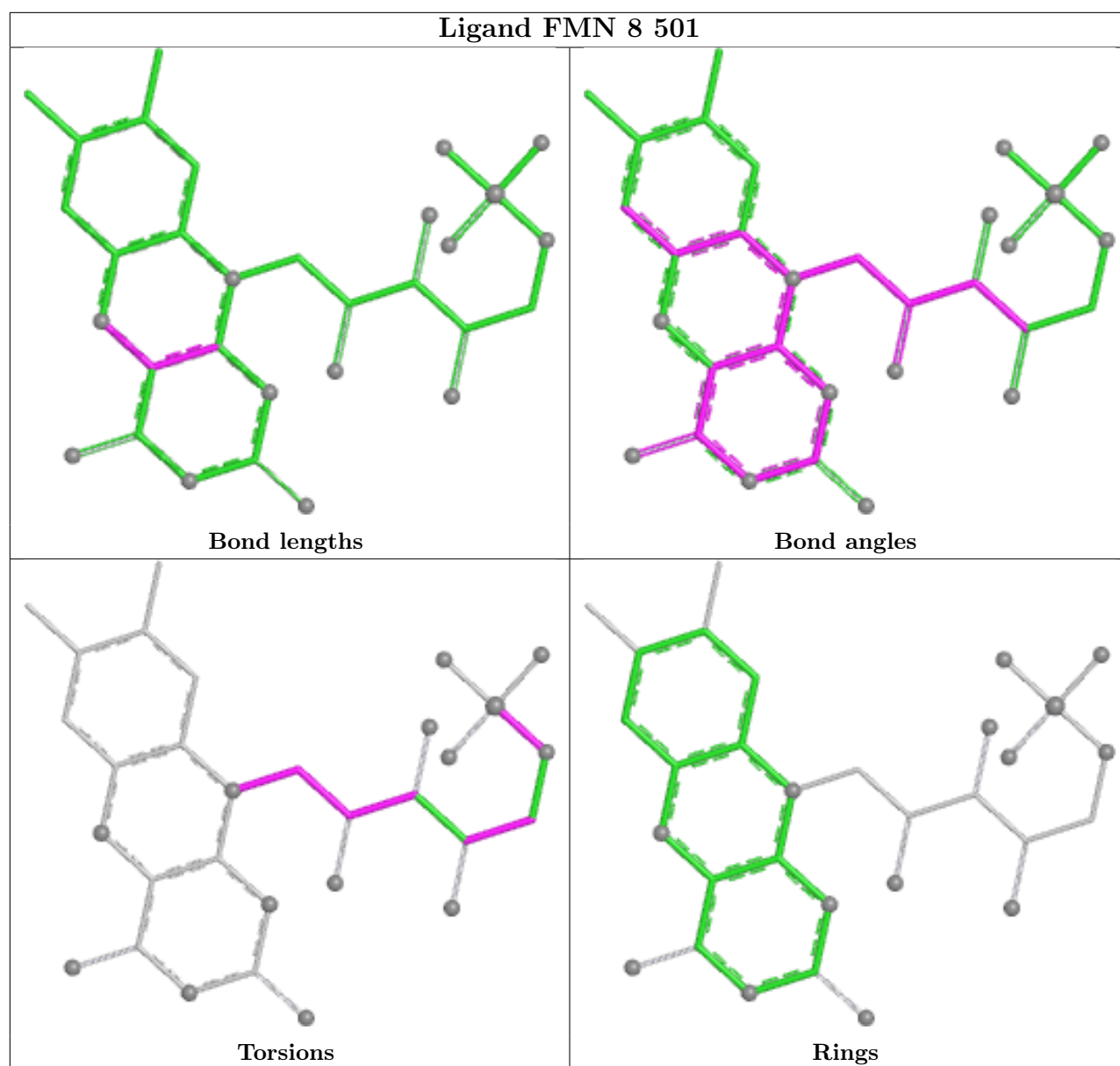
Ligand HEA A9 602

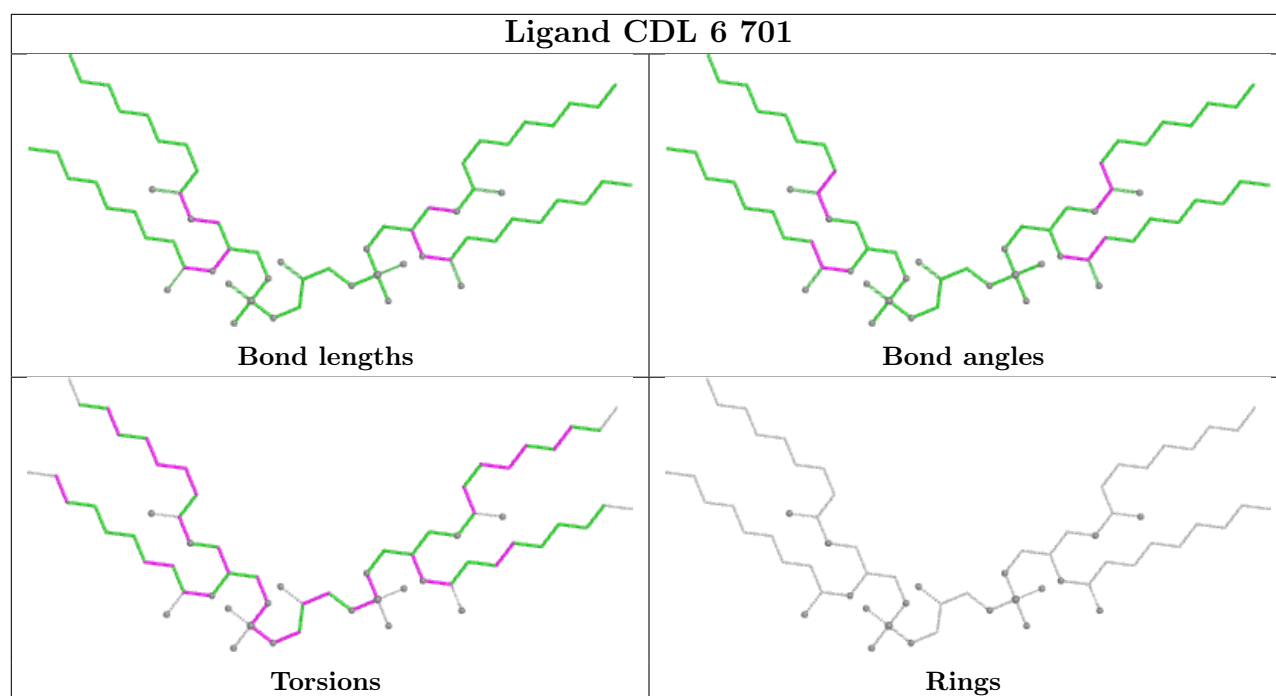


Ligand HEM y 401

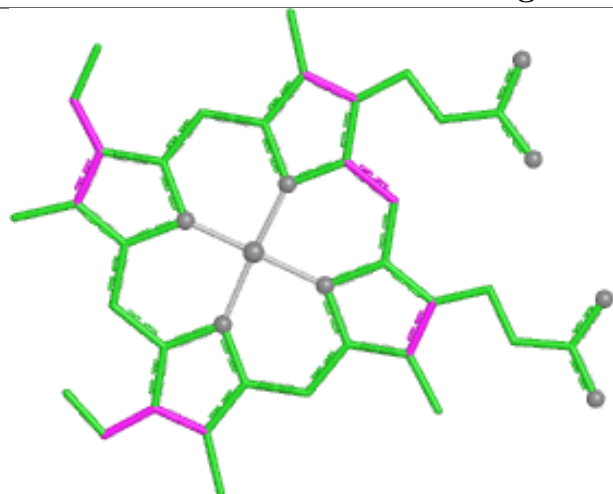




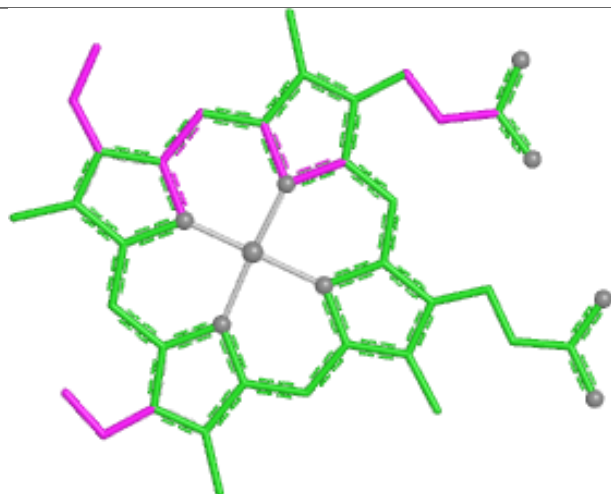




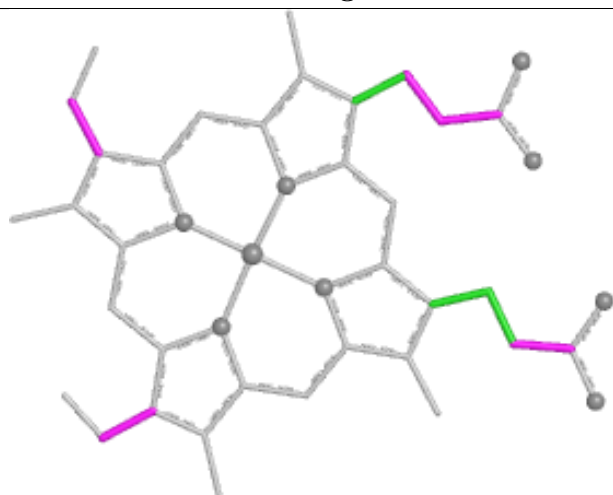
Ligand HEC z 301



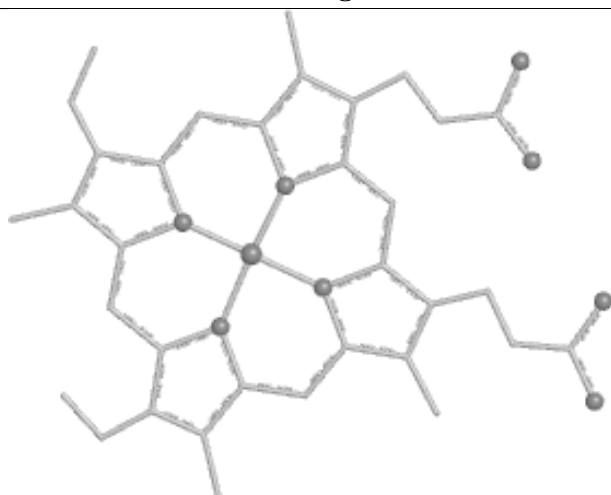
Bond lengths



Bond angles

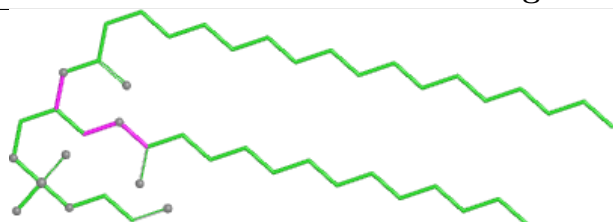


Torsions

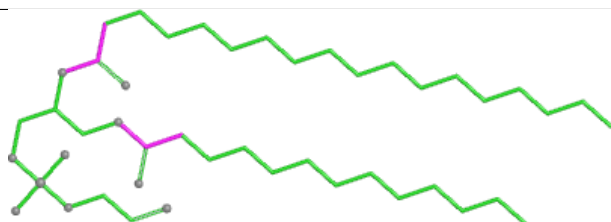


Rings

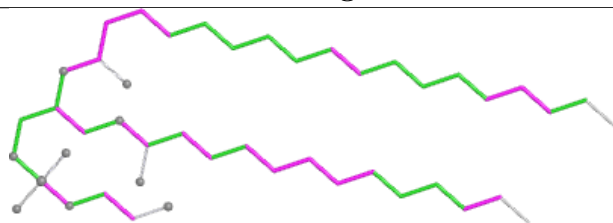
Ligand 3PE 2 401



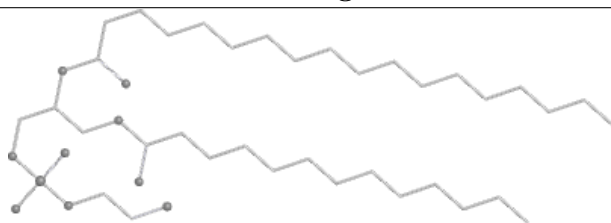
Bond lengths



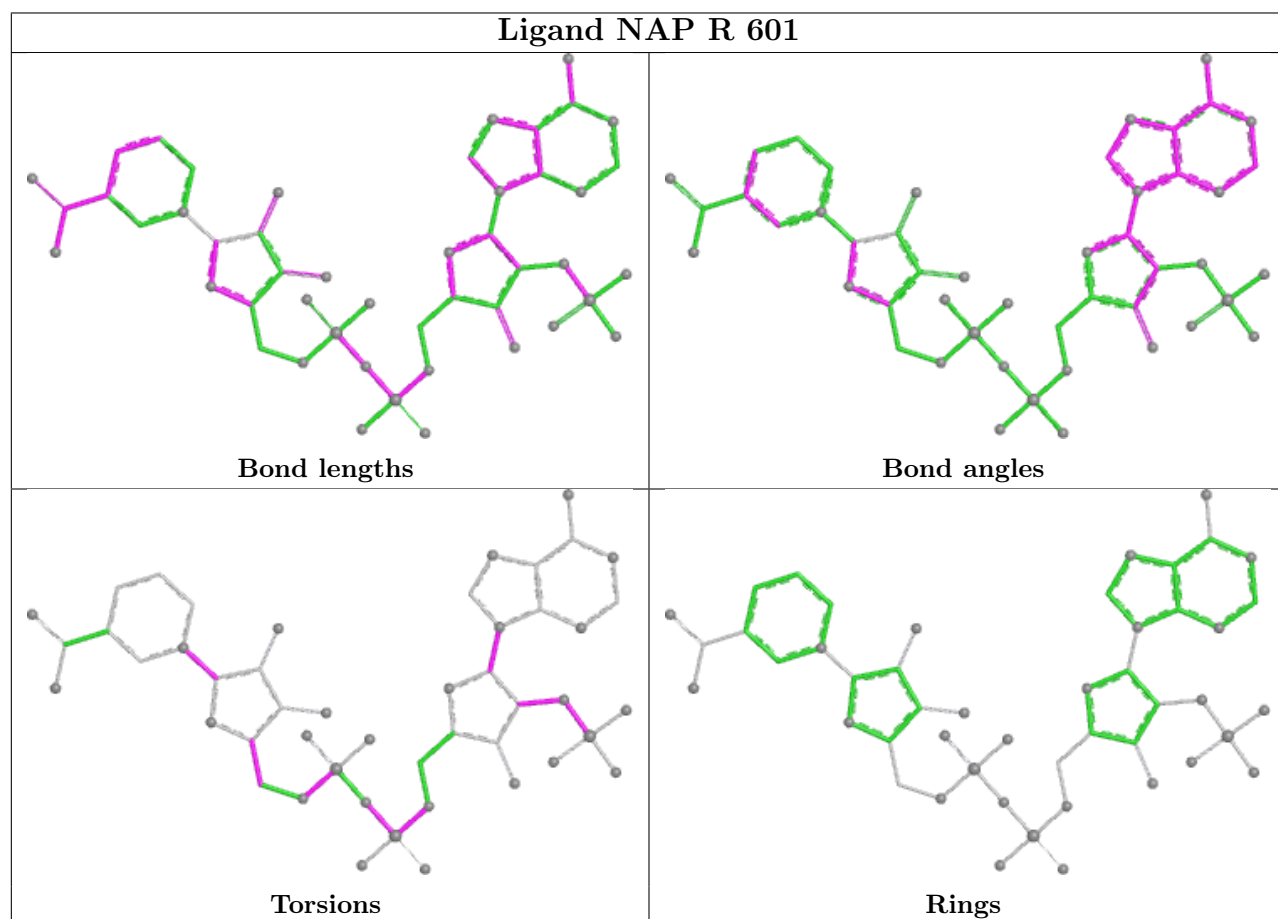
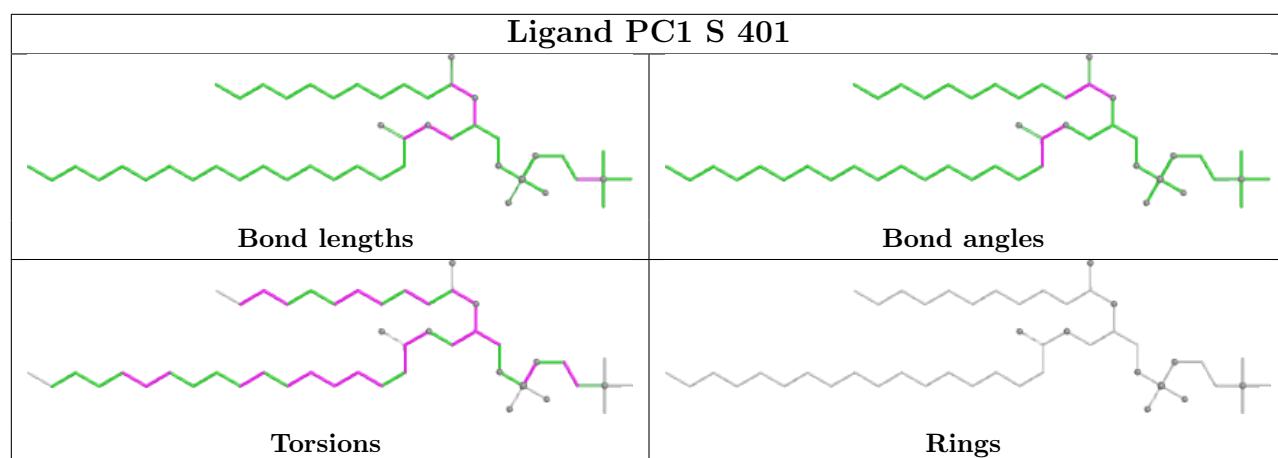
Bond angles

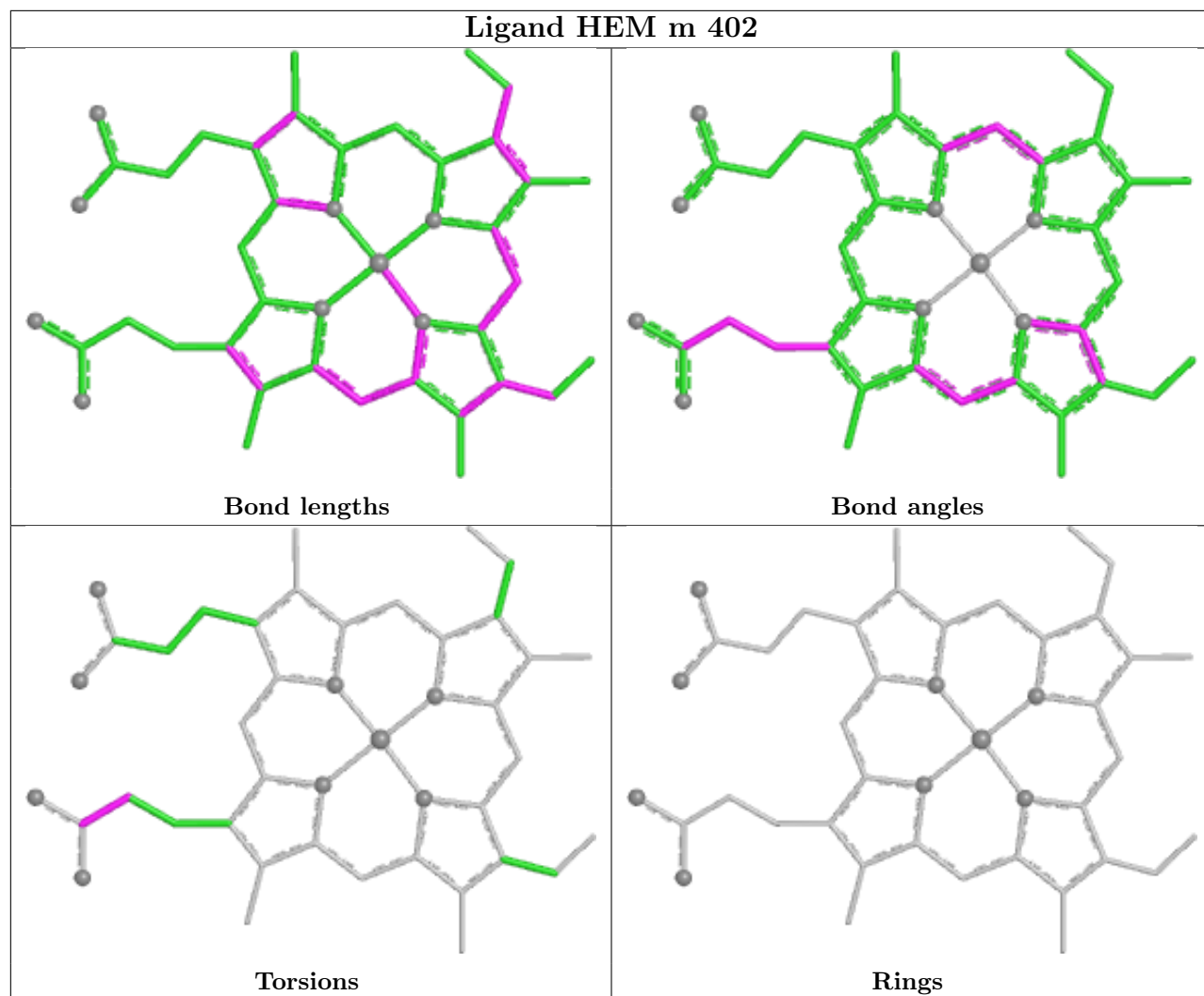


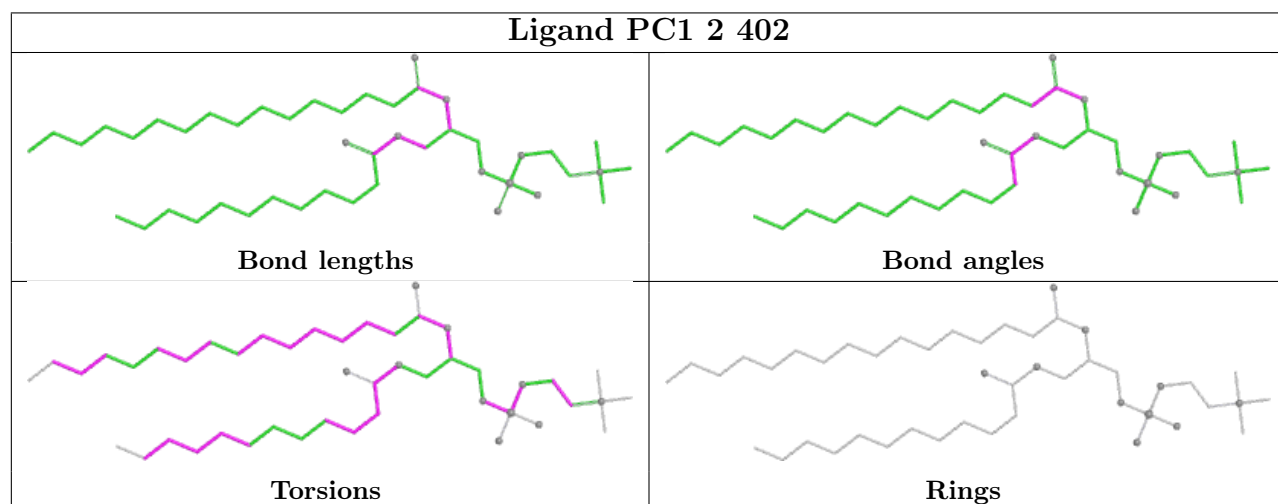
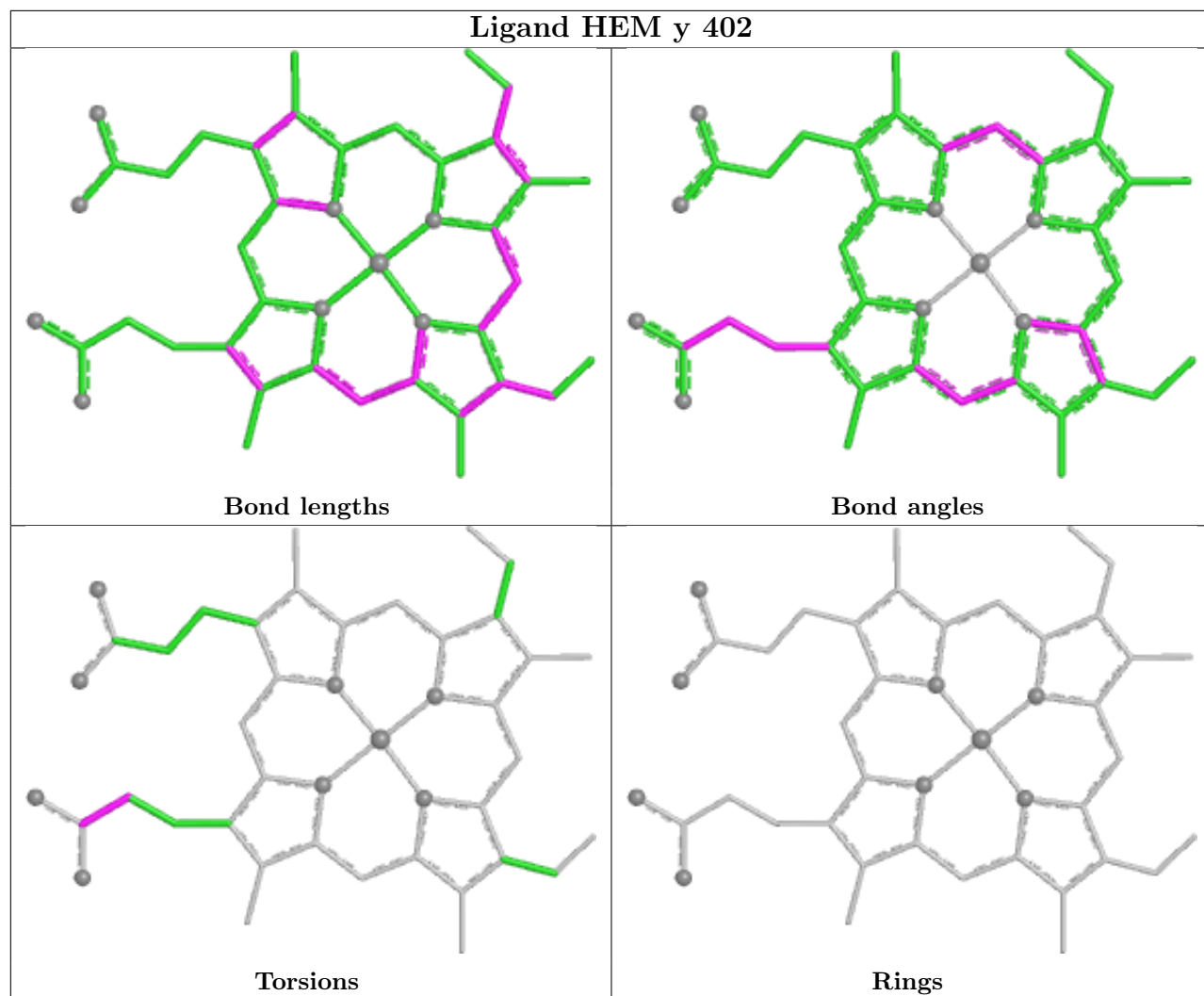
Torsions

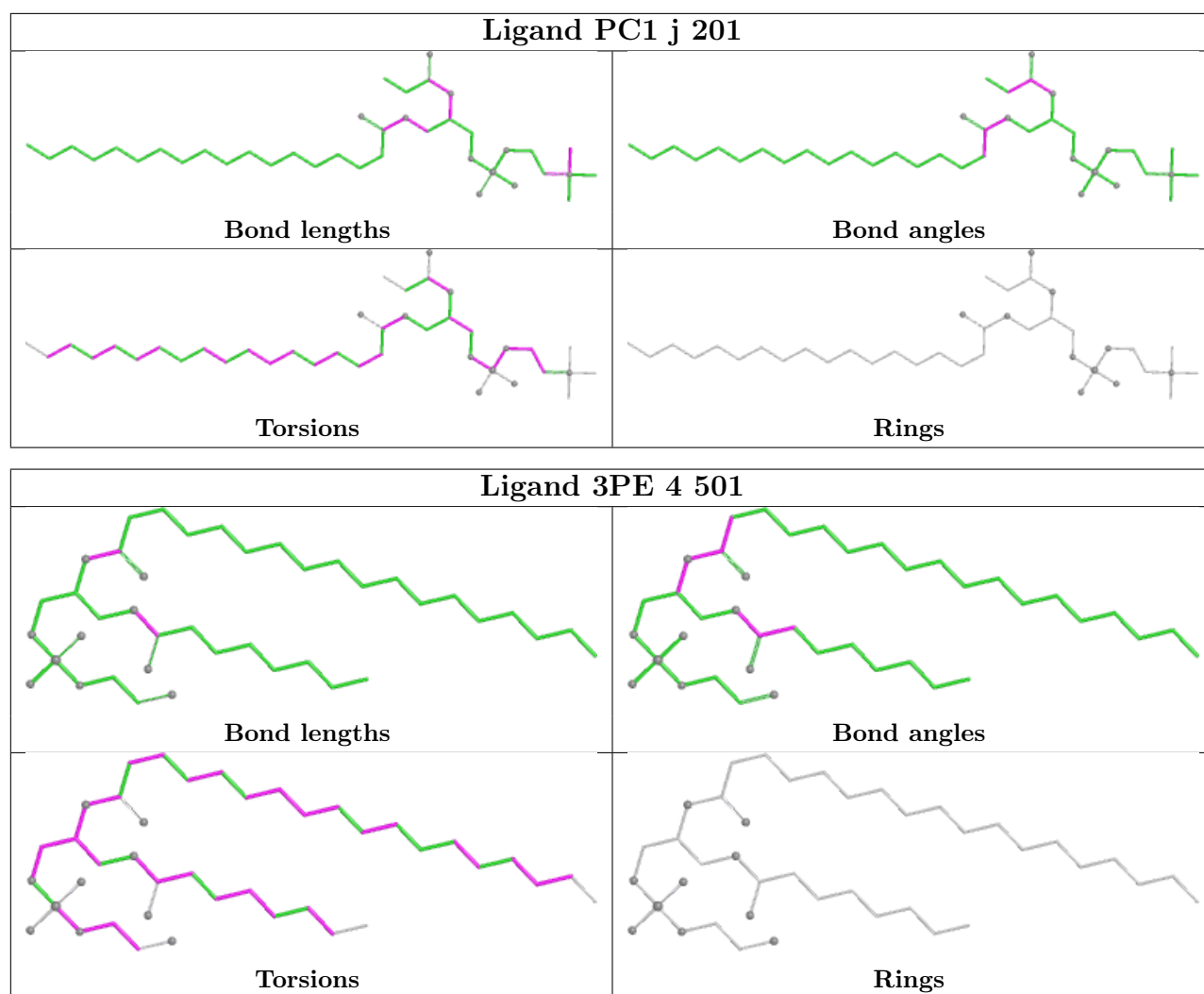


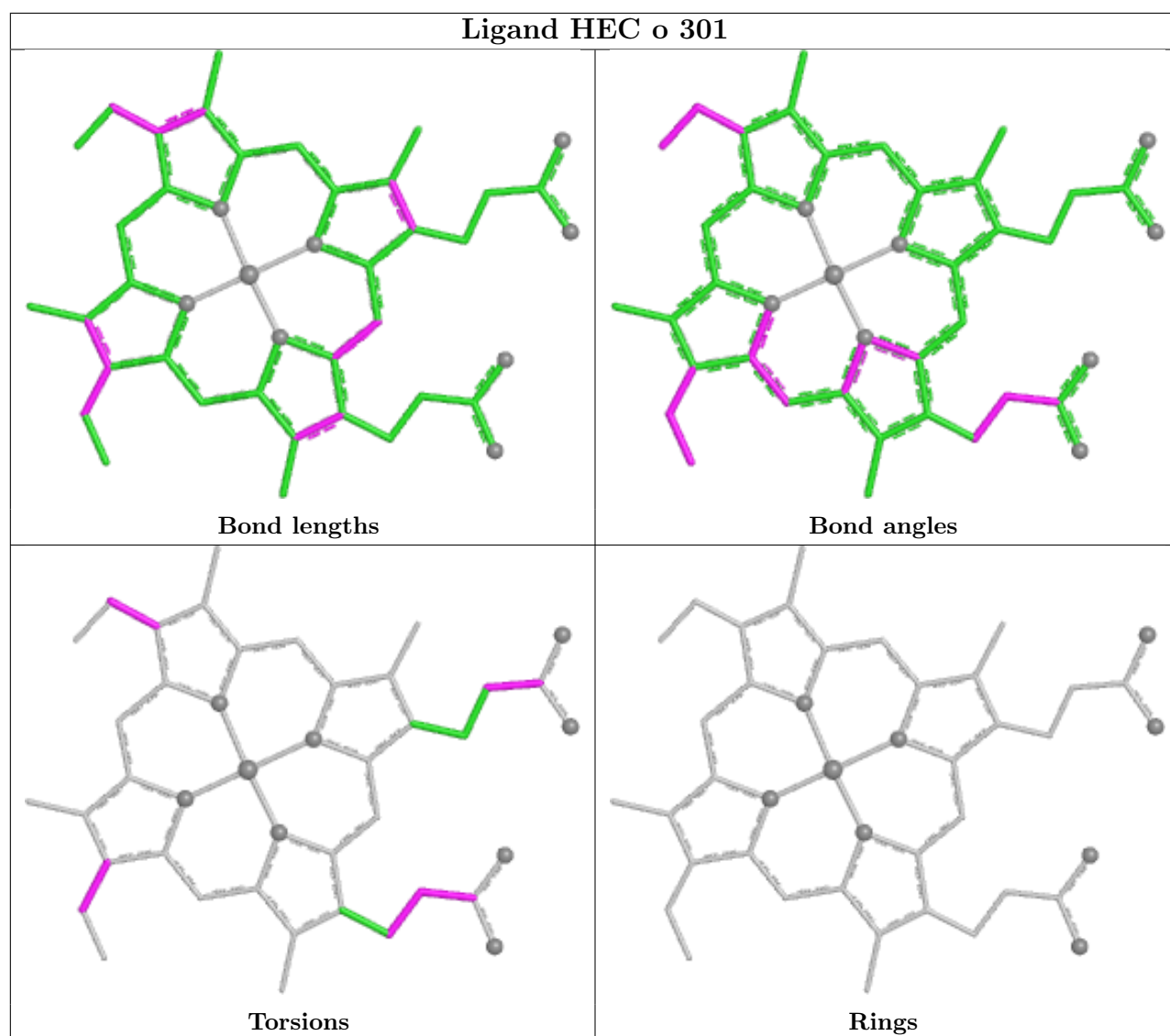
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

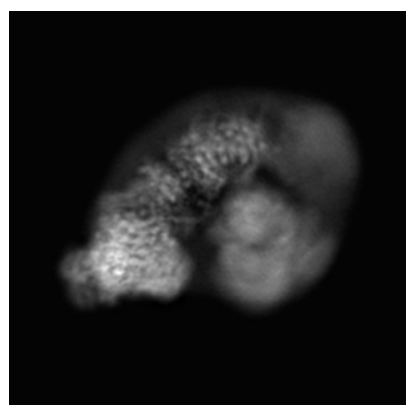
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30674. These allow visual inspection of the internal detail of the map and identification of artifacts.

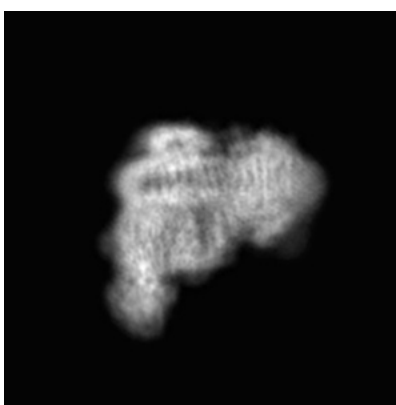
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

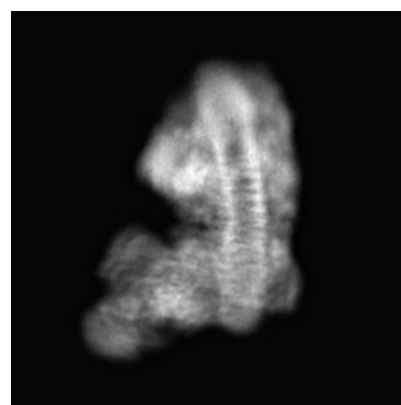
6.1.1 Primary map



X



Y

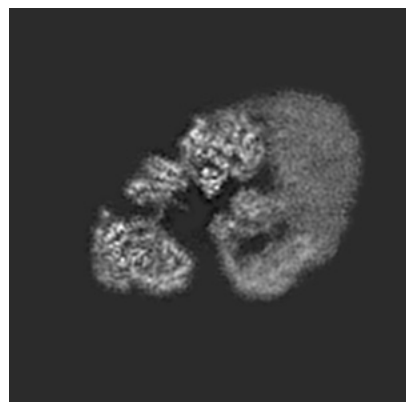


Z

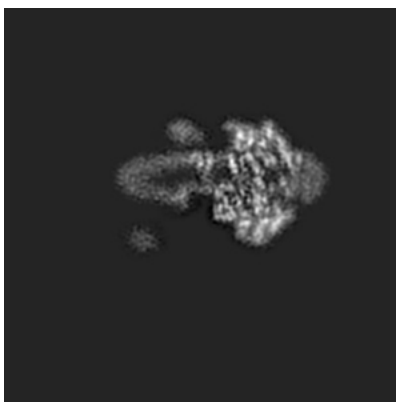
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

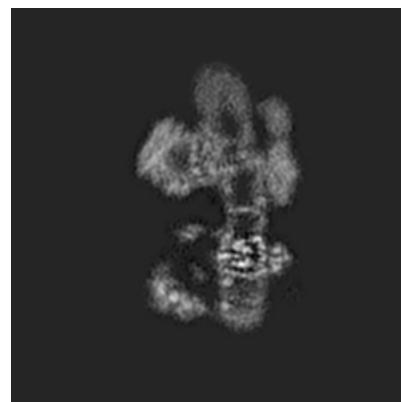
6.2.1 Primary map



X Index: 140



Y Index: 140

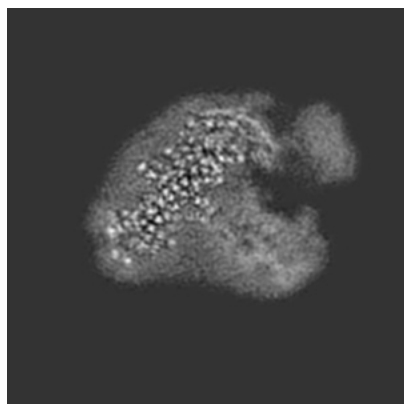


Z Index: 140

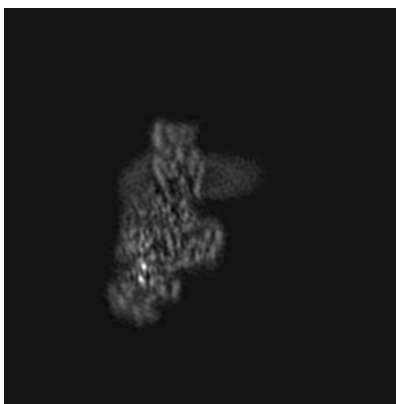
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

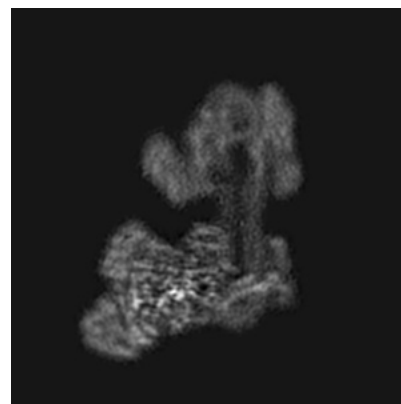
6.3.1 Primary map



X Index: 173



Y Index: 75

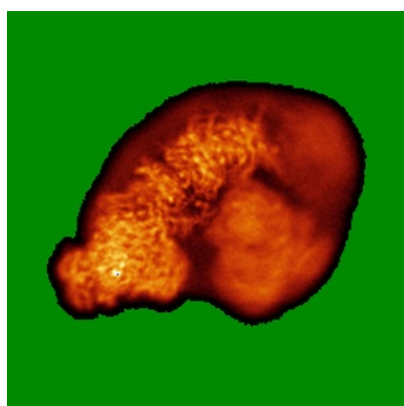


Z Index: 103

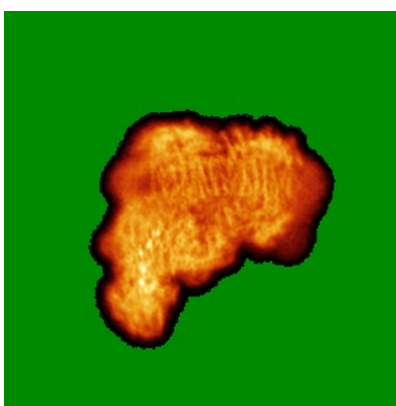
The images above show the largest variance slices of the map in three orthogonal directions.

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

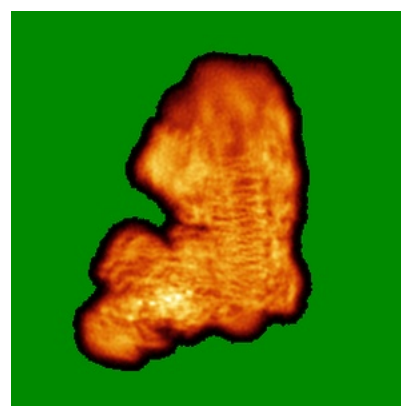
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

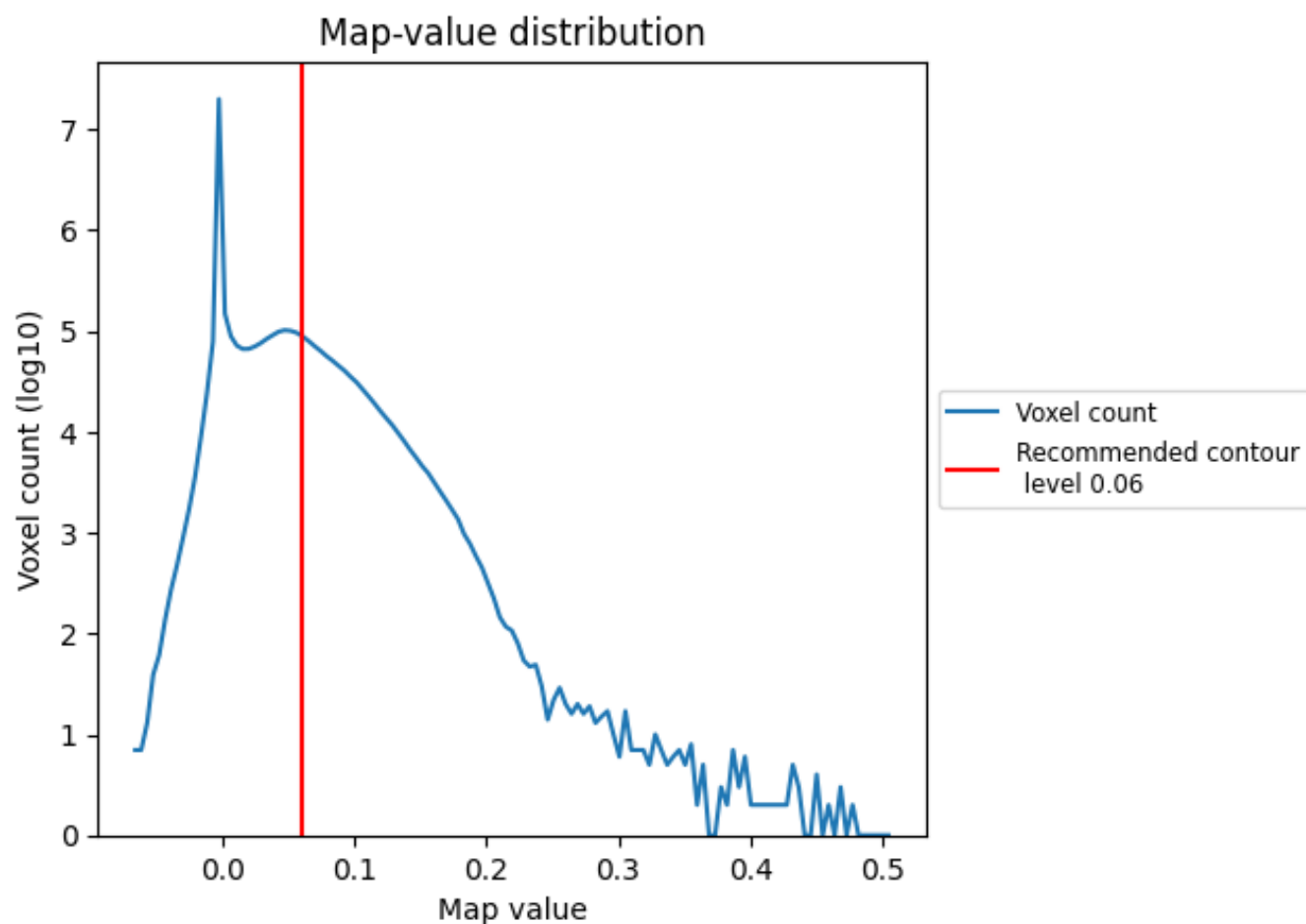
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

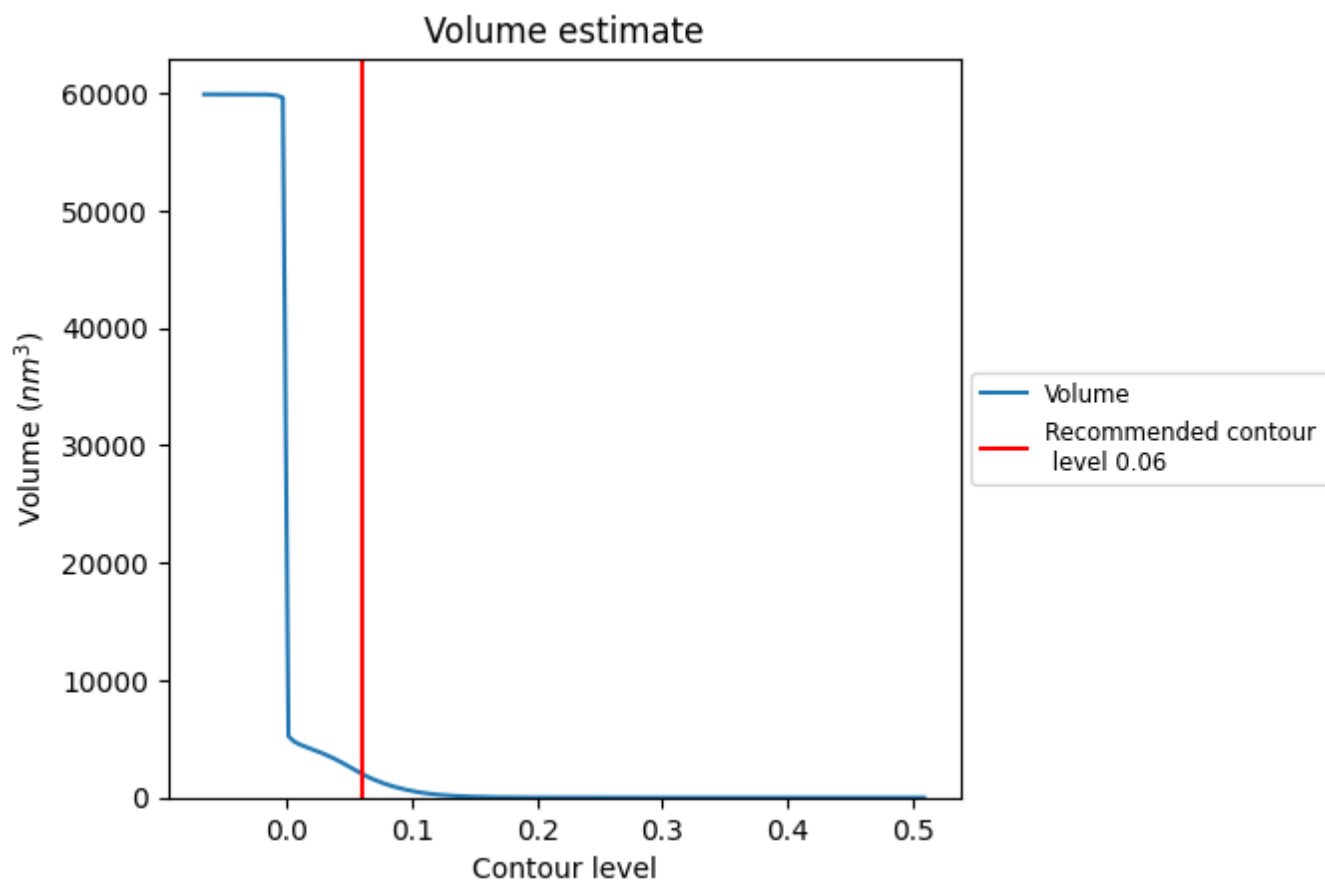
This section contains the results of statistical analysis of the map.

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.

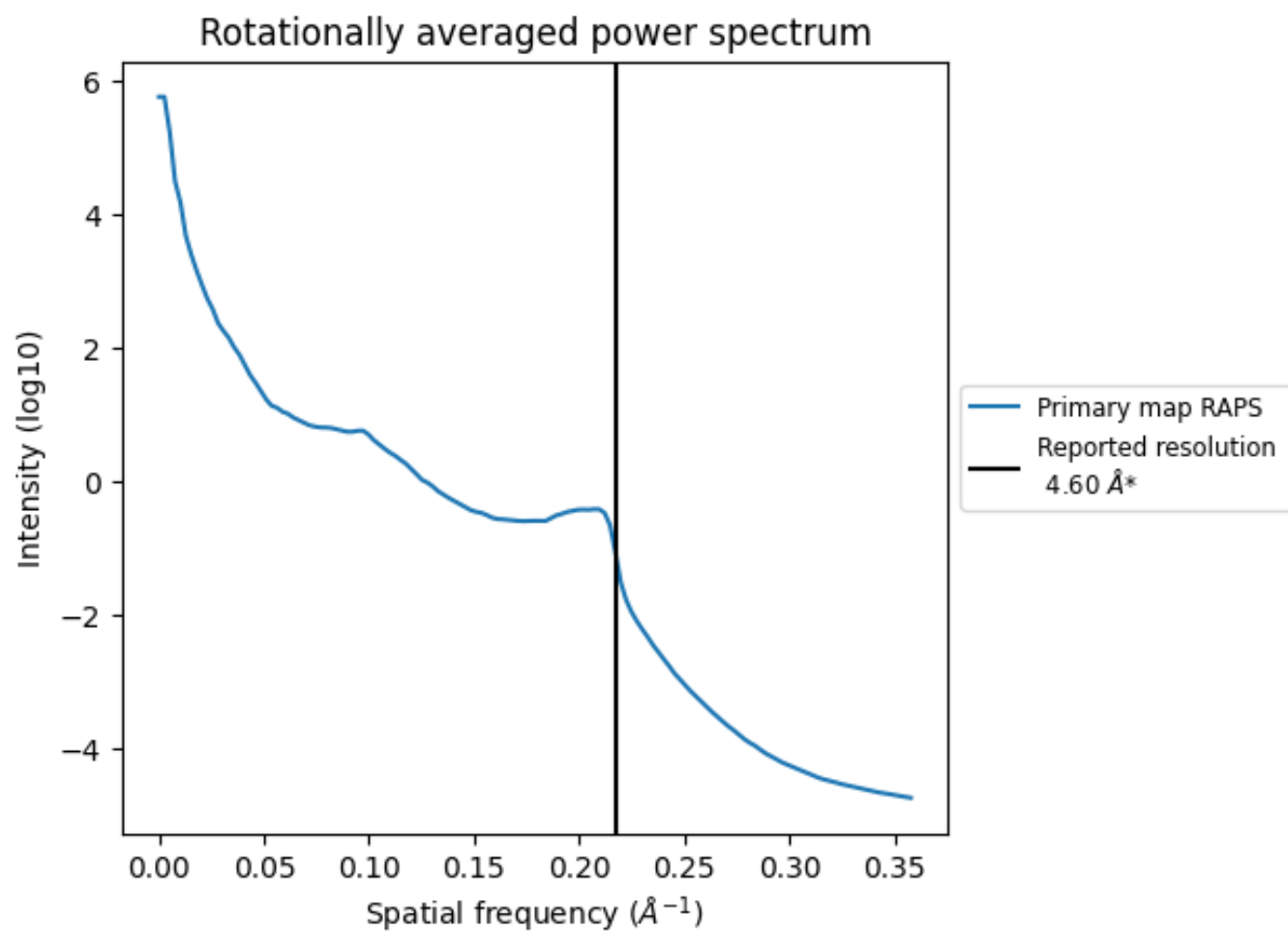
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2007 nm³; this corresponds to an approximate mass of 1813 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

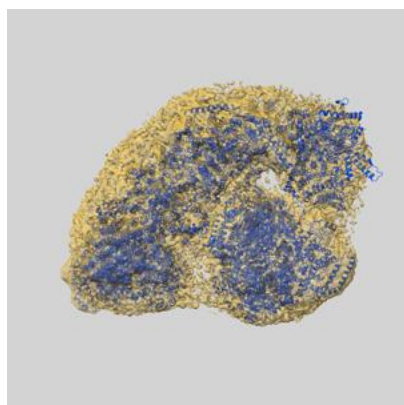
8 Fourier-Shell correlation ⓘ

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

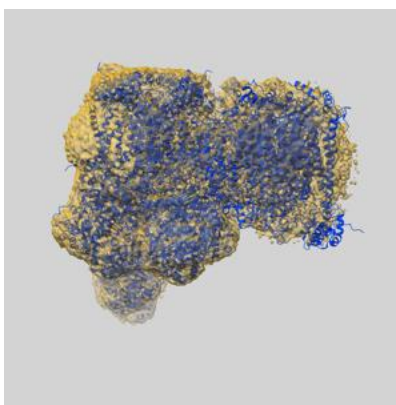
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30674 and PDB model 7DGR. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

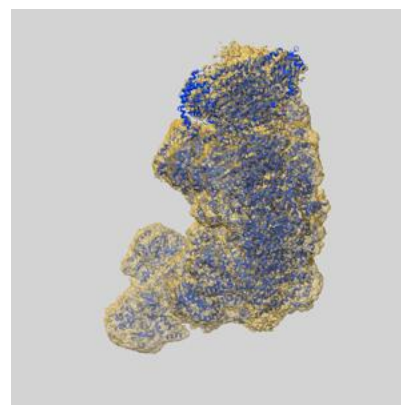
9.1 Map-model overlay [i](#)



X



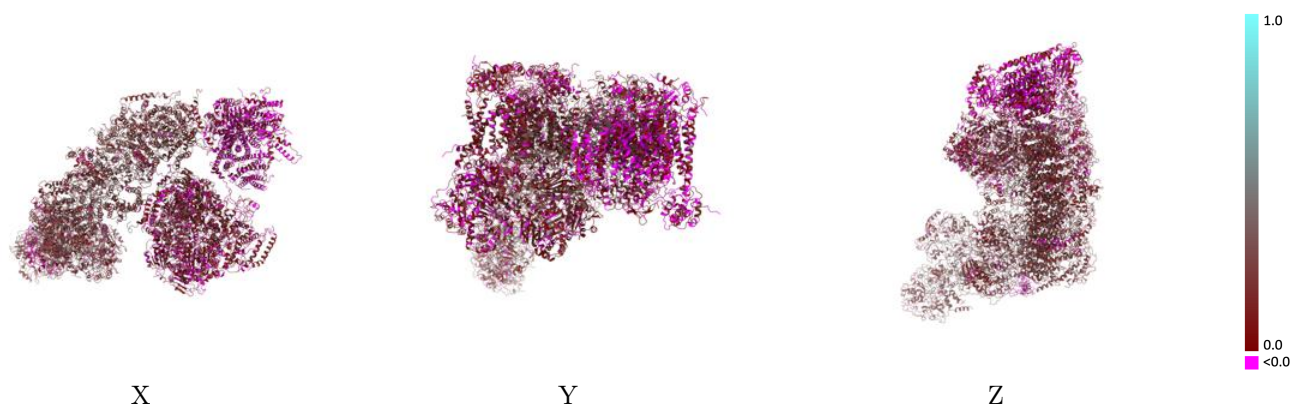
Y



Z

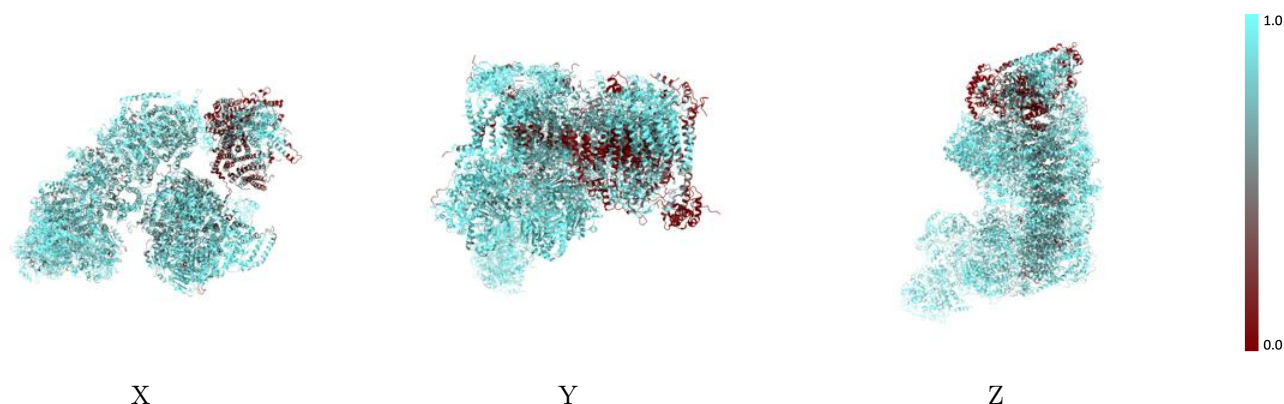
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



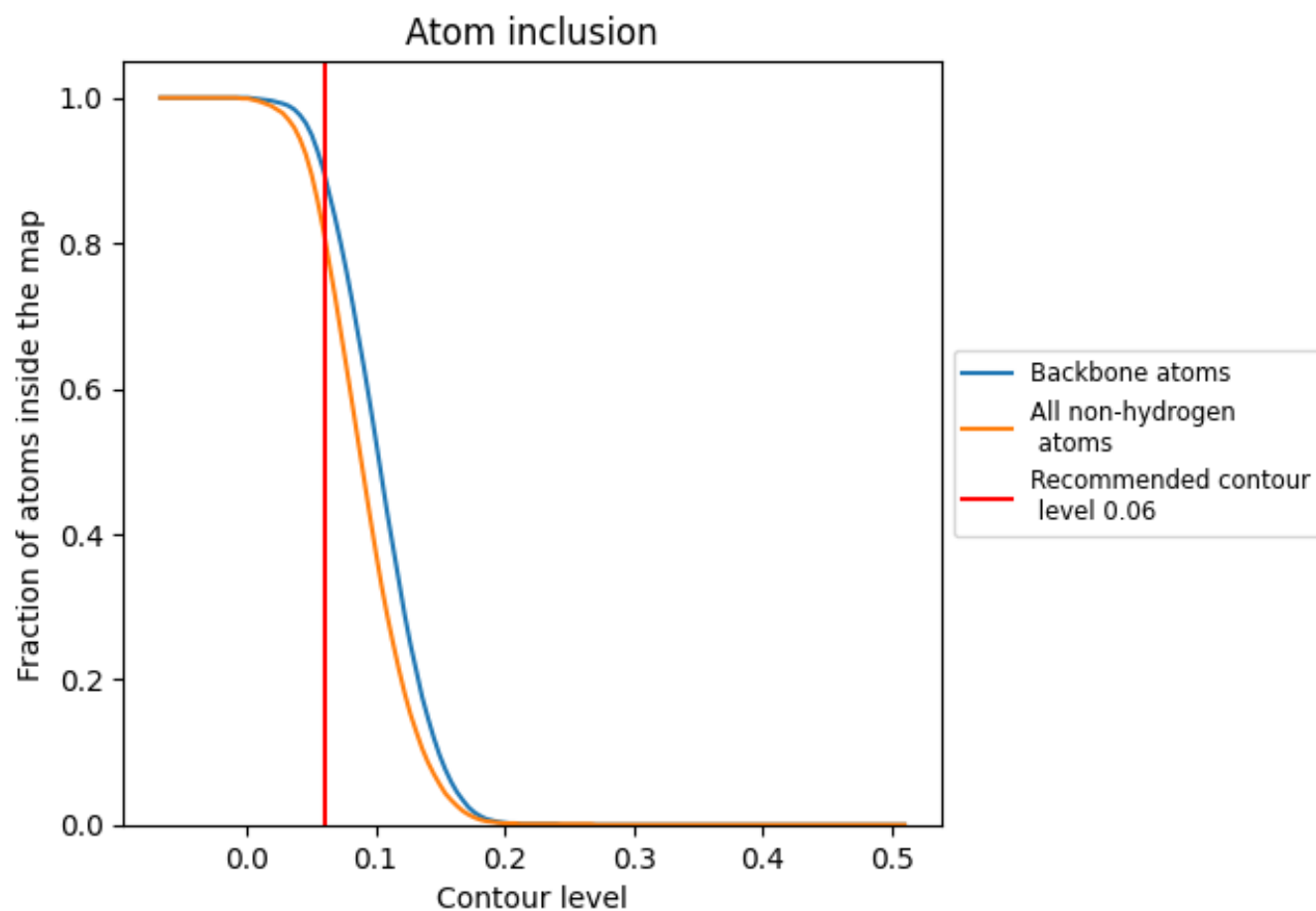
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.1780
1	 0.8290	 0.2630
2	 0.8070	 0.2820
3	 0.7050	 0.2230
4	 0.7840	 0.2760
5	 0.7910	 0.2750
6	 0.7760	 0.2350
7	 0.7750	 0.2410
8	 0.9830	 0.2200
9	 0.9630	 0.2180
A	 0.9670	 0.2460
A0	 0.7870	 0.1230
A1	 0.7440	 0.1590
A2	 0.6870	 0.1430
A3	 0.6470	 0.1640
A4	 0.1930	 0.0300
A5	 0.5640	 0.0450
A6	 0.3280	 0.0150
A7	 0.2770	 0.0260
A8	 0.2680	 0.0780
A9	 0.5820	 0.0150
B	 0.8680	 0.2900
B0	 0.3550	 0.0390
B1	 0.8120	 0.1000
B2	 0.5710	 0.1400
B3	 0.7510	 0.0800
B4	 0.3910	 0.0290
C	 0.9200	 0.2310
C0	 0.1480	 0.0420
C1	 0.3260	 0.0240
C2	 0.4270	 0.0210
C3	 0.1820	 0.0190
C4	 0.7760	 0.0260
D	 0.9030	 0.3030
E	 0.9120	 0.1400



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Chain	Atom inclusion	Q-score
F	 0.9120	 0.1510
G	 0.9280	 0.2900
H	 0.9530	 0.2880
I	 0.8980	 0.2440
J	 0.9350	 0.2190
K	 0.9730	 0.1990
L	 0.8100	 0.2180
M	 0.8680	 0.2270
N	 0.9160	 0.1760
O	 0.8670	 0.1790
P	 0.8340	 0.1560
Q	 0.9570	 0.2550
R	 0.8840	 0.2300
S	 0.9040	 0.2270
T	 0.8080	 0.2450
U	 0.6760	 0.0490
V	 0.9460	 0.2580
W	 0.9800	 0.2310
X	 0.8990	 0.2630
Y	 0.9500	 0.2510
Z	 0.9280	 0.2100
a	 0.7950	 0.1490
b	 0.9460	 0.2950
c	 0.9540	 0.2300
d	 0.9770	 0.1890
e	 0.9170	 0.2890
f	 0.9650	 0.2730
g	 0.9350	 0.2480
h	 0.9230	 0.2550
i	 0.9230	 0.2540
j	 0.7830	 0.1210
k	 0.9270	 0.0920
l	 0.9110	 0.1020
m	 0.7760	 0.1460
o	 0.9360	 0.1160
p	 0.8970	 0.0940
q	 0.8840	 0.1250
r	 0.7960	 0.1150
s	 0.8790	 0.1230
t	 0.7310	 0.0810
u	 0.8400	 0.0760
v	 0.8390	 0.0170

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Chain	Atom inclusion	Q-score
w	 0.8910	 0.1790
x	 0.9430	 0.1400
y	 0.7240	 0.1610
z	 0.8810	 0.1340