



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:25 AM JST

PDB ID : 7DGS / pdb_00007dgs
EMDB ID : EMD-30675
Title : Activity optimized supercomplex state3
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 : 7.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

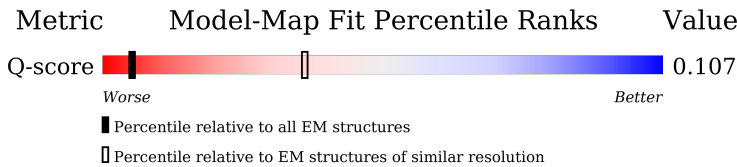
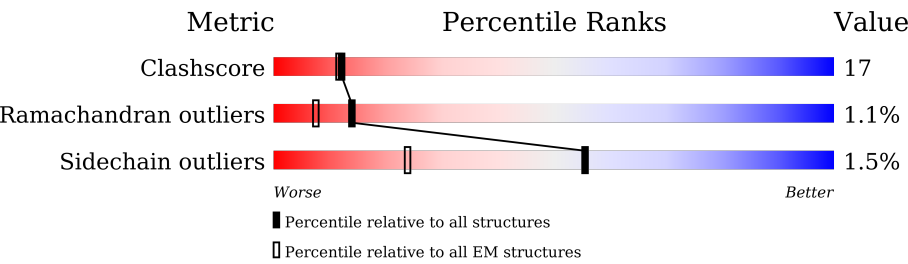
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.80 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	370 (7.30 - 8.30)

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	71%22%• 5%
2	7	175	7% 86%10%• •
3	6	606	8% 86%14%•
4	2	347	• 86%12%• •

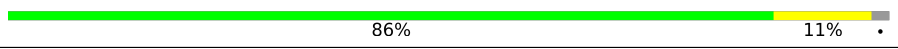
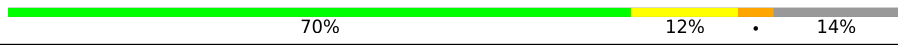
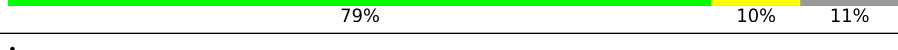
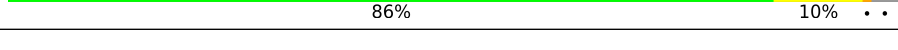
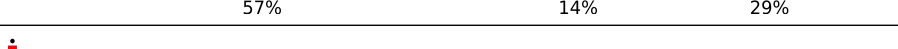
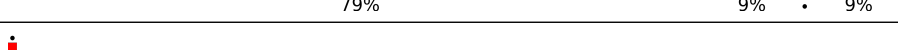
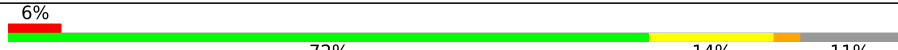
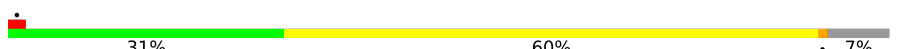
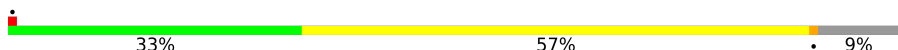
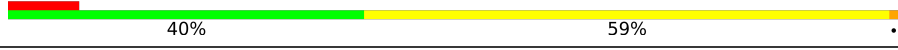
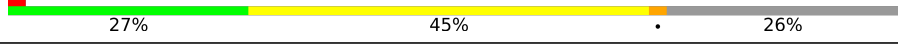
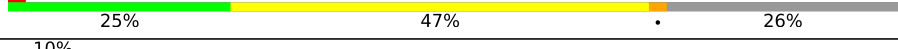
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Mol	Chain	Length	Quality of chain
5	4	459	
6	5	98	
7	8	444	
8	1	318	
9	3	115	
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	

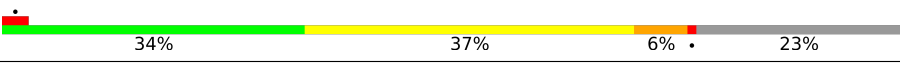
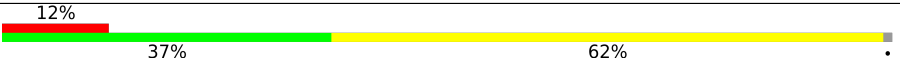
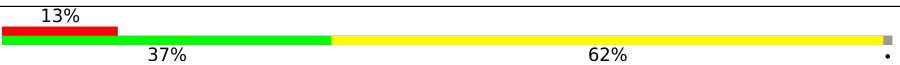
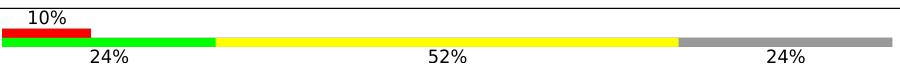
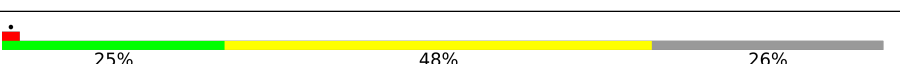
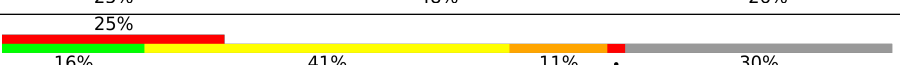
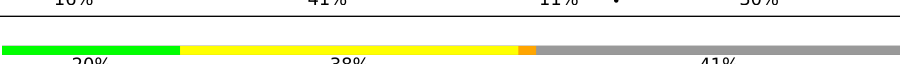
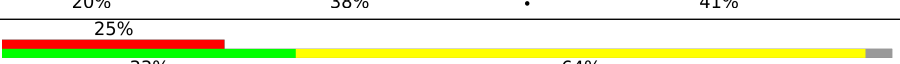
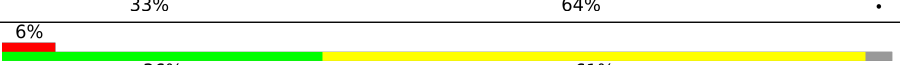
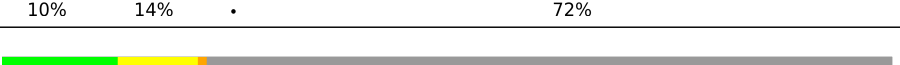
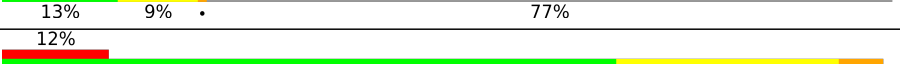
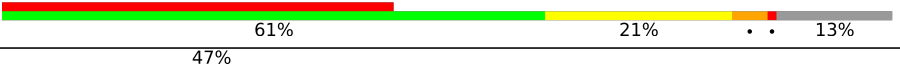
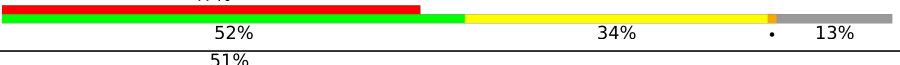
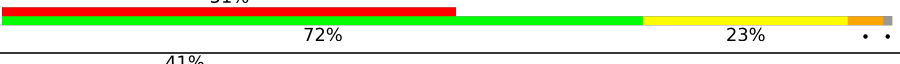
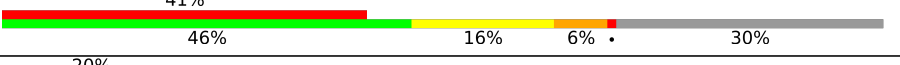
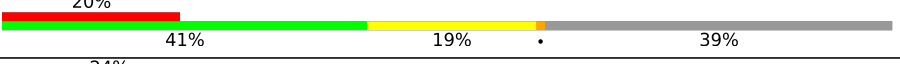
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Mol	Chain	Length	Quality of chain
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	
34	Z	97	
35	a	128	
36	b	143	
37	c	127	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	325	
48	z	325	
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	B5	91	
52	s	91	
53	A3	56	
53	t	56	
54	B4	64	
54	u	64	
55	B3	78	
55	v	78	
56	A9	514	
57	B9	227	
58	B7	261	
59	A7	169	
60	A6	152	
61	B2	129	
62	A4	97	
63	A5	86	
64	B6	74	
65	B8	80	
66	B0	80	
67	B1	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
78	HEC	o	301	X	-	-	-
78	HEC	z	301	X	-	-	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 106778 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
			1534	978	261	285	10		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	172	Total	C	N	O	S	0	0
			1186	798	179	202	7		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	344	Total	C	N	O	S	0	0
			2582	1707	404	437	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	458	Total	C	N	O	S	1	0
			3447	2293	548	574	32		

- 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
			697	454	109	124	10		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	427	Total	C	N	O	S	0	0
			2965	1864	552	534	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	317	Total	C	N	O	S	0	0
			2499	1676	384	416	23		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	112	Total	C	N	O	S	0	0
			862	580	127	150	5		

- 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
			5179	3252	914	977	36		

- 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
			3416	2179	589	623	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
			1705	1102	294	306	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
			1200	769	209	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
			1388	874	239	264	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	0	0
			183	116	32	35		

- 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
			981	619	177	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
			530	331	99	97	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
			652	409	125	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
			698	442	128	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
			2297	1455	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
			922	584	161	171	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
			708	445	134	125	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
			892	587	149	153	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	B5	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
			304	202	55	47		

- 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	B4	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	B3	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	B9	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	B7	261	Total	C	N	O	S	0	0
			2125	1421	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	A6	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	B2	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	B6	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	B8	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		

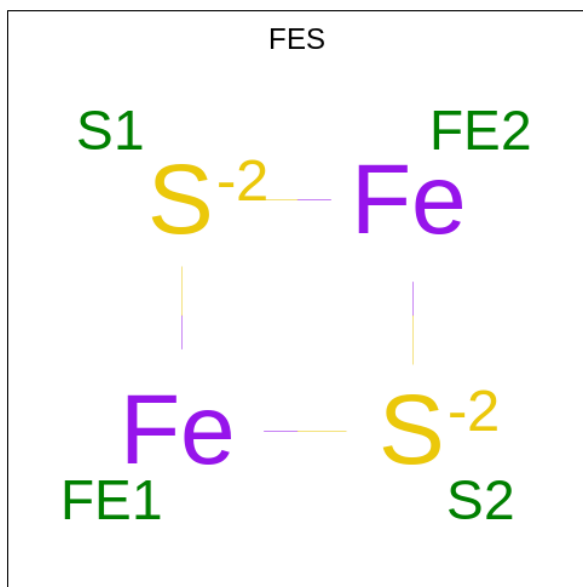
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	B1	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.

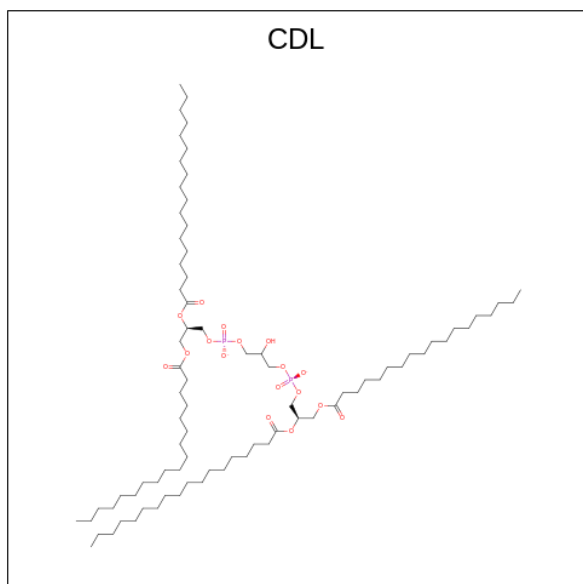
Mol	Chain	Residues	Atoms				AltConf	Trace
68	A8	43	Total	C	N	O	0	0
			335	223	53	59		

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



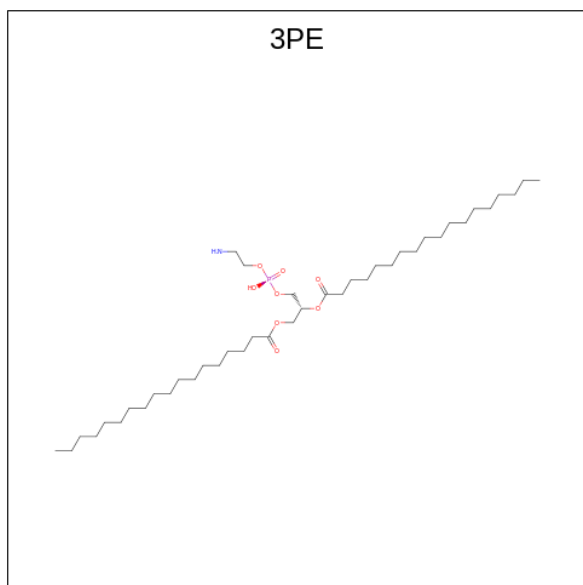
Mol	Chain	Residues	Atoms			AltConf
69	9	1	Total	Fe	S	0
			4	2	2	
69	A	1	Total	Fe	S	0
			4	2	2	
69	m	1	Total	Fe	S	0
			4	2	2	

- Molecule 70 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



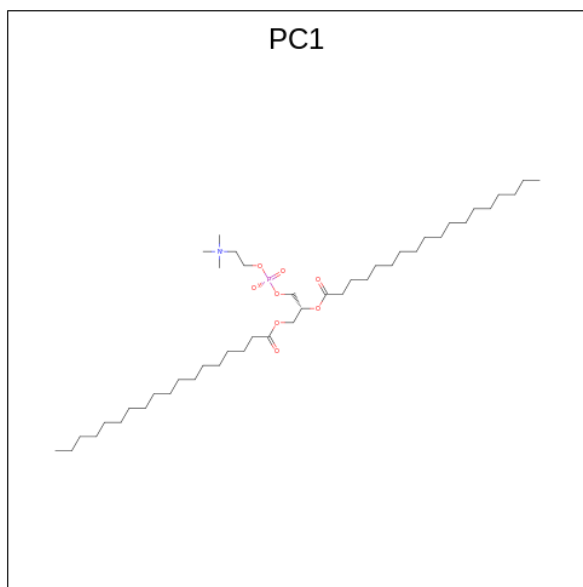
Mol	Chain	Residues	Atoms				AltConf
70	6	1	Total	C	O	P	0
			64	45	17	2	
70	4	1	Total	C	O	P	0
			82	63	17	2	
70	J	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



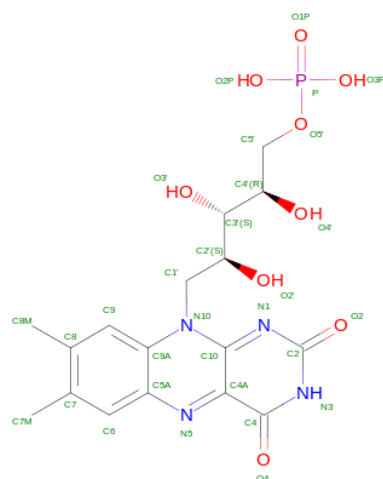
Mol	Chain	Residues	Atoms					AltConf
71	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	j	1	Total	C	N	O	P	0
			46	36	1	8	1	

- 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).



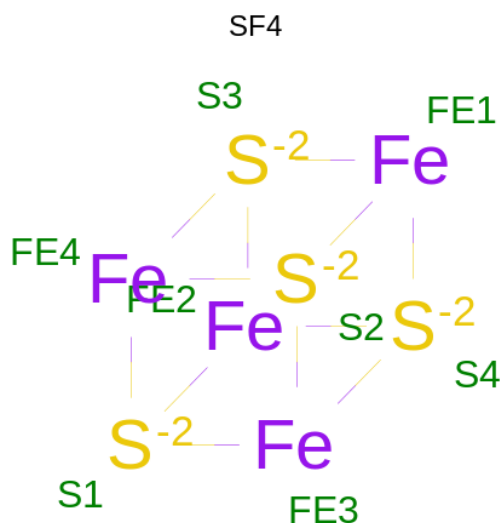
Mol	Chain	Residues	Atoms					AltConf
72	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf
73	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

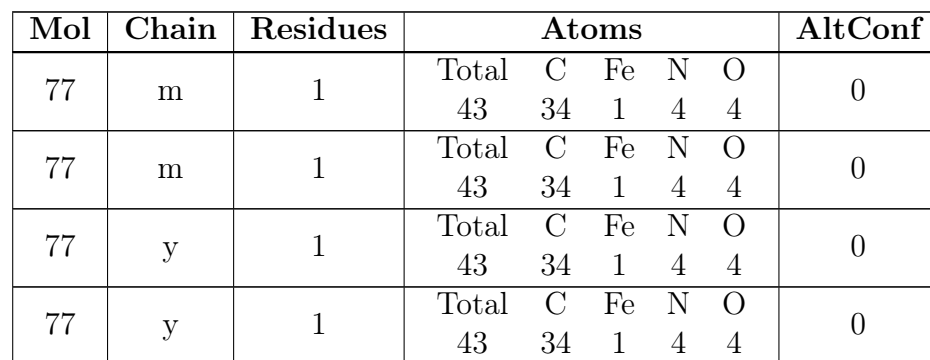
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Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total 8	Fe 4	S 4	0
74	E	1	Total 8	Fe 4	S 4	0
74	E	1	Total 8	Fe 4	S 4	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 75 | I | 1 | Total Zn
1 1 | 0 |
| 75 | B2 | 1 | Total Zn
1 1 | 0 |

- # NAP

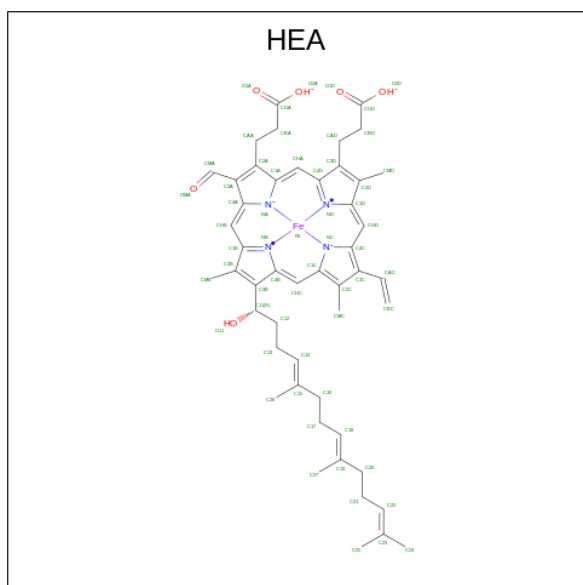
- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- [illegible]

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	B9	2	Total	Cu	0
			2	2	

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

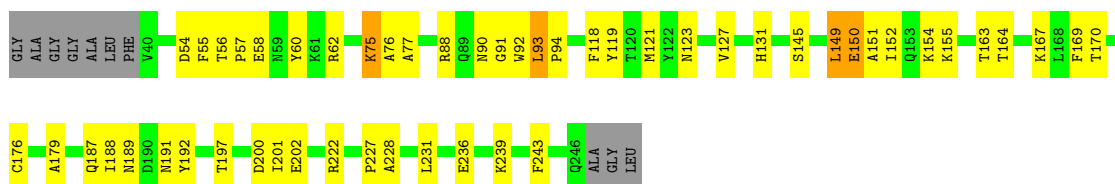
Mol	Chain	Residues	Atoms		AltConf
81	A9	1	Total	Mg	0
			1	1	

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

Chain 9: 



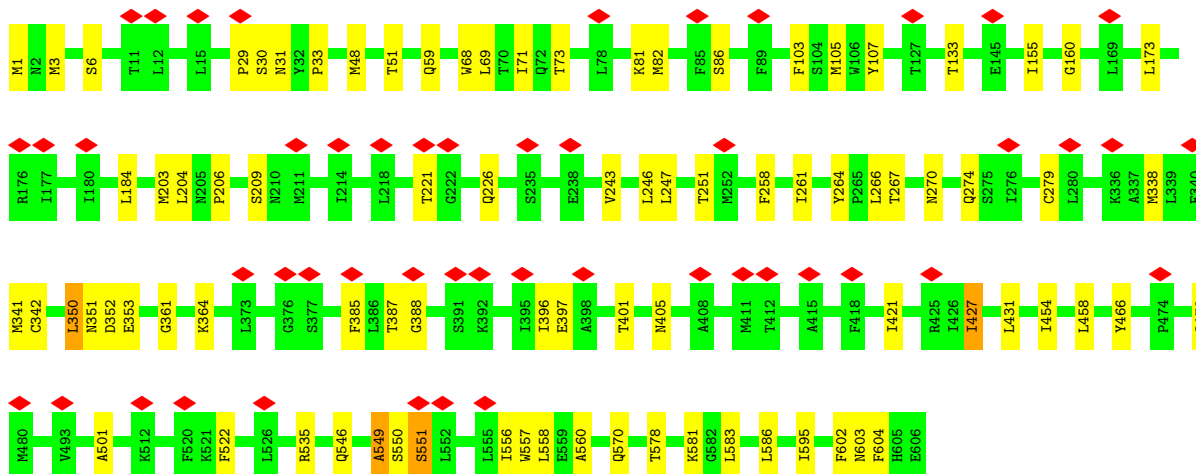
- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

Chain 7: 



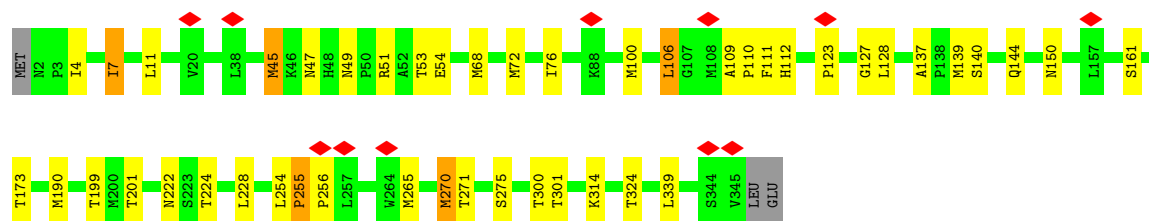
- Molecule 3: NADH-ubiquinone oxidoreductase chain 5

Chain 6: 



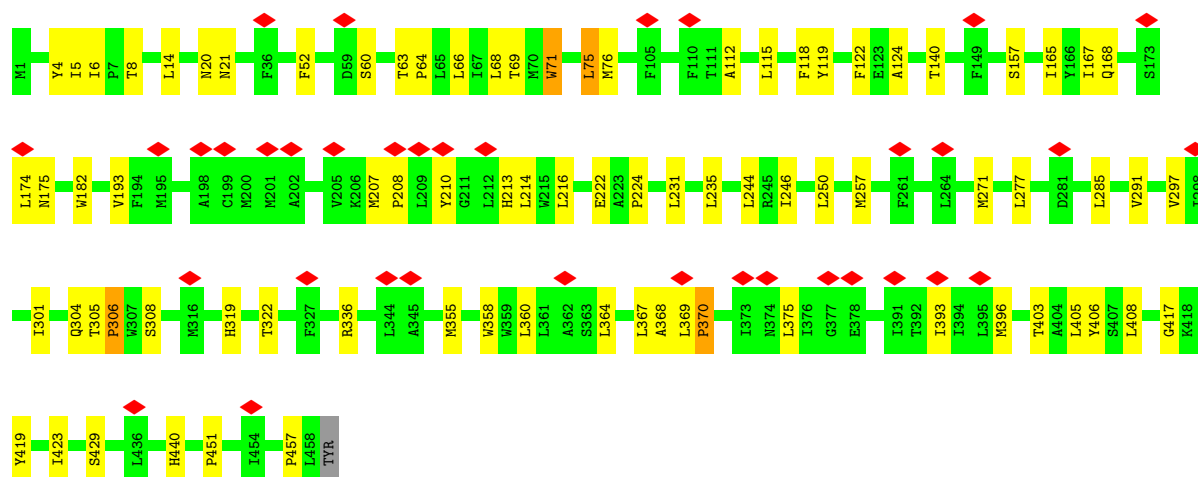
- Molecule 4: NADH-ubiquinone oxidoreductase chain 2

Chain 2:  86% 12% ..



- Molecule 5: NADH-ubiquinone oxidoreductase chain 4

Chain 4:  8% 82% 17% .



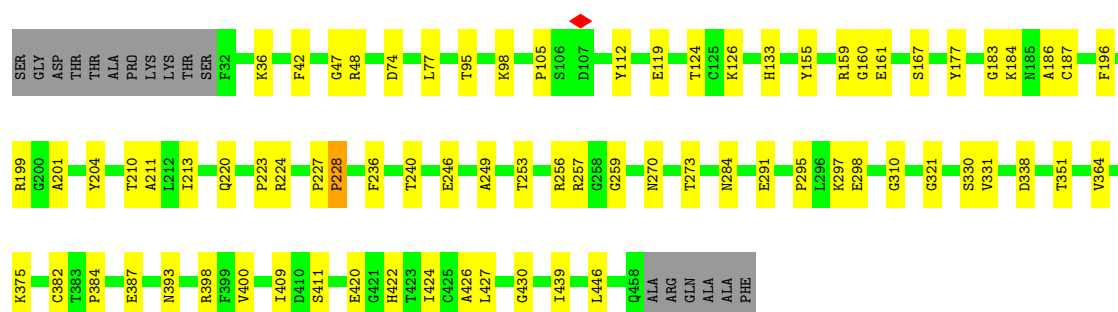
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5:  78% 19% ..



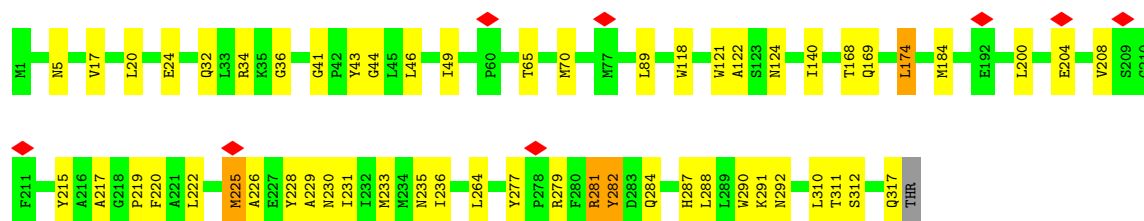
- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 8:  79% 17% .



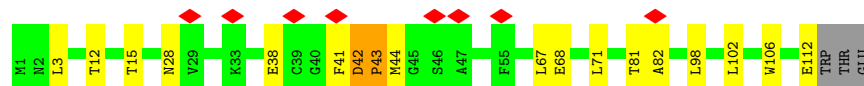
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1: 



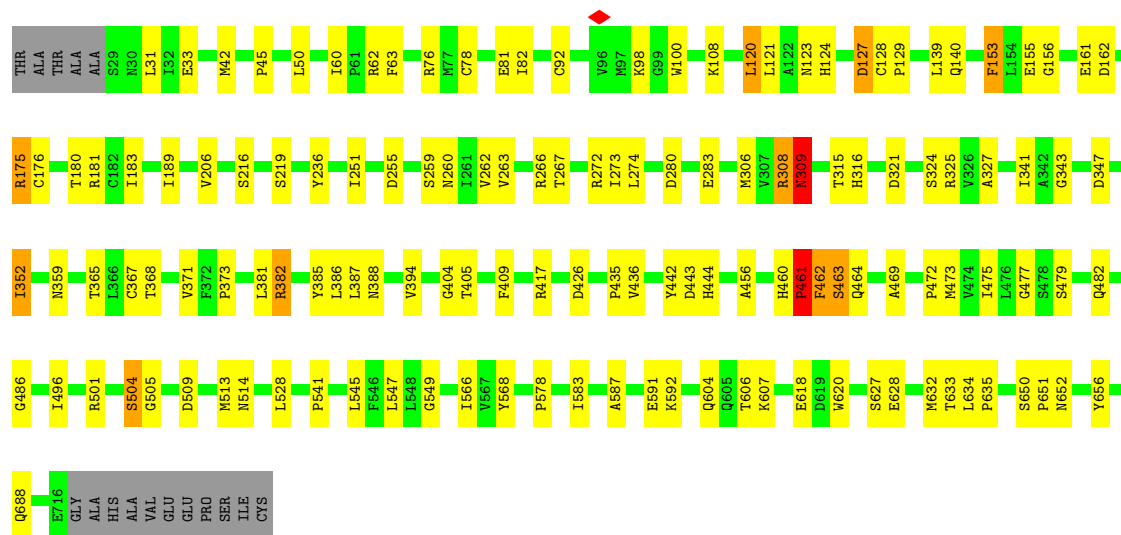
- Molecule 9: NADH-ubiquinone oxidoreductase chain 3

Chain 3: 



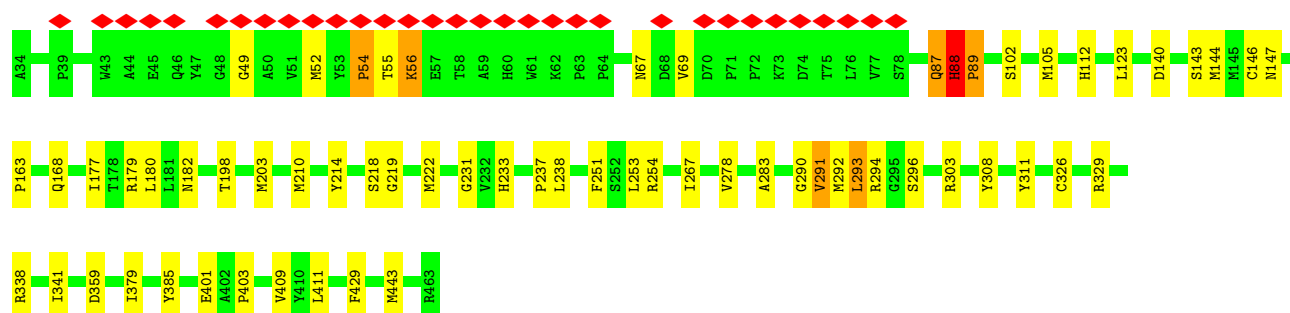
- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A: 



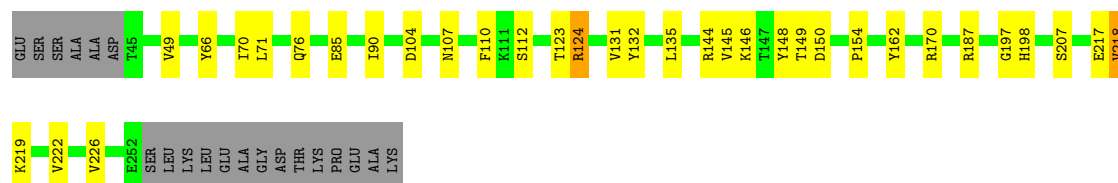
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B: 



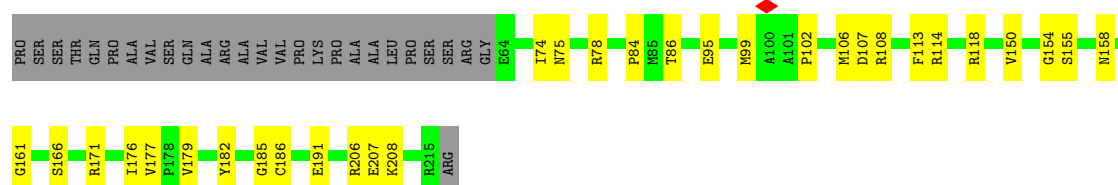
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  76% 14% 9%



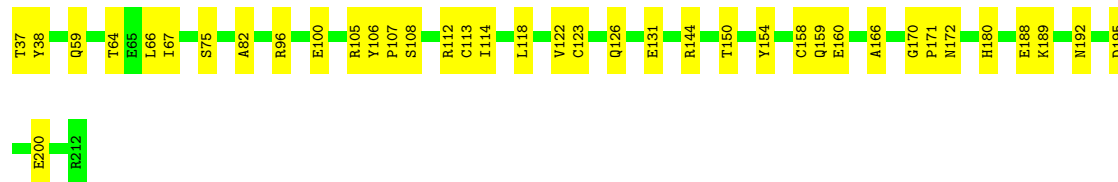
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D:  68% 17% 15%



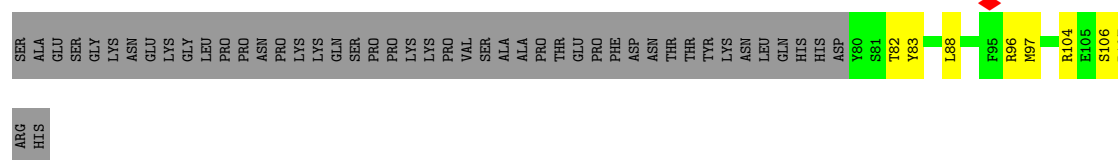
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E:  78% 22%



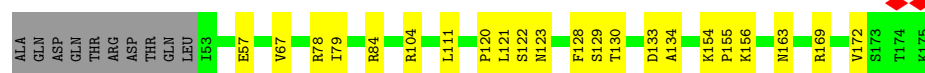
- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:  27% 11% 63%

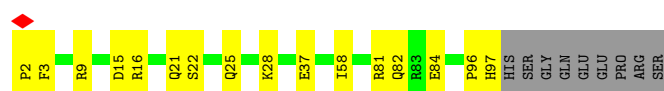
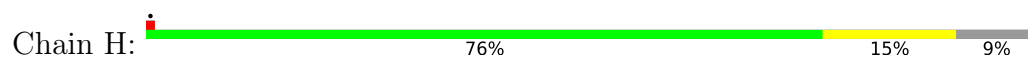


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

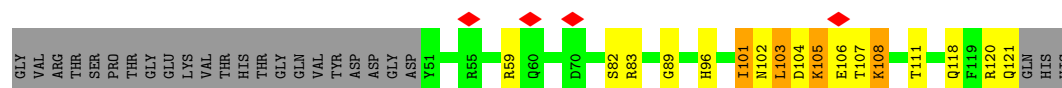
Chain G:  76% 17% 8%



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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



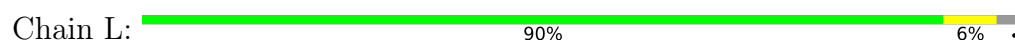
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



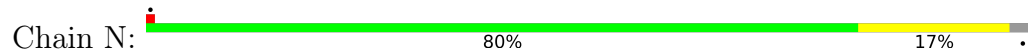
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



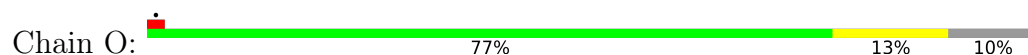
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



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



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

Chain P: 



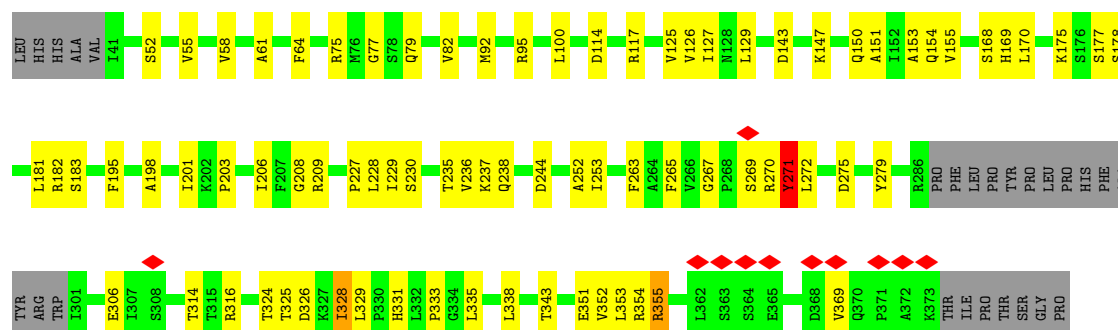
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Q: 



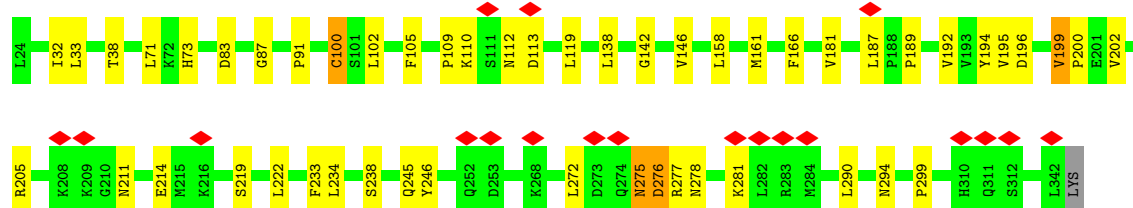
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R: 



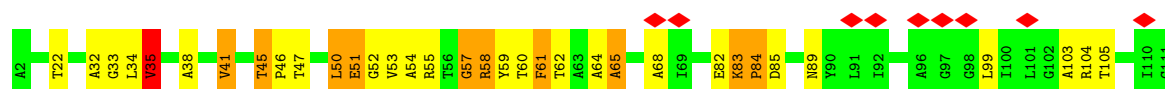
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

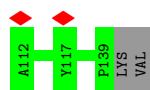
Chain S: 



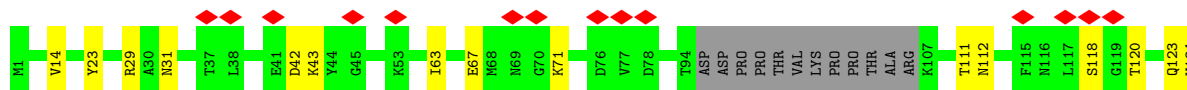
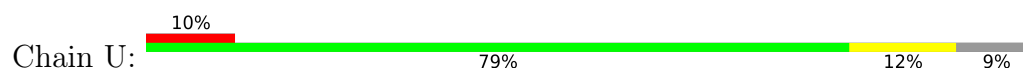
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T: 

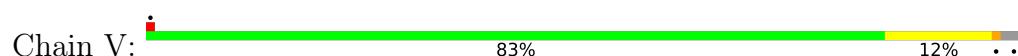




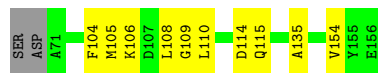
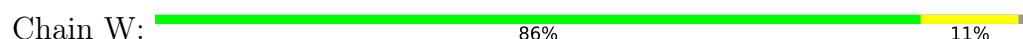
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Molecule 31: Acyl carrier protein, mitochondrial



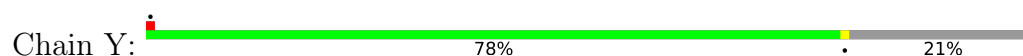
- Molecule 31: Acyl carrier protein, mitochondrial

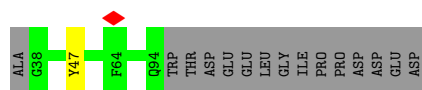


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

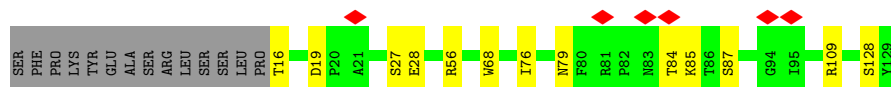
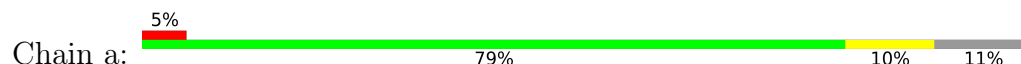




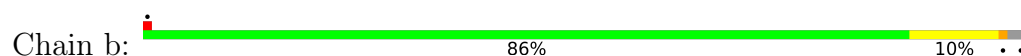
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



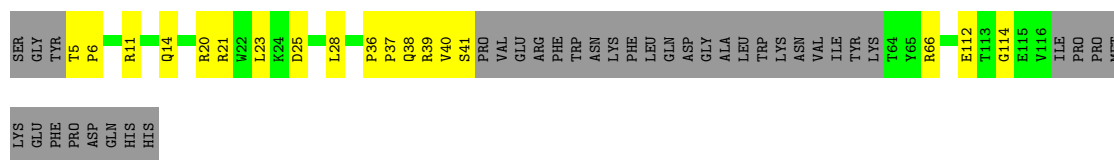
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



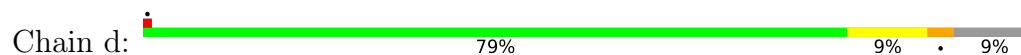
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



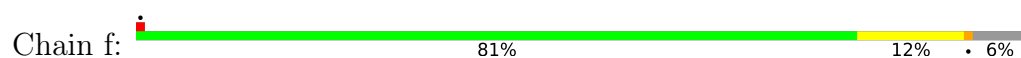
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



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

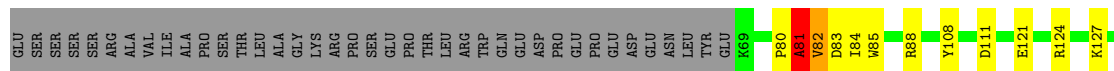


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

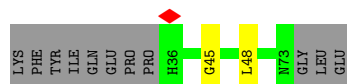




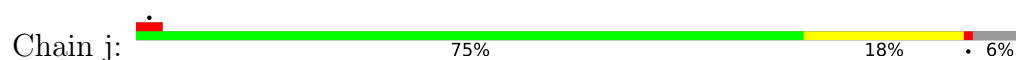
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



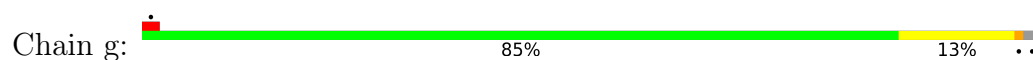
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



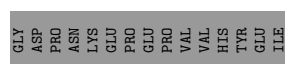
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

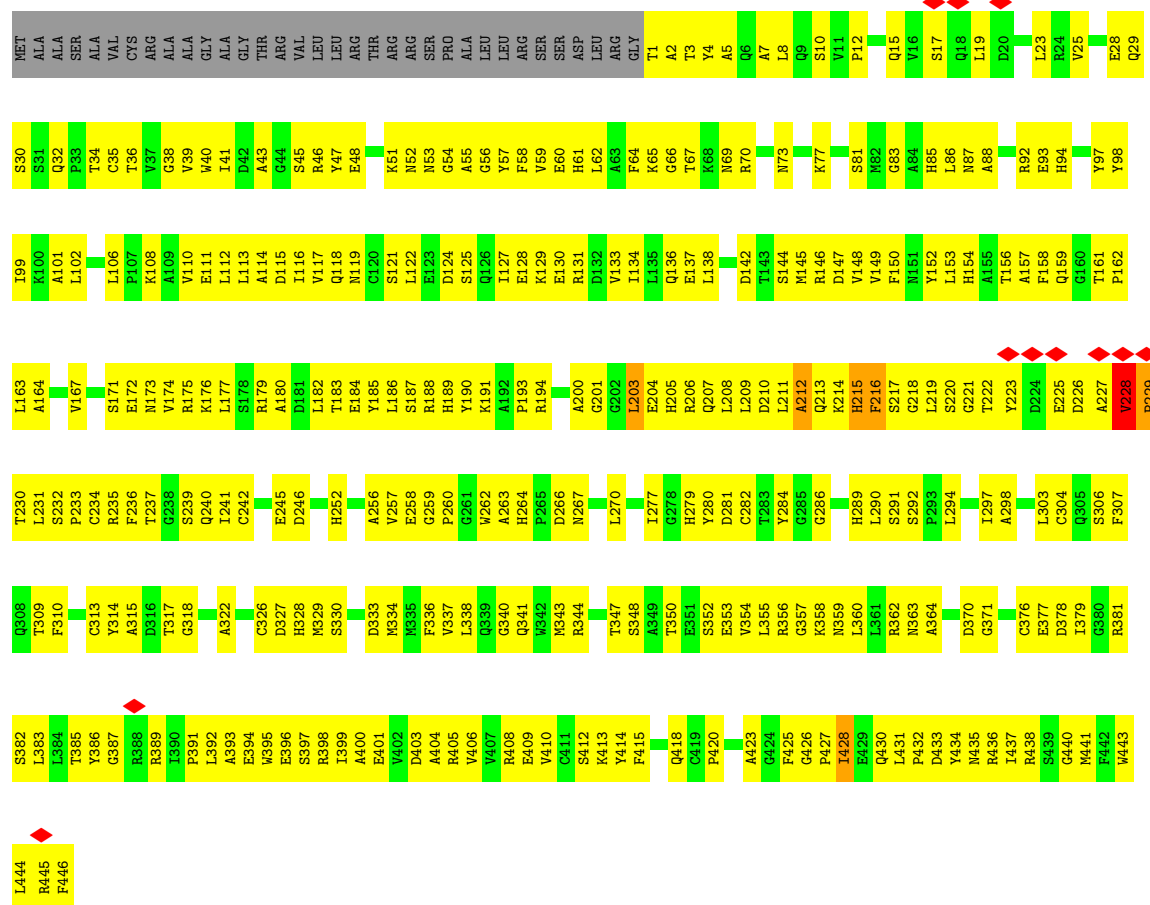


- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



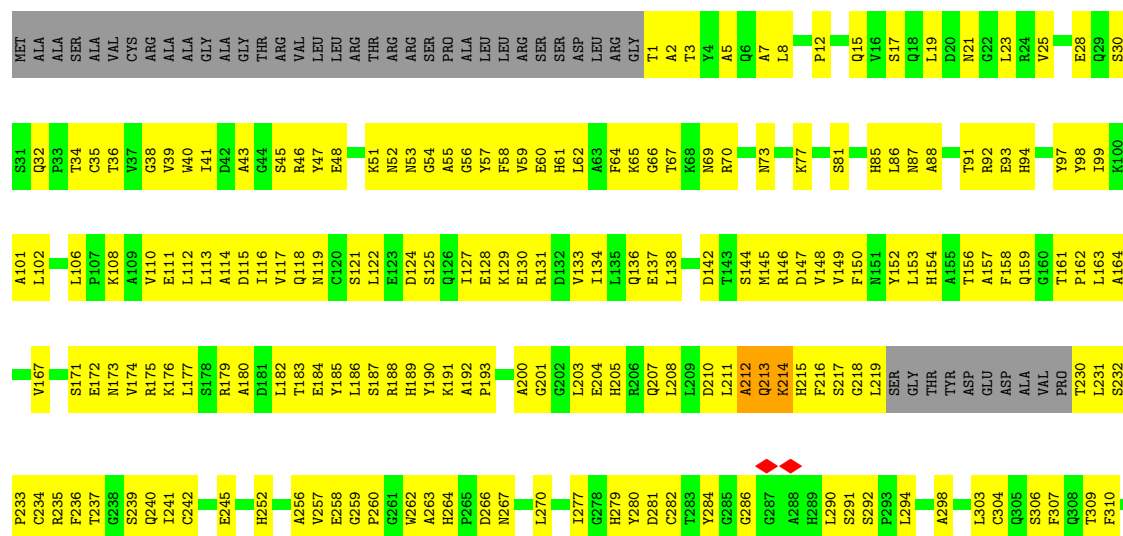
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

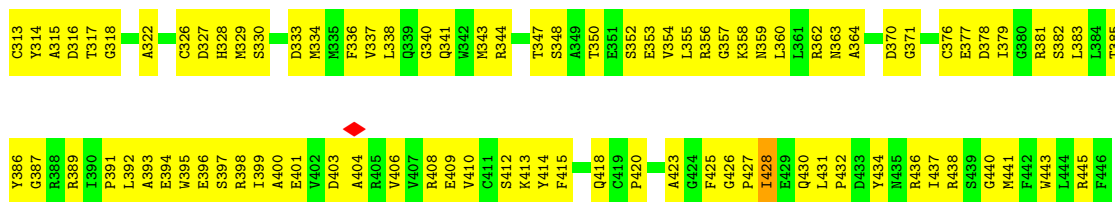
Chain k: 



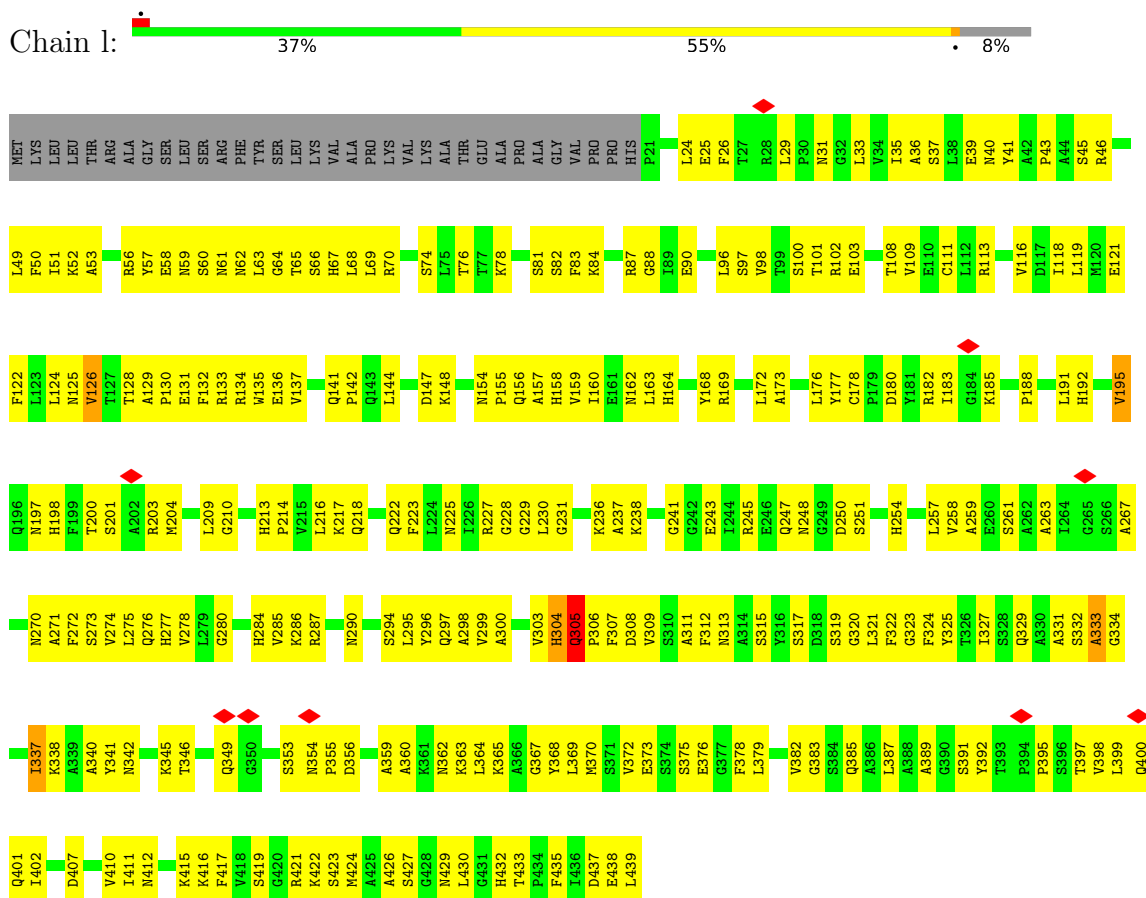
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain w: 

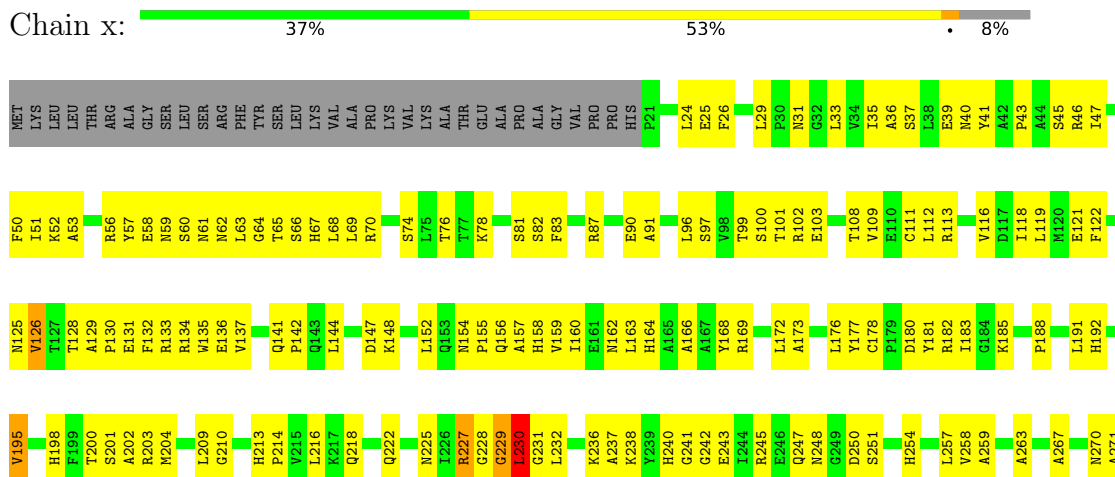


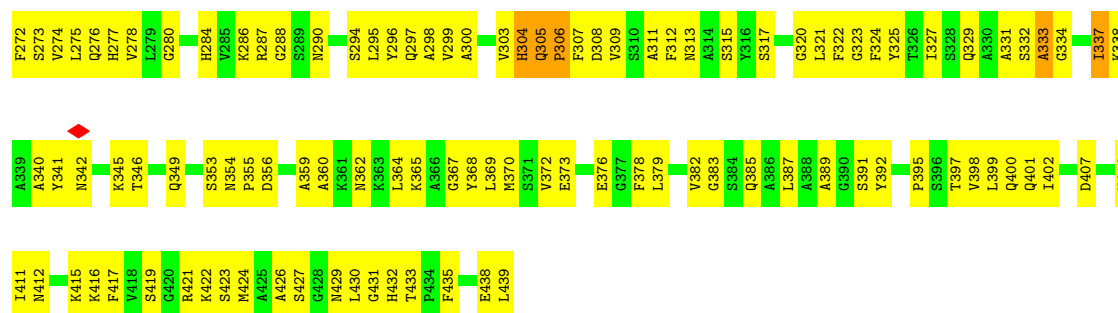


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

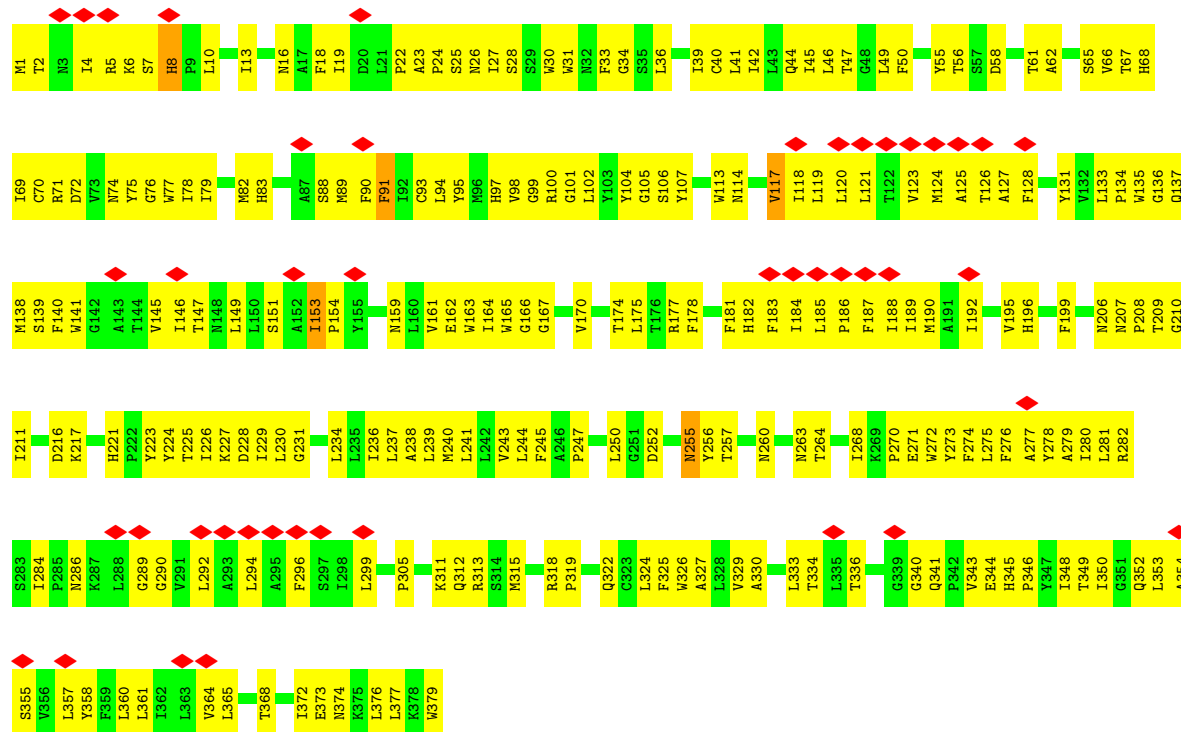
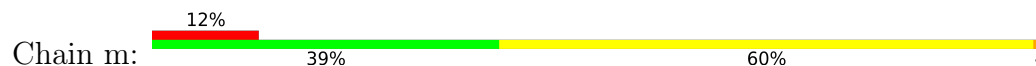


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

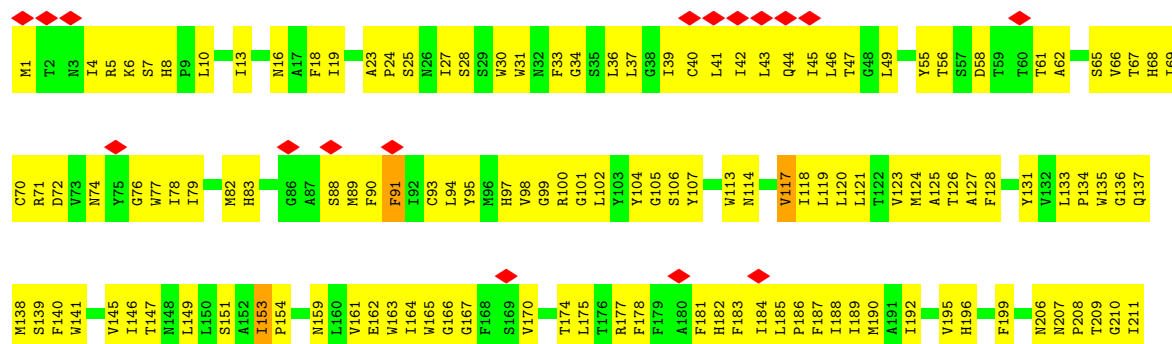
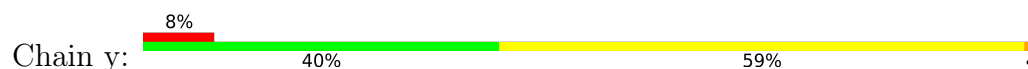


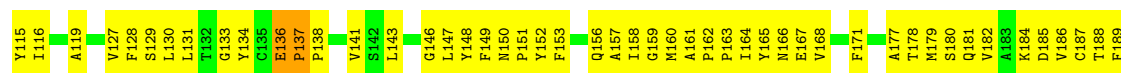


• Molecule 47: Cytochrome b



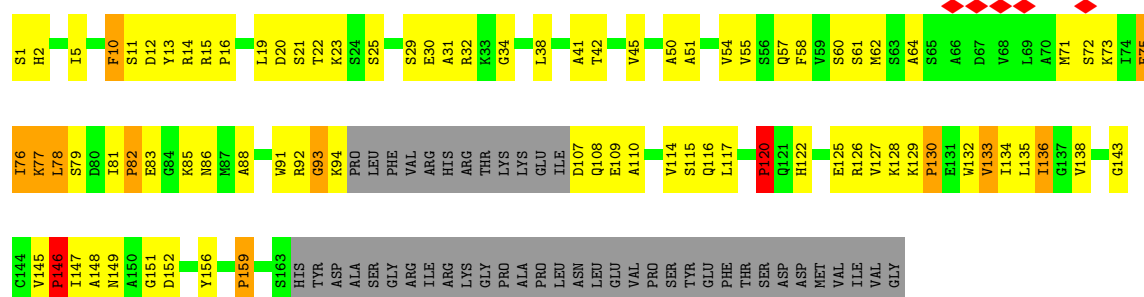
• Molecule 47: Cytochrome b



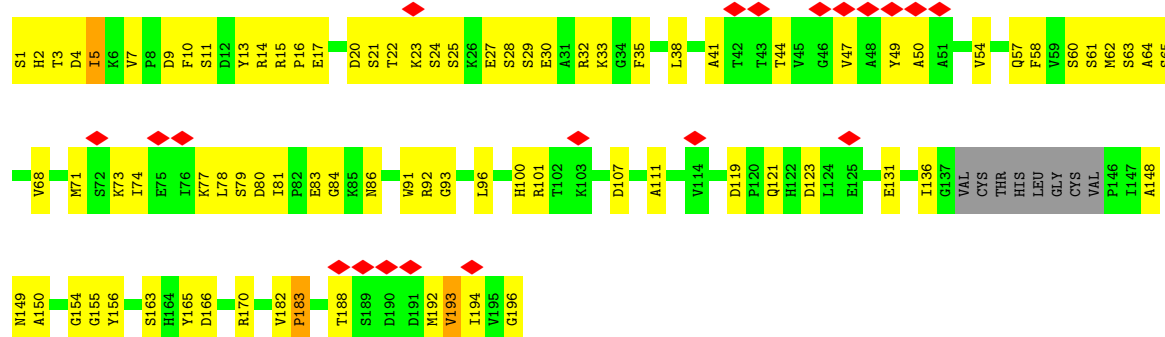




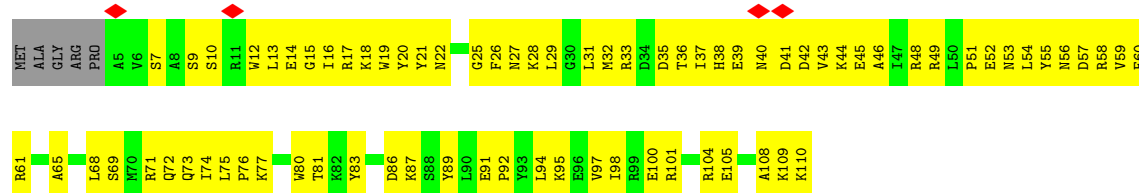
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



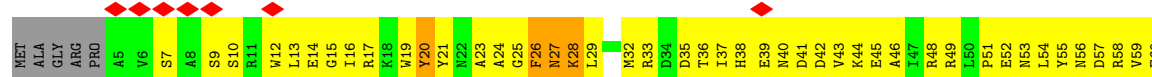
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



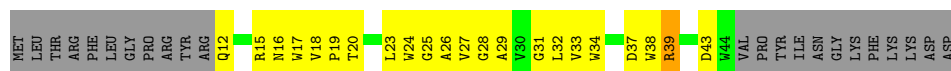
- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7

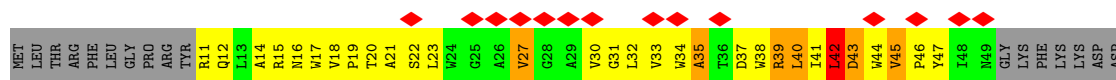


Chain t: 20% 38% . 41%



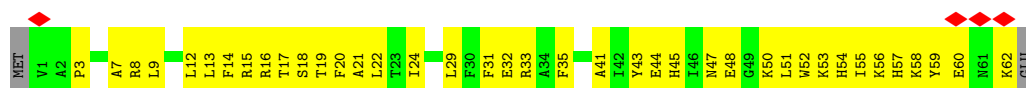
- Molecule 53: Cytochrome b-c1 complex subunit 10

Chain A3: 16% 25% 41% 11% . 30%



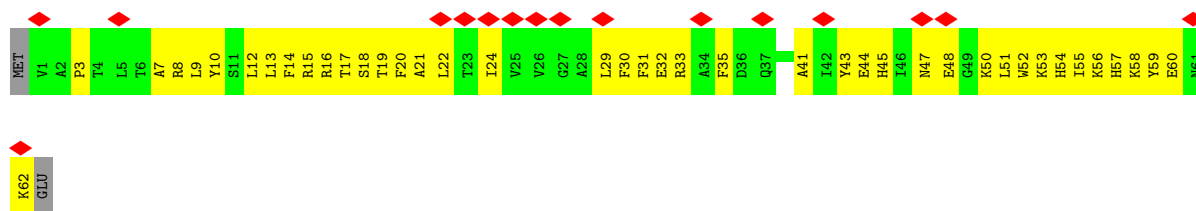
- Molecule 54: Cytochrome b-c1 complex subunit 9

Chain u: 6% 36% 61% .



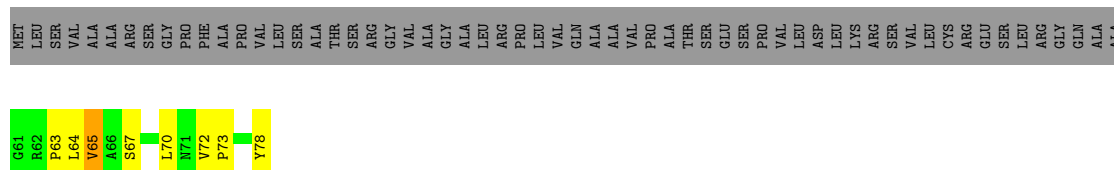
- Molecule 54: Cytochrome b-c1 complex subunit 9

Chain B4: 25% 33% 64% .



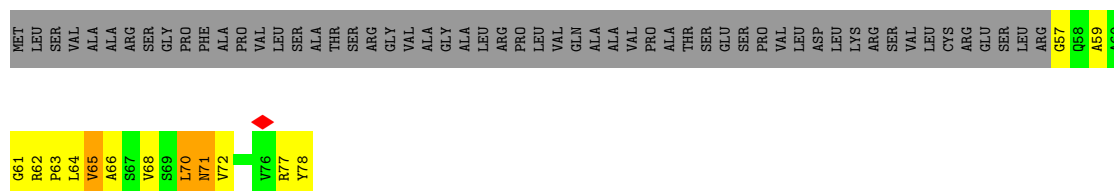
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain v: 13% 9% . 77%

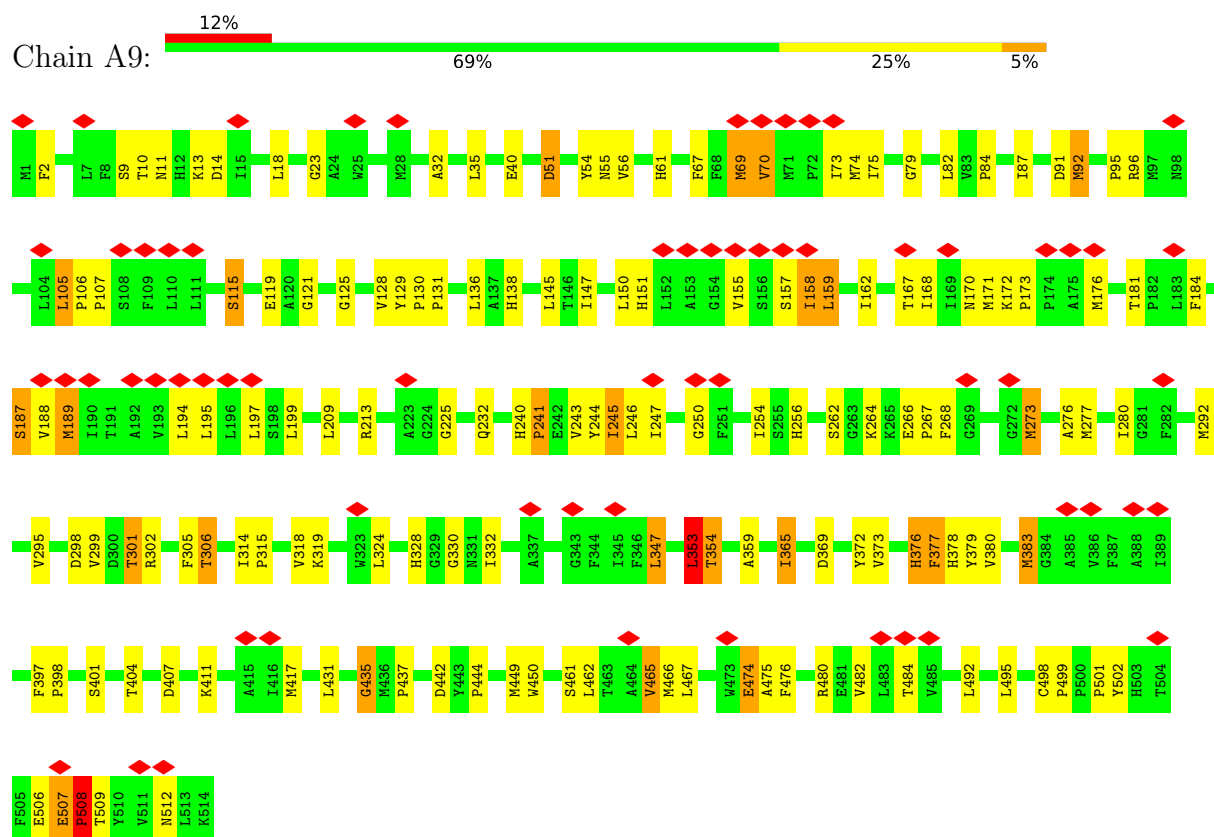


- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

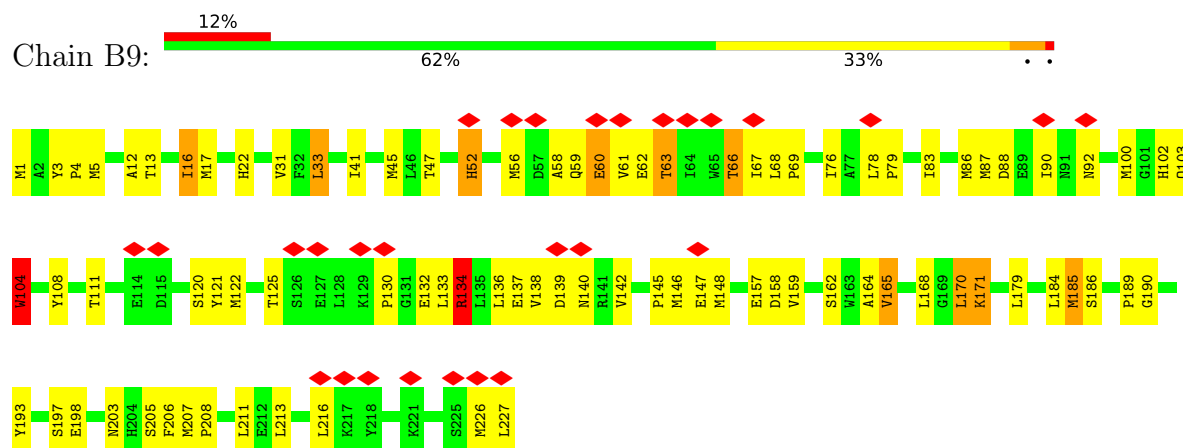
Chain B3: 10% 14% . 72%



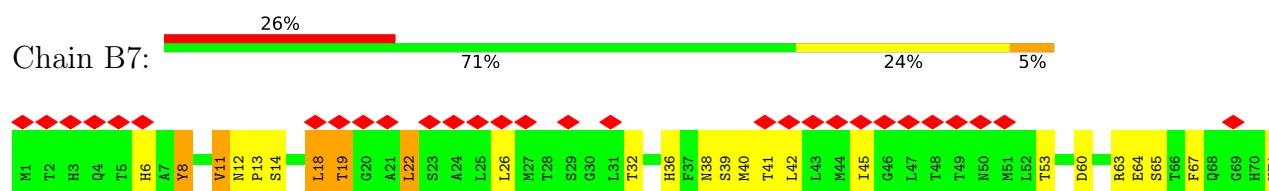
- Molecule 56: Cytochrome c oxidase subunit 1

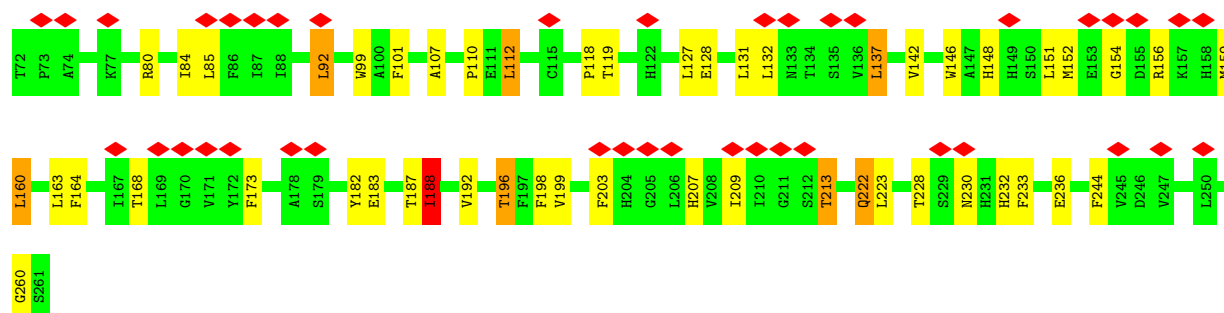


- Molecule 57: Cytochrome c oxidase subunit 2

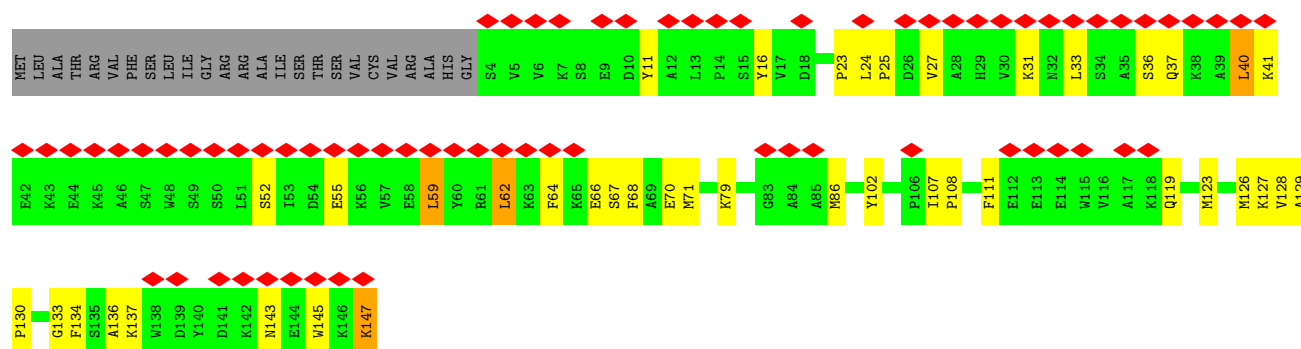
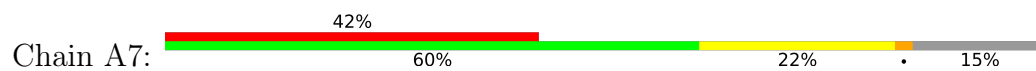


- Molecule 58: Cytochrome c oxidase subunit 3

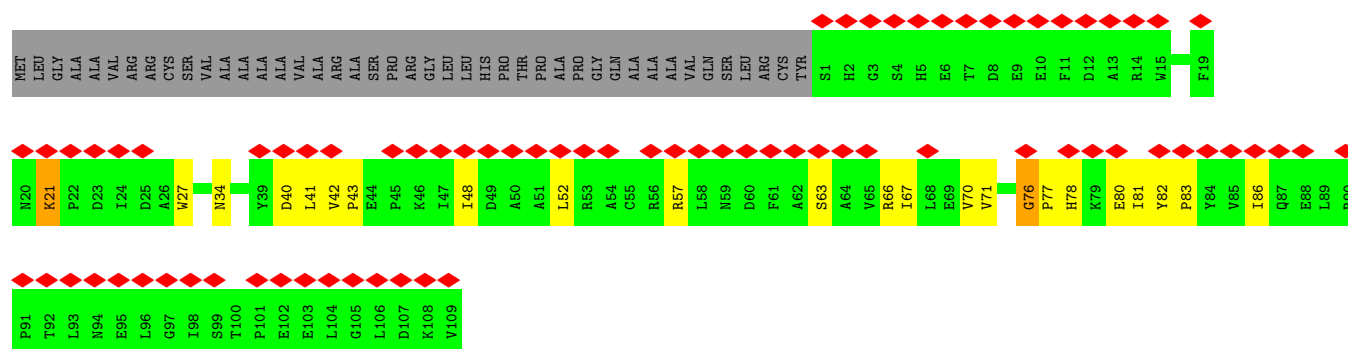




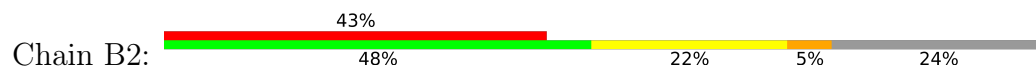
- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

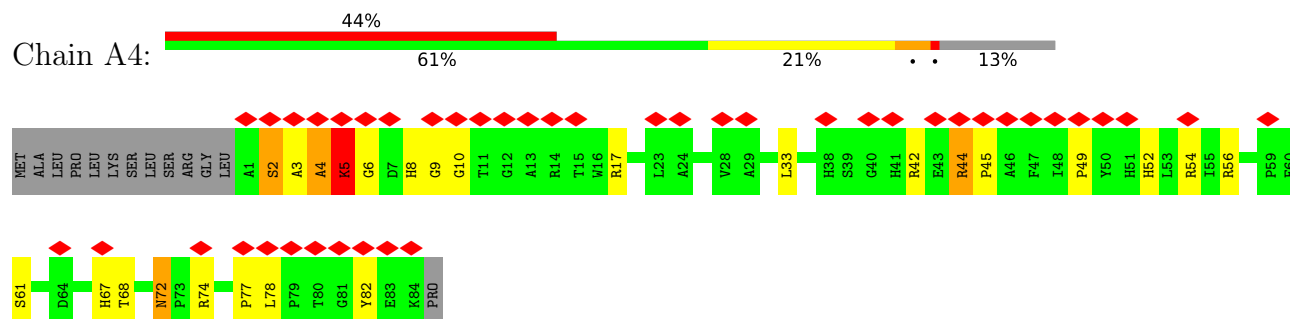


- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial



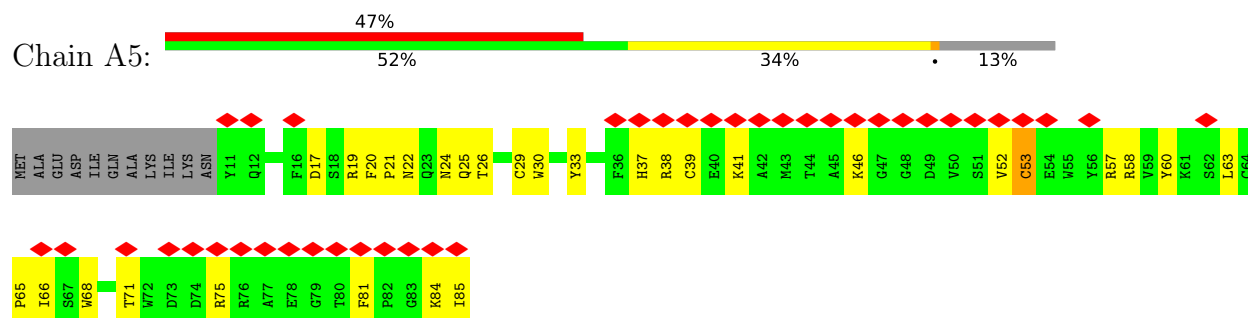
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain A4:



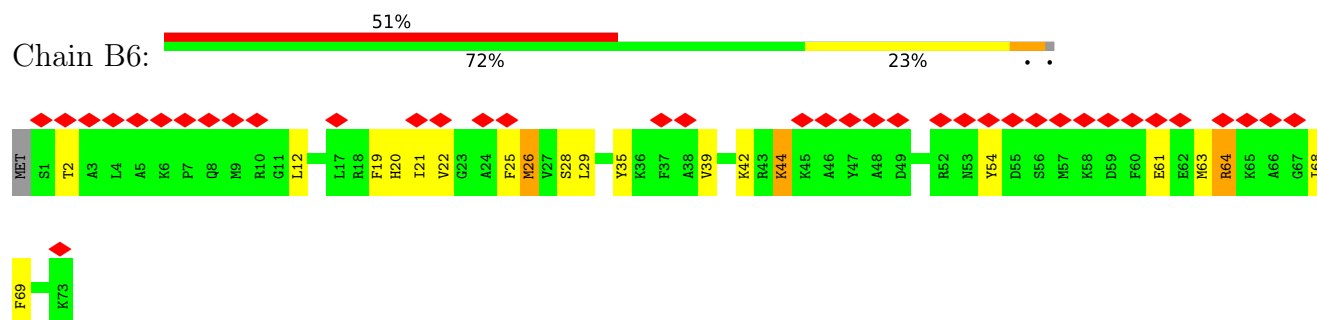
- Molecule 63: Cytochrome c oxidase subunit 6B1

Chain A5:



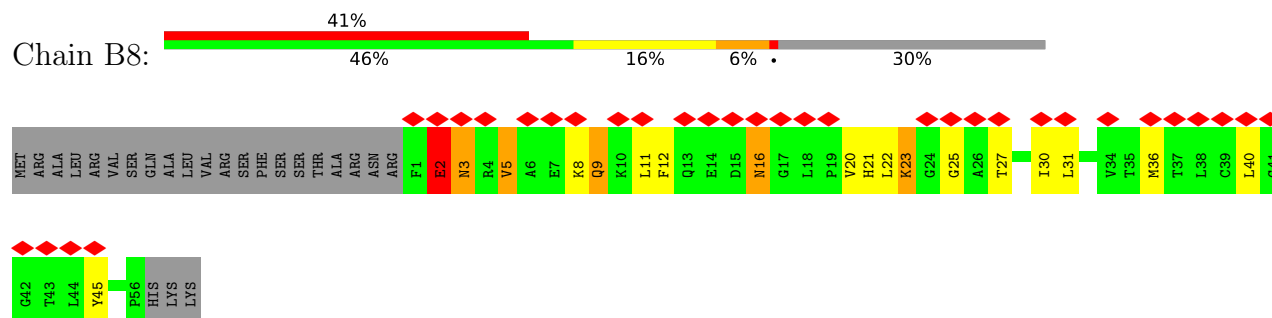
- Molecule 64: Cytochrome c oxidase subunit 6C

Chain B6:



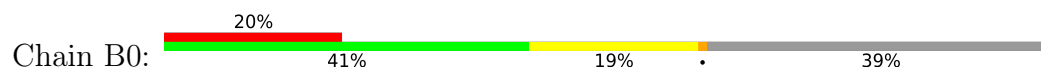
- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial

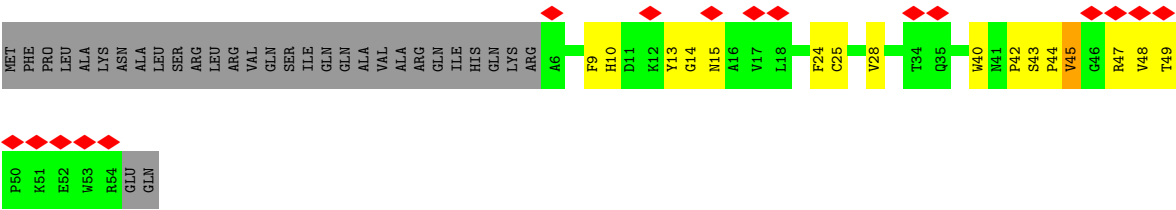
Chain B8:



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

Chain B0:





● 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	24810	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	0.368	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	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: SF4, PC1, CU, HEA, FES, FMN, ZN, HEM, NAP, HEC, MG, CDL, 3PE

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	0.29	0/1571	0.76	0/2149
2	7	0.34	0/1213	0.83	4/1659 (0.2%)
3	6	0.30	0/4892	0.73	4/6660 (0.1%)
4	2	0.41	0/2646	0.85	3/3618 (0.1%)
5	4	0.38	0/3538	0.86	10/4845 (0.2%)
6	5	0.36	0/706	0.82	0/960
7	8	0.31	0/3035	0.76	6/4130 (0.1%)
8	1	0.40	0/2571	0.83	1/3512 (0.0%)
9	3	0.34	0/885	0.89	5/1213 (0.4%)
10	A	0.36	0/5265	0.78	12/7147 (0.2%)
11	B	0.46	0/3505	0.86	5/4752 (0.1%)
12	C	0.39	0/1756	0.75	2/2394 (0.1%)
13	D	0.47	0/1231	0.85	1/1669 (0.1%)
14	E	0.45	0/1418	0.83	3/1922 (0.2%)
15	F	0.37	0/188	1.28	5/259 (1.9%)
16	G	0.41	0/1004	0.84	2/1359 (0.1%)
17	H	0.33	0/800	0.79	1/1076 (0.1%)
18	I	0.31	0/538	0.74	0/722
19	J	0.30	0/545	0.63	0/740
20	K	0.28	0/663	0.72	0/896
21	L	0.33	0/623	0.81	2/862 (0.2%)
22	N	0.27	0/882	0.72	0/1203
23	O	0.31	0/948	0.68	2/1279 (0.2%)
24	P	0.33	0/719	0.80	0/981
25	Q	0.29	0/1381	0.84	2/1869 (0.1%)
26	R	0.32	0/2465	0.85	4/3349 (0.1%)
27	S	0.31	0/2345	0.85	7/3193 (0.2%)
28	T	0.37	0/938	0.89	3/1279 (0.2%)
29	U	0.27	0/1053	0.78	3/1439 (0.2%)
30	V	0.31	0/1115	0.69	0/1508
31	M	0.27	0/651	0.77	2/876 (0.2%)
31	W	0.25	0/624	0.82	0/847

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X	0.31	0/383	0.94	4/523 (0.8%)
33	Y	0.26	0/428	0.60	0/592
34	Z	0.37	0/506	1.03	6/688 (0.9%)
35	a	0.29	0/878	0.82	5/1195 (0.4%)
36	b	0.32	0/1058	0.83	5/1434 (0.3%)
37	c	0.36	0/632	1.07	9/871 (1.0%)
38	d	0.25	0/724	0.73	2/989 (0.2%)
39	f	0.25	0/1191	0.77	2/1639 (0.1%)
40	h	0.33	0/679	0.87	0/926
41	i	0.22	0/286	0.48	0/392
42	j	0.31	0/922	0.83	5/1254 (0.4%)
43	g	0.27	0/1380	0.75	5/1872 (0.3%)
44	e	0.30	0/888	0.94	6/1234 (0.5%)
45	k	0.43	0/3527	0.69	4/4787 (0.1%)
45	w	0.42	0/3455	0.65	1/4685 (0.0%)
46	l	0.40	0/3192	0.65	3/4329 (0.1%)
46	x	0.40	0/3198	0.68	5/4336 (0.1%)
47	m	0.55	0/3108	0.68	0/4252
47	y	0.55	0/3108	0.68	0/4252
48	o	0.48	0/1978	0.71	2/2684 (0.1%)
48	z	0.48	0/1965	0.69	2/2669 (0.1%)
49	A0	0.38	0/1124	0.85	1/1538 (0.1%)
49	p	0.48	0/945	1.13	12/1288 (0.9%)
50	A1	0.52	0/935	0.70	1/1253 (0.1%)
50	q	0.52	0/935	0.64	0/1253
51	A2	0.40	0/698	0.64	0/944
51	r	0.39	0/704	0.64	0/951
52	B5	0.34	0/571	0.67	0/765
52	s	0.35	0/553	0.67	0/741
53	A3	0.44	0/314	0.74	0/434
53	t	0.28	0/272	0.54	0/377
54	B4	0.37	0/524	0.58	0/707
54	u	0.37	0/524	0.58	0/707
55	B3	0.55	0/149	1.32	1/203 (0.5%)
55	v	0.45	0/114	1.13	0/156
56	A9	0.86	7/4164 (0.2%)	1.16	35/5688 (0.6%)
57	B9	0.77	0/1868	1.12	10/2544 (0.4%)
58	B7	0.74	0/2212	1.02	8/3025 (0.3%)
59	A7	0.67	0/1229	0.96	3/1658 (0.2%)
60	A6	0.64	0/898	1.02	6/1218 (0.5%)
61	B2	0.73	0/765	1.13	3/1038 (0.3%)
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	B6	0.71	0/611	0.94	2/810 (0.2%)
65	B8	0.71	0/451	1.04	3/610 (0.5%)
66	B0	0.75	0/398	1.01	0/546
67	B1	0.77	0/399	0.98	2/534 (0.4%)
68	A8	0.69	0/345	0.99	1/470 (0.2%)
All	All	0.46	7/108248 (0.0%)	0.82	254/147255 (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	4
2	7	0	5
3	6	0	6
4	2	0	9
5	4	0	6
6	5	0	3
7	8	0	1
8	1	0	1
10	A	0	12
11	B	0	6
12	C	0	1
13	D	0	4
14	E	0	1
17	H	0	1
22	N	0	1
24	P	0	2
25	Q	0	1
26	R	0	4
27	S	0	4
28	T	0	2
29	U	0	1
30	V	0	3
31	M	0	1
31	W	0	1
36	b	0	3
38	d	0	1
39	f	0	1
40	h	0	2
42	j	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	g	0	1
44	e	0	5
45	k	0	6
45	w	0	3
46	l	0	3
46	x	0	3
47	m	0	4
47	y	0	2
48	o	0	4
48	z	0	4
49	A0	0	6
49	p	0	6
53	A3	0	1
55	B3	0	1
All	All	0	138

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A9	61	HIS	CG-CD2	7.53	1.44	1.35
56	A9	378	HIS	ND1-CE1	7.07	1.39	1.32
56	A9	378	HIS	CE1-NE2	-6.52	1.26	1.32
56	A9	69	MET	SD-CE	-6.28	1.63	1.79
56	A9	61	HIS	ND1-CE1	5.59	1.38	1.32

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	x	230	LEU	N-CA-C	12.17	128.14	110.24
56	A9	376	HIS	ND1-CE1-NE2	10.36	118.76	108.40
9	3	42	ASP	CA-C-N	9.84	132.14	119.84
9	3	42	ASP	C-N-CA	9.84	132.14	119.84
63	A5	52	VAL	N-CA-C	8.97	121.26	108.17

There are no chirality outliers.

5 of 138 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	7	24	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	9	179	ALA	Peptide
1	9	75	LYS	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	1534	0	1488	33	0
2	7	1186	0	1123	11	0
3	6	4765	0	4894	51	0
4	2	2582	0	2612	28	0
5	4	3447	0	3442	46	0
6	5	697	0	708	12	0
7	8	2965	0	2596	47	0
8	1	2499	0	2612	49	0
9	3	862	0	860	14	0
10	A	5179	0	5173	76	0
11	B	3416	0	3335	52	0
12	C	1705	0	1645	24	0
13	D	1200	0	1195	22	0
14	E	1388	0	1340	24	0
15	F	183	0	132	5	0
16	G	981	0	965	14	0
17	H	780	0	753	10	0
18	I	530	0	508	22	0
19	J	530	0	503	4	0
20	K	652	0	636	7	0
21	L	602	0	592	4	0
22	N	862	0	868	11	0
23	O	925	0	907	11	0
24	P	698	0	659	11	0
25	Q	1345	0	1282	19	0
26	R	2407	0	2296	52	0
27	S	2297	0	2022	28	0
28	T	922	0	852	64	0
29	U	1019	0	900	10	0
30	V	1087	0	1037	14	0
31	M	642	0	642	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	W	616	0	579	11	0
32	X	372	0	314	4	0
33	Y	409	0	318	1	0
34	Z	493	0	395	5	0
35	a	857	0	765	9	0
36	b	1032	0	954	9	0
37	c	617	0	492	10	0
38	d	708	0	514	7	0
39	f	1156	0	892	16	0
40	h	658	0	584	10	0
41	i	277	0	240	1	0
42	j	892	0	835	13	0
43	g	1351	0	1262	16	0
44	e	864	0	567	13	0
45	k	3454	0	3350	303	0
45	w	3385	0	3293	276	0
46	l	3135	0	3112	243	0
46	x	3141	0	3123	256	0
47	m	3011	0	3077	252	0
47	y	3011	0	3077	246	0
48	o	1919	0	1870	186	0
48	z	1906	0	1841	189	0
49	A0	1117	0	808	80	0
49	p	938	0	733	72	0
50	A1	916	0	911	116	0
50	q	916	0	911	89	0
51	A2	676	0	668	74	0
51	r	682	0	679	49	0
52	B5	566	0	542	47	0
52	s	548	0	530	49	0
53	A3	304	0	299	49	0
53	t	262	0	250	25	0
54	B4	511	0	518	62	0
54	u	511	0	518	56	0
55	B3	148	0	154	18	0
55	v	114	0	107	9	0
56	A9	4025	0	4003	86	0
57	B9	1822	0	1834	73	0
58	B7	2125	0	2046	52	0
59	A7	1195	0	1183	35	0
60	A6	878	0	868	21	0
61	B2	748	0	728	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	A4	671	0	645	29	0
63	A5	628	0	582	24	0
64	B6	598	0	612	16	0
65	B8	441	0	439	17	0
66	B0	384	0	366	12	0
67	B1	386	0	388	8	0
68	A8	335	0	352	12	0
69	9	4	0	0	0	0
69	A	4	0	0	0	0
69	m	4	0	0	0	0
70	4	82	0	114	1	0
70	6	64	0	72	2	0
70	J	58	0	60	1	0
71	2	41	0	59	1	0
71	4	41	0	59	1	0
71	B	51	0	82	2	0
71	V	51	0	82	0	0
71	j	46	0	69	1	0
72	2	46	0	66	2	0
72	L	47	0	71	2	0
72	Q	46	0	66	1	0
72	S	47	0	71	3	0
72	j	39	0	55	1	0
73	8	31	0	19	3	0
74	8	8	0	0	0	0
74	A	16	0	0	1	0
74	D	8	0	0	0	0
74	E	16	0	0	1	0
75	B2	1	0	0	0	0
75	I	1	0	0	0	0
76	R	48	0	23	3	0
77	m	86	0	60	28	0
77	y	86	0	60	30	0
78	o	43	0	32	10	0
78	z	43	0	32	10	0
79	A9	120	0	108	4	0
80	A9	1	0	0	0	0
80	B9	2	0	0	0	0
81	A9	1	0	0	0	0
All	All	106778	0	102965	3613	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 17.

The worst 5 of 3613 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)
8:1:17:VAL:HG21	8:1:225:MET:CE	1.21	1.57
8:1:17:VAL:CG2	8:1:225:MET:CE	1.78	1.47
50:A1:24:ALA:HB1	51:A2:47:ARG:NH2	1.33	1.43
50:A1:24:ALA:CB	51:A2:47:ARG:HH21	1.36	1.36
11:B:52:MET:O	11:B:54:PRO:HD3	1.17	1.31

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%)	166 (81%)	38 (18%)	1 (0%)	24	63
2	7	170/175 (97%)	135 (79%)	31 (18%)	4 (2%)	4	27
3	6	604/606 (100%)	518 (86%)	82 (14%)	4 (1%)	18	56
4	2	342/347 (99%)	298 (87%)	44 (13%)	0	100	100
5	4	457/459 (100%)	374 (82%)	77 (17%)	6 (1%)	9	42
6	5	94/98 (96%)	80 (85%)	14 (15%)	0	100	100
7	8	425/444 (96%)	343 (81%)	80 (19%)	2 (0%)	24	63
8	1	315/318 (99%)	270 (86%)	43 (14%)	2 (1%)	21	59
9	3	110/115 (96%)	92 (84%)	16 (14%)	2 (2%)	6	34
10	A	686/704 (97%)	563 (82%)	118 (17%)	5 (1%)	18	56
11	B	428/430 (100%)	357 (83%)	64 (15%)	7 (2%)	7	38
12	C	206/228 (90%)	175 (85%)	31 (15%)	0	100	100
13	D	150/179 (84%)	133 (89%)	17 (11%)	0	100	100
14	E	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	F	26/75 (35%)	17 (65%)	9 (35%)	0	100	100
16	G	121/133 (91%)	99 (82%)	20 (16%)	2 (2%)	7	36
17	H	94/105 (90%)	74 (79%)	19 (20%)	1 (1%)	11	46
18	I	69/96 (72%)	57 (83%)	11 (16%)	1 (1%)	9	40
19	J	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8	40
20	K	82/98 (84%)	62 (76%)	20 (24%)	0	100	100
21	L	78/83 (94%)	68 (87%)	10 (13%)	0	100	100
22	N	109/115 (95%)	91 (84%)	18 (16%)	0	100	100
23	O	112/127 (88%)	98 (88%)	14 (12%)	0	100	100
24	P	86/112 (77%)	66 (77%)	20 (23%)	0	100	100
25	Q	166/171 (97%)	117 (70%)	47 (28%)	2 (1%)	10	44
26	R	315/345 (91%)	249 (79%)	64 (20%)	2 (1%)	21	59
27	S	317/320 (99%)	249 (78%)	64 (20%)	4 (1%)	9	42
28	T	136/140 (97%)	112 (82%)	16 (12%)	8 (6%)	1	13
29	U	128/145 (88%)	101 (79%)	27 (21%)	0	100	100
30	V	136/143 (95%)	119 (88%)	15 (11%)	2 (2%)	8	40
31	M	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
31	W	84/88 (96%)	66 (79%)	18 (21%)	0	100	100
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
33	Y	55/72 (76%)	44 (80%)	11 (20%)	0	100	100
34	Z	72/97 (74%)	49 (68%)	23 (32%)	0	100	100
35	a	112/128 (88%)	87 (78%)	25 (22%)	0	100	100
36	b	137/143 (96%)	118 (86%)	19 (14%)	0	100	100
37	c	86/127 (68%)	67 (78%)	19 (22%)	0	100	100
38	d	105/117 (90%)	77 (73%)	24 (23%)	4 (4%)	2	19
39	f	165/178 (93%)	126 (76%)	38 (23%)	1 (1%)	21	59
40	h	82/125 (66%)	57 (70%)	23 (28%)	2 (2%)	4	27
41	i	36/49 (74%)	34 (94%)	2 (6%)	0	100	100
42	j	111/120 (92%)	95 (86%)	16 (14%)	0	100	100
43	g	171/176 (97%)	143 (84%)	28 (16%)	0	100	100
44	e	139/158 (88%)	80 (58%)	52 (37%)	7 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	k	444/480 (92%)	401 (90%)	42 (10%)	1 (0%)	43	78
45	w	432/480 (90%)	397 (92%)	33 (8%)	2 (0%)	24	63
46	l	417/453 (92%)	380 (91%)	31 (7%)	6 (1%)	9	40
46	x	417/453 (92%)	379 (91%)	31 (7%)	7 (2%)	7	36
47	m	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	36	72
47	y	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	36	72
48	o	239/325 (74%)	211 (88%)	24 (10%)	4 (2%)	7	36
48	z	239/325 (74%)	211 (88%)	23 (10%)	5 (2%)	5	30
49	A0	184/196 (94%)	135 (73%)	45 (24%)	4 (2%)	5	29
49	p	147/196 (75%)	93 (63%)	40 (27%)	14 (10%)	0	8
50	A1	104/111 (94%)	94 (90%)	7 (7%)	3 (3%)	3	23
50	q	104/111 (94%)	98 (94%)	6 (6%)	0	100	100
51	A2	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
51	r	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
52	B5	67/91 (74%)	57 (85%)	9 (13%)	1 (2%)	8	40
52	s	65/91 (71%)	55 (85%)	9 (14%)	1 (2%)	8	40
53	A3	37/56 (66%)	26 (70%)	7 (19%)	4 (11%)	0	6
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	3	21
54	B4	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
54	u	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
55	B3	20/78 (26%)	9 (45%)	9 (45%)	2 (10%)	0	7
55	v	16/78 (20%)	7 (44%)	8 (50%)	1 (6%)	1	13
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
57	B9	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
58	B7	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	A6	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	B2	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	40
64	B6	71/74 (96%)	65 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	B8	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	20
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	B1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13637/15129 (90%)	11563 (85%)	1924 (14%)	150 (1%)	14	46

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	7	171	ILE
9	3	43	PRO
10	A	463	SER
11	B	54	PRO
11	B	56	LYS

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	159/183 (87%)	157 (99%)	2 (1%)	61	74
2	7	104/142 (73%)	104 (100%)	0	100	100
3	6	523/534 (98%)	521 (100%)	2 (0%)	84	84
4	2	274/316 (87%)	273 (100%)	1 (0%)	84	84
5	4	351/413 (85%)	350 (100%)	1 (0%)	86	86
6	5	75/86 (87%)	75 (100%)	0	100	100
7	8	236/353 (67%)	236 (100%)	0	100	100
8	1	273/275 (99%)	269 (98%)	4 (2%)	57	72
9	3	89/101 (88%)	88 (99%)	1 (1%)	65	76
10	A	550/588 (94%)	548 (100%)	2 (0%)	84	84
11	B	362/371 (98%)	361 (100%)	1 (0%)	86	86
12	C	183/204 (90%)	182 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	D	126/150 (84%)	125 (99%)	1 (1%)	73	80
14	E	145/151 (96%)	145 (100%)	0	100	100
15	F	13/69 (19%)	13 (100%)	0	100	100
16	G	105/119 (88%)	105 (100%)	0	100	100
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	52/79 (66%)	49 (94%)	3 (6%)	18	40
19	J	50/59 (85%)	50 (100%)	0	100	100
20	K	66/81 (82%)	66 (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	72/96 (75%)	72 (100%)	0	100	100
25	Q	142/154 (92%)	139 (98%)	3 (2%)	47	65
26	R	232/298 (78%)	229 (99%)	3 (1%)	61	74
27	S	204/283 (72%)	203 (100%)	1 (0%)	81	83
28	T	75/101 (74%)	73 (97%)	2 (3%)	39	61
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%)	56 (98%)	1 (2%)	51	68
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/75 (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	45/121 (37%)	45 (100%)	0	100	100
38	d	42/107 (39%)	42 (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	88/106 (83%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	g	130/157 (83%)	130 (100%)	0	100	100
44	e	44/141 (31%)	44 (100%)	0	100	100
45	k	369/394 (94%)	368 (100%)	1 (0%)	86	86
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%)	325 (99%)	2 (1%)	78	83
47	y	327/327 (100%)	325 (99%)	2 (1%)	78	83
48	o	206/257 (80%)	205 (100%)	1 (0%)	81	83
48	z	202/257 (79%)	201 (100%)	1 (0%)	81	83
49	A0	64/168 (38%)	63 (98%)	1 (2%)	55	70
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	95 (99%)	1 (1%)	68	78
50	q	96/99 (97%)	96 (100%)	0	100	100
51	A2	70/72 (97%)	70 (100%)	0	100	100
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B5	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	28/46 (61%)	25 (89%)	3 (11%)	6	21
53	t	24/46 (52%)	23 (96%)	1 (4%)	26	48
54	B4	52/54 (96%)	51 (98%)	1 (2%)	50	67
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B3	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	B9	211/211 (100%)	192 (91%)	19 (9%)	9	27
58	B7	226/226 (100%)	200 (88%)	26 (12%)	5	18
59	A7	128/148 (86%)	119 (93%)	9 (7%)	14	35
60	A6	95/123 (77%)	95 (100%)	0	100	100
61	B2	81/103 (79%)	77 (95%)	4 (5%)	22	43
62	A4	68/79 (86%)	66 (97%)	2 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	A5	67/76 (88%)	64 (96%)	3 (4%)	24	46
64	B6	58/59 (98%)	54 (93%)	4 (7%)	14	36
65	B8	47/68 (69%)	43 (92%)	4 (8%)	10	29
66	B0	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	B1	40/55 (73%)	40 (100%)	0	100	100
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10623/12909 (82%)	10463 (98%)	160 (2%)	55	72

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	B7	128	GLU
63	A5	29	CYS
58	B7	142	VAL
59	A7	36	SER
65	B8	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
45	w	267	ASN
56	A9	4	ASN
46	x	254	HIS
47	y	374	ASN
56	A9	256	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 38 ligands modelled in this entry, 6 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
77	HEM	m	402	47	50,50,50	1.90	18 (36%)	66,82,82	1.41	7 (10%)
77	HEM	y	402	47	50,50,50	1.89	17 (34%)	66,82,82	1.40	7 (10%)
71	3PE	j	202	-	45,45,50	0.91	4 (8%)	48,50,55	1.05	2 (4%)
72	PC1	Q	201	-	45,45,53	1.00	4 (8%)	51,53,61	1.07	2 (3%)
72	PC1	2	402	-	45,45,53	1.00	3 (6%)	51,53,61	1.03	2 (3%)
74	SF4	A	802	-	0,12,12	-	-	-	-	-
79	HEA	A9	602	56	66,67,67	1.22	7 (10%)	78,103,103	1.36	11 (14%)
79	HEA	A9	601	56	66,67,67	1.10	3 (4%)	78,103,103	1.38	11 (14%)
71	3PE	4	502	-	40,40,50	0.93	3 (7%)	43,45,55	1.37	3 (6%)
72	PC1	j	201	-	38,38,53	1.12	4 (10%)	44,46,61	1.10	2 (4%)
78	HEC	o	301	48	50,50,50	1.68	7 (14%)	68,82,82	1.56	11 (16%)
76	NAP	R	601	-	49,52,52	4.36	22 (44%)	69,80,80	1.86	15 (21%)
71	3PE	V	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
74	SF4	E	302	-	0,12,12	-	-	-	-	-
71	3PE	B	501	11	50,50,50	0.85	4 (8%)	53,55,55	1.12	2 (3%)
77	HEM	m	401	47	50,50,50	1.91	20 (40%)	66,82,82	1.70	12 (18%)
69	FES	9	301	-	0,4,4	-	-	-	-	-
74	SF4	8	502	-	0,12,12	-	-	-	-	-
69	FES	A	803	-	0,4,4	-	-	-	-	-
74	SF4	A	801	-	0,12,12	-	-	-	-	-
72	PC1	S	401	-	46,46,53	0.99	4 (8%)	52,54,61	0.99	2 (3%)
70	CDL	6	701	-	63,63,99	1.07	7 (11%)	69,75,111	1.28	4 (5%)
72	PC1	L	200	-	46,46,53	1.02	4 (8%)	52,54,61	1.06	2 (3%)
73	FMN	8	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.62	11 (22%)
74	SF4	E	301	-	0,12,12	-	-	-	-	-
70	CDL	J	101	-	57,57,99	1.14	7 (12%)	63,69,111	1.19	4 (6%)
77	HEM	y	401	47	50,50,50	1.90	20 (40%)	66,82,82	1.70	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	3PE	2	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.18	2 (4%)
74	SF4	D	301	-	0,12,12	-	-	-	-	-
70	CDL	4	501	-	81,81,99	0.97	6 (7%)	87,93,111	1.10	5 (5%)
78	HEC	z	301	48	50,50,50	1.68	7 (14%)	68,82,82	1.56	11 (16%)
69	FES	m	403	-	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEM	m	402	47	-	2/14/54/54	-
77	HEM	y	402	47	-	2/14/54/54	-
71	3PE	j	202	-	-	24/49/49/54	-
72	PC1	Q	201	-	-	20/49/49/57	-
72	PC1	2	402	-	-	20/49/49/57	-
74	SF4	A	802	-	-	-	0/6/5/5
79	HEA	A9	602	56	-	7/36/76/76	-
79	HEA	A9	601	56	-	9/36/76/76	-
71	3PE	4	502	-	-	24/44/44/54	-
72	PC1	j	201	-	-	23/42/42/57	-
78	HEC	o	301	48	1/1/3/7	3/14/54/54	-
76	NAP	R	601	-	-	16/35/67/67	0/5/5/5
71	3PE	V	201	-	-	21/54/54/54	-
77	HEM	m	401	47	-	4/14/54/54	-
71	3PE	B	501	11	-	26/54/54/54	-
74	SF4	E	302	-	-	-	0/6/5/5
69	FES	9	301	-	-	-	0/1/1/1
74	SF4	8	502	-	-	-	0/6/5/5
69	FES	A	803	-	-	-	0/1/1/1
74	SF4	A	801	-	-	-	0/6/5/5
72	PC1	S	401	-	-	32/50/50/57	-
70	CDL	6	701	-	-	42/74/74/110	-
72	PC1	L	200	-	-	23/50/50/57	-
73	FMN	8	501	-	-	10/18/18/18	0/3/3/3
74	SF4	E	301	-	-	-	0/6/5/5
70	CDL	J	101	-	-	31/68/68/110	-

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEM	y	401	47	-	4/14/54/54	-
71	3PE	2	401	-	-	21/44/44/54	-
74	SF4	D	301	-	-	-	0/6/5/5
70	CDL	4	501	-	-	39/92/92/110	-
78	HEC	z	301	48	1/1/3/7	3/14/54/54	-
69	FES	m	403	-	-	-	0/1/1/1

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	O4D-C1D	16.09	1.63	1.41
76	R	601	NAP	C2D-C1D	-14.41	1.31	1.53
76	R	601	NAP	C2B-C1B	-9.13	1.29	1.53
76	R	601	NAP	O4B-C1B	8.26	1.61	1.42
76	R	601	NAP	C7N-N7N	6.91	1.46	1.33

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	R	601	NAP	N3A-C2A-N1A	-6.02	119.19	128.60
77	y	401	HEM	C1C-CHC-C4B	-5.74	113.67	126.06
77	m	401	HEM	C1C-CHC-C4B	-5.72	113.72	126.06
77	m	401	HEM	C1A-CHA-C4D	-5.57	113.13	126.34
77	y	401	HEM	C1A-CHA-C4D	-5.53	113.22	126.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
78	o	301	HEC	NA
78	z	301	HEC	NA

5 of 406 torsion outliers are listed below:

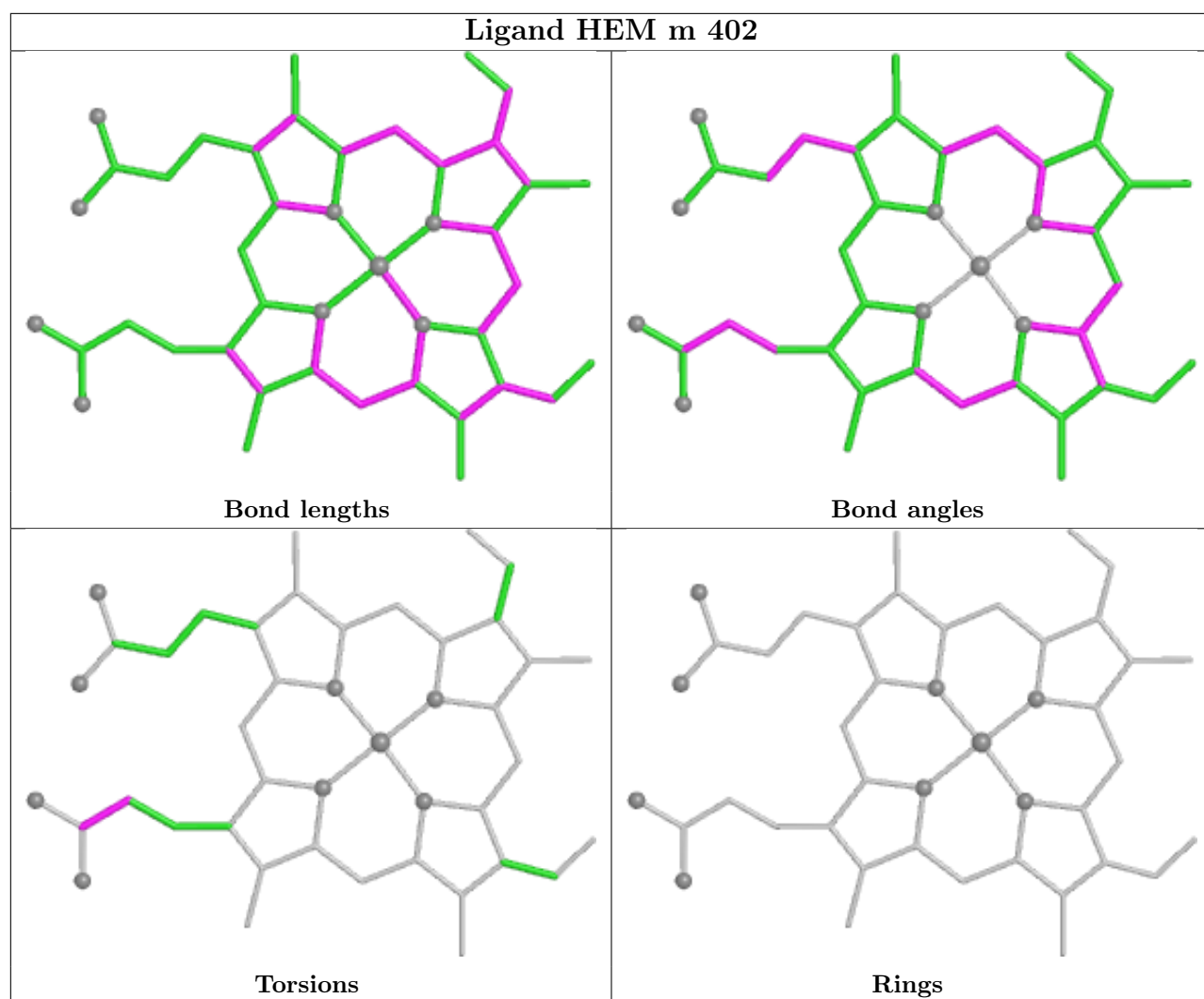
Mol	Chain	Res	Type	Atoms
70	6	701	CDL	CB2-C1-CA2-OA2
70	6	701	CDL	CA3-OA5-PA1-OA2
70	6	701	CDL	CA3-OA5-PA1-OA3
70	6	701	CDL	CA3-OA5-PA1-OA4
70	6	701	CDL	CB2-OB2-PB2-OB3

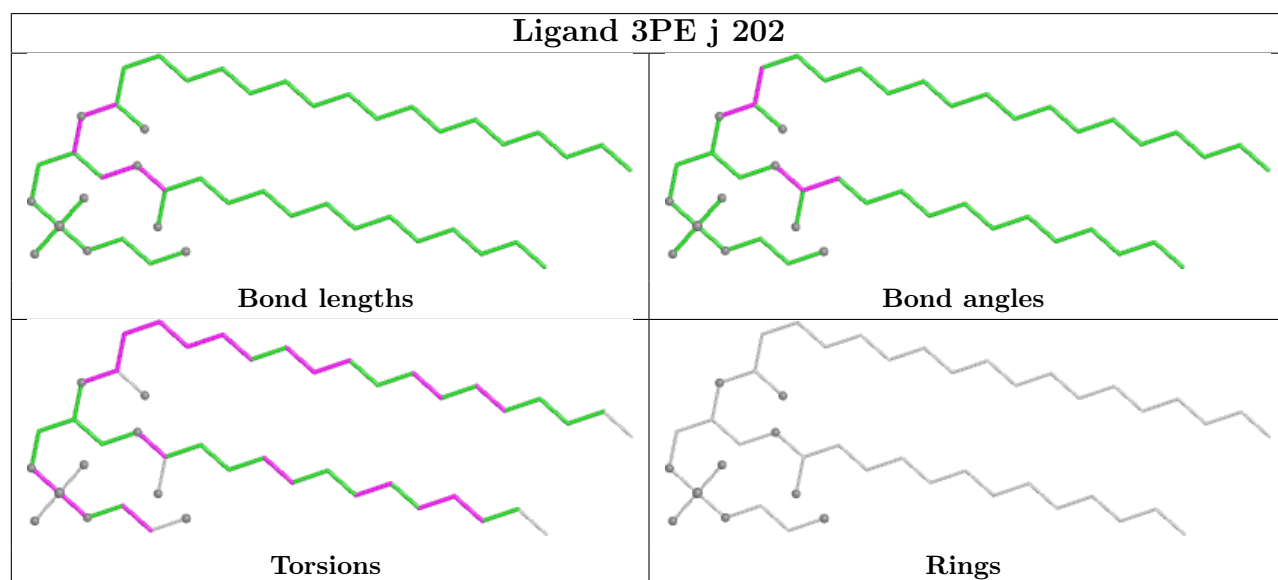
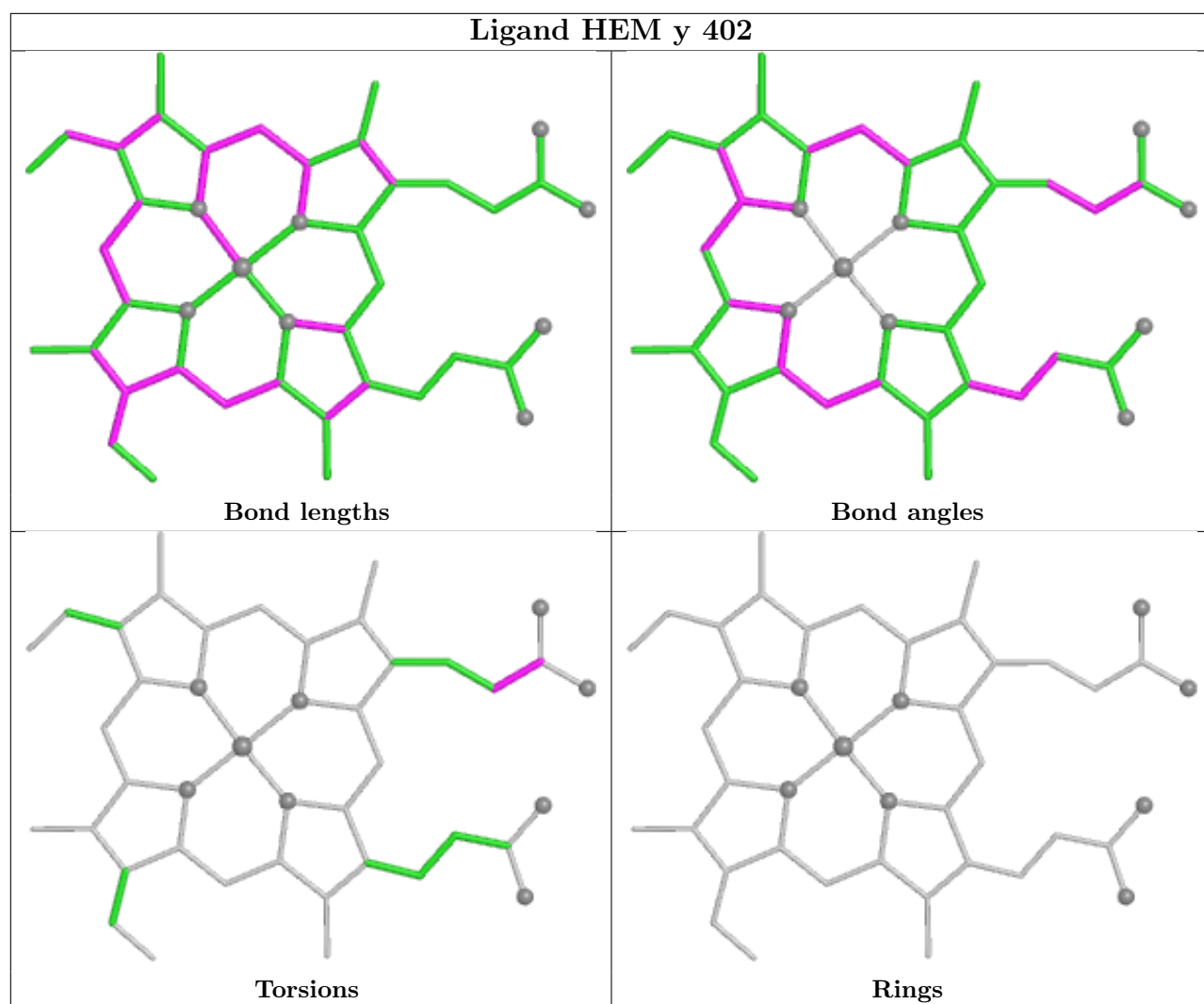
There are no ring outliers.

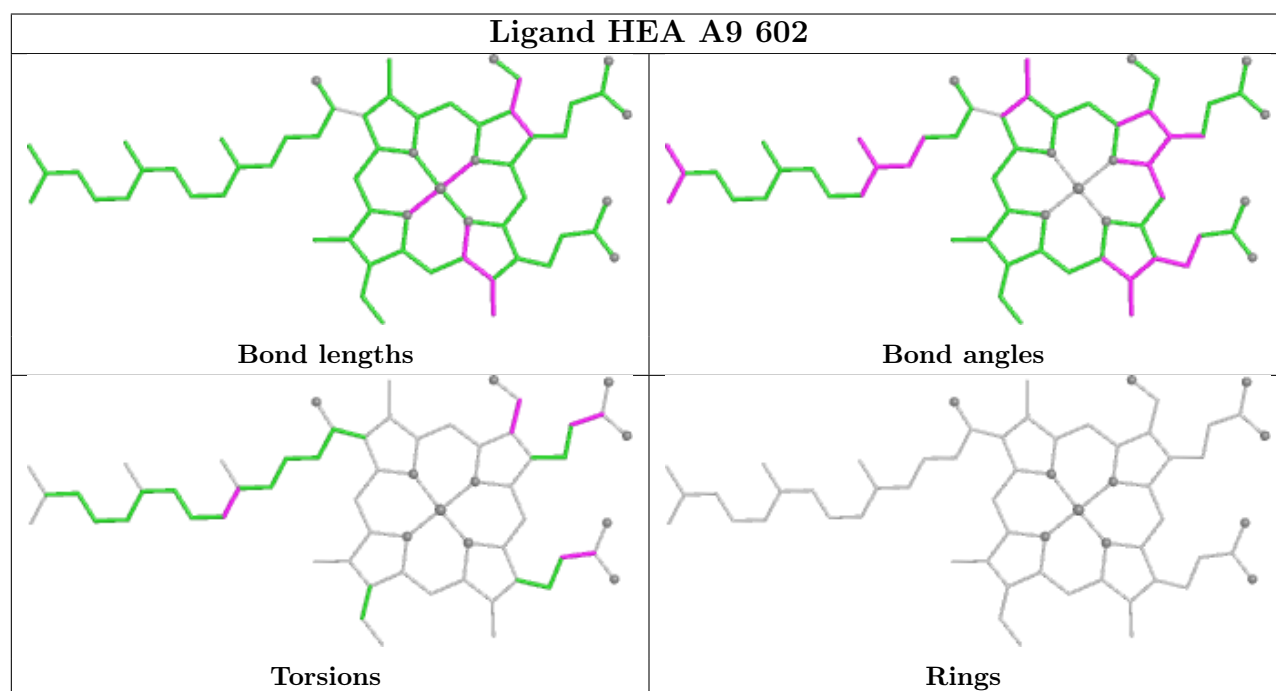
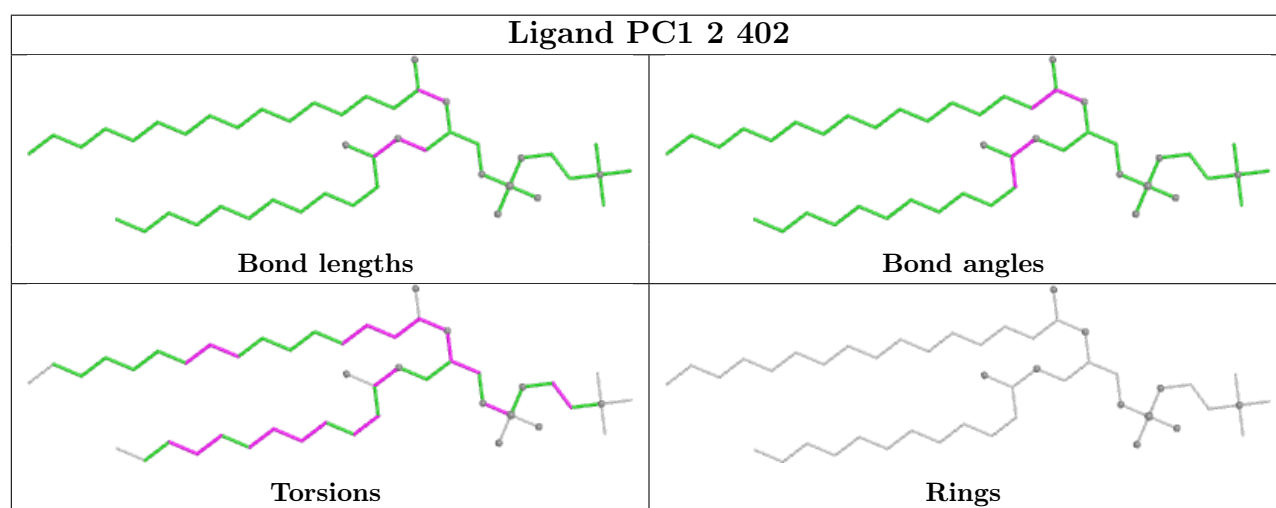
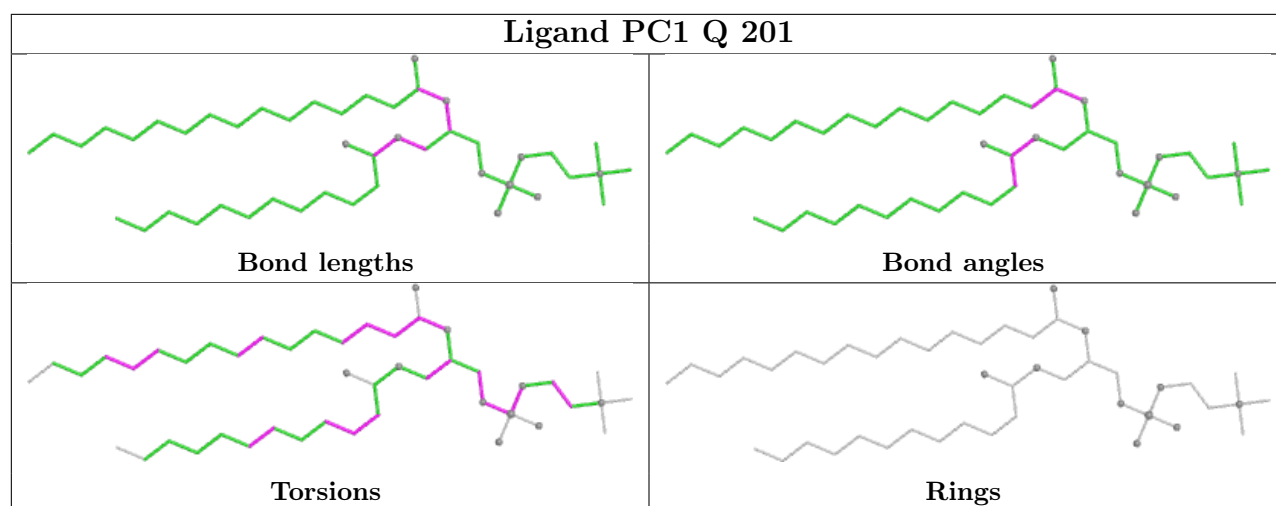
24 monomers are involved in 108 short contacts:

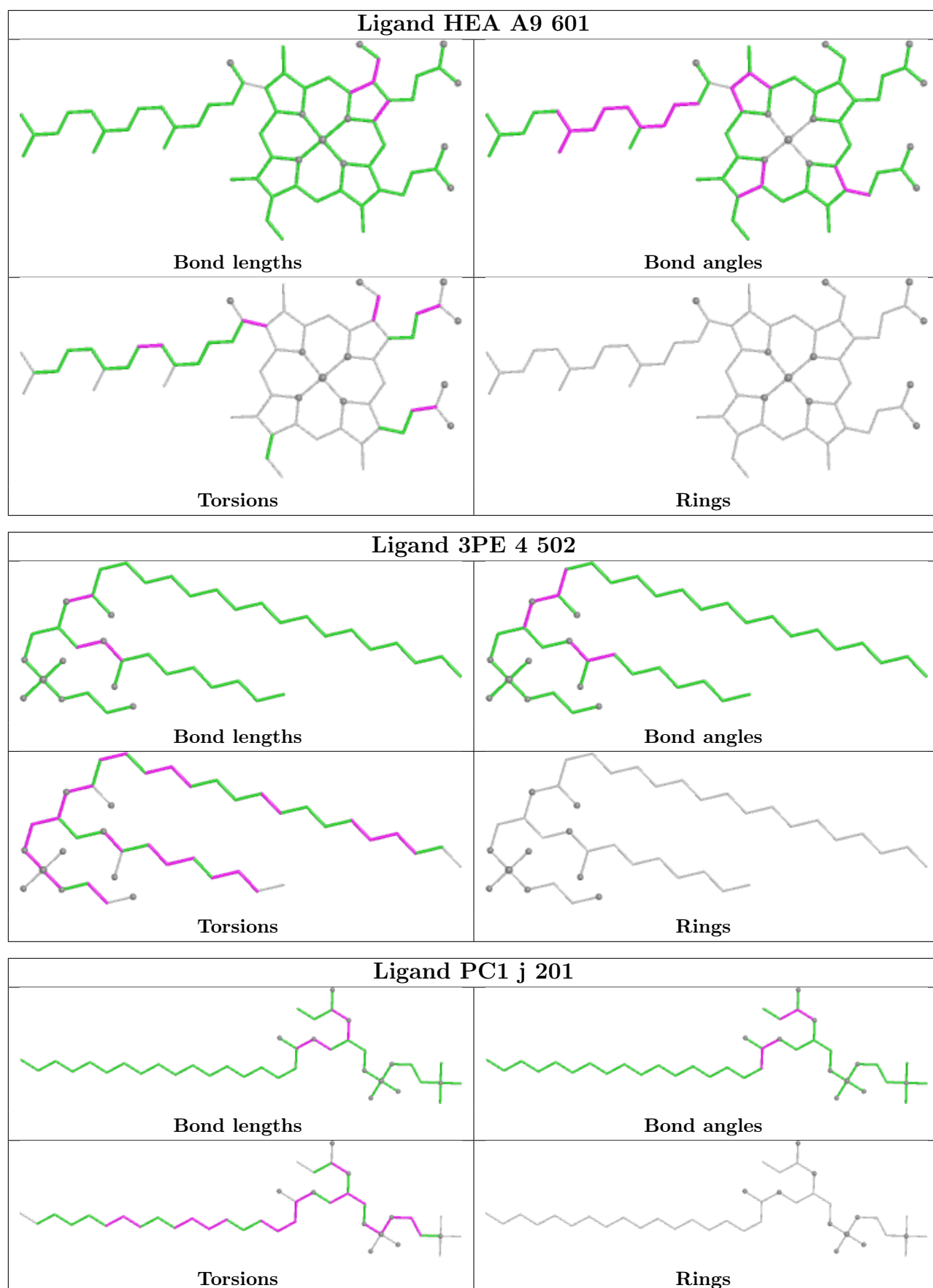
Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	m	402	HEM	17	0
77	y	402	HEM	19	0
71	j	202	3PE	1	0
72	Q	201	PC1	1	0
72	2	402	PC1	2	0
79	A9	602	HEA	3	0
79	A9	601	HEA	1	0
71	4	502	3PE	1	0
72	j	201	PC1	1	0
78	o	301	HEC	10	0
76	R	601	NAP	3	0
74	E	302	SF4	1	0
71	B	501	3PE	2	0
77	m	401	HEM	11	0
74	A	801	SF4	1	0
72	S	401	PC1	3	0
70	6	701	CDL	2	0
72	L	200	PC1	2	0
73	8	501	FMN	3	0
70	J	101	CDL	1	0
77	y	401	HEM	11	0
71	2	401	3PE	1	0
70	4	501	CDL	1	0
78	z	301	HEC	10	0

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

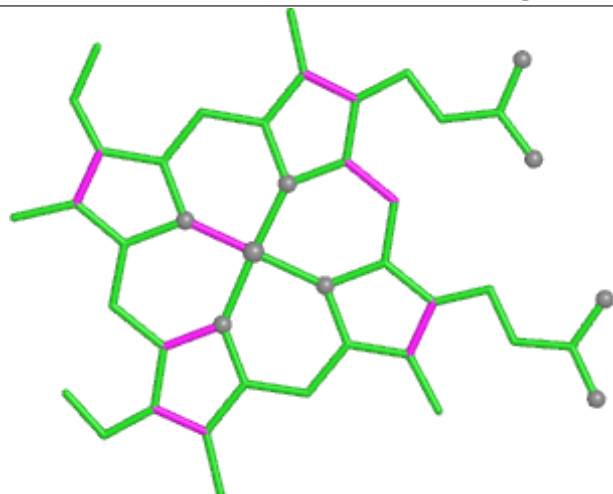




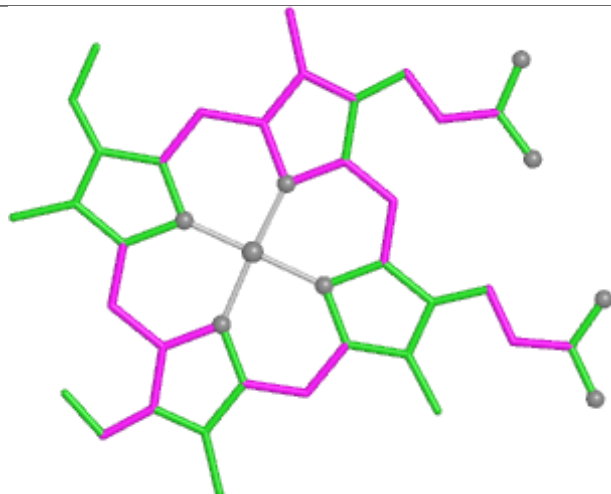




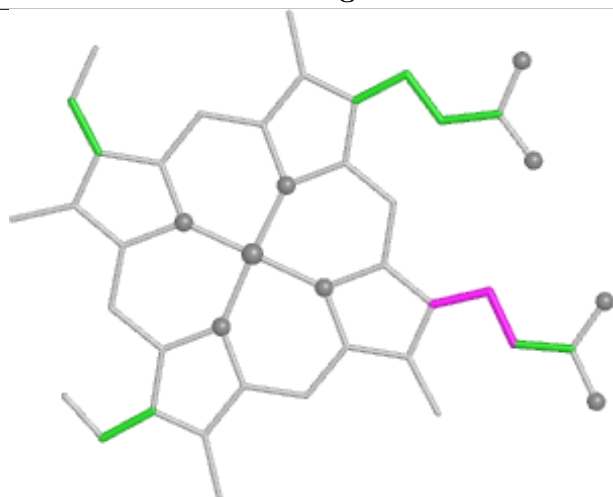
Ligand HEC o 301



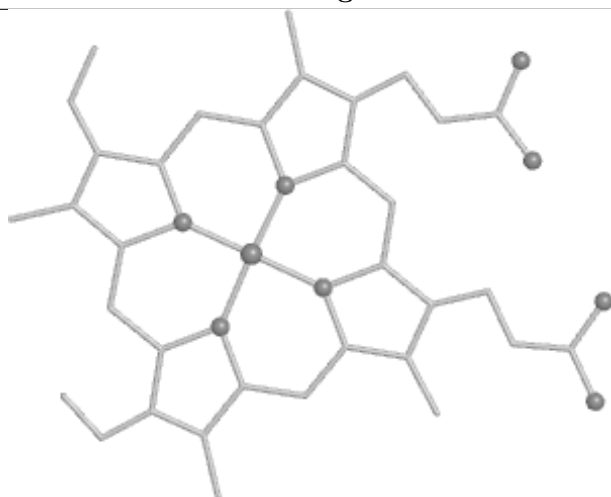
Bond lengths



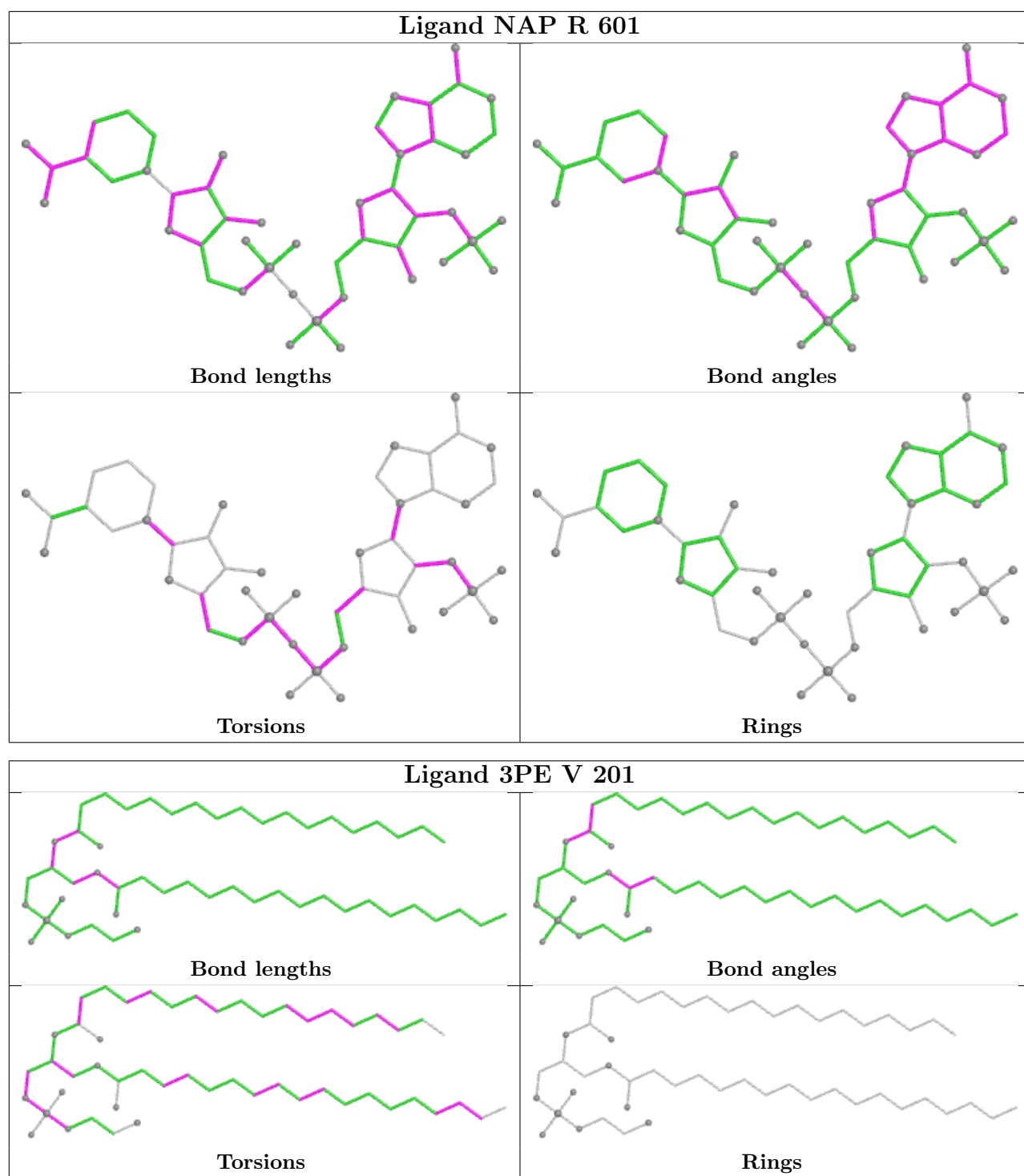
Bond angles

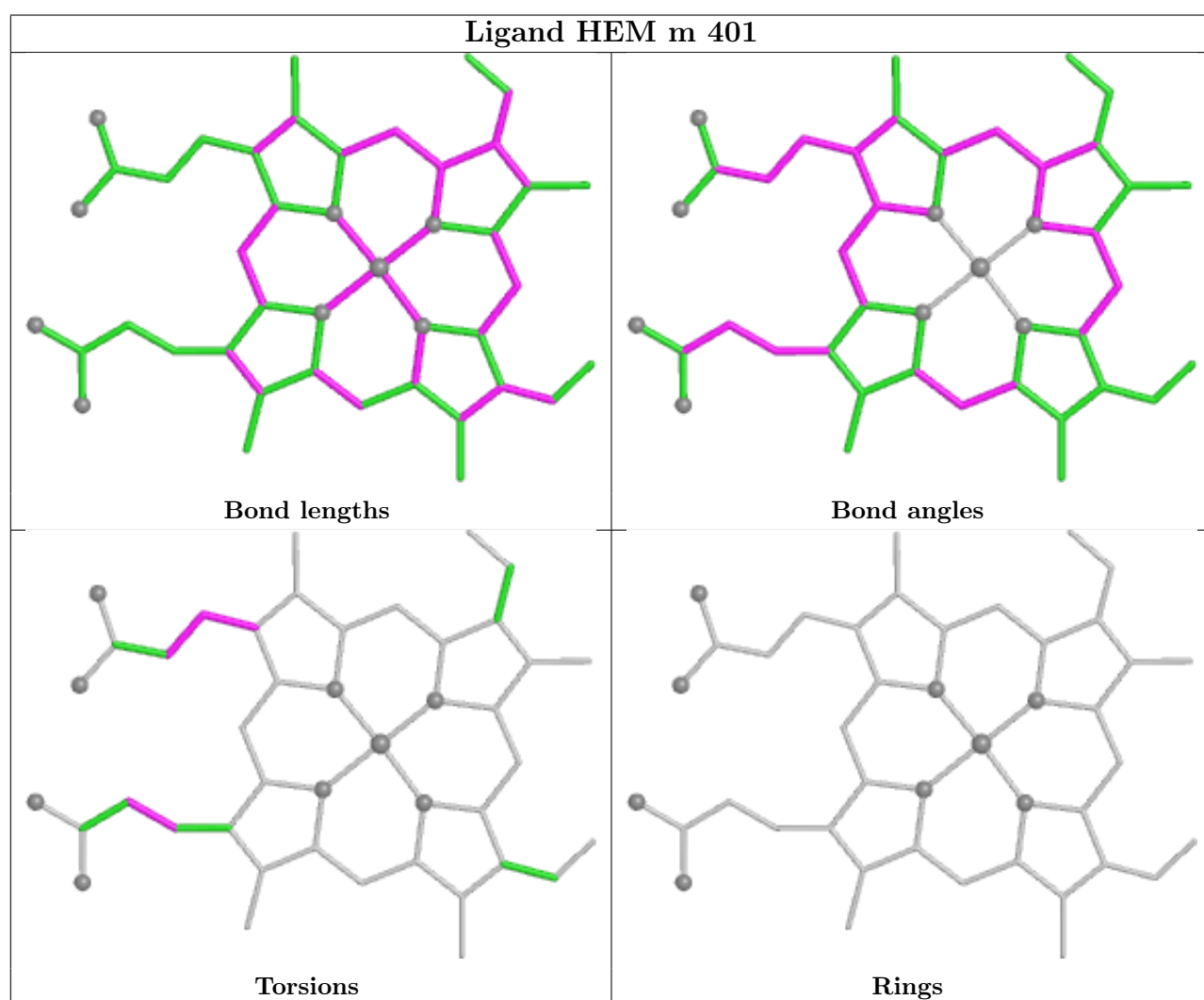
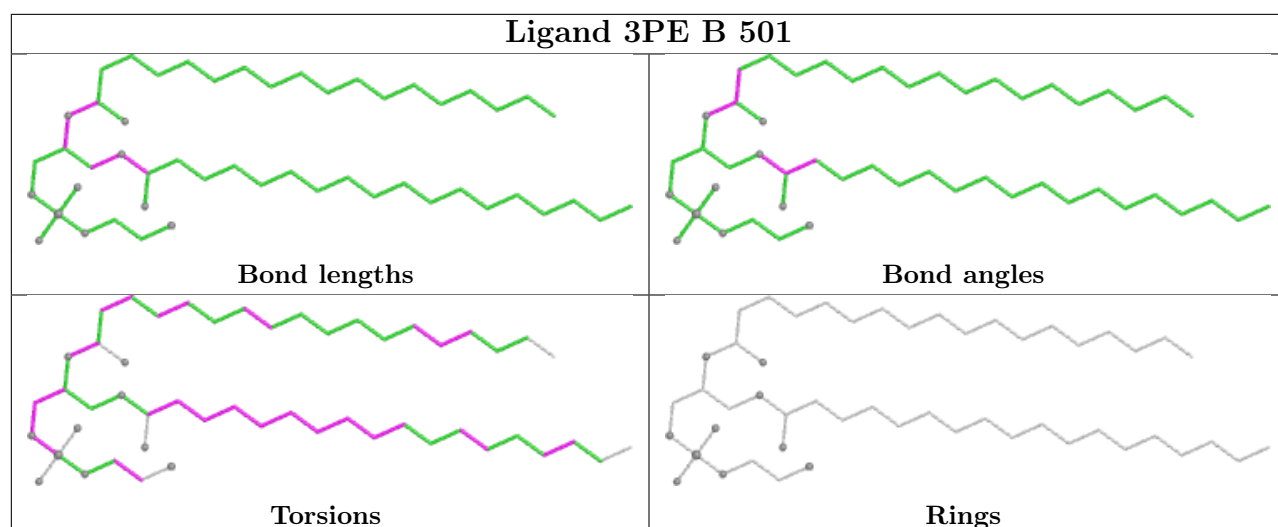


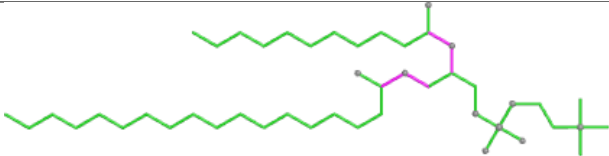
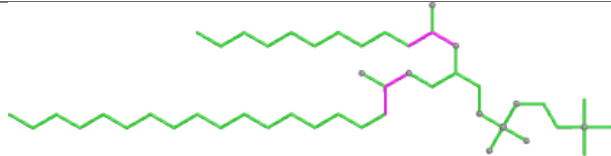
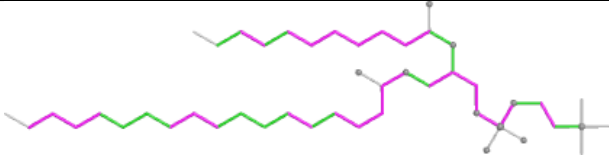
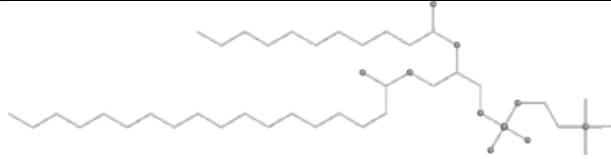
Torsions

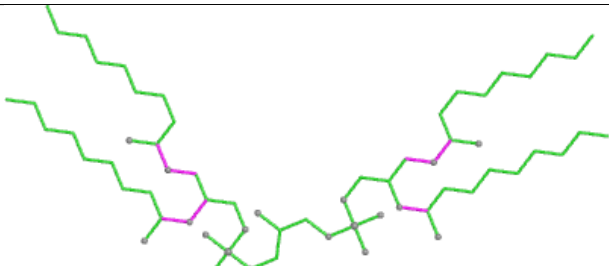
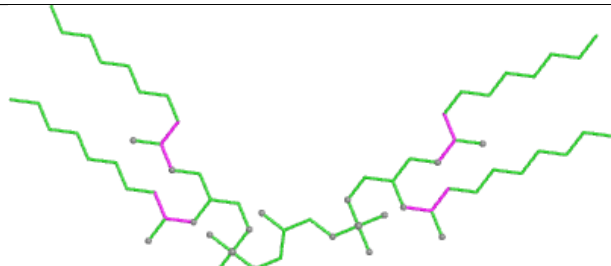
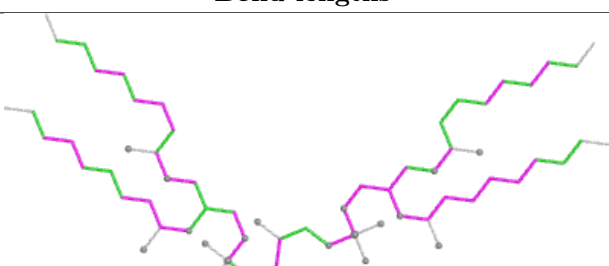
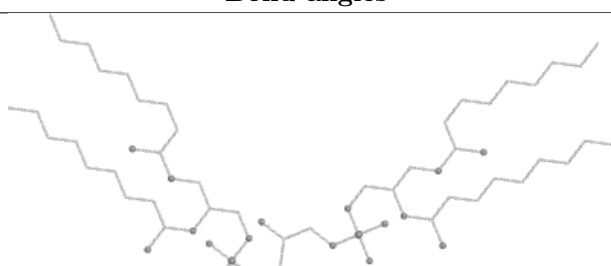


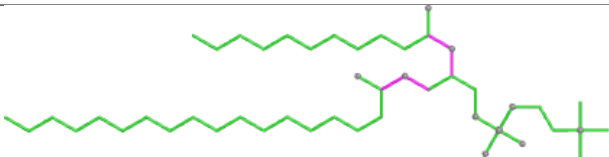
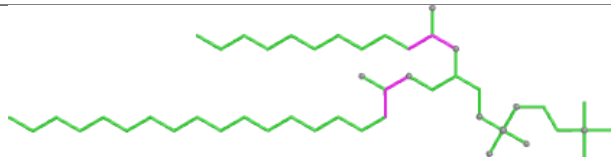
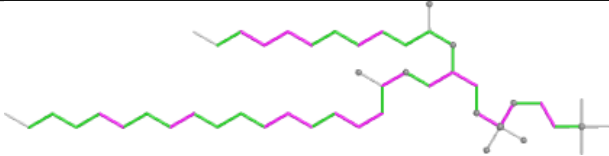
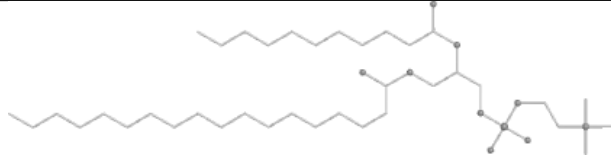
Rings

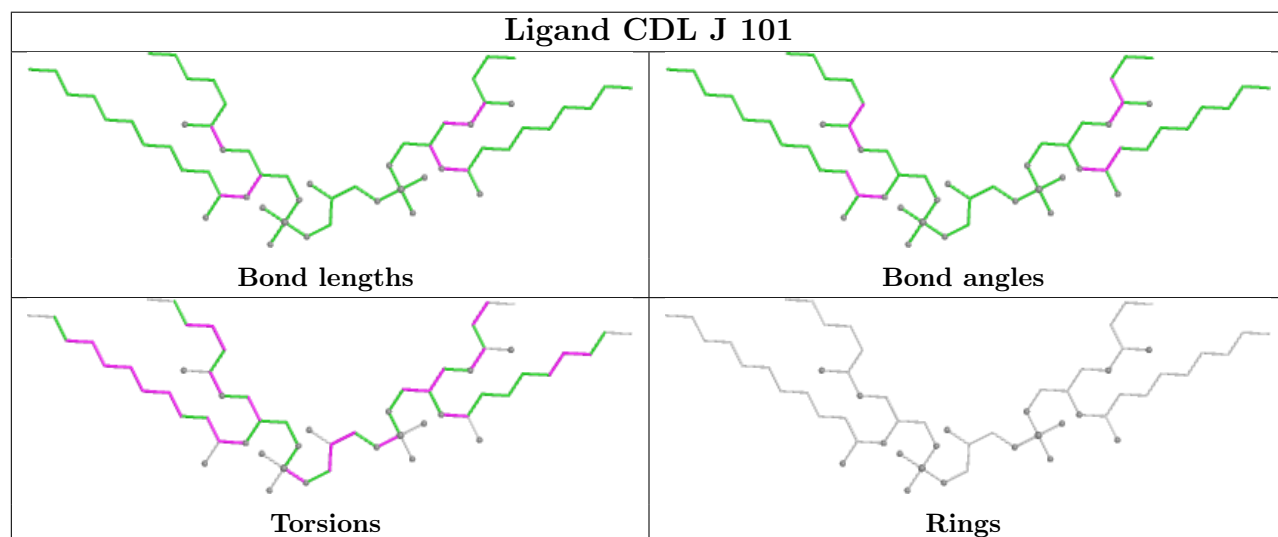
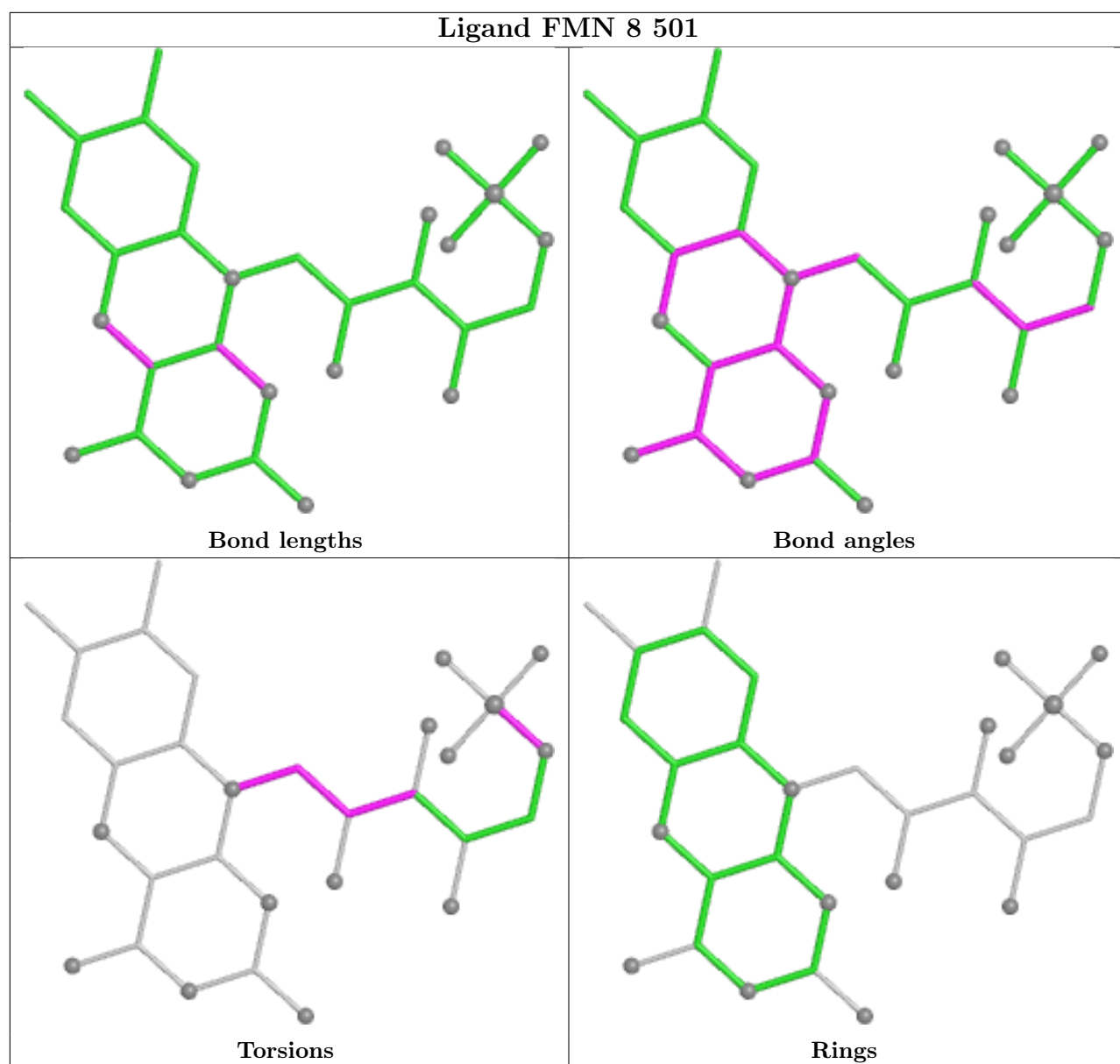


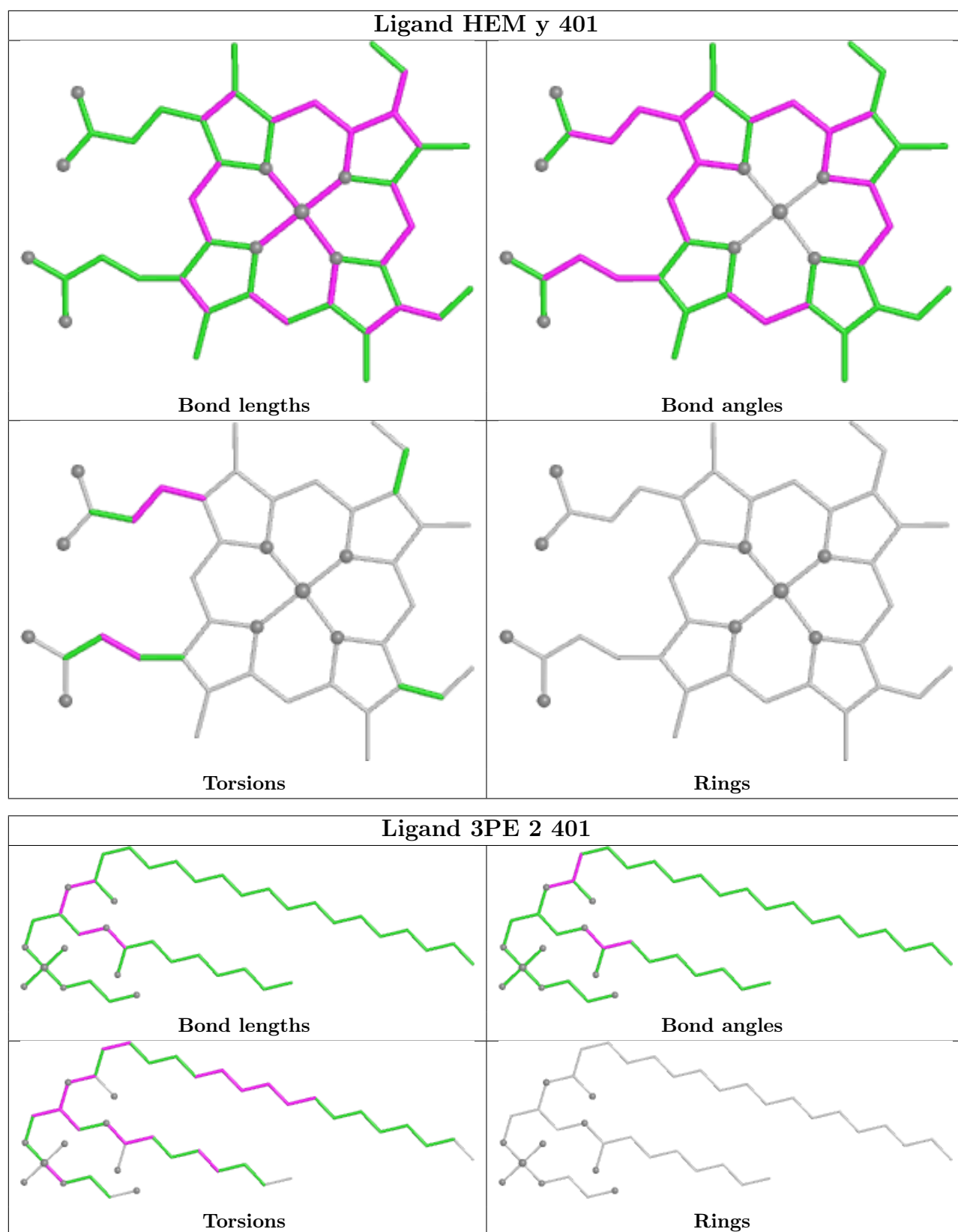


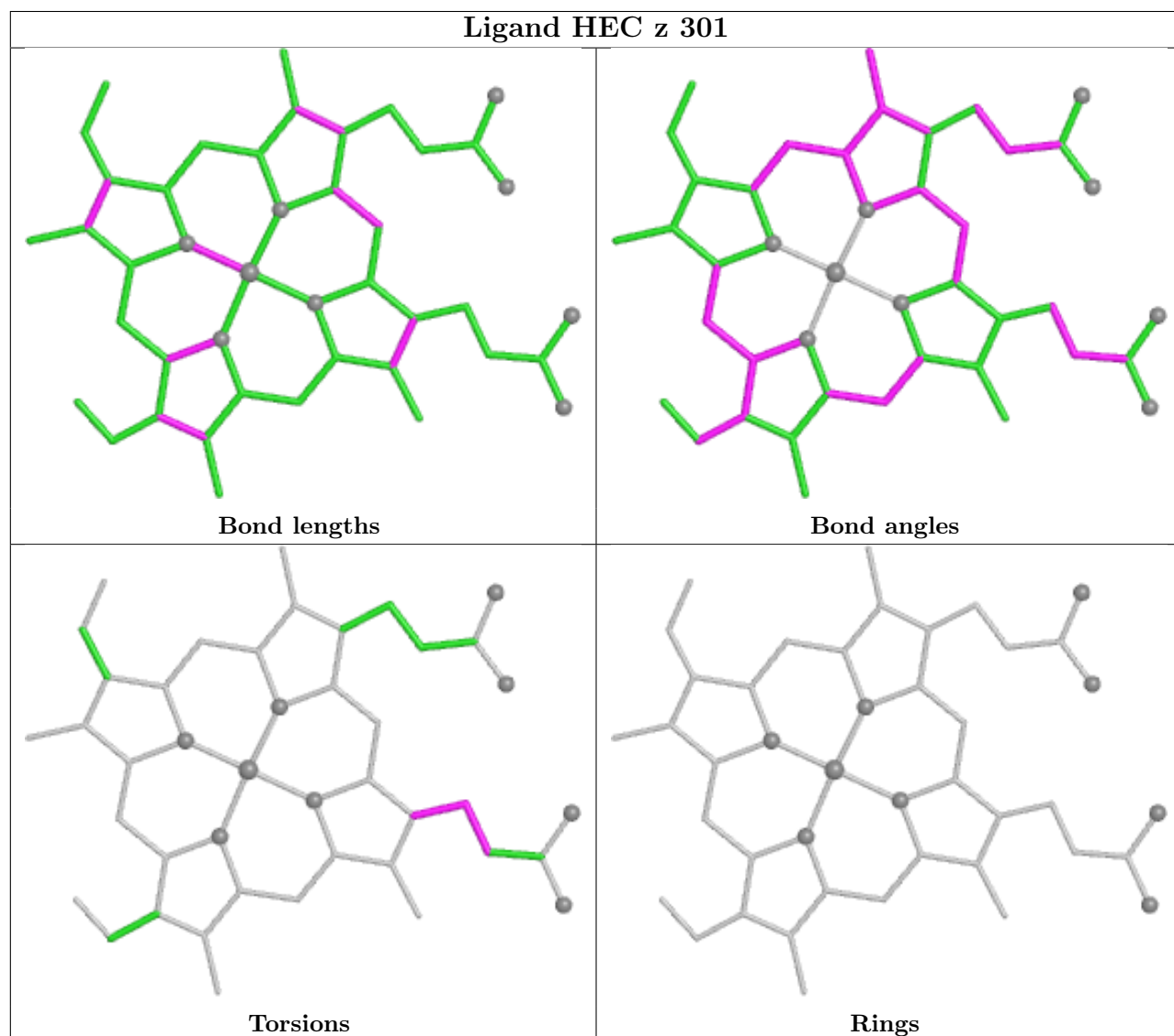
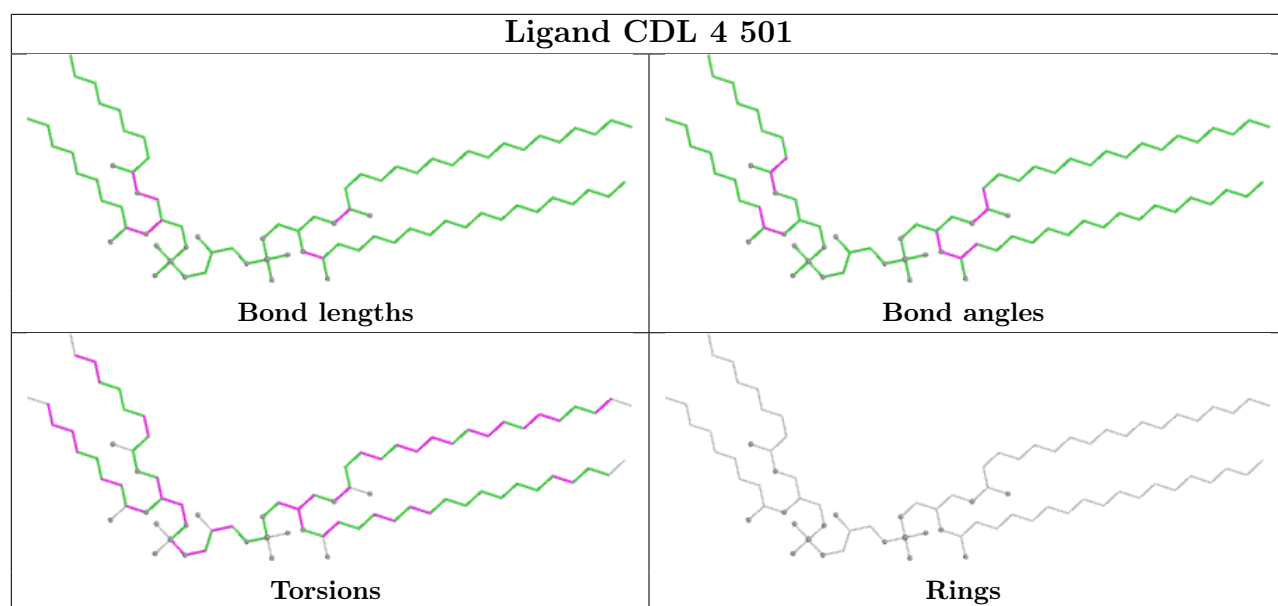
Ligand PC1 S 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL 6 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 L 200	
	
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.

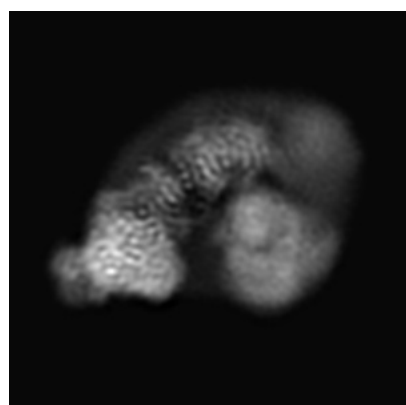
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30675. These allow visual inspection of the internal detail of the map and identification of artifacts.

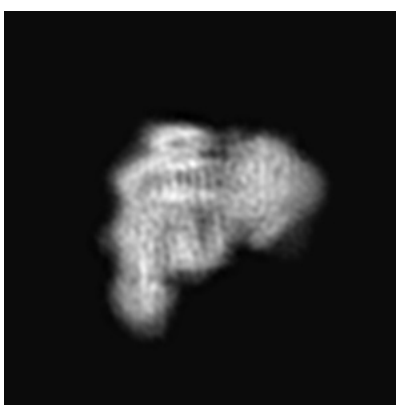
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

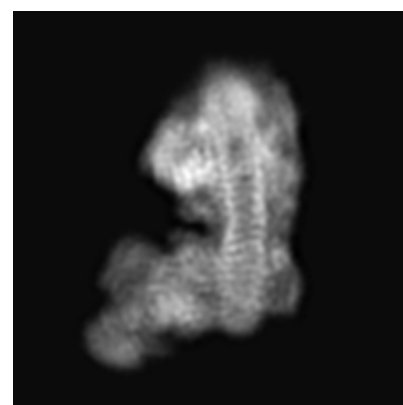
6.1.1 Primary map



X



Y

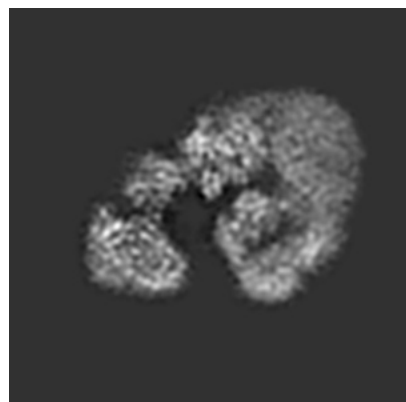


Z

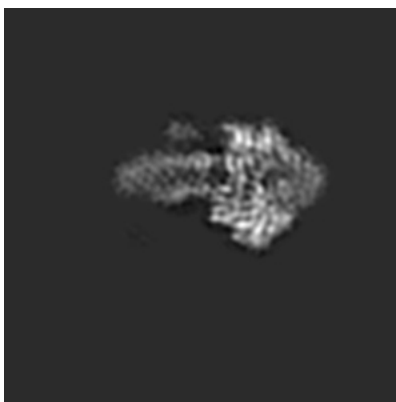
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

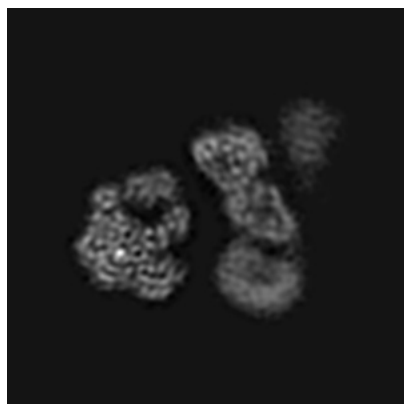


Z Index: 140

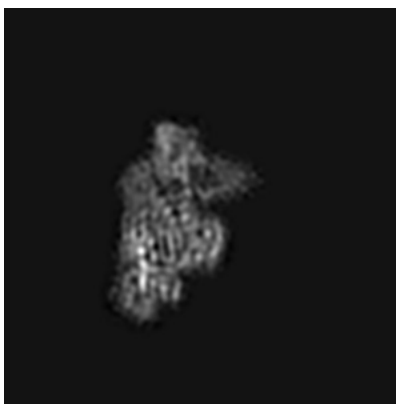
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 123



Y Index: 71



Z Index: 97

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

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

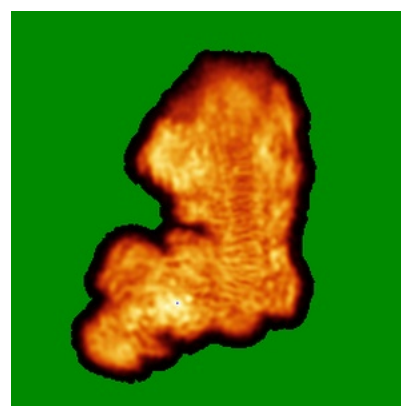
6.4.1 Primary map



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

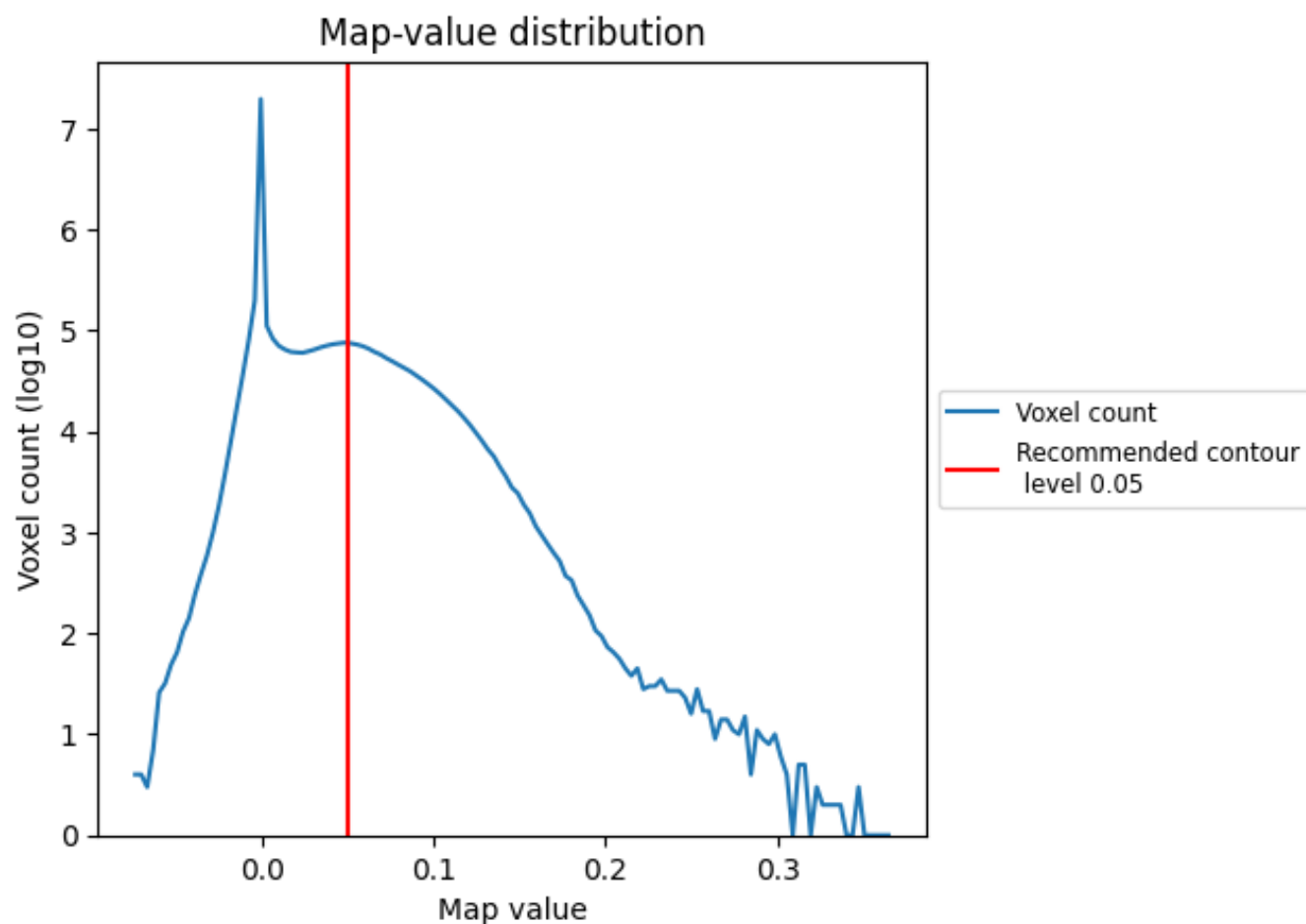
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

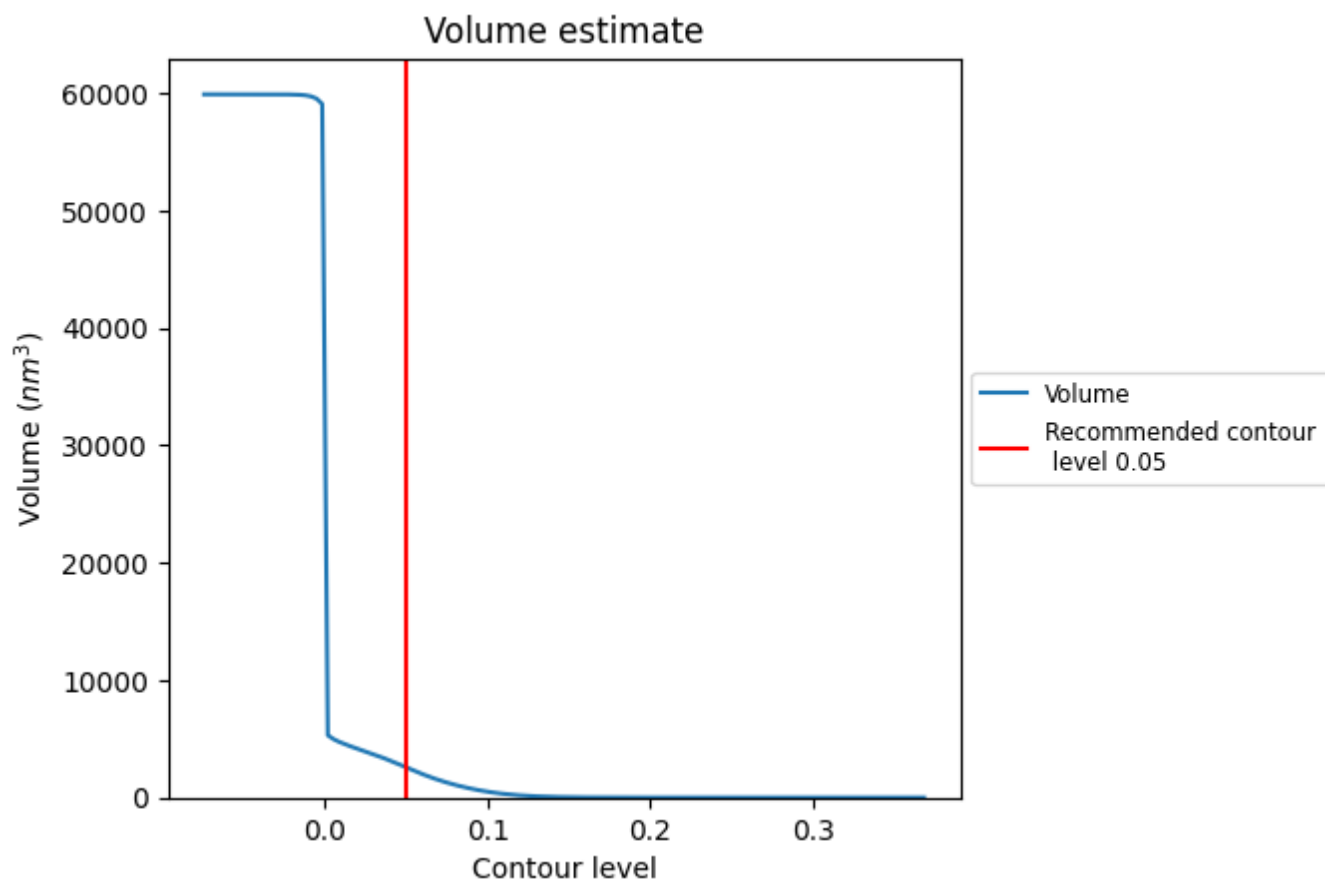
This section contains the results of statistical analysis of the map.

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.

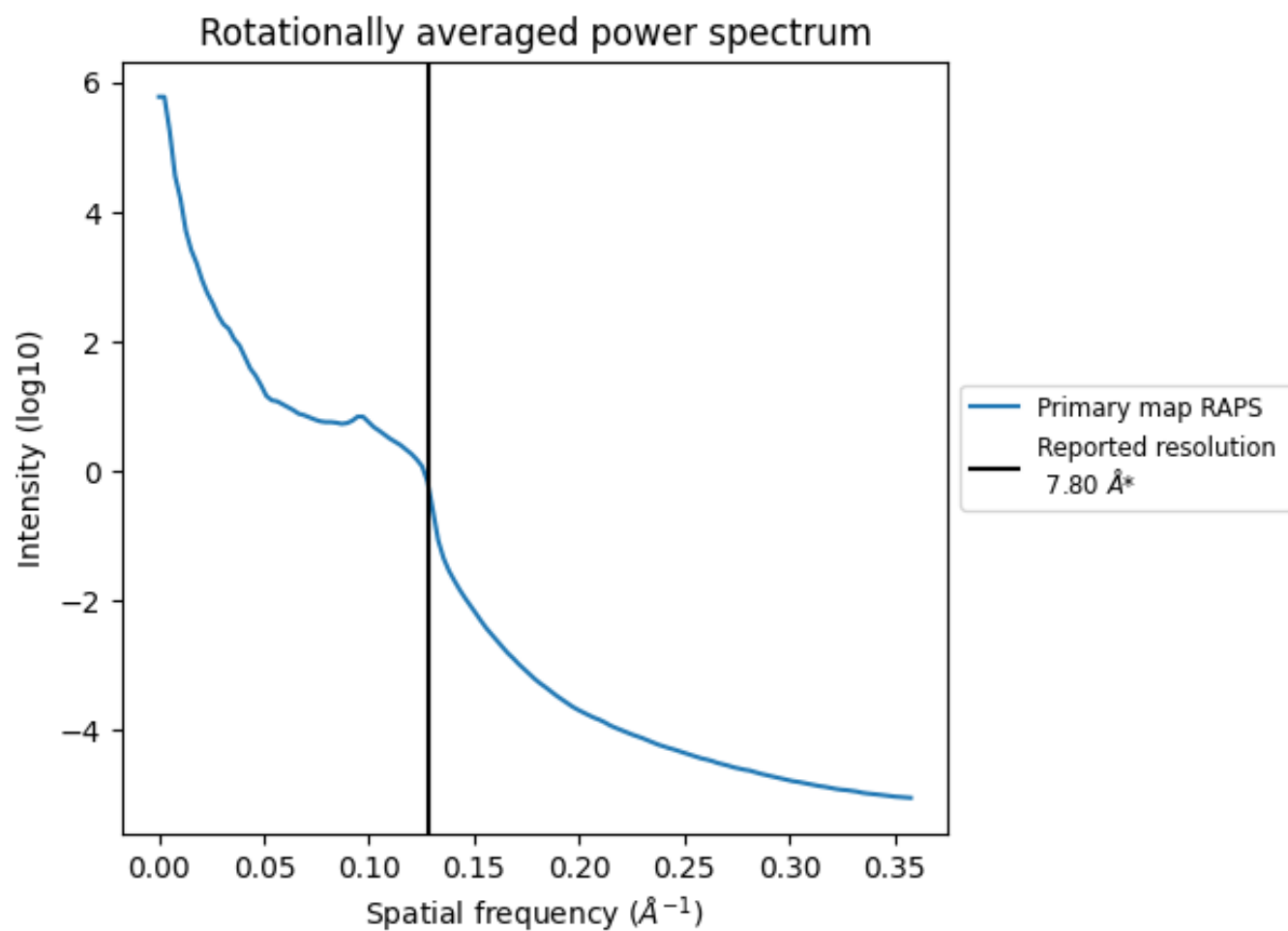
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2566 nm³; this corresponds to an approximate mass of 2318 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 0.128 Å⁻¹

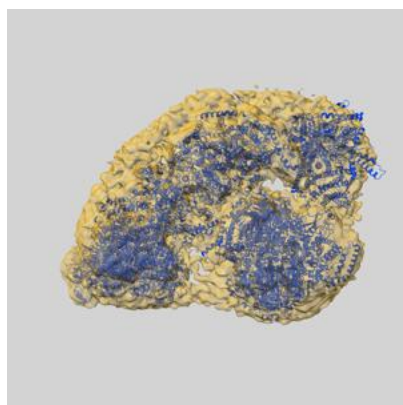
8 Fourier-Shell correlation

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

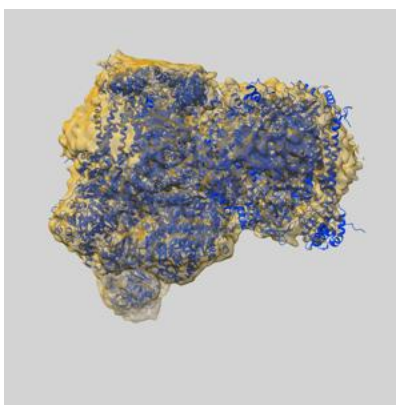
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30675 and PDB model 7DGS. Per-residue inclusion information can be found in section 3 on page 25.

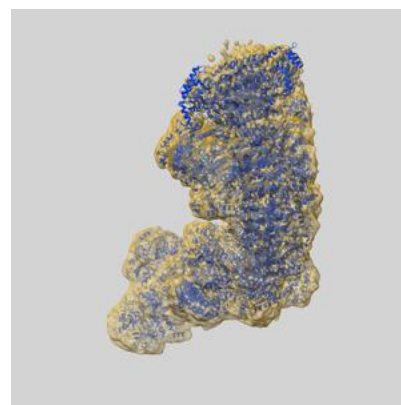
9.1 Map-model overlay [i](#)



X



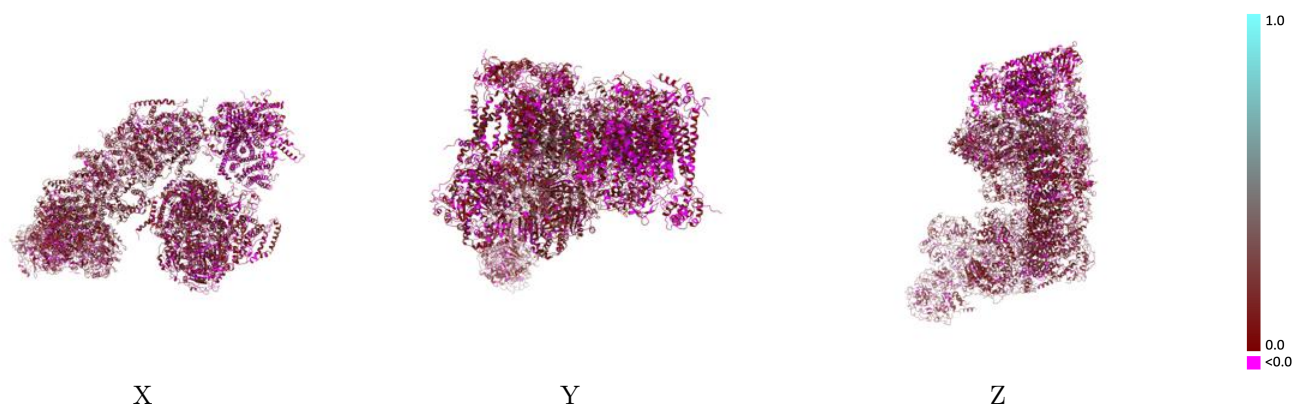
Y



Z

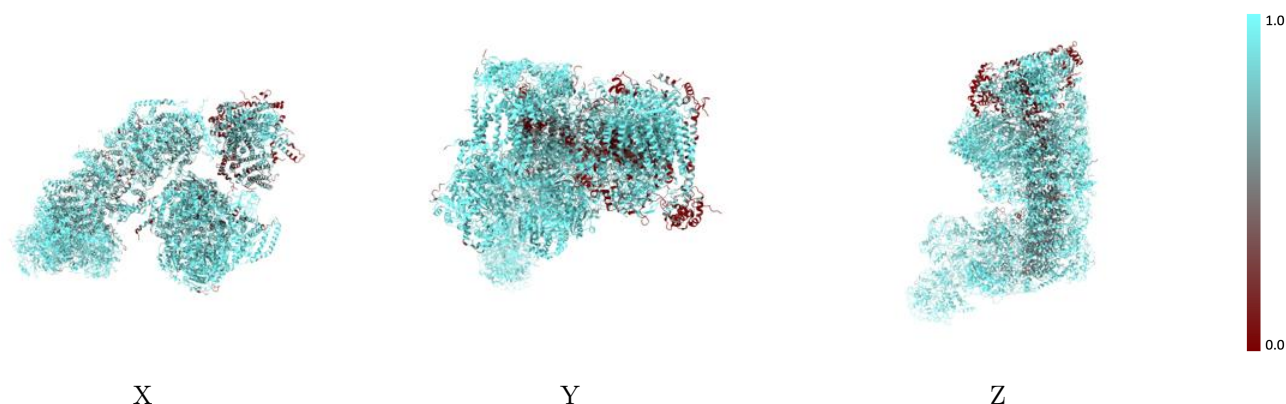
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



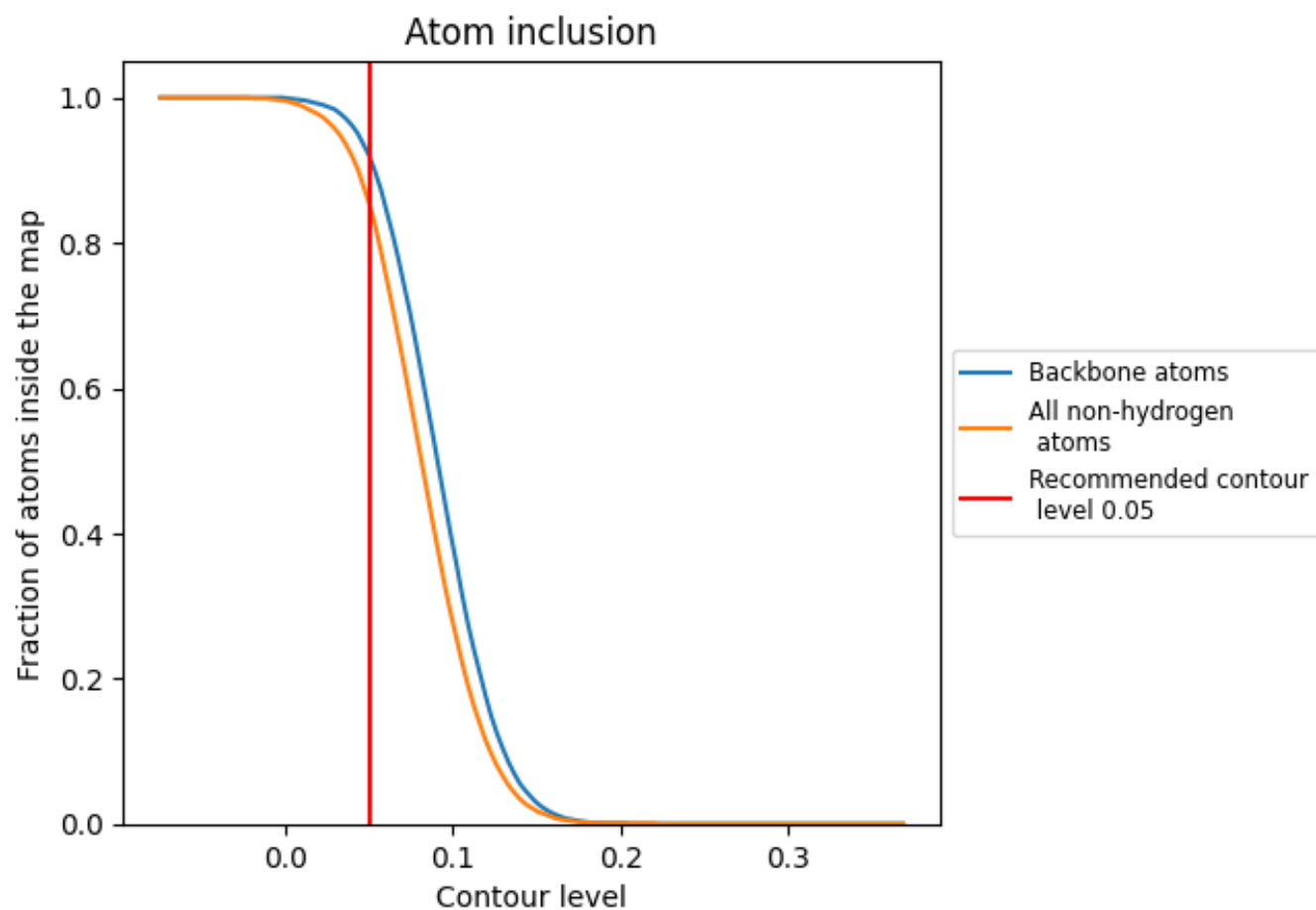
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.1070
1	 0.8100	 0.1090
2	 0.7720	 0.1360
3	 0.7320	 0.1250
4	 0.7440	 0.1310
5	 0.7720	 0.1370
6	 0.7790	 0.1090
7	 0.7820	 0.1390
8	 0.9880	 0.1220
9	 0.9760	 0.1210
A	 0.9760	 0.1180
A0	 0.8540	 0.1070
A1	 0.8090	 0.1020
A2	 0.8050	 0.1220
A3	 0.6250	 0.1390
A4	 0.4460	 0.0290
A5	 0.4850	 0.0270
A6	 0.2510	 0.0430
A7	 0.4570	 0.0200
A8	 0.5750	 0.0720
A9	 0.8320	 0.0150
B	 0.8540	 0.1110
B0	 0.6290	 0.0590
B1	 0.6550	 0.0110
B2	 0.3770	 0.0100
B3	 0.8960	 -0.0200
B4	 0.6470	 0.1520
B5	 0.7730	 0.0990
B6	 0.4400	 0.0530
B7	 0.7020	 0.0260
B8	 0.3880	 0.0110
B9	 0.8100	 0.0390
C	 0.9520	 0.1320
D	 0.9060	 0.1050
E	 0.9600	 0.1020



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Chain	Atom inclusion	Q-score
F	 0.9440	 0.0600
G	 0.9300	 0.1290
H	 0.9120	 0.1270
I	 0.8940	 0.0830
J	 0.9700	 0.1380
K	 0.9530	 0.1230
L	 0.8870	 0.1490
M	 0.8880	 0.1500
N	 0.9820	 0.1550
O	 0.9180	 0.1580
P	 0.9360	 0.1390
Q	 0.9260	 0.1460
R	 0.9260	 0.1230
S	 0.8460	 0.1300
T	 0.7900	 0.1700
U	 0.8580	 0.0850
V	 0.9380	 0.1590
W	 0.9540	 0.1440
X	 0.9100	 0.1290
Y	 0.9480	 0.1790
Z	 0.9090	 0.1270
a	 0.8210	 0.1530
b	 0.9360	 0.1410
c	 0.9470	 0.1590
d	 0.9800	 0.1240
e	 0.8620	 0.1390
f	 0.9380	 0.1520
g	 0.9550	 0.1270
h	 0.8890	 0.1200
i	 0.9190	 0.1820
j	 0.8490	 0.1320
k	 0.9560	 0.0600
l	 0.9550	 0.0930
m	 0.8260	 0.1030
o	 0.9470	 0.0840
p	 0.9450	 0.0970
q	 0.9290	 0.1420
r	 0.8370	 0.0960
s	 0.9120	 0.0940
t	 0.9090	 0.1090
u	 0.9020	 0.0550
v	 0.9460	 -0.0380

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Chain	Atom inclusion	Q-score
w	 0.9540	 0.1330
x	 0.9820	 0.1330
y	 0.8200	 0.1220
z	 0.9160	 0.1010