



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:31 AM UTC

PDB ID : 5XTH / pdb_00005xth
EMDB ID : EMD-6775
Title : Cryo-EM structure of human respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.90 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

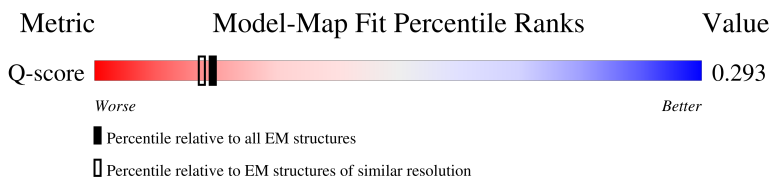
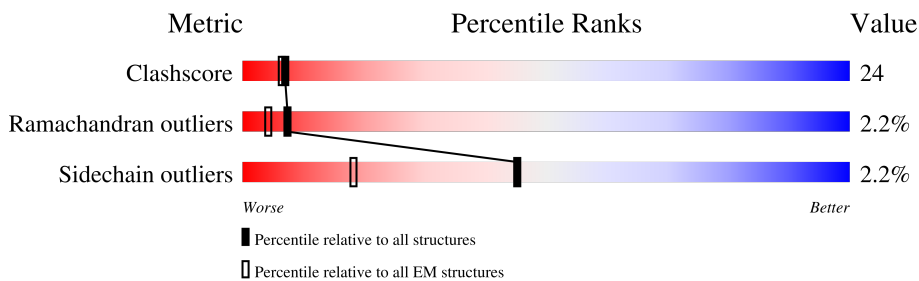
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	A	431	<p>6% (red), 47% (green), 51% (yellow), . (grey)</p>
2	B	176	<p>45% (green), 53% (yellow), . (grey)</p>
3	C	156	<p>51% (green), 48% (yellow), . (grey)</p>
4	E	113	<p>12% (red), 44% (green), 53% (yellow), . (grey)</p>

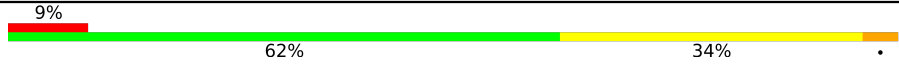


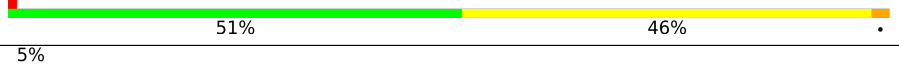
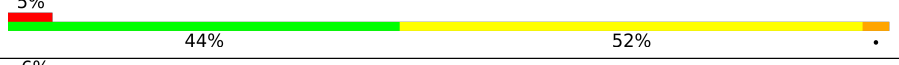
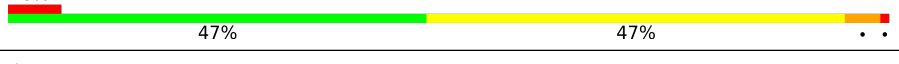
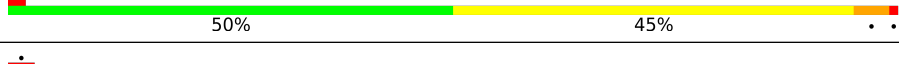


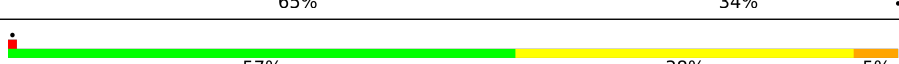
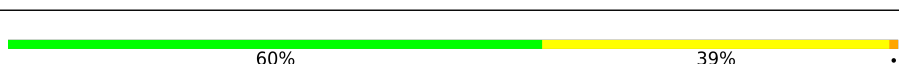
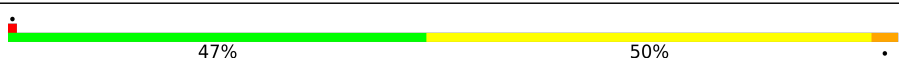

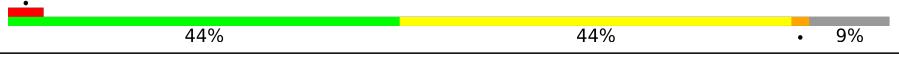







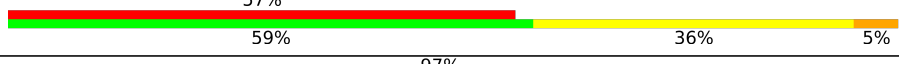



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Mol	Chain	Length	Quality of chain
5	F	83	5% 49% 51%
6	G	85	46% 47% 51%
6	X	85	53% 45%
7	H	112	10% 52% 45%
8	I	110	5% 45% 35% 6% 14%
9	J	337	45% 51%
10	K	33	12% 45% 45% 9%
11	L	118	9% 44% 54%
12	M	687	46% 51%
13	N	143	58% 38%
14	O	212	38% 59%
15	P	208	47% 48% 5%
16	Q	430	6% 43% 54%
17	S	70	60% 37%
18	T	95	54% 43%
19	U	83	75% 25%
20	V	140	63% 36%
21	W	138	65% 30%
22	Y	59	31% 47% 19%
23	Z	80	74% 26%
24	a	138	59% 37%
25	b	124	44% 47% 10%
26	c	153	50% 48%
27	d	171	63% 33%
28	e	97	6% 68% 32%

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Mol	Chain	Length	Quality of chain
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	122	
44	w	320	
45	x	514	
46	y	227	
47	z	261	
48	0	144	
49	1	109	
50	2	98	
51	3	84	
52	4	75	
53	5	73	

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Mol	Chain	Length	Quality of chain
54	6	56	54% 62% 25% 11% .
55	7	49	96% 65% 33% .
56	8	47	79% 74% 23% .
57	9	43	91% 67% 30% .
58	AA	81	. 63% 30% 7%
58	AN	81	20% 74% 25% .
59	AB	57	75% 51% 46% .
59	AO	57	86% 53% 42% 5%
60	AC	196	20% 70% 28% .
60	AP	196	15% 63% 35% .
61	AD	62	16% 76% 24%
61	AQ	62	19% 61% 37% .
62	AE	74	14% 69% 28% ..
62	AR	74	18% 74% 22% .
63	AF	106	10% 56% 32% 12%
63	AS	106	7% 61% 39%
64	AG	51	16% 71% 27% .
64	AT	51	14% 65% 29% 6%
65	AH	241	. 70% 29% .
65	AU	241	. 69% 29% .
66	AJ	378	. 65% 34% .
66	AV	378	. 60% 37% .
67	AK	419	. 62% 37% .
67	AW	419	16% 63% 35% .
68	AL	446	. 62% 37% .

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Mol	Chain	Length	Quality of chain
68	AY	446	

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	SF4	A	501	-	-	X	-
69	SF4	B	302	-	-	X	-
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
71	PLX	b	201	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	301	-	-	X	-
74	FES	O	301	-	-	X	-
75	CDL	AG	101	-	-	X	-
75	CDL	AL	502	-	-	X	-
76	PEE	AH	401	-	-	X	-
76	PEE	AL	503	-	-	X	-
76	PEE	AU	401	-	-	X	-
76	PEE	AV	403	-	-	X	-
76	PEE	AY	502	-	-	X	-
76	PEE	V	202	-	-	X	-
76	PEE	l	701	-	-	X	-

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 115642 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3322	2096	594	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1420	893	243	271	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1249	794	227	214	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	968	623	178	162	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	83	670	422	124	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	85	672	434	99	134	5	0	0
6	X	85	686	442	101	138	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	922	593	157	169	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	95	769	483	146	138	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	337	2712	1759	482	463	8	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	274	173	47	53	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	964	608	173	179	4	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	5274	3310	917	1009	38	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	1195	770	210	212	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	212	1643	1047	276	310	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1730	1117	297	313	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3460	2214	599	624	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	568	367	101	96	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	95	742	459	138	142	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	83	647	427	105	113	2	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	140	1038	668	178	187	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	138	1135	727	202	200	6	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	59	533	354	87	91	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	80	648	426	110	110	2	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	138	1174	771	199	202	2	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	124	1059	697	181	176	5	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	153	1236	795	208	222	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	171	1418	885	262	259	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	97	810	522	132	152	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	47	405	269	69	67	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	119	1004	658	173	169	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	104	863	546	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2735	1819	421	470	25	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	115	919	626	132	152	9	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	97	740	487	113	127	13	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4717	3119	742	823	33	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	174	1313	879	194	229	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	473	305	85	80	3	0	0

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

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	128	1066	685	192	187	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	172	1495	961	265	261	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3629	2411	569	619	30	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	318	2509	1678	380	435	16	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	169	1394	886	247	252	9	0	0

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	111	921	569	187	156	9	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AG	51	Total	C	N	O	0	0
			425	287	72	66		
64	AT	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

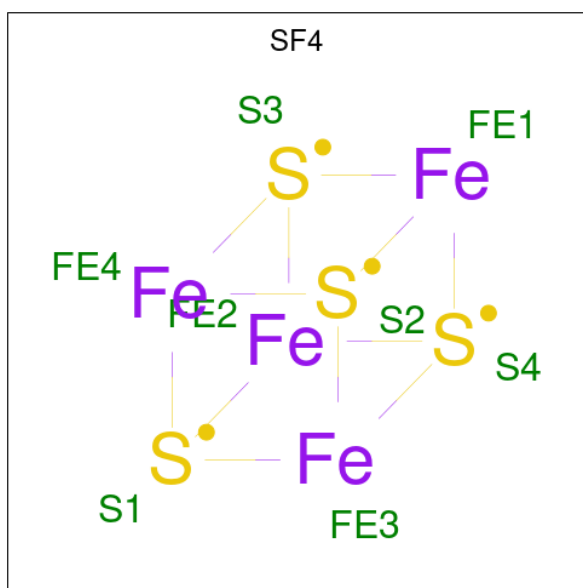
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
68	AY	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 69 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



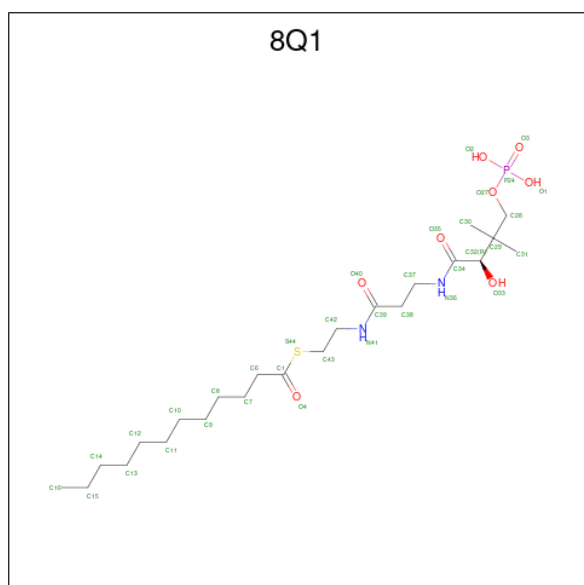
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
71	V	1	Total 52	C 42	N 1	O 8	P 1	0
71	b	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	r	1	Total 52	C 42	N 1	O 8	P 1	0
71	r	1	Total 52	C 42	N 1	O 8	P 1	0
71	AL	1	Total 52	C 42	N 1	O 8	P 1	0
71	AQ	1	Total 52	C 42	N 1	O 8	P 1	0
71	AT	1	Total 52	C 42	N 1	O 8	P 1	0

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



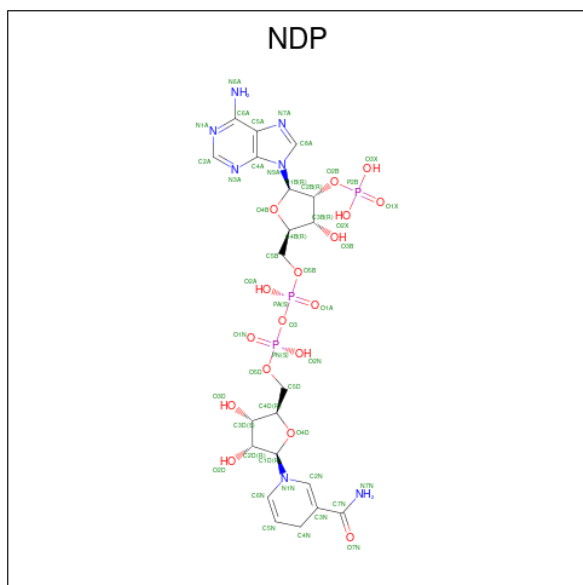
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
72	E	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

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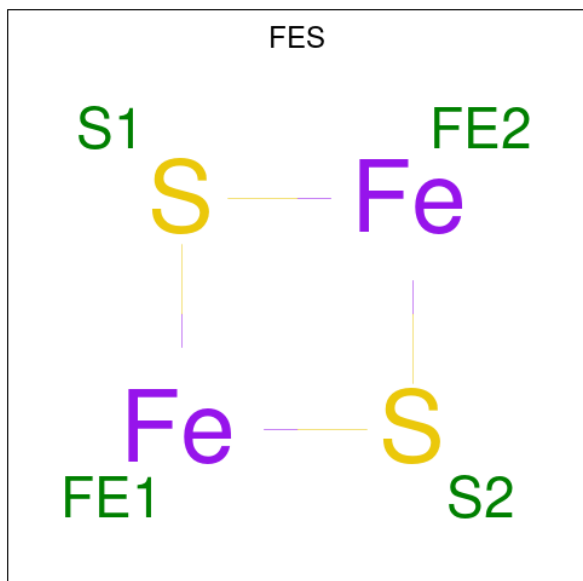
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
72	p	1	35	23	2	8	1	1	0

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



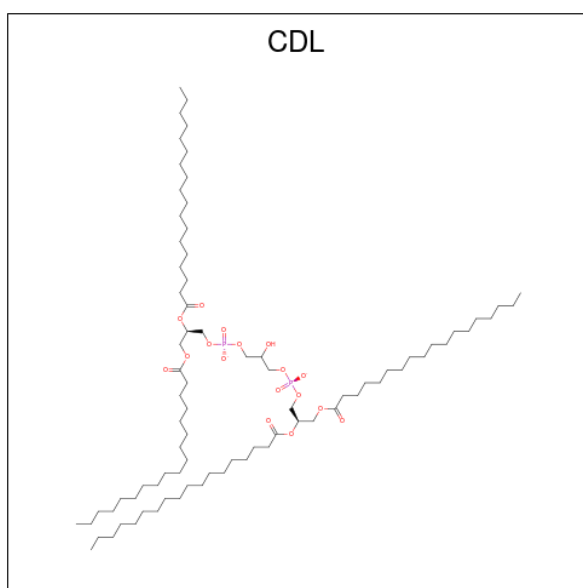
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	J	1	48	21	7	17	3	0

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



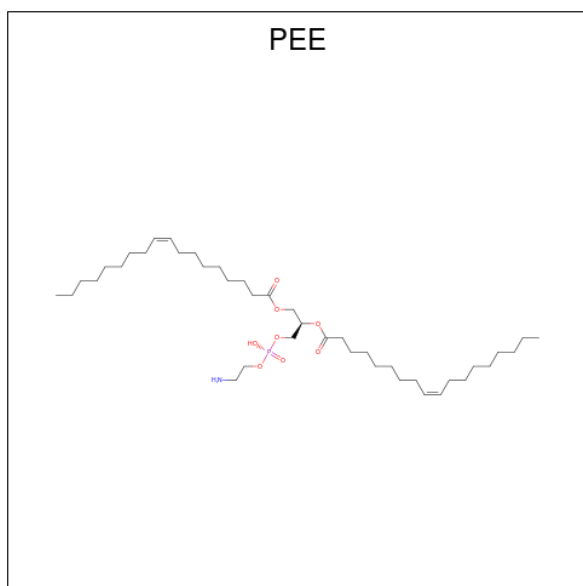
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total	C	O	P	0
			64	45	17	2	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	AJ	1	Total 64	C 45	O 17	P 2	0
75	AJ	1	Total 64	C 45	O 17	P 2	0
75	AL	1	Total 64	C 45	O 17	P 2	0
75	AN	1	Total 64	C 45	O 17	P 2	0
75	AU	1	Total 64	C 45	O 17	P 2	0
75	AY	1	Total 64	C 45	O 17	P 2	0

- Molecule 76 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	V	1	Total 51	C 41	N 1	O 8	P 1	0
76	W	1	Total 51	C 41	N 1	O 8	P 1	0
76	1	1	Total 49	C 39	N 1	O 8	P 1	0
76	1	1	Total 51	C 41	N 1	O 8	P 1	0
76	AH	1	Total 49	C 39	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	

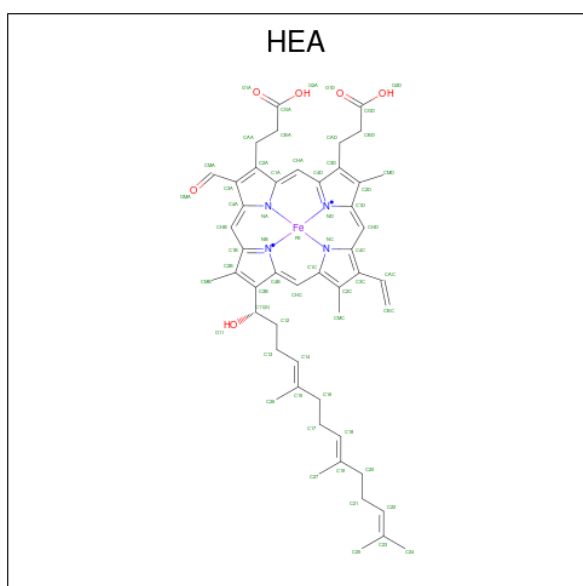
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

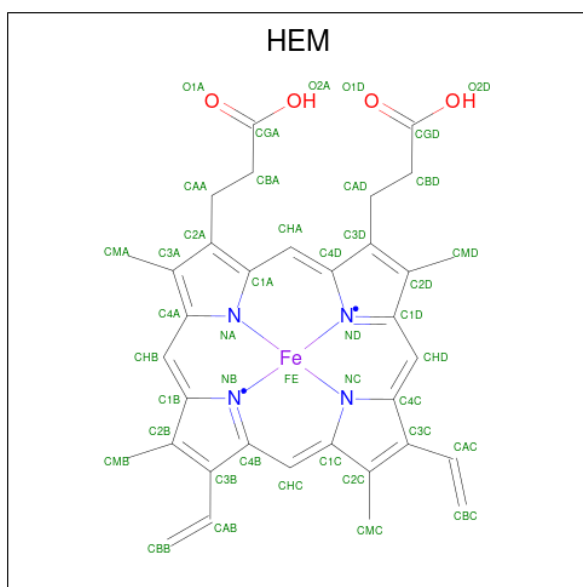
Mol	Chain	Residues	Atoms		AltConf
77	x	1	Total	Cu	0
			1	1	
77	y	2	Total	Cu	0
			2	2	

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	x	1	Total	Mg	0
			1	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



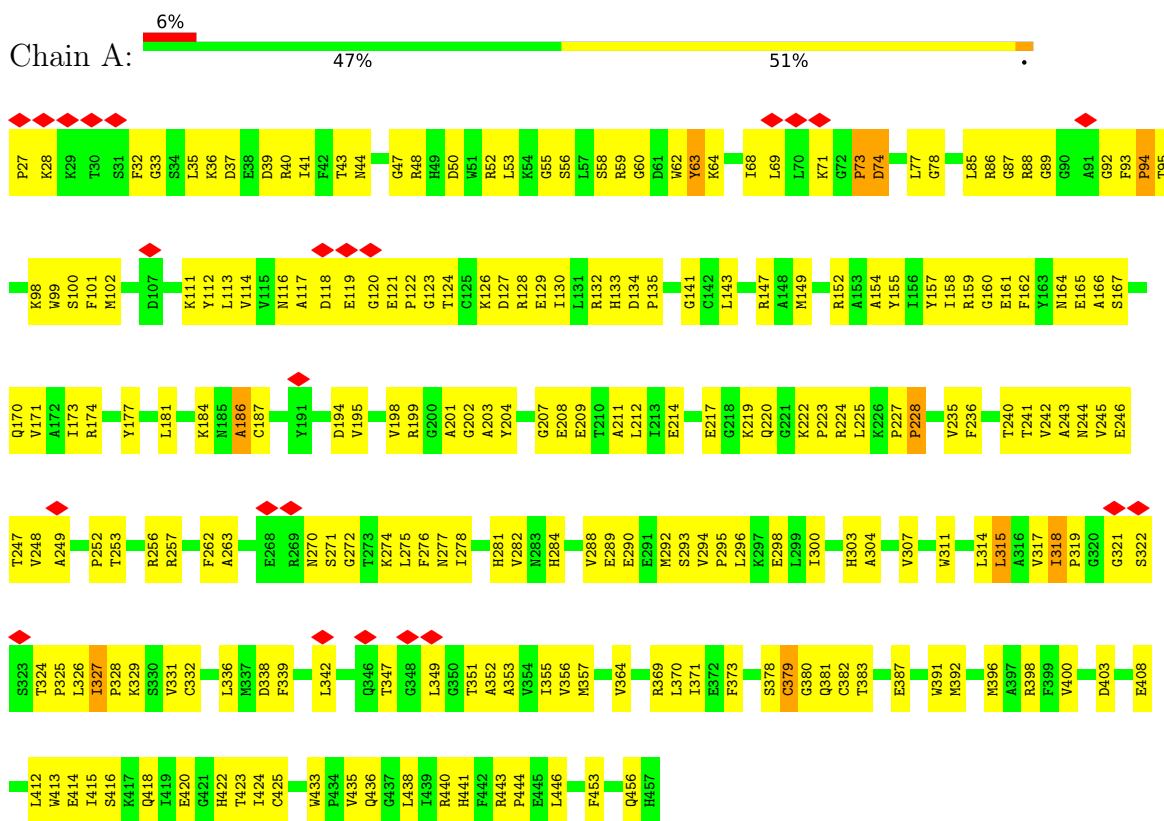


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
82	AJ	1	43	34	1	4	4	0
82	AJ	1	43	34	1	4	4	0
82	AV	1	43	34	1	4	4	0
82	AV	1	43	34	1	4	4	0

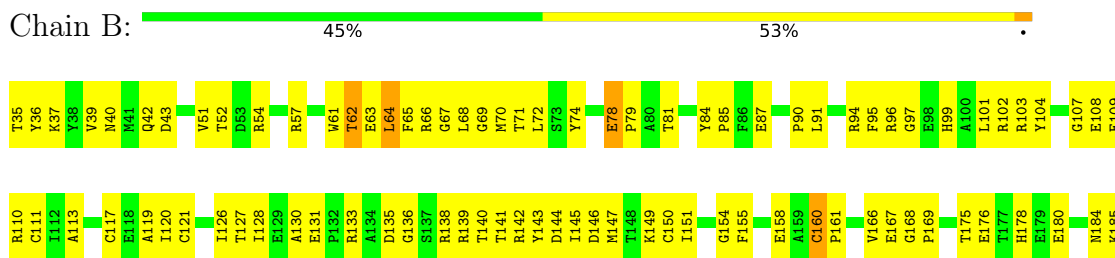
3 Residue-property plots [i](#)

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

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

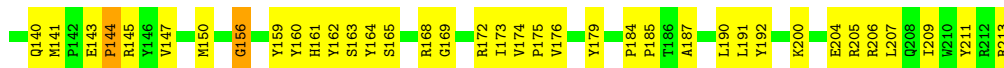
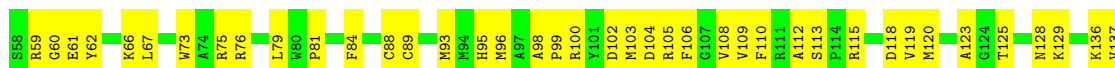


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

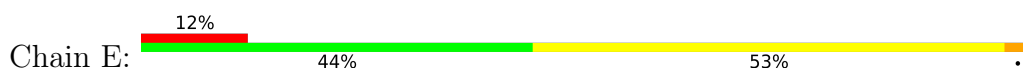




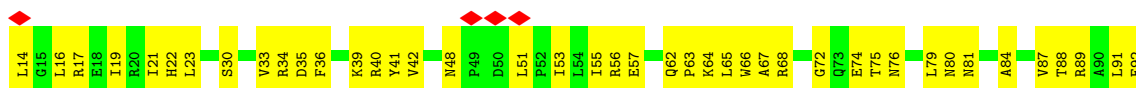
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



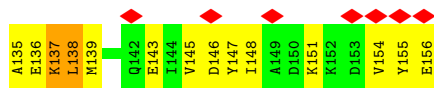
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial

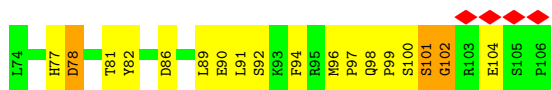


- Molecule 6: Acyl carrier protein, mitochondrial

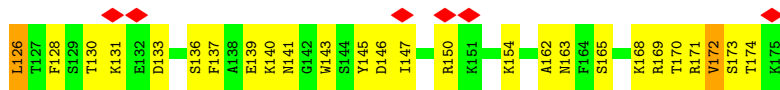




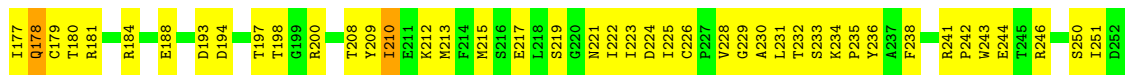
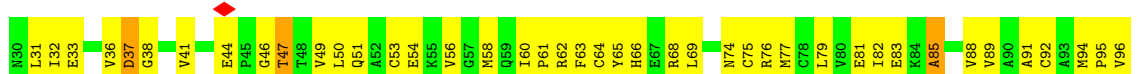
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

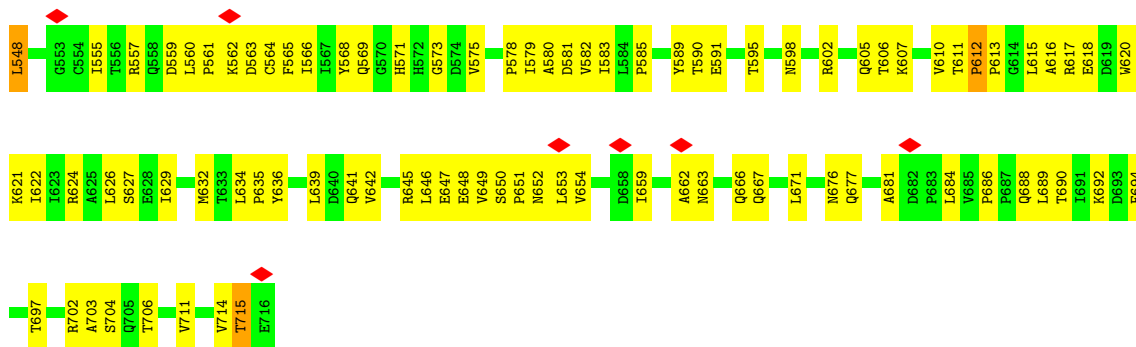


• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

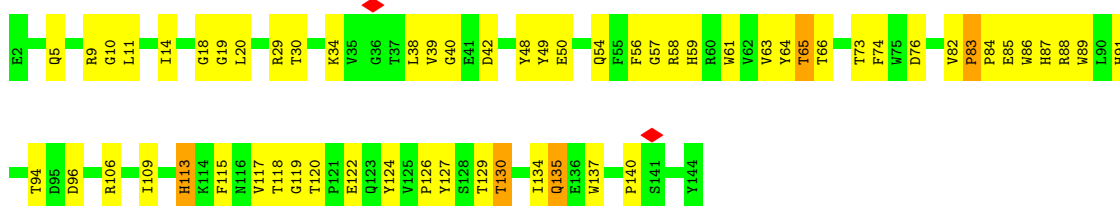


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

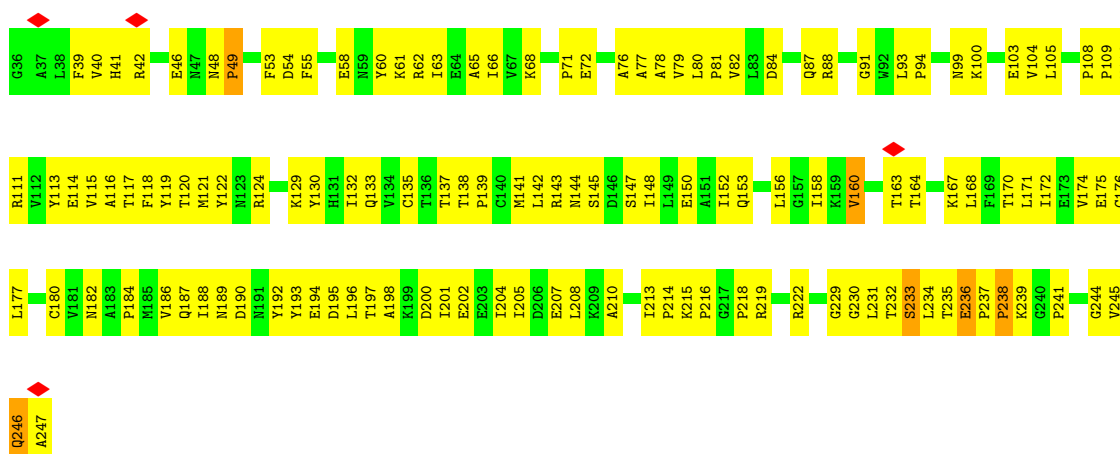




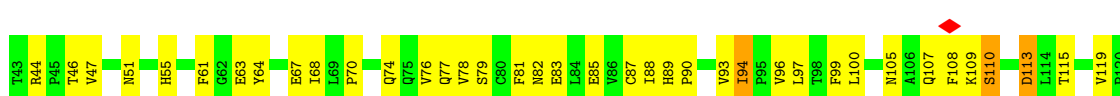
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

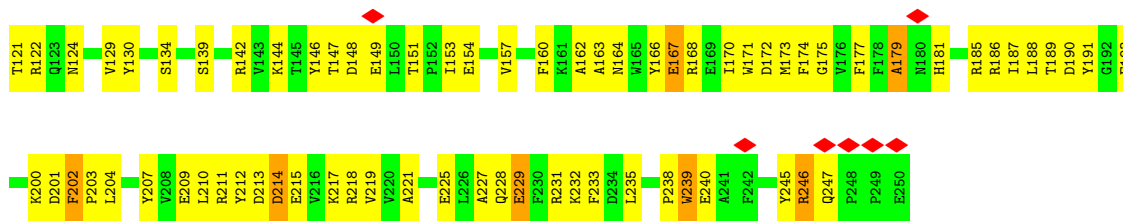


• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

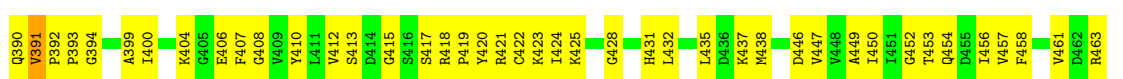
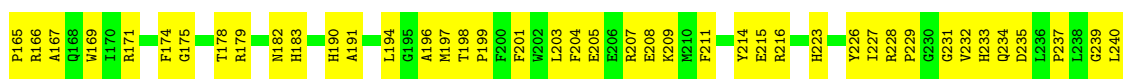
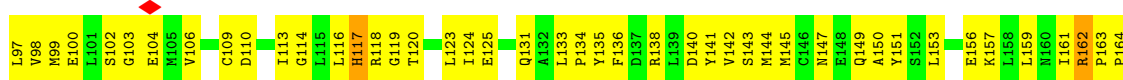
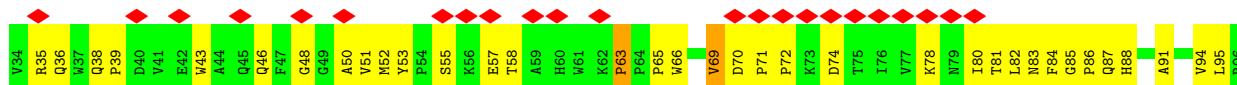


• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial




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



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



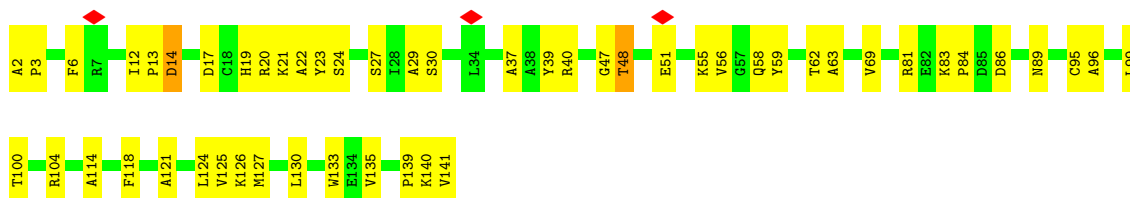
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  75% 25%



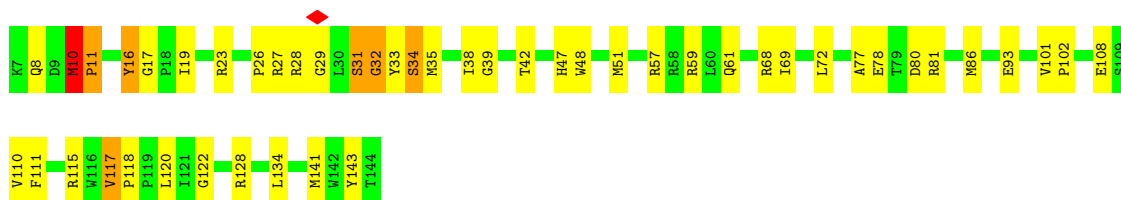
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  63% 36%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  65% 30%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  31% 47% 19%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  74% 26%



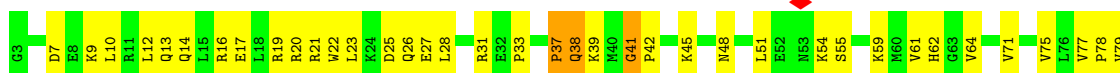
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  59% 37%

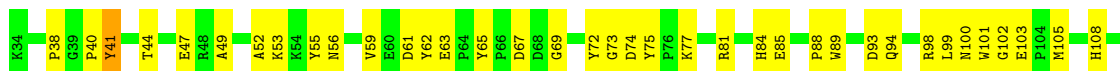




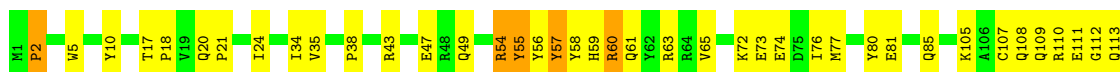
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



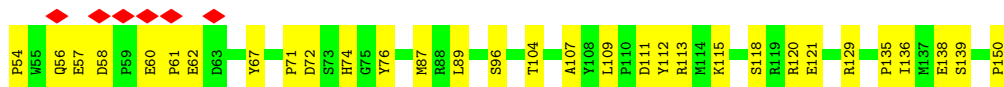
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

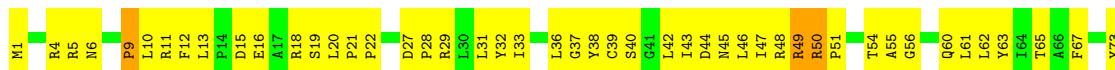


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

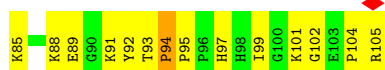




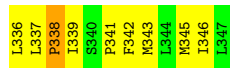
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

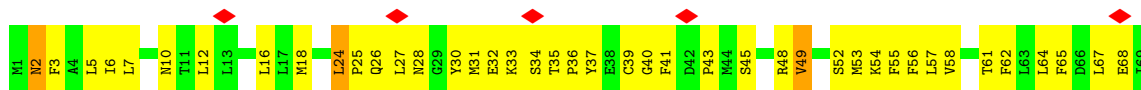


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

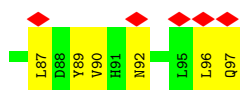
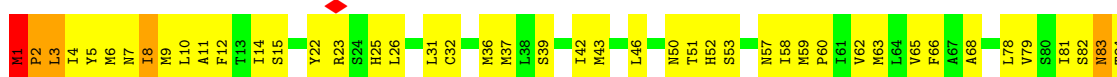


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

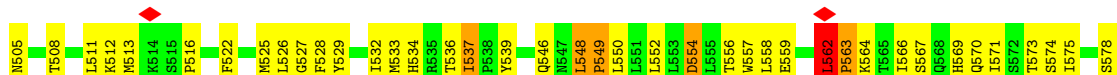
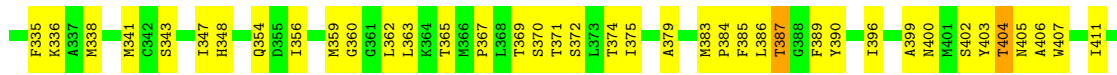
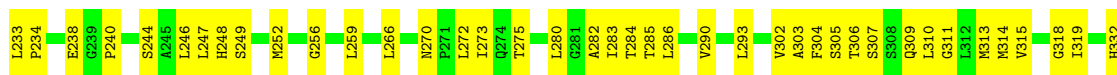




• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

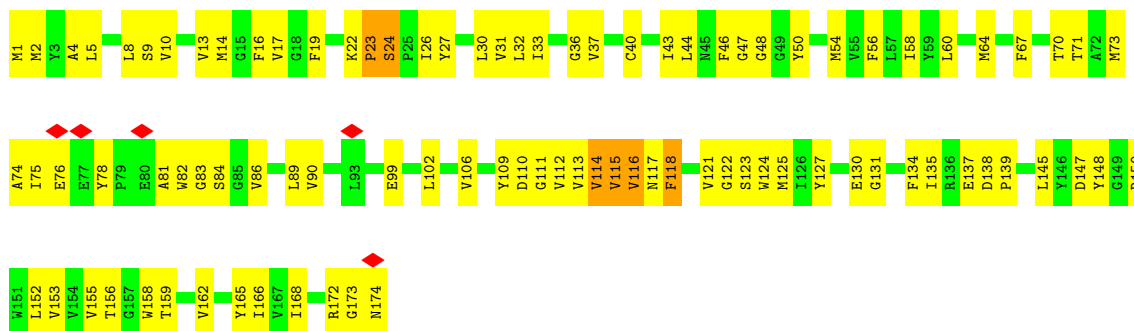


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



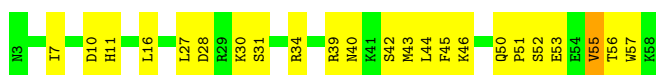
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  47% 50%



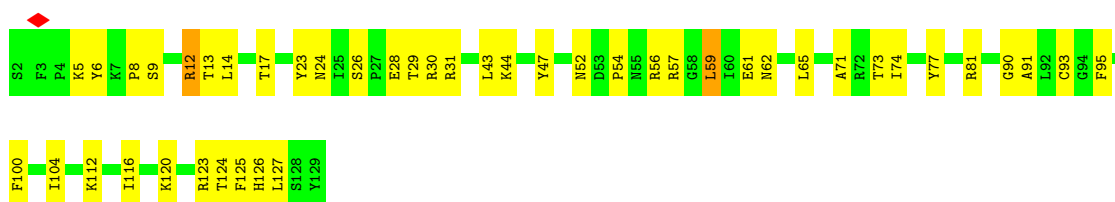
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  59% 39%



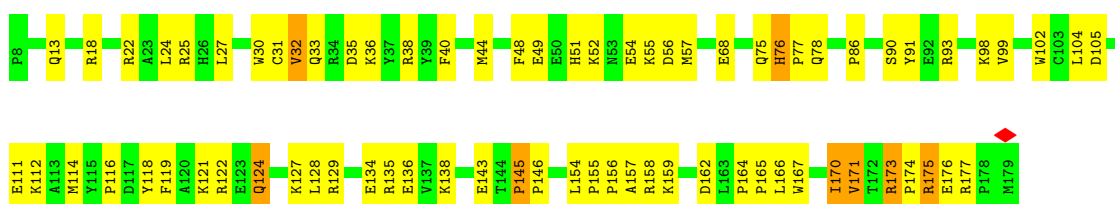
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  65% 34%



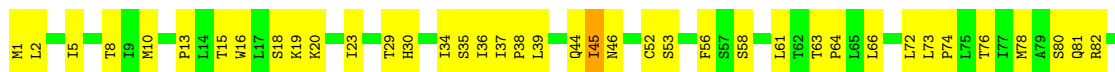
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

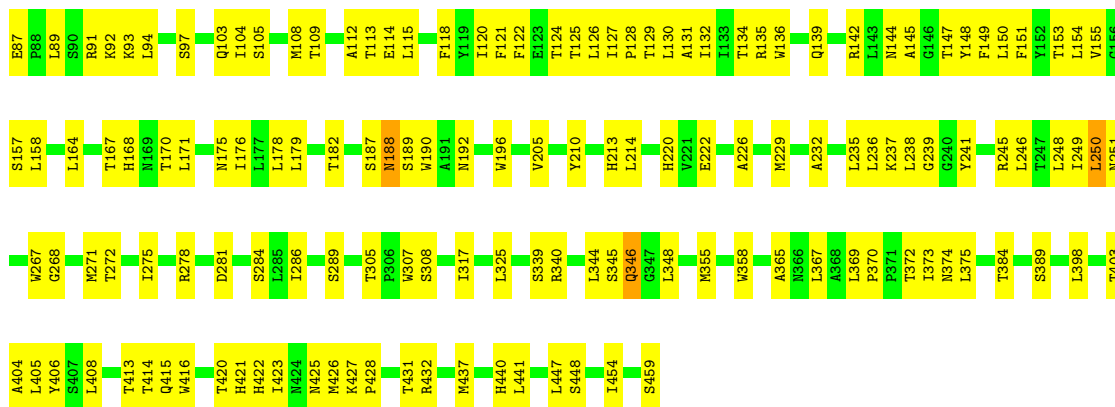
Chain p:  57% 38% 5%



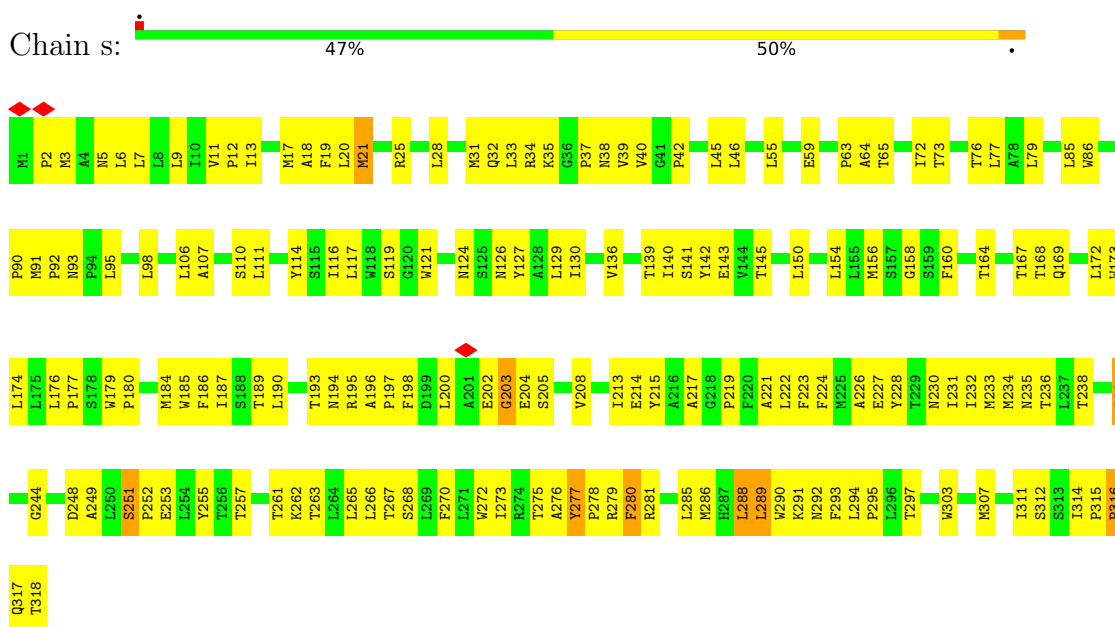
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  60% 39%

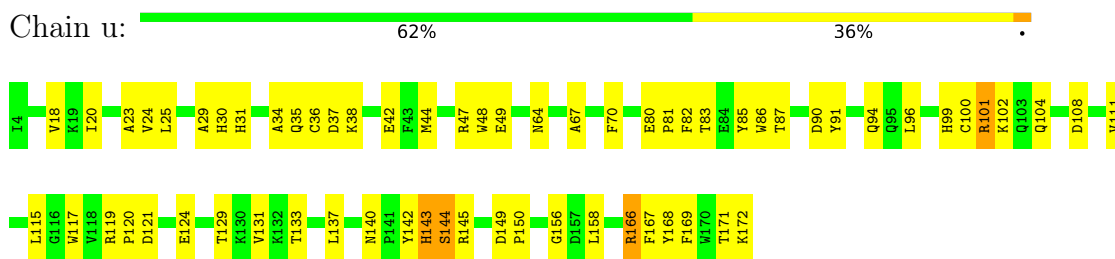




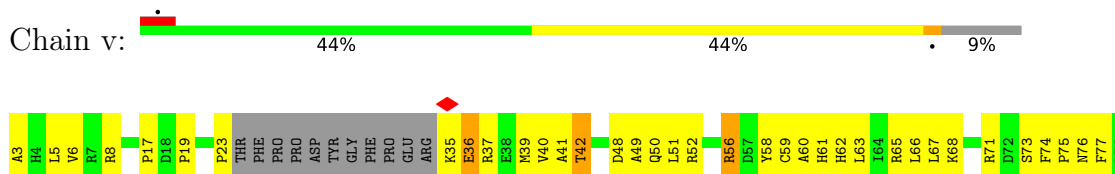
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

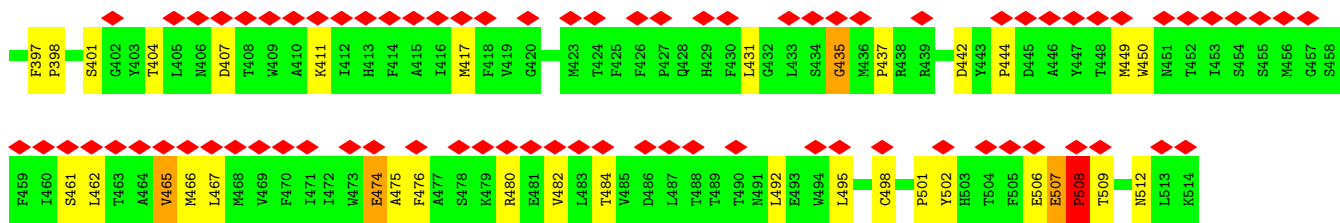


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

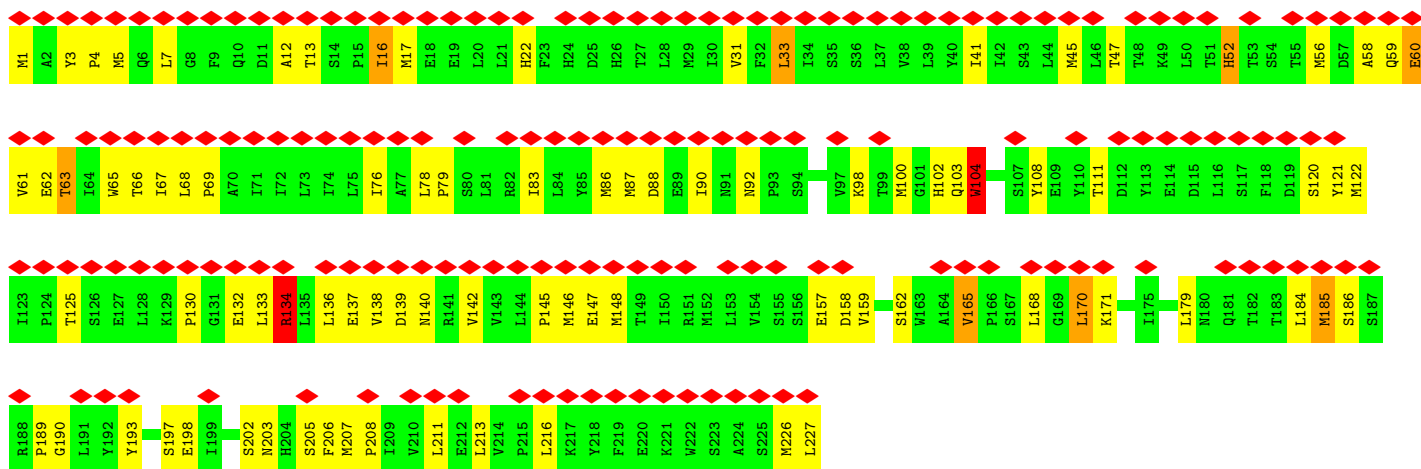
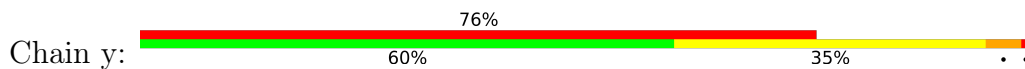


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

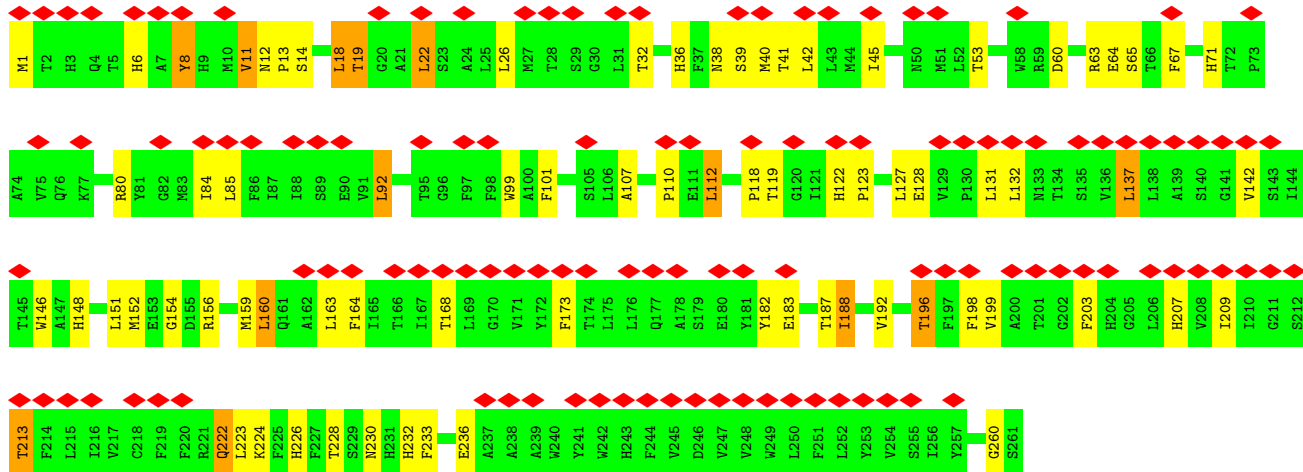




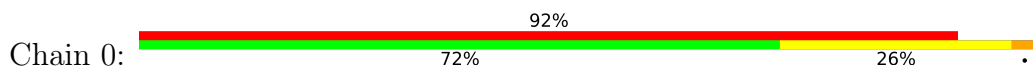
• Molecule 46: Cytochrome c oxidase subunit 2

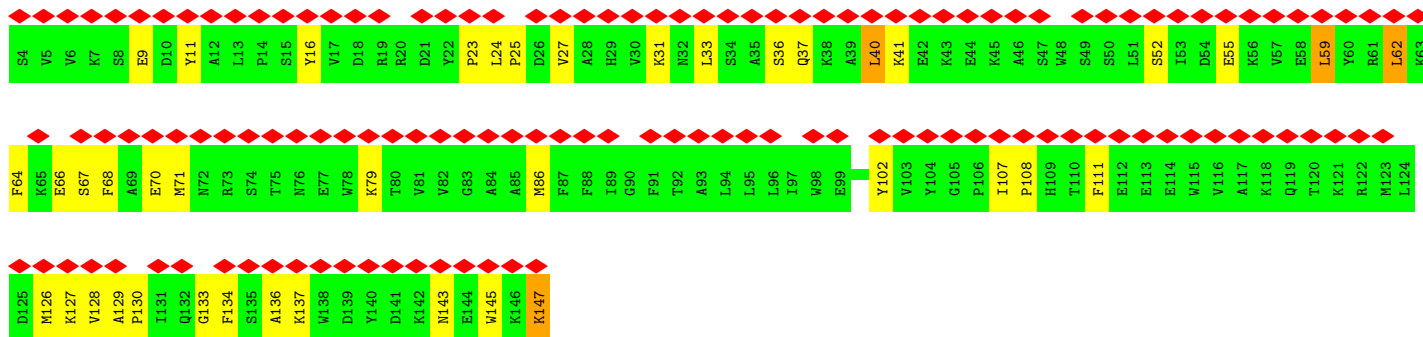


• Molecule 47: Cytochrome c oxidase subunit 3

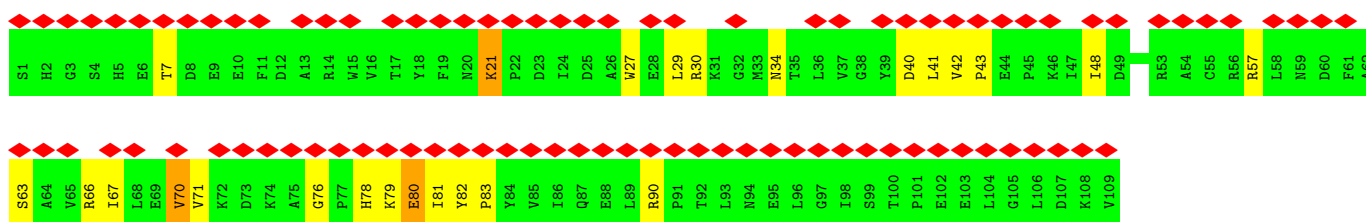
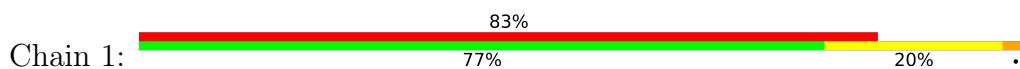


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

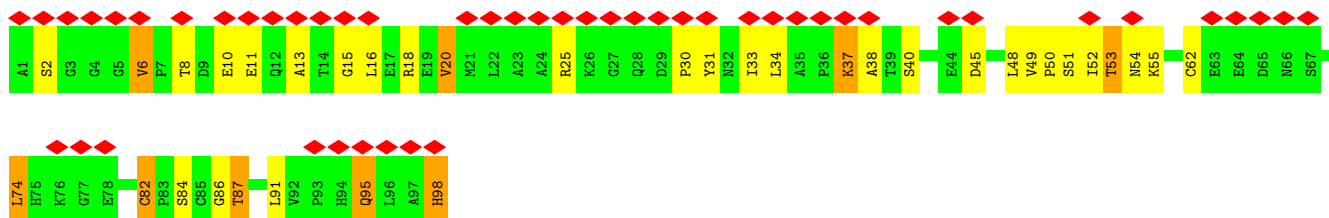




- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial

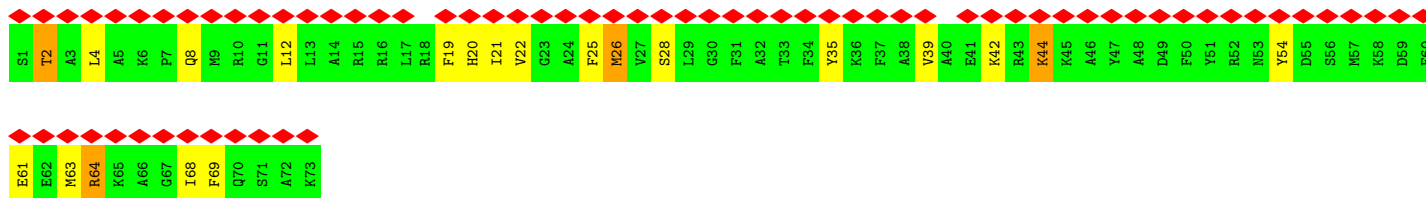


- Molecule 52: Cytochrome c oxidase subunit 6B1

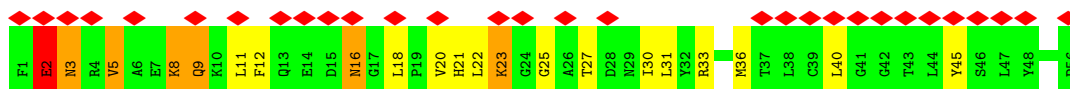




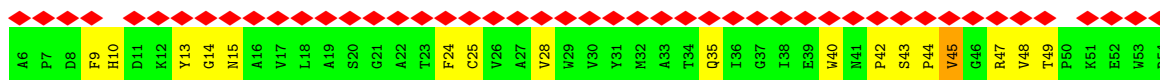
• Molecule 53: Cytochrome c oxidase subunit 6C



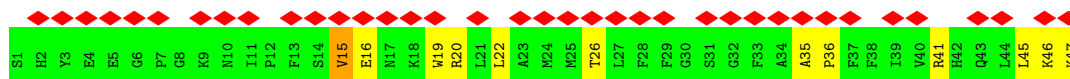
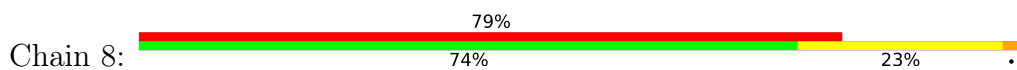
• Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



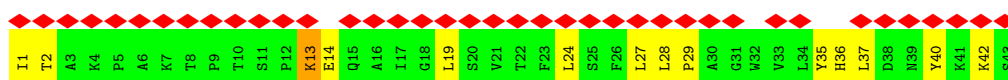
• Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial

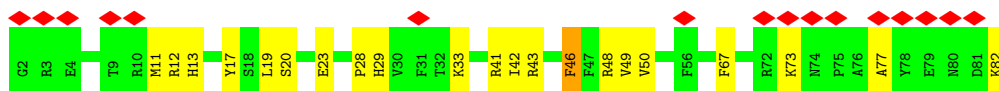
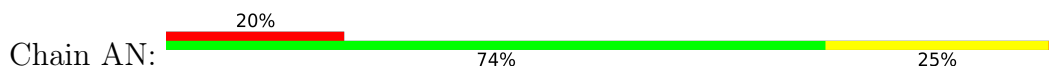


• Molecule 58: Cytochrome b-c1 complex subunit 8

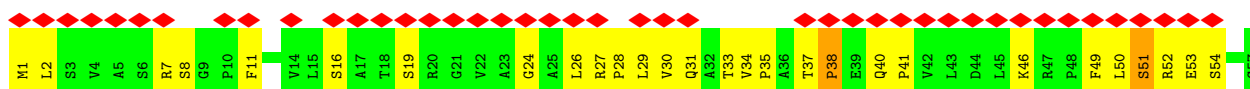
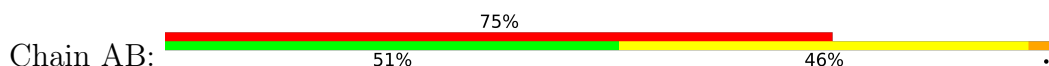




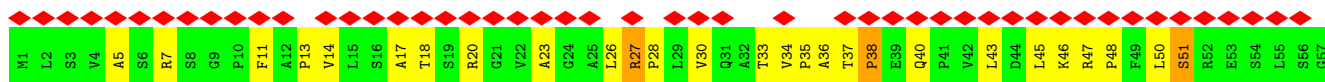
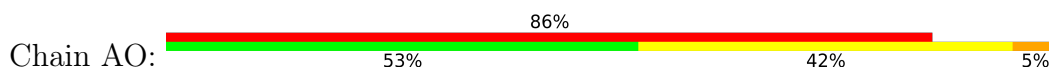
- Molecule 58: Cytochrome b-c1 complex subunit 8



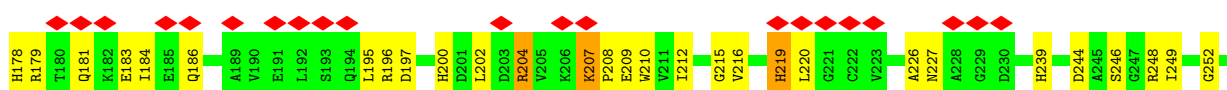
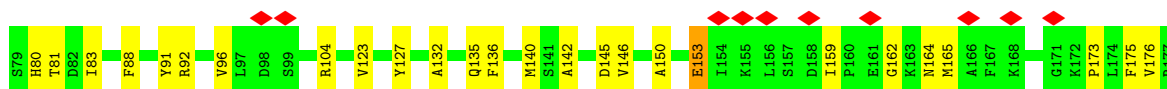
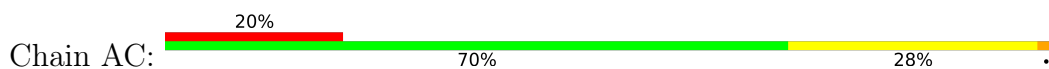
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



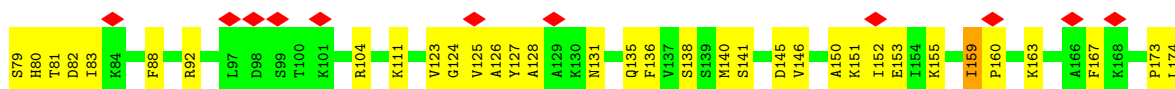
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

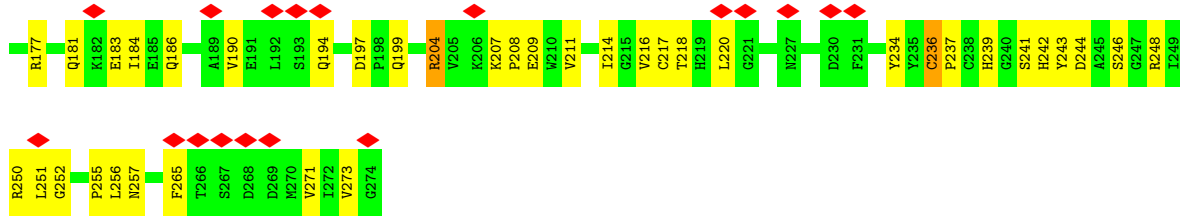


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

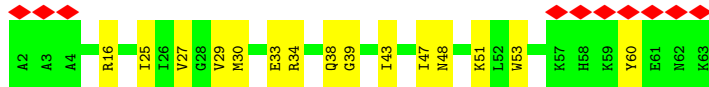
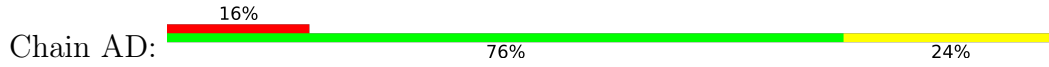


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

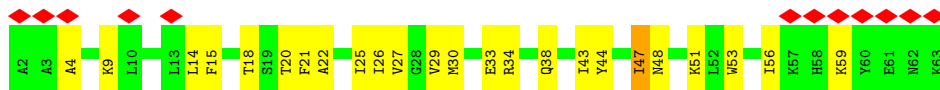




• Molecule 61: Cytochrome b-c1 complex subunit 9



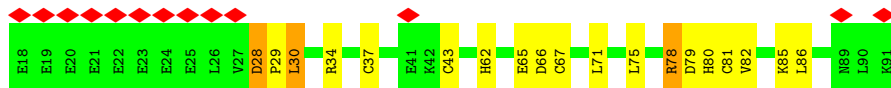
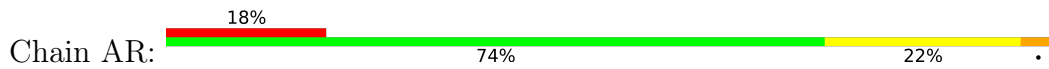
• Molecule 61: Cytochrome b-c1 complex subunit 9



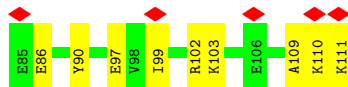
• Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



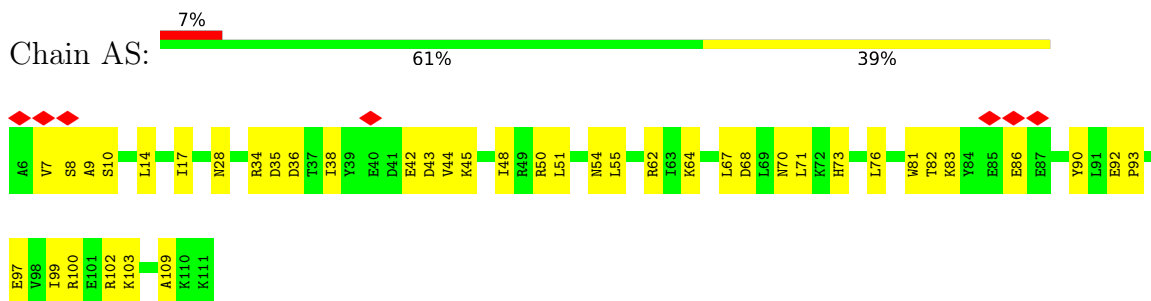
• Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



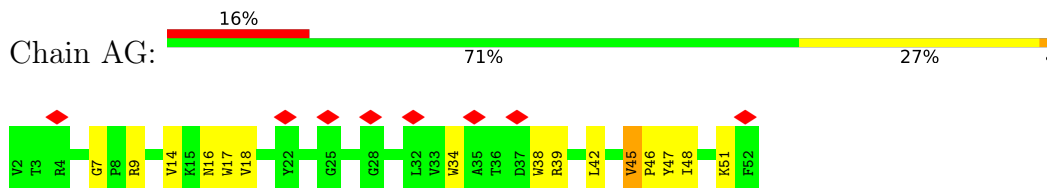
• Molecule 63: Cytochrome b-c1 complex subunit 7



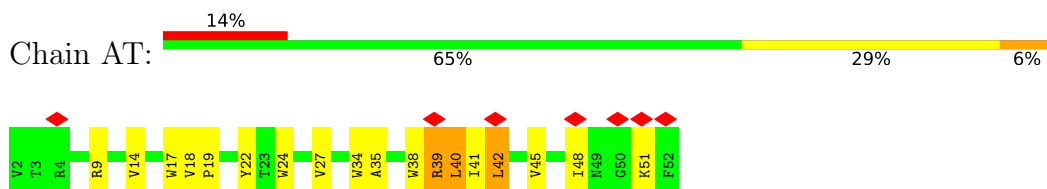
• Molecule 63: Cytochrome b-c1 complex subunit 7



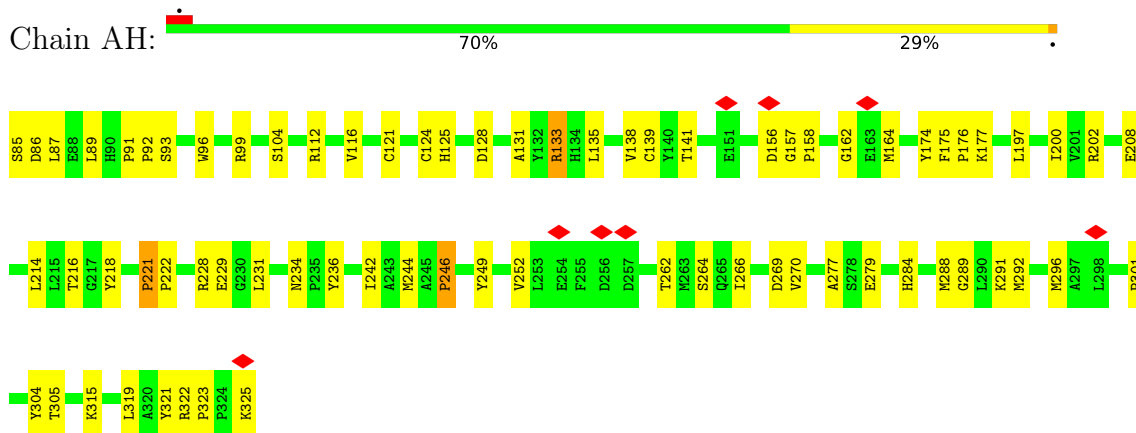
- Molecule 64: Cytochrome b-c1 complex subunit 10



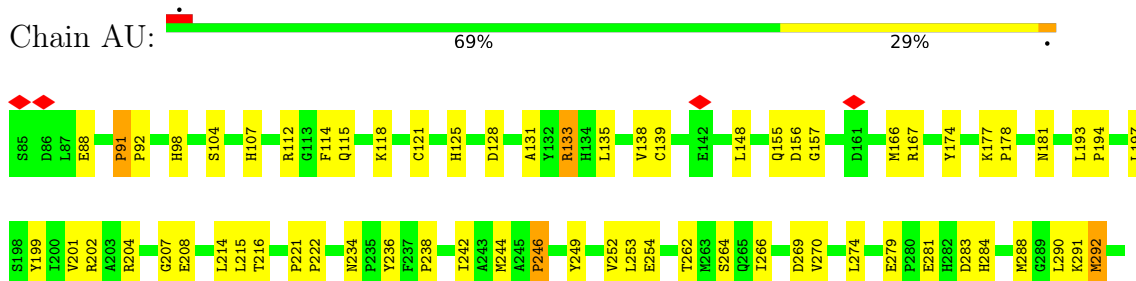
- Molecule 64: Cytochrome b-c1 complex subunit 10



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

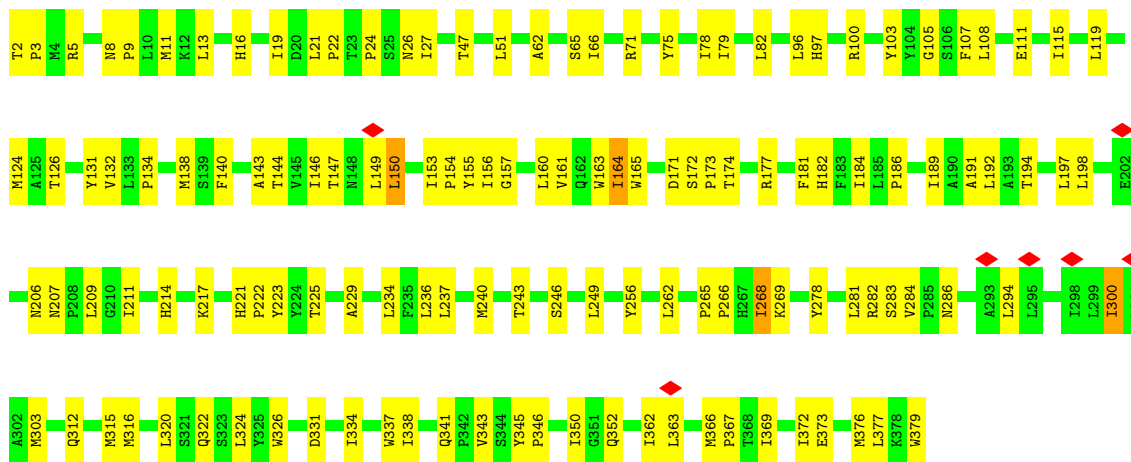


- Molecule 65: Cytochrome c1, heme protein, mitochondrial

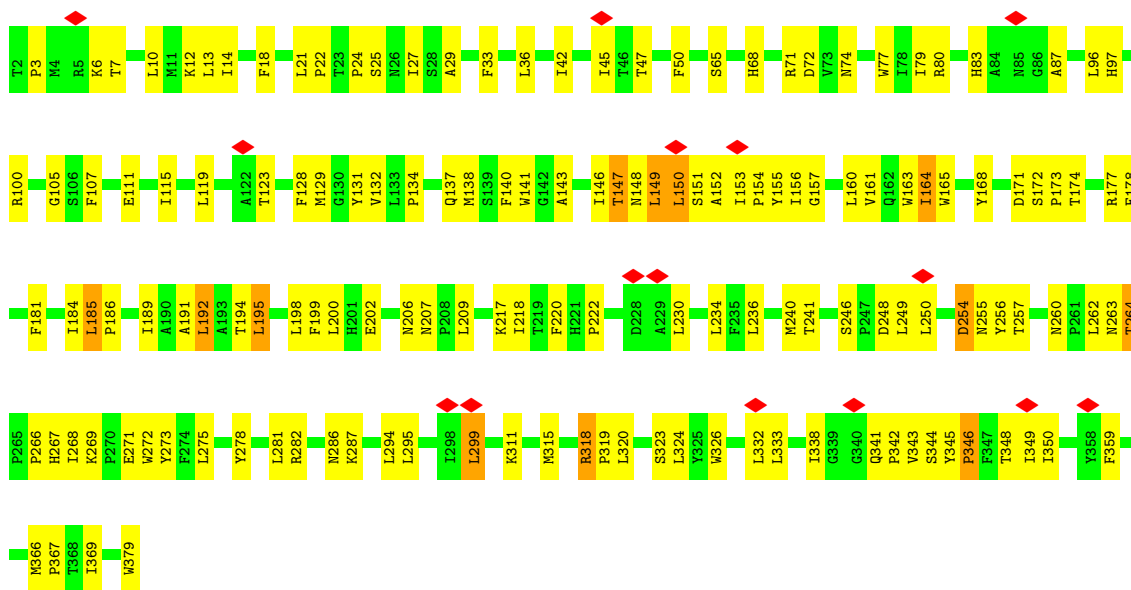




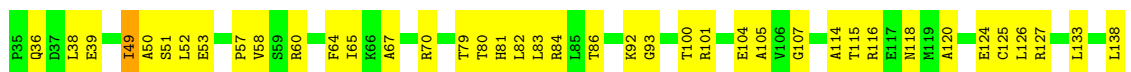
• Molecule 66: Cytochrome b

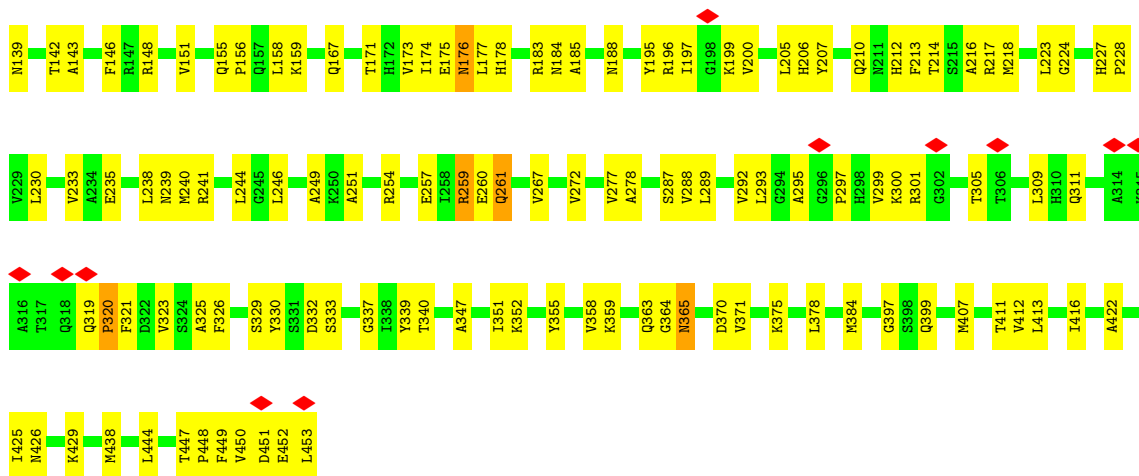


• Molecule 66: Cytochrome b

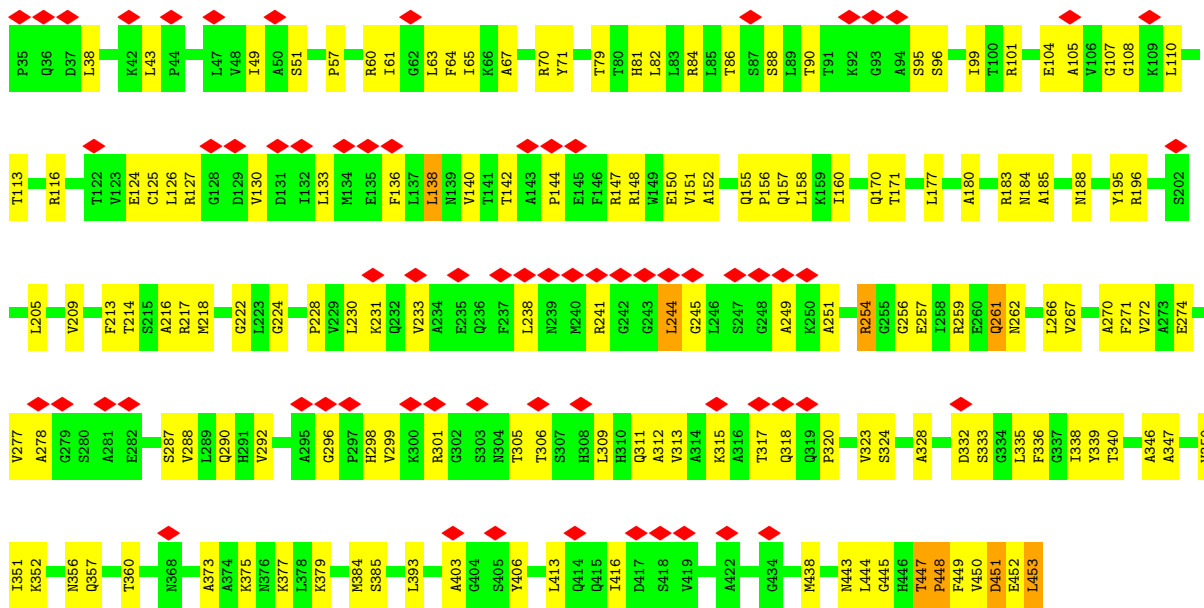


• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

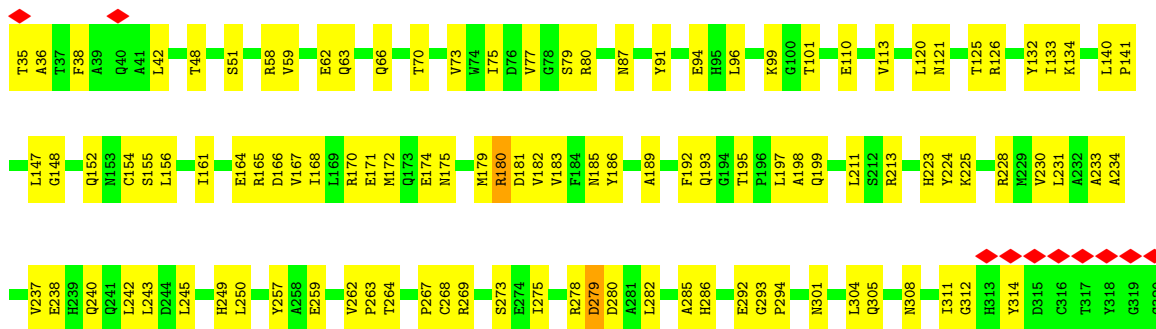


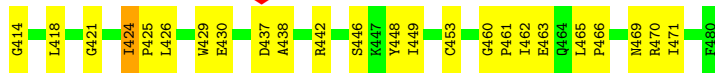


• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

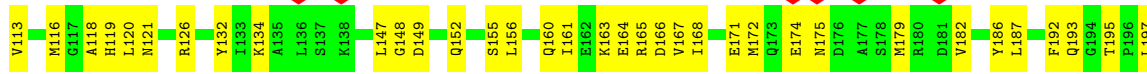
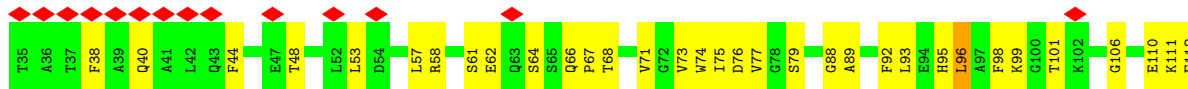


• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial





• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	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 ($e^-/\text{\AA}^2$)	1.25	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	0.385	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0354	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEM, HEC, PEE, FMN, SF4, FES, CU, PLX, CDL, 8Q1, ZN, NDP, HEA

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	A	0.39	0/3398	0.87	6/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.37	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	H	0.45	0/941	0.87	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	6/1681 (0.4%)
14	O	0.40	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.55	0/3552	1.01	14/4815 (0.3%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	T	0.37	0/755	0.79	0/1017
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	W	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
22	Y	0.61	0/559	1.16	7/763 (0.9%)
23	Z	0.56	0/669	0.82	0/899
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	d	0.78	0/1445	0.97	3/1945 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	l	0.84	4/4840 (0.1%)	1.04	29/6611 (0.4%)
36	m	0.82	0/1346	0.99	5/1832 (0.3%)
37	n	0.63	0/484	0.99	0/652
38	o	0.71	0/1093	0.89	0/1479
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	v	0.64	0/934	1.00	4/1241 (0.3%)
44	w	0.54	1/2533 (0.0%)	0.91	8/3440 (0.2%)
45	x	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
46	y	0.78	0/1868	1.12	11/2544 (0.4%)
47	z	0.75	0/2211	1.02	7/3023 (0.2%)
48	0	0.68	0/1229	0.96	3/1658 (0.2%)
49	1	0.64	0/898	1.02	6/1218 (0.5%)
50	2	0.72	0/765	1.13	3/1038 (0.3%)
51	3	0.69	0/699	1.10	6/950 (0.6%)
52	4	0.67	0/648	1.17	5/877 (0.6%)
53	5	0.71	0/611	0.94	2/810 (0.2%)
54	6	0.70	0/451	1.04	3/610 (0.5%)
55	7	0.76	0/398	1.01	1/546 (0.2%)
56	8	0.78	0/399	0.97	2/534 (0.4%)
57	9	0.69	0/345	0.99	1/470 (0.2%)
58	AA	0.44	0/715	0.83	1/964 (0.1%)
58	AN	0.37	0/707	0.86	2/953 (0.2%)
59	AB	0.37	0/421	0.91	0/574
59	AO	0.40	0/417	0.98	0/569
60	AC	0.32	0/1554	0.81	6/2104 (0.3%)
60	AP	0.30	0/1554	0.84	6/2104 (0.3%)
61	AD	0.30	0/521	0.63	0/699
61	AQ	0.31	0/521	0.67	0/699
62	AE	0.48	1/587 (0.2%)	0.84	2/789 (0.3%)
62	AR	0.37	0/587	0.77	2/789 (0.3%)
63	AF	0.61	2/942 (0.2%)	0.85	3/1263 (0.2%)
63	AS	0.33	0/942	0.65	0/1263
64	AG	0.38	0/442	0.82	4/608 (0.7%)
64	AT	0.40	0/442	0.80	1/608 (0.2%)
65	AH	0.35	0/1983	0.84	6/2691 (0.2%)
65	AU	0.35	0/1983	0.79	4/2691 (0.1%)
66	AJ	0.42	2/3108 (0.1%)	0.82	7/4254 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
66	AV	0.46	4/3108 (0.1%)	0.86	11/4254 (0.3%)
67	AK	0.36	0/3217	0.79	0/4361
67	AW	0.39	2/3220 (0.1%)	0.81	4/4365 (0.1%)
68	AL	0.37	0/3527	0.82	8/4788 (0.2%)
68	AY	0.40	2/3527 (0.1%)	0.82	6/4788 (0.1%)
All	All	0.61	32/115987 (0.0%)	0.94	394/157444 (0.3%)

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
44	w	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.60	1.50	1.54
45	x	61	HIS	CG-CD2	7.48	1.44	1.35
45	x	378	HIS	ND1-CE1	7.38	1.40	1.32
62	AE	28	ASP	C-N	7.28	1.41	1.34
45	x	378	HIS	CE1-NE2	-6.50	1.26	1.32

The worst 5 of 394 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	31	SER	N-CA-C	-16.80	92.09	112.59
21	W	10	MET	CA-C-N	-10.86	109.19	120.38
21	W	10	MET	C-N-CA	-10.86	109.19	120.38
8	I	38	PRO	CA-C-N	10.33	130.64	119.28
8	I	38	PRO	C-N-CA	10.33	130.64	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

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	A	3322	0	3289	212	0
2	B	1420	0	1371	121	0
3	C	1249	0	1253	83	0
4	E	968	0	982	66	0
5	F	670	0	679	37	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	H	922	0	950	58	0
8	I	769	0	788	46	0
9	J	2712	0	2757	236	0
10	K	274	0	257	24	0
11	L	964	0	962	63	0
12	M	5274	0	5312	335	0
13	N	1195	0	1155	49	0
14	O	1643	0	1646	114	0
15	P	1730	0	1685	113	0
16	Q	3460	0	3419	310	0
17	S	568	0	567	42	0
18	T	742	0	723	39	0
19	U	647	0	653	16	0
20	V	1038	0	1027	37	0
21	W	1135	0	1129	60	0
22	Y	533	0	475	97	0
23	Z	648	0	627	18	0
24	a	1174	0	1177	106	0
25	b	1059	0	1079	125	0
26	c	1236	0	1092	81	0
27	d	1418	0	1375	121	0
28	e	810	0	772	35	0
29	f	405	0	407	19	0
30	g	1004	0	1008	65	0
31	h	863	0	861	66	0
32	i	2735	0	2893	187	0
33	j	919	0	968	83	0
34	k	740	0	792	90	0
35	l	4717	0	4893	409	0
36	m	1313	0	1330	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	473	0	480	30	0
38	o	1066	0	1086	62	0
39	p	1495	0	1440	101	0
40	r	3629	0	3825	163	0
41	s	2509	0	2617	166	0
42	u	1394	0	1367	60	0
43	v	921	0	892	90	0
44	w	2474	0	2304	115	0
45	x	4025	0	4003	84	0
46	y	1822	0	1834	72	0
47	z	2124	0	2042	52	0
48	0	1195	0	1183	34	0
49	1	878	0	868	18	0
50	2	748	0	728	24	0
51	3	672	0	645	31	0
52	4	628	0	582	22	0
53	5	598	0	612	15	0
54	6	441	0	439	26	0
55	7	384	0	366	13	0
56	8	386	0	388	8	0
57	9	335	0	352	13	0
58	AA	694	0	683	46	0
58	AN	687	0	676	24	0
59	AB	413	0	438	25	0
59	AO	409	0	432	26	0
60	AC	1521	0	1505	54	0
60	AP	1521	0	1505	61	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	24	0
62	AE	580	0	526	52	0
62	AR	580	0	526	34	0
63	AF	921	0	909	73	0
63	AS	921	0	910	30	0
64	AG	425	0	422	14	0
64	AT	425	0	422	30	0
65	AH	1924	0	1874	64	0
65	AU	1924	0	1874	81	0
66	AJ	3009	0	3065	113	0
66	AV	3009	0	3065	176	0
67	AK	3159	0	3130	154	0
67	AW	3162	0	3139	130	0
68	AL	3453	0	3370	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	AY	3453	0	3368	161	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	3	0
70	A	31	0	19	16	0
71	AL	52	0	88	3	0
71	AQ	52	0	88	7	0
71	AT	52	0	88	3	0
71	B	52	0	88	2	0
71	U	52	0	88	3	0
71	V	52	0	88	5	0
71	b	52	0	88	38	0
71	g	156	0	264	13	0
71	r	104	0	176	23	0
72	E	35	0	0	4	0
72	p	35	0	0	12	0
73	J	48	0	26	27	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	1	0
75	AG	64	0	72	29	0
75	AH	64	0	72	6	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	23	0
75	AN	64	0	72	8	0
75	AU	64	0	72	12	0
75	AY	64	0	72	4	0
75	V	63	0	68	8	0
75	i	64	0	72	3	0
75	l	128	0	144	4	0
75	n	64	0	72	10	0
76	AH	49	0	75	31	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	38	0
76	AU	41	0	56	24	0
76	AV	49	0	75	21	0
76	AY	49	0	75	22	0
76	V	51	0	82	21	0
76	W	51	0	82	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	l	100	0	157	68	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	x	1	0	0	0	0
79	x	120	0	108	5	0
80	2	1	0	0	0	0
81	AH	43	0	32	5	0
81	AU	43	0	32	6	0
82	AJ	86	0	60	7	0
82	AV	86	0	60	13	0
All	All	115642	0	115742	5541	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 24.

The worst 5 of 5541 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)
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.65
68:AY:296:TRP:CD1	68:AY:419:THR:CG2	1.74	1.60
63:AF:29:LYS:CD	63:AF:75:ILE:HD11	1.31	1.58
35:l:533:MET:CE	76:l:702:PEE:H36	1.25	1.58
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.56

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	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5 31
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	25
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	29
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	18
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	19
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	14
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	31
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	8
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	24
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	24
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	18
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	24
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	17
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	36
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	26
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	20
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	41
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	31
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	22
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	31
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	20
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	19
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	55
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	25
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	31
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	17
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	15
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	28
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	25
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	35
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	16
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	22
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	25
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	32
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	27
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	26
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	27
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	27
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	50
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	40
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	20
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	15
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	38
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	22
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	29
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	9	40
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	17
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	6
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	28
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	4	27
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	38
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	12	45
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16	50
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	50
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16	50
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16	50
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	10	41
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	10	41
68	AL	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	9	38
68	AY	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	7	36
All	All	14029/14219 (99%)	12872 (92%)	849 (6%)	308 (2%)	7	31

5 of 308 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

5.3.2 Protein sidechains [i](#)

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	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	75
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	71
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	85
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	77
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	20
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	77
25	b	118/118 (100%)	113 (96%)	5 (4%)	26	50
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	45
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	85
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	75
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	48
35	l	531/532 (100%)	511 (96%)	20 (4%)	29	52
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	71
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	x	427/427 (100%)	387 (91%)	40 (9%)	8	29
46	y	211/211 (100%)	191 (90%)	20 (10%)	8	29
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	21
48	0	128/128 (100%)	118 (92%)	10 (8%)	11	36
49	1	95/95 (100%)	89 (94%)	6 (6%)	16	42
50	2	81/81 (100%)	73 (90%)	8 (10%)	7	28
51	3	68/68 (100%)	52 (76%)	16 (24%)	1	5
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	19
53	5	58/58 (100%)	51 (88%)	7 (12%)	5	21
54	6	47/47 (100%)	41 (87%)	6 (13%)	4	20
55	7	39/39 (100%)	36 (92%)	3 (8%)	12	37
56	8	40/40 (100%)	37 (92%)	3 (8%)	12	38
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	35
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	35
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	51 (98%)	1 (2%)	50	66
62	AE	61/71 (86%)	59 (97%)	2 (3%)	33	56
62	AR	61/71 (86%)	58 (95%)	3 (5%)	22	47
63	AF	95/95 (100%)	83 (87%)	12 (13%)	4	20
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	23	48
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	81	82
66	AJ	330/330 (100%)	326 (99%)	4 (1%)	63	72
66	AV	330/330 (100%)	321 (97%)	9 (3%)	39	60
67	AK	334/335 (100%)	330 (99%)	4 (1%)	63	72
67	AW	335/335 (100%)	331 (99%)	4 (1%)	63	72
68	AL	367/367 (100%)	367 (100%)	0	100	100
68	AY	367/367 (100%)	362 (99%)	5 (1%)	59	71
All	All	12164/12289 (99%)	11894 (98%)	270 (2%)	45	64

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	AF	40	GLU
66	AJ	150	LEU
66	AV	299	LEU
45	x	509	THR
45	x	474	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 274 such sidechains are listed below:

Mol	Chain	Res	Type
68	AL	66	GLN
68	AL	335	ASN
67	AW	298	HIS
32	i	83	GLN

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Mol	Chain	Res	Type
30	g	45	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 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
75	CDL	AN	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.04	4 (5%)
71	PLX	g	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
75	CDL	l	703	-	63,63,99	1.22	5 (7%)	69,75,111	1.08	4 (5%)
75	CDL	AL	502	-	63,63,99	1.26	5 (7%)	69,75,111	1.07	4 (5%)
69	SF4	C	301	3	0,12,12	-	-	-		
74	FES	O	301	14	0,4,4	-	-	-		
76	PEE	AY	502	-	48,48,50	1.41	4 (8%)	51,53,55	0.97	2 (3%)
69	SF4	M	802	12	0,12,12	-	-	-		
71	PLX	b	201	-	51,51,51	0.55	0	53,59,59	0.64	0
76	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
71	PLX	V	203	-	51,51,51	0.80	1 (1%)	53,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PEE	AL	503	-	48,48,50	1.40	4 (8%)	51,53,55	0.93	2 (3%)
75	CDL	AJ	404	-	63,63,99	1.26	5 (7%)	69,75,111	1.04	4 (5%)
71	PLX	g	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.60	1 (1%)
71	PLX	AQ	101	-	51,51,51	0.80	1 (1%)	53,59,59	0.63	2 (3%)
76	PEE	AU	401	-	40,40,50	1.48	4 (10%)	43,45,55	0.95	2 (4%)
71	PLX	AL	501	-	51,51,51	0.80	1 (1%)	53,59,59	0.64	1 (1%)
76	PEE	l	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
75	CDL	AY	501	-	63,63,99	1.26	5 (7%)	69,75,111	1.02	4 (5%)
81	HEC	AU	402	65	46,50,50	1.84	5 (10%)	58,82,82	1.84	4 (6%)
82	HEM	AV	402	66	50,50,50	1.79	9 (18%)	67,82,82	1.25	6 (8%)
75	CDL	n	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
70	FMN	A	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	8 (16%)
71	PLX	r	502	-	51,51,51	0.62	0	53,59,59	0.66	1 (1%)
71	PLX	AT	101	-	51,51,51	0.78	1 (1%)	53,59,59	0.61	1 (1%)
74	FES	AP	301	60	0,4,4	-	-	-	-	-
71	PLX	U	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
72	8Q1	E	201	-	32,34,34	1.58	6 (18%)	39,43,43	1.42	7 (17%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.23	5 (7%)
82	HEM	AV	401	66	50,50,50	1.82	9 (18%)	67,82,82	1.21	3 (4%)
75	CDL	AU	403	-	63,63,99	1.26	6 (9%)	69,75,111	1.06	4 (5%)
69	SF4	B	301	2	0,12,12	-	-	-	-	-
69	SF4	A	501	1	0,12,12	-	-	-	-	-
71	PLX	g	202	-	51,51,51	0.77	1 (1%)	53,59,59	0.62	1 (1%)
76	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
82	HEM	AJ	402	66	50,50,50	1.82	9 (18%)	67,82,82	1.22	6 (8%)
75	CDL	l	704	-	63,63,99	1.28	5 (7%)	69,75,111	1.02	4 (5%)
75	CDL	AH	403	-	63,63,99	1.27	5 (7%)	69,75,111	1.05	4 (5%)
79	HEA	x	604	45	67,67,67	1.20	7 (10%)	81,103,103	1.35	11 (13%)
72	8Q1	p	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
81	HEC	AH	402	65	46,50,50	1.82	5 (10%)	58,82,82	1.86	5 (8%)
79	HEA	x	603	45	67,67,67	1.20	4 (5%)	81,103,103	1.33	10 (12%)
69	SF4	M	801	12	0,12,12	-	-	-	-	-
76	PEE	AH	401	-	48,48,50	1.37	4 (8%)	51,53,55	0.97	2 (3%)
82	HEM	AJ	401	66	50,50,50	1.80	9 (18%)	67,82,82	1.19	2 (2%)
75	CDL	AA	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.09	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PLX	B	303	-	51,51,51	0.79	1 (1%)	53,59,59	0.69	1 (1%)
76	PEE	AJ	403	-	48,48,50	1.35	4 (8%)	51,53,55	1.00	2 (3%)
76	PEE	W	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
74	FES	M	803	-	0,4,4	-	-	-	-	-
75	CDL	V	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.18	6 (8%)
71	PLX	r	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
76	PEE	AV	403	-	48,48,50	1.36	4 (8%)	51,53,55	1.05	2 (3%)
73	NDP	J	401	-	51,52,52	1.15	5 (9%)	71,80,80	1.57	10 (14%)
75	CDL	i	401	-	63,63,99	1.22	5 (7%)	69,75,111	1.06	5 (7%)
69	SF4	B	302	2	0,12,12	-	-	-	-	-
74	FES	AC	301	60	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
75	CDL	AN	101	-	-	39/74/74/110	-
71	PLX	g	201	-	-	24/55/55/55	-
69	SF4	B	302	2	-	-	0/6/5/5
75	CDL	l	703	-	-	36/74/74/110	-
75	CDL	AL	502	-	-	42/74/74/110	-
69	SF4	C	301	3	-	-	0/6/5/5
74	FES	O	301	14	-	-	0/1/1/1
76	PEE	AY	502	-	-	18/52/52/54	-
69	SF4	M	802	12	-	-	0/6/5/5
71	PLX	b	201	-	-	26/55/55/55	-
76	PEE	V	202	-	-	26/54/54/54	-
71	PLX	V	203	-	-	26/55/55/55	-
74	FES	AC	301	60	-	-	0/1/1/1
76	PEE	AL	503	-	-	21/52/52/54	-
75	CDL	AJ	404	-	-	32/74/74/110	-
71	PLX	g	203	-	-	22/55/55/55	-
71	PLX	AQ	101	-	-	24/55/55/55	-
76	PEE	AU	401	-	-	17/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	AL	501	-	-	23/55/55/55	-
76	PEE	l	702	-	-	27/54/54/54	-
75	CDL	AY	501	-	-	35/74/74/110	-
81	HEC	AU	402	65	-	4/14/54/54	-
82	HEM	AV	402	66	-	4/14/54/54	-
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
71	PLX	r	502	-	-	36/55/55/55	-
71	PLX	AT	101	-	-	22/55/55/55	-
74	FES	AP	301	60	-	-	0/1/1/1
71	PLX	U	101	-	-	22/55/55/55	-
72	8Q1	E	201	-	-	18/41/41/41	-
75	CDL	AJ	405	-	-	25/74/74/110	-
82	HEM	AV	401	66	-	5/14/54/54	-
75	CDL	AU	403	-	-	46/74/74/110	-
69	SF4	B	301	2	-	-	0/6/5/5
69	SF4	A	501	1	-	-	0/6/5/5
71	PLX	g	202	-	-	26/55/55/55	-
76	PEE	l	701	-	-	31/52/52/54	-
82	HEM	AJ	402	66	-	2/14/54/54	-
75	CDL	l	704	-	-	42/74/74/110	-
75	CDL	AH	403	-	-	40/74/74/110	-
79	HEA	x	604	45	-	7/36/76/76	-
72	8Q1	p	201	-	-	19/41/41/41	-
81	HEC	AH	402	65	-	6/14/54/54	-
79	HEA	x	603	45	-	7/36/76/76	-
69	SF4	M	801	12	-	-	0/6/5/5
76	PEE	AH	401	-	-	25/52/52/54	-
82	HEM	AJ	401	66	-	1/14/54/54	-
75	CDL	AA	101	-	-	35/74/74/110	-
71	PLX	B	303	-	-	22/55/55/55	-
76	PEE	AJ	403	-	-	18/52/52/54	-
74	FES	M	803	-	-	-	0/1/1/1
75	CDL	V	201	-	-	40/69/69/110	-
75	CDL	AG	101	-	-	37/74/74/110	-
71	PLX	r	501	-	-	27/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	PEE	AV	403	-	-	29/52/52/54	-
73	NDP	J	401	-	-	15/34/77/77	0/5/5/5
75	CDL	i	401	-	-	39/74/74/110	-
75	CDL	n	101	-	-	32/74/74/110	-
76	PEE	W	201	-	-	29/54/54/54	-

The worst 5 of 203 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AJ	401	HEM	C3D-C2D	7.73	1.53	1.36
82	AV	402	HEM	C3D-C2D	7.72	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.68	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.63	1.53	1.36
81	AU	402	HEC	CAB-C3B	6.21	1.55	1.35

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	CBC-CAC-C3C	-8.70	110.05	127.43
81	AH	402	HEC	CBC-CAC-C3C	-7.92	111.60	127.43
81	AH	402	HEC	CBB-CAB-C3B	-7.82	111.80	127.43
81	AU	402	HEC	CBB-CAB-C3B	-7.09	113.27	127.43
72	p	201	8Q1	C6-C1-S44	5.93	120.47	113.40

There are no chirality outliers.

5 of 1156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'
71	B	303	PLX	C2-O1-P1-O4

There are no ring outliers.

56 monomers are involved in 561 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	AN	101	CDL	8	0
71	g	201	PLX	2	0

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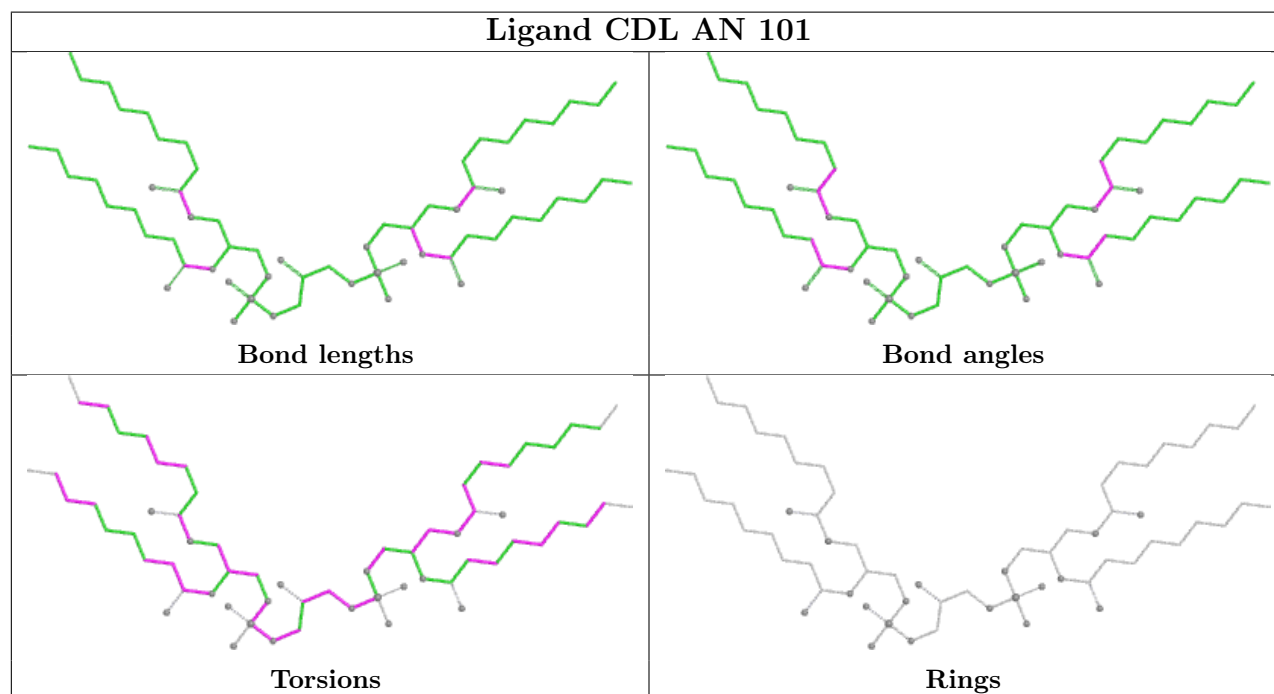
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	l	703	CDL	2	0
75	AL	502	CDL	23	0
74	O	301	FES	2	0
76	AY	502	PEE	22	0
71	b	201	PLX	38	0
76	V	202	PEE	21	0
71	V	203	PLX	5	0
76	AL	503	PEE	38	0
75	AJ	404	CDL	6	0
71	g	203	PLX	8	0
71	AQ	101	PLX	7	0
76	AU	401	PEE	24	0
71	AL	501	PLX	3	0
76	l	702	PEE	18	0
75	AY	501	CDL	4	0
81	AU	402	HEC	6	0
82	AV	402	HEM	6	0
75	n	101	CDL	10	0
70	A	502	FMN	16	0
71	r	502	PLX	17	0
71	AT	101	PLX	3	0
74	AP	301	FES	2	0
71	U	101	PLX	3	0
72	E	201	8Q1	4	0
75	AJ	405	CDL	17	0
82	AV	401	HEM	7	0
75	AU	403	CDL	12	0
69	B	301	SF4	1	0
69	A	501	SF4	6	0
71	g	202	PLX	3	0
76	l	701	PEE	50	0
82	AJ	402	HEM	4	0
75	l	704	CDL	2	0
75	AH	403	CDL	6	0
79	x	604	HEA	3	0
72	p	201	8Q1	12	0
81	AH	402	HEC	5	0
79	x	603	HEA	2	0
69	M	801	SF4	3	0
76	AH	401	PEE	31	0
82	AJ	401	HEM	3	0
75	AA	101	CDL	1	0

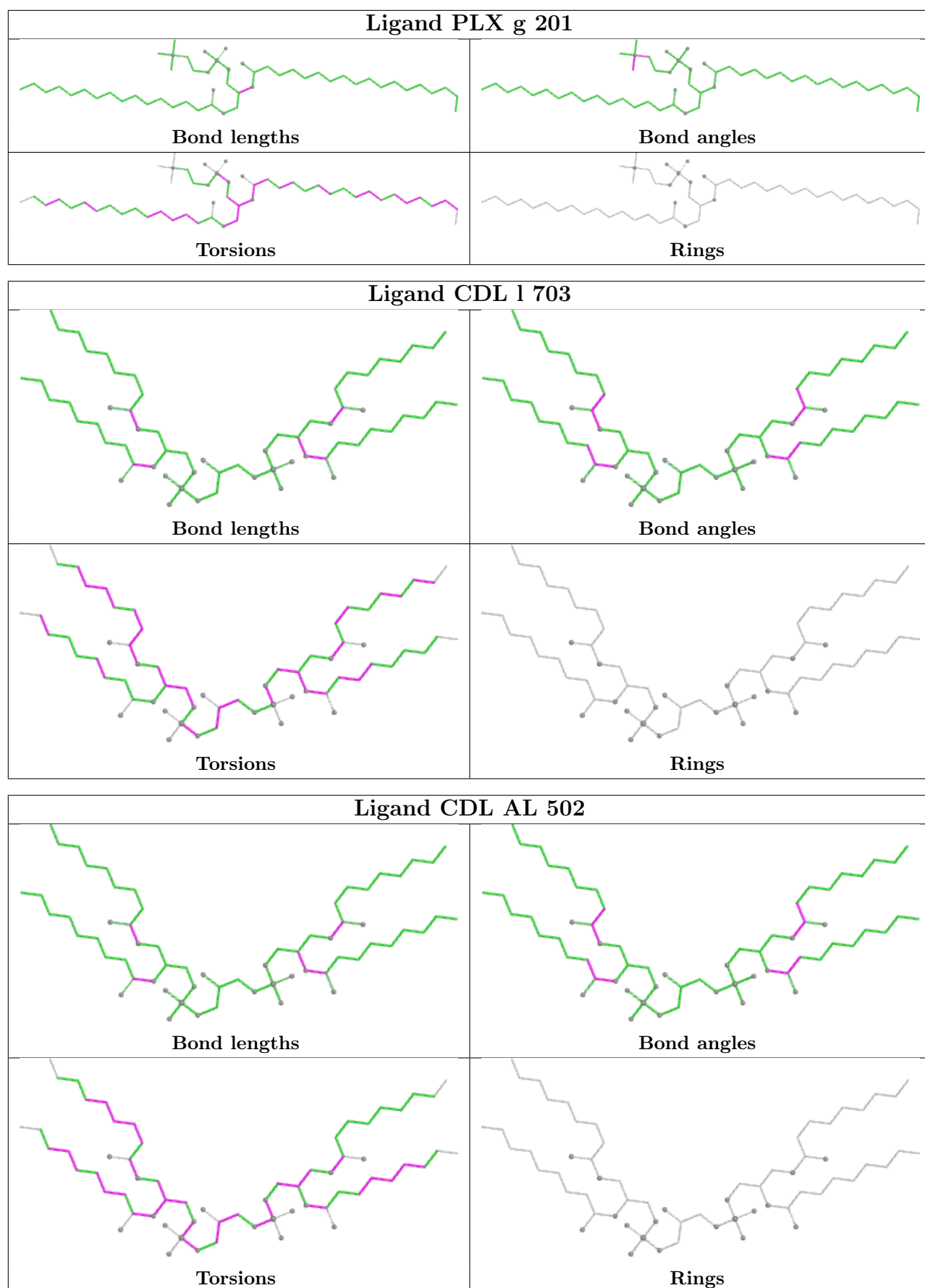
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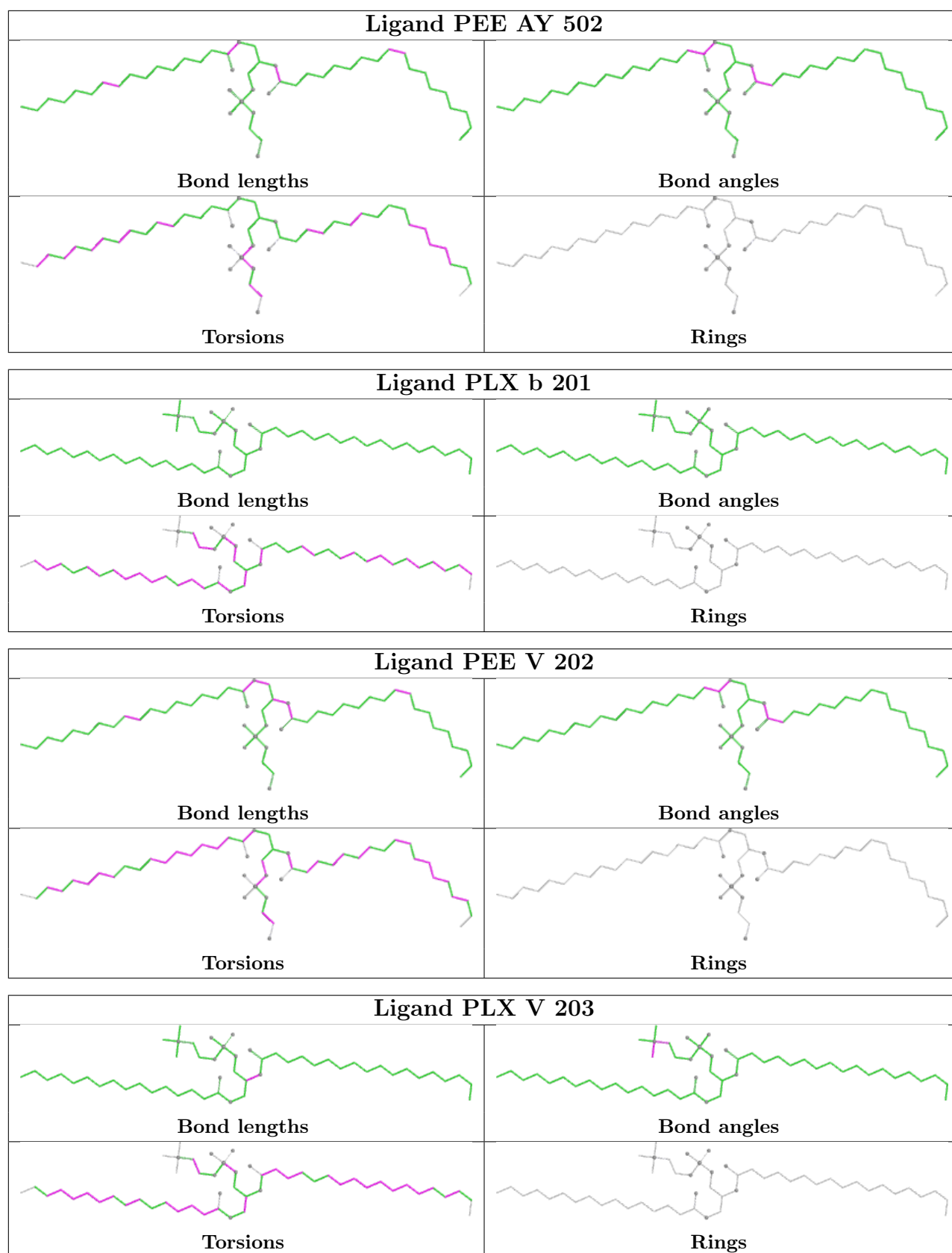
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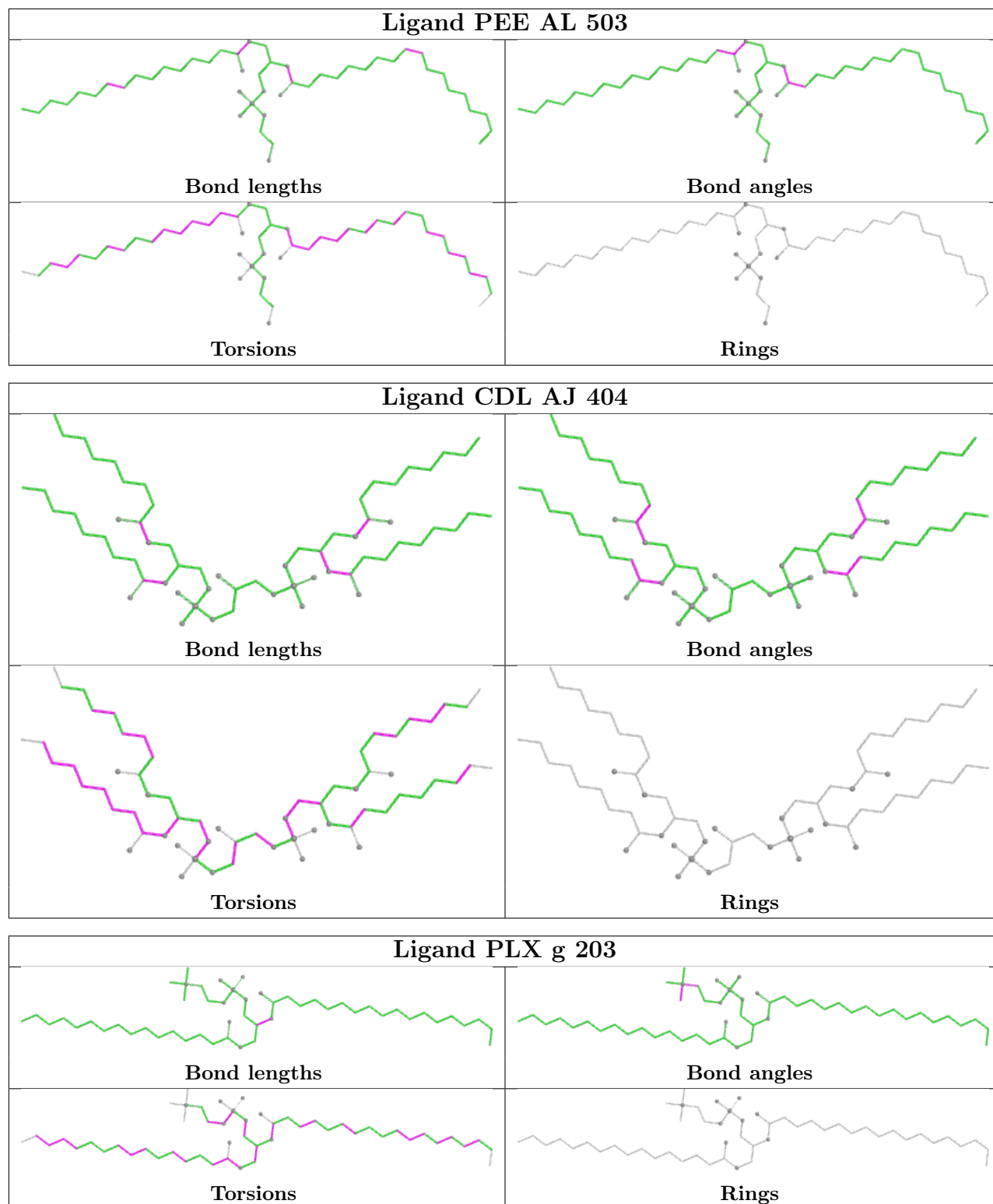
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	B	303	PLX	2	0
76	AJ	403	PEE	8	0
76	W	201	PEE	19	0
74	M	803	FES	1	0
75	V	201	CDL	8	0
75	AG	101	CDL	29	0
71	r	501	PLX	6	0
76	AV	403	PEE	21	0
73	J	401	NDP	27	0
75	i	401	CDL	3	0
69	B	302	SF4	2	0
74	AC	301	FES	3	0

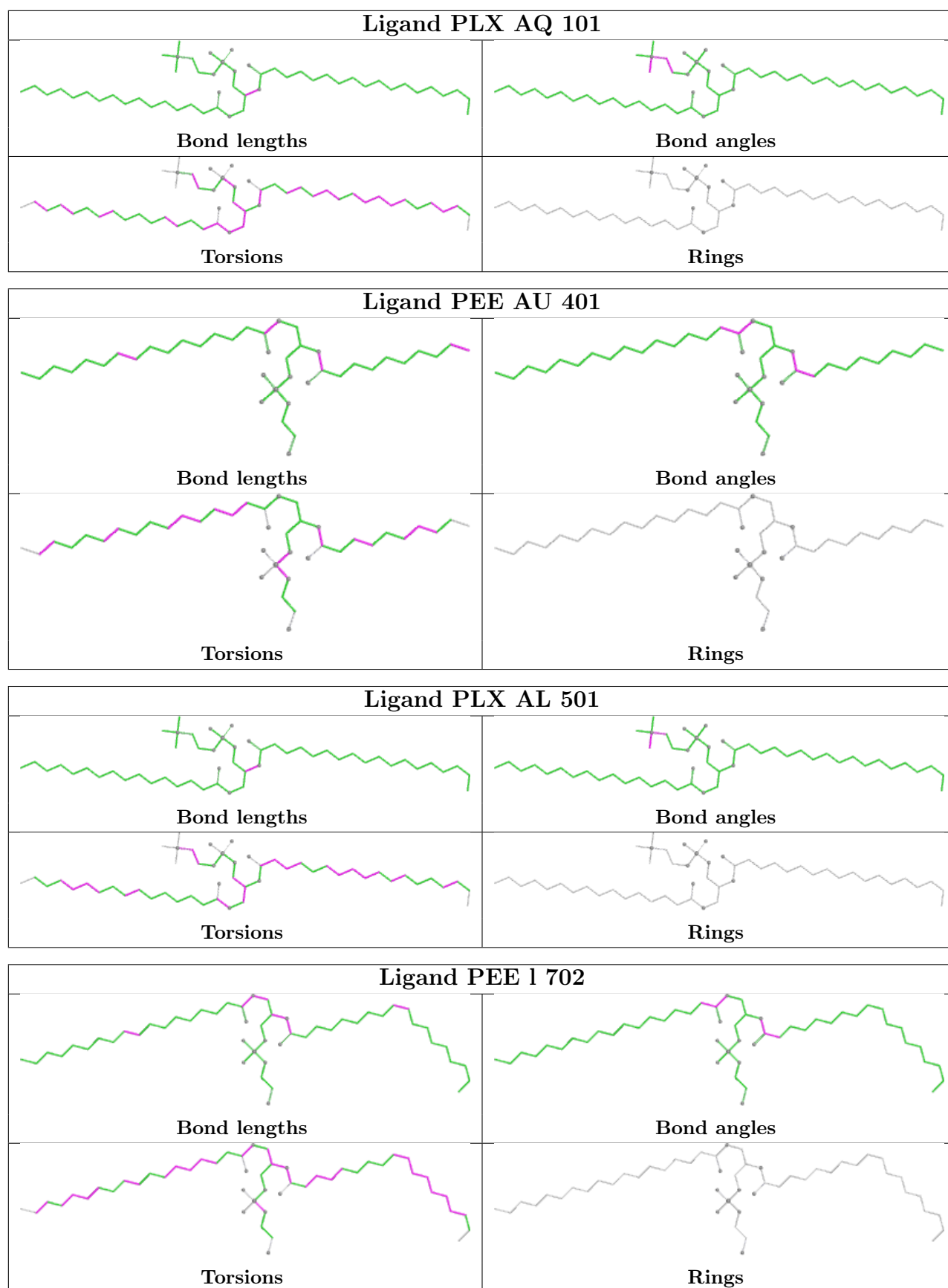
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

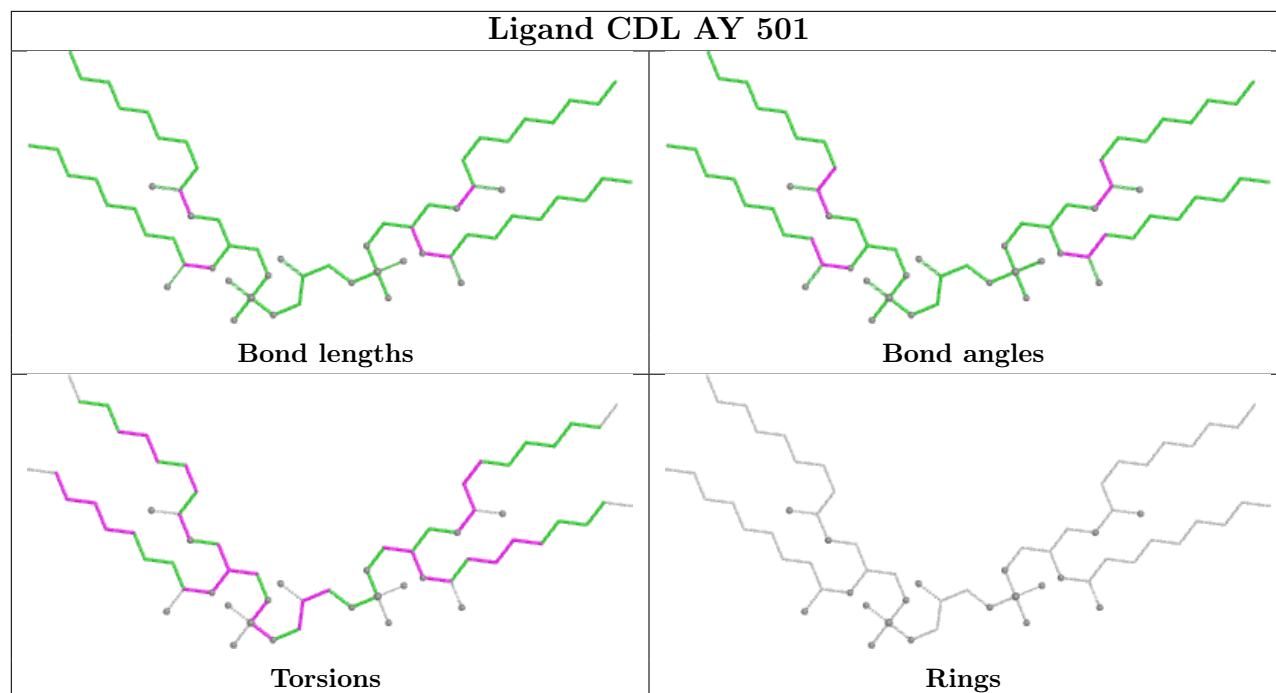


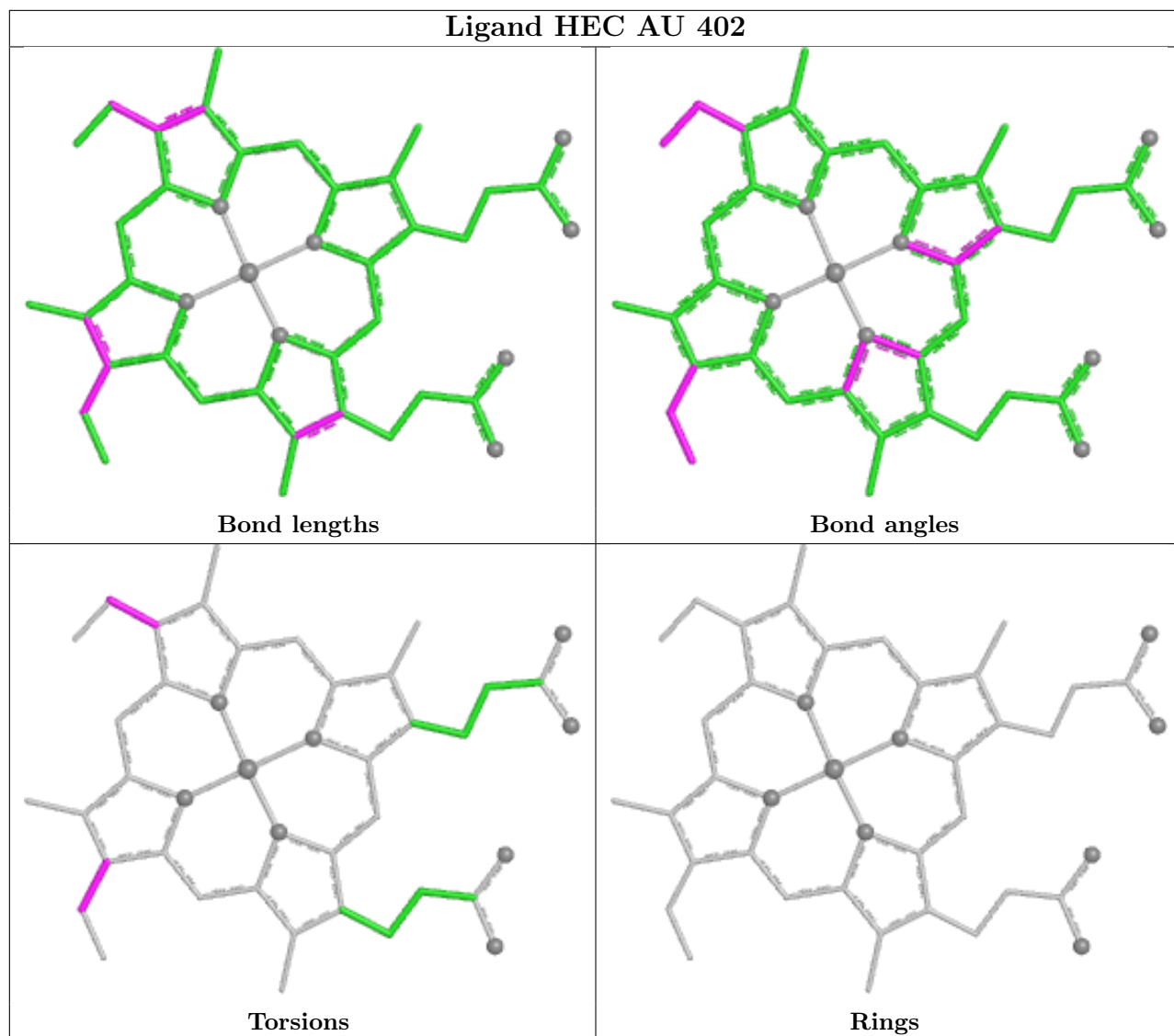


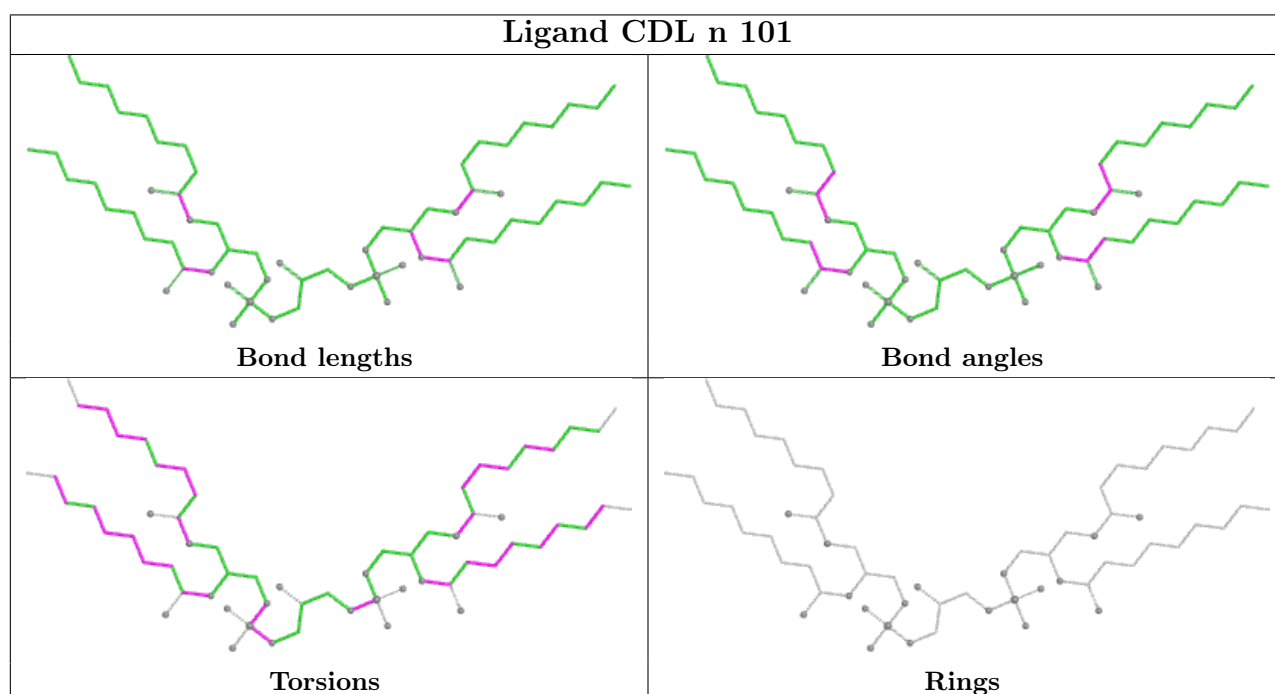
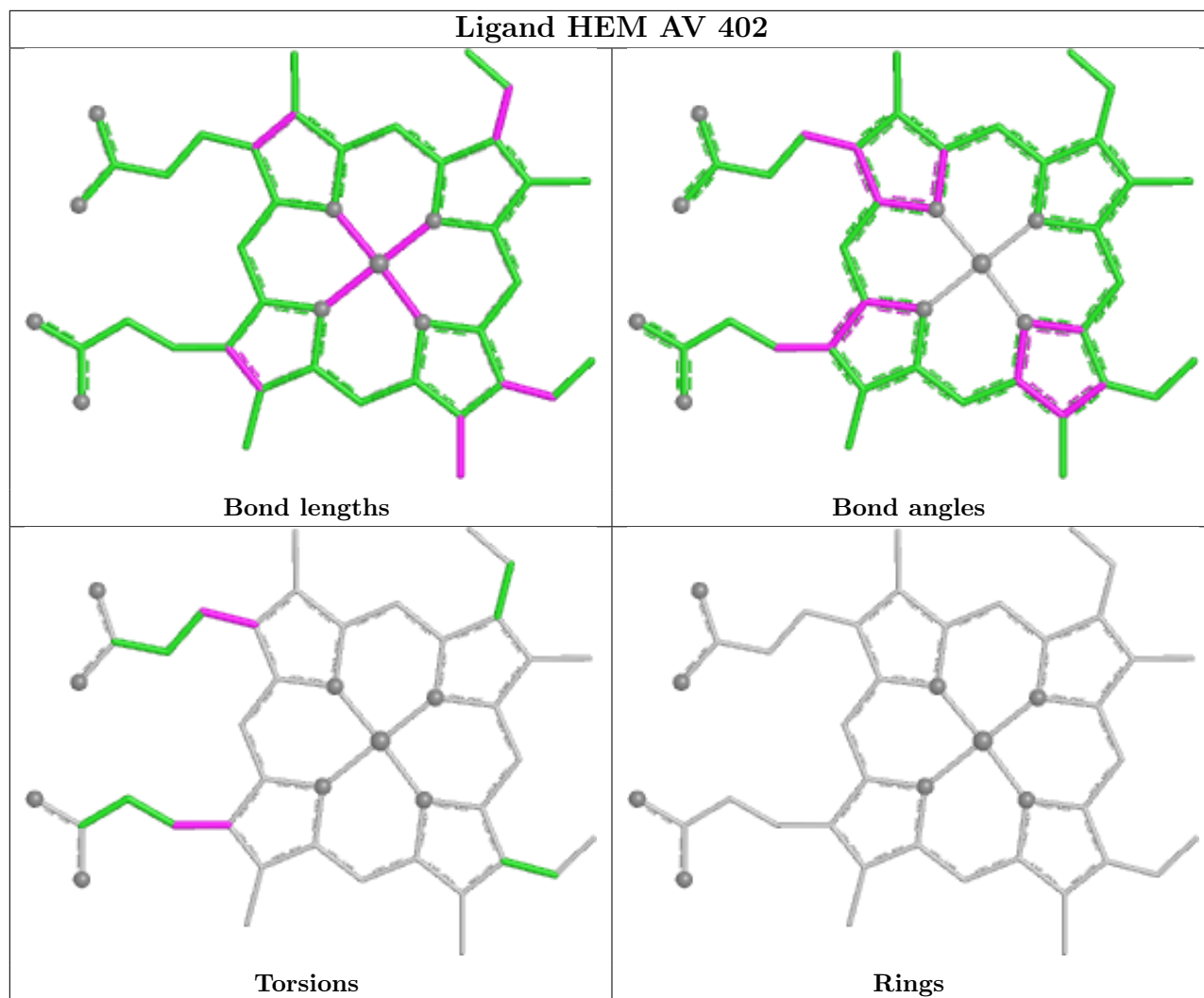


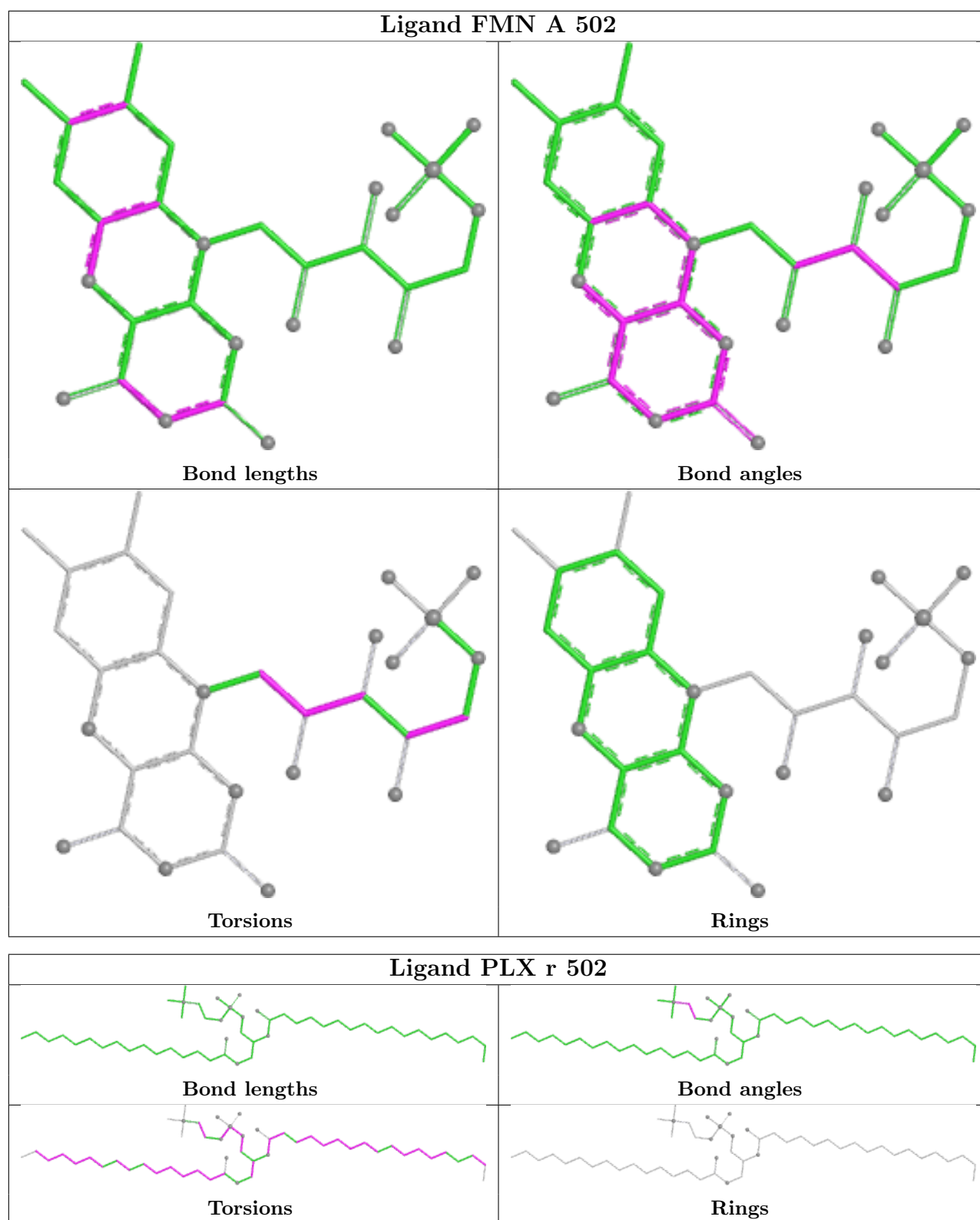


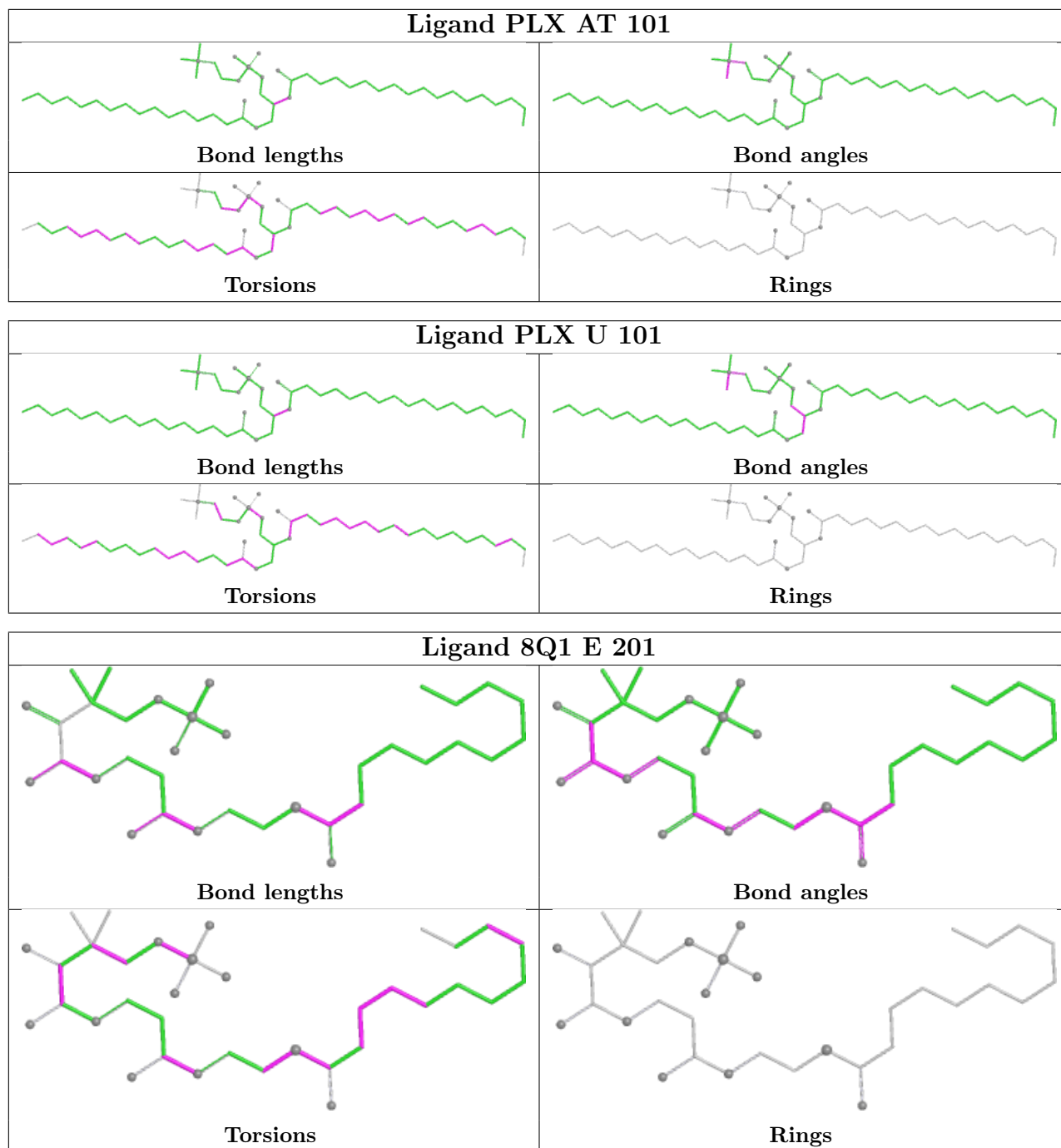


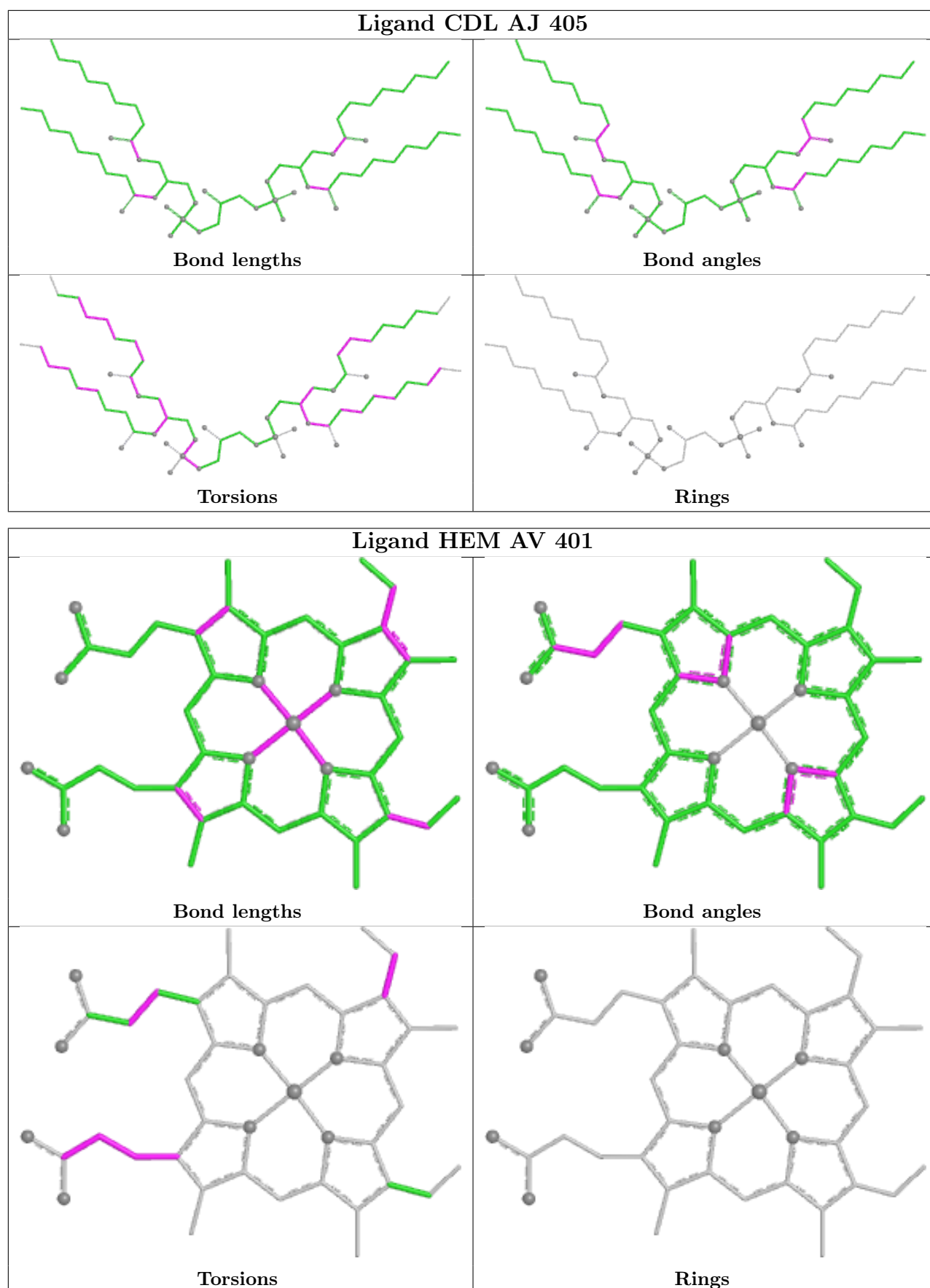


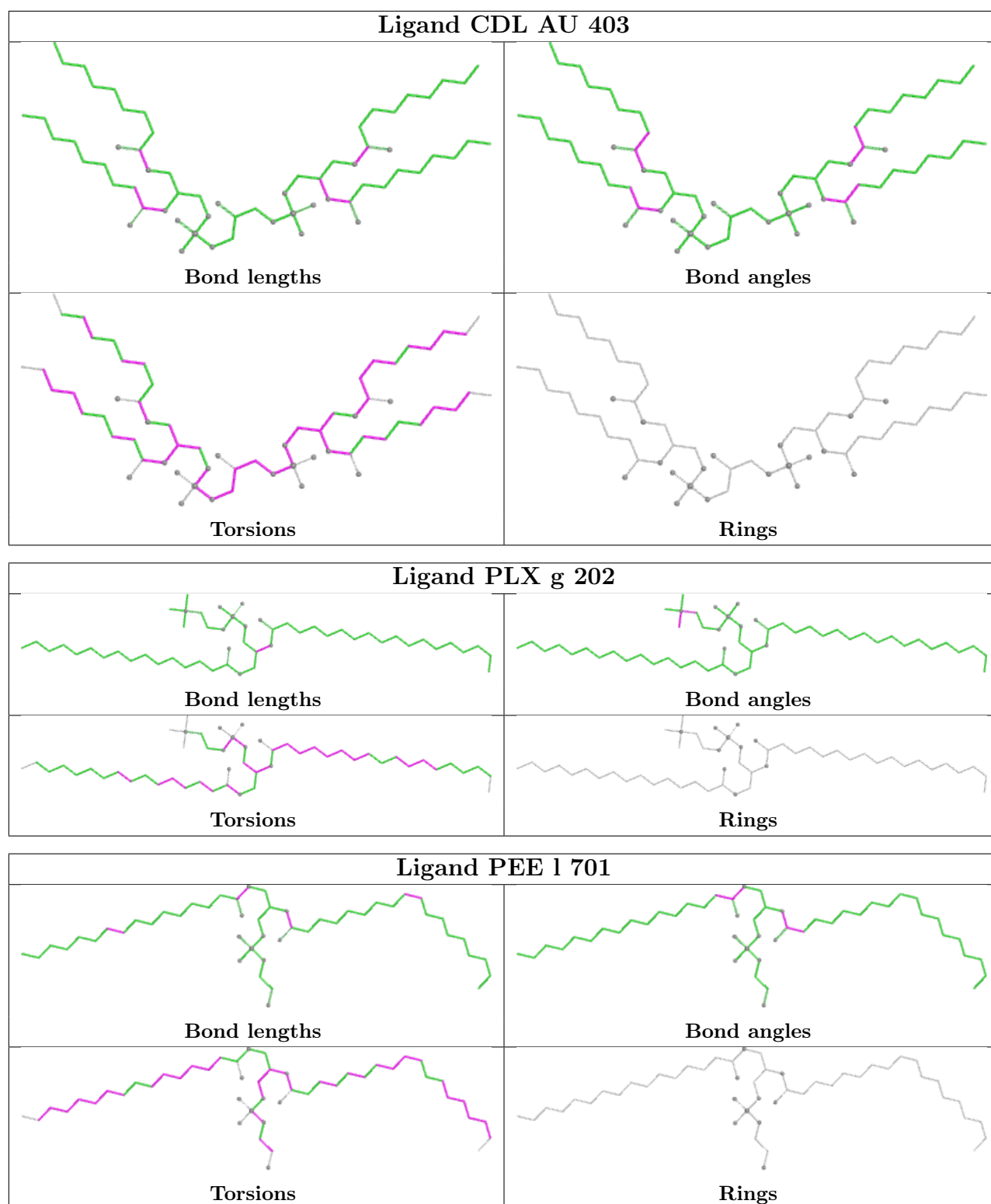


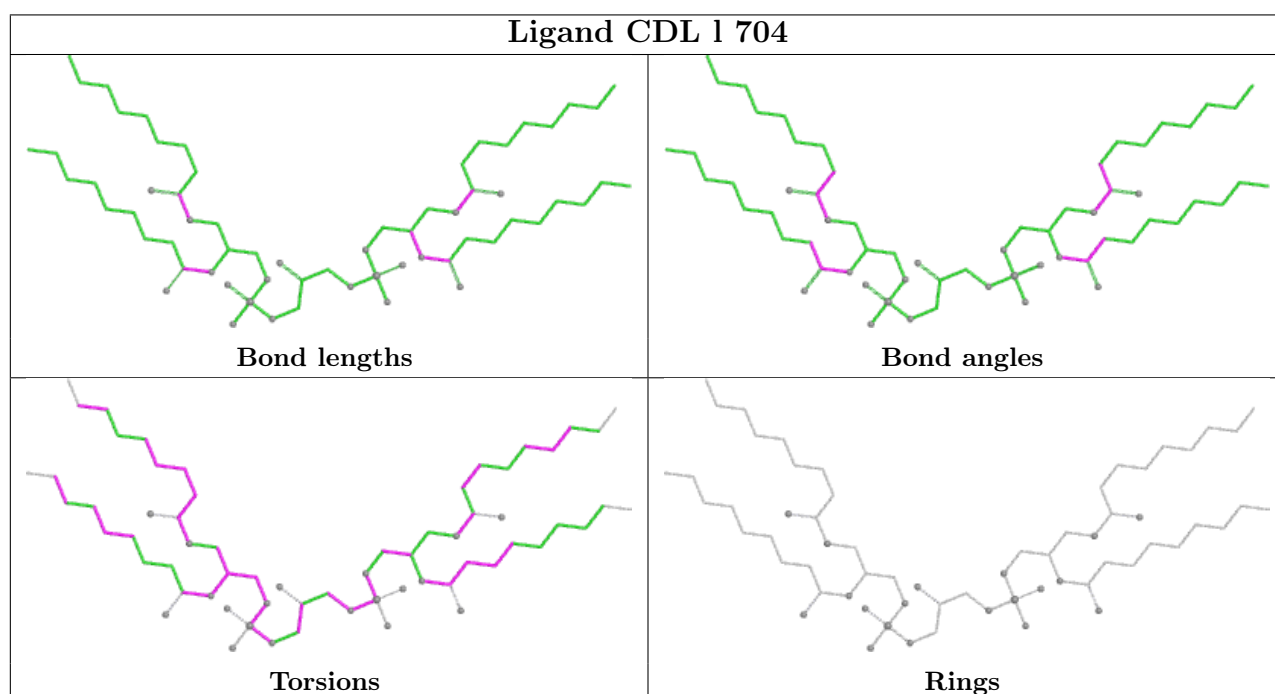
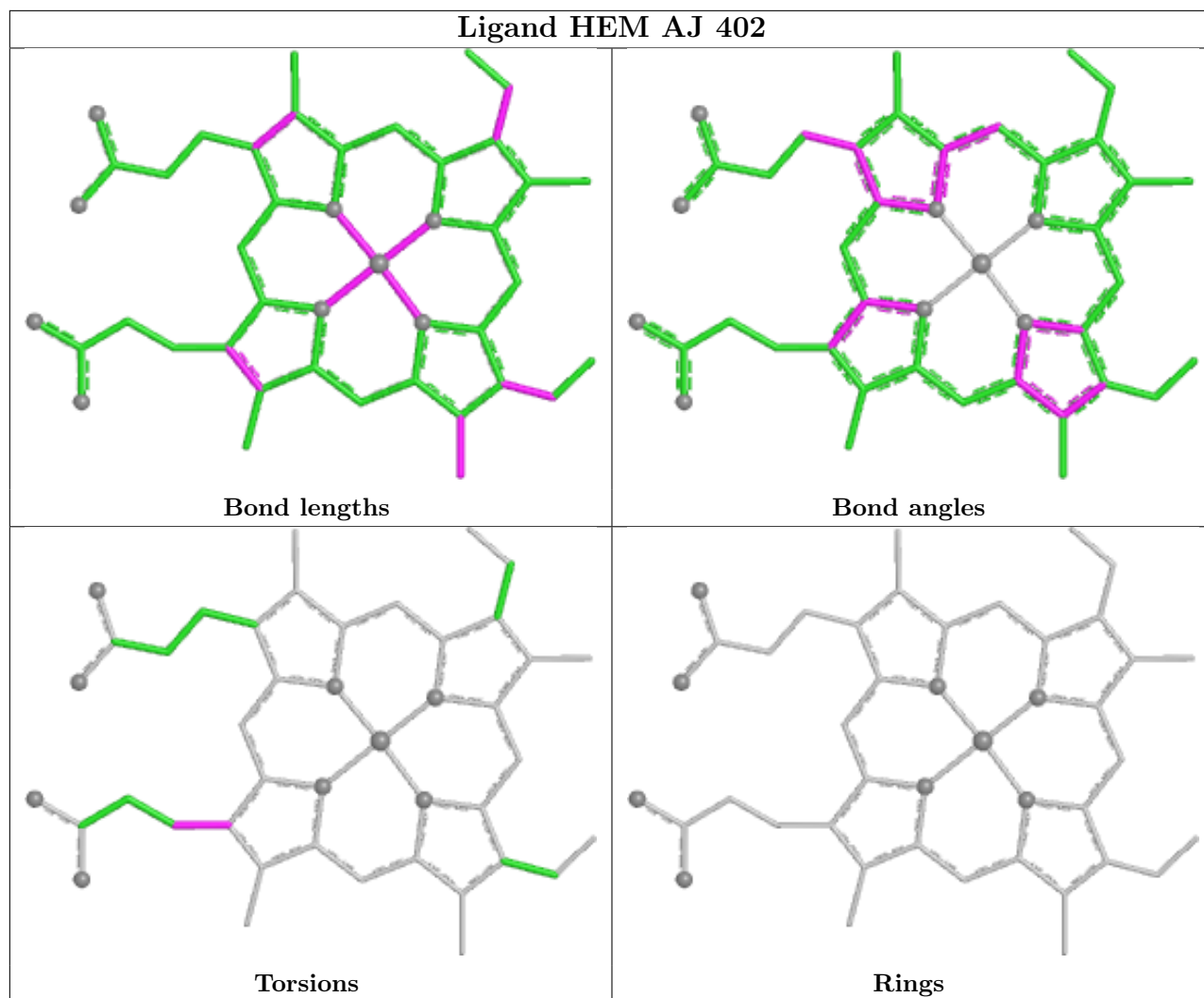


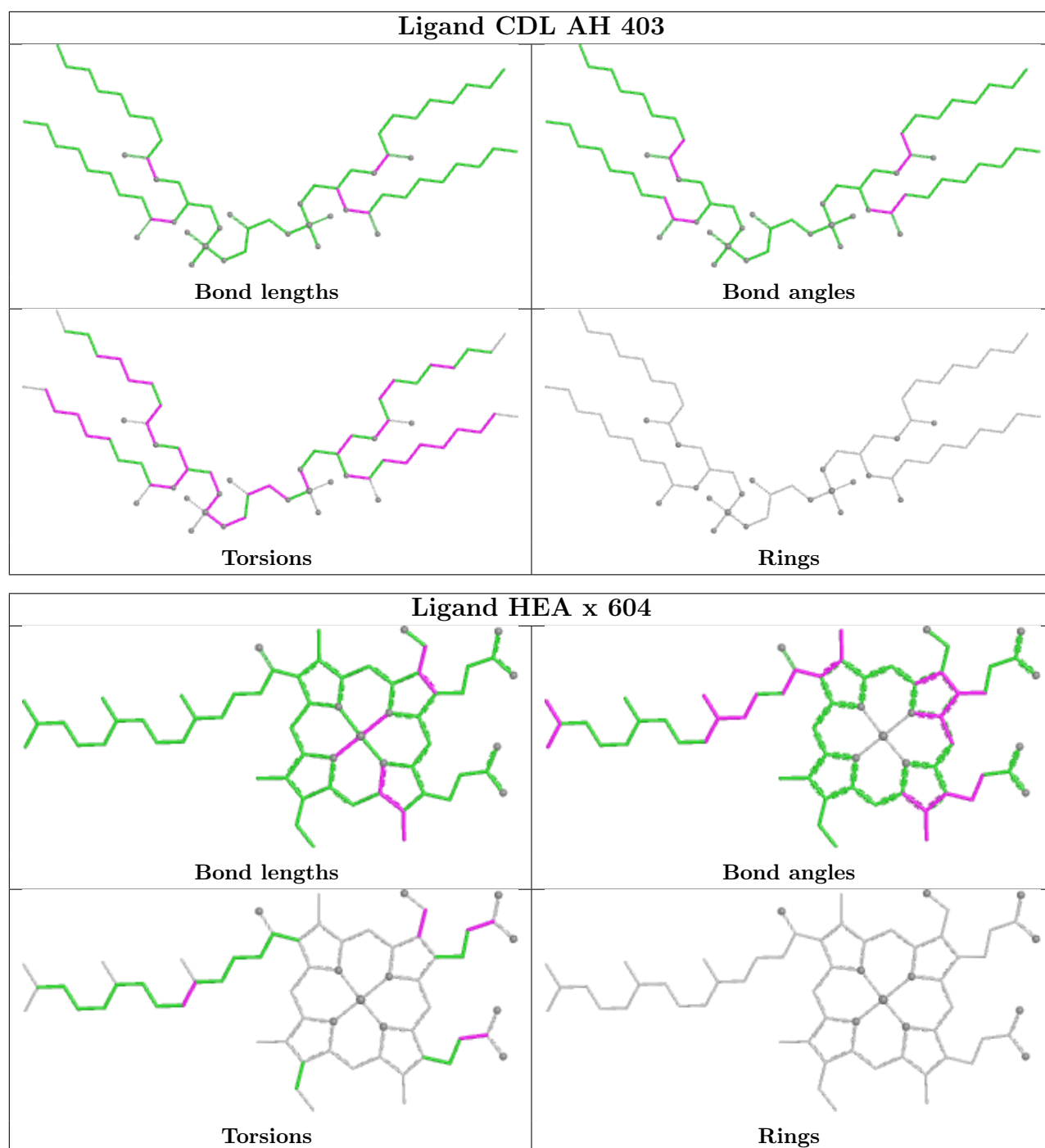


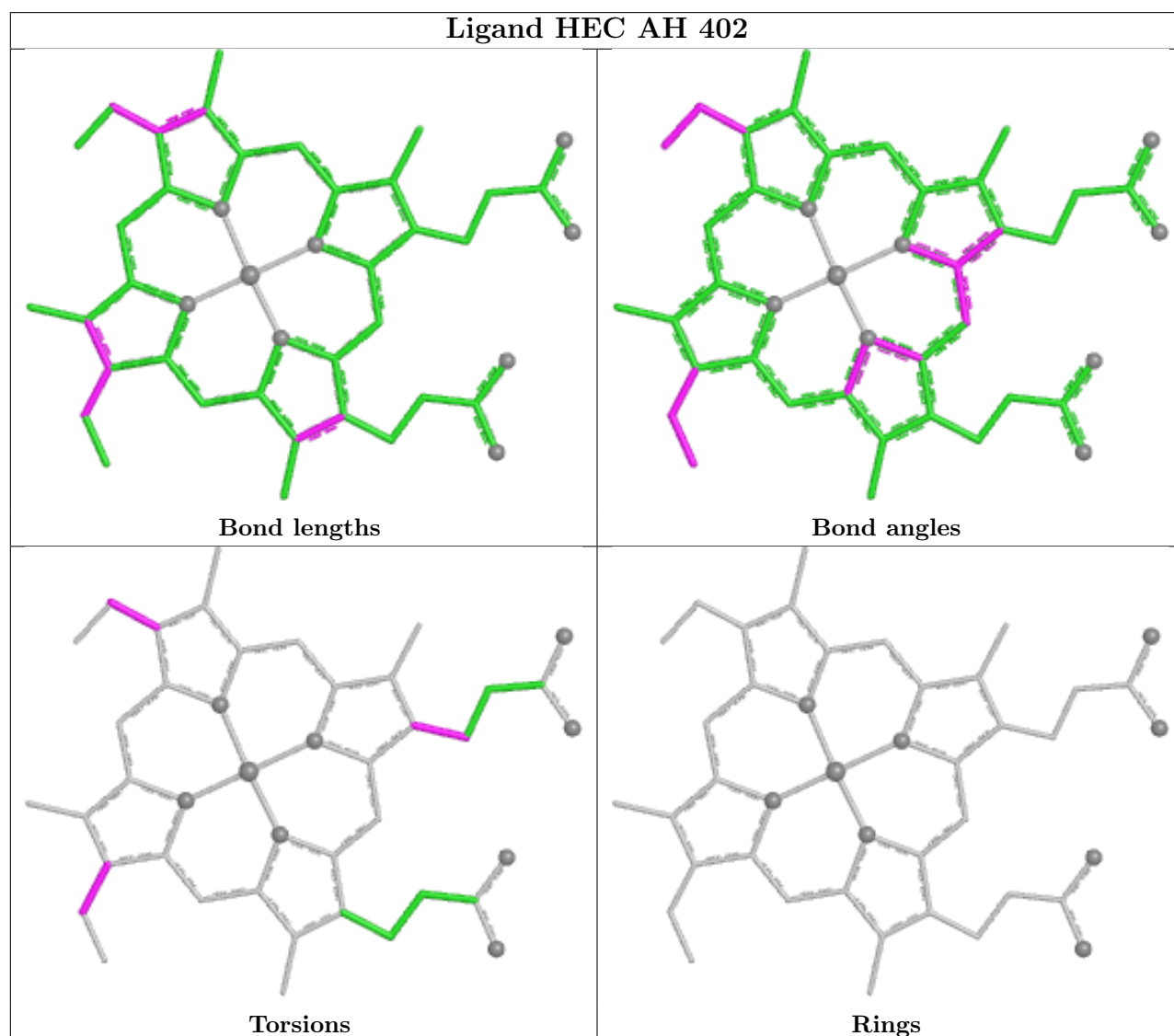
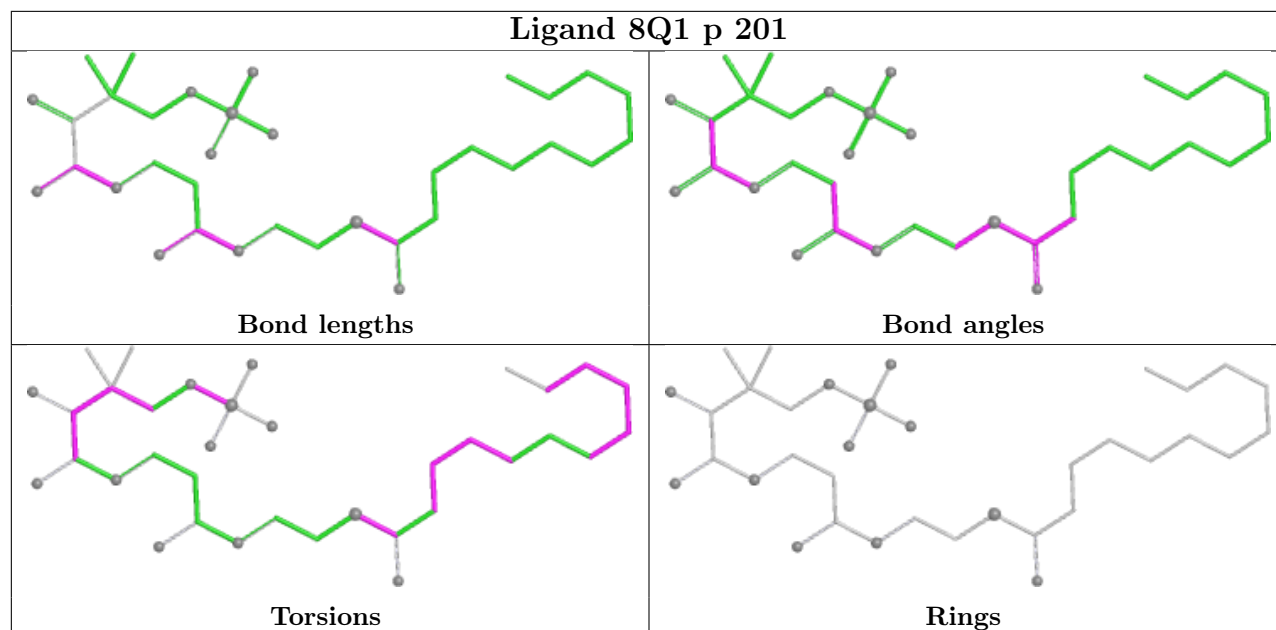


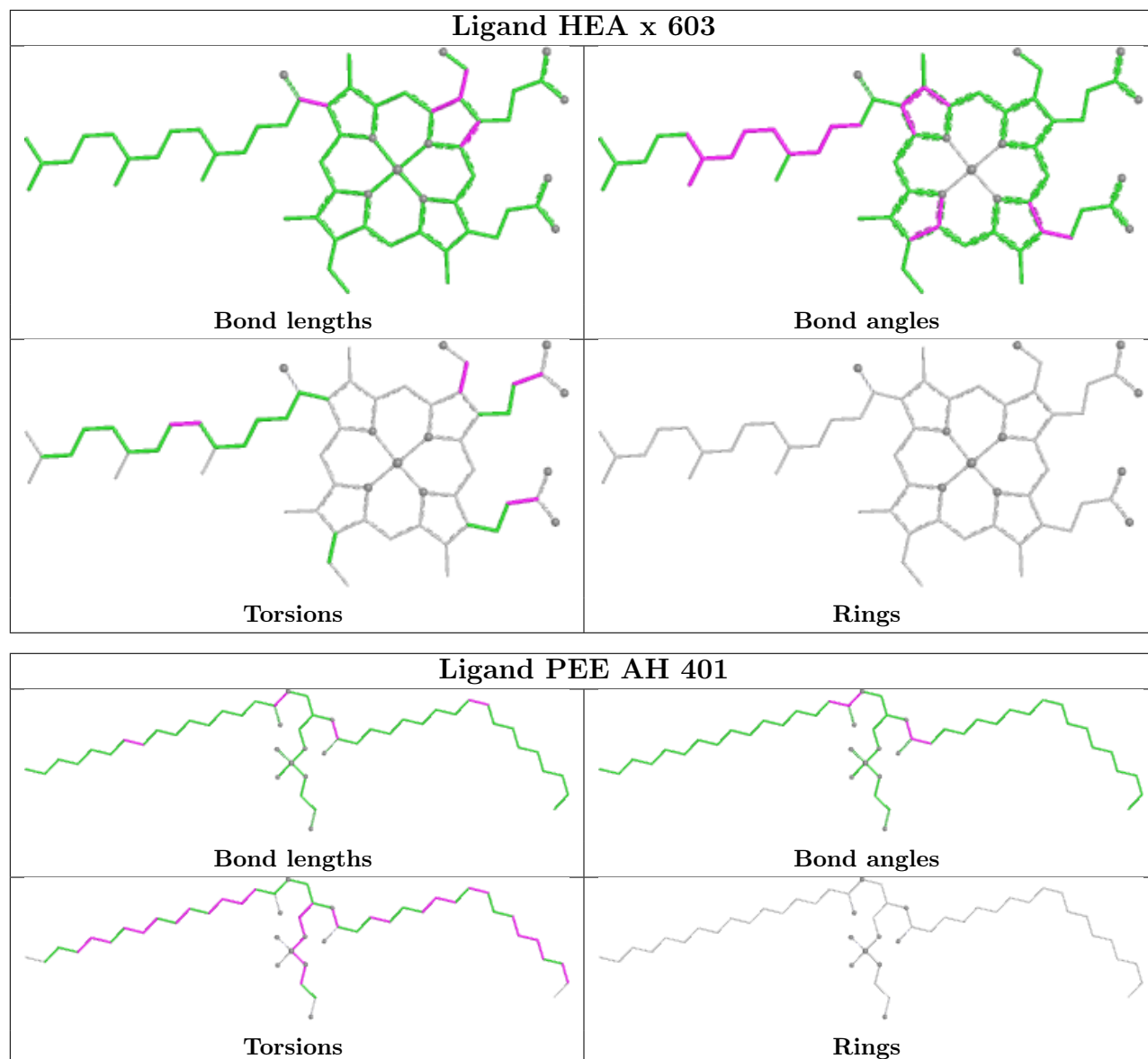


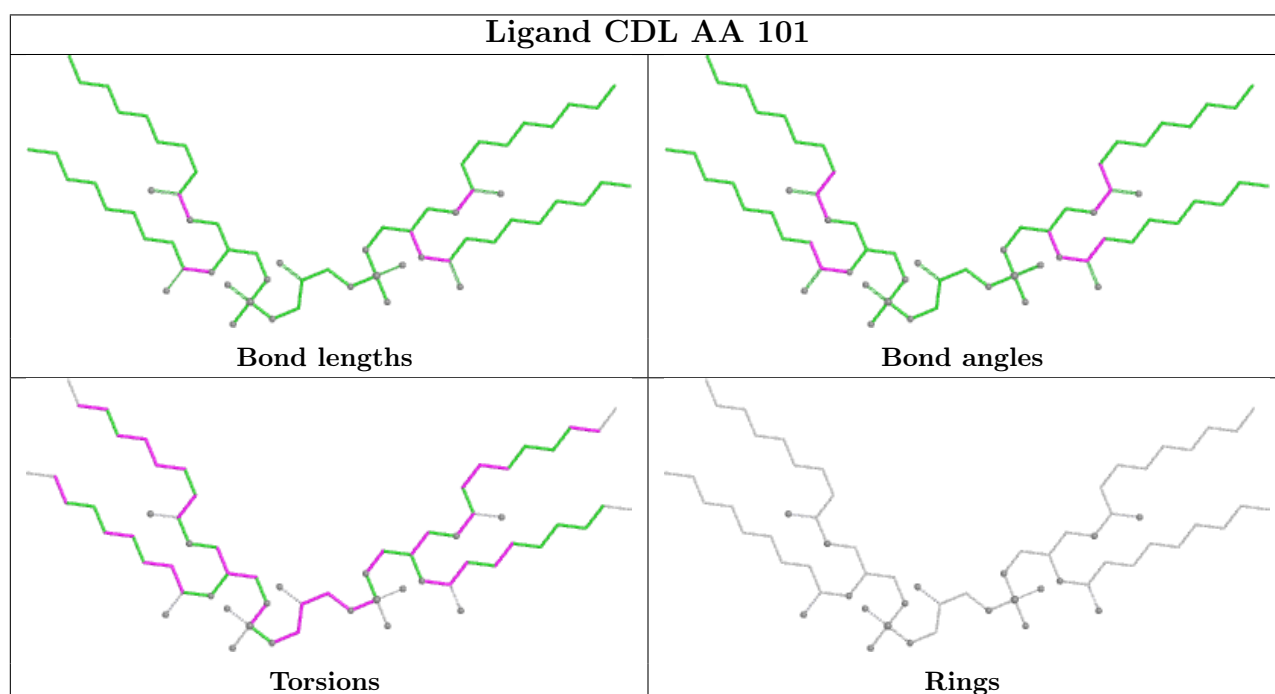
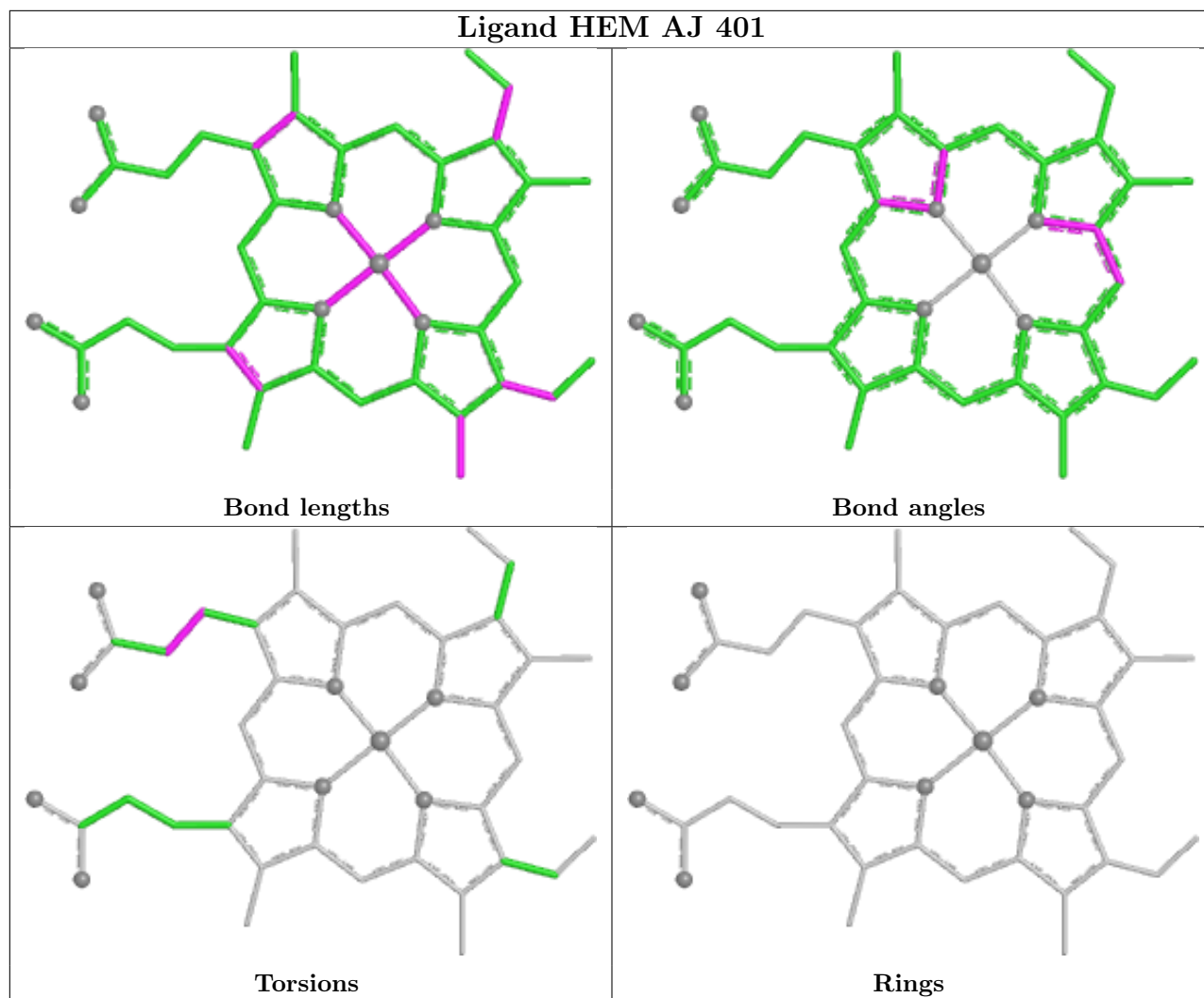


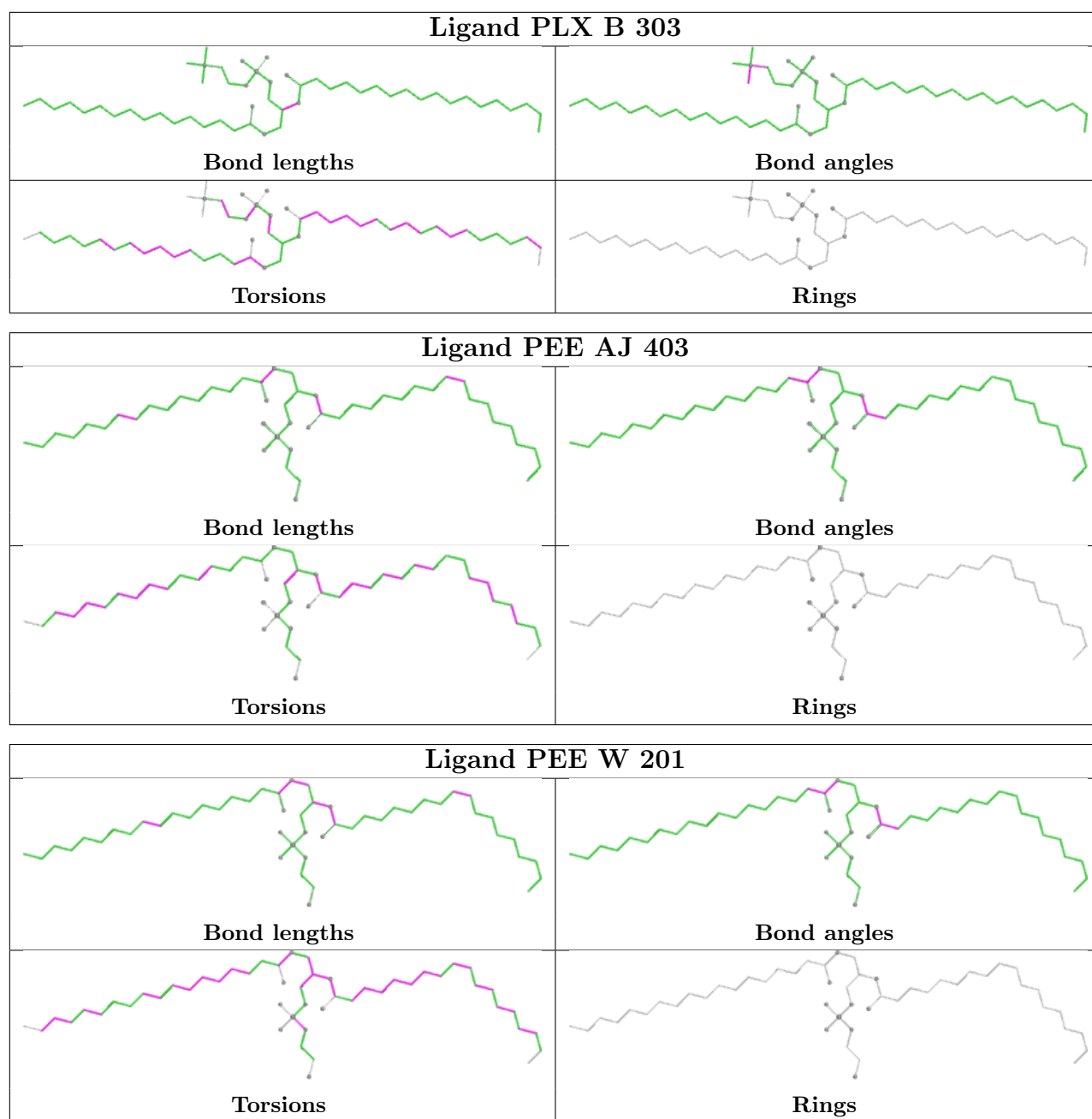


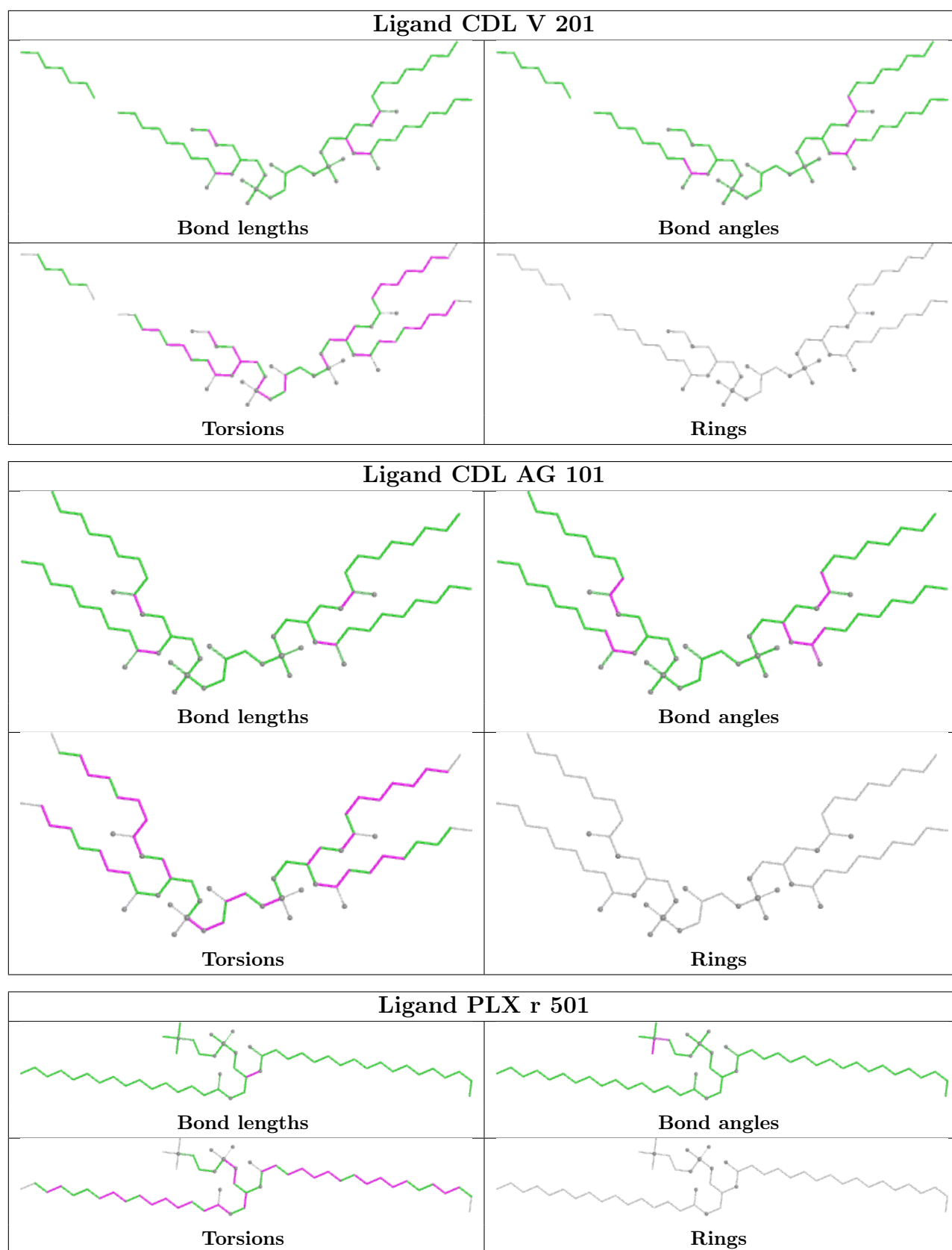


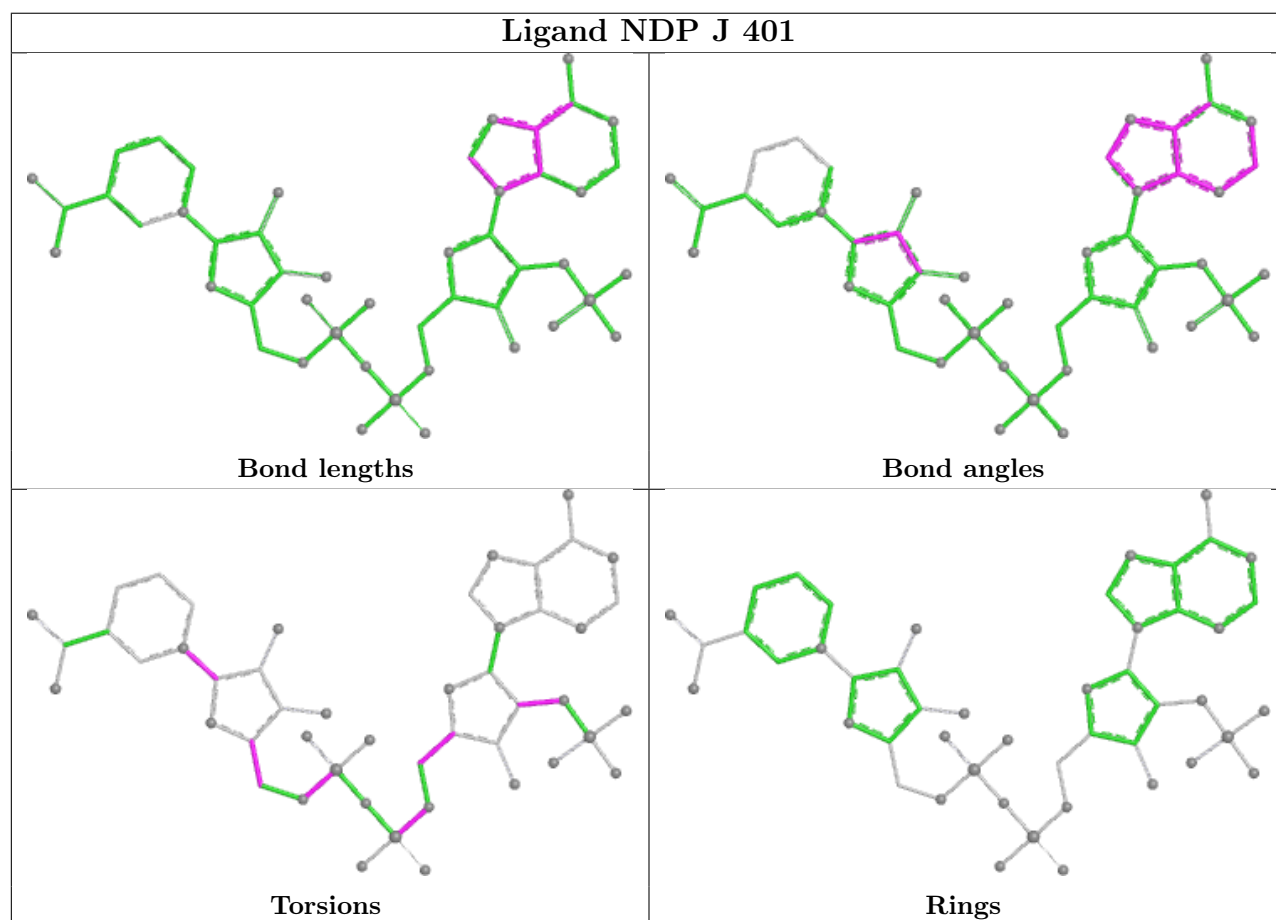
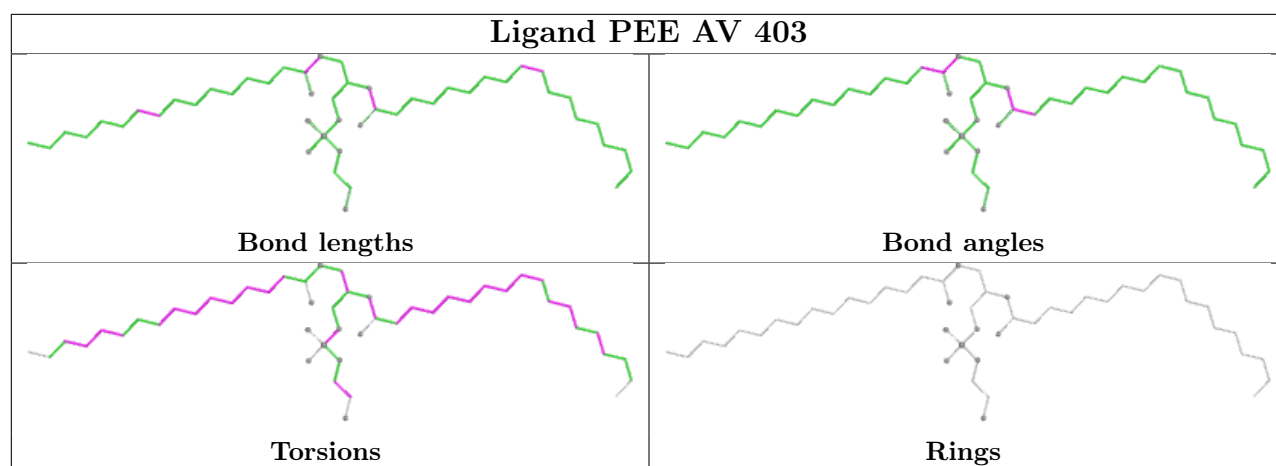


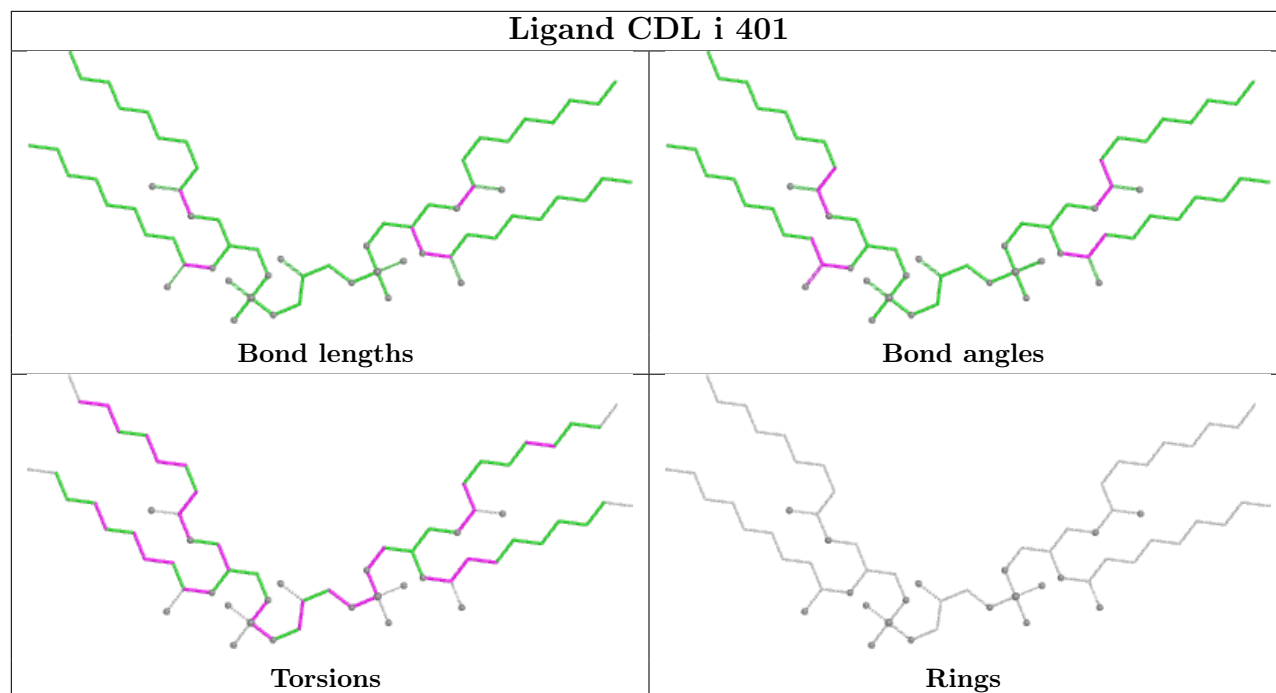












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

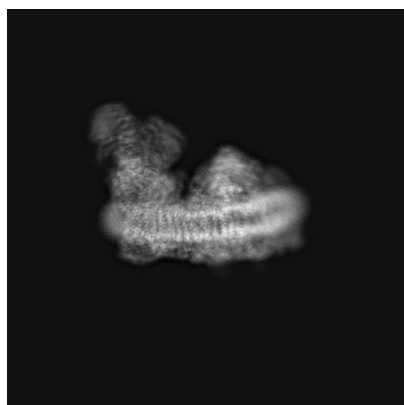
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6775. These allow visual inspection of the internal detail of the map and identification of artifacts.

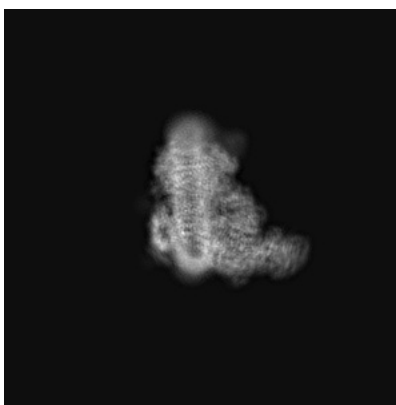
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

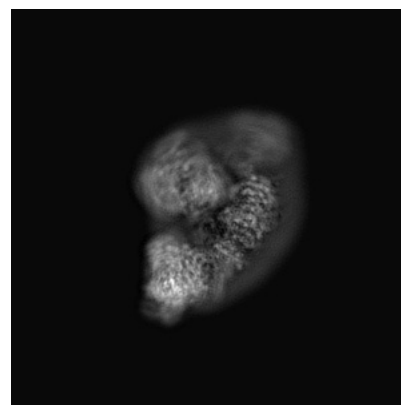
6.1.1 Primary map



X



Y

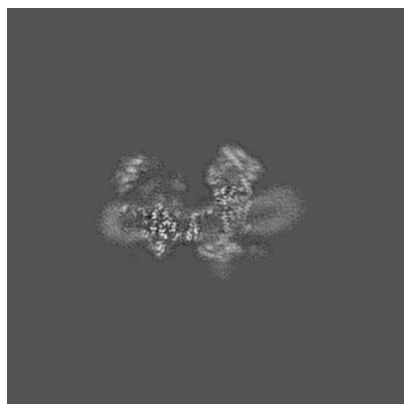


Z

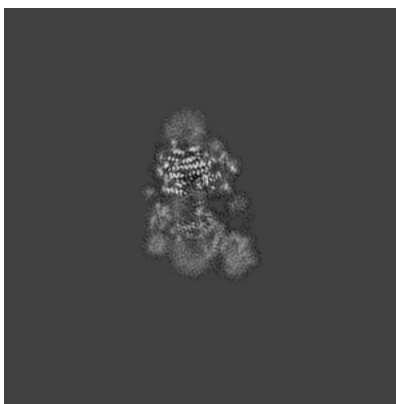
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

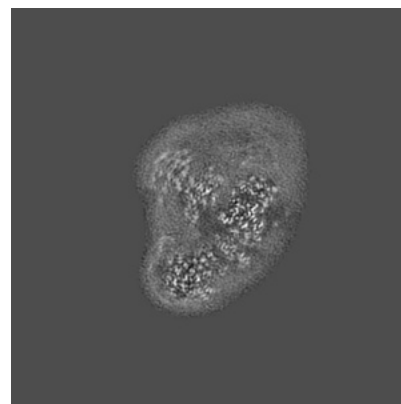
6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

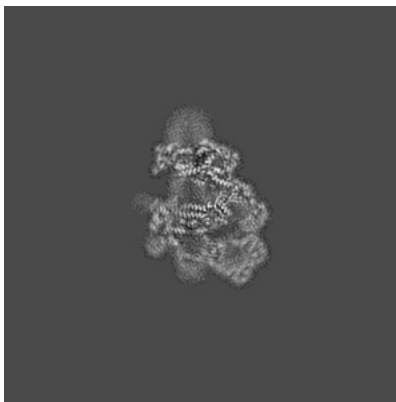
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

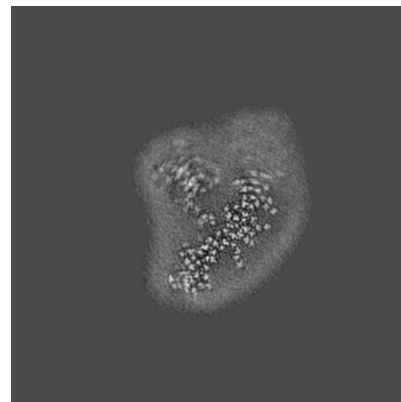
6.3.1 Primary map



X Index: 194



Y Index: 261

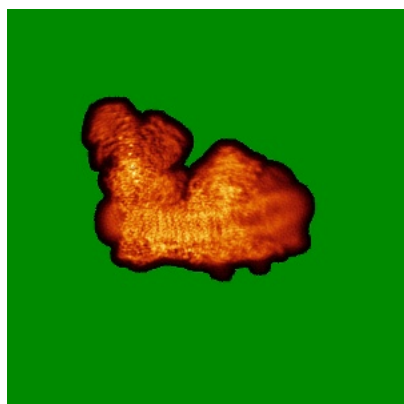


Z Index: 214

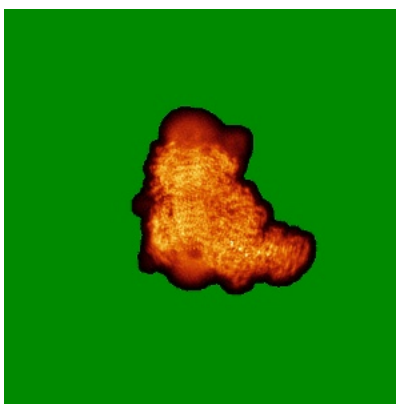
The images above show the largest variance slices of the map in three orthogonal directions.

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

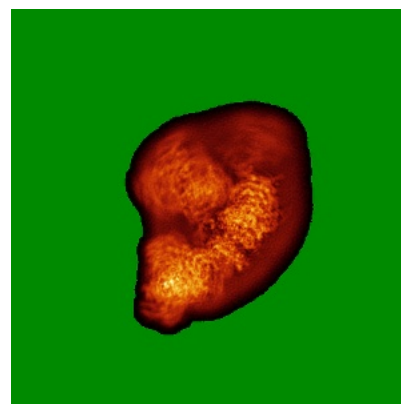
6.4.1 Primary map



X



Y

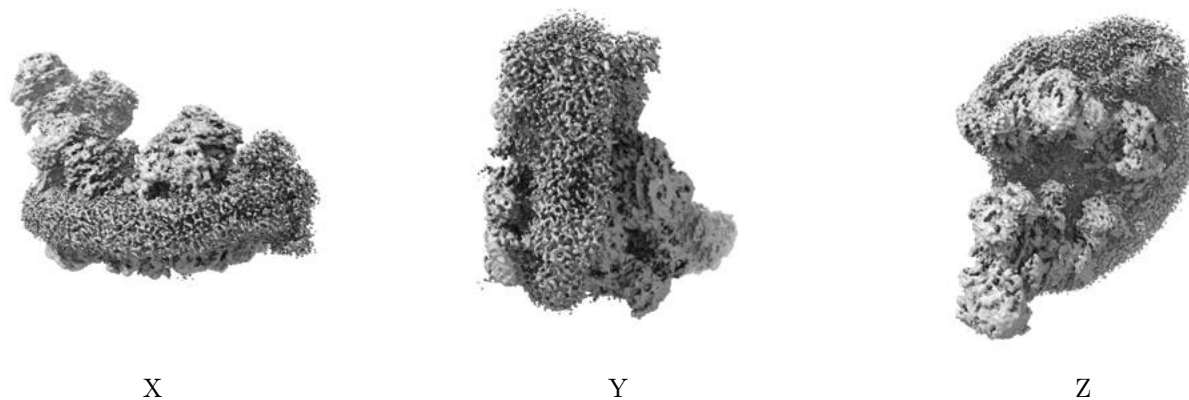


Z

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 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

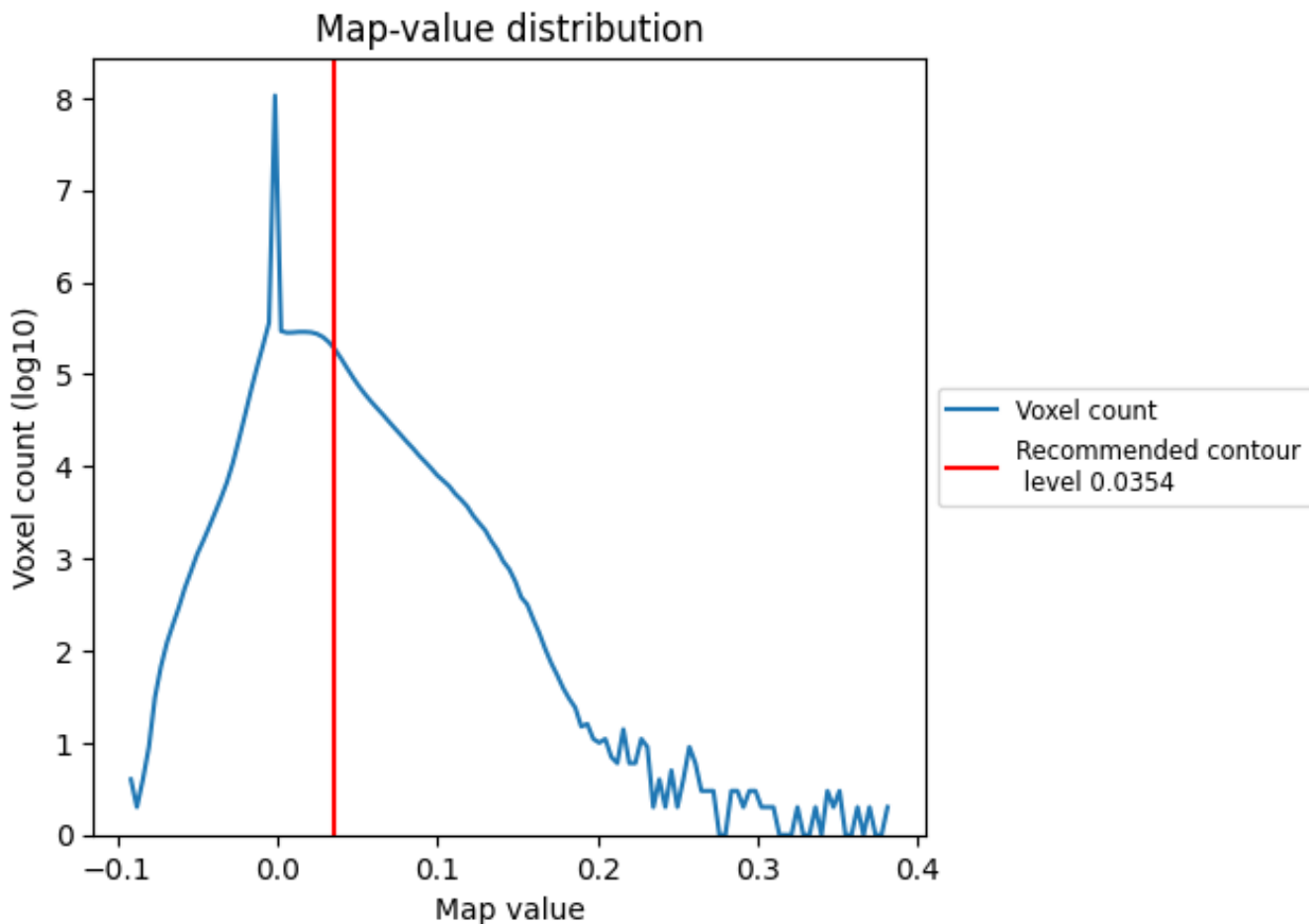
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

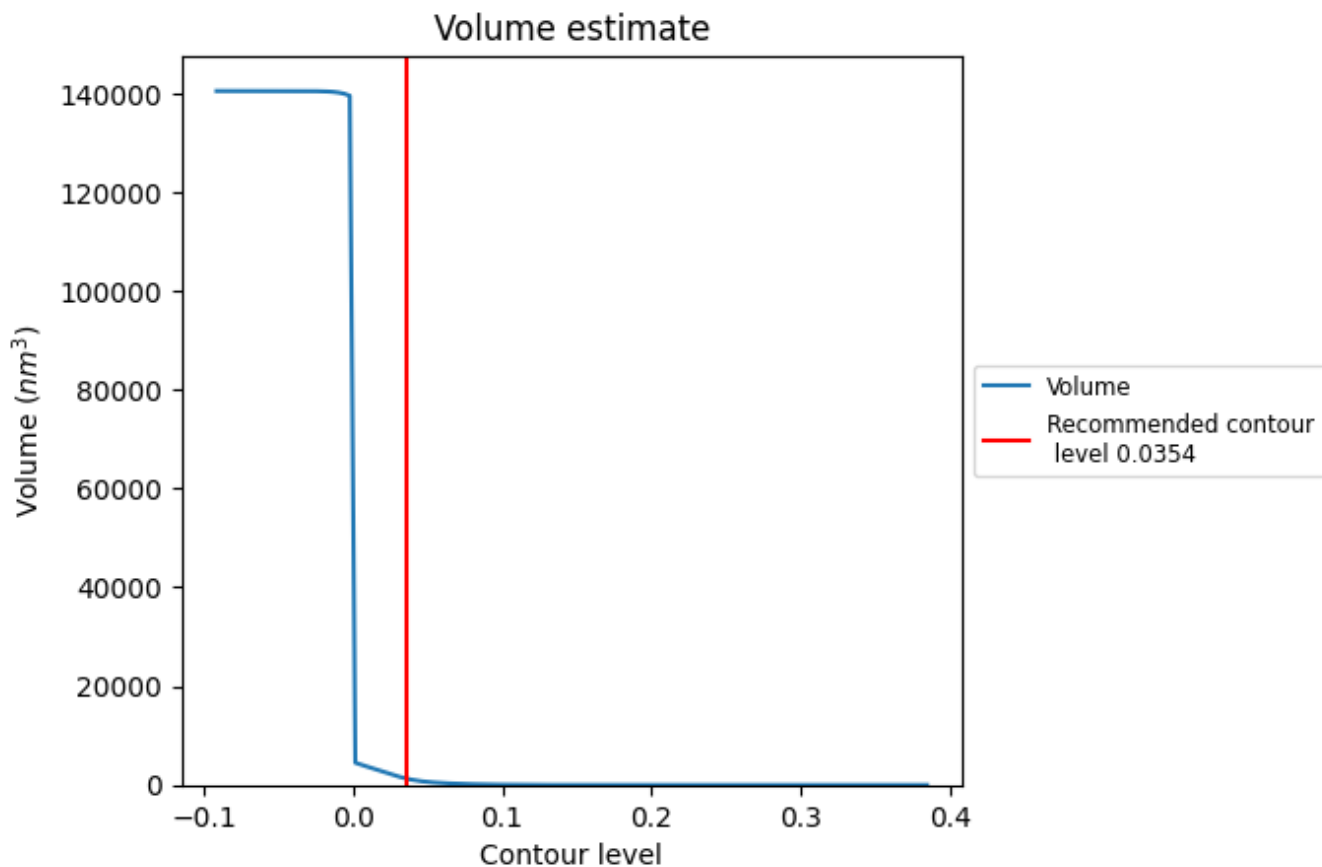
This section contains the results of statistical analysis of the map.

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.

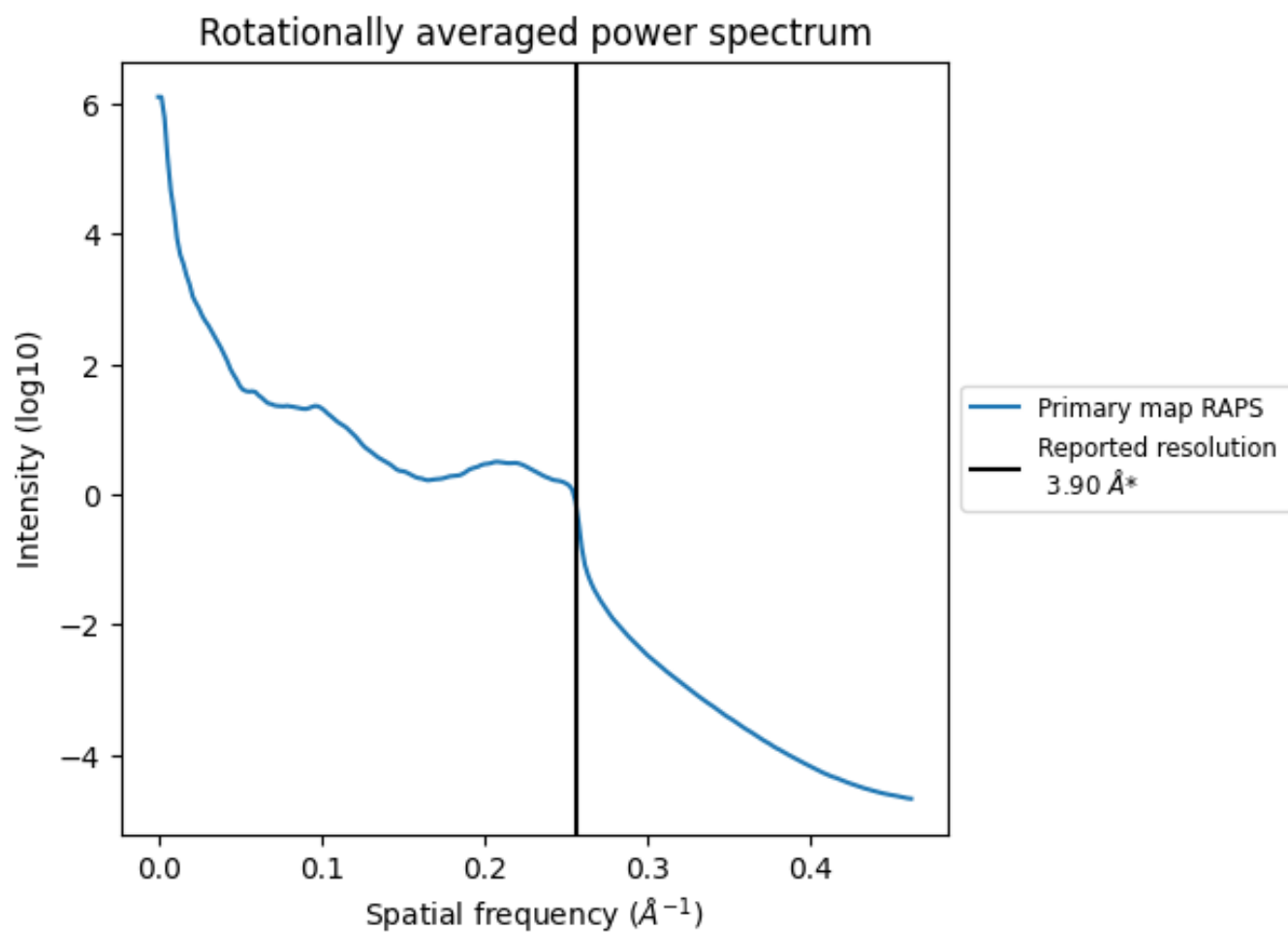
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1319 nm³; this corresponds to an approximate mass of 1191 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256\AA^{-1}

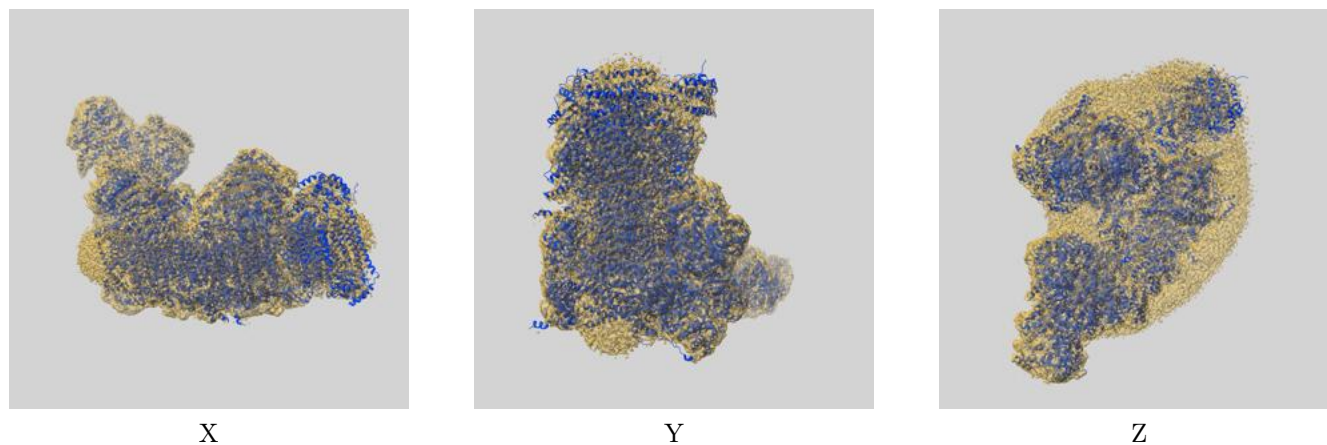
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

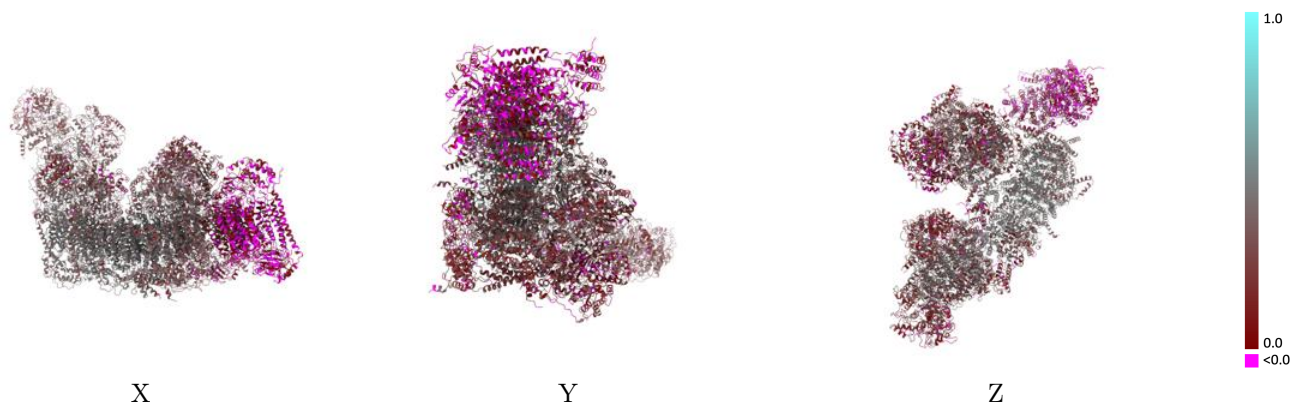
This section contains information regarding the fit between EMDB map EMD-6775 and PDB model 5XTH. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



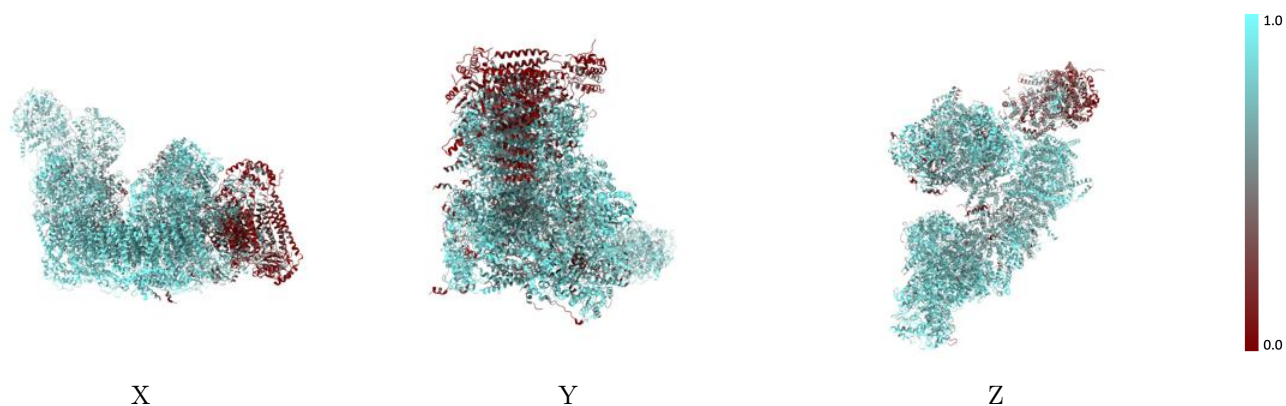
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



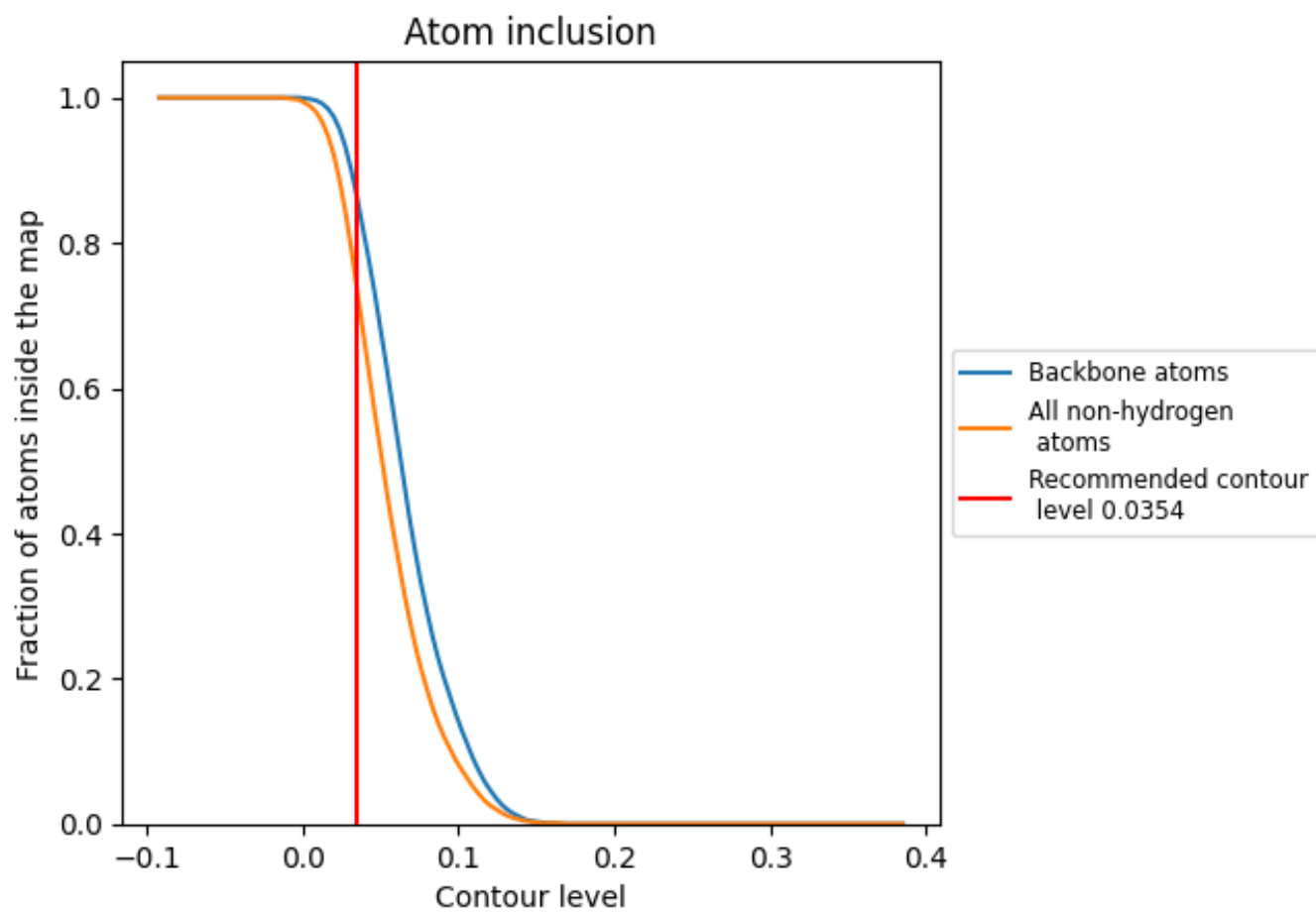
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0354).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.2930
0	 0.1290	 0.0250
1	 0.1760	 0.0530
2	 0.4300	 0.0700
3	 0.2680	 0.0410
4	 0.3500	 0.0370
5	 0.0950	 0.0310
6	 0.3420	 0.0880
7	 0.1040	 0.0240
8	 0.2820	 0.0120
9	 0.1360	 0.0240
A	 0.7830	 0.2470
AA	 0.7190	 0.3250
AB	 0.2280	 0.0740
AC	 0.6510	 0.2070
AD	 0.6410	 0.2820
AE	 0.7310	 0.2250
AF	 0.7020	 0.2830
AG	 0.6360	 0.2600
AH	 0.7730	 0.2990
AJ	 0.7420	 0.3490
AK	 0.8260	 0.2600
AL	 0.7960	 0.3320
AN	 0.6850	 0.1970
AO	 0.1150	 -0.0360
AP	 0.6980	 0.1840
AQ	 0.6500	 0.1980
AR	 0.7170	 0.1870
AS	 0.7790	 0.2640
AT	 0.6440	 0.1700
AU	 0.7820	 0.2360
AV	 0.7580	 0.3070
AW	 0.6950	 0.1790
AY	 0.7270	 0.1890
B	 0.8840	 0.4270











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Chain	Atom inclusion	Q-score
C	 0.9010	 0.4360
E	 0.6870	 0.2550
F	 0.7820	 0.1840
G	 0.4550	 0.1620
H	 0.7200	 0.2130
I	 0.7930	 0.3150
J	 0.8070	 0.2950
K	 0.7540	 0.2440
L	 0.7280	 0.3180
M	 0.7950	 0.2910
N	 0.8210	 0.3440
O	 0.8010	 0.2630
P	 0.7980	 0.3200
Q	 0.8200	 0.3830
S	 0.9090	 0.4250
T	 0.7840	 0.3430
U	 0.8790	 0.4120
V	 0.7820	 0.4030
W	 0.8900	 0.4140
X	 0.8660	 0.3870
Y	 0.8900	 0.3530
Z	 0.8520	 0.3550
a	 0.9170	 0.4530
b	 0.8370	 0.3440
c	 0.8960	 0.4430
d	 0.8900	 0.4060
e	 0.8320	 0.4170
f	 0.7970	 0.3270
g	 0.8480	 0.4350
h	 0.8830	 0.4310
i	 0.8500	 0.4610
j	 0.7550	 0.3810
k	 0.7920	 0.4260
l	 0.8170	 0.4190
m	 0.7980	 0.4080
n	 0.8530	 0.3850
o	 0.8560	 0.4240
p	 0.8950	 0.4010
r	 0.8720	 0.4660
s	 0.8480	 0.4340
u	 0.9120	 0.4080
v	 0.8310	 0.3020

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Chain	Atom inclusion	Q-score
w	 0.8350	 0.3410
x	 0.3690	 0.0410
y	 0.2580	 0.0090
z	 0.4570	 0.0910