



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 04:46 PM JST

PDB ID : 5GUP / pdb_00005gup
EMDB ID : EMD-9539
Title : Cryo-EM structure of mammalian respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on : 2016-08-30
Resolution : 4.00 Å(reported)

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

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

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:

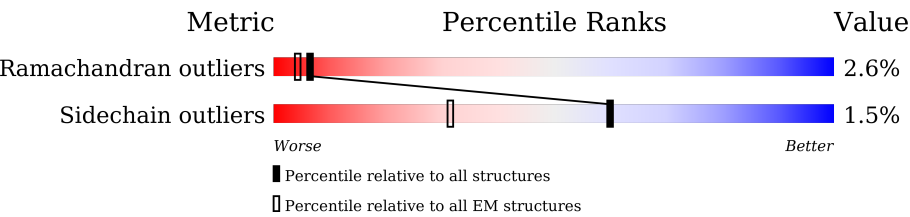
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	73	<div><div>100%</div><div><div></div><div></div><div></div><div></div></div><div>93%7%</div></div>
2	B	464	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>85%12%</div></div>
3	C	463	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%7%</div></div>
4	D	264	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%5%21%</div></div>
5	E	249	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>76%21%</div></div>
6	F	123	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>33%64%</div></div>
7	G	727	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>88%5%7%</div></div>
8	H	212	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>83%17%</div></div>
9	I	216	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>68%28%</div></div>

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Mol	Chain	Length	Quality of chain
10	J	175	
11	K	145	
11	R	145	
12	L	377	
13	M	113	
14	N	116	
15	O	156	
15	X	156	
16	P	99	
17	Q	128	
18	S	70	
19	T	84	
20	U	357	
21	V	141	
22	W	144	
23	Y	105	
24	Z	98	
25	a	189	
26	b	128	
27	c	186	
28	d	176	
29	e	154	
30	f	76	
31	g	122	
32	h	106	

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Mol	Chain	Length	Quality of chain
33	i	347	99% .
34	j	115	10% 97% ..
35	k	98	96% ..
36	l	606	97% .
37	m	175	9% 97% ..
38	n	58	81% 19%
39	o	129	94% 5% .
40	p	179	89% 6% . .
41	q	459	98% .
42	r	318	99% .
43	s	172	94% 5% .
44	t	137	7% 78% 6% 16%
45	5	480	45% 92% . 7%
45	u	480	11% 91% . 7%
46	6	453	56% 92% . 8%
46	v	453	22% 91% . 8%
47	7	379	39% 98% .
47	w	379	29% 98% .
48	8	326	26% 73% . 26%
48	x	326	25% 72% . 26%
49	9	111	34% 95% 5%
49	y	111	50% 95% 5%
50	Aa	82	40% 98% .
50	z	82	33% 95% . .
51	0	91	24% 70% 30%

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Mol	Chain	Length	Quality of chain
51	Ab	91	
52	1	64	
52	Ac	64	
53	2	274	
53	4	274	
54	3	56	
54	Ad	56	
55	Ae	78	
55	Af	78	
56	Ag	46	
57	Ah	59	
58	Ai	56	
59	Aj	47	
60	Ak	514	
61	Al	227	
62	Am	261	
63	An	147	
64	Ao	109	
65	Ap	98	
66	Aq	84	
67	Ar	85	

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 109982 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 Cytochrome c oxidase subunit 6C.

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

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3128	1975	558	575	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	430	Total	C	N	O	S	0	0
			3391	2167	583	617	24		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1679	1088	290	299	2		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	197	Total	C	N	O	S	0	0
			1463	935	246	273	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	44	Total	C	N	O	S	0	0
			242	145	49	47	1		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	673	Total	C	N	O	S	0	0
			5005	3133	875	959	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	176	Total	C	N	O	S	0	0
			1408	884	242	269	13		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	156	Total	C	N	O	S	0	0
			1241	792	227	208	14		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	109	Total	C	N	O	S	0	0
			877	557	154	163	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O		0	0
			520	314	104	102			
11	R	18	Total	C	N	O		0	0
			90	54	18	18			

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	337	Total	C	N	O	S	0	0
			2665	1726	462	468	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	94	Total	C	N	O	S	0	0
			685	433	129	121	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	112	Total	C	N	O	S	0	0
			895	577	152	163	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	85	Total	C	N	O	S	0	0
			647	417	97	128	5		
15	X	85	Total	C	N	O	S	0	0
			663	428	98	132	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			673	423	125	123	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			942	600	174	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	82	Total	C	N	O	S	0	0
			622	404	104	113	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	281	Total	C	N	O	S	0	0
			1941	1228	342	366	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	140	Total	C	N	O	S	0	0
			1009	644	172	187	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	138	Total	C	N	O	S	0	0
			1122	724	193	197	8		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	S	0	0
			400	262	70	67	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	78	Total	C	N	O	0	0
			550	363	92	95		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	138	Total	C	N	O	S	0	0
			1124	736	190	195	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	b	113	Total	C	N	O	0	0
			741	478	137	126		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	148	Total	C	N	O	S	0	0
			1073	696	185	185	7		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	169	Total	C	N	O	S	0	0
			1233	763	233	229	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	97	Total	C	N	O	S	0	0
			757	490	127	136	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	36	Total	C	N	O	0	0
			300	201	51	48		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	121	Total	C	N	O	S	0	0
			996	648	173	169	6		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	104	Total	C	N	O	S	0	0
			798	501	150	141	6		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	347	Total	C	N	O	S	0	0
			2706	1779	419	462	46		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	114	Total	C	N	O	S	0	0
			893	601	130	155	7		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	97	Total	C	N	O	S	0	0
			718	473	109	123	13		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	606	Total	C	N	O	S	0	0
			4790	3177	742	821	50		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	174	Total	C	N	O	S	0	0
			1280	855	187	226	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	47	Total	C	N	O	S	0	0
			359	233	66	59	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	128	Total	C	N	O	S	0	0
			1021	666	179	176			

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	171	Total	C	N	O	S	0	0
			1415	904	263	240	8		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	459	Total	C	N	O	S	0	0
			3627	2408	572	609	38		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	169	Total	C	N	O	S	0	0
			1350	858	247	235	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	115	Total	C	N	O	S	0	0
			749	463	151	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	446	Total	C	N	O	S	0	0
			3452	2157	603	673	19		
45	5	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		
46	6	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
47	7	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		
48	8	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 7.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
50	Aa	80	Total	C	N	O	S	0	0
			679	442	124	111	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
51	Ab	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	62	Total	C	N	O	S	0	0
			507	331	90	86			
52	Ac	62	Total	C	N	O	S	0	0
			507	331	90	86			

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		
53	4	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	51	Total	C	N	O	S	0	0
			414	277	74	63			
54	Ad	49	Total	C	N	O	S	0	0
			395	262	71	61	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ae	57	Total	C	N	O	S	0	0
			394	243	74	75	2		
55	Af	57	Total	C	N	O	S	0	0
			389	240	71	76	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 57 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ah	56	Total	C	N	O	S	0	0
			431	277	73	78	3		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

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

- Molecule 59 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 60 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 61 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 62 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 63 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 64 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 65 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

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

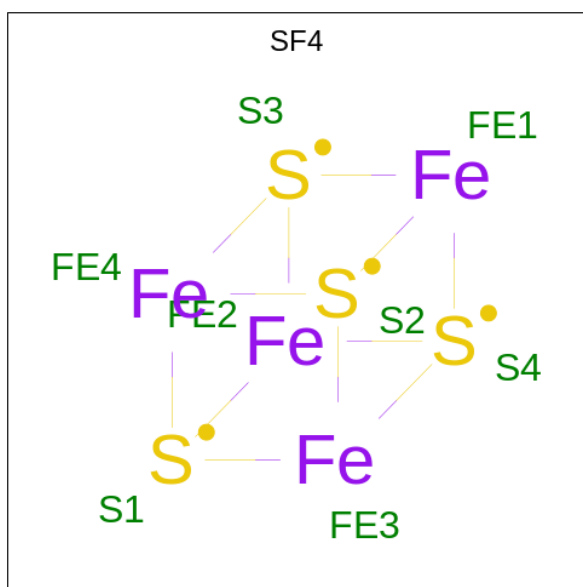
- Molecule 66 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

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

- Molecule 67 is a protein called Cytochrome c oxidase subunit 6B1.

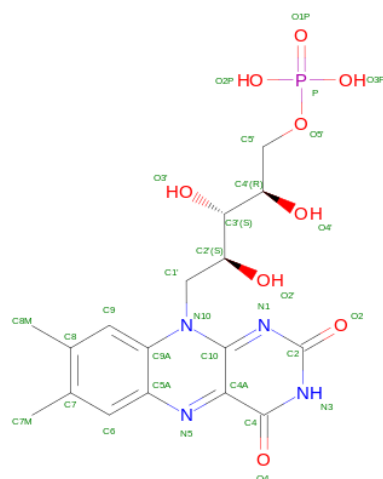
Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ar	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 68 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



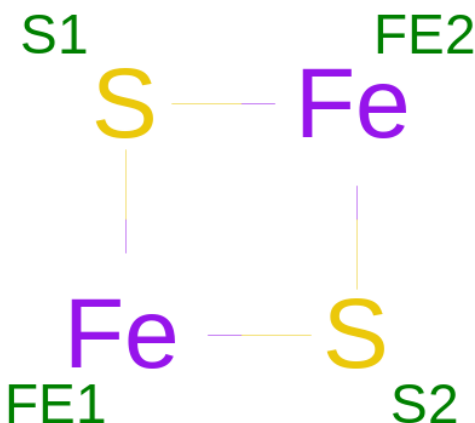
Mol	Chain	Residues	Atoms			AltConf
68	B	1	Total	Fe	S	0
			8	4	4	
68	G	1	Total	Fe	S	
			8	4	4	
68	G	1	Total	Fe	S	
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 69 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 70 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



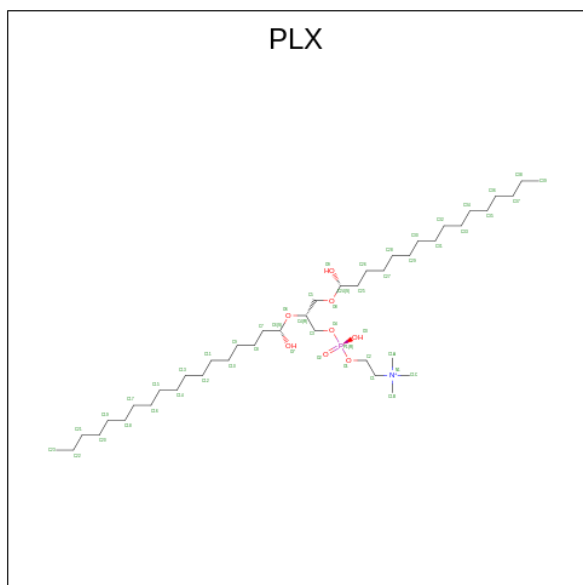
Mol	Chain	Residues	Atoms			AltConf
70	E	1	Total 4	Fe 2	S 2	0
70	G	1	Total 4	Fe 2	S 2	0
70	2	1	Total 4	Fe 2	S 2	0

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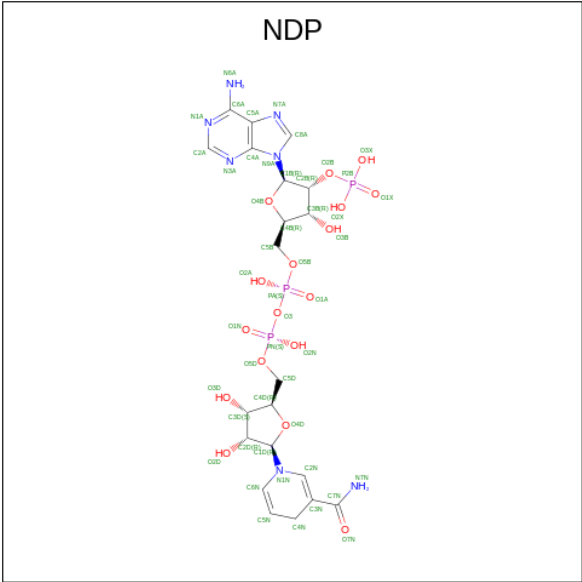
Mol	Chain	Residues	Atoms			AltConf
70	4	1	Total	Fe	S	0
			4	2	2	

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
71	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	2	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	4	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



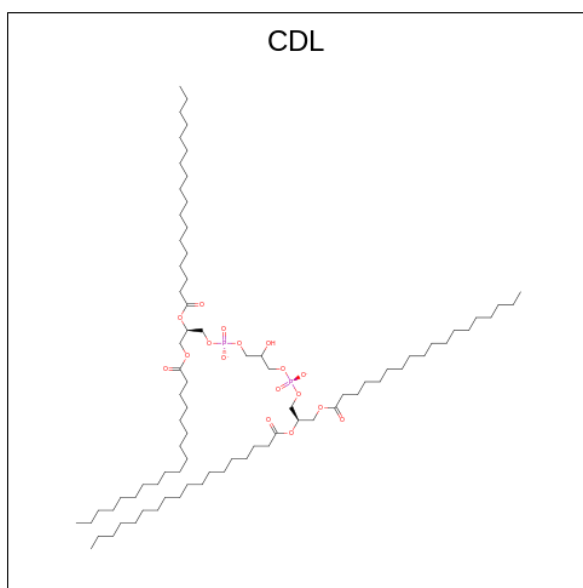
Mol	Chain	Residues	Atoms					AltConf
72	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 73 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



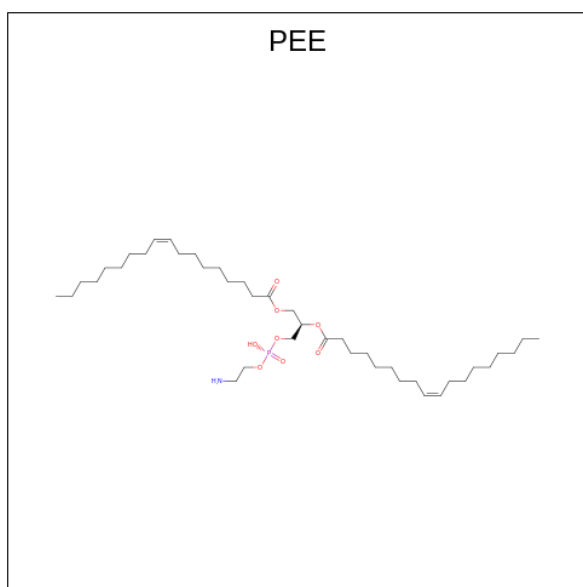
Mol	Chain	Residues	Atoms						AltConf
73	Q	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
73	X	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 74 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



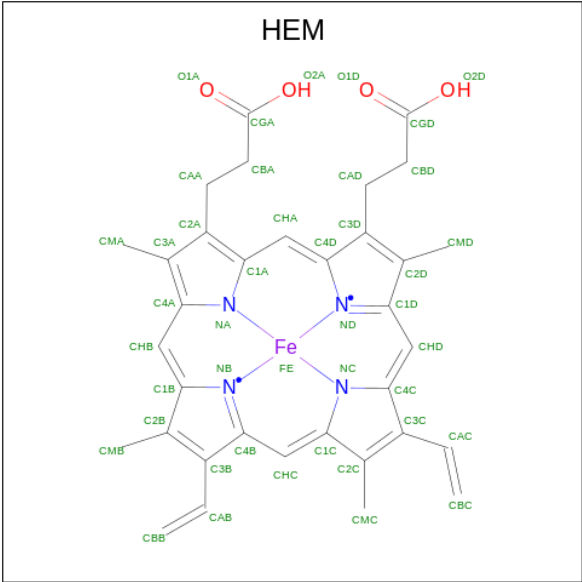
Mol	Chain	Residues	Atoms				AltConf
74	V	1	Total	C	O	P	0
			63	44	17	2	
74	i	1	Total	C	O	P	0
			64	45	17	2	
74	l	1	Total	C	O	P	0
			64	45	17	2	
74	s	1	Total	C	O	P	0
			64	45	17	2	
74	u	1	Total	C	O	P	0
			64	45	17	2	
74	x	1	Total	C	O	P	0
			64	45	17	2	
74	z	1	Total	C	O	P	0
			64	45	17	2	
74	5	1	Total	C	O	P	0
			64	45	17	2	
74	8	1	Total	C	O	P	0
			64	45	17	2	
74	Aa	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 75 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



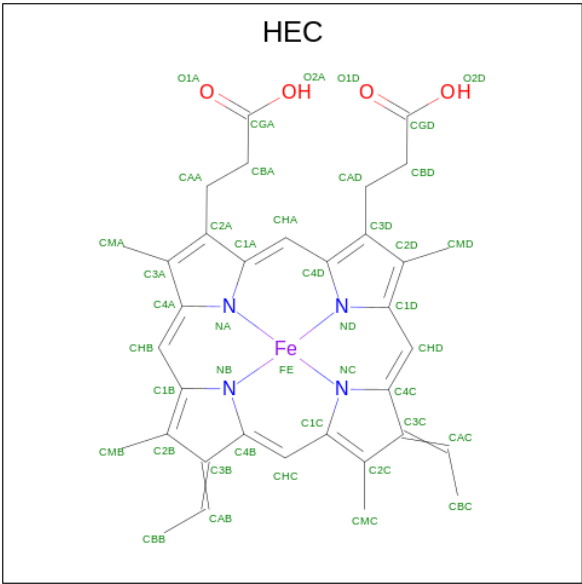
Mol	Chain	Residues	Atoms					AltConf
75	W	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	i	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	l	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	q	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	u	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	w	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	2	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	5	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	7	1	Total	C	N	O	P	0
			41	31	1	8	1	
75	7	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 76 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



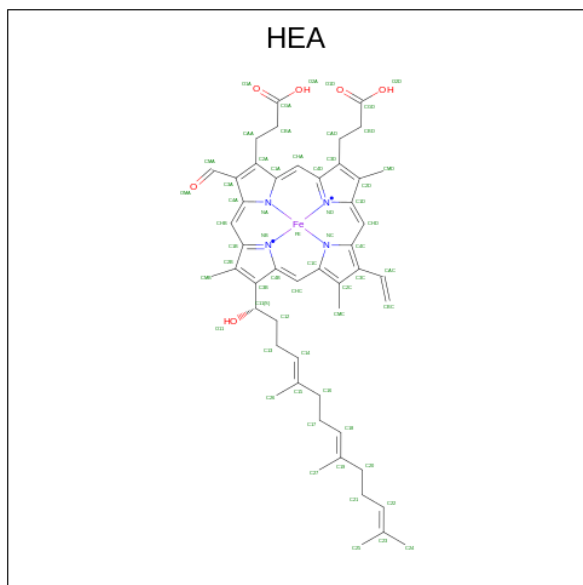
Mol	Chain	Residues	Atoms					AltConf
76	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
76	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
76	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
76	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 77 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
77	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
79	Ak	1	Total	Cu	0
			1	1	
79	Al	2	Total	Cu	0
			2	2	

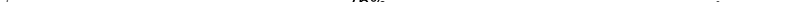
- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	Ak	1	Total	Mg	0
			1	1	

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Ap	1	Total	Zn	0
			1	1	

G192	F193	E194		F202	E215	P223	E229	W239	R246	Q247	E250	ASP	LEU	LYS	LYS	PRO	GLU	THR	LYS									
MET	ALA	ALA	ALA	ALA	ALA	ARG	CYS	TRP	ARG	GLY	LEU	VAL	GLY	PRO	ALA	ALA	ASP	T43	R44	R50	N105	T121	R122	Q123	N138	E149	E154	Y161

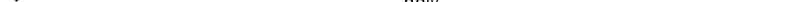
- Chain E:  76% 21%

The diagram illustrates the distribution of 150,000 SNPs across the human genome. The genome is represented as a horizontal bar divided into segments of different colors (grey, green, yellow, red). Above the bar, red diamond markers indicate the positions of SNPs. Below the bar, the names of the chromosomes are listed in a column.

Chromosome	SNP Count (approx.)
1	10,000
2	10,000
3	10,000
4	10,000
5	10,000
6	10,000
7	10,000
8	10,000
9	10,000
10	10,000
11	10,000
12	10,000
13	10,000
14	10,000
15	10,000
16	10,000
17	10,000
18	10,000
19	10,000
20	10,000
21	10,000
22	10,000
23	10,000
24	10,000
25	10,000
26	10,000
27	10,000
28	10,000
29	10,000
30	10,000
31	10,000
32	10,000
33	10,000
34	10,000
35	10,000
36	10,000
37	10,000
38	10,000
39	10,000
40	10,000
41	10,000
42	10,000
43	10,000
44	10,000
45	10,000
46	10,000
47	10,000
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83	10,000
84	10,000
85	10,000
86	10,000
87	10,000
88	10,000
89	10,000
90	10,000
91	10,000
92	10,000
93	10,000
94	10,000
95	10,000
96	10,000
97	10,000
98	10,000
99	10,000
100	10,000

- Chain F:  7% 33% 64%

[illegible]

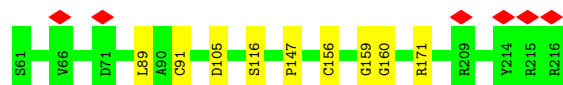
- Chain G:  10% 88% 5% 7%

Protein	Residue	Score	Annotation
Protein 1	L626	0.85	Conserved
	M632	0.78	Conserved
	D637	0.82	Conserved
	D640	0.88	Conserved
	S644	0.75	Conserved
	S650	0.80	Conserved
	V654	0.72	Conserved
	D658	0.85	Conserved
	V659	0.82	Conserved
	E660	0.88	Conserved
Protein 2	G661	0.75	Conserved
	A662	0.82	Conserved
	N663	0.88	Conserved
	Y664	0.72	Conserved
	F665	0.78	Conserved
	N676	0.85	Conserved
	Q677	0.75	Conserved
	A681	0.82	Conserved
	D682	0.88	Conserved
	P683	0.72	Conserved
Protein 3	L684	0.78	Conserved
	V685	0.85	Conserved
	L689	0.75	Conserved
	D693	0.82	Conserved
	E716	0.88	Conserved
	GLY	0.72	Conserved
	ILE	0.78	Conserved
	GLN	0.85	Conserved
	ALA	0.75	Conserved
	VAL	0.82	Conserved
Protein 4	GLU	0.78	Conserved
	PRO	0.85	Conserved
	SER	0.72	Conserved
	ILE	0.78	Conserved
	CYS	0.85	Conserved
	F462	0.82	Conserved
	A469	0.75	Conserved
	S478	0.88	Conserved
	Q482	0.72	Conserved
	R483	0.85	Conserved
Protein 5	S484	0.78	Conserved
	G505	0.85	Conserved
	VAL	0.72	Conserved
	THR	0.78	Conserved
	GLY	0.85	Conserved
	ASP	0.75	Conserved
	TRP	0.82	Conserved
	LYS	0.78	Conserved
	VAL	0.85	Conserved
	MET	0.72	Conserved
Protein 6	ASN	0.78	Conserved
	ILE	0.85	Conserved
	LEU	0.72	Conserved
	HIS	0.78	Conserved
	ARG	0.85	Conserved
	ILE	0.72	Conserved
	A520	0.88	Conserved
	L528	0.75	Conserved
	P532	0.82	Conserved
	I537	0.78	Conserved
Protein 7	P541	0.85	Conserved
	L545	0.72	Conserved
	F546	0.78	Conserved
	D551	0.85	Conserved
	G552	0.72	Conserved
	G553	0.82	Conserved
	C554	0.78	Conserved
	I555	0.85	Conserved
	VAL	0.72	Conserved
	T556	0.88	Conserved
Protein 8	K562	0.75	Conserved
	I567	0.82	Conserved
	V575	0.78	Conserved
	A576	0.85	Conserved
	G577	0.72	Conserved
	V582	0.88	Conserved
	G601	0.75	Conserved
	D619	0.82	Conserved
	G458	0.78	Conserved
	K621	0.85	Conserved
Protein 9	E283	0.82	Conserved
	S287	0.75	Conserved
	D288	0.88	Conserved
	T307	0.72	Conserved
	E310	0.85	Conserved
	K311	0.78	Conserved
	L314	0.85	Conserved
	E320	0.72	Conserved
	D321	0.88	Conserved
	S324	0.75	Conserved
Protein 10	A327	0.82	Conserved
	G328	0.75	Conserved
	H329	0.88	Conserved
	L330	0.72	Conserved
	THR	0.85	Conserved
	ALA	0.78	Conserved
	THR	0.85	Conserved
	ALA	0.72	Conserved
	ALA	0.88	Conserved
	SER	0.75	Conserved
Protein 11	N30	0.82	Conserved
	D37	0.75	Conserved
	M42	0.88	Conserved
	T47	0.72	Conserved
	L69	0.85	Conserved
	K84	0.78	Conserved
	N164	0.85	Conserved
	T174	0.72	Conserved
	R181	0.88	Conserved
	D194	0.75	Conserved
Protein 12	I210	0.82	Conserved
	M254	0.75	Conserved
	D255	0.88	Conserved
	G258	0.72	Conserved
	T267	0.85	Conserved
	I281	0.78	Conserved
	N282	0.85	Conserved
	S457	0.72	Conserved
	G458	0.88	Conserved
	H459	0.75	Conserved

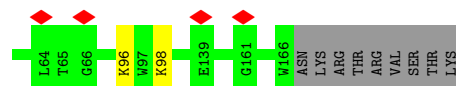
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MET	ARG	CYS	LEU	SER	THR	PRO	MET	LEU	LEU	ARG	ALA	ALA	GLN	GLN	ALA	ALA	ALA	HTS	ALA	GLY	HTS	PRO	SER	ALA	ALA	ARG	THR	LEU	HTS	SER	SER	VAL	ALA	ALA	ALA	ALA	T37	M43	R44	E46	M48	F175	R212
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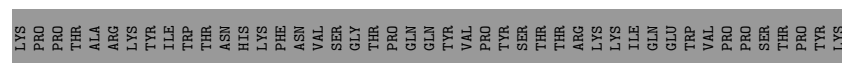
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | ALA | LEU | ALA | ALA | SER | GLY | LEU | LEU | ARG | ARG | SER | SER | MET | GLY | ALA | ALA | ALA | VAL | GLN | VAL | ARG | ARG | PHE | VAL | HIS | PRO | SER | ALA | ALA | THR | ASP | SER | SER | PRO | SER | SER | SER | SER | GLN | PRO | ALA | ALA | VAL | VAL | VAL | GLY | ALA | VAL | VAL | VAL | VAL | VAL | LYS | PRO | THR | THR | LEU | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



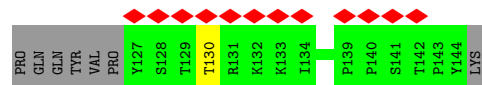
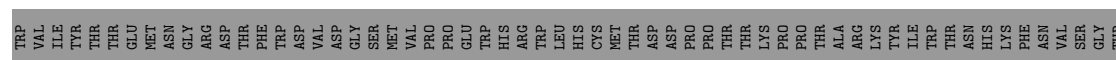
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | VAL | SER | MET | SER | VAL | ALA | LEU | LYS | GLN | ALA | LEU | TRP | GLY | ARG | ARG | ALA | ALA | ALA | VAL | GLY | ALA | VAL | SER | SER | LYS | VAL | PRO | THR | THR | ARG | LEU | LEU | SER | SER | THR | SER | THR | TRP | LYS | LEU | LEU | GLN | ASP | GLN | GLN | THR | THR | GLN | GLN | ASP | THR | GLN | ILE | LEU | VAL | VAL | ASP | GLU | K58 | L59 | ... |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



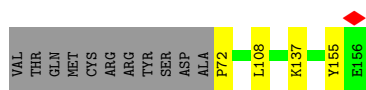
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|----------|-------|
| M1 | 10 |
| L7 | 10 |
| R8 | 10 |
| Q12 | 10 |
| Q13 | 10 |
| V14 | 10 |
| S15 | 10 |
| S16 | 10 |
| H17 | 10 |
| L24 | 10 |
| R25 | 10 |
| V26 | 10 |
| L27 | 10 |
| F28 | 10 |
| N31 | 10 |
| D32 | 10 |
| G36 | 10 |
| T37 | 10 |
| L38 | 10 |
| V39 | 10 |
| G40 | 10 |
| E41 | 10 |
| Y49 | 10 |
| F55 | 10 |
| W61 | 10 |
| V62 | 10 |
| I63 | 10 |
| Y64 | 10 |
| T65 | 10 |
| T66 | 10 |
| E67 | 10 |
| M68 | 10 |
| N69 | 10 |
| G70 | 10 |
| R71 | 10 |
| D72 | 10 |
| T73 | 10 |
| F74 | 10 |
| W75 | 10 |
| D76 | 10 |
| V77 | 10 |
| M81 | 10 |
| C92 | 10 |
| M93 | 10 |
| T94 | 10 |
| P97 | 10 |
| THR | 10 |
| THR | 10 |



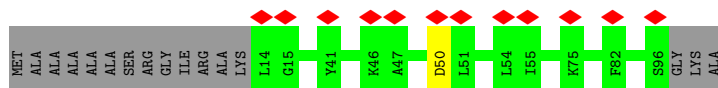
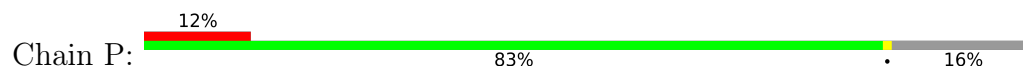
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| MET | GLU | LEU | VAL | GLN | VAL | LEU | ARG | ARG | GLY | LEU | GLN | GLN | VAL | SER | GLY | HIS | GLY | LEU | ARG | VAL | VAL | LEU | PHE | ARG | ALA | ASN | ASP | VAL | VAL | ARG | VAL | GLY | GLU | ASP | LYS | TYR | GLY | ASN | LYS | TYR | GLU | ASP | PHE | GLN | GLN | PHE | GLY | ARG | HIS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



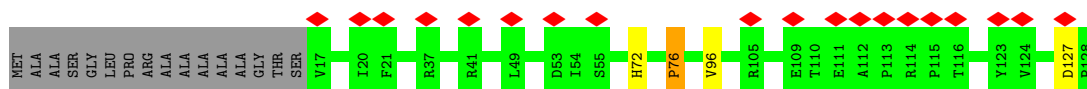
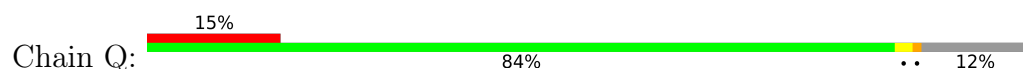
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | ALA | ARG | VAL | LEU | CYS | ALA | CYS | VAL | ARG | ARG | LEU | PRO | ALA | ALA | PHE | ALA | PRO | LEU | PRO | ARG | ARG | ILE | PRO | THR | THR | VAL | VAL | ALA | ALA | ALA | ARG | PRO | PRO | LEU | LEU | SER | SER | THR | THR | LEU | PHE | PRO | PRO | THR | GLY | GLN | ALA | ALA | ARG | ARG | SER | SER | ARG | ALA | ALA | LEU | PRO | ALA | ALA | VAL | LEU | LEU | GLN | GLN | GLN | GLN | PRO | PRO | ALA | ALA | PRO | PRO | GLY | CYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



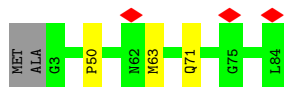
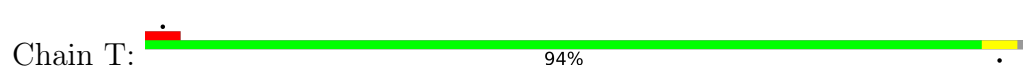
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



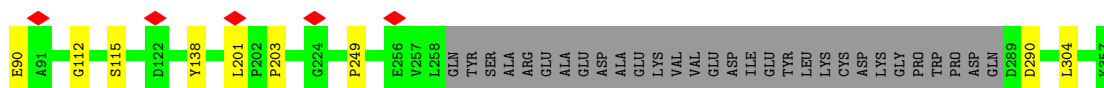
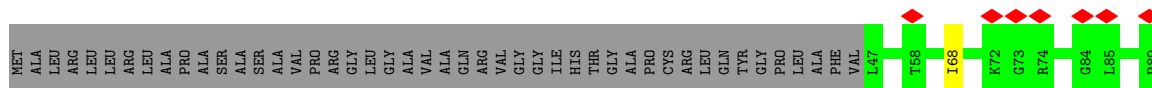
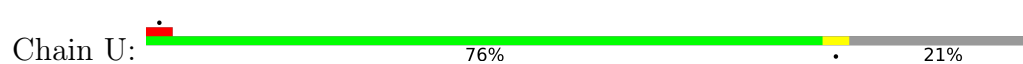
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

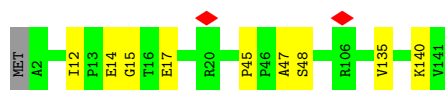


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

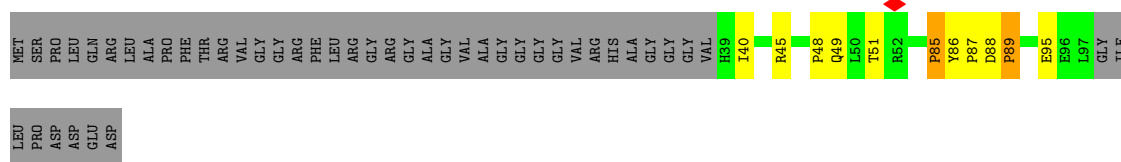




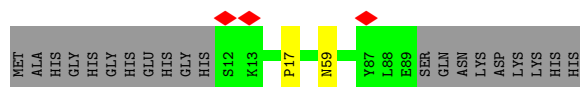
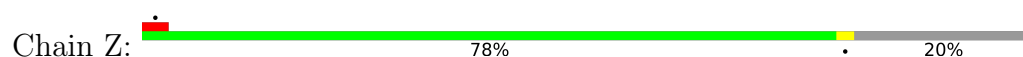
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



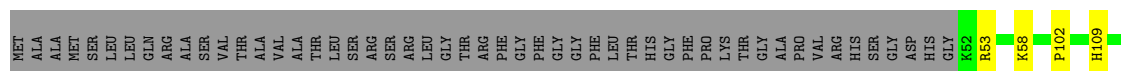
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



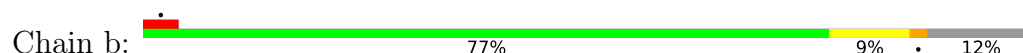
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



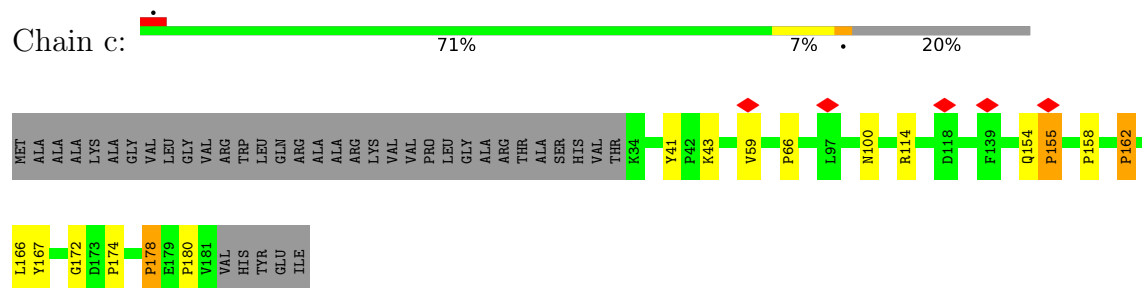
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



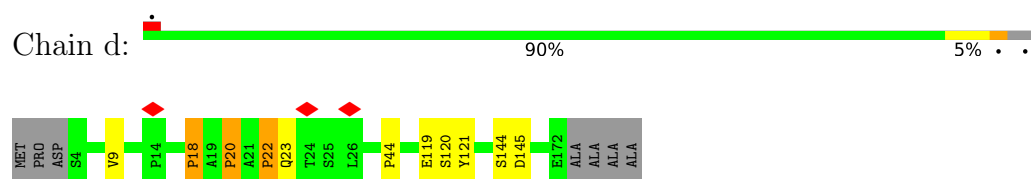
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



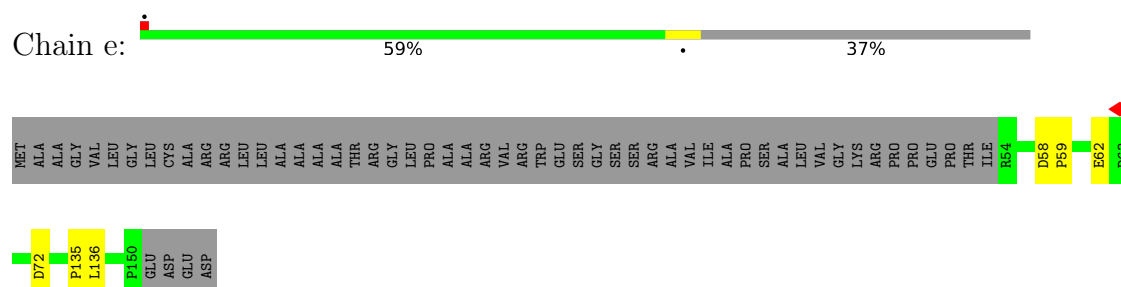
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



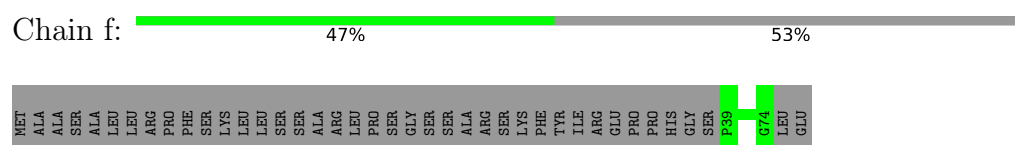
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



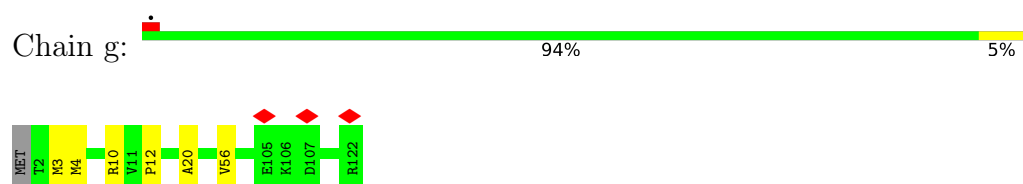
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

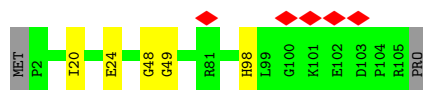


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5





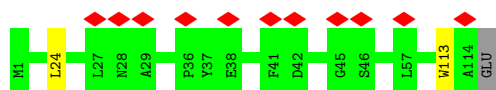
- Molecule 33: NADH-ubiquinone oxidoreductase chain 2

Chain i: 99%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 3

Chain j: 10% 97%



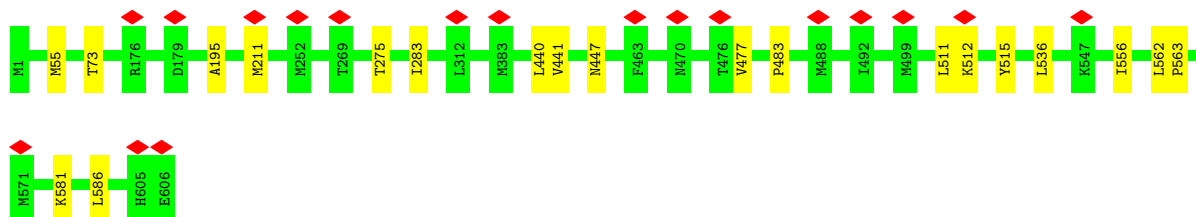
- Molecule 35: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 96%



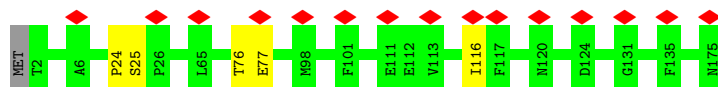
- Molecule 36: NADH-ubiquinone oxidoreductase chain 5

Chain l: 97%



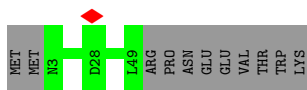
- Molecule 37: NADH-ubiquinone oxidoreductase chain 6

Chain m: 9% 97%



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

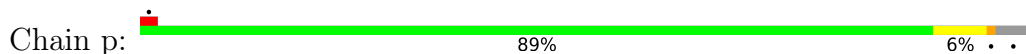
Chain n: 81% 19%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



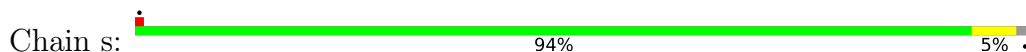
- Molecule 41: NADH-ubiquinone oxidoreductase chain 4



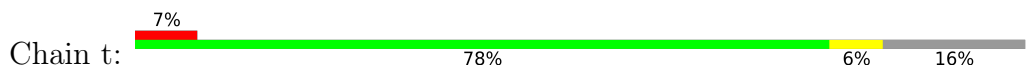
- Molecule 42: NADH-ubiquinone oxidoreductase chain 1



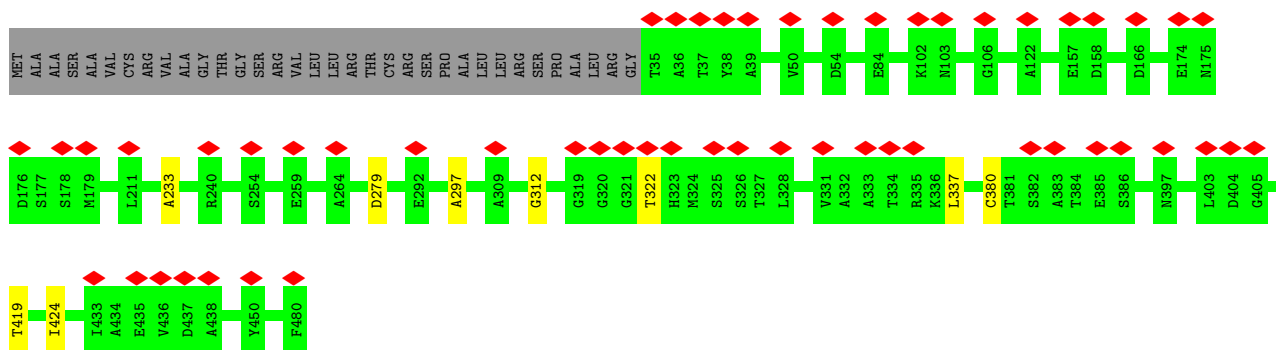
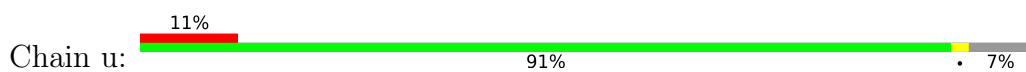
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



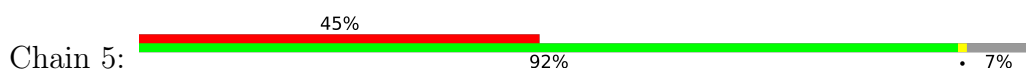
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



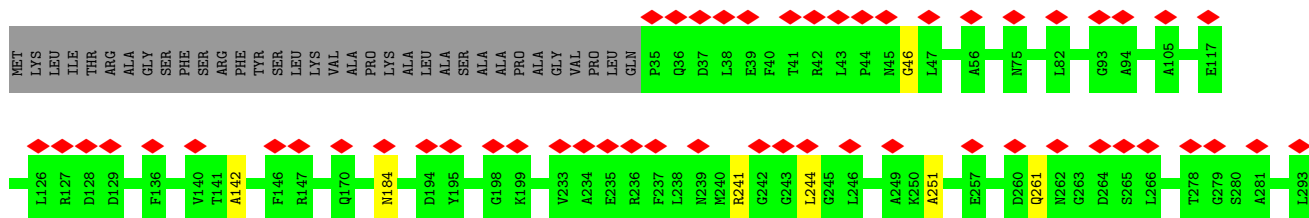
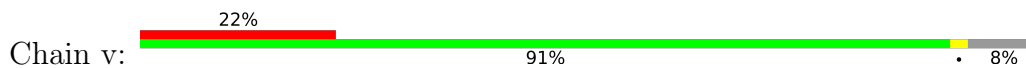
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

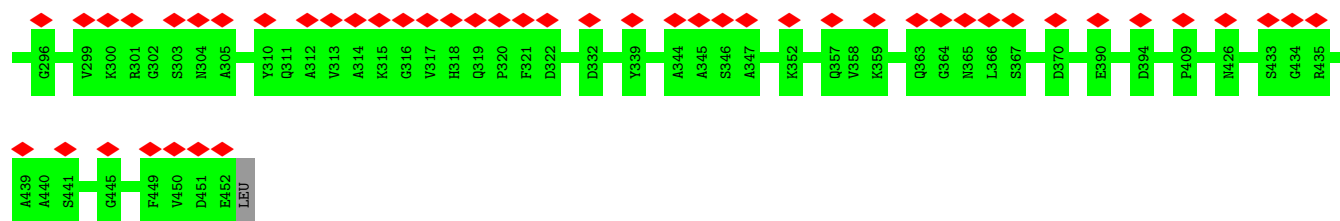


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

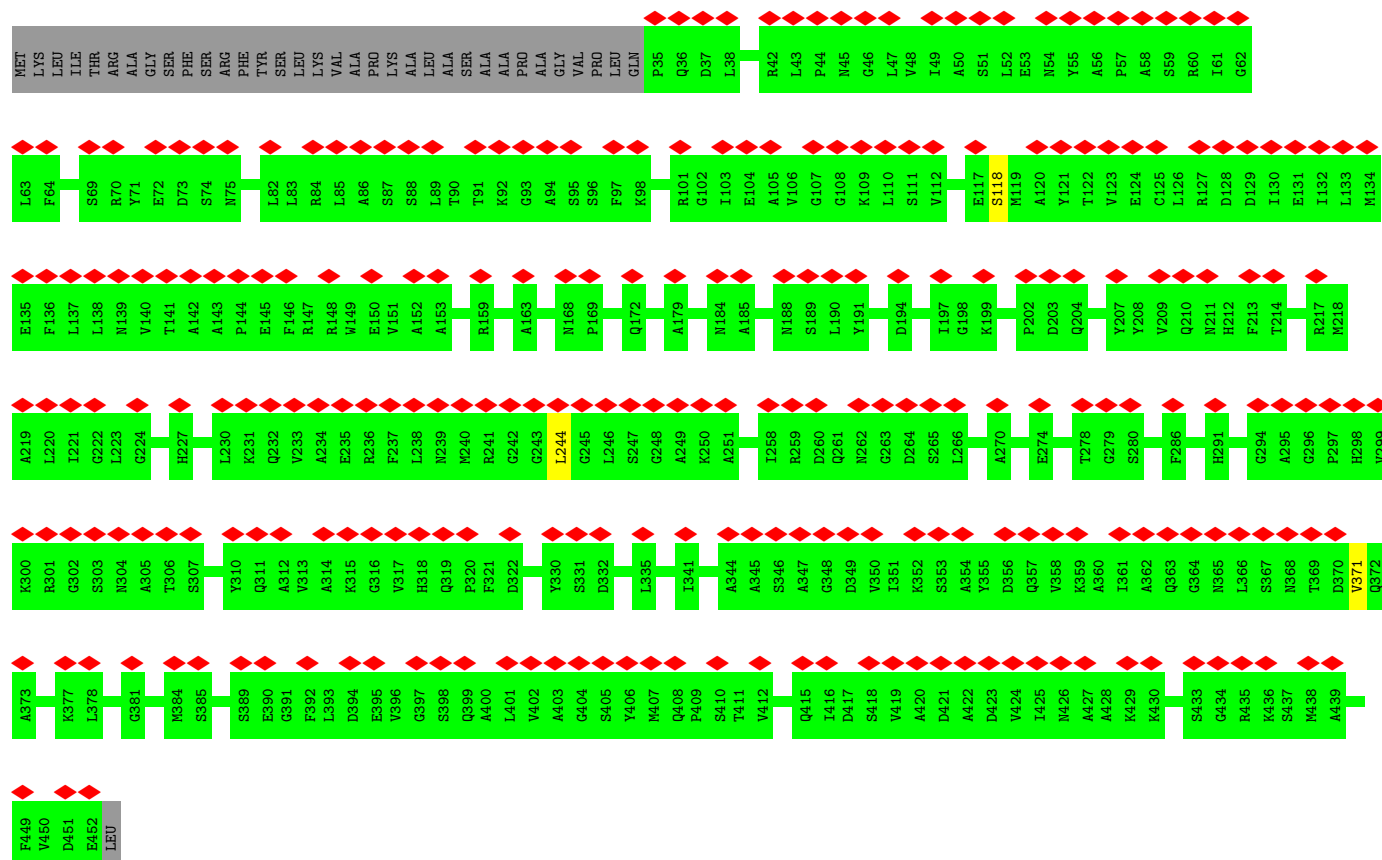


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

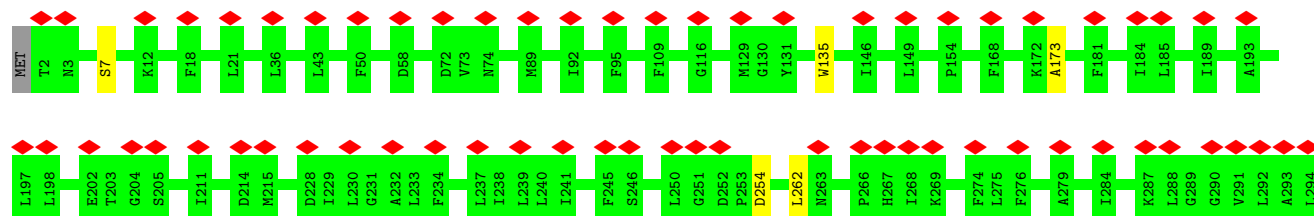


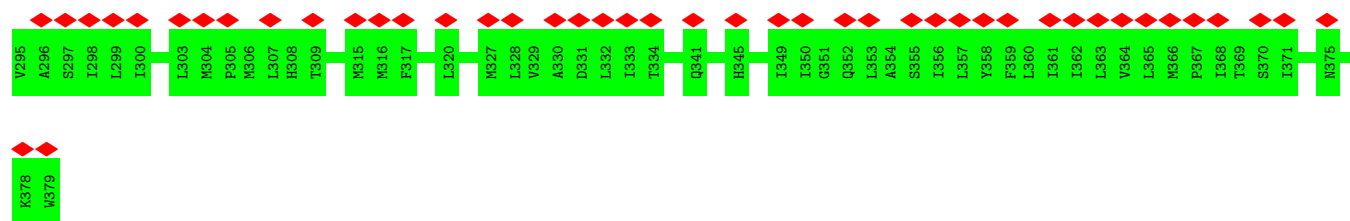


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

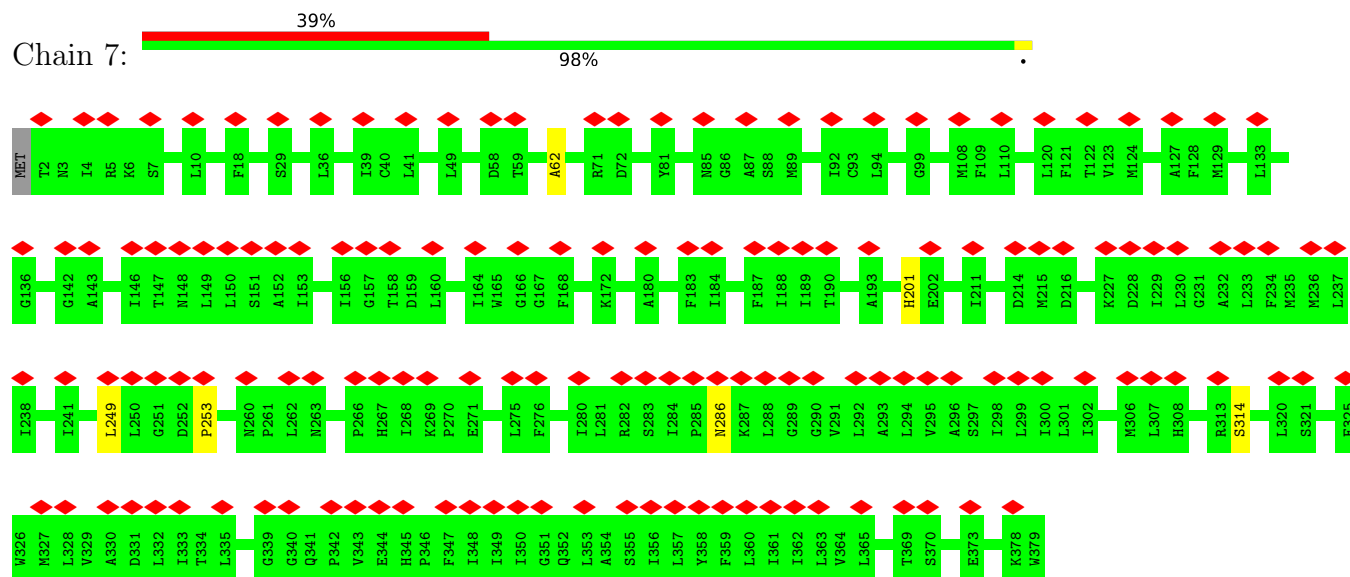


• Molecule 47: Cytochrome b

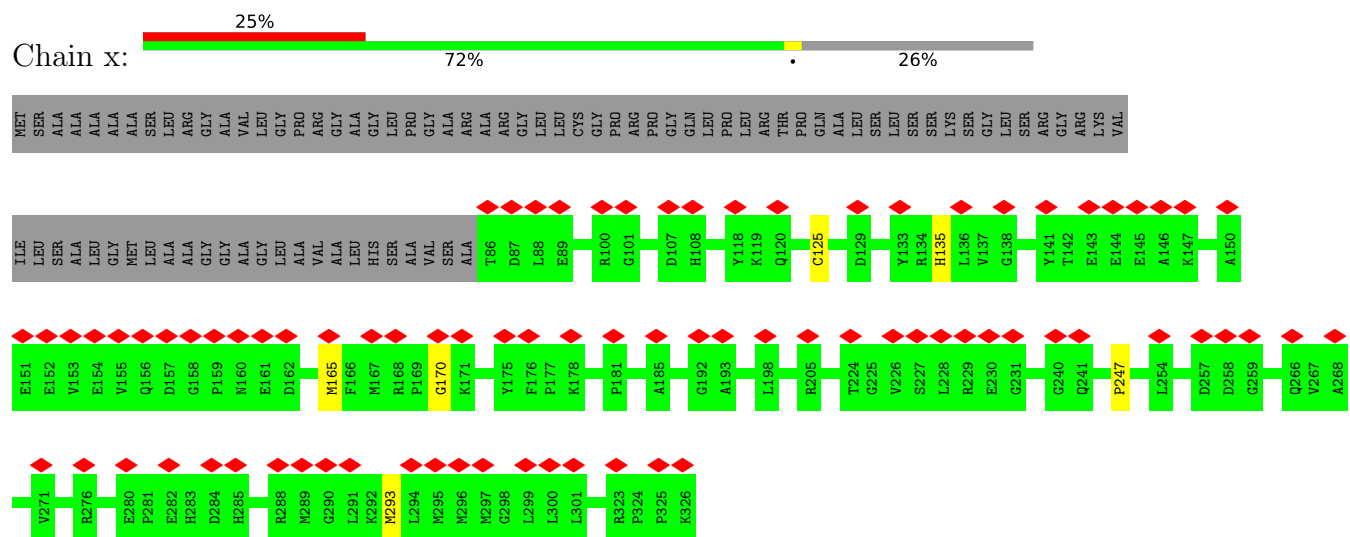




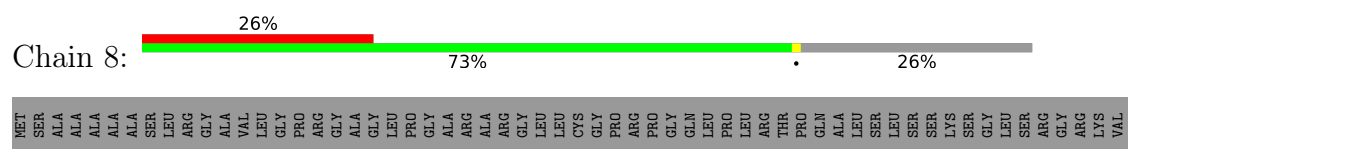
• Molecule 47: Cytochrome b

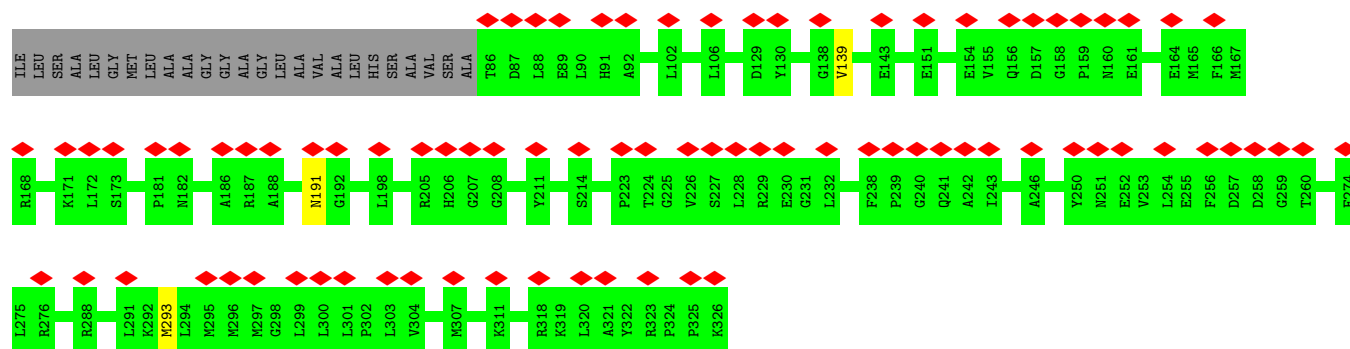


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

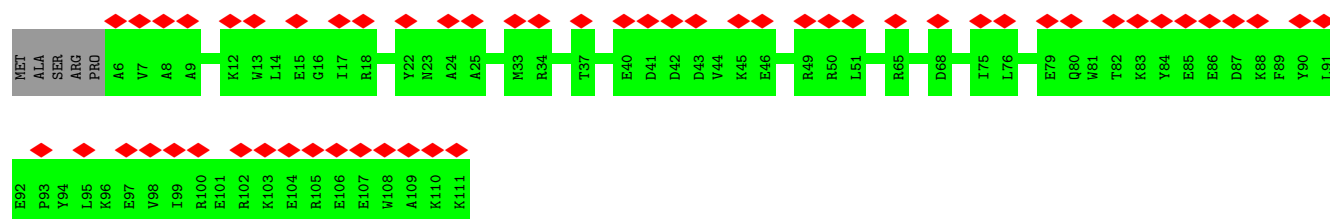


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

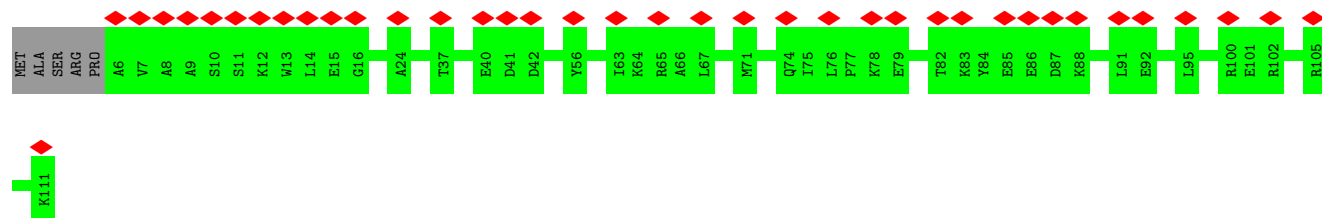




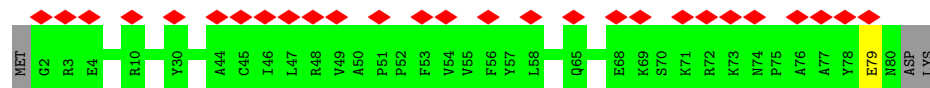
• Molecule 49: Cytochrome b-c1 complex subunit 7



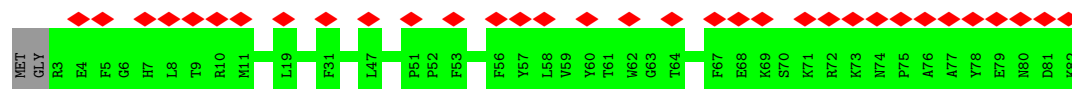
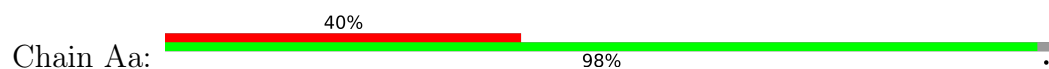
• Molecule 49: Cytochrome b-c1 complex subunit 7



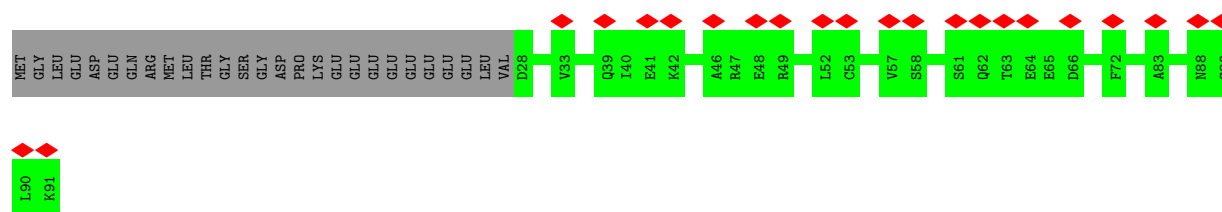
• Molecule 50: Cytochrome b-c1 complex subunit 8



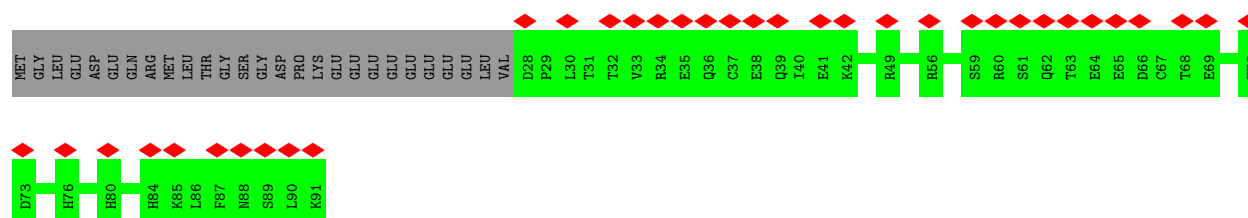
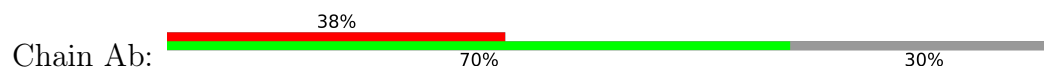
• Molecule 50: Cytochrome b-c1 complex subunit 8



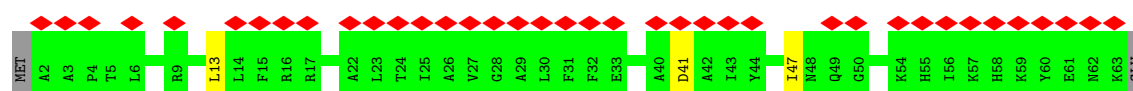
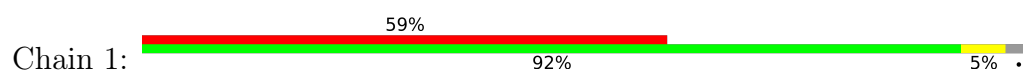
• Molecule 51: Cytochrome b-c1 complex subunit 6, mitochondrial



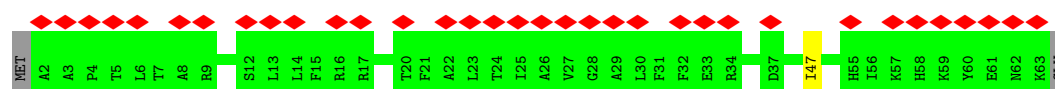
- Molecule 51: Cytochrome b-c1 complex subunit 6, mitochondrial



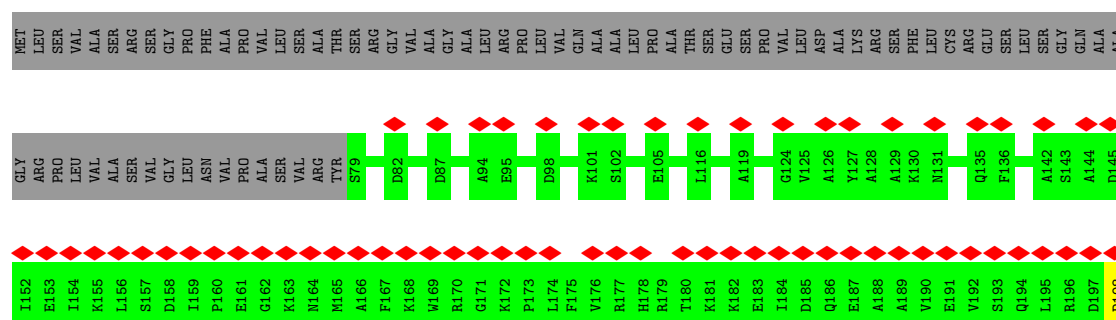
- Molecule 52: Cytochrome b-c1 complex subunit 9



- Molecule 52: Cytochrome b-c1 complex subunit 9

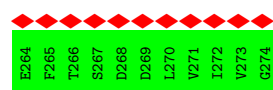
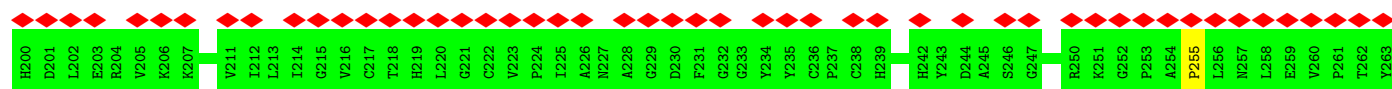
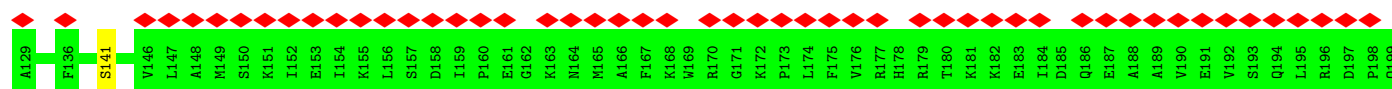
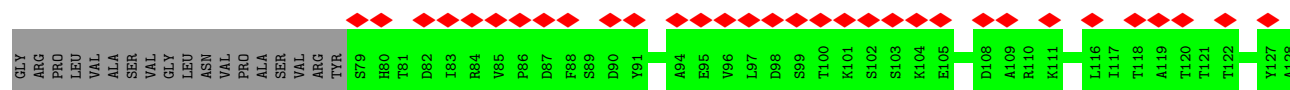
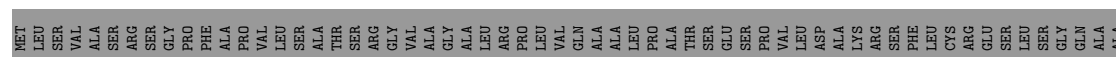


- Molecule 53: Cytochrome b-c1 complex subunit Rieske, mitochondrial

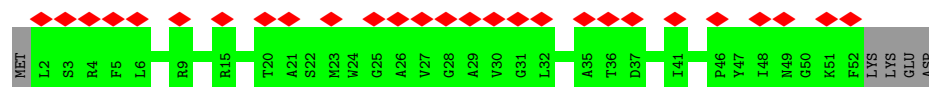
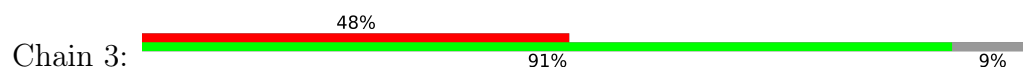




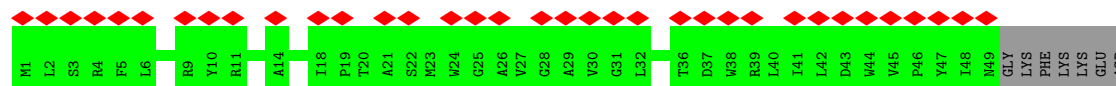
- Molecule 53: Cytochrome b-c1 complex subunit Rieske, mitochondrial



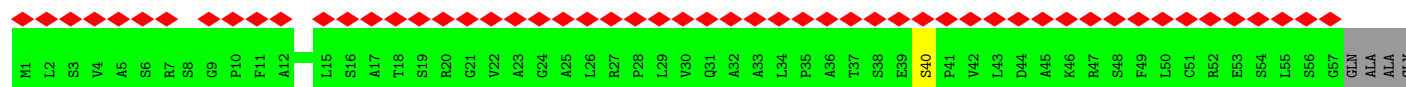
- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 54: Cytochrome b-c1 complex subunit 10



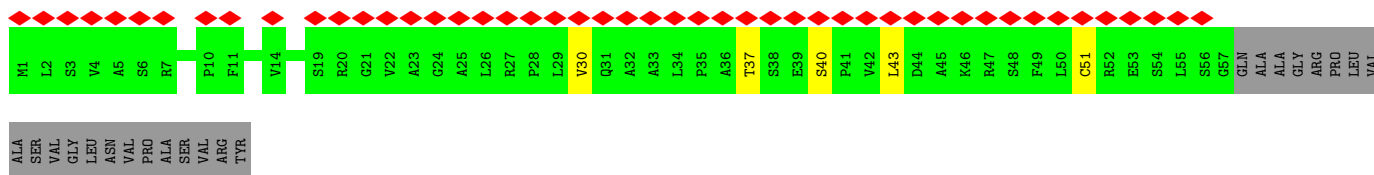
- Molecule 55: Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial



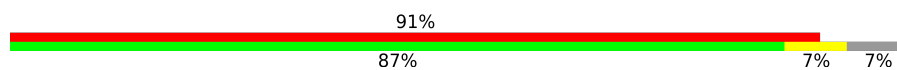
ARG PRO LEU VAL ALA SER VAL GLY LEU ASN VAL PRO ALA SER VAL ARG TYR

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

Chain Af: 

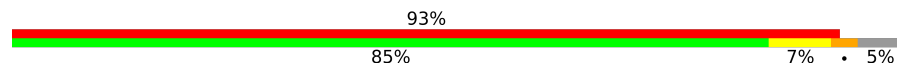


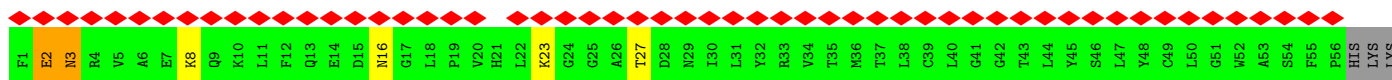
- Molecule 56: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Ag: 




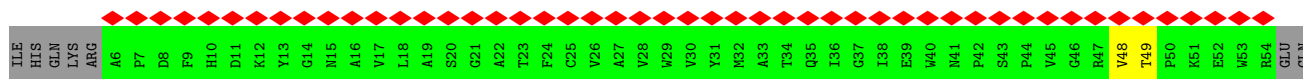
- Molecule 57: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain Ah: 

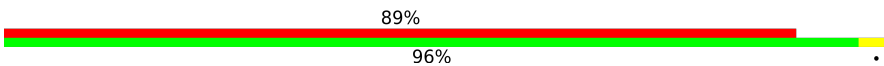



- Molecule 58: Cytochrome c oxidase subunit 7B, mitochondrial

Chain Ai: 



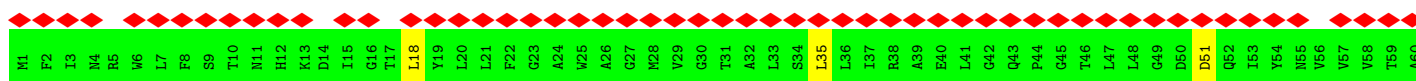
- Molecule 59: Cytochrome c oxidase subunit 7C, mitochondrial

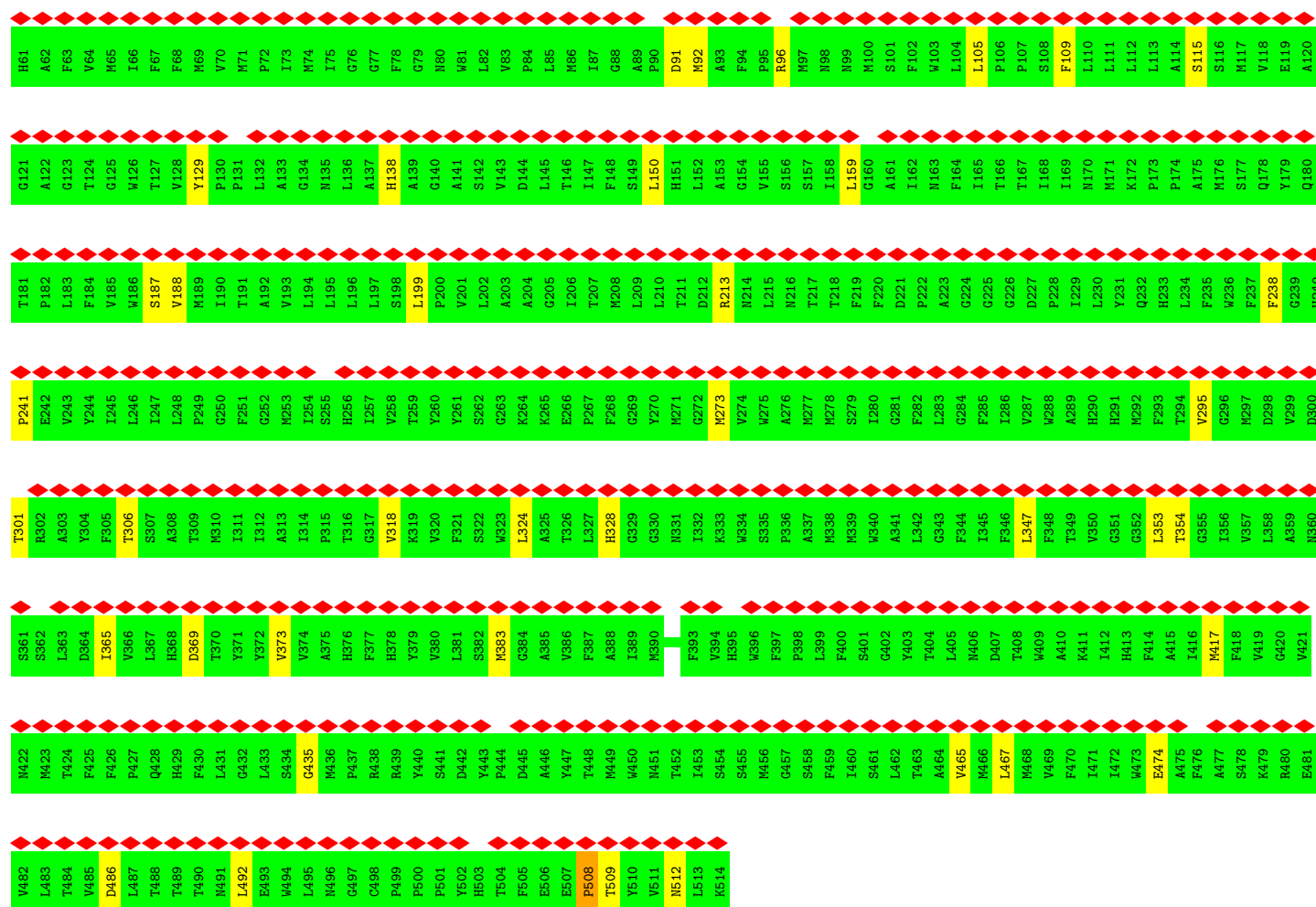
Chain Aj: 



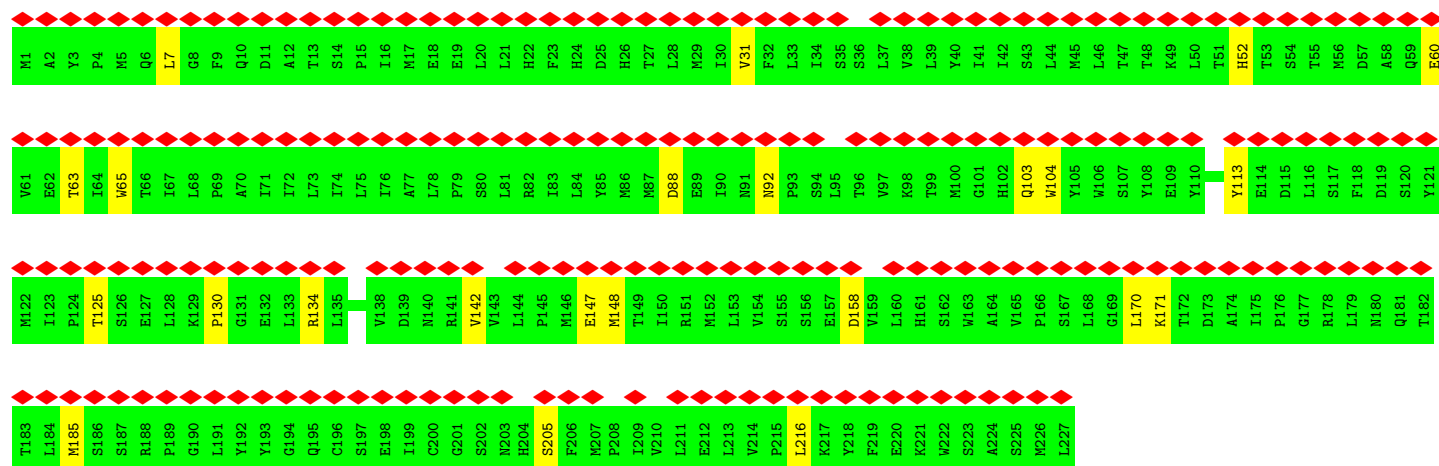
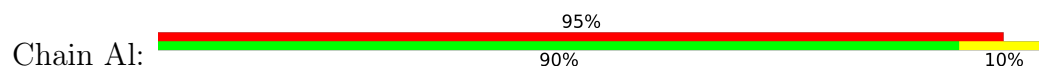
- Molecule 60: Cytochrome c oxidase subunit 1

Chain Ak: 



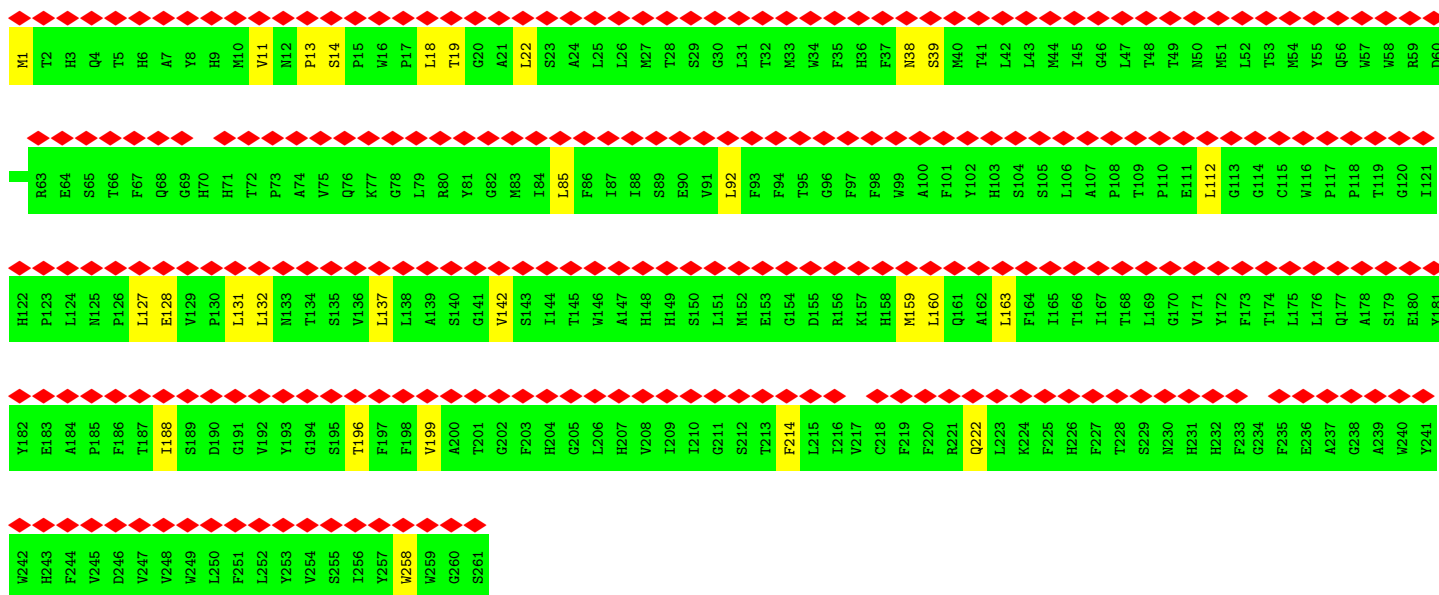


• Molecule 61: Cytochrome c oxidase subunit 2

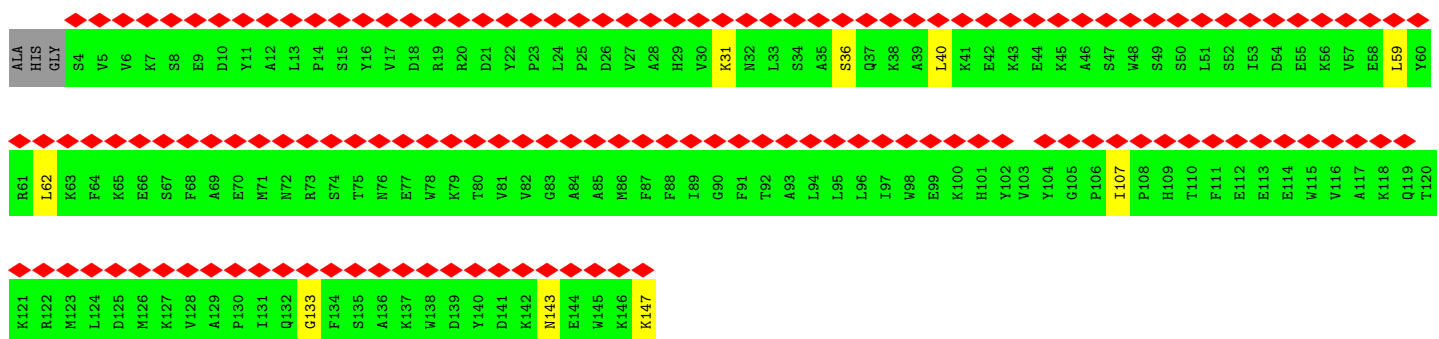


• Molecule 62: Cytochrome c oxidase subunit 3

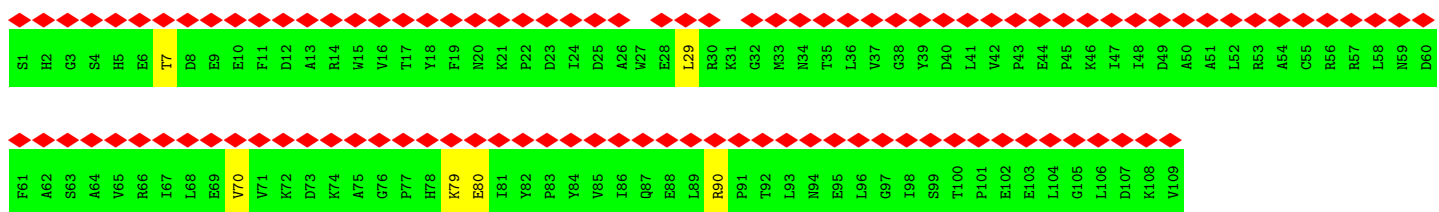




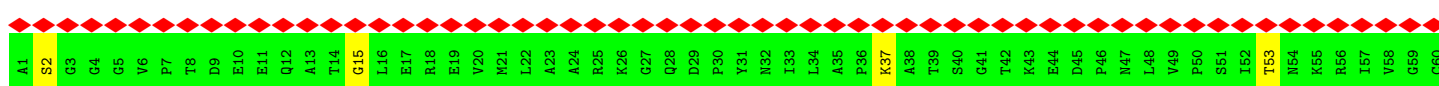
- Molecule 63: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

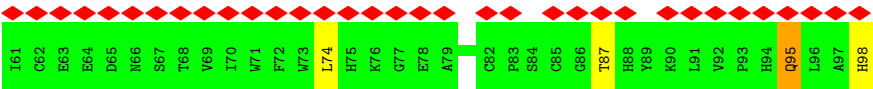


- Molecule 64: Cytochrome c oxidase subunit 5A, mitochondrial

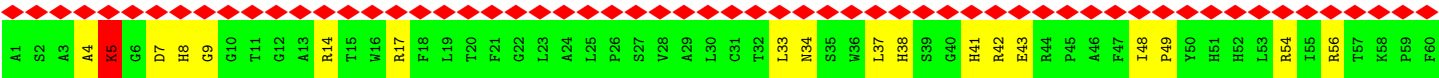
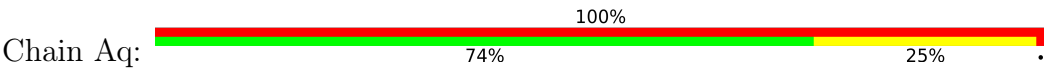


- Molecule 65: Cytochrome c oxidase subunit 5B, mitochondrial

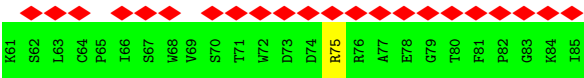
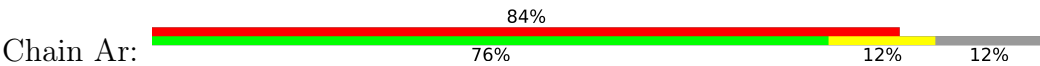




• Molecule 66: Cytochrome c oxidase subunit 6A, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 6B1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161912	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	0.519	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0504	Depositor
Map size (\AA)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.60	0/611	0.65	0/810
2	B	0.37	0/3199	0.55	0/4327
3	C	0.59	0/3479	0.64	2/4718 (0.0%)
4	D	0.45	0/1727	0.65	0/2355
5	E	0.39	0/1367	0.60	2/1860 (0.1%)
6	F	0.49	0/244	0.63	1/332 (0.3%)
7	G	0.43	0/5084	0.61	3/6898 (0.0%)
8	H	0.62	0/1439	0.61	0/1948
9	I	0.68	0/1272	0.64	0/1721
10	J	0.42	0/900	0.56	0/1218
11	K	0.42	0/526	0.56	1/728 (0.1%)
11	R	0.24	0/89	0.69	0/123
12	L	0.38	0/2740	0.57	2/3721 (0.1%)
13	M	0.36	0/702	0.56	0/959
14	N	0.38	0/914	0.58	0/1241
15	O	0.36	0/656	0.56	1/890 (0.1%)
15	X	0.47	0/673	0.62	1/912 (0.1%)
16	P	0.33	0/684	0.56	0/922
17	Q	0.40	0/965	0.62	1/1301 (0.1%)
18	S	0.47	0/582	0.56	0/783
19	T	0.44	0/643	0.59	0/886
20	U	0.43	0/1981	0.59	2/2711 (0.1%)
21	V	0.49	0/1030	0.62	0/1397
22	W	0.48	0/1153	0.59	0/1561
23	Y	0.46	0/412	0.66	3/567 (0.5%)
24	Z	0.42	0/567	0.51	0/777
25	a	0.52	0/1157	0.59	0/1571
26	b	0.46	0/756	0.76	8/1042 (0.8%)
27	c	0.53	0/1115	0.71	6/1535 (0.4%)
28	d	0.50	0/1253	0.64	4/1697 (0.2%)
29	e	0.54	0/778	0.55	0/1059
30	f	0.49	0/308	0.51	0/415

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	g	0.51	0/1027	0.62	0/1389
32	h	0.48	0/812	0.58	0/1087
33	i	0.63	0/2769	0.70	0/3764
34	j	0.51	0/916	0.60	0/1253
35	k	0.61	0/728	0.72	0/988
36	l	0.50	0/4919	0.63	1/6693 (0.0%)
37	m	0.57	0/1312	0.62	0/1784
38	n	0.44	0/368	0.55	0/499
39	o	0.50	0/1050	0.58	0/1430
40	p	0.51	0/1463	0.63	3/1984 (0.2%)
41	q	0.59	0/3718	0.70	0/5070
42	r	0.57	0/2581	0.68	0/3529
43	s	0.44	0/1387	0.57	0/1876
44	t	0.41	0/758	0.61	4/1032 (0.4%)
45	5	0.30	0/3531	0.51	0/4793
45	u	0.39	0/3523	0.54	0/4782
46	6	0.29	0/3179	0.51	0/4303
46	v	0.32	0/3179	0.53	0/4303
47	7	0.36	0/3115	0.54	0/4259
47	w	0.40	0/3115	0.58	0/4259
48	8	0.32	0/1976	0.51	0/2681
48	x	0.35	0/1976	0.55	0/2681
49	9	0.32	0/941	0.52	0/1262
49	y	0.33	0/941	0.50	0/1262
50	Aa	0.31	0/701	0.51	0/948
50	z	0.37	0/688	0.57	0/931
51	0	0.31	0/534	0.52	0/714
51	Ab	0.30	0/534	0.49	0/714
52	1	0.31	0/520	0.51	0/701
52	Ac	0.29	0/520	0.51	0/701
53	2	0.30	0/1549	0.51	0/2095
53	4	0.29	0/1549	0.49	0/2095
54	3	0.29	0/430	0.50	0/590
54	Ad	0.28	0/410	0.51	0/564
55	Ae	0.25	0/399	0.53	0/542
55	Af	0.26	0/394	0.59	0/536
56	Ag	0.51	0/345	0.65	0/470
57	Ah	0.60	0/440	0.72	0/596
58	Ai	0.57	0/398	0.66	0/546
59	Aj	0.63	0/399	0.62	0/534
60	Ak	0.60	0/4164	0.76	2/5688 (0.0%)
61	Al	0.58	0/1868	0.80	0/2544
62	Am	0.56	0/2211	0.69	0/3023

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
63	An	0.57	0/1229	0.65	1/1658 (0.1%)
64	Ao	0.50	0/898	0.66	0/1218
65	Ap	0.56	0/765	0.81	0/1038
66	Aq	0.55	0/699	0.73	1/950 (0.1%)
67	Ar	0.55	0/648	0.73	0/877
All	All	0.47	0/110582	0.61	49/150221 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	1
10	J	0	1
21	V	0	1
25	a	0	1
All	All	0	5

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	An	133	GLY	N-CA-C	6.44	129.20	113.10
26	b	30	PRO	N-CA-CB	6.38	110.95	103.30
26	b	124	PRO	N-CA-CB	6.29	110.85	103.30
40	p	155	PRO	N-CA-CB	6.28	110.84	103.30
28	d	44	PRO	N-CA-CB	6.22	110.77	103.30
28	d	18	PRO	N-CA-CB	6.22	110.76	103.30
27	c	180	PRO	N-CA-CB	6.18	110.72	103.30
27	c	174	PRO	N-CA-CB	6.15	110.68	103.30
5	E	218	PRO	N-CA-CB	6.14	110.67	103.30
44	t	27	PRO	N-CA-CB	6.12	110.64	103.30
26	b	36	PRO	N-CA-CB	6.06	110.57	103.30
15	X	72	PRO	N-CA-CB	6.00	110.50	103.30
7	G	449	PRO	N-CA-CB	6.00	110.49	103.30
3	C	72	PRO	N-CA-CB	5.99	110.48	103.30
6	F	75	PRO	N-CA-CB	5.96	110.45	103.30
26	b	37	PRO	N-CA-CB	5.95	110.44	103.30
15	O	72	PRO	N-CA-CB	5.94	110.43	103.30
27	c	178	PRO	N-CA-CB	5.89	110.37	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	33	PRO	N-CA-CB	5.85	110.31	103.30
44	t	23	PRO	N-CA-CB	5.85	110.32	103.30
17	Q	76	PRO	N-CA-CB	5.83	110.30	103.30
23	Y	85	PRO	N-CA-CB	5.83	110.29	103.30
44	t	26	PRO	N-CA-CB	5.81	110.27	103.30
44	t	75	PRO	N-CA-CB	5.78	110.23	103.30
7	G	435	PRO	N-CA-CB	5.76	110.22	103.30
27	c	158	PRO	N-CA-CB	5.75	110.20	103.30
27	c	162	PRO	N-CA-CB	5.73	110.18	103.30
20	U	249	PRO	N-CA-CB	5.66	110.09	103.30
5	E	49	PRO	N-CA-CB	5.63	110.06	103.30
23	Y	89	PRO	N-CA-CB	5.63	110.06	103.30
40	p	156	PRO	N-CA-CB	5.59	110.01	103.30
26	b	56	PRO	N-CA-CB	5.58	110.00	103.30
26	b	106	PRO	N-CA-CB	5.56	109.97	103.30
11	K	97	PRO	N-CA-CB	5.52	109.92	103.30
28	d	20	PRO	N-CA-CB	5.51	109.92	103.30
23	Y	87	PRO	N-CA-CB	5.47	109.86	103.30
28	d	22	PRO	N-CA-CB	5.47	109.86	103.30
36	l	556	ILE	CG1-CB-CG2	-5.46	99.38	111.40
26	b	118	PRO	N-CA-CB	5.40	109.78	103.30
12	L	134	TRP	N-CA-C	5.32	125.36	111.00
3	C	71	PRO	N-CA-CB	5.26	109.62	103.30
66	Aq	5	LYS	N-CA-C	5.24	125.15	111.00
12	L	55	VAL	N-CA-C	-5.23	96.87	111.00
40	p	149	PRO	N-CA-CB	5.23	109.58	103.30
60	Ak	435	GLY	N-CA-C	5.22	126.15	113.10
20	U	290	ASP	CB-CG-OD2	5.21	122.99	118.30
27	c	155	PRO	N-CA-CB	5.13	109.46	103.30
7	G	346	VAL	C-N-CA	5.01	134.24	121.70
60	Ak	129	TYR	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	327	ILE	Peptide
4	D	223	PRO	Peptide
10	J	98	LYS	Peptide
21	V	12	ILE	Peptide
25	a	109	HIS	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
2	B	408/464 (88%)	365 (90%)	30 (7%)	13 (3%)	3	26
3	C	428/463 (92%)	388 (91%)	28 (6%)	12 (3%)	4	28
4	D	206/264 (78%)	164 (80%)	29 (14%)	13 (6%)	1	16
5	E	170/249 (68%)	154 (91%)	11 (6%)	5 (3%)	3	27
6	F	42/123 (34%)	29 (69%)	10 (24%)	3 (7%)	1	14
7	G	669/727 (92%)	574 (86%)	66 (10%)	29 (4%)	2	21
8	H	174/212 (82%)	166 (95%)	7 (4%)	1 (1%)	22	58
9	I	154/216 (71%)	134 (87%)	12 (8%)	8 (5%)	1	19
10	J	107/175 (61%)	94 (88%)	12 (11%)	1 (1%)	14	49
11	K	95/145 (66%)	74 (78%)	14 (15%)	7 (7%)	1	13
11	R	16/145 (11%)	13 (81%)	2 (12%)	1 (6%)	1	16
12	L	335/377 (89%)	308 (92%)	15 (4%)	12 (4%)	3	24
13	M	90/113 (80%)	76 (84%)	6 (7%)	8 (9%)	0	11
14	N	110/116 (95%)	99 (90%)	6 (6%)	5 (4%)	2	21
15	O	83/156 (53%)	77 (93%)	2 (2%)	4 (5%)	2	20
15	X	83/156 (53%)	76 (92%)	4 (5%)	3 (4%)	3	24
16	P	81/99 (82%)	74 (91%)	6 (7%)	1 (1%)	11	43
17	Q	110/128 (86%)	99 (90%)	7 (6%)	4 (4%)	3	24
18	S	68/70 (97%)	63 (93%)	2 (3%)	3 (4%)	2	21
19	T	80/84 (95%)	69 (86%)	8 (10%)	3 (4%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	U	277/357 (78%)	249 (90%)	22 (8%)	6 (2%)	5	32
21	V	138/141 (98%)	127 (92%)	3 (2%)	8 (6%)	1	17
22	W	136/144 (94%)	124 (91%)	9 (7%)	3 (2%)	5	32
23	Y	57/105 (54%)	42 (74%)	5 (9%)	10 (18%)	0	2
24	Z	76/98 (78%)	71 (93%)	3 (4%)	2 (3%)	4	30
25	a	136/189 (72%)	118 (87%)	14 (10%)	4 (3%)	3	27
26	b	109/128 (85%)	95 (87%)	4 (4%)	10 (9%)	0	10
27	c	146/186 (78%)	119 (82%)	14 (10%)	13 (9%)	0	11
28	d	167/176 (95%)	151 (90%)	6 (4%)	10 (6%)	1	16
29	e	95/154 (62%)	83 (87%)	6 (6%)	6 (6%)	1	16
30	f	34/76 (45%)	29 (85%)	5 (15%)	0	100	100
31	g	119/122 (98%)	106 (89%)	7 (6%)	6 (5%)	1	19
32	h	102/106 (96%)	89 (87%)	8 (8%)	5 (5%)	2	19
33	i	345/347 (99%)	325 (94%)	17 (5%)	3 (1%)	14	49
34	j	112/115 (97%)	101 (90%)	9 (8%)	2 (2%)	7	36
35	k	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	3	26
36	l	604/606 (100%)	545 (90%)	41 (7%)	18 (3%)	3	27
37	m	172/175 (98%)	156 (91%)	11 (6%)	5 (3%)	3	27
38	n	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
39	o	126/129 (98%)	108 (86%)	11 (9%)	7 (6%)	1	18
40	p	167/179 (93%)	145 (87%)	13 (8%)	9 (5%)	1	19
41	q	457/459 (100%)	426 (93%)	21 (5%)	10 (2%)	5	32
42	r	316/318 (99%)	285 (90%)	27 (8%)	4 (1%)	10	42
43	s	167/172 (97%)	149 (89%)	14 (8%)	4 (2%)	5	31
44	t	111/137 (81%)	100 (90%)	8 (7%)	3 (3%)	4	29
45	5	444/480 (92%)	412 (93%)	29 (6%)	3 (1%)	19	55
45	u	444/480 (92%)	407 (92%)	28 (6%)	9 (2%)	6	34
46	6	416/453 (92%)	383 (92%)	30 (7%)	3 (1%)	19	55
46	v	416/453 (92%)	379 (91%)	30 (7%)	7 (2%)	7	37
47	7	376/379 (99%)	348 (93%)	22 (6%)	6 (2%)	8	38
47	w	376/379 (99%)	352 (94%)	19 (5%)	5 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	8	239/326 (73%)	221 (92%)	16 (7%)	2 (1%)	16	53
48	x	239/326 (73%)	219 (92%)	15 (6%)	5 (2%)	5	33
49	9	104/111 (94%)	102 (98%)	2 (2%)	0	100	100
49	y	104/111 (94%)	100 (96%)	4 (4%)	0	100	100
50	Aa	78/82 (95%)	70 (90%)	8 (10%)	0	100	100
50	z	77/82 (94%)	70 (91%)	6 (8%)	1 (1%)	10	42
51	0	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
51	Ab	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
52	1	60/64 (94%)	55 (92%)	2 (3%)	3 (5%)	1	19
52	Ac	60/64 (94%)	57 (95%)	2 (3%)	1 (2%)	7	37
53	2	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	13	47
53	4	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	13	47
54	3	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
54	Ad	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
55	Ae	55/78 (70%)	41 (74%)	13 (24%)	1 (2%)	7	36
55	Af	55/78 (70%)	40 (73%)	10 (18%)	5 (9%)	0	11
56	Ag	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
57	Ah	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	23
58	Ai	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
59	Aj	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
60	Ak	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
61	Al	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	10	42
62	Am	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
63	An	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
64	Ao	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
65	Ap	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	22
66	Aq	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	16
67	Ar	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	40
All	All	13723/15851 (87%)	12412 (90%)	950 (7%)	361 (3%)	6	30

All (361) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	PRO
2	B	105	PRO
2	B	121	GLU
2	B	379	CYS
3	C	84	PHE
4	D	50	ARG
4	D	229	GLU
5	E	183	ALA
6	F	114	CYS
7	G	37	ASP
7	G	47	THR
7	G	181	ARG
7	G	287	SER
7	G	347	ASP
7	G	448	SER
7	G	482	GLN
11	K	62	VAL
12	L	135	GLU
16	P	50	ASP
18	S	52	ARG
18	S	60	TYR
19	T	63	MET
19	T	71	GLN
20	U	201	LEU
21	V	135	VAL
21	V	140	LYS
23	Y	51	THR
23	Y	85	PRO
23	Y	88	ASP
23	Y	89	PRO
24	Z	17	PRO
26	b	29	SER
26	b	33	PRO
26	b	124	PRO
27	c	100	ASN
27	c	155	PRO
27	c	178	PRO
28	d	9	VAL
28	d	18	PRO
28	d	20	PRO
28	d	121	TYR
29	e	59	PRO
31	g	3	MET

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Mol	Chain	Res	Type
31	g	10	ARG
31	g	20	ALA
36	l	562	LEU
36	l	581	LYS
37	m	76	THR
39	o	57	LEU
39	o	83	THR
40	p	156	PRO
40	p	175	ARG
41	q	429	SER
42	r	208	VAL
43	s	49	GLU
45	u	337	LEU
46	v	142	ALA
52	1	13	LEU
45	5	105	PRO
45	5	249	HIS
47	7	62	ALA
57	Ah	2	GLU
60	Ak	328	HIS
60	Ak	508	PRO
65	Ap	2	SER
65	Ap	87	THR
65	Ap	95	GLN
66	Aq	4	ALA
66	Aq	9	GLY
67	Ar	46	LYS
2	B	50	ASP
2	B	331	VAL
2	B	378	SER
3	C	104	GLU
3	C	265	ASN
3	C	273	VAL
3	C	386	THR
4	D	138	ASN
4	D	192	GLY
7	G	210	ILE
7	G	288	ASP
7	G	336	ASN
7	G	368	THR
7	G	450	LYS
7	G	541	PRO

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Mol	Chain	Res	Type
7	G	555	ILE
11	K	32	ASP
11	K	37	THR
12	L	86	CYS
12	L	230	SER
12	L	239	PRO
12	L	310	PHE
13	M	40	LYS
13	M	72	SER
14	N	9	THR
14	N	41	ASN
15	O	137	LYS
15	O	139	MET
17	Q	76	PRO
19	T	50	PRO
20	U	90	GLU
20	U	115	SER
20	U	203	PRO
21	V	14	GLU
21	V	47	ALA
22	W	11	PRO
22	W	16	TYR
23	Y	40	ILE
23	Y	45	ARG
23	Y	48	PRO
23	Y	49	GLN
25	a	185	THR
26	b	112	GLU
26	b	118	PRO
27	c	59	VAL
27	c	154	GLN
28	d	22	PRO
28	d	119	GLU
28	d	120	SER
29	e	58	ASP
31	g	12	PRO
32	h	20	ILE
32	h	24	GLU
32	h	48	GLY
32	h	49	GLY
33	i	86	ILE
34	j	113	TRP

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Mol	Chain	Res	Type
35	k	22	TYR
36	l	73	THR
36	l	440	LEU
36	l	586	LEU
37	m	24	PRO
39	o	5	LYS
40	p	106	ASP
41	q	22	MET
41	q	139	GLN
41	q	188	ASN
45	u	297	ALA
45	u	312	GLY
45	u	380	CYS
47	w	7	SER
47	w	254	ASP
48	x	125	CYS
52	1	47	ILE
53	4	141	SER
53	4	255	PRO
45	5	279	ASP
47	7	201	HIS
48	8	139	VAL
66	Aq	5	LYS
2	B	236	PHE
3	C	102	SER
3	C	139	LEU
3	C	197	MET
3	C	233	HIS
4	D	194	GLU
4	D	246	ARG
5	E	176	CYS
6	F	110	THR
7	G	174	THR
7	G	283	GLU
7	G	377	ALA
7	G	663	ASN
7	G	665	PHE
7	G	677	GLN
7	G	689	LEU
9	I	105	ASP
9	I	116	SER
9	I	156	CYS

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Mol	Chain	Res	Type
11	K	17	HIS
12	L	178	SER
12	L	205	ASP
12	L	259	LYS
13	M	107	SER
15	O	138	LEU
20	U	112	GLY
21	V	48	SER
15	X	108	LEU
23	Y	86	TYR
23	Y	95	GLU
24	Z	59	ASN
25	a	188	ASP
26	b	88	TYR
26	b	101	LYS
26	b	119	LEU
27	c	43	LYS
27	c	167	TYR
28	d	23	GLN
28	d	144	SER
28	d	145	ASP
29	e	62	GLU
29	e	136	LEU
31	g	4	MET
34	j	24	LEU
35	k	50	ASN
36	l	55	MET
36	l	447	ASN
37	m	77	GLU
37	m	116	ILE
39	o	80	PHE
39	o	126	ASN
40	p	8	ALA
40	p	51	HIS
41	q	251	ASN
41	q	353	PRO
42	r	60	PRO
44	t	56	ARG
45	u	322	THR
46	v	244	LEU
46	v	251	ALA
46	v	261	GLN

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Mol	Chain	Res	Type
48	x	165	MET
48	x	247	PRO
46	6	118	SER
46	6	244	LEU
47	7	249	LEU
55	Af	40	SER
61	Al	104	TRP
66	Aq	61	SER
2	B	186	ALA
2	B	237	GLY
4	D	105	ASN
4	D	121	THR
4	D	202	PHE
5	E	160	VAL
7	G	69	LEU
7	G	337	ASP
7	G	575	VAL
7	G	650	SER
8	H	175	PHE
9	I	89	LEU
12	L	102	GLN
12	L	370	LYS
13	M	108	LYS
14	N	76	GLN
14	N	103	LEU
14	N	105	GLU
15	O	155	TYR
17	Q	72	HIS
11	R	130	THR
18	S	51	ASP
21	V	15	GLY
21	V	17	GLU
22	W	118	THR
15	X	155	TYR
25	a	58	LYS
27	c	41	TYR
27	c	66	PRO
27	c	114	ARG
27	c	162	PRO
27	c	166	LEU
29	e	72	ASP
33	i	48	PHE

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Mol	Chain	Res	Type
33	i	81	SER
35	k	96	LEU
36	l	477	VAL
36	l	511	LEU
36	l	512	LYS
36	l	536	LEU
37	m	25	SER
39	o	81	ARG
40	p	32	VAL
40	p	145	PRO
42	r	196	ALA
43	s	37	ASP
43	s	139	GLU
44	t	42	THR
46	v	184	ASN
48	x	135	HIS
52	1	41	ASP
53	2	266	THR
47	7	286	ASN
48	8	191	ASN
55	Af	43	LEU
55	Af	51	CYS
60	Ak	51	ASP
5	E	214	PRO
6	F	81	SER
7	G	281	ILE
7	G	582	VAL
7	G	654	VAL
10	J	96	LYS
11	K	41	GLU
12	L	330	PRO
13	M	31	ILE
13	M	70	MET
17	Q	127	ASP
20	U	68	ILE
15	X	137	LYS
25	a	102	PRO
26	b	105	PHE
27	c	172	GLY
32	h	98	HIS
36	l	195	ALA
36	l	211	MET

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Mol	Chain	Res	Type
36	l	441	VAL
40	p	76	HIS
40	p	87	GLY
41	q	85	SER
41	q	368	ALA
42	r	281	ARG
43	s	79	ALA
45	u	233	ALA
46	v	241	ARG
47	w	135	TRP
47	7	314	SER
52	Ac	47	ILE
55	Af	37	THR
57	Ah	3	ASN
61	Al	103	GLN
2	B	74	ASP
3	C	94	VAL
4	D	122	ARG
4	D	191	TYR
4	D	239	TRP
7	G	267	THR
9	I	159	GLY
9	I	171	ARG
11	K	55	PHE
11	K	64	TYR
12	L	83	PRO
13	M	92	LYS
13	M	93	LYS
17	Q	96	VAL
26	b	115	GLU
36	l	275	THR
45	u	279	ASP
45	u	419	THR
47	w	173	ALA
47	w	262	LEU
50	z	79	GLU
60	Ak	91	ASP
61	Al	158	ASP
66	Aq	49	PRO
46	6	371	VAL
2	B	94	PRO
9	I	160	GLY

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Mol	Chain	Res	Type
36	l	563	PRO
39	o	94	GLY
55	Af	30	VAL
3	C	85	GLY
3	C	319	PRO
4	D	44	ARG
9	I	147	PRO
31	g	56	VAL
36	l	515	TYR
41	q	172	GLY
41	q	249	ILE
45	u	424	ILE
53	2	198	PRO
47	7	253	PRO
65	Ap	15	GLY
2	B	221	GLY
21	V	45	PRO
44	t	74	PHE
48	x	170	GLY
55	Ae	40	SER
5	E	216	PRO
46	v	46	GLY
36	l	483	PRO
29	e	135	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/58 (100%)	53 (91%)	5 (9%)	8	30
2	B	322/368 (88%)	321 (100%)	1 (0%)	91	92
3	C	351/393 (89%)	350 (100%)	1 (0%)	91	92
4	D	176/228 (77%)	176 (100%)	0	100	100
5	E	145/173 (84%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	9/97 (9%)	9 (100%)	0	100	100
7	G	518/610 (85%)	517 (100%)	1 (0%)	92	93
8	H	150/176 (85%)	150 (100%)	0	100	100
9	I	129/177 (73%)	128 (99%)	1 (1%)	79	84
10	J	95/152 (62%)	95 (100%)	0	100	100
11	K	11/131 (8%)	11 (100%)	0	100	100
12	L	280/323 (87%)	277 (99%)	3 (1%)	70	80
13	M	65/98 (66%)	65 (100%)	0	100	100
14	N	95/101 (94%)	95 (100%)	0	100	100
15	O	66/132 (50%)	66 (100%)	0	100	100
15	X	71/132 (54%)	71 (100%)	0	100	100
16	P	75/82 (92%)	75 (100%)	0	100	100
17	Q	101/112 (90%)	101 (100%)	0	100	100
18	S	58/58 (100%)	58 (100%)	0	100	100
19	T	65/70 (93%)	65 (100%)	0	100	100
20	U	151/307 (49%)	149 (99%)	2 (1%)	65	77
21	V	98/102 (96%)	98 (100%)	0	100	100
22	W	114/124 (92%)	114 (100%)	0	100	100
23	Y	24/84 (29%)	24 (100%)	0	100	100
24	Z	41/76 (54%)	41 (100%)	0	100	100
25	a	114/158 (72%)	113 (99%)	1 (1%)	75	83
26	b	46/121 (38%)	46 (100%)	0	100	100
27	c	87/160 (54%)	87 (100%)	0	100	100
28	d	99/156 (64%)	99 (100%)	0	100	100
29	e	74/129 (57%)	74 (100%)	0	100	100
30	f	31/66 (47%)	31 (100%)	0	100	100
31	g	107/109 (98%)	107 (100%)	0	100	100
32	h	75/94 (80%)	75 (100%)	0	100	100
33	i	310/311 (100%)	310 (100%)	0	100	100
34	j	97/100 (97%)	97 (100%)	0	100	100
35	k	78/85 (92%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	l	534/540 (99%)	533 (100%)	1 (0%)	92	93
37	m	129/141 (92%)	129 (100%)	0	100	100
38	n	33/55 (60%)	33 (100%)	0	100	100
39	o	101/114 (89%)	101 (100%)	0	100	100
40	p	134/160 (84%)	133 (99%)	1 (1%)	81	86
41	q	408/409 (100%)	407 (100%)	1 (0%)	92	93
42	r	275/275 (100%)	275 (100%)	0	100	100
43	s	142/154 (92%)	138 (97%)	4 (3%)	38	59
44	t	41/120 (34%)	40 (98%)	1 (2%)	44	63
45	5	372/397 (94%)	372 (100%)	0	100	100
45	u	370/397 (93%)	370 (100%)	0	100	100
46	6	326/354 (92%)	326 (100%)	0	100	100
46	v	326/354 (92%)	326 (100%)	0	100	100
47	7	331/332 (100%)	331 (100%)	0	100	100
47	w	331/332 (100%)	331 (100%)	0	100	100
48	8	205/259 (79%)	204 (100%)	1 (0%)	86	89
48	x	205/259 (79%)	204 (100%)	1 (0%)	86	89
49	9	95/99 (96%)	95 (100%)	0	100	100
49	y	95/99 (96%)	95 (100%)	0	100	100
50	Aa	72/73 (99%)	72 (100%)	0	100	100
50	z	70/73 (96%)	70 (100%)	0	100	100
51	0	61/85 (72%)	61 (100%)	0	100	100
51	Ab	61/85 (72%)	61 (100%)	0	100	100
52	1	50/52 (96%)	50 (100%)	0	100	100
52	Ac	50/52 (96%)	50 (100%)	0	100	100
53	2	165/225 (73%)	165 (100%)	0	100	100
53	4	165/225 (73%)	165 (100%)	0	100	100
54	3	39/46 (85%)	39 (100%)	0	100	100
54	Ad	37/46 (80%)	37 (100%)	0	100	100
55	Ae	41/59 (70%)	41 (100%)	0	100	100
55	Af	41/59 (70%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	Ag	37/38 (97%)	34 (92%)	3 (8%)	9	32
57	Ah	45/50 (90%)	39 (87%)	6 (13%)	3	17
58	Ai	39/46 (85%)	37 (95%)	2 (5%)	20	43
59	Aj	40/40 (100%)	38 (95%)	2 (5%)	20	44
60	Ak	427/427 (100%)	389 (91%)	38 (9%)	8	28
61	Al	211/211 (100%)	191 (90%)	20 (10%)	7	24
62	Am	226/226 (100%)	199 (88%)	27 (12%)	4	19
63	An	128/129 (99%)	120 (94%)	8 (6%)	15	38
64	Ao	95/95 (100%)	89 (94%)	6 (6%)	15	38
65	Ap	81/81 (100%)	76 (94%)	5 (6%)	15	38
66	Aq	68/68 (100%)	50 (74%)	18 (26%)	0	3
67	Ar	67/75 (89%)	58 (87%)	9 (13%)	3	17
All	All	11155/13269 (84%)	10986 (98%)	169 (2%)	60	75

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	GLN
1	A	26	MET
1	A	44	LYS
1	A	64	ARG
2	B	118	ASP
3	C	84	PHE
7	G	478	SER
9	I	91	CYS
12	L	67	ARG
12	L	134	TRP
12	L	242	ILE
20	U	138	TYR
20	U	304	LEU
25	a	53	ARG
36	l	283	ILE
40	p	108	HIS
41	q	96	ILE
43	s	46	CYS
43	s	47	ARG
43	s	48	TRP

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Mol	Chain	Res	Type
43	s	103	GLN
44	t	111	ARG
48	x	293	MET
48	8	293	MET
56	Ag	13	LYS
56	Ag	42	LYS
56	Ag	43	SER
57	Ah	2	GLU
57	Ah	3	ASN
57	Ah	8	LYS
57	Ah	16	ASN
57	Ah	23	LYS
57	Ah	27	THR
58	Ai	48	VAL
58	Ai	49	THR
59	Aj	15	VAL
59	Aj	22	LEU
60	Ak	18	LEU
60	Ak	35	LEU
60	Ak	92	MET
60	Ak	96	ARG
60	Ak	105	LEU
60	Ak	109	PHE
60	Ak	115	SER
60	Ak	138	HIS
60	Ak	150	LEU
60	Ak	159	LEU
60	Ak	187	SER
60	Ak	188	VAL
60	Ak	199	LEU
60	Ak	213	ARG
60	Ak	238	PHE
60	Ak	241	PRO
60	Ak	273	MET
60	Ak	295	VAL
60	Ak	301	THR
60	Ak	306	THR
60	Ak	318	VAL
60	Ak	324	LEU
60	Ak	347	LEU
60	Ak	353	LEU
60	Ak	354	THR

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Mol	Chain	Res	Type
60	Ak	365	ILE
60	Ak	369	ASP
60	Ak	373	VAL
60	Ak	383	MET
60	Ak	417	MET
60	Ak	465	VAL
60	Ak	467	LEU
60	Ak	474	GLU
60	Ak	486	ASP
60	Ak	492	LEU
60	Ak	508	PRO
60	Ak	509	THR
60	Ak	512	ASN
61	Al	7	LEU
61	Al	31	VAL
61	Al	52	HIS
61	Al	60	GLU
61	Al	63	THR
61	Al	65	TRP
61	Al	88	ASP
61	Al	92	ASN
61	Al	113	TYR
61	Al	125	THR
61	Al	130	PRO
61	Al	134	ARG
61	Al	142	VAL
61	Al	147	GLU
61	Al	148	MET
61	Al	170	LEU
61	Al	171	LYS
61	Al	185	MET
61	Al	205	SER
61	Al	216	LEU
62	Am	1	MET
62	Am	11	VAL
62	Am	13	PRO
62	Am	14	SER
62	Am	18	LEU
62	Am	19	THR
62	Am	22	LEU
62	Am	38	ASN
62	Am	39	SER

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Mol	Chain	Res	Type
62	Am	85	LEU
62	Am	92	LEU
62	Am	112	LEU
62	Am	127	LEU
62	Am	128	GLU
62	Am	131	LEU
62	Am	132	LEU
62	Am	137	LEU
62	Am	142	VAL
62	Am	159	MET
62	Am	160	LEU
62	Am	163	LEU
62	Am	188	ILE
62	Am	196	THR
62	Am	199	VAL
62	Am	214	PHE
62	Am	222	GLN
62	Am	258	TRP
63	An	31	LYS
63	An	36	SER
63	An	40	LEU
63	An	59	LEU
63	An	62	LEU
63	An	107	ILE
63	An	143	ASN
63	An	147	LYS
64	Ao	7	THR
64	Ao	29	LEU
64	Ao	70	VAL
64	Ao	79	LYS
64	Ao	80	GLU
64	Ao	90	ARG
65	Ap	37	LYS
65	Ap	53	THR
65	Ap	74	LEU
65	Ap	95	GLN
65	Ap	98	HIS
66	Aq	5	LYS
66	Aq	7	ASP
66	Aq	8	HIS
66	Aq	14	ARG
66	Aq	17	ARG

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Mol	Chain	Res	Type
66	Aq	33	LEU
66	Aq	34	ASN
66	Aq	37	LEU
66	Aq	38	HIS
66	Aq	41	HIS
66	Aq	42	ARG
66	Aq	43	GLU
66	Aq	48	ILE
66	Aq	54	ARG
66	Aq	56	ARG
66	Aq	68	THR
66	Aq	69	PHE
66	Aq	78	LEU
67	Ar	19	ARG
67	Ar	24	ASN
67	Ar	28	ASN
67	Ar	29	CYS
67	Ar	51	SER
67	Ar	53	CYS
67	Ar	57	ARG
67	Ar	60	TYR
67	Ar	75	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	220	GLN
2	B	393	ASN
2	B	441	HIS
3	C	38	GLN
3	C	92	HIS
3	C	131	GLN
3	C	250	ASN
3	C	270	ASN
3	C	339	GLN
3	C	381	HIS
3	C	442	HIS
4	D	55	HIS
4	D	107	GLN
4	D	181	HIS
5	E	59	ASN
5	E	90	ASN

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Mol	Chain	Res	Type
5	E	99	ASN
5	E	123	ASN
5	E	153	GLN
5	E	187	GLN
5	E	189	ASN
5	E	191	ASN
7	G	142	GLN
7	G	569	GLN
7	G	705	GLN
9	I	75	ASN
9	I	98	HIS
9	I	164	HIS
10	J	71	HIS
10	J	88	GLN
12	L	71	ASN
12	L	102	GLN
12	L	154	GLN
12	L	171	ASN
14	N	50	GLN
14	N	111	GLN
16	P	22	HIS
16	P	62	GLN
16	P	93	ASN
17	Q	51	GLN
17	Q	70	ASN
17	Q	99	GLN
18	S	27	HIS
18	S	68	ASN
19	T	69	HIS
20	U	134	GLN
20	U	144	GLN
20	U	188	HIS
20	U	294	HIS
22	W	112	HIS
15	X	115	GLN
25	a	132	ASN
28	d	100	GLN
28	d	114	GLN
28	d	131	GLN
31	g	61	HIS
33	i	120	GLN
33	i	134	GLN

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Mol	Chain	Res	Type
33	i	144	GLN
33	i	172	GLN
33	i	221	HIS
33	i	273	ASN
33	i	310	ASN
33	i	319	HIS
34	j	2	ASN
35	k	7	ASN
36	l	165	ASN
36	l	194	ASN
36	l	296	ASN
36	l	328	HIS
36	l	332	HIS
36	l	541	ASN
36	l	546	GLN
36	l	570	GLN
37	m	46	ASN
37	m	120	ASN
37	m	175	ASN
40	p	13	GLN
40	p	14	GLN
40	p	75	GLN
40	p	139	GLN
41	q	81	GLN
41	q	220	HIS
41	q	251	ASN
41	q	304	GLN
41	q	331	ASN
41	q	390	ASN
41	q	434	ASN
42	r	5	ASN
42	r	124	ASN
42	r	230	ASN
42	r	235	ASN
42	r	284	GLN
42	r	317	GLN
43	s	30	HIS
43	s	31	HIS
43	s	77	HIS
43	s	95	GLN
43	s	151	ASN
44	t	55	GLN

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Mol	Chain	Res	Type
44	t	85	HIS
45	u	52	GLN
45	u	87	ASN
45	u	95	HIS
45	u	188	HIS
45	u	207	ASN
45	u	223	HIS
45	u	247	GLN
45	u	277	HIS
45	u	286	HIS
45	u	301	ASN
45	u	305	GLN
45	u	308	ASN
45	u	342	GLN
46	v	36	GLN
46	v	45	ASN
46	v	139	ASN
46	v	167	GLN
46	v	206	HIS
46	v	291	HIS
46	v	311	GLN
46	v	343	GLN
46	v	399	GLN
46	v	446	HIS
47	w	8	HIS
47	w	32	ASN
47	w	114	ASN
47	w	182	HIS
47	w	255	ASN
48	x	266	GLN
48	x	285	HIS
49	y	28	ASN
52	1	49	GLN
53	2	164	ASN
53	4	219	HIS
53	4	227	ASN
45	5	52	GLN
45	5	87	ASN
45	5	121	ASN
45	5	128	HIS
45	5	153	ASN
45	5	170	GLN

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Mol	Chain	Res	Type
45	5	188	HIS
45	5	193	GLN
45	5	207	ASN
45	5	277	HIS
45	5	305	GLN
45	5	313	HIS
45	5	357	HIS
45	5	375	GLN
45	5	397	ASN
45	5	402	HIS
45	5	464	GLN
45	5	469	ASN
46	6	155	GLN
46	6	178	HIS
46	6	188	ASN
46	6	204	GLN
46	6	212	HIS
46	6	227	HIS
46	6	261	GLN
46	6	311	GLN
46	6	343	GLN
46	6	376	ASN
47	7	44	GLN
47	7	68	HIS
47	7	255	ASN
47	7	322	GLN
48	8	108	HIS
48	8	116	GLN
48	8	191	ASN
48	8	266	GLN
48	8	283	HIS
49	9	28	ASN
49	9	74	GLN
50	Aa	24	GLN
51	Ab	84	HIS
52	Ac	49	GLN
52	Ac	58	HIS
54	Ad	49	ASN
56	Ag	39	ASN
57	Ah	3	ASN
57	Ah	16	ASN
58	Ai	10	HIS

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Mol	Chain	Res	Type
58	Ai	15	ASN
58	Ai	41	ASN
59	Aj	42	HIS
60	Ak	11	ASN
60	Ak	12	HIS
60	Ak	43	GLN
60	Ak	99	ASN
60	Ak	170	ASN
60	Ak	256	HIS
60	Ak	360	ASN
60	Ak	413	HIS
60	Ak	512	ASN
61	Al	103	GLN
61	Al	203	ASN
62	Am	6	HIS
62	Am	12	ASN
62	Am	133	ASN
62	Am	148	HIS
62	Am	207	HIS
62	Am	222	GLN
62	Am	232	HIS
63	An	109	HIS
64	Ao	34	ASN
65	Ap	66	ASN
66	Aq	52	HIS
67	Ar	23	GLN
67	Ar	24	ASN
67	Ar	25	GLN
67	Ar	28	ASN
67	Ar	37	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 5 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	HEC	8	402	48	32,50,50	2.23	3 (9%)	24,82,82	1.49	4 (16%)
71	PLX	V	202	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	i	502	-	51,51,51	0.75	1 (1%)	55,59,59	0.65	1 (1%)
75	PEE	W	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.98	2 (3%)
74	CDL	z	101	-	63,63,99	1.22	5 (7%)	69,75,111	1.08	6 (8%)
76	HEM	7	403	47	41,50,50	4.58	12 (29%)	45,82,82	3.73	26 (57%)
72	NDP	L	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.32	4 (7%)
74	CDL	u	501	-	63,63,99	1.25	5 (7%)	69,75,111	1.00	4 (5%)
71	PLX	4	301	-	51,51,51	0.79	1 (1%)	55,59,59	0.61	1 (1%)
69	FMN	B	502	-	33,33,33	1.42	6 (18%)	48,50,50	1.30	8 (16%)
73	ZMP	X	201	-	27,33,36	1.96	6 (22%)	32,40,45	1.98	7 (21%)
73	ZMP	Q	201	-	27,33,36	1.94	5 (18%)	32,40,45	1.89	6 (18%)
75	PEE	i	501	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
74	CDL	Aa	101	-	63,63,99	1.27	5 (7%)	69,75,111	1.13	5 (7%)
70	FES	2	303	-	0,4,4	-	-	-	-	-
75	PEE	7	402	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
68	SF4	H	301	8	0,12,12	-	-	-	-	-
74	CDL	l	702	-	63,63,99	1.22	5 (7%)	69,75,111	1.06	4 (5%)
74	CDL	5	501	-	63,63,99	1.24	5 (7%)	69,75,111	0.99	4 (5%)
68	SF4	B	501	2	0,12,12	-	-	-	-	-
68	SF4	G	802	7	0,12,12	-	-	-	-	-
74	CDL	x	402	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	5 (7%)
68	SF4	G	801	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	CDL	8	401	-	63,63,99	1.24	6 (9%)	69,75,111	0.99	4 (5%)
74	CDL	s	201	-	63,63,99	1.23	5 (7%)	69,75,111	1.04	4 (5%)
75	PEE	2	302	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
68	SF4	H	302	8	0,12,12	-	-	-	-	-
78	HEA	Ak	601	60	57,67,67	1.24	6 (10%)	61,103,103	1.47	11 (18%)
75	PEE	w	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.98	2 (3%)
75	PEE	7	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
76	HEM	w	402	47	41,50,50	4.55	13 (31%)	45,82,82	3.39	22 (48%)
76	HEM	7	404	-	41,50,50	4.58	12 (29%)	45,82,82	3.46	18 (40%)
70	FES	4	302	53	0,4,4	-	-	-	-	-
68	SF4	I	301	9	0,12,12	-	-	-	-	-
70	FES	G	803	7	0,4,4	-	-	-	-	-
71	PLX	H	303	-	51,51,51	0.78	1 (1%)	55,59,59	0.63	1 (1%)
75	PEE	5	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
74	CDL	V	201	-	61,61,99	1.18	5 (8%)	64,71,111	1.11	4 (6%)
75	PEE	q	501	-	48,48,50	1.35	4 (8%)	51,53,55	0.92	2 (3%)
77	HEC	x	401	48	32,50,50	2.37	3 (9%)	24,82,82	1.64	5 (20%)
70	FES	E	301	-	0,4,4	-	-	-	-	-
75	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.94	2 (3%)
71	PLX	2	301	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
76	HEM	w	401	47	41,50,50	4.55	12 (29%)	45,82,82	3.37	22 (48%)
78	HEA	Ak	602	60	57,67,67	1.48	6 (10%)	61,103,103	1.46	12 (19%)
74	CDL	i	503	-	63,63,99	1.22	5 (7%)	69,75,111	1.07	4 (5%)
75	PEE	u	502	-	48,48,50	1.38	4 (8%)	51,53,55	0.91	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEC	8	402	48	-	4/10/54/54	-
71	PLX	V	202	-	-	32/55/55/55	-
71	PLX	i	502	-	-	25/55/55/55	-
75	PEE	W	401	-	-	21/52/52/54	-
74	CDL	z	101	-	-	44/74/74/110	-
76	HEM	7	403	47	-	8/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	NDP	L	401	-	-	15/30/77/77	0/5/5/5
74	CDL	u	501	-	-	38/74/74/110	-
71	PLX	4	301	-	-	26/55/55/55	-
69	FMN	B	502	-	-	4/18/18/18	0/3/3/3
73	ZMP	X	201	-	-	7/38/40/43	-
73	ZMP	Q	201	-	-	11/38/40/43	-
75	PEE	i	501	-	-	32/52/52/54	-
74	CDL	Aa	101	-	-	32/74/74/110	-
70	FES	2	303	-	-	-	0/1/1/1
75	PEE	7	402	-	-	30/52/52/54	-
68	SF4	H	301	8	-	-	0/6/5/5
74	CDL	5	501	-	-	40/74/74/110	-
74	CDL	8	401	-	-	37/74/74/110	-
74	CDL	x	402	-	-	44/74/74/110	-
74	CDL	l	702	-	-	25/74/74/110	-
75	PEE	2	302	-	-	27/52/52/54	-
78	HEA	Ak	601	60	-	7/32/76/76	-
68	SF4	B	501	2	-	-	0/6/5/5
74	CDL	s	201	-	-	40/74/74/110	-
68	SF4	G	801	7	-	-	0/6/5/5
68	SF4	G	802	7	-	-	0/6/5/5
68	SF4	H	302	8	-	-	0/6/5/5
75	PEE	w	403	-	-	20/52/52/54	-
75	PEE	7	401	-	-	17/44/44/54	-
76	HEM	w	402	47	-	5/12/54/54	-
76	HEM	7	404	-	-	5/12/54/54	-
70	FES	4	302	53	-	-	0/1/1/1
68	SF4	I	301	9	-	-	0/6/5/5
71	PLX	H	303	-	-	33/55/55/55	-
75	PEE	5	502	-	-	20/52/52/54	-
70	FES	G	803	7	-	-	0/1/1/1
74	CDL	V	201	-	-	28/69/69/110	-
75	PEE	q	501	-	-	22/52/52/54	-
77	HEC	x	401	48	-	6/10/54/54	-
70	FES	E	301	-	-	-	0/1/1/1
75	PEE	l	701	-	-	30/52/52/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	2	301	-	-	27/55/55/55	-
76	HEM	w	401	47	-	5/12/54/54	-
78	HEA	Ak	602	60	-	5/32/76/76	-
74	CDL	i	503	-	-	41/74/74/110	-
75	PEE	u	502	-	-	22/52/52/54	-

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7	403	HEM	C4A-CHB	13.21	1.77	1.41
76	7	404	HEM	C4A-CHB	12.89	1.76	1.41
76	w	401	HEM	C4A-CHB	12.72	1.76	1.41
76	w	402	HEM	C4A-CHB	12.54	1.75	1.41
76	w	401	HEM	C1A-CHA	12.36	1.75	1.41
76	7	404	HEM	C1A-CHA	12.26	1.75	1.41
76	7	403	HEM	C1A-CHA	12.21	1.74	1.41
76	w	402	HEM	C1A-CHA	12.14	1.74	1.41
76	7	403	HEM	CHD-C1D	10.78	1.72	1.41
76	7	404	HEM	CHD-C1D	10.70	1.72	1.41
76	w	401	HEM	CHD-C1D	10.52	1.71	1.41
76	w	402	HEM	CHD-C1D	10.37	1.71	1.41
76	w	401	HEM	CHC-C4B	10.00	1.70	1.41
76	7	404	HEM	CHC-C4B	9.97	1.69	1.41
76	w	402	HEM	CHC-C4B	9.92	1.69	1.41
76	w	401	HEM	CHB-C1B	9.66	1.59	1.35
76	7	403	HEM	CHC-C4B	9.62	1.68	1.41
76	w	402	HEM	CHA-C4D	9.50	1.59	1.35
76	7	403	HEM	CHB-C1B	9.47	1.59	1.35
76	7	404	HEM	CHA-C4D	9.45	1.59	1.35
76	w	402	HEM	CHB-C1B	9.41	1.59	1.35
76	7	403	HEM	CHA-C4D	9.38	1.59	1.35
76	7	404	HEM	CHB-C1B	9.29	1.58	1.35
76	w	401	HEM	CHA-C4D	9.22	1.58	1.35
77	x	401	HEC	C2B-C3B	-8.14	1.32	1.40
76	w	401	HEM	C4D-ND	-6.92	1.28	1.40
76	w	402	HEM	C4D-ND	-6.92	1.28	1.40
77	8	402	HEC	C3C-C2C	-6.86	1.33	1.40
76	7	404	HEM	C4D-ND	-6.76	1.28	1.40
76	7	403	HEM	C1B-NB	-6.67	1.28	1.40
76	7	403	HEM	C4D-ND	-6.67	1.28	1.40
73	Q	201	ZMP	C16-N2	6.62	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	x	401	HEC	C3C-C2C	-6.59	1.33	1.40
76	w	402	HEM	C1B-NB	-6.56	1.29	1.40
76	7	404	HEM	C1B-NB	-6.55	1.29	1.40
78	Ak	602	HEA	C3A-C2A	-6.51	1.31	1.40
77	8	402	HEC	C2B-C3B	-6.49	1.34	1.40
73	X	201	ZMP	C16-N2	6.34	1.47	1.33
76	w	401	HEM	C1B-NB	-6.13	1.29	1.40
77	x	401	HEC	C3D-C2D	5.35	1.53	1.37
77	8	402	HEC	C3D-C2D	5.26	1.53	1.37
69	B	502	FMN	C9A-C5A	4.56	1.48	1.41
74	x	402	CDL	OB8-CB7	4.45	1.46	1.33
73	X	201	ZMP	C9-C10	4.39	1.55	1.50
74	x	402	CDL	OA6-CA5	4.37	1.46	1.34
74	8	401	CDL	OB8-CB7	4.36	1.46	1.33
74	Aa	101	CDL	OB8-CB7	4.34	1.46	1.33
75	5	502	PEE	C39-C38	4.30	1.56	1.31
74	Aa	101	CDL	OA6-CA5	4.28	1.46	1.34
75	7	401	PEE	C39-C38	4.27	1.56	1.31
75	u	502	PEE	O3-C30	4.27	1.45	1.33
75	7	402	PEE	C39-C38	4.25	1.56	1.31
75	q	501	PEE	C39-C38	4.25	1.56	1.31
74	l	702	CDL	OB8-CB7	4.24	1.45	1.33
75	u	502	PEE	C39-C38	4.24	1.56	1.31
75	w	403	PEE	C39-C38	4.24	1.56	1.31
75	5	502	PEE	O3-C30	4.24	1.45	1.33
75	2	302	PEE	C39-C38	4.23	1.56	1.31
74	z	101	CDL	OB8-CB7	4.22	1.45	1.33
75	W	401	PEE	C18-C19	4.21	1.56	1.31
75	W	401	PEE	C39-C38	4.21	1.56	1.31
75	5	502	PEE	C18-C19	4.21	1.56	1.31
75	l	701	PEE	C18-C19	4.21	1.56	1.31
74	s	201	CDL	OA6-CA5	4.20	1.46	1.34
75	2	302	PEE	O3-C30	4.20	1.45	1.33
75	l	701	PEE	C39-C38	4.20	1.56	1.31
75	u	502	PEE	C18-C19	4.20	1.56	1.31
74	5	501	CDL	OB8-CB7	4.20	1.45	1.33
74	8	401	CDL	OA6-CA5	4.19	1.46	1.34
75	2	302	PEE	C18-C19	4.18	1.56	1.31
75	q	501	PEE	C18-C19	4.18	1.56	1.31
74	u	501	CDL	OB8-CB7	4.18	1.45	1.33
74	u	501	CDL	OA6-CA5	4.18	1.46	1.34
75	l	701	PEE	O3-C30	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	5	501	CDL	OA6-CA5	4.17	1.46	1.34
75	i	501	PEE	C39-C38	4.16	1.55	1.31
75	w	403	PEE	C18-C19	4.14	1.55	1.31
74	i	503	CDL	OA6-CA5	4.13	1.46	1.34
75	i	501	PEE	O3-C30	4.13	1.45	1.33
75	i	501	PEE	C18-C19	4.13	1.55	1.31
75	7	402	PEE	O3-C30	4.12	1.45	1.33
75	W	401	PEE	O3-C30	4.12	1.45	1.33
74	i	503	CDL	OB8-CB7	4.12	1.45	1.33
75	7	402	PEE	C18-C19	4.11	1.55	1.31
74	V	201	CDL	OB8-CB7	4.11	1.45	1.33
74	l	702	CDL	OA6-CA5	4.09	1.45	1.34
74	V	201	CDL	OA6-CA5	4.09	1.45	1.34
75	7	401	PEE	O3-C30	4.07	1.45	1.33
74	u	501	CDL	OA8-CA7	4.07	1.45	1.33
74	z	101	CDL	OA6-CA5	4.06	1.45	1.34
75	7	401	PEE	C19-C18	4.06	1.56	1.28
73	Q	201	ZMP	C13-N1	4.05	1.42	1.33
75	q	501	PEE	O3-C30	4.05	1.45	1.33
74	s	201	CDL	OB8-CB7	4.04	1.45	1.33
73	X	201	ZMP	C13-N1	4.02	1.42	1.33
73	Q	201	ZMP	C9-C10	4.02	1.54	1.50
74	Aa	101	CDL	OA8-CA7	4.01	1.45	1.33
75	w	403	PEE	O3-C30	3.99	1.45	1.33
74	8	401	CDL	OA8-CA7	3.98	1.45	1.33
74	x	402	CDL	OA8-CA7	3.96	1.44	1.33
74	5	501	CDL	OA8-CA7	3.94	1.44	1.33
78	Ak	602	HEA	C3A-CMA	-3.90	1.37	1.46
74	s	201	CDL	OA8-CA7	3.87	1.44	1.33
74	l	702	CDL	OA8-CA7	3.86	1.44	1.33
74	i	503	CDL	OA8-CA7	3.82	1.44	1.33
74	z	101	CDL	OA8-CA7	3.76	1.44	1.33
76	w	402	HEM	FE-NB	-3.64	1.78	1.96
76	7	404	HEM	FE-NB	-3.56	1.79	1.96
75	u	502	PEE	O2-C10	3.48	1.44	1.34
76	w	401	HEM	FE-NB	-3.45	1.79	1.96
75	5	502	PEE	O2-C10	3.44	1.44	1.34
76	7	403	HEM	FE-NB	-3.42	1.80	1.96
74	l	702	CDL	OB6-CB5	3.38	1.43	1.34
76	7	404	HEM	FE-ND	-3.37	1.80	1.96
75	q	501	PEE	O2-C10	3.34	1.43	1.34
74	i	503	CDL	OB6-CB5	3.33	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	w	402	HEM	FE-ND	-3.31	1.80	1.96
75	l	701	PEE	O2-C10	3.31	1.43	1.34
76	7	403	HEM	FE-ND	-3.31	1.80	1.96
75	i	501	PEE	O2-C10	3.30	1.43	1.34
78	Ak	601	HEA	C3C-C2C	-3.26	1.35	1.40
74	V	201	CDL	OB6-CB5	3.26	1.43	1.34
75	w	403	PEE	O2-C10	3.26	1.43	1.34
74	8	401	CDL	OB6-CB5	3.25	1.43	1.34
74	Aa	101	CDL	OB6-CB5	3.23	1.43	1.34
75	W	401	PEE	O2-C10	3.23	1.43	1.34
75	7	401	PEE	O2-C10	3.20	1.43	1.34
69	B	502	FMN	C8-C7	3.17	1.48	1.40
74	s	201	CDL	OB6-CB5	3.16	1.43	1.34
74	5	501	CDL	OB6-CB5	3.14	1.43	1.34
75	7	402	PEE	O2-C10	3.13	1.43	1.34
74	u	501	CDL	OB6-CB5	3.13	1.43	1.34
74	z	101	CDL	OB6-CB5	3.12	1.43	1.34
76	w	401	HEM	FE-ND	-3.11	1.81	1.96
72	L	401	NDP	C6N-C5N	3.10	1.38	1.33
75	2	302	PEE	O2-C10	3.10	1.43	1.34
74	x	402	CDL	OB6-CB5	3.06	1.42	1.34
69	B	502	FMN	C4-N3	-3.03	1.33	1.38
74	V	201	CDL	OA8-CA7	3.01	1.44	1.33
78	Ak	601	HEA	C3A-CMA	-2.94	1.39	1.46
71	H	303	PLX	O6-C4	-2.86	1.40	1.44
71	V	202	PLX	O6-C4	-2.84	1.40	1.44
76	w	402	HEM	C1D-C2D	-2.80	1.39	1.44
71	4	301	PLX	O6-C4	-2.78	1.40	1.44
78	Ak	602	HEA	C3C-C2C	-2.74	1.36	1.40
78	Ak	601	HEA	C4C-NC	2.70	1.41	1.36
78	Ak	602	HEA	C1D-C2D	2.69	1.49	1.44
73	Q	201	ZMP	C10-S1	-2.68	1.69	1.76
74	s	201	CDL	OB6-CB4	-2.68	1.39	1.46
74	x	402	CDL	OB6-CB4	-2.67	1.39	1.46
74	u	501	CDL	OB6-CB4	-2.67	1.39	1.46
74	5	501	CDL	OB6-CB4	-2.66	1.39	1.46
78	Ak	602	HEA	C1D-ND	-2.65	1.35	1.40
74	z	101	CDL	OB6-CB4	-2.63	1.40	1.46
73	X	201	ZMP	C10-S1	-2.61	1.69	1.76
74	i	503	CDL	OB6-CB4	-2.61	1.40	1.46
74	Aa	101	CDL	OB6-CB4	-2.59	1.40	1.46
71	i	502	PLX	O6-C4	-2.56	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	2	301	PLX	O6-C4	-2.47	1.41	1.44
74	8	401	CDL	OB6-CB4	-2.43	1.40	1.46
74	V	201	CDL	OB6-CB4	-2.40	1.40	1.46
69	B	502	FMN	C5A-N5	-2.30	1.35	1.39
74	l	702	CDL	OB6-CB4	-2.29	1.40	1.46
78	Ak	602	HEA	CMD-C2D	2.25	1.55	1.50
76	w	401	HEM	C1D-C2D	-2.25	1.40	1.44
76	7	403	HEM	C3B-C4B	-2.24	1.40	1.44
78	Ak	601	HEA	C3A-C2A	-2.19	1.37	1.40
78	Ak	601	HEA	C1C-NC	2.18	1.40	1.36
73	X	201	ZMP	O5-C21	-2.14	1.39	1.44
69	B	502	FMN	C4A-N5	2.14	1.34	1.30
76	w	401	HEM	C2A-C3A	2.14	1.44	1.37
76	7	403	HEM	C2A-C3A	2.14	1.44	1.37
69	B	502	FMN	C2-N3	-2.13	1.34	1.39
76	7	404	HEM	C1D-C2D	-2.12	1.40	1.44
76	w	402	HEM	C2A-C3A	2.12	1.43	1.37
73	X	201	ZMP	O4-C17	-2.07	1.38	1.42
76	7	404	HEM	C2A-C3A	2.07	1.43	1.37
76	w	402	HEM	C3B-C4B	-2.07	1.40	1.44
78	Ak	601	HEA	CHD-C1D	2.06	1.40	1.35
72	L	401	NDP	C5A-C4A	2.05	1.46	1.40
73	Q	201	ZMP	O4-C17	-2.01	1.38	1.42
74	8	401	CDL	C11-CA5	2.00	1.56	1.50

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	403	HEM	C4A-C3A-C2A	-12.30	98.44	107.00
76	7	403	HEM	C4B-CHC-C1C	-10.37	108.87	122.56
76	w	402	HEM	C4C-CHD-C1D	-9.52	109.99	122.56
76	7	404	HEM	C4A-C3A-C2A	-9.50	100.39	107.00
76	7	404	HEM	C4B-CHC-C1C	-9.41	110.14	122.56
76	w	401	HEM	C4C-CHD-C1D	-9.37	110.19	122.56
76	w	402	HEM	C4B-CHC-C1C	-9.35	110.22	122.56
76	w	401	HEM	C4B-CHC-C1C	-9.17	110.46	122.56
76	7	404	HEM	C4C-CHD-C1D	-9.01	110.67	122.56
76	7	403	HEM	C4C-CHD-C1D	-8.52	111.31	122.56
76	w	402	HEM	C4A-C3A-C2A	-7.54	101.75	107.00
76	7	404	HEM	C2B-C1B-NB	6.46	117.50	109.84
76	w	401	HEM	C3D-C4D-ND	6.08	116.94	110.17
76	w	401	HEM	C4A-C3A-C2A	-6.04	102.79	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	403	HEM	C3D-C4D-ND	6.04	116.89	110.17
73	X	201	ZMP	C11-S1-C10	6.04	120.67	101.87
76	w	402	HEM	C2B-C1B-NB	6.02	116.97	109.84
76	7	404	HEM	C3D-C4D-ND	5.75	116.56	110.17
76	7	403	HEM	C2B-C1B-NB	5.75	116.65	109.84
73	Q	201	ZMP	C9-C10-S1	5.66	120.05	113.46
76	w	401	HEM	C2B-C1B-NB	5.56	116.42	109.84
76	w	401	HEM	C2C-C3C-C4C	-5.49	103.07	106.90
73	X	201	ZMP	C9-C10-S1	5.39	119.73	113.46
76	w	402	HEM	C3D-C4D-ND	5.36	116.14	110.17
76	w	402	HEM	C2C-C3C-C4C	-5.26	103.22	106.90
72	L	401	NDP	PN-O3-PA	-5.21	114.94	132.83
73	Q	201	ZMP	C11-S1-C10	5.11	117.78	101.87
76	7	404	HEM	C3B-C2B-C1B	-5.10	102.70	106.49
76	w	402	HEM	C3B-C2B-C1B	-4.94	102.82	106.49
74	V	201	CDL	OA6-CA5-C11	4.93	122.12	111.50
76	7	403	HEM	CHC-C4B-C3B	-4.65	117.45	124.57
76	7	403	HEM	C4B-C3B-C2B	-4.60	103.46	107.11
76	7	404	HEM	C2C-C3C-C4C	-4.55	103.72	106.90
74	Aa	101	CDL	OB6-CB5-C51	4.53	121.27	111.50
76	w	401	HEM	C4B-C3B-C2B	-4.49	103.55	107.11
74	x	402	CDL	OA6-CA5-C11	4.48	121.16	111.50
74	V	201	CDL	OB6-CB5-C51	4.44	121.07	111.50
76	7	404	HEM	C4B-C3B-C2B	-4.43	103.60	107.11
76	w	402	HEM	CHD-C1D-C2D	-4.40	118.11	124.98
76	7	403	HEM	C3B-C2B-C1B	-4.39	103.23	106.49
76	w	401	HEM	C2D-C1D-ND	4.37	115.11	109.88
74	Aa	101	CDL	OA6-CA5-C11	4.34	120.85	111.50
75	5	502	PEE	O2-C10-C11	4.29	120.74	111.50
74	i	503	CDL	OA6-CA5-C11	4.27	120.71	111.50
74	8	401	CDL	OB6-CB5-C51	4.21	120.58	111.50
76	w	402	HEM	C2D-C1D-ND	4.20	114.92	109.88
75	W	401	PEE	O2-C10-C11	4.16	120.47	111.50
74	s	201	CDL	OA6-CA5-C11	4.11	120.35	111.50
75	w	403	PEE	O2-C10-C11	4.01	120.13	111.50
74	z	101	CDL	OA6-CA5-C11	4.00	120.13	111.50
75	i	501	PEE	O2-C10-C11	4.00	120.11	111.50
76	w	401	HEM	C4D-ND-C1D	-3.97	100.97	105.07
74	i	503	CDL	OB6-CB5-C51	3.97	120.05	111.50
78	Ak	601	HEA	C17-C18-C19	-3.96	118.13	127.66
75	7	402	PEE	O2-C10-C11	3.92	119.96	111.50
74	z	101	CDL	OB6-CB5-C51	3.91	119.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	403	HEM	C1B-NB-C4B	-3.91	101.03	105.07
76	w	401	HEM	CHD-C1D-C2D	-3.91	118.88	124.98
74	8	401	CDL	OA6-CA5-C11	3.89	119.88	111.50
75	l	701	PEE	O2-C10-C11	3.88	119.86	111.50
75	q	501	PEE	O2-C10-C11	3.86	119.82	111.50
74	u	501	CDL	OA6-CA5-C11	3.86	119.82	111.50
74	x	402	CDL	OB6-CB5-C51	3.85	119.80	111.50
76	7	403	HEM	C2C-C3C-C4C	-3.84	104.21	106.90
76	7	404	HEM	C1B-NB-C4B	-3.84	101.10	105.07
73	Q	201	ZMP	O1-C10-C9	-3.83	119.47	123.99
74	l	702	CDL	OA6-CA5-C11	3.80	119.69	111.50
76	7	404	HEM	CHC-C4B-C3B	-3.79	118.77	124.57
74	s	201	CDL	OB6-CB5-C51	3.79	119.67	111.50
72	L	401	NDP	N3A-C2A-N1A	-3.78	122.77	128.68
74	5	501	CDL	OB6-CB5-C51	3.78	119.64	111.50
76	w	401	HEM	C3B-C2B-C1B	-3.76	103.69	106.49
74	l	702	CDL	OB6-CB5-C51	3.73	119.54	111.50
76	7	403	HEM	C2D-C1D-ND	3.70	114.32	109.88
74	5	501	CDL	OA6-CA5-C11	3.70	119.47	111.50
76	w	401	HEM	CHC-C4B-C3B	-3.70	118.91	124.57
76	7	404	HEM	C2D-C1D-ND	3.66	114.26	109.88
77	x	401	HEC	CMC-C2C-C1C	-3.65	122.85	128.46
76	w	402	HEM	CHC-C4B-C3B	-3.64	118.99	124.57
74	u	501	CDL	OB6-CB5-C51	3.61	119.29	111.50
76	w	401	HEM	C1B-NB-C4B	-3.58	101.38	105.07
78	Ak	602	HEA	C4A-CHB-C1B	3.57	127.26	122.56
75	2	302	PEE	O2-C10-C11	3.55	119.15	111.50
73	Q	201	ZMP	C15-C14-C13	3.54	118.25	112.36
76	w	402	HEM	C4B-C3B-C2B	-3.54	104.31	107.11
73	X	201	ZMP	O1-C10-C9	-3.52	119.84	123.99
75	u	502	PEE	O2-C10-C11	3.47	118.98	111.50
76	w	402	HEM	C1B-NB-C4B	-3.43	101.53	105.07
76	7	403	HEM	C4D-ND-C1D	-3.43	101.53	105.07
76	7	404	HEM	CHD-C1D-C2D	-3.36	119.73	124.98
75	7	401	PEE	O2-C10-C11	3.26	118.53	111.50
76	w	401	HEM	C1D-C2D-C3D	-3.18	103.61	106.96
74	l	702	CDL	OB8-CB7-C71	3.16	121.83	111.91
77	x	401	HEC	C1D-C2D-C3D	-3.16	104.80	107.00
78	Ak	601	HEA	C13-C14-C15	-3.14	120.10	127.66
76	w	402	HEM	C4D-ND-C1D	-3.09	101.89	105.07
75	7	402	PEE	O3-C30-C31	3.07	121.54	111.91
76	7	403	HEM	CHD-C1D-C2D	-3.07	120.19	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	404	HEM	C4D-ND-C1D	-3.06	101.92	105.07
76	7	404	HEM	CHB-C1B-C2B	-3.02	118.37	126.72
73	X	201	ZMP	C15-C14-C13	2.92	117.23	112.36
74	u	501	CDL	OA8-CA7-C31	2.89	120.96	111.91
76	w	402	HEM	CHB-C1B-C2B	-2.88	118.75	126.72
78	Ak	601	HEA	C1B-C2B-C3B	2.87	110.23	106.80
76	w	401	HEM	CHA-C4D-ND	-2.86	120.84	124.38
76	7	403	HEM	CMB-C2B-C1B	2.86	129.40	125.04
69	B	502	FMN	C4A-C10-N1	-2.86	118.09	124.73
78	Ak	602	HEA	CBA-CAA-C2A	2.84	117.39	112.60
74	x	402	CDL	OB8-CB7-C71	2.83	120.79	111.91
74	Aa	101	CDL	OB8-CB7-C71	2.83	120.78	111.91
76	w	402	HEM	C1D-C2D-C3D	-2.80	104.02	106.96
76	7	404	HEM	C4D-C3D-C2D	-2.76	102.87	106.90
76	7	403	HEM	CMC-C2C-C3C	2.71	129.75	124.68
74	s	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
76	w	402	HEM	C4D-C3D-C2D	-2.69	102.97	106.90
77	8	402	HEC	CMC-C2C-C1C	-2.69	124.33	128.46
69	B	502	FMN	C4-C4A-N5	2.68	122.05	118.23
76	7	403	HEM	C4D-C3D-C2D	-2.67	103.00	106.90
74	i	503	CDL	OB8-CB7-C71	2.67	120.27	111.91
76	w	401	HEM	CMB-C2B-C1B	2.65	129.07	125.04
74	s	201	CDL	OA8-CA7-C31	2.64	120.18	111.91
78	Ak	602	HEA	C4D-CHA-C1A	2.63	126.03	122.56
75	2	302	PEE	O3-C30-C31	2.63	120.17	111.91
76	7	404	HEM	CAD-C3D-C4D	2.63	129.25	124.66
76	7	403	HEM	C1D-C2D-C3D	-2.62	104.21	106.96
77	8	402	HEC	CMB-C2B-C1B	-2.61	124.44	128.46
76	w	402	HEM	CHA-C4D-ND	-2.61	121.16	124.38
78	Ak	602	HEA	CMD-C2D-C1D	2.59	128.99	125.04
74	5	501	CDL	OA8-CA7-C31	2.59	120.04	111.91
74	5	501	CDL	OB8-CB7-C71	2.58	120.02	111.91
74	V	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
74	z	101	CDL	OB8-CB7-C71	2.58	120.01	111.91
75	l	701	PEE	O3-C30-C31	2.57	119.98	111.91
74	u	501	CDL	OB8-CB7-C71	2.56	119.95	111.91
74	x	402	CDL	OA8-CA7-C31	2.56	119.95	111.91
74	z	101	CDL	OA8-CA7-C31	2.56	119.94	111.91
77	8	402	HEC	CBD-CAD-C3D	-2.55	108.27	112.62
76	7	403	HEM	CHA-C4D-C3D	-2.54	120.56	125.33
75	W	401	PEE	O3-C30-C31	2.52	119.81	111.91
76	7	403	HEM	CMA-C3A-C4A	-2.51	124.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	i	503	CDL	OA8-CA7-C31	2.49	119.72	111.91
75	q	501	PEE	O3-C30-C31	2.49	119.71	111.91
74	l	702	CDL	OA8-CA7-C31	2.48	119.70	111.91
71	4	301	PLX	C1C-N1-C1	2.48	120.07	109.92
76	7	404	HEM	C1D-C2D-C3D	-2.48	104.35	106.96
74	Aa	101	CDL	OA8-CA7-C31	2.48	119.69	111.91
76	w	402	HEM	CMB-C2B-C1B	2.48	128.81	125.04
72	L	401	NDP	C4A-C5A-N7A	-2.47	106.82	109.40
77	x	401	HEC	C2B-C3B-C4B	2.47	109.02	106.35
76	w	401	HEM	CHB-C1B-C2B	-2.47	119.88	126.72
75	u	502	PEE	O3-C30-C31	2.47	119.66	111.91
78	Ak	602	HEA	CMC-C2C-C3C	2.46	129.28	124.68
76	w	401	HEM	C4D-C3D-C2D	-2.46	103.32	106.90
78	Ak	602	HEA	C1D-C2D-C3D	-2.45	104.38	106.96
74	Aa	101	CDL	CB4-OB6-CB5	-2.44	111.78	117.79
71	i	502	PLX	C1C-N1-C1	2.43	119.84	109.92
78	Ak	601	HEA	C17-C16-C15	-2.42	105.01	112.98
78	Ak	601	HEA	C20-C19-C18	2.41	125.99	121.12
73	X	201	ZMP	C15-N2-C16	-2.40	118.30	122.59
71	H	303	PLX	C1C-N1-C1	2.40	119.75	109.92
76	7	403	HEM	CBA-CAA-C2A	2.40	116.71	112.62
76	7	403	HEM	CHC-C4B-NB	2.39	127.03	124.43
75	w	403	PEE	O3-C30-C31	2.38	119.36	111.91
78	Ak	602	HEA	C25-C23-C24	2.36	119.82	114.60
76	7	404	HEM	CHA-C4D-ND	-2.36	121.47	124.38
78	Ak	602	HEA	CMB-C2B-C3B	-2.36	125.85	130.34
74	z	101	CDL	CA4-OA6-CA5	-2.35	112.01	117.79
78	Ak	601	HEA	CAD-C3D-C4D	2.35	128.76	124.66
78	Ak	601	HEA	C16-C17-C18	-2.35	104.16	111.88
76	w	402	HEM	CHD-C1D-ND	2.33	126.96	124.43
73	X	201	ZMP	C20-C18-C17	2.33	112.86	108.82
76	w	401	HEM	CMC-C2C-C3C	2.33	129.03	124.68
76	w	401	HEM	CAD-C3D-C4D	2.32	128.72	124.66
75	i	501	PEE	O3-C30-C31	2.32	119.19	111.91
69	B	502	FMN	C4A-C4-N3	2.32	119.07	113.19
76	7	403	HEM	CAD-C3D-C4D	2.31	128.70	124.66
75	7	401	PEE	O3-C30-C31	2.31	119.16	111.91
75	5	502	PEE	O3-C30-C31	2.30	119.12	111.91
71	2	301	PLX	C1C-N1-C1	2.30	119.31	109.92
74	8	401	CDL	OA8-CA7-C31	2.29	119.10	111.91
78	Ak	602	HEA	C13-C14-C15	-2.27	122.19	127.66
76	7	403	HEM	CHB-C1B-NB	-2.27	121.58	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	B	502	FMN	C4-N3-C2	-2.26	121.47	125.64
77	8	402	HEC	C1D-C2D-C3D	-2.24	105.44	107.00
71	V	202	PLX	C1C-N1-C1	2.24	119.09	109.92
74	x	402	CDL	CB4-OB6-CB5	-2.23	112.29	117.79
69	B	502	FMN	C10-N1-C2	2.23	121.36	116.90
72	L	401	NDP	C3D-C2D-C1D	2.22	105.65	101.43
76	w	402	HEM	CAD-C3D-C4D	2.22	128.53	124.66
69	B	502	FMN	O4-C4-C4A	-2.21	120.73	126.60
73	Q	201	ZMP	C14-C15-N2	-2.21	107.43	111.90
78	Ak	602	HEA	C26-C15-C16	2.21	118.99	115.27
76	w	401	HEM	CAA-CBA-CGA	-2.21	107.58	113.76
73	X	201	ZMP	O3-C16-N2	-2.20	118.26	122.99
74	8	401	CDL	OB8-CB7-C71	2.19	118.79	111.91
78	Ak	601	HEA	C4B-C3B-C2B	-2.18	103.68	107.41
77	x	401	HEC	CAA-CBA-CGA	-2.17	107.67	113.76
78	Ak	601	HEA	C12-C13-C14	-2.16	106.53	112.23
75	7	401	PEE	C17-C18-C19	-2.15	112.23	126.84
76	7	403	HEM	CMD-C2D-C1D	2.11	128.26	125.04
73	Q	201	ZMP	C11-C12-N1	-2.11	107.98	112.42
76	7	403	HEM	O2D-CGD-CBD	2.10	120.79	114.03
74	V	201	CDL	CA4-OA6-CA5	-2.10	112.62	117.79
76	w	401	HEM	CAA-C2A-C3A	-2.09	121.25	127.25
78	Ak	602	HEA	CBD-CAD-C3D	2.08	118.41	112.63
76	w	402	HEM	CHC-C4B-NB	2.08	126.69	124.43
69	B	502	FMN	C4A-C10-N10	2.07	119.51	116.48
76	7	403	HEM	CHB-C1B-C2B	-2.07	121.00	126.72
78	Ak	601	HEA	C27-C19-C18	-2.07	118.37	123.68
78	Ak	601	HEA	C4A-CHB-C1B	2.06	125.27	122.56
76	w	402	HEM	O2A-CGA-CBA	2.05	120.62	114.03
74	z	101	CDL	CB4-OB6-CB5	-2.02	112.81	117.79
78	Ak	602	HEA	CMC-C2C-C1C	-2.01	125.37	128.46
77	x	401	HEC	CMD-C2D-C3D	2.01	128.72	124.94
69	B	502	FMN	N3-C2-N1	2.00	123.31	119.38

There are no chirality outliers.

All (835) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	B	502	FMN	C1'-C2'-C3'-C4'
69	B	502	FMN	C3'-C4'-C5'-O5'
69	B	502	FMN	O4'-C4'-C5'-O5'
71	H	303	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
71	H	303	PLX	O9-C24-O8-C5
71	H	303	PLX	O9-C24-C25-C26
71	V	202	PLX	O7-C6-O6-C4
71	V	202	PLX	N1-C1-C2-O1
71	V	202	PLX	C25-C24-O8-C5
71	V	202	PLX	O9-C24-C25-C26
71	i	502	PLX	O7-C6-O6-C4
71	i	502	PLX	C3-O4-P1-O2
71	i	502	PLX	C2-O1-P1-O2
71	2	301	PLX	O7-C6-C7-C8
71	2	301	PLX	O7-C6-O6-C4
71	2	301	PLX	C3-O4-P1-O2
71	2	301	PLX	C3-O4-P1-O3
71	2	301	PLX	N1-C1-C2-O1
71	2	301	PLX	C25-C24-O8-C5
71	4	301	PLX	C7-C6-O6-C4
71	4	301	PLX	O7-C6-O6-C4
71	4	301	PLX	C3-O4-P1-O2
71	4	301	PLX	C3-O4-P1-O3
71	4	301	PLX	C2-O1-P1-O4
71	4	301	PLX	C2-O1-P1-O2
71	4	301	PLX	C2-O1-P1-O3
72	L	401	NDP	C5B-O5B-PA-O1A
72	L	401	NDP	C5D-O5D-PN-O1N
73	Q	201	ZMP	C17-C16-N2-C15
73	X	201	ZMP	O3-C16-C17-C18
73	X	201	ZMP	N2-C16-C17-C18
73	X	201	ZMP	O3-C16-C17-O4
73	X	201	ZMP	N2-C16-C17-O4
73	X	201	ZMP	S1-C11-C12-N1
74	V	201	CDL	CA3-OA5-PA1-OA2
74	V	201	CDL	OA5-CA3-CA4-OA6
74	V	201	CDL	CA4-CA6-OA8-CA7
74	V	201	CDL	CB2-OB2-PB2-OB3
74	V	201	CDL	CB2-OB2-PB2-OB4
74	V	201	CDL	OB7-CB5-OB6-CB4
74	V	201	CDL	OB9-CB7-OB8-CB6
74	V	201	CDL	C71-CB7-OB8-CB6
74	i	503	CDL	OA7-CA5-OA6-CA4
74	i	503	CDL	C11-CA5-OA6-CA4
74	i	503	CDL	CB2-OB2-PB2-OB3
74	i	503	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
74	i	503	CDL	CB3-OB5-PB2-OB4
74	l	702	CDL	CA3-OA5-PA1-OA4
74	l	702	CDL	CB2-OB2-PB2-OB3
74	l	702	CDL	CB3-OB5-PB2-OB3
74	l	702	CDL	CB3-OB5-PB2-OB4
74	s	201	CDL	CA3-OA5-PA1-OA3
74	s	201	CDL	OA7-CA5-OA6-CA4
74	s	201	CDL	C11-CA5-OA6-CA4
74	s	201	CDL	CB3-OB5-PB2-OB4
74	u	501	CDL	CB2-C1-CA2-OA2
74	u	501	CDL	OA5-CA3-CA4-OA6
74	u	501	CDL	OA7-CA5-OA6-CA4
74	u	501	CDL	C11-CA5-OA6-CA4
74	x	402	CDL	O1-C1-CA2-OA2
74	x	402	CDL	C11-CA5-OA6-CA4
74	x	402	CDL	CB3-OB5-PB2-OB2
74	x	402	CDL	CB3-OB5-PB2-OB4
74	x	402	CDL	OB7-CB5-OB6-CB4
74	x	402	CDL	C51-CB5-OB6-CB4
74	z	101	CDL	CB2-C1-CA2-OA2
74	z	101	CDL	CB3-OB5-PB2-OB3
74	z	101	CDL	CB3-OB5-PB2-OB4
74	z	101	CDL	C51-CB5-OB6-CB4
74	5	501	CDL	CA2-OA2-PA1-OA3
74	5	501	CDL	OA5-CA3-CA4-OA6
74	5	501	CDL	C11-CA5-OA6-CA4
74	5	501	CDL	CB3-OB5-PB2-OB4
74	8	401	CDL	O1-C1-CB2-OB2
74	8	401	CDL	CA2-OA2-PA1-OA3
74	8	401	CDL	CA2-OA2-PA1-OA4
74	8	401	CDL	CA3-OA5-PA1-OA2
74	8	401	CDL	CA3-OA5-PA1-OA3
74	8	401	CDL	C11-CA5-OA6-CA4
74	Aa	101	CDL	CA2-OA2-PA1-OA3
74	Aa	101	CDL	CA3-OA5-PA1-OA3
74	Aa	101	CDL	CA3-OA5-PA1-OA4
74	Aa	101	CDL	OA7-CA5-OA6-CA4
74	Aa	101	CDL	C11-CA5-OA6-CA4
74	Aa	101	CDL	CB2-OB2-PB2-OB4
75	W	401	PEE	C11-C10-O2-C2
75	W	401	PEE	C5-C4-O4P-P
75	W	401	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
75	i	501	PEE	C11-C10-O2-C2
75	i	501	PEE	C4-O4P-P-O2P
75	i	501	PEE	C4-O4P-P-O1P
75	l	701	PEE	C5-C4-O4P-P
75	u	502	PEE	C11-C10-O2-C2
75	u	502	PEE	O4-C10-O2-C2
75	w	403	PEE	C37-C38-C39-C40
75	2	302	PEE	C4-O4P-P-O2P
75	5	502	PEE	C1-O3P-P-O2P
75	5	502	PEE	C4-O4P-P-O3P
75	5	502	PEE	C4-O4P-P-O2P
75	5	502	PEE	C4-O4P-P-O1P
75	7	401	PEE	C11-C10-O2-C2
75	7	401	PEE	C1-O3P-P-O2P
75	7	401	PEE	C1-O3P-P-O1P
75	7	401	PEE	C4-O4P-P-O2P
75	7	402	PEE	O4P-C4-C5-N
75	7	402	PEE	C39-C40-C41-C42
76	w	401	HEM	C2B-C3B-CAB-CBB
76	w	401	HEM	C4B-C3B-CAB-CBB
76	w	402	HEM	C2B-C3B-CAB-CBB
76	w	402	HEM	C4B-C3B-CAB-CBB
76	7	403	HEM	C1A-C2A-CAA-CBA
76	7	404	HEM	C3A-C2A-CAA-CBA
77	x	401	HEC	C1A-C2A-CAA-CBA
77	x	401	HEC	C3A-C2A-CAA-CBA
77	x	401	HEC	C2D-C3D-CAD-CBD
77	x	401	HEC	C4D-C3D-CAD-CBD
78	Ak	601	HEA	C12-C11-C3B-C2B
74	x	402	CDL	OB9-CB7-OB8-CB6
74	5	501	CDL	OB9-CB7-OB8-CB6
74	x	402	CDL	C71-CB7-OB8-CB6
74	5	501	CDL	C71-CB7-OB8-CB6
74	Aa	101	CDL	C71-CB7-OB8-CB6
74	s	201	CDL	OA9-CA7-OA8-CA6
74	Aa	101	CDL	OA9-CA7-OA8-CA6
74	Aa	101	CDL	OB9-CB7-OB8-CB6
74	x	402	CDL	OA7-CA5-OA6-CA4
74	z	101	CDL	OB7-CB5-OB6-CB4
74	5	501	CDL	OA7-CA5-OA6-CA4
74	8	401	CDL	OA7-CA5-OA6-CA4
75	W	401	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
75	i	501	PEE	O4-C10-O2-C2
75	7	401	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C31-CA7-OA8-CA6
74	V	201	CDL	C51-CB5-OB6-CB4
74	z	101	CDL	OB9-CB7-OB8-CB6
74	i	503	CDL	C31-CA7-OA8-CA6
74	s	201	CDL	C31-CA7-OA8-CA6
74	x	402	CDL	C31-CA7-OA8-CA6
75	i	501	PEE	C37-C38-C39-C40
74	u	501	CDL	OA9-CA7-OA8-CA6
74	x	402	CDL	OA9-CA7-OA8-CA6
74	u	501	CDL	O1-C1-CA2-OA2
74	5	501	CDL	O1-C1-CA2-OA2
73	Q	201	ZMP	O3-C16-N2-C15
74	i	503	CDL	C51-CB5-OB6-CB4
74	l	702	CDL	C11-CA5-OA6-CA4
75	q	501	PEE	C11-C10-O2-C2
74	8	401	CDL	CB4-CB6-OB8-CB7
74	x	402	CDL	C31-C32-C33-C34
75	7	401	PEE	C31-C32-C33-C34
75	i	501	PEE	C32-C33-C34-C35
72	L	401	NDP	O4B-C4B-C5B-O5B
72	L	401	NDP	C3B-C4B-C5B-O5B
74	u	501	CDL	C31-CA7-OA8-CA6
74	z	101	CDL	C71-CB7-OB8-CB6
76	w	402	HEM	C3D-CAD-CBD-CGD
74	l	702	CDL	C73-C74-C75-C76
74	i	503	CDL	OA9-CA7-OA8-CA6
78	Ak	601	HEA	C15-C16-C17-C18
72	L	401	NDP	C1B-C2B-O2B-P2B
74	x	402	CDL	C53-C54-C55-C56
74	z	101	CDL	CA2-C1-CB2-OB2
74	8	401	CDL	CA2-C1-CB2-OB2
74	i	503	CDL	OB7-CB5-OB6-CB4
74	l	702	CDL	OA7-CA5-OA6-CA4
74	5	501	CDL	C31-CA7-OA8-CA6
75	l	701	PEE	C31-C30-O3-C3
71	V	202	PLX	C16-C17-C18-C19
74	8	401	CDL	C12-C13-C14-C15
71	4	301	PLX	C30-C31-C32-C33
75	i	501	PEE	C34-C35-C36-C37
74	z	101	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
74	i	503	CDL	OB6-CB4-CB6-OB8
75	q	501	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C51-CB5-OB6-CB4
74	8	401	CDL	CA7-C31-C32-C33
71	2	301	PLX	C7-C8-C9-C10
77	8	402	HEC	C3D-CAD-CBD-CGD
75	l	701	PEE	C17-C18-C19-C20
75	q	501	PEE	C17-C18-C19-C20
75	2	302	PEE	C37-C38-C39-C40
71	H	303	PLX	C19-C20-C21-C22
74	i	503	CDL	CA7-C31-C32-C33
74	s	201	CDL	CA5-C11-C12-C13
74	z	101	CDL	CA5-C11-C12-C13
74	Aa	101	CDL	CB7-C71-C72-C73
75	i	501	PEE	C30-C31-C32-C33
75	7	402	PEE	C10-C11-C12-C13
74	V	201	CDL	C1-CA2-OA2-PA1
71	4	301	PLX	C2-C1-N1-C1C
74	i	503	CDL	CB5-C51-C52-C53
75	l	701	PEE	C30-C31-C32-C33
74	z	101	CDL	C11-CA5-OA6-CA4
74	5	501	CDL	OA9-CA7-OA8-CA6
74	s	201	CDL	CB7-C71-C72-C73
75	u	502	PEE	C30-C31-C32-C33
74	s	201	CDL	O1-C1-CA2-OA2
72	L	401	NDP	C3B-C2B-O2B-P2B
75	l	701	PEE	O5-C30-O3-C3
75	i	501	PEE	C39-C40-C41-C42
75	i	501	PEE	C17-C18-C19-C20
71	2	301	PLX	C3-O4-P1-O1
71	4	301	PLX	C3-O4-P1-O1
74	V	201	CDL	CB2-OB2-PB2-OB5
74	i	503	CDL	CA3-OA5-PA1-OA2
74	i	503	CDL	CB2-OB2-PB2-OB5
74	i	503	CDL	CB3-OB5-PB2-OB2
74	l	702	CDL	CA3-OA5-PA1-OA2
74	l	702	CDL	CB2-OB2-PB2-OB5
74	l	702	CDL	CB3-OB5-PB2-OB2
74	s	201	CDL	CA3-OA5-PA1-OA2
74	u	501	CDL	CB2-OB2-PB2-OB5
74	z	101	CDL	CB3-OB5-PB2-OB2
74	5	501	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
74	5	501	CDL	CB3-OB5-PB2-OB2
74	8	401	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CA3-OA5-PA1-OA2
74	Aa	101	CDL	CB2-OB2-PB2-OB5
75	i	501	PEE	C4-O4P-P-O3P
75	l	701	PEE	C1-O3P-P-O4P
75	2	302	PEE	C4-O4P-P-O3P
75	5	502	PEE	C1-O3P-P-O4P
75	7	401	PEE	C1-O3P-P-O4P
75	7	401	PEE	C4-O4P-P-O3P
74	x	402	CDL	CB2-C1-CA2-OA2
74	5	501	CDL	CB2-C1-CA2-OA2
74	z	101	CDL	OA7-CA5-OA6-CA4
74	Aa	101	CDL	OB7-CB5-OB6-CB4
71	H	303	PLX	C2-C1-N1-C1C
71	H	303	PLX	C2-C1-N1-C1A
71	V	202	PLX	O6-C6-C7-C8
71	2	301	PLX	O6-C6-C7-C8
71	4	301	PLX	C9-C10-C11-C12
74	i	503	CDL	C53-C54-C55-C56
74	s	201	CDL	C51-C52-C53-C54
74	z	101	CDL	C12-C13-C14-C15
74	z	101	CDL	C13-C14-C15-C16
75	i	501	PEE	C22-C23-C24-C25
75	l	701	PEE	C34-C35-C36-C37
71	H	303	PLX	C15-C16-C17-C18
71	V	202	PLX	C10-C11-C12-C13
74	V	201	CDL	C13-C14-C15-C16
74	s	201	CDL	C14-C15-C16-C17
74	u	501	CDL	C52-C53-C54-C55
75	l	701	PEE	C23-C24-C25-C26
75	l	701	PEE	C14-C15-C16-C17
75	w	403	PEE	C20-C21-C22-C23
75	5	502	PEE	C11-C12-C13-C14
74	5	501	CDL	CA6-CA4-OA6-CA5
74	8	401	CDL	CA6-CA4-OA6-CA5
75	W	401	PEE	C33-C34-C35-C36
74	Aa	101	CDL	CB4-CB3-OB5-PB2
71	i	502	PLX	C17-C18-C19-C20
71	i	502	PLX	C34-C35-C36-C37
74	z	101	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
75	i	501	PEE	C21-C22-C23-C24
74	i	503	CDL	O1-C1-CA2-OA2
74	l	702	CDL	O1-C1-CB2-OB2
74	z	101	CDL	O1-C1-CB2-OB2
71	i	502	PLX	C26-C27-C28-C29
74	z	101	CDL	C73-C74-C75-C76
74	V	201	CDL	CB5-C51-C52-C53
74	i	503	CDL	C12-C13-C14-C15
74	u	501	CDL	C53-C54-C55-C56
75	q	501	PEE	C41-C42-C43-C44
71	2	301	PLX	C12-C13-C14-C15
75	w	403	PEE	C13-C14-C15-C16
75	w	403	PEE	C11-C12-C13-C14
75	2	302	PEE	C21-C22-C23-C24
71	V	202	PLX	C30-C31-C32-C33
71	i	502	PLX	C10-C11-C12-C13
74	s	201	CDL	C71-C72-C73-C74
74	u	501	CDL	C13-C14-C15-C16
74	x	402	CDL	C73-C74-C75-C76
74	Aa	101	CDL	C33-C34-C35-C36
75	u	502	PEE	C32-C33-C34-C35
74	8	401	CDL	C73-C74-C75-C76
75	q	501	PEE	C20-C21-C22-C23
75	q	501	PEE	C13-C14-C15-C16
75	2	302	PEE	C11-C12-C13-C14
71	4	301	PLX	C12-C13-C14-C15
75	l	701	PEE	C33-C34-C35-C36
75	2	302	PEE	C22-C23-C24-C25
75	7	401	PEE	C11-C12-C13-C14
75	q	501	PEE	C35-C36-C37-C38
75	5	502	PEE	C19-C20-C21-C22
75	7	402	PEE	C35-C36-C37-C38
75	u	502	PEE	C11-C12-C13-C14
75	w	403	PEE	C22-C23-C24-C25
71	V	202	PLX	C27-C28-C29-C30
73	Q	201	ZMP	C6-C7-C8-C9
74	i	503	CDL	C31-C32-C33-C34
74	Aa	101	CDL	C32-C33-C34-C35
74	Aa	101	CDL	C34-C35-C36-C37
74	Aa	101	CDL	C71-C72-C73-C74
75	5	502	PEE	C22-C23-C24-C25
71	H	303	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
71	2	301	PLX	C32-C33-C34-C35
75	q	501	PEE	C11-C12-C13-C14
74	l	702	CDL	C32-C33-C34-C35
74	u	501	CDL	C11-C12-C13-C14
71	V	202	PLX	C12-C13-C14-C15
71	V	202	PLX	C26-C27-C28-C29
71	4	301	PLX	C7-C8-C9-C10
75	i	501	PEE	C20-C21-C22-C23
75	u	502	PEE	C34-C35-C36-C37
75	w	403	PEE	C32-C33-C34-C35
76	7	404	HEM	C2A-CAA-CBA-CGA
74	5	501	CDL	C71-C72-C73-C74
75	7	402	PEE	C32-C33-C34-C35
71	2	301	PLX	C17-C18-C19-C20
74	x	402	CDL	C33-C34-C35-C36
75	2	302	PEE	C32-C33-C34-C35
71	4	301	PLX	C28-C29-C30-C31
71	i	502	PLX	C7-C8-C9-C10
71	V	202	PLX	C17-C18-C19-C20
71	2	301	PLX	C26-C27-C28-C29
74	x	402	CDL	C13-C14-C15-C16
74	z	101	CDL	C71-C72-C73-C74
74	Aa	101	CDL	C31-C32-C33-C34
75	W	401	PEE	C35-C36-C37-C38
74	i	503	CDL	C73-C74-C75-C76
75	i	501	PEE	C41-C42-C43-C44
74	l	702	CDL	CA2-C1-CB2-OB2
75	i	501	PEE	C13-C14-C15-C16
75	l	701	PEE	C11-C12-C13-C14
75	l	701	PEE	C42-C43-C44-C45
74	5	501	CDL	C31-C32-C33-C34
75	7	402	PEE	C41-C42-C43-C44
71	H	303	PLX	C2-C1-N1-C1B
75	7	402	PEE	C30-C31-C32-C33
71	H	303	PLX	C25-C26-C27-C28
74	8	401	CDL	C71-CB7-OB8-CB6
75	2	302	PEE	C11-C10-O2-C2
71	i	502	PLX	C12-C13-C14-C15
74	z	101	CDL	C72-C73-C74-C75
74	s	201	CDL	CB5-C51-C52-C53
74	5	501	CDL	CA7-C31-C32-C33
75	u	502	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
71	4	301	PLX	C10-C11-C12-C13
75	7	402	PEE	C12-C13-C14-C15
74	i	503	CDL	C55-C56-C57-C58
75	7	401	PEE	C33-C34-C35-C36
75	u	502	PEE	C37-C38-C39-C40
71	2	301	PLX	C28-C29-C30-C31
74	z	101	CDL	C15-C16-C17-C18
75	i	501	PEE	C15-C16-C17-C18
75	l	701	PEE	C19-C20-C21-C22
75	q	501	PEE	C15-C16-C17-C18
74	l	702	CDL	OB7-CB5-OB6-CB4
75	7	402	PEE	O4-C10-O2-C2
74	u	501	CDL	CB7-C71-C72-C73
74	u	501	CDL	C71-CB7-OB8-CB6
71	i	502	PLX	C33-C34-C35-C36
74	s	201	CDL	C73-C74-C75-C76
74	x	402	CDL	CB7-C71-C72-C73
71	i	502	PLX	C30-C31-C32-C33
75	5	502	PEE	C20-C21-C22-C23
73	Q	201	ZMP	C4-C5-C6-C7
74	u	501	CDL	C51-C52-C53-C54
71	2	301	PLX	C9-C10-C11-C12
74	x	402	CDL	C34-C35-C36-C37
75	W	401	PEE	C12-C13-C14-C15
74	l	702	CDL	C51-CB5-OB6-CB4
75	7	402	PEE	C11-C10-O2-C2
74	8	401	CDL	OB9-CB7-OB8-CB6
71	H	303	PLX	C10-C11-C12-C13
71	V	202	PLX	C9-C10-C11-C12
74	i	503	CDL	C71-C72-C73-C74
74	8	401	CDL	C71-C72-C73-C74
75	q	501	PEE	C31-C32-C33-C34
75	7	402	PEE	C40-C41-C42-C43
75	2	302	PEE	O4-C10-O2-C2
75	W	401	PEE	C21-C22-C23-C24
71	V	202	PLX	O6-C4-C5-O8
74	8	401	CDL	C13-C14-C15-C16
75	u	502	PEE	C12-C13-C14-C15
71	4	301	PLX	C2-C1-N1-C1B
71	4	301	PLX	C2-C1-N1-C1A
75	q	501	PEE	C23-C24-C25-C26
75	7	401	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
75	7	402	PEE	C19-C20-C21-C22
74	u	501	CDL	C71-C72-C73-C74
74	x	402	CDL	C15-C16-C17-C18
75	W	401	PEE	C11-C12-C13-C14
71	H	303	PLX	C9-C10-C11-C12
71	V	202	PLX	C18-C19-C20-C21
73	Q	201	ZMP	C2-C3-C4-C5
74	u	501	CDL	C32-C33-C34-C35
71	H	303	PLX	C16-C17-C18-C19
71	2	301	PLX	C13-C14-C15-C16
74	5	501	CDL	C13-C14-C15-C16
75	W	401	PEE	C31-C32-C33-C34
75	i	501	PEE	C23-C24-C25-C26
75	i	501	PEE	C40-C41-C42-C43
75	i	501	PEE	C16-C17-C18-C19
71	H	303	PLX	C2-O1-P1-O4
74	s	201	CDL	CB3-OB5-PB2-OB2
74	5	501	CDL	CA2-OA2-PA1-OA5
75	7	402	PEE	C1-O3P-P-O4P
75	7	402	PEE	C33-C34-C35-C36
75	2	302	PEE	C2-C1-O3P-P
74	V	201	CDL	OA5-CA3-CA4-CA6
74	i	503	CDL	OB5-CB3-CB4-CB6
74	l	702	CDL	OB5-CB3-CB4-CB6
74	u	501	CDL	OB5-CB3-CB4-CB6
75	i	501	PEE	O3P-C1-C2-C3
75	l	701	PEE	O3P-C1-C2-C3
75	w	403	PEE	O3P-C1-C2-C3
74	z	101	CDL	CA7-C31-C32-C33
75	u	502	PEE	C21-C22-C23-C24
75	q	501	PEE	C39-C40-C41-C42
74	V	201	CDL	C22-C23-C24-C25
74	i	503	CDL	CB2-C1-CA2-OA2
74	Aa	101	CDL	C51-C52-C53-C54
71	H	303	PLX	C11-C12-C13-C14
71	4	301	PLX	C3-C4-C5-O8
74	u	501	CDL	CA3-CA4-CA6-OA8
74	z	101	CDL	CA3-CA4-CA6-OA8
74	z	101	CDL	CB3-CB4-CB6-OB8
74	8	401	CDL	CB3-CB4-CB6-OB8
75	7	402	PEE	C1-C2-C3-O3
74	u	501	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
74	s	201	CDL	C74-C75-C76-C77
75	l	701	PEE	C40-C41-C42-C43
75	5	502	PEE	C33-C34-C35-C36
74	l	702	CDL	C13-C14-C15-C16
75	w	403	PEE	C41-C42-C43-C44
75	q	501	PEE	C10-C11-C12-C13
71	i	502	PLX	O6-C6-C7-C8
73	Q	201	ZMP	O3-C16-C17-O4
71	4	301	PLX	C31-C32-C33-C34
75	w	403	PEE	C35-C36-C37-C38
75	w	403	PEE	C39-C40-C41-C42
75	7	401	PEE	C15-C16-C17-C18
75	7	402	PEE	C15-C16-C17-C18
74	x	402	CDL	C12-C13-C14-C15
74	Aa	101	CDL	C15-C16-C17-C18
75	5	502	PEE	C42-C43-C44-C45
71	V	202	PLX	C13-C14-C15-C16
74	u	501	CDL	CA6-CA4-OA6-CA5
75	i	501	PEE	C42-C43-C44-C45
75	i	501	PEE	C2-C1-O3P-P
71	H	303	PLX	C28-C29-C30-C31
74	z	101	CDL	C75-C76-C77-C78
74	x	402	CDL	C11-C12-C13-C14
74	i	503	CDL	OA6-CA4-CA6-OA8
73	X	201	ZMP	C5-C6-C7-C8
75	2	302	PEE	C34-C35-C36-C37
75	2	302	PEE	C30-C31-C32-C33
71	i	502	PLX	C11-C10-C9-C8
75	2	302	PEE	C24-C25-C26-C27
75	7	402	PEE	C13-C14-C15-C16
71	2	301	PLX	C11-C10-C9-C8
74	8	401	CDL	C52-C53-C54-C55
74	i	503	CDL	C11-C12-C13-C14
71	H	303	PLX	O4-C3-C4-C5
71	V	202	PLX	O4-C3-C4-C5
74	s	201	CDL	OB5-CB3-CB4-CB6
75	2	302	PEE	C20-C21-C22-C23
75	l	701	PEE	O4P-C4-C5-N
71	i	502	PLX	C20-C21-C22-C23
71	2	301	PLX	C14-C15-C16-C17
74	8	401	CDL	C1-CA2-OA2-PA1
71	V	202	PLX	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
74	u	501	CDL	C75-C76-C77-C78
74	z	101	CDL	C33-C34-C35-C36
75	w	403	PEE	C40-C41-C42-C43
71	H	303	PLX	C29-C30-C31-C32
76	7	403	HEM	C3D-CAD-CBD-CGD
74	l	702	CDL	C34-C35-C36-C37
71	V	202	PLX	C3-C4-C5-O8
71	2	301	PLX	C3-C4-C5-O8
74	V	201	CDL	CA3-CA4-CA6-OA8
74	i	503	CDL	CB3-CB4-CB6-OB8
74	x	402	CDL	CA3-CA4-CA6-OA8
75	l	701	PEE	C20-C21-C22-C23
75	7	402	PEE	C22-C23-C24-C25
74	l	702	CDL	C53-C54-C55-C56
71	H	303	PLX	C3-C4-O6-C6
71	V	202	PLX	C5-C4-O6-C6
74	s	201	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CB3-OB5-PB2-OB2
75	7	402	PEE	C4-O4P-P-O3P
74	l	702	CDL	OB5-CB3-CB4-OB6
74	u	501	CDL	OB5-CB3-CB4-OB6
74	z	101	CDL	OB5-CB3-CB4-OB6
75	w	403	PEE	O3P-C1-C2-O2
71	V	202	PLX	C28-C29-C30-C31
74	z	101	CDL	C11-C12-C13-C14
75	q	501	PEE	C24-C25-C26-C27
74	u	501	CDL	OA6-CA4-CA6-OA8
74	x	402	CDL	OA6-CA4-CA6-OA8
74	z	101	CDL	OB6-CB4-CB6-OB8
74	5	501	CDL	C75-C76-C77-C78
75	u	502	PEE	C14-C15-C16-C17
74	5	501	CDL	C51-CB5-OB6-CB4
71	i	502	PLX	C29-C30-C31-C32
74	s	201	CDL	CB4-CB3-OB5-PB2
74	u	501	CDL	C1-CA2-OA2-PA1
74	z	101	CDL	CB4-CB3-OB5-PB2
74	Aa	101	CDL	C1-CA2-OA2-PA1
71	i	502	PLX	C35-C36-C37-C38
71	2	301	PLX	C19-C20-C21-C22
75	7	402	PEE	C34-C35-C36-C37
71	2	301	PLX	C25-C26-C27-C28
75	l	701	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
74	i	503	CDL	C13-C14-C15-C16
71	V	202	PLX	C36-C37-C38-C39
71	i	502	PLX	C9-C10-C11-C12
71	V	202	PLX	O8-C24-C25-C26
74	s	201	CDL	C31-C32-C33-C34
75	7	402	PEE	C20-C21-C22-C23
71	2	301	PLX	O4-C3-C4-C5
74	s	201	CDL	OA5-CA3-CA4-CA6
74	u	501	CDL	OA5-CA3-CA4-CA6
74	z	101	CDL	OB5-CB3-CB4-CB6
74	8	401	CDL	OB5-CB3-CB4-CB6
74	8	401	CDL	C32-C33-C34-C35
75	5	502	PEE	C14-C15-C16-C17
75	7	402	PEE	C16-C17-C18-C19
71	4	301	PLX	C27-C28-C29-C30
75	2	302	PEE	C39-C40-C41-C42
75	7	402	PEE	C11-C12-C13-C14
75	l	701	PEE	C22-C23-C24-C25
73	Q	201	ZMP	N2-C16-C17-O4
74	8	401	CDL	C75-C76-C77-C78
75	i	501	PEE	C31-C32-C33-C34
71	H	303	PLX	C27-C28-C29-C30
74	l	702	CDL	CB6-CB4-OB6-CB5
76	7	403	HEM	C2B-C3B-CAB-CBB
74	5	501	CDL	C72-C73-C74-C75
75	u	502	PEE	C31-C32-C33-C34
74	x	402	CDL	CA4-CA3-OA5-PA1
74	5	501	CDL	CB3-CB4-CB6-OB8
71	V	202	PLX	O4-C3-C4-O6
74	i	503	CDL	OB5-CB3-CB4-OB6
74	s	201	CDL	OA5-CA3-CA4-OA6
74	s	201	CDL	OB5-CB3-CB4-OB6
74	8	401	CDL	C72-C71-CB7-OB8
74	x	402	CDL	C14-C15-C16-C17
74	z	101	CDL	C74-C75-C76-C77
71	H	303	PLX	C6-C7-C8-C9
71	i	502	PLX	C6-C7-C8-C9
74	s	201	CDL	CB2-C1-CA2-OA2
74	5	501	CDL	OB7-CB5-OB6-CB4
74	V	201	CDL	OA6-CA4-CA6-OA8
74	5	501	CDL	OB6-CB4-CB6-OB8
72	L	401	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
72	L	401	NDP	C5D-O5D-PN-O3
74	s	201	CDL	C13-C14-C15-C16
75	2	302	PEE	C15-C16-C17-C18
75	w	403	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C14-C15-C16-C17
73	Q	201	ZMP	C2-C1-C22-C23
74	i	503	CDL	C52-C53-C54-C55
75	i	501	PEE	C24-C25-C26-C27
71	i	502	PLX	C18-C19-C20-C21
74	Aa	101	CDL	C13-C14-C15-C16
71	2	301	PLX	C34-C35-C36-C37
74	i	503	CDL	C35-C36-C37-C38
71	V	202	PLX	C11-C12-C13-C14
74	s	201	CDL	C33-C34-C35-C36
71	H	303	PLX	C24-C25-C26-C27
71	H	303	PLX	C3-O4-P1-O1
71	i	502	PLX	C3-O4-P1-O1
75	W	401	PEE	C1-O3P-P-O4P
75	q	501	PEE	C4-O4P-P-O3P
74	i	503	CDL	O1-C1-CB2-OB2
74	x	402	CDL	C1-CA2-OA2-PA1
74	z	101	CDL	C1-CA2-OA2-PA1
74	8	401	CDL	CA4-CA3-OA5-PA1
75	l	701	PEE	C2-C1-O3P-P
71	H	303	PLX	C3-O4-P1-O3
71	H	303	PLX	C2-O1-P1-O2
72	L	401	NDP	C5B-O5B-PA-O2A
72	L	401	NDP	C5D-O5D-PN-O2N
74	V	201	CDL	CA2-OA2-PA1-OA4
74	V	201	CDL	CA3-OA5-PA1-OA4
74	V	201	CDL	CB3-OB5-PB2-OB3
74	i	503	CDL	CA3-OA5-PA1-OA3
74	i	503	CDL	CA3-OA5-PA1-OA4
74	s	201	CDL	CB3-OB5-PB2-OB3
74	u	501	CDL	CB2-OB2-PB2-OB4
74	x	402	CDL	CA2-OA2-PA1-OA3
74	x	402	CDL	CB3-OB5-PB2-OB3
74	5	501	CDL	CB2-OB2-PB2-OB3
74	5	501	CDL	CB3-OB5-PB2-OB3
75	l	701	PEE	C1-O3P-P-O2P
75	q	501	PEE	C4-O4P-P-O2P
75	q	501	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
75	2	302	PEE	C4-O4P-P-O1P
75	5	502	PEE	C1-O3P-P-O1P
75	7	401	PEE	C4-O4P-P-O1P
75	7	402	PEE	C1-O3P-P-O2P
75	7	402	PEE	C1-O3P-P-O1P
74	5	501	CDL	OA5-CA3-CA4-CA6
71	4	301	PLX	C18-C19-C20-C21
75	1	701	PEE	C38-C39-C40-C41
75	2	302	PEE	C17-C18-C19-C20
75	7	402	PEE	C17-C18-C19-C20
71	i	502	PLX	C36-C37-C38-C39
71	4	301	PLX	C25-C24-O8-C5
75	2	302	PEE	C5-C4-O4P-P
75	W	401	PEE	C13-C14-C15-C16
71	H	303	PLX	C12-C13-C14-C15
71	i	502	PLX	C27-C28-C29-C30
71	H	303	PLX	O4-C3-C4-O6
71	2	301	PLX	O4-C3-C4-O6
74	5	501	CDL	OB5-CB3-CB4-OB6
75	i	501	PEE	O3P-C1-C2-O2
74	s	201	CDL	C15-C16-C17-C18
74	l	702	CDL	C15-C16-C17-C18
75	w	403	PEE	C11-C10-O2-C2
75	2	302	PEE	C14-C15-C16-C17
74	l	702	CDL	CB5-C51-C52-C53
74	z	101	CDL	C12-C11-CA5-OA6
71	H	303	PLX	N1-C1-C2-O1
74	V	201	CDL	OA9-CA7-OA8-CA6
74	i	503	CDL	CA3-CA4-CA6-OA8
74	u	501	CDL	CB3-CB4-CB6-OB8
74	5	501	CDL	CA3-CA4-CA6-OA8
76	w	401	HEM	C3A-C2A-CAA-CBA
77	8	402	HEC	C1A-C2A-CAA-CBA
77	8	402	HEC	C3A-C2A-CAA-CBA
71	4	301	PLX	O6-C4-C5-O8
74	u	501	CDL	OB6-CB4-CB6-OB8
74	z	101	CDL	OA6-CA4-CA6-OA8
74	5	501	CDL	OA6-CA4-CA6-OA8
74	8	401	CDL	OB6-CB4-CB6-OB8
75	7	402	PEE	O2-C2-C3-O3
74	V	201	CDL	C15-C16-C17-C18
74	8	401	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
74	i	503	CDL	C33-C34-C35-C36
71	V	202	PLX	O7-C6-C7-C8
71	i	502	PLX	O7-C6-C7-C8
74	x	402	CDL	C35-C36-C37-C38
72	L	401	NDP	O4D-C1D-N1N-C6N
75	u	502	PEE	C33-C34-C35-C36
71	4	301	PLX	C33-C34-C35-C36
75	l	701	PEE	C41-C42-C43-C44
74	V	201	CDL	C12-C11-CA5-OA6
74	x	402	CDL	CA3-CA4-OA6-CA5
75	i	501	PEE	C3-C2-O2-C10
74	8	401	CDL	OB5-CB3-CB4-OB6
75	l	701	PEE	O3P-C1-C2-O2
71	2	301	PLX	C29-C30-C31-C32
75	2	302	PEE	C31-C32-C33-C34
75	5	502	PEE	C38-C39-C40-C41
71	i	502	PLX	C2-O1-P1-O4
74	u	501	CDL	CA3-OA5-PA1-OA2
74	x	402	CDL	CA3-OA5-PA1-OA2
74	z	101	CDL	CA2-OA2-PA1-OA5
74	z	101	CDL	CB2-OB2-PB2-OB5
74	5	501	CDL	CA3-OA5-PA1-OA2
75	i	501	PEE	C1-O3P-P-O4P
75	u	502	PEE	C4-O4P-P-O3P
75	2	302	PEE	C1-O3P-P-O4P
73	Q	201	ZMP	C22-C1-C2-C3
74	x	402	CDL	C74-C75-C76-C77
74	8	401	CDL	C55-C56-C57-C58
75	5	502	PEE	C40-C41-C42-C43
75	7	402	PEE	C31-C32-C33-C34
74	x	402	CDL	C52-C53-C54-C55
71	4	301	PLX	C4-C3-O4-P1
74	i	503	CDL	C32-C31-CA7-OA8
71	V	202	PLX	C33-C34-C35-C36
74	s	201	CDL	C71-CB7-OB8-CB6
75	l	701	PEE	C15-C16-C17-C18
72	L	401	NDP	C2D-C1D-N1N-C6N
75	i	501	PEE	O4P-C4-C5-N
75	5	502	PEE	O4P-C4-C5-N
74	5	501	CDL	C55-C56-C57-C58
71	V	202	PLX	C7-C8-C9-C10
74	5	501	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
71	V	202	PLX	C32-C33-C34-C35
74	i	503	CDL	C74-C75-C76-C77
74	z	101	CDL	CB7-C71-C72-C73
74	s	201	CDL	OA6-CA4-CA6-OA8
73	Q	201	ZMP	C5-C6-C7-C8
74	i	503	CDL	CB4-CB3-OB5-PB2
75	q	501	PEE	C18-C19-C20-C21
74	8	401	CDL	C54-C55-C56-C57
71	H	303	PLX	C3-C4-C5-O8
74	Aa	101	CDL	CB2-C1-CA2-OA2
78	Ak	601	HEA	CAD-CBD-CGD-O1D
75	W	401	PEE	C41-C42-C43-C44
75	w	403	PEE	C15-C16-C17-C18
76	w	402	HEM	CAA-CBA-CGA-O1A
74	V	201	CDL	C54-C55-C56-C57
75	l	701	PEE	C31-C32-C33-C34
74	x	402	CDL	C55-C56-C57-C58
76	w	401	HEM	CAD-CBD-CGD-O1D
76	7	404	HEM	CAD-CBD-CGD-O1D
74	8	401	CDL	C31-CA7-OA8-CA6
71	i	502	PLX	C32-C33-C34-C35
74	5	501	CDL	OB5-CB3-CB4-CB6
74	x	402	CDL	C75-C76-C77-C78
76	7	403	HEM	CAA-CBA-CGA-O2A
76	7	404	HEM	CAD-CBD-CGD-O2D
78	Ak	602	HEA	CAD-CBD-CGD-O1D
78	Ak	602	HEA	CAD-CBD-CGD-O2D
74	5	501	CDL	CB5-C51-C52-C53
71	4	301	PLX	C13-C14-C15-C16
77	x	401	HEC	CAA-CBA-CGA-O2A
74	s	201	CDL	OB9-CB7-OB8-CB6
75	7	401	PEE	C30-C31-C32-C33
76	7	403	HEM	CAA-CBA-CGA-O1A
75	W	401	PEE	C39-C40-C41-C42
75	u	502	PEE	C19-C20-C21-C22
75	7	402	PEE	C14-C15-C16-C17
75	W	401	PEE	C37-C38-C39-C40
75	u	502	PEE	C40-C41-C42-C43
78	Ak	601	HEA	CAA-CBA-CGA-O1A
78	Ak	601	HEA	CAD-CBD-CGD-O2D
75	u	502	PEE	C16-C17-C18-C19
74	z	101	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
74	8	401	CDL	OA9-CA7-OA8-CA6
74	i	503	CDL	C1-CB2-OB2-PB2
75	q	501	PEE	O2-C10-C11-C12
74	5	501	CDL	C14-C15-C16-C17
75	l	701	PEE	C32-C33-C34-C35
75	q	501	PEE	C36-C37-C38-C39
75	w	403	PEE	C36-C37-C38-C39
76	w	402	HEM	CAA-CBA-CGA-O2A
71	H	303	PLX	O8-C24-C25-C26
77	x	401	HEC	CAA-CBA-CGA-O1A
69	B	502	FMN	O2'-C2'-C3'-C4'
76	7	403	HEM	CAD-CBD-CGD-O1D
76	7	403	HEM	CAD-CBD-CGD-O2D
71	2	301	PLX	O6-C4-C5-O8
75	u	502	PEE	C23-C24-C25-C26
75	5	502	PEE	C36-C37-C38-C39
71	V	202	PLX	C20-C21-C22-C23
74	Aa	101	CDL	CA5-C11-C12-C13
75	7	401	PEE	C14-C15-C16-C17
75	7	401	PEE	C42-C43-C44-C45
74	x	402	CDL	C72-C71-CB7-OB8
75	w	403	PEE	C19-C20-C21-C22
74	l	702	CDL	C35-C36-C37-C38
75	q	501	PEE	C38-C39-C40-C41
75	7	401	PEE	C38-C39-C40-C41
75	2	302	PEE	C40-C41-C42-C43
74	V	201	CDL	C72-C71-CB7-OB8
74	5	501	CDL	C72-C71-CB7-OB8
73	Q	201	ZMP	C3-C4-C5-C6
75	W	401	PEE	C18-C19-C20-C21
75	7	402	PEE	C36-C37-C38-C39
74	s	201	CDL	CA3-CA4-CA6-OA8
75	2	302	PEE	O3P-C1-C2-O2
74	x	402	CDL	C52-C51-CB5-OB6
74	V	201	CDL	CA5-C11-C12-C13
74	V	201	CDL	C20-C21-C22-C23
76	7	403	HEM	C4B-C3B-CAB-CBB
72	L	401	NDP	O4D-C4D-C5D-O5D
76	w	401	HEM	CAD-CBD-CGD-O2D
78	Ak	602	HEA	CAA-CBA-CGA-O2A
75	W	401	PEE	C38-C39-C40-C41
72	L	401	NDP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
78	Ak	602	HEA	CAA-CBA-CGA-O1A
74	x	402	CDL	C32-C31-CA7-OA8
74	z	101	CDL	C52-C51-CB5-OB6
74	s	201	CDL	C72-C73-C74-C75
74	5	501	CDL	C15-C16-C17-C18
71	H	303	PLX	O6-C4-C5-O8
74	l	702	CDL	OB6-CB4-CB6-OB8
75	2	302	PEE	C36-C37-C38-C39
74	u	501	CDL	C12-C11-CA5-OA6
74	s	201	CDL	C32-C31-CA7-OA8
75	l	701	PEE	O4-C10-O2-C2
75	W	401	PEE	C16-C17-C18-C19
75	i	501	PEE	C38-C39-C40-C41
74	u	501	CDL	C32-C31-CA7-OA8
75	W	401	PEE	O2-C10-C11-C12
74	5	501	CDL	C72-C71-CB7-OB9
75	u	502	PEE	O2-C10-C11-C12
74	V	201	CDL	C72-C71-CB7-OB9
74	x	402	CDL	C72-C71-CB7-OB9
74	8	401	CDL	C72-C71-CB7-OB9
74	s	201	CDL	C52-C51-CB5-OB6
75	u	502	PEE	C41-C42-C43-C44
75	5	502	PEE	C21-C22-C23-C24
78	Ak	601	HEA	CAA-CBA-CGA-O2A
71	H	303	PLX	C2-O1-P1-O3
74	u	501	CDL	CA3-OA5-PA1-OA3
74	u	501	CDL	CB2-OB2-PB2-OB3
74	x	402	CDL	CA3-OA5-PA1-OA3
74	x	402	CDL	CB2-OB2-PB2-OB4
74	z	101	CDL	CA2-OA2-PA1-OA3
74	z	101	CDL	CA3-OA5-PA1-OA4
74	z	101	CDL	CB2-OB2-PB2-OB3
74	Aa	101	CDL	CB3-OB5-PB2-OB4
75	W	401	PEE	C4-O4P-P-O1P
75	q	501	PEE	C1-O3P-P-O1P
75	w	403	PEE	C4-O4P-P-O2P
75	2	302	PEE	C1-O3P-P-O1P
74	x	402	CDL	C32-C31-CA7-OA9
75	i	501	PEE	C33-C34-C35-C36
75	w	403	PEE	O4P-C4-C5-N
75	l	701	PEE	C21-C22-C23-C24
75	W	401	PEE	O4-C10-C11-C12

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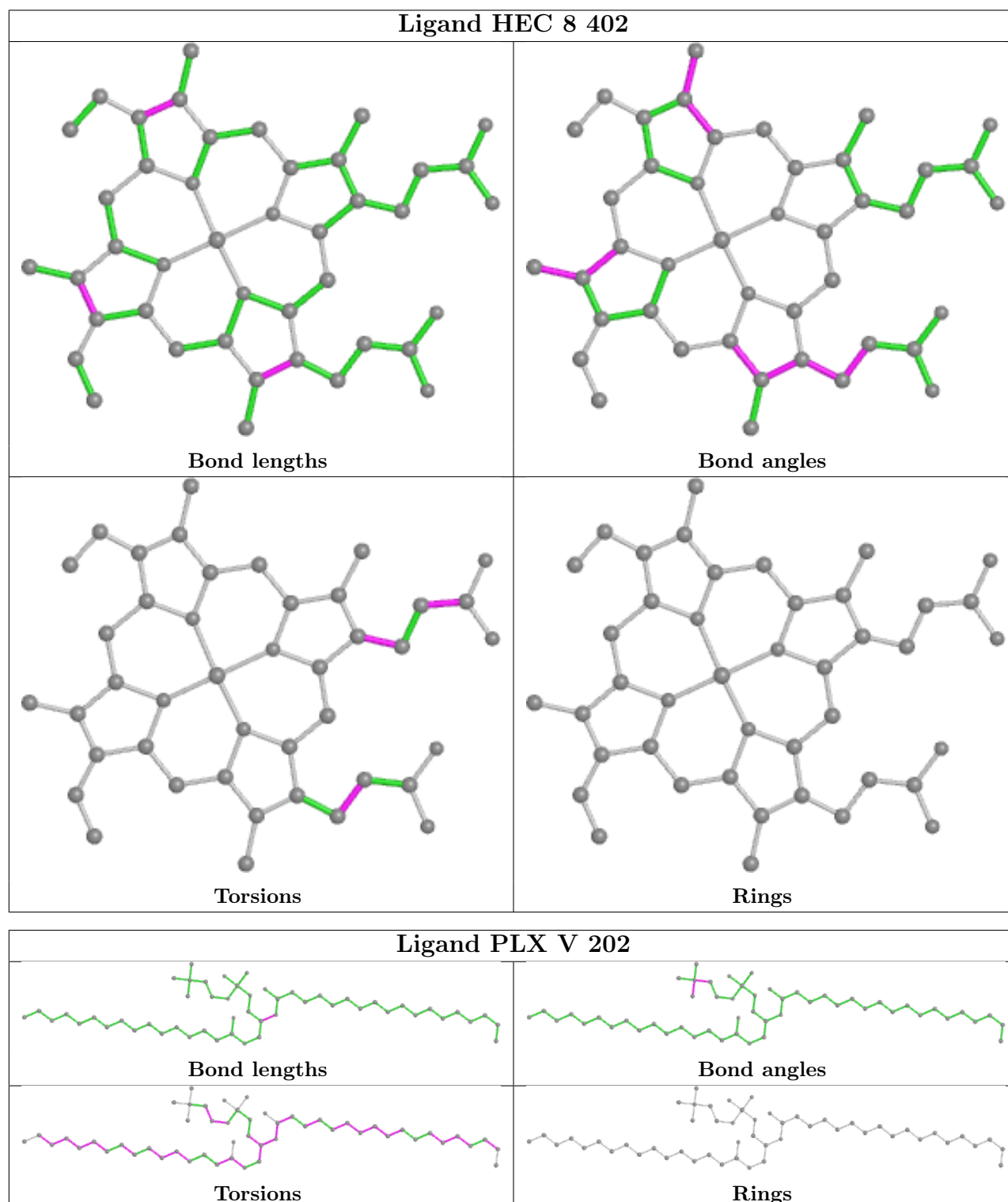
Mol	Chain	Res	Type	Atoms
78	Ak	602	HEA	C26-C15-C16-C17
71	V	202	PLX	C1-C2-O1-P1
71	2	301	PLX	C1-C2-O1-P1
75	w	403	PEE	C10-C11-C12-C13
74	s	201	CDL	C32-C31-CA7-OA9
74	x	402	CDL	C52-C51-CB5-OB7
74	z	101	CDL	C52-C51-CB5-OB7
72	L	401	NDP	C2D-C1D-N1N-C2N
75	5	502	PEE	O3-C30-C31-C32
71	H	303	PLX	C34-C35-C36-C37
71	V	202	PLX	C35-C36-C37-C38
74	8	401	CDL	C52-C51-CB5-OB6
74	Aa	101	CDL	C32-C31-CA7-OA8
75	u	502	PEE	O3-C30-C31-C32
74	u	501	CDL	CA2-C1-CB2-OB2
74	8	401	CDL	CB2-C1-CA2-OA2
74	s	201	CDL	C54-C55-C56-C57
74	u	501	CDL	C12-C11-CA5-OA7
74	u	501	CDL	C32-C31-CA7-OA9
75	u	502	PEE	O4-C10-C11-C12
78	Ak	601	HEA	O11-C11-C3B-C2B
74	s	201	CDL	C72-C71-CB7-OB8
74	u	501	CDL	C52-C51-CB5-OB6
75	2	302	PEE	O2-C10-C11-C12
75	i	501	PEE	C11-C12-C13-C14
75	5	502	PEE	O5-C30-C31-C32
73	X	201	ZMP	C6-C7-C8-C9
74	8	401	CDL	C52-C51-CB5-OB7
76	7	404	HEM	CAA-CBA-CGA-O2A
75	l	701	PEE	C36-C37-C38-C39
74	s	201	CDL	C72-C71-CB7-OB9
74	i	503	CDL	C52-C51-CB5-OB6
77	8	402	HEC	CAA-CBA-CGA-O2A

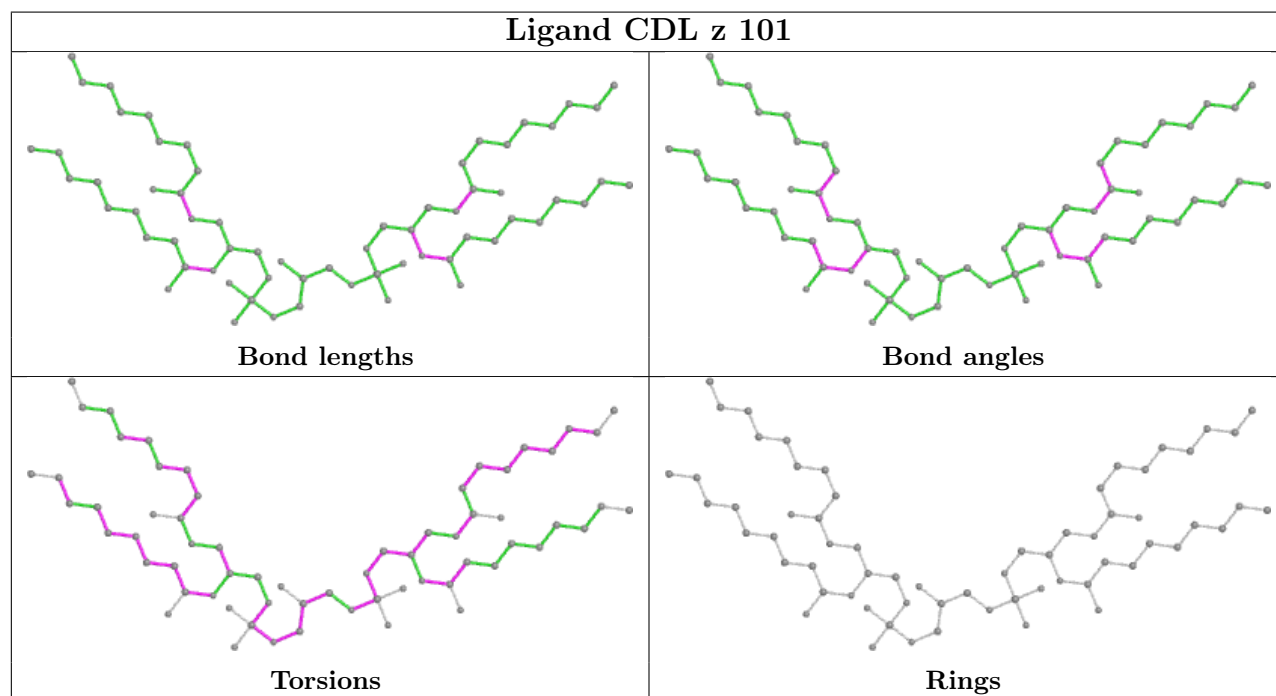
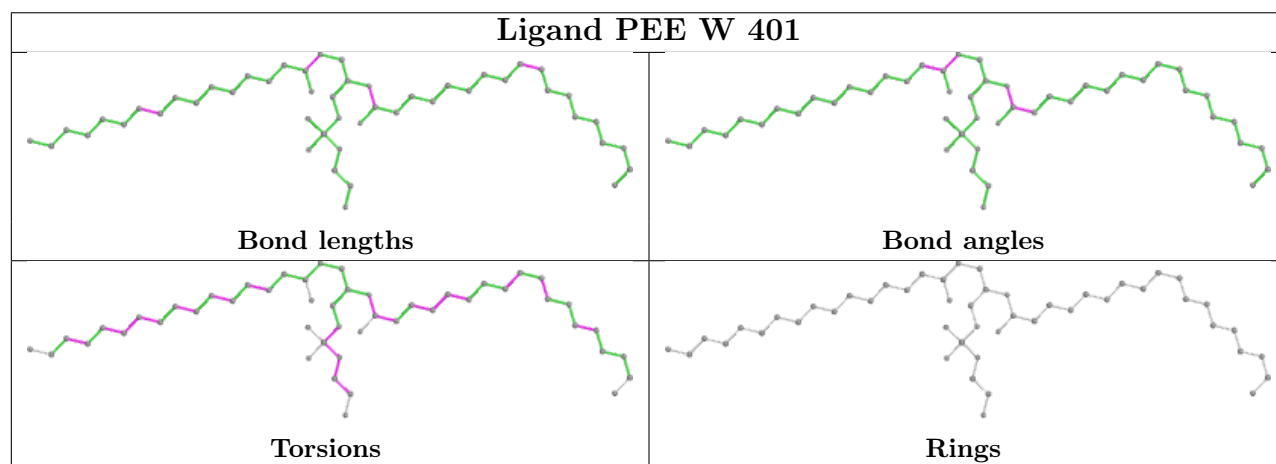
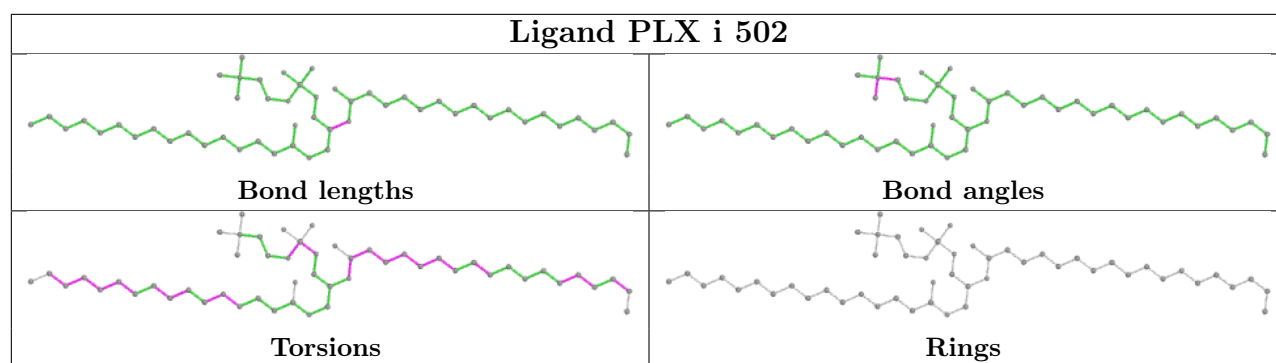
There are no ring outliers.

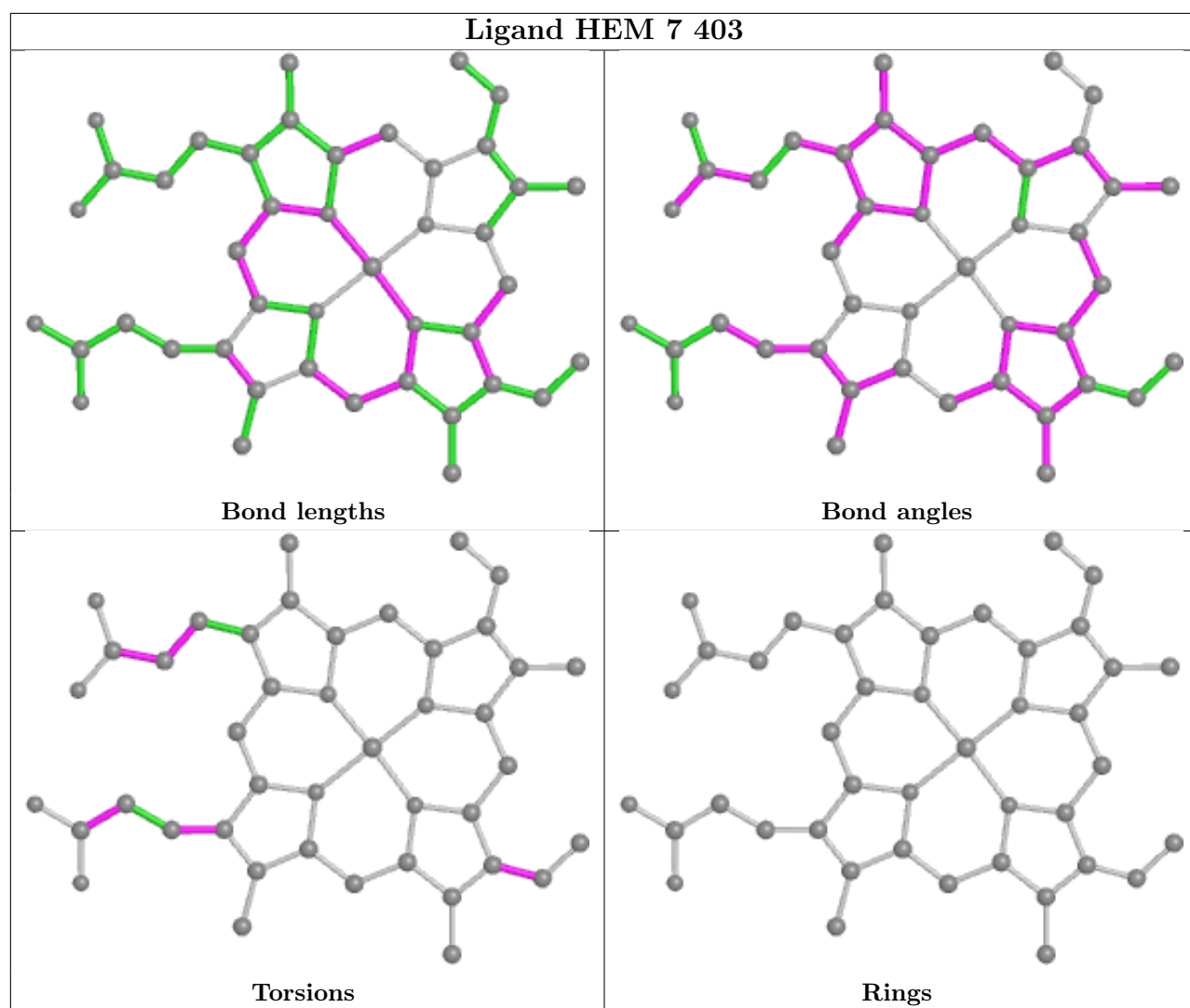
No monomer is involved in short contacts.

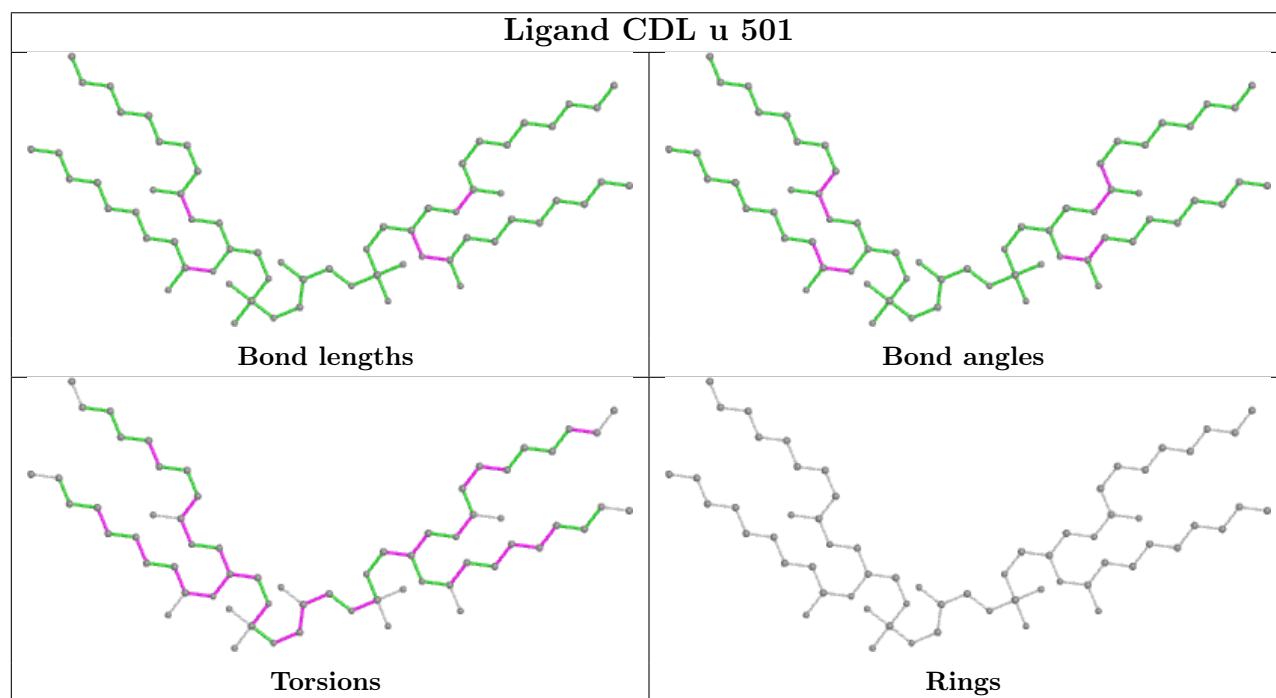
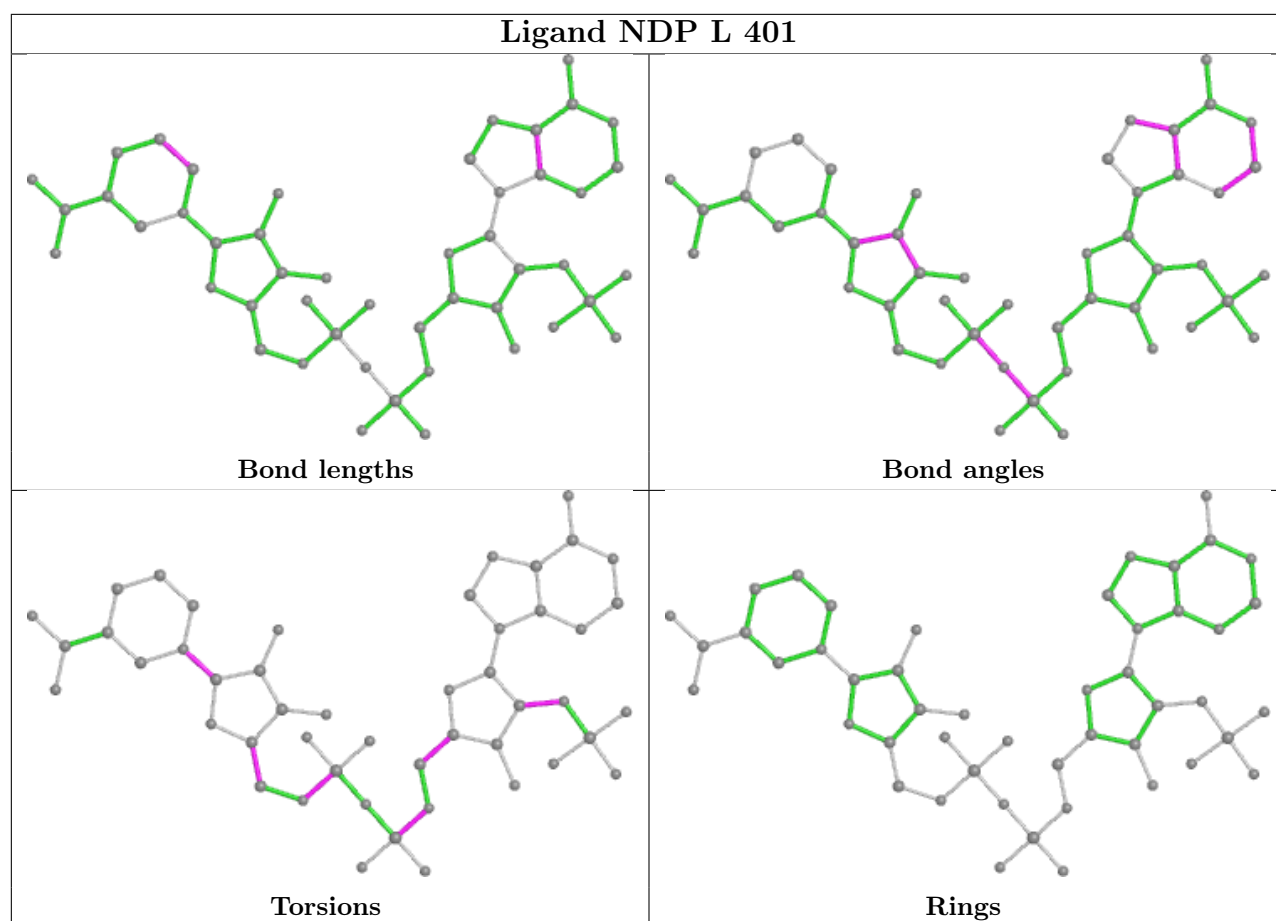
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

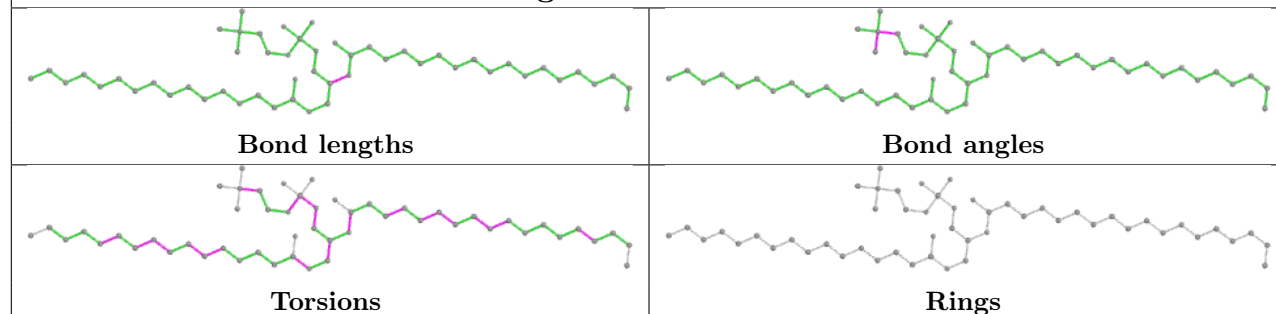
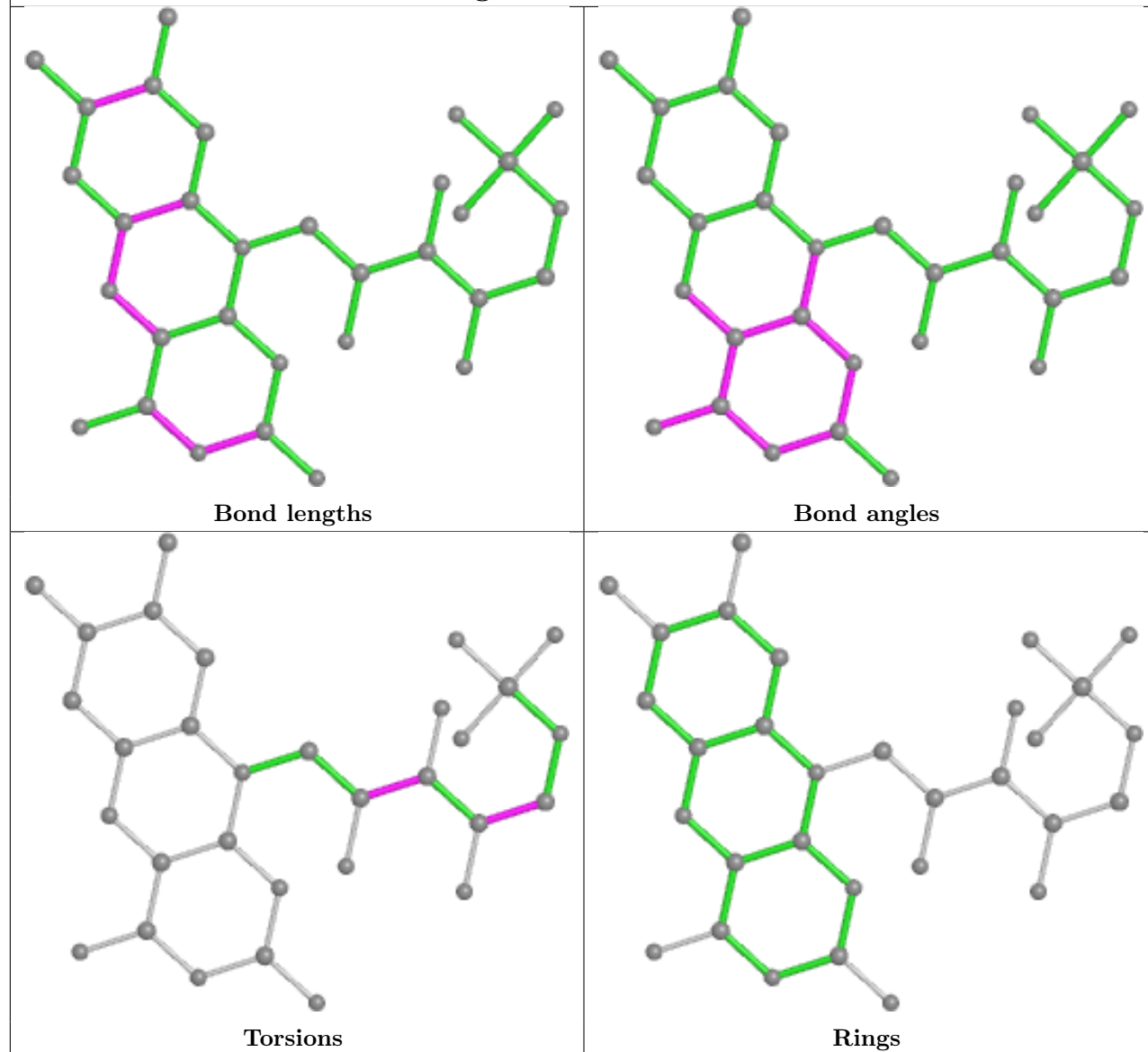
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

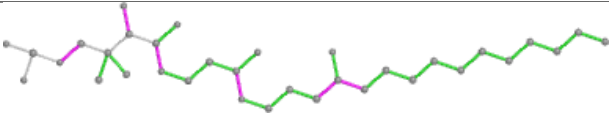
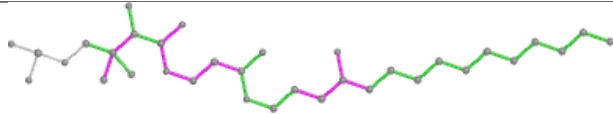
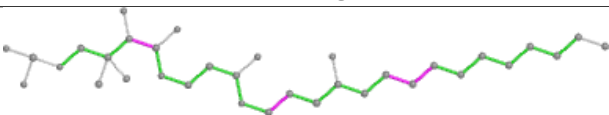
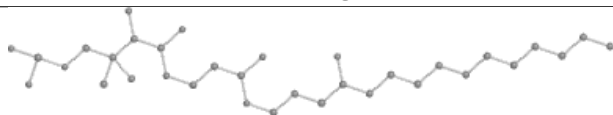


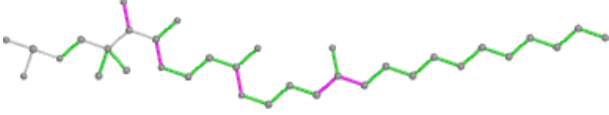
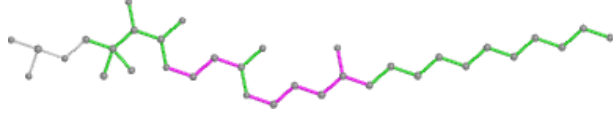
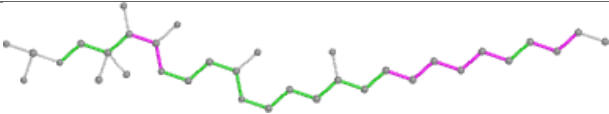
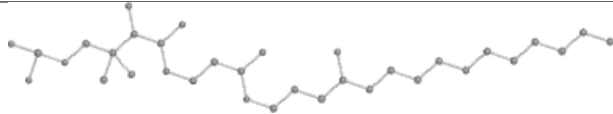


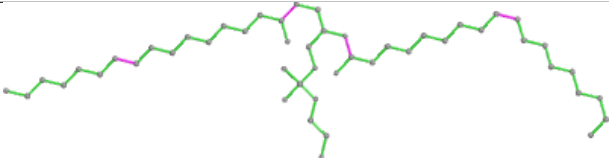
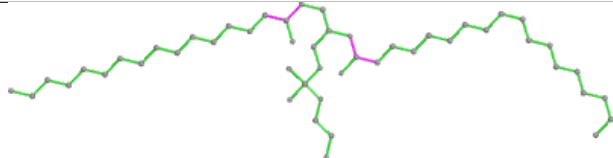
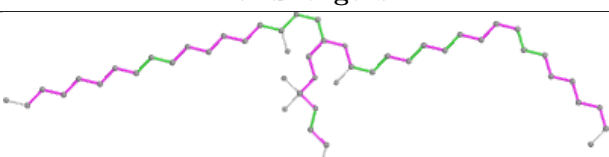
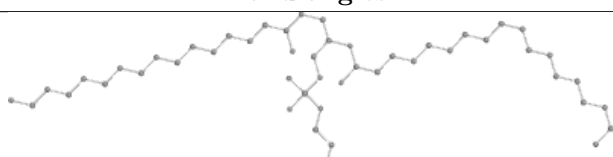


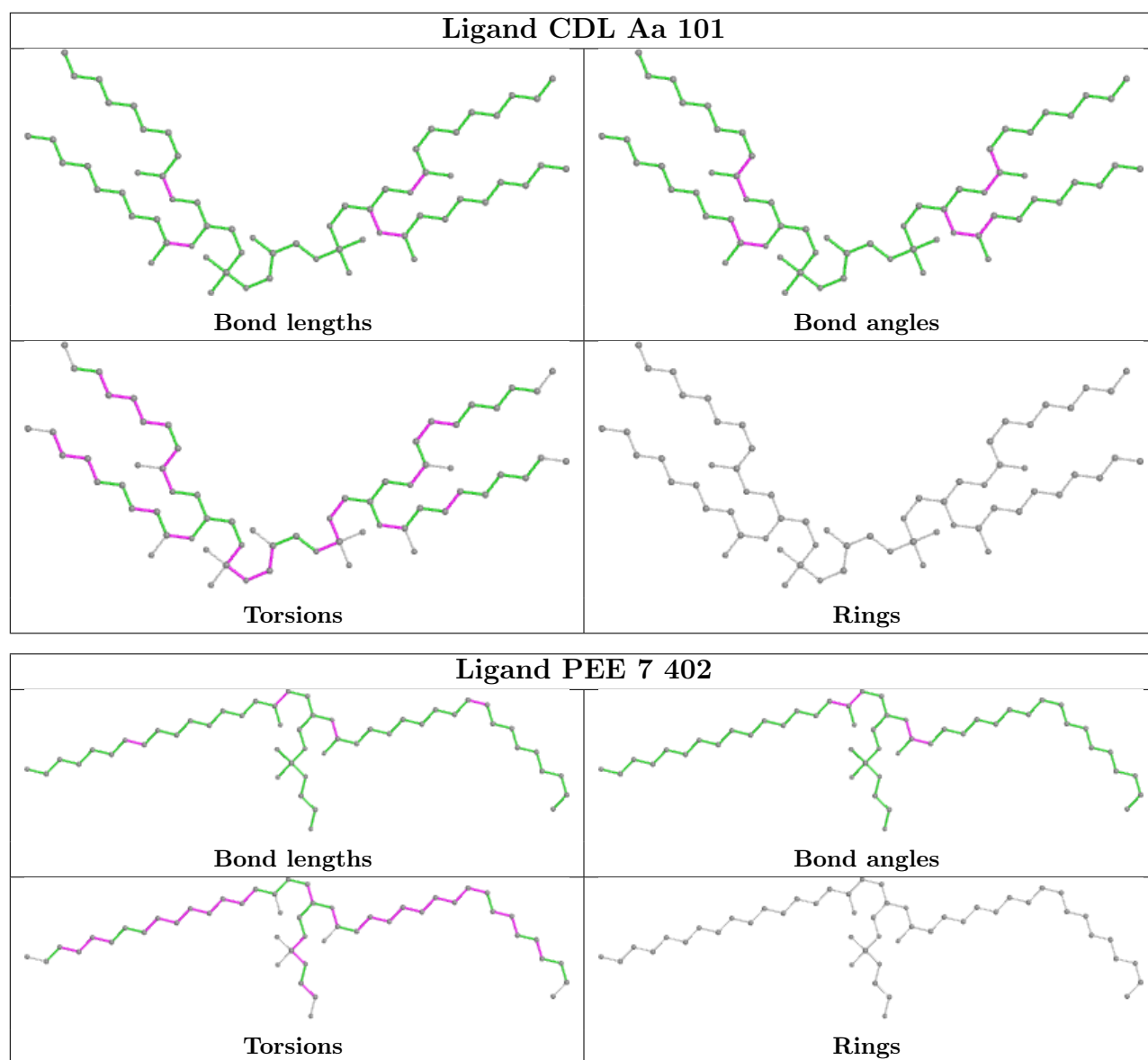


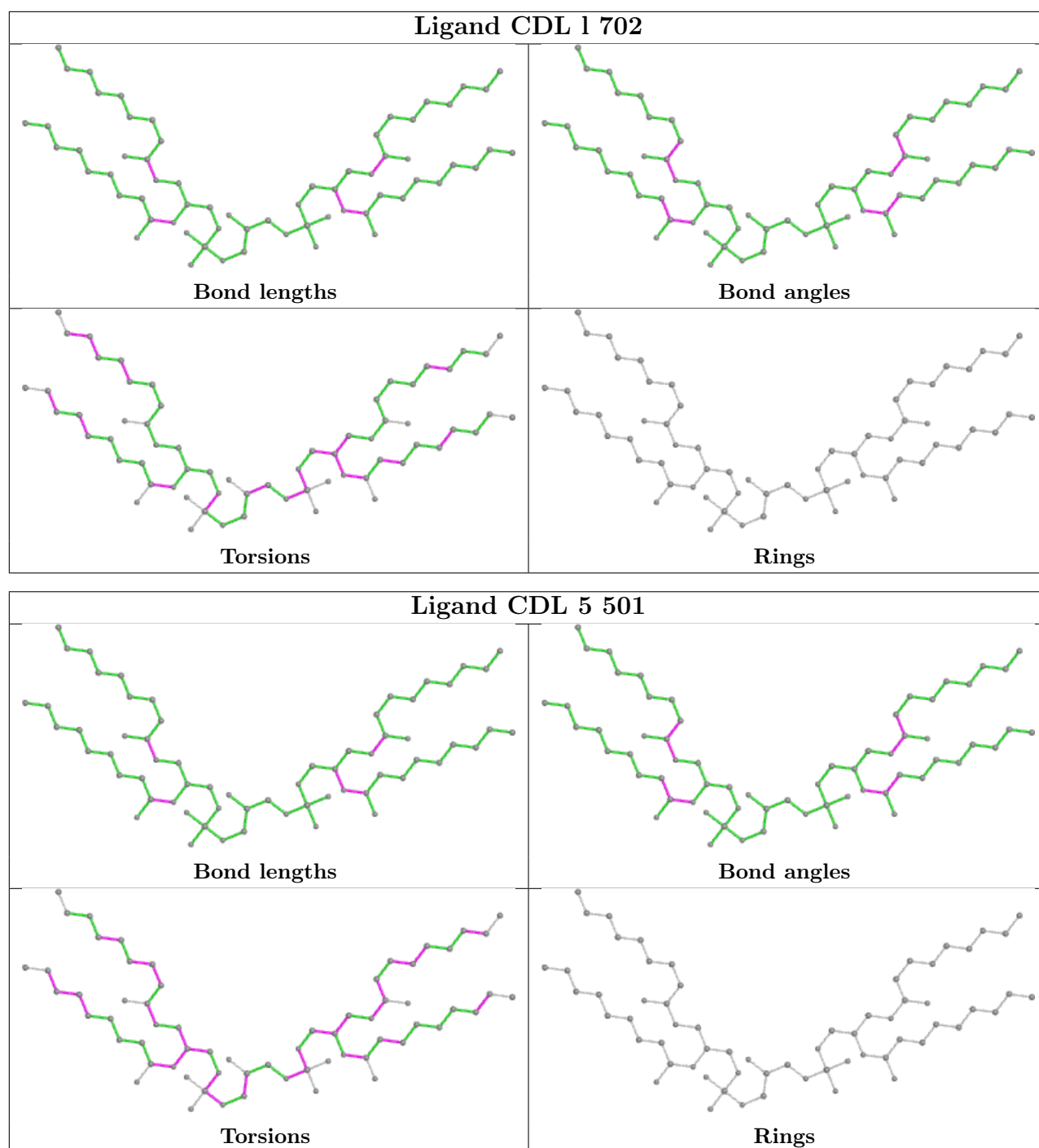
Ligand PLX 4 301**Ligand FMN B 502**

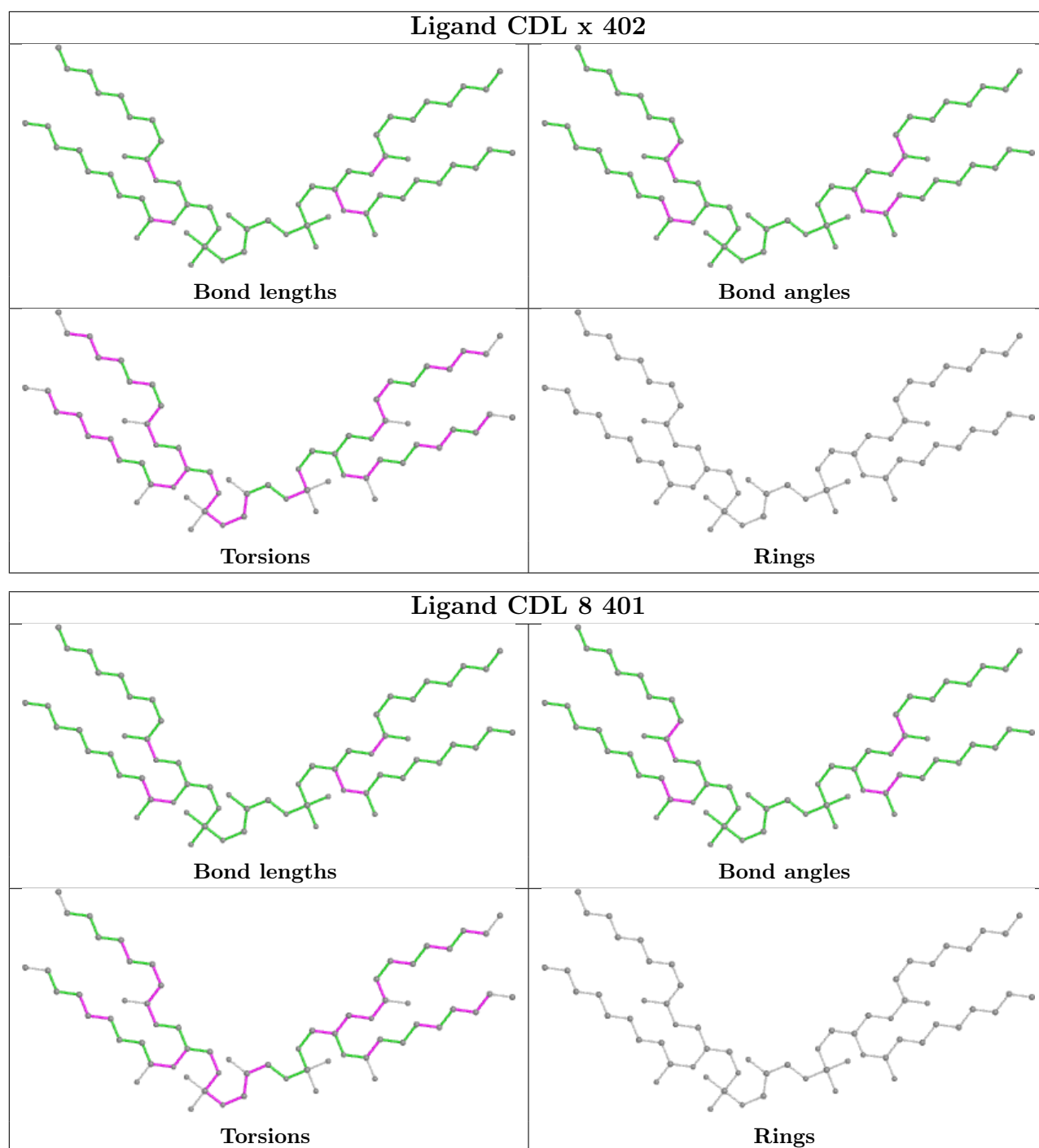
Ligand ZMP X 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

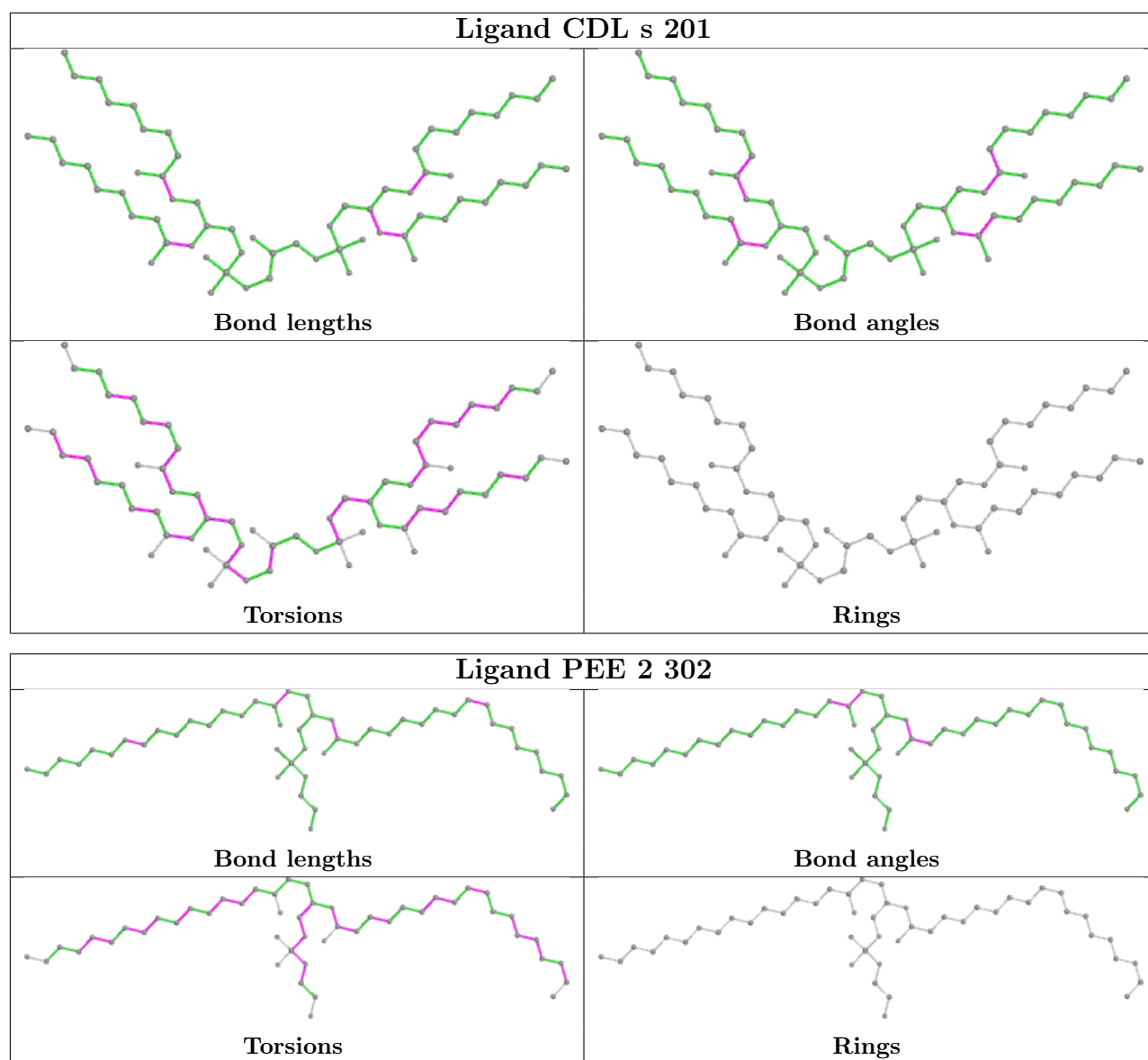
Ligand ZMP Q 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

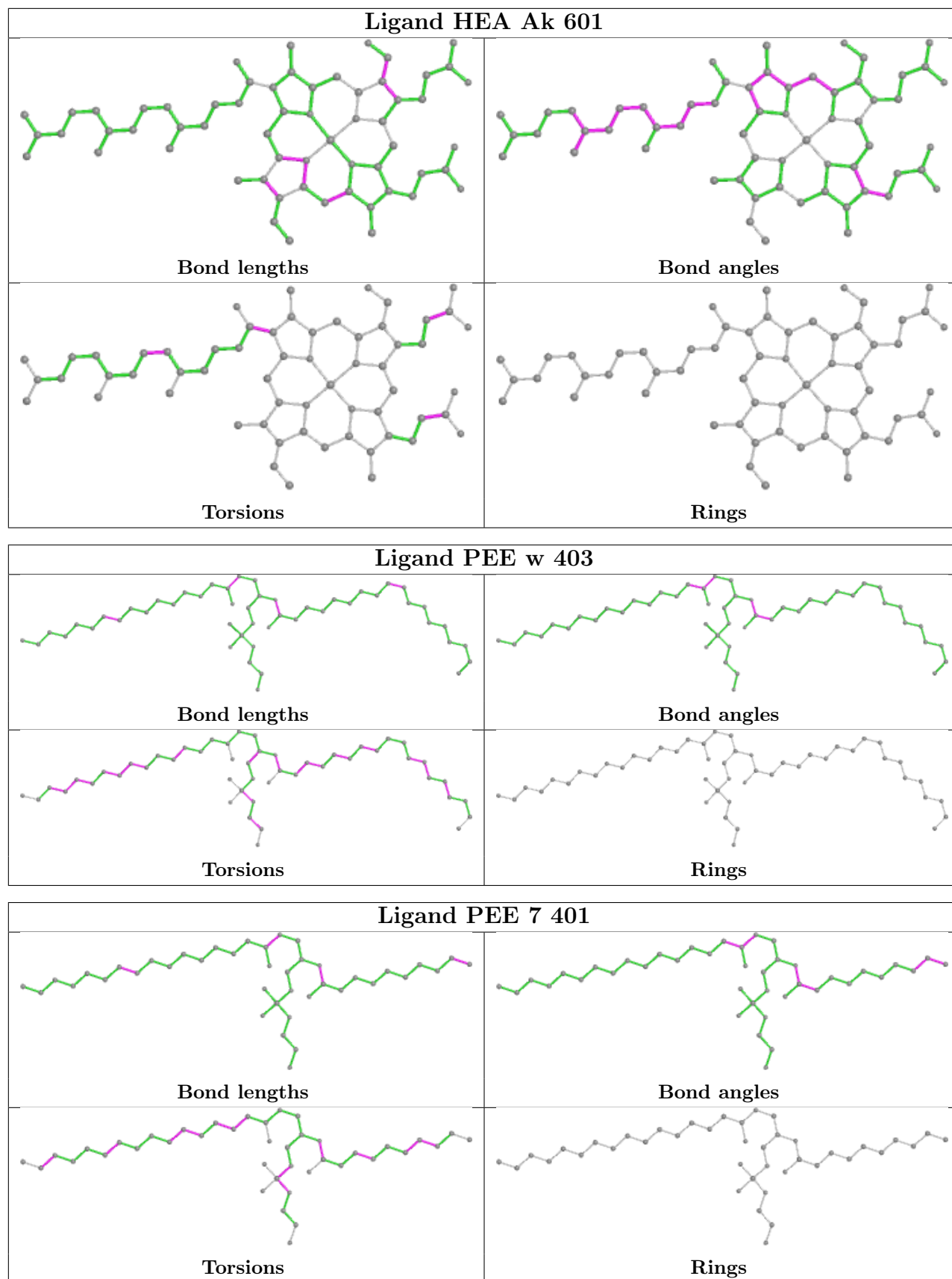
Ligand PEE i 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

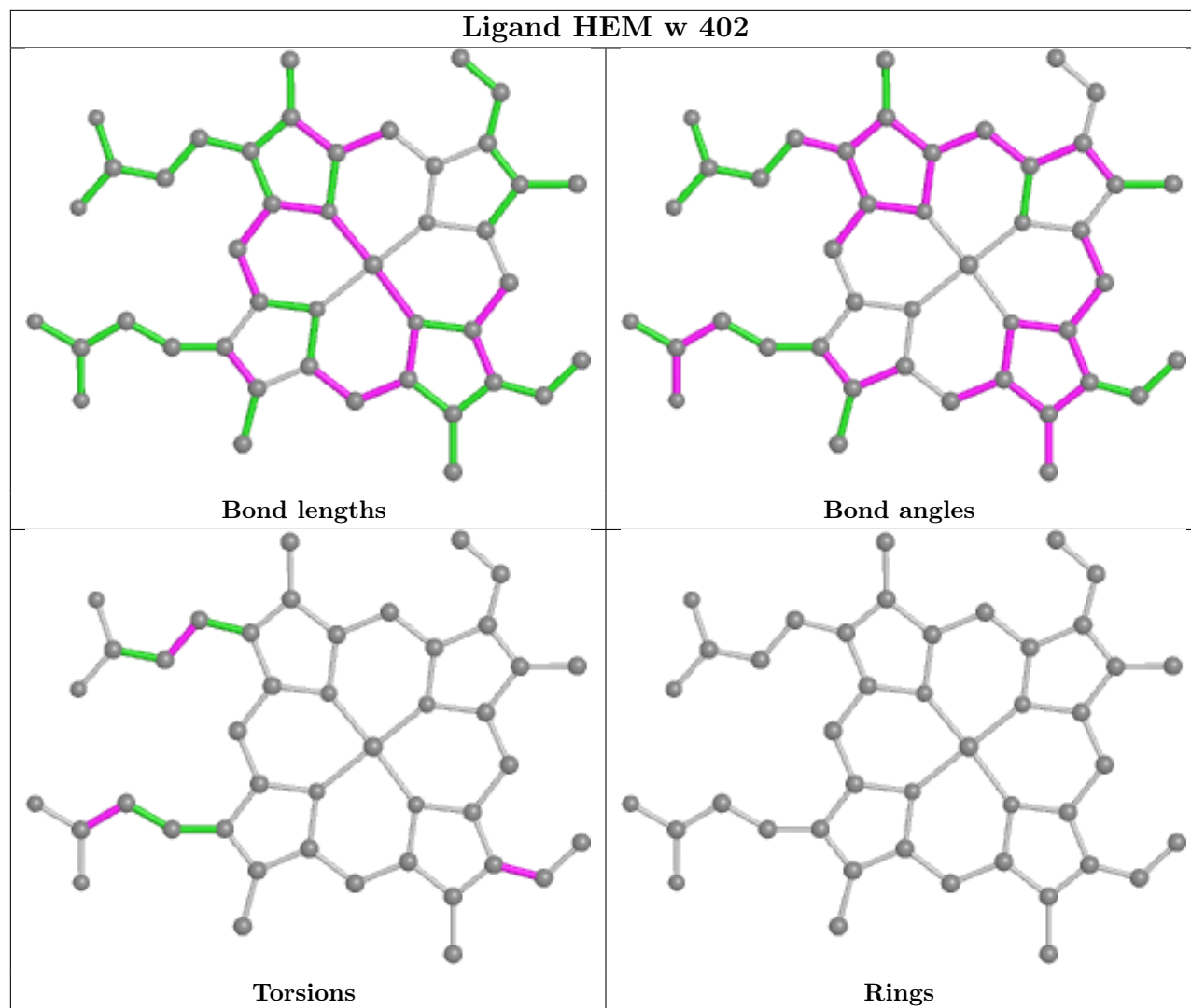


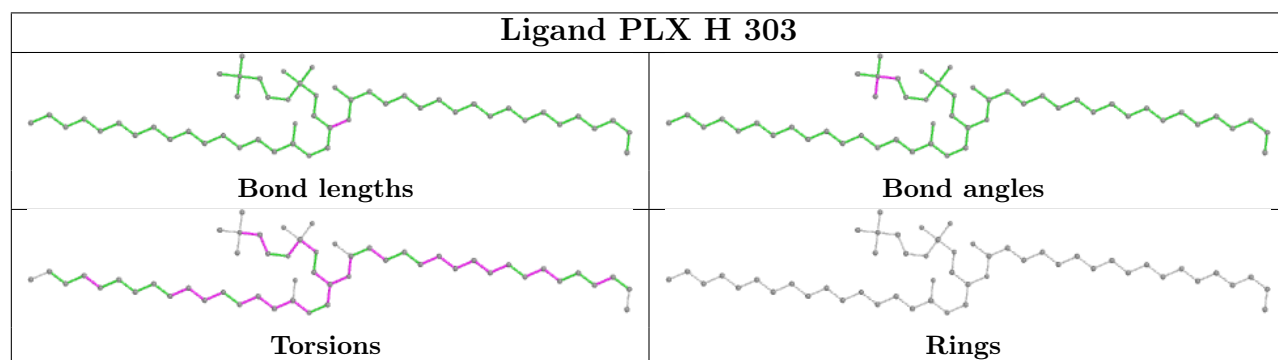
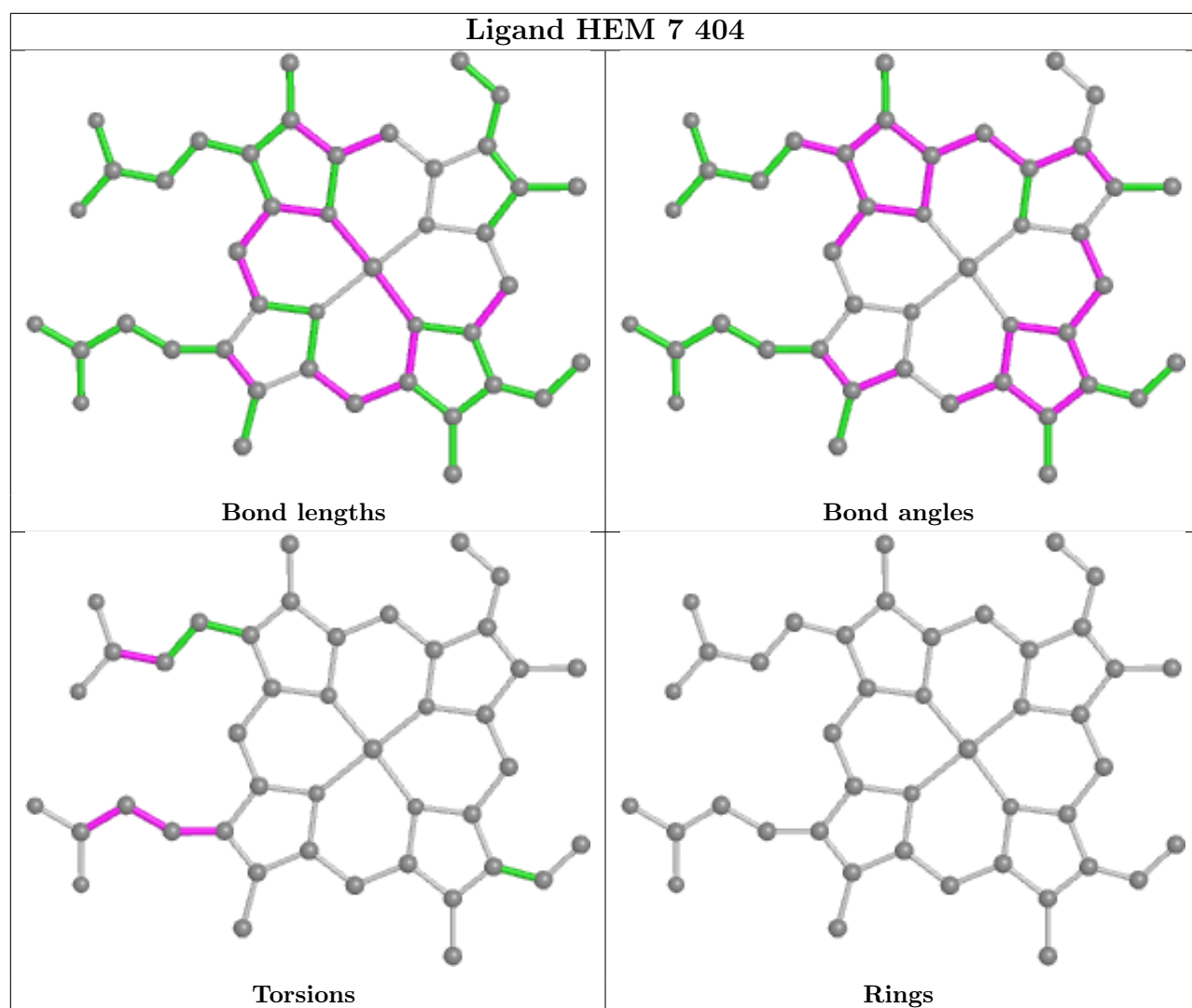


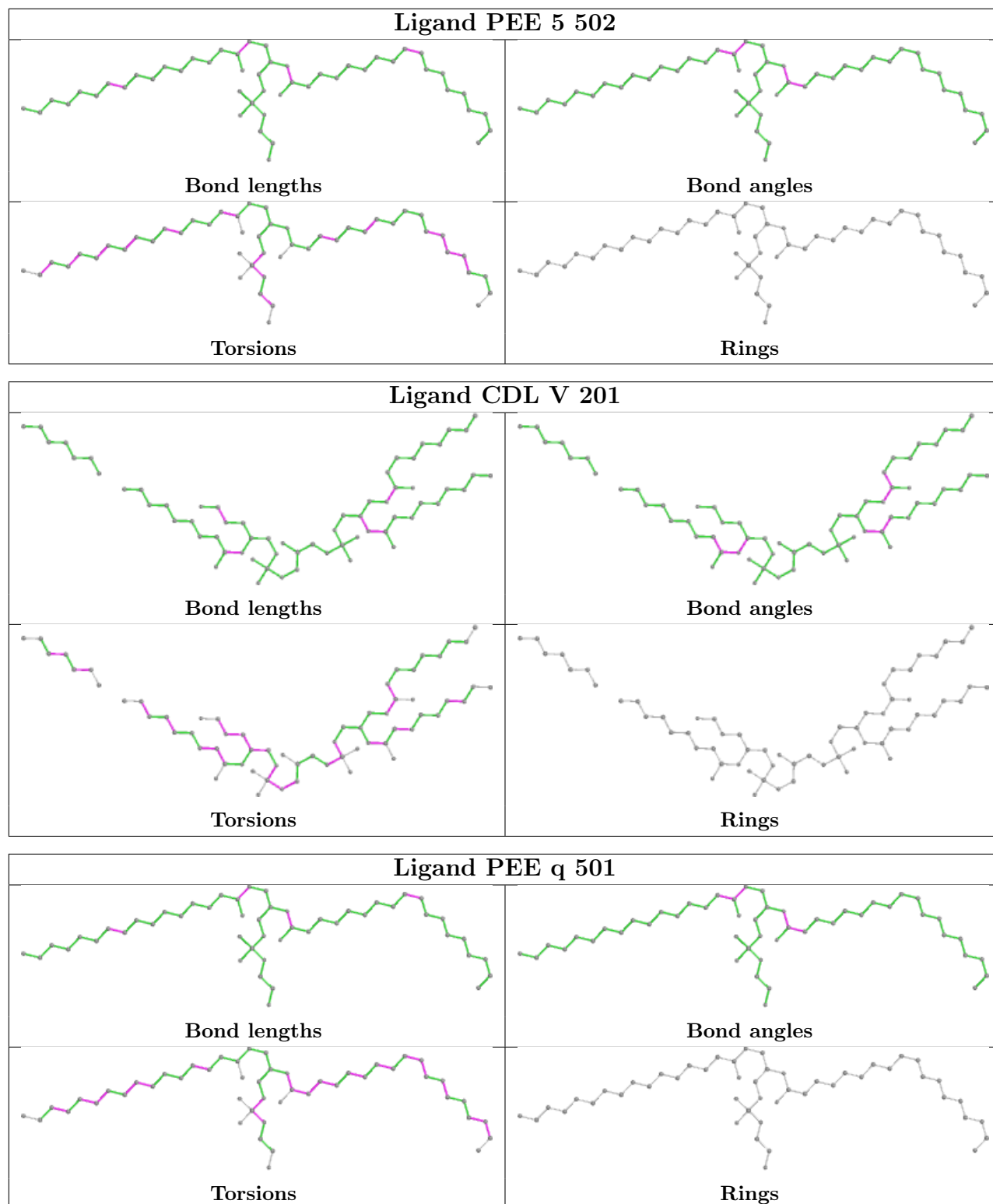


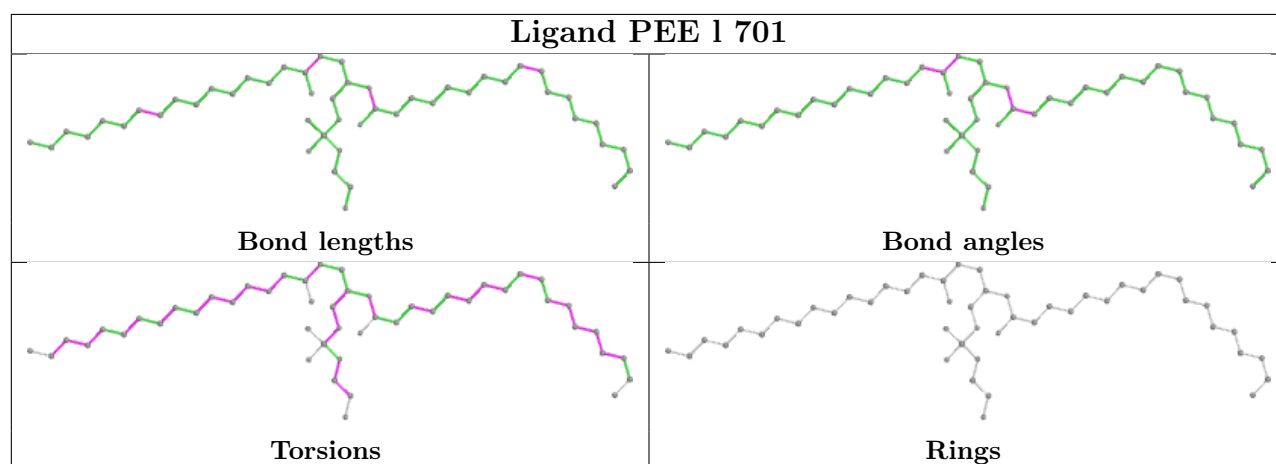
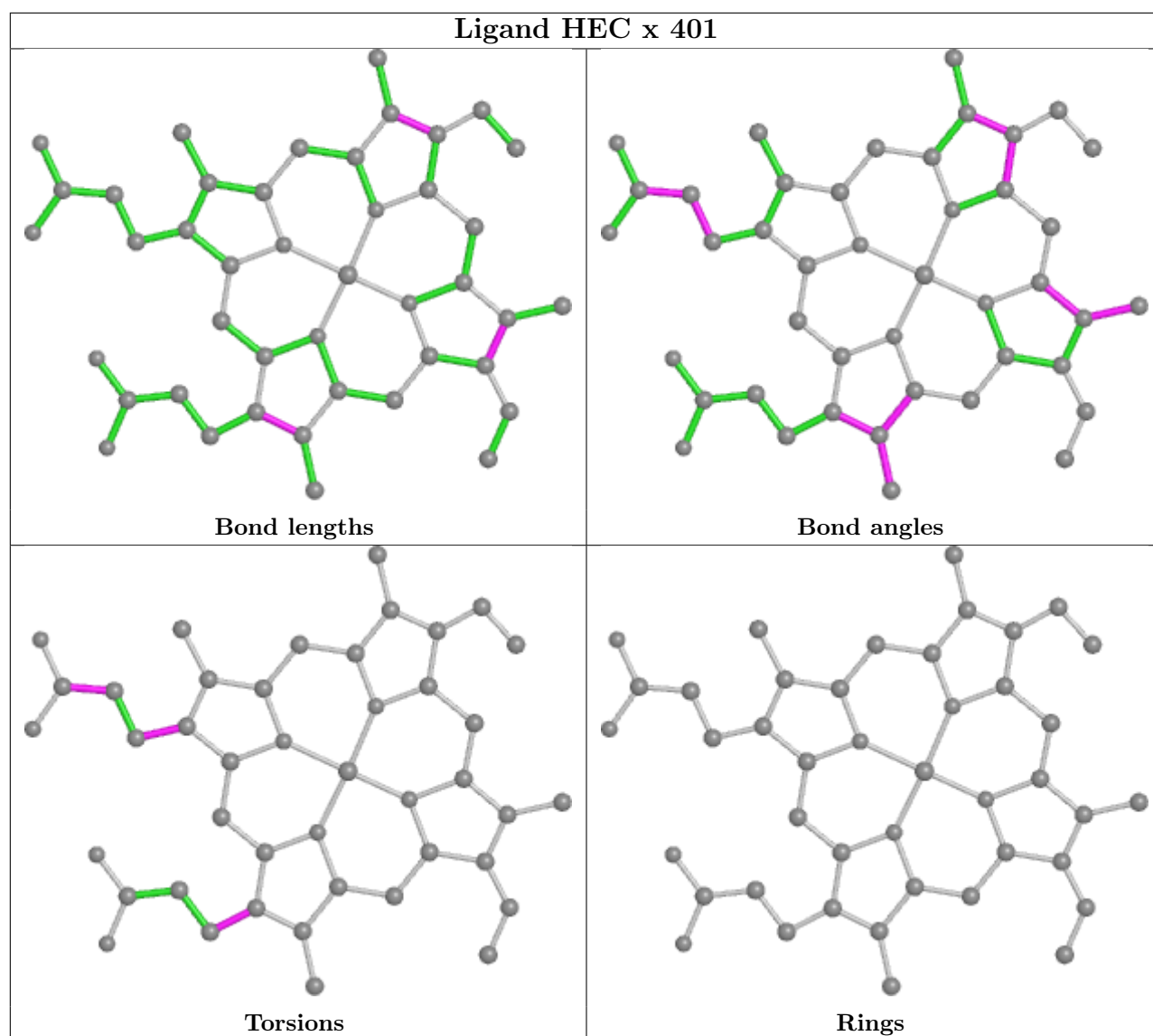


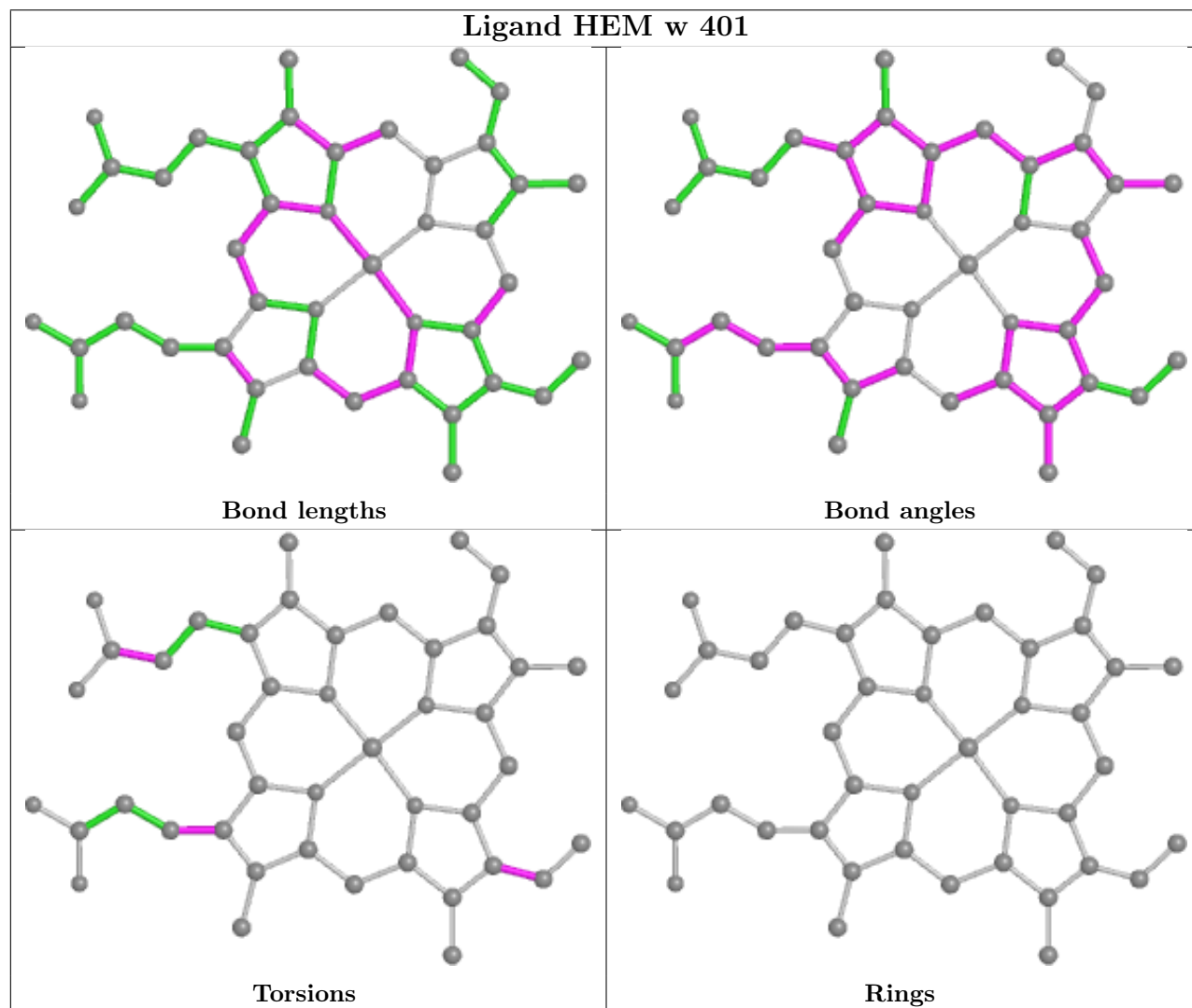
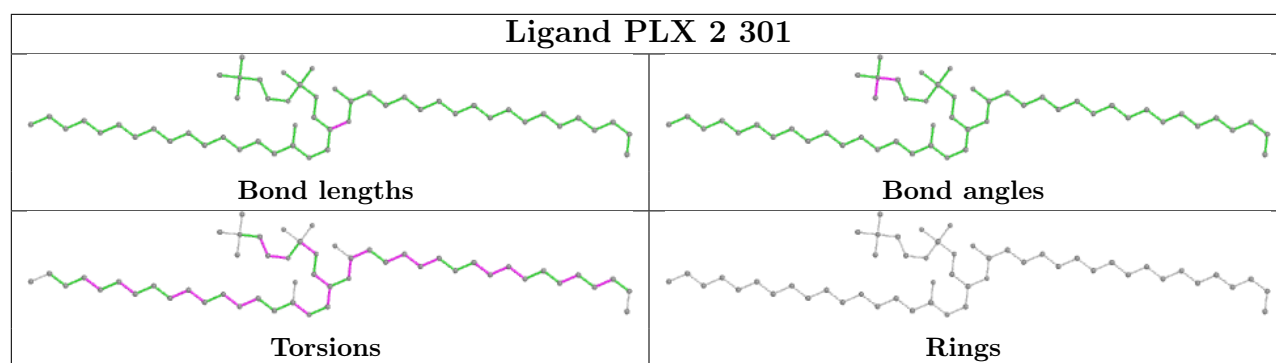


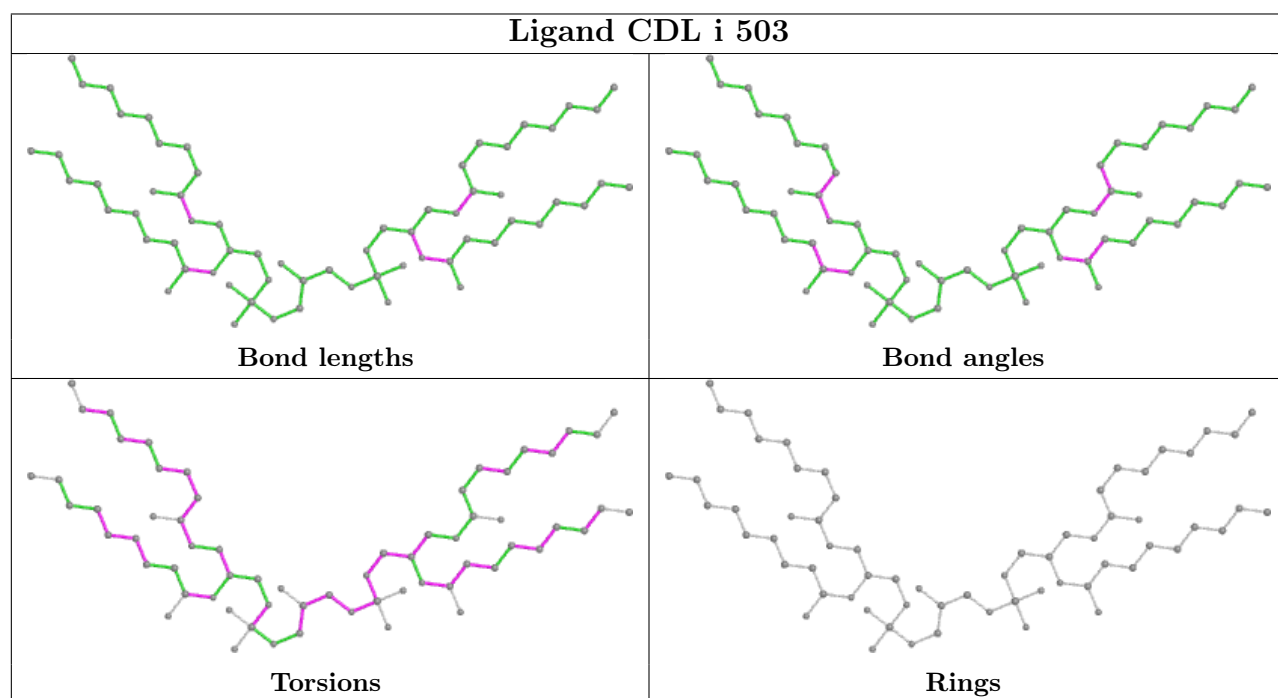
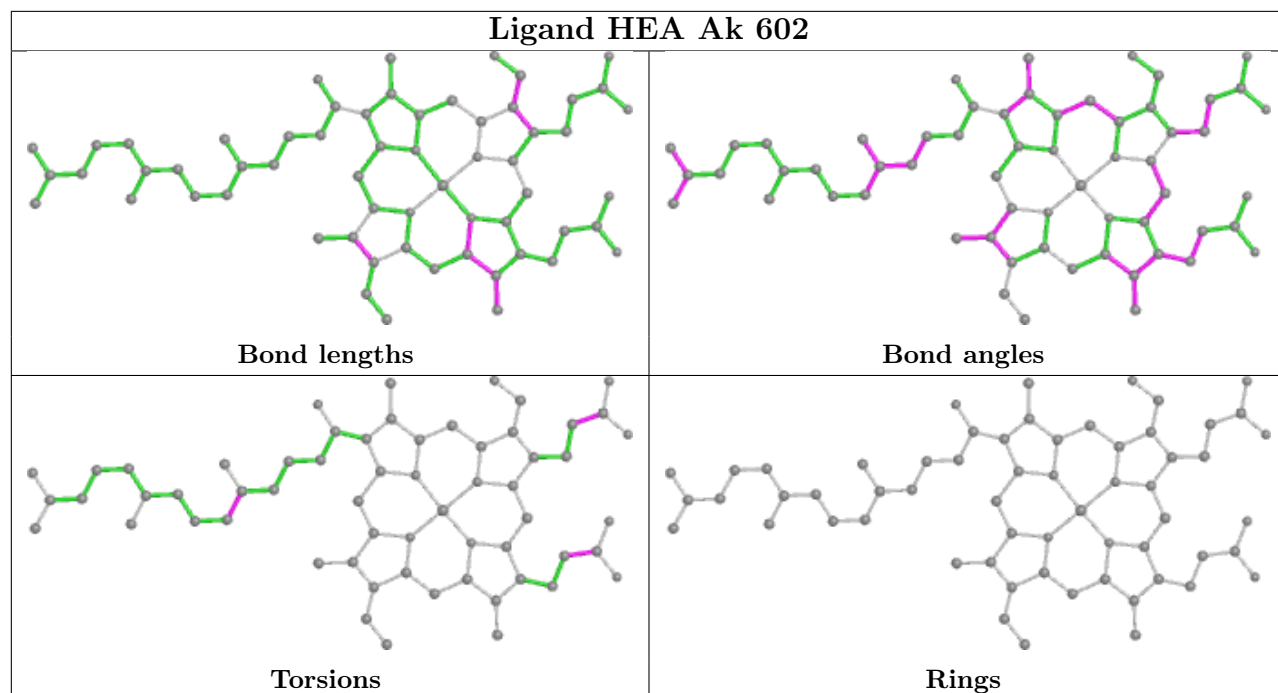


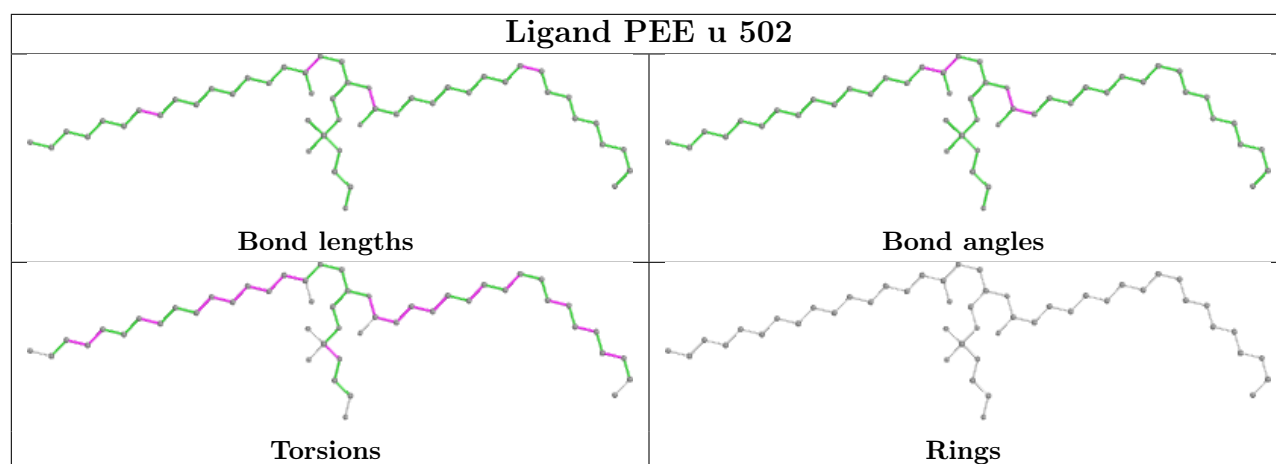












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

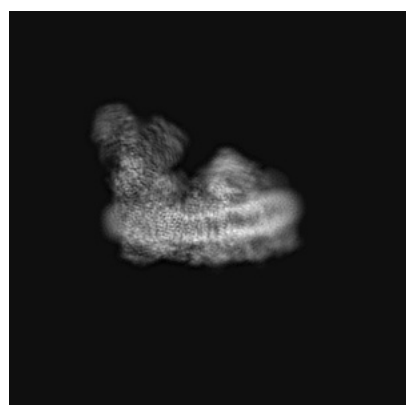
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9539. These allow visual inspection of the internal detail of the map and identification of artifacts.

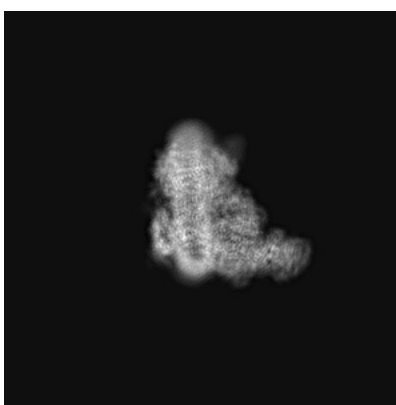
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

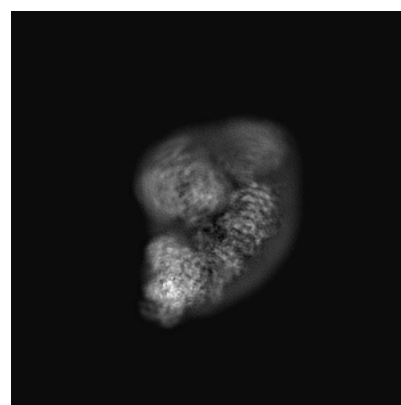
6.1.1 Primary map



X



Y



Z

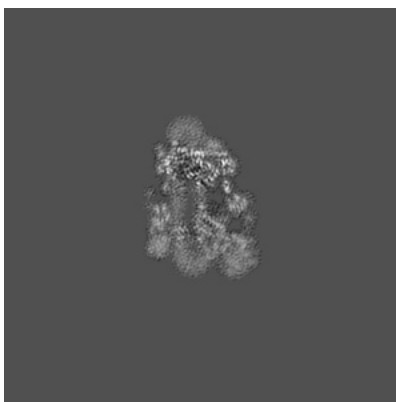
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

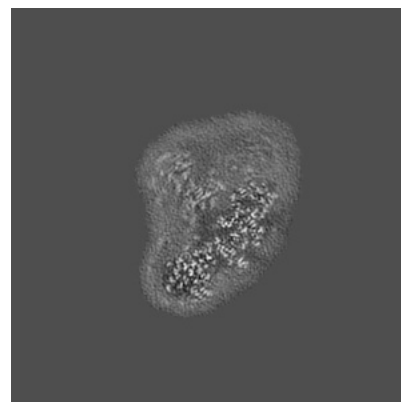
6.2.1 Primary map



X Index: 240



Y Index: 240

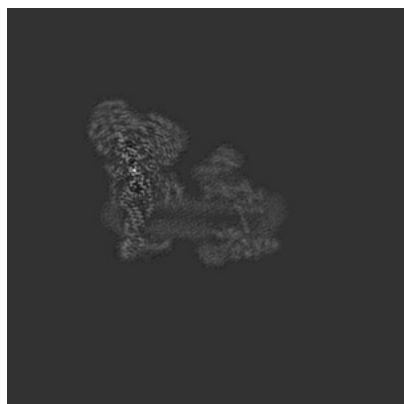


Z Index: 240

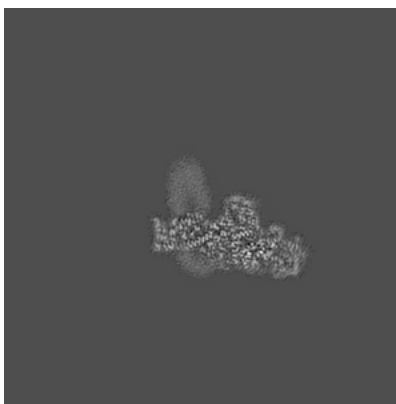
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

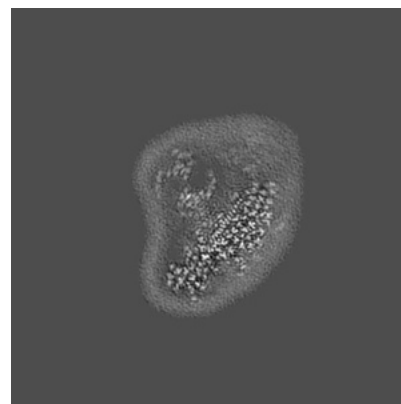
6.3.1 Primary map



X Index: 191



Y Index: 145

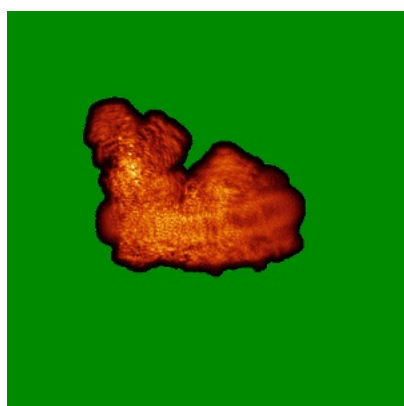


Z Index: 231

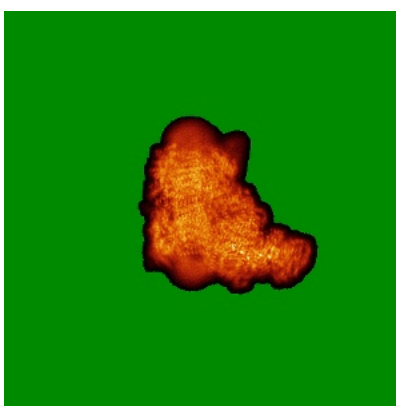
The images above show the largest variance slices of the map in three orthogonal directions.

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

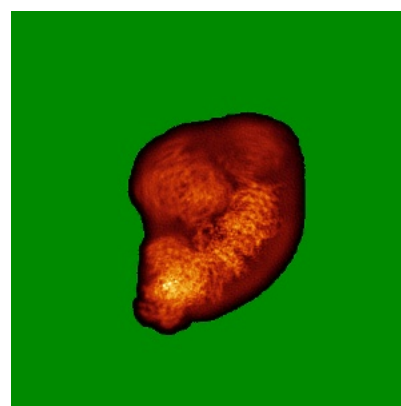
6.4.1 Primary map



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 0.0504. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

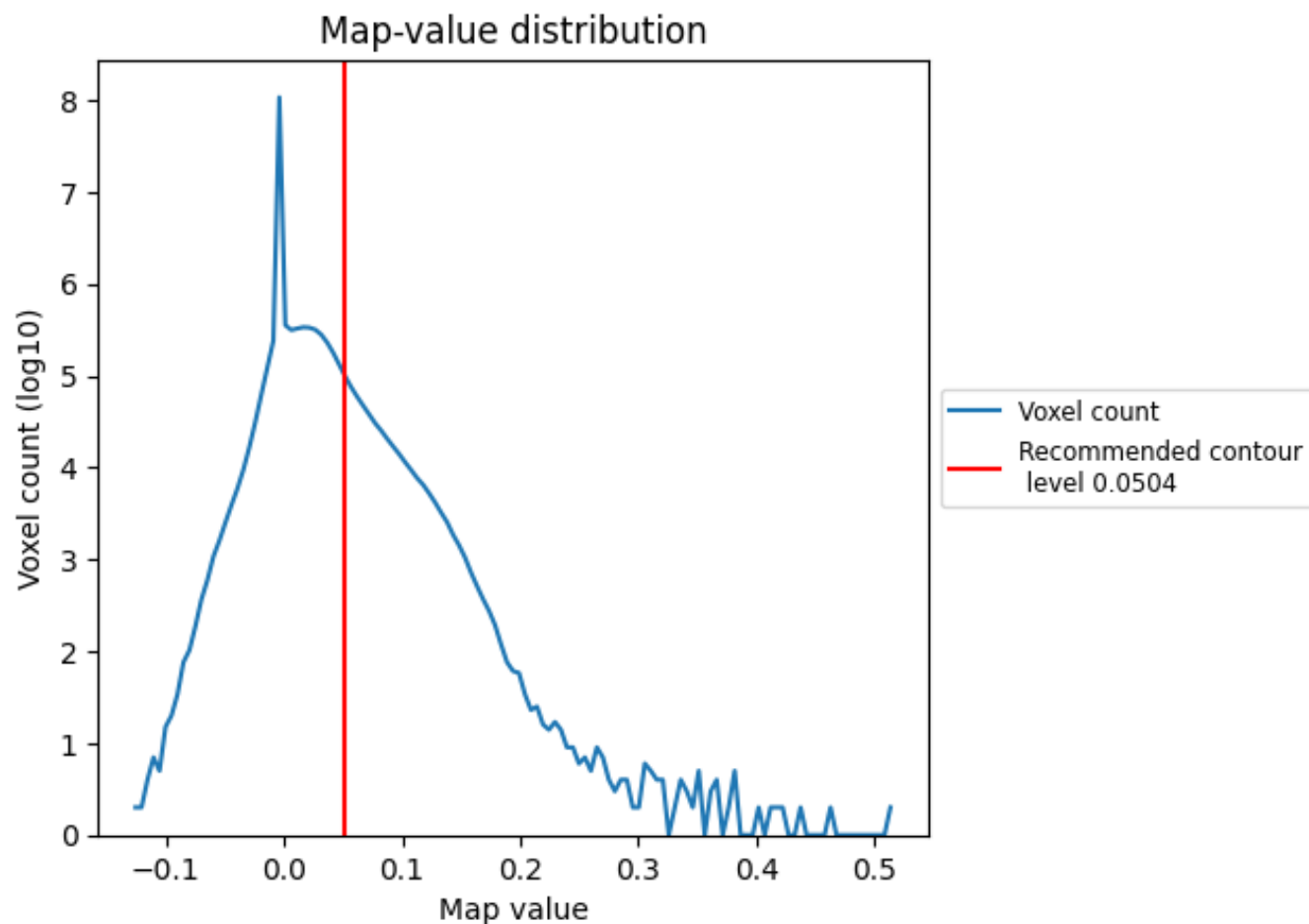
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

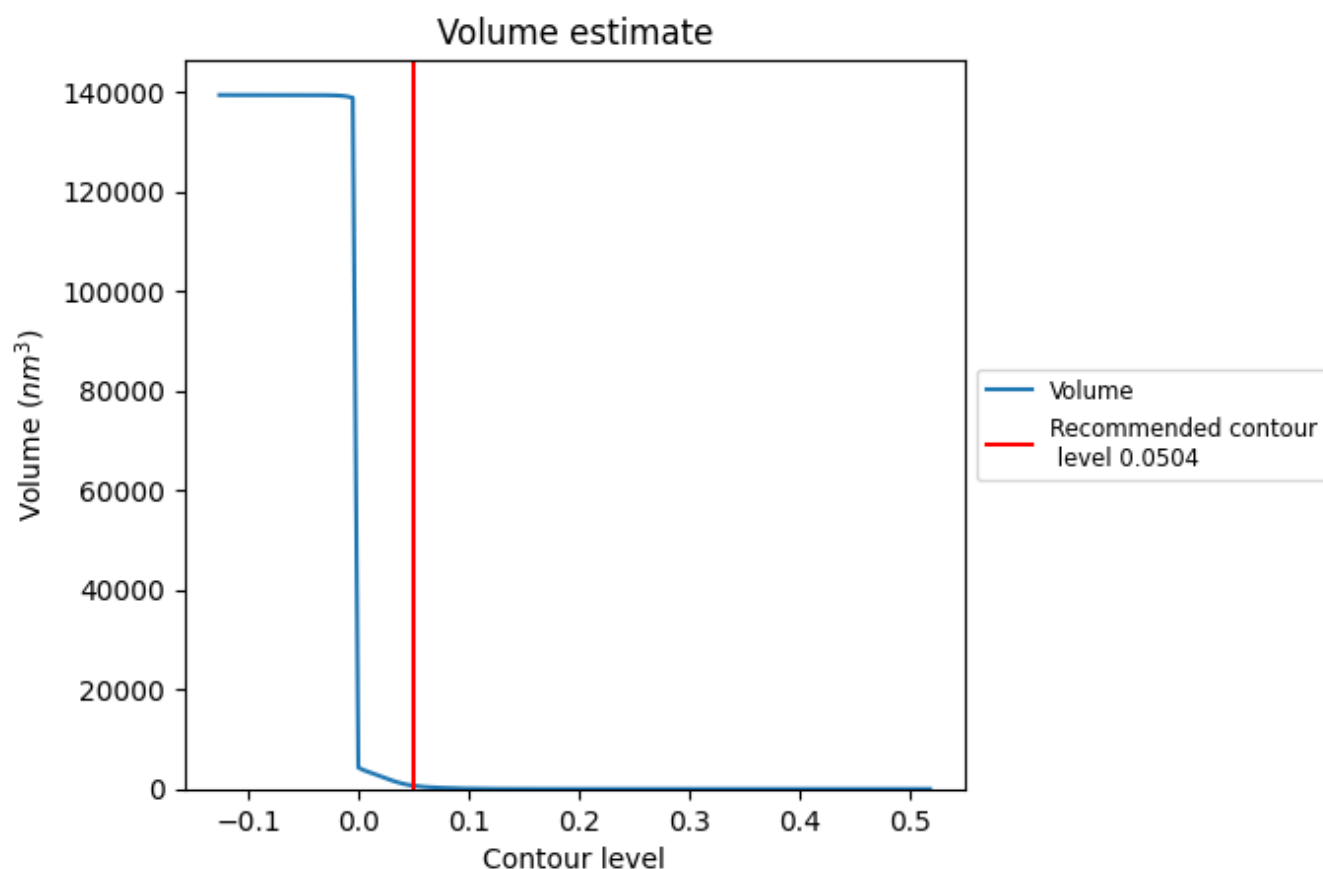
This section contains the results of statistical analysis of the map.

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.

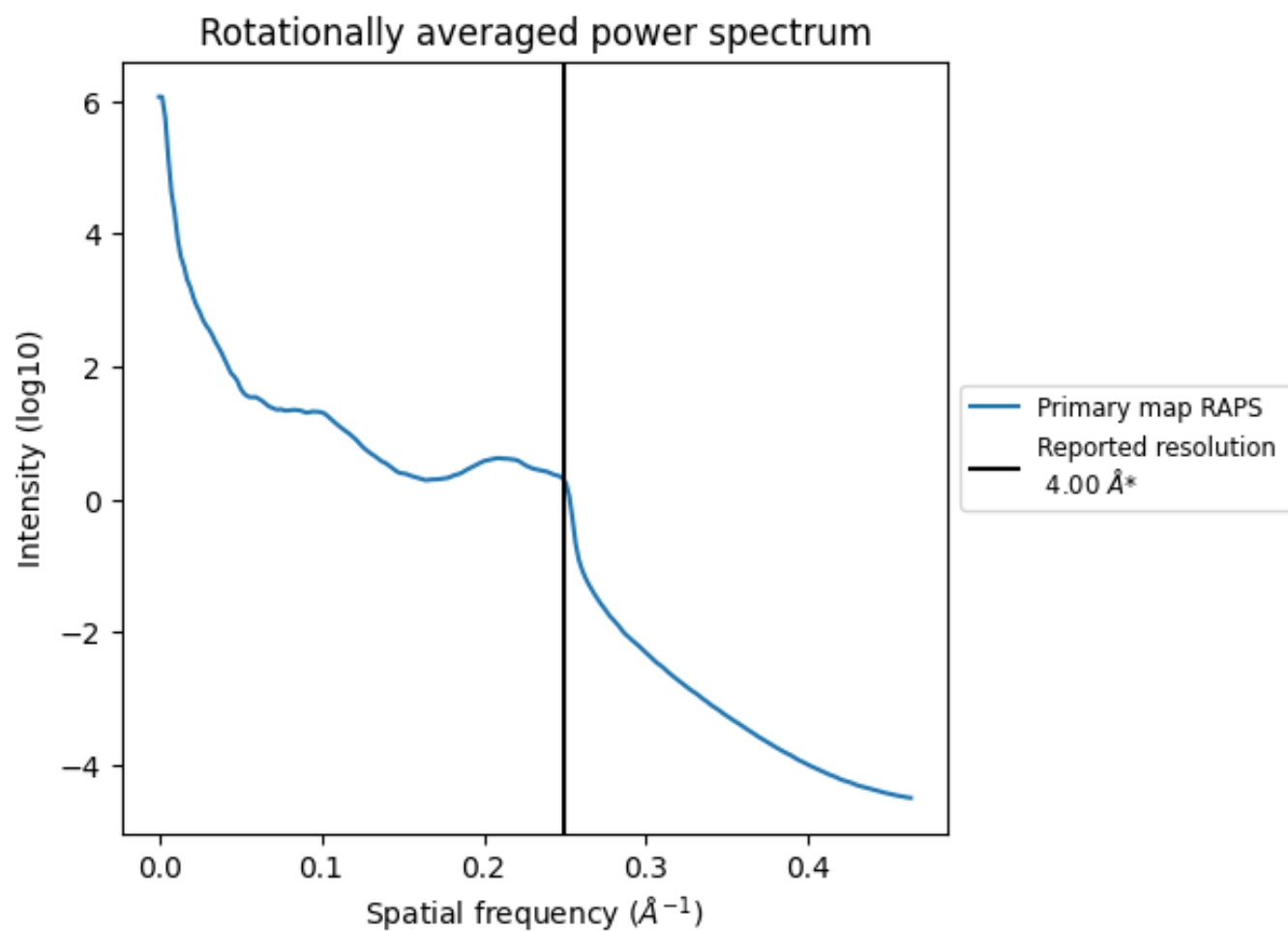
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 645 nm^3 ; this corresponds to an approximate mass of 583 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

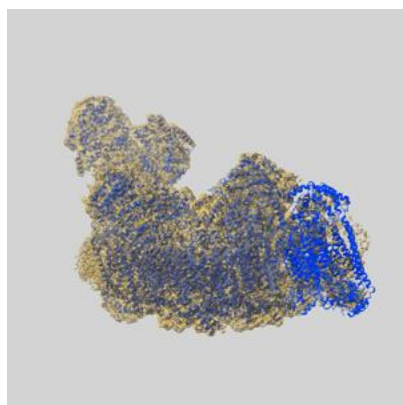
8 Fourier-Shell correlation

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

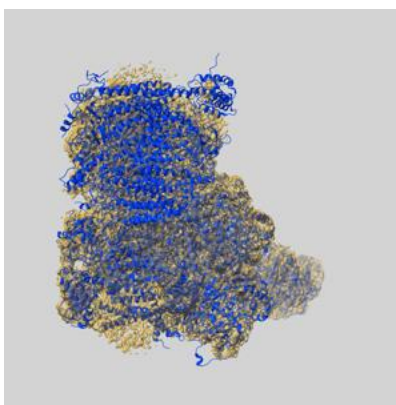
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9539 and PDB model 5GUP. Per-residue inclusion information can be found in section [3](#) on page [26](#).

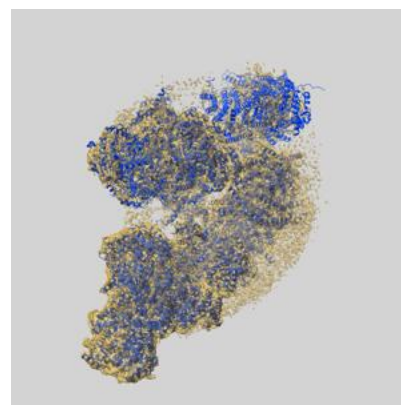
9.1 Map-model overlay [i](#)



X



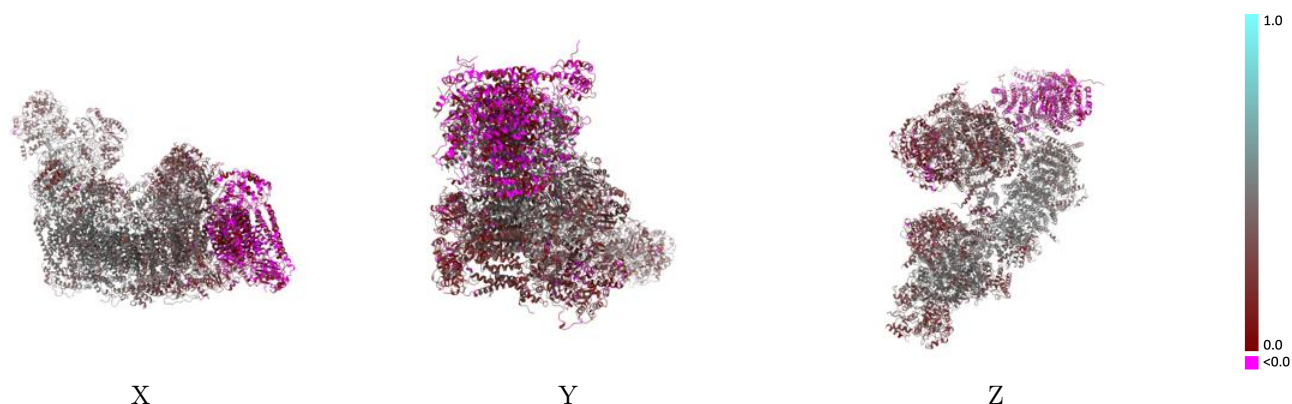
Y



Z

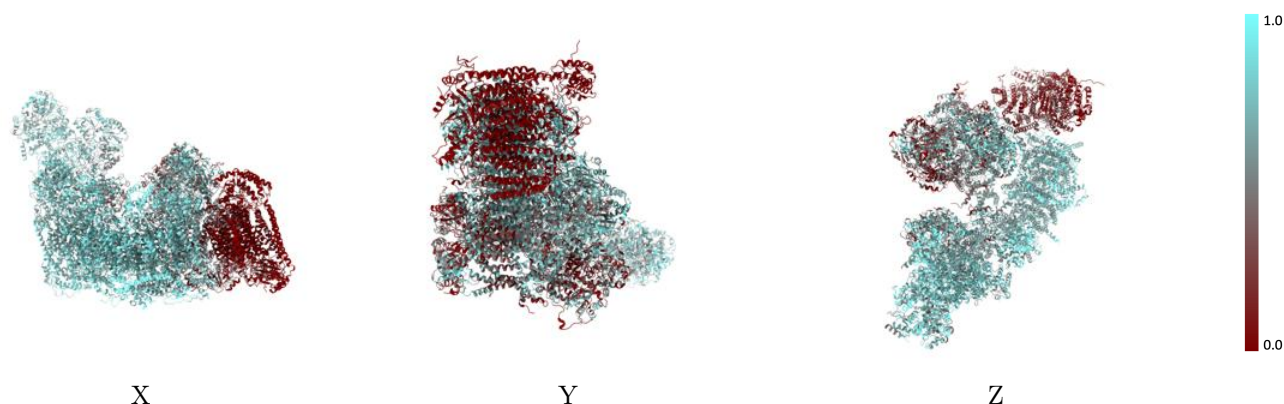
The images above show the 3D surface view of the map at the recommended contour level 0.0504 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



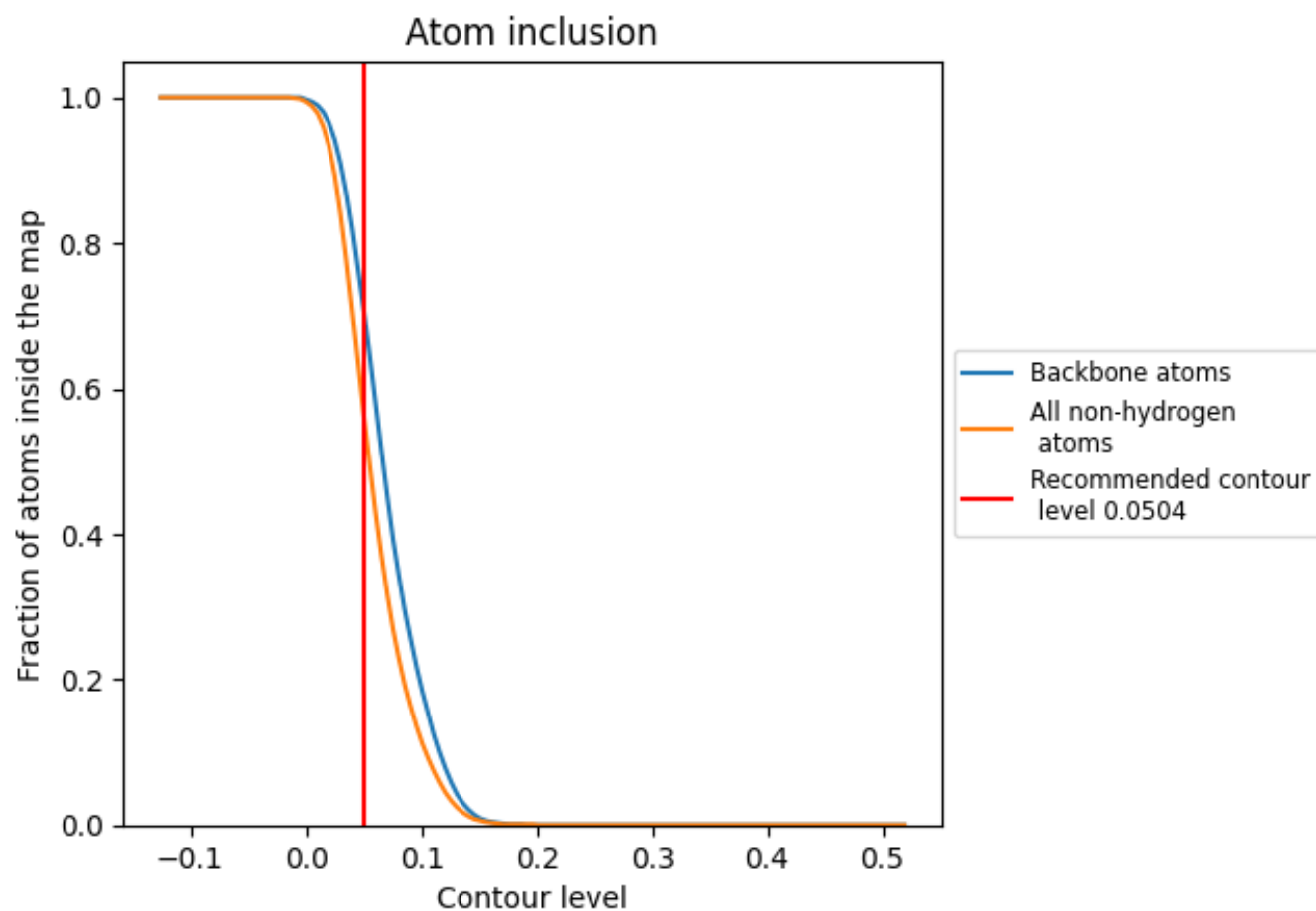
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0504).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 56% 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 (0.0504) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5630	 0.3210
0	 0.5190	 0.2820
1	 0.3490	 0.2500
2	 0.2290	 0.2380
3	 0.4180	 0.3100
4	 0.2310	 0.2150
5	 0.4020	 0.2360
6	 0.3350	 0.2240
7	 0.4720	 0.3060
8	 0.5010	 0.2670
9	 0.5120	 0.2880
A	 0.0090	 0.0280
Aa	 0.4200	 0.2560
Ab	 0.3860	 0.2050
Ac	 0.4020	 0.2340
Ad	 0.2830	 0.2220
Ae	 0.0550	 0.1380
Af	 0.1310	 0.2360
Ag	 0.0630	 0.0600
Ah	 0.0350	 -0.0050
Ai	 0.0080	 -0.0150
Aj	 0.1320	 0.0390
Ak	 0.0560	 0.0150
Al	 0.0760	 0.0170
Am	 0.0400	 0.0350
An	 0.0380	 0.0370
Ao	 0.0340	 0.0210
Ap	 0.0640	 0.0150
Aq	 0.0080	 -0.0050
Ar	 0.0480	 0.0160
B	 0.7030	 0.3330
C	 0.7990	 0.4620
D	 0.7920	 0.4200
E	 0.7200	 0.3530
F	 0.7660	 0.3820











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Chain	Atom inclusion	Q-score
G	 0.7160	 0.3650
H	 0.8140	 0.4740
I	 0.7820	 0.4530
J	 0.7020	 0.4110
K	 0.5310	 0.3890
L	 0.6070	 0.3330
M	 0.6570	 0.4030
N	 0.6690	 0.3080
O	 0.4760	 0.2630
P	 0.6540	 0.2970
Q	 0.6320	 0.3480
R	 0.4000	 0.3430
S	 0.7430	 0.4220
T	 0.7790	 0.4160
U	 0.8140	 0.4130
V	 0.6730	 0.4320
W	 0.7710	 0.4210
X	 0.7570	 0.4130
Y	 0.8420	 0.4200
Z	 0.7900	 0.3920
a	 0.8130	 0.4420
b	 0.8330	 0.4090
c	 0.8310	 0.4510
d	 0.8390	 0.4140
e	 0.7800	 0.4310
f	 0.7530	 0.3890
g	 0.8030	 0.4500
h	 0.7790	 0.4240
i	 0.7810	 0.4840
j	 0.6500	 0.4360
k	 0.7770	 0.4640
l	 0.7240	 0.4290
m	 0.6480	 0.4130
n	 0.7970	 0.4250
o	 0.7690	 0.4440
p	 0.8140	 0.4270
q	 0.7820	 0.4750
r	 0.7300	 0.4580
s	 0.8040	 0.4260
t	 0.7890	 0.3280
u	 0.6340	 0.3640
v	 0.5800	 0.3020

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Chain	Atom inclusion	Q-score
w	 0.5450	 0.3340
x	 0.5320	 0.2960
y	 0.4060	 0.2970
z	 0.5060	 0.3470