



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 03:01 AM JST

PDB ID : 8GZU / pdb_00008gzu
EMDB ID : EMD-34403
Title : Cryo-EM structure of Tetrahymena thermophila respiratory Megacomplex MC (IV2+I+III2+II)2
Authors : Wu, M.C.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on : 2022-09-27
Resolution : 4.18 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:

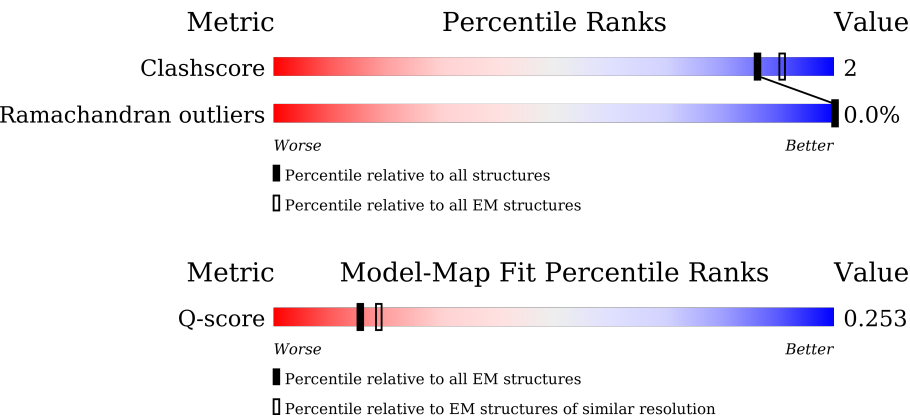
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.18 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	5389 (3.68 - 4.68)

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	00	490	15% 89% • 8%
1	55	490	21% 90% • 8%
1	A	490	89% • 8%
1	a	490	90% • 8%
2	01	473	39% 86% 5% 10%
2	56	473	21% 84% 6% 10%

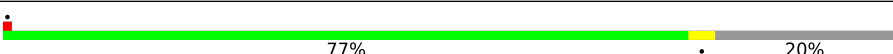
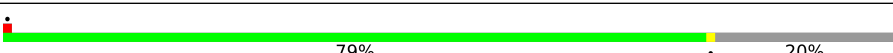
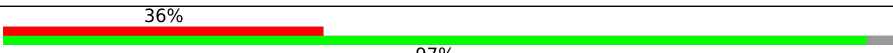
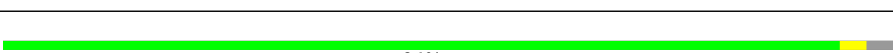
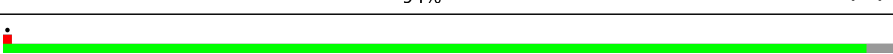
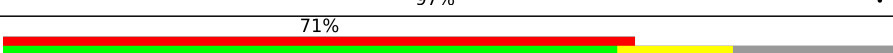
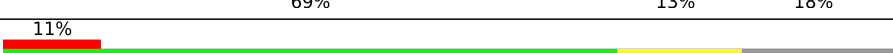
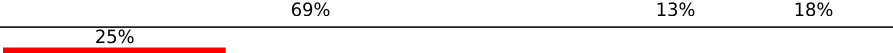
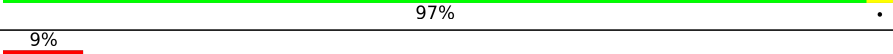
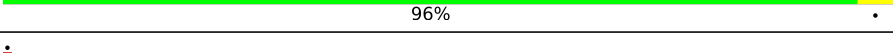
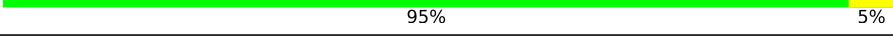
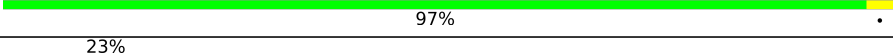
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Mol	Chain	Length	Quality of chain
2	B	473	
2	b	473	
3	02	212	
3	57	212	
3	C	212	
3	c	212	
4	03	402	
4	58	402	
4	D	402	
4	d	402	
5	04	385	
5	59	385	
5	E	385	
5	e	385	
6	05	348	
6	60	348	
6	F	348	
6	f	348	
7	06	318	
7	61	318	
7	G	318	
7	g	318	
8	07	318	
8	62	318	
8	H	318	

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Mol	Chain	Length	Quality of chain
8	h	318	
9	08	252	
9	63	252	
9	I	252	
9	i	252	
10	09	234	
10	64	234	
10	J	234	
10	j	234	
11	0A	72	
11	45	72	
11	6T	72	
11	6t	72	
12	0B	462	
12	46	462	
12	BP	462	
12	bp	462	
13	0C	188	
13	47	188	
13	FS	188	
13	fs	188	
14	0D	127	
14	48	127	
14	4A	127	
14	4a	127	

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Mol	Chain	Length	Quality of chain
15	0E	453	
15	49	453	
15	Y7	453	
15	y7	453	
16	0F	190	
16	50	190	
16	Y5	190	
16	y5	190	
17	0G	89	
17	51	89	
17	Y0	89	
17	y0	89	
18	0H	100	
18	52	100	
18	Z1	100	
18	z1	100	
19	0I	92	
19	53	92	
19	U1	92	
19	u1	92	
20	0J	17	
20	54	17	
20	QM	17	
20	Qm	17	
20	U2	17	

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Mol	Chain	Length	Quality of chain
20	qM	17	
20	qm	17	
20	u2	17	
21	10	231	
21	65	231	
21	K	231	
21	k	231	
22	11	222	
22	66	222	
22	L	222	
22	l	222	
23	12	220	
23	67	220	
23	M	220	
23	m	220	
24	13	210	
24	68	210	
24	N	210	
24	n	210	
25	14	193	
25	69	193	
25	O	193	
25	o	193	
26	15	175	
26	70	175	

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Mol	Chain	Length	Quality of chain
26	P	175	98%
26	p	175	99%
27	16	173	39%
27	71	173	21%
27	Q	173	100%
27	q	173	100%
28	17	173	68%
28	72	173	25%
28	R	173	98%
28	r	173	99%
29	18	170	68%
29	73	170	18%
29	S	170	96%
29	s	170	98%
30	19	158	32%
30	74	158	29%
30	T	158	96%
30	t	158	97%
31	1B	59	100%
31	1b	59	19%
32	20	154	9%
32	75	154	70%
32	U	154	98%
32	u	154	97%
33	21	149	11%

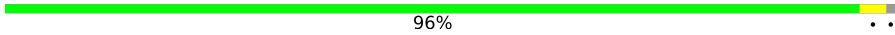
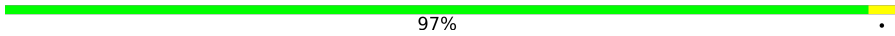
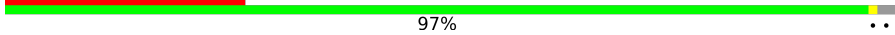
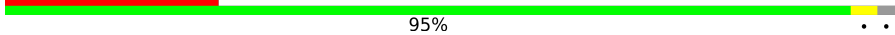
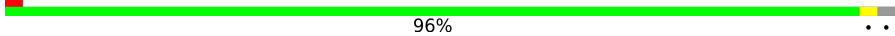
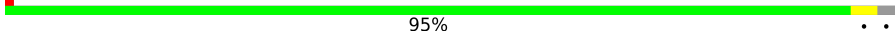
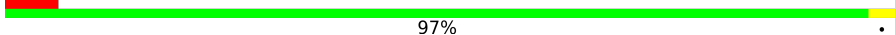
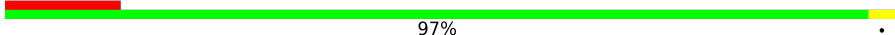
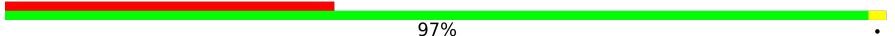
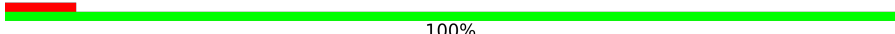
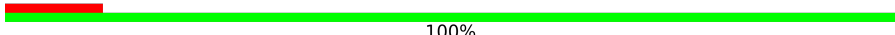
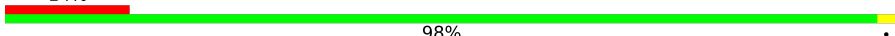
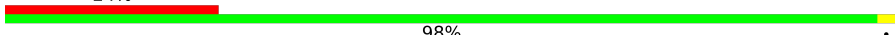
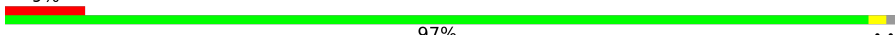
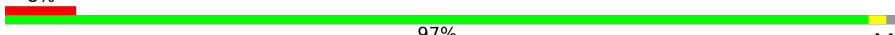
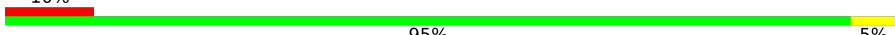
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Mol	Chain	Length	Quality of chain
33	76	149	54% 96%
33	V	149	96%
33	v	149	96%
34	22	124	40% 96%
34	77	124	52% 95%
34	W	124	96%
34	w	124	95%
35	23	122	49% 98%
35	78	122	18% 100%
35	X	122	98%
35	x	122	100%
36	24	105	49% 97%
36	79	105	58% 99%
36	Y	105	97%
36	y	105	99%
37	25	90	84% 94%
37	80	90	49% 97%
37	Z	90	94%
37	z	90	6% 97%
38	26	688	21% 97%
38	81	688	51% 96%
38	C1	688	97%
38	c1	688	96%
39	27	604	35% 96%
39	82	604	58% 97%

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Mol	Chain	Length	Quality of chain
39	C2	604	 96%
39	c2	604	 97%
40	28	594	 27% 97%
40	83	594	 24% 95%
40	C3	594	 96%
40	c3	594	 95%
41	29	637	 22% 85% 13%
41	84	637	 19% 85% 13%
41	VB	637	 85% 13%
41	vb	637	 86% 13%
42	2B	178	 6% 97%
42	2b	178	 13% 97%
43	2E	322	 37% 97%
43	2e	322	 23% 97%
44	2F	296	 10% 73% 27%
44	2f	296	 11% 73% 27%
45	2G	198	 8% 100%
45	2g	198	 11% 100%
46	2H	195	 11% 51% 48%
46	2h	195	 8% 51% 48%
47	2I	114	 14% 98%
47	2i	114	 24% 98%
48	2J	103	 9% 97%
48	2j	103	 8% 97%
49	2K	93	 10% 95% 5%

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Mol	Chain	Length	Quality of chain
49	2k	93	
50	2L	89	
50	2l	89	
51	2M	76	
51	2m	76	
52	2N	62	
52	2n	62	
53	2O	46	
53	2o	46	
54	30	130	
54	6A	130	
54	6a	130	
54	85	130	
55	31	230	
55	6B	230	
55	6b	230	
55	86	230	
56	32	103	
56	6C	103	
56	6c	103	
56	87	103	
57	33	88	
57	6L	88	
57	6l	88	
57	88	88	

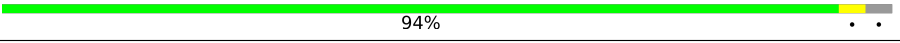
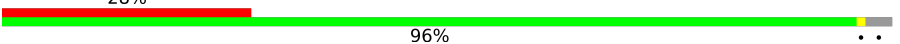
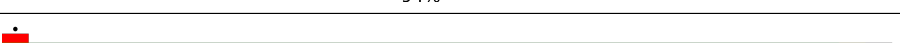
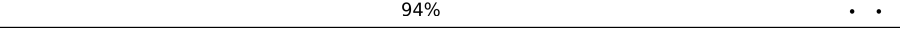
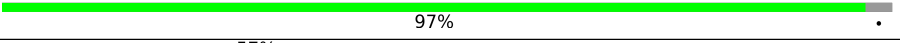
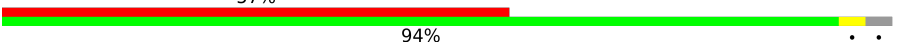
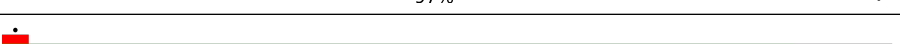
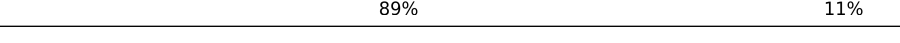
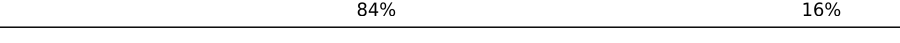
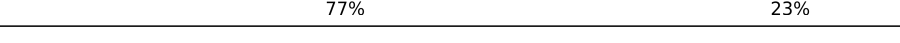
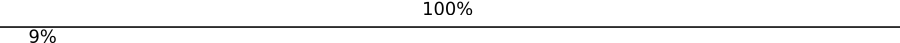
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Mol	Chain	Length	Quality of chain
58	34	133	
58	7A	133	
58	7a	133	
58	89	133	
59	35	236	
59	7C	236	
59	7c	236	
59	90	236	
60	36	990	
60	7L	990	
60	7l	990	
60	91	990	
61	37	346	
61	92	346	
61	M1	346	
61	m1	346	
62	38	318	
62	93	318	
62	M2	318	
62	m2	318	
63	39	330	
63	94	330	
63	M3	330	
63	m3	330	
64	1T	72	

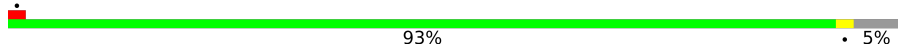
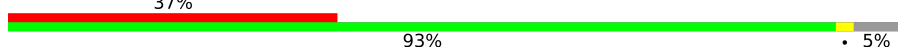
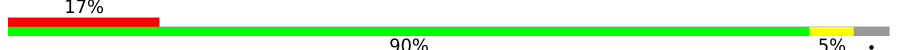
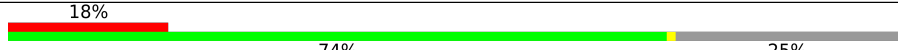
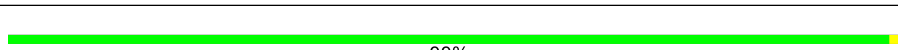
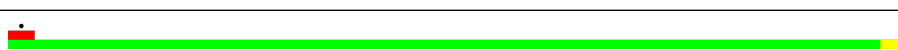
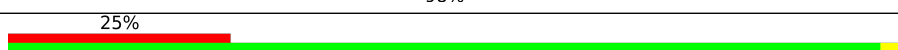
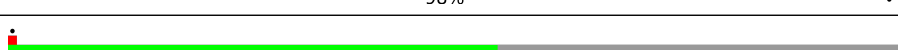
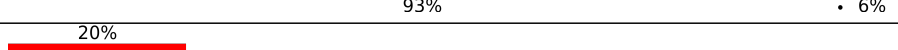
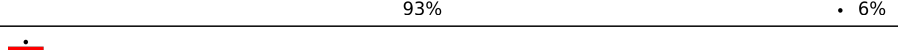
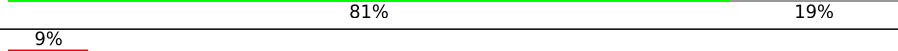
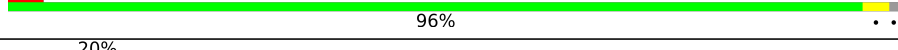
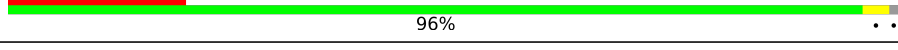
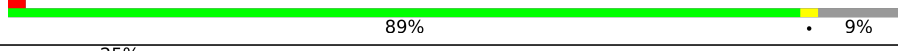
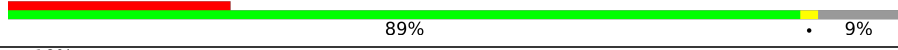
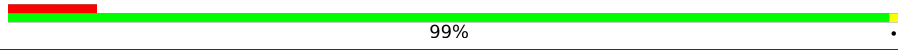
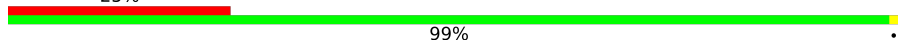
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Mol	Chain	Length	Quality of chain
64	1t	72	
64	40	72	
64	95	72	
65	2T	72	
65	2t	72	
65	41	72	
65	96	72	
66	3T	93	
66	3t	93	
66	42	93	
66	97	93	
67	43	68	
67	4T	68	
67	4t	68	
67	98	68	
68	44	81	
68	5T	81	
68	5t	81	
68	99	81	
69	4L	116	
69	4l	116	
70	5B	100	
70	5b	100	
71	A1	94	
71	a1	94	

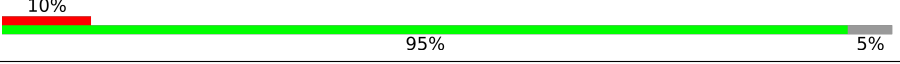
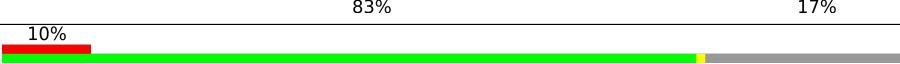
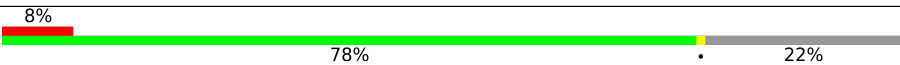
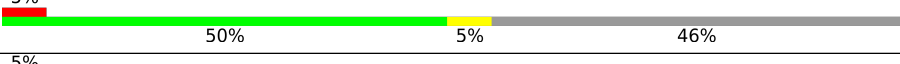
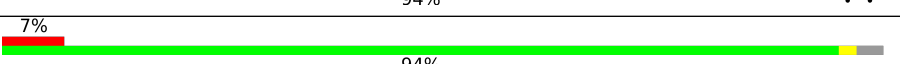
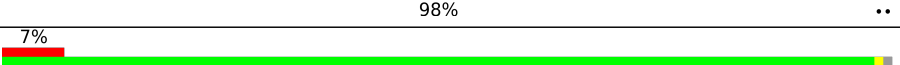
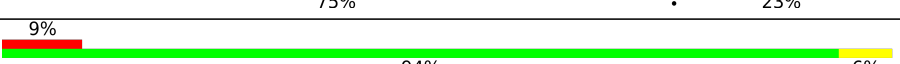
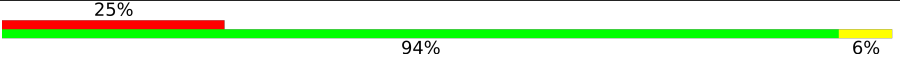
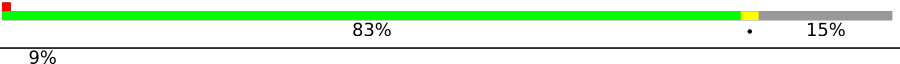
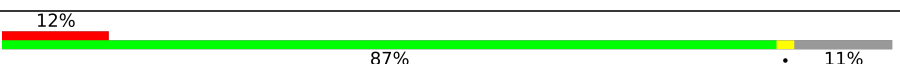
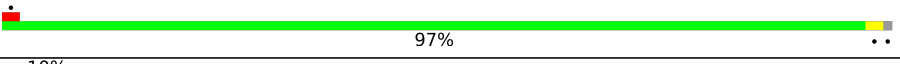
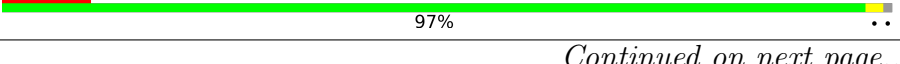
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Mol	Chain	Length	Quality of chain
72	A2	103	
72	a2	103	
73	A3	135	
73	a3	135	
74	A5	206	
74	a5	206	
75	A6	172	
75	a6	172	
76	A7	282	
76	a7	282	
77	A8	238	
77	a8	238	
78	A9	362	
78	a9	362	
79	AB	138	
79	ab	138	
80	AC	133	
80	ac	133	
81	AL	194	
81	al	194	
82	AM	175	
82	am	175	
83	AN	231	
83	an	231	
84	B2	126	

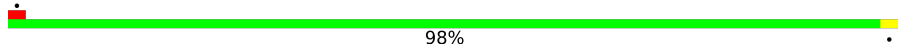
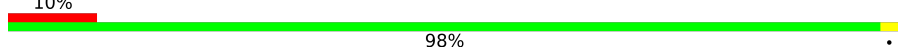
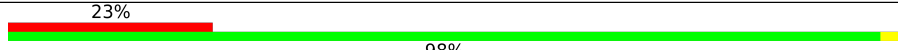
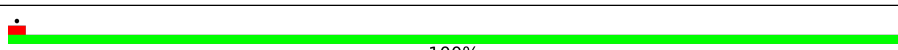
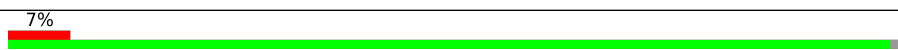
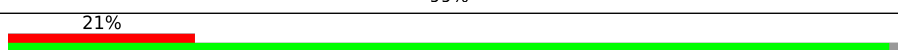
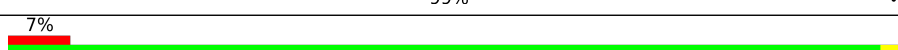
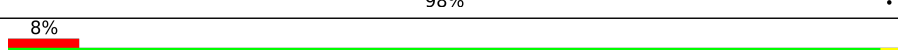
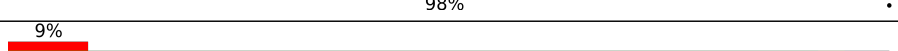
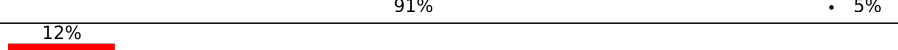
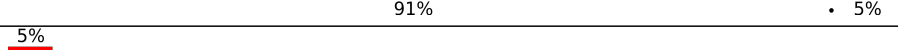
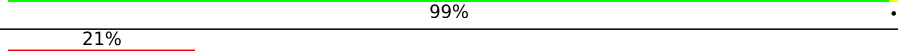
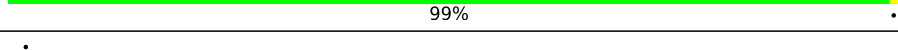
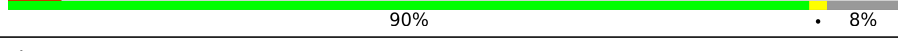
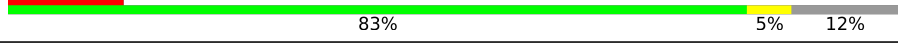
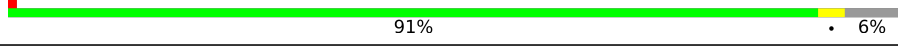
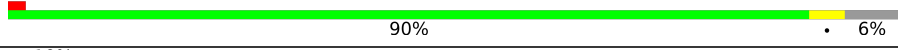
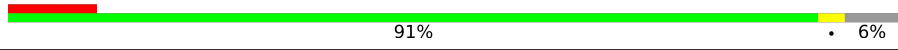
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Mol	Chain	Length	Quality of chain
84	b2	126	
85	B3	83	
85	b3	83	
86	B4	147	
86	b4	147	
87	B6	129	
87	b6	129	
88	B7	120	
88	b7	120	
89	B8	207	
89	b8	207	
90	B9	189	
90	b9	189	
91	BL	188	
91	bl	188	
92	BM	214	
92	bm	214	
93	C4	102	
93	c4	102	
94	FX	172	
94	fx	172	
95	G1	257	
95	g1	257	
96	G2	233	
96	g2	233	

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Mol	Chain	Length	Quality of chain
97	G3	346	
97	g3	346	
98	J1	317	
98	j1	317	
99	N1	284	
99	n1	284	
100	N2	360	
100	n2	360	
101	N3	121	
101	n3	121	
102	N4	505	
102	n4	505	
103	N5	750	
103	n5	750	
104	N6	255	
104	n6	255	
105	P1	251	
105	p1	251	
106	P2	189	
106	p2	189	
107	QA	482	
107	Qa	482	
107	qA	482	
107	qa	482	
108	QB	513	

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Mol	Chain	Length	Quality of chain
108	Qb	513	
108	qB	513	
108	qb	513	
109	QC	426	
109	Qc	426	
109	qC	426	
109	qc	426	
110	QD	319	
110	Qd	319	
110	qD	319	
110	qd	319	
111	QE	269	
111	Qe	269	
111	qE	269	
111	qe	269	
112	QF	90	
112	Qf	90	
112	qF	90	
112	qf	90	
113	QG	328	
113	Qg	328	
113	qG	328	
113	qg	328	
114	QH	130	
114	Qh	130	

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Mol	Chain	Length	Quality of chain
114	qH	130	12% 96% ..
114	qh	130	25% 96% ..
115	QI	119	94% ..
115	Qi	119	6% 95% ..
115	qI	119	8% 94% ..
115	qi	119	39% 95% ..
116	QJ	62	5% 90% 10%
116	Qj	62	15% 89% 5% 6%
116	qJ	62	10% 90% 10%
116	qj	62	18% 89% 5% 6%
117	QL	41	7% 78% 22%
117	Ql	41	5% 78% 22%
117	qL	41	12% 78% 22%
117	ql	41	10% 78% 22%
118	S1	718	6% 92% ..
118	s1	718	54% 92% ..
119	S2	442	.. 96% .
119	s2	442	25% 96% .
120	S3	198	.. 96% .
120	s3	198	25% 97% .
121	S4	185	15% 97% ..
121	s4	185	55% 97% ..
122	S5	94	12% 99% .
122	s5	94	44% 99% .
123	S6	132	62% 8% 30%

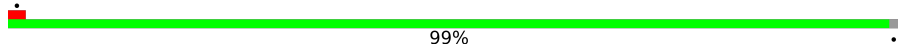
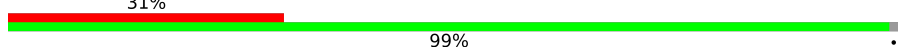
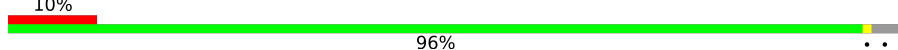
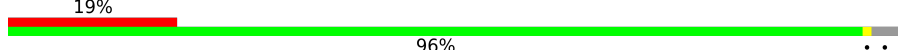
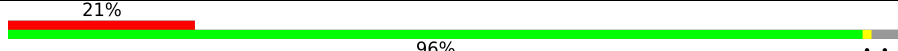
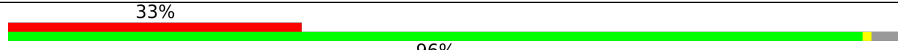
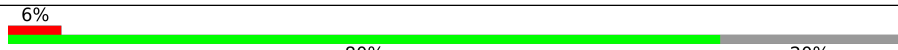
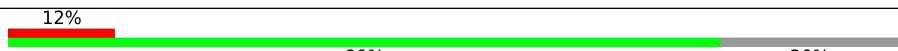
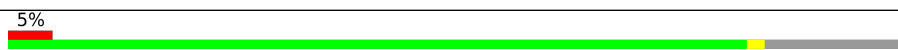
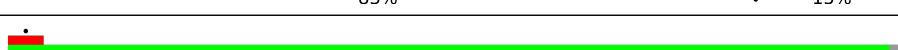
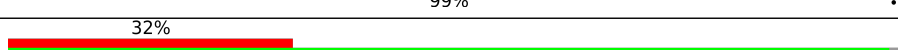
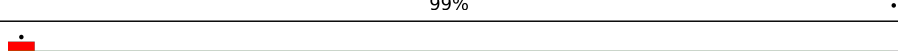
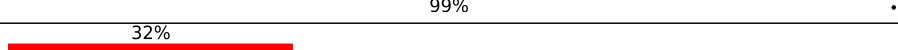
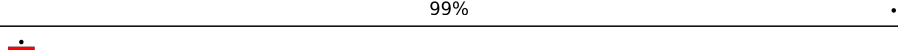
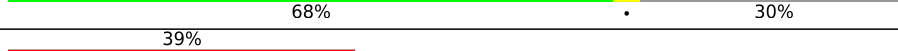
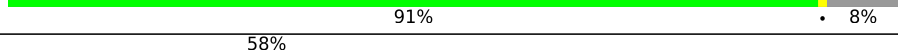
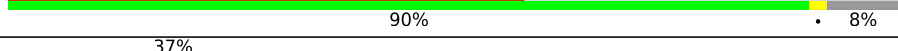
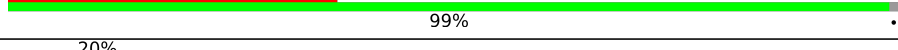
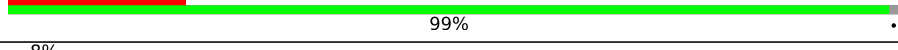
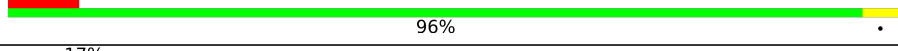
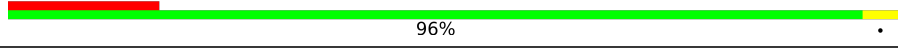
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Mol	Chain	Length	Quality of chain
123	s6	132	
124	S7	162	
124	s7	162	
125	S8	236	
125	s8	236	
126	SA	636	
126	sa	636	
127	SB	312	
127	sb	312	
128	SC	60	
128	sc	60	
129	SD	44	
129	sd	44	
130	T1	516	
130	t1	516	
131	T2	333	
131	t2	333	
132	T3	311	
132	t3	311	
133	T4	212	
133	t4	212	
134	T5	205	
134	t5	205	
135	T6	144	
135	t6	144	

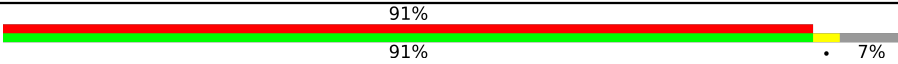
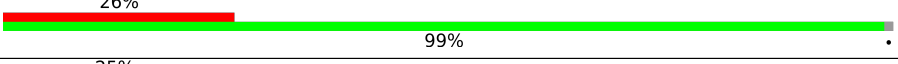
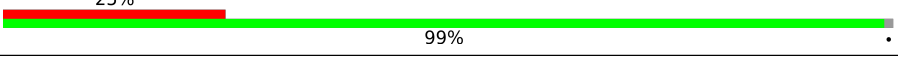
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Mol	Chain	Length	Quality of chain
136	T7	143	
136	t7	143	
137	T8	135	
137	t8	135	
138	T9	136	
138	t9	136	
139	TA	127	
139	ta	127	
140	TB	113	
140	tb	113	
141	TC	93	
141	tc	93	
142	TD	73	
142	td	73	
143	TE	71	
143	te	71	
144	TF	236	
144	tf	236	
145	TG	135	
145	tg	135	
146	TH	124	
146	th	124	
147	TX	166	
147	tx	166	
148	V1	474	

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Mol	Chain	Length	Quality of chain
148	v1	474	
149	V2	274	
149	v2	274	
150	X1	150	
150	x1	150	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
151	FES	fs	202	-	-	X	-
157	HEC	2E	401	X	-	-	-
157	HEC	2e	401	X	-	-	-
157	HEC	QD	401	X	-	-	-
157	HEC	Qd	401	X	-	-	-
157	HEC	qD	401	X	-	-	-
157	HEC	qd	401	X	-	-	-

2 Entry composition

There are 164 unique types of molecules in this entry. The entry contains 447736 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 Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	00	449	Total	C	N	O	0	0
			2228	1330	449	449		
1	55	449	Total	C	N	O	0	0
			2228	1330	449	449		
1	a	449	Total	C	N	O	0	0
			2228	1330	449	449		
1	A	449	Total	C	N	O	0	0
			2228	1330	449	449		

- Molecule 2 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	01	428	Total	C	N	O	0	0
			2116	1260	428	428		
2	56	428	Total	C	N	O	0	0
			2116	1260	428	428		
2	b	428	Total	C	N	O	0	0
			2116	1260	428	428		
2	B	428	Total	C	N	O	0	0
			2116	1260	428	428		

- Molecule 3 is a protein called COXTT3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	02	203	Total	C	N	O	0	0
			1003	597	203	203		
3	57	203	Total	C	N	O	0	0
			1003	597	203	203		
3	c	203	Total	C	N	O	0	0
			1003	597	203	203		
3	C	203	Total	C	N	O	0	0
			1003	597	203	203		

- Molecule 4 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	03	289	Total	C	N	O	0	0
			1427	849	289	289		
4	58	289	Total	C	N	O	0	0
			1427	849	289	289		
4	d	289	Total	C	N	O	0	0
			1427	849	289	289		
4	D	289	Total	C	N	O	0	0
			1427	849	289	289		

- Molecule 5 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	04	384	Total	C	N	O	0	0
			1905	1137	384	384		
5	59	384	Total	C	N	O	0	0
			1905	1137	384	384		
5	e	384	Total	C	N	O	0	0
			1905	1137	384	384		
5	E	384	Total	C	N	O	0	0
			1905	1137	384	384		

- Molecule 6 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	05	243	Total	C	N	O	0	0
			1205	719	243	243		
6	60	243	Total	C	N	O	0	0
			1205	719	243	243		
6	f	243	Total	C	N	O	0	0
			1205	719	243	243		
6	F	243	Total	C	N	O	0	0
			1205	719	243	243		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	06	293	Total	C	N	O	0	0
			1454	868	293	293		
7	61	293	Total	C	N	O	0	0
			1454	868	293	293		
7	g	293	Total	C	N	O	0	0
			1454	868	293	293		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	293	Total	C	N	O	0	0
			1454	868	293	293		

- Molecule 8 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	07	298	Total	C	N	O	0	0
			1469	873	298	298		
8	62	298	Total	C	N	O	0	0
			1469	873	298	298		
8	h	298	Total	C	N	O	0	0
			1469	873	298	298		
8	H	298	Total	C	N	O	0	0
			1469	873	298	298		

- Molecule 9 is a protein called COXTT9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	08	231	Total	C	N	O	0	0
			1141	679	231	231		
9	63	231	Total	C	N	O	0	0
			1141	679	231	231		
9	i	231	Total	C	N	O	0	0
			1141	679	231	231		
9	I	231	Total	C	N	O	0	0
			1141	679	231	231		

- Molecule 10 is a protein called COXTT10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	09	187	Total	C	N	O	0	0
			931	557	187	187		
10	64	187	Total	C	N	O	0	0
			931	557	187	187		
10	j	187	Total	C	N	O	0	0
			931	557	187	187		
10	J	187	Total	C	N	O	0	0
			931	557	187	187		

- Molecule 11 is a protein called Annexin.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	0A	70	Total	C	N	O	0	0
			346	206	70	70		
11	45	70	Total	C	N	O	0	0
			346	206	70	70		
11	6t	70	Total	C	N	O	0	0
			346	206	70	70		
11	6T	70	Total	C	N	O	0	0
			346	206	70	70		

- Molecule 12 is a protein called Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	0B	381	Total	C	N	O	0	0
			1858	1096	381	381		
12	46	381	Total	C	N	O	0	0
			1858	1096	381	381		
12	bp	381	Total	C	N	O	0	0
			1858	1096	381	381		
12	BP	381	Total	C	N	O	0	0
			1858	1096	381	381		

- Molecule 13 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	0C	188	Total	C	N	O	0	0
			928	552	188	188		
13	47	188	Total	C	N	O	0	0
			928	552	188	188		
13	fs	188	Total	C	N	O	0	0
			928	552	188	188		
13	FS	188	Total	C	N	O	0	0
			928	552	188	188		

- Molecule 14 is a protein called Phage protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	0D	100	Total	C	N	O	0	0
			494	294	100	100		
14	48	100	Total	C	N	O	0	0
			494	294	100	100		
14	4A	100	Total	C	N	O	0	0
			494	294	100	100		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	4a	100	Total	C	N	O	0	0
			494	294	100	100		

- Molecule 15 is a protein called Ymf67.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	0E	343	Total	C	N	O	0	0
			1711	1025	343	343		
15	49	343	Total	C	N	O	0	0
			1711	1025	343	343		
15	y7	343	Total	C	N	O	0	0
			1711	1025	343	343		
15	Y7	343	Total	C	N	O	0	0
			1711	1025	343	343		

- Molecule 16 is a protein called Ymf75.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	0F	190	Total	C	N	O	0	0
			947	567	190	190		
16	50	190	Total	C	N	O	0	0
			947	567	190	190		
16	y5	190	Total	C	N	O	0	0
			947	567	190	190		
16	Y5	190	Total	C	N	O	0	0
			947	567	190	190		

- Molecule 17 is a protein called Ymf70.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	0G	89	Total	C	N	O	0	0
			444	266	89	89		
17	51	89	Total	C	N	O	0	0
			444	266	89	89		
17	y0	89	Total	C	N	O	0	0
			444	266	89	89		
17	Y0	89	Total	C	N	O	0	0
			444	266	89	89		

- Molecule 18 is a protein called COXTT28.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	0H	97	Total	C	N	O	0	0
			479	285	97	97		
18	52	97	Total	C	N	O	0	0
			479	285	97	97		
18	z1	97	Total	C	N	O	0	0
			479	285	97	97		
18	Z1	97	Total	C	N	O	0	0
			479	285	97	97		

- Molecule 19 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	0I	92	Total	C	N	O	0	0
			460	276	92	92		
19	53	92	Total	C	N	O	0	0
			460	276	92	92		
19	u1	92	Total	C	N	O	0	0
			460	276	92	92		
19	U1	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 20 is a protein called unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	0J	17	Total	C	N	O	0	0
			85	51	17	17		
20	54	17	Total	C	N	O	0	0
			85	51	17	17		
20	qM	17	Total	C	N	O	0	0
			85	51	17	17		
20	qm	17	Total	C	N	O	0	0
			85	51	17	17		
20	QM	17	Total	C	N	O	0	0
			85	51	17	17		
20	Qm	17	Total	C	N	O	0	0
			85	51	17	17		
20	u2	17	Total	C	N	O	0	0
			85	51	17	17		
20	U2	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 21 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	10	208	Total	C	N	O	0	0
			1032	616	208	208		
21	65	208	Total	C	N	O	0	0
			1032	616	208	208		
21	k	208	Total	C	N	O	0	0
			1032	616	208	208		
21	K	208	Total	C	N	O	0	0
			1032	616	208	208		

- Molecule 22 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	11	194	Total	C	N	O	0	0
			965	577	194	194		
22	66	194	Total	C	N	O	0	0
			965	577	194	194		
22	l	194	Total	C	N	O	0	0
			965	577	194	194		
22	L	194	Total	C	N	O	0	0
			965	577	194	194		

- Molecule 23 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	12	219	Total	C	N	O	0	0
			1083	645	219	219		
23	67	219	Total	C	N	O	0	0
			1083	645	219	219		
23	m	219	Total	C	N	O	0	0
			1083	645	219	219		
23	M	219	Total	C	N	O	0	0
			1083	645	219	219		

- Molecule 24 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	13	206	Total	C	N	O	0	0
			1016	604	206	206		
24	68	206	Total	C	N	O	0	0
			1016	604	206	206		
24	n	206	Total	C	N	O	0	0
			1016	604	206	206		

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Mol	Chain	Residues	Atoms				AltConf	Trace
24	N	206	Total	C	N	O	0	0
			1016	604	206	206		

- Molecule 25 is a protein called Mobilization protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	14	129	Total	C	N	O	0	0
			641	383	129	129		
25	69	129	Total	C	N	O	0	0
			641	383	129	129		
25	o	129	Total	C	N	O	0	0
			641	383	129	129		
25	O	129	Total	C	N	O	0	0
			641	383	129	129		

- Molecule 26 is a protein called YfiT domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	15	175	Total	C	N	O	0	0
			865	515	175	175		
26	70	175	Total	C	N	O	0	0
			865	515	175	175		
26	p	175	Total	C	N	O	0	0
			865	515	175	175		
26	P	175	Total	C	N	O	0	0
			865	515	175	175		

- Molecule 27 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	16	173	Total	C	N	O	0	0
			855	509	173	173		
27	71	173	Total	C	N	O	0	0
			855	509	173	173		
27	q	173	Total	C	N	O	0	0
			855	509	173	173		
27	Q	173	Total	C	N	O	0	0
			855	509	173	173		

- Molecule 28 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	17	172	Total	C	N	O	0	0
			852	508	172	172		
28	72	172	Total	C	N	O	0	0
			852	508	172	172		
28	r	172	Total	C	N	O	0	0
			852	508	172	172		
28	R	172	Total	C	N	O	0	0
			852	508	172	172		

- Molecule 29 is a protein called Complex III subunit VII.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	18	169	Total	C	N	O	0	0
			841	503	169	169		
29	73	169	Total	C	N	O	0	0
			841	503	169	169		
29	s	169	Total	C	N	O	0	0
			841	503	169	169		
29	S	169	Total	C	N	O	0	0
			841	503	169	169		

- Molecule 30 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	19	156	Total	C	N	O	0	0
			771	459	156	156		
30	74	156	Total	C	N	O	0	0
			771	459	156	156		
30	t	156	Total	C	N	O	0	0
			771	459	156	156		
30	T	156	Total	C	N	O	0	0
			771	459	156	156		

- Molecule 31 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	1b	59	Total	C	N	O	0	0
			293	175	59	59		
31	1B	59	Total	C	N	O	0	0
			293	175	59	59		

- Molecule 32 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	20	153	Total	C	N	O	0	0
			757	451	153	153		
32	75	153	Total	C	N	O	0	0
			757	451	153	153		
32	u	153	Total	C	N	O	0	0
			757	451	153	153		
32	U	153	Total	C	N	O	0	0
			757	451	153	153		

- Molecule 33 is a protein called COXTT22.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	21	146	Total	C	N	O	0	0
			722	430	146	146		
33	76	146	Total	C	N	O	0	0
			722	430	146	146		
33	v	146	Total	C	N	O	0	0
			722	430	146	146		
33	V	146	Total	C	N	O	0	0
			722	430	146	146		

- Molecule 34 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	22	123	Total	C	N	O	0	0
			612	366	123	123		
34	77	123	Total	C	N	O	0	0
			612	366	123	123		
34	w	123	Total	C	N	O	0	0
			612	366	123	123		
34	W	123	Total	C	N	O	0	0
			612	366	123	123		

- Molecule 35 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	23	122	Total	C	N	O	0	0
			602	358	122	122		
35	78	122	Total	C	N	O	0	0
			602	358	122	122		
35	x	122	Total	C	N	O	0	0
			602	358	122	122		

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Mol	Chain	Residues	Atoms				AltConf	Trace
35	X	122	Total	C	N	O	0	0
			602	358	122	122		

- Molecule 36 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	24	105	Total	C	N	O	0	0
			517	307	105	105		
36	79	105	Total	C	N	O	0	0
			517	307	105	105		
36	y	105	Total	C	N	O	0	0
			517	307	105	105		
36	Y	105	Total	C	N	O	0	0
			517	307	105	105		

- Molecule 37 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	25	87	Total	C	N	O	0	0
			429	255	87	87		
37	80	87	Total	C	N	O	0	0
			429	255	87	87		
37	z	87	Total	C	N	O	0	0
			429	255	87	87		
37	Z	87	Total	C	N	O	0	0
			429	255	87	87		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	26	674	Total	C	N	O	0	0
			3328	1980	674	674		
38	81	674	Total	C	N	O	0	0
			3328	1980	674	674		
38	c1	674	Total	C	N	O	0	0
			3328	1980	674	674		
38	C1	674	Total	C	N	O	0	0
			3328	1980	674	674		

- Molecule 39 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	27	599	Total	C	N	O	0	0
			2975	1777	599	599		
39	82	599	Total	C	N	O	0	0
			2975	1777	599	599		
39	c2	599	Total	C	N	O	0	0
			2975	1777	599	599		
39	C2	599	Total	C	N	O	0	0
			2975	1777	599	599		

- Molecule 40 is a protein called Ymf68.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	28	582	Total	C	N	O	0	0
			2894	1730	582	582		
40	83	582	Total	C	N	O	0	0
			2894	1730	582	582		
40	c3	582	Total	C	N	O	0	0
			2894	1730	582	582		
40	C3	582	Total	C	N	O	0	0
			2894	1730	582	582		

- Molecule 41 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	29	555	Total	C	N	O	P	0	0
			2765	1645	555	563	2		
41	84	555	Total	C	N	O	P	0	0
			2765	1645	555	563	2		
41	vb	555	Total	C	N	O	P	0	0
			2765	1645	555	563	2		
41	VB	555	Total	C	N	O	P	0	0
			2765	1645	555	563	2		

- Molecule 42 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2b	178	Total	C	N	O	0	0
			884	528	178	178		
42	2B	178	Total	C	N	O	0	0
			884	528	178	178		

- Molecule 43 is a protein called NmrA domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2e	321	Total	C	N	O	0	0
			1591	949	321	321		
43	2E	321	Total	C	N	O	0	0
			1591	949	321	321		

- Molecule 44 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2f	217	Total	C	N	O	0	0
			1077	643	217	217		
44	2F	217	Total	C	N	O	0	0
			1077	643	217	217		

- Molecule 45 is a protein called SDHTT3.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	2g	198	Total	C	N	O	0	0
			984	588	198	198		
45	2G	198	Total	C	N	O	0	0
			984	588	198	198		

- Molecule 46 is a protein called Dipthamide synthesis protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	2h	102	Total	C	N	O	0	0
			507	303	102	102		
46	2H	102	Total	C	N	O	0	0
			507	303	102	102		

- Molecule 47 is a protein called DUF4885 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	2i	114	Total	C	N	O	0	0
			564	336	114	114		
47	2I	114	Total	C	N	O	0	0
			564	336	114	114		

- Molecule 48 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	2j	102	Total	C	N	O	0	0
			505	301	102	102		

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Mol	Chain	Residues	Atoms				AltConf	Trace
48	2J	102	Total	C	N	O	0	0
			505	301	102	102		

- Molecule 49 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	2k	93	Total	C	N	O	0	0
			462	276	93	93		
49	2K	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 50 is a protein called Transposase.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	2l	83	Total	C	N	O	0	0
			415	249	83	83		
50	2L	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 51 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	2m	75	Total	C	N	O	0	0
			370	220	75	75		
51	2M	75	Total	C	N	O	0	0
			370	220	75	75		

- Molecule 52 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	2n	61	Total	C	N	O	0	0
			302	180	61	61		
52	2N	61	Total	C	N	O	0	0
			302	180	61	61		

- Molecule 53 is a protein called SDHTT11.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	2o	42	Total	C	N	O	0	0
			210	126	42	42		
53	2O	42	Total	C	N	O	0	0
			210	126	42	42		

- Molecule 54 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	30	126	Total	C	N	O	0	0
			624	372	126	126		
54	85	126	Total	C	N	O	0	0
			624	372	126	126		
54	6a	126	Total	C	N	O	0	0
			624	372	126	126		
54	6A	126	Total	C	N	O	0	0
			624	372	126	126		

- Molecule 55 is a protein called Structural protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	31	222	Total	C	N	O	0	0
			1101	657	222	222		
55	86	222	Total	C	N	O	0	0
			1101	657	222	222		
55	6b	222	Total	C	N	O	0	0
			1101	657	222	222		
55	6B	222	Total	C	N	O	0	0
			1101	657	222	222		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	32	101	Total	C	N	O	0	0
			499	297	101	101		
56	87	101	Total	C	N	O	0	0
			499	297	101	101		
56	6c	101	Total	C	N	O	0	0
			499	297	101	101		
56	6C	101	Total	C	N	O	0	0
			499	297	101	101		

- Molecule 57 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	33	77	Total	C	N	O	0	0
			383	229	77	77		
57	88	77	Total	C	N	O	0	0
			383	229	77	77		
57	6l	77	Total	C	N	O	0	0
			383	229	77	77		

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Mol	Chain	Residues	Atoms				AltConf	Trace
57	6L	77	Total	C	N	O	0	0
			383	229	77	77		

- Molecule 58 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	34	133	Total	C	N	O	0	0
			659	393	133	133		
58	89	133	Total	C	N	O	0	0
			659	393	133	133		
58	7a	133	Total	C	N	O	0	0
			659	393	133	133		
58	7A	133	Total	C	N	O	0	0
			659	393	133	133		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	35	211	Total	C	N	O	P	0	0
			1052	625	211	215	1		
59	90	211	Total	C	N	O	P	0	0
			1052	625	211	215	1		
59	7c	211	Total	C	N	O	P	0	0
			1052	625	211	215	1		
59	7C	211	Total	C	N	O	P	0	0
			1052	625	211	215	1		

- Molecule 60 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	36	131	Total	C	N	O	0	0
			654	392	131	131		
60	91	131	Total	C	N	O	0	0
			654	392	131	131		
60	7l	131	Total	C	N	O	0	0
			654	392	131	131		
60	7L	131	Total	C	N	O	0	0
			654	392	131	131		

- Molecule 61 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	37	346	Total	C	N	O	0	0
			1709	1017	346	346		
61	92	346	Total	C	N	O	0	0
			1709	1017	346	346		
61	m1	346	Total	C	N	O	0	0
			1709	1017	346	346		
61	M1	346	Total	C	N	O	0	0
			1709	1017	346	346		

- Molecule 62 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	38	318	Total	C	N	O	0	0
			1561	925	318	318		
62	93	318	Total	C	N	O	0	0
			1561	925	318	318		
62	m2	318	Total	C	N	O	0	0
			1561	925	318	318		
62	M2	318	Total	C	N	O	0	0
			1561	925	318	318		

- Molecule 63 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	39	329	Total	C	N	O	0	0
			1624	966	329	329		
63	94	329	Total	C	N	O	0	0
			1624	966	329	329		
63	m3	329	Total	C	N	O	0	0
			1624	966	329	329		
63	M3	329	Total	C	N	O	0	0
			1624	966	329	329		

- Molecule 64 is a protein called Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	40	70	Total	C	N	O	0	0
			349	209	70	70		
64	95	70	Total	C	N	O	0	0
			349	209	70	70		
64	1t	70	Total	C	N	O	0	0
			349	209	70	70		

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Mol	Chain	Residues	Atoms				AltConf	Trace
64	1T	70	Total	C	N	O	0	0
			349	209	70	70		

- Molecule 65 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	41	70	Total	C	N	O	0	0
			348	208	70	70		
65	96	70	Total	C	N	O	0	0
			348	208	70	70		
65	2T	70	Total	C	N	O	0	0
			348	208	70	70		
65	2t	70	Total	C	N	O	0	0
			348	208	70	70		

- Molecule 66 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	42	83	Total	C	N	O	0	0
			413	247	83	83		
66	97	83	Total	C	N	O	0	0
			413	247	83	83		
66	3T	83	Total	C	N	O	0	0
			413	247	83	83		
66	3t	83	Total	C	N	O	0	0
			413	247	83	83		

- Molecule 67 is a protein called Transposase.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	43	57	Total	C	N	O	0	0
			285	171	57	57		
67	98	57	Total	C	N	O	0	0
			285	171	57	57		
67	4T	57	Total	C	N	O	0	0
			285	171	57	57		
67	4t	57	Total	C	N	O	0	0
			285	171	57	57		

- Molecule 68 is a protein called Cullin domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	44	62	Total	C	N	O	0	0
			309	185	62	62		
68	99	62	Total	C	N	O	0	0
			309	185	62	62		
68	5t	62	Total	C	N	O	0	0
			309	185	62	62		
68	5T	62	Total	C	N	O	0	0
			309	185	62	62		

- Molecule 69 is a protein called Ymf58.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	4l	116	Total	C	N	O	0	0
			576	344	116	116		
69	4L	116	Total	C	N	O	0	0
			576	344	116	116		

- Molecule 70 is a protein called Ymf57.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	5b	100	Total	C	N	O	0	0
			498	298	100	100		
70	5B	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 71 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	a1	93	Total	C	N	O	0	0
			463	277	93	93		
71	A1	93	Total	C	N	O	0	0
			463	277	93	93		

- Molecule 72 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	a2	98	Total	C	N	O	0	0
			487	291	98	98		
72	A2	98	Total	C	N	O	0	0
			487	291	98	98		

- Molecule 73 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	a3	129	Total	C	N	O	0	0
			633	375	129	129		
73	A3	129	Total	C	N	O	0	0
			633	375	129	129		

- Molecule 74 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	a5	155	Total	C	N	O	0	0
			771	461	155	155		
74	A5	155	Total	C	N	O	0	0
			771	461	155	155		

- Molecule 75 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	a6	172	Total	C	N	O	0	0
			847	503	172	172		
75	A6	172	Total	C	N	O	0	0
			847	503	172	172		

- Molecule 76 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	a7	282	Total	C	N	O	0	0
			1404	840	282	282		
76	A7	282	Total	C	N	O	0	0
			1404	840	282	282		

- Molecule 77 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	a8	132	Total	C	N	O	0	0
			658	394	132	132		
77	A8	132	Total	C	N	O	0	0
			658	394	132	132		

- Molecule 78 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	a9	340	Total	C	N	O	0	0
			1678	998	340	340		

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Mol	Chain	Residues	Atoms				AltConf	Trace
78	A9	340	Total	C	N	O	0	0
			1678	998	340	340		

- Molecule 79 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	ab	112	Total	C	N	O	0	0
			557	333	112	112		
79	AB	112	Total	C	N	O	0	0
			557	333	112	112		

- Molecule 80 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
80	ac	98	Total	C	N	O	0	0
			488	292	98	98		
80	AC	98	Total	C	N	O	0	0
			488	292	98	98		

- Molecule 81 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	al	193	Total	C	N	O	0	0
			949	563	193	193		
81	AL	193	Total	C	N	O	0	0
			949	563	193	193		

- Molecule 82 is a protein called NDUA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	am	160	Total	C	N	O	0	0
			794	474	160	160		
82	AM	160	Total	C	N	O	0	0
			794	474	160	160		

- Molecule 83 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	an	231	Total	C	N	O	0	0
			1135	673	231	231		

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Mol	Chain	Residues	Atoms				AltConf	Trace
83	AN	231	Total	C	N	O	0	0
			1135	673	231	231		

- Molecule 84 is a protein called NDUB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	b2	120	Total	C	N	O	0	0
			590	350	120	120		
84	B2	120	Total	C	N	O	0	0
			590	350	120	120		

- Molecule 85 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	b3	69	Total	C	N	O	0	0
			342	204	69	69		
85	B3	69	Total	C	N	O	0	0
			342	204	69	69		

- Molecule 86 is a protein called NDUB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	b4	115	Total	C	N	O	0	0
			568	338	115	115		
86	B4	115	Total	C	N	O	0	0
			568	338	115	115		

- Molecule 87 is a protein called NDUB6.

Mol	Chain	Residues	Atoms				AltConf	Trace
87	b6	70	Total	C	N	O	0	0
			348	208	70	70		
87	B6	70	Total	C	N	O	0	0
			348	208	70	70		

- Molecule 88 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	b7	116	Total	C	N	O	0	0
			572	340	116	116		
88	B7	116	Total	C	N	O	0	0
			572	340	116	116		

- Molecule 89 is a protein called NDUB8.

Mol	Chain	Residues	Atoms				AltConf	Trace
89	b8	175	Total	C	N	O	0	0
			862	512	175	175		
89	B8	175	Total	C	N	O	0	0
			862	512	175	175		

- Molecule 90 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
90	b9	188	Total	C	N	O	0	0
			935	559	188	188		
90	B9	188	Total	C	N	O	0	0
			935	559	188	188		

- Molecule 91 is a protein called NDUB10.

Mol	Chain	Residues	Atoms				AltConf	Trace
91	bl	175	Total	C	N	O	0	0
			869	519	175	175		
91	BL	175	Total	C	N	O	0	0
			869	519	175	175		

- Molecule 92 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
92	bm	164	Total	C	N	O	0	0
			810	482	164	164		
92	BM	164	Total	C	N	O	0	0
			810	482	164	164		

- Molecule 93 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms				AltConf	Trace
93	c4	102	Total	C	N	O	0	0
			507	303	102	102		
93	C4	102	Total	C	N	O	0	0
			507	303	102	102		

- Molecule 94 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
94	fx	146	Total	C	N	O	0	0
			722	430	146	146		
94	FX	146	Total	C	N	O	0	0
			722	430	146	146		

- Molecule 95 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms				AltConf	Trace
95	g1	229	Total	C	N	O	0	0
			1126	668	229	229		
95	G1	229	Total	C	N	O	0	0
			1126	668	229	229		

- Molecule 96 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms				AltConf	Trace
96	g2	230	Total	C	N	O	0	0
			1129	669	230	230		
96	G2	230	Total	C	N	O	0	0
			1129	669	230	230		

- Molecule 97 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
97	g3	346	Total	C	N	O	0	0
			1711	1019	346	346		
97	G3	346	Total	C	N	O	0	0
			1711	1019	346	346		

- Molecule 98 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
98	j1	265	Total	C	N	O	0	0
			1306	776	265	265		
98	J1	265	Total	C	N	O	0	0
			1306	776	265	265		

- Molecule 99 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
99	n1	283	Total	C	N	O	0	0
			1397	831	283	283		

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Mol	Chain	Residues	Atoms				AltConf	Trace
99	N1	283	Total	C	N	O	0	0
			1397	831	283	283		

- Molecule 100 is a protein called Ymf65.

Mol	Chain	Residues	Atoms				AltConf	Trace
100	n2	360	Total	C	N	O	0	0
			1793	1073	360	360		
100	N2	360	Total	C	N	O	0	0
			1793	1073	360	360		

- Molecule 101 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
101	n3	120	Total	C	N	O	0	0
			596	356	120	120		
101	N3	120	Total	C	N	O	0	0
			596	356	120	120		

- Molecule 102 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
102	n4	505	Total	C	N	O	0	0
			2502	1492	505	505		
102	N4	505	Total	C	N	O	0	0
			2502	1492	505	505		

- Molecule 103 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
103	n5	709	Total	C	N	O	0	0
			3517	2099	709	709		
103	N5	709	Total	C	N	O	0	0
			3517	2099	709	709		

- Molecule 104 is a protein called Ymf62.

Mol	Chain	Residues	Atoms				AltConf	Trace
104	n6	255	Total	C	N	O	0	0
			1269	759	255	255		
104	N6	255	Total	C	N	O	0	0
			1269	759	255	255		

- Molecule 105 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
105	p1	230	Total	C	N	O	0	0
			1139	679	230	230		
105	P1	230	Total	C	N	O	0	0
			1139	679	230	230		

- Molecule 106 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms				AltConf	Trace
106	p2	167	Total	C	N	O	0	0
			831	497	167	167		
106	P2	167	Total	C	N	O	0	0
			831	497	167	167		

- Molecule 107 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
107	qA	454	Total	C	N	O	0	0
			2246	1338	454	454		
107	qa	454	Total	C	N	O	0	0
			2246	1338	454	454		
107	QA	454	Total	C	N	O	0	0
			2246	1338	454	454		
107	Qa	454	Total	C	N	O	0	0
			2246	1338	454	454		

- Molecule 108 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
108	qB	480	Total	C	N	O	0	0
			2370	1410	480	480		
108	qb	480	Total	C	N	O	0	0
			2370	1410	480	480		
108	QB	480	Total	C	N	O	0	0
			2370	1410	480	480		
108	Qb	480	Total	C	N	O	0	0
			2370	1410	480	480		

- Molecule 109 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms				AltConf	Trace
109	qC	426	Total	C	N	O	0	0
			2109	1257	426	426		
109	qc	425	Total	C	N	O	0	0
			2104	1254	425	425		
109	QC	426	Total	C	N	O	0	0
			2109	1257	426	426		
109	Qc	425	Total	C	N	O	0	0
			2104	1254	425	425		

- Molecule 110 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms				AltConf	Trace
110	qD	295	Total	C	N	O	0	0
			1448	858	295	295		
110	qd	295	Total	C	N	O	0	0
			1448	858	295	295		
110	QD	295	Total	C	N	O	0	0
			1448	858	295	295		
110	Qd	295	Total	C	N	O	0	0
			1448	858	295	295		

- Molecule 111 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
111	qE	230	Total	C	N	O	0	0
			1131	671	230	230		
111	qe	219	Total	C	N	O	0	0
			1077	639	219	219		
111	QE	230	Total	C	N	O	0	0
			1131	671	230	230		
111	Qe	219	Total	C	N	O	0	0
			1077	639	219	219		

- Molecule 112 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
112	qF	89	Total	C	N	O	0	0
			441	263	89	89		
112	qf	80	Total	C	N	O	0	0
			397	237	80	80		
112	QF	89	Total	C	N	O	0	0
			441	263	89	89		

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Mol	Chain	Residues	Atoms				AltConf	Trace
112	Qf	80	Total	C	N	O	0	0
			397	237	80	80		

- Molecule 113 is a protein called Sulphotransf domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
113	qG	327	Total	C	N	O	0	0
			1621	967	327	327		
113	qg	326	Total	C	N	O	0	0
			1616	964	326	326		
113	QG	327	Total	C	N	O	0	0
			1621	967	327	327		
113	Qg	326	Total	C	N	O	0	0
			1616	964	326	326		

- Molecule 114 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
114	qH	129	Total	C	N	O	0	0
			635	377	129	129		
114	qh	129	Total	C	N	O	0	0
			635	377	129	129		
114	QH	129	Total	C	N	O	0	0
			635	377	129	129		
114	Qh	129	Total	C	N	O	0	0
			635	377	129	129		

- Molecule 115 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
115	qI	114	Total	C	N	O	0	0
			567	339	114	114		
115	qi	114	Total	C	N	O	0	0
			567	339	114	114		
115	QI	114	Total	C	N	O	0	0
			567	339	114	114		
115	Qi	114	Total	C	N	O	0	0
			567	339	114	114		

- Molecule 116 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
116	qJ	56	Total	C	N	O	0	0
			277	165	56	56		
116	qj	58	Total	C	N	O	0	0
			287	171	58	58		
116	QJ	56	Total	C	N	O	0	0
			277	165	56	56		
116	Qj	58	Total	C	N	O	0	0
			287	171	58	58		

- Molecule 117 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms				AltConf	Trace
117	qL	32	Total	C	N	O	0	0
			160	96	32	32		
117	ql	32	Total	C	N	O	0	0
			160	96	32	32		
117	QL	32	Total	C	N	O	0	0
			160	96	32	32		
117	Ql	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 118 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
118	s1	689	Total	C	N	O	0	0
			3400	2022	689	689		
118	S1	689	Total	C	N	O	0	0
			3400	2022	689	689		

- Molecule 119 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
119	s2	442	Total	C	N	O	0	0
			2185	1301	442	442		
119	S2	442	Total	C	N	O	0	0
			2185	1301	442	442		

- Molecule 120 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
120	s3	198	Total	C	N	O	0	0
			988	592	198	198		

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Mol	Chain	Residues	Atoms				AltConf	Trace
120	S3	198	Total	C	N	O	0	0
			988	592	198	198		

- Molecule 121 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
121	s4	182	Total	C	N	O	0	0
			900	536	182	182		
121	S4	182	Total	C	N	O	0	0
			900	536	182	182		

- Molecule 122 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
122	s5	93	Total	C	N	O	0	0
			462	276	93	93		
122	S5	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 123 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
123	s6	92	Total	C	N	O	0	0
			455	271	92	92		
123	S6	92	Total	C	N	O	0	0
			455	271	92	92		

- Molecule 124 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
124	s7	161	Total	C	N	O	0	0
			792	470	161	161		
124	S7	161	Total	C	N	O	0	0
			792	470	161	161		

- Molecule 125 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
125	s8	218	Total	C	N	O	0	0
			1080	644	218	218		

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Mol	Chain	Residues	Atoms				AltConf	Trace
125	S8	218	Total	C	N	O	0	0
			1080	644	218	218		

- Molecule 126 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
126	sa	599	Total	C	N	O	0	0
			2937	1739	599	599		
126	SA	599	Total	C	N	O	0	0
			2937	1739	599	599		

- Molecule 127 is a protein called Succinate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms				AltConf	Trace
127	sb	279	Total	C	N	O	0	0
			1384	826	279	279		
127	SB	279	Total	C	N	O	0	0
			1384	826	279	279		

- Molecule 128 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
128	sc	58	Total	C	N	O	0	0
			286	170	58	58		
128	SC	58	Total	C	N	O	0	0
			286	170	58	58		

- Molecule 129 is a protein called SDHD.

Mol	Chain	Residues	Atoms				AltConf	Trace
129	sd	44	Total	C	N	O	0	0
			220	132	44	44		
129	SD	44	Total	C	N	O	0	0
			220	132	44	44		

- Molecule 130 is a protein called Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms				AltConf	Trace
130	t1	502	Total	C	N	O	0	0
			2490	1486	502	502		

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Mol	Chain	Residues	Atoms				AltConf	Trace
130	T1	502	Total	C	N	O	0	0
			2490	1486	502	502		

- Molecule 131 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms				AltConf	Trace
131	t2	279	Total	C	N	O	0	0
			1376	818	279	279		
131	T2	279	Total	C	N	O	0	0
			1376	818	279	279		

- Molecule 132 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
132	t3	310	Total	C	N	O	0	0
			1541	921	310	310		
132	T3	310	Total	C	N	O	0	0
			1541	921	310	310		

- Molecule 133 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
133	t4	198	Total	C	N	O	0	0
			981	585	198	198		
133	T4	198	Total	C	N	O	0	0
			981	585	198	198		

- Molecule 134 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
134	t5	141	Total	C	N	O	0	0
			698	416	141	141		
134	T5	141	Total	C	N	O	0	0
			698	416	141	141		

- Molecule 135 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
135	t6	109	Total	C	N	O	0	0
			542	324	109	109		
135	T6	109	Total	C	N	O	0	0
			542	324	109	109		

- Molecule 136 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
136	t7	142	Total	C	N	O	0	0
			702	418	142	142		
136	T7	142	Total	C	N	O	0	0
			702	418	142	142		

- Molecule 137 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
137	t8	131	Total	C	N	O	0	0
			651	389	131	131		
137	T8	131	Total	C	N	O	0	0
			651	389	131	131		

- Molecule 138 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
138	t9	132	Total	C	N	O	0	0
			651	387	132	132		
138	T9	132	Total	C	N	O	0	0
			651	387	132	132		

- Molecule 139 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
139	ta	102	Total	C	N	O	0	0
			504	300	102	102		
139	TA	102	Total	C	N	O	0	0
			504	300	102	102		

- Molecule 140 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
140	tb	96	Total	C	N	O	0	0
			475	283	96	96		
140	TB	96	Total	C	N	O	0	0
			475	283	96	96		

- Molecule 141 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
141	tc	92	Total	C	N	O	0	0
			458	274	92	92		
141	TC	92	Total	C	N	O	0	0
			458	274	92	92		

- Molecule 142 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
142	td	72	Total	C	N	O	0	0
			359	215	72	72		
142	TD	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 143 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
143	te	50	Total	C	N	O	0	0
			248	148	50	50		
143	TE	50	Total	C	N	O	0	0
			248	148	50	50		

- Molecule 144 is a protein called NDUTT15.

Mol	Chain	Residues	Atoms				AltConf	Trace
144	tf	216	Total	C	N	O	0	0
			1074	642	216	216		
144	TF	216	Total	C	N	O	0	0
			1074	642	216	216		

- Molecule 145 is a protein called NDUTT16.

Mol	Chain	Residues	Atoms				AltConf	Trace
145	tg	134	Total	C	N	O	0	0
			665	397	134	134		
145	TG	134	Total	C	N	O	0	0
			665	397	134	134		

- Molecule 146 is a protein called NDUTT17.

Mol	Chain	Residues	Atoms				AltConf	Trace
146	th	124	Total	C	N	O	0	0
			611	363	124	124		

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Mol	Chain	Residues	Atoms				AltConf	Trace
146	TH	124	Total	C	N	O	0	0
			611	363	124	124		

- Molecule 147 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
147	tx	144	Total	C	N	O	0	0
			715	427	144	144		
147	TX	144	Total	C	N	O	0	0
			715	427	144	144		

- Molecule 148 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
148	v1	442	Total	C	N	O	0	0
			2163	1279	442	442		
148	V1	442	Total	C	N	O	0	0
			2163	1279	442	442		

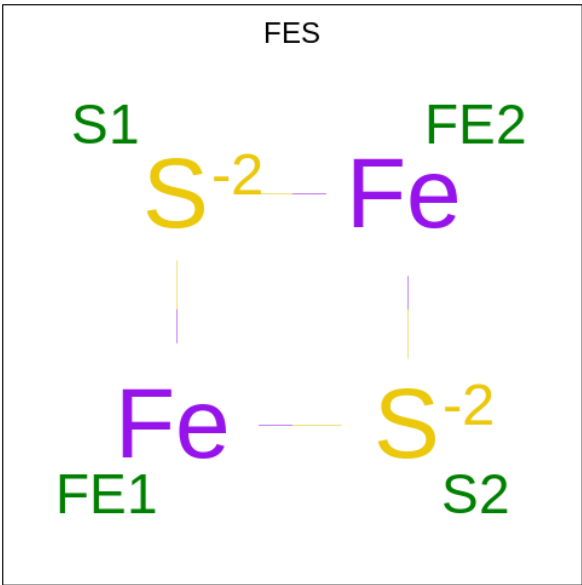
- Molecule 149 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
149	v2	231	Total	C	N	O	0	0
			1144	682	231	231		
149	V2	231	Total	C	N	O	0	0
			1144	682	231	231		

- Molecule 150 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
150	x1	149	Total	C	N	O	0	0
			732	434	149	149		
150	X1	149	Total	C	N	O	0	0
			732	434	149	149		

- Molecule 151 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



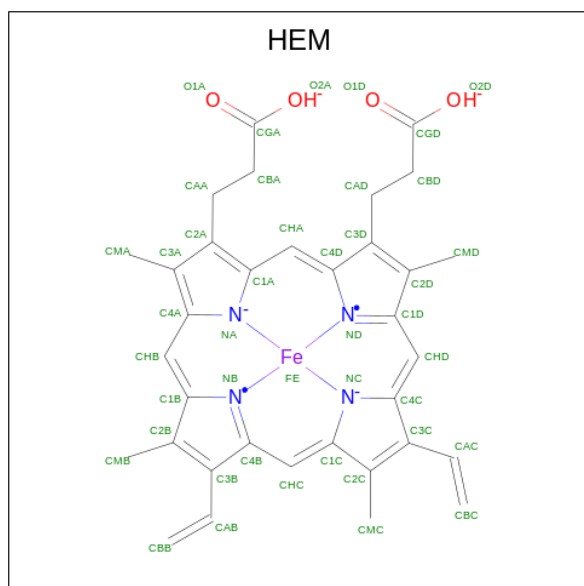
Mol	Chain	Residues	Atoms			AltConf
151	0C	1	Total	Fe	S	0
			4	2	2	
151	0C	1	Total	Fe	S	0
			4	2	2	
151	47	1	Total	Fe	S	0
			4	2	2	
151	47	1	Total	Fe	S	0
			4	2	2	
151	fx	1	Total	Fe	S	0
			4	2	2	
151	qE	1	Total	Fe	S	0
			4	2	2	
151	qe	1	Total	Fe	S	0
			4	2	2	
151	s1	1	Total	Fe	S	0
			4	2	2	
151	sb	1	Total	Fe	S	0
			4	2	2	
151	v2	1	Total	Fe	S	0
			4	2	2	
151	QE	1	Total	Fe	S	0
			4	2	2	
151	Qe	1	Total	Fe	S	0
			4	2	2	
151	SB	1	Total	Fe	S	0
			4	2	2	
151	S1	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
151	V2	1	Total	Fe	S	0
			4	2	2	
151	FX	1	Total	Fe	S	0
			4	2	2	
151	fs	1	Total	Fe	S	0
			4	2	2	
151	fs	1	Total	Fe	S	0
			4	2	2	
151	FS	1	Total	Fe	S	0
			4	2	2	
151	FS	1	Total	Fe	S	0
			4	2	2	

- Molecule 152 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



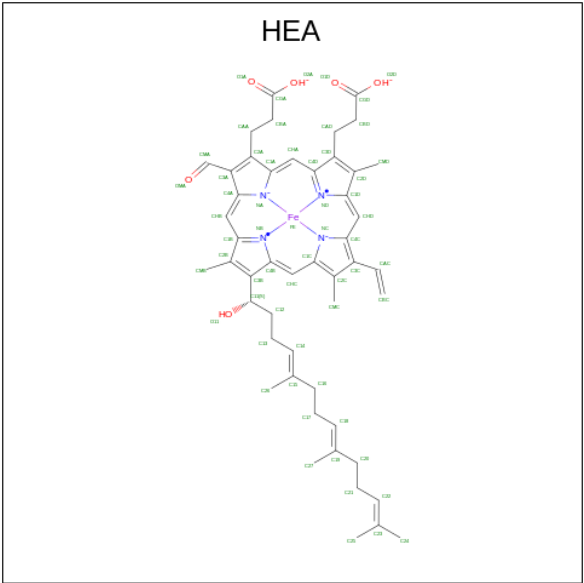
Mol	Chain	Residues	Atoms					AltConf
152	0F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	50	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
152	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	y5	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
152	Y5	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 153 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
153	26	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
153	26	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
153	81	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
153	81	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
153	c1	1	Total 60	C 49	Fe 1	N 4	O 6	0
153	c1	1	Total 60	C 49	Fe 1	N 4	O 6	0
153	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
153	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 154 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
154	26	1	Total	Cu	0
			1	1	
154	27	2	Total	Cu	0
			2	2	
154	81	1	Total	Cu	0
			1	1	
154	82	2	Total	Cu	0
			2	2	
154	c1	1	Total	Cu	0
			1	1	
154	c2	2	Total	Cu	0
			2	2	
154	C1	1	Total	Cu	0
			1	1	
154	C2	2	Total	Cu	0
			2	2	

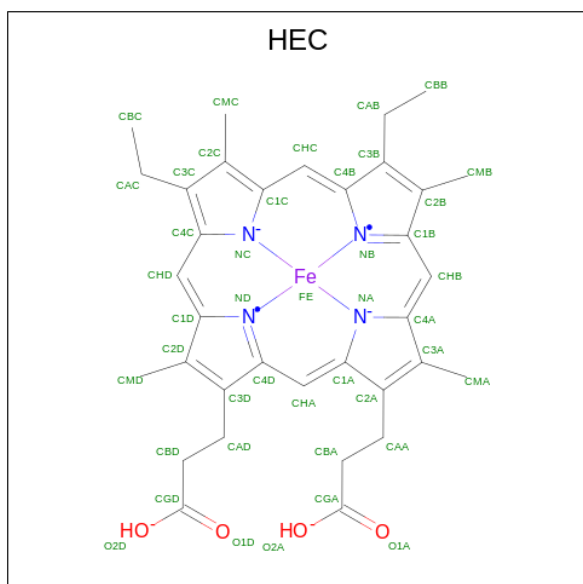
- Molecule 155 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
155	26	1	Total	Mg	0
			1	1	
155	81	1	Total	Mg	0
			1	1	
155	c1	1	Total	Mg	0
			1	1	
155	C1	1	Total	Mg	0
			1	1	

- Molecule 156 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
156	29	2	Total 2	Zn 2	0
156	84	2	Total 2	Zn 2	0
156	s6	1	Total 1	Zn 1	0
156	S6	1	Total 1	Zn 1	0
156	vb	2	Total 2	Zn 2	0
156	VB	2	Total 2	Zn 2	0

- Molecule 157 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



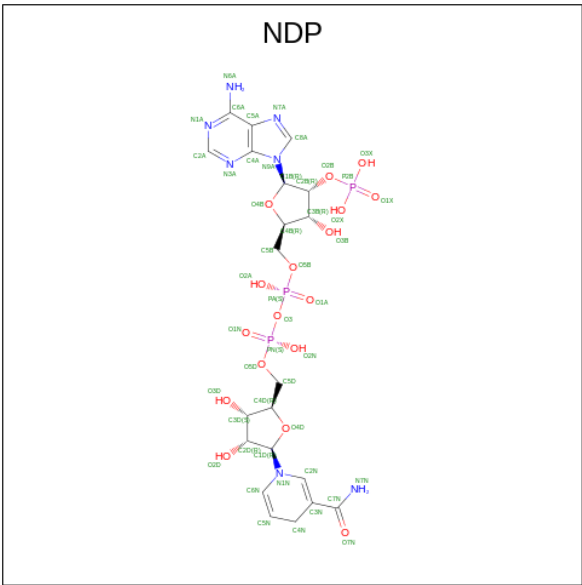
Mol	Chain	Residues	Atoms					AltConf
157	2e	1	Total 43	C 34	Fe 1	N 4	O 4	0
157	qD	1	Total 43	C 34	Fe 1	N 4	O 4	0
157	qd	1	Total 43	C 34	Fe 1	N 4	O 4	0
157	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
157	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

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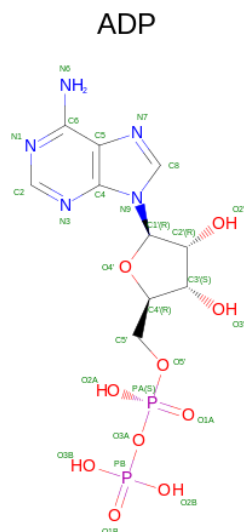
Mol	Chain	Residues	Atoms					AltConf
157	2E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 158 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



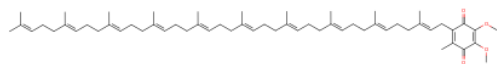
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
158	a9	1	48	21	7	17	3	0
158	A9	1	48	21	7	17	3	0

- Molecule 159 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
159	b8	1	Total 27	C 10	N 5	O 10	P 2	0
159	B8	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 160 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



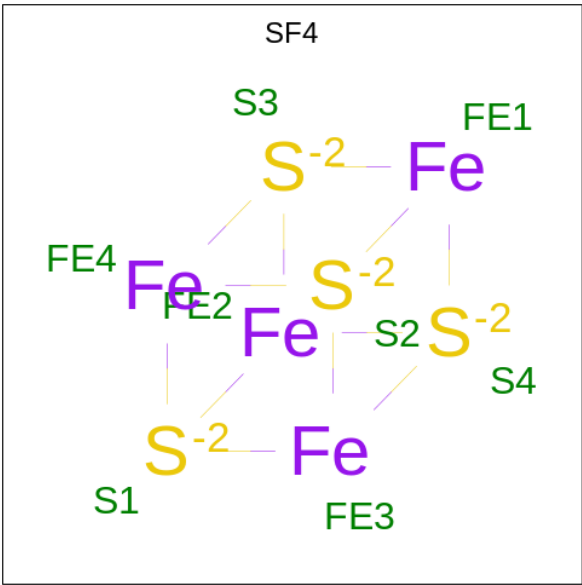
Mol	Chain	Residues	Atoms	AltConf
160	qc	1	Total C 26 26	0

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Mol	Chain	Residues	Atoms		AltConf
160	Qc	1	Total	C	0
			26	26	

- Molecule 161 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



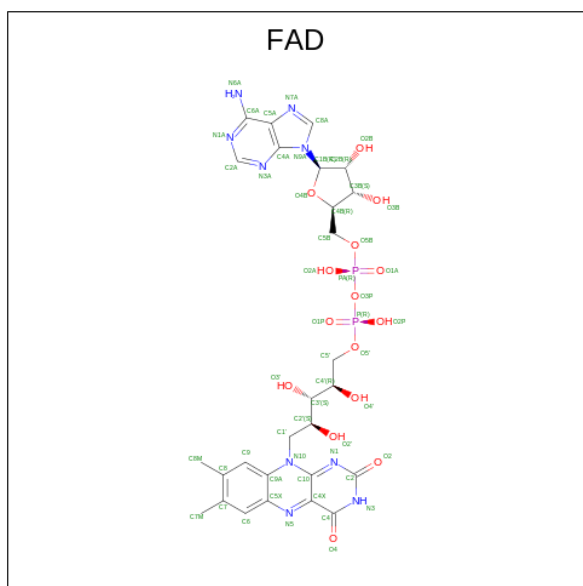
Mol	Chain	Residues	Atoms			AltConf
161	s1	1	Total	Fe	S	0
			8	4	4	
161	s1	1	Total	Fe	S	0
			8	4	4	
161	s7	1	Total	Fe	S	0
			8	4	4	
161	s8	1	Total	Fe	S	0
			8	4	4	
161	s8	1	Total	Fe	S	0
			8	4	4	
161	sb	1	Total	Fe	S	0
			8	4	4	
161	v1	1	Total	Fe	S	0
			8	4	4	
161	SB	1	Total	Fe	S	0
			8	4	4	
161	S1	1	Total	Fe	S	0
			8	4	4	
161	S1	1	Total	Fe	S	0
			8	4	4	

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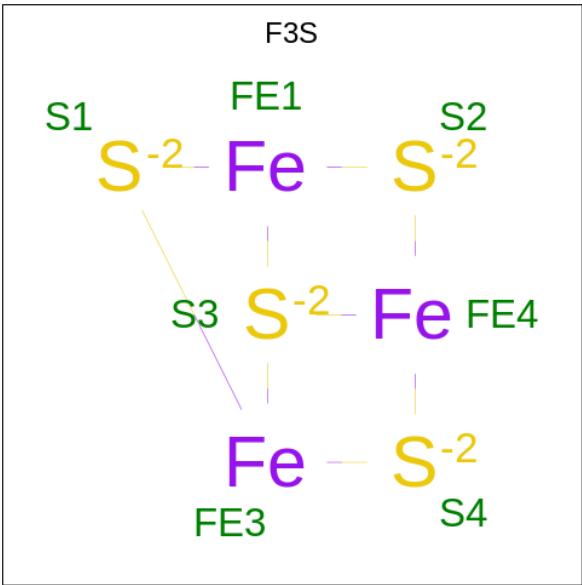
Mol	Chain	Residues	Atoms			AltConf
161	S7	1	Total	Fe	S	0
			8	4	4	
161	S8	1	Total	Fe	S	0
			8	4	4	
161	S8	1	Total	Fe	S	0
			8	4	4	
161	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 162 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



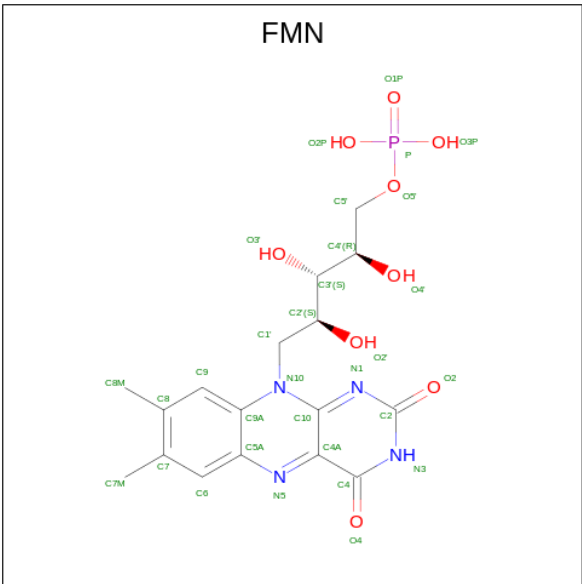
Mol	Chain	Residues	Atoms					AltConf
162	sa	1	Total	C	N	O	P	0
			53	27	9	15	2	
162	SA	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 163 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
163	sb	1	Total	Fe	S	0
			7	3	4	
163	SB	1	Total	Fe	S	0
			7	3	4	

- Molecule 164 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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

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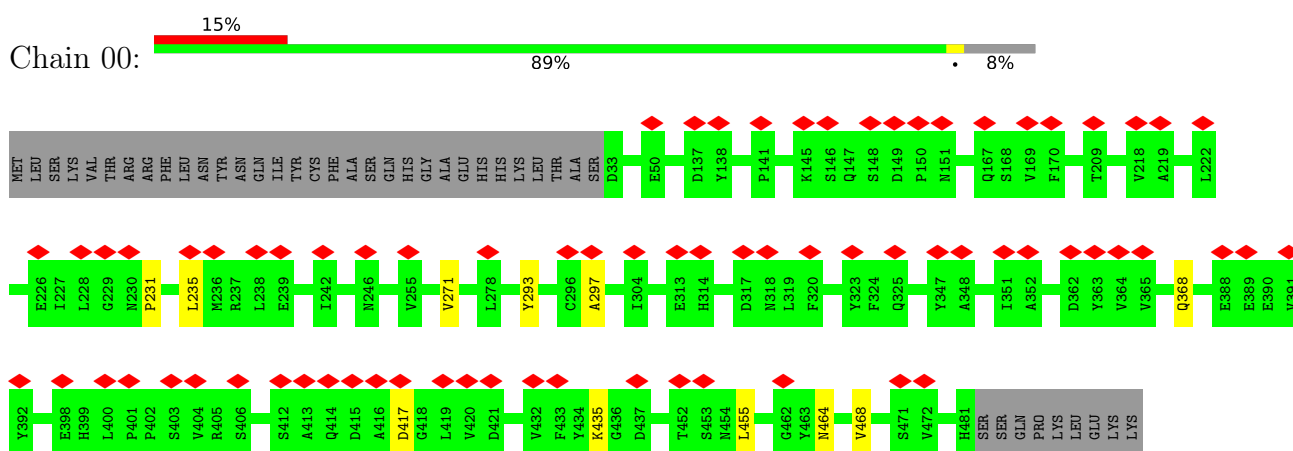
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
164	V1	1	31	17	4	9	1	0

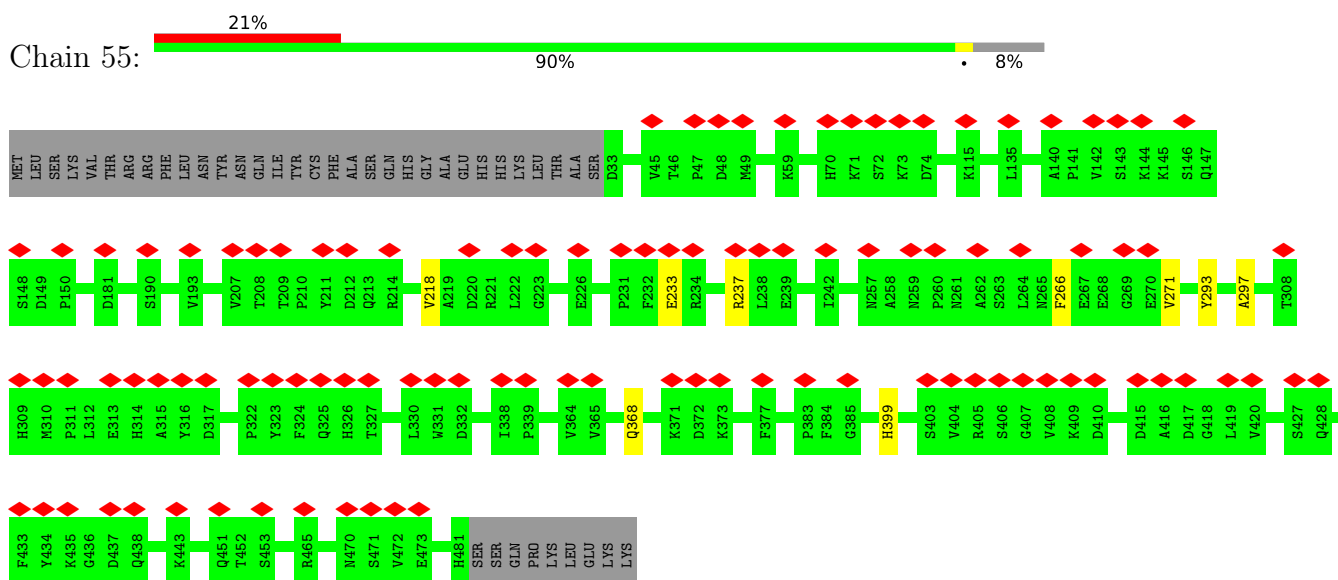
3 Residue-property plots

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

- Molecule 1: Transmembrane protein, putative

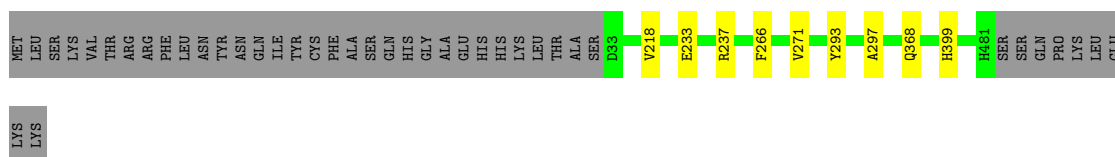


- Molecule 1: Transmembrane protein, putative



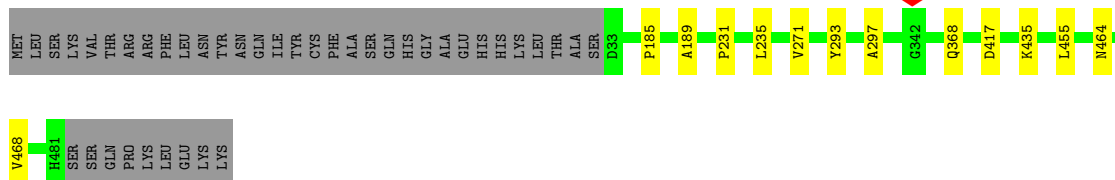
- Molecule 1: Transmembrane protein, putative





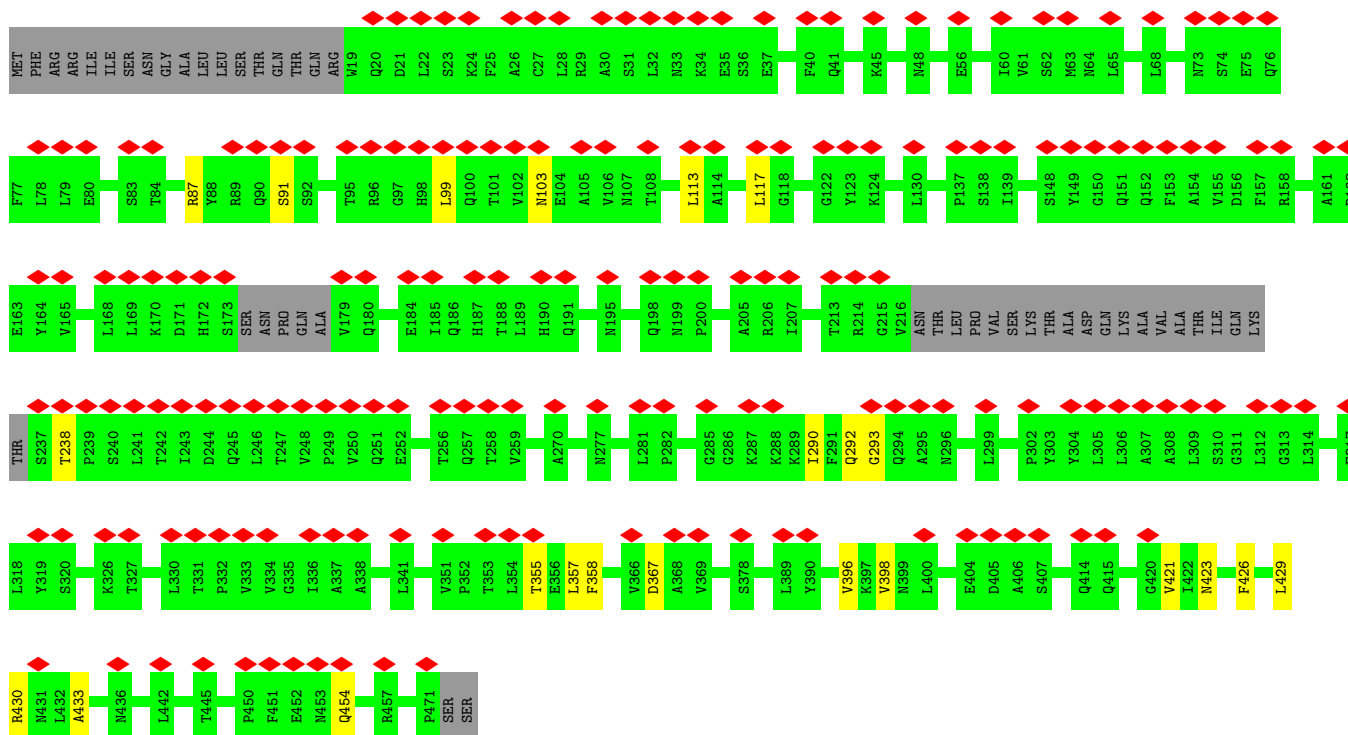
- Molecule 1: Transmembrane protein, putative

Chain A: 89% 8%



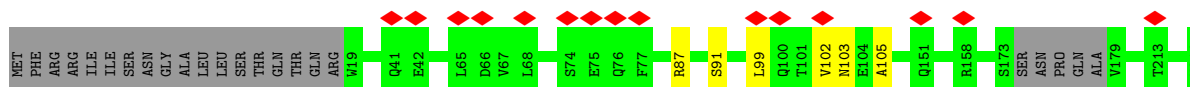
- Molecule 2: Protein phosphatase 2C, putative

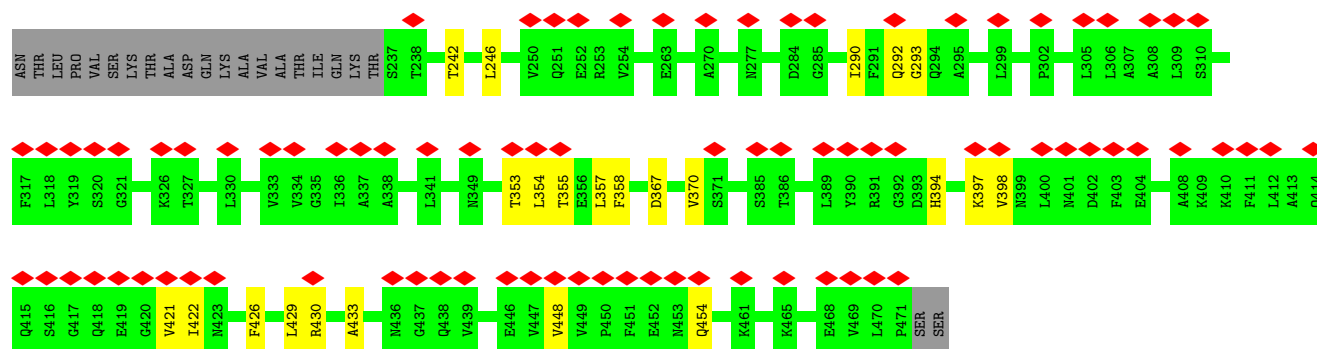
Chain 01: 39% 86% 5% 10%



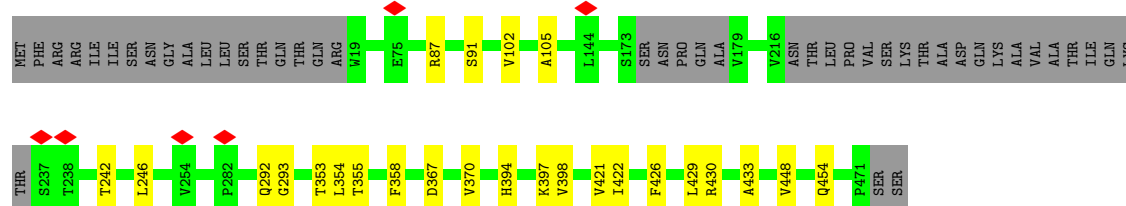
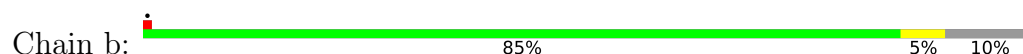
- Molecule 2: Protein phosphatase 2C, putative

Chain 56: 21% 84% 6% 10%

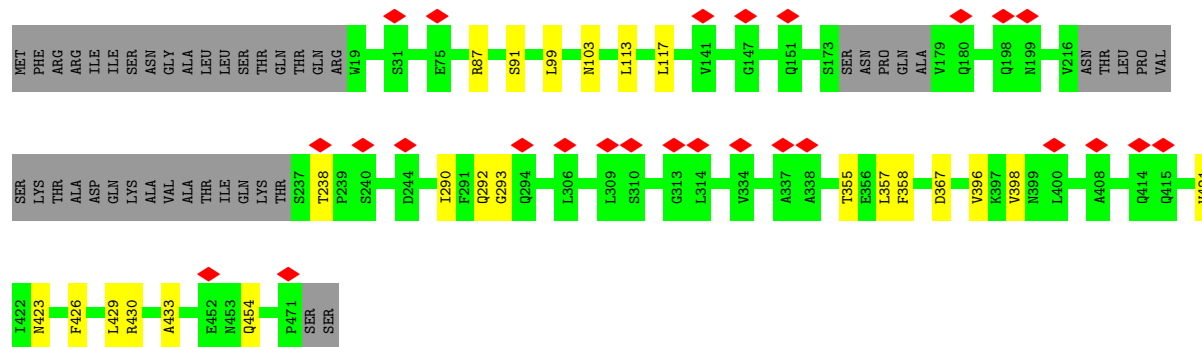
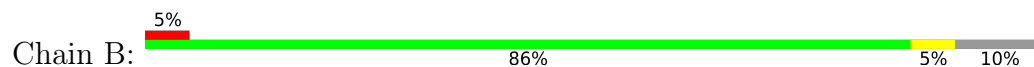




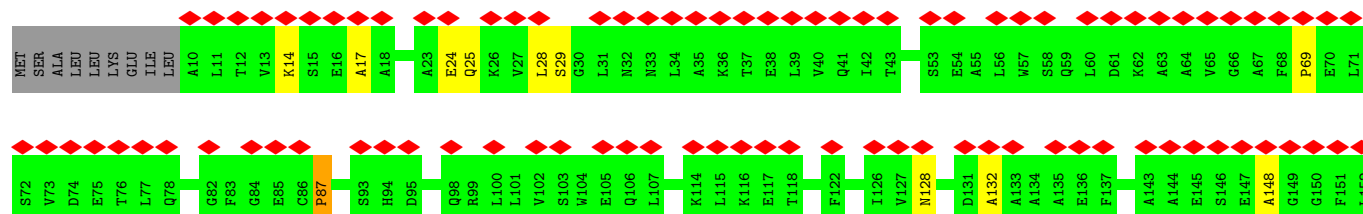
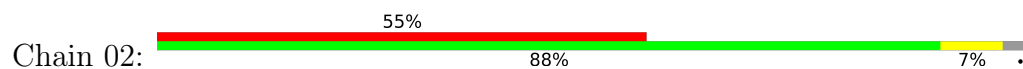
- Molecule 2: Protein phosphatase 2C, putative

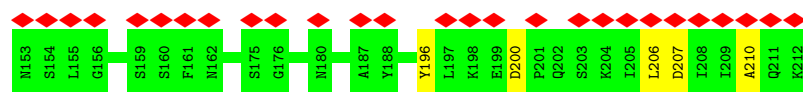


- Molecule 2: Protein phosphatase 2C, putative

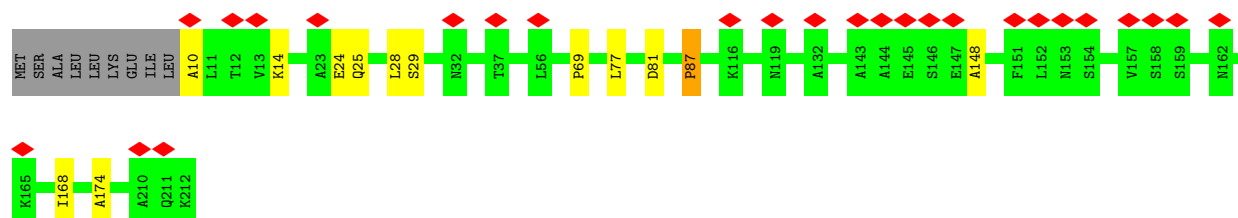


- Molecule 3: COXTT3

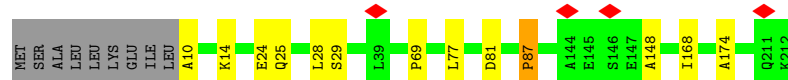




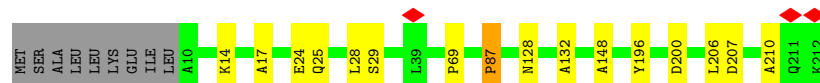
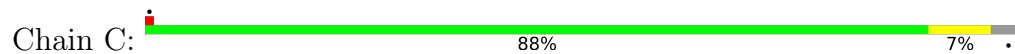
• Molecule 3: COXTT3



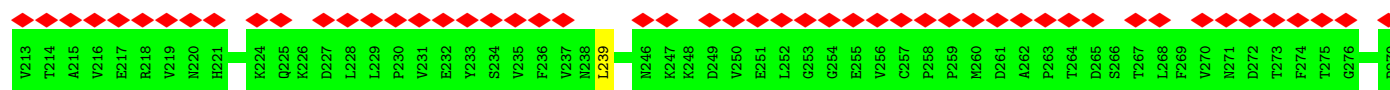
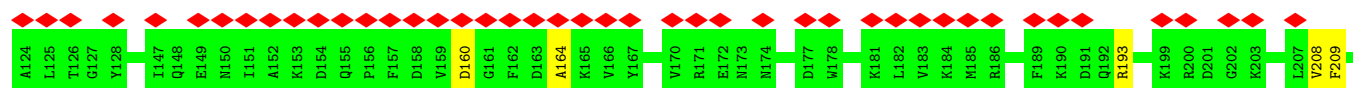
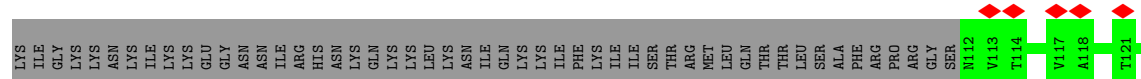
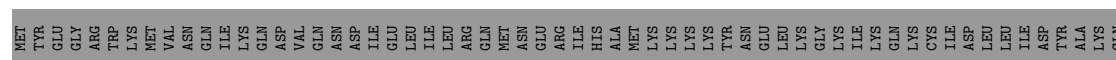
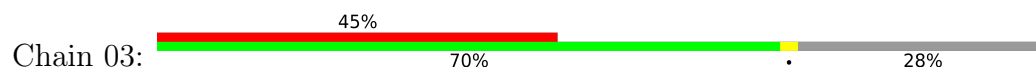
• Molecule 3: COXTT3

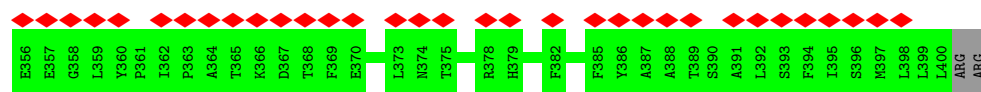


• Molecule 3: COXTT3

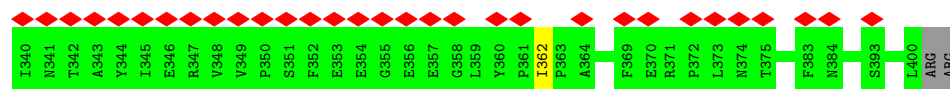
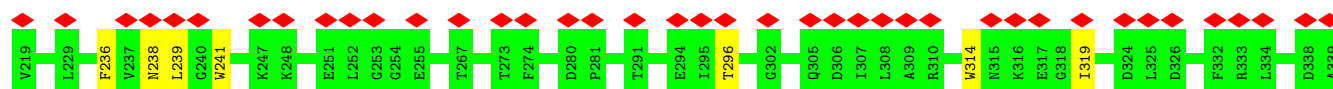
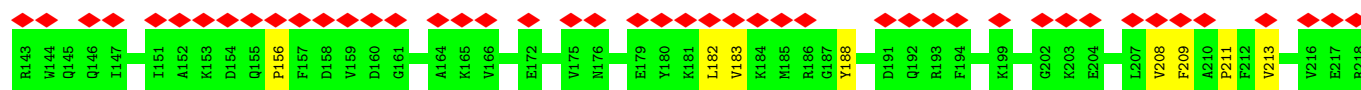
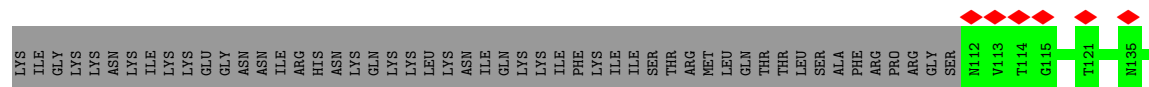
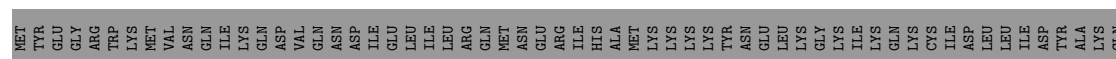


• Molecule 4: SURF1-like protein

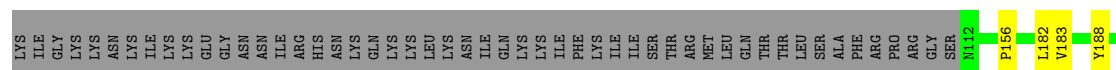
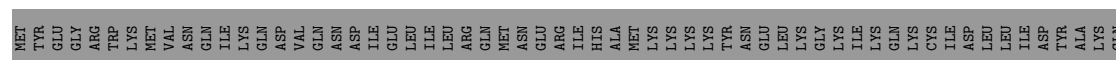




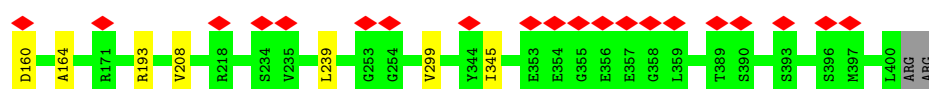
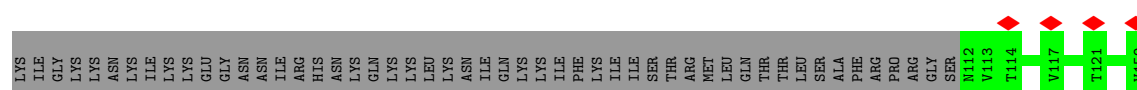
• Molecule 4: SURF1-like protein



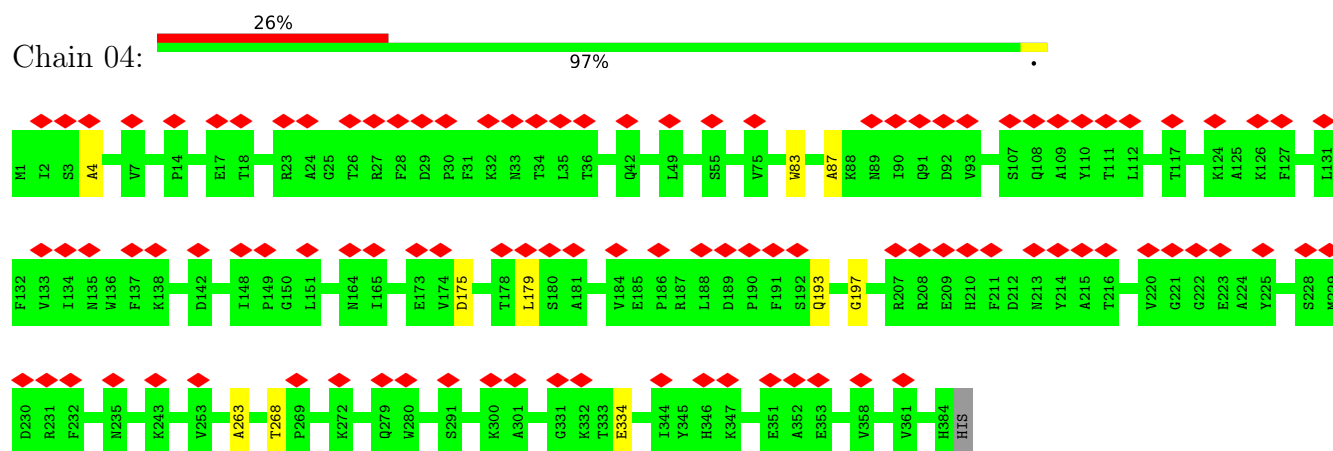
• Molecule 4: SURF1-like protein



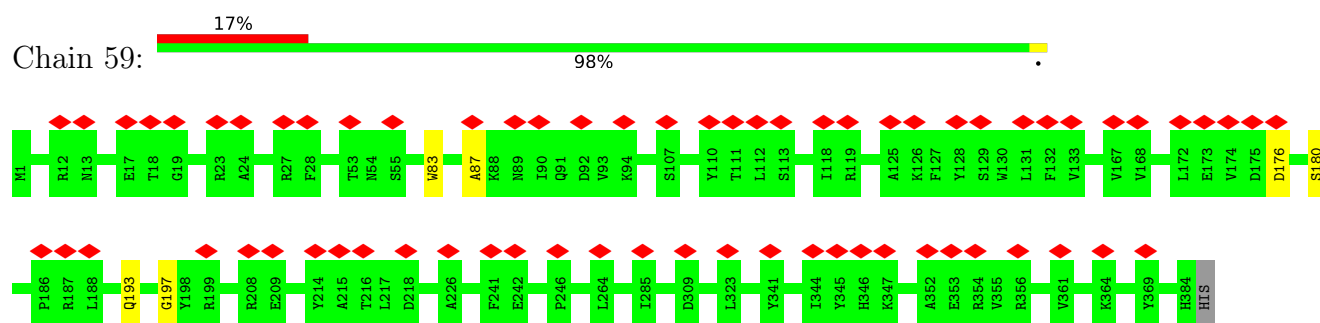
• Molecule 4: SURF1-like protein



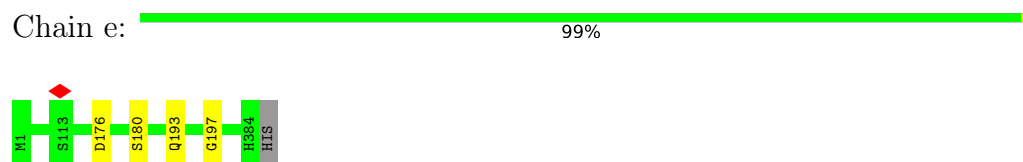
- Molecule 5: TraB family protein



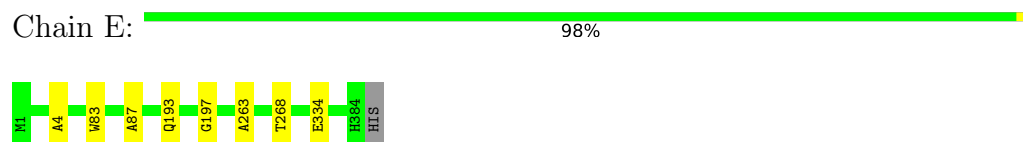
- Molecule 5: TraB family protein



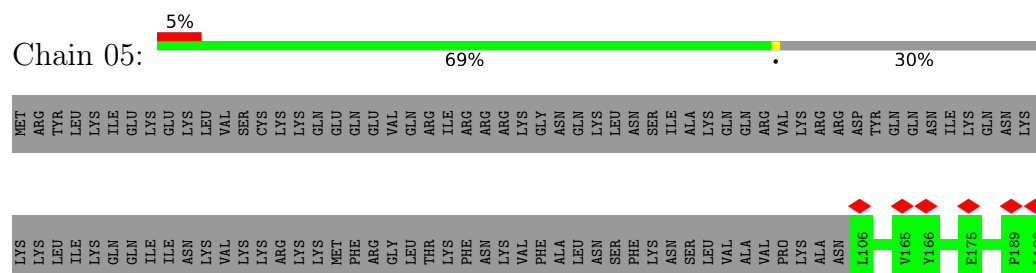
- Molecule 5: TraB family protein

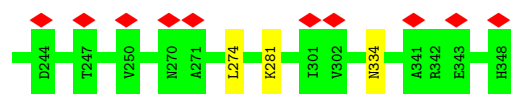


- Molecule 5: TraB family protein

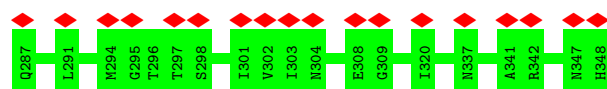
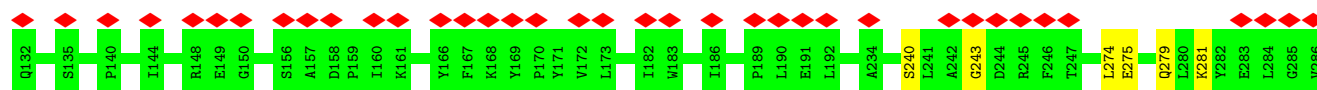
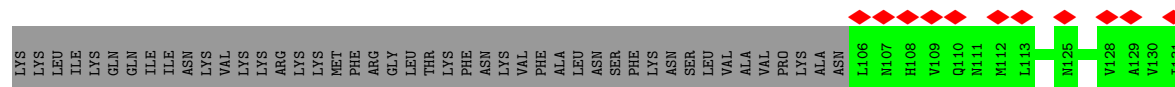
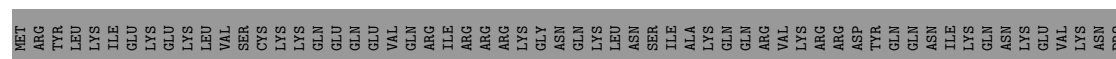


- Molecule 6: Transmembrane protein, putative

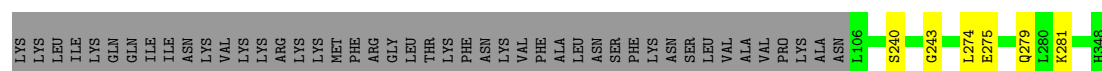
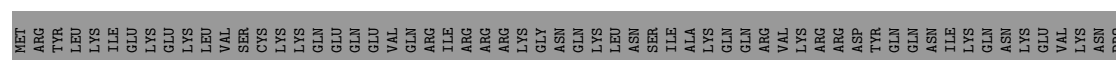




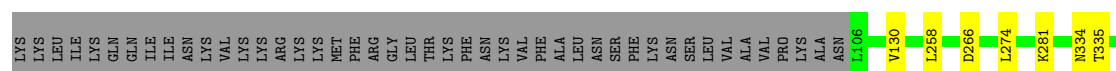
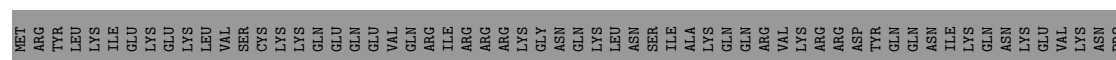
- Molecule 6: Transmembrane protein, putative



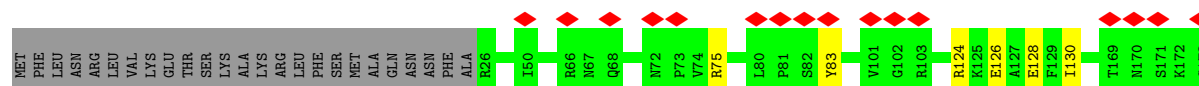
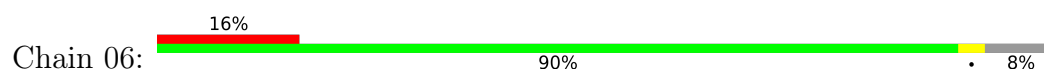
- Molecule 6: Transmembrane protein, putative

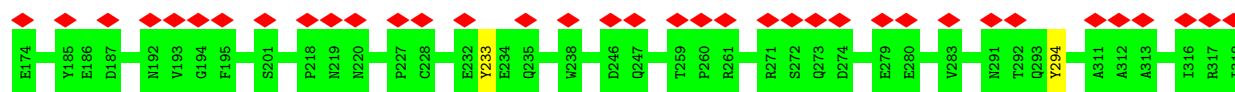


- Molecule 6: Transmembrane protein, putative

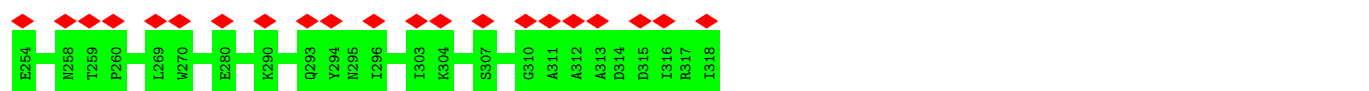
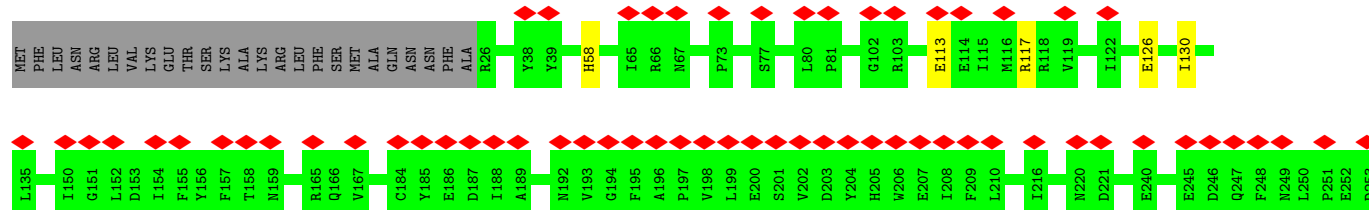


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

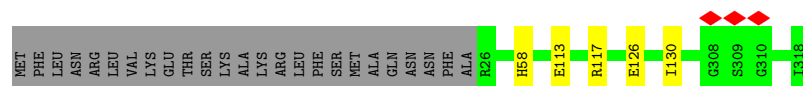
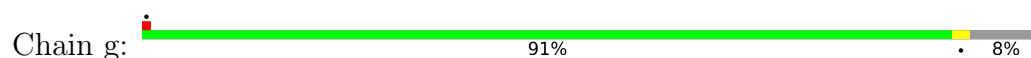




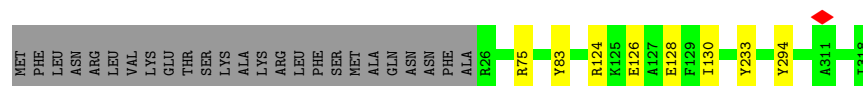
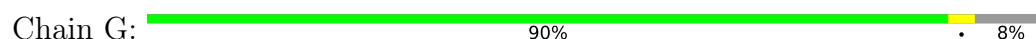
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial



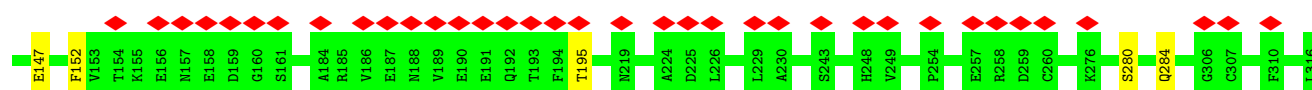
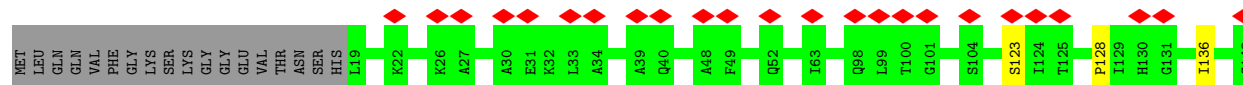
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

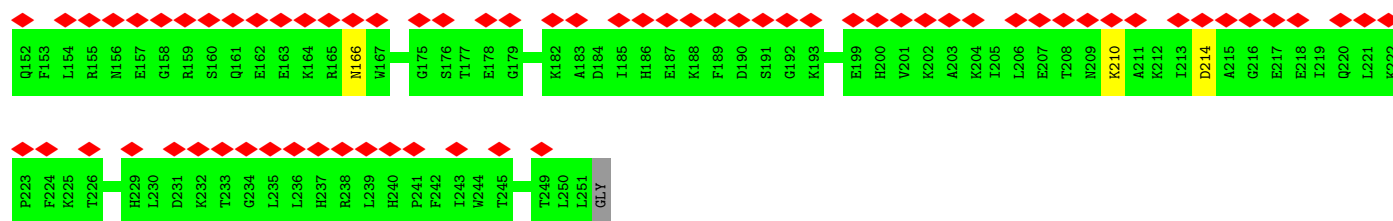


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

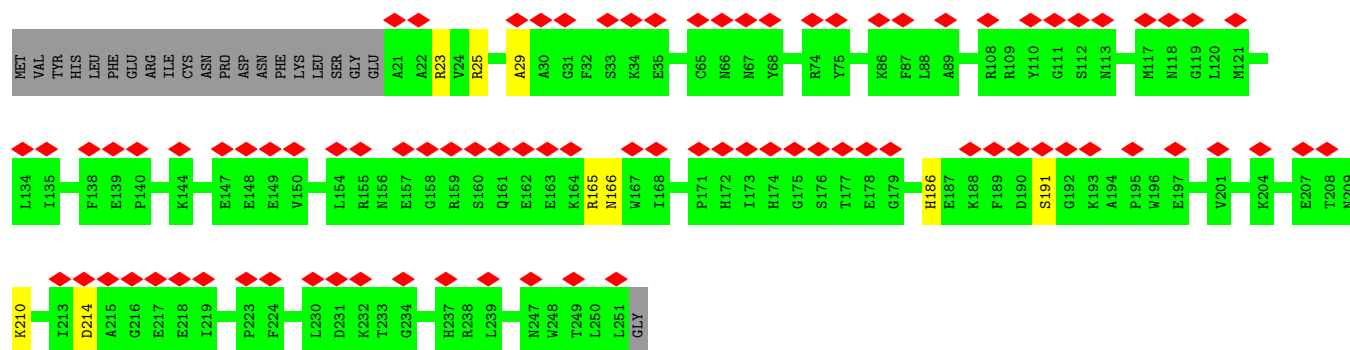
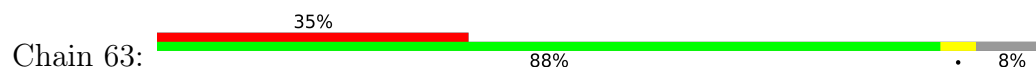


- Molecule 8: SURF1-like protein

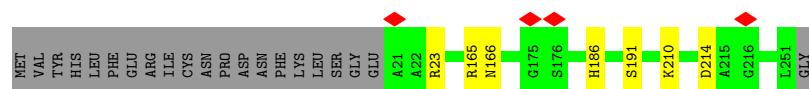
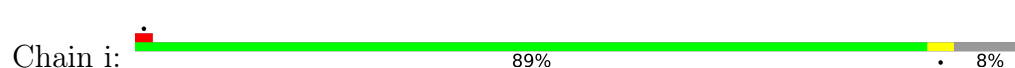




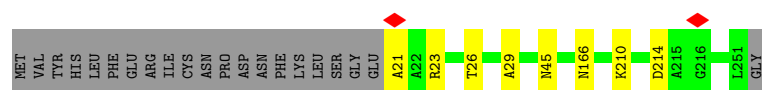
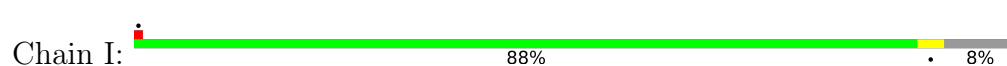
• Molecule 9: COXTT9



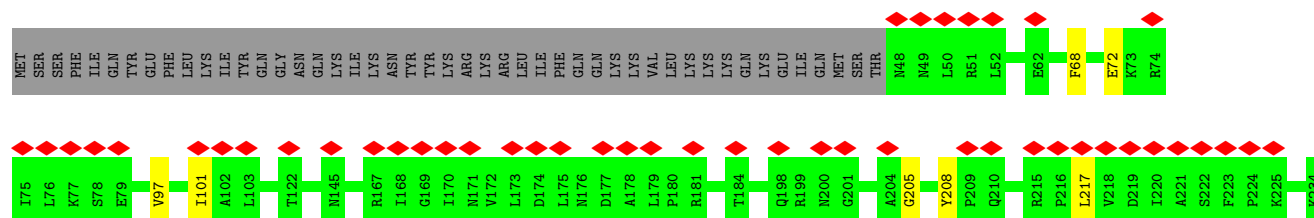
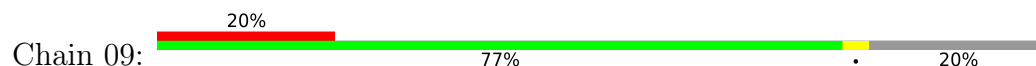
• Molecule 9: COXTT9



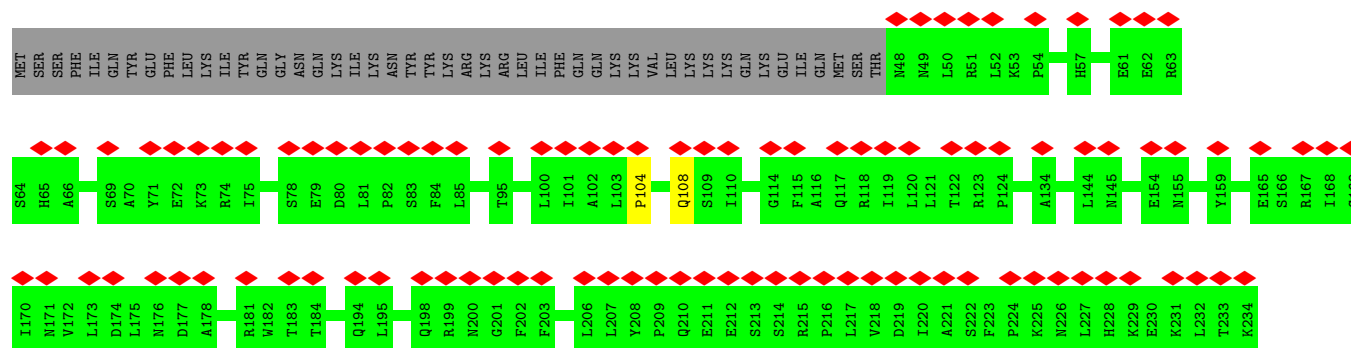
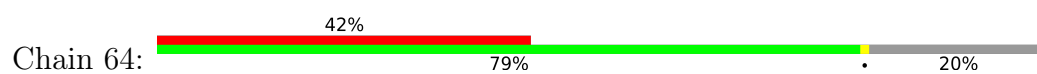
• Molecule 9: COXTT9



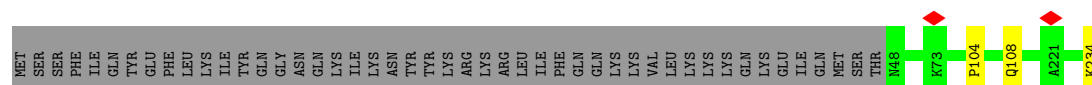
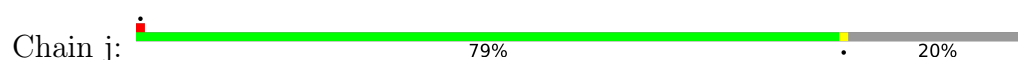
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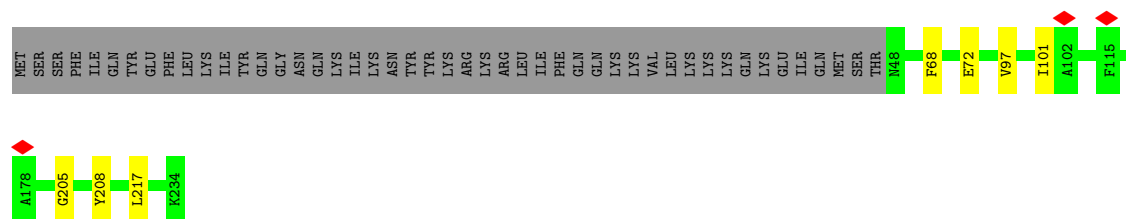
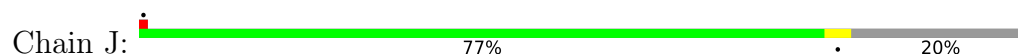
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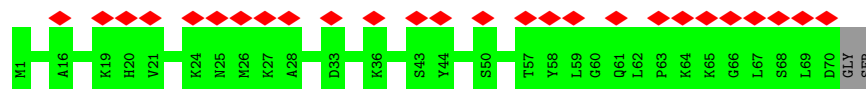
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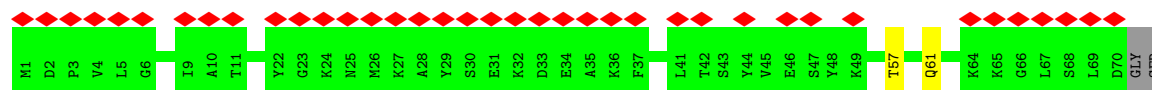
• Molecule 10: COXTT10



• Molecule 11: Annexin

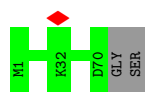


• Molecule 11: Annexin



• Molecule 11: Annexin





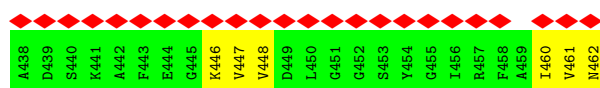
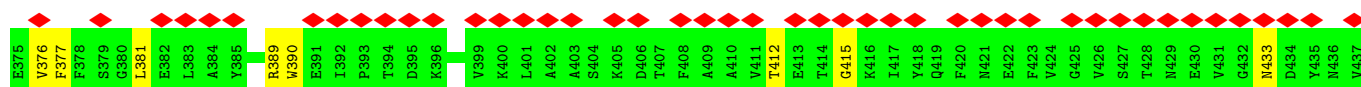
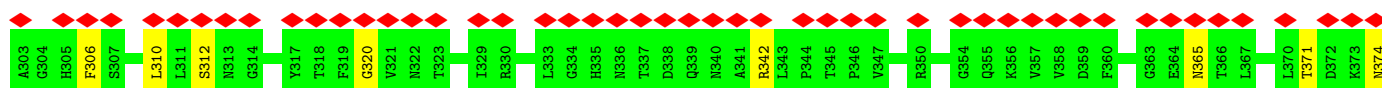
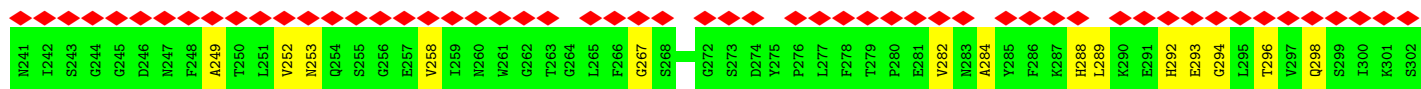
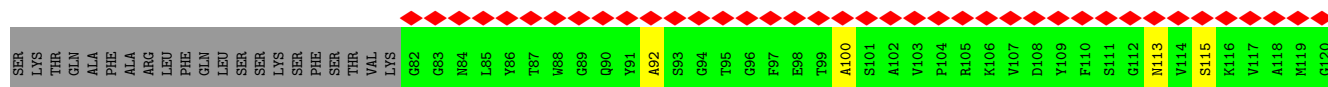
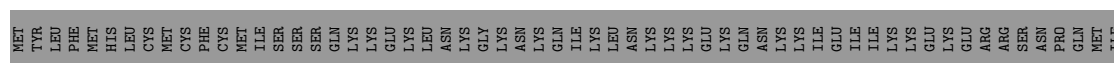
- Molecule 11: Annexin

Chain 6T: 94%



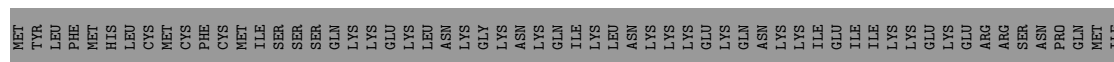
- Molecule 12: Chromosome condensation regulator RCC1 repeat protein

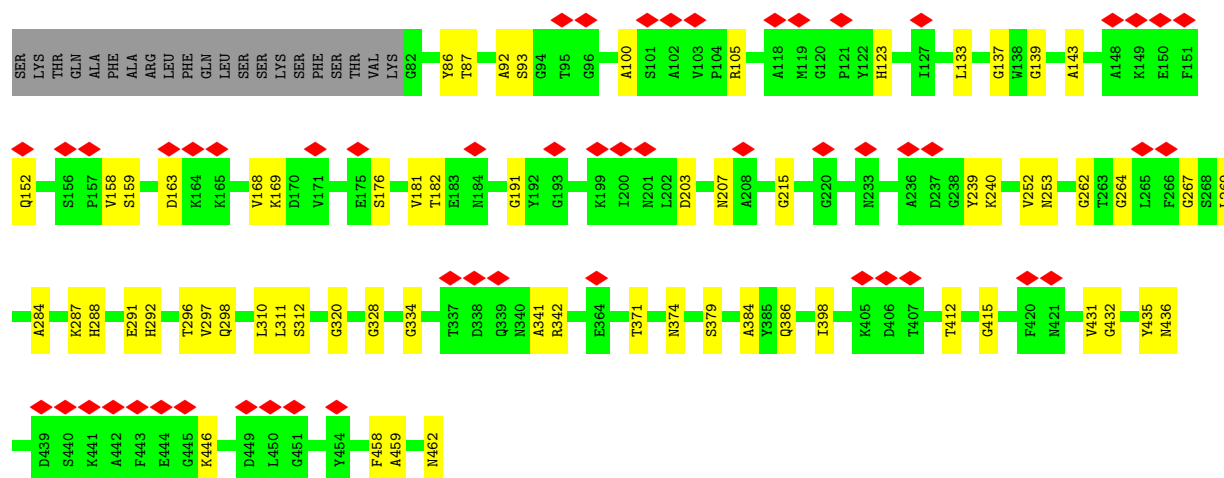
Chain 0B: 71%
69% 13% 18%



- Molecule 12: Chromosome condensation regulator RCC1 repeat protein

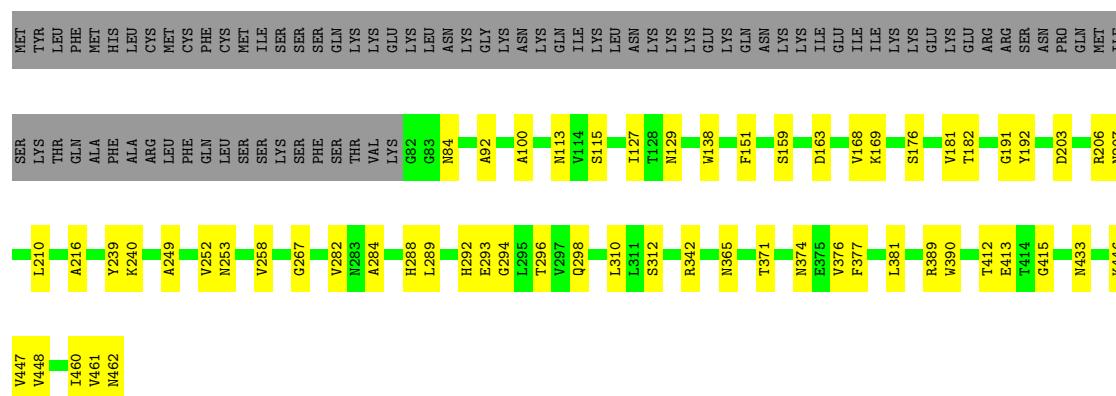
Chain 46: 11%
69% 14% 18%





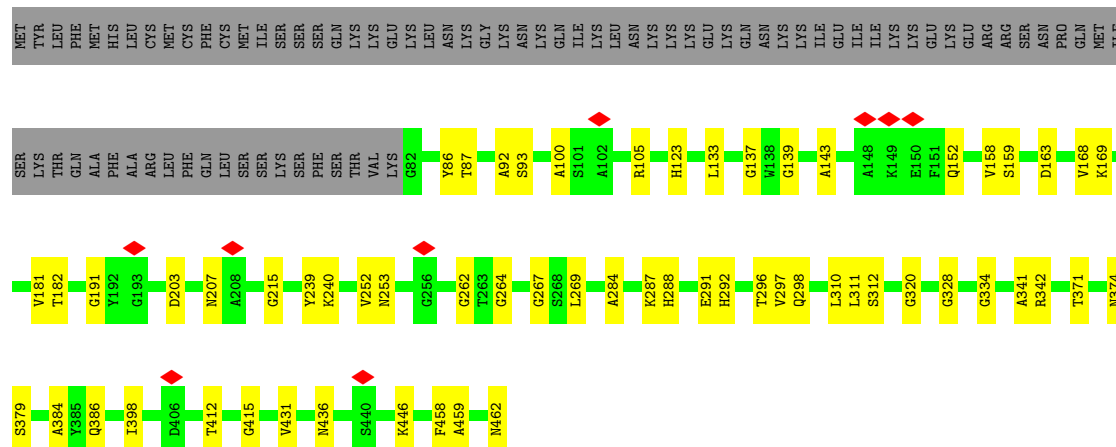
- Molecule 12: Chromosome condensation regulator RCC1 repeat protein

Chain bp: 69% 13% 18%

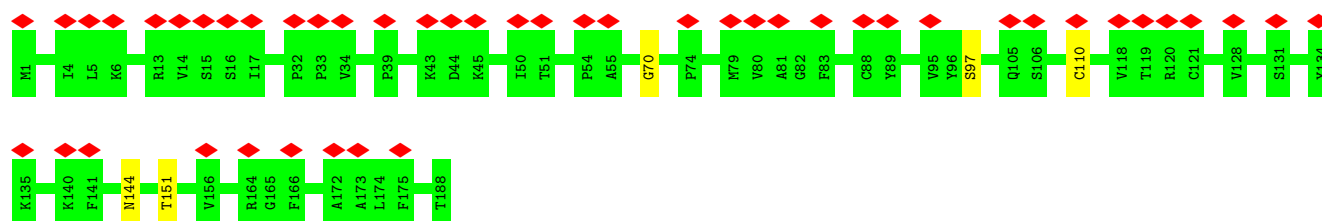


- Molecule 12: Chromosome condensation regulator RCC1 repeat protein

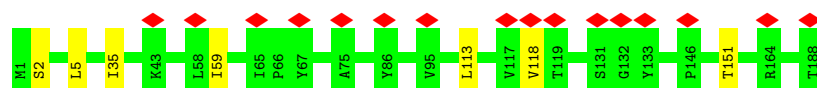
Chain BP: 69% 13% 18%



- Molecule 13: Iron-binding zinc finger CDGSH type protein



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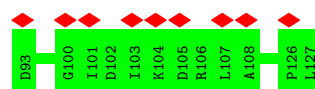
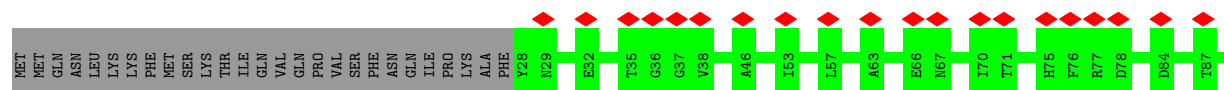
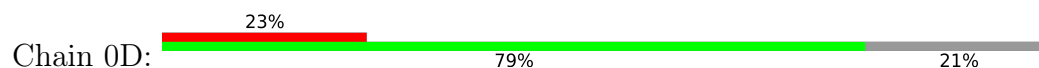
- Molecule 13: Iron-binding zinc finger CDGSH type protein



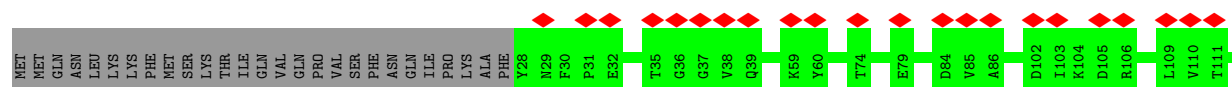
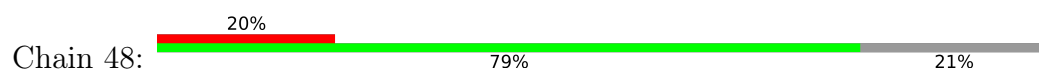
- Molecule 13: Iron-binding zinc finger CDGSH type protein

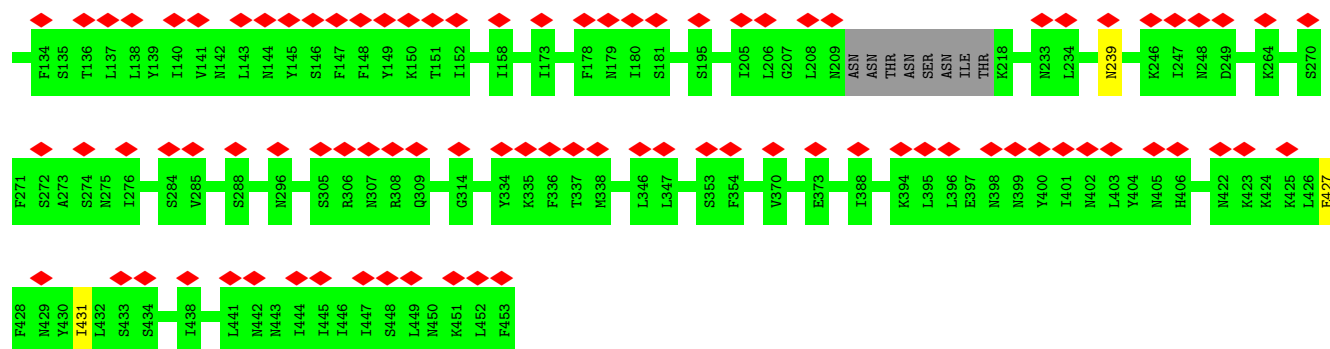


- Molecule 14: Phage protein

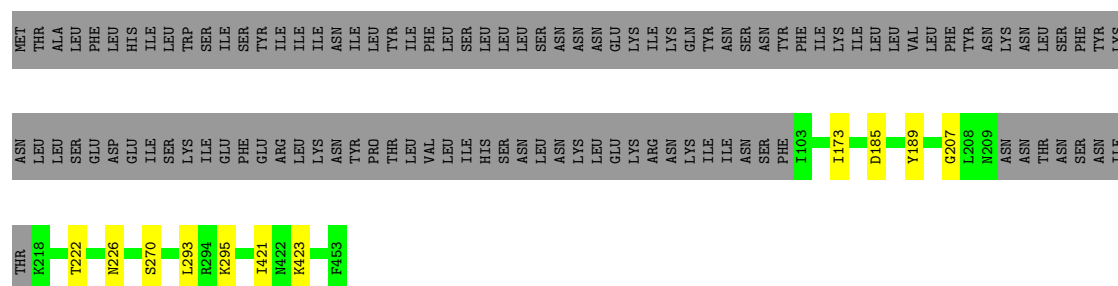
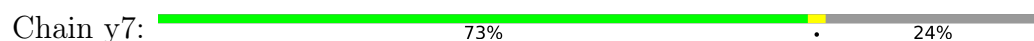


- Molecule 14: Phage protein

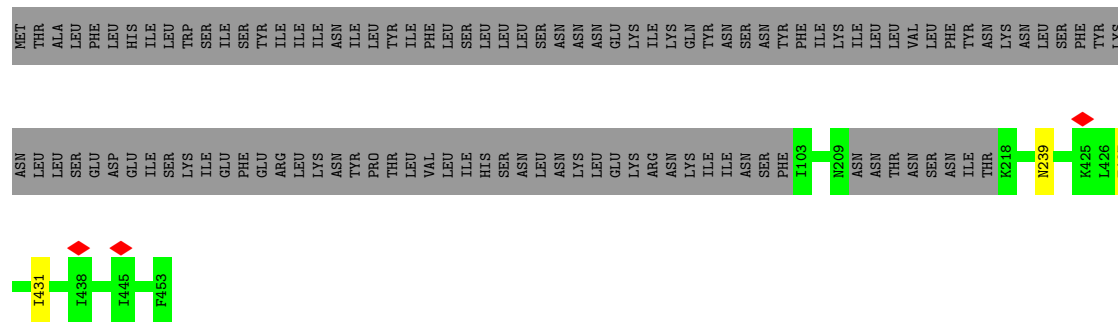
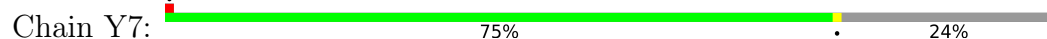




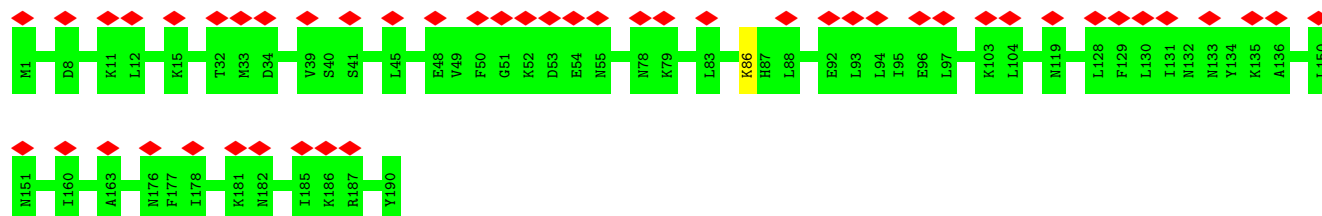
- Molecule 15: Ymf67



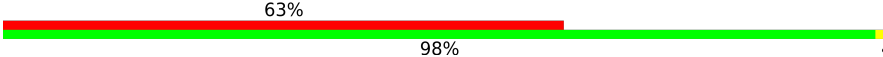
- Molecule 15: Ymf67

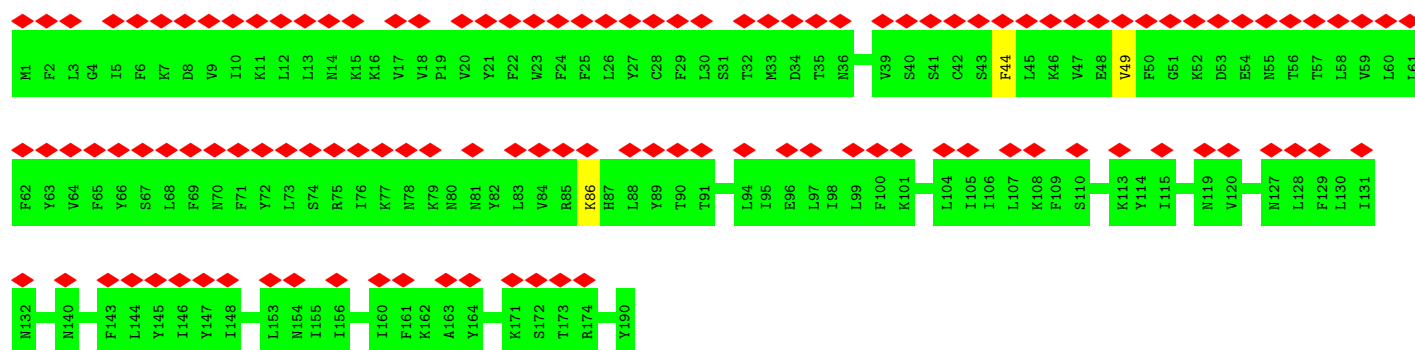


- Molecule 16: Ymf75

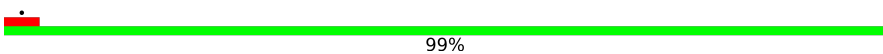


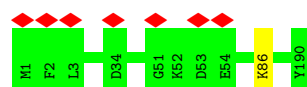
- Molecule 16: Ymf75

Chain 50: 

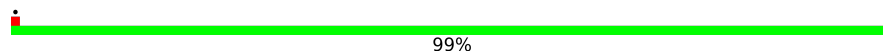


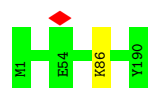
• Molecule 16: Ymf75

Chain y5: 



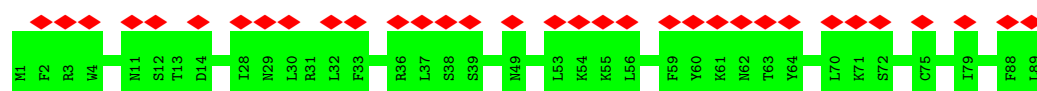
• Molecule 16: Ymf75

Chain Y5: 



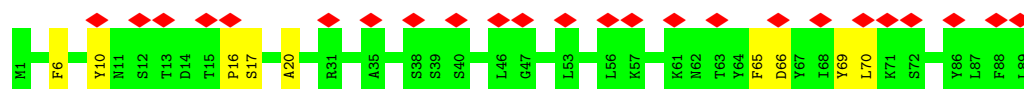
• Molecule 17: Ymf70

Chain 0G: 



• Molecule 17: Ymf70

Chain 51: 



• Molecule 17: Ymf70

Chain y0: 

There are no outlier residues recorded for this chain.

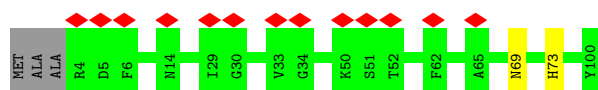
• Molecule 17: Ymf70

Chain Y0:  90% 10%



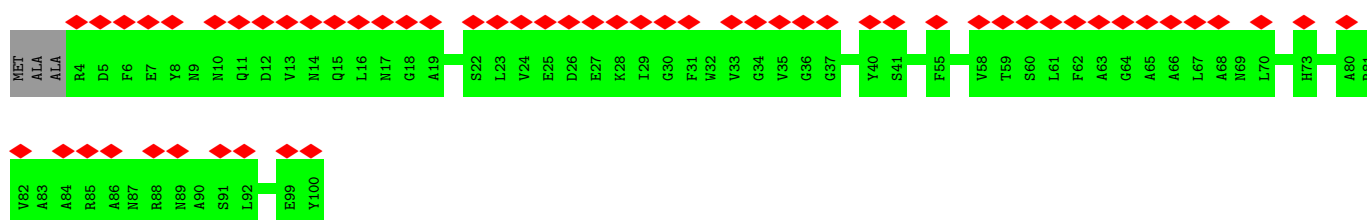
- Molecule 18: COXTT28

Chain 0H:  13% 95%



- Molecule 18: COXTT28

Chain 52:  57% 97%

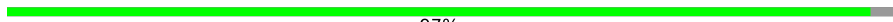


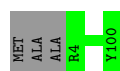
- Molecule 18: COXTT28

Chain z1:  95%



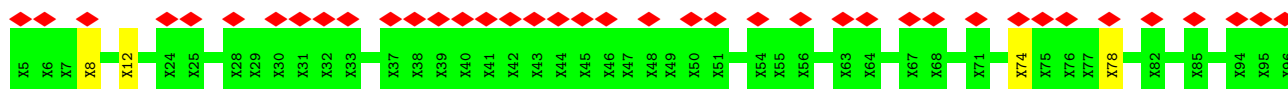
- Molecule 18: COXTT28

Chain Z1:  97%



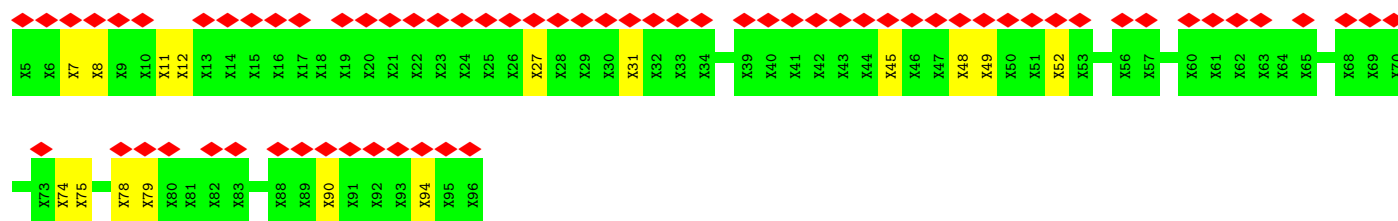
- Molecule 19: Unknown peptide

Chain 0I:  42% 96%

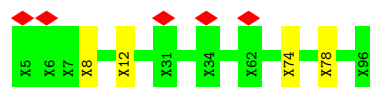


- Molecule 19: Unknown peptide

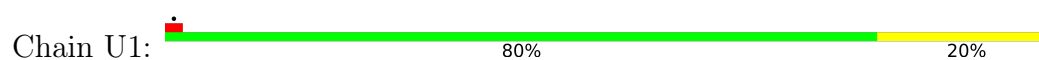
Chain 53:  73% 83% 17%



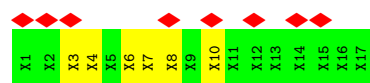
- Molecule 19: Unknown peptide



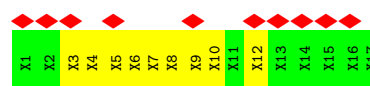
- Molecule 19: Unknown peptide



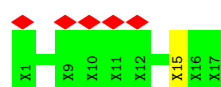
- Molecule 20: unknown peptide



- Molecule 20: unknown peptide

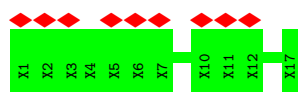


- Molecule 20: unknown peptide

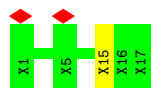


- Molecule 20: unknown peptide





- Molecule 20: unknown peptide



- Molecule 20: unknown peptide

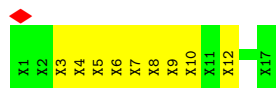


There are no outlier residues recorded for this chain.

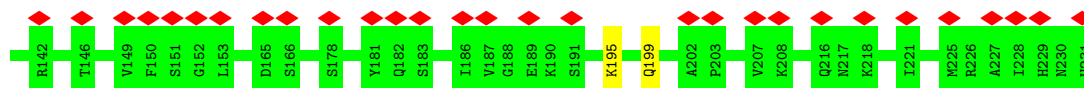
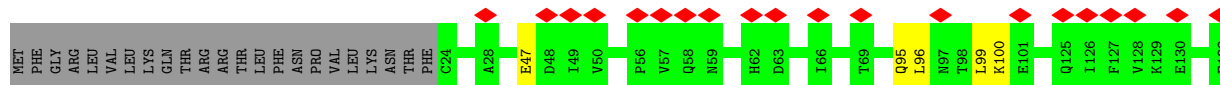
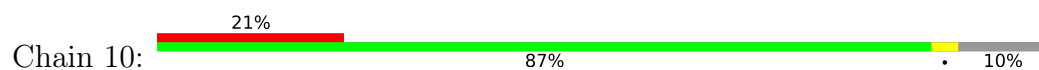
- Molecule 20: unknown peptide



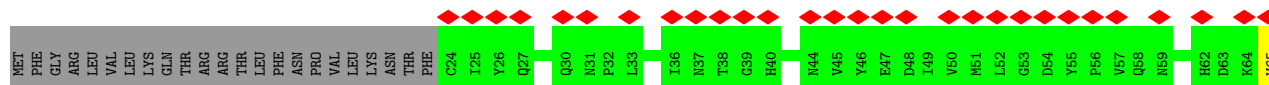
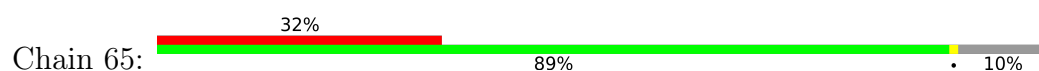
- Molecule 20: unknown peptide

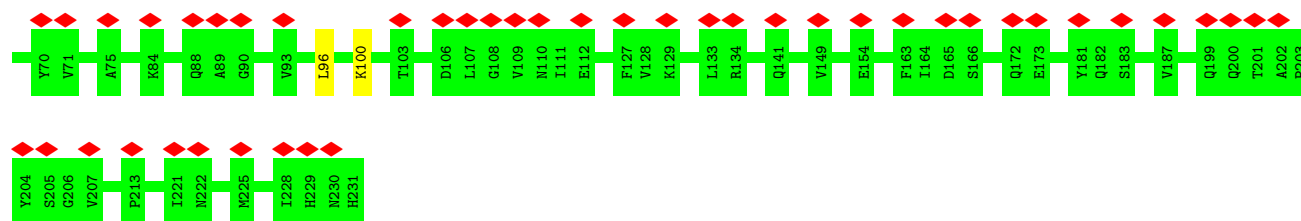


- Molecule 21: 39S ribosomal protein L9, mitochondrial



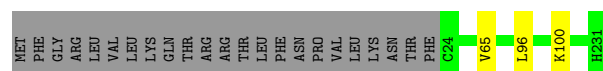
- Molecule 21: 39S ribosomal protein L9, mitochondrial





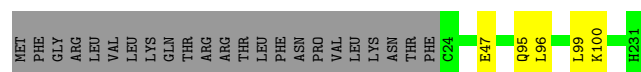
- Molecule 21: 39S ribosomal protein L9, mitochondrial

Chain k: 89% 10%



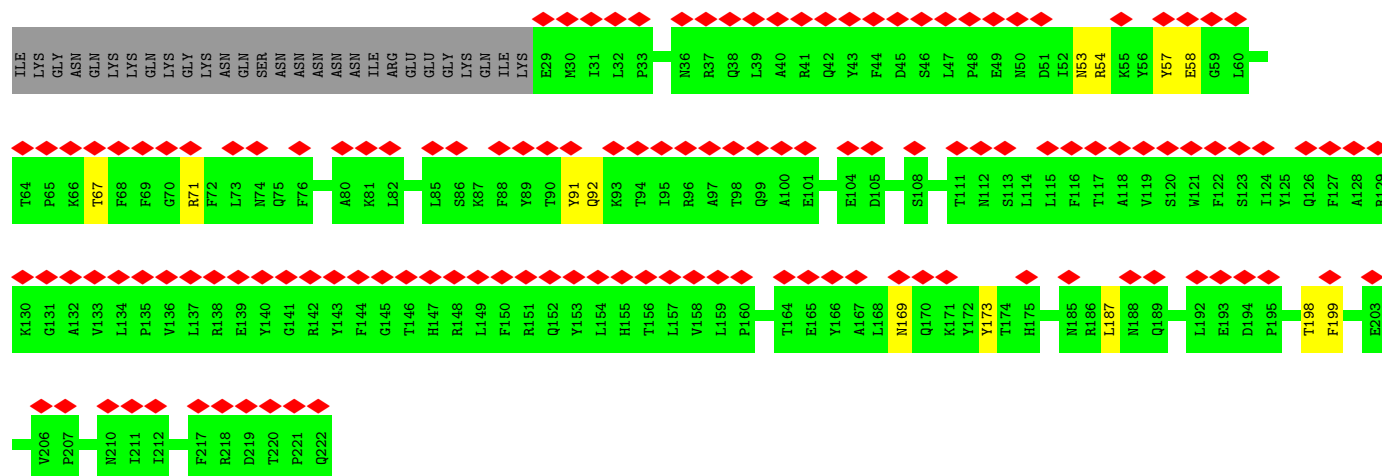
- Molecule 21: 39S ribosomal protein L9, mitochondrial

Chain K: 88% 10%



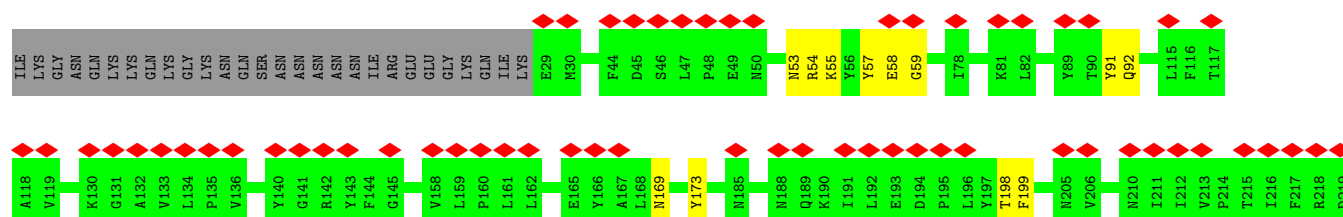
- Molecule 22: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain 11: 60% 82% 6% 13%



- Molecule 22: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

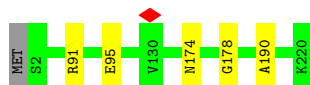
Chain 66: 28% 82% 5% 13%





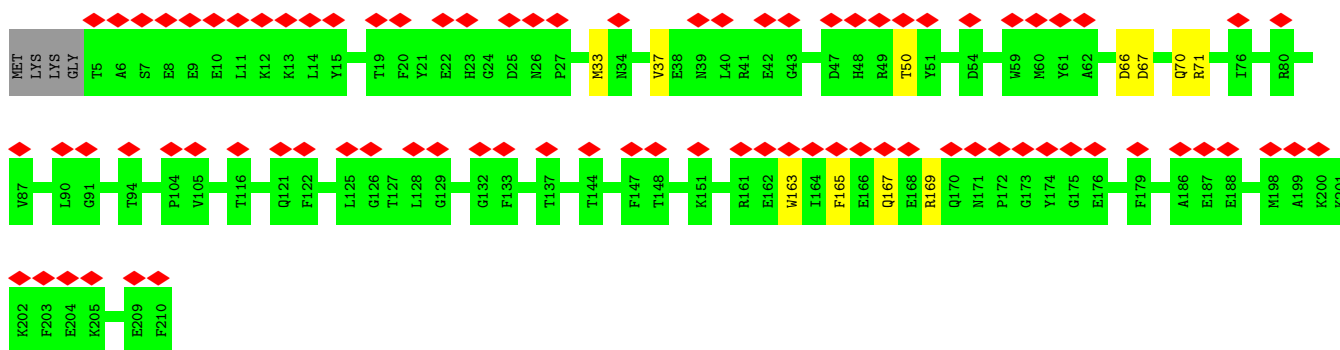
- Molecule 23: Transmembrane protein, putative

Chain M: 97% .



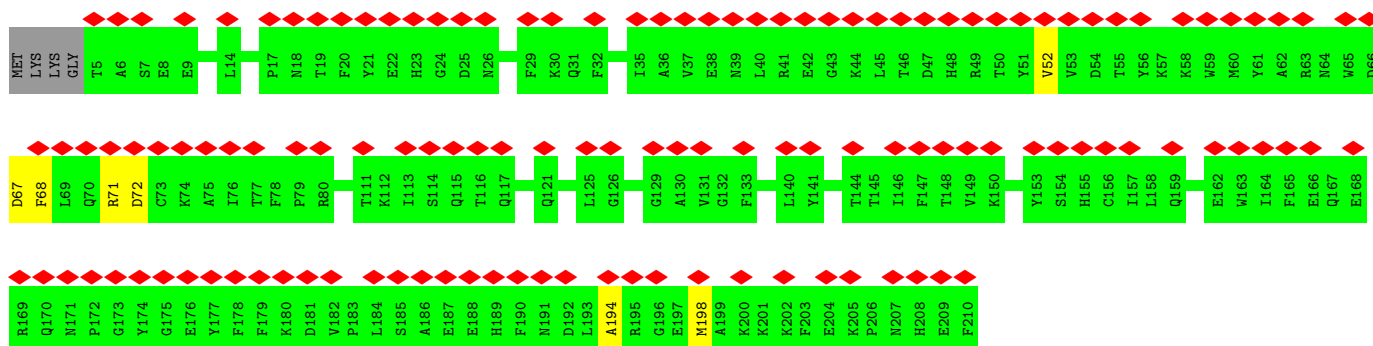
- Molecule 24: Transmembrane protein, putative

Chain 13: 40% 93% 5% .



- Molecule 24: Transmembrane protein, putative

Chain 68: 61% 95% . .

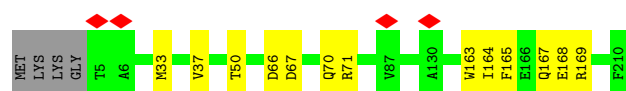


- Molecule 24: Transmembrane protein, putative

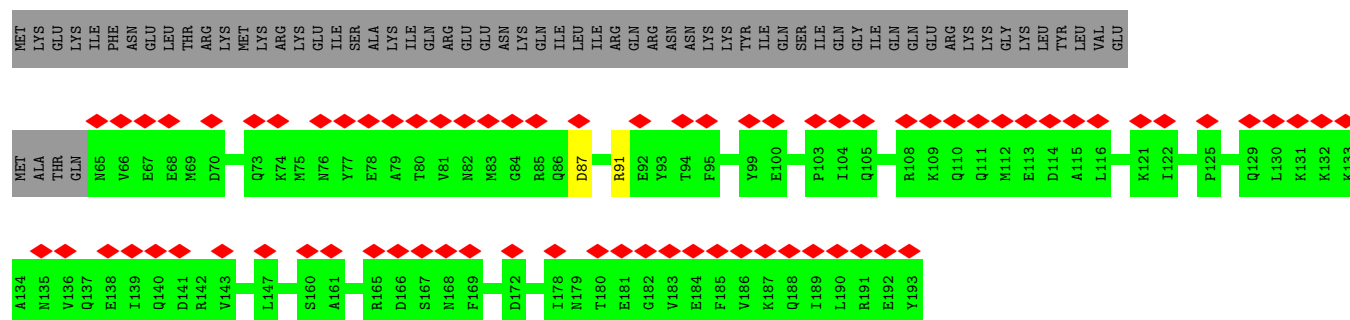
Chain n: 95% . .



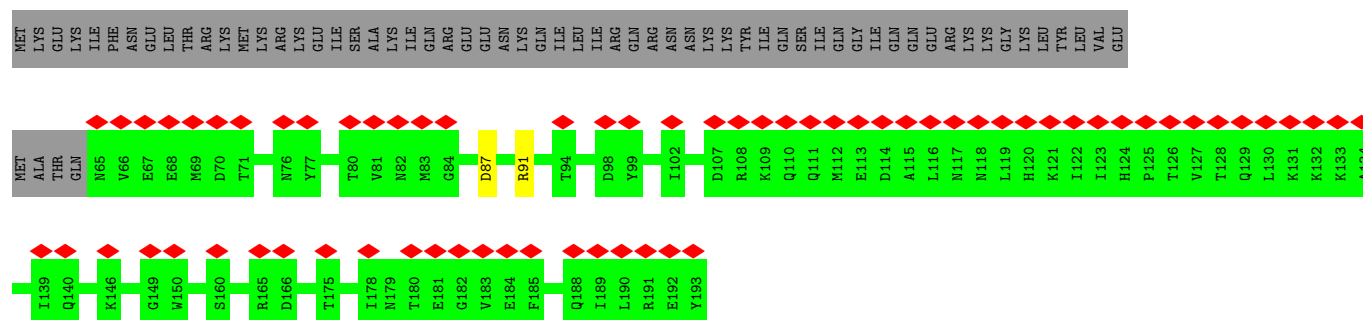
- Molecule 24: Transmembrane protein, putative



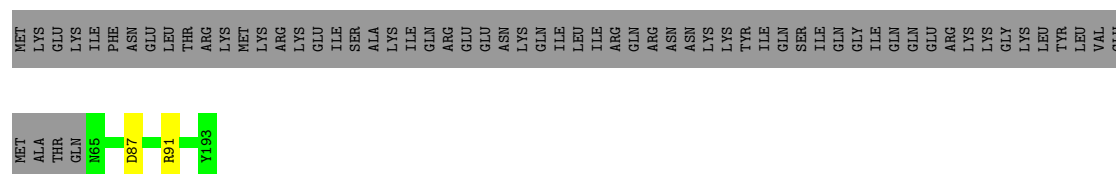
Chain 14: 38% 66% 33%



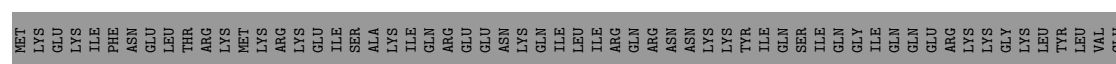
Chain 69: 35% 66% 33%

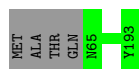


Chain o: 66% 33%



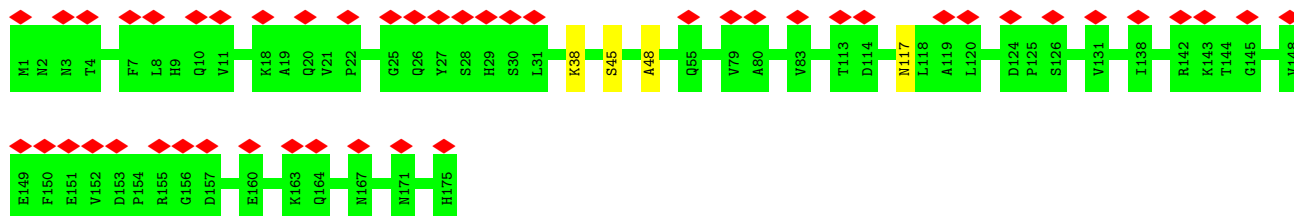
Chain O: 67% 33%





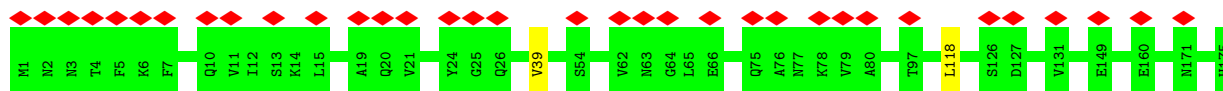
- Molecule 26: YfIT domain-containing protein

Chain 15: 27% 98%



- Molecule 26: YfIT domain-containing protein

Chain 70: 19% 99%



- Molecule 26: YfIT domain-containing protein

Chain p: 99%



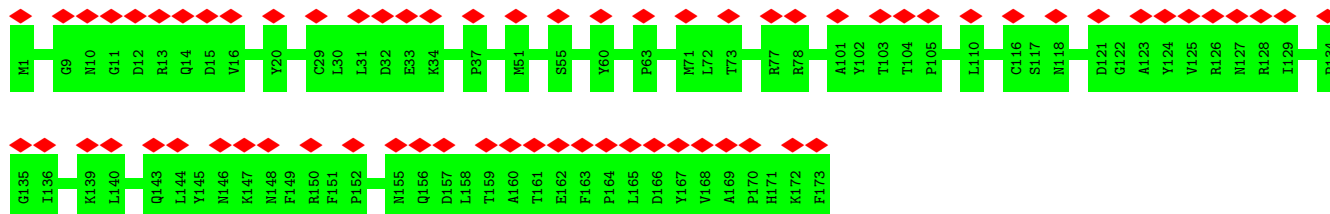
- Molecule 26: YfIT domain-containing protein

Chain P: 98%

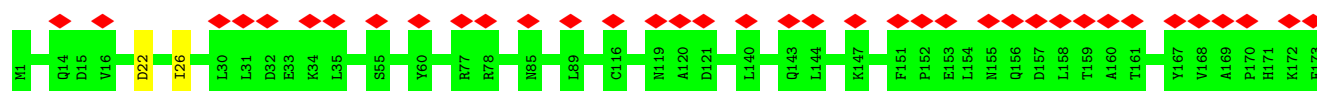


- Molecule 27: Transmembrane protein, putative

Chain 16: 39% 100%



- Molecule 27: Transmembrane protein, putative

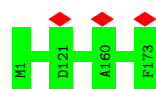


- Molecule 27: Transmembrane protein, putative

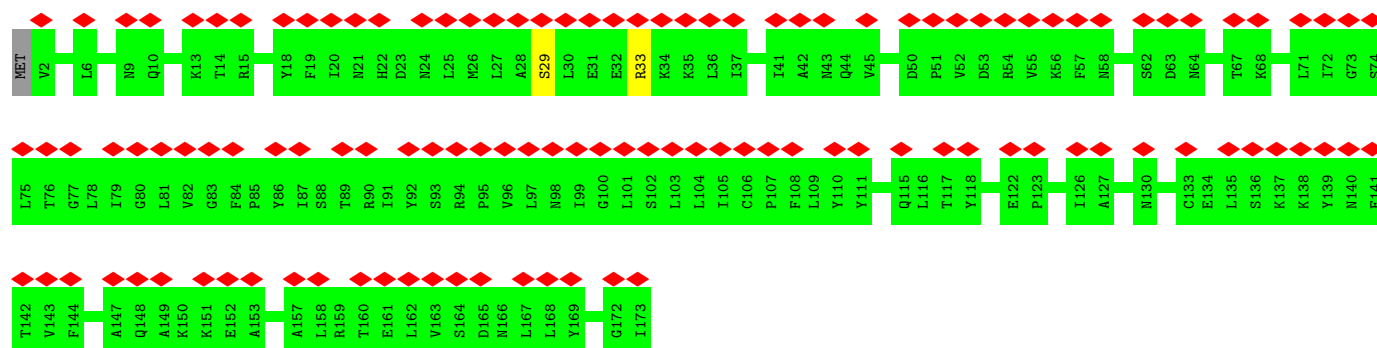


There are no outlier residues recorded for this chain.

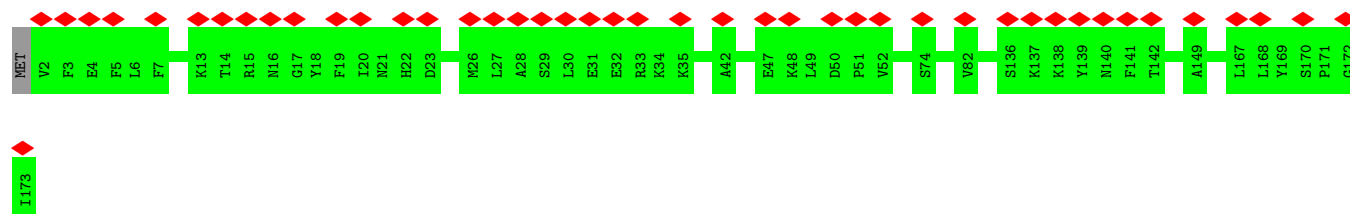
- Molecule 27: Transmembrane protein, putative



- Molecule 28: Transmembrane protein



- Molecule 28: Transmembrane protein



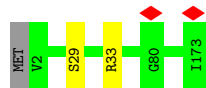
- Molecule 28: Transmembrane protein





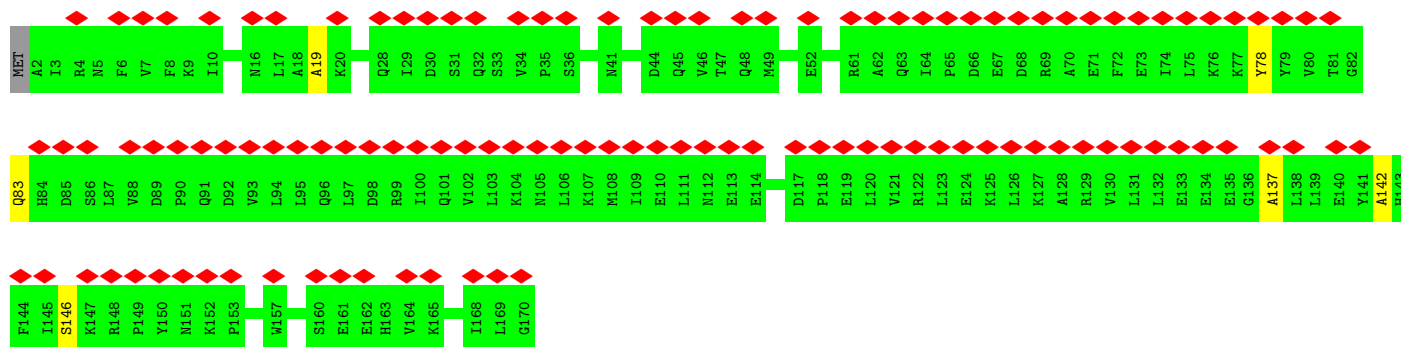
- Molecule 28: Transmembrane protein

Chain R: 98%



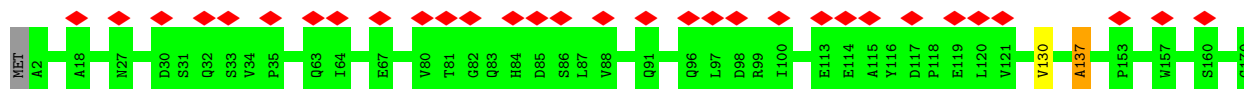
- Molecule 29: Complex III subunit VII

Chain 18: 68% 96%



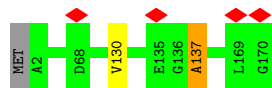
- Molecule 29: Complex III subunit VII

Chain 73: 18% 98%



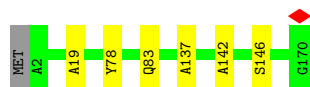
- Molecule 29: Complex III subunit VII

Chain s: 98%

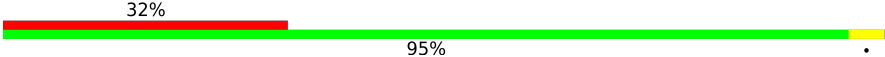


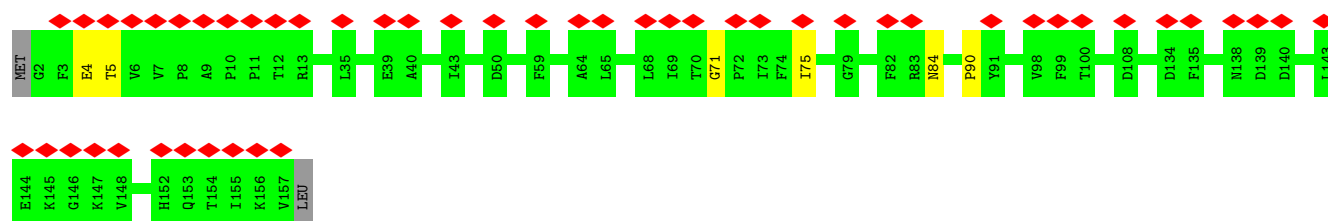
- Molecule 29: Complex III subunit VII

Chain S: 96%

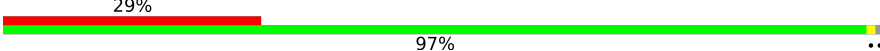


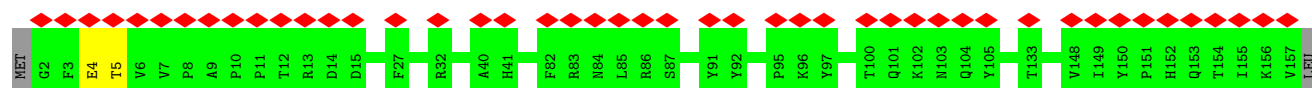
- Molecule 30: Transmembrane protein, putative

Chain 19: 

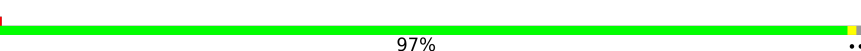


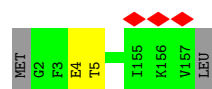
- Molecule 30: Transmembrane protein, putative

Chain 74: 

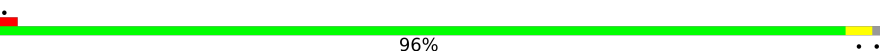


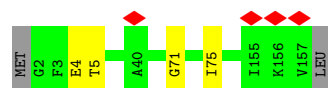
- Molecule 30: Transmembrane protein, putative

Chain t: 

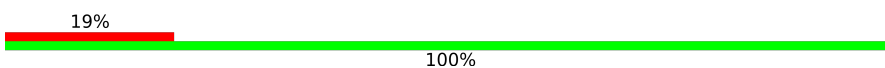


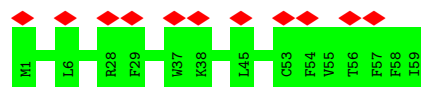
- Molecule 30: Transmembrane protein, putative

Chain T: 

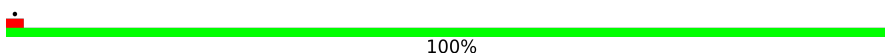


- Molecule 31: NADH dehydrogenase subunit 1

Chain 1b: 

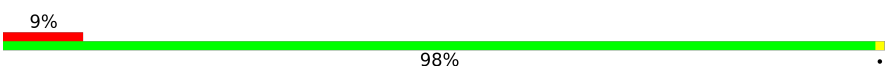


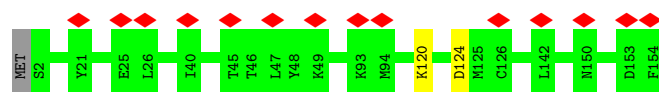
- Molecule 31: NADH dehydrogenase subunit 1

Chain 1B: 



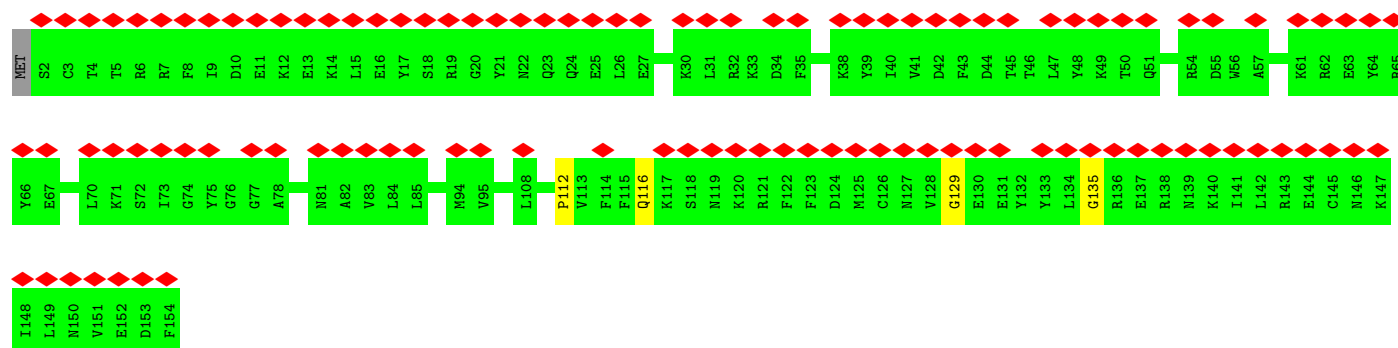
- Molecule 32: Transmembrane protein, putative

Chain 20: 



- Molecule 32: Transmembrane protein, putative

Chain 75: 70%
97%



- Molecule 32: Transmembrane protein, putative

Chain u: 97%



- Molecule 32: Transmembrane protein, putative

Chain U: 98%



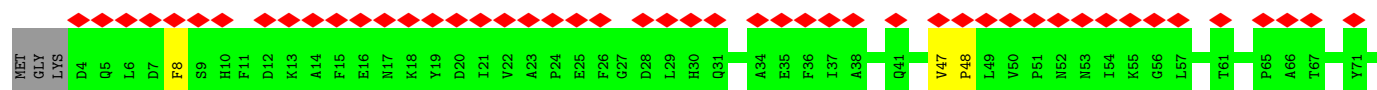
- Molecule 33: COXTT22

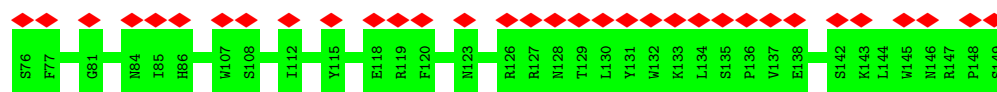
Chain 21: 11%
96%



- Molecule 33: COXTT22

Chain 76: 54%
96%





- Molecule 33: COXTT22

Chain v: 96%



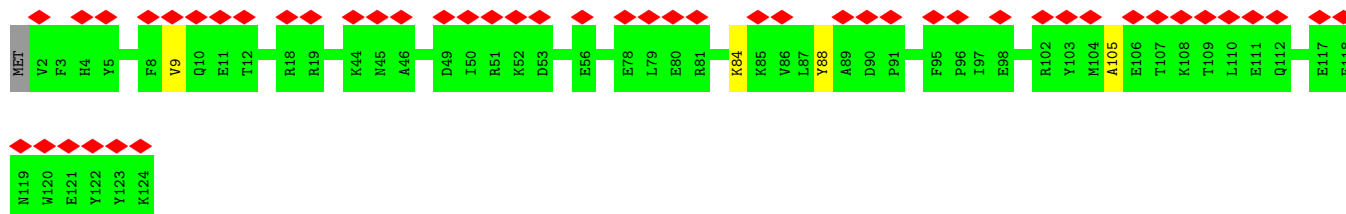
- Molecule 33: COXTT22

Chain V: 96%



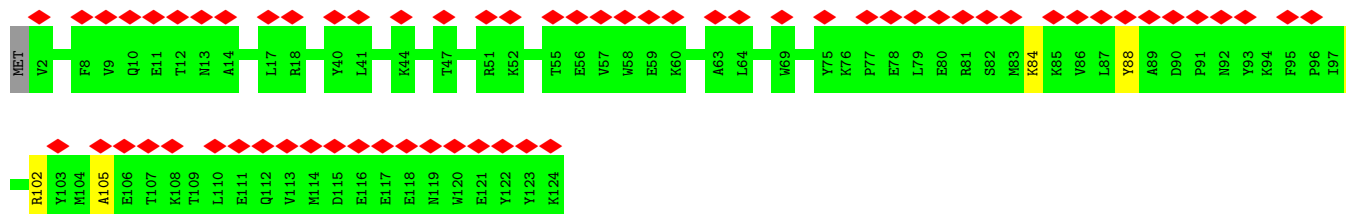
- Molecule 34: Transmembrane protein, putative

Chain 22: 40% 96%



- Molecule 34: Transmembrane protein, putative

Chain 77: 52% 95%

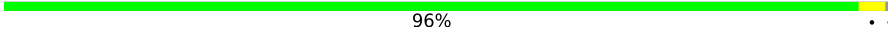


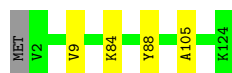
- Molecule 34: Transmembrane protein, putative

Chain w: 95%

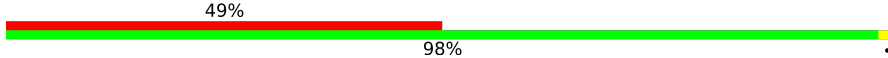


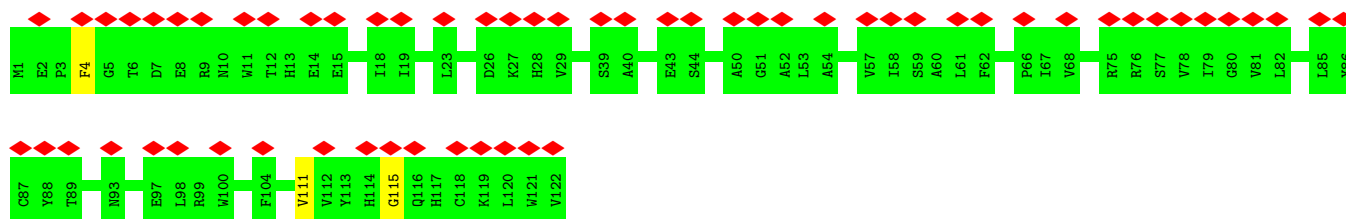
- Molecule 34: Transmembrane protein, putative

Chain W:  96%



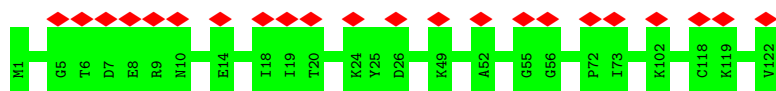
- Molecule 35: Transmembrane protein, putative

Chain 23:  49% 98%

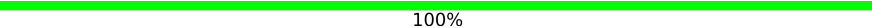


- Molecule 35: Transmembrane protein, putative

Chain 78:  18% 100%

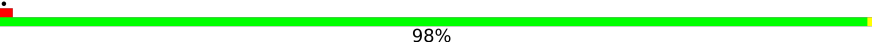


- Molecule 35: Transmembrane protein, putative

Chain x:  100%

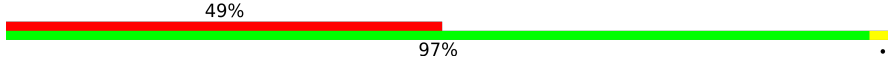
There are no outlier residues recorded for this chain.

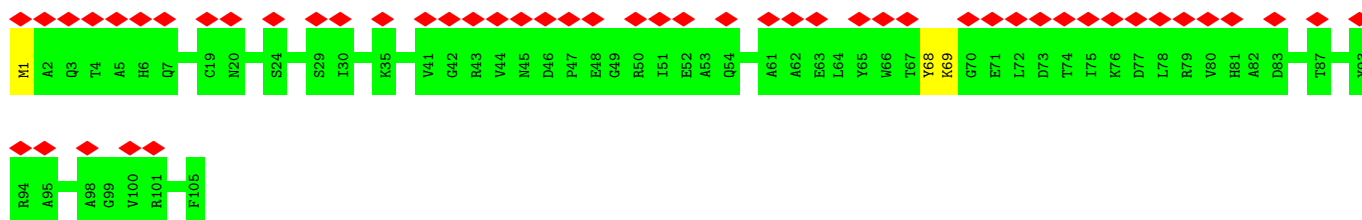
- Molecule 35: Transmembrane protein, putative

Chain X:  98%

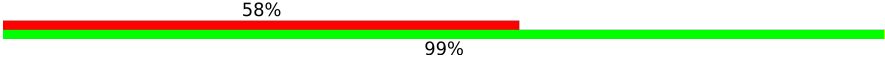


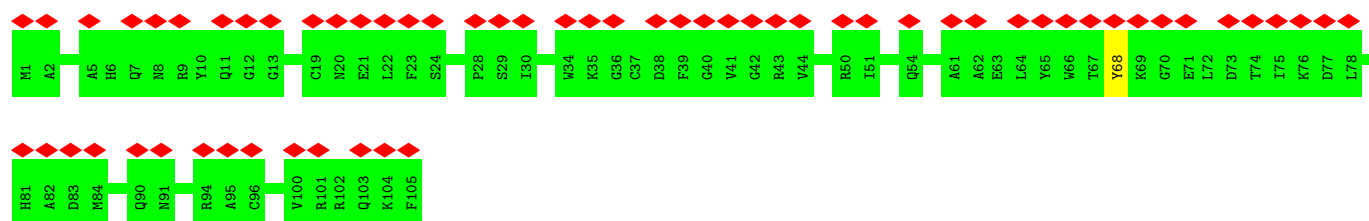
- Molecule 36: Lysozyme

Chain 24:  49% 97%

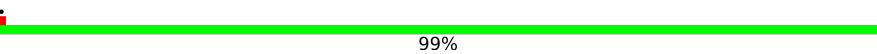


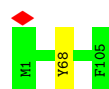
- Molecule 36: Lysozyme

Chain 79: 

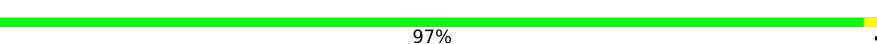


• Molecule 36: Lysozyme

Chain y: 

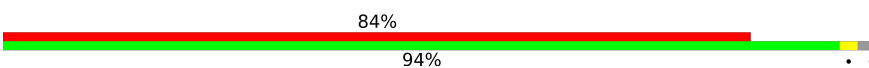


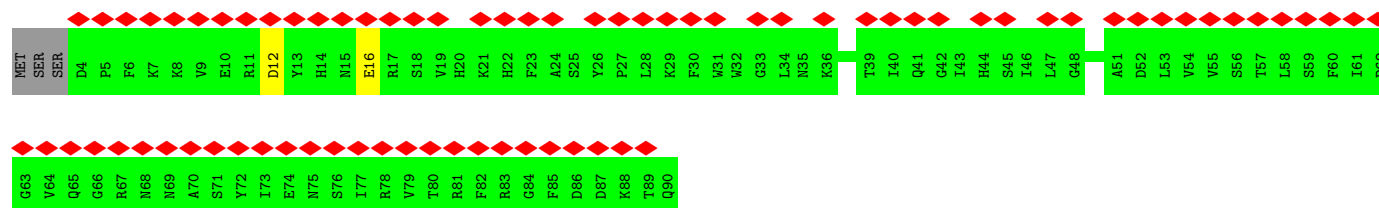
• Molecule 36: Lysozyme

Chain Y: 

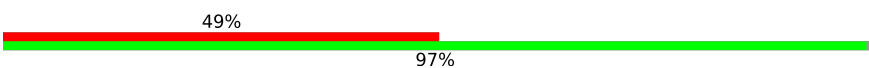


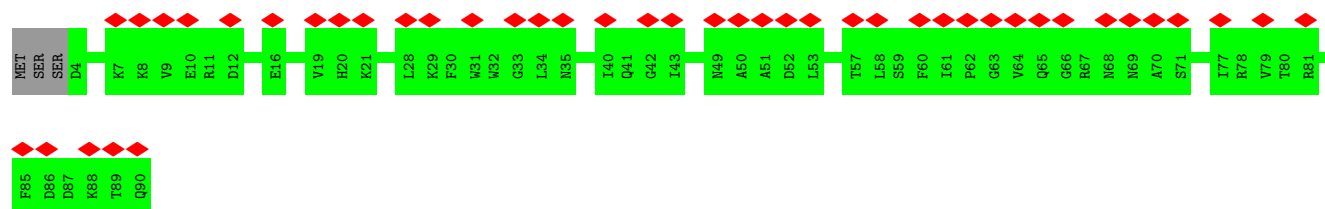
• Molecule 37: ABC transporter

Chain 25: 

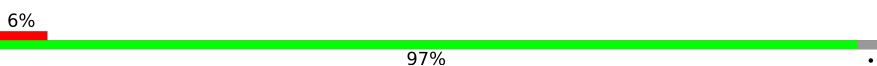


• Molecule 37: ABC transporter

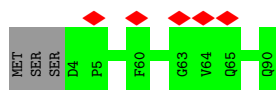
Chain 80: 



• Molecule 37: ABC transporter

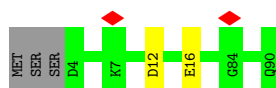
Chain z: 





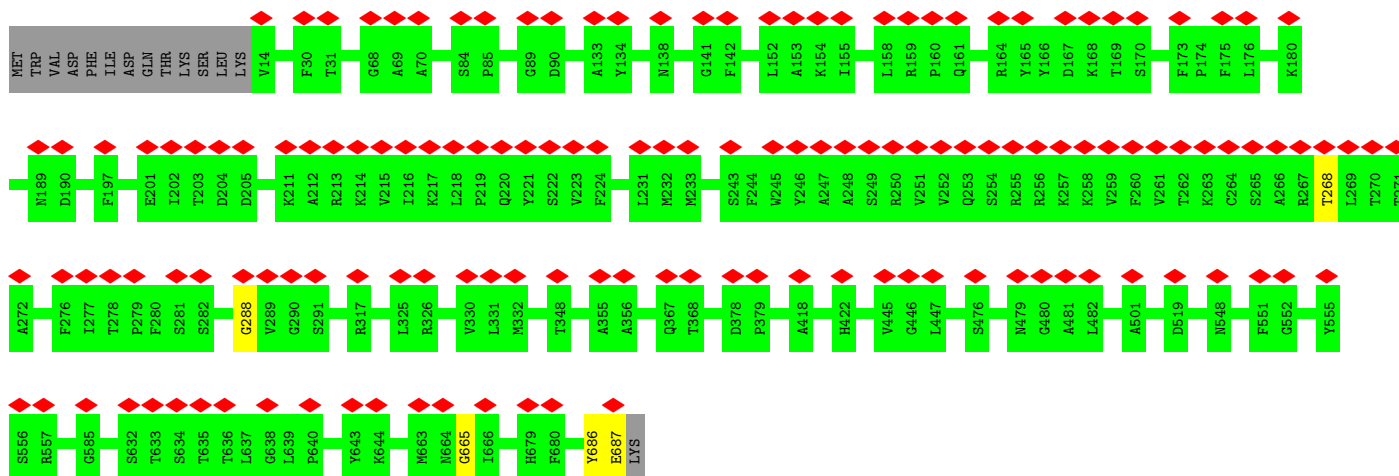
- Molecule 37: ABC transporter

Chain Z: 94%



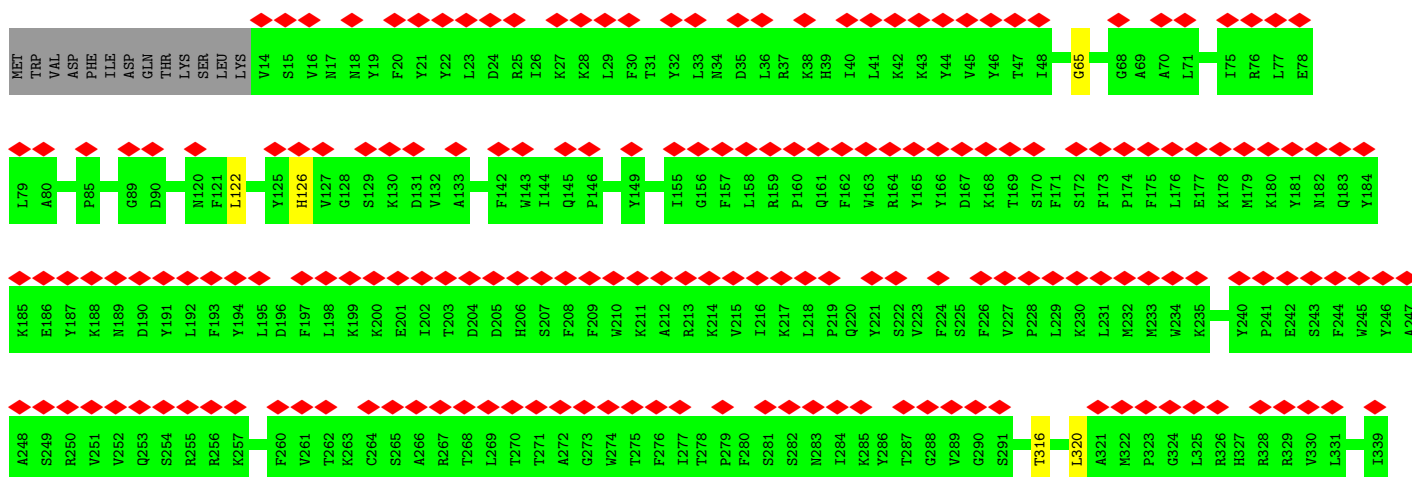
- Molecule 38: Cytochrome c oxidase subunit 1

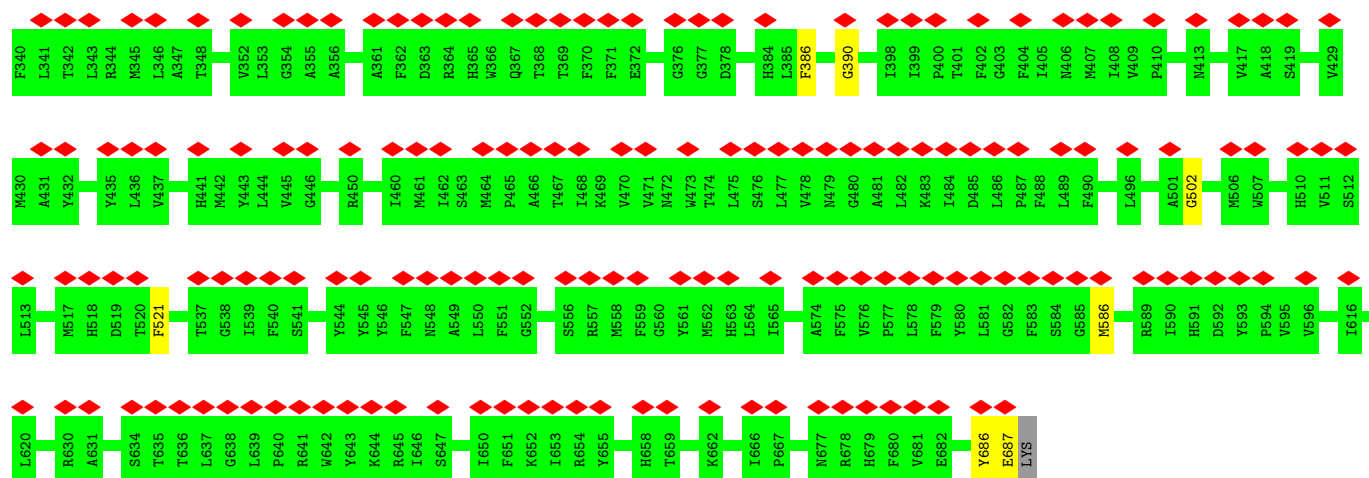
Chain 26: 21% 97%



- Molecule 38: Cytochrome c oxidase subunit 1

Chain 81: 51% 96%





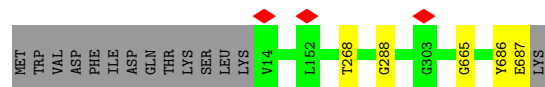
• Molecule 38: Cytochrome c oxidase subunit 1

Chain c1: 96%



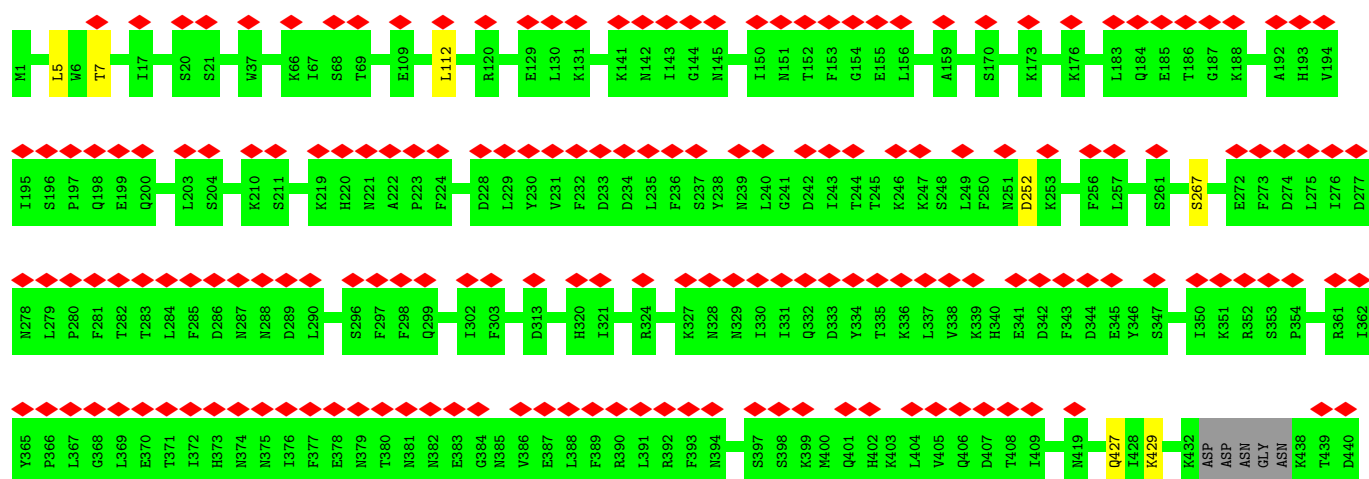
• Molecule 38: Cytochrome c oxidase subunit 1

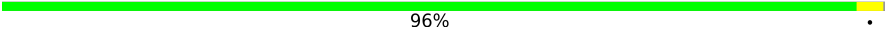
Chain C1: 97%

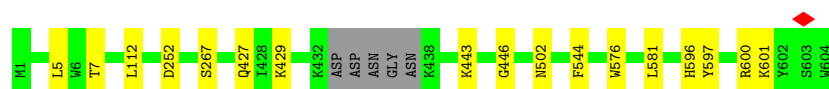


• Molecule 39: Cytochrome c oxidase subunit 2

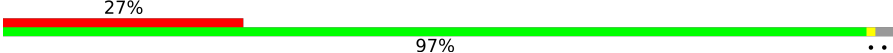
Chain 27: 35% 96%

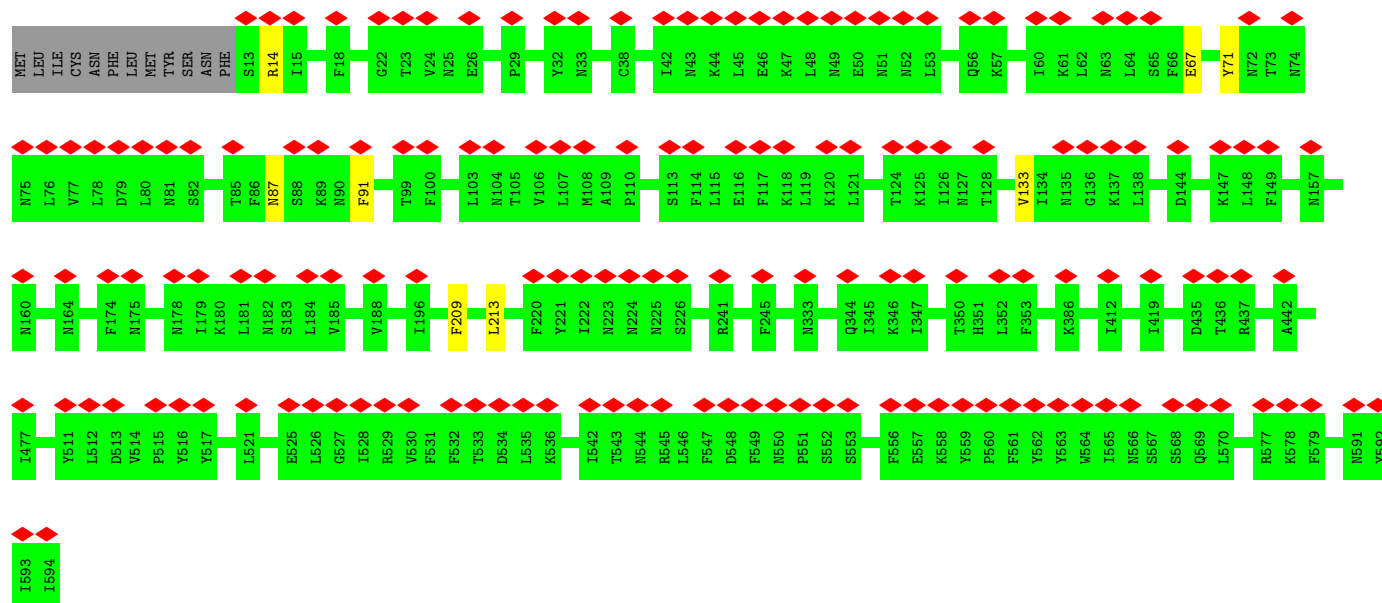


Chain C2:  96%

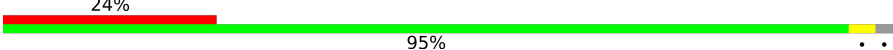


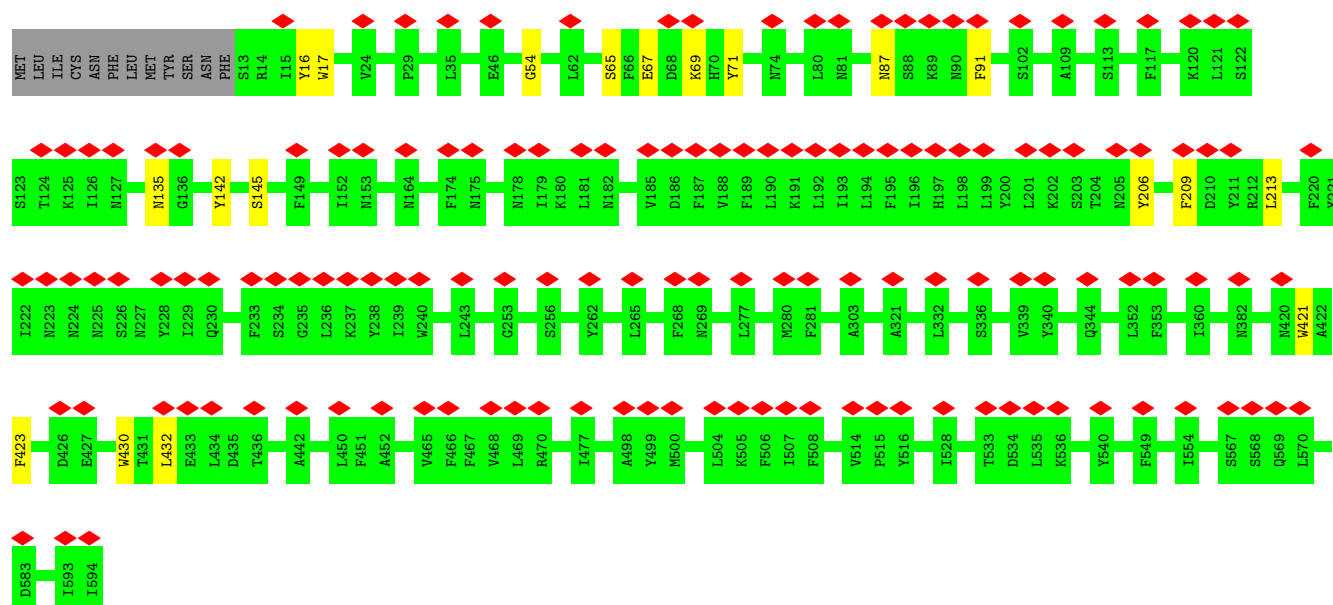
• Molecule 40: Ymf68

Chain 28:  27% 97%

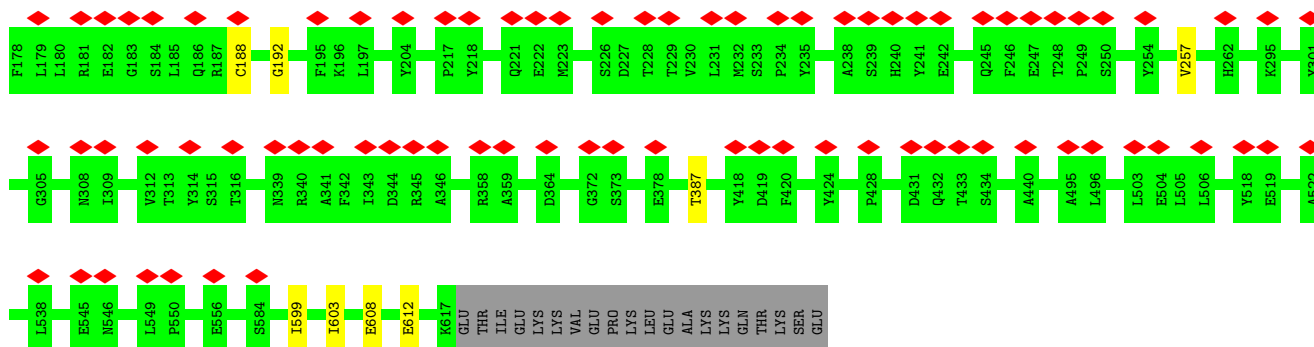


• Molecule 40: Ymf68

Chain 83:  24% 95%



• Molecule 40: Ymf68



• Molecule 41: Cytochrome C oxidase subunit Vb protein

Chain vb: 86% 13%



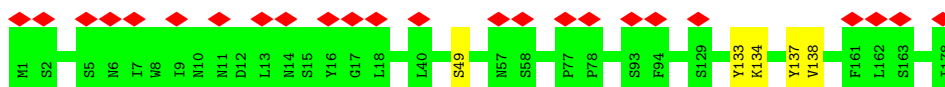
• Molecule 41: Cytochrome C oxidase subunit Vb protein

Chain VB: 85% 13%



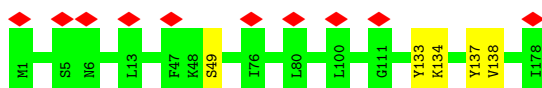
• Molecule 42: NADH dehydrogenase subunit 2

Chain 2b: 13% 97%



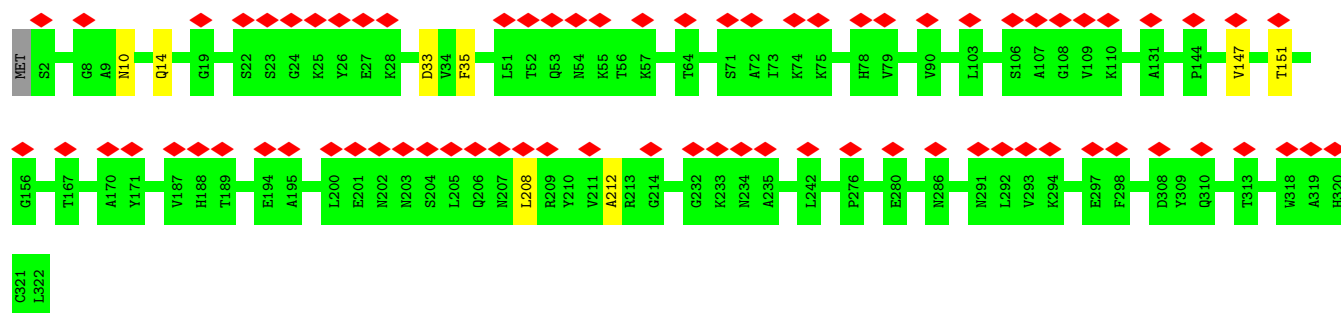
• Molecule 42: NADH dehydrogenase subunit 2

Chain 2B: 6% 97%

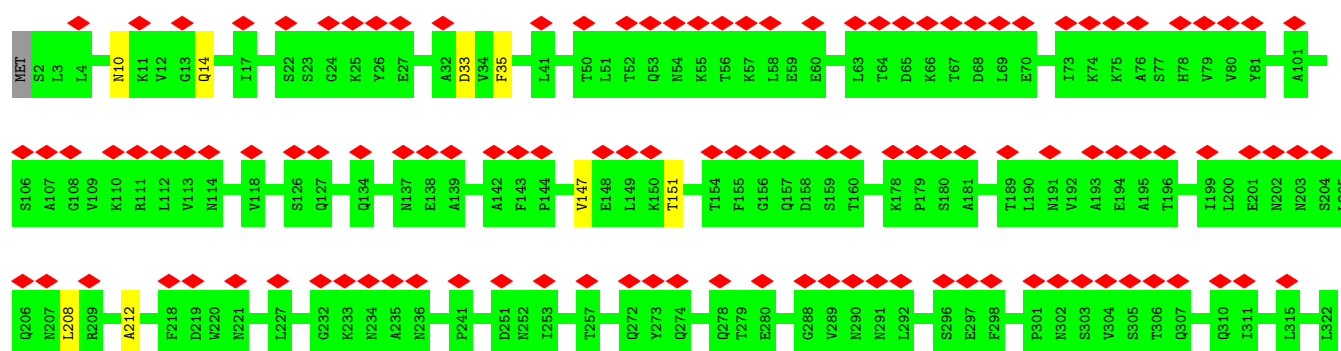


• Molecule 43: NmrA domain-containing protein

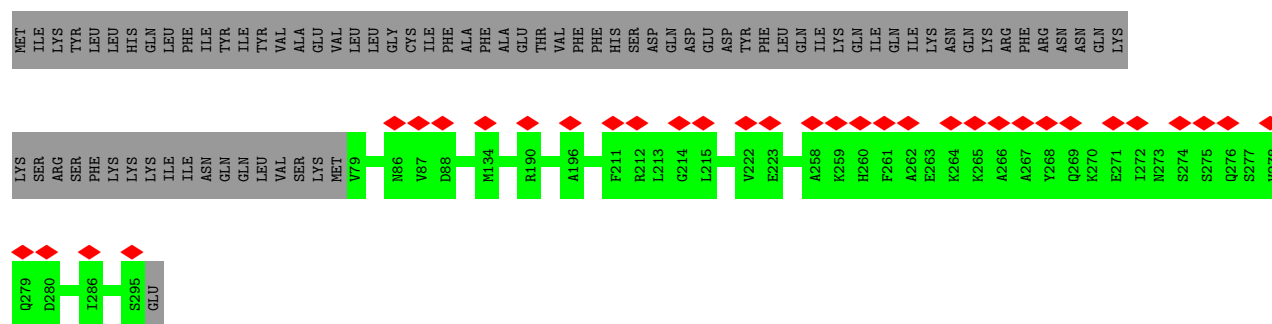
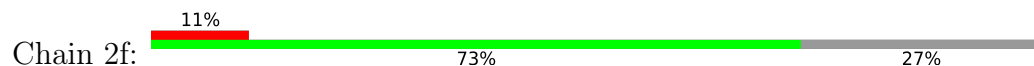
Chain 2e: 23% 97%



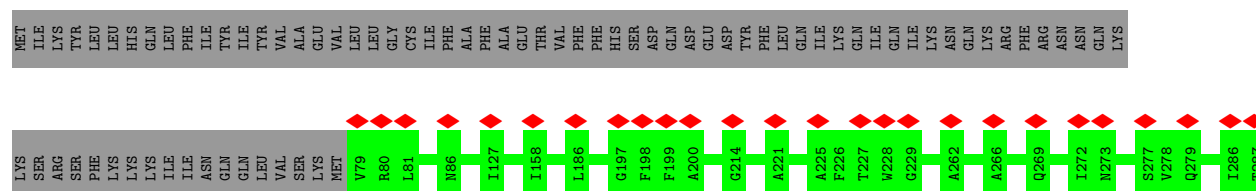
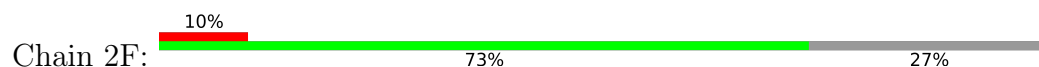
- Molecule 43: NmrA domain-containing protein

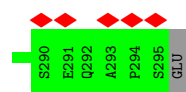


- Molecule 44: Transmembrane protein, putative

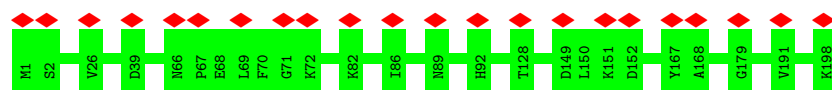


- Molecule 44: Transmembrane protein, putative

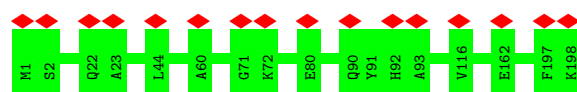




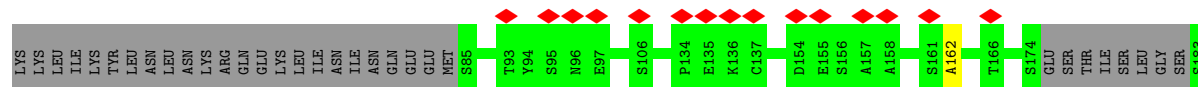
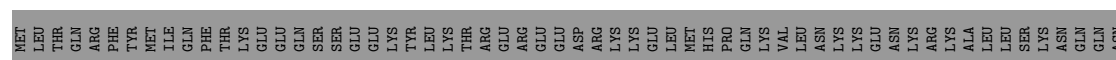
- Molecule 45: SDHTT3



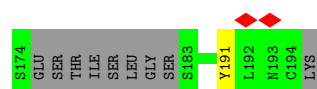
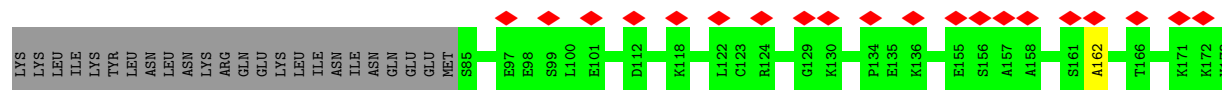
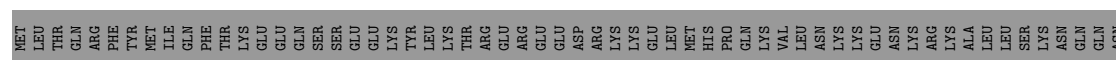
- Molecule 45: SDHTT3



- Molecule 46: Diphthamide synthesis protein

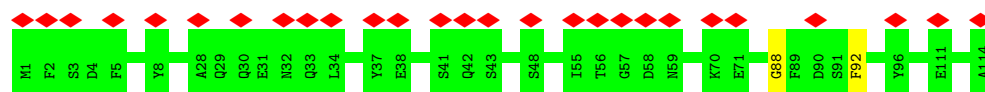


- Molecule 46: Diphthamide synthesis protein

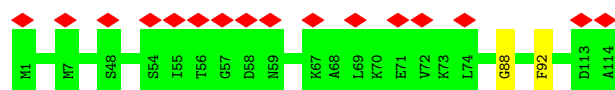


- Molecule 47: DUF4885 domain-containing protein

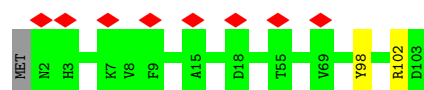




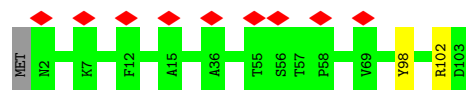
- Molecule 47: DUF4885 domain-containing protein



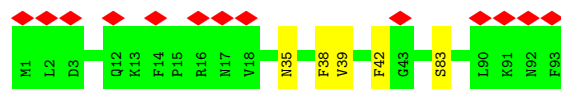
- Molecule 48: Transmembrane protein, putative



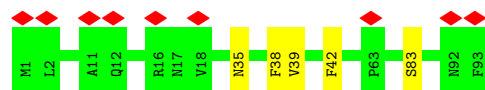
- Molecule 48: Transmembrane protein, putative



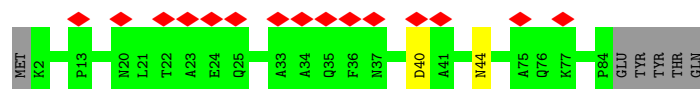
- Molecule 49: Transmembrane protein, putative



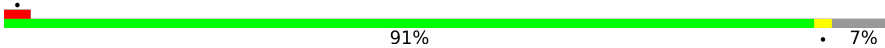
- Molecule 49: Transmembrane protein, putative

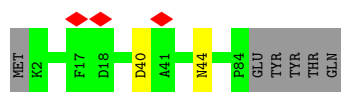


- Molecule 50: Transposase

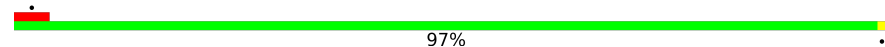


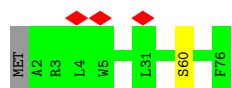
- Molecule 50: Transposase

Chain 2L:  91% 7%

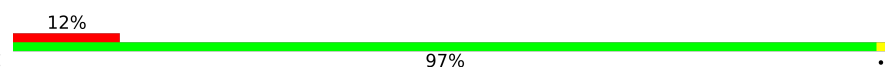


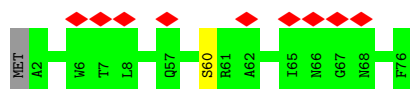
- Molecule 51: Transmembrane protein, putative

Chain 2m:  97%

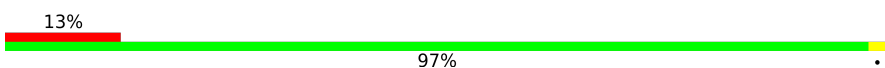


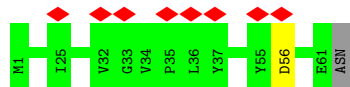
- Molecule 51: Transmembrane protein, putative

Chain 2M:  12% 97%

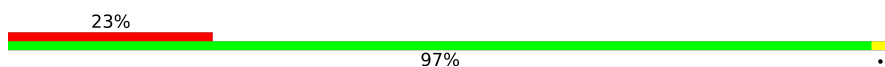


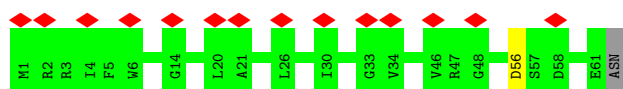
- Molecule 52: Transmembrane protein, putative

Chain 2n:  13% 97%

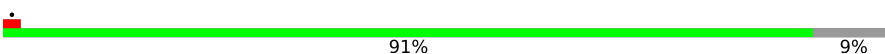


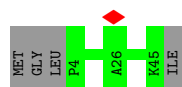
- Molecule 52: Transmembrane protein, putative

Chain 2N:  23% 97%

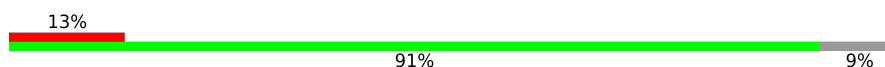


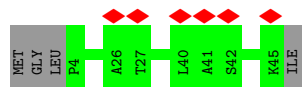
- Molecule 53: SDHTT11

Chain 2o:  91% 9%

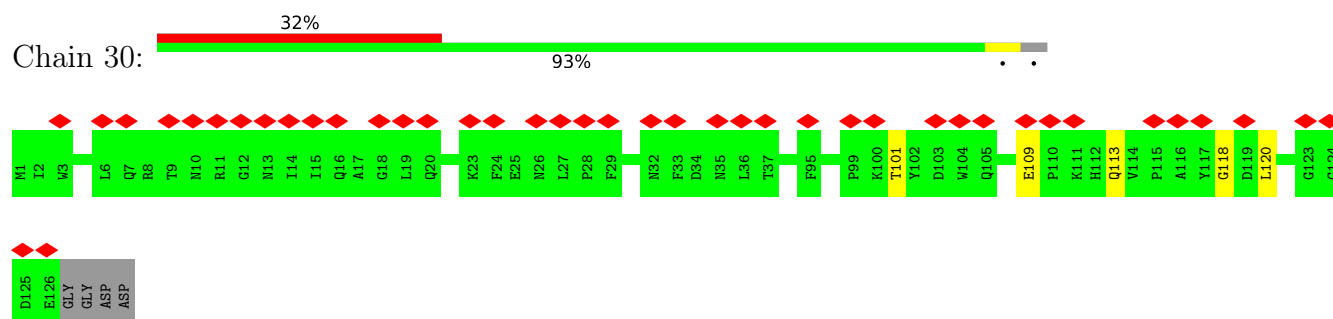


- Molecule 53: SDHTT11

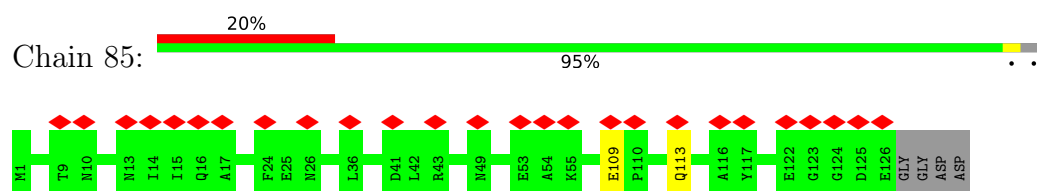
Chain 2O:  13% 91% 9%



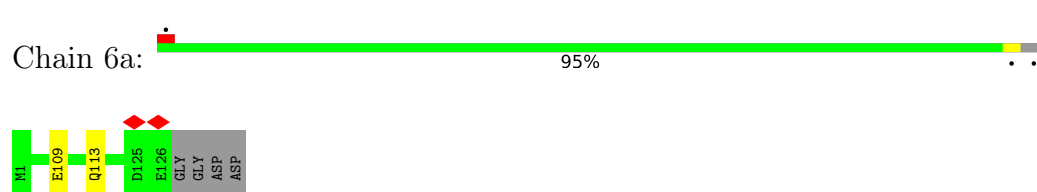
- Molecule 54: Transmembrane protein, putative



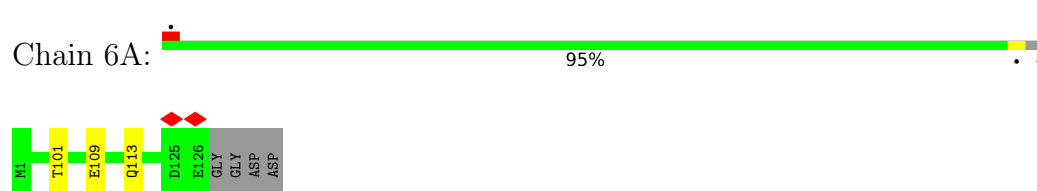
- Molecule 54: Transmembrane protein, putative



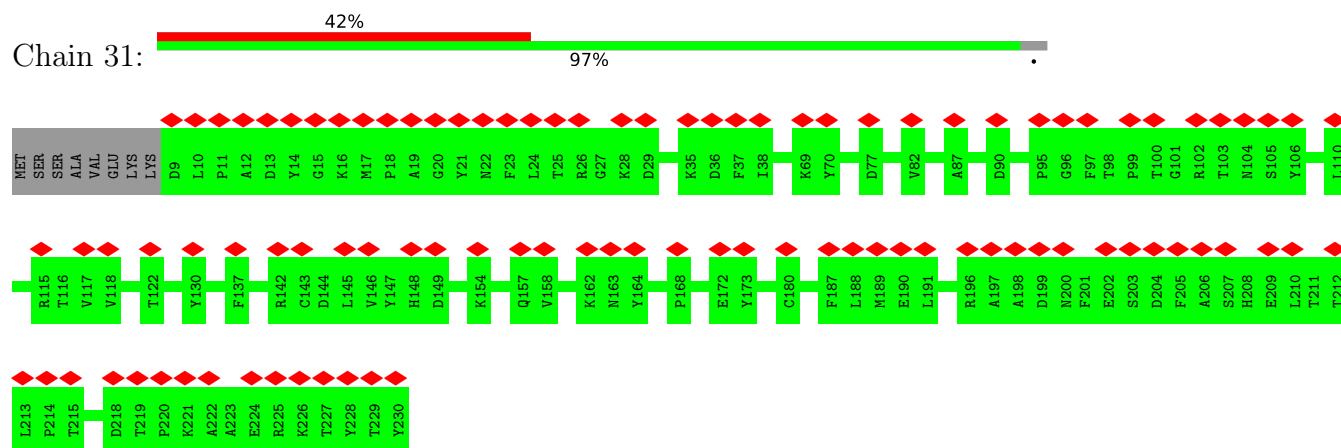
- Molecule 54: Transmembrane protein, putative



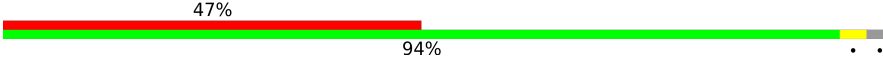
- Molecule 54: Transmembrane protein, putative

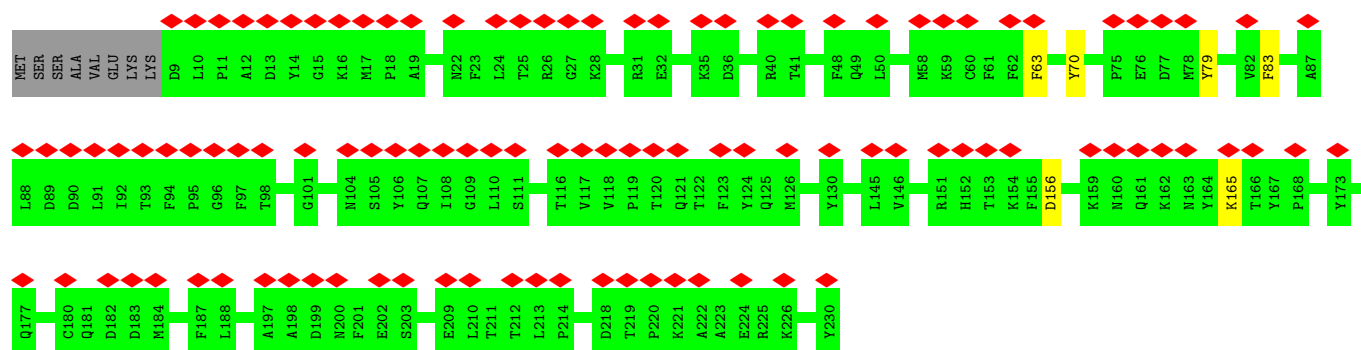


- Molecule 55: Structural protein

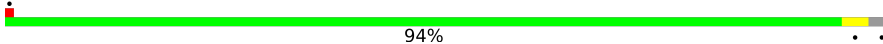


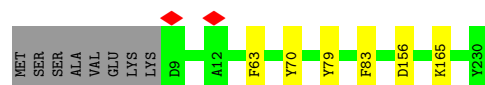
- Molecule 55: Structural protein

Chain 86: 

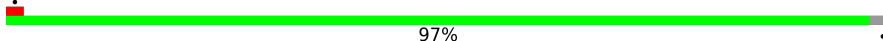


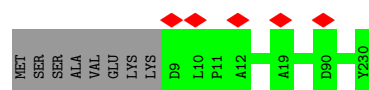
- Molecule 55: Structural protein

Chain 6b: 

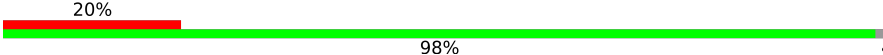


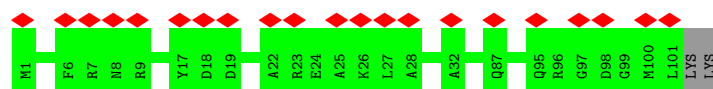
- Molecule 55: Structural protein

Chain 6B: 

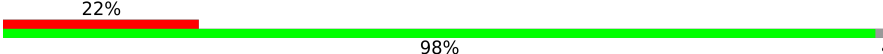


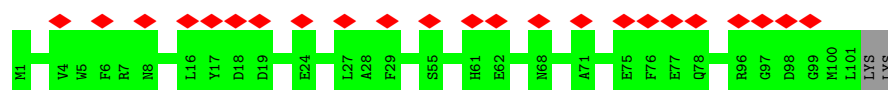
- Molecule 56: Transmembrane protein, putative

Chain 32: 

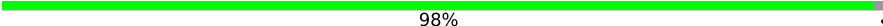


- Molecule 56: Transmembrane protein, putative

Chain 87: 

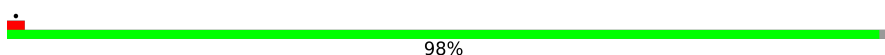


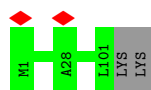
- Molecule 56: Transmembrane protein, putative

Chain 6c: 



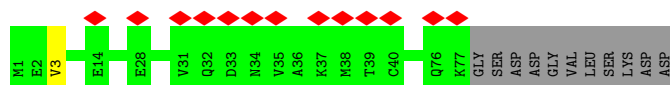
- Molecule 56: Transmembrane protein, putative

Chain 6C:  98%



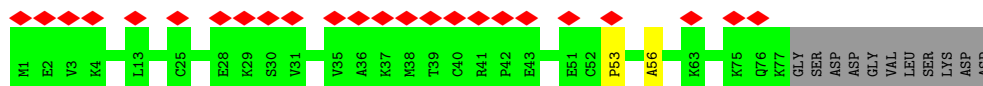
- Molecule 57: Decapping nuclease

Chain 33:  15% 86% 13%



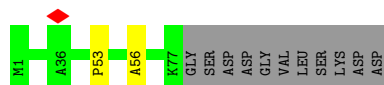
- Molecule 57: Decapping nuclease

Chain 88:  27% 85% 13%



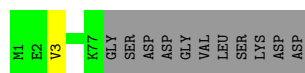
- Molecule 57: Decapping nuclease

Chain 6I:  85% 13%

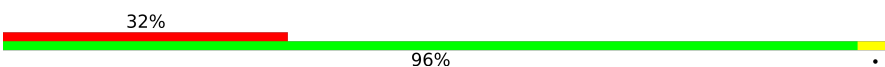


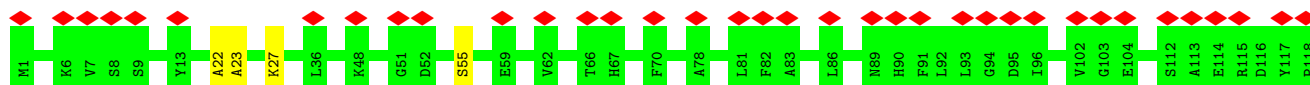
- Molecule 57: Decapping nuclease

Chain 6L:  86% 13%

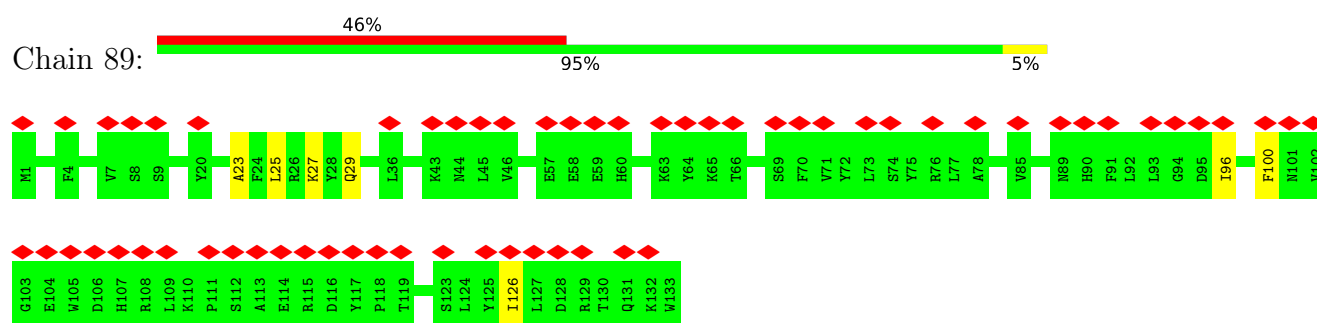


- Molecule 58: Transmembrane protein, putative

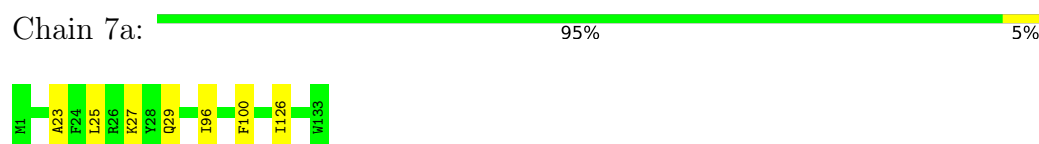
Chain 34:  32% 96% 13%



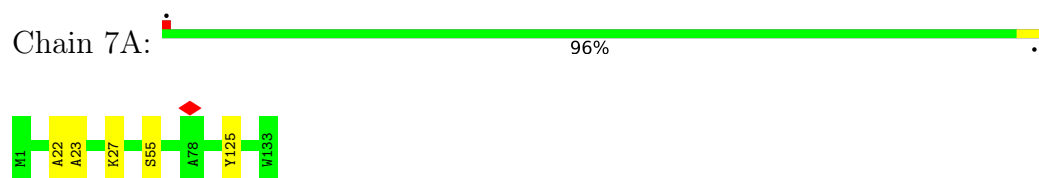
- Molecule 58: Transmembrane protein, putative



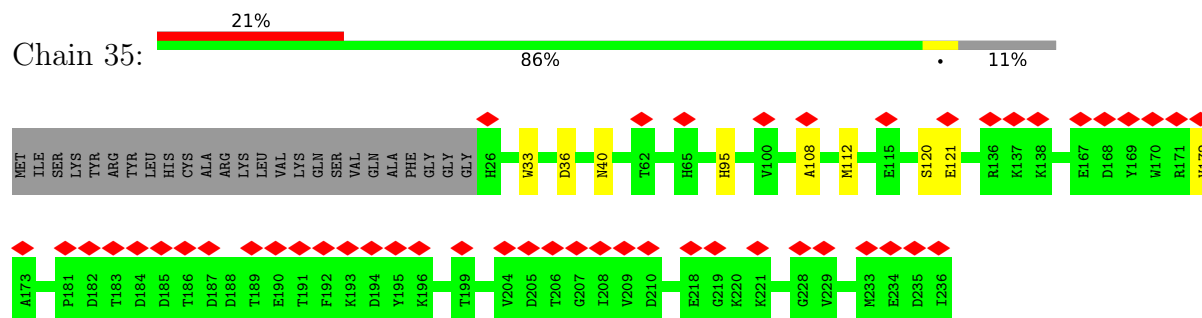
- Molecule 58: Transmembrane protein, putative



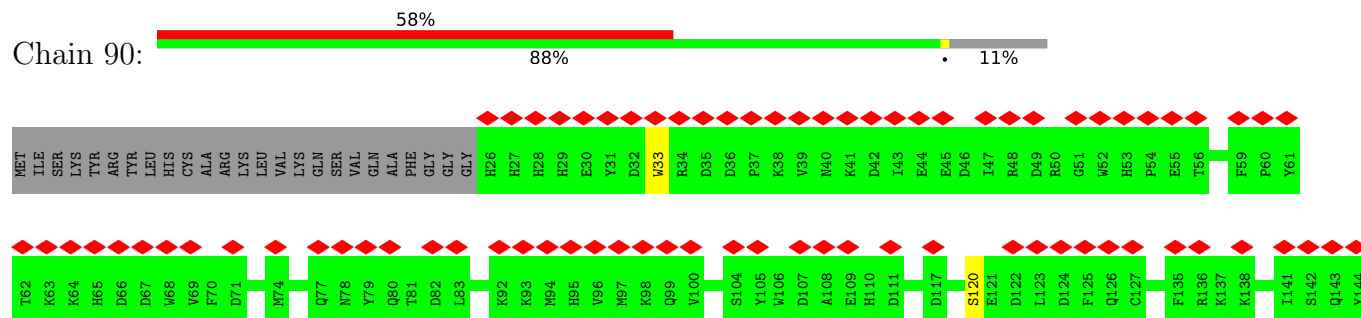
- Molecule 58: Transmembrane protein, putative

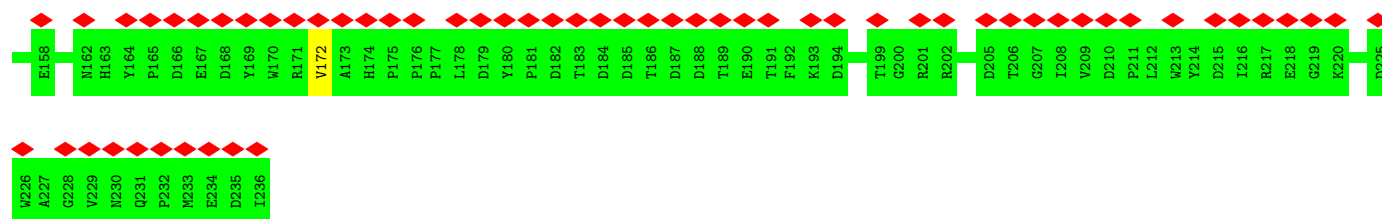


- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



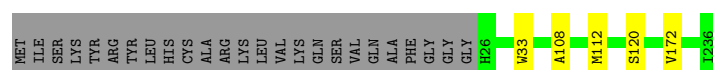
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





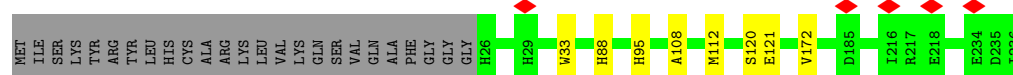
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 7c: 87% 11%



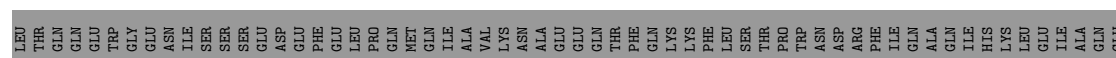
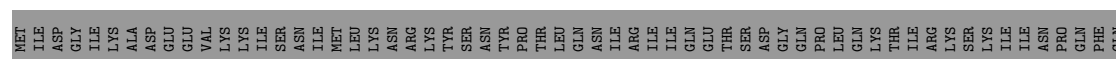
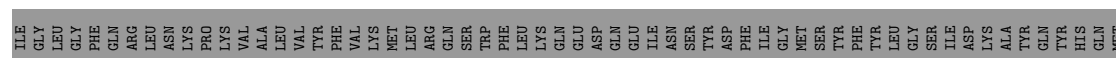
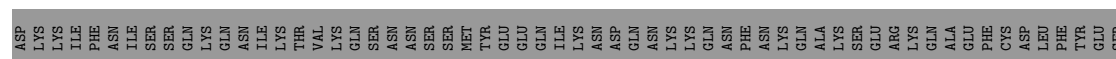
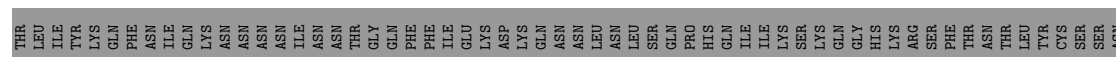
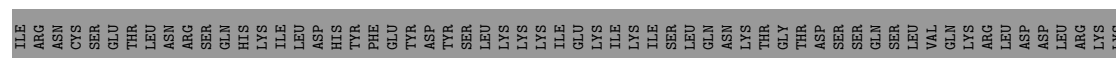
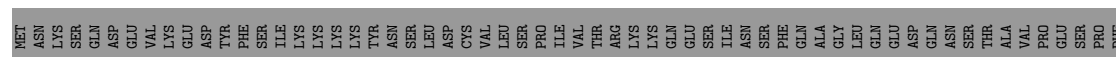
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

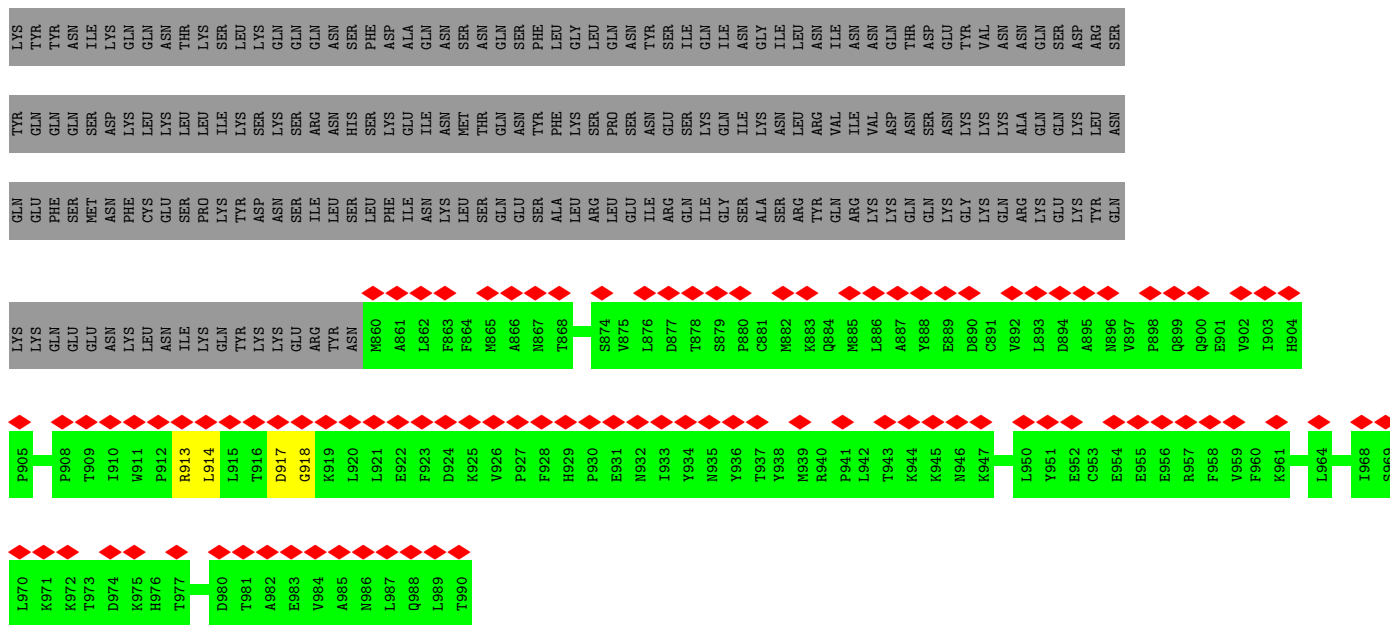
Chain 7C: 86% 11%



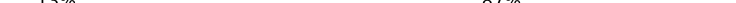
- Molecule 60: CTF/NF-I domain-containing protein

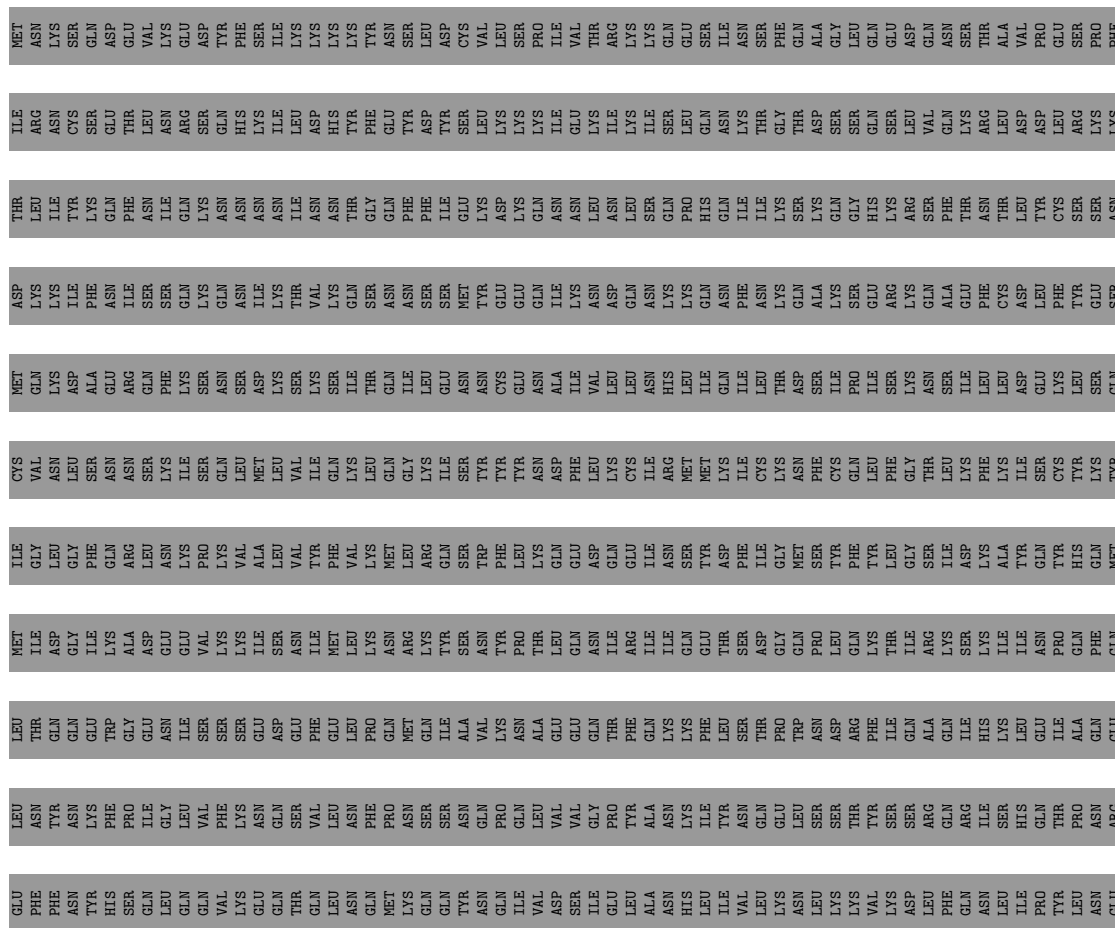
Chain 36: 5% 13% 87%

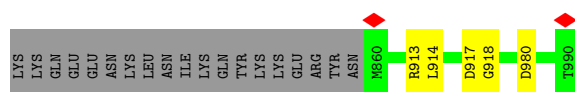




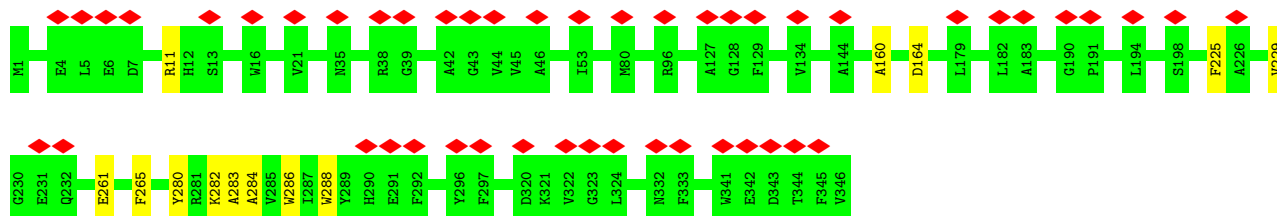
- Molecule 60: CTF/NF-I domain-containing protein

Chain 7l:  13% 87%

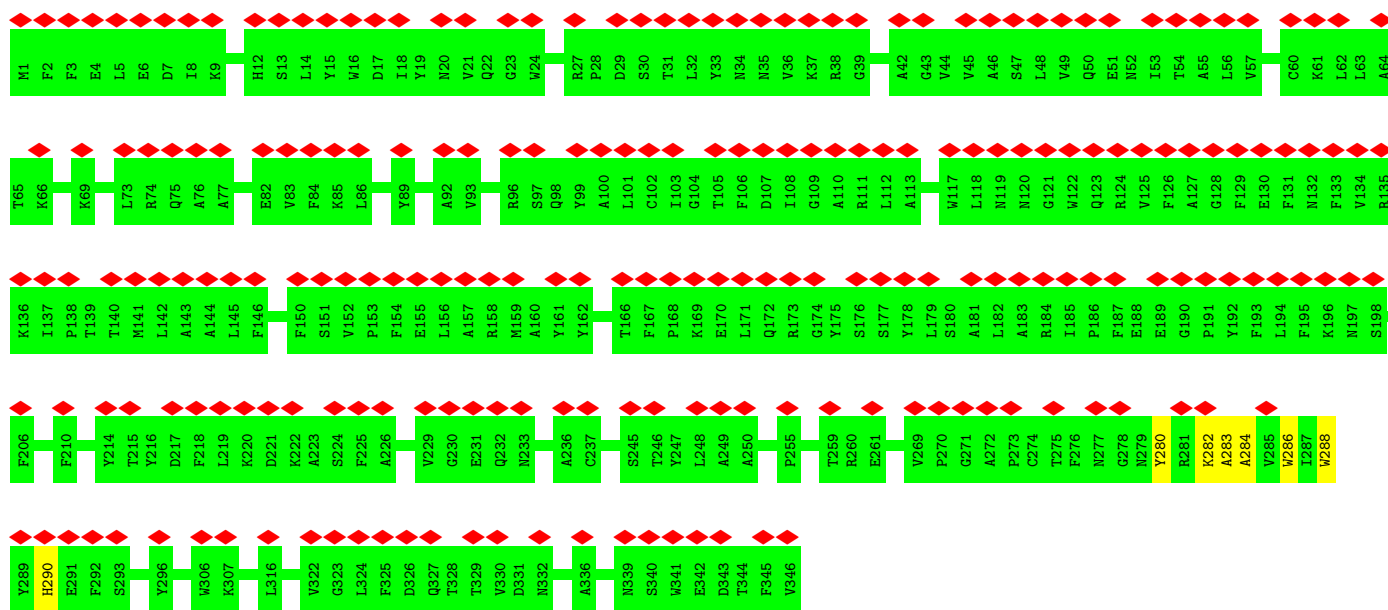




- Molecule 61: Oxoglutarate/malate translocator protein, putative



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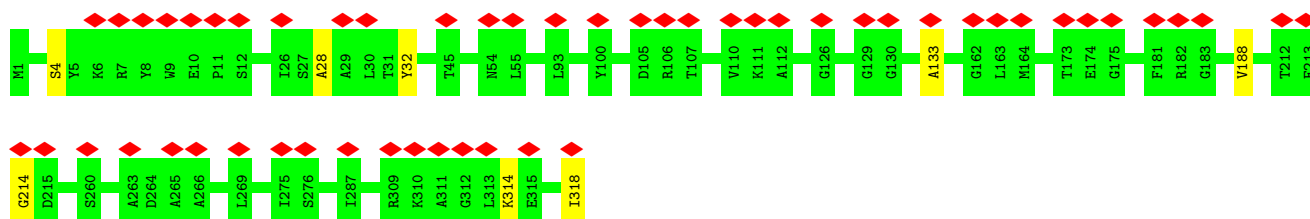


- Molecule 61: Oxoglutarate/malate translocator protein, putative

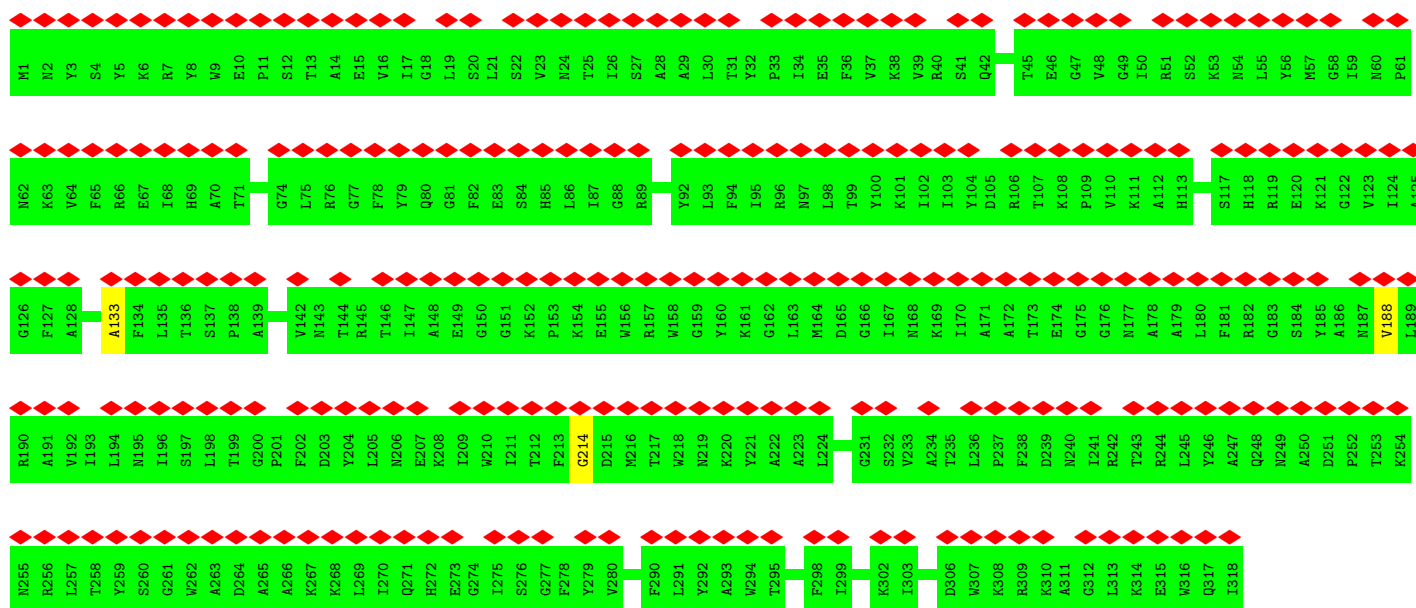
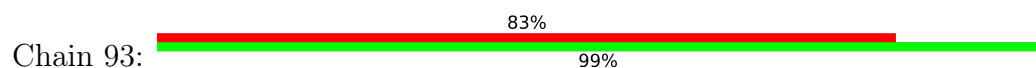




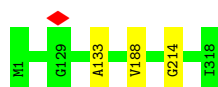
- Molecule 62: 2-oxoglutarate/malate carrier protein



- Molecule 62: 2-oxoglutarate/malate carrier protein

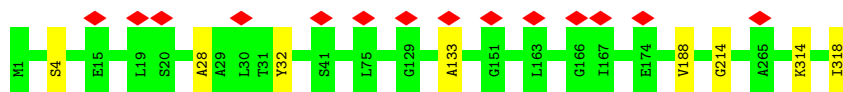


- Molecule 62: 2-oxoglutarate/malate carrier protein

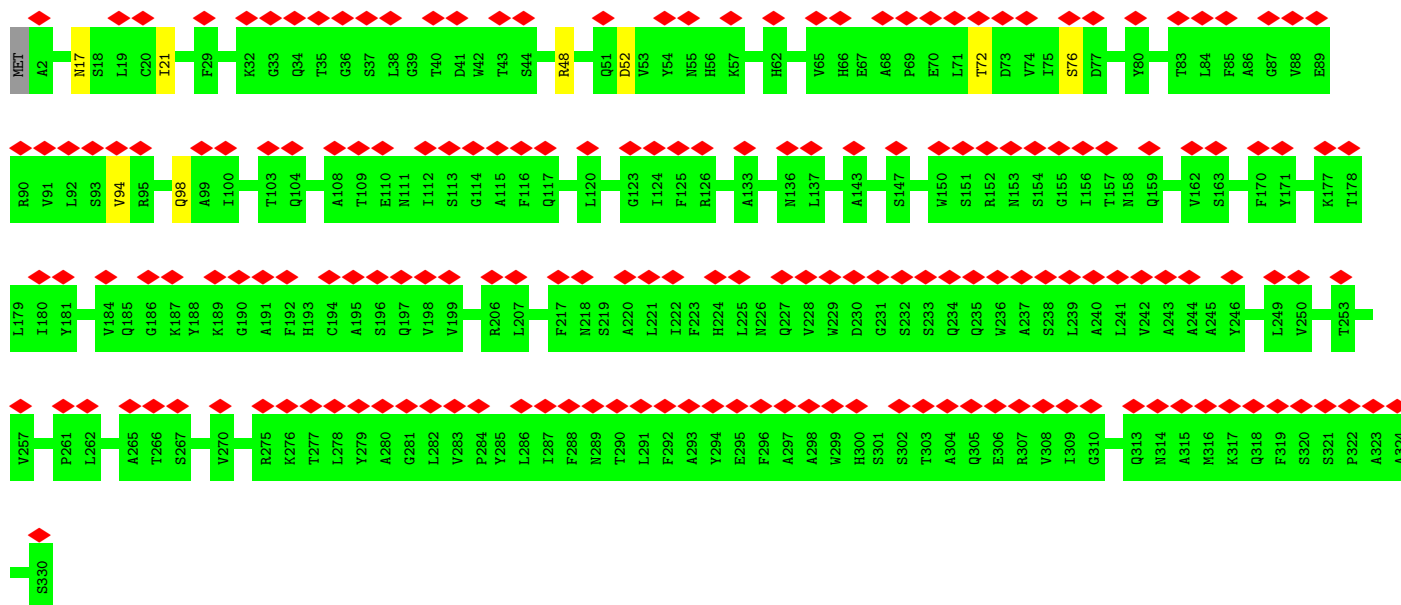


- Molecule 62: 2-oxoglutarate/malate carrier protein

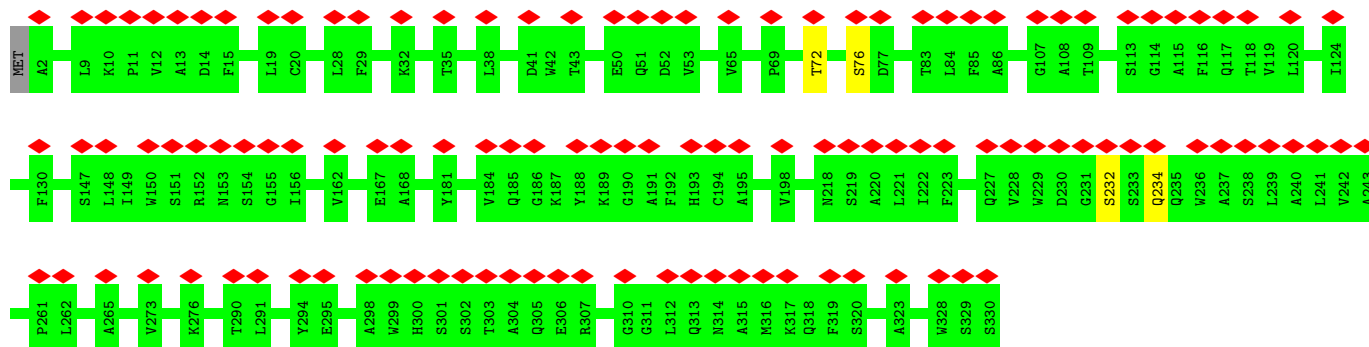




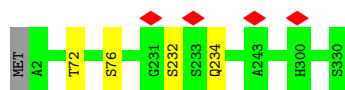
- Molecule 63: Carrier protein



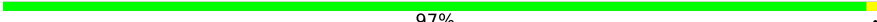
- Molecule 63: Carrier protein



- Molecule 63: Carrier protein



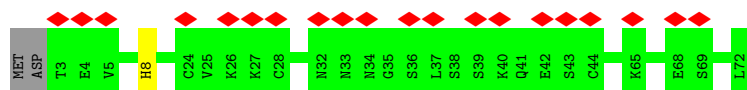
- Molecule 63: Carrier protein

Chain M3:  97%



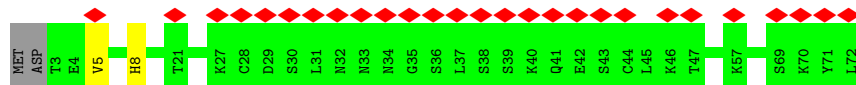
- Molecule 64: Tim10/DDP family zinc finger protein

Chain 40:  28% 96%



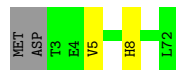
- Molecule 64: Tim10/DDP family zinc finger protein

Chain 95:  38% 94%

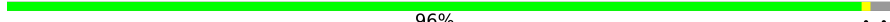


- Molecule 64: Tim10/DDP family zinc finger protein

Chain 1t:  94%



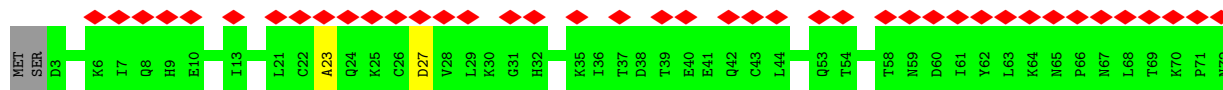
- Molecule 64: Tim10/DDP family zinc finger protein

Chain 1T:  96%



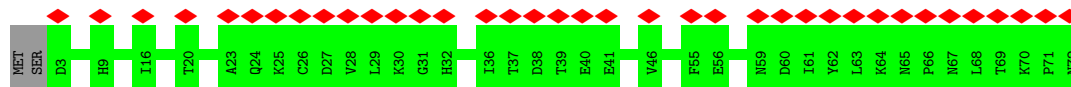
- Molecule 65: Zf-Tim10_DDP domain-containing protein

Chain 41:  57% 94%

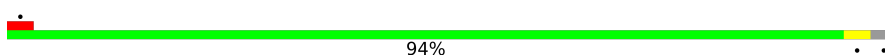


- Molecule 65: Zf-Tim10_DDP domain-containing protein

Chain 96:  51% 97%

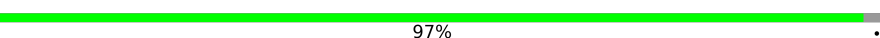


- Molecule 65: Zf-Tim10_DDP domain-containing protein

Chain 2T:  94%

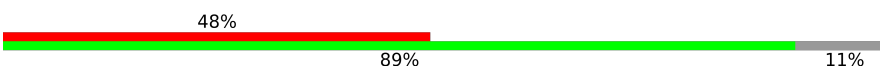


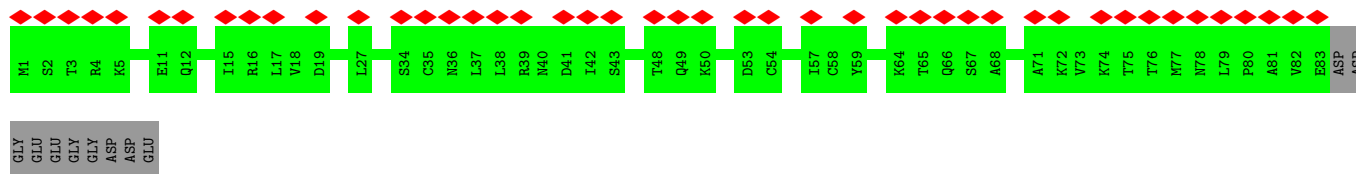
- Molecule 65: Zf-Tim10_DDP domain-containing protein

Chain 2t:  97%



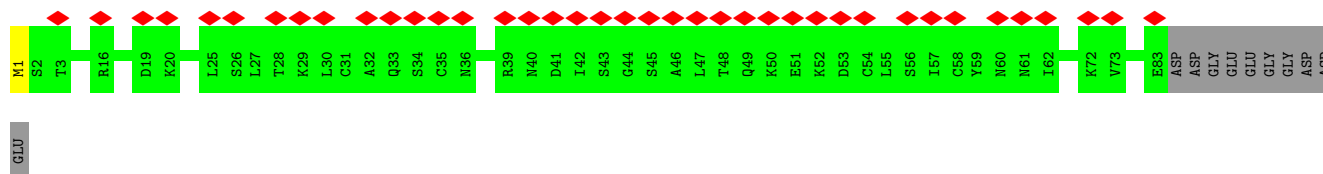
- Molecule 66: Zf-Tim10_DDP domain-containing protein

Chain 42:  48%
89% 11%



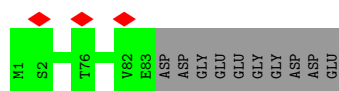
- Molecule 66: Zf-Tim10_DDP domain-containing protein

Chain 97:  42%
88% 11%



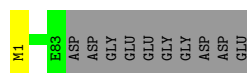
- Molecule 66: Zf-Tim10_DDP domain-containing protein

Chain 3T:  89% 11%

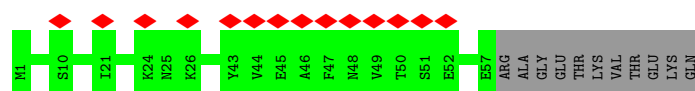
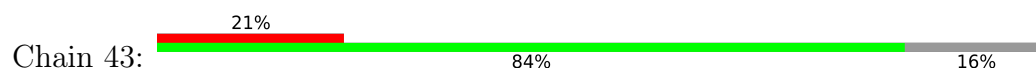


- Molecule 66: Zf-Tim10_DDP domain-containing protein

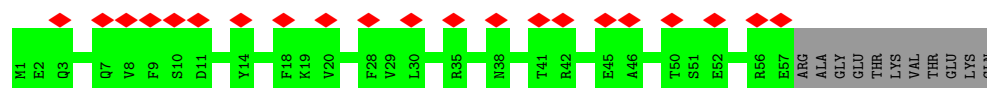
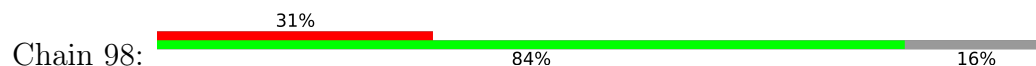
Chain 3t:  88% 11%



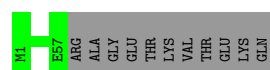
- Molecule 67: Transposase



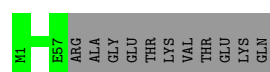
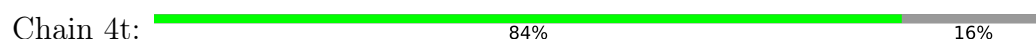
- Molecule 67: Transposase



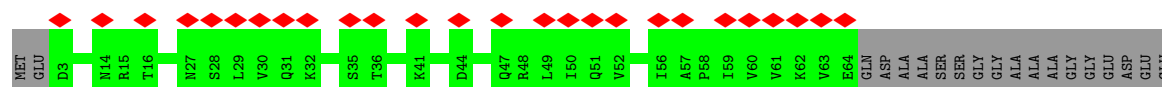
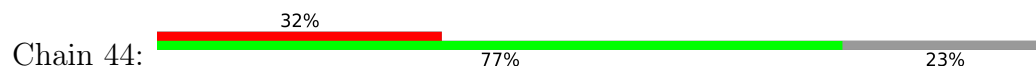
- Molecule 67: Transposase



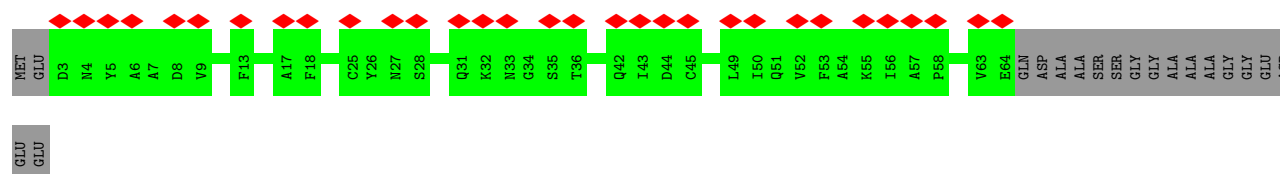
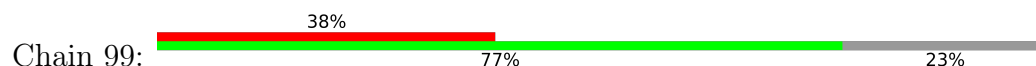
- Molecule 67: Transposase



- Molecule 68: Cullin domain-containing protein

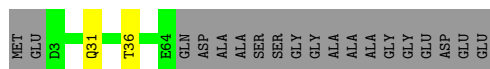


- Molecule 68: Cullin domain-containing protein



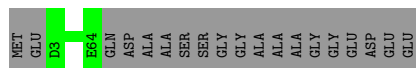
- Molecule 68: Cullin domain-containing protein





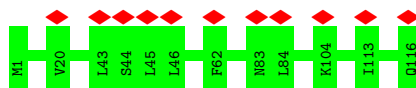
- Molecule 68: Cullin domain-containing protein

Chain 5T: 77% 23%



- Molecule 69: Ymf58

Chain 4L: 9% 100%



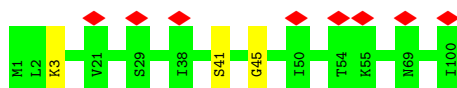
- Molecule 69: Ymf58

Chain 4L: 100%



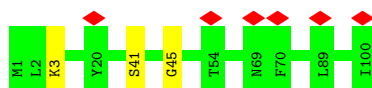
- Molecule 70: Ymf57

Chain 5b: 8% 97%



- Molecule 70: Ymf57

Chain 5B: 6% 97%



- Molecule 71: Transmembrane protein, putative

Chain a1: 26% 99%

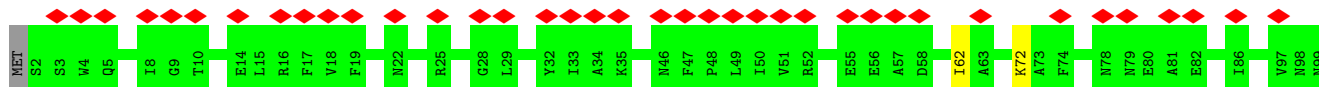


- Molecule 71: Transmembrane protein, putative

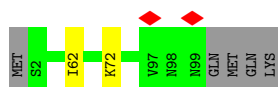
Chain A1: 99%



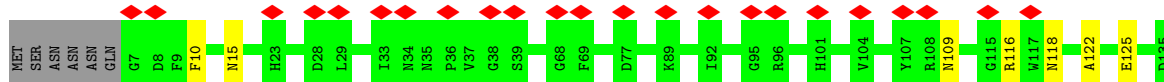
- Molecule 72: Ribosomal protein L51/S25/CI-B8 domain protein



- Molecule 72: Ribosomal protein L51/S25/CI-B8 domain protein



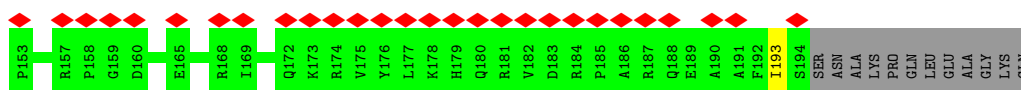
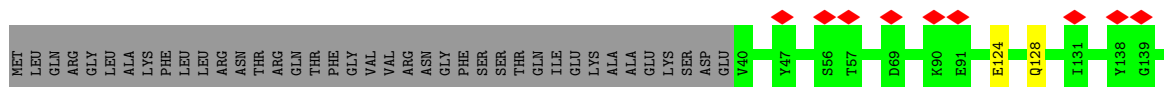
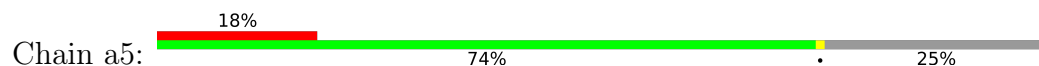
- Molecule 73: Transmembrane protein, putative



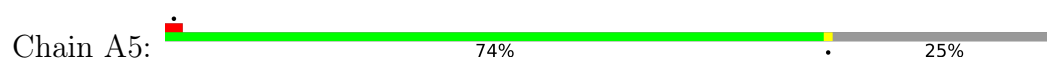
- Molecule 73: Transmembrane protein, putative

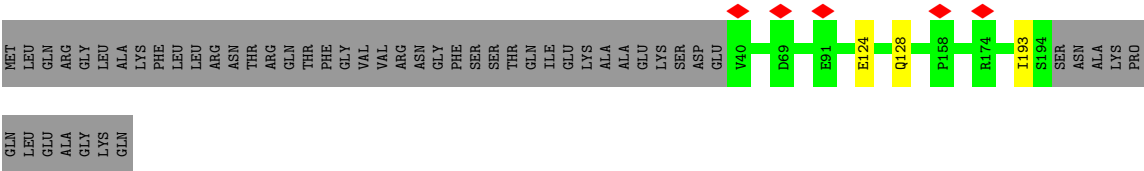


- Molecule 74: ETC complex I subunit motif protein

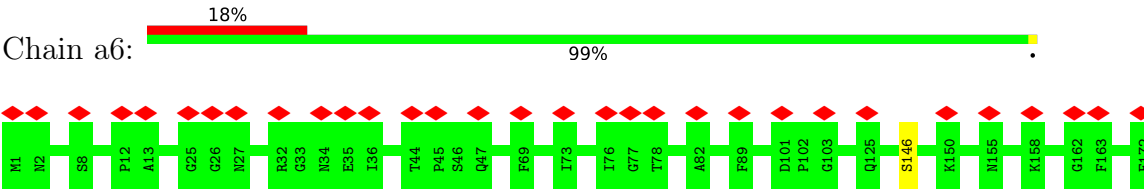


- Molecule 74: ETC complex I subunit motif protein

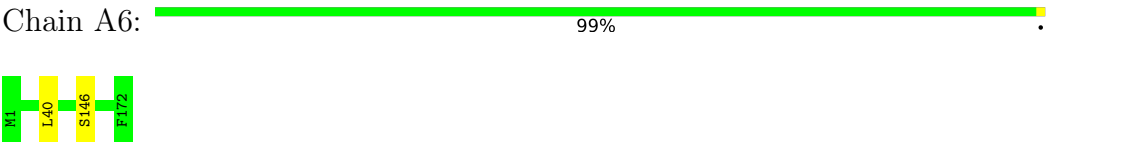




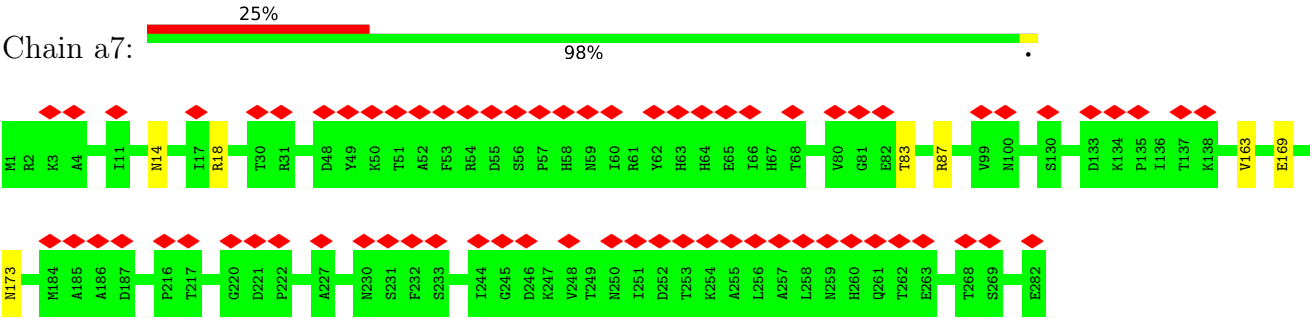
• Molecule 75: NADH dehydrogenase, putative



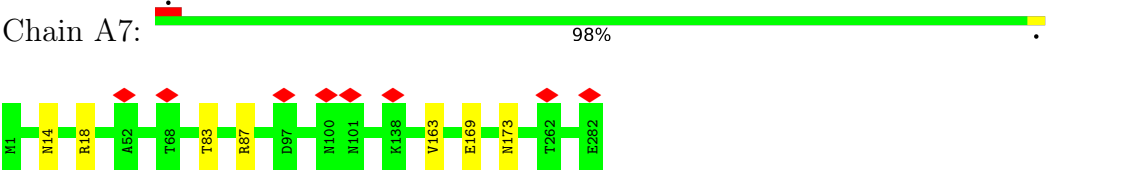
• Molecule 75: NADH dehydrogenase, putative



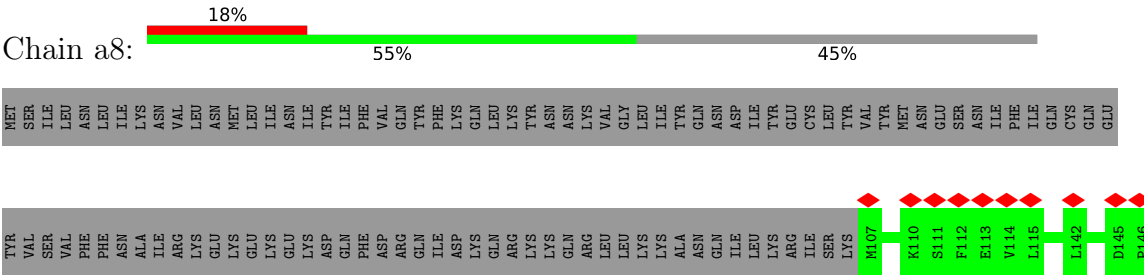
• Molecule 76: 37S ribosomal protein S25, mitochondrial

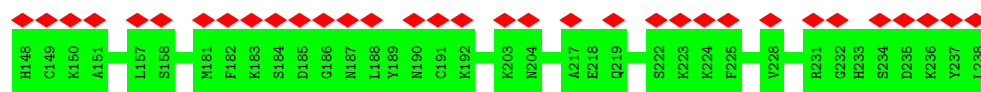


• Molecule 76: 37S ribosomal protein S25, mitochondrial



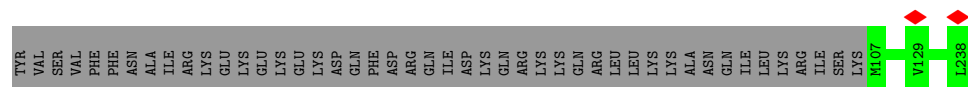
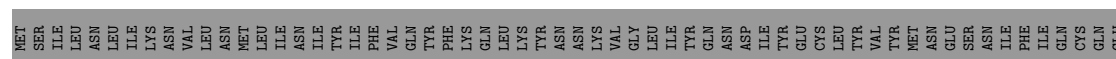
• Molecule 77: CX9C domain-containing protein





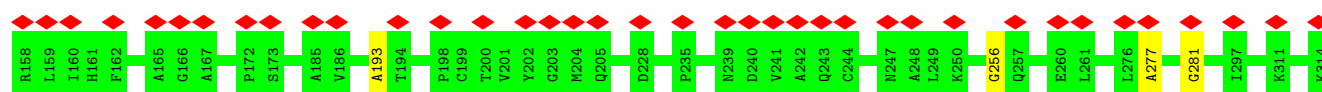
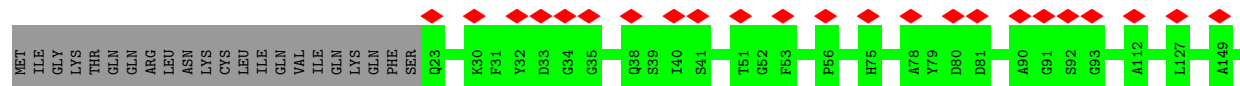
- Molecule 77: CX9C domain-containing protein

Chain A8: 55% 45%



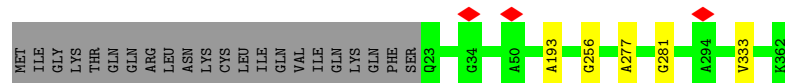
- Molecule 78: NAD-dependent epimerase/dehydratase family protein

Chain a9: 20% 93% 6%



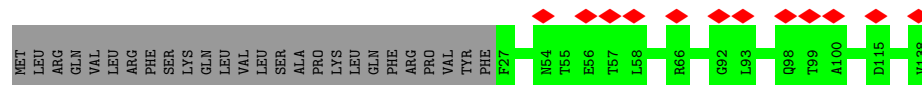
- Molecule 78: NAD-dependent epimerase/dehydratase family protein

Chain A9: 93% 6%



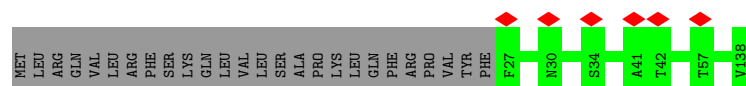
- Molecule 79: Acyl carrier protein

Chain ab: 9% 81% 19%



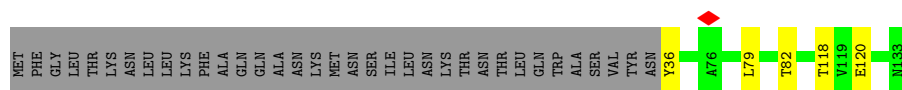
- Molecule 79: Acyl carrier protein

Chain AB: 81% 19%



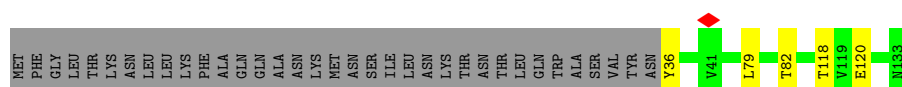
- Molecule 80: Acyl carrier protein

Chain ac:  70% 26%

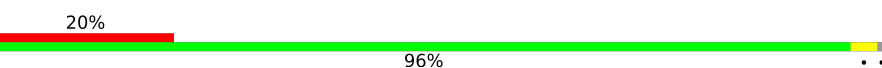


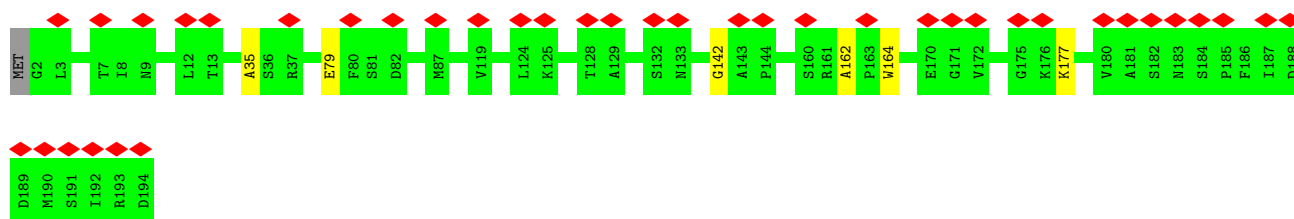
- Molecule 80: Acyl carrier protein

Chain AC:  70% 26%

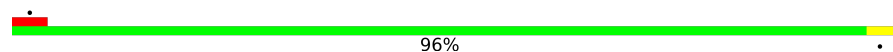


- Molecule 81: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain al:  20% 96%

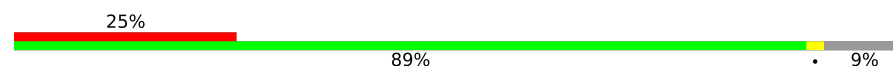


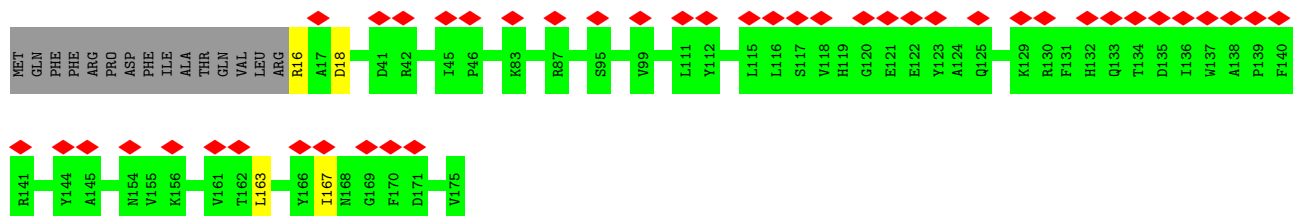
- Molecule 81: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:  96%

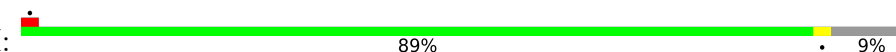


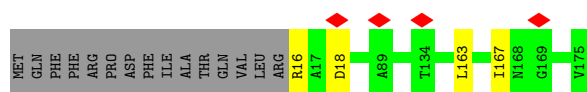
- Molecule 82: NDUA13

Chain am:  25% 89% 9%

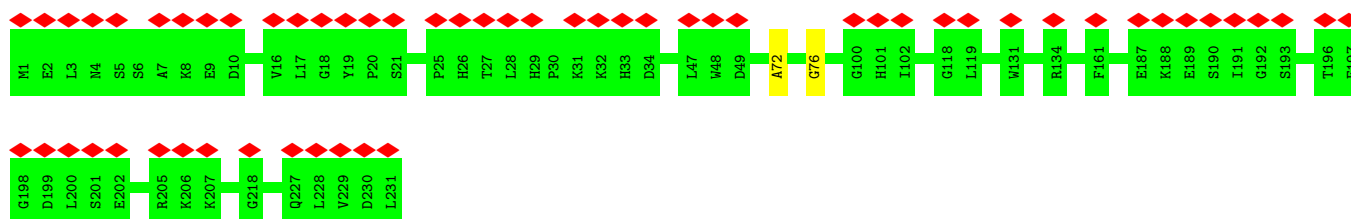


- Molecule 82: NDUA13

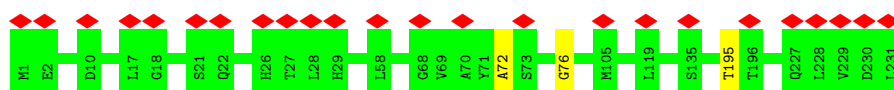
Chain AM:  89% 9%



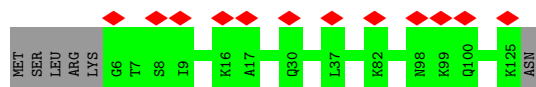
- Molecule 83: Transmembrane protein, putative



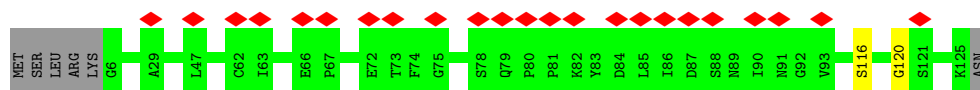
- Molecule 83: Transmembrane protein, putative



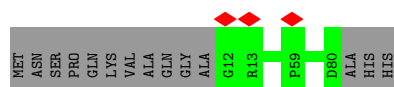
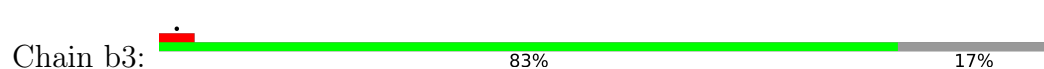
- Molecule 84: NDUB2



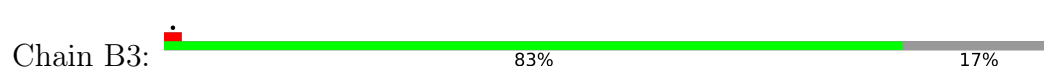
- Molecule 84: NDUB2

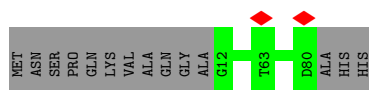


- Molecule 85: Transmembrane protein, putative

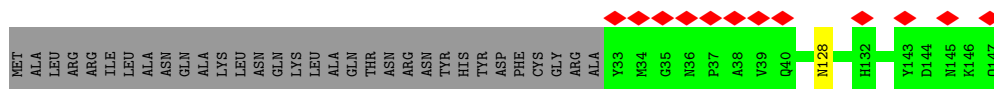
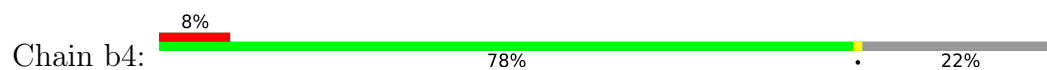


- Molecule 85: Transmembrane protein, putative

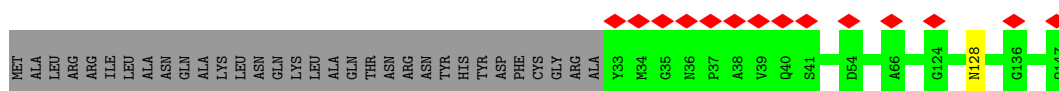
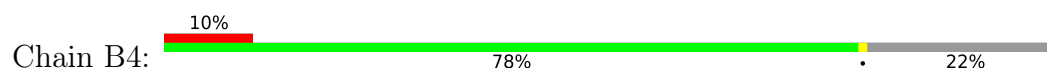




- Molecule 86: NDUB4



- Molecule 86: NDUB4



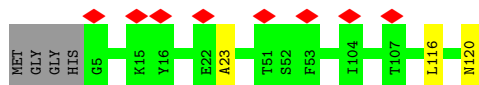
- Molecule 87: NDUB6



- Molecule 87: NDUB6

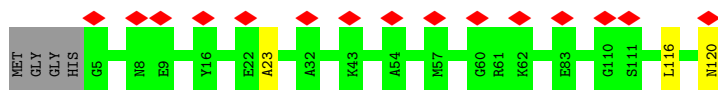


- Molecule 88: CHCH domain-containing protein

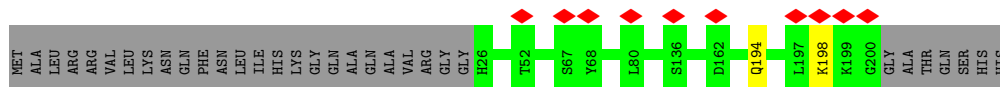
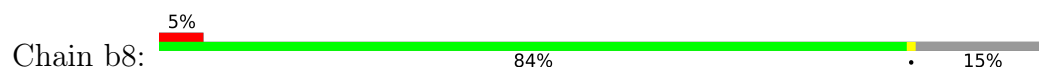


- Molecule 88: CHCH domain-containing protein

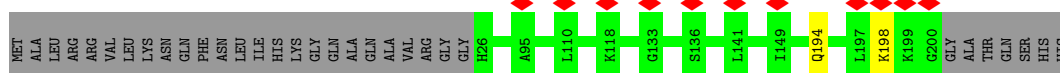
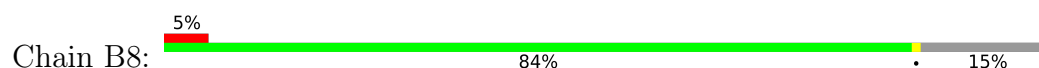




- Molecule 89: NDUB8



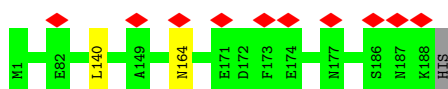
- Molecule 89: NDUB8



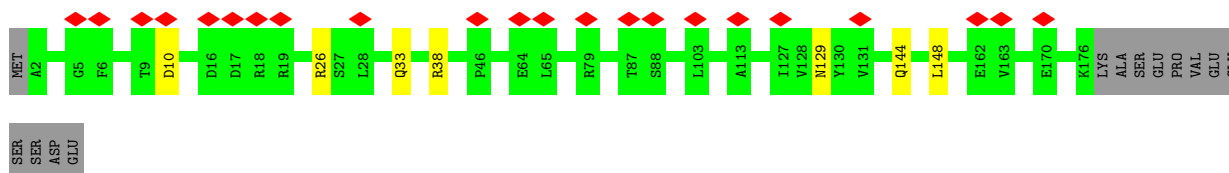
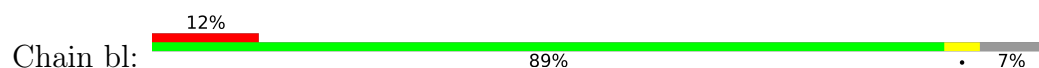
- Molecule 90: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 90: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



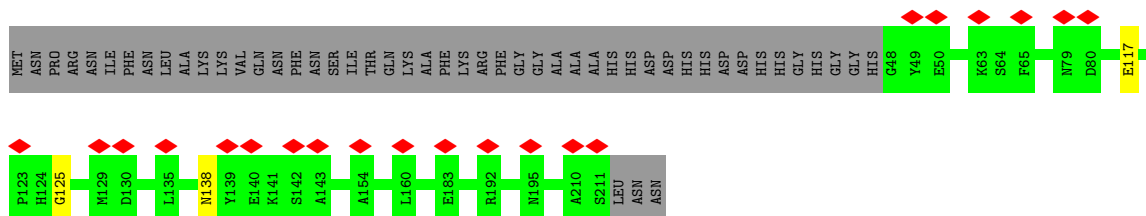
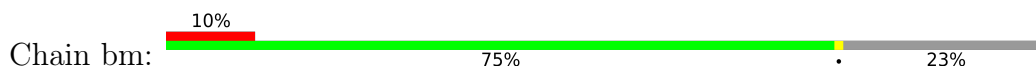
- Molecule 91: NDUB10



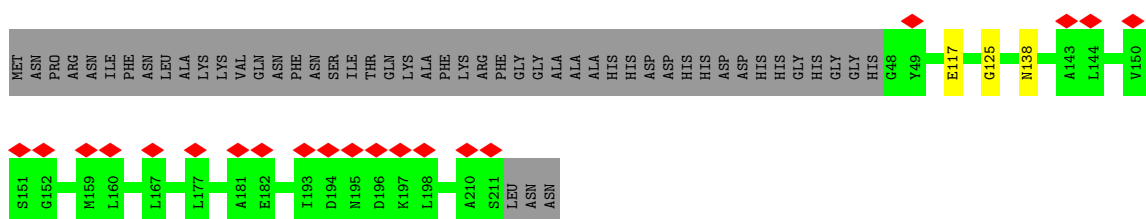
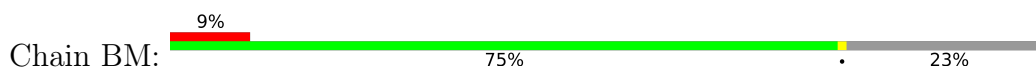
- Molecule 91: NDUB10



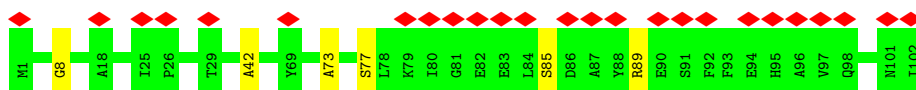
- Molecule 92: Transmembrane protein, putative



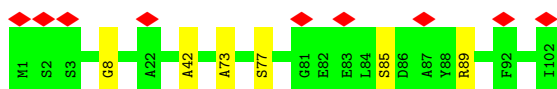
- Molecule 92: Transmembrane protein, putative



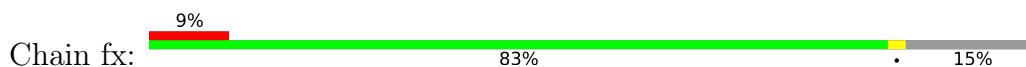
- Molecule 93: Complex I-MNLL



- Molecule 93: Complex I-MNLL



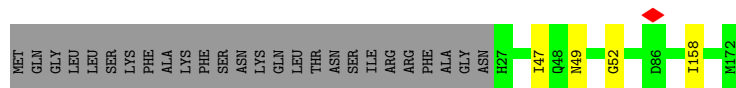
- Molecule 94: 2 iron, 2 sulfur cluster-binding protein





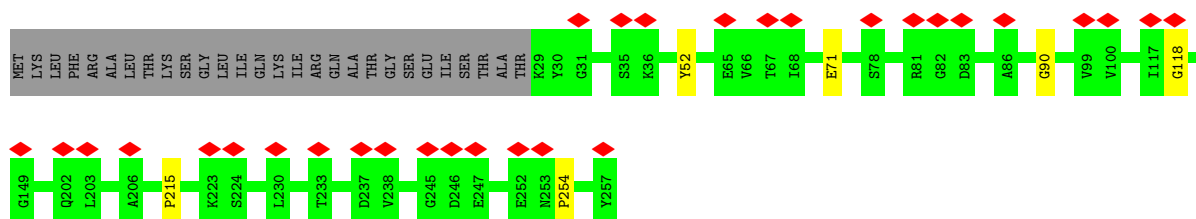
- Molecule 94: 2 iron, 2 sulfur cluster-binding protein

Chain FX: 83% 15%



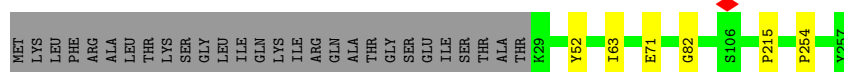
- Molecule 95: Gamma-carbonic anhydrase

Chain g1: 12% 87% 11%



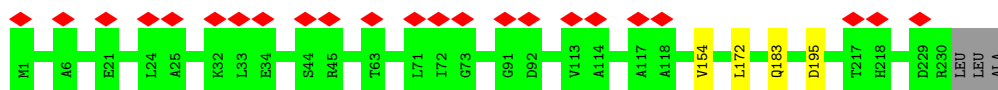
- Molecule 95: Gamma-carbonic anhydrase

Chain G1: 87% 11%



- Molecule 96: Gamma-carbonic anhydrase

Chain g2: 10% 97% ..



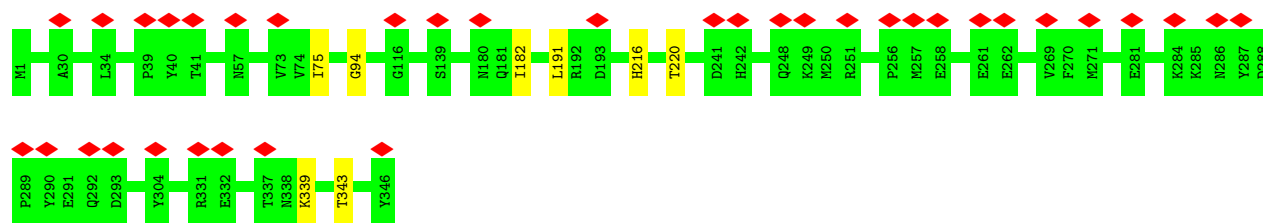
- Molecule 96: Gamma-carbonic anhydrase

Chain G2: 97% ..



- Molecule 97: Transcription factor apf protein, putative

Chain g3: 10% 98% .



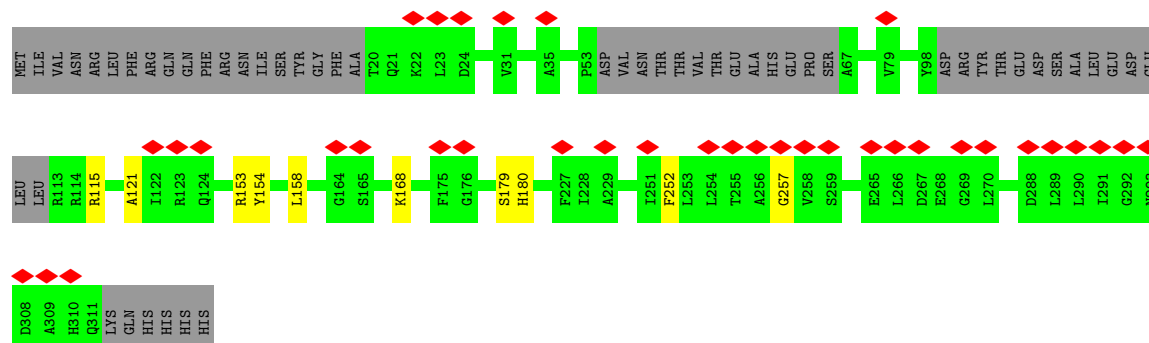
- Molecule 97: Transcription factor apfi protein, putative

Chain G3: 98%



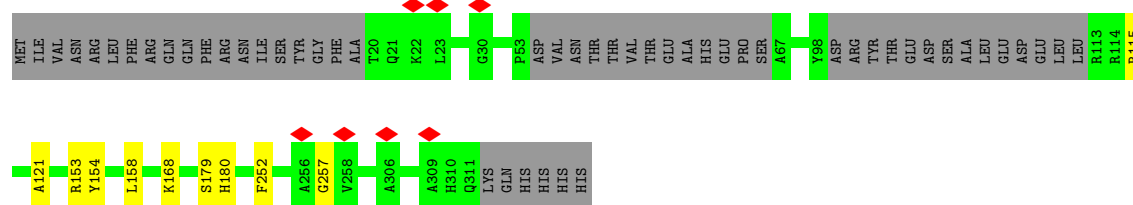
- Molecule 98: DnaJ domain protein

Chain j1: 13% 80% 16%



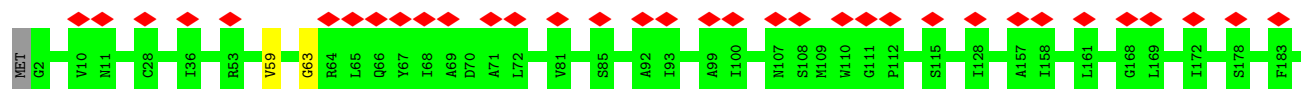
- Molecule 98: DnaJ domain protein

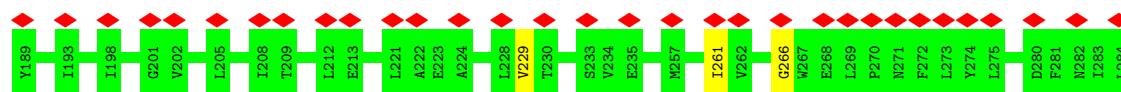
Chain J1: 80% 16%



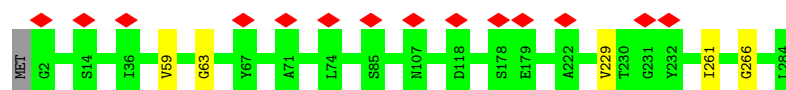
- Molecule 99: NADH-ubiquinone oxidoreductase chain 1

Chain n1: 23% 98%

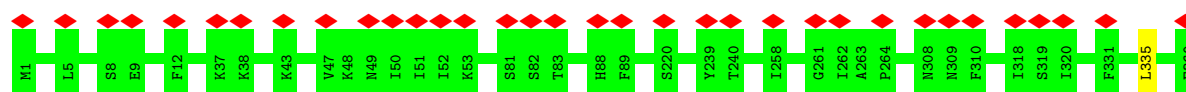




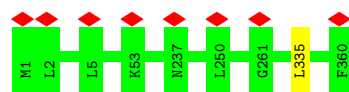
- Molecule 99: NADH-ubiquinone oxidoreductase chain 1



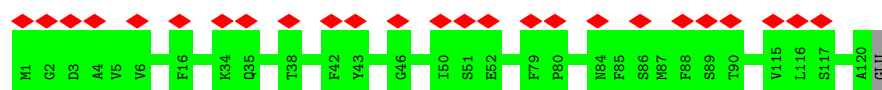
- Molecule 100: Ymf65



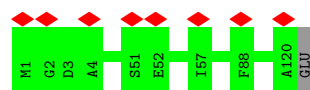
- Molecule 100: Ymf65



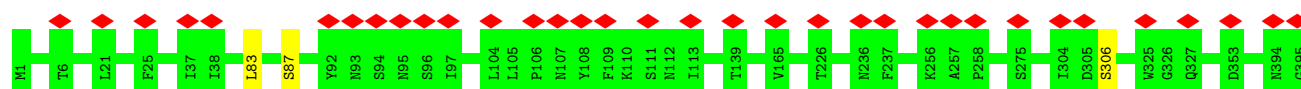
- Molecule 101: NADH-ubiquinone oxidoreductase chain 3

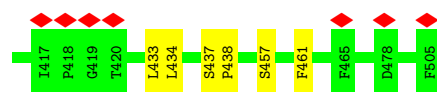


- Molecule 101: NADH-ubiquinone oxidoreductase chain 3

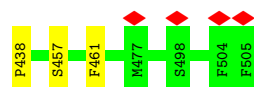
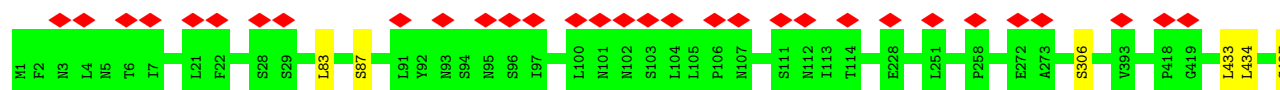


- Molecule 102: NADH-ubiquinone oxidoreductase chain 4

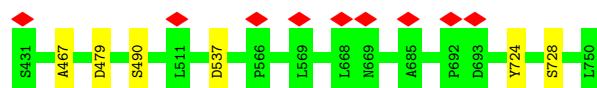
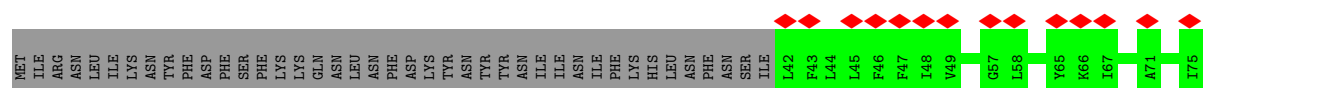
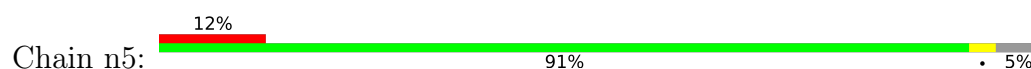




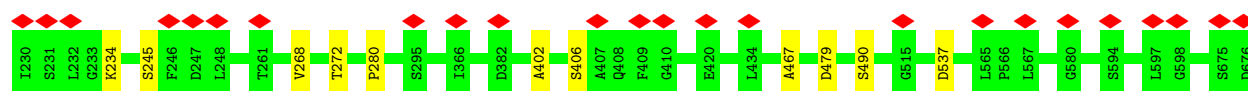
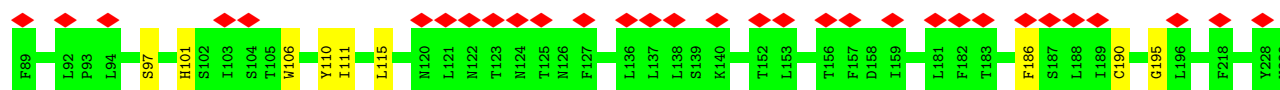
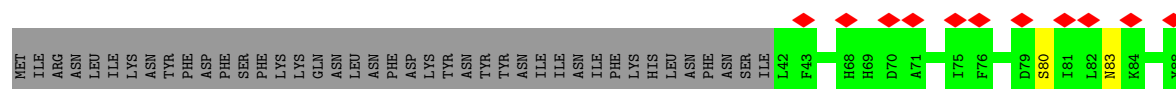
- Molecule 102: NADH-ubiquinone oxidoreductase chain 4



- Molecule 103: NADH dehydrogenase subunit 5

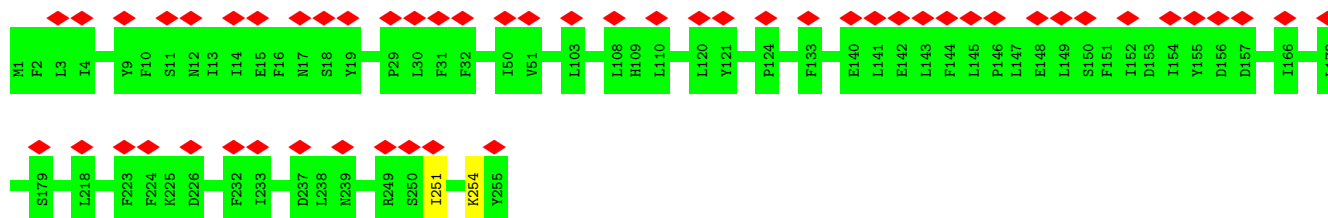


- Molecule 103: NADH dehydrogenase subunit 5

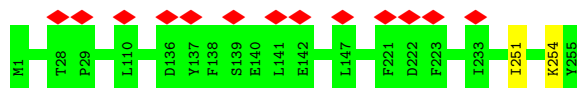




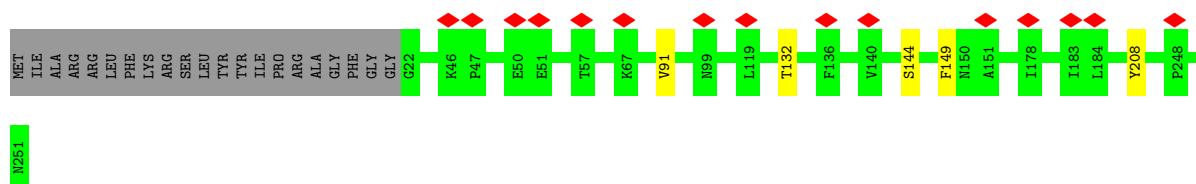
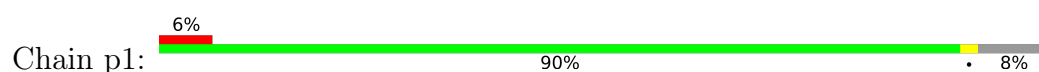
- Molecule 104: Ymf62



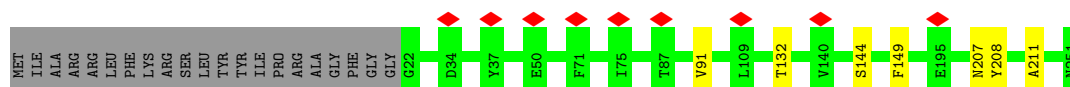
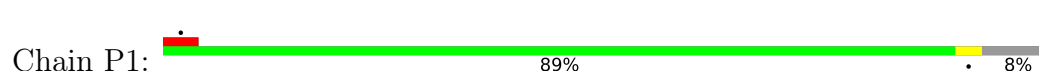
- Molecule 104: Ymf62



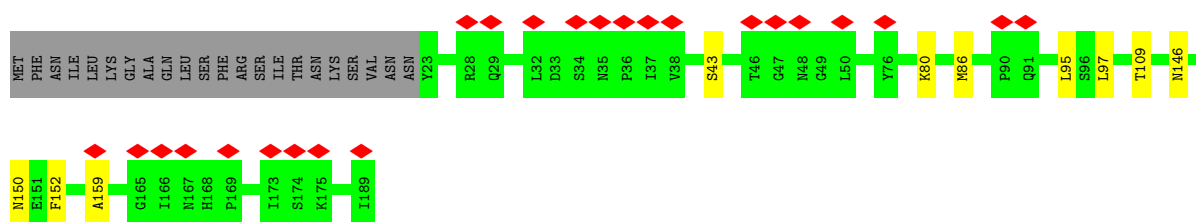
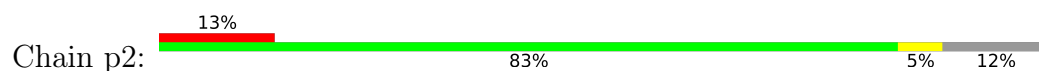
- Molecule 105: Transmembrane protein, putative



- Molecule 105: Transmembrane protein, putative

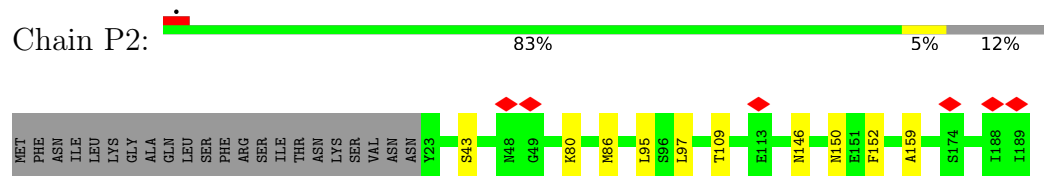


- Molecule 106: NDUPH2



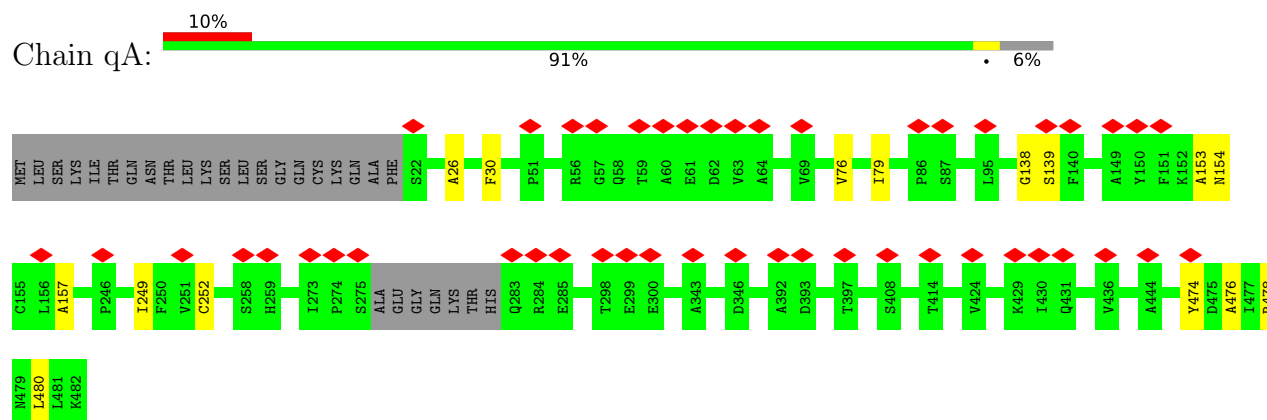
- Molecule 106: NDUPH2

Chain P2:



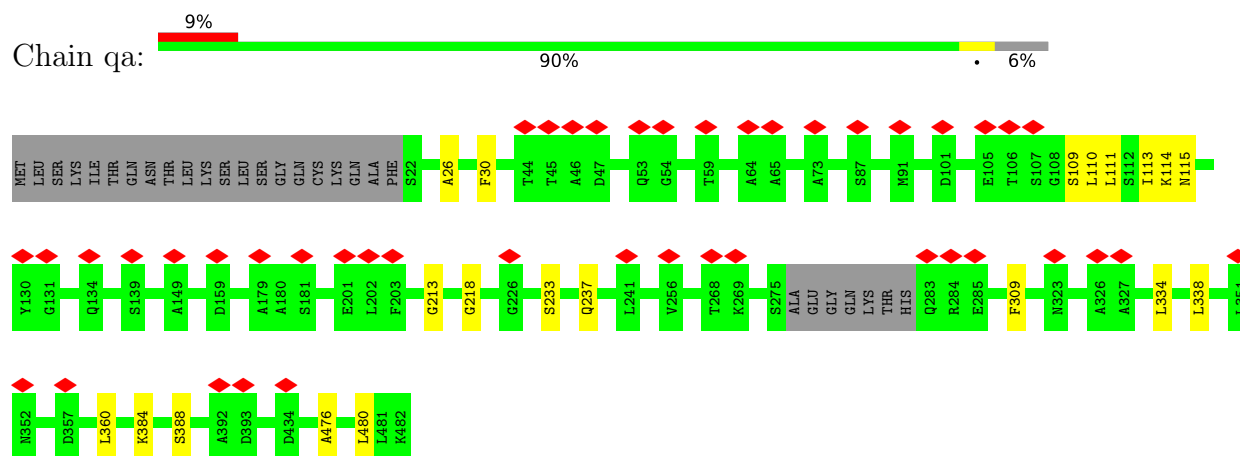
- Molecule 107: M16 family peptidase, putative

Chain qA:



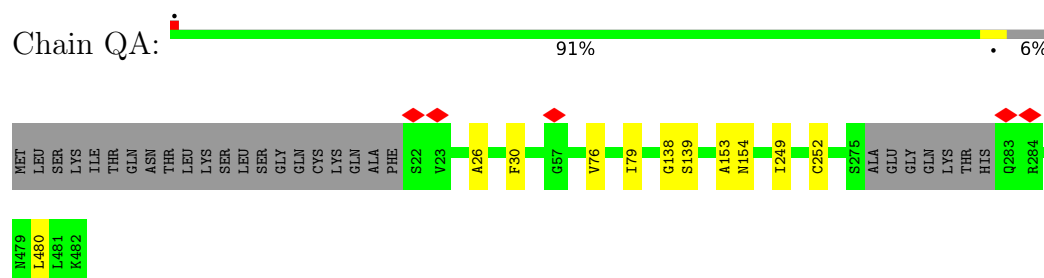
- Molecule 107: M16 family peptidase, putative

Chain qa:



- Molecule 107: M16 family peptidase, putative

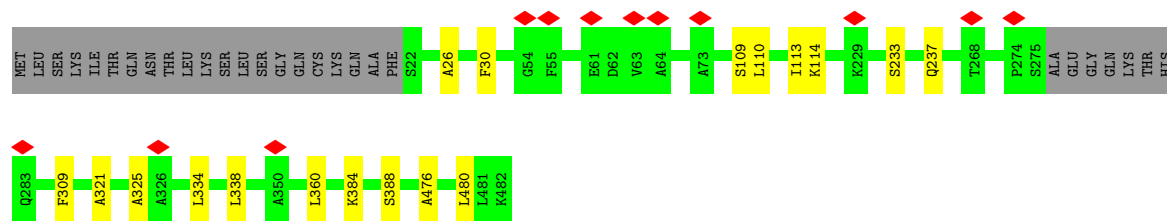
Chain QA:



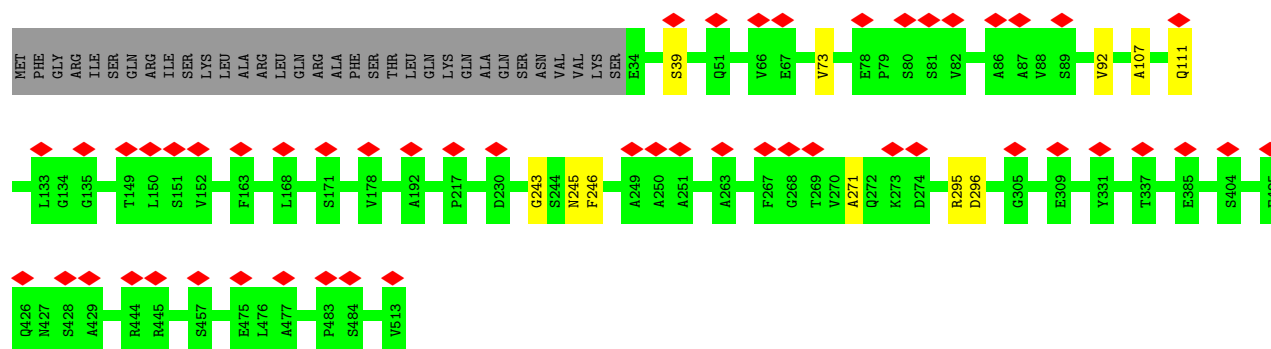
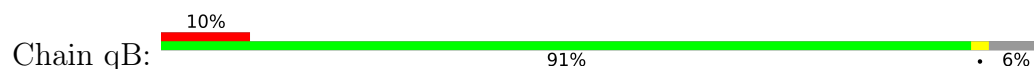
- Molecule 107: M16 family peptidase, putative

Chain Qa:

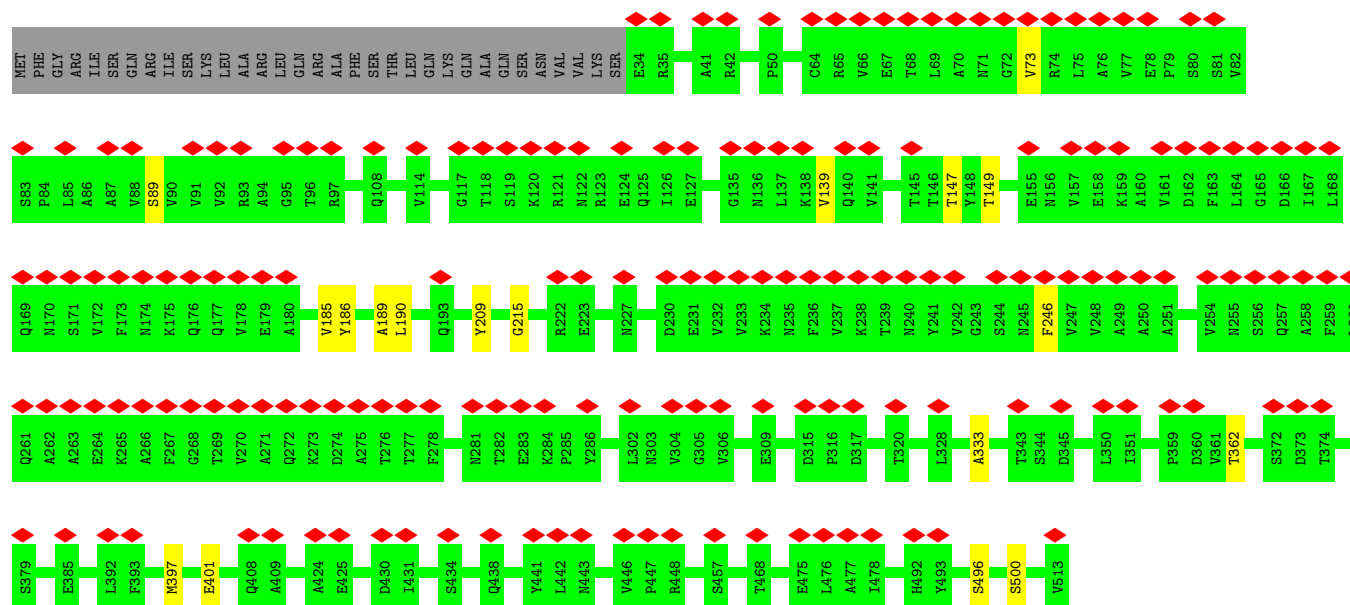
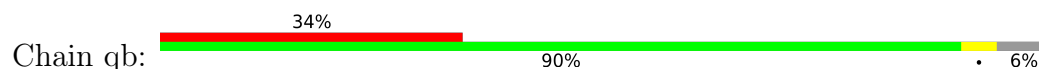




- Molecule 108: Peptidase M16 inactive domain protein



- Molecule 108: Peptidase M16 inactive domain protein



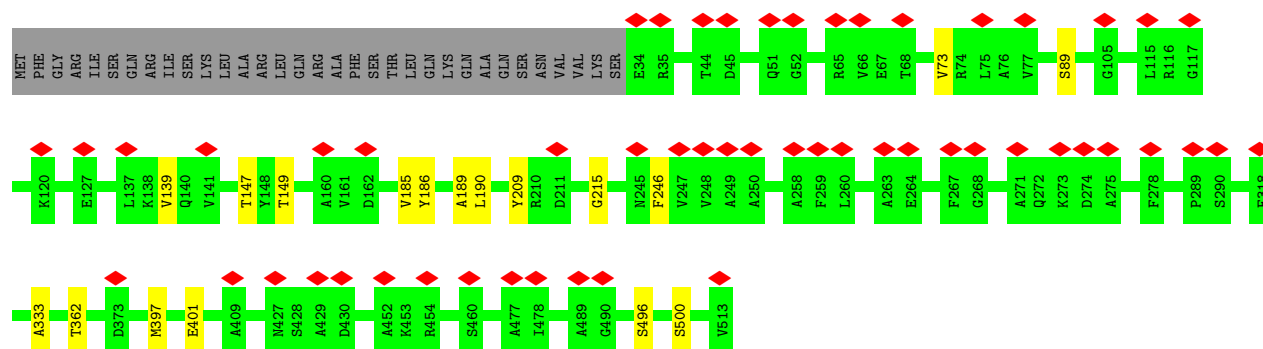
- Molecule 108: Peptidase M16 inactive domain protein





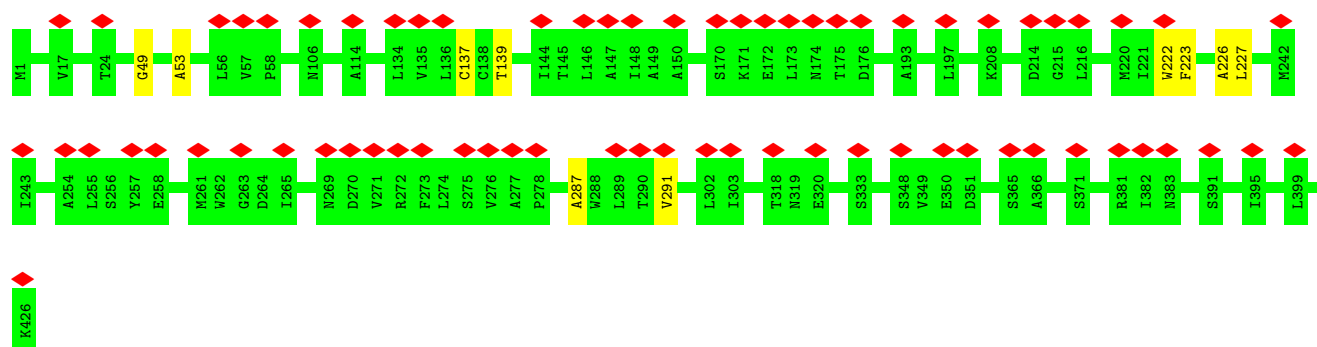
- Molecule 108: Peptidase M16 inactive domain protein

Chain Qb: 11% 90% 6%



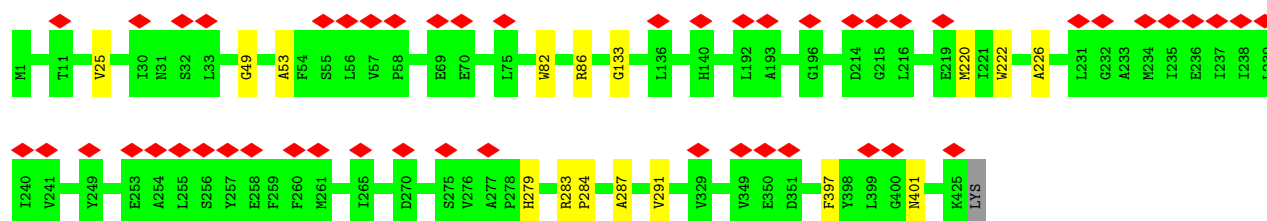
- Molecule 109: Apocytochrome b

Chain qC: 16% 98%

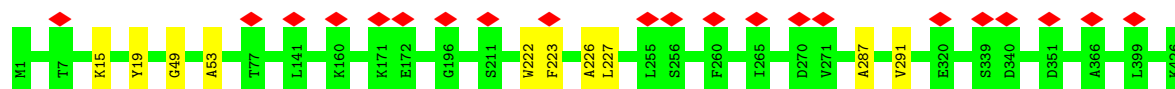


- Molecule 109: Apocytochrome b

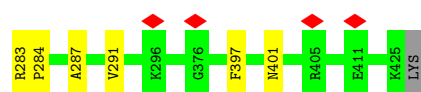
Chain qc: 12% 96%



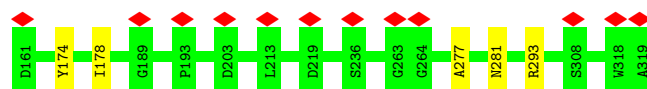
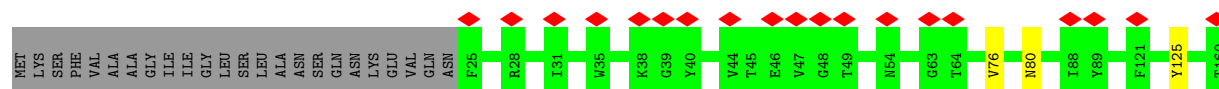
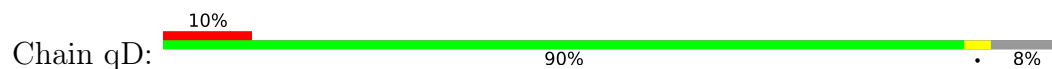
- Molecule 109: Apocytochrome b



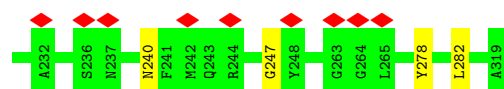
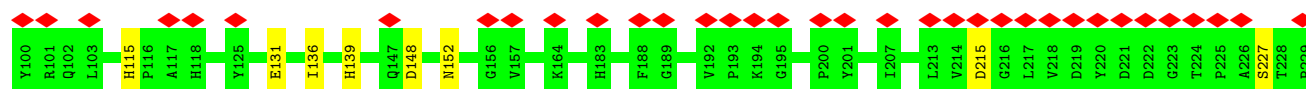
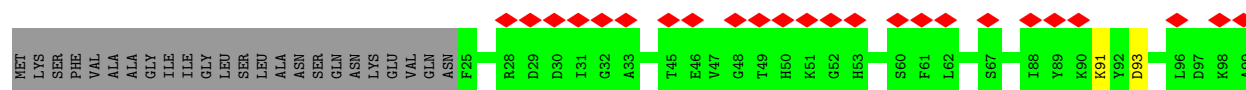
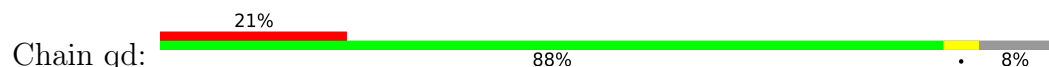
• Molecule 109: Apocytochrome b



• Molecule 110: Cytochrome protein c1

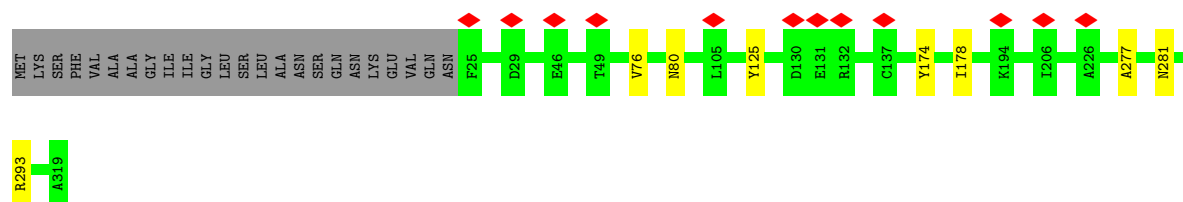


• Molecule 110: Cytochrome protein c1

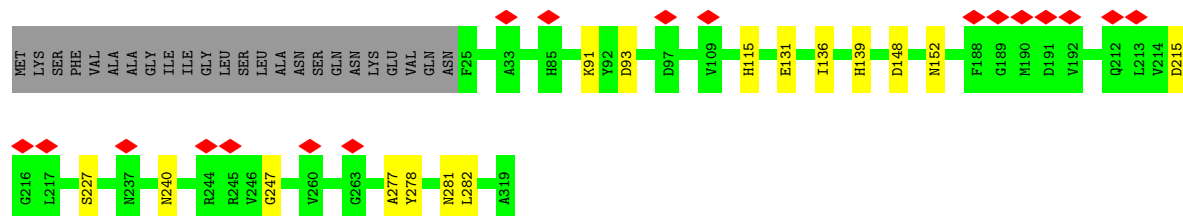
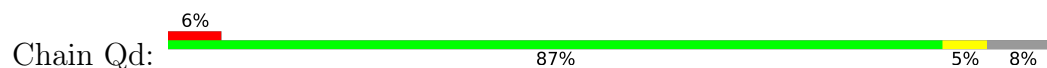


• Molecule 110: Cytochrome protein c1

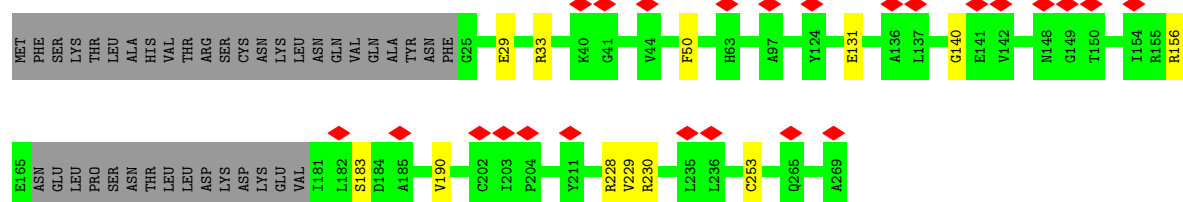
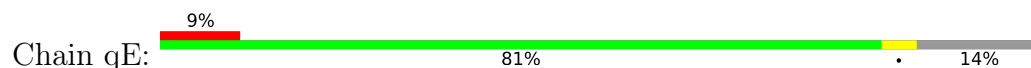




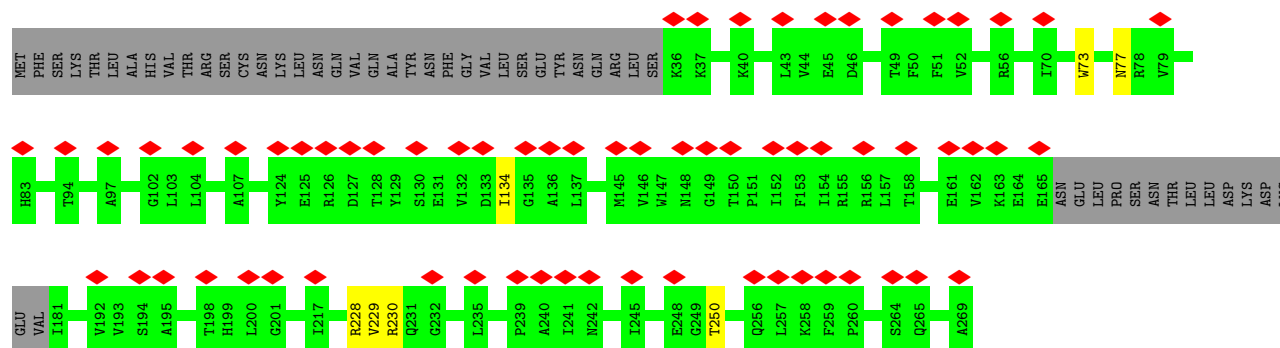
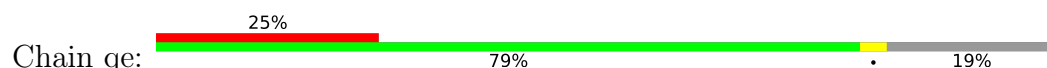
- Molecule 110: Cytochrome protein c1



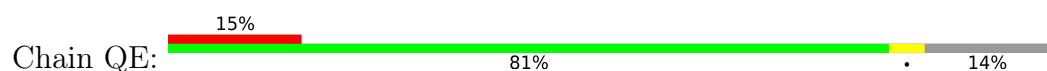
- Molecule 111: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

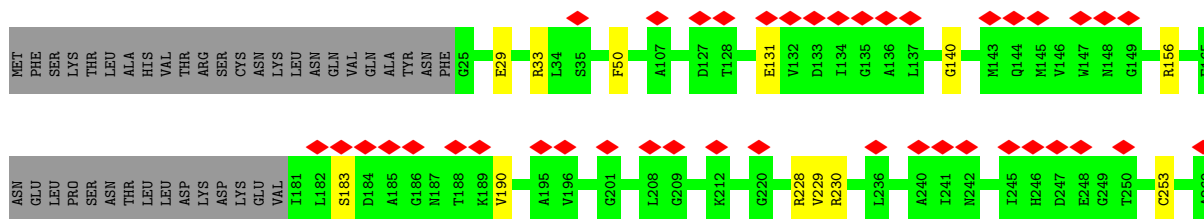


- Molecule 111: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

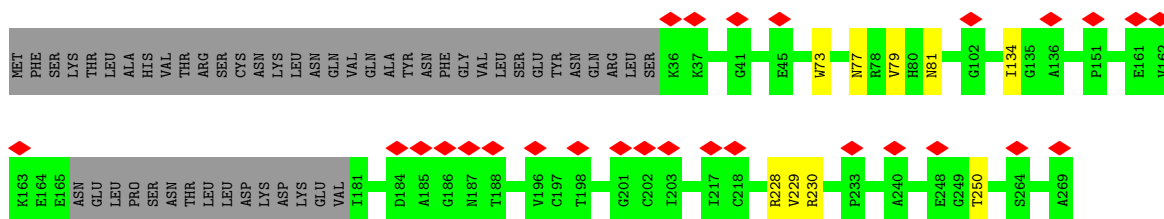
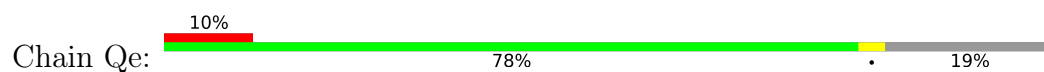


- Molecule 111: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

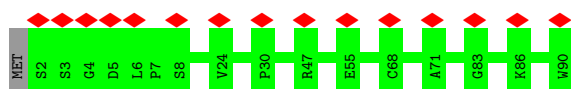




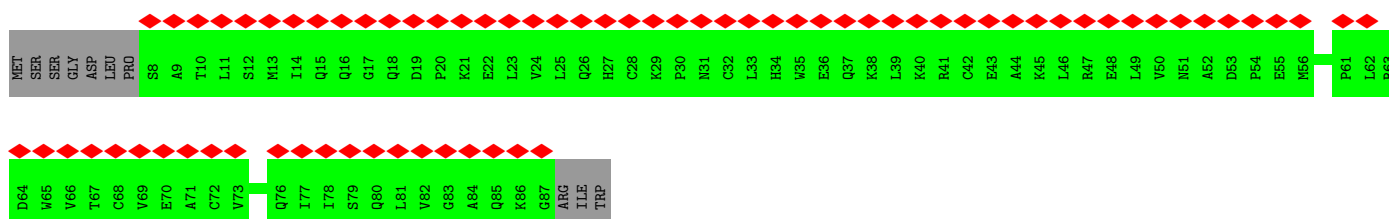
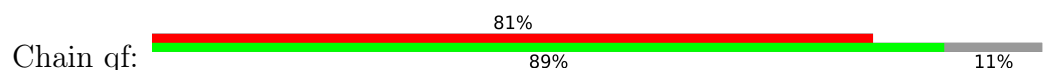
- Molecule 111: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



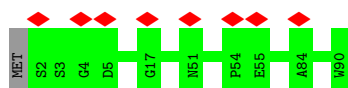
- Molecule 112: Ubiquinol-cytochrome C reductase hinge protein



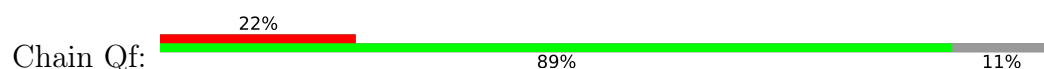
- Molecule 112: Ubiquinol-cytochrome C reductase hinge protein

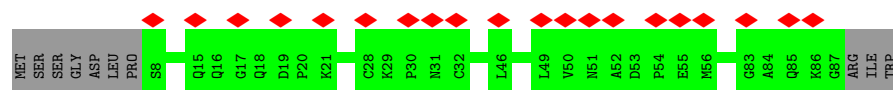


- Molecule 112: Ubiquinol-cytochrome C reductase hinge protein

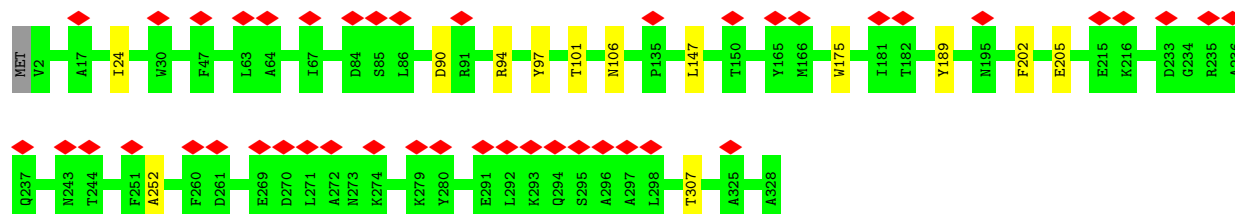


- Molecule 112: Ubiquinol-cytochrome C reductase hinge protein

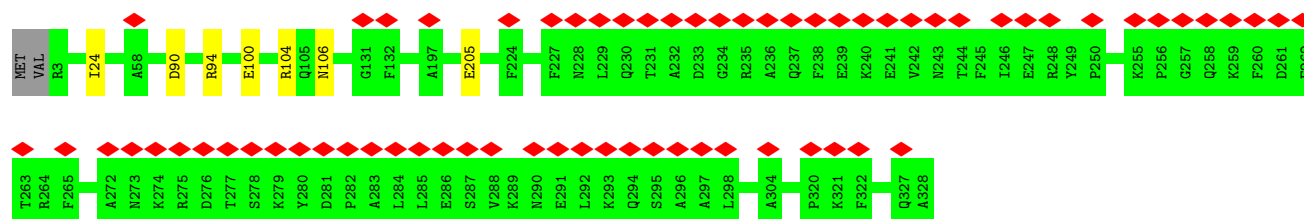




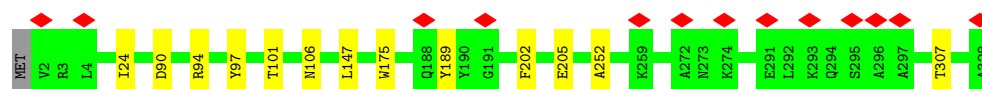
- Molecule 113: Sulphotransf domain-containing protein



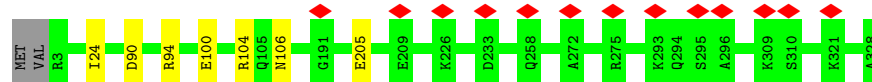
- Molecule 113: Sulphotransf domain-containing protein



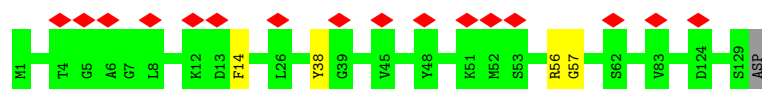
- Molecule 113: Sulphotransf domain-containing protein



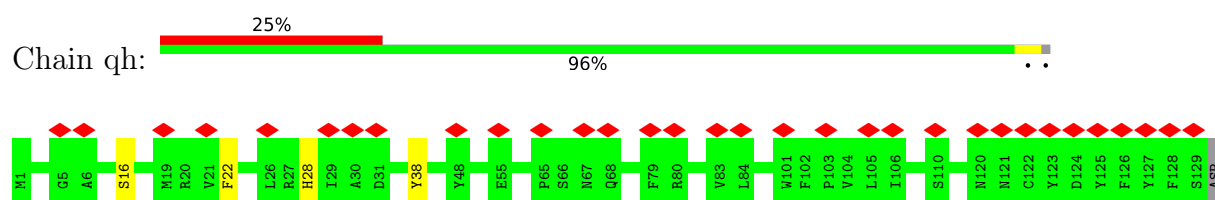
- Molecule 113: Sulphotransf domain-containing protein



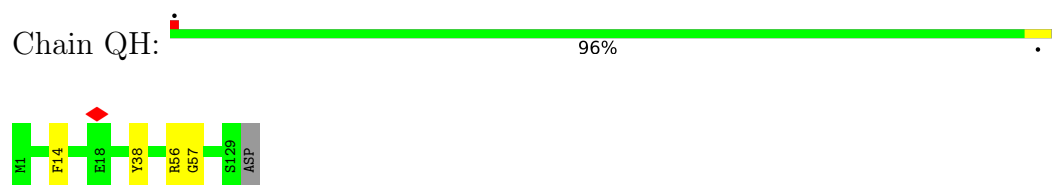
- Molecule 114: Transmembrane protein, putative



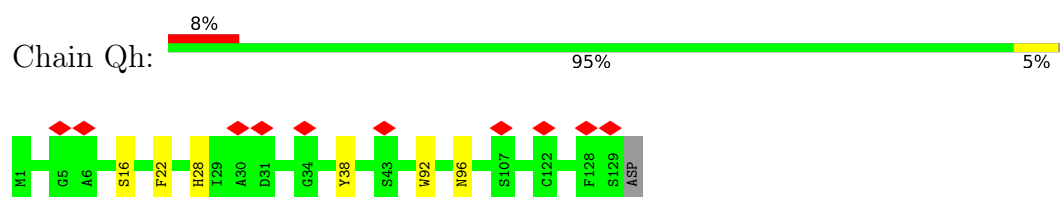
- Molecule 114: Transmembrane protein, putative



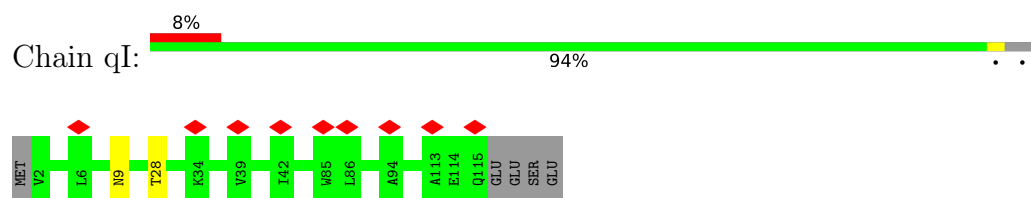
- Molecule 114: Transmembrane protein, putative



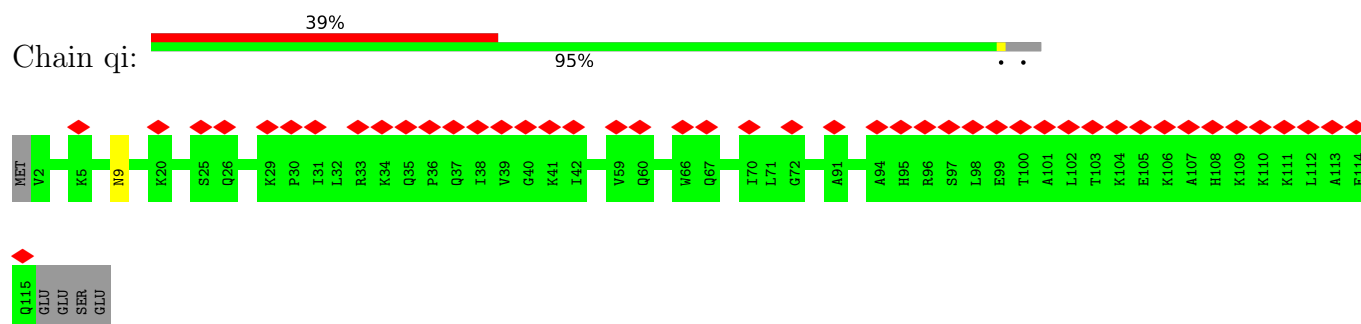
- Molecule 114: Transmembrane protein, putative



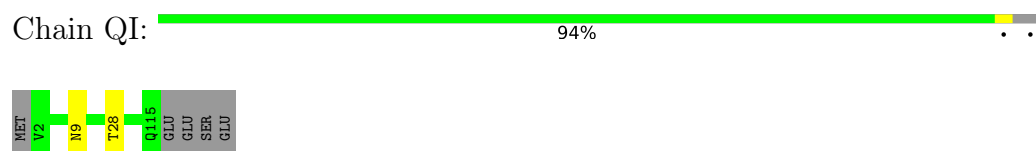
- Molecule 115: Transmembrane protein, putative



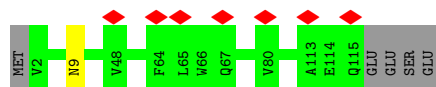
- Molecule 115: Transmembrane protein, putative



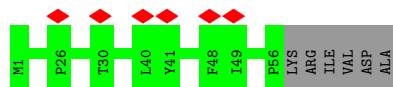
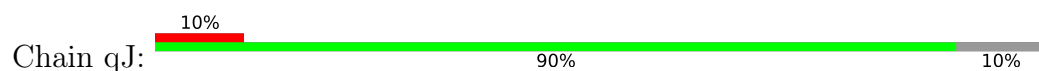
- Molecule 115: Transmembrane protein, putative



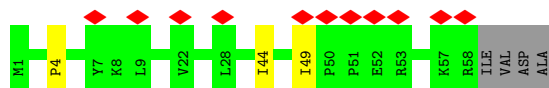
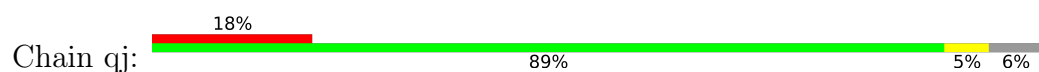
- Molecule 115: Transmembrane protein, putative



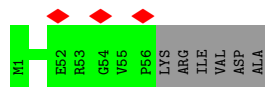
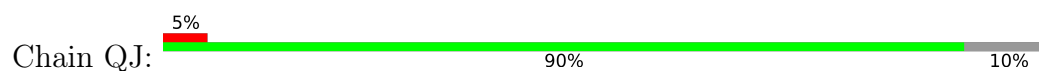
- Molecule 116: Transmembrane protein, putative



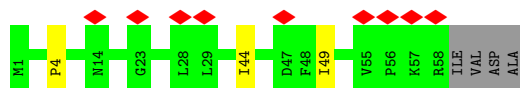
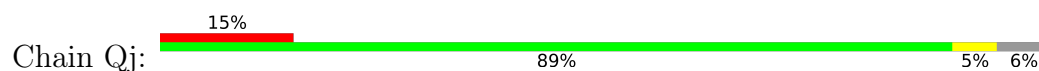
- Molecule 116: Transmembrane protein, putative



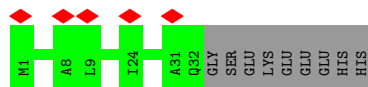
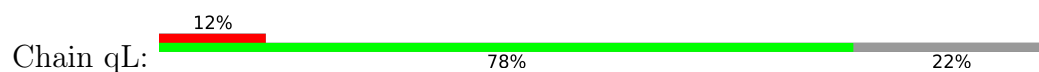
- Molecule 116: Transmembrane protein, putative



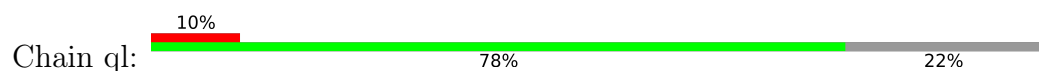
- Molecule 116: Transmembrane protein, putative

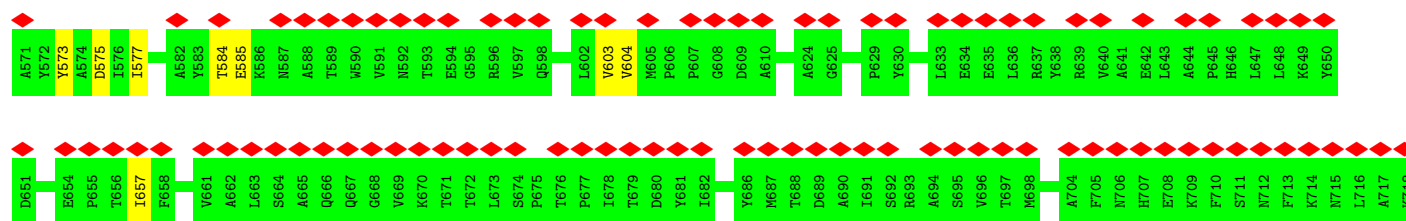


- Molecule 117: UQCRTT2



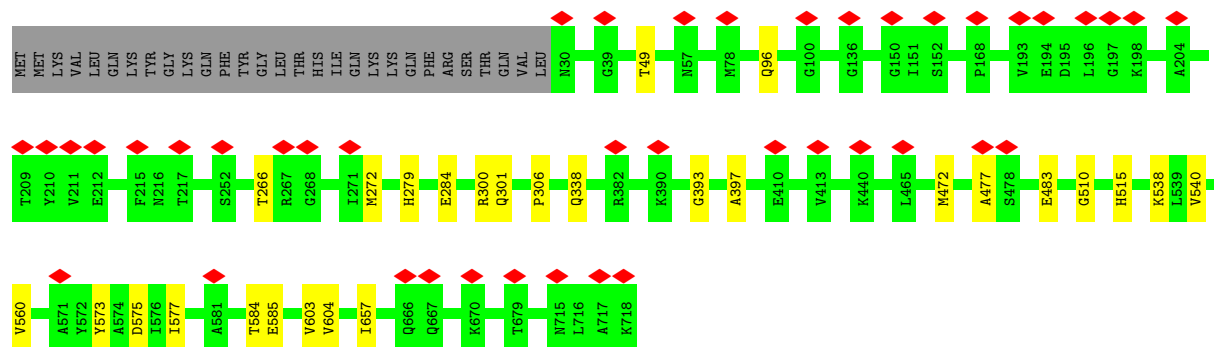
- Molecule 117: UQCRTT2





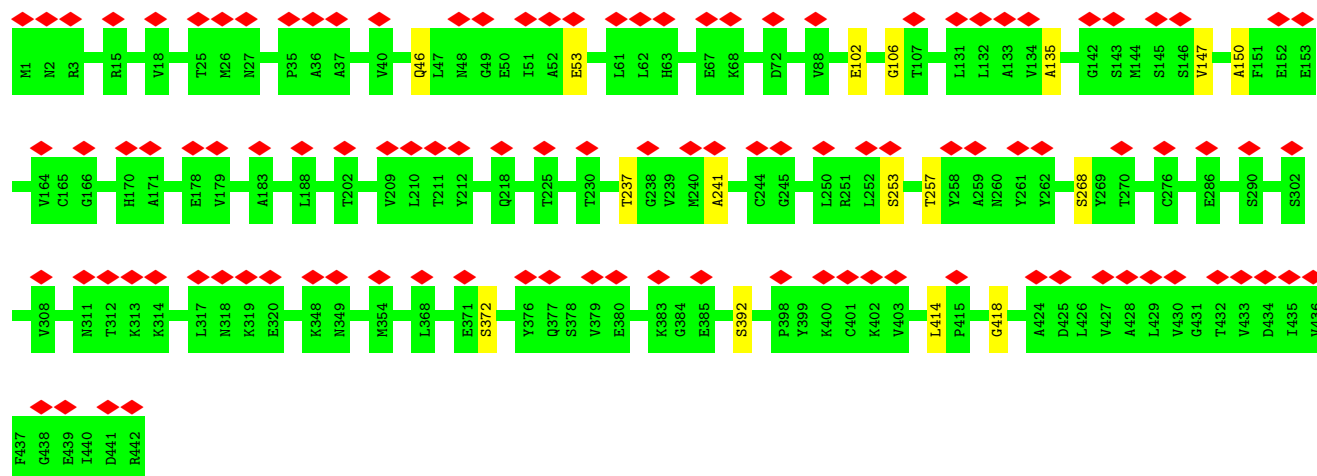
• Molecule 118: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain S1: 6% 92%



• Molecule 119: NADH dehydrogenase subunit 7

Chain S2: 25% 96%

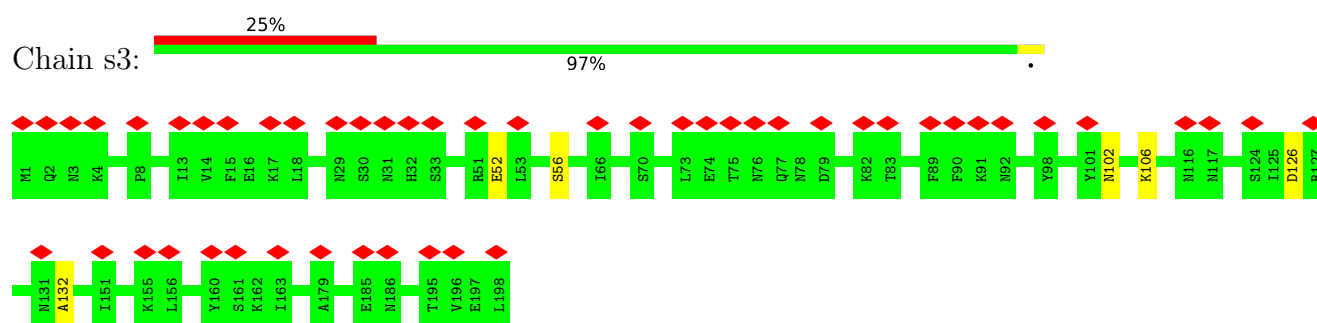


• Molecule 119: NADH dehydrogenase subunit 7

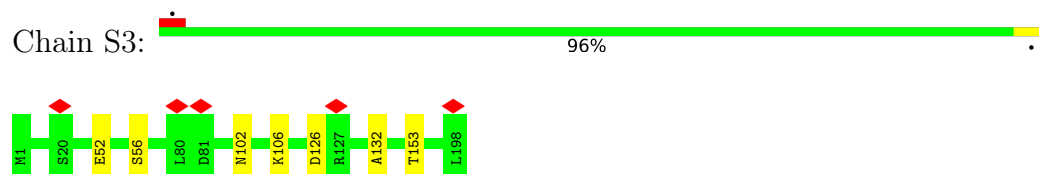
Chain S2: 25% 96%



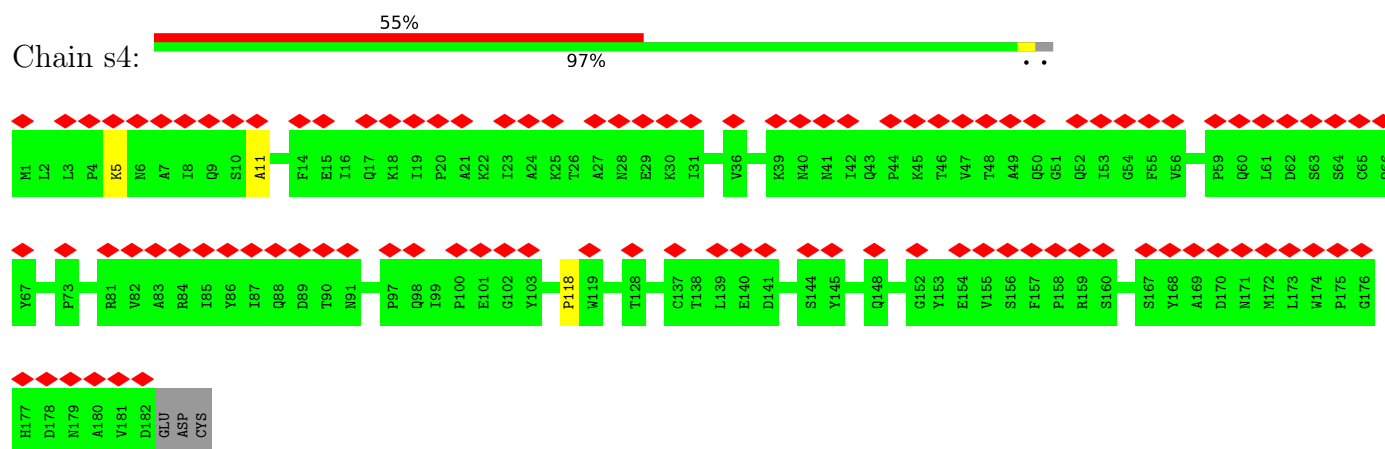
• Molecule 120: NADH dehydrogenase subunit 9



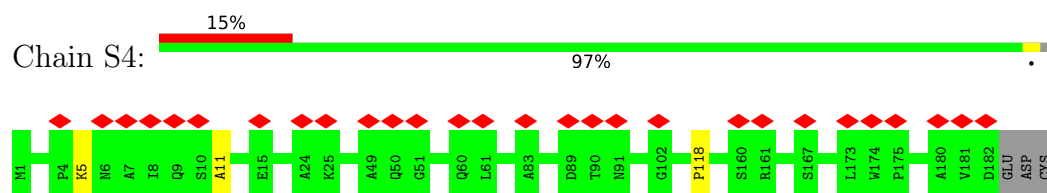
- Molecule 120: NADH dehydrogenase subunit 9



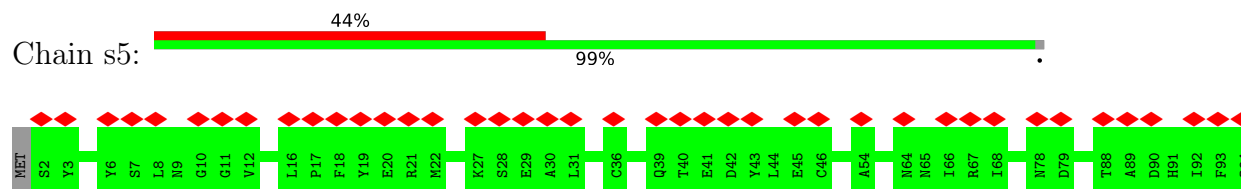
- Molecule 121: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 121: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

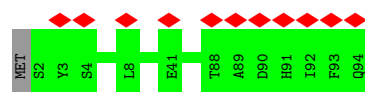


- Molecule 122: GRAM domain protein

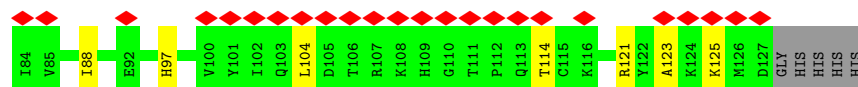
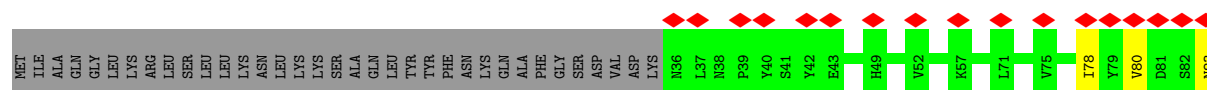


- Molecule 122: GRAM domain protein

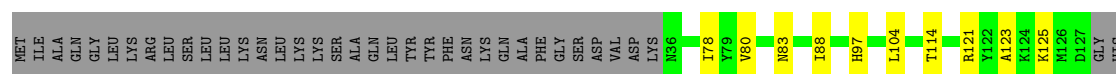




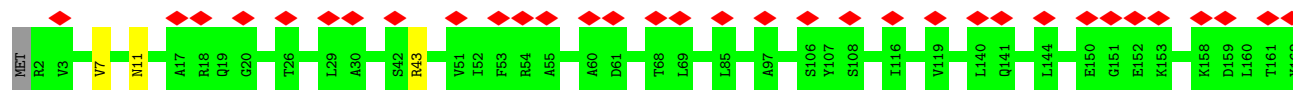
- Molecule 123: Zinc-finger protein



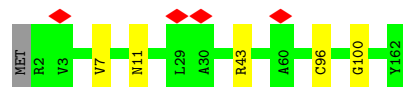
- Molecule 123: Zinc-finger protein



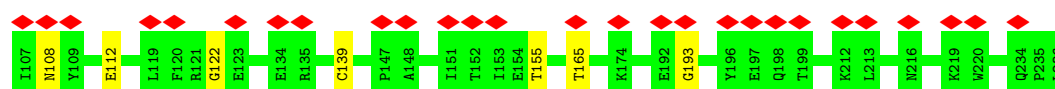
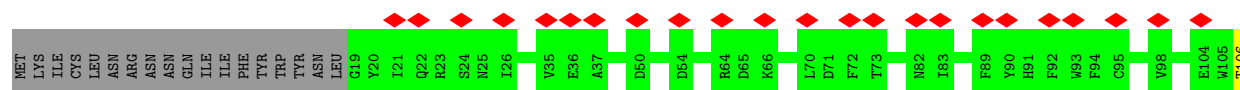
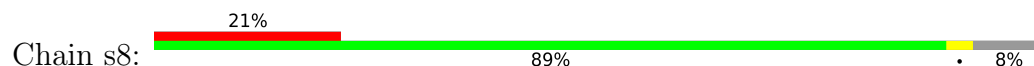
- Molecule 124: NADH dehydrogenase subunit 10



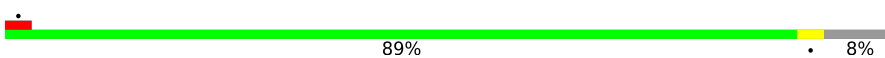
- Molecule 124: NADH dehydrogenase subunit 10

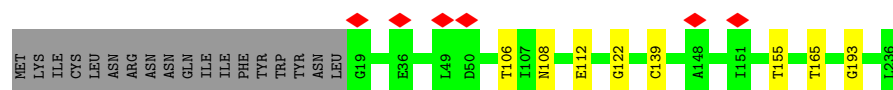


- Molecule 125: NADH-ubiquinone oxidoreductase 1, chain, putative

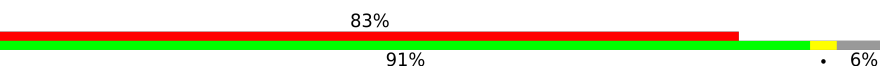


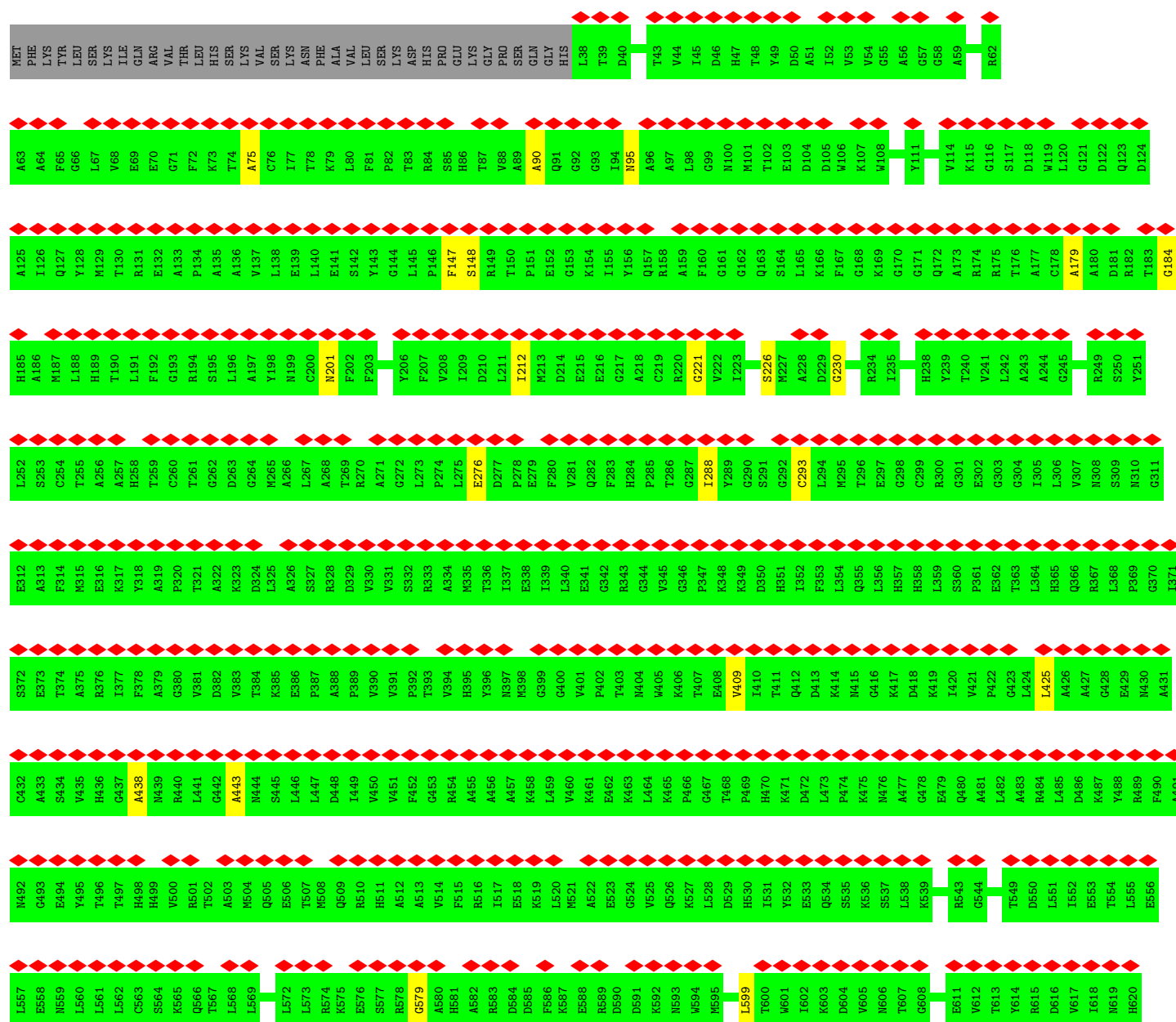
- Molecule 125: NADH-ubiquinone oxidoreductase 1, chain, putative

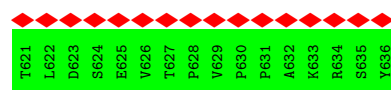
Chain S8:  89% 8%



- Molecule 126: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

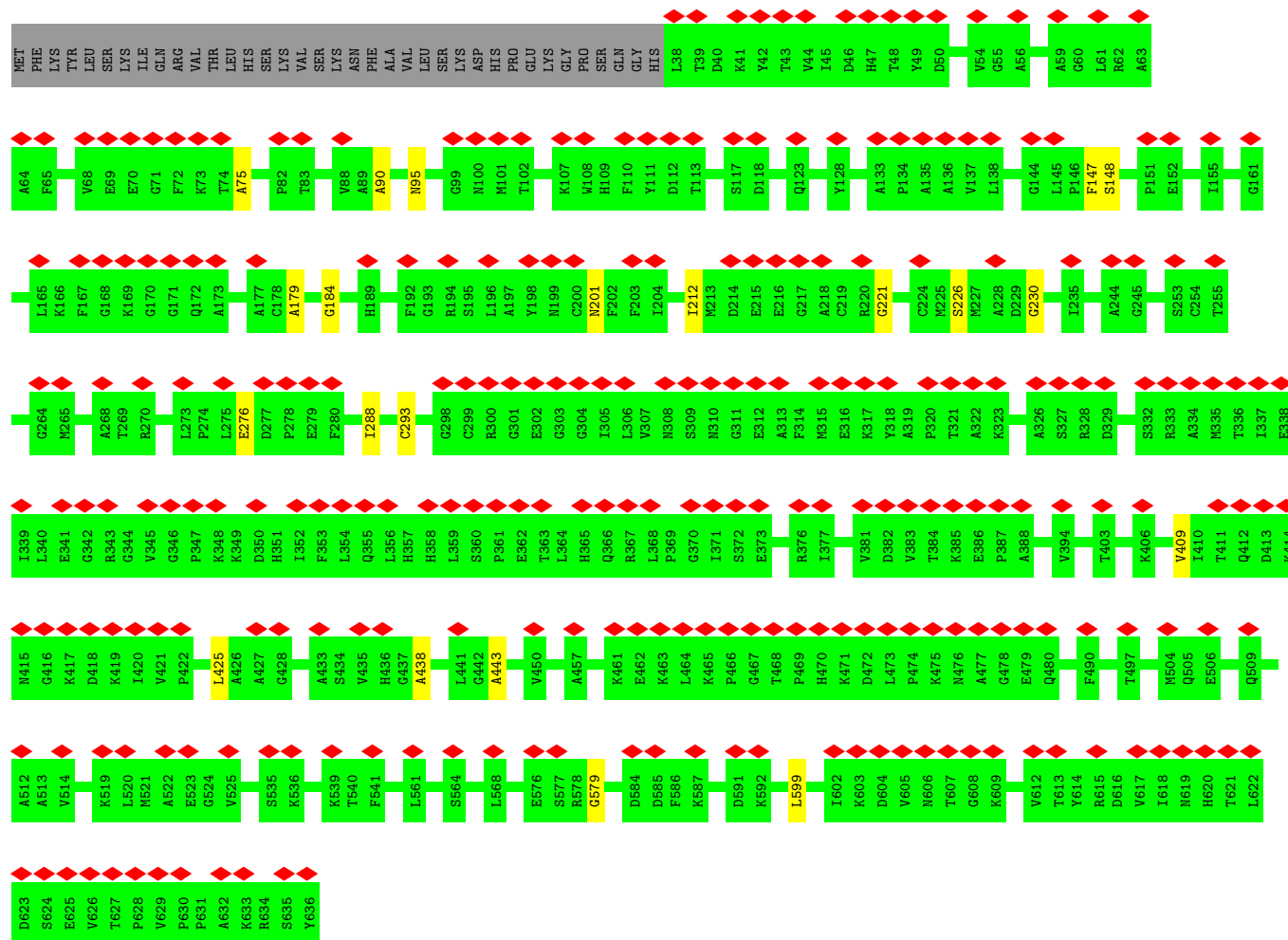
Chain sa:  83% 91% 6%





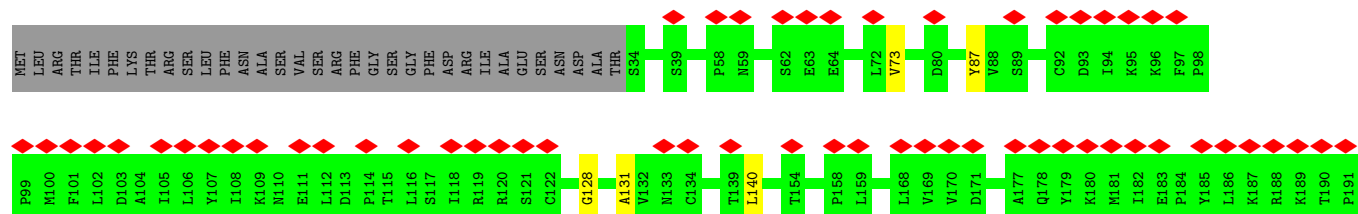
- Molecule 126: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

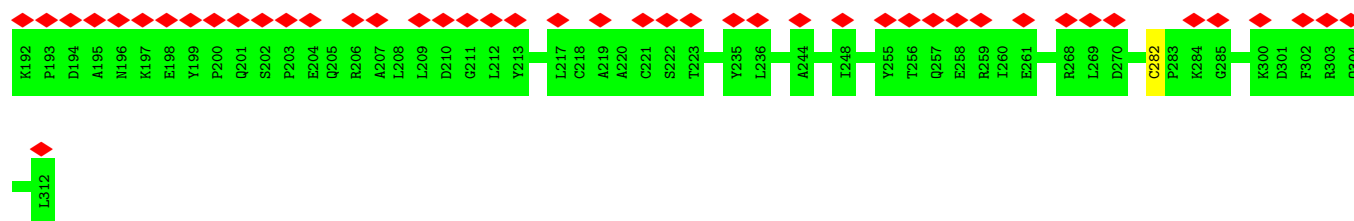
Chain SA: 42% 91% 6%



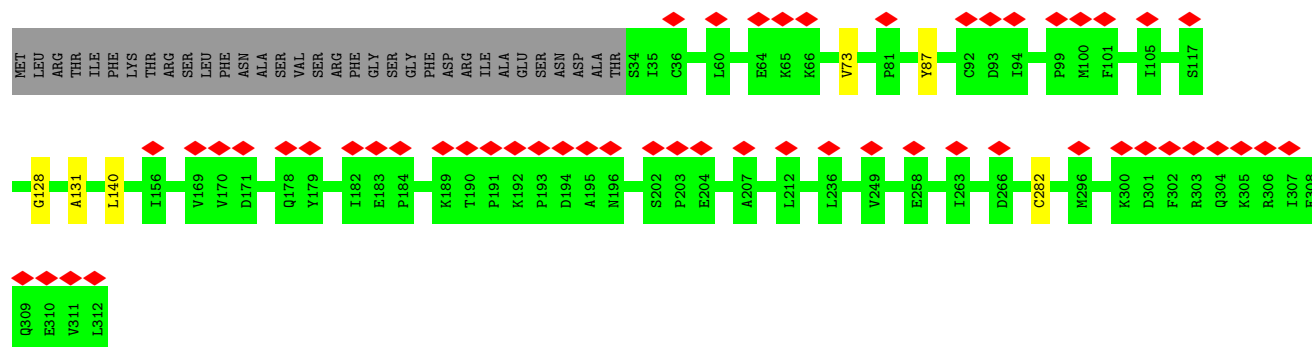
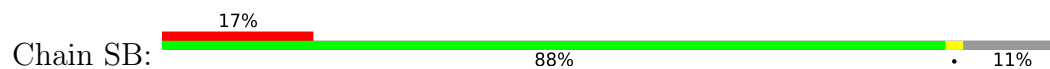
- Molecule 127: Succinate dehydrogenase (quinone)

Chain sb: 33% 88% 11%

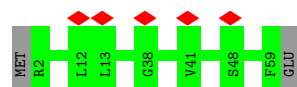




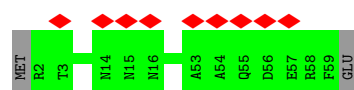
- Molecule 127: Succinate dehydrogenase (quinone)



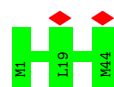
- Molecule 128: Cytochrome b-c1 complex subunit 8



- Molecule 128: Cytochrome b-c1 complex subunit 8

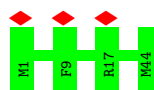


- Molecule 129: SDHD



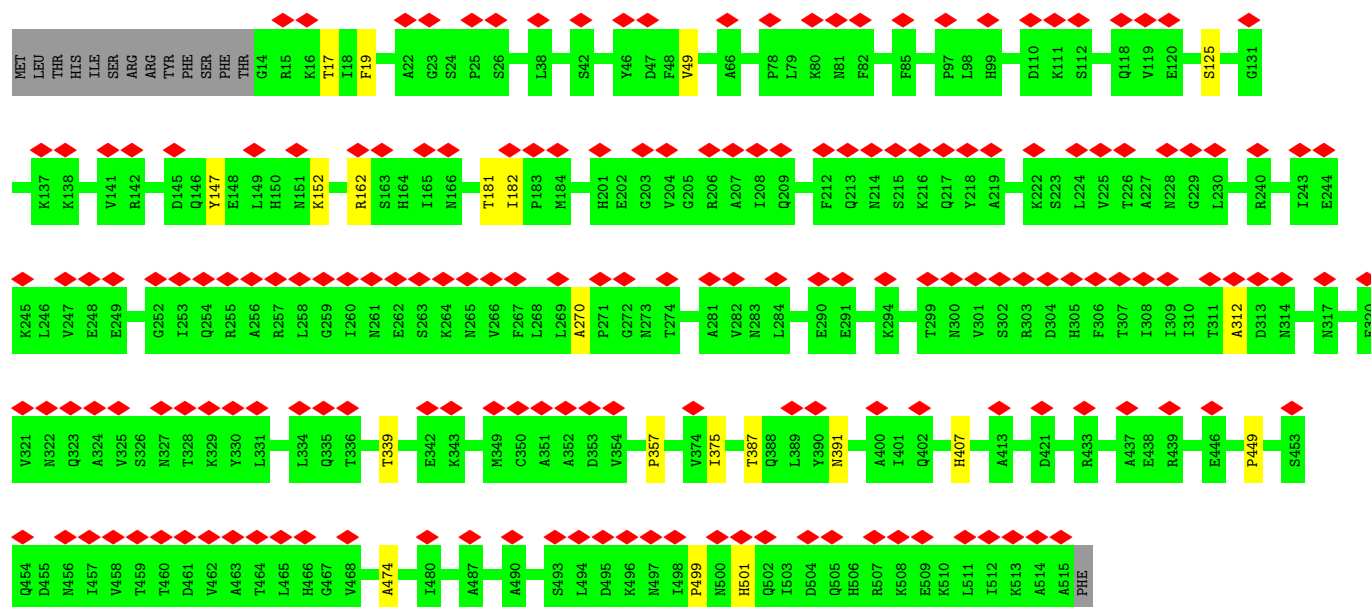
- Molecule 129: SDHD





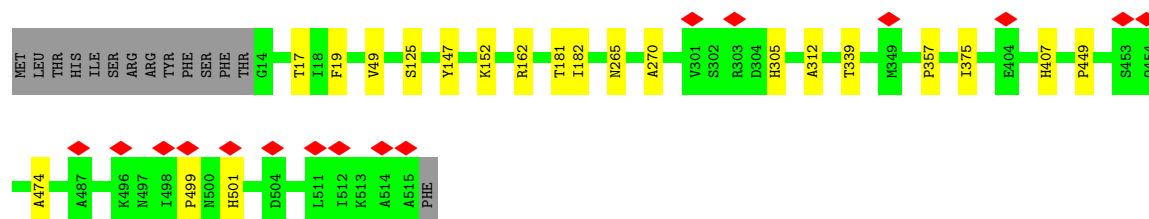
• Molecule 130: Lipid-A-disaccharide synthase

Chain t1: 35% 93%



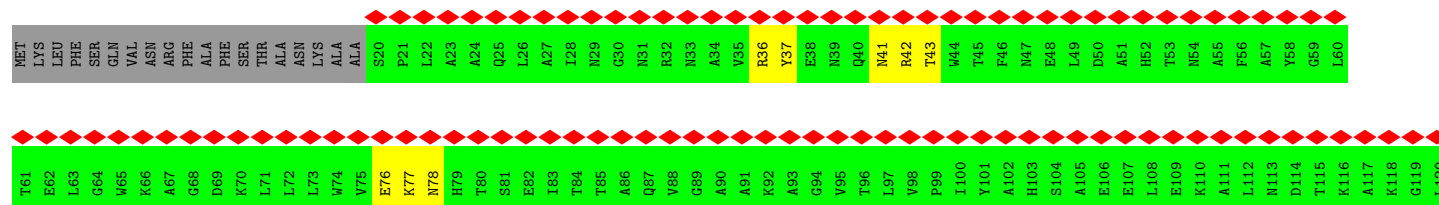
• Molecule 130: Lipid-A-disaccharide synthase

Chain T1: 93%

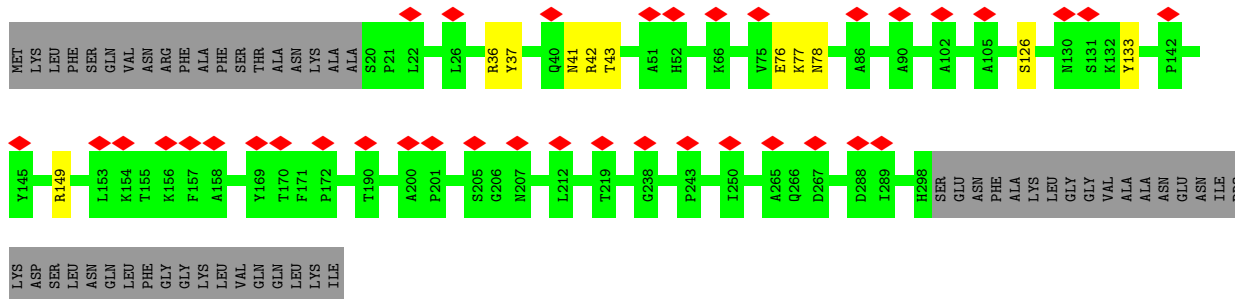
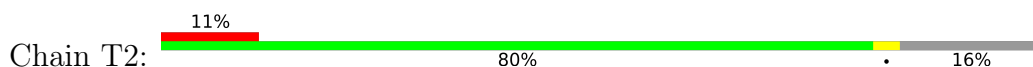


• Molecule 131: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

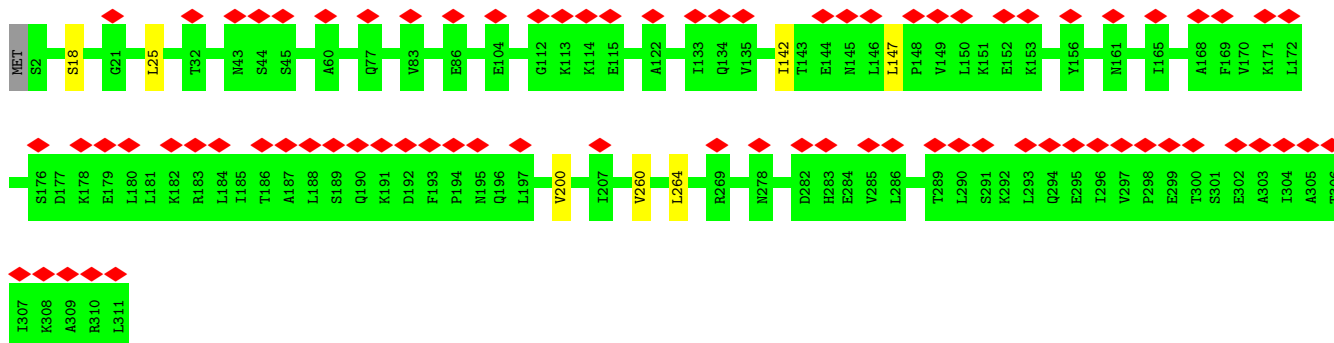
Chain t2: 80% 16%



- Molecule 131: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II



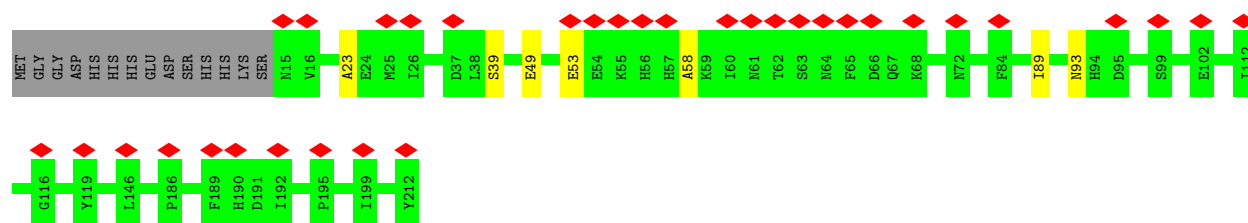
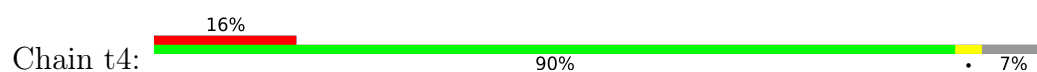
- Molecule 132: RNase III domain-containing protein



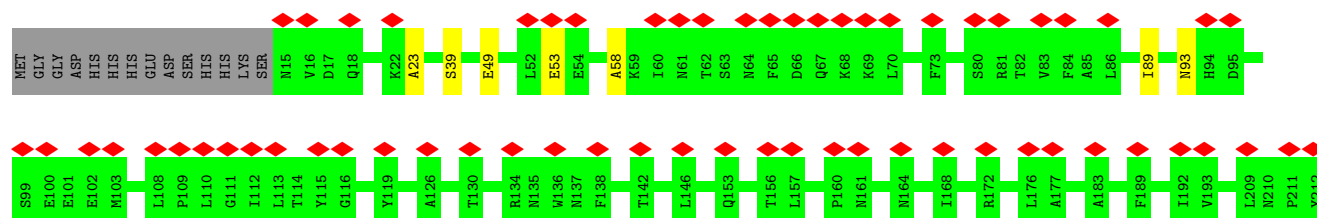
- Molecule 132: RNase III domain-containing protein



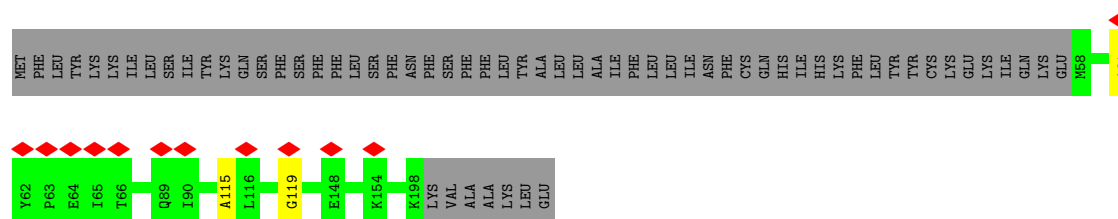
- Molecule 133: Transmembrane protein



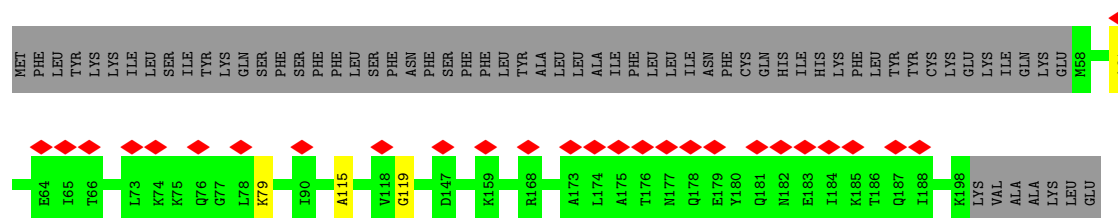
- Molecule 133: Transmembrane protein



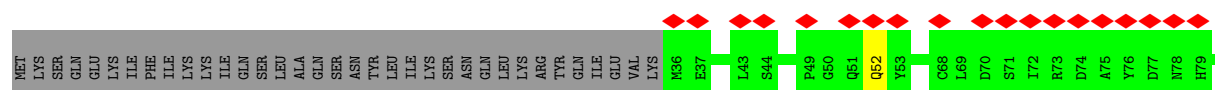
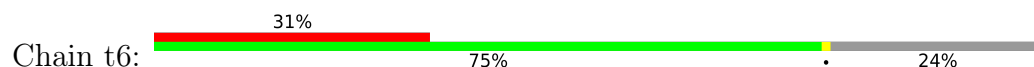
- Molecule 134: Transmembrane protein, putative

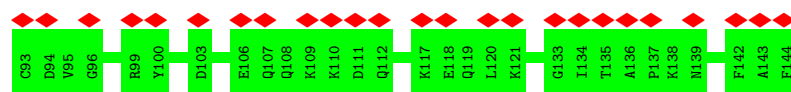


- Molecule 134: Transmembrane protein, putative

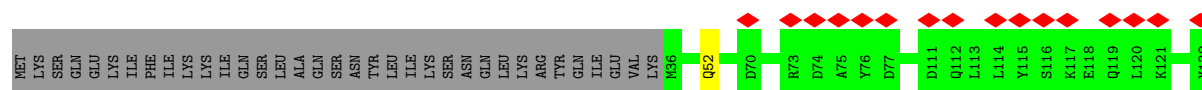
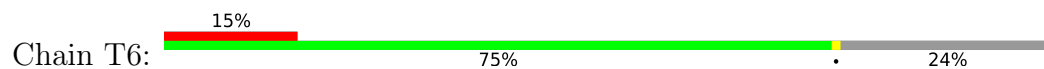


- Molecule 135: COX assembly mitochondrial protein

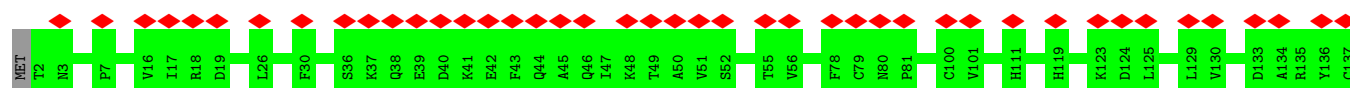




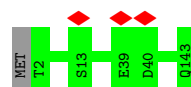
- Molecule 135: COX assembly mitochondrial protein



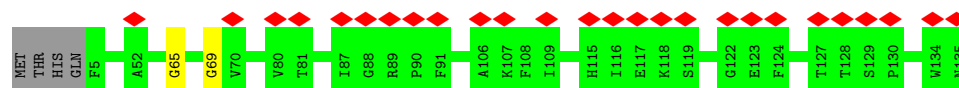
- Molecule 136: Transmembrane protein, putative



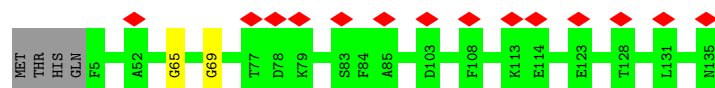
- Molecule 136: Transmembrane protein, putative



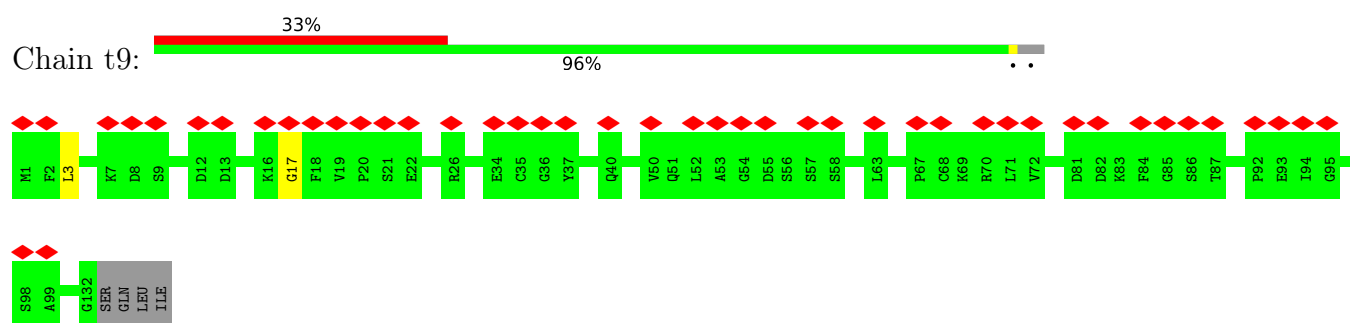
- Molecule 137: PH domain-containing protein



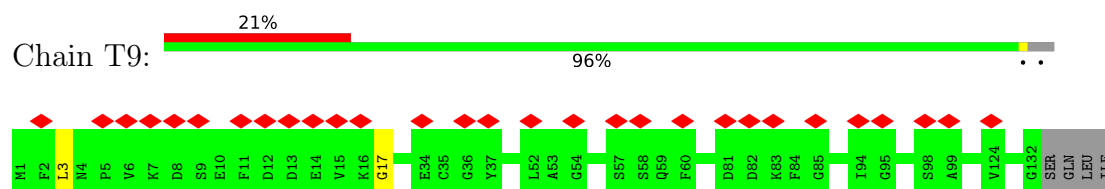
- Molecule 137: PH domain-containing protein



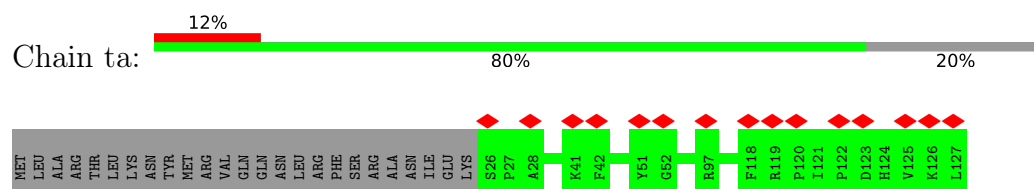
- Molecule 138: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



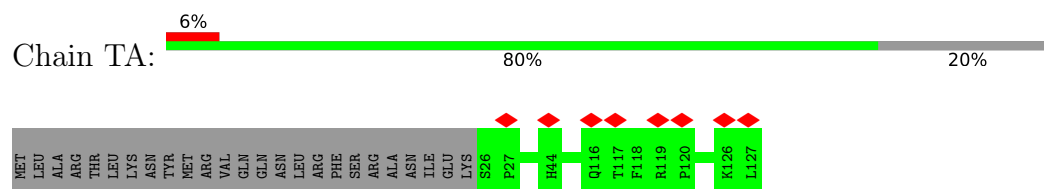
- Molecule 138: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



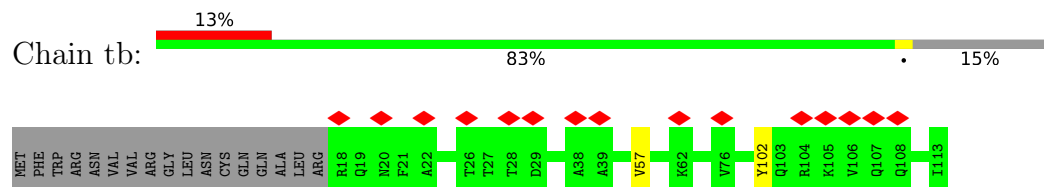
- Molecule 139: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



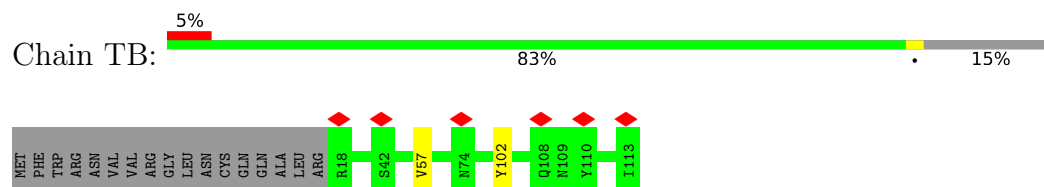
- Molecule 139: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 140: Transmembrane protein, putative

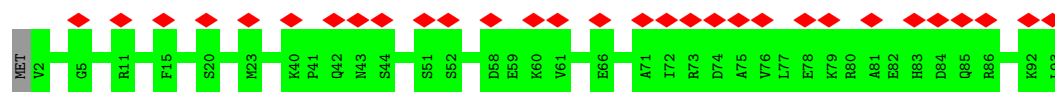


- Molecule 140: Transmembrane protein, putative



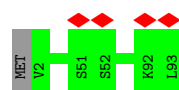
- Molecule 141: ATP synthase subunit e, mitochondrial





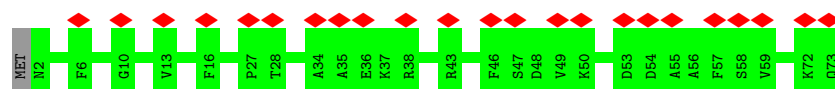
- Molecule 141: ATP synthase subunit e, mitochondrial

Chain TC: 99%



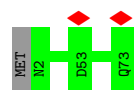
- Molecule 142: Transmembrane protein, putative

Chain td: 32% 99%



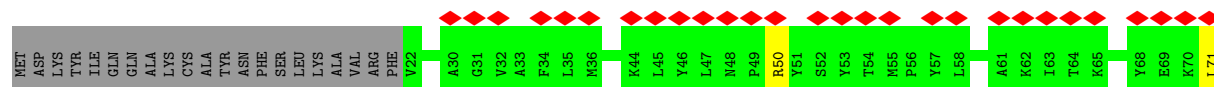
- Molecule 142: Transmembrane protein, putative

Chain TD: 99%



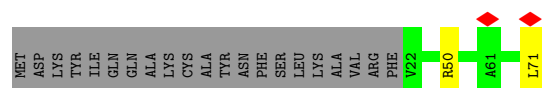
- Molecule 143: Transmembrane protein, putative

Chain te: 39% 68% 30%



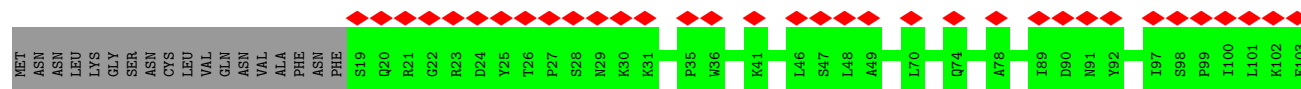
- Molecule 143: Transmembrane protein, putative

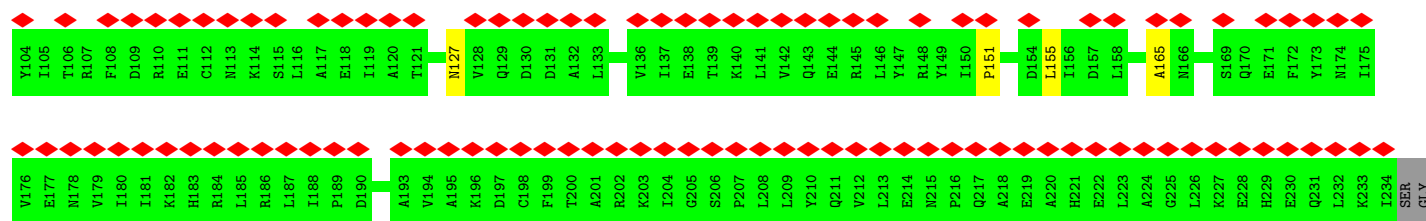
Chain TE: 68% 30%



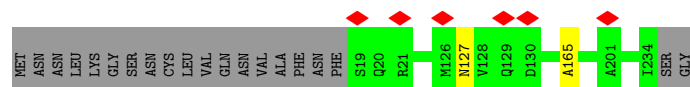
- Molecule 144: NDUTT15

Chain tf: 58% 90% 8%

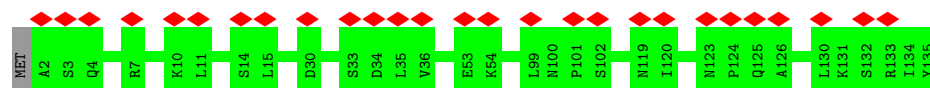




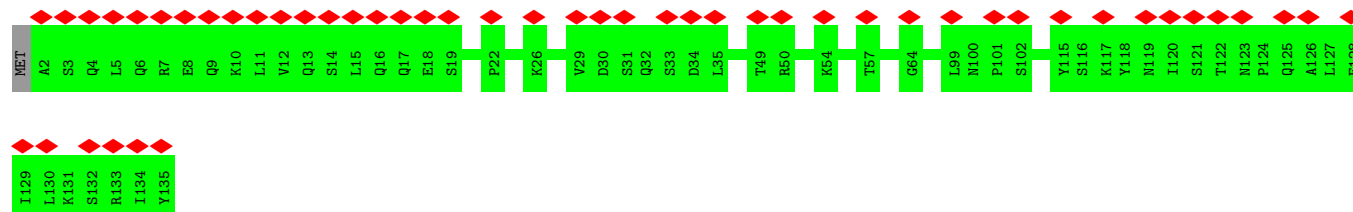
• Molecule 144: NDUTT15



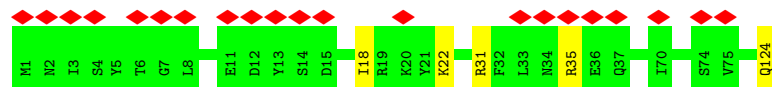
• Molecule 145: NDUTT16



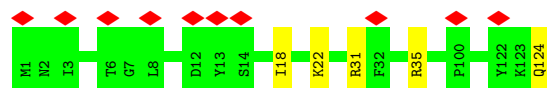
• Molecule 145: NDUTT16



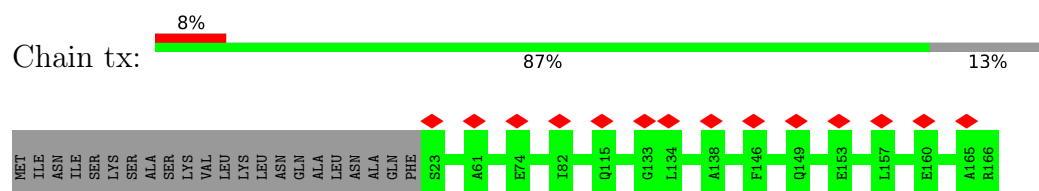
• Molecule 146: NDUTT17



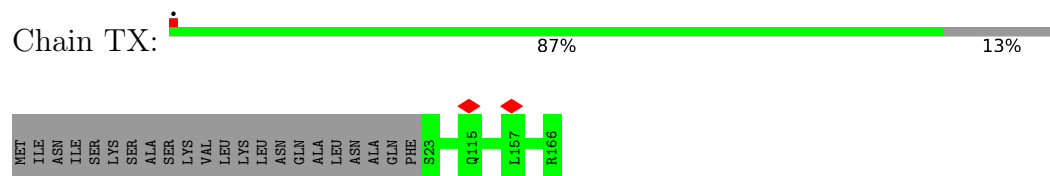
• Molecule 146: NDUTT17



• Molecule 147: Thioredoxin



- Molecule 147: Thioredoxin

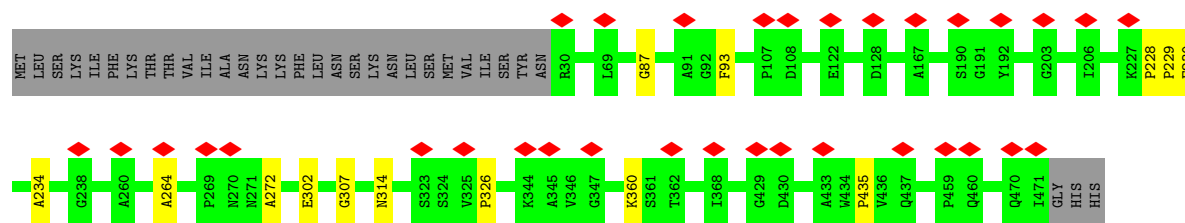


- Molecule 148: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

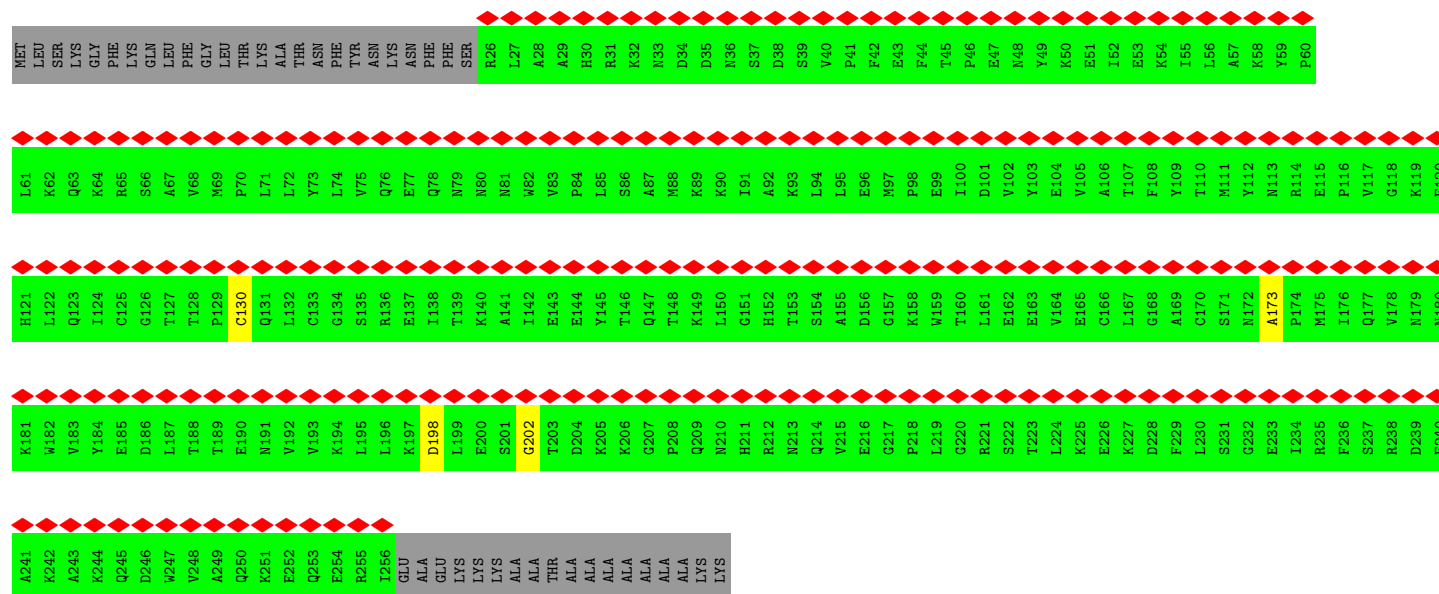
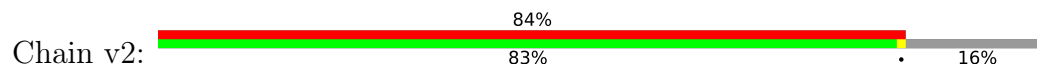


- Molecule 148: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

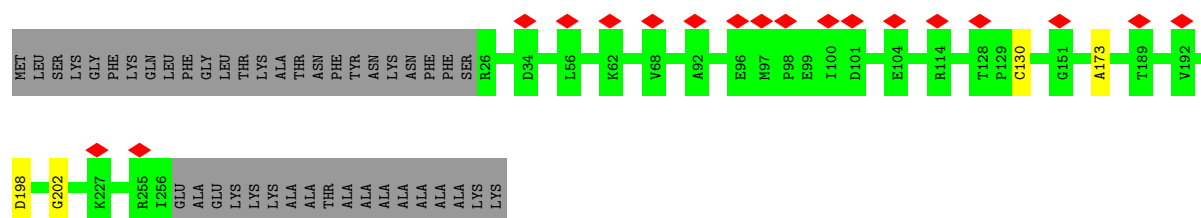
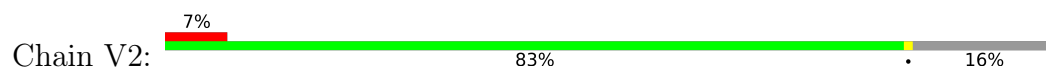




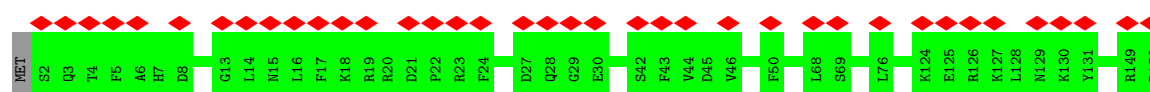
• Molecule 149: NADH-ubiquinone oxidoreductase 24 kDa subunit



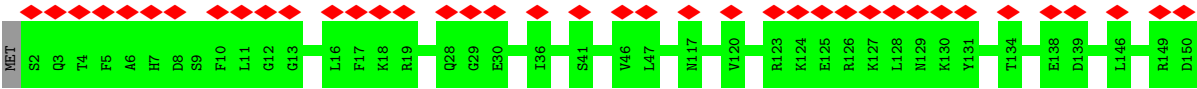
• Molecule 149: NADH-ubiquinone oxidoreductase 24 kDa subunit



• Molecule 150: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit



• Molecule 150: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	25.410	Depositor
Minimum map value	-12.625	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.096	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	840.00006, 840.00006, 840.00006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CU, ADP, FMN, TPO, ZN, NDP, F3S, MG, HEC, FES, U10, SF4, FAD, HEA, SEP

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	00	0.14	0/2227	0.40	0/3106
1	55	0.15	0/2227	0.42	3/3106 (0.1%)
1	A	0.13	0/2227	0.39	0/3106
1	a	0.14	0/2227	0.42	3/3106 (0.1%)
2	01	0.13	0/2113	0.34	0/2939
2	56	0.13	0/2113	0.33	0/2939
2	B	0.13	0/2113	0.34	0/2939
2	b	0.13	0/2113	0.33	0/2939
3	02	0.16	0/1002	0.46	2/1394 (0.1%)
3	57	0.17	0/1002	0.47	2/1394 (0.1%)
3	C	0.16	0/1002	0.46	2/1394 (0.1%)
3	c	0.17	0/1002	0.47	2/1394 (0.1%)
4	03	0.14	0/1426	0.35	0/1984
4	58	0.15	0/1426	0.37	0/1984
4	D	0.14	0/1426	0.35	0/1984
4	d	0.15	0/1426	0.37	0/1984
5	04	0.15	0/1904	0.38	0/2655
5	59	0.14	0/1904	0.39	0/2655
5	E	0.15	0/1904	0.38	0/2655
5	e	0.14	0/1904	0.39	0/2655
6	05	0.14	0/1204	0.38	0/1678
6	60	0.14	0/1204	0.39	0/1678
6	F	0.14	0/1204	0.38	0/1678
6	f	0.14	0/1204	0.39	0/1678
7	06	0.14	0/1453	0.40	0/2026
7	61	0.14	0/1453	0.38	0/2026
7	G	0.14	0/1453	0.40	0/2026
7	g	0.13	0/1453	0.38	0/2026
8	07	0.15	0/1468	0.34	0/2041
8	62	0.15	0/1468	0.34	0/2041
8	H	0.15	0/1468	0.34	0/2041
8	h	0.15	0/1468	0.34	0/2041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	08	0.14	0/1140	0.35	0/1586
9	63	0.14	0/1140	0.36	0/1586
9	I	0.14	0/1140	0.35	0/1586
9	i	0.14	0/1140	0.36	0/1586
10	09	0.13	0/930	0.37	0/1298
10	64	0.12	0/930	0.37	0/1298
10	J	0.13	0/930	0.37	0/1298
10	j	0.12	0/930	0.37	0/1298
11	0A	0.12	0/345	0.31	0/479
11	45	0.13	0/345	0.33	0/479
11	6T	0.12	0/345	0.33	0/479
11	6t	0.12	0/345	0.31	0/479
12	0B	0.17	0/1857	0.47	0/2570
12	46	0.17	0/1857	0.43	0/2570
12	BP	0.16	0/1857	0.43	0/2570
12	bp	0.17	0/1857	0.47	0/2570
13	0C	0.17	0/927	0.41	0/1289
13	47	0.16	0/927	0.38	0/1289
13	FS	0.16	0/927	0.38	0/1289
13	fs	0.17	0/927	0.41	0/1289
14	0D	0.11	0/493	0.29	0/685
14	48	0.12	0/493	0.32	0/685
14	4A	0.11	0/493	0.32	0/685
14	4a	0.11	0/493	0.29	0/685
15	0E	0.11	0/1709	0.32	0/2387
15	49	0.13	0/1709	0.33	0/2387
15	Y7	0.12	0/1709	0.33	0/2387
15	y7	0.11	0/1709	0.32	0/2387
16	0F	0.12	0/946	0.32	0/1321
16	50	0.12	0/946	0.34	0/1321
16	Y5	0.12	0/946	0.34	0/1321
16	y5	0.11	0/946	0.32	0/1321
17	0G	0.13	0/443	0.35	0/618
17	51	0.13	0/443	0.35	0/618
17	Y0	0.13	0/443	0.35	0/618
17	y0	0.12	0/443	0.35	0/618
18	0H	0.14	0/478	0.26	0/664
18	52	0.15	0/478	0.27	0/664
18	Z1	0.15	0/478	0.27	0/664
18	z1	0.14	0/478	0.26	0/664
21	10	0.13	0/1031	0.40	0/1437
21	65	0.13	0/1031	0.40	0/1437
21	K	0.12	0/1031	0.39	0/1437

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	k	0.13	0/1031	0.40	0/1437
22	11	0.16	0/964	0.33	0/1345
22	66	0.15	0/964	0.34	0/1345
22	L	0.15	0/964	0.33	0/1345
22	l	0.15	0/964	0.34	0/1345
23	12	0.14	0/1082	0.39	0/1506
23	67	0.14	0/1082	0.37	0/1506
23	M	0.14	0/1082	0.39	0/1506
23	m	0.13	0/1082	0.37	0/1506
24	13	0.12	0/1015	0.37	0/1411
24	68	0.13	0/1015	0.38	0/1411
24	N	0.12	0/1015	0.37	0/1411
24	n	0.13	0/1015	0.38	0/1411
25	14	0.14	0/640	0.30	0/892
25	69	0.14	0/640	0.29	0/892
25	O	0.14	0/640	0.30	0/892
25	o	0.13	0/640	0.29	0/892
26	15	0.13	0/864	0.35	0/1202
26	70	0.14	0/864	0.37	0/1202
26	P	0.13	0/864	0.35	0/1202
26	p	0.13	0/864	0.37	0/1202
27	16	0.13	0/854	0.35	0/1188
27	71	0.14	0/854	0.40	0/1188
27	Q	0.12	0/854	0.35	0/1188
27	q	0.14	0/854	0.40	0/1188
28	17	0.12	0/851	0.32	0/1185
28	72	0.11	0/851	0.30	0/1185
28	R	0.11	0/851	0.32	0/1185
28	r	0.11	0/851	0.29	0/1185
29	18	0.14	0/840	0.33	0/1172
29	73	0.14	0/840	0.32	0/1172
29	S	0.14	0/840	0.33	0/1172
29	s	0.14	0/840	0.32	0/1172
30	19	0.13	0/770	0.32	0/1071
30	74	0.13	0/770	0.31	0/1071
30	T	0.12	0/770	0.32	0/1071
30	t	0.13	0/770	0.31	0/1071
31	1B	0.08	0/292	0.31	0/406
31	1b	0.09	0/292	0.31	0/406
32	20	0.13	0/756	0.30	0/1052
32	75	0.13	0/756	0.33	0/1052
32	U	0.12	0/756	0.30	0/1052
32	u	0.13	0/756	0.34	0/1052

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	21	0.14	0/721	0.39	0/1003
33	76	0.14	0/721	0.39	0/1003
33	V	0.13	0/721	0.39	0/1003
33	v	0.14	0/721	0.38	0/1003
34	22	0.11	0/611	0.32	0/852
34	77	0.13	0/611	0.34	0/852
34	W	0.10	0/611	0.32	0/852
34	w	0.12	0/611	0.34	0/852
35	23	0.12	0/601	0.29	0/835
35	78	0.11	0/601	0.31	0/835
35	X	0.11	0/601	0.29	0/835
35	x	0.10	0/601	0.31	0/835
36	24	0.13	0/516	0.30	0/716
36	79	0.12	0/516	0.32	0/716
36	Y	0.12	0/516	0.30	0/716
36	y	0.11	0/516	0.32	0/716
37	25	0.14	0/428	0.36	0/594
37	80	0.13	0/428	0.32	0/594
37	Z	0.14	0/428	0.35	0/594
37	z	0.13	0/428	0.32	0/594
38	26	0.14	0/3327	0.38	0/4631
38	81	0.14	0/3327	0.38	0/4631
38	C1	0.13	0/3327	0.38	0/4631
38	c1	0.14	0/3327	0.38	0/4631
39	27	0.14	0/2973	0.37	0/4147
39	82	0.14	0/2973	0.39	0/4147
39	C2	0.13	0/2973	0.37	0/4147
39	c2	0.14	0/2973	0.38	0/4147
40	28	0.14	0/2893	0.38	0/4039
40	83	0.13	0/2893	0.34	0/4039
40	C3	0.14	0/2893	0.37	0/4039
40	c3	0.13	0/2893	0.34	0/4039
41	29	0.13	0/2741	0.34	0/3820
41	84	0.13	0/2741	0.34	0/3820
41	VB	0.13	0/2741	0.33	0/3820
41	vb	0.12	0/2741	0.34	0/3820
42	2B	0.11	0/883	0.29	0/1231
42	2b	0.11	0/883	0.29	0/1231
43	2E	0.11	0/1590	0.31	0/2216
43	2e	0.12	0/1590	0.31	0/2216
44	2F	0.12	0/1076	0.33	0/1500
44	2f	0.12	0/1076	0.33	0/1500
45	2G	0.12	0/983	0.30	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
45	2g	0.12	0/983	0.30	0/1371
46	2H	0.10	0/505	0.30	0/702
46	2h	0.10	0/505	0.30	0/702
47	2I	0.10	0/563	0.27	0/783
47	2i	0.10	0/563	0.27	0/783
48	2J	0.11	0/504	0.32	0/701
48	2j	0.11	0/504	0.32	0/701
49	2K	0.12	0/461	0.34	0/642
49	2k	0.12	0/461	0.34	0/642
50	2L	0.11	0/414	0.37	0/578
50	2l	0.12	0/414	0.37	0/578
51	2M	0.10	0/369	0.36	0/512
51	2m	0.11	0/369	0.36	0/512
52	2N	0.14	0/301	0.46	0/418
52	2n	0.15	0/301	0.46	0/418
53	2O	0.10	0/209	0.29	0/291
53	2o	0.10	0/209	0.29	0/291
54	30	0.17	0/623	0.36	0/867
54	6A	0.16	0/623	0.36	0/867
54	6a	0.17	0/623	0.36	0/867
54	85	0.17	0/623	0.36	0/867
55	31	0.13	0/1100	0.36	0/1533
55	6B	0.12	0/1100	0.36	0/1533
55	6b	0.12	0/1100	0.34	0/1533
55	86	0.13	0/1100	0.34	0/1533
56	32	0.19	0/498	0.37	0/692
56	6C	0.19	0/498	0.36	0/692
56	6c	0.21	0/498	0.38	0/692
56	87	0.21	0/498	0.38	0/692
57	33	0.12	0/382	0.29	0/532
57	6L	0.12	0/382	0.29	0/532
57	6l	0.13	0/382	0.33	0/532
57	88	0.13	0/382	0.33	0/532
58	34	0.13	0/658	0.39	0/916
58	7A	0.13	0/658	0.39	0/916
58	7a	0.13	0/658	0.36	0/916
58	89	0.13	0/658	0.36	0/916
59	35	0.13	0/1040	0.37	0/1448
59	7C	0.12	0/1040	0.37	0/1448
59	7c	0.13	0/1040	0.37	0/1448
59	90	0.13	0/1040	0.37	0/1448
60	36	0.14	0/653	0.35	0/912
60	7L	0.13	0/653	0.35	0/912

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	7l	0.14	0/653	0.36	0/912
60	91	0.14	0/653	0.36	0/912
61	37	0.14	0/1708	0.42	0/2377
61	92	0.14	0/1708	0.41	0/2377
61	M1	0.14	0/1708	0.42	0/2377
61	m1	0.14	0/1708	0.41	0/2377
62	38	0.12	0/1560	0.32	0/2165
62	93	0.12	0/1560	0.32	0/2165
62	M2	0.12	0/1560	0.32	0/2165
62	m2	0.12	0/1560	0.32	0/2165
63	39	0.13	0/1623	0.38	0/2258
63	94	0.13	0/1623	0.36	0/2258
63	M3	0.13	0/1623	0.38	0/2258
63	m3	0.12	0/1623	0.36	0/2258
64	1T	0.11	0/348	0.25	0/485
64	1t	0.10	0/348	0.25	0/485
64	40	0.11	0/348	0.26	0/485
64	95	0.11	0/348	0.25	0/485
65	2T	0.12	0/347	0.31	0/483
65	2t	0.09	0/347	0.29	0/483
65	41	0.12	0/347	0.31	0/483
65	96	0.10	0/347	0.29	0/483
66	3T	0.11	0/412	0.29	0/574
66	3t	0.11	0/412	0.28	0/574
66	42	0.12	0/412	0.29	0/574
66	97	0.12	0/412	0.28	0/574
67	43	0.10	0/284	0.32	0/396
67	4T	0.10	0/284	0.32	0/396
67	4t	0.12	0/284	0.27	0/396
67	98	0.12	0/284	0.27	0/396
68	44	0.15	0/308	0.29	0/429
68	5T	0.14	0/308	0.29	0/429
68	5t	0.14	0/308	0.32	0/429
68	99	0.14	0/308	0.32	0/429
69	4L	0.10	0/575	0.33	0/801
69	4l	0.10	0/575	0.33	0/801
70	5B	0.12	0/497	0.34	0/693
70	5b	0.13	0/497	0.34	0/693
71	A1	0.11	0/462	0.40	0/644
71	a1	0.11	0/462	0.40	0/644
72	A2	0.11	0/486	0.33	0/677
72	a2	0.12	0/486	0.34	0/677
73	A3	0.11	0/632	0.29	0/876

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
73	a3	0.11	0/632	0.29	0/876
74	A5	0.10	0/770	0.27	0/1074
74	a5	0.10	0/770	0.27	0/1074
75	A6	0.11	0/846	0.39	0/1175
75	a6	0.12	0/846	0.39	0/1175
76	A7	0.13	0/1403	0.32	0/1959
76	a7	0.13	0/1403	0.32	0/1959
77	A8	0.10	0/657	0.30	0/917
77	a8	0.10	0/657	0.30	0/917
78	A9	0.13	0/1677	0.34	0/2333
78	a9	0.13	0/1677	0.34	0/2333
79	AB	0.13	0/556	0.35	0/775
79	ab	0.13	0/556	0.35	0/775
80	AC	0.10	0/487	0.32	0/679
80	ac	0.11	0/487	0.32	0/679
81	AL	0.11	0/948	0.34	0/1316
81	al	0.12	0/948	0.34	0/1316
82	AM	0.12	0/793	0.33	0/1105
82	am	0.12	0/793	0.33	0/1105
83	AN	0.11	0/1134	0.30	0/1574
83	an	0.12	0/1134	0.30	0/1574
84	B2	0.12	0/589	0.32	0/817
84	b2	0.12	0/589	0.32	0/817
85	B3	0.11	0/341	0.37	0/474
85	b3	0.11	0/341	0.38	0/474
86	B4	0.10	0/567	0.28	0/788
86	b4	0.10	0/567	0.28	0/788
87	B6	0.13	0/347	0.34	0/483
87	b6	0.13	0/347	0.34	0/483
88	B7	0.11	0/571	0.31	0/793
88	b7	0.12	0/571	0.31	0/793
89	B8	0.13	0/861	0.32	0/1196
89	b8	0.13	0/861	0.33	0/1196
90	B9	0.11	0/934	0.31	0/1303
90	b9	0.12	0/934	0.31	0/1303
91	BL	0.12	0/868	0.30	0/1210
91	bl	0.12	0/868	0.30	0/1210
92	BM	0.11	0/809	0.31	0/1125
92	bm	0.12	0/809	0.31	0/1125
93	C4	0.12	0/506	0.30	0/705
93	c4	0.13	0/506	0.30	0/705
94	FX	0.11	0/721	0.37	0/1003
94	fx	0.12	0/721	0.37	0/1003

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
95	G1	0.12	0/1125	0.34	0/1562
95	g1	0.13	0/1125	0.34	0/1562
96	G2	0.12	0/1128	0.31	0/1565
96	g2	0.12	0/1128	0.31	0/1565
97	G3	0.11	0/1710	0.31	0/2381
97	g3	0.12	0/1710	0.31	0/2381
98	J1	0.11	0/1303	0.30	0/1808
98	j1	0.12	0/1303	0.30	0/1808
99	N1	0.11	0/1396	0.35	0/1942
99	n1	0.12	0/1396	0.35	0/1942
100	N2	0.11	0/1792	0.33	0/2503
100	n2	0.11	0/1792	0.33	0/2503
101	N3	0.12	0/595	0.30	0/829
101	n3	0.12	0/595	0.30	0/829
102	N4	0.13	0/2501	0.33	0/3486
102	n4	0.13	0/2501	0.33	0/3486
103	N5	0.12	0/3516	0.33	0/4904
103	n5	0.12	0/3516	0.33	0/4904
104	N6	0.10	0/1268	0.32	0/1770
104	n6	0.11	0/1268	0.32	0/1770
105	P1	0.13	0/1138	0.40	0/1585
105	p1	0.13	0/1138	0.41	0/1585
106	P2	0.13	0/830	0.38	0/1158
106	p2	0.13	0/830	0.38	0/1158
107	QA	0.11	0/2244	0.33	0/3124
107	Qa	0.12	0/2244	0.32	0/3124
107	qA	0.12	0/2244	0.33	0/3124
107	qa	0.12	0/2244	0.33	0/3124
108	QB	0.13	0/2369	0.35	0/3297
108	Qb	0.13	0/2369	0.35	0/3297
108	qB	0.13	0/2369	0.35	0/3297
108	qb	0.13	0/2369	0.35	0/3297
109	QC	0.12	0/2108	0.36	0/2937
109	Qc	0.13	0/2103	0.32	0/2930
109	qC	0.13	0/2108	0.36	0/2937
109	qc	0.13	0/2103	0.32	0/2930
110	QD	0.12	0/1447	0.36	0/2008
110	Qd	0.12	0/1447	0.36	0/2008
110	qD	0.13	0/1447	0.36	0/2008
110	qd	0.13	0/1447	0.36	0/2008
111	QE	0.13	0/1129	0.34	0/1566
111	Qe	0.13	0/1075	0.34	0/1491
111	qE	0.14	0/1129	0.34	0/1566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
111	qe	0.14	0/1075	0.34	0/1491
112	QF	0.12	0/440	0.36	0/612
112	Qf	0.12	0/396	0.36	0/551
112	qF	0.13	0/440	0.37	0/612
112	qf	0.13	0/396	0.36	0/551
113	QG	0.12	0/1620	0.35	0/2258
113	Qg	0.11	0/1615	0.32	0/2251
113	qG	0.13	0/1620	0.35	0/2258
113	qg	0.11	0/1615	0.33	0/2251
114	QH	0.12	0/634	0.34	0/880
114	Qh	0.14	0/634	0.37	0/880
114	qH	0.12	0/634	0.34	0/880
114	qh	0.14	0/634	0.37	0/880
115	QI	0.12	0/566	0.31	0/789
115	Qi	0.11	0/566	0.31	0/789
115	qI	0.13	0/566	0.31	0/789
115	qi	0.12	0/566	0.31	0/789
116	QJ	0.15	0/276	0.37	0/383
116	Qj	0.08	0/286	0.27	0/397
116	qJ	0.16	0/276	0.36	0/383
116	qj	0.09	0/286	0.27	0/397
117	QL	0.08	0/159	0.24	0/221
117	Ql	0.10	0/159	0.23	0/221
117	qL	0.09	0/159	0.24	0/221
117	ql	0.11	0/159	0.23	0/221
118	S1	0.12	0/3399	0.34	0/4730
118	s1	0.13	0/3399	0.34	0/4730
119	S2	0.13	0/2184	0.35	0/3041
119	s2	0.14	0/2184	0.35	0/3041
120	S3	0.13	0/987	0.35	0/1379
120	s3	0.13	0/987	0.35	0/1379
121	S4	0.11	0/899	0.31	0/1251
121	s4	0.11	0/899	0.31	0/1251
122	S5	0.11	0/461	0.32	0/642
122	s5	0.12	0/461	0.32	0/642
123	S6	0.13	0/454	0.34	0/631
123	s6	0.13	0/454	0.34	0/631
124	S7	0.14	0/791	0.36	0/1098
124	s7	0.14	0/791	0.36	0/1098
125	S8	0.14	0/1079	0.34	0/1503
125	s8	0.15	0/1079	0.34	0/1503
126	SA	0.12	0/2936	0.36	0/4074
126	sa	0.13	0/2936	0.36	0/4074

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
127	SB	0.14	0/1383	0.37	0/1928
127	sb	0.14	0/1383	0.37	0/1928
128	SC	0.16	0/285	0.34	0/395
128	sc	0.17	0/285	0.34	0/395
129	SD	0.08	0/219	0.27	0/305
129	sd	0.09	0/219	0.27	0/305
130	T1	0.12	0/2489	0.33	0/3471
130	t1	0.12	0/2489	0.33	0/3471
131	T2	0.12	0/1375	0.32	0/1912
131	t2	0.12	0/1375	0.32	0/1912
132	T3	0.11	0/1540	0.30	0/2149
132	t3	0.11	0/1540	0.30	0/2149
133	T4	0.11	0/980	0.31	0/1365
133	t4	0.12	0/980	0.31	0/1365
134	T5	0.12	0/697	0.31	0/970
134	t5	0.12	0/697	0.31	0/970
135	T6	0.10	0/541	0.28	0/754
135	t6	0.10	0/541	0.27	0/754
136	T7	0.09	0/701	0.25	0/975
136	t7	0.10	0/701	0.25	0/975
137	T8	0.11	0/650	0.31	0/906
137	t8	0.11	0/650	0.31	0/906
138	T9	0.11	0/650	0.32	0/903
138	t9	0.12	0/650	0.32	0/903
139	TA	0.11	0/503	0.30	0/699
139	ta	0.12	0/503	0.30	0/699
140	TB	0.10	0/474	0.30	0/659
140	tb	0.11	0/474	0.30	0/659
141	TC	0.10	0/457	0.29	0/637
141	tc	0.10	0/457	0.29	0/637
142	TD	0.09	0/358	0.31	0/499
142	td	0.10	0/358	0.31	0/499
143	TE	0.10	0/247	0.28	0/343
143	te	0.10	0/247	0.28	0/343
144	TF	0.10	0/1073	0.29	0/1497
144	tf	0.11	0/1073	0.29	0/1497
145	TG	0.10	0/664	0.28	0/925
145	tg	0.11	0/664	0.28	0/925
146	TH	0.09	0/610	0.26	0/847
146	th	0.09	0/610	0.26	0/847
147	TX	0.12	0/714	0.30	0/995
147	tx	0.12	0/714	0.30	0/995
148	V1	0.12	0/2162	0.38	2/2997 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
148	v1	0.12	0/2162	0.38	2/2997 (0.1%)
149	V2	0.11	0/1143	0.33	0/1592
149	v2	0.12	0/1143	0.33	0/1592
150	X1	0.10	0/731	0.30	0/1014
150	x1	0.10	0/731	0.30	0/1014
All	All	0.13	0/442770	0.35	18/616418 (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
148	V1	0	1
148	v1	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	57	87	PRO	N-CA-CB	7.96	111.61	103.25
3	c	87	PRO	N-CA-CB	7.94	111.59	103.25
3	02	87	PRO	N-CA-CB	7.82	111.46	103.25
3	C	87	PRO	N-CA-CB	7.81	111.45	103.25
3	c	69	PRO	N-CA-CB	7.26	110.10	103.20
3	57	69	PRO	N-CA-CB	7.25	110.09	103.20
3	C	69	PRO	N-CA-CB	6.66	110.14	102.88
3	02	69	PRO	N-CA-CB	6.60	110.08	102.88
148	V1	229	PRO	CA-C-N	-5.73	110.05	120.94
148	V1	229	PRO	C-N-CA	-5.73	110.05	120.94
148	v1	229	PRO	CA-C-N	-5.71	110.08	120.94
148	v1	229	PRO	C-N-CA	-5.71	110.08	120.94
1	a	399	HIS	CA-C-N	-5.23	113.82	123.65
1	a	399	HIS	C-N-CA	-5.23	113.82	123.65
1	55	399	HIS	CA-C-N	-5.21	113.85	123.65
1	55	399	HIS	C-N-CA	-5.21	113.85	123.65
1	55	218	VAL	N-CA-C	-5.10	108.30	113.20
1	a	218	VAL	N-CA-C	-5.08	108.32	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
148	V1	228	PRO	Peptide
148	v1	228	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	00	2228	0	956	6	0
1	55	2228	0	956	5	0
1	A	2228	0	956	7	0
1	a	2228	0	956	5	0
2	01	2116	0	954	12	0
2	56	2116	0	954	16	0
2	B	2116	0	954	11	0
2	b	2116	0	954	14	0
3	02	1003	0	475	8	0
3	57	1003	0	475	7	0
3	C	1003	0	475	8	0
3	c	1003	0	475	7	0
4	03	1427	0	633	5	0
4	58	1427	0	633	8	0
4	D	1427	0	633	4	0
4	d	1427	0	633	8	0
5	04	1905	0	847	6	0
5	59	1905	0	847	3	0
5	E	1905	0	847	5	0
5	e	1905	0	847	2	0
6	05	1205	0	528	2	0
6	60	1205	0	528	3	0
6	F	1205	0	528	5	0
6	f	1205	0	528	3	0
7	06	1454	0	617	6	0
7	61	1454	0	617	3	0
7	G	1454	0	617	6	0
7	g	1454	0	617	3	0
8	07	1469	0	665	4	0
8	62	1469	0	665	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1469	0	665	5	0
8	h	1469	0	665	11	0
9	08	1141	0	519	6	0
9	63	1141	0	519	5	0
9	I	1141	0	519	6	0
9	i	1141	0	519	4	0
10	09	931	0	406	4	0
10	64	931	0	406	1	0
10	J	931	0	406	4	0
10	j	931	0	406	2	0
11	0A	346	0	156	0	0
11	45	346	0	156	1	0
11	6T	346	0	156	1	0
11	6t	346	0	156	0	0
12	0B	1858	0	873	32	0
12	46	1858	0	873	37	0
12	BP	1858	0	873	36	0
12	bp	1858	0	873	33	0
13	0C	928	0	408	3	0
13	47	928	0	408	6	0
13	FS	928	0	408	8	0
13	fs	928	0	408	4	0
14	0D	494	0	221	0	0
14	48	494	0	221	0	0
14	4A	494	0	221	0	0
14	4a	494	0	221	0	0
15	0E	1711	0	704	8	0
15	49	1711	0	704	2	0
15	Y7	1711	0	704	2	0
15	y7	1711	0	704	8	0
16	0F	947	0	389	1	0
16	50	947	0	389	2	0
16	Y5	947	0	389	1	0
16	y5	947	0	389	1	0
17	0G	444	0	191	0	0
17	51	444	0	191	5	0
17	Y0	444	0	191	5	0
17	y0	444	0	191	0	0
18	0H	479	0	241	1	0
18	52	479	0	241	0	0
18	Z1	479	0	241	0	0
18	z1	479	0	241	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	0I	460	0	94	2	0
19	53	460	0	94	8	0
19	U1	460	0	94	9	0
19	u1	460	0	94	2	0
20	0J	85	0	19	3	0
20	54	85	0	19	5	0
20	QM	85	0	19	1	0
20	Qm	85	0	19	0	0
20	U2	85	0	19	5	0
20	qM	85	0	19	1	0
20	qm	85	0	19	0	0
20	u2	85	0	19	3	0
21	10	1032	0	443	4	0
21	65	1032	0	443	2	0
21	K	1032	0	443	3	0
21	k	1032	0	443	2	0
22	11	965	0	406	7	0
22	66	965	0	406	6	0
22	L	965	0	406	7	0
22	l	965	0	406	6	0
23	12	1083	0	467	3	0
23	67	1083	0	467	0	0
23	M	1083	0	467	3	0
23	m	1083	0	467	0	0
24	13	1016	0	459	6	0
24	68	1016	0	459	4	0
24	N	1016	0	459	7	0
24	n	1016	0	459	4	0
25	14	641	0	274	1	0
25	69	641	0	274	1	0
25	O	641	0	274	0	0
25	o	641	0	274	1	0
26	15	865	0	380	2	0
26	70	865	0	380	1	0
26	P	865	0	380	2	0
26	p	865	0	380	1	0
27	16	855	0	366	0	0
27	71	855	0	366	1	0
27	Q	855	0	366	0	0
27	q	855	0	366	0	0
28	17	852	0	368	1	0
28	72	852	0	368	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	R	852	0	368	1	0
28	r	852	0	368	0	0
29	18	841	0	371	3	0
29	73	841	0	371	1	0
29	S	841	0	371	3	0
29	s	841	0	371	1	0
30	19	771	0	340	4	0
30	74	771	0	340	2	0
30	T	771	0	340	3	0
30	t	771	0	340	2	0
31	1B	293	0	126	0	0
31	1b	293	0	126	0	0
32	20	757	0	334	1	0
32	75	757	0	334	2	0
32	U	757	0	334	1	0
32	u	757	0	334	2	0
33	21	722	0	303	3	0
33	76	722	0	303	3	0
33	V	722	0	303	3	0
33	v	722	0	303	3	0
34	22	612	0	267	4	0
34	77	612	0	267	3	0
34	W	612	0	267	4	0
34	w	612	0	267	3	0
35	23	602	0	277	2	0
35	78	602	0	277	0	0
35	X	602	0	277	2	0
35	x	602	0	277	0	0
36	24	517	0	243	3	0
36	79	517	0	243	1	0
36	Y	517	0	243	3	0
36	y	517	0	243	1	0
37	25	429	0	188	1	0
37	80	429	0	188	0	0
37	Z	429	0	188	1	0
37	z	429	0	188	0	0
38	26	3328	0	1462	4	0
38	81	3328	0	1462	9	0
38	C1	3328	0	1462	4	0
38	c1	3328	0	1462	10	0
39	27	2975	0	1241	9	0
39	82	2975	0	1241	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C2	2975	0	1241	9	0
39	c2	2975	0	1241	10	0
40	28	2894	0	1207	4	0
40	83	2894	0	1207	10	0
40	C3	2894	0	1207	6	0
40	c3	2894	0	1207	11	0
41	29	2765	0	1203	7	0
41	84	2765	0	1203	7	0
41	VB	2765	0	1203	7	0
41	vb	2765	0	1203	6	0
42	2B	884	0	368	3	0
42	2b	884	0	368	3	0
43	2E	1591	0	708	4	0
43	2e	1591	0	708	5	0
44	2F	1077	0	481	0	0
44	2f	1077	0	481	0	0
45	2G	984	0	433	0	0
45	2g	984	0	433	0	0
46	2H	507	0	220	1	0
46	2h	507	0	220	1	0
47	2I	564	0	269	1	0
47	2i	564	0	269	1	0
48	2J	505	0	241	1	0
48	2j	505	0	241	1	0
49	2K	462	0	201	3	0
49	2k	462	0	201	3	0
50	2L	415	0	181	1	0
50	2l	415	0	181	1	0
51	2M	370	0	165	1	0
51	2m	370	0	165	1	0
52	2N	302	0	132	0	0
52	2n	302	0	132	0	0
53	2O	210	0	97	0	0
53	2o	210	0	97	0	0
54	30	624	0	273	3	0
54	6A	624	0	273	2	0
54	6a	624	0	273	1	0
54	85	624	0	273	1	0
55	31	1101	0	481	0	0
55	6B	1101	0	481	0	0
55	6b	1101	0	481	3	0
55	86	1101	0	481	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	32	499	0	235	0	0
56	6C	499	0	235	0	0
56	6c	499	0	235	0	0
56	87	499	0	235	0	0
57	33	383	0	163	1	0
57	6L	383	0	163	1	0
57	6l	383	0	163	1	0
57	88	383	0	163	1	0
58	34	659	0	293	4	0
58	7A	659	0	293	4	0
58	7a	659	0	293	4	0
58	89	659	0	293	4	0
59	35	1052	0	428	6	0
59	7C	1052	0	428	6	0
59	7c	1052	0	428	3	0
59	90	1052	0	428	2	0
60	36	654	0	277	3	0
60	7L	654	0	277	4	0
60	7l	654	0	277	3	0
60	91	654	0	277	3	0
61	37	1709	0	794	7	0
61	92	1709	0	794	4	0
61	M1	1709	0	794	7	0
61	m1	1709	0	794	4	0
62	38	1561	0	745	5	0
62	93	1561	0	745	2	0
62	M2	1561	0	745	5	0
62	m2	1561	0	745	2	0
63	39	1624	0	768	4	0
63	94	1624	0	768	2	0
63	M3	1624	0	768	4	0
63	m3	1624	0	768	2	0
64	1T	349	0	164	1	0
64	1t	349	0	164	2	0
64	40	349	0	164	1	0
64	95	349	0	164	2	0
65	2T	348	0	148	1	0
65	2t	348	0	148	0	0
65	41	348	0	148	1	0
65	96	348	0	148	0	0
66	3T	413	0	184	0	0
66	3t	413	0	184	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	42	413	0	184	0	0
66	97	413	0	184	1	0
67	43	285	0	124	0	0
67	4T	285	0	124	0	0
67	4t	285	0	124	0	0
67	98	285	0	124	0	0
68	44	309	0	138	0	0
68	5T	309	0	138	0	0
68	5t	309	0	138	1	0
68	99	309	0	138	0	0
69	4L	576	0	248	0	0
69	4l	576	0	248	0	0
70	5B	498	0	204	3	0
70	5b	498	0	204	3	0
71	A1	463	0	189	0	0
71	a1	463	0	189	0	0
72	A2	487	0	216	1	0
72	a2	487	0	216	1	0
73	A3	633	0	291	4	0
73	a3	633	0	291	4	0
74	A5	771	0	325	2	0
74	a5	771	0	325	2	0
75	A6	847	0	366	2	0
75	a6	847	0	366	1	0
76	A7	1404	0	613	4	0
76	a7	1404	0	613	4	0
77	A8	658	0	287	0	0
77	a8	658	0	287	0	0
78	A9	1678	0	771	5	0
78	a9	1678	0	771	5	0
79	AB	557	0	239	0	0
79	ab	557	0	239	0	0
80	AC	488	0	217	3	0
80	ac	488	0	217	3	0
81	AL	949	0	416	5	0
81	al	949	0	416	5	0
82	AM	794	0	356	2	0
82	am	794	0	356	2	0
83	AN	1135	0	514	2	0
83	an	1135	0	514	1	0
84	B2	590	0	267	1	0
84	b2	590	0	267	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	B3	342	0	144	0	0
85	b3	342	0	144	0	0
86	B4	568	0	247	1	0
86	b4	568	0	247	1	0
87	B6	348	0	145	6	0
87	b6	348	0	145	5	0
88	B7	572	0	268	2	0
88	b7	572	0	268	2	0
89	B8	862	0	374	1	0
89	b8	862	0	374	1	0
90	B9	935	0	409	2	0
90	b9	935	0	409	2	0
91	BL	869	0	376	5	0
91	bl	869	0	376	4	0
92	BM	810	0	367	3	0
92	bm	810	0	367	3	0
93	C4	507	0	236	3	0
93	c4	507	0	236	3	0
94	FX	722	0	316	2	0
94	fx	722	0	316	2	0
95	G1	1126	0	510	3	0
95	g1	1126	0	510	3	0
96	G2	1129	0	516	2	0
96	g2	1129	0	516	2	0
97	G3	1711	0	748	4	0
97	g3	1711	0	748	4	0
98	J1	1306	0	610	6	0
98	j1	1306	0	610	6	0
99	N1	1397	0	623	2	0
99	n1	1397	0	623	2	0
100	N2	1793	0	745	1	0
100	n2	1793	0	745	1	0
101	N3	596	0	260	0	0
101	n3	596	0	260	0	0
102	N4	2502	0	1081	5	0
102	n4	2502	0	1081	5	0
103	N5	3517	0	1517	13	0
103	n5	3517	0	1517	13	0
104	N6	1269	0	528	2	0
104	n6	1269	0	528	2	0
105	P1	1139	0	495	5	0
105	p1	1139	0	495	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
106	P2	831	0	344	5	0
106	p2	831	0	344	5	0
107	QA	2246	0	1055	8	0
107	Qa	2246	0	1055	9	0
107	qA	2246	0	1055	9	0
107	qa	2246	0	1055	10	0
108	QB	2370	0	1090	5	0
108	Qb	2370	0	1090	9	0
108	qB	2370	0	1090	7	0
108	qb	2370	0	1090	9	0
109	QC	2109	0	920	5	0
109	Qc	2104	0	918	12	0
109	qC	2109	0	920	5	0
109	qc	2104	0	918	10	0
110	QD	1448	0	640	5	0
110	Qd	1448	0	640	8	0
110	qD	1448	0	640	5	0
110	qd	1448	0	640	7	0
111	QE	1131	0	499	6	0
111	Qe	1077	0	476	4	0
111	qE	1131	0	499	6	0
111	qe	1077	0	476	3	0
112	QF	441	0	190	0	0
112	Qf	397	0	172	0	0
112	qF	441	0	190	0	0
112	qf	397	0	172	0	0
113	QG	1621	0	728	8	0
113	Qg	1616	0	726	4	0
113	qG	1621	0	728	8	0
113	qg	1616	0	726	4	0
114	QH	635	0	274	4	0
114	Qh	635	0	274	4	0
114	qH	635	0	274	4	0
114	qh	635	0	274	3	0
115	QI	567	0	244	2	0
115	Qi	567	0	244	1	0
115	qI	567	0	244	2	0
115	qi	567	0	244	1	0
116	QJ	277	0	117	0	0
116	Qj	287	0	121	2	0
116	qJ	277	0	117	0	0
116	qj	287	0	121	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
117	QL	160	0	76	0	0
117	Ql	160	0	76	0	0
117	qL	160	0	76	0	0
117	ql	160	0	76	0	0
118	S1	3400	0	1552	17	0
118	s1	3400	0	1552	17	0
119	S2	2185	0	952	9	0
119	s2	2185	0	952	9	0
120	S3	988	0	412	4	0
120	s3	988	0	412	3	0
121	S4	900	0	402	2	0
121	s4	900	0	402	2	0
122	S5	462	0	207	0	0
122	s5	462	0	207	0	0
123	S6	455	0	199	6	0
123	s6	455	0	199	6	0
124	S7	792	0	361	3	0
124	s7	792	0	361	2	0
125	S8	1080	0	462	5	0
125	s8	1080	0	462	5	0
126	SA	2937	0	1413	13	0
126	sa	2937	0	1413	13	0
127	SB	1384	0	588	4	0
127	sb	1384	0	588	4	0
128	SC	286	0	134	0	0
128	sc	286	0	134	0	0
129	SD	220	0	93	0	0
129	sd	220	0	93	0	0
130	T1	2490	0	1129	11	0
130	t1	2490	0	1129	11	0
131	T2	1376	0	636	6	0
131	t2	1376	0	636	6	0
132	T3	1541	0	699	4	0
132	t3	1541	0	699	4	0
133	T4	981	0	430	4	0
133	t4	981	0	430	4	0
134	T5	698	0	325	3	0
134	t5	698	0	325	2	0
135	T6	542	0	244	1	0
135	t6	542	0	244	1	0
136	T7	702	0	316	0	0
136	t7	702	0	316	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
137	T8	651	0	285	1	0
137	t8	651	0	285	1	0
138	T9	651	0	285	2	0
138	t9	651	0	285	2	0
139	TA	504	0	209	0	0
139	ta	504	0	209	0	0
140	TB	475	0	219	2	0
140	tb	475	0	219	2	0
141	TC	458	0	202	0	0
141	tc	458	0	202	0	0
142	TD	359	0	162	0	0
142	td	359	0	162	0	0
143	TE	248	0	107	1	0
143	te	248	0	107	1	0
144	TF	1074	0	474	1	0
144	tf	1074	0	474	2	0
145	TG	665	0	292	0	0
145	tg	665	0	292	0	0
146	TH	611	0	276	3	0
146	th	611	0	276	3	0
147	TX	715	0	320	0	0
147	tx	715	0	320	0	0
148	V1	2163	0	1005	6	0
148	v1	2163	0	1005	6	0
149	V2	1144	0	503	2	0
149	v2	1144	0	503	2	0
150	X1	732	0	317	0	0
150	x1	732	0	317	0	0
151	0C	8	0	0	1	0
151	47	8	0	0	2	0
151	FS	8	0	0	2	0
151	FX	4	0	0	0	0
151	QE	4	0	0	0	0
151	Qe	4	0	0	0	0
151	S1	4	0	0	0	0
151	SB	4	0	0	1	0
151	V2	4	0	0	0	0
151	fs	8	0	0	2	0
151	fx	4	0	0	0	0
151	qE	4	0	0	0	0
151	qe	4	0	0	0	0
151	s1	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
151	sb	4	0	0	1	0
151	v2	4	0	0	0	0
152	0F	43	0	30	0	0
152	50	43	0	30	0	0
152	QC	86	0	60	0	0
152	Qc	86	0	60	2	0
152	Y5	43	0	30	0	0
152	qC	86	0	60	0	0
152	qc	86	0	60	2	0
152	y5	43	0	30	0	0
153	26	120	0	108	4	0
153	81	120	0	108	9	0
153	C1	120	0	108	4	0
153	c1	120	0	108	9	0
154	26	1	0	0	0	0
154	27	2	0	0	0	0
154	81	1	0	0	0	0
154	82	2	0	0	0	0
154	C1	1	0	0	0	0
154	C2	2	0	0	0	0
154	c1	1	0	0	0	0
154	c2	2	0	0	0	0
155	26	1	0	0	0	0
155	81	1	0	0	0	0
155	C1	1	0	0	0	0
155	c1	1	0	0	0	0
156	29	2	0	0	0	0
156	84	2	0	0	0	0
156	S6	1	0	0	0	0
156	VB	2	0	0	0	0
156	s6	1	0	0	0	0
156	vb	2	0	0	0	0
157	2E	43	0	32	0	0
157	2e	43	0	32	0	0
157	QD	43	0	32	0	0
157	Qd	43	0	32	0	0
157	qD	43	0	32	0	0
157	qd	43	0	32	0	0
158	A9	48	0	26	1	0
158	a9	48	0	26	1	0
159	B8	27	0	12	0	0
159	b8	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
160	Qc	26	0	35	1	0
160	qc	26	0	35	1	0
161	S1	16	0	0	0	0
161	S7	8	0	0	0	0
161	S8	16	0	0	1	0
161	SB	8	0	0	1	0
161	V1	8	0	0	0	0
161	s1	16	0	0	0	0
161	s7	8	0	0	0	0
161	s8	16	0	0	1	0
161	sb	8	0	0	1	0
161	v1	8	0	0	0	0
162	SA	53	0	31	1	0
162	sa	53	0	31	1	0
163	SB	7	0	0	0	0
163	sb	7	0	0	0	0
164	V1	31	0	19	1	0
164	v1	31	0	19	0	0
All	All	447736	0	197816	1361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (1361) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:398:VAL:O	2:b:421:VAL:HA	1.63	0.99
2:56:398:VAL:O	2:56:421:VAL:HA	1.63	0.98
98:J1:154:TYR:O	98:J1:179:SER:N	2.18	0.77
98:j1:154:TYR:O	98:j1:179:SER:N	2.18	0.77
15:0E:207:GLY:HA3	3:57:168:ILE:HA	1.68	0.76
3:c:168:ILE:HA	15:y7:207:GLY:HA3	1.68	0.75
12:bp:169:LYS:N	12:bp:181:VAL:O	2.20	0.74
12:BP:169:LYS:N	12:BP:181:VAL:O	2.21	0.74
153:c1:703:HEA:HBA1	153:c1:703:HEA:HHA	1.70	0.73
12:0B:169:LYS:N	12:0B:181:VAL:O	2.20	0.73
12:46:169:LYS:N	12:46:181:VAL:O	2.21	0.72
99:n1:261:ILE:HA	99:n1:266:GLY:HA2	1.70	0.72
99:N1:261:ILE:HA	99:N1:266:GLY:HA2	1.70	0.72
108:qB:73:VAL:HA	108:qB:246:PHE:O	1.89	0.72
118:S1:306:PRO:HA	118:S1:577:ILE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:81:703:HEA:HHA	153:81:703:HEA:HBA1	1.70	0.71
108:QB:73:VAL:HA	108:QB:246:PHE:O	1.89	0.71
103:N5:479:ASP:HA	103:N5:537:ASP:HA	1.72	0.71
118:s1:306:PRO:HA	118:s1:577:ILE:O	1.90	0.71
103:n5:479:ASP:HA	103:n5:537:ASP:HA	1.71	0.70
23:M:190:ALA:O	36:Y:1:MET:N	2.25	0.70
12:46:267:GLY:HA3	12:46:342:ARG:HA	1.75	0.69
2:B:398:VAL:O	2:B:421:VAL:HA	1.92	0.69
12:bp:115:SER:N	12:bp:127:ILE:O	2.22	0.69
23:12:190:ALA:O	36:24:1:MET:N	2.25	0.69
2:01:398:VAL:O	2:01:421:VAL:HA	1.92	0.68
12:0B:115:SER:N	12:0B:127:ILE:O	2.22	0.68
12:BP:267:GLY:HA3	12:BP:342:ARG:HA	1.75	0.68
106:P2:146:ASN:O	106:P2:150:ASN:N	2.27	0.68
106:p2:146:ASN:O	106:p2:150:ASN:N	2.27	0.68
126:sa:226:SER:O	126:sa:230:GLY:N	2.27	0.68
59:35:172:VAL:H	62:38:214:GLY:HA3	1.58	0.68
59:7C:172:VAL:H	62:M2:214:GLY:HA3	1.58	0.68
118:S1:49:THR:HA	118:S1:96:GLN:HA	1.76	0.67
12:0B:412:THR:O	12:0B:415:GLY:N	2.28	0.67
131:T2:76:GLU:O	131:T2:78:ASN:N	2.27	0.67
2:56:426:PHE:O	2:56:430:ARG:N	2.28	0.67
118:s1:49:THR:HA	118:s1:96:GLN:HA	1.76	0.67
131:t2:76:GLU:O	131:t2:78:ASN:N	2.27	0.67
103:N5:80:SER:O	103:N5:83:ASN:N	2.27	0.67
126:SA:226:SER:O	126:SA:230:GLY:N	2.27	0.67
12:bp:412:THR:O	12:bp:415:GLY:N	2.28	0.67
12:46:284:ALA:O	12:46:288:HIS:N	2.26	0.67
33:21:48:PRO:HA	38:26:686:TYR:HA	1.78	0.66
2:b:426:PHE:O	2:b:430:ARG:N	2.28	0.66
61:M1:261:GLU:O	61:M1:265:PHE:N	2.29	0.66
22:66:92:GLN:HA	22:66:198:THR:HA	1.77	0.66
132:T3:260:VAL:O	132:T3:264:LEU:N	2.29	0.66
12:46:398:ILE:HA	12:46:412:THR:HA	1.77	0.66
132:t3:260:VAL:O	132:t3:264:LEU:N	2.29	0.66
12:0B:267:GLY:HA3	12:0B:342:ARG:HA	1.78	0.65
22:l:92:GLN:HA	22:l:198:THR:HA	1.77	0.65
38:C1:686:TYR:HA	33:V:48:PRO:HA	1.78	0.65
61:37:261:GLU:O	61:37:265:PHE:N	2.29	0.65
12:46:412:THR:O	12:46:415:GLY:N	2.29	0.65
103:n5:80:SER:O	103:n5:83:ASN:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:l:53:ASN:O	22:l:57:TYR:N	2.28	0.65
12:BP:284:ALA:O	12:BP:288:HIS:N	2.26	0.65
12:BP:412:THR:O	12:BP:415:GLY:N	2.29	0.65
12:0B:203:ASP:O	12:0B:207:ASN:N	2.27	0.65
60:36:913:ARG:O	60:36:918:GLY:N	2.22	0.65
19:u1:74:UNK:O	19:u1:78:UNK:N	2.29	0.65
2:B:290:ILE:N	2:B:357:LEU:O	2.30	0.65
2:01:290:ILE:N	2:01:357:LEU:O	2.30	0.64
13:0C:70:GLY:HA2	13:0C:144:ASN:HA	1.79	0.64
93:C4:8:GLY:HA3	93:C4:42:ALA:HA	1.79	0.64
12:bp:267:GLY:HA3	12:bp:342:ARG:HA	1.79	0.64
9:i:210:LYS:O	9:i:214:ASP:N	2.29	0.64
12:BP:398:ILE:HA	12:BP:412:THR:HA	1.77	0.64
20:U2:6:UNK:O	20:U2:10:UNK:N	2.30	0.64
133:T4:89:ILE:O	133:T4:93:ASN:N	2.31	0.64
12:BP:240:LYS:N	12:BP:252:VAL:O	2.30	0.64
109:qc:222:TRP:HA	109:qc:226:ALA:HB3	1.80	0.64
22:11:53:ASN:O	22:11:57:TYR:N	2.26	0.64
12:46:240:LYS:N	12:46:252:VAL:O	2.31	0.64
9:63:210:LYS:O	9:63:214:ASP:N	2.29	0.64
108:qB:243:GLY:N	108:qB:271:ALA:O	2.28	0.64
108:QB:296:ASP:HA	114:QH:56:ARG:HA	1.80	0.64
21:k:96:LEU:O	21:k:100:LYS:N	2.31	0.64
21:65:96:LEU:O	21:65:100:LYS:N	2.31	0.64
108:qB:296:ASP:HA	114:qH:56:ARG:HA	1.80	0.64
13:fs:70:GLY:HA2	13:fs:144:ASN:HA	1.79	0.64
22:L:53:ASN:O	22:L:57:TYR:N	2.26	0.64
19:0L:74:UNK:O	19:0L:78:UNK:N	2.29	0.64
43:2e:151:THR:HA	43:2e:212:ALA:HB3	1.80	0.64
20:54:6:UNK:O	20:54:10:UNK:N	2.30	0.64
39:82:576:TRP:O	39:82:581:LEU:N	2.31	0.64
61:92:280:TYR:O	61:92:283:ALA:HB3	1.98	0.64
39:c2:576:TRP:O	39:c2:581:LEU:N	2.31	0.64
133:t4:89:ILE:O	133:t4:93:ASN:N	2.31	0.63
109:qc:49:GLY:O	109:qc:53:ALA:N	2.31	0.63
126:sa:90:ALA:HB3	126:sa:184:GLY:HA3	1.79	0.63
126:SA:90:ALA:HB3	126:SA:184:GLY:HA3	1.79	0.63
12:bp:168:VAL:HA	12:bp:182:THR:HA	1.80	0.63
2:B:429:LEU:O	2:B:433:ALA:N	2.30	0.63
12:0B:168:VAL:HA	12:0B:182:THR:HA	1.80	0.63
43:2E:151:THR:HA	43:2E:212:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:m1:280:TYR:O	61:m1:283:ALA:HB3	1.98	0.63
12:BP:298:GLN:N	12:BP:310:LEU:O	2.32	0.63
12:BP:334:GLY:O	21:K:47:GLU:N	2.32	0.63
21:10:47:GLU:N	12:46:334:GLY:O	2.32	0.62
12:46:159:SER:O	12:46:163:ASP:N	2.32	0.62
93:c4:8:GLY:HA3	93:c4:42:ALA:HA	1.79	0.62
109:Qc:222:TRP:HA	109:Qc:226:ALA:HB3	1.80	0.62
39:C2:112:LEU:N	39:C2:502:ASN:O	2.31	0.62
12:46:133:LEU:O	12:46:158:VAL:N	2.31	0.62
109:Qc:49:GLY:O	109:Qc:53:ALA:N	2.31	0.62
153:c1:703:HEA:HBA1	153:c1:703:HEA:CHA	2.28	0.62
94:fx:47:ILE:HA	94:fx:158:ILE:O	1.98	0.62
12:46:298:GLN:N	12:46:310:LEU:O	2.32	0.62
94:FX:47:ILE:HA	94:FX:158:ILE:O	1.98	0.62
153:81:703:HEA:HBA1	153:81:703:HEA:CHA	2.28	0.62
61:37:11:ARG:N	62:38:4:SER:O	2.31	0.62
108:QB:243:GLY:N	108:QB:271:ALA:O	2.28	0.62
12:BP:159:SER:O	12:BP:163:ASP:N	2.32	0.62
73:a3:10:PHE:HA	73:a3:15:ASN:HA	1.81	0.62
153:26:701:HEA:HMA	153:26:701:HEA:HBA2	1.82	0.61
73:A3:10:PHE:HA	73:A3:15:ASN:HA	1.81	0.61
94:FX:49:ASN:O	94:FX:52:GLY:N	2.33	0.61
103:n5:268:VAL:O	103:n5:272:THR:N	2.33	0.61
43:2e:33:ASP:O	43:2e:35:PHE:N	2.25	0.61
12:BP:133:LEU:O	12:BP:158:VAL:N	2.31	0.61
153:C1:701:HEA:HMA	153:C1:701:HEA:HBA2	1.82	0.61
5:E:193:GLN:O	5:E:197:GLY:N	2.31	0.61
49:2k:35:ASN:O	49:2k:39:VAL:N	2.25	0.61
94:fx:49:ASN:O	94:fx:52:GLY:N	2.33	0.61
95:g1:52:TYR:O	95:g1:71:GLU:N	2.31	0.61
4:d:211:PRO:HA	4:d:236:PHE:HA	1.82	0.61
5:04:193:GLN:O	5:04:197:GLY:N	2.31	0.61
60:7L:913:ARG:O	60:7L:918:GLY:N	2.22	0.61
39:82:7:THR:O	39:82:544:PHE:N	2.24	0.60
22:L:92:GLN:HA	22:L:198:THR:HA	1.83	0.60
43:2e:10:ASN:O	43:2e:14:GLN:N	2.33	0.60
22:11:92:GLN:HA	22:11:198:THR:HA	1.83	0.60
126:SA:276:GLU:HA	126:SA:599:LEU:HA	1.83	0.60
149:V2:198:ASP:O	149:V2:202:GLY:N	2.35	0.60
126:sa:276:GLU:HA	126:sa:599:LEU:HA	1.83	0.60
149:v2:198:ASP:O	149:v2:202:GLY:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
103:N5:186:PHE:O	103:N5:190:CYS:N	2.34	0.60
49:2K:35:ASN:O	49:2K:39:VAL:N	2.25	0.60
103:N5:268:VAL:O	103:N5:272:THR:N	2.33	0.60
2:B:293:GLY:N	2:B:355:THR:O	2.34	0.60
43:2E:10:ASN:O	43:2E:14:GLN:N	2.33	0.60
80:ac:79:LEU:O	80:ac:120:GLU:N	2.34	0.60
39:27:112:LEU:N	39:27:502:ASN:O	2.31	0.60
99:n1:59:VAL:O	99:n1:63:GLY:HA2	2.02	0.60
102:n4:433:LEU:O	102:n4:437:SER:N	2.33	0.60
6:F:274:LEU:HA	6:F:281:LYS:H	1.67	0.60
3:57:77:LEU:O	3:57:81:ASP:N	2.34	0.59
109:QC:49:GLY:O	109:QC:53:ALA:N	2.35	0.59
6:05:274:LEU:HA	6:05:281:LYS:H	1.67	0.59
1:55:293:TYR:O	1:55:297:ALA:HB3	2.02	0.59
12:0B:239:TYR:HA	12:0B:253:ASN:HA	1.83	0.59
4:58:211:PRO:HA	4:58:236:PHE:HA	1.82	0.59
109:qc:284:PRO:O	109:qc:287:ALA:HB3	2.03	0.59
97:G3:75:ILE:O	97:G3:94:GLY:N	2.28	0.59
12:bp:239:TYR:HA	12:bp:253:ASN:HA	1.83	0.59
22:66:53:ASN:O	22:66:57:TYR:N	2.28	0.59
103:n5:186:PHE:O	103:n5:190:CYS:N	2.34	0.59
109:qC:49:GLY:O	109:qC:53:ALA:N	2.35	0.59
12:bp:376:VAL:O	12:bp:390:TRP:N	2.33	0.59
3:c:77:LEU:O	3:c:81:ASP:N	2.34	0.59
12:0B:92:ALA:HB2	12:0B:100:ALA:HB2	1.84	0.59
109:Qc:284:PRO:O	109:Qc:287:ALA:HB3	2.03	0.59
43:2E:147:VAL:HA	43:2E:208:LEU:O	2.02	0.59
12:0B:176:SER:O	12:0B:191:GLY:HA3	2.03	0.59
12:46:264:GLY:HA2	12:46:269:LEU:H	1.68	0.59
43:2E:33:ASP:O	43:2E:35:PHE:N	2.25	0.59
38:c1:122:LEU:O	38:c1:126:HIS:N	2.27	0.59
4:03:208:VAL:O	4:03:239:LEU:N	2.36	0.59
2:56:354:LEU:HA	2:56:370:VAL:HA	1.84	0.59
43:2e:147:VAL:HA	43:2e:208:LEU:O	2.02	0.59
2:b:354:LEU:HA	2:b:370:VAL:HA	1.84	0.59
4:D:208:VAL:O	4:D:239:LEU:N	2.36	0.59
12:46:86:TYR:N	12:46:459:ALA:O	2.32	0.59
12:46:203:ASP:O	12:46:207:ASN:N	2.28	0.59
33:76:48:PRO:HA	38:81:686:TYR:HA	1.85	0.59
99:N1:59:VAL:O	99:N1:63:GLY:HA2	2.02	0.59
1:a:293:TYR:O	1:a:297:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:bp:240:LYS:N	12:bp:252:VAL:O	2.36	0.59
12:bp:92:ALA:HB2	12:bp:100:ALA:HB2	1.84	0.58
2:b:429:LEU:O	2:b:433:ALA:N	2.32	0.58
40:c3:67:GLU:O	40:c3:71:TYR:N	2.34	0.58
20:54:3:UNK:O	20:54:7:UNK:N	2.37	0.58
60:7l:914:LEU:HA	60:7l:918:GLY:HA2	1.86	0.58
12:bp:176:SER:O	12:bp:191:GLY:HA3	2.03	0.58
12:0B:240:LYS:N	12:0B:252:VAL:O	2.36	0.58
40:83:87:ASN:O	40:83:91:PHE:CB	2.52	0.58
113:qG:147:LEU:N	113:qG:252:ALA:O	2.35	0.58
59:7c:33:TRP:N	33:v:8:PHE:O	2.25	0.58
12:46:296:THR:O	12:46:312:SER:N	2.37	0.58
41:84:599:ILE:O	41:84:603:ILE:N	2.30	0.58
107:QA:138:GLY:HA3	107:QA:154:ASN:O	2.04	0.58
95:G1:52:TYR:O	95:G1:71:GLU:N	2.31	0.58
2:b:394:HIS:O	2:b:426:PHE:N	2.36	0.58
153:26:701:HEA:HBA2	153:26:701:HEA:CMA	2.34	0.58
1:a:271:VAL:HA	1:a:368:GLN:HA	1.86	0.58
20:U2:3:UNK:O	20:U2:7:UNK:N	2.37	0.58
12:0B:376:VAL:O	12:0B:390:TRP:N	2.33	0.58
23:12:174:ASN:O	23:12:178:GLY:N	2.31	0.58
132:t3:25:LEU:O	132:t3:200:VAL:N	2.37	0.58
61:M1:11:ARG:N	62:M2:4:SER:O	2.31	0.58
39:82:112:LEU:N	39:82:502:ASN:O	2.36	0.58
60:91:914:LEU:HA	60:91:918:GLY:HA2	1.86	0.58
132:T3:25:LEU:O	132:T3:200:VAL:N	2.37	0.58
24:N:165:PHE:O	24:N:169:ARG:N	2.37	0.58
78:A9:193:ALA:O	78:A9:256:GLY:HA2	2.04	0.58
12:bp:284:ALA:O	12:bp:288:HIS:N	2.30	0.58
38:c1:686:TYR:HA	33:v:48:PRO:HA	1.85	0.58
153:C1:701:HEA:HBA2	153:C1:701:HEA:CMA	2.34	0.58
24:N:163:TRP:O	24:N:167:GLN:N	2.32	0.58
12:0B:288:HIS:O	12:0B:292:HIS:N	2.37	0.57
33:76:8:PHE:O	59:90:33:TRP:N	2.25	0.57
107:qa:109:SER:O	107:qa:113:ILE:N	2.33	0.57
80:AC:79:LEU:O	80:AC:120:GLU:N	2.34	0.57
93:C4:73:ALA:O	93:C4:77:SER:N	2.37	0.57
2:01:293:GLY:N	2:01:355:THR:O	2.34	0.57
38:81:122:LEU:O	38:81:126:HIS:N	2.27	0.57
40:83:67:GLU:O	40:83:71:TYR:N	2.34	0.57
97:g3:75:ILE:O	97:g3:94:GLY:N	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:c1:502:GLY:O	153:c1:703:HEA:H263	2.04	0.57
39:c2:112:LEU:N	39:c2:502:ASN:O	2.36	0.57
40:c3:87:ASN:O	40:c3:91:PHE:CB	2.52	0.57
24:13:165:PHE:O	24:13:169:ARG:N	2.37	0.57
107:qA:138:GLY:HA3	107:qA:154:ASN:O	2.04	0.57
12:0B:159:SER:O	12:0B:163:ASP:N	2.38	0.57
34:22:84:LYS:O	34:22:88:TYR:N	2.29	0.57
93:c4:73:ALA:O	93:c4:77:SER:N	2.37	0.57
12:bp:203:ASP:O	12:bp:207:ASN:N	2.27	0.57
34:W:84:LYS:O	34:W:88:TYR:N	2.29	0.57
20:54:8:UNK:O	20:54:12:UNK:N	2.38	0.57
2:56:394:HIS:O	2:56:426:PHE:N	2.36	0.57
108:qb:89:SER:HA	108:qb:149:THR:HA	1.87	0.57
58:7a:23:ALA:O	58:7a:27:LYS:N	2.36	0.57
12:BP:264:GLY:HA2	12:BP:269:LEU:H	1.68	0.57
12:bp:159:SER:O	12:bp:163:ASP:N	2.38	0.57
63:M3:72:THR:O	63:M3:76:SER:N	2.36	0.57
12:46:168:VAL:HA	12:46:182:THR:HA	1.87	0.57
63:94:72:THR:O	63:94:76:SER:N	2.34	0.57
9:08:23:ARG:O	9:08:26:THR:N	2.37	0.57
106:p2:80:LYS:HA	106:p2:152:PHE:O	2.04	0.57
108:Qb:89:SER:HA	108:Qb:149:THR:HA	1.87	0.57
131:T2:36:ARG:HA	131:T2:43:THR:HA	1.86	0.57
12:BP:296:THR:O	12:BP:312:SER:N	2.37	0.57
12:46:92:ALA:HB2	12:46:100:ALA:HB2	1.86	0.57
38:81:502:GLY:O	153:81:703:HEA:H263	2.04	0.57
78:a9:193:ALA:O	78:a9:256:GLY:HA2	2.04	0.57
134:t5:115:ALA:O	134:t5:119:GLY:N	2.37	0.57
102:N4:433:LEU:O	102:N4:437:SER:N	2.33	0.57
2:B:358:PHE:N	2:B:367:ASP:O	2.38	0.57
21:10:96:LEU:O	21:10:100:LYS:N	2.38	0.57
26:15:38:LYS:O	26:15:117:ASN:N	2.38	0.57
61:37:280:TYR:O	61:37:283:ALA:HB3	2.05	0.57
1:A:417:ASP:HA	1:A:435:LYS:O	2.05	0.57
26:P:38:LYS:O	26:P:117:ASN:N	2.38	0.57
1:00:417:ASP:HA	1:00:435:LYS:O	2.05	0.56
143:TE:50:ARG:O	143:TE:71:LEU:N	2.37	0.56
22:L:67:THR:O	22:L:71:ARG:N	2.29	0.56
1:55:271:VAL:HA	1:55:368:GLN:HA	1.86	0.56
12:BP:92:ALA:HB2	12:BP:100:ALA:HB2	1.86	0.56
22:11:67:THR:O	22:11:71:ARG:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:82:267:SER:O	64:95:8:HIS:N	2.35	0.56
54:85:109:GLU:O	54:85:113:GLN:N	2.37	0.56
109:qc:279:HIS:O	109:qc:283:ARG:N	2.36	0.56
131:t2:36:ARG:HA	131:t2:43:THR:HA	1.85	0.56
110:QD:76:VAL:O	110:QD:80:ASN:N	2.36	0.56
106:P2:80:LYS:HA	106:P2:152:PHE:O	2.04	0.56
102:N4:83:LEU:O	102:N4:87:SER:N	2.38	0.56
61:M1:280:TYR:O	61:M1:283:ALA:HB3	2.05	0.56
29:18:19:ALA:HB2	41:29:594:ALA:HB1	1.87	0.56
3:57:25:GLN:O	3:57:29:SER:N	2.37	0.56
19:U1:45:UNK:O	19:U1:49:UNK:N	2.39	0.56
12:BP:168:VAL:HA	12:BP:182:THR:HA	1.87	0.56
41:29:599:ILE:O	41:29:603:ILE:N	2.32	0.56
110:QD:174:TYR:O	110:QD:178:ILE:N	2.34	0.56
64:1t:8:HIS:N	39:c2:267:SER:O	2.35	0.56
39:c2:7:THR:O	39:c2:544:PHE:N	2.24	0.56
21:K:96:LEU:O	21:K:100:LYS:N	2.38	0.56
20:U2:8:UNK:O	20:U2:12:UNK:N	2.38	0.56
19:53:45:UNK:O	19:53:49:UNK:N	2.39	0.56
120:S3:102:ASN:O	120:S3:106:LYS:N	2.39	0.56
130:T1:270:ALA:HB3	130:T1:357:PRO:HA	1.87	0.56
76:A7:14:ASN:O	76:A7:18:ARG:N	2.39	0.56
2:01:358:PHE:N	2:01:367:ASP:O	2.38	0.56
78:a9:193:ALA:O	78:a9:256:GLY:CA	2.53	0.56
127:sb:73:VAL:O	127:sb:87:TYR:HA	2.06	0.56
127:SB:73:VAL:O	127:SB:87:TYR:HA	2.06	0.56
34:77:84:LYS:O	34:77:88:TYR:N	2.28	0.56
76:a7:14:ASN:O	76:a7:18:ARG:N	2.39	0.56
81:al:162:ALA:HB3	118:s1:300:ARG:HA	1.87	0.56
107:qa:334:LEU:O	107:qa:338:LEU:N	2.39	0.56
78:A9:193:ALA:O	78:A9:256:GLY:CA	2.53	0.56
2:B:292:GLN:N	2:B:454:GLN:O	2.39	0.56
2:56:353:THR:HA	2:56:448:VAL:H	1.71	0.56
143:te:50:ARG:O	143:te:71:LEU:N	2.37	0.56
109:Qc:82:TRP:O	109:Qc:86:ARG:N	2.35	0.56
70:5B:41:SER:O	70:5B:45:GLY:HA3	2.06	0.56
15:0E:173:ILE:HA	3:57:174:ALA:H	1.71	0.55
58:34:23:ALA:O	58:34:27:LYS:N	2.35	0.55
93:c4:85:SER:O	93:c4:89:ARG:N	2.39	0.55
93:C4:85:SER:O	93:C4:89:ARG:N	2.39	0.55
12:BP:203:ASP:O	12:BP:207:ASN:N	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:27:267:SER:O	64:40:8:HIS:N	2.35	0.55
90:b9:164:ASN:HA	92:bm:138:ASN:HA	1.89	0.55
110:qD:174:TYR:O	110:qD:178:ILE:N	2.34	0.55
131:t2:37:TYR:N	131:t2:42:ARG:O	2.36	0.55
118:S1:300:ARG:HA	81:AL:162:ALA:HB3	1.87	0.55
54:6a:109:GLU:O	54:6a:113:GLN:N	2.37	0.55
3:c:174:ALA:H	15:y7:173:ILE:HA	1.71	0.55
102:n4:83:LEU:O	102:n4:87:SER:N	2.38	0.55
132:T3:142:ILE:O	132:T3:147:LEU:N	2.31	0.55
12:bp:288:HIS:O	12:bp:292:HIS:N	2.37	0.55
59:7C:108:ALA:O	59:7C:112:MET:N	2.31	0.55
75:a6:146:SER:HA	78:a9:333:VAL:HA	1.89	0.55
29:S:19:ALA:HB2	41:VB:594:ALA:HB1	1.87	0.55
32:U:120:LYS:O	32:U:124:ASP:N	2.33	0.55
2:01:113:LEU:O	2:01:117:LEU:N	2.39	0.55
2:01:292:GLN:N	2:01:454:GLN:O	2.39	0.55
120:s3:102:ASN:O	120:s3:106:LYS:N	2.39	0.55
126:SA:226:SER:O	126:SA:230:GLY:CA	2.55	0.55
34:w:105:ALA:HB3	36:y:68:TYR:HA	1.88	0.55
9:63:166:ASN:N	30:74:4:GLU:O	2.39	0.55
34:77:105:ALA:HB3	36:79:68:TYR:HA	1.88	0.55
74:a5:193:ILE:N	118:s1:657:ILE:O	2.40	0.55
130:T1:375:ILE:N	130:T1:407:HIS:O	2.36	0.55
58:7A:23:ALA:O	58:7A:27:LYS:N	2.35	0.55
12:BP:86:TYR:N	12:BP:459:ALA:O	2.32	0.55
3:02:196:TYR:O	3:02:200:ASP:N	2.33	0.55
3:C:196:TYR:O	3:C:200:ASP:N	2.33	0.55
3:C:207:ASP:O	3:C:210:ALA:HB3	2.07	0.55
12:0B:284:ALA:O	12:0B:288:HIS:N	2.30	0.55
126:sa:226:SER:O	126:sa:230:GLY:CA	2.55	0.55
113:Qg:24:ILE:HA	113:Qg:205:GLU:HA	1.89	0.55
118:S1:657:ILE:O	74:A5:193:ILE:N	2.40	0.55
9:i:166:ASN:N	30:t:4:GLU:O	2.39	0.55
2:B:113:LEU:O	2:B:117:LEU:N	2.39	0.55
2:01:429:LEU:O	2:01:433:ALA:N	2.30	0.55
13:0C:97:SER:O	13:0C:110:CYS:N	2.40	0.55
12:46:297:VAL:HA	12:46:311:LEU:HA	1.89	0.55
70:5b:41:SER:O	70:5b:45:GLY:HA3	2.06	0.55
110:qD:76:VAL:O	110:qD:80:ASN:N	2.36	0.55
130:t1:270:ALA:HB3	130:t1:357:PRO:HA	1.87	0.55
105:P1:144:SER:O	105:P1:149:PHE:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:6b:79:TYR:O	55:6b:83:PHE:N	2.40	0.55
63:m3:72:THR:O	63:m3:76:SER:N	2.34	0.55
118:s1:338:GLN:O	118:s1:538:LYS:N	2.40	0.55
111:QE:183:SER:O	111:QE:190:VAL:N	2.34	0.55
41:vb:599:ILE:O	41:vb:603:ILE:N	2.30	0.55
39:C2:7:THR:O	39:C2:544:PHE:N	2.32	0.55
3:02:207:ASP:O	3:02:210:ALA:HB3	2.07	0.54
34:w:84:LYS:O	34:w:88:TYR:N	2.28	0.54
63:39:72:THR:O	63:39:76:SER:N	2.36	0.54
73:a3:116:ARG:O	73:a3:125:GLU:N	2.36	0.54
109:qC:222:TRP:O	109:qC:226:ALA:HB3	2.08	0.54
113:qg:24:ILE:HA	113:qg:205:GLU:HA	1.89	0.54
123:s6:80:VAL:N	123:s6:123:ALA:O	2.38	0.54
107:Qa:334:LEU:O	107:Qa:338:LEU:N	2.39	0.54
118:S1:338:GLN:O	118:S1:538:LYS:N	2.40	0.54
2:b:358:PHE:O	2:b:367:ASP:N	2.33	0.54
8:H:280:SER:O	8:H:284:GLN:N	2.41	0.54
24:N:67:ASP:O	24:N:71:ARG:N	2.38	0.54
12:46:137:GLY:N	12:46:152:GLN:O	2.35	0.54
109:qc:25:VAL:O	109:qc:220:MET:N	2.39	0.54
109:qc:287:ALA:O	109:qc:291:VAL:N	2.39	0.54
34:W:105:ALA:HB3	36:Y:68:TYR:HA	1.89	0.54
8:07:280:SER:O	8:07:284:GLN:N	2.41	0.54
24:13:67:ASP:O	24:13:71:ARG:N	2.38	0.54
97:g3:216:HIS:O	97:g3:220:THR:N	2.36	0.54
111:qE:50:PHE:O	115:qI:28:THR:N	2.35	0.54
114:QH:38:TYR:O	114:Qh:16:SER:N	2.41	0.54
4:D:193:ARG:O	10:J:217:LEU:N	2.41	0.54
118:s1:477:ALA:HB2	118:s1:515:HIS:HA	1.88	0.54
130:t1:449:PRO:O	130:t1:474:ALA:N	2.39	0.54
109:Qc:25:VAL:O	109:Qc:220:MET:N	2.39	0.54
118:S1:477:ALA:HB2	118:S1:515:HIS:HA	1.88	0.54
75:A6:146:SER:HA	78:A9:333:VAL:HA	1.89	0.54
12:0B:289:LEU:O	12:0B:294:GLY:N	2.40	0.54
34:22:105:ALA:HB3	36:24:68:TYR:HA	1.89	0.54
119:S2:372:SER:HA	119:S2:392:SER:O	2.08	0.54
54:30:109:GLU:O	54:30:113:GLN:N	2.40	0.54
109:QC:222:TRP:O	109:QC:226:ALA:HB3	2.08	0.54
73:A3:116:ARG:O	73:A3:125:GLU:N	2.36	0.54
2:b:353:THR:HA	2:b:448:VAL:H	1.71	0.54
12:BP:297:VAL:HA	12:BP:311:LEU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:03:193:ARG:O	10:09:217:LEU:N	2.41	0.54
118:s1:483:GLU:N	131:t2:149:ARG:O	2.34	0.54
120:S3:52:GLU:O	120:S3:56:SER:N	2.41	0.54
33:21:8:PHE:O	59:35:33:TRP:N	2.34	0.54
105:p1:144:SER:O	105:p1:149:PHE:N	2.40	0.54
2:B:426:PHE:O	2:B:430:ARG:N	2.39	0.54
12:0B:433:ASN:O	40:83:206:TYR:N	2.30	0.53
38:26:665:GLY:HA2	59:35:95:HIS:H	1.73	0.53
8:62:123:SER:HA	8:62:195:THR:HA	1.90	0.53
24:68:67:ASP:O	24:68:71:ARG:N	2.38	0.53
107:qA:76:VAL:HA	107:qA:249:ILE:O	2.08	0.53
113:QG:147:LEU:N	113:QG:252:ALA:O	2.35	0.53
107:Qa:476:ALA:O	107:Qa:480:LEU:N	2.37	0.53
4:d:188:TYR:O	4:d:213:VAL:N	2.34	0.53
9:I:23:ARG:O	9:I:26:THR:N	2.37	0.53
114:qH:38:TYR:O	114:qh:16:SER:N	2.41	0.53
107:QA:26:ALA:O	107:QA:30:PHE:N	2.42	0.53
4:d:314:TRP:N	4:d:319:ILE:O	2.42	0.53
118:s1:560:VAL:O	118:s1:575:ASP:N	2.41	0.53
120:s3:52:GLU:O	120:s3:56:SER:N	2.41	0.53
149:v2:130:CYS:HA	149:v2:173:ALA:HB1	1.90	0.53
4:d:241:TRP:O	4:d:362:ILE:N	2.41	0.53
61:92:282:LYS:O	61:92:286:TRP:N	2.30	0.53
87:b6:77:ASN:H	103:n5:195:GLY:HA3	1.73	0.53
125:s8:122:GLY:HA3	125:s8:193:GLY:O	2.08	0.53
137:t8:65:GLY:HA2	137:t8:69:GLY:HA3	1.90	0.53
108:Qb:333:ALA:HB2	108:Qb:362:THR:HA	1.90	0.53
87:B6:77:ASN:H	103:N5:195:GLY:HA3	1.73	0.53
2:01:426:PHE:O	2:01:430:ARG:N	2.39	0.53
15:0E:185:ASP:O	15:0E:189:TYR:N	2.39	0.53
106:p2:43:SER:H	106:p2:159:ALA:HA	1.72	0.53
119:s2:372:SER:HA	119:s2:392:SER:O	2.08	0.53
106:P2:43:SER:H	106:P2:159:ALA:HA	1.72	0.53
90:B9:164:ASN:HA	92:BM:138:ASN:HA	1.89	0.53
64:1T:8:HIS:N	39:C2:267:SER:O	2.35	0.53
4:58:241:TRP:O	4:58:362:ILE:N	2.41	0.53
33:76:47:VAL:O	38:81:687:GLU:N	2.42	0.53
137:T8:65:GLY:HA2	137:T8:69:GLY:HA3	1.89	0.53
59:7C:33:TRP:N	33:V:8:PHE:O	2.34	0.53
131:t2:37:TYR:O	131:t2:41:ASN:N	2.42	0.53
125:S8:122:GLY:HA3	125:S8:193:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:123:SER:HA	8:h:195:THR:HA	1.90	0.53
23:M:174:ASN:O	23:M:178:GLY:N	2.31	0.53
107:QA:76:VAL:HA	107:QA:249:ILE:O	2.08	0.53
110:Qd:278:TYR:O	110:Qd:282:LEU:N	2.42	0.53
123:S6:80:VAL:N	123:S6:123:ALA:O	2.38	0.53
130:T1:449:PRO:O	130:T1:474:ALA:N	2.39	0.53
134:T5:115:ALA:O	134:T5:119:GLY:N	2.37	0.53
12:bp:289:LEU:O	12:bp:294:GLY:N	2.40	0.53
39:C2:427:GLN:N	39:C2:446:GLY:O	2.42	0.53
39:C2:576:TRP:O	39:C2:581:LEU:N	2.29	0.53
111:Qe:134:ILE:N	111:Qe:250:THR:O	2.39	0.53
3:c:25:GLN:O	3:c:29:SER:N	2.37	0.53
38:c1:687:GLU:N	33:v:47:VAL:O	2.42	0.53
105:p1:91:VAL:HA	132:t3:18:SER:HA	1.91	0.53
108:qb:496:SER:O	108:qb:500:SER:N	2.42	0.53
120:s3:126:ASP:HA	120:s3:132:ALA:HB3	1.90	0.53
132:t3:142:ILE:O	132:t3:147:LEU:N	2.31	0.53
107:Qa:109:SER:O	107:Qa:113:ILE:N	2.33	0.53
108:Qb:496:SER:O	108:Qb:500:SER:N	2.42	0.53
49:2K:83:SER:N	51:2M:60:SER:O	2.31	0.53
13:fs:97:SER:O	13:fs:110:CYS:N	2.40	0.53
12:BP:137:GLY:N	12:BP:152:GLN:O	2.35	0.53
40:28:14:ARG:O	40:28:133:VAL:N	2.31	0.52
108:qB:107:ALA:O	108:qB:111:GLN:N	2.41	0.52
110:qd:278:TYR:O	110:qd:282:LEU:N	2.42	0.52
118:S1:560:VAL:O	118:S1:575:ASP:N	2.41	0.52
149:V2:130:CYS:HA	149:V2:173:ALA:HB1	1.90	0.52
34:22:105:ALA:O	36:24:69:LYS:N	2.40	0.52
4:58:314:TRP:N	4:58:319:ILE:O	2.42	0.52
130:t1:375:ILE:N	130:t1:407:HIS:O	2.36	0.52
9:I:166:ASN:N	30:T:4:GLU:O	2.39	0.52
24:13:163:TRP:O	24:13:167:GLN:N	2.32	0.52
109:Qc:287:ALA:O	109:Qc:291:VAL:N	2.39	0.52
59:35:108:ALA:O	59:35:112:MET:N	2.31	0.52
111:qE:183:SER:O	111:qE:190:VAL:N	2.34	0.52
105:P1:91:VAL:HA	132:T3:18:SER:HA	1.91	0.52
138:T9:3:LEU:HA	138:T9:17:GLY:HA2	1.91	0.52
12:bp:113:ASN:O	12:bp:129:ASN:N	2.34	0.52
12:bp:447:VAL:HA	12:bp:461:VAL:HA	1.92	0.52
12:0B:447:VAL:HA	12:0B:461:VAL:HA	1.92	0.52
110:qd:91:LYS:HA	110:qd:139:HIS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:qe:73:TRP:O	111:qe:77:ASN:N	2.42	0.52
108:QB:107:ALA:O	108:QB:111:GLN:N	2.41	0.52
81:AL:35:ALA:HB2	81:AL:79:GLU:HA	1.91	0.52
111:qE:228:ARG:O	111:qE:230:ARG:N	2.43	0.52
40:c3:17:TRP:N	40:c3:54:GLY:O	2.32	0.52
3:C:206:LEU:O	3:C:210:ALA:N	2.43	0.52
12:0B:113:ASN:O	12:0B:129:ASN:N	2.34	0.52
8:62:201:GLY:O	8:62:205:SER:N	2.41	0.52
81:al:35:ALA:HB2	81:al:79:GLU:HA	1.91	0.52
138:t9:3:LEU:HA	138:t9:17:GLY:HA2	1.91	0.52
95:G1:215:PRO:HA	95:G1:254:PRO:HA	1.92	0.52
39:27:427:GLN:N	39:27:446:GLY:O	2.42	0.52
63:39:94:VAL:O	63:39:98:GLN:N	2.43	0.52
120:S3:126:ASP:HA	120:S3:132:ALA:HB3	1.90	0.52
12:46:176:SER:O	12:46:191:GLY:HA3	2.10	0.52
4:58:188:TYR:O	4:58:213:VAL:N	2.34	0.52
29:73:130:VAL:HA	29:73:137:ALA:HB1	1.91	0.52
88:b7:116:LEU:HA	88:b7:120:ASN:HA	1.91	0.52
113:qG:24:ILE:HA	113:qG:205:GLU:HA	1.91	0.52
60:7l:913:ARG:O	60:7l:918:GLY:N	2.37	0.52
107:qA:26:ALA:O	107:qA:30:PHE:N	2.42	0.52
111:Qe:73:TRP:O	111:Qe:77:ASN:N	2.42	0.52
49:2K:38:PHE:O	49:2K:42:PHE:CB	2.58	0.52
131:T2:37:TYR:O	131:T2:41:ASN:N	2.42	0.52
140:TB:102:TYR:N	146:TH:124:GLN:O	2.42	0.52
88:B7:116:LEU:HA	88:B7:120:ASN:HA	1.91	0.52
8:h:201:GLY:O	8:h:205:SER:N	2.42	0.52
20:0J:3:UNK:O	20:0J:7:UNK:N	2.44	0.51
49:2k:38:PHE:O	49:2k:42:PHE:CB	2.58	0.51
2:56:358:PHE:O	2:56:367:ASP:N	2.33	0.51
107:qa:476:ALA:O	107:qa:480:LEU:N	2.37	0.51
108:qb:333:ALA:HB2	108:qb:362:THR:HA	1.90	0.51
111:QE:50:PHE:O	115:QI:28:THR:N	2.35	0.51
144:TF:127:ASN:HA	144:TF:165:ALA:HB2	1.92	0.51
59:7C:95:HIS:H	38:C1:665:GLY:HA2	1.73	0.51
12:BP:176:SER:O	12:BP:191:GLY:HA3	2.10	0.51
12:0B:138:TRP:HA	12:0B:151:PHE:HA	1.93	0.51
87:B6:74:TRP:N	103:N5:280:PRO:O	2.43	0.51
8:h:101:GLY:O	8:h:105:GLN:N	2.37	0.51
29:s:130:VAL:HA	29:s:137:ALA:HB1	1.91	0.51
12:BP:320:GLY:O	12:BP:341:ALA:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:56:397:LYS:HA	2:56:422:ILE:O	2.10	0.51
2:56:429:LEU:O	2:56:433:ALA:N	2.32	0.51
144:tf:127:ASN:HA	144:tf:165:ALA:HB2	1.92	0.51
148:v1:264:ALA:HA	148:v1:272:ALA:HB1	1.93	0.51
58:7a:126:ILE:O	24:n:52:VAL:N	2.42	0.51
1:a:266:PHE:O	21:k:65:VAL:N	2.43	0.51
22:11:91:TYR:O	22:11:199:PHE:N	2.41	0.51
23:12:91:ARG:O	23:12:95:GLU:N	2.43	0.51
61:37:282:LYS:O	61:37:286:TRP:N	2.33	0.51
113:QG:24:ILE:HA	113:QG:205:GLU:HA	1.91	0.51
126:SA:438:ALA:HB1	126:SA:579:GLY:HA3	1.93	0.51
20:u2:3:UNK:O	20:u2:7:UNK:N	2.44	0.51
63:M3:94:VAL:O	63:M3:98:GLN:N	2.43	0.51
9:08:166:ASN:N	30:19:4:GLU:O	2.39	0.51
11:45:57:THR:O	11:45:61:GLN:N	2.41	0.51
114:qH:14:PHE:O	114:qh:38:TYR:N	2.44	0.51
110:Qd:91:LYS:HA	110:Qd:139:HIS:HA	1.90	0.51
2:b:397:LYS:HA	2:b:422:ILE:O	2.10	0.51
41:vb:188:CYS:O	41:vb:192:GLY:N	2.44	0.51
37:25:12:ASP:O	37:25:16:GLU:N	2.39	0.51
19:53:48:UNK:O	19:53:52:UNK:N	2.43	0.51
83:an:72:ALA:HA	83:an:76:GLY:HA3	1.93	0.51
87:b6:74:TRP:N	103:n5:280:PRO:O	2.43	0.51
109:qc:82:TRP:O	109:qc:86:ARG:N	2.35	0.51
19:U1:48:UNK:O	19:U1:52:UNK:N	2.43	0.51
3:02:206:LEU:O	3:02:210:ALA:N	2.43	0.51
126:sa:438:ALA:HB1	126:sa:579:GLY:HA3	1.93	0.51
111:QE:228:ARG:O	111:QE:230:ARG:N	2.43	0.51
131:T2:37:TYR:N	131:T2:42:ARG:O	2.36	0.51
83:AN:72:ALA:HA	83:AN:76:GLY:HA3	1.93	0.51
12:bp:433:ASN:O	40:c3:206:TYR:N	2.30	0.51
1:A:293:TYR:O	1:A:297:ALA:HB3	2.10	0.51
1:00:293:TYR:O	1:00:297:ALA:HB3	2.10	0.51
9:08:210:LYS:O	9:08:214:ASP:N	2.44	0.51
125:s8:155:THR:HA	125:s8:165:THR:HA	1.93	0.51
130:T1:19:PHE:HA	130:T1:49:VAL:O	2.10	0.51
25:o:87:ASP:O	25:o:91:ARG:N	2.44	0.51
89:b8:194:GLN:O	89:b8:198:LYS:N	2.41	0.51
130:t1:19:PHE:HA	130:t1:49:VAL:O	2.10	0.51
140:tb:102:TYR:N	146:th:124:GLN:O	2.42	0.51
118:S1:483:GLU:N	131:T2:149:ARG:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:293:GLY:N	2:b:355:THR:O	2.43	0.51
24:68:52:VAL:N	58:89:126:ILE:O	2.42	0.50
95:g1:215:PRO:HA	95:g1:254:PRO:HA	1.92	0.50
113:qg:100:GLU:O	113:qg:104:ARG:N	2.43	0.50
126:sa:75:ALA:HA	126:sa:201:ASN:O	2.12	0.50
130:t1:17:THR:O	130:t1:125:SER:N	2.45	0.50
40:c3:16:TYR:O	40:c3:135:ASN:N	2.42	0.50
11:6T:57:THR:O	11:6T:61:GLN:N	2.41	0.50
9:I:210:LYS:O	9:I:214:ASP:N	2.44	0.50
23:M:91:ARG:O	23:M:95:GLU:N	2.43	0.50
35:X:111:VAL:O	35:X:115:GLY:N	2.45	0.50
35:23:111:VAL:O	35:23:115:GLY:N	2.45	0.50
123:s6:88:ILE:O	123:s6:97:HIS:N	2.36	0.50
97:G3:216:HIS:O	97:G3:220:THR:N	2.36	0.50
12:bp:371:THR:O	12:bp:374:ASN:N	2.45	0.50
17:Y0:17:SER:O	17:Y0:20:ALA:HB3	2.11	0.50
42:2b:49:SER:HA	100:n2:335:LEU:HA	1.92	0.50
12:46:215:GLY:C	12:46:262:GLY:HA2	2.36	0.50
12:46:320:GLY:O	12:46:341:ALA:N	2.36	0.50
55:86:79:TYR:O	55:86:83:PHE:N	2.40	0.50
148:V1:264:ALA:HA	148:V1:272:ALA:HB1	1.93	0.50
12:0B:371:THR:O	12:0B:374:ASN:N	2.44	0.50
63:39:17:ASN:O	63:39:21:ILE:N	2.43	0.50
17:51:17:SER:O	17:51:20:ALA:HB3	2.11	0.50
25:69:87:ASP:O	25:69:91:ARG:N	2.44	0.50
63:M3:17:ASN:O	63:M3:21:ILE:N	2.43	0.50
17:Y0:6:PHE:O	17:Y0:10:TYR:N	2.45	0.50
39:27:7:THR:O	39:27:544:PHE:N	2.32	0.50
24:n:67:ASP:O	24:n:71:ARG:N	2.38	0.50
41:VB:188:CYS:O	41:VB:192:GLY:N	2.45	0.50
8:62:101:GLY:O	8:62:105:GLN:N	2.37	0.50
22:L:91:TYR:O	22:L:199:PHE:N	2.41	0.50
61:M1:282:LYS:O	61:M1:286:TRP:N	2.33	0.50
17:51:6:PHE:O	17:51:10:TYR:N	2.45	0.50
41:84:188:CYS:O	41:84:192:GLY:N	2.44	0.50
125:S8:155:THR:HA	125:S8:165:THR:HA	1.93	0.50
42:2B:49:SER:HA	100:N2:335:LEU:HA	1.92	0.50
86:B4:128:ASN:O	102:N4:306:SER:N	2.35	0.50
12:BP:215:GLY:C	12:BP:262:GLY:HA2	2.37	0.50
39:C2:429:LYS:O	39:C2:443:LYS:N	2.45	0.50
39:27:429:LYS:O	39:27:443:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:36:913:ARG:O	60:36:917:ASP:N	2.44	0.50
12:46:446:LYS:O	12:46:462:ASN:N	2.44	0.50
103:n5:97:SER:O	103:n5:101:HIS:N	2.37	0.50
109:Qc:279:HIS:O	109:Qc:283:ARG:N	2.36	0.50
15:y7:185:ASP:O	15:y7:189:TYR:N	2.39	0.50
12:BP:86:TYR:O	12:BP:459:ALA:N	2.33	0.50
61:37:284:ALA:O	61:37:288:TRP:N	2.43	0.50
5:59:193:GLN:O	5:59:197:GLY:N	2.45	0.50
57:88:53:PRO:O	57:88:56:ALA:HB3	2.12	0.50
103:n5:724:TYR:O	103:n5:728:SER:N	2.42	0.50
108:Qb:185:VAL:O	108:Qb:189:ALA:N	2.45	0.50
73:A3:118:ASN:O	73:A3:122:ALA:N	2.45	0.50
12:bp:138:TRP:HA	12:bp:151:PHE:HA	1.93	0.50
19:53:75:UNK:O	19:53:79:UNK:N	2.45	0.49
73:a3:118:ASN:O	73:a3:122:ALA:N	2.45	0.49
111:qe:134:ILE:N	111:qe:250:THR:O	2.39	0.49
140:TB:57:VAL:HA	90:B9:140:LEU:HA	1.94	0.49
54:6A:109:GLU:O	54:6A:113:GLN:N	2.40	0.49
12:46:123:HIS:HA	12:46:137:GLY:HA3	1.94	0.49
1:55:266:PHE:O	21:65:65:VAL:N	2.43	0.49
60:91:913:ARG:O	60:91:918:GLY:N	2.37	0.49
108:qb:185:VAL:O	108:qb:189:ALA:N	2.45	0.49
57:6l:53:PRO:O	57:6l:56:ALA:HB3	2.12	0.49
34:W:105:ALA:O	36:Y:69:LYS:N	2.40	0.49
133:t4:49:GLU:O	133:t4:53:GLU:N	2.46	0.49
12:bp:446:LYS:O	12:bp:462:ASN:N	2.42	0.49
8:h:136:ILE:O	8:h:147:GLU:N	2.32	0.49
61:m1:282:LYS:O	61:m1:286:TRP:N	2.30	0.49
40:C3:14:ARG:O	40:C3:133:VAL:N	2.31	0.49
13:47:113:LEU:N	151:47:201:FES:S2	2.86	0.49
41:vb:160:GLY:HA2	41:vb:177:PHE:HA	1.94	0.49
60:7L:913:ARG:O	60:7L:917:ASP:N	2.44	0.49
1:00:231:PRO:O	1:00:235:LEU:N	2.40	0.49
12:0B:446:LYS:O	12:0B:462:ASN:N	2.42	0.49
39:27:576:TRP:O	39:27:581:LEU:N	2.29	0.49
19:53:74:UNK:O	19:53:78:UNK:N	2.46	0.49
38:81:521:PHE:N	38:81:586:MET:O	2.40	0.49
41:84:160:GLY:HA2	41:84:177:PHE:HA	1.94	0.49
123:s6:83:ASN:O	123:s6:104:LEU:N	2.43	0.49
126:SA:75:ALA:HA	126:SA:201:ASN:O	2.12	0.49
3:02:25:GLN:O	3:02:29:SER:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
130:T1:17:THR:O	130:T1:125:SER:N	2.45	0.49
12:BP:446:LYS:O	12:BP:462:ASN:N	2.44	0.49
19:U1:74:UNK:O	19:U1:78:UNK:N	2.46	0.49
19:U1:75:UNK:O	19:U1:79:UNK:N	2.45	0.49
61:m1:284:ALA:O	61:m1:288:TRP:N	2.44	0.49
41:29:188:CYS:O	41:29:192:GLY:N	2.45	0.49
41:29:609:GLU:O	41:29:613:ALA:N	2.46	0.49
40:83:16:TYR:O	40:83:135:ASN:N	2.42	0.49
58:89:23:ALA:O	58:89:27:LYS:N	2.36	0.49
107:qa:233:SER:O	107:qa:237:GLN:N	2.39	0.49
131:T2:126:SER:O	131:T2:133:TYR:N	2.42	0.49
89:B8:194:GLN:O	89:B8:198:LYS:N	2.41	0.49
103:N5:402:ALA:O	103:N5:406:SER:N	2.44	0.49
20:u2:6:UNK:O	20:u2:10:UNK:N	2.46	0.49
10:J:68:PHE:O	10:J:72:GLU:N	2.41	0.49
37:Z:12:ASP:O	37:Z:16:GLU:N	2.39	0.49
20:0J:6:UNK:O	20:0J:10:UNK:N	2.45	0.49
24:13:66:ASP:O	24:13:70:GLN:N	2.46	0.49
90:b9:140:LEU:HA	140:tb:57:VAL:HA	1.94	0.49
119:S2:253:SER:O	119:S2:257:THR:N	2.45	0.49
5:e:193:GLN:O	5:e:197:GLY:N	2.45	0.49
41:VB:599:ILE:O	41:VB:603:ILE:N	2.32	0.49
60:7L:914:LEU:HA	60:7L:918:GLY:HA2	1.95	0.49
2:B:99:LEU:O	2:B:103:ASN:N	2.36	0.49
3:C:25:GLN:O	3:C:29:SER:N	2.46	0.49
21:K:95:GLN:O	21:K:99:LEU:N	2.44	0.49
41:VB:609:GLU:O	41:VB:613:ALA:N	2.46	0.49
12:46:86:TYR:O	12:46:459:ALA:N	2.33	0.48
4:58:209:PHE:HA	4:58:238:ASN:HA	1.95	0.48
7:61:113:GLU:O	7:61:117:ARG:N	2.40	0.48
124:S7:7:VAL:O	124:S7:11:ASN:N	2.37	0.48
57:6L:3:VAL:HA	39:C2:5:LEU:HA	1.94	0.48
13:FS:113:LEU:N	151:FS:201:FES:S2	2.86	0.48
22:L:54:ARG:O	22:L:58:GLU:N	2.45	0.48
7:06:83:TYR:N	13:47:59:ILE:O	2.46	0.48
32:20:120:LYS:O	32:20:124:ASP:N	2.33	0.48
12:46:287:LYS:O	12:46:291:GLU:N	2.46	0.48
110:Qd:240:ASN:O	110:Qd:247:GLY:HA2	2.12	0.48
113:Qg:100:GLU:O	113:Qg:104:ARG:N	2.43	0.48
24:N:66:ASP:O	24:N:70:GLN:N	2.46	0.48
13:47:151:THR:N	151:47:202:FES:S2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:165:ARG:HA	30:t:5:THR:HA	1.96	0.48
62:m2:133:ALA:HB3	62:m2:188:VAL:HA	1.95	0.48
22:L:169:ASN:O	22:L:173:TYR:CB	2.61	0.48
4:03:299:VAL:HA	4:03:345:ILE:HA	1.95	0.48
22:11:169:ASN:O	22:11:173:TYR:CB	2.61	0.48
108:Qb:139:VAL:HA	108:Qb:147:THR:O	2.13	0.48
133:T4:49:GLU:O	133:T4:53:GLU:N	2.46	0.48
7:g:113:GLU:O	7:g:117:ARG:N	2.40	0.48
17:Y0:65:PHE:O	17:Y0:69:TYR:N	2.41	0.48
12:0B:365:ASN:O	12:0B:381:LEU:N	2.46	0.48
22:11:54:ARG:O	22:11:58:GLU:N	2.45	0.48
39:27:5:LEU:HA	57:33:3:VAL:HA	1.94	0.48
42:2b:133:TYR:HA	42:2b:138:VAL:HA	1.94	0.48
49:2k:83:SER:N	51:2m:60:SER:O	2.31	0.48
63:94:232:SER:C	63:94:234:GLN:H	2.21	0.48
110:Qd:215:ASP:O	110:Qd:227:SER:HA	2.14	0.48
42:2B:133:TYR:HA	42:2B:138:VAL:HA	1.94	0.48
12:bp:365:ASN:O	12:bp:381:LEU:N	2.46	0.48
4:D:299:VAL:HA	4:D:345:ILE:HA	1.95	0.48
1:00:271:VAL:HA	1:00:368:GLN:HA	1.96	0.48
12:0B:176:SER:CB	12:0B:192:TYR:O	2.62	0.48
60:36:914:LEU:HA	60:36:918:GLY:HA2	1.95	0.48
2:56:87:ARG:O	2:56:91:SER:N	2.47	0.48
113:qg:106:ASN:O	115:qi:9:ASN:N	2.44	0.48
119:s2:253:SER:O	119:s2:257:THR:N	2.45	0.48
119:s2:414:LEU:O	119:s2:418:GLY:N	2.44	0.48
12:bp:298:GLN:N	12:bp:310:LEU:O	2.47	0.48
12:BP:93:SER:O	12:BP:137:GLY:HA2	2.14	0.48
12:BP:123:HIS:HA	12:BP:137:GLY:HA3	1.94	0.48
8:07:136:ILE:O	8:07:147:GLU:N	2.36	0.48
12:46:93:SER:O	12:46:137:GLY:HA2	2.13	0.48
40:83:209:PHE:O	40:83:213:LEU:N	2.45	0.48
110:qd:240:ASN:O	110:qd:247:GLY:HA2	2.12	0.48
118:S1:584:THR:O	118:S1:603:VAL:N	2.46	0.48
38:c1:386:PHE:O	38:c1:390:GLY:N	2.47	0.48
12:BP:287:LYS:O	12:BP:291:GLU:N	2.46	0.48
34:22:9:VAL:HA	41:29:168:ASP:HA	1.95	0.48
40:28:209:PHE:O	40:28:213:LEU:N	2.44	0.48
108:qb:139:VAL:HA	108:qb:147:THR:O	2.13	0.48
113:QG:90:ASP:O	113:QG:94:ARG:N	2.46	0.48
40:c3:421:TRP:HA	40:c3:432:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:m3:232:SER:C	63:m3:234:GLN:H	2.21	0.48
41:VB:168:ASP:HA	34:W:9:VAL:HA	1.95	0.48
38:81:386:PHE:O	38:81:390:GLY:N	2.47	0.48
62:93:133:ALA:HB3	62:93:188:VAL:HA	1.95	0.48
110:qd:215:ASP:O	110:qd:227:SER:HA	2.14	0.48
103:N5:724:TYR:O	103:N5:728:SER:N	2.42	0.48
2:b:87:ARG:O	2:b:91:SER:N	2.47	0.48
6:f:240:SER:O	6:f:243:GLY:N	2.47	0.48
8:h:97:ILE:O	8:h:122:VAL:HA	2.14	0.48
13:FS:151:THR:N	151:FS:202:FES:S2	2.87	0.48
119:s2:135:ALA:HB2	119:s2:150:ALA:HB3	1.96	0.47
40:83:17:TRP:N	40:83:54:GLY:O	2.32	0.47
107:qA:476:ALA:O	107:qA:480:LEU:N	2.45	0.47
110:QD:125:TYR:O	20:QM:15:UNK:N	2.47	0.47
114:Qh:22:PHE:HA	114:Qh:28:HIS:HA	1.97	0.47
2:B:87:ARG:O	2:B:91:SER:N	2.47	0.47
3:02:24:GLU:O	3:02:28:LEU:N	2.35	0.47
2:56:293:GLY:N	2:56:355:THR:O	2.43	0.47
8:62:97:ILE:O	8:62:122:VAL:HA	2.14	0.47
22:66:54:ARG:O	22:66:58:GLU:N	2.48	0.47
40:83:421:TRP:HA	40:83:432:LEU:HA	1.95	0.47
110:qD:125:TYR:O	20:qM:15:UNK:N	2.47	0.47
111:qE:131:GLU:HA	111:qE:253:CYS:HA	1.96	0.47
114:qh:22:PHE:HA	114:qh:28:HIS:HA	1.97	0.47
118:s1:584:THR:O	118:s1:603:VAL:N	2.46	0.47
64:1t:5:VAL:O	39:c2:271:ASN:N	2.46	0.47
12:bp:176:SER:CB	12:bp:192:TYR:O	2.62	0.47
39:c2:1:MET:HA	39:c2:7:THR:H	1.79	0.47
39:c2:260:TYR:O	39:c2:264:ASN:N	2.45	0.47
4:d:209:PHE:HA	4:d:238:ASN:HA	1.95	0.47
20:0J:4:UNK:O	20:0J:8:UNK:N	2.47	0.47
12:46:87:THR:HA	12:46:458:PHE:HA	1.97	0.47
153:81:701:HEA:HBA2	153:81:701:HEA:CMA	2.44	0.47
86:b4:128:ASN:O	102:n4:306:SER:N	2.35	0.47
103:n5:402:ALA:O	103:n5:406:SER:N	2.44	0.47
111:QE:131:GLU:HA	111:QE:253:CYS:HA	1.96	0.47
123:S6:88:ILE:O	123:S6:97:HIS:N	2.36	0.47
20:u2:4:UNK:O	20:u2:8:UNK:N	2.47	0.47
15:y7:421:ILE:O	15:y7:423:LYS:N	2.46	0.47
12:0B:448:VAL:N	12:0B:460:ILE:O	2.48	0.47
15:0E:421:ILE:O	15:0E:423:LYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:82:260:TYR:O	39:82:264:ASN:N	2.45	0.47
78:a9:193:ALA:O	78:a9:256:GLY:N	2.47	0.47
13:FS:59:ILE:O	7:G:83:TYR:N	2.46	0.47
22:66:169:ASN:O	22:66:173:TYR:CB	2.63	0.47
107:Qa:233:SER:O	107:Qa:237:GLN:N	2.39	0.47
38:c1:65:GLY:C	153:c1:701:HEA:H273	2.40	0.47
153:c1:701:HEA:CMA	153:c1:701:HEA:HBA2	2.44	0.47
2:01:87:ARG:O	2:01:91:SER:N	2.47	0.47
17:51:16:PRO:O	17:51:20:ALA:N	2.48	0.47
32:75:112:PRO:O	32:75:116:GLN:N	2.47	0.47
39:82:1:MET:HA	39:82:7:THR:H	1.80	0.47
91:bl:129:ASN:CB	138:t9:17:GLY:HA3	2.45	0.47
110:qD:277:ALA:O	110:qD:281:ASN:N	2.41	0.47
130:t1:162:ARG:O	130:t1:182:ILE:N	2.36	0.47
111:Qe:228:ARG:O	111:Qe:230:ARG:N	2.48	0.47
78:A9:193:ALA:O	78:A9:256:GLY:N	2.47	0.47
1:A:231:PRO:O	1:A:235:LEU:N	2.40	0.47
9:I:26:THR:O	9:I:29:ALA:HB3	2.15	0.47
24:68:68:PHE:O	24:68:72:ASP:N	2.48	0.47
123:S6:83:ASN:O	123:S6:104:LEU:N	2.43	0.47
138:T9:17:GLY:HA3	91:BL:129:ASN:CB	2.45	0.47
1:A:271:VAL:HA	1:A:368:GLN:HA	1.96	0.47
12:BP:87:THR:HA	12:BP:458:PHE:HA	1.96	0.47
19:U1:27:UNK:O	19:U1:31:UNK:N	2.48	0.47
5:04:83:TRP:O	5:04:87:ALA:N	2.42	0.47
10:09:68:PHE:O	10:09:72:GLU:N	2.41	0.47
12:0B:298:GLN:N	12:0B:310:LEU:O	2.47	0.47
15:0E:295:LYS:N	41:84:257:VAL:O	2.47	0.47
21:10:95:GLN:O	21:10:99:LEU:N	2.44	0.47
3:57:10:ALA:O	3:57:14:LYS:N	2.45	0.47
8:62:136:ILE:O	8:62:147:GLU:N	2.32	0.47
9:63:165:ARG:HA	30:74:5:THR:HA	1.96	0.47
38:81:316:THR:O	38:81:320:LEU:N	2.47	0.47
123:s6:78:ILE:O	123:s6:123:ALA:N	2.45	0.47
12:bp:448:VAL:N	12:bp:460:ILE:O	2.48	0.47
1:00:464:ASN:O	1:00:468:VAL:N	2.46	0.47
2:01:99:LEU:O	2:01:103:ASN:N	2.36	0.47
6:60:240:SER:O	6:60:243:GLY:N	2.47	0.47
22:l:169:ASN:O	22:l:173:TYR:CB	2.63	0.47
19:53:8:UNK:O	19:53:12:UNK:N	2.48	0.46
8:62:138:ALA:O	8:62:145:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:81:703:HEA:H271	153:81:703:HEA:H211	1.36	0.46
113:qG:90:ASP:O	113:qG:94:ARG:N	2.46	0.46
130:t1:312:ALA:N	130:t1:339:THR:O	2.49	0.46
24:n:68:PHE:O	24:n:72:ASP:N	2.48	0.46
32:u:112:PRO:O	32:u:116:GLN:N	2.47	0.46
12:BP:431:VAL:HA	12:BP:436:ASN:HA	1.97	0.46
33:21:47:VAL:O	38:26:687:GLU:N	2.40	0.46
5:59:176:ASP:O	5:59:180:SER:N	2.42	0.46
102:n4:434:LEU:HA	102:n4:438:PRO:HA	1.97	0.46
111:qe:228:ARG:O	111:qe:230:ARG:N	2.48	0.46
19:U1:8:UNK:O	19:U1:12:UNK:N	2.48	0.46
12:46:431:VAL:HA	12:46:436:ASN:HA	1.97	0.46
116:Qj:44:ILE:O	116:Qj:49:ILE:N	2.46	0.46
119:S2:135:ALA:HB2	119:S2:150:ALA:HB3	1.96	0.46
119:S2:414:LEU:O	119:S2:418:GLY:N	2.44	0.46
62:38:133:ALA:HB3	62:38:188:VAL:HA	1.97	0.46
12:46:371:THR:O	12:46:374:ASN:N	2.48	0.46
124:s7:7:VAL:O	124:s7:11:ASN:N	2.37	0.46
148:V1:230:PHE:O	148:V1:234:ALA:N	2.36	0.46
153:C1:702:HEA:H211	153:C1:702:HEA:H271	1.40	0.46
62:M2:133:ALA:HB3	62:M2:188:VAL:HA	1.97	0.46
9:08:26:THR:O	9:08:29:ALA:HB3	2.15	0.46
24:68:194:ALA:O	24:68:198:MET:N	2.39	0.46
38:81:65:GLY:C	153:81:701:HEA:H273	2.40	0.46
55:86:156:ASP:N	55:86:165:LYS:O	2.49	0.46
113:qG:97:TYR:O	113:qG:101:THR:N	2.37	0.46
113:QG:106:ASN:O	115:QI:9:ASN:N	2.39	0.46
6:f:275:GLU:N	6:f:279:GLN:O	2.37	0.46
22:l:54:ARG:O	22:l:58:GLU:N	2.48	0.46
12:BP:371:THR:O	12:BP:374:ASN:N	2.48	0.46
19:53:27:UNK:O	19:53:31:UNK:N	2.48	0.46
40:83:65:SER:O	40:83:69:LYS:N	2.48	0.46
97:g3:182:ILE:O	97:g3:191:LEU:N	2.44	0.46
124:s7:43:ARG:HA	125:s8:106:THR:HA	1.97	0.46
107:QA:476:ALA:O	107:QA:480:LEU:N	2.45	0.46
38:c1:521:PHE:N	38:c1:586:MET:O	2.40	0.46
59:7C:88:HIS:N	6:F:130:VAL:O	2.46	0.46
17:Y0:16:PRO:O	17:Y0:20:ALA:N	2.48	0.46
7:06:126:GLU:O	7:06:130:ILE:N	2.47	0.46
6:60:275:GLU:N	6:60:279:GLN:O	2.37	0.46
39:82:271:ASN:N	64:95:5:VAL:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:90:172:VAL:H	62:93:214:GLY:HA3	1.81	0.46
118:s1:393:GLY:O	118:s1:397:ALA:N	2.34	0.46
108:Qb:209:TYR:O	108:Qb:215:GLY:HA3	2.16	0.46
110:Qd:93:ASP:N	110:Qd:136:ILE:O	2.48	0.46
133:T4:23:ALA:HB2	133:T4:58:ALA:HB2	1.98	0.46
72:A2:62:ILE:HA	72:A2:72:LYS:HA	1.97	0.46
102:N4:434:LEU:HA	102:N4:438:PRO:HA	1.98	0.46
15:Y7:427:GLU:O	15:Y7:431:ILE:N	2.49	0.46
24:13:50:THR:H	58:34:125:TYR:HA	1.81	0.46
119:s2:135:ALA:HB1	119:s2:147:VAL:HA	1.97	0.46
12:BP:215:GLY:O	12:BP:262:GLY:HA2	2.16	0.46
19:U1:7:UNK:O	19:U1:11:UNK:N	2.49	0.46
12:46:215:GLY:O	12:46:262:GLY:HA2	2.16	0.46
12:46:328:GLY:HA2	12:46:386:GLN:HA	1.97	0.46
17:51:65:PHE:O	17:51:69:TYR:N	2.41	0.46
70:5b:41:SER:O	70:5b:45:GLY:CA	2.64	0.46
158:a9:401:NDP:H51A	158:a9:401:NDP:H8A	1.98	0.46
126:SA:212:ILE:N	126:SA:221:GLY:O	2.38	0.46
119:S2:135:ALA:HB1	119:S2:147:VAL:HA	1.97	0.46
158:A9:401:NDP:H8A	158:A9:401:NDP:H51A	1.98	0.46
97:G3:182:ILE:O	97:G3:191:LEU:N	2.44	0.46
103:N5:97:SER:O	103:N5:101:HIS:N	2.37	0.46
8:07:128:PRO:HA	8:07:152:PHE:HA	1.98	0.45
39:82:515:SER:O	39:82:549:CYS:HA	2.16	0.45
98:J1:158:LEU:O	98:J1:168:LYS:N	2.37	0.45
55:6b:63:PHE:HA	55:6b:70:TYR:HA	1.99	0.45
55:6b:156:ASP:N	55:6b:165:LYS:O	2.49	0.45
58:7a:25:LEU:O	58:7a:29:GLN:N	2.49	0.45
40:c3:142:TYR:N	40:c3:145:SER:O	2.42	0.45
8:h:138:ALA:O	8:h:145:GLY:N	2.49	0.45
8:H:128:PRO:HA	8:H:152:PHE:HA	1.98	0.45
15:49:427:GLU:O	15:49:431:ILE:N	2.49	0.45
107:Qa:321:ALA:O	107:Qa:325:ALA:N	2.45	0.45
70:5B:41:SER:O	70:5B:45:GLY:CA	2.64	0.45
3:c:24:GLU:O	3:c:28:LEU:N	2.40	0.45
15:y7:222:THR:O	15:y7:226:ASN:N	2.43	0.45
12:BP:328:GLY:HA2	12:BP:386:GLN:HA	1.97	0.45
61:M1:284:ALA:O	61:M1:288:TRP:N	2.43	0.45
48:2j:98:TYR:O	48:2j:102:ARG:N	2.49	0.45
19:53:7:UNK:O	19:53:11:UNK:N	2.49	0.45
4:58:183:VAL:O	4:58:296:THR:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:82:13:LEU:HA	39:82:481:PRO:HA	1.99	0.45
40:83:142:TYR:N	40:83:145:SER:O	2.42	0.45
81:al:142:GLY:HA3	121:s4:118:PRO:O	2.17	0.45
81:al:164:TRP:HA	118:s1:301:GLN:HA	1.98	0.45
113:qG:106:ASN:O	115:qI:9:ASN:N	2.39	0.45
110:qd:93:ASP:N	110:qd:136:ILE:O	2.48	0.45
48:2J:98:TYR:O	48:2J:102:ARG:N	2.49	0.45
39:c2:515:SER:O	39:c2:549:CYS:HA	2.16	0.45
41:29:608:GLU:O	41:29:612:GLU:N	2.38	0.45
50:2l:40:ASP:O	50:2l:44:ASN:N	2.41	0.45
76:a7:83:THR:O	76:a7:87:ARG:N	2.42	0.45
107:qa:110:LEU:O	107:qa:114:LYS:N	2.45	0.45
148:v1:227:LYS:HA	148:v1:228:PRO:HA	1.75	0.45
160:Qc:501:U10:H1M1	160:Qc:501:U10:H71	1.80	0.45
123:S6:78:ILE:O	123:S6:123:ALA:N	2.45	0.45
153:C1:701:HEA:H271	153:C1:701:HEA:H211	1.38	0.45
40:C3:17:TRP:N	40:C3:54:GLY:O	2.25	0.45
124:S7:43:ARG:HA	125:S8:106:THR:HA	1.97	0.45
24:n:194:ALA:O	24:n:198:MET:N	2.39	0.45
1:A:464:ASN:O	1:A:468:VAL:N	2.46	0.45
38:C1:268:THR:O	38:C1:288:GLY:N	2.40	0.45
2:01:396:VAL:O	2:01:423:ASN:HA	2.16	0.45
72:a2:62:ILE:HA	72:a2:72:LYS:HA	1.97	0.45
104:n6:251:ILE:N	119:s2:268:SER:O	2.38	0.45
133:t4:23:ALA:HB2	133:t4:58:ALA:HB2	1.98	0.45
113:QG:202:PHE:HA	116:Qj:4:PRO:HA	1.98	0.45
130:T1:162:ARG:O	130:T1:181:THR:N	2.49	0.45
164:V1:501:FMN:H4'	164:V1:501:FMN:H1'2	1.83	0.45
63:M3:48:ARG:O	63:M3:52:ASP:N	2.49	0.45
61:92:286:TRP:O	61:92:290:HIS:N	2.50	0.45
113:qG:202:PHE:HA	116:qj:4:PRO:HA	1.98	0.45
130:T1:312:ALA:N	130:T1:339:THR:O	2.49	0.45
153:c1:701:HEA:H211	153:c1:701:HEA:H271	1.30	0.45
39:c2:13:LEU:HA	39:c2:481:PRO:HA	1.99	0.45
4:d:183:VAL:O	4:d:296:THR:HA	2.15	0.45
10:j:104:PRO:O	10:j:108:GLN:N	2.49	0.45
7:06:233:TYR:O	13:47:118:VAL:N	2.50	0.45
18:0H:69:ASN:O	18:0H:73:HIS:N	2.49	0.45
108:qb:209:TYR:O	108:qb:215:GLY:HA3	2.16	0.45
108:QB:295:ARG:O	114:QH:57:GLY:N	2.50	0.45
108:Qb:186:TYR:O	108:Qb:190:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:c1:502:GLY:C	153:c1:703:HEA:H263	2.42	0.45
13:fs:151:THR:N	151:fs:202:FES:S2	2.90	0.45
58:7A:22:ALA:HB1	1:A:455:LEU:HA	1.98	0.45
153:26:702:HEA:H271	153:26:702:HEA:H211	1.40	0.45
20:54:5:UNK:O	20:54:9:UNK:N	2.50	0.45
82:am:163:LEU:O	82:am:167:ILE:N	2.45	0.45
105:P1:208:TYR:H	70:5B:3:LYS:HA	1.82	0.45
106:P2:95:LEU:O	106:P2:109:THR:HA	2.17	0.45
118:S1:279:HIS:N	118:S1:284:GLU:O	2.43	0.45
7:G:124:ARG:O	7:G:128:GLU:N	2.40	0.45
62:M2:314:LYS:O	62:M2:318:ILE:N	2.49	0.45
106:p2:86:MET:HA	106:p2:97:LEU:HA	1.99	0.45
130:t1:147:TYR:O	130:t1:152:LYS:N	2.40	0.45
130:t1:162:ARG:O	130:t1:181:THR:N	2.49	0.45
107:Qa:110:LEU:O	107:Qa:114:LYS:N	2.45	0.45
127:SB:131:ALA:HA	127:SB:140:LEU:HA	1.98	0.45
59:7c:172:VAL:H	62:m2:214:GLY:HA3	1.81	0.45
18:z1:69:ASN:O	18:z1:73:HIS:N	2.49	0.45
2:B:396:VAL:O	2:B:423:ASN:HA	2.16	0.45
3:C:24:GLU:O	3:C:28:LEU:N	2.35	0.45
13:FS:118:VAL:N	7:G:233:TYR:O	2.50	0.45
8:H:136:ILE:O	8:H:147:GLU:N	2.36	0.45
5:04:334:GLU:O	7:06:75:ARG:N	2.47	0.44
13:0C:151:THR:N	151:0C:202:FES:S2	2.90	0.44
15:0E:222:THR:O	15:0E:226:ASN:N	2.43	0.44
47:2i:88:GLY:O	47:2i:92:PHE:N	2.49	0.44
70:5b:3:LYS:HA	105:p1:208:TYR:H	1.82	0.44
10:64:104:PRO:O	10:64:108:GLN:N	2.49	0.44
58:89:25:LEU:O	58:89:29:GLN:N	2.49	0.44
110:QD:277:ALA:O	110:QD:281:ASN:N	2.41	0.44
106:P2:86:MET:HA	106:P2:97:LEU:HA	1.99	0.44
121:S4:118:PRO:O	81:AL:142:GLY:HA3	2.17	0.44
58:7A:125:TYR:HA	24:N:50:THR:H	1.81	0.44
41:VB:615:LEU:O	15:Y7:239:ASN:N	2.50	0.44
10:09:97:VAL:O	10:09:101:ILE:N	2.51	0.44
108:qb:186:TYR:O	108:qb:190:LEU:N	2.49	0.44
107:QA:138:GLY:CA	107:QA:154:ASN:O	2.65	0.44
114:QH:14:PHE:O	114:Qh:38:TYR:N	2.44	0.44
148:V1:326:PRO:HA	148:V1:435:PRO:HA	2.00	0.44
38:c1:316:THR:O	38:c1:320:LEU:N	2.47	0.44
1:00:455:LEU:HA	58:34:22:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:46:432:GLY:N	12:46:435:TYR:O	2.41	0.44
7:61:126:GLU:O	7:61:130:ILE:N	2.42	0.44
106:p2:95:LEU:O	106:p2:109:THR:HA	2.17	0.44
127:sb:131:ALA:HA	127:sb:140:LEU:HA	1.98	0.44
108:Qb:397:MET:O	108:Qb:401:GLU:N	2.46	0.44
47:2I:88:GLY:O	47:2I:92:PHE:N	2.49	0.44
96:G2:183:GLN:HA	96:G2:195:ASP:HA	2.00	0.44
9:i:186:HIS:O	9:i:191:SER:N	2.31	0.44
19:U1:90:UNK:O	19:U1:94:UNK:N	2.50	0.44
3:02:148:ALA:HB2	16:50:86:LYS:HA	1.98	0.44
38:26:268:THR:O	38:26:288:GLY:N	2.40	0.44
8:62:128:PRO:HA	8:62:152:PHE:HA	1.99	0.44
96:g2:183:GLN:HA	96:g2:195:ASP:HA	2.00	0.44
98:j1:153:ARG:HA	98:j1:180:HIS:O	2.17	0.44
98:j1:158:LEU:N	98:j1:168:LYS:O	2.49	0.44
108:qB:295:ARG:O	114:qH:57:GLY:N	2.50	0.44
148:V1:302:GLU:HA	148:V1:307:GLY:HA2	1.99	0.44
8:h:128:PRO:HA	8:h:152:PHE:HA	1.99	0.44
61:m1:286:TRP:O	61:m1:290:HIS:N	2.50	0.44
41:vb:257:VAL:O	15:y7:295:LYS:N	2.47	0.44
12:46:239:TYR:HA	12:46:253:ASN:HA	1.99	0.44
38:81:502:GLY:C	153:81:703:HEA:H263	2.42	0.44
131:t2:126:SER:O	131:t2:133:TYR:N	2.42	0.44
2:b:102:VAL:O	2:b:105:ALA:HB3	2.18	0.44
5:E:83:TRP:O	5:E:87:ALA:N	2.42	0.44
30:T:71:GLY:O	30:T:75:ILE:N	2.51	0.44
29:18:78:TYR:O	29:18:83:GLN:N	2.46	0.44
41:29:615:LEU:O	15:49:239:ASN:N	2.51	0.44
110:qd:148:ASP:O	110:qd:152:ASN:N	2.51	0.44
118:s1:585:GLU:HA	118:s1:604:VAL:O	2.17	0.44
148:v1:326:PRO:HA	148:v1:435:PRO:HA	2.00	0.44
107:QA:79:ILE:O	107:QA:252:CYS:HA	2.17	0.44
12:0B:296:THR:O	12:0B:312:SER:N	2.51	0.44
107:qA:79:ILE:O	107:qA:252:CYS:HA	2.17	0.44
118:S1:301:GLN:HA	81:AL:164:TRP:HA	1.98	0.44
98:J1:252:PHE:O	98:J1:257:GLY:N	2.41	0.44
3:C:148:ALA:HB2	16:Y5:86:LYS:HA	1.98	0.44
41:VB:608:GLU:O	41:VB:612:GLU:N	2.38	0.44
19:53:90:UNK:O	19:53:94:UNK:N	2.50	0.44
55:86:63:PHE:HA	55:86:70:TYR:HA	1.99	0.44
103:N5:111:ILE:O	103:N5:115:LEU:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:bp:296:THR:O	12:bp:312:SER:N	2.51	0.44
29:S:78:TYR:O	29:S:83:GLN:N	2.46	0.44
12:0B:206:ARG:O	12:0B:210:LEU:N	2.50	0.44
30:19:71:GLY:O	30:19:75:ILE:N	2.51	0.44
61:37:160:ALA:O	61:37:164:ASP:N	2.50	0.44
2:56:242:THR:O	2:56:246:LEU:N	2.50	0.44
39:82:278:ASN:C	66:97:1:MET:H3	2.26	0.44
113:QG:97:TYR:O	113:QG:101:THR:N	2.37	0.44
82:AM:163:LEU:O	82:AM:167:ILE:N	2.45	0.44
98:J1:153:ARG:HA	98:J1:180:HIS:O	2.17	0.44
2:b:242:THR:O	2:b:246:LEU:N	2.50	0.44
61:M1:160:ALA:O	61:M1:164:ASP:N	2.50	0.44
20:U2:5:UNK:O	20:U2:9:UNK:N	2.50	0.44
146:th:31:ARG:O	146:th:35:ARG:N	2.51	0.43
39:c2:278:ASN:C	66:3t:1:MET:H3	2.26	0.43
40:c3:65:SER:O	40:c3:69:LYS:N	2.48	0.43
29:18:142:ALA:O	29:18:146:SER:N	2.49	0.43
63:39:48:ARG:O	63:39:52:ASP:N	2.49	0.43
110:Qd:277:ALA:O	110:Qd:281:ASN:N	2.37	0.43
104:N6:254:LYS:N	76:A7:163:VAL:O	2.50	0.43
146:TH:18:ILE:O	146:TH:22:LYS:N	2.52	0.43
103:N5:106:TRP:O	103:N5:110:TYR:N	2.37	0.43
12:bp:258:VAL:O	12:bp:282:VAL:HA	2.19	0.43
40:c3:423:PHE:HA	40:c3:430:TRP:HA	2.00	0.43
22:l:91:TYR:O	22:l:199:PHE:N	2.49	0.43
5:04:4:ALA:HB1	7:06:294:TYR:HA	2.00	0.43
62:38:28:ALA:O	62:38:32:TYR:N	2.51	0.43
153:81:701:HEA:CMA	153:81:701:HEA:CBA	2.97	0.43
76:a7:163:VAL:O	104:n6:254:LYS:N	2.50	0.43
148:v1:302:GLU:HA	148:v1:307:GLY:HA2	1.99	0.43
111:QE:29:GLU:O	111:QE:33:ARG:N	2.49	0.43
107:Qa:26:ALA:O	107:Qa:30:PHE:N	2.50	0.43
110:Qd:148:ASP:O	110:Qd:152:ASN:N	2.51	0.43
113:Qg:106:ASN:O	115:Qi:9:ASN:N	2.44	0.43
126:SA:409:VAL:H	126:SA:425:LEU:HA	1.83	0.43
104:N6:251:ILE:N	119:S2:268:SER:O	2.38	0.43
2:56:358:PHE:N	2:56:367:ASP:O	2.45	0.43
26:70:39:VAL:HA	26:70:118:LEU:O	2.18	0.43
108:qb:397:MET:O	108:qb:401:GLU:N	2.46	0.43
107:Qa:384:LYS:O	107:Qa:388:SER:N	2.50	0.43
7:g:58:HIS:O	15:y7:270:SER:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:vb:608:GLU:O	41:vb:612:GLU:N	2.43	0.43
8:H:123:SER:HA	8:H:195:THR:HA	2.00	0.43
15:0E:270:SER:N	7:61:58:HIS:O	2.44	0.43
61:37:225:PHE:O	61:37:229:VAL:N	2.52	0.43
62:38:314:LYS:O	62:38:318:ILE:N	2.49	0.43
2:56:102:VAL:O	2:56:105:ALA:HB3	2.18	0.43
98:j1:115:ARG:HA	98:j1:121:ALA:HA	2.00	0.43
107:qA:138:GLY:CA	107:qA:154:ASN:O	2.65	0.43
110:qD:293:ARG:O	113:qG:307:THR:N	2.51	0.43
118:S1:585:GLU:HA	118:S1:604:VAL:O	2.17	0.43
146:TH:31:ARG:O	146:TH:35:ARG:N	2.51	0.43
42:2B:134:LYS:N	42:2B:137:TYR:O	2.48	0.43
87:B6:70:HIS:HA	92:BM:125:GLY:HA3	2.00	0.43
97:G3:339:LYS:O	97:G3:343:THR:N	2.52	0.43
12:bp:216:ALA:HB1	12:bp:249:ALA:HB2	2.00	0.43
26:p:39:VAL:HA	26:p:118:LEU:O	2.18	0.43
19:u1:8:UNK:O	19:u1:12:UNK:N	2.51	0.43
7:G:126:GLU:O	7:G:130:ILE:N	2.47	0.43
153:26:701:HEA:HMB1	153:26:701:HEA:HHB	1.81	0.43
61:92:284:ALA:O	61:92:288:TRP:N	2.44	0.43
87:b6:70:HIS:HA	92:bm:125:GLY:HA3	2.00	0.43
126:sa:409:VAL:H	126:sa:425:LEU:HA	1.83	0.43
126:SA:148:SER:H	126:SA:179:ALA:HA	1.84	0.43
60:7l:913:ARG:O	60:7l:917:ASP:N	2.43	0.43
40:c3:209:PHE:O	40:c3:213:LEU:N	2.45	0.43
19:0I:8:UNK:O	19:0I:12:UNK:N	2.51	0.43
103:n5:234:LYS:HA	103:n5:245:SER:HA	2.01	0.43
121:S4:5:LYS:O	121:S4:11:ALA:HB2	2.19	0.43
98:J1:115:ARG:HA	98:J1:121:ALA:HA	2.00	0.43
10:J:97:VAL:O	10:J:101:ILE:N	2.51	0.43
12:0B:258:VAL:O	12:0B:282:VAL:HA	2.19	0.43
6:60:274:LEU:HA	6:60:281:LYS:H	1.83	0.43
40:83:423:PHE:HA	40:83:430:TRP:HA	2.00	0.43
41:84:608:GLU:O	41:84:612:GLU:N	2.43	0.43
126:SA:147:PHE:HA	126:SA:179:ALA:HA	2.01	0.43
1:a:233:GLU:O	1:a:237:ARG:N	2.52	0.43
153:c1:701:HEA:CMA	153:c1:701:HEA:CBA	2.97	0.43
5:E:4:ALA:HB1	7:G:294:TYR:HA	2.00	0.43
6:F:335:THR:N	13:FS:34:VAL:O	2.49	0.43
62:M2:28:ALA:O	62:M2:32:TYR:N	2.51	0.43
15:0E:293:LEU:O	41:84:257:VAL:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:27:597:TYR:O	39:27:601:LYS:N	2.52	0.43
40:28:67:GLU:O	40:28:71:TYR:N	2.42	0.43
111:qE:29:GLU:O	111:qE:33:ARG:N	2.49	0.43
109:Qc:397:PHE:O	109:Qc:401:ASN:N	2.37	0.43
126:SA:95:ASN:N	126:SA:443:ALA:O	2.49	0.43
58:7a:96:ILE:O	58:7a:100:PHE:N	2.52	0.43
12:BP:239:TYR:HA	12:BP:253:ASN:HA	1.99	0.43
12:0B:216:ALA:HB1	12:0B:249:ALA:HB2	2.00	0.43
9:63:25:ARG:O	9:63:29:ALA:N	2.46	0.43
153:81:701:HEA:H211	153:81:701:HEA:H271	1.30	0.43
81:al:177:LYS:HA	118:s1:573:TYR:HA	2.01	0.43
103:N5:234:LYS:HA	103:N5:245:SER:HA	2.01	0.43
39:C2:597:TYR:O	39:C2:601:LYS:N	2.52	0.43
5:04:175:ASP:O	5:04:179:LEU:N	2.37	0.42
3:57:24:GLU:O	3:57:28:LEU:N	2.40	0.42
78:a9:277:ALA:O	78:a9:281:GLY:N	2.45	0.42
105:p1:132:THR:HA	133:t4:39:SER:HA	2.01	0.42
103:N5:467:ALA:HA	103:N5:490:SER:HA	2.00	0.42
12:46:288:HIS:O	12:46:292:HIS:N	2.53	0.42
20:54:4:UNK:O	20:54:8:UNK:N	2.52	0.42
107:qA:474:TYR:O	107:qA:478:ARG:N	2.38	0.42
146:th:18:ILE:O	146:th:22:LYS:N	2.52	0.42
109:Qc:79:ASP:O	109:Qc:83:LEU:N	2.40	0.42
118:S1:266:THR:HA	118:S1:272:MET:H	1.84	0.42
12:bp:289:LEU:O	12:bp:293:GLU:N	2.52	0.42
5:e:176:ASP:O	5:e:180:SER:N	2.42	0.42
9:I:21:ALA:HB3	9:I:45:ASN:HA	2.00	0.42
8:07:123:SER:HA	8:07:195:THR:HA	2.00	0.42
9:08:166:ASN:H	30:19:5:THR:HA	1.84	0.42
65:41:23:ALA:O	65:41:27:ASP:N	2.52	0.42
1:55:233:GLU:O	1:55:237:ARG:N	2.52	0.42
58:89:96:ILE:O	58:89:100:PHE:N	2.52	0.42
107:qa:26:ALA:O	107:qa:30:PHE:N	2.50	0.42
110:QD:293:ARG:O	113:QG:307:THR:N	2.51	0.42
118:S1:573:TYR:HA	81:AL:177:LYS:HA	2.01	0.42
123:S6:114:THR:HA	123:S6:121:ARG:HA	2.01	0.42
82:AM:16:ARG:C	82:AM:18:ASP:H	2.27	0.42
8:h:156:GLU:HA	8:h:163:GLN:HA	2.02	0.42
12:BP:139:GLY:HA2	12:BP:143:ALA:HB3	2.02	0.42
12:BP:288:HIS:O	12:BP:292:HIS:N	2.53	0.42
61:M1:225:PHE:O	61:M1:229:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:46:139:GLY:HA2	12:46:143:ALA:HB3	2.02	0.42
116:qj:44:ILE:O	116:qj:49:ILE:N	2.46	0.42
121:s4:5:LYS:O	121:s4:11:ALA:HB2	2.19	0.42
123:s6:80:VAL:O	123:s6:125:LYS:N	2.53	0.42
123:s6:114:THR:HA	123:s6:121:ARG:HA	2.01	0.42
148:v1:230:PHE:O	148:v1:234:ALA:N	2.36	0.42
119:S2:46:GLN:O	119:S2:53:GLU:N	2.37	0.42
76:A7:83:THR:O	76:A7:87:ARG:N	2.42	0.42
95:G1:63:ILE:O	95:G1:82:GLY:N	2.39	0.42
8:h:196:CYS:HA	8:h:248:HIS:HA	2.01	0.42
12:BP:379:SER:HA	12:BP:384:ALA:HB3	2.01	0.42
10:J:205:GLY:N	10:J:208:TYR:O	2.35	0.42
60:91:913:ARG:O	60:91:917:ASP:N	2.43	0.42
103:n5:111:ILE:O	103:n5:115:LEU:N	2.47	0.42
127:sb:128:GLY:N	151:sb:401:FES:S2	2.91	0.42
127:sb:282:CYS:HA	161:sb:402:SF4:S4	2.60	0.42
134:T5:61:ALA:HB2	87:B6:126:ALA:HB2	2.01	0.42
6:f:274:LEU:HA	6:f:281:LYS:H	1.83	0.42
9:I:166:ASN:H	30:T:5:THR:HA	1.84	0.42
1:55:293:TYR:O	1:55:297:ALA:CB	2.67	0.42
97:g3:339:LYS:O	97:g3:343:THR:N	2.52	0.42
111:qE:140:GLY:N	111:qE:156:ARG:O	2.47	0.42
110:qd:115:HIS:HA	110:qd:131:GLU:HA	2.01	0.42
2:56:292:GLN:N	2:56:454:GLN:O	2.53	0.42
103:n5:467:ALA:HA	103:n5:490:SER:HA	2.00	0.42
113:QG:175:TRP:HA	113:QG:189:TYR:HA	2.02	0.42
78:A9:277:ALA:O	78:A9:281:GLY:N	2.45	0.42
1:a:293:TYR:O	1:a:297:ALA:CB	2.67	0.42
40:c3:430:TRP:O	10:j:234:LYS:N	2.46	0.42
42:2b:134:LYS:N	42:2b:137:TYR:O	2.48	0.42
17:51:66:ASP:O	17:51:70:LEU:N	2.53	0.42
5:59:83:TRP:O	5:59:87:ALA:N	2.39	0.42
8:62:156:GLU:HA	8:62:163:GLN:HA	2.02	0.42
8:62:196:CYS:HA	8:62:248:HIS:HA	2.01	0.42
118:s1:266:THR:HA	118:s1:272:MET:H	1.84	0.42
118:s1:279:HIS:N	118:s1:284:GLU:O	2.43	0.42
107:QA:139:SER:O	107:QA:153:ALA:HA	2.20	0.42
50:2L:40:ASP:O	50:2L:44:ASN:N	2.41	0.42
126:SA:90:ALA:HA	162:SA:701:FAD:C5X	2.50	0.42
98:J1:158:LEU:N	98:J1:168:LYS:O	2.49	0.42
41:vb:257:VAL:N	15:y7:293:LEU:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:2T:23:ALA:O	65:2T:27:ASP:N	2.52	0.42
24:13:33:MET:O	24:13:37:VAL:N	2.50	0.42
74:a5:124:GLU:HA	74:a5:128:GLN:HA	2.02	0.42
102:n4:457:SER:O	102:n4:461:PHE:N	2.39	0.42
107:qA:139:SER:O	107:qA:153:ALA:HA	2.20	0.42
109:qc:397:PHE:O	109:qc:401:ASN:N	2.37	0.42
144:tf:151:PRO:O	144:tf:155:LEU:N	2.39	0.42
107:QA:474:TYR:O	107:QA:478:ARG:N	2.38	0.42
127:SB:282:CYS:HA	161:SB:402:SF4:S4	2.60	0.42
130:T1:265:ASN:N	130:T1:305:HIS:O	2.48	0.42
74:A5:124:GLU:HA	74:A5:128:GLN:HA	2.02	0.42
91:BL:10:ASP:O	91:BL:26:ARG:N	2.53	0.42
2:b:358:PHE:N	2:b:367:ASP:O	2.45	0.42
40:C3:67:GLU:O	40:C3:71:TYR:N	2.42	0.42
4:03:160:ASP:HA	4:03:164:ALA:HB2	2.02	0.42
9:08:21:ALA:HB3	9:08:45:ASN:HA	2.01	0.42
46:2h:162:ALA:HB1	46:2h:191:TYR:HA	2.01	0.42
82:am:16:ARG:C	82:am:18:ASP:H	2.27	0.42
87:b6:126:ALA:HB2	134:t5:61:ALA:HB2	2.01	0.42
119:s2:46:GLN:O	119:s2:53:GLU:N	2.37	0.42
126:sa:147:PHE:HA	126:sa:179:ALA:HA	2.01	0.42
109:Qc:133:GLY:HA3	152:Qc:502:HEM:C1D	2.55	0.42
5:E:334:GLU:O	7:G:75:ARG:N	2.47	0.42
20:U2:4:UNK:O	20:U2:8:UNK:N	2.52	0.42
58:34:55:SER:HA	59:35:120:SEP:OG	2.20	0.41
4:58:156:PRO:HA	4:58:182:LEU:O	2.20	0.41
160:qc:501:U10:H1M1	160:qc:501:U10:H71	1.80	0.41
110:Qd:115:HIS:HA	110:Qd:131:GLU:HA	2.01	0.41
126:SA:288:ILE:N	126:SA:293:CYS:O	2.44	0.41
120:S3:153:THR:N	75:A6:40:LEU:O	2.45	0.41
124:S7:96:CYS:HA	124:S7:100:GLY:C	2.45	0.41
125:S8:139:CYS:N	161:S8:302:SF4:S1	2.93	0.41
135:T6:52:GLN:H	73:A3:109:ASN:HA	1.85	0.41
68:5t:31:GLN:N	68:5t:36:THR:O	2.52	0.41
13:FS:89:TYR:HA	13:FS:133:TYR:HA	2.02	0.41
24:N:33:MET:O	24:N:37:VAL:N	2.50	0.41
91:bl:10:ASP:O	91:bl:26:ARG:N	2.53	0.41
109:qC:287:ALA:O	109:qC:291:VAL:N	2.53	0.41
107:qa:384:LYS:O	107:qa:388:SER:N	2.50	0.41
108:qb:73:VAL:HA	108:qb:246:PHE:O	2.20	0.41
126:sa:95:ASN:N	126:sa:443:ALA:O	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
148:v1:314:ASN:O	148:v1:360:LYS:N	2.53	0.41
80:AC:82:THR:HA	80:AC:118:THR:HA	2.02	0.41
96:G2:154:VAL:O	96:G2:172:LEU:HA	2.20	0.41
12:bp:84:ASN:N	12:bp:461:VAL:O	2.53	0.41
58:7A:55:SER:HA	59:7C:120:SEP:OG	2.20	0.41
3:C:128:ASN:O	3:C:132:ALA:HB2	2.20	0.41
4:D:160:ASP:HA	4:D:164:ALA:HB2	2.02	0.41
12:46:379:SER:HA	12:46:384:ALA:HB3	2.01	0.41
109:qc:133:GLY:HA3	152:qc:502:HEM:C1D	2.55	0.41
109:qc:133:GLY:HA3	152:qc:502:HEM:C2D	2.56	0.41
126:sa:148:SER:H	126:sa:179:ALA:HA	1.84	0.41
105:P1:132:THR:HA	133:T4:39:SER:HA	2.01	0.41
8:h:137:PRO:HA	8:h:146:PHE:HA	2.02	0.41
5:E:263:ALA:O	5:E:268:THR:N	2.53	0.41
2:01:292:GLN:O	2:01:454:GLN:N	2.46	0.41
2:56:99:LEU:O	2:56:103:ASN:N	2.41	0.41
98:j1:252:PHE:O	98:j1:257:GLY:N	2.41	0.41
113:qg:90:ASP:O	113:qg:94:ARG:N	2.53	0.41
125:s8:108:ASN:O	125:s8:112:GLU:N	2.53	0.41
126:sa:90:ALA:HA	162:sa:701:FAD:C5X	2.50	0.41
108:Qb:73:VAL:HA	108:Qb:246:PHE:O	2.21	0.41
59:35:36:ASP:O	59:35:40:ASN:N	2.46	0.41
91:bl:33:GLN:O	91:bl:38:ARG:N	2.39	0.41
96:g2:154:VAL:O	96:g2:172:LEU:HA	2.20	0.41
126:sa:212:ILE:N	126:sa:221:GLY:O	2.38	0.41
125:S8:108:ASN:O	125:S8:112:GLU:N	2.53	0.41
3:c:148:ALA:HB2	16:y5:86:LYS:HA	2.03	0.41
4:d:156:PRO:HA	4:d:182:LEU:O	2.19	0.41
40:C3:87:ASN:O	40:C3:91:PHE:CB	2.69	0.41
6:F:258:LEU:HA	6:F:266:ASP:H	1.85	0.41
22:L:57:TYR:HA	22:L:187:LEU:O	2.20	0.41
5:04:263:ALA:O	5:04:268:THR:N	2.53	0.41
6:05:334:ASN:HA	13:47:35:ILE:HA	2.03	0.41
12:0B:289:LEU:O	12:0B:293:GLU:N	2.52	0.41
8:62:137:PRO:HA	8:62:146:PHE:HA	2.02	0.41
9:63:186:HIS:O	9:63:191:SER:N	2.31	0.41
109:qC:223:PHE:O	109:qC:227:LEU:CB	2.68	0.41
123:S6:80:VAL:O	123:S6:125:LYS:N	2.52	0.41
84:B2:116:SER:O	84:B2:120:GLY:N	2.48	0.41
29:S:142:ALA:O	29:S:146:SER:N	2.49	0.41
17:Y0:66:ASP:O	17:Y0:70:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:11:57:TYR:HA	22:11:187:LEU:O	2.20	0.41
13:47:2:SER:O	13:47:5:LEU:CB	2.68	0.41
41:84:162:THR:O	41:84:173:HIS:N	2.34	0.41
118:s1:540:VAL:O	118:s1:560:VAL:HA	2.21	0.41
109:QC:15:LYS:O	109:QC:19:TYR:N	2.54	0.41
113:Qg:90:ASP:O	113:Qg:94:ARG:N	2.53	0.41
134:T5:79:LYS:O	87:B6:115:TYR:N	2.51	0.41
8:h:133:GLY:HA2	8:h:150:VAL:HA	2.02	0.41
13:FS:2:SER:O	13:FS:5:LEU:CB	2.68	0.41
119:s2:102:GLU:O	119:s2:106:GLY:N	2.54	0.41
125:s8:139:CYS:N	161:s8:302:SF4:S1	2.93	0.41
130:t1:387:THR:O	130:t1:391:ASN:N	2.54	0.41
118:S1:472:MET:HA	118:S1:510:GLY:HA3	2.01	0.41
148:V1:87:GLY:N	148:V1:93:PHE:O	2.51	0.41
76:A7:169:GLU:O	76:A7:173:ASN:N	2.54	0.41
2:b:292:GLN:N	2:b:454:GLN:O	2.53	0.41
3:c:10:ALA:O	3:c:14:LYS:N	2.45	0.41
34:w:98:GLU:O	34:w:102:ARG:N	2.54	0.41
1:A:185:PRO:O	1:A:189:ALA:N	2.46	0.41
39:C2:596:HIS:O	39:C2:600:ARG:N	2.54	0.41
24:N:164:ILE:O	24:N:168:GLU:N	2.41	0.41
3:02:128:ASN:O	3:02:132:ALA:HB2	2.20	0.41
28:17:29:SER:O	28:17:33:ARG:N	2.42	0.41
16:50:44:PHE:O	16:50:49:VAL:N	2.54	0.41
80:ac:36:TYR:N	92:bm:117:GLU:O	2.54	0.41
87:b6:113:GLY:HA2	88:b7:23:ALA:HB1	2.03	0.41
91:bl:144:GLN:O	91:bl:148:LEU:N	2.46	0.41
98:j1:158:LEU:O	98:j1:168:LYS:N	2.37	0.41
107:qA:157:ALA:O	108:qB:39:SER:N	2.53	0.41
109:qC:137:CYS:O	109:qC:139:THR:N	2.53	0.41
113:qG:175:TRP:HA	113:qG:189:TYR:HA	2.02	0.41
107:qa:111:LEU:O	107:qa:115:ASN:N	2.39	0.41
118:s1:472:MET:HA	118:s1:510:GLY:HA3	2.02	0.41
111:QE:140:GLY:N	111:QE:156:ARG:O	2.47	0.41
109:Qc:133:GLY:HA3	152:Qc:502:HEM:C2D	2.56	0.41
111:Qe:79:VAL:O	111:Qe:81:ASN:N	2.54	0.41
114:Qh:92:TRP:O	114:Qh:96:ASN:N	2.37	0.41
127:SB:128:GLY:N	151:SB:401:FES:S2	2.91	0.41
118:S1:540:VAL:O	118:S1:560:VAL:HA	2.21	0.41
130:T1:162:ARG:O	130:T1:182:ILE:N	2.36	0.41
80:AC:36:TYR:N	92:BM:117:GLU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:BL:144:GLN:O	91:BL:148:LEU:N	2.46	0.41
12:bp:206:ARG:O	12:bp:210:LEU:N	2.51	0.41
12:bp:413:GLU:C	12:bp:415:GLY:H	2.29	0.41
153:c1:703:HEA:HHA	153:c1:703:HEA:CBA	2.47	0.41
22:l:55:LYS:O	22:l:59:GLY:N	2.54	0.41
60:7L:980:ASP:O	8:H:267:SER:N	2.51	0.41
38:C1:687:GLU:N	33:V:47:VAL:O	2.40	0.41
40:C3:209:PHE:O	40:C3:213:LEU:N	2.44	0.41
3:02:14:LYS:O	3:02:17:ALA:HB3	2.21	0.41
10:09:205:GLY:N	10:09:208:TYR:O	2.35	0.41
40:28:87:ASN:O	40:28:91:PHE:CB	2.69	0.41
43:2e:33:ASP:C	43:2e:35:PHE:H	2.24	0.41
12:46:86:TYR:HA	12:46:105:ARG:O	2.21	0.41
22:66:55:LYS:O	22:66:59:GLY:N	2.54	0.41
76:a7:169:GLU:O	76:a7:173:ASN:N	2.54	0.41
107:qa:309:PHE:O	107:qa:360:LEU:HA	2.21	0.41
119:s2:237:THR:HA	119:s2:241:ALA:HB2	2.03	0.41
126:sa:288:ILE:N	126:sa:293:CYS:O	2.44	0.41
107:Qa:309:PHE:O	107:Qa:360:LEU:HA	2.21	0.41
105:P1:207:ASN:O	105:P1:211:ALA:N	2.53	0.41
130:T1:147:TYR:O	130:T1:152:LYS:N	2.40	0.41
148:V1:314:ASN:O	148:V1:360:LYS:N	2.53	0.41
12:bp:377:PHE:HA	12:bp:389:ARG:HA	2.03	0.41
38:c1:528:HIS:O	38:c1:532:SER:N	2.53	0.41
32:u:129:GLY:O	32:u:135:GLY:HA3	2.21	0.41
16:0F:86:LYS:HA	3:57:148:ALA:HB2	2.03	0.40
21:10:195:LYS:O	21:10:199:GLN:N	2.49	0.40
30:19:84:ASN:HA	30:19:90:PRO:HA	2.03	0.40
2:56:290:ILE:N	2:56:357:LEU:O	2.49	0.40
95:g1:90:GLY:HA3	95:g1:118:GLY:O	2.22	0.40
119:S2:102:GLU:O	119:S2:106:GLY:N	2.54	0.40
59:7c:108:ALA:O	59:7c:112:MET:N	2.33	0.40
12:BP:86:TYR:HA	12:BP:105:ARG:O	2.21	0.40
6:F:334:ASN:HA	13:FS:35:ILE:HA	2.03	0.40
19:U1:50:UNK:O	19:U1:54:UNK:N	2.54	0.40
4:03:209:PHE:HA	4:03:239:LEU:H	1.86	0.40
12:0B:306:PHE:HA	12:0B:320:GLY:HA3	2.03	0.40
8:62:133:GLY:HA2	8:62:150:VAL:HA	2.02	0.40
22:66:91:TYR:O	22:66:199:PHE:N	2.49	0.40
102:N4:457:SER:O	102:N4:461:PHE:N	2.39	0.40
3:C:14:LYS:O	3:C:17:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:39:VAL:HA	26:P:118:LEU:O	2.21	0.40
39:27:596:HIS:O	39:27:600:ARG:N	2.54	0.40
32:75:129:GLY:O	32:75:135:GLY:HA3	2.21	0.40
73:a3:109:ASN:HA	135:t6:52:GLN:H	1.85	0.40
130:t1:499:PRO:C	130:t1:501:HIS:H	2.28	0.40
109:QC:287:ALA:O	109:QC:291:VAL:N	2.53	0.40
46:2H:162:ALA:HB1	46:2H:191:TYR:HA	2.01	0.40
87:B6:113:GLY:HA2	88:B7:23:ALA:HB1	2.03	0.40
91:BL:145:PHE:HA	91:BL:146:PRO:HA	1.88	0.40
7:g:126:GLU:O	7:g:130:ILE:N	2.42	0.40
54:6A:101:THR:O	35:X:4:PHE:HA	2.21	0.40
7:06:124:ARG:O	7:06:128:GLU:N	2.40	0.40
12:0B:377:PHE:HA	12:0B:389:ARG:HA	2.03	0.40
25:14:87:ASP:O	25:14:91:ARG:N	2.55	0.40
35:23:4:PHE:HA	54:30:101:THR:O	2.21	0.40
27:71:22:ASP:O	27:71:26:ILE:N	2.42	0.40
34:77:98:GLU:O	34:77:102:ARG:N	2.54	0.40
80:ac:82:THR:HA	80:ac:118:THR:HA	2.02	0.40
103:n5:106:TRP:O	103:n5:110:TYR:N	2.37	0.40
109:QC:223:PHE:O	109:QC:227:LEU:CB	2.68	0.40
118:S1:393:GLY:O	118:S1:397:ALA:N	2.34	0.40
119:S2:237:THR:HA	119:S2:241:ALA:HB2	2.03	0.40
130:T1:499:PRO:C	130:T1:501:HIS:H	2.28	0.40
83:AN:195:THR:O	91:BL:22:ILE:N	2.49	0.40
28:R:29:SER:O	28:R:33:ARG:N	2.42	0.40
26:15:45:SER:H	26:15:48:ALA:HB3	1.86	0.40
54:30:118:GLY:C	54:30:120:LEU:H	2.29	0.40
4:58:208:VAL:O	4:58:239:LEU:N	2.55	0.40
108:qB:92:VAL:HA	108:qB:245:ASN:O	2.22	0.40
107:qa:213:GLY:O	107:qa:218:GLY:HA3	2.21	0.40
109:Qc:130:VAL:O	109:Qc:134:LEU:N	2.54	0.40
4:d:208:VAL:O	4:d:239:LEU:N	2.55	0.40
13:fs:138:ASN:N	151:fs:202:FES:S1	2.87	0.40
40:C3:140:ILE:O	40:C3:146:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

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	00	447/490 (91%)	434 (97%)	13 (3%)	0	100	100
1	55	447/490 (91%)	433 (97%)	14 (3%)	0	100	100
1	A	447/490 (91%)	434 (97%)	13 (3%)	0	100	100
1	a	447/490 (91%)	433 (97%)	14 (3%)	0	100	100
2	01	422/473 (89%)	403 (96%)	18 (4%)	1 (0%)	43	77
2	56	422/473 (89%)	407 (96%)	15 (4%)	0	100	100
2	B	422/473 (89%)	402 (95%)	19 (4%)	1 (0%)	43	77
2	b	422/473 (89%)	407 (96%)	15 (4%)	0	100	100
3	02	201/212 (95%)	190 (94%)	10 (5%)	1 (0%)	24	62
3	57	201/212 (95%)	195 (97%)	5 (2%)	1 (0%)	24	62
3	C	201/212 (95%)	190 (94%)	10 (5%)	1 (0%)	24	62
3	c	201/212 (95%)	195 (97%)	5 (2%)	1 (0%)	24	62
4	03	287/402 (71%)	282 (98%)	5 (2%)	0	100	100
4	58	287/402 (71%)	275 (96%)	12 (4%)	0	100	100
4	D	287/402 (71%)	282 (98%)	5 (2%)	0	100	100
4	d	287/402 (71%)	275 (96%)	12 (4%)	0	100	100
5	04	382/385 (99%)	366 (96%)	16 (4%)	0	100	100
5	59	382/385 (99%)	365 (96%)	17 (4%)	0	100	100
5	E	382/385 (99%)	366 (96%)	16 (4%)	0	100	100
5	e	382/385 (99%)	365 (96%)	17 (4%)	0	100	100
6	05	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
6	60	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
6	F	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
6	f	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
7	06	291/318 (92%)	279 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	61	291/318 (92%)	283 (97%)	8 (3%)	0	100	100
7	G	291/318 (92%)	279 (96%)	12 (4%)	0	100	100
7	g	291/318 (92%)	283 (97%)	8 (3%)	0	100	100
8	07	296/318 (93%)	286 (97%)	10 (3%)	0	100	100
8	62	296/318 (93%)	290 (98%)	6 (2%)	0	100	100
8	H	296/318 (93%)	287 (97%)	9 (3%)	0	100	100
8	h	296/318 (93%)	290 (98%)	6 (2%)	0	100	100
9	08	229/252 (91%)	219 (96%)	10 (4%)	0	100	100
9	63	229/252 (91%)	220 (96%)	8 (4%)	1 (0%)	30	66
9	I	229/252 (91%)	218 (95%)	11 (5%)	0	100	100
9	i	229/252 (91%)	219 (96%)	9 (4%)	1 (0%)	30	66
10	09	185/234 (79%)	180 (97%)	5 (3%)	0	100	100
10	64	185/234 (79%)	179 (97%)	6 (3%)	0	100	100
10	J	185/234 (79%)	180 (97%)	5 (3%)	0	100	100
10	j	185/234 (79%)	179 (97%)	6 (3%)	0	100	100
11	0A	68/72 (94%)	68 (100%)	0	0	100	100
11	45	68/72 (94%)	68 (100%)	0	0	100	100
11	6T	68/72 (94%)	68 (100%)	0	0	100	100
11	6t	68/72 (94%)	68 (100%)	0	0	100	100
12	0B	379/462 (82%)	356 (94%)	23 (6%)	0	100	100
12	46	379/462 (82%)	359 (95%)	20 (5%)	0	100	100
12	BP	379/462 (82%)	359 (95%)	20 (5%)	0	100	100
12	bp	379/462 (82%)	356 (94%)	23 (6%)	0	100	100
13	0C	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
13	47	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
13	FS	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
13	fs	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
14	0D	98/127 (77%)	96 (98%)	2 (2%)	0	100	100
14	48	98/127 (77%)	96 (98%)	2 (2%)	0	100	100
14	4A	98/127 (77%)	96 (98%)	2 (2%)	0	100	100
14	4a	98/127 (77%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	0E	339/453 (75%)	330 (97%)	9 (3%)	0	100	100
15	49	339/453 (75%)	330 (97%)	9 (3%)	0	100	100
15	Y7	339/453 (75%)	330 (97%)	9 (3%)	0	100	100
15	y7	339/453 (75%)	330 (97%)	9 (3%)	0	100	100
16	0F	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
16	50	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
16	Y5	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
16	y5	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
17	0G	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
17	51	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
17	Y0	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
17	y0	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
18	0H	95/100 (95%)	95 (100%)	0	0	100	100
18	52	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
18	Z1	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
18	z1	95/100 (95%)	95 (100%)	0	0	100	100
21	10	206/231 (89%)	200 (97%)	6 (3%)	0	100	100
21	65	206/231 (89%)	202 (98%)	4 (2%)	0	100	100
21	K	206/231 (89%)	200 (97%)	6 (3%)	0	100	100
21	k	206/231 (89%)	200 (97%)	6 (3%)	0	100	100
22	11	192/222 (86%)	188 (98%)	4 (2%)	0	100	100
22	66	192/222 (86%)	188 (98%)	4 (2%)	0	100	100
22	L	192/222 (86%)	188 (98%)	4 (2%)	0	100	100
22	l	192/222 (86%)	188 (98%)	4 (2%)	0	100	100
23	12	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
23	67	217/220 (99%)	206 (95%)	11 (5%)	0	100	100
23	M	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
23	m	217/220 (99%)	206 (95%)	11 (5%)	0	100	100
24	13	204/210 (97%)	201 (98%)	3 (2%)	0	100	100
24	68	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
24	N	204/210 (97%)	200 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	n	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
25	14	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
25	69	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
25	O	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
25	o	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
26	15	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
26	70	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
26	P	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
26	p	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
27	16	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
27	71	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
27	Q	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
27	q	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
28	17	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
28	72	170/173 (98%)	164 (96%)	6 (4%)	0	100	100
28	R	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
28	r	170/173 (98%)	164 (96%)	6 (4%)	0	100	100
29	18	167/170 (98%)	162 (97%)	4 (2%)	1 (1%)	21	58
29	73	167/170 (98%)	161 (96%)	5 (3%)	1 (1%)	21	58
29	S	167/170 (98%)	162 (97%)	4 (2%)	1 (1%)	21	58
29	s	167/170 (98%)	161 (96%)	5 (3%)	1 (1%)	21	58
30	19	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
30	74	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
30	T	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
30	t	154/158 (98%)	151 (98%)	3 (2%)	0	100	100
31	1B	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
31	1b	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
32	20	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
32	75	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
32	U	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
32	u	151/154 (98%)	146 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	21	144/149 (97%)	136 (94%)	8 (6%)	0	100	100
33	76	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
33	V	144/149 (97%)	136 (94%)	8 (6%)	0	100	100
33	v	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
34	22	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
34	77	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
34	W	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
34	w	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
35	23	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
35	78	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
35	X	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
35	x	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
36	24	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
36	79	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
36	Y	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
36	y	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
37	25	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
37	80	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
37	Z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
37	z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
38	26	672/688 (98%)	654 (97%)	18 (3%)	0	100	100
38	81	672/688 (98%)	651 (97%)	21 (3%)	0	100	100
38	C1	672/688 (98%)	654 (97%)	18 (3%)	0	100	100
38	c1	672/688 (98%)	651 (97%)	21 (3%)	0	100	100
39	27	595/604 (98%)	574 (96%)	20 (3%)	1 (0%)	43	77
39	82	595/604 (98%)	572 (96%)	23 (4%)	0	100	100
39	C2	595/604 (98%)	574 (96%)	20 (3%)	1 (0%)	43	77
39	c2	595/604 (98%)	572 (96%)	23 (4%)	0	100	100
40	28	580/594 (98%)	557 (96%)	23 (4%)	0	100	100
40	83	580/594 (98%)	559 (96%)	21 (4%)	0	100	100
40	C3	580/594 (98%)	558 (96%)	22 (4%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	c3	580/594 (98%)	559 (96%)	21 (4%)	0	100	100
41	29	551/637 (86%)	538 (98%)	13 (2%)	0	100	100
41	84	551/637 (86%)	532 (97%)	19 (3%)	0	100	100
41	VB	551/637 (86%)	538 (98%)	13 (2%)	0	100	100
41	vb	551/637 (86%)	532 (97%)	19 (3%)	0	100	100
42	2B	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
42	2b	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
43	2E	319/322 (99%)	305 (96%)	14 (4%)	0	100	100
43	2e	319/322 (99%)	305 (96%)	14 (4%)	0	100	100
44	2F	215/296 (73%)	212 (99%)	3 (1%)	0	100	100
44	2f	215/296 (73%)	212 (99%)	3 (1%)	0	100	100
45	2G	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
45	2g	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
46	2H	98/195 (50%)	94 (96%)	4 (4%)	0	100	100
46	2h	98/195 (50%)	94 (96%)	4 (4%)	0	100	100
47	2I	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
47	2i	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
48	2J	100/103 (97%)	98 (98%)	2 (2%)	0	100	100
48	2j	100/103 (97%)	98 (98%)	2 (2%)	0	100	100
49	2K	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	2k	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
50	2L	81/89 (91%)	81 (100%)	0	0	100	100
50	2l	81/89 (91%)	81 (100%)	0	0	100	100
51	2M	73/76 (96%)	67 (92%)	6 (8%)	0	100	100
51	2m	73/76 (96%)	67 (92%)	6 (8%)	0	100	100
52	2N	59/62 (95%)	53 (90%)	5 (8%)	1 (2%)	7	35
52	2n	59/62 (95%)	53 (90%)	5 (8%)	1 (2%)	7	35
53	2O	40/46 (87%)	40 (100%)	0	0	100	100
53	2o	40/46 (87%)	40 (100%)	0	0	100	100
54	30	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
54	6A	124/130 (95%)	118 (95%)	6 (5%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	6a	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
54	85	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
55	31	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
55	6B	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
55	6b	220/230 (96%)	208 (94%)	12 (6%)	0	100	100
55	86	220/230 (96%)	208 (94%)	12 (6%)	0	100	100
56	32	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
56	6C	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
56	6c	99/103 (96%)	96 (97%)	3 (3%)	0	100	100
56	87	99/103 (96%)	96 (97%)	3 (3%)	0	100	100
57	33	75/88 (85%)	75 (100%)	0	0	100	100
57	6L	75/88 (85%)	74 (99%)	1 (1%)	0	100	100
57	6l	75/88 (85%)	71 (95%)	4 (5%)	0	100	100
57	88	75/88 (85%)	71 (95%)	4 (5%)	0	100	100
58	34	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
58	7A	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
58	7a	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
58	89	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
59	35	208/236 (88%)	203 (98%)	4 (2%)	1 (0%)	24	62
59	7C	208/236 (88%)	203 (98%)	4 (2%)	1 (0%)	24	62
59	7c	208/236 (88%)	201 (97%)	7 (3%)	0	100	100
59	90	208/236 (88%)	201 (97%)	7 (3%)	0	100	100
60	36	129/990 (13%)	122 (95%)	7 (5%)	0	100	100
60	7L	129/990 (13%)	122 (95%)	7 (5%)	0	100	100
60	7l	129/990 (13%)	121 (94%)	8 (6%)	0	100	100
60	91	129/990 (13%)	121 (94%)	8 (6%)	0	100	100
61	37	344/346 (99%)	331 (96%)	13 (4%)	0	100	100
61	92	344/346 (99%)	335 (97%)	9 (3%)	0	100	100
61	M1	344/346 (99%)	331 (96%)	13 (4%)	0	100	100
61	m1	344/346 (99%)	335 (97%)	9 (3%)	0	100	100
62	38	316/318 (99%)	306 (97%)	10 (3%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	93	316/318 (99%)	312 (99%)	4 (1%)	0	100	100
62	M2	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
62	m2	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
63	39	327/330 (99%)	313 (96%)	14 (4%)	0	100	100
63	94	327/330 (99%)	319 (98%)	8 (2%)	0	100	100
63	M3	327/330 (99%)	313 (96%)	14 (4%)	0	100	100
63	m3	327/330 (99%)	319 (98%)	8 (2%)	0	100	100
64	1T	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
64	1t	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
64	40	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
64	95	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
65	2T	68/72 (94%)	68 (100%)	0	0	100	100
65	2t	68/72 (94%)	68 (100%)	0	0	100	100
65	41	68/72 (94%)	68 (100%)	0	0	100	100
65	96	68/72 (94%)	68 (100%)	0	0	100	100
66	3T	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
66	3t	81/93 (87%)	80 (99%)	1 (1%)	0	100	100
66	42	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
66	97	81/93 (87%)	80 (99%)	1 (1%)	0	100	100
67	43	55/68 (81%)	54 (98%)	1 (2%)	0	100	100
67	4T	55/68 (81%)	54 (98%)	1 (2%)	0	100	100
67	4t	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
67	98	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
68	44	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
68	5T	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
68	5t	60/81 (74%)	60 (100%)	0	0	100	100
68	99	60/81 (74%)	60 (100%)	0	0	100	100
69	4L	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
69	4l	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
70	5B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
70	5b	98/100 (98%)	94 (96%)	4 (4%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	A1	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
71	a1	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
72	A2	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
72	a2	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
73	A3	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
73	a3	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
74	A5	153/206 (74%)	153 (100%)	0	0	100	100
74	a5	153/206 (74%)	153 (100%)	0	0	100	100
75	A6	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
75	a6	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
76	A7	280/282 (99%)	277 (99%)	3 (1%)	0	100	100
76	a7	280/282 (99%)	277 (99%)	3 (1%)	0	100	100
77	A8	130/238 (55%)	128 (98%)	2 (2%)	0	100	100
77	a8	130/238 (55%)	128 (98%)	2 (2%)	0	100	100
78	A9	338/362 (93%)	325 (96%)	13 (4%)	0	100	100
78	a9	338/362 (93%)	325 (96%)	13 (4%)	0	100	100
79	AB	110/138 (80%)	110 (100%)	0	0	100	100
79	ab	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
80	AC	96/133 (72%)	92 (96%)	4 (4%)	0	100	100
80	ac	96/133 (72%)	92 (96%)	4 (4%)	0	100	100
81	AL	191/194 (98%)	184 (96%)	7 (4%)	0	100	100
81	al	191/194 (98%)	184 (96%)	7 (4%)	0	100	100
82	AM	158/175 (90%)	151 (96%)	7 (4%)	0	100	100
82	am	158/175 (90%)	151 (96%)	7 (4%)	0	100	100
83	AN	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
83	an	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
84	B2	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
84	b2	118/126 (94%)	114 (97%)	4 (3%)	0	100	100
85	B3	67/83 (81%)	64 (96%)	3 (4%)	0	100	100
85	b3	67/83 (81%)	64 (96%)	3 (4%)	0	100	100
86	B4	113/147 (77%)	111 (98%)	2 (2%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	b4	113/147 (77%)	111 (98%)	2 (2%)	0	100	100
87	B6	68/129 (53%)	67 (98%)	1 (2%)	0	100	100
87	b6	68/129 (53%)	67 (98%)	1 (2%)	0	100	100
88	B7	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
88	b7	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
89	B8	173/207 (84%)	165 (95%)	8 (5%)	0	100	100
89	b8	173/207 (84%)	165 (95%)	8 (5%)	0	100	100
90	B9	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
90	b9	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
91	BL	173/188 (92%)	169 (98%)	4 (2%)	0	100	100
91	bl	173/188 (92%)	169 (98%)	4 (2%)	0	100	100
92	BM	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
92	bm	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
93	C4	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
93	c4	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
94	FX	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
94	fx	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
95	G1	227/257 (88%)	220 (97%)	7 (3%)	0	100	100
95	g1	227/257 (88%)	220 (97%)	7 (3%)	0	100	100
96	G2	228/233 (98%)	225 (99%)	3 (1%)	0	100	100
96	g2	228/233 (98%)	225 (99%)	3 (1%)	0	100	100
97	G3	344/346 (99%)	336 (98%)	8 (2%)	0	100	100
97	g3	344/346 (99%)	336 (98%)	8 (2%)	0	100	100
98	J1	259/317 (82%)	252 (97%)	7 (3%)	0	100	100
98	j1	259/317 (82%)	252 (97%)	7 (3%)	0	100	100
99	N1	281/284 (99%)	271 (96%)	9 (3%)	1 (0%)	30	66
99	n1	281/284 (99%)	272 (97%)	8 (3%)	1 (0%)	30	66
100	N2	358/360 (99%)	354 (99%)	4 (1%)	0	100	100
100	n2	358/360 (99%)	354 (99%)	4 (1%)	0	100	100
101	N3	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
101	n3	118/121 (98%)	115 (98%)	3 (2%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
102	N4	503/505 (100%)	492 (98%)	11 (2%)	0	100	100
102	n4	503/505 (100%)	492 (98%)	11 (2%)	0	100	100
103	N5	707/750 (94%)	682 (96%)	25 (4%)	0	100	100
103	n5	707/750 (94%)	682 (96%)	25 (4%)	0	100	100
104	N6	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
104	n6	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
105	P1	228/251 (91%)	223 (98%)	5 (2%)	0	100	100
105	p1	228/251 (91%)	223 (98%)	5 (2%)	0	100	100
106	P2	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
106	p2	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
107	QA	450/482 (93%)	441 (98%)	9 (2%)	0	100	100
107	Qa	450/482 (93%)	437 (97%)	13 (3%)	0	100	100
107	qA	450/482 (93%)	441 (98%)	9 (2%)	0	100	100
107	qa	450/482 (93%)	437 (97%)	13 (3%)	0	100	100
108	QB	478/513 (93%)	463 (97%)	15 (3%)	0	100	100
108	Qb	478/513 (93%)	461 (96%)	17 (4%)	0	100	100
108	qB	478/513 (93%)	462 (97%)	16 (3%)	0	100	100
108	qb	478/513 (93%)	461 (96%)	17 (4%)	0	100	100
109	QC	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
109	Qc	423/426 (99%)	404 (96%)	19 (4%)	0	100	100
109	qC	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
109	qc	423/426 (99%)	404 (96%)	19 (4%)	0	100	100
110	QD	293/319 (92%)	282 (96%)	11 (4%)	0	100	100
110	Qd	293/319 (92%)	276 (94%)	17 (6%)	0	100	100
110	qD	293/319 (92%)	282 (96%)	11 (4%)	0	100	100
110	qd	293/319 (92%)	276 (94%)	17 (6%)	0	100	100
111	QE	226/269 (84%)	212 (94%)	13 (6%)	1 (0%)	30	66
111	Qe	215/269 (80%)	200 (93%)	14 (6%)	1 (0%)	24	62
111	qE	226/269 (84%)	212 (94%)	13 (6%)	1 (0%)	30	66
111	qe	215/269 (80%)	201 (94%)	13 (6%)	1 (0%)	24	62
112	QF	87/90 (97%)	84 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
112	Qf	78/90 (87%)	75 (96%)	3 (4%)	0	100	100
112	qF	87/90 (97%)	84 (97%)	3 (3%)	0	100	100
112	qf	78/90 (87%)	75 (96%)	3 (4%)	0	100	100
113	QG	325/328 (99%)	315 (97%)	10 (3%)	0	100	100
113	Qg	324/328 (99%)	316 (98%)	8 (2%)	0	100	100
113	qG	325/328 (99%)	315 (97%)	10 (3%)	0	100	100
113	qg	324/328 (99%)	317 (98%)	7 (2%)	0	100	100
114	QH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
114	Qh	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
114	qH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
114	qh	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
115	QI	112/119 (94%)	106 (95%)	6 (5%)	0	100	100
115	Qi	112/119 (94%)	112 (100%)	0	0	100	100
115	qI	112/119 (94%)	106 (95%)	6 (5%)	0	100	100
115	qi	112/119 (94%)	112 (100%)	0	0	100	100
116	QJ	54/62 (87%)	54 (100%)	0	0	100	100
116	Qj	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
116	qJ	54/62 (87%)	54 (100%)	0	0	100	100
116	qj	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
117	QL	30/41 (73%)	30 (100%)	0	0	100	100
117	Ql	30/41 (73%)	29 (97%)	1 (3%)	0	100	100
117	qL	30/41 (73%)	30 (100%)	0	0	100	100
117	ql	30/41 (73%)	29 (97%)	1 (3%)	0	100	100
118	S1	687/718 (96%)	663 (96%)	24 (4%)	0	100	100
118	s1	687/718 (96%)	663 (96%)	24 (4%)	0	100	100
119	S2	440/442 (100%)	426 (97%)	14 (3%)	0	100	100
119	s2	440/442 (100%)	425 (97%)	15 (3%)	0	100	100
120	S3	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
120	s3	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
121	S4	180/185 (97%)	176 (98%)	4 (2%)	0	100	100
121	s4	180/185 (97%)	176 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
122	S5	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
122	s5	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
123	S6	90/132 (68%)	85 (94%)	5 (6%)	0	100	100
123	s6	90/132 (68%)	85 (94%)	5 (6%)	0	100	100
124	S7	159/162 (98%)	153 (96%)	6 (4%)	0	100	100
124	s7	159/162 (98%)	153 (96%)	6 (4%)	0	100	100
125	S8	216/236 (92%)	211 (98%)	5 (2%)	0	100	100
125	s8	216/236 (92%)	211 (98%)	5 (2%)	0	100	100
126	SA	597/636 (94%)	573 (96%)	24 (4%)	0	100	100
126	sa	597/636 (94%)	573 (96%)	24 (4%)	0	100	100
127	SB	277/312 (89%)	263 (95%)	14 (5%)	0	100	100
127	sb	277/312 (89%)	263 (95%)	14 (5%)	0	100	100
128	SC	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
128	sc	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
129	SD	42/44 (96%)	42 (100%)	0	0	100	100
129	sd	42/44 (96%)	42 (100%)	0	0	100	100
130	T1	500/516 (97%)	491 (98%)	9 (2%)	0	100	100
130	t1	500/516 (97%)	491 (98%)	9 (2%)	0	100	100
131	T2	277/333 (83%)	268 (97%)	8 (3%)	1 (0%)	30	66
131	t2	277/333 (83%)	268 (97%)	8 (3%)	1 (0%)	30	66
132	T3	308/311 (99%)	300 (97%)	8 (3%)	0	100	100
132	t3	308/311 (99%)	300 (97%)	8 (3%)	0	100	100
133	T4	196/212 (92%)	190 (97%)	6 (3%)	0	100	100
133	t4	196/212 (92%)	190 (97%)	6 (3%)	0	100	100
134	T5	139/205 (68%)	137 (99%)	2 (1%)	0	100	100
134	t5	139/205 (68%)	137 (99%)	2 (1%)	0	100	100
135	T6	107/144 (74%)	105 (98%)	2 (2%)	0	100	100
135	t6	107/144 (74%)	105 (98%)	2 (2%)	0	100	100
136	T7	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
136	t7	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
137	T8	129/135 (96%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
137	t8	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
138	T9	130/136 (96%)	125 (96%)	5 (4%)	0	100	100
138	t9	130/136 (96%)	125 (96%)	5 (4%)	0	100	100
139	TA	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
139	ta	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
140	TB	94/113 (83%)	94 (100%)	0	0	100	100
140	tb	94/113 (83%)	94 (100%)	0	0	100	100
141	TC	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
141	tc	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
142	TD	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
142	td	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
143	TE	48/71 (68%)	44 (92%)	4 (8%)	0	100	100
143	te	48/71 (68%)	44 (92%)	4 (8%)	0	100	100
144	TF	214/236 (91%)	210 (98%)	4 (2%)	0	100	100
144	tf	214/236 (91%)	210 (98%)	4 (2%)	0	100	100
145	TG	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
145	tg	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
146	TH	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
146	th	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
147	TX	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
147	tx	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
148	V1	440/474 (93%)	423 (96%)	17 (4%)	0	100	100
148	v1	440/474 (93%)	423 (96%)	17 (4%)	0	100	100
149	V2	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
149	v2	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
150	X1	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
150	x1	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
All	All	88644/100386 (88%)	85881 (97%)	2737 (3%)	26 (0%)	100	100

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	02	87	PRO

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Mol	Chain	Res	Type
3	57	87	PRO
131	t2	77	LYS
131	T2	77	LYS
3	c	87	PRO
3	C	87	PRO
99	n1	229	VAL
99	N1	229	VAL
59	35	121	GLU
9	63	23	ARG
29	73	137	ALA
9	i	23	ARG
29	s	137	ALA
59	7C	121	GLU
2	01	238	THR
29	18	137	ALA
52	2n	56	ASP
52	2N	56	ASP
2	B	238	THR
29	S	137	ALA
39	27	252	ASP
39	C2	252	ASP
111	qE	229	VAL
111	qe	229	VAL
111	QE	229	VAL
111	Qe	229	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	TPO	29	387	41	8,10,11	1.21	1 (12%)	10,14,16	1.06	0
59	SEP	35	120	59	8,9,10	0.88	0	8,12,14	0.98	0
41	SEP	84	520	41	8,9,10	0.87	0	8,12,14	0.81	0
41	SEP	29	520	41	8,9,10	0.88	0	8,12,14	0.72	0
59	SEP	90	120	59	8,9,10	0.87	0	8,12,14	1.09	1 (12%)
59	SEP	7c	120	59	8,9,10	0.87	0	8,12,14	1.09	1 (12%)
41	SEP	vb	520	41	8,9,10	0.87	0	8,12,14	0.80	0
59	SEP	7C	120	59	8,9,10	0.88	0	8,12,14	1.00	0
41	TPO	vb	387	41	8,10,11	1.25	1 (12%)	10,14,16	1.05	1 (10%)
41	TPO	84	387	41	8,10,11	1.26	1 (12%)	10,14,16	1.05	1 (10%)
41	SEP	VB	520	41	8,9,10	0.87	0	8,12,14	0.72	0
41	TPO	VB	387	41	8,10,11	1.21	1 (12%)	10,14,16	1.04	0

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
41	TPO	29	387	41	-	1/9/11/13	-
59	SEP	35	120	59	-	3/5/8/10	-
41	SEP	84	520	41	-	4/5/8/10	-
41	SEP	29	520	41	-	3/5/8/10	-
59	SEP	90	120	59	-	3/5/8/10	-
59	SEP	7c	120	59	-	3/5/8/10	-
41	SEP	vb	520	41	-	4/5/8/10	-
59	SEP	7C	120	59	-	3/5/8/10	-
41	TPO	vb	387	41	-	1/9/11/13	-
41	TPO	84	387	41	-	1/9/11/13	-
41	SEP	VB	520	41	-	3/5/8/10	-
41	TPO	VB	387	41	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	84	387	TPO	P-OG1	3.18	1.65	1.59
41	vb	387	TPO	P-OG1	3.14	1.65	1.59
41	29	387	TPO	P-OG1	3.02	1.65	1.59
41	VB	387	TPO	P-OG1	3.00	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	7c	120	SEP	OG-CB-CA	-2.34	105.87	108.14
59	90	120	SEP	OG-CB-CA	-2.33	105.88	108.14
41	84	387	TPO	CG2-CB-CA	-2.03	109.15	113.16
41	vb	387	TPO	CG2-CB-CA	-2.03	109.17	113.16

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	29	520	SEP	CB-OG-P-O1P
41	29	520	SEP	CB-OG-P-O2P
41	29	520	SEP	CB-OG-P-O3P
59	35	120	SEP	CB-OG-P-O1P
59	35	120	SEP	CB-OG-P-O2P
59	35	120	SEP	CB-OG-P-O3P
41	84	387	TPO	O-C-CA-CB
41	84	520	SEP	N-CA-CB-OG
41	84	520	SEP	CB-OG-P-O2P
41	84	520	SEP	CB-OG-P-O3P
59	90	120	SEP	CB-OG-P-O1P
59	90	120	SEP	CB-OG-P-O2P
59	90	120	SEP	CB-OG-P-O3P
59	7c	120	SEP	CB-OG-P-O1P
59	7c	120	SEP	CB-OG-P-O2P
59	7c	120	SEP	CB-OG-P-O3P
41	vb	387	TPO	O-C-CA-CB
41	vb	520	SEP	N-CA-CB-OG
41	vb	520	SEP	CB-OG-P-O2P
41	vb	520	SEP	CB-OG-P-O3P
59	7C	120	SEP	CB-OG-P-O2P
59	7C	120	SEP	CB-OG-P-O3P
41	VB	520	SEP	CB-OG-P-O1P
41	VB	520	SEP	CB-OG-P-O2P
41	VB	520	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
41	84	520	SEP	CB-OG-P-O1P
41	vb	520	SEP	CB-OG-P-O1P
59	7C	120	SEP	CB-OG-P-O1P
41	29	387	TPO	O-C-CA-CB
41	VB	387	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	35	120	SEP	1	0
59	7C	120	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 26 are monoatomic - leaving 72 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	$\# Z > 2$
161	SF4	S1	801	-	0,12,12	-	-	-		
151	FES	s1	803	-	0,4,4	-	-	-		
152	HEM	QC	501	-	50,50,50	1.30	5 (10%)	66,82,82	1.78	16 (24%)
160	U10	Qc	501	-	25,25,63	2.25	5 (20%)	27,29,79	1.85	8 (29%)
152	HEM	Y5	201	-	50,50,50	1.28	6 (12%)	66,82,82	1.71	13 (19%)
159	ADP	b8	301	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
152	HEM	50	201	-	50,50,50	1.28	6 (12%)	66,82,82	1.71	14 (21%)
151	FES	fx	201	-	0,4,4	-	-	-		
153	HEA	81	701	-	66,67,67	2.16	21 (31%)	78,103,103	2.63	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	HEA	26	702	-	66,67,67	2.32	25 (37%)	78,103,103	2.77	27 (34%)
161	SF4	v1	500	-	0,12,12	-	-	-		
151	FES	QE	301	-	0,4,4	-	-	-		
152	HEM	qC	501	-	50,50,50	1.30	5 (10%)	66,82,82	1.78	16 (24%)
153	HEA	C1	702	-	66,67,67	2.32	25 (37%)	78,103,103	2.77	27 (34%)
151	FES	SB	401	-	0,4,4	-	-	-		
152	HEM	Qc	503	-	50,50,50	1.30	6 (12%)	66,82,82	1.69	15 (22%)
151	FES	sb	401	-	0,4,4	-	-	-		
152	HEM	qC	502	-	50,50,50	1.31	7 (14%)	66,82,82	1.73	14 (21%)
153	HEA	c1	703	-	66,67,67	2.25	22 (33%)	78,103,103	2.61	32 (41%)
153	HEA	81	703	-	66,67,67	2.25	22 (33%)	78,103,103	2.61	31 (39%)
161	SF4	s1	801	-	0,12,12	-	-	-		
157	HEC	qD	401	-	50,50,50	1.30	6 (12%)	68,82,82	1.36	10 (14%)
151	FES	qe	301	-	0,4,4	-	-	-		
161	SF4	S8	302	-	0,12,12	-	-	-		
151	FES	OC	202	-	0,4,4	-	-	-		
159	ADP	B8	301	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
160	U10	qc	501	-	25,25,63	2.25	5 (20%)	27,29,79	1.84	8 (29%)
161	SF4	s7	201	-	0,12,12	-	-	-		
161	SF4	V1	500	-	0,12,12	-	-	-		
151	FES	qE	301	-	0,4,4	-	-	-		
151	FES	FS	202	-	0,4,4	-	-	-		
152	HEM	qc	502	-	50,50,50	1.30	6 (12%)	66,82,82	1.75	17 (25%)
151	FES	Qe	301	-	0,4,4	-	-	-		
152	HEM	Qc	502	-	50,50,50	1.30	6 (12%)	66,82,82	1.75	17 (25%)
153	HEA	c1	701	-	66,67,67	2.16	21 (31%)	78,103,103	2.63	28 (35%)
158	NDP	A9	401	-	49,52,52	0.36	0	66,80,80	0.43	0
153	HEA	26	701	-	66,67,67	2.27	25 (37%)	78,103,103	2.88	35 (44%)
151	FES	fs	202	-	0,4,4	-	-	-		
151	FES	FX	201	-	0,4,4	-	-	-		
151	FES	fs	201	-	0,4,4	-	-	-		
164	FMN	V1	501	-	33,33,33	0.17	0	48,50,50	0.44	0
152	HEM	QC	502	-	50,50,50	1.31	7 (14%)	66,82,82	1.72	13 (19%)
157	HEC	2e	401	-	50,50,50	1.32	9 (18%)	68,82,82	1.18	6 (8%)
158	NDP	a9	401	-	49,52,52	0.36	0	66,80,80	0.43	0
161	SF4	s8	302	-	0,12,12	-	-	-		
151	FES	47	202	-	0,4,4	-	-	-		
151	FES	S1	803	-	0,4,4	-	-	-		
157	HEC	QD	401	-	50,50,50	1.30	6 (12%)	68,82,82	1.36	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
161	SF4	S7	201	-	0,12,12	-	-	-		
152	HEM	0F	201	-	50,50,50	1.28	6 (12%)	66,82,82	1.70	14 (21%)
151	FES	47	201	-	0,4,4	-	-	-		
157	HEC	qd	401	-	50,50,50	1.32	7 (14%)	68,82,82	1.15	7 (10%)
161	SF4	S8	301	-	0,12,12	-	-	-		
162	FAD	SA	701	-	56,58,58	0.27	0	81,89,89	0.35	1 (1%)
151	FES	0C	201	-	0,4,4	-	-	-		
153	HEA	C1	701	-	66,67,67	2.27	23 (34%)	78,103,103	2.88	34 (43%)
157	HEC	Qd	401	-	50,50,50	1.32	8 (16%)	68,82,82	1.14	7 (10%)
161	SF4	s1	802	-	0,12,12	-	-	-		
152	HEM	y5	201	-	50,50,50	1.28	6 (12%)	66,82,82	1.69	14 (21%)
151	FES	v2	300	-	0,4,4	-	-	-		
151	FES	V2	300	-	0,4,4	-	-	-		
152	HEM	qc	503	-	50,50,50	1.29	6 (12%)	66,82,82	1.68	15 (22%)
161	SF4	s8	301	-	0,12,12	-	-	-		
161	SF4	sb	402	-	0,12,12	-	-	-		
161	SF4	SB	402	-	0,12,12	-	-	-		
162	FAD	sa	701	-	56,58,58	0.28	0	81,89,89	0.35	1 (1%)
151	FES	FS	201	-	0,4,4	-	-	-		
161	SF4	S1	802	-	0,12,12	-	-	-		
163	F3S	sb	403	-	0,9,9	-	-	-		
163	F3S	SB	403	-	0,9,9	-	-	-		
157	HEC	2E	401	-	50,50,50	1.31	9 (18%)	68,82,82	1.18	6 (8%)
164	FMN	v1	501	-	33,33,33	0.17	0	48,50,50	0.44	1 (2%)

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
161	SF4	S1	801	-	-	-	0/6/5/5
152	HEM	QC	501	-	-	6/14/54/54	-
151	FES	s1	803	-	-	-	0/1/1/1
160	U10	Qc	501	-	-	6/28/28/87	-
152	HEM	Y5	201	-	-	6/14/54/54	-
159	ADP	b8	301	-	-	4/16/32/32	0/3/3/3
152	HEM	50	201	-	-	6/14/54/54	-
153	HEA	81	701	-	-	15/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
151	FES	fx	201	-	-	-	0/1/1/1
153	HEA	26	702	-	-	12/36/76/76	-
161	SF4	S8	301	-	-	-	0/6/5/5
161	SF4	v1	500	-	-	-	0/6/5/5
151	FES	QE	301	-	-	-	0/1/1/1
152	HEM	qC	501	-	-	6/14/54/54	-
153	HEA	C1	702	-	-	12/36/76/76	-
151	FES	SB	401	-	-	-	0/1/1/1
152	HEM	Qc	503	-	-	8/14/54/54	-
151	FES	sb	401	-	-	-	0/1/1/1
152	HEM	qC	502	-	-	7/14/54/54	-
153	HEA	c1	703	-	-	19/36/76/76	-
153	HEA	81	703	-	-	19/36/76/76	-
161	SF4	s1	801	-	-	-	0/6/5/5
157	HEC	qD	401	-	1/1/3/7	7/14/54/54	-
151	FES	qe	301	-	-	-	0/1/1/1
161	SF4	S8	302	-	-	-	0/6/5/5
159	ADP	B8	301	-	-	5/16/32/32	0/3/3/3
151	FES	0C	202	-	-	-	0/1/1/1
160	U10	qc	501	-	-	6/28/28/87	-
161	SF4	s7	201	-	-	-	0/6/5/5
161	SF4	V1	500	-	-	-	0/6/5/5
151	FES	qE	301	-	-	-	0/1/1/1
151	FES	FS	202	-	-	-	0/1/1/1
152	HEM	qc	502	-	-	4/14/54/54	-
152	HEM	Qc	502	-	-	4/14/54/54	-
158	NDP	A9	401	-	-	6/34/77/77	0/5/5/5
153	HEA	c1	701	-	-	15/36/76/76	-
151	FES	Qe	301	-	-	-	0/1/1/1
153	HEA	26	701	-	-	13/36/76/76	-
151	FES	fs	202	-	-	-	0/1/1/1
151	FES	FX	201	-	-	-	0/1/1/1
151	FES	fs	201	-	-	-	0/1/1/1
152	HEM	QC	502	-	-	7/14/54/54	-
157	HEC	2e	401	-	1/1/3/7	3/14/54/54	-
158	NDP	a9	401	-	-	6/34/77/77	0/5/5/5
161	SF4	s8	302	-	-	-	0/6/5/5
157	HEC	QD	401	-	1/1/3/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
151	FES	47	202	-	-	-	0/1/1/1
151	FES	S1	803	-	-	-	0/1/1/1
161	SF4	S7	201	-	-	-	0/6/5/5
152	HEM	0F	201	-	-	7/14/54/54	-
151	FES	47	201	-	-	-	0/1/1/1
157	HEC	qd	401	-	1/1/3/7	3/14/54/54	-
162	FAD	SA	701	-	-	12/34/50/50	0/6/6/6
161	SF4	S1	802	-	-	-	0/6/5/5
157	HEC	Qd	401	-	1/1/3/7	3/14/54/54	-
153	HEA	C1	701	-	-	13/36/76/76	-
164	FMN	V1	501	-	-	4/18/18/18	0/3/3/3
151	FES	0C	201	-	-	-	0/1/1/1
152	HEM	y5	201	-	-	7/14/54/54	-
151	FES	v2	300	-	-	-	0/1/1/1
151	FES	V2	300	-	-	-	0/1/1/1
152	HEM	qc	503	-	-	8/14/54/54	-
161	SF4	s1	802	-	-	-	0/6/5/5
162	FAD	sa	701	-	-	12/34/50/50	0/6/6/6
161	SF4	s8	301	-	-	-	0/6/5/5
161	SF4	sb	402	-	-	-	0/6/5/5
151	FES	FS	201	-	-	-	0/1/1/1
161	SF4	SB	402	-	-	-	0/6/5/5
163	F3S	sb	403	-	-	-	0/3/3/3
163	F3S	SB	403	-	-	-	0/3/3/3
157	HEC	2E	401	-	1/1/3/7	3/14/54/54	-
164	FMN	v1	501	-	-	4/18/18/18	0/3/3/3

All (319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
160	qc	501	U10	C6-C1	8.74	1.53	1.33
160	Qc	501	U10	C6-C1	8.72	1.53	1.33
153	C1	701	HEA	FE-ND	6.20	2.14	1.94
153	26	701	HEA	FE-ND	6.18	2.14	1.94
153	C1	701	HEA	C1D-ND	-5.91	1.30	1.40
153	26	701	HEA	C1D-ND	-5.90	1.30	1.40
153	81	703	HEA	C4B-NB	-5.78	1.30	1.40
153	c1	703	HEA	C4B-NB	-5.76	1.30	1.40
153	C1	702	HEA	C4B-NB	-5.69	1.30	1.40
153	26	702	HEA	C4B-NB	-5.68	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	c1	703	HEA	FE-NB	5.68	2.12	1.94
153	81	703	HEA	FE-NB	5.66	2.12	1.94
153	c1	701	HEA	FE-NB	5.49	2.11	1.94
153	81	701	HEA	FE-NB	5.47	2.11	1.94
153	81	701	HEA	C3B-C2B	5.36	1.46	1.34
153	c1	701	HEA	C3B-C2B	5.36	1.46	1.34
153	C1	702	HEA	FE-NC	5.34	2.13	1.95
153	26	702	HEA	FE-NC	5.31	2.13	1.95
153	C1	702	HEA	C3B-C2B	5.31	1.46	1.34
153	26	702	HEA	C3B-C2B	5.30	1.46	1.34
153	C1	701	HEA	C3A-C2A	4.92	1.47	1.36
153	26	701	HEA	C3A-C2A	4.92	1.47	1.36
153	C1	702	HEA	FE-NB	4.89	2.10	1.94
153	26	702	HEA	FE-NB	4.88	2.10	1.94
153	c1	703	HEA	C1B-NB	-4.77	1.29	1.38
153	81	703	HEA	C1B-NB	-4.76	1.29	1.38
153	C1	701	HEA	C3B-C2B	4.75	1.45	1.34
153	26	701	HEA	C3B-C2B	4.73	1.45	1.34
153	81	703	HEA	C3B-C2B	4.72	1.45	1.34
153	c1	703	HEA	C3B-C2B	4.71	1.45	1.34
153	26	702	HEA	FE-ND	4.62	2.09	1.94
153	C1	702	HEA	FE-ND	4.62	2.09	1.94
159	b8	301	ADP	C5-C4	4.56	1.47	1.39
153	c1	703	HEA	C3D-C2D	4.56	1.46	1.36
159	B8	301	ADP	C5-C4	4.55	1.47	1.39
153	81	703	HEA	C3D-C2D	4.55	1.46	1.36
153	c1	701	HEA	C3D-C2D	4.53	1.46	1.36
153	81	701	HEA	C3D-C2D	4.52	1.46	1.36
153	c1	703	HEA	FE-NC	4.35	2.09	1.95
153	81	703	HEA	FE-NC	4.33	2.09	1.95
153	C1	701	HEA	FE-NC	4.22	2.09	1.95
153	26	701	HEA	FE-NC	4.21	2.09	1.95
153	c1	703	HEA	C3A-C2A	4.17	1.45	1.36
153	26	702	HEA	C3D-C2D	4.14	1.45	1.36
153	81	703	HEA	C3A-C2A	4.14	1.45	1.36
153	81	701	HEA	FE-ND	4.12	2.07	1.94
153	C1	702	HEA	C3D-C2D	4.12	1.45	1.36
153	c1	701	HEA	FE-ND	4.11	2.07	1.94
153	81	701	HEA	C3A-C2A	4.10	1.45	1.36
153	c1	701	HEA	C3A-C2A	4.08	1.45	1.36
153	C1	701	HEA	C4B-NB	-4.07	1.33	1.40
153	26	702	HEA	C3A-C2A	4.05	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	26	701	HEA	C4B-NB	-4.03	1.33	1.40
153	C1	702	HEA	C3A-C2A	4.02	1.45	1.36
153	C1	701	HEA	C4C-NC	-3.89	1.32	1.39
153	26	701	HEA	C4C-NC	-3.88	1.32	1.39
153	c1	701	HEA	CHC-C4B	3.88	1.46	1.38
153	81	701	HEA	CHC-C4B	3.87	1.46	1.38
153	81	701	HEA	FE-NC	3.85	2.08	1.95
153	c1	701	HEA	FE-NC	3.85	2.08	1.95
153	c1	703	HEA	C1C-NC	-3.83	1.32	1.39
153	81	703	HEA	C1C-NC	-3.83	1.32	1.39
153	C1	701	HEA	C3D-C2D	3.82	1.44	1.36
153	26	701	HEA	C3D-C2D	3.80	1.44	1.36
152	QC	501	HEM	C4D-ND	-3.80	1.33	1.40
152	qC	501	HEM	C4D-ND	-3.79	1.33	1.40
153	C1	701	HEA	CHA-C1A	3.78	1.45	1.38
153	26	701	HEA	CHA-C1A	3.77	1.45	1.38
153	c1	701	HEA	C1C-NC	-3.74	1.32	1.39
153	81	701	HEA	C1C-NC	-3.73	1.32	1.39
152	qc	503	HEM	C4D-ND	-3.69	1.33	1.40
152	Qc	503	HEM	C4D-ND	-3.69	1.33	1.40
153	81	701	HEA	CHA-C1A	3.68	1.45	1.38
152	Qc	502	HEM	C4D-ND	-3.68	1.34	1.40
153	C1	702	HEA	CHC-C4B	3.68	1.46	1.38
152	QC	502	HEM	C4D-ND	-3.67	1.34	1.40
152	0F	201	HEM	C4D-ND	-3.66	1.34	1.40
152	qc	502	HEM	C4D-ND	-3.66	1.34	1.40
153	26	702	HEA	CHC-C4B	3.66	1.46	1.38
152	qC	502	HEM	C4D-ND	-3.65	1.34	1.40
152	y5	201	HEM	C4D-ND	-3.65	1.34	1.40
153	81	701	HEA	C4B-NB	-3.65	1.34	1.40
153	c1	701	HEA	CHA-C1A	3.64	1.45	1.38
153	c1	701	HEA	C4B-NB	-3.64	1.34	1.40
153	26	702	HEA	C4C-NC	-3.58	1.32	1.39
153	C1	702	HEA	C4C-NC	-3.58	1.32	1.39
153	c1	703	HEA	C1A-NA	3.54	1.46	1.39
153	81	703	HEA	C1A-NA	3.54	1.46	1.39
152	50	201	HEM	C4D-ND	-3.53	1.34	1.40
153	26	701	HEA	FE-NB	3.52	2.05	1.94
153	C1	701	HEA	FE-NB	3.52	2.05	1.94
153	26	702	HEA	C4B-C3B	3.51	1.50	1.44
153	C1	702	HEA	CHD-C1D	3.51	1.45	1.38
153	C1	702	HEA	C4B-C3B	3.49	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	26	702	HEA	CHB-C4A	3.49	1.45	1.38
152	Y5	201	HEM	C4D-ND	-3.49	1.34	1.40
153	26	702	HEA	CHD-C1D	3.48	1.45	1.38
153	C1	702	HEA	CHB-C4A	3.47	1.45	1.38
157	2E	401	HEC	CBC-CAC	-3.45	1.36	1.51
157	2e	401	HEC	CBC-CAC	-3.45	1.36	1.51
153	C1	701	HEA	CHC-C4B	3.44	1.45	1.38
153	26	701	HEA	CHC-C4B	3.42	1.45	1.38
153	26	702	HEA	C1D-ND	-3.39	1.34	1.40
153	c1	703	HEA	FE-ND	3.38	2.05	1.94
153	81	703	HEA	FE-ND	3.37	2.05	1.94
153	C1	702	HEA	C1D-ND	-3.37	1.34	1.40
153	c1	703	HEA	CHC-C4B	3.37	1.45	1.38
153	81	703	HEA	CHC-C4B	3.37	1.45	1.38
153	81	703	HEA	CHC-C1C	3.34	1.46	1.39
153	c1	703	HEA	CHC-C1C	3.30	1.46	1.39
153	c1	703	HEA	CHB-C4A	3.30	1.44	1.38
153	c1	703	HEA	CHA-C4D	3.29	1.46	1.39
153	c1	701	HEA	C1D-ND	-3.28	1.34	1.40
153	81	703	HEA	CHB-C4A	3.28	1.44	1.38
152	qc	502	HEM	C1B-NB	-3.27	1.34	1.40
153	C1	702	HEA	CHC-C1C	3.27	1.46	1.39
153	81	701	HEA	C1D-ND	-3.27	1.34	1.40
153	81	703	HEA	CHA-C4D	3.26	1.46	1.39
157	Qd	401	HEC	CBC-CAC	-3.25	1.37	1.51
153	26	702	HEA	CHC-C1C	3.25	1.46	1.39
152	Qc	502	HEM	C1B-NB	-3.25	1.34	1.40
157	qd	401	HEC	CBC-CAC	-3.25	1.37	1.51
153	C1	702	HEA	C1B-NB	-3.24	1.32	1.38
153	26	702	HEA	C1B-NB	-3.24	1.32	1.38
153	c1	701	HEA	CHB-C1B	3.24	1.46	1.39
152	qC	501	HEM	C1B-NB	-3.24	1.34	1.40
157	QD	401	HEC	CBC-CAC	-3.23	1.37	1.51
152	QC	501	HEM	C1B-NB	-3.23	1.34	1.40
157	qD	401	HEC	CBC-CAC	-3.23	1.37	1.51
153	C1	702	HEA	C1C-NC	-3.22	1.33	1.39
153	81	701	HEA	CHB-C1B	3.22	1.46	1.39
153	c1	701	HEA	C1B-NB	-3.21	1.32	1.38
153	26	702	HEA	C1C-NC	-3.18	1.33	1.39
153	C1	701	HEA	CHB-C1B	3.17	1.46	1.39
153	81	701	HEA	C1B-NB	-3.17	1.32	1.38
153	26	701	HEA	CHB-C1B	3.17	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	c1	703	HEA	CHD-C1D	3.16	1.44	1.38
153	81	703	HEA	CHD-C1D	3.15	1.44	1.38
153	26	702	HEA	C1A-NA	3.08	1.45	1.39
152	Qc	503	HEM	C1B-NB	-3.08	1.35	1.40
152	qC	502	HEM	C1B-NB	-3.07	1.35	1.40
152	QC	502	HEM	C1B-NB	-3.06	1.35	1.40
153	C1	702	HEA	CHA-C1A	3.04	1.44	1.38
152	qc	503	HEM	C1B-NB	-3.04	1.35	1.40
153	C1	702	HEA	C1A-NA	3.03	1.45	1.39
152	0F	201	HEM	C1B-NB	-3.03	1.35	1.40
152	y5	201	HEM	C1B-NB	-3.03	1.35	1.40
152	Y5	201	HEM	C1B-NB	-3.00	1.35	1.40
153	26	702	HEA	CHA-C1A	2.99	1.44	1.38
153	C1	701	HEA	CHD-C1D	2.98	1.44	1.38
153	26	701	HEA	CHD-C1D	2.96	1.44	1.38
152	50	201	HEM	C1B-NB	-2.92	1.35	1.40
153	C1	701	HEA	CHD-C4C	2.90	1.45	1.39
153	26	701	HEA	CHD-C4C	2.87	1.45	1.39
153	81	701	HEA	CHC-C1C	2.87	1.45	1.39
153	c1	701	HEA	CHC-C1C	2.87	1.45	1.39
153	81	703	HEA	CHA-C1A	2.83	1.43	1.38
153	81	701	HEA	CHD-C4C	2.83	1.45	1.39
153	c1	703	HEA	CHA-C1A	2.83	1.43	1.38
153	26	702	HEA	CHA-C4D	2.82	1.45	1.39
153	c1	701	HEA	CHD-C4C	2.81	1.45	1.39
153	C1	702	HEA	CHA-C4D	2.79	1.45	1.39
157	qD	401	HEC	CAC-C3C	2.78	1.58	1.51
157	QD	401	HEC	CAC-C3C	2.77	1.58	1.51
157	qd	401	HEC	CAC-C3C	2.76	1.58	1.51
153	81	701	HEA	CHB-C4A	2.76	1.43	1.38
153	c1	701	HEA	C1A-NA	2.75	1.45	1.39
152	QC	501	HEM	C1D-ND	-2.75	1.33	1.38
157	Qd	401	HEC	CAC-C3C	2.74	1.58	1.51
153	c1	701	HEA	CHB-C4A	2.74	1.43	1.38
152	qC	501	HEM	C1D-ND	-2.73	1.33	1.38
153	81	701	HEA	C1A-NA	2.72	1.45	1.39
153	c1	703	HEA	C4C-NC	-2.70	1.34	1.39
159	B8	301	ADP	C5-C6	2.68	1.48	1.41
153	26	702	HEA	C1C-C2C	2.68	1.49	1.43
152	qC	502	HEM	C1D-ND	-2.68	1.33	1.38
152	Qc	502	HEM	C1D-ND	-2.68	1.33	1.38
153	81	703	HEA	C4C-NC	-2.67	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	C1	702	HEA	C1C-C2C	2.67	1.49	1.43
159	b8	301	ADP	C5-C6	2.67	1.48	1.41
153	26	701	HEA	CHA-C4D	2.66	1.45	1.39
152	qc	502	HEM	C1D-ND	-2.65	1.33	1.38
153	C1	701	HEA	CHA-C4D	2.65	1.45	1.39
152	QC	502	HEM	C1D-ND	-2.64	1.33	1.38
153	c1	701	HEA	CHA-C4D	2.62	1.45	1.39
160	qc	501	U10	C21-C19	2.62	1.56	1.51
160	Qc	501	U10	C21-C19	2.62	1.56	1.51
153	81	701	HEA	CHA-C4D	2.61	1.45	1.39
153	c1	701	HEA	C4D-ND	-2.59	1.33	1.38
153	81	701	HEA	C4D-ND	-2.58	1.33	1.38
153	C1	701	HEA	C4A-NA	2.58	1.44	1.39
152	qc	503	HEM	C1D-ND	-2.57	1.33	1.38
152	Qc	503	HEM	C1D-ND	-2.55	1.33	1.38
152	qC	502	HEM	C1C-C2C	-2.55	1.40	1.45
153	26	701	HEA	C4A-NA	2.55	1.44	1.39
152	0F	201	HEM	C1D-ND	-2.54	1.33	1.38
152	Y5	201	HEM	C1C-C2C	-2.53	1.40	1.45
152	QC	502	HEM	C1C-C2C	-2.53	1.40	1.45
153	C1	701	HEA	CHC-C1C	2.53	1.45	1.39
153	26	701	HEA	CHC-C1C	2.52	1.45	1.39
152	50	201	HEM	C1C-C2C	-2.51	1.40	1.45
153	C1	701	HEA	O2A-CGA	-2.51	1.22	1.30
152	Y5	201	HEM	C1D-ND	-2.51	1.33	1.38
153	26	701	HEA	O2A-CGA	-2.51	1.22	1.30
153	81	703	HEA	CHB-C1B	2.51	1.44	1.39
152	QC	501	HEM	C1C-C2C	-2.51	1.40	1.45
152	y5	201	HEM	C1D-ND	-2.51	1.33	1.38
153	26	701	HEA	CHB-C4A	2.51	1.43	1.38
152	50	201	HEM	C1D-ND	-2.50	1.33	1.38
153	c1	703	HEA	CHB-C1B	2.50	1.44	1.39
153	26	701	HEA	C1A-NA	2.50	1.44	1.39
153	C1	701	HEA	CHB-C4A	2.50	1.43	1.38
152	qC	501	HEM	C1C-C2C	-2.49	1.40	1.45
152	qc	502	HEM	C1C-C2C	-2.49	1.40	1.45
152	Qc	502	HEM	C1C-C2C	-2.48	1.40	1.45
152	Qc	503	HEM	C1C-C2C	-2.47	1.40	1.45
157	2e	401	HEC	CAB-C3B	2.47	1.57	1.51
157	2e	401	HEC	CAC-C3C	2.47	1.57	1.51
152	qc	503	HEM	C1C-C2C	-2.47	1.40	1.45
153	C1	701	HEA	C1A-NA	2.47	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
153	c1	703	HEA	CHD-C4C	2.46	1.44	1.39
157	2E	401	HEC	CAB-C3B	2.46	1.57	1.51
153	81	703	HEA	CHD-C4C	2.46	1.44	1.39
153	C1	701	HEA	C4B-C3B	2.46	1.48	1.44
153	C1	701	HEA	C4D-ND	-2.44	1.33	1.38
153	26	701	HEA	C4D-ND	-2.44	1.33	1.38
152	Y5	201	HEM	FE-NB	2.44	2.02	1.94
157	2E	401	HEC	CAC-C3C	2.44	1.57	1.51
153	26	701	HEA	C4B-C3B	2.44	1.48	1.44
152	0F	201	HEM	C1C-C2C	-2.44	1.40	1.45
152	y5	201	HEM	C1C-C2C	-2.44	1.40	1.45
152	50	201	HEM	FE-NB	2.43	2.02	1.94
152	qC	502	HEM	FE-NB	2.42	2.02	1.94
152	QC	502	HEM	FE-NB	2.41	2.02	1.94
153	C1	702	HEA	O2D-CGD	-2.39	1.22	1.30
153	26	702	HEA	O2D-CGD	-2.38	1.22	1.30
157	Qd	401	HEC	CBB-CAB	-2.37	1.40	1.51
152	y5	201	HEM	FE-NB	2.36	2.02	1.94
152	Qc	503	HEM	FE-NB	2.36	2.02	1.94
152	0F	201	HEM	FE-NB	2.36	2.02	1.94
157	qd	401	HEC	CBB-CAB	-2.36	1.41	1.51
152	qc	503	HEM	FE-NB	2.34	2.02	1.94
159	b8	301	ADP	C8-N7	2.34	1.36	1.31
159	B8	301	ADP	C8-N7	2.34	1.36	1.31
153	C1	702	HEA	C4A-NA	2.33	1.44	1.39
153	26	701	HEA	O2D-CGD	-2.33	1.22	1.30
153	C1	701	HEA	O2D-CGD	-2.32	1.22	1.30
157	2E	401	HEC	CMB-C2B	2.31	1.55	1.50
157	2e	401	HEC	CMB-C2B	2.31	1.55	1.50
160	Qc	501	U10	C11-C9	2.30	1.56	1.51
153	26	702	HEA	C4A-NA	2.30	1.44	1.39
153	81	703	HEA	O2D-CGD	-2.29	1.23	1.30
157	QD	401	HEC	CBB-CAB	-2.29	1.41	1.51
160	qc	501	U10	C11-C9	2.29	1.56	1.51
157	qD	401	HEC	CBB-CAB	-2.28	1.41	1.51
153	26	702	HEA	O2A-CGA	-2.27	1.23	1.30
153	c1	703	HEA	O2D-CGD	-2.27	1.23	1.30
153	C1	702	HEA	O2A-CGA	-2.26	1.23	1.30
153	26	702	HEA	CHB-C1B	2.25	1.44	1.39
153	c1	701	HEA	O2D-CGD	-2.24	1.23	1.30
153	81	701	HEA	O2D-CGD	-2.24	1.23	1.30
157	2e	401	HEC	CMA-C3A	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
152	50	201	HEM	FE-ND	2.23	2.01	1.94
152	Y5	201	HEM	FE-ND	2.23	2.01	1.94
153	C1	702	HEA	CHB-C1B	2.23	1.44	1.39
157	2E	401	HEC	CMA-C3A	2.23	1.55	1.50
160	qc	501	U10	C16-C14	2.21	1.55	1.51
157	qd	401	HEC	CMD-C2D	2.21	1.55	1.50
157	Qd	401	HEC	CAB-C3B	2.19	1.56	1.51
160	Qc	501	U10	C16-C14	2.19	1.55	1.51
159	B8	301	ADP	C5-N7	-2.19	1.34	1.39
157	qd	401	HEC	CAB-C3B	2.18	1.56	1.51
153	c1	703	HEA	O2A-CGA	-2.18	1.23	1.30
153	81	703	HEA	O2A-CGA	-2.18	1.23	1.30
157	2E	401	HEC	CBB-CAB	-2.17	1.41	1.51
152	qc	502	HEM	FE-NB	2.17	2.01	1.94
157	qD	401	HEC	CMD-C2D	2.17	1.55	1.50
157	2e	401	HEC	CBB-CAB	-2.17	1.41	1.51
157	QD	401	HEC	CAB-C3B	2.17	1.56	1.51
157	qD	401	HEC	CAB-C3B	2.17	1.56	1.51
153	81	701	HEA	O2A-CGA	-2.17	1.23	1.30
152	qC	502	HEM	FE-ND	2.16	2.01	1.94
157	qD	401	HEC	CMA-C3A	2.16	1.55	1.50
157	QD	401	HEC	CMD-C2D	2.16	1.55	1.50
152	Qc	502	HEM	FE-NB	2.15	2.01	1.94
152	QC	502	HEM	FE-ND	2.15	2.01	1.94
159	b8	301	ADP	C5-N7	-2.15	1.35	1.39
153	c1	701	HEA	O2A-CGA	-2.15	1.23	1.30
157	Qd	401	HEC	CMD-C2D	2.15	1.55	1.50
152	qc	503	HEM	FE-ND	2.14	2.01	1.94
157	QD	401	HEC	CMA-C3A	2.14	1.55	1.50
160	qc	501	U10	C22-C23	2.14	1.57	1.50
160	Qc	501	U10	C22-C23	2.13	1.57	1.50
152	QC	501	HEM	FE-NB	2.13	2.01	1.94
152	Qc	503	HEM	FE-ND	2.12	2.01	1.94
152	qC	501	HEM	FE-NB	2.12	2.01	1.94
152	qC	502	HEM	C3C-C4C	-2.12	1.42	1.46
152	0F	201	HEM	FE-ND	2.12	2.01	1.94
153	c1	703	HEA	C1C-C2C	2.11	1.48	1.43
153	81	703	HEA	C1C-C2C	2.11	1.48	1.43
152	y5	201	HEM	FE-ND	2.09	2.01	1.94
152	QC	502	HEM	C3C-C4C	-2.09	1.42	1.46
157	2e	401	HEC	CMD-C2D	2.07	1.55	1.50
157	qd	401	HEC	FE-ND	2.07	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
157	2E	401	HEC	FE-ND	2.07	2.01	1.94
157	Qd	401	HEC	FE-ND	2.06	2.01	1.94
157	qd	401	HEC	CMB-C2B	2.06	1.55	1.50
157	2e	401	HEC	FE-ND	2.06	2.01	1.94
157	2E	401	HEC	CMD-C2D	2.05	1.55	1.50
152	qc	502	HEM	C4B-NB	-2.05	1.34	1.38
157	2e	401	HEC	CMC-C2C	2.05	1.55	1.50
157	Qd	401	HEC	CMB-C2B	2.05	1.55	1.50
152	Qc	502	HEM	C4B-NB	-2.03	1.34	1.38
157	2E	401	HEC	CMC-C2C	2.03	1.55	1.50
153	26	701	HEA	C1C-NC	-2.02	1.35	1.39
153	26	702	HEA	CHD-C4C	2.01	1.43	1.39
153	C1	702	HEA	CHD-C4C	2.01	1.43	1.39
153	26	701	HEA	C1D-C2D	2.00	1.48	1.44
157	Qd	401	HEC	CMA-C3A	2.00	1.55	1.50

All (507) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
153	C1	701	HEA	C3C-C4C-NC	8.73	115.62	110.25
153	26	701	HEA	C3C-C4C-NC	8.72	115.61	110.25
153	81	703	HEA	CAD-CBD-CGD	-8.56	95.19	113.60
153	c1	703	HEA	CAD-CBD-CGD	-8.54	95.24	113.60
153	26	702	HEA	CAD-CBD-CGD	-8.41	95.51	113.60
153	C1	702	HEA	CAD-CBD-CGD	-8.41	95.51	113.60
153	26	702	HEA	C3C-C4C-NC	8.24	115.32	110.25
153	C1	702	HEA	C3C-C4C-NC	8.18	115.28	110.25
153	81	701	HEA	CAD-CBD-CGD	-8.06	96.26	113.60
153	c1	701	HEA	CAD-CBD-CGD	-8.05	96.29	113.60
153	26	701	HEA	CAD-CBD-CGD	-7.43	97.61	113.60
153	C1	701	HEA	CAD-CBD-CGD	-7.41	97.66	113.60
153	C1	701	HEA	CAA-CBA-CGA	-7.01	98.51	113.60
153	26	701	HEA	CAA-CBA-CGA	-7.00	98.54	113.60
153	26	702	HEA	C3D-C4D-ND	6.47	116.62	110.36
153	C1	702	HEA	C3D-C4D-ND	6.46	116.61	110.36
153	C1	701	HEA	C2B-C1B-NB	6.42	117.57	109.88
153	81	703	HEA	C3C-C2C-C1C	-6.38	99.46	107.16
153	26	701	HEA	C2B-C1B-NB	6.37	117.51	109.88
153	c1	703	HEA	C3C-C2C-C1C	-6.35	99.49	107.16
153	81	701	HEA	C3C-C4C-NC	6.24	114.09	110.25
153	c1	701	HEA	C3C-C4C-NC	6.21	114.07	110.25
159	B8	301	ADP	C5-C4-N3	-6.12	118.76	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
159	b8	301	ADP	C5-C4-N3	-6.12	118.76	126.75
153	26	701	HEA	C13-C12-C11	-5.98	105.37	114.35
153	C1	701	HEA	C13-C12-C11	-5.97	105.38	114.35
153	26	702	HEA	CHB-C1B-C2B	-5.90	115.77	124.98
153	C1	702	HEA	CHB-C1B-C2B	-5.90	115.77	124.98
153	c1	703	HEA	C2D-C1D-ND	5.86	116.78	109.84
153	81	703	HEA	C2D-C1D-ND	5.85	116.77	109.84
153	81	701	HEA	C13-C12-C11	-5.85	105.57	114.35
153	c1	701	HEA	C13-C12-C11	-5.84	105.58	114.35
153	81	703	HEA	C1D-C2D-C3D	-5.71	100.96	106.96
153	c1	703	HEA	C1D-C2D-C3D	-5.69	100.97	106.96
153	C1	701	HEA	CHB-C1B-C2B	-5.69	116.09	124.98
153	26	701	HEA	CHB-C1B-C2B	-5.69	116.10	124.98
153	c1	701	HEA	C2B-C1B-NB	5.68	116.68	109.88
153	81	701	HEA	C2B-C1B-NB	5.65	116.66	109.88
153	26	702	HEA	C2D-C1D-ND	5.61	116.49	109.84
153	C1	702	HEA	C2D-C1D-ND	5.61	116.49	109.84
153	C1	701	HEA	C3B-C4B-NB	5.58	116.45	109.84
153	26	701	HEA	C3B-C4B-NB	5.56	116.43	109.84
153	C1	701	HEA	C3C-C2C-C1C	-5.45	100.58	107.16
153	26	701	HEA	C3C-C2C-C1C	-5.44	100.60	107.16
153	c1	703	HEA	CAA-CBA-CGA	-5.30	102.19	113.60
153	81	703	HEA	CAA-CBA-CGA	-5.30	102.20	113.60
153	C1	702	HEA	C3C-C2C-C1C	-5.29	100.77	107.16
153	c1	701	HEA	C3D-C4D-ND	5.27	115.46	110.36
153	26	702	HEA	C3C-C2C-C1C	-5.26	100.82	107.16
153	81	701	HEA	C3D-C4D-ND	5.25	115.44	110.36
153	26	702	HEA	CAA-CBA-CGA	-5.17	102.49	113.60
153	C1	702	HEA	CAA-CBA-CGA	-5.16	102.50	113.60
153	C1	702	HEA	C13-C12-C11	-5.07	106.73	114.35
153	26	702	HEA	C13-C12-C11	-5.07	106.74	114.35
153	81	701	HEA	C1D-C2D-C3D	-4.98	101.72	106.96
153	c1	701	HEA	C1D-C2D-C3D	-4.95	101.75	106.96
159	b8	301	ADP	N3-C4-N9	4.93	135.21	127.08
152	Y5	201	HEM	CHC-C4B-NB	4.92	129.77	124.42
152	qC	502	HEM	CHC-C4B-NB	4.92	129.77	124.42
159	B8	301	ADP	N3-C4-N9	4.91	135.17	127.08
153	c1	703	HEA	C3D-C4D-ND	4.91	115.11	110.36
152	50	201	HEM	CHC-C4B-NB	4.90	129.74	124.42
153	81	703	HEA	C3D-C4D-ND	4.89	115.09	110.36
153	c1	701	HEA	CHB-C1B-C2B	-4.88	117.35	124.98
153	81	701	HEA	CHB-C1B-C2B	-4.88	117.36	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
152	QC	502	HEM	CHC-C4B-NB	4.87	129.71	124.42
153	81	701	HEA	C3B-C4B-NB	4.79	115.51	109.84
153	c1	701	HEA	C3B-C4B-NB	4.79	115.51	109.84
152	QC	502	HEM	CHD-C4C-NC	4.76	129.59	124.44
152	qC	502	HEM	CHD-C4C-NC	4.75	129.58	124.44
153	26	701	HEA	CHA-C4D-C3D	-4.74	117.88	124.84
153	C1	701	HEA	CHA-C4D-C3D	-4.73	117.89	124.84
152	Y5	201	HEM	CHD-C4C-NC	4.63	129.45	124.44
152	50	201	HEM	CHD-C4C-NC	4.58	129.39	124.44
153	81	701	HEA	C2D-C1D-ND	4.57	115.26	109.84
153	81	701	HEA	C3C-C2C-C1C	-4.57	101.64	107.16
153	c1	701	HEA	C3C-C2C-C1C	-4.57	101.65	107.16
153	c1	701	HEA	C2D-C1D-ND	4.56	115.24	109.84
153	C1	702	HEA	C1D-C2D-C3D	-4.55	102.17	106.96
153	c1	701	HEA	C2C-C1C-NC	4.54	116.99	110.08
153	26	702	HEA	C1D-C2D-C3D	-4.53	102.19	106.96
153	81	701	HEA	C2C-C1C-NC	4.51	116.95	110.08
152	Qc	503	HEM	CHC-C4B-NB	4.46	129.27	124.42
153	81	703	HEA	C2B-C1B-NB	4.44	115.20	109.88
152	0F	201	HEM	CHC-C4B-NB	4.44	129.24	124.42
153	26	702	HEA	C2B-C1B-NB	4.44	115.20	109.88
153	C1	702	HEA	C2B-C1B-NB	4.44	115.20	109.88
152	y5	201	HEM	CHC-C4B-NB	4.43	129.24	124.42
152	qc	503	HEM	CHC-C4B-NB	4.42	129.22	124.42
153	c1	703	HEA	C2B-C1B-NB	4.40	115.16	109.88
153	26	701	HEA	CHC-C4B-NB	-4.39	118.96	124.37
152	qC	501	HEM	C4D-ND-C1D	4.39	109.61	105.07
152	Qc	503	HEM	CHD-C4C-NC	4.38	129.18	124.44
153	C1	701	HEA	CHC-C4B-NB	-4.38	118.98	124.37
152	QC	501	HEM	C4D-ND-C1D	4.37	109.59	105.07
153	C1	701	HEA	C1D-C2D-C3D	-4.36	102.37	106.96
152	qc	503	HEM	CHD-C4C-NC	4.34	129.13	124.44
153	26	701	HEA	C1D-C2D-C3D	-4.34	102.40	106.96
152	QC	501	HEM	C1B-NB-C4B	4.32	109.53	105.07
153	c1	703	HEA	CHB-C1B-C2B	-4.31	118.25	124.98
153	81	703	HEA	CHB-C1B-C2B	-4.31	118.25	124.98
152	0F	201	HEM	CHD-C4C-NC	4.30	129.09	124.44
153	81	703	HEA	C2C-C1C-NC	4.30	116.62	110.08
152	y5	201	HEM	CHD-C4C-NC	4.28	129.07	124.44
152	qC	501	HEM	C1B-NB-C4B	4.28	109.49	105.07
152	Qc	502	HEM	C4D-ND-C1D	4.28	109.49	105.07
152	qc	502	HEM	C4D-ND-C1D	4.26	109.48	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
153	c1	703	HEA	C2C-C1C-NC	4.26	116.57	110.08
153	c1	701	HEA	CHA-C4D-C3D	-4.26	118.58	124.84
153	26	702	HEA	CHB-C1B-NB	4.25	129.03	124.42
153	C1	702	HEA	CHB-C1B-NB	4.25	129.03	124.42
153	81	701	HEA	CHA-C4D-C3D	-4.23	118.62	124.84
152	qC	501	HEM	CHD-C4C-NC	4.22	129.00	124.44
152	QC	501	HEM	CHD-C4C-NC	4.22	129.00	124.44
153	26	701	HEA	C3D-C4D-ND	4.19	114.41	110.36
153	C1	701	HEA	C3D-C4D-ND	4.18	114.40	110.36
152	qc	502	HEM	C1B-NB-C4B	4.14	109.35	105.07
152	qc	502	HEM	CHC-C4B-NB	4.12	128.90	124.42
153	c1	701	HEA	C4B-C3B-C2B	-4.10	100.40	107.41
152	Qc	502	HEM	C1B-NB-C4B	4.09	109.30	105.07
152	Qc	502	HEM	CHC-C4B-NB	4.08	128.85	124.42
153	81	701	HEA	C4B-C3B-C2B	-4.07	100.45	107.41
152	QC	501	HEM	CHC-C4B-NB	4.07	128.84	124.42
152	Y5	201	HEM	CHB-C1B-NB	4.06	129.39	124.37
152	qC	501	HEM	CHC-C4B-NB	4.06	128.83	124.42
152	qc	502	HEM	CHD-C4C-NC	4.06	128.83	124.44
152	50	201	HEM	CHB-C1B-NB	4.05	129.37	124.37
152	Qc	502	HEM	CHD-C4C-NC	4.05	128.82	124.44
153	C1	701	HEA	C2C-C1C-NC	4.01	116.19	110.08
153	c1	703	HEA	C13-C12-C11	-4.01	108.32	114.35
153	26	701	HEA	C2C-C1C-NC	4.00	116.17	110.08
153	81	703	HEA	C13-C12-C11	-4.00	108.34	114.35
152	QC	501	HEM	C4C-NC-C1C	3.94	109.20	105.35
152	qC	501	HEM	C4C-NC-C1C	3.93	109.20	105.35
152	qC	502	HEM	CHB-C1B-NB	3.90	129.18	124.37
152	QC	502	HEM	CHB-C1B-NB	3.88	129.16	124.37
153	C1	701	HEA	C4B-NB-C1B	-3.87	101.07	105.07
152	Qc	503	HEM	CHB-C1B-NB	3.87	129.14	124.37
153	26	701	HEA	C4B-NB-C1B	-3.86	101.09	105.07
152	0F	201	HEM	C4D-ND-C1D	3.84	109.04	105.07
153	26	702	HEA	CHA-C4D-C3D	-3.83	119.20	124.84
152	qc	503	HEM	CHB-C1B-NB	3.83	129.09	124.37
153	C1	702	HEA	CHA-C4D-C3D	-3.82	119.22	124.84
159	b8	301	ADP	C2-N3-C4	3.81	120.74	111.75
159	B8	301	ADP	C2-N3-C4	3.80	120.73	111.75
153	81	703	HEA	C4B-C3B-C2B	-3.77	100.96	107.41
152	y5	201	HEM	C4D-ND-C1D	3.77	108.97	105.07
153	c1	703	HEA	C4B-C3B-C2B	-3.77	100.97	107.41
153	C1	702	HEA	C1D-ND-C4D	-3.70	101.25	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
152	y5	201	HEM	CHB-C1B-NB	3.69	128.92	124.37
153	26	702	HEA	C1D-ND-C4D	-3.69	101.26	105.07
152	0F	201	HEM	CHB-C1B-NB	3.68	128.91	124.37
153	81	703	HEA	C3B-C4B-NB	3.65	114.17	109.84
153	c1	703	HEA	C3B-C4B-NB	3.61	114.12	109.84
152	0F	201	HEM	C1B-NB-C4B	3.61	108.80	105.07
152	y5	201	HEM	C1B-NB-C4B	3.60	108.79	105.07
152	QC	501	HEM	CHB-C1B-NB	3.59	128.80	124.37
152	qc	502	HEM	CHB-C1B-NB	3.59	128.80	124.37
152	Qc	502	HEM	CHB-C1B-NB	3.57	128.77	124.37
153	81	703	HEA	C3C-C4C-NC	3.56	112.44	110.25
153	C1	701	HEA	C4B-C3B-C2B	-3.56	101.32	107.41
153	c1	703	HEA	C3C-C4C-NC	3.56	112.44	110.25
152	qC	501	HEM	CHB-C1B-NB	3.55	128.76	124.37
153	26	701	HEA	C4B-C3B-C2B	-3.55	101.35	107.41
159	B8	301	ADP	PA-O3A-PB	-3.52	120.76	132.83
159	b8	301	ADP	PA-O3A-PB	-3.52	120.76	132.83
152	Qc	502	HEM	C4C-NC-C1C	3.49	108.77	105.35
153	C1	702	HEA	C4B-C3B-C2B	-3.48	101.47	107.41
153	26	702	HEA	C4B-C3B-C2B	-3.48	101.47	107.41
152	qc	503	HEM	C4D-ND-C1D	3.46	108.65	105.07
152	qc	502	HEM	C4C-NC-C1C	3.46	108.74	105.35
152	Qc	503	HEM	C4D-ND-C1D	3.46	108.64	105.07
152	qC	501	HEM	C4A-NA-C1A	3.43	108.71	105.35
160	qc	501	U10	C1M-C1-C2	3.43	119.90	115.98
160	Qc	501	U10	C1M-C1-C2	3.42	119.90	115.98
152	QC	501	HEM	C4A-NA-C1A	3.41	108.69	105.35
153	26	702	HEA	C13-C14-C15	-3.39	119.50	127.66
153	C1	702	HEA	C2C-C1C-NC	3.39	115.24	110.08
153	26	702	HEA	C2C-C1C-NC	3.37	115.21	110.08
153	C1	702	HEA	C13-C14-C15	-3.36	119.56	127.66
153	c1	703	HEA	CMB-C2B-C1B	-3.34	119.96	125.04
152	qC	502	HEM	C1B-NB-C4B	3.33	108.51	105.07
153	81	703	HEA	CMB-C2B-C1B	-3.32	119.98	125.04
153	81	701	HEA	CHC-C4B-NB	-3.30	120.31	124.37
153	c1	701	HEA	CHC-C4B-NB	-3.30	120.31	124.37
152	Qc	503	HEM	C1B-NB-C4B	3.30	108.48	105.07
152	QC	502	HEM	C1B-NB-C4B	3.30	108.48	105.07
153	c1	701	HEA	CAA-CBA-CGA	-3.28	106.55	113.60
153	81	701	HEA	CAA-CBA-CGA	-3.27	106.57	113.60
160	Qc	501	U10	C25-C24-C26	3.27	119.72	115.98
152	qc	503	HEM	C1B-NB-C4B	3.24	108.42	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
152	Y5	201	HEM	C4D-ND-C1D	3.24	108.42	105.07
153	C1	702	HEA	C3B-C4B-NB	3.24	113.67	109.84
160	qc	501	U10	C25-C24-C26	3.23	119.67	115.98
153	26	702	HEA	C3B-C4B-NB	3.22	113.66	109.84
153	C1	701	HEA	C2D-C1D-ND	3.22	113.65	109.84
152	50	201	HEM	C4D-ND-C1D	3.21	108.39	105.07
153	c1	703	HEA	CHA-C4D-C3D	-3.19	120.14	124.84
153	26	701	HEA	C2D-C1D-ND	3.19	113.62	109.84
160	Qc	501	U10	C12-C13-C14	-3.19	119.98	127.66
152	qc	502	HEM	C4A-NA-C1A	3.19	108.47	105.35
160	qc	501	U10	C12-C13-C14	-3.19	119.98	127.66
152	Qc	502	HEM	C4A-NA-C1A	3.19	108.47	105.35
153	81	703	HEA	CHA-C4D-C3D	-3.19	120.16	124.84
160	Qc	501	U10	C17-C18-C19	-3.17	120.04	127.66
160	qc	501	U10	C17-C18-C19	-3.16	120.05	127.66
153	81	703	HEA	CMB-C2B-C3B	3.16	136.37	130.34
152	qC	502	HEM	C4D-ND-C1D	3.16	108.33	105.07
153	c1	703	HEA	CMB-C2B-C3B	3.16	136.36	130.34
152	QC	502	HEM	C4D-ND-C1D	3.14	108.32	105.07
159	B8	301	ADP	C4-C5-N7	-3.13	106.80	110.62
159	b8	301	ADP	C4-C5-N7	-3.13	106.81	110.62
152	qC	502	HEM	CHA-C4D-ND	3.12	128.22	124.37
159	B8	301	ADP	N3-C2-N1	-3.10	123.75	128.60
153	81	703	HEA	C1D-ND-C4D	-3.10	101.87	105.07
152	Y5	201	HEM	C1B-NB-C4B	3.10	108.28	105.07
152	QC	502	HEM	CHA-C4D-ND	3.10	128.20	124.37
159	b8	301	ADP	N3-C2-N1	-3.10	123.75	128.60
153	c1	703	HEA	C1D-ND-C4D	-3.10	101.87	105.07
152	50	201	HEM	C1B-NB-C4B	3.07	108.25	105.07
160	qc	501	U10	C22-C23-C24	-3.03	120.36	127.66
160	Qc	501	U10	C22-C23-C24	-3.03	120.37	127.66
153	C1	701	HEA	CHA-C4D-ND	3.03	127.70	124.42
153	26	701	HEA	CHA-C4D-ND	3.02	127.70	124.42
152	0F	201	HEM	C4C-NC-C1C	3.01	108.29	105.35
152	qC	502	HEM	CHA-C1A-NA	2.98	129.32	123.85
152	QC	502	HEM	CHA-C1A-NA	2.97	129.31	123.85
152	y5	201	HEM	C4C-NC-C1C	2.97	108.25	105.35
153	C1	702	HEA	C27-C19-C20	2.95	120.24	115.27
153	26	702	HEA	C27-C19-C20	2.93	120.21	115.27
157	qD	401	HEC	C4B-NB-C1B	2.92	108.08	105.07
157	2e	401	HEC	O1D-CGD-CBD	-2.91	113.73	123.08
157	2E	401	HEC	O1D-CGD-CBD	-2.91	113.73	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
153	c1	703	HEA	CHD-C4C-NC	2.90	129.19	123.85
153	81	703	HEA	CHD-C4C-NC	2.88	129.15	123.85
153	81	703	HEA	C26-C15-C16	2.88	120.11	115.27
152	50	201	HEM	CHA-C4D-ND	2.87	127.92	124.37
157	QD	401	HEC	C4B-NB-C1B	2.87	108.03	105.07
152	Qc	503	HEM	C4C-NC-C1C	2.86	108.15	105.35
153	C1	701	HEA	CMC-C2C-C1C	2.86	129.73	125.37
153	C1	702	HEA	C1B-C2B-C3B	-2.86	103.38	106.80
152	qc	503	HEM	C4C-NC-C1C	2.85	108.14	105.35
153	c1	703	HEA	C26-C15-C16	2.85	120.07	115.27
153	26	702	HEA	C1B-C2B-C3B	-2.85	103.39	106.80
153	26	701	HEA	CMC-C2C-C1C	2.84	129.69	125.37
153	c1	701	HEA	C13-C14-C15	-2.84	120.82	127.66
152	Y5	201	HEM	CHA-C4D-ND	2.84	127.87	124.37
152	qc	503	HEM	CHA-C4D-ND	2.84	127.87	124.37
153	C1	701	HEA	C1B-C2B-C3B	-2.83	103.42	106.80
153	81	701	HEA	C13-C14-C15	-2.83	120.85	127.66
153	26	701	HEA	C27-C19-C20	2.82	120.02	115.27
152	QC	501	HEM	C1C-CHC-C4B	-2.81	119.99	126.06
157	qD	401	HEC	O1D-CGD-CBD	-2.81	114.06	123.08
152	Qc	503	HEM	CHA-C4D-ND	2.81	127.83	124.37
153	C1	701	HEA	C27-C19-C20	2.81	119.99	115.27
153	26	701	HEA	C1B-C2B-C3B	-2.80	103.45	106.80
152	qC	501	HEM	C1C-CHC-C4B	-2.80	120.02	126.06
157	QD	401	HEC	O1D-CGD-CBD	-2.79	114.12	123.08
152	qc	503	HEM	CHA-C1A-NA	2.77	128.94	123.85
152	Qc	503	HEM	CHA-C1A-NA	2.76	128.93	123.85
152	0F	201	HEM	C4A-NA-C1A	2.76	108.05	105.35
152	qc	502	HEM	C1C-CHC-C4B	-2.75	120.13	126.06
152	50	201	HEM	CHA-C1A-NA	2.75	128.90	123.85
153	C1	701	HEA	C4C-NC-C1C	-2.75	102.66	105.35
160	Qc	501	U10	C15-C14-C16	2.74	119.89	115.27
152	Qc	502	HEM	C1C-CHC-C4B	-2.74	120.15	126.06
159	b8	301	ADP	C4-N9-C8	2.74	108.69	105.73
153	26	701	HEA	C4C-NC-C1C	-2.73	102.67	105.35
153	81	703	HEA	C27-C19-C20	2.73	119.86	115.27
152	Y5	201	HEM	CHA-C1A-NA	2.73	128.87	123.85
153	c1	703	HEA	C27-C19-C20	2.73	119.86	115.27
153	c1	701	HEA	C17-C18-C19	-2.73	121.10	127.66
152	y5	201	HEM	C4A-NA-C1A	2.73	108.02	105.35
153	81	703	HEA	CHB-C4A-NA	-2.72	121.49	124.44
160	qc	501	U10	C15-C14-C16	2.72	119.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
159	B8	301	ADP	C4-N9-C8	2.72	108.68	105.73
157	Qd	401	HEC	O1D-CGD-CBD	-2.72	114.35	123.08
153	81	701	HEA	C17-C18-C19	-2.72	121.12	127.66
157	qd	401	HEC	O1D-CGD-CBD	-2.72	114.36	123.08
153	c1	703	HEA	CHB-C4A-NA	-2.71	121.50	124.44
153	c1	703	HEA	CMD-C2D-C1D	2.71	129.16	125.04
159	B8	301	ADP	C5-N7-C8	2.70	107.35	103.51
152	qc	502	HEM	CAD-CBD-CGD	-2.70	107.79	113.60
152	Y5	201	HEM	CHD-C1D-ND	2.70	127.36	124.42
153	26	702	HEA	C17-C18-C19	-2.70	121.16	127.66
152	Qc	502	HEM	CAD-CBD-CGD	-2.70	107.80	113.60
153	c1	701	HEA	C27-C19-C20	2.70	119.81	115.27
153	C1	702	HEA	C17-C18-C19	-2.69	121.17	127.66
160	Qc	501	U10	C20-C19-C21	2.69	119.80	115.27
160	qc	501	U10	C20-C19-C21	2.69	119.80	115.27
153	81	701	HEA	C27-C19-C20	2.68	119.78	115.27
153	81	703	HEA	CMD-C2D-C1D	2.68	129.12	125.04
159	b8	301	ADP	C5-N7-C8	2.67	107.31	103.51
152	0F	201	HEM	CHA-C4D-ND	2.67	127.67	124.37
152	qC	502	HEM	CHD-C1D-ND	2.67	127.32	124.42
152	50	201	HEM	CHD-C1D-ND	2.67	127.32	124.42
153	c1	701	HEA	OMA-CMA-C3A	-2.66	119.66	125.69
152	QC	502	HEM	CHD-C1D-ND	2.66	127.31	124.42
160	Qc	501	U10	C10-C9-C11	2.64	119.72	115.27
153	26	702	HEA	OMA-CMA-C3A	-2.64	119.72	125.69
153	c1	703	HEA	C17-C18-C19	-2.64	121.31	127.66
153	81	703	HEA	C1B-C2B-C3B	-2.64	103.65	106.80
152	y5	201	HEM	CHA-C4D-ND	2.63	127.62	124.37
153	81	701	HEA	OMA-CMA-C3A	-2.63	119.73	125.69
153	81	703	HEA	C17-C18-C19	-2.63	121.33	127.66
153	C1	702	HEA	OMA-CMA-C3A	-2.63	119.75	125.69
160	qc	501	U10	C10-C9-C11	2.62	119.68	115.27
153	81	703	HEA	CMC-C2C-C3C	2.62	132.92	126.59
153	26	701	HEA	C13-C14-C15	-2.61	121.38	127.66
153	c1	703	HEA	C1B-C2B-C3B	-2.61	103.68	106.80
153	C1	701	HEA	C13-C14-C15	-2.60	121.41	127.66
153	c1	703	HEA	CMC-C2C-C3C	2.59	132.87	126.59
157	2e	401	HEC	C1D-ND-C4D	2.59	107.75	105.07
157	2E	401	HEC	C1D-ND-C4D	2.59	107.75	105.07
152	0F	201	HEM	CHA-C1A-NA	2.58	128.60	123.85
153	C1	701	HEA	OMA-CMA-C3A	-2.58	119.85	125.69
153	26	702	HEA	C26-C15-C16	2.58	119.61	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
153	26	701	HEA	OMA-CMA-C3A	-2.57	119.87	125.69
153	C1	702	HEA	C26-C15-C16	2.57	119.59	115.27
152	y5	201	HEM	CHA-C1A-NA	2.56	128.56	123.85
153	26	701	HEA	C17-C18-C19	-2.56	121.50	127.66
153	C1	701	HEA	C17-C18-C19	-2.55	121.51	127.66
152	QC	502	HEM	C4C-NC-C1C	2.55	107.85	105.35
152	Qc	503	HEM	CHD-C1D-ND	2.55	127.19	124.42
152	qC	502	HEM	C4C-NC-C1C	2.54	107.84	105.35
159	b8	301	ADP	C3'-C2'-C1'	2.54	106.25	101.43
159	B8	301	ADP	C3'-C2'-C1'	2.54	106.25	101.43
152	qc	503	HEM	CHD-C1D-ND	2.53	127.17	124.42
153	81	703	HEA	C13-C14-C15	-2.53	121.58	127.66
153	c1	703	HEA	C13-C14-C15	-2.51	121.61	127.66
157	QD	401	HEC	CAA-C2A-C3A	2.49	132.51	127.88
153	81	703	HEA	O1D-CGD-CBD	-2.48	115.11	123.08
152	0F	201	HEM	CHD-C1D-ND	2.47	127.11	124.42
153	c1	703	HEA	O1D-CGD-CBD	-2.47	115.14	123.08
157	qD	401	HEC	CAA-C2A-C3A	2.47	132.48	127.88
162	SA	701	FAD	P-O3P-PA	-2.46	124.38	132.83
153	26	701	HEA	CMB-C2B-C3B	2.46	135.03	130.34
152	Qc	503	HEM	C4A-NA-C1A	2.45	107.75	105.35
153	81	701	HEA	CBA-CAA-C2A	-2.45	105.82	112.63
162	sa	701	FAD	P-O3P-PA	-2.45	124.42	132.83
152	qc	503	HEM	C4A-NA-C1A	2.45	107.75	105.35
152	qc	502	HEM	C2A-C1A-NA	-2.45	107.41	110.15
153	C1	701	HEA	CMB-C2B-C3B	2.45	135.01	130.34
153	c1	701	HEA	CBA-CAA-C2A	-2.44	105.84	112.63
152	50	201	HEM	CAA-CBA-CGA	-2.43	108.37	113.60
153	c1	701	HEA	C4C-NC-C1C	-2.43	102.97	105.35
152	qc	502	HEM	CHA-C1A-NA	2.43	128.32	123.85
152	Y5	201	HEM	C4C-NC-C1C	2.42	107.72	105.35
152	Qc	502	HEM	C2A-C1A-NA	-2.42	107.44	110.15
153	C1	701	HEA	C3A-C2A-C1A	-2.42	104.77	107.08
153	81	701	HEA	C4C-NC-C1C	-2.42	102.98	105.35
152	Qc	502	HEM	CHA-C1A-NA	2.42	128.29	123.85
152	Y5	201	HEM	CAA-CBA-CGA	-2.42	108.41	113.60
152	y5	201	HEM	CHD-C1D-ND	2.41	127.03	124.42
152	QC	501	HEM	C4A-CHB-C1B	-2.41	120.63	126.34
157	2E	401	HEC	O1A-CGA-CBA	-2.40	115.36	123.08
152	50	201	HEM	C4C-NC-C1C	2.40	107.70	105.35
157	2e	401	HEC	O1A-CGA-CBA	-2.40	115.38	123.08
153	26	701	HEA	C3A-C2A-C1A	-2.40	104.79	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
152	qC	501	HEM	C4A-CHB-C1B	-2.38	120.69	126.34
153	26	702	HEA	C4D-C3D-C2D	-2.38	103.43	106.90
152	QC	501	HEM	CHA-C4D-ND	2.37	127.30	124.37
157	qD	401	HEC	CHC-C4B-NB	2.37	127.30	124.37
157	qD	401	HEC	CAA-C2A-C1A	-2.36	120.44	124.89
157	QD	401	HEC	CAA-C2A-C1A	-2.36	120.44	124.89
153	26	702	HEA	CHD-C1D-ND	-2.36	121.46	124.37
152	QC	501	HEM	C2A-C1A-NA	-2.36	107.51	110.15
152	qC	501	HEM	C2A-C1A-NA	-2.36	107.51	110.15
152	Y5	201	HEM	CHB-C1B-C2B	-2.35	120.19	126.73
153	C1	702	HEA	CHD-C1D-ND	-2.35	121.47	124.37
152	qC	501	HEM	CHA-C1A-NA	2.35	128.17	123.85
152	0F	201	HEM	C1C-CHC-C4B	-2.35	120.99	126.06
152	Qc	503	HEM	CAD-CBD-CGD	-2.35	108.55	113.60
152	y5	201	HEM	C1C-CHC-C4B	-2.34	121.00	126.06
152	Qc	502	HEM	CAA-CBA-CGA	-2.34	108.56	113.60
153	C1	702	HEA	C4D-C3D-C2D	-2.34	103.48	106.90
152	qc	503	HEM	CAD-CBD-CGD	-2.34	108.57	113.60
157	qD	401	HEC	CBA-CAA-C2A	2.34	119.12	112.63
152	qC	501	HEM	CHA-C4D-ND	2.34	127.26	124.37
157	QD	401	HEC	CBA-CAA-C2A	2.34	119.12	112.63
152	50	201	HEM	CHB-C1B-C2B	-2.34	120.24	126.73
157	QD	401	HEC	CHC-C4B-NB	2.33	127.25	124.37
152	qc	502	HEM	CAA-CBA-CGA	-2.33	108.59	113.60
152	QC	501	HEM	CHA-C1A-NA	2.32	128.12	123.85
153	26	701	HEA	O1D-CGD-CBD	-2.31	115.64	123.08
153	C1	701	HEA	O1D-CGD-CBD	-2.31	115.65	123.08
153	81	703	HEA	O1A-CGA-CBA	-2.31	115.66	123.08
153	26	701	HEA	CMB-C2B-C1B	-2.31	121.52	125.04
153	c1	703	HEA	O1A-CGA-CBA	-2.30	115.68	123.08
153	C1	701	HEA	C4A-C3A-C2A	2.29	108.63	106.75
152	Qc	503	HEM	C4A-CHB-C1B	-2.28	120.92	126.34
157	Qd	401	HEC	CHC-C4B-NB	2.28	127.19	124.37
152	qc	502	HEM	C4A-CHB-C1B	-2.28	120.93	126.34
153	26	701	HEA	C4A-C3A-C2A	2.28	108.62	106.75
152	Qc	502	HEM	CHA-C4D-ND	2.28	127.18	124.37
152	50	201	HEM	C1C-CHC-C4B	-2.28	121.15	126.06
152	Qc	502	HEM	C4A-CHB-C1B	-2.28	120.94	126.34
153	C1	701	HEA	CMB-C2B-C1B	-2.27	121.58	125.04
152	qc	502	HEM	CHA-C4D-ND	2.27	127.17	124.37
152	Y5	201	HEM	C1C-CHC-C4B	-2.26	121.17	126.06
152	Qc	503	HEM	CHB-C1B-C2B	-2.26	120.44	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
157	qd	401	HEC	CHC-C4B-NB	2.26	127.17	124.37
153	c1	703	HEA	CHD-C1D-C2D	-2.26	120.45	126.73
152	QC	501	HEM	CAD-CBD-CGD	-2.26	108.74	113.60
153	26	701	HEA	C4D-C3D-C2D	-2.26	103.61	106.90
157	qD	401	HEC	C1D-ND-C4D	2.26	107.40	105.07
153	81	701	HEA	C26-C15-C16	2.26	119.06	115.27
152	qC	501	HEM	CAD-CBD-CGD	-2.25	108.75	113.60
153	C1	701	HEA	C27-C19-C18	-2.25	117.89	123.68
157	qD	401	HEC	O1A-CGA-CBA	-2.25	115.84	123.08
153	26	701	HEA	C27-C19-C18	-2.25	117.90	123.68
157	QD	401	HEC	O1A-CGA-CBA	-2.25	115.85	123.08
152	qc	503	HEM	C4A-CHB-C1B	-2.25	121.00	126.34
153	C1	701	HEA	C4D-C3D-C2D	-2.25	103.62	106.90
157	qd	401	HEC	O1A-CGA-CBA	-2.25	115.86	123.08
153	81	703	HEA	CHD-C1D-C2D	-2.25	120.49	126.73
152	qc	503	HEM	CHB-C1B-C2B	-2.24	120.50	126.73
157	QD	401	HEC	C1D-ND-C4D	2.24	107.39	105.07
153	C1	701	HEA	C26-C15-C16	2.24	119.04	115.27
153	c1	701	HEA	C26-C15-C16	2.24	119.03	115.27
153	26	701	HEA	C26-C15-C16	2.23	119.03	115.27
157	Qd	401	HEC	O1A-CGA-CBA	-2.23	115.91	123.08
153	c1	701	HEA	C4D-C3D-C2D	-2.23	103.65	106.90
152	qC	502	HEM	CHB-C1B-C2B	-2.22	120.56	126.73
152	QC	502	HEM	CHB-C1B-C2B	-2.21	120.59	126.73
153	c1	701	HEA	O1D-CGD-CBD	-2.21	115.98	123.08
153	81	701	HEA	O1D-CGD-CBD	-2.21	115.99	123.08
152	qC	502	HEM	C1C-CHC-C4B	-2.20	121.31	126.06
152	y5	201	HEM	C4A-CHB-C1B	-2.20	121.12	126.34
152	0F	201	HEM	C4A-CHB-C1B	-2.20	121.13	126.34
152	QC	502	HEM	C1C-CHC-C4B	-2.19	121.34	126.06
153	81	701	HEA	C4D-C3D-C2D	-2.19	103.71	106.90
152	QC	501	HEM	CAA-CBA-CGA	-2.18	108.92	113.60
152	y5	201	HEM	C2A-C1A-NA	-2.17	107.72	110.15
152	qC	501	HEM	CAA-CBA-CGA	-2.17	108.93	113.60
157	2e	401	HEC	O2A-CGA-O1A	2.17	128.71	123.30
152	qc	503	HEM	C1C-CHC-C4B	-2.17	121.38	126.06
152	Qc	502	HEM	C1A-CHA-C4D	-2.17	121.20	126.34
157	qD	401	HEC	C3B-C4B-NB	-2.17	107.75	110.17
152	qc	502	HEM	C1A-CHA-C4D	-2.17	121.20	126.34
152	0F	201	HEM	C2A-C1A-NA	-2.16	107.73	110.15
152	QC	501	HEM	C4C-CHD-C1D	-2.16	121.39	126.06
157	QD	401	HEC	C3B-C4B-NB	-2.16	107.76	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
152	Qc	503	HEM	C1C-CHC-C4B	-2.16	121.40	126.06
157	2E	401	HEC	O2A-CGA-O1A	2.15	128.66	123.30
152	qC	501	HEM	C4C-CHD-C1D	-2.15	121.43	126.06
152	qc	502	HEM	O2D-CGD-CBD	2.14	120.92	114.03
152	Qc	502	HEM	O2D-CGD-CBD	2.14	120.91	114.03
157	qd	401	HEC	O2A-CGA-O1A	2.13	128.60	123.30
157	Qd	401	HEC	O2A-CGA-O1A	2.12	128.59	123.30
152	qC	502	HEM	C4A-NA-C1A	2.12	107.42	105.35
152	QC	502	HEM	C4A-NA-C1A	2.12	107.42	105.35
153	81	701	HEA	CMB-C2B-C1B	-2.11	121.83	125.04
152	QC	501	HEM	C1A-CHA-C4D	-2.10	121.35	126.34
152	qC	501	HEM	C1A-CHA-C4D	-2.10	121.35	126.34
153	c1	703	HEA	CHD-C4C-C3C	-2.10	118.36	127.71
153	81	701	HEA	C1B-C2B-C3B	-2.10	104.29	106.80
153	c1	701	HEA	CHC-C1C-C2C	-2.10	121.31	127.24
153	c1	701	HEA	CMB-C2B-C1B	-2.10	121.85	125.04
153	81	703	HEA	CHD-C4C-C3C	-2.09	118.40	127.71
153	81	701	HEA	CHC-C1C-C2C	-2.09	121.33	127.24
153	c1	701	HEA	C1B-C2B-C3B	-2.08	104.31	106.80
157	qd	401	HEC	CBD-CAD-C3D	2.08	118.40	112.63
157	Qd	401	HEC	CBD-CAD-C3D	2.08	118.39	112.63
153	26	702	HEA	C27-C19-C18	-2.07	118.36	123.68
152	y5	201	HEM	CHB-C1B-C2B	-2.07	120.97	126.73
152	0F	201	HEM	CHB-C1B-C2B	-2.07	120.97	126.73
153	C1	702	HEA	C27-C19-C18	-2.07	118.36	123.68
152	Y5	201	HEM	CAD-CBD-CGD	-2.07	109.15	113.60
157	2e	401	HEC	C3D-C4D-ND	-2.06	108.36	110.36
157	2E	401	HEC	C3D-C4D-ND	-2.06	108.36	110.36
153	c1	701	HEA	CMC-C2C-C1C	2.06	128.51	125.37
159	b8	301	ADP	C6-C5-N7	2.06	135.86	132.02
157	qd	401	HEC	C1D-ND-C4D	2.06	107.20	105.07
159	B8	301	ADP	C6-C5-N7	2.06	135.85	132.02
152	50	201	HEM	CAD-CBD-CGD	-2.05	109.18	113.60
159	B8	301	ADP	N9-C8-N7	-2.05	111.11	113.91
153	26	701	HEA	CHC-C1C-C2C	-2.05	121.45	127.24
157	qD	401	HEC	O2A-CGA-O1A	2.05	128.40	123.30
157	QD	401	HEC	O2A-CGA-O1A	2.04	128.40	123.30
153	81	701	HEA	CMC-C2C-C1C	2.04	128.48	125.37
153	C1	701	HEA	CHC-C1C-C2C	-2.04	121.48	127.24
157	Qd	401	HEC	C1D-ND-C4D	2.04	107.18	105.07
153	c1	703	HEA	C27-C19-C18	-2.04	118.46	123.68
153	81	703	HEA	C27-C19-C18	-2.03	118.46	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
157	2E	401	HEC	CBD-CAD-C3D	2.03	118.28	112.63
157	2e	401	HEC	CBD-CAD-C3D	2.03	118.27	112.63
153	C1	702	HEA	O1D-CGD-CBD	-2.03	116.55	123.08
157	Qd	401	HEC	CMC-C2C-C3C	2.03	130.00	125.61
153	26	702	HEA	O1D-CGD-CBD	-2.03	116.57	123.08
157	qd	401	HEC	CMC-C2C-C3C	2.03	129.99	125.61
152	qC	502	HEM	C4A-CHB-C1B	-2.02	121.55	126.34
153	C1	701	HEA	O2D-CGD-CBD	2.02	120.52	114.03
153	26	701	HEA	O2D-CGD-CBD	2.02	120.51	114.03
159	b8	301	ADP	N9-C8-N7	-2.02	111.16	113.91
152	Qc	502	HEM	CHD-C1D-ND	2.01	126.61	124.42
152	Qc	503	HEM	C2A-C1A-NA	-2.01	107.90	110.15
152	QC	502	HEM	C4A-CHB-C1B	-2.01	121.57	126.34
153	26	701	HEA	O1A-CGA-CBA	-2.01	116.62	123.08
164	v1	501	FMN	P-O5'-C5'	2.01	123.83	118.30
152	qC	502	HEM	O2A-CGA-CBA	2.01	120.48	114.03
152	qc	503	HEM	C2A-C1A-NA	-2.01	107.90	110.15
153	C1	702	HEA	CMB-C2B-C3B	2.01	134.17	130.34
153	c1	703	HEA	CHB-C1B-NB	2.01	126.60	124.42
152	50	201	HEM	C4A-CHB-C1B	-2.01	121.58	126.34
153	26	702	HEA	CMB-C2B-C3B	2.01	134.16	130.34
152	qc	502	HEM	CHD-C1D-ND	2.00	126.59	124.42

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
157	2e	401	HEC	NA
157	qD	401	HEC	NA
157	qd	401	HEC	NA
157	QD	401	HEC	NA
157	Qd	401	HEC	NA
157	2E	401	HEC	NA

All (285) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
152	0F	201	HEM	C2B-C3B-CAB-CBB
152	0F	201	HEM	C4B-C3B-CAB-CBB
152	50	201	HEM	C2B-C3B-CAB-CBB
152	50	201	HEM	C4B-C3B-CAB-CBB
152	50	201	HEM	C2C-C3C-CAC-CBC
152	qC	501	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
152	qC	501	HEM	C4B-C3B-CAB-CBB
152	qC	501	HEM	C2C-C3C-CAC-CBC
152	qC	501	HEM	C4C-C3C-CAC-CBC
152	qC	502	HEM	C2B-C3B-CAB-CBB
152	qC	502	HEM	C4B-C3B-CAB-CBB
152	qC	502	HEM	C2C-C3C-CAC-CBC
152	qC	502	HEM	C4C-C3C-CAC-CBC
152	qc	502	HEM	C2C-C3C-CAC-CBC
152	qc	502	HEM	C4C-C3C-CAC-CBC
152	qc	503	HEM	C2B-C3B-CAB-CBB
152	qc	503	HEM	C4B-C3B-CAB-CBB
152	QC	501	HEM	C2B-C3B-CAB-CBB
152	QC	501	HEM	C4B-C3B-CAB-CBB
152	QC	501	HEM	C2C-C3C-CAC-CBC
152	QC	501	HEM	C4C-C3C-CAC-CBC
152	QC	502	HEM	C2B-C3B-CAB-CBB
152	QC	502	HEM	C4B-C3B-CAB-CBB
152	QC	502	HEM	C2C-C3C-CAC-CBC
152	QC	502	HEM	C4C-C3C-CAC-CBC
152	Qc	502	HEM	C2C-C3C-CAC-CBC
152	Qc	502	HEM	C4C-C3C-CAC-CBC
152	Qc	503	HEM	C2B-C3B-CAB-CBB
152	Qc	503	HEM	C4B-C3B-CAB-CBB
152	y5	201	HEM	C2B-C3B-CAB-CBB
152	y5	201	HEM	C4B-C3B-CAB-CBB
152	Y5	201	HEM	C2B-C3B-CAB-CBB
152	Y5	201	HEM	C4B-C3B-CAB-CBB
152	Y5	201	HEM	C2C-C3C-CAC-CBC
153	26	701	HEA	C1A-C2A-CAA-CBA
153	26	701	HEA	C3A-C2A-CAA-CBA
153	26	701	HEA	C2A-C3A-CMA-OMA
153	26	701	HEA	C4A-C3A-CMA-OMA
153	26	701	HEA	C27-C19-C20-C21
153	26	701	HEA	C19-C20-C21-C22
153	26	701	HEA	C21-C22-C23-C25
153	26	702	HEA	C2A-C3A-CMA-OMA
153	26	702	HEA	C4A-C3A-CMA-OMA
153	26	702	HEA	C18-C19-C20-C21
153	26	702	HEA	C19-C20-C21-C22
153	81	701	HEA	C3A-C2A-CAA-CBA
153	81	701	HEA	C2A-C3A-CMA-OMA
153	81	701	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
153	81	701	HEA	C19-C20-C21-C22
153	81	701	HEA	C21-C22-C23-C25
153	81	703	HEA	C2A-C3A-CMA-OMA
153	81	703	HEA	C4A-C3A-CMA-OMA
153	81	703	HEA	C3B-C11-C12-C13
153	81	703	HEA	O11-C11-C12-C13
153	81	703	HEA	C11-C12-C13-C14
153	81	703	HEA	C19-C20-C21-C22
153	c1	701	HEA	C3A-C2A-CAA-CBA
153	c1	701	HEA	C2A-C3A-CMA-OMA
153	c1	701	HEA	C15-C16-C17-C18
153	c1	701	HEA	C19-C20-C21-C22
153	c1	701	HEA	C21-C22-C23-C25
153	c1	703	HEA	C2A-C3A-CMA-OMA
153	c1	703	HEA	C4A-C3A-CMA-OMA
153	c1	703	HEA	C3B-C11-C12-C13
153	c1	703	HEA	O11-C11-C12-C13
153	c1	703	HEA	C11-C12-C13-C14
153	c1	703	HEA	C19-C20-C21-C22
153	C1	701	HEA	C1A-C2A-CAA-CBA
153	C1	701	HEA	C3A-C2A-CAA-CBA
153	C1	701	HEA	C2A-C3A-CMA-OMA
153	C1	701	HEA	C4A-C3A-CMA-OMA
153	C1	701	HEA	C27-C19-C20-C21
153	C1	701	HEA	C19-C20-C21-C22
153	C1	701	HEA	C21-C22-C23-C25
153	C1	702	HEA	C2A-C3A-CMA-OMA
153	C1	702	HEA	C4A-C3A-CMA-OMA
153	C1	702	HEA	C18-C19-C20-C21
153	C1	702	HEA	C19-C20-C21-C22
157	qD	401	HEC	C3A-C2A-CAA-CBA
157	QD	401	HEC	C3A-C2A-CAA-CBA
159	b8	301	ADP	C5'-O5'-PA-O2A
159	b8	301	ADP	C5'-O5'-PA-O3A
159	B8	301	ADP	C5'-O5'-PA-O3A
162	sa	701	FAD	C5B-O5B-PA-O1A
162	sa	701	FAD	C5B-O5B-PA-O2A
162	sa	701	FAD	C5B-O5B-PA-O3P
162	sa	701	FAD	C2'-C3'-C4'-O4'
162	sa	701	FAD	C2'-C3'-C4'-C5'
162	sa	701	FAD	O3'-C3'-C4'-O4'
162	sa	701	FAD	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
162	SA	701	FAD	C5B-O5B-PA-O1A
162	SA	701	FAD	C5B-O5B-PA-O2A
162	SA	701	FAD	C5B-O5B-PA-O3P
162	SA	701	FAD	C2'-C3'-C4'-O4'
162	SA	701	FAD	C2'-C3'-C4'-C5'
162	SA	701	FAD	O3'-C3'-C4'-O4'
162	SA	701	FAD	O3'-C3'-C4'-C5'
164	v1	501	FMN	N10-C1'-C2'-O2'
164	V1	501	FMN	N10-C1'-C2'-O2'
153	26	701	HEA	C21-C22-C23-C24
153	81	701	HEA	C21-C22-C23-C24
153	c1	701	HEA	C21-C22-C23-C24
153	C1	701	HEA	C21-C22-C23-C24
153	26	702	HEA	C27-C19-C20-C21
153	C1	702	HEA	C27-C19-C20-C21
153	81	701	HEA	C1A-C2A-CAA-CBA
153	c1	701	HEA	C1A-C2A-CAA-CBA
157	qD	401	HEC	C1A-C2A-CAA-CBA
157	QD	401	HEC	C1A-C2A-CAA-CBA
162	sa	701	FAD	O4B-C4B-C5B-O5B
162	SA	701	FAD	O4B-C4B-C5B-O5B
153	81	701	HEA	C27-C19-C20-C21
153	81	703	HEA	C27-C19-C20-C21
153	c1	701	HEA	C27-C19-C20-C21
153	c1	703	HEA	C27-C19-C20-C21
153	26	701	HEA	C18-C19-C20-C21
153	81	701	HEA	C18-C19-C20-C21
153	81	703	HEA	C18-C19-C20-C21
153	c1	701	HEA	C18-C19-C20-C21
153	c1	703	HEA	C18-C19-C20-C21
153	C1	701	HEA	C18-C19-C20-C21
153	26	701	HEA	C15-C16-C17-C18
153	26	702	HEA	C15-C16-C17-C18
153	C1	701	HEA	C15-C16-C17-C18
153	C1	702	HEA	C15-C16-C17-C18
160	qc	501	U10	C14-C16-C17-C18
160	qc	501	U10	C19-C21-C22-C23
160	Qc	501	U10	C14-C16-C17-C18
160	Qc	501	U10	C19-C21-C22-C23
153	26	701	HEA	C17-C18-C19-C27
153	81	703	HEA	C17-C18-C19-C27
153	c1	703	HEA	C17-C18-C19-C27

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Mol	Chain	Res	Type	Atoms
153	C1	701	HEA	C17-C18-C19-C27
153	81	701	HEA	C2A-CAA-CBA-CGA
153	c1	701	HEA	C2A-CAA-CBA-CGA
153	81	703	HEA	C15-C16-C17-C18
153	c1	703	HEA	C15-C16-C17-C18
153	81	703	HEA	C1A-C2A-CAA-CBA
153	c1	703	HEA	C1A-C2A-CAA-CBA
153	81	703	HEA	C3A-C2A-CAA-CBA
153	c1	703	HEA	C3A-C2A-CAA-CBA
152	qC	502	HEM	C2A-CAA-CBA-CGA
152	QC	502	HEM	C2A-CAA-CBA-CGA
157	2e	401	HEC	C3D-CAD-CBD-CGD
157	2E	401	HEC	C3D-CAD-CBD-CGD
152	0F	201	HEM	C2C-C3C-CAC-CBC
152	y5	201	HEM	C2C-C3C-CAC-CBC
152	50	201	HEM	C4C-C3C-CAC-CBC
152	Y5	201	HEM	C4C-C3C-CAC-CBC
159	b8	301	ADP	O4'-C4'-C5'-O5'
159	b8	301	ADP	C3'-C4'-C5'-O5'
159	B8	301	ADP	O4'-C4'-C5'-O5'
159	B8	301	ADP	C3'-C4'-C5'-O5'
153	81	701	HEA	C11-C12-C13-C14
153	c1	701	HEA	C11-C12-C13-C14
164	v1	501	FMN	C5'-O5'-P-O1P
164	V1	501	FMN	C5'-O5'-P-O1P
160	qc	501	U10	C12-C11-C9-C10
160	Qc	501	U10	C12-C11-C9-C10
152	qC	501	HEM	C2A-CAA-CBA-CGA
152	QC	501	HEM	C2A-CAA-CBA-CGA
162	sa	701	FAD	C3B-C4B-C5B-O5B
162	SA	701	FAD	C3B-C4B-C5B-O5B
158	a9	401	NDP	C2B-O2B-P2B-O1X
158	A9	401	NDP	C2B-O2B-P2B-O1X
152	qc	503	HEM	C2C-C3C-CAC-CBC
152	Qc	503	HEM	C2C-C3C-CAC-CBC
152	0F	201	HEM	C4C-C3C-CAC-CBC
152	y5	201	HEM	C4C-C3C-CAC-CBC
158	a9	401	NDP	PA-O3-PN-O1N
158	A9	401	NDP	PA-O3-PN-O1N
159	B8	301	ADP	C5'-O5'-PA-O1A
160	qc	501	U10	C23-C24-C26-C27
160	Qc	501	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
164	v1	501	FMN	N10-C1'-C2'-C3'
164	V1	501	FMN	N10-C1'-C2'-C3'
153	81	701	HEA	C4A-C3A-CMA-OMA
153	c1	701	HEA	C4A-C3A-CMA-OMA
158	a9	401	NDP	C4B-C5B-O5B-PA
158	A9	401	NDP	C4B-C5B-O5B-PA
160	qc	501	U10	C12-C11-C9-C8
160	Qc	501	U10	C12-C11-C9-C8
152	0F	201	HEM	CAA-CBA-CGA-O1A
152	y5	201	HEM	CAA-CBA-CGA-O1A
162	sa	701	FAD	C2B-C1B-N9A-C8A
162	SA	701	FAD	C2B-C1B-N9A-C8A
158	a9	401	NDP	O4D-C1D-N1N-C6N
158	A9	401	NDP	O4D-C1D-N1N-C6N
152	qc	503	HEM	C4C-C3C-CAC-CBC
152	Qc	503	HEM	C4C-C3C-CAC-CBC
152	50	201	HEM	CAA-CBA-CGA-O1A
152	Y5	201	HEM	CAA-CBA-CGA-O1A
152	qC	502	HEM	CAA-CBA-CGA-O2A
152	QC	502	HEM	CAA-CBA-CGA-O2A
152	Qc	503	HEM	CAA-CBA-CGA-O1A
152	qc	503	HEM	CAD-CBD-CGD-O1D
152	Qc	503	HEM	CAD-CBD-CGD-O1D
152	qc	503	HEM	CAA-CBA-CGA-O1A
152	qC	502	HEM	CAA-CBA-CGA-O1A
152	QC	502	HEM	CAA-CBA-CGA-O1A
153	81	703	HEA	CAD-CBD-CGD-O2D
153	c1	703	HEA	CAD-CBD-CGD-O2D
152	Qc	503	HEM	CAA-CBA-CGA-O2A
152	qc	503	HEM	CAA-CBA-CGA-O2A
153	26	702	HEA	CAD-CBD-CGD-O1D
153	C1	702	HEA	CAD-CBD-CGD-O1D
153	81	703	HEA	C13-C14-C15-C26
157	qD	401	HEC	C3D-CAD-CBD-CGD
157	QD	401	HEC	C3D-CAD-CBD-CGD
152	0F	201	HEM	CAA-CBA-CGA-O2A
152	qc	503	HEM	CAD-CBD-CGD-O2D
152	Qc	503	HEM	CAD-CBD-CGD-O2D
152	y5	201	HEM	CAA-CBA-CGA-O2A
157	Qd	401	HEC	CAA-CBA-CGA-O1A
153	26	702	HEA	CAD-CBD-CGD-O2D
153	C1	702	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
157	qd	401	HEC	CAA-CBA-CGA-O1A
152	50	201	HEM	CAA-CBA-CGA-O2A
152	Y5	201	HEM	CAA-CBA-CGA-O2A
153	c1	703	HEA	C13-C14-C15-C26
153	81	703	HEA	CAD-CBD-CGD-O1D
153	c1	703	HEA	CAD-CBD-CGD-O1D
159	B8	301	ADP	PB-O3A-PA-O2A
157	qd	401	HEC	CAA-CBA-CGA-O2A
157	Qd	401	HEC	CAA-CBA-CGA-O2A
152	0F	201	HEM	C2A-CAA-CBA-CGA
152	qC	501	HEM	C3D-CAD-CBD-CGD
152	QC	501	HEM	C3D-CAD-CBD-CGD
152	y5	201	HEM	C2A-CAA-CBA-CGA
153	81	703	HEA	CAA-CBA-CGA-O2A
153	c1	703	HEA	CAA-CBA-CGA-O2A
157	qD	401	HEC	CAA-CBA-CGA-O2A
157	QD	401	HEC	CAA-CBA-CGA-O2A
162	sa	701	FAD	PA-O3P-P-O5'
162	SA	701	FAD	PA-O3P-P-O5'
157	2e	401	HEC	CAA-CBA-CGA-O2A
157	qD	401	HEC	CAD-CBD-CGD-O2D
157	2E	401	HEC	CAA-CBA-CGA-O2A
153	81	703	HEA	C21-C22-C23-C25
157	QD	401	HEC	CAD-CBD-CGD-O2D
157	qD	401	HEC	CAA-CBA-CGA-O1A
157	QD	401	HEC	CAA-CBA-CGA-O1A
153	c1	703	HEA	C21-C22-C23-C25
164	v1	501	FMN	C5'-O5'-P-O3P
164	V1	501	FMN	C5'-O5'-P-O3P
153	c1	703	HEA	C2A-CAA-CBA-CGA
153	26	701	HEA	CAD-CBD-CGD-O2D
153	26	702	HEA	CAA-CBA-CGA-O1A
153	C1	702	HEA	CAA-CBA-CGA-O1A
157	2e	401	HEC	CAA-CBA-CGA-O1A
157	2E	401	HEC	CAA-CBA-CGA-O1A
152	qc	502	HEM	C2B-C3B-CAB-CBB
152	Qc	502	HEM	C2B-C3B-CAB-CBB
153	C1	701	HEA	CAD-CBD-CGD-O2D
153	81	703	HEA	CAA-CBA-CGA-O1A
153	c1	703	HEA	CAA-CBA-CGA-O1A
153	C1	702	HEA	CAA-CBA-CGA-O2A
152	qc	502	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
152	Qc	502	HEM	C4B-C3B-CAB-CBB
153	26	702	HEA	CAA-CBA-CGA-O2A
153	81	701	HEA	CAD-CBD-CGD-O1D
153	c1	701	HEA	CAD-CBD-CGD-O1D
153	81	703	HEA	C2A-CAA-CBA-CGA
153	81	701	HEA	C17-C18-C19-C20
153	c1	701	HEA	C17-C18-C19-C20
153	81	701	HEA	CAD-CBD-CGD-O2D
153	c1	701	HEA	CAD-CBD-CGD-O2D
158	a9	401	NDP	PA-O3-PN-O2N
158	A9	401	NDP	PA-O3-PN-O2N
157	qD	401	HEC	CAD-CBD-CGD-O1D
157	QD	401	HEC	CAD-CBD-CGD-O1D
153	26	701	HEA	CAD-CBD-CGD-O1D
153	C1	701	HEA	CAD-CBD-CGD-O1D
157	qd	401	HEC	CAD-CBD-CGD-O2D
157	Qd	401	HEC	CAD-CBD-CGD-O2D
160	qc	501	U10	C6-C7-C8-C9
160	Qc	501	U10	C6-C7-C8-C9
158	a9	401	NDP	O4B-C4B-C5B-O5B
158	A9	401	NDP	O4B-C4B-C5B-O5B
153	26	702	HEA	C3B-C11-C12-C13
153	C1	702	HEA	C3B-C11-C12-C13
153	26	702	HEA	C26-C15-C16-C17
153	C1	702	HEA	C26-C15-C16-C17
162	sa	701	FAD	O4'-C4'-C5'-O5'
162	SA	701	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 50 short contacts:

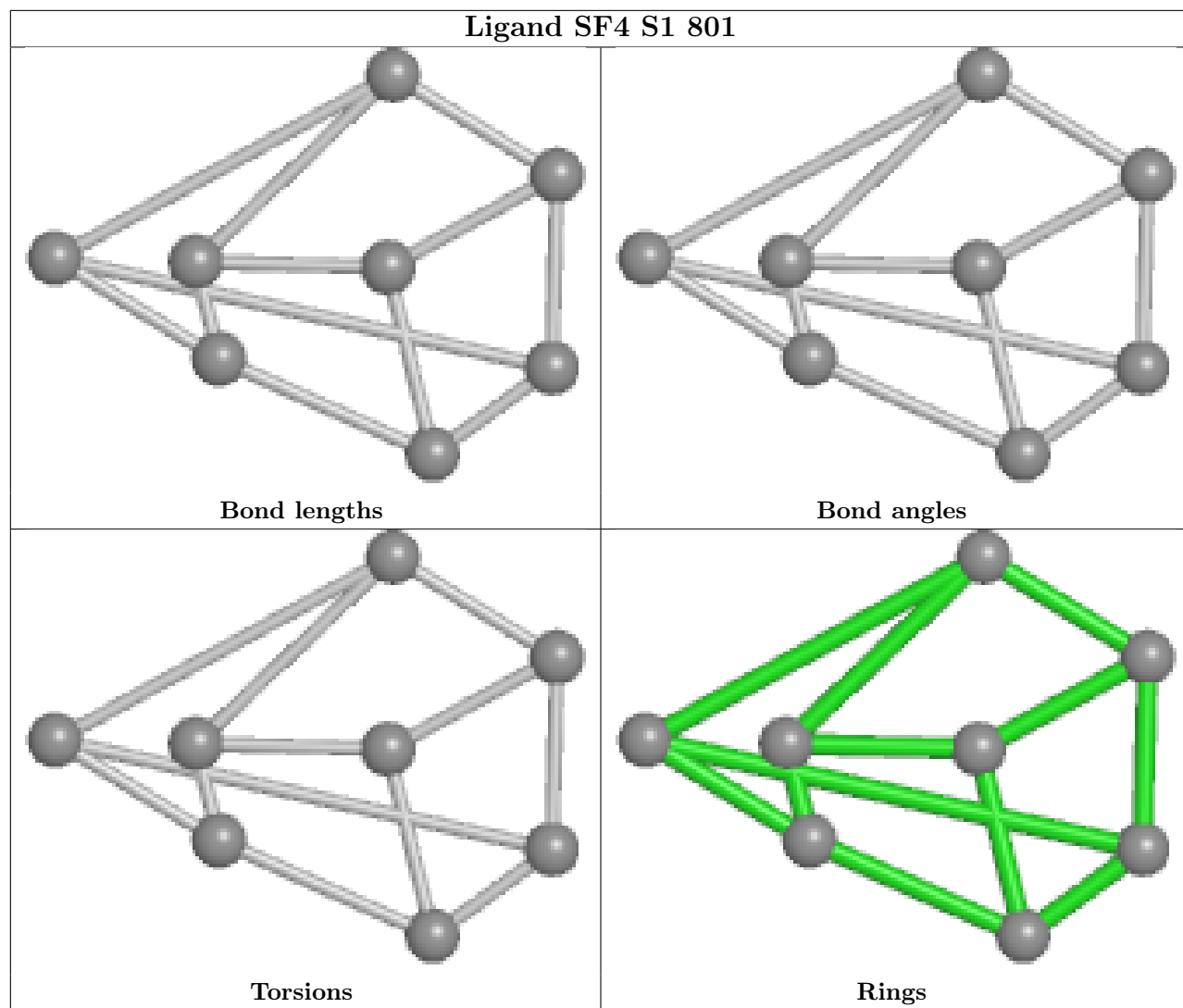
Mol	Chain	Res	Type	Clashes	Symm-Clashes
160	Qc	501	U10	1	0
153	81	701	HEA	4	0
153	26	702	HEA	1	0
153	C1	702	HEA	1	0
151	SB	401	FES	1	0
151	sb	401	FES	1	0
153	c1	703	HEA	5	0
153	81	703	HEA	5	0
161	S8	302	SF4	1	0
151	0C	202	FES	1	0

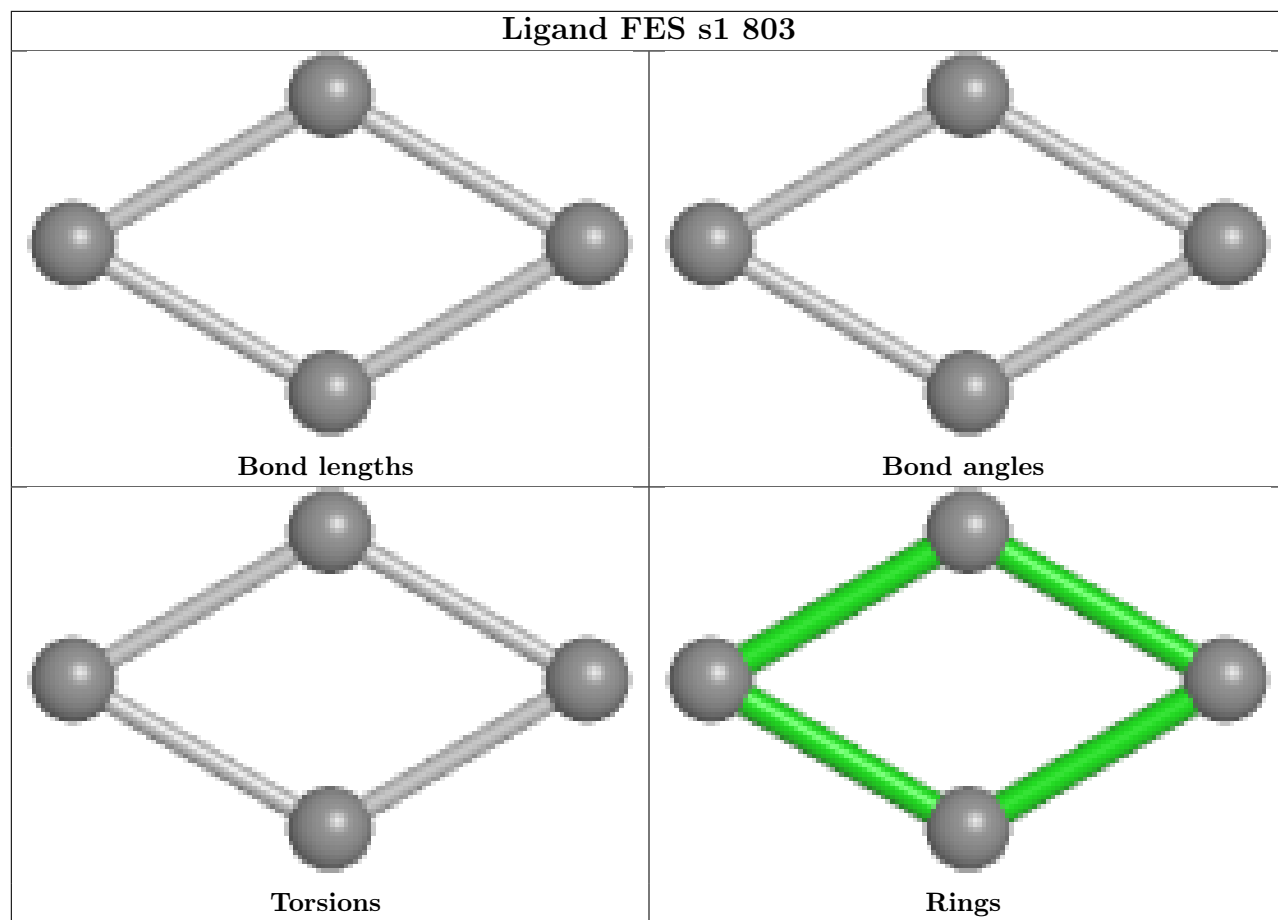
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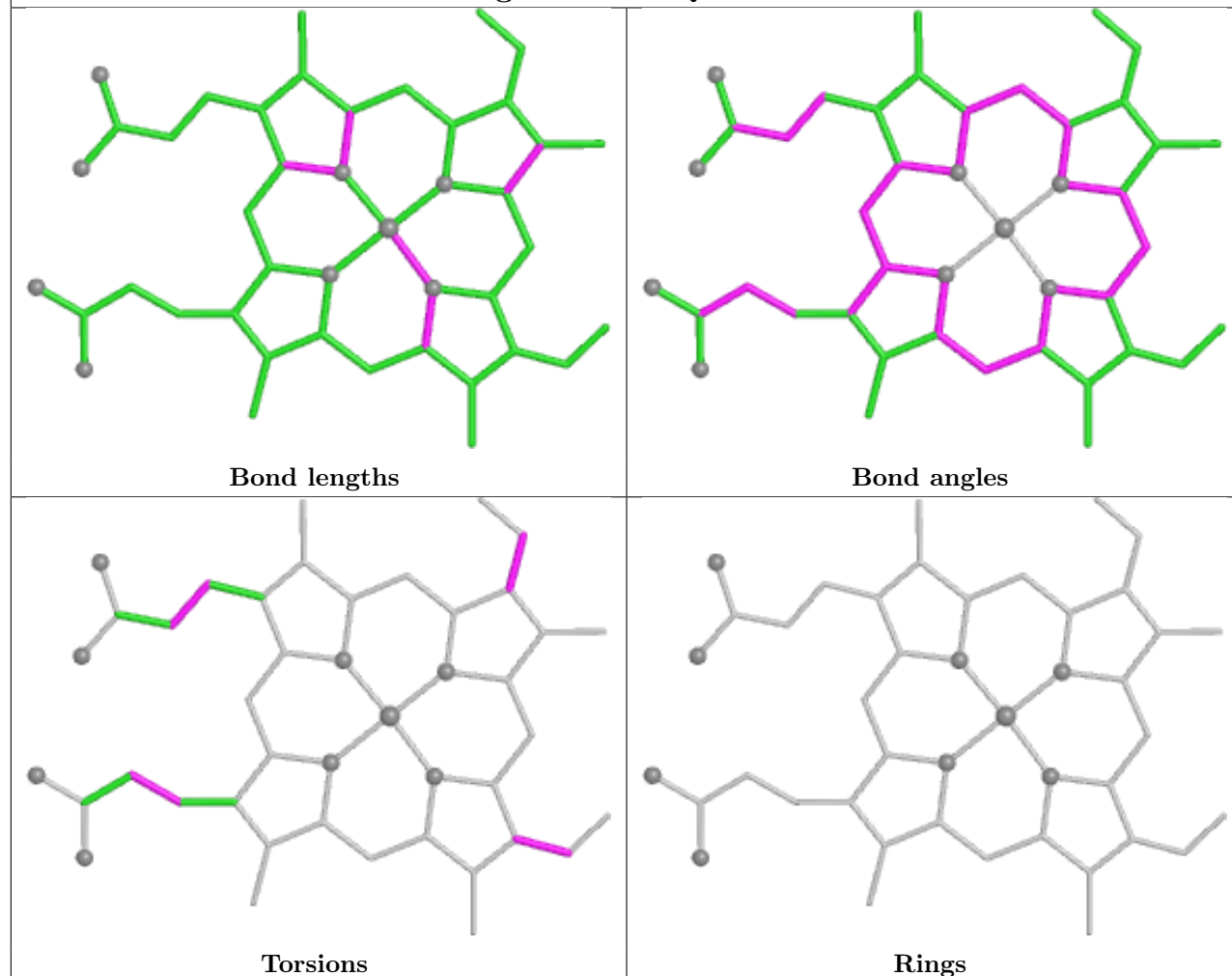
Mol	Chain	Res	Type	Clashes	Symm-Clashes
160	qc	501	U10	1	0
151	FS	202	FES	1	0
152	qc	502	HEM	2	0
152	Qc	502	HEM	2	0
153	c1	701	HEA	4	0
158	A9	401	NDP	1	0
153	26	701	HEA	3	0
151	fs	202	FES	2	0
164	V1	501	FMN	1	0
158	a9	401	NDP	1	0
161	s8	302	SF4	1	0
151	47	202	FES	1	0
151	47	201	FES	1	0
162	SA	701	FAD	1	0
153	C1	701	HEA	3	0
161	sb	402	SF4	1	0
161	SB	402	SF4	1	0
162	sa	701	FAD	1	0
151	FS	201	FES	1	0

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

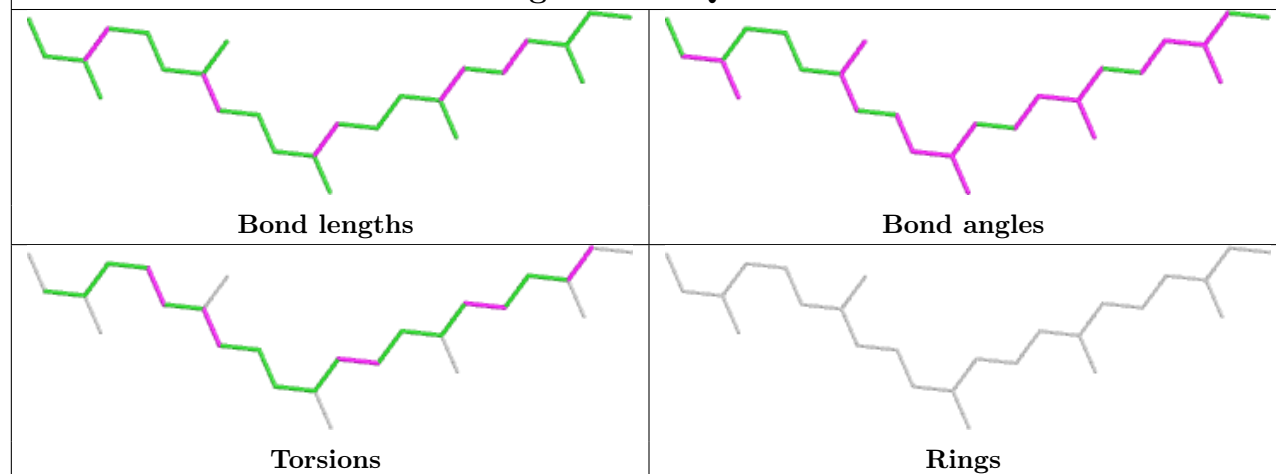




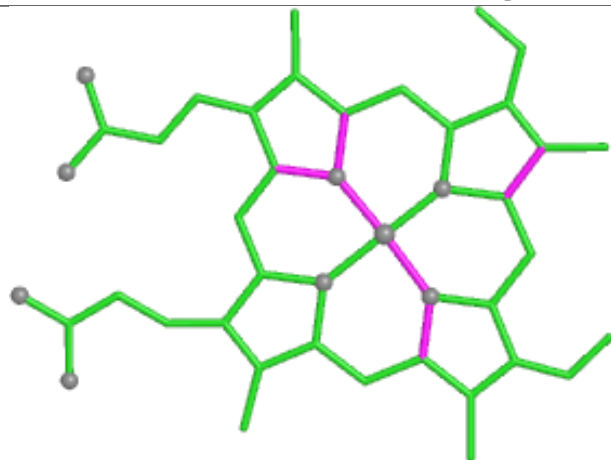
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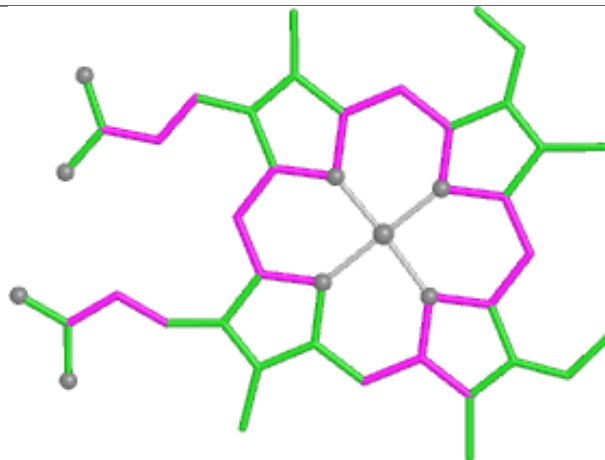
Ligand U10 Qc 501



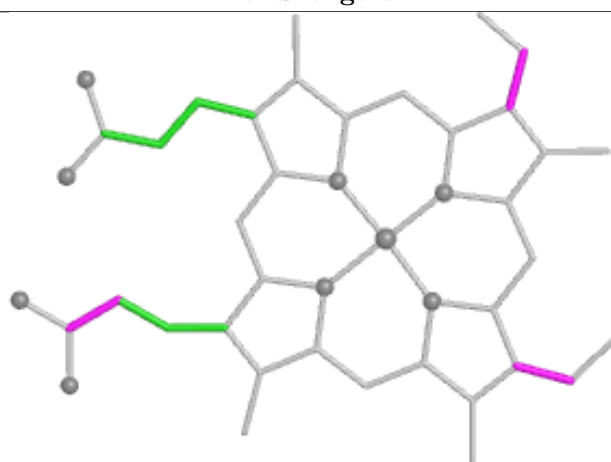
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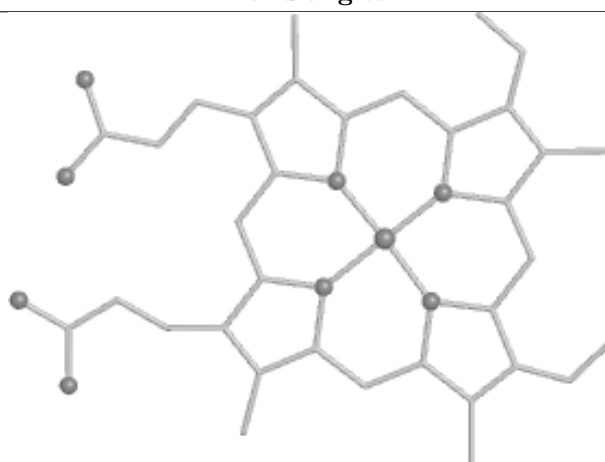
Bond lengths



Bond angles

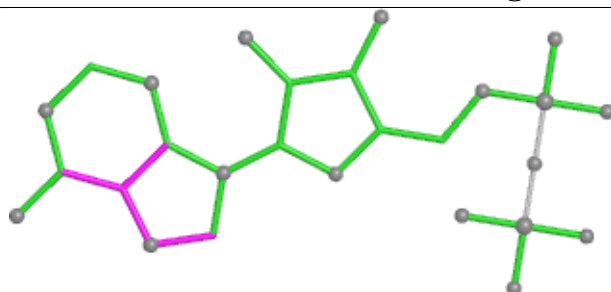


Torsions

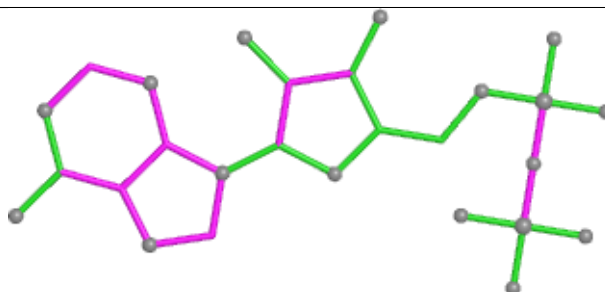


Rings

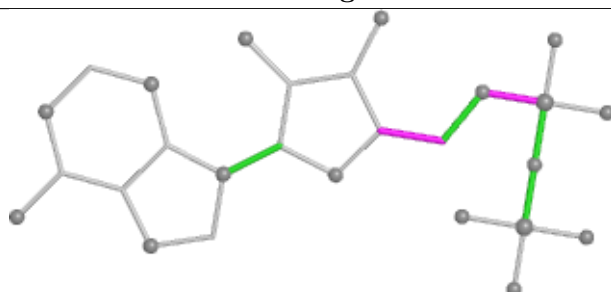
Ligand ADP b8 301



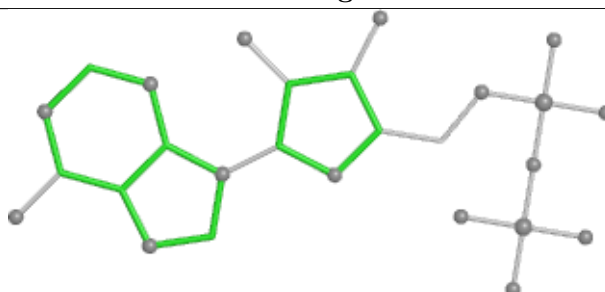
Bond lengths



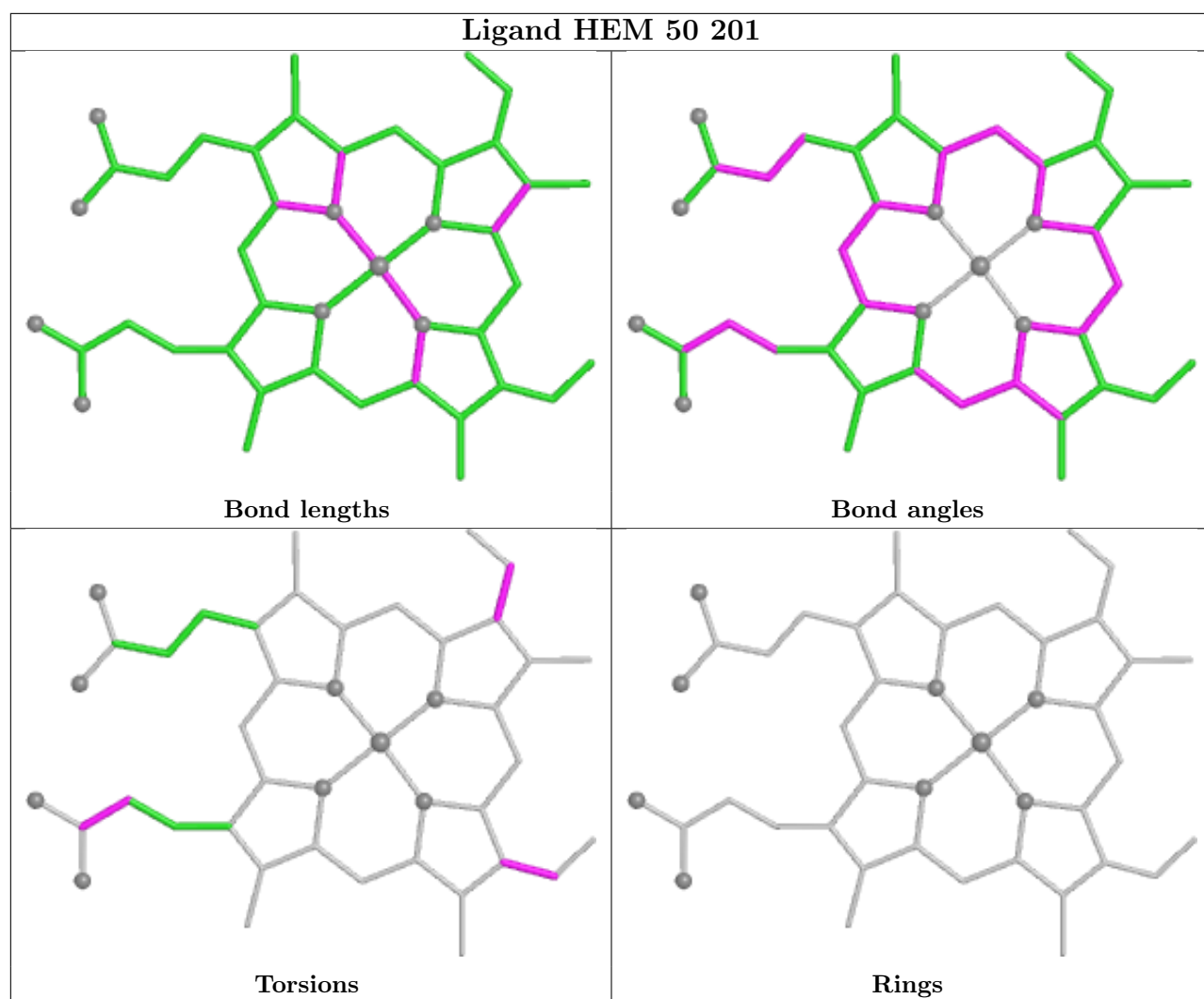
Bond angles

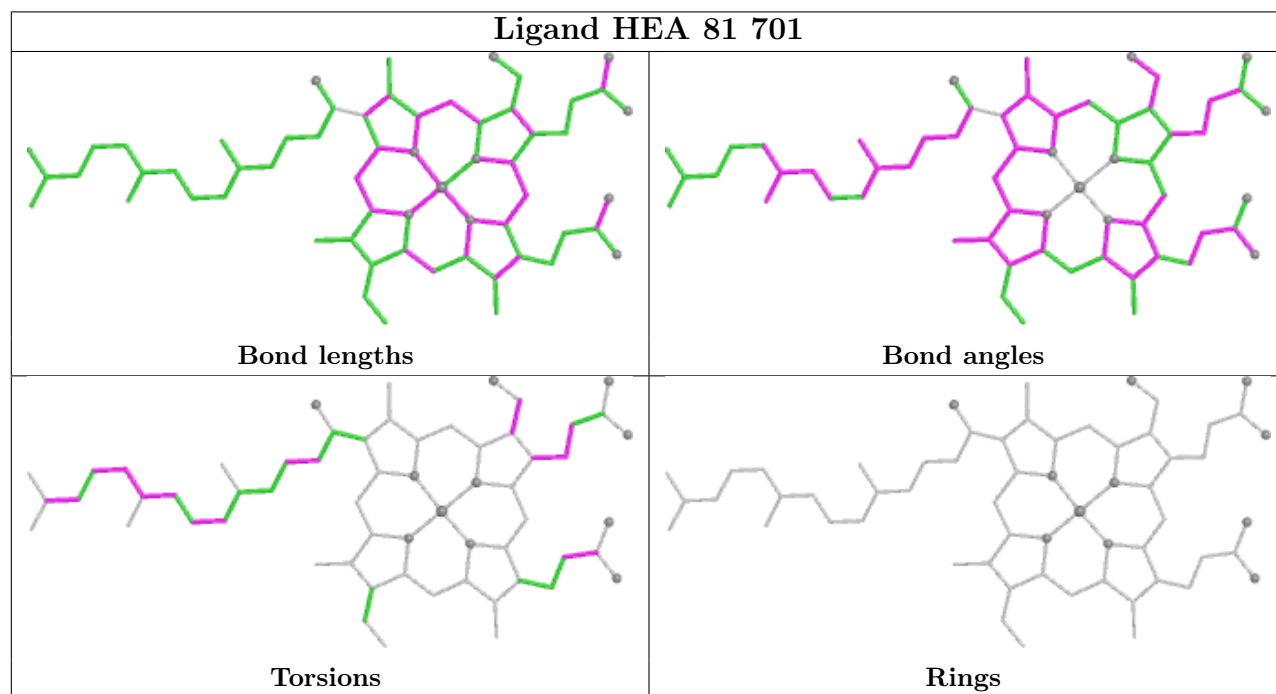
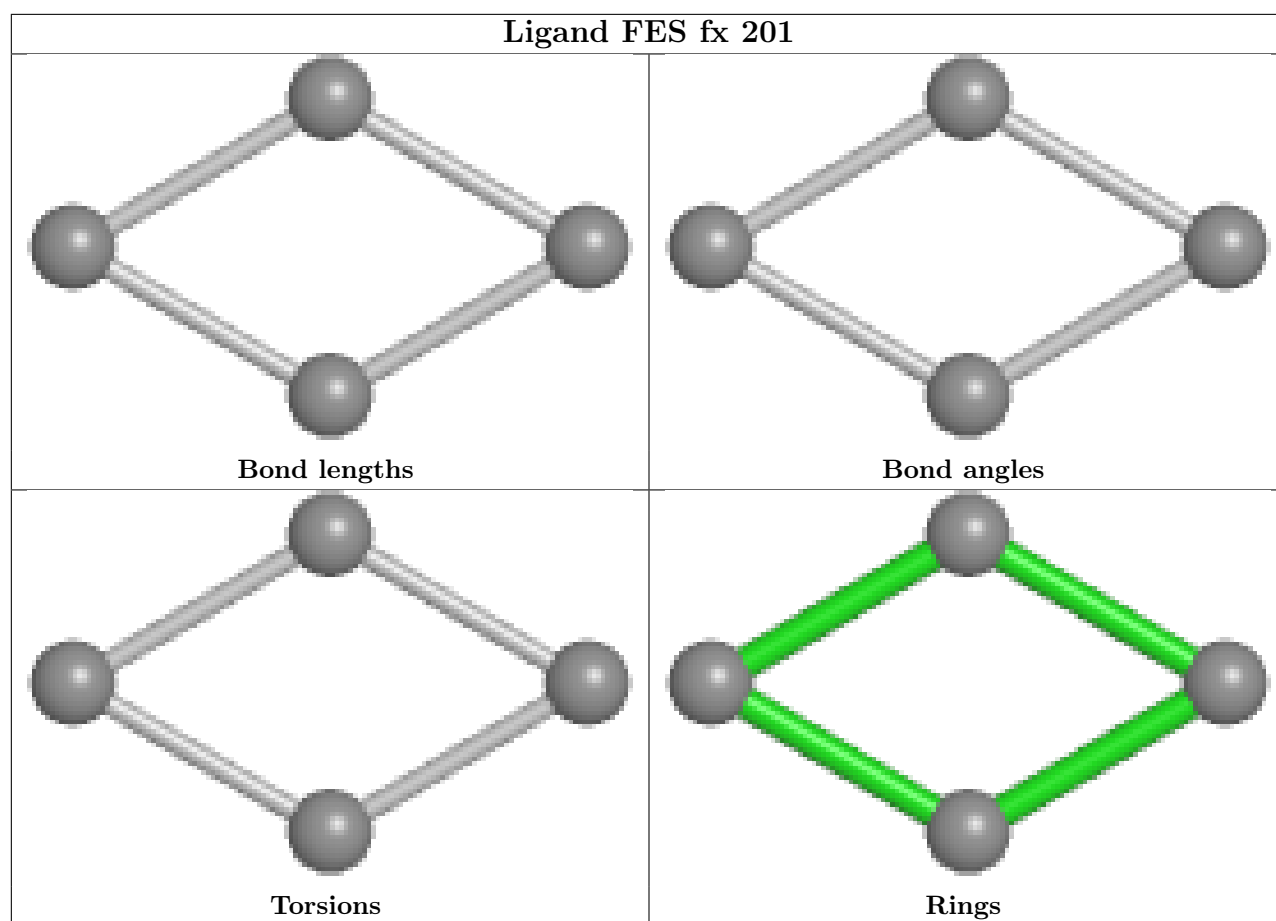


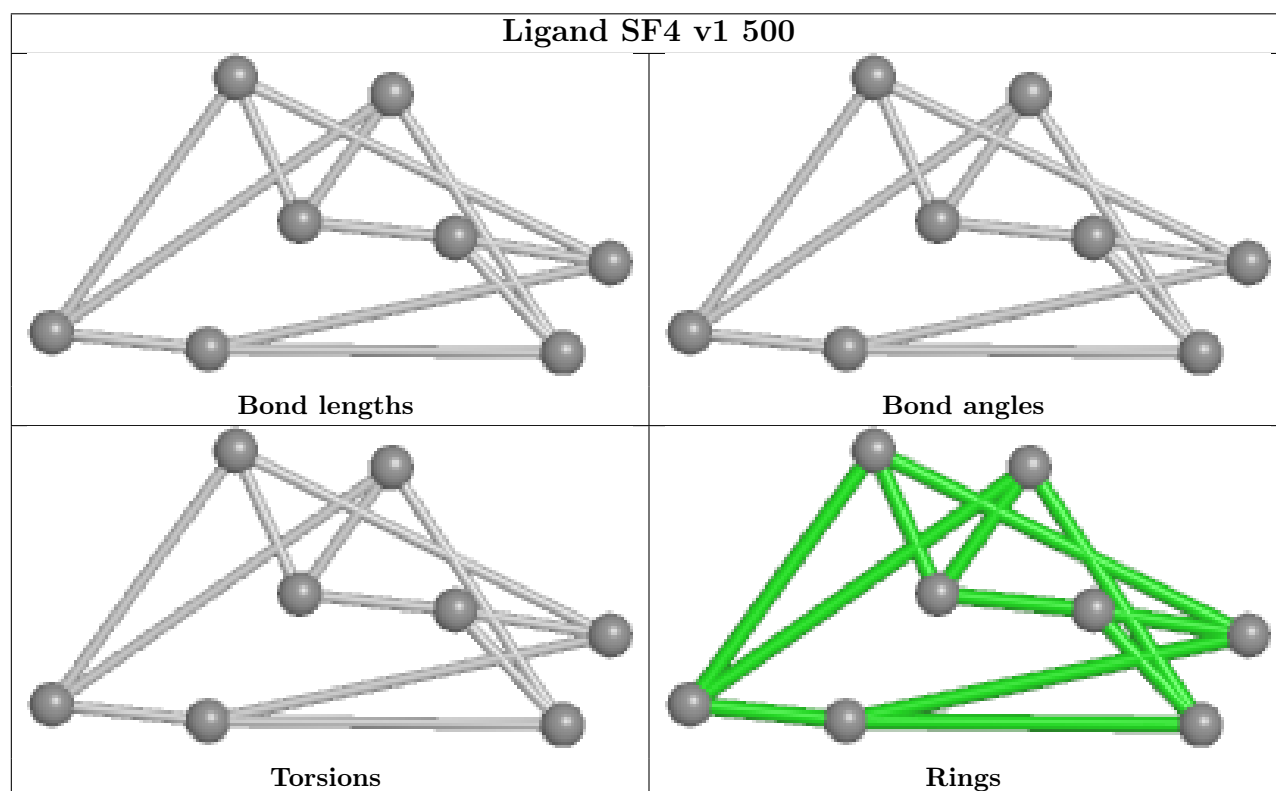
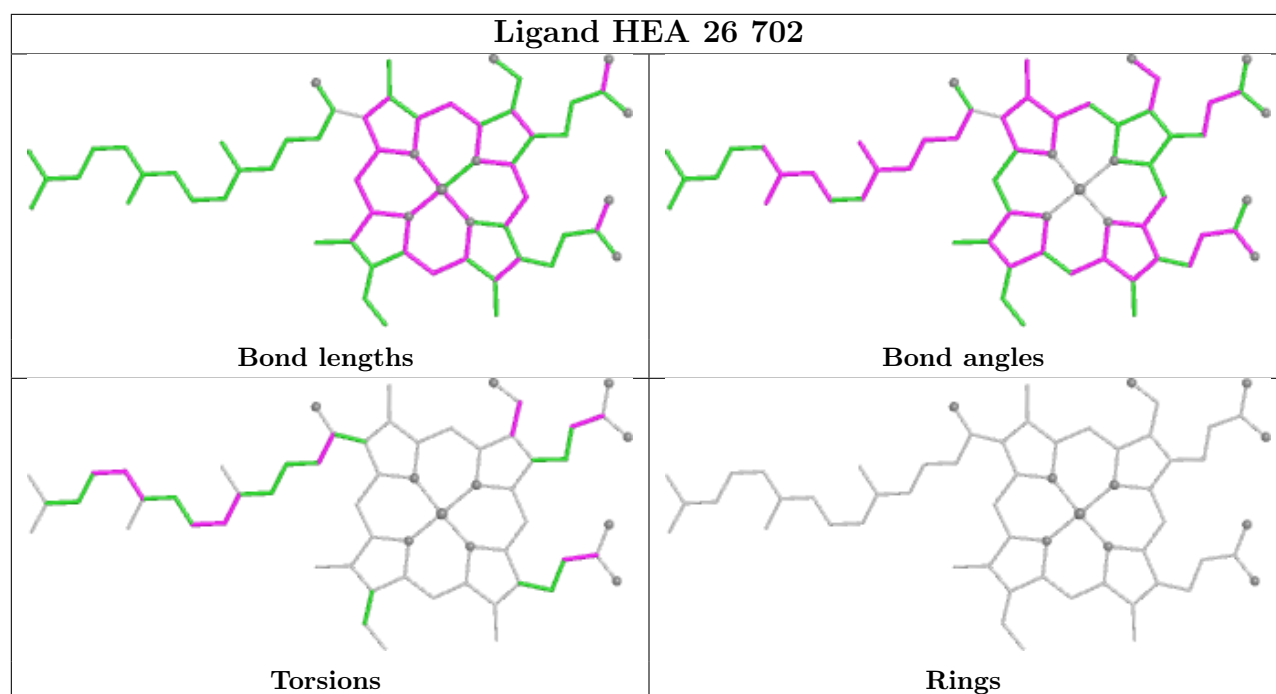
Torsions

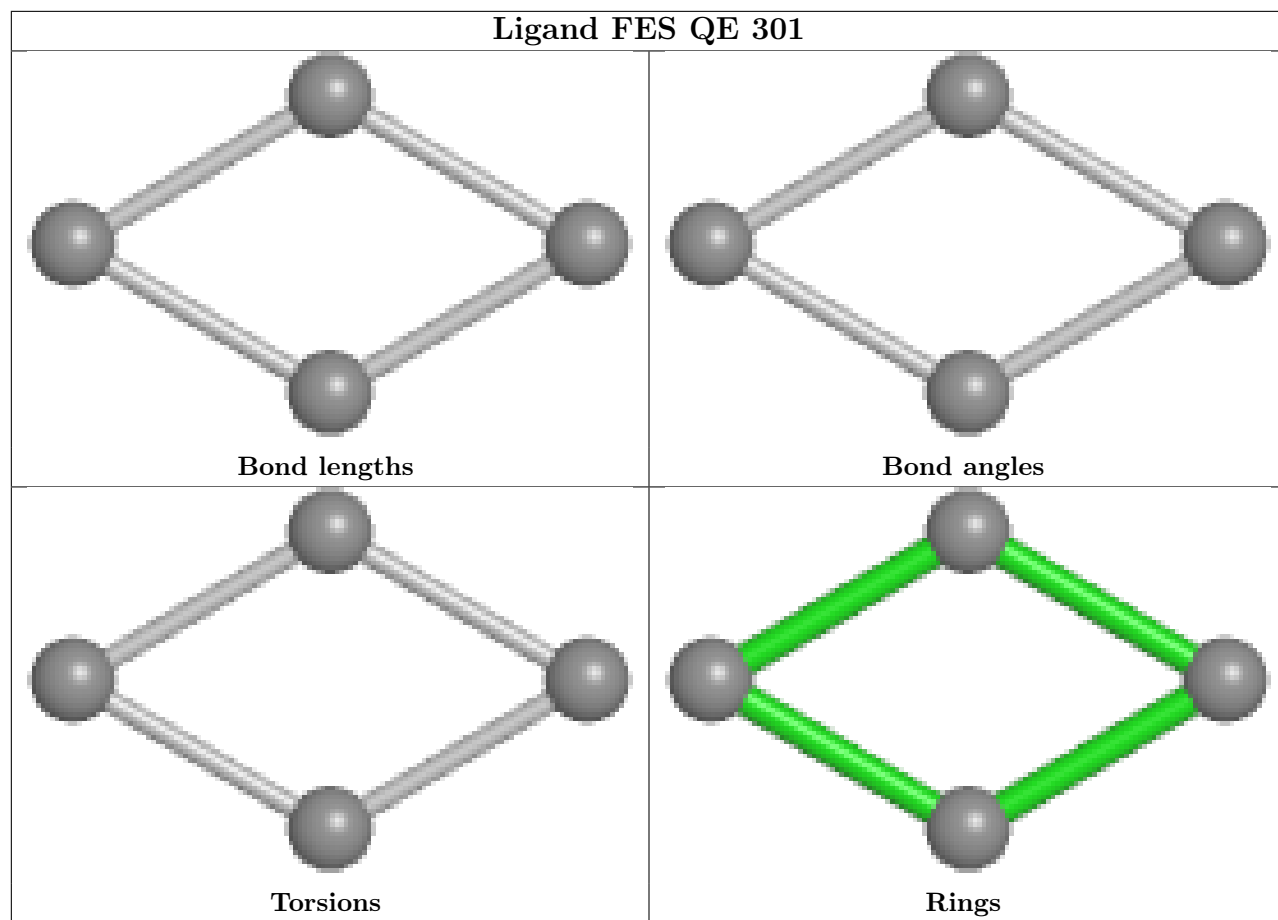


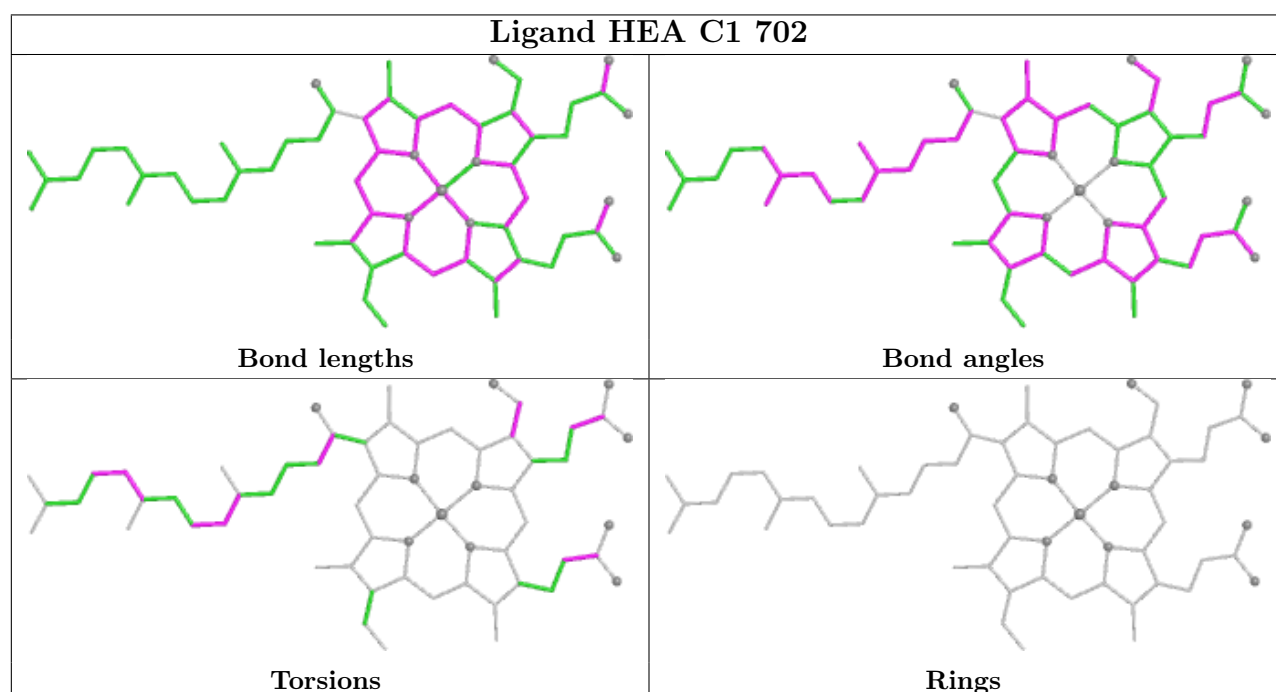
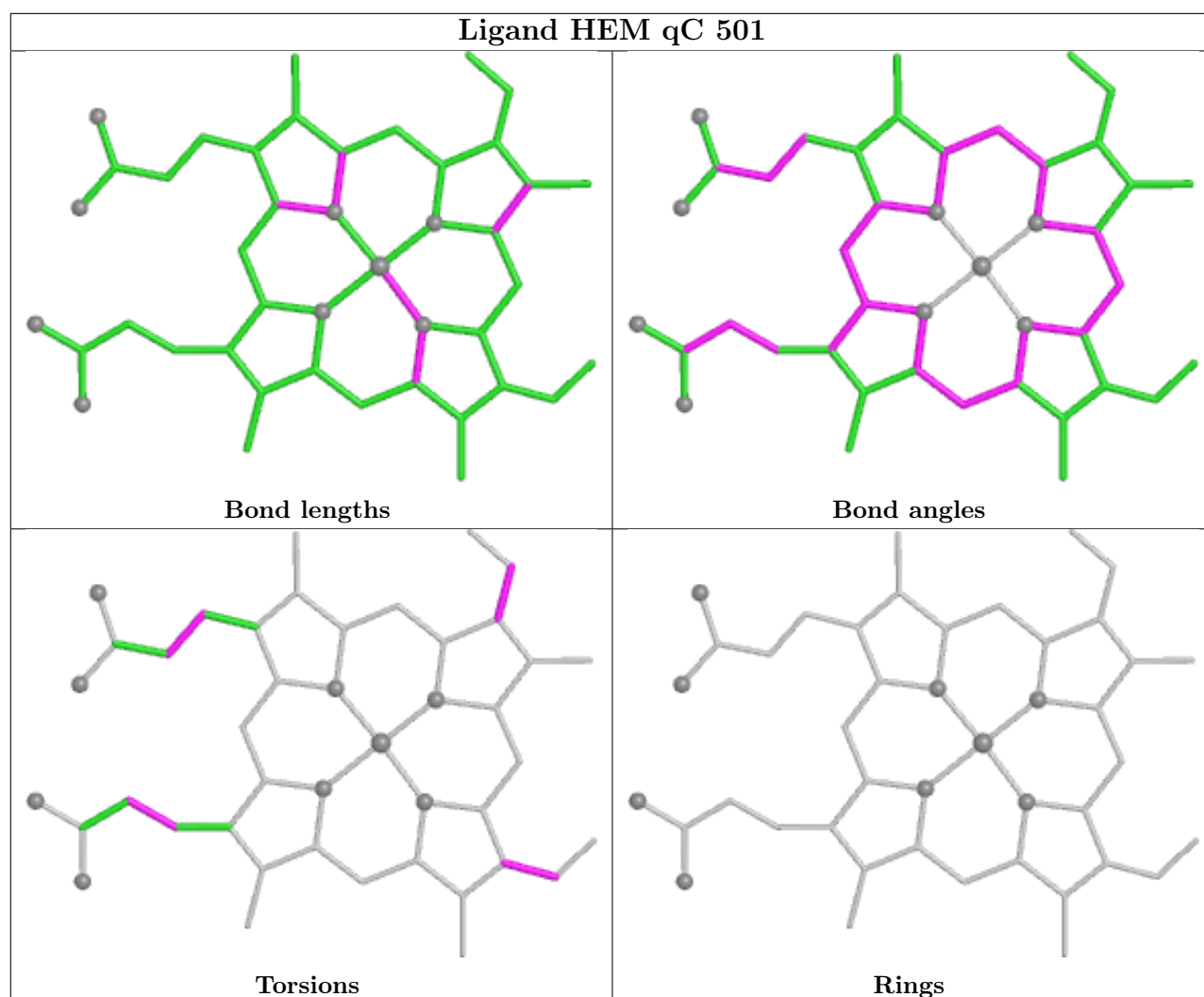
Rings

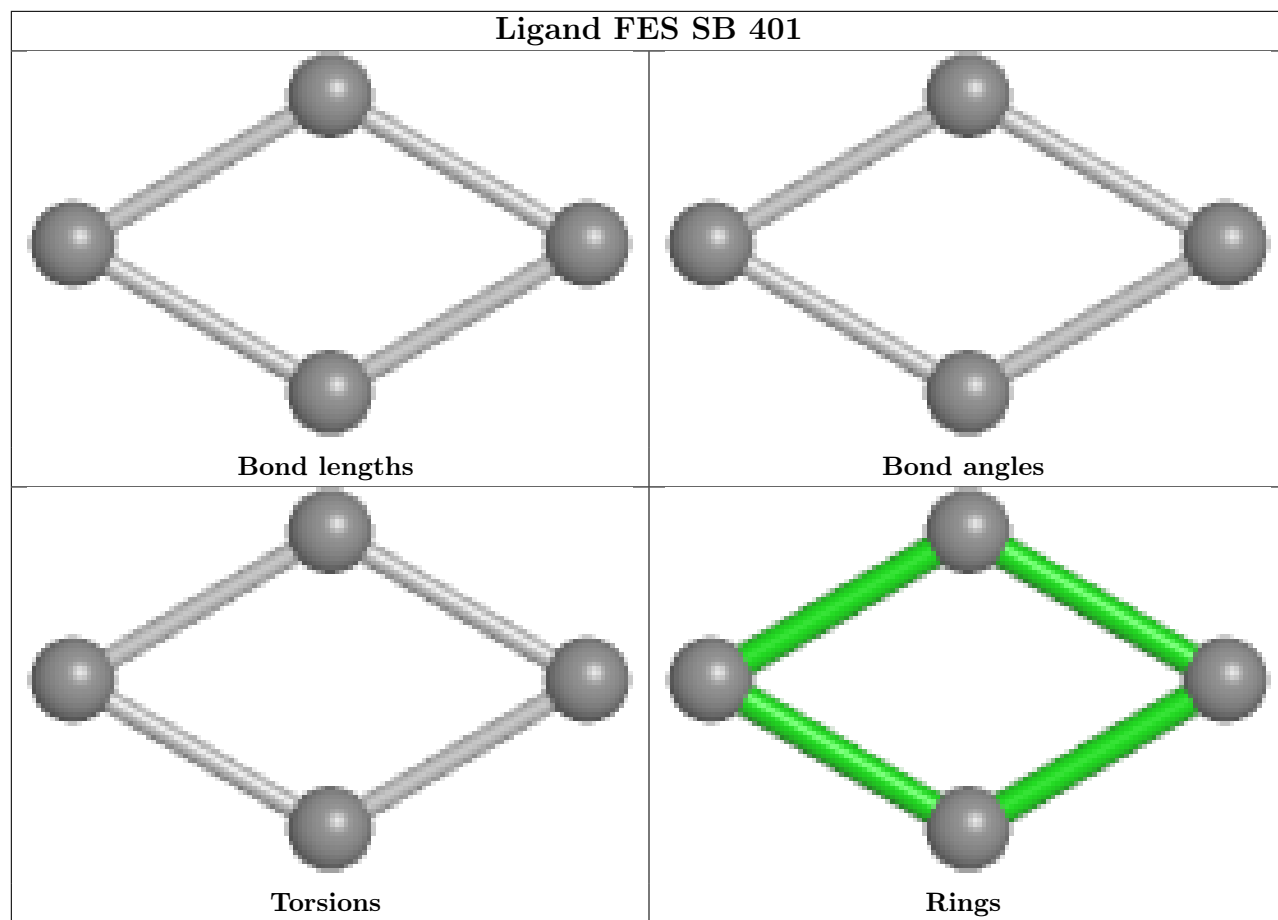


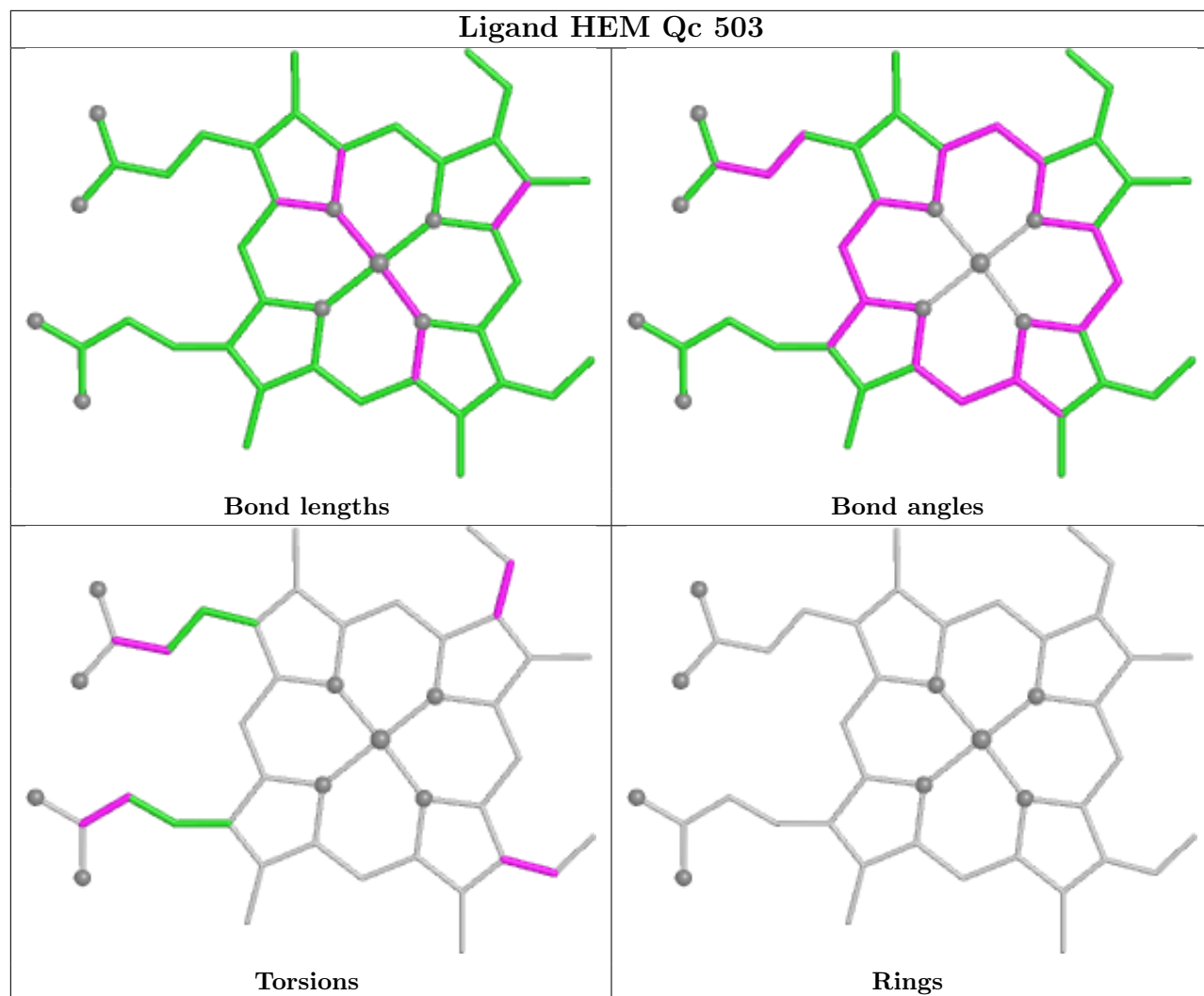


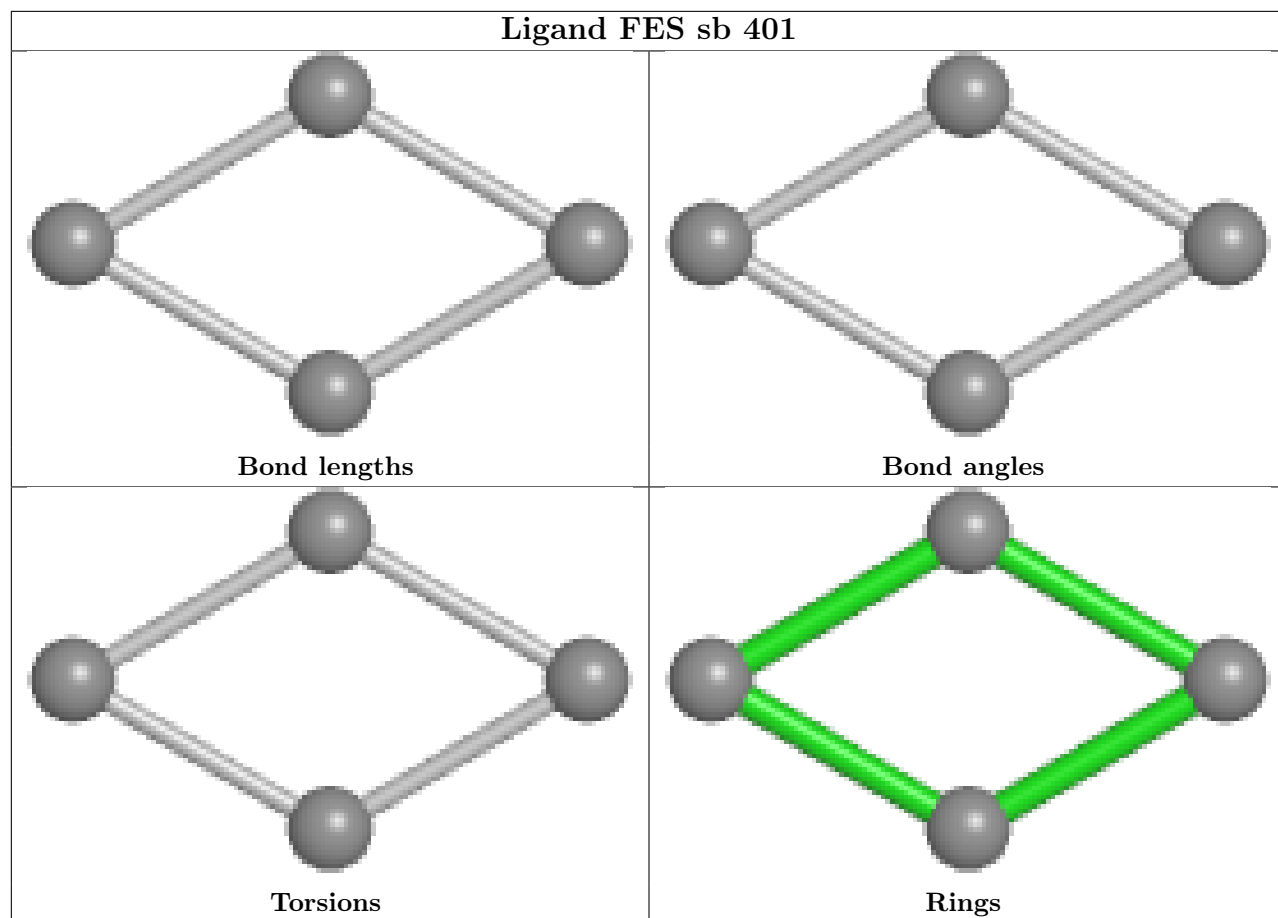




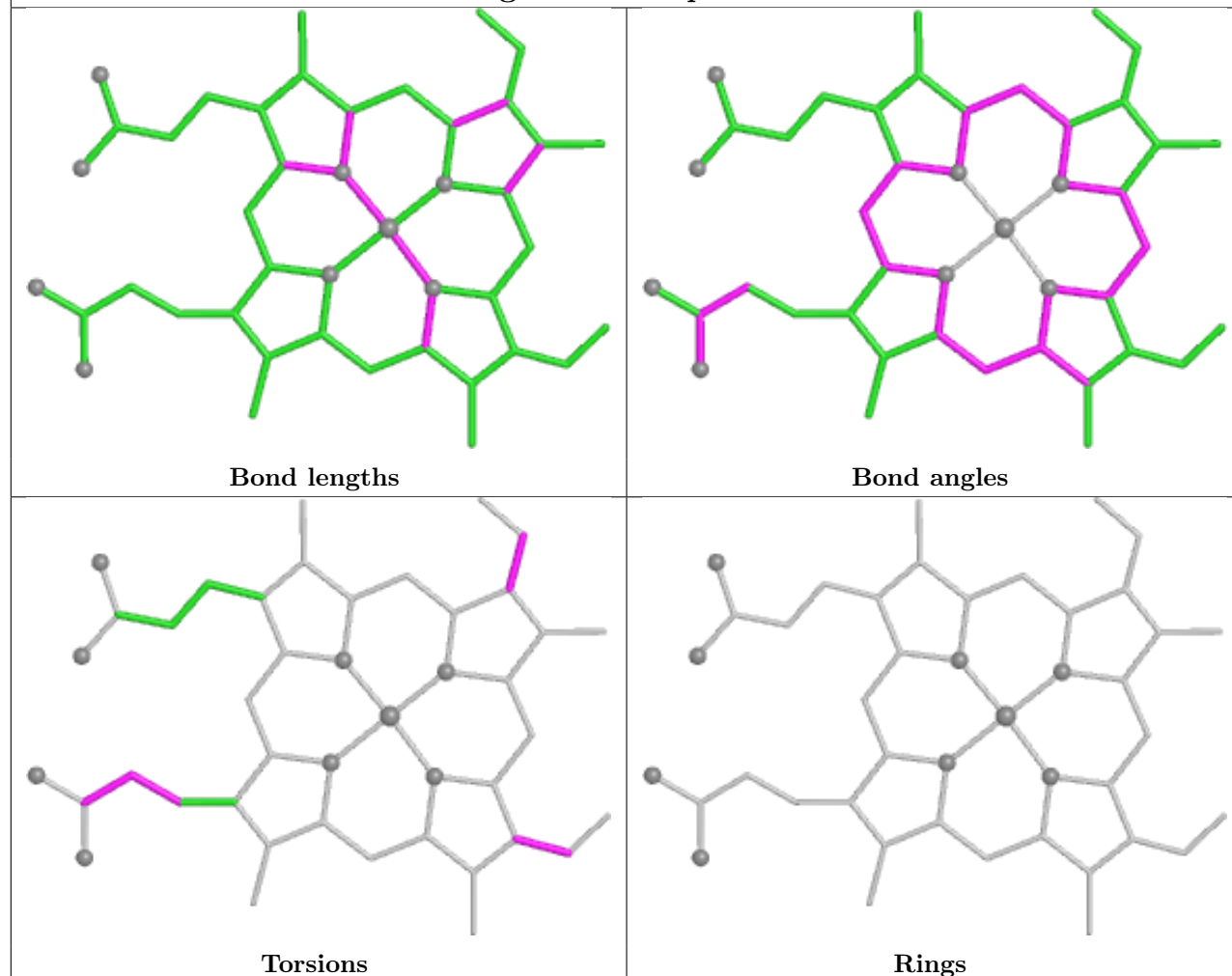




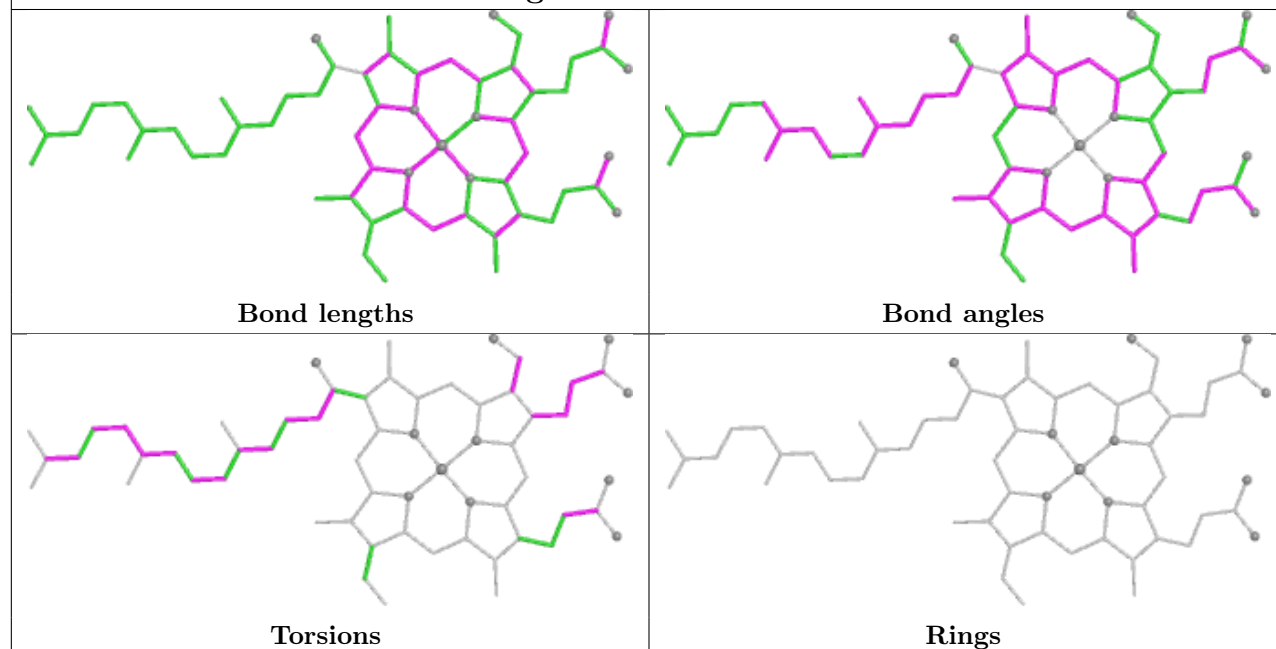


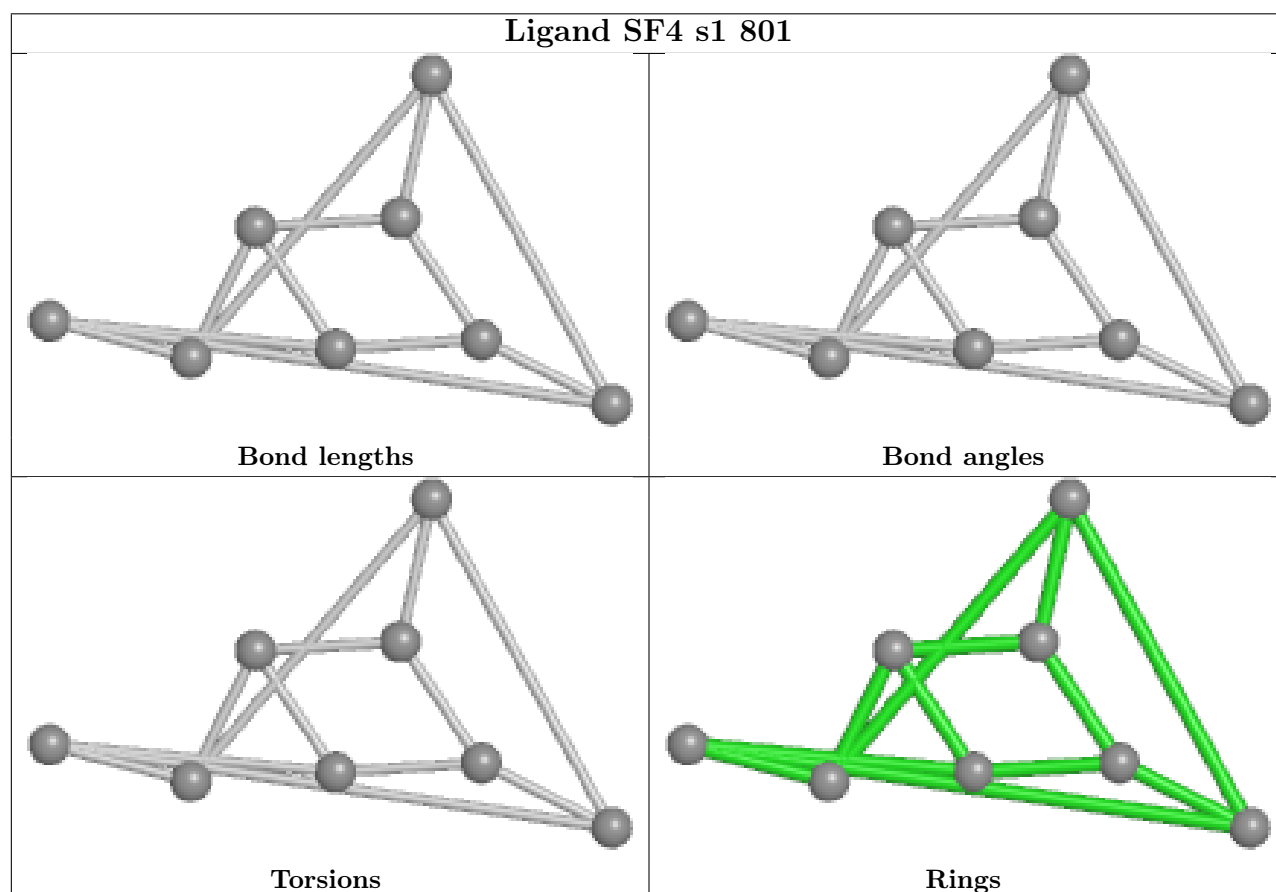
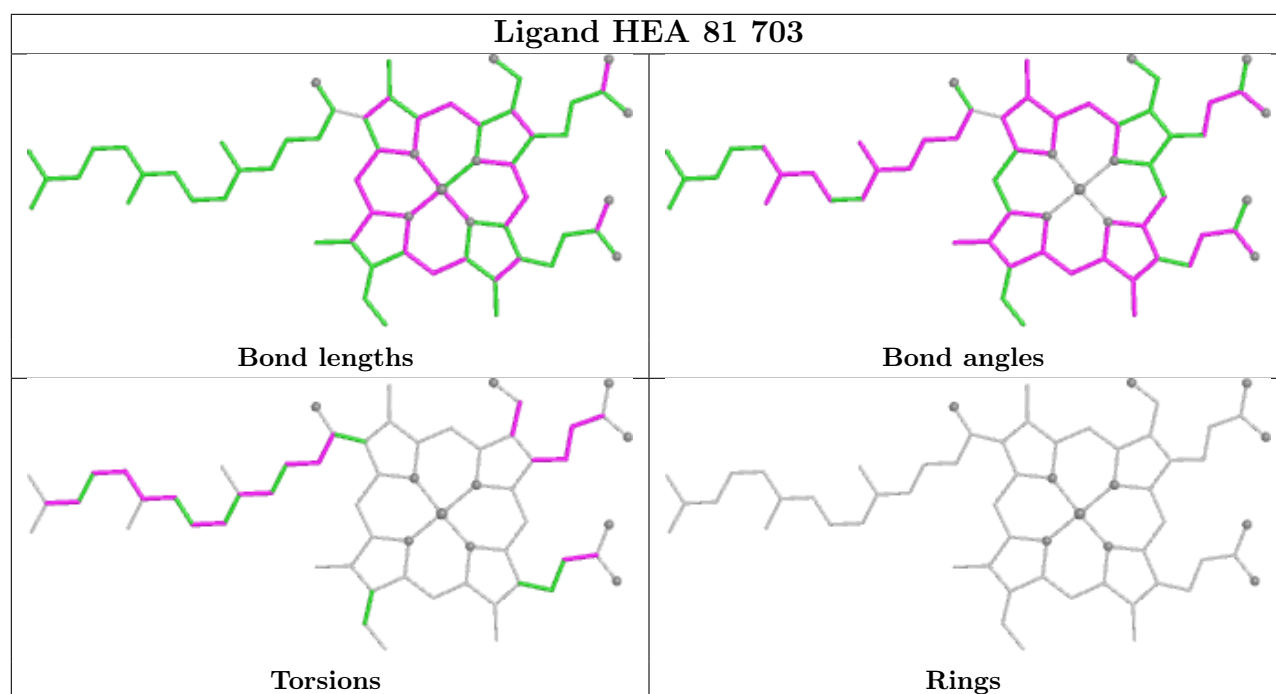


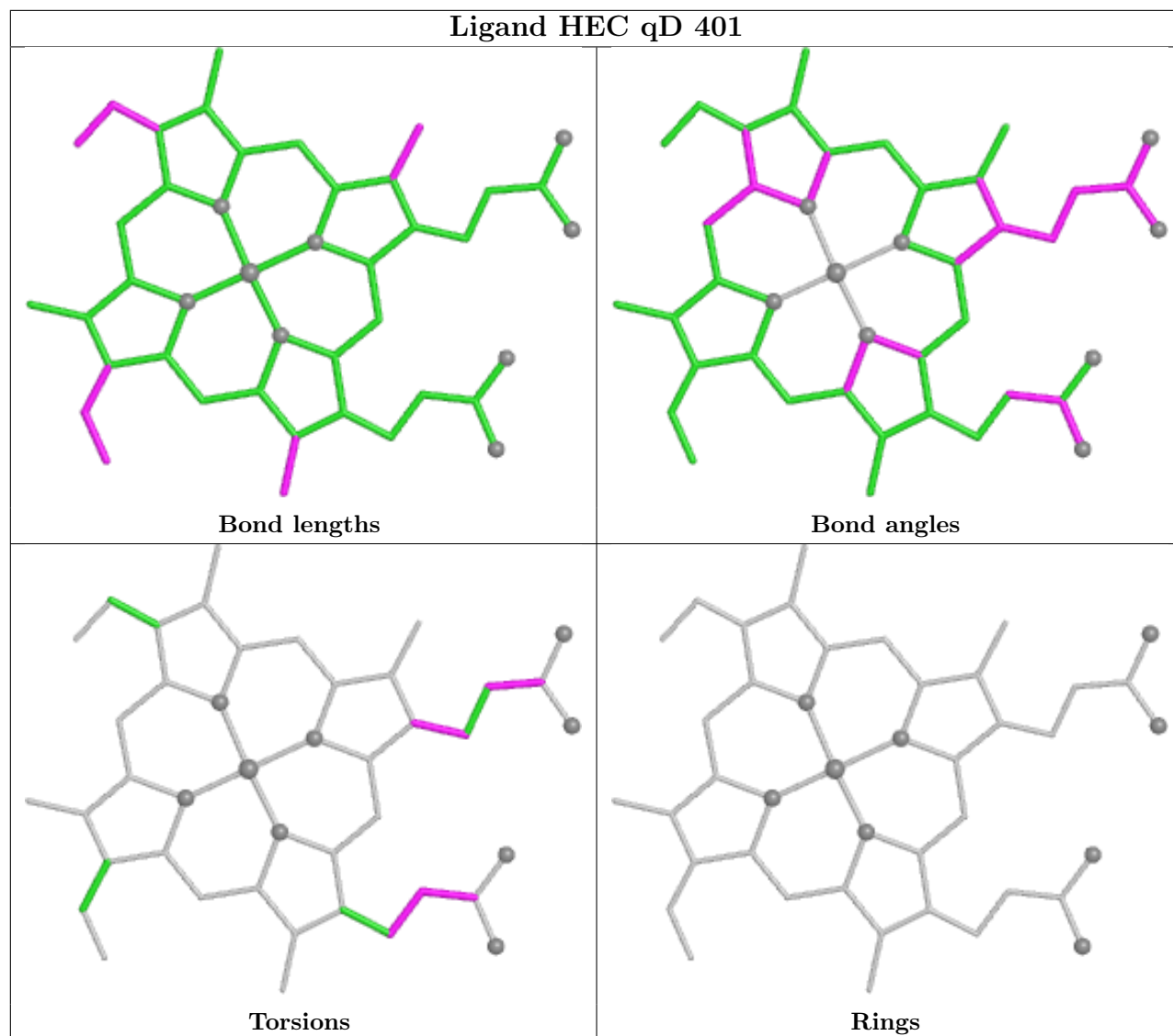
Ligand HEM qC 502

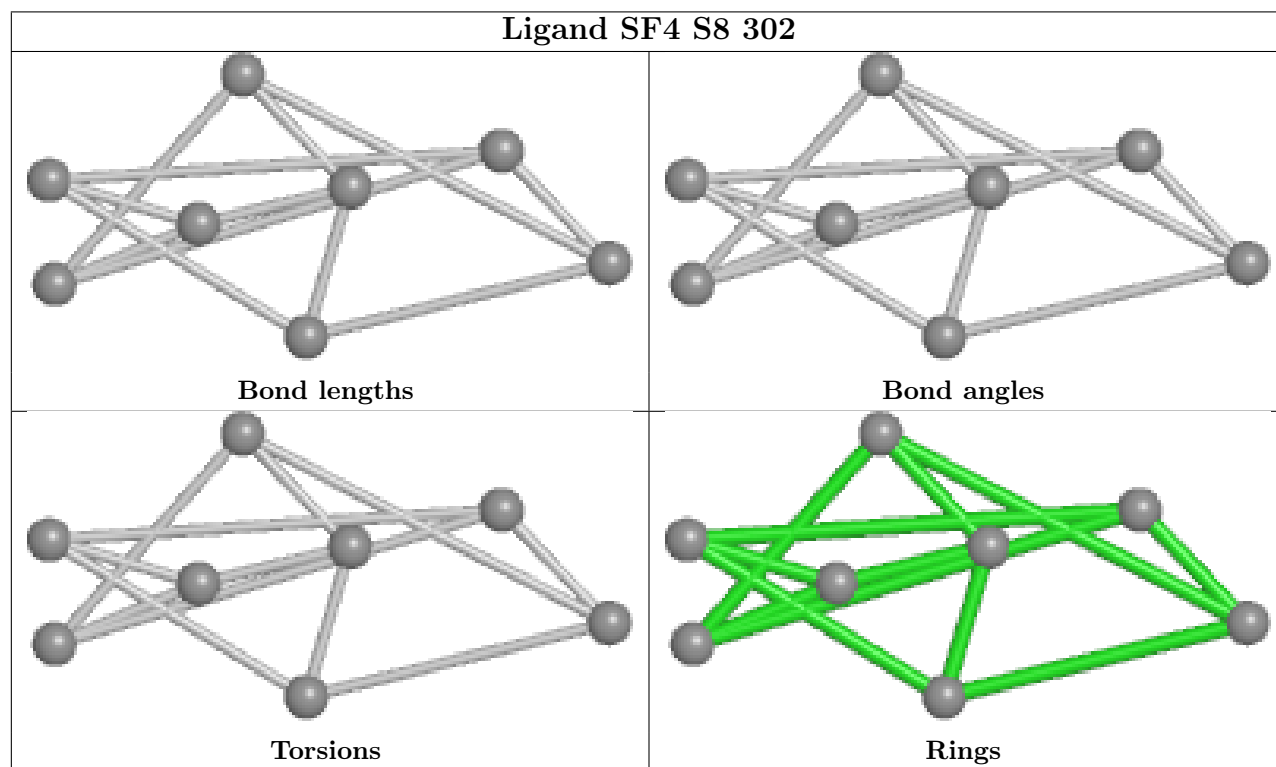
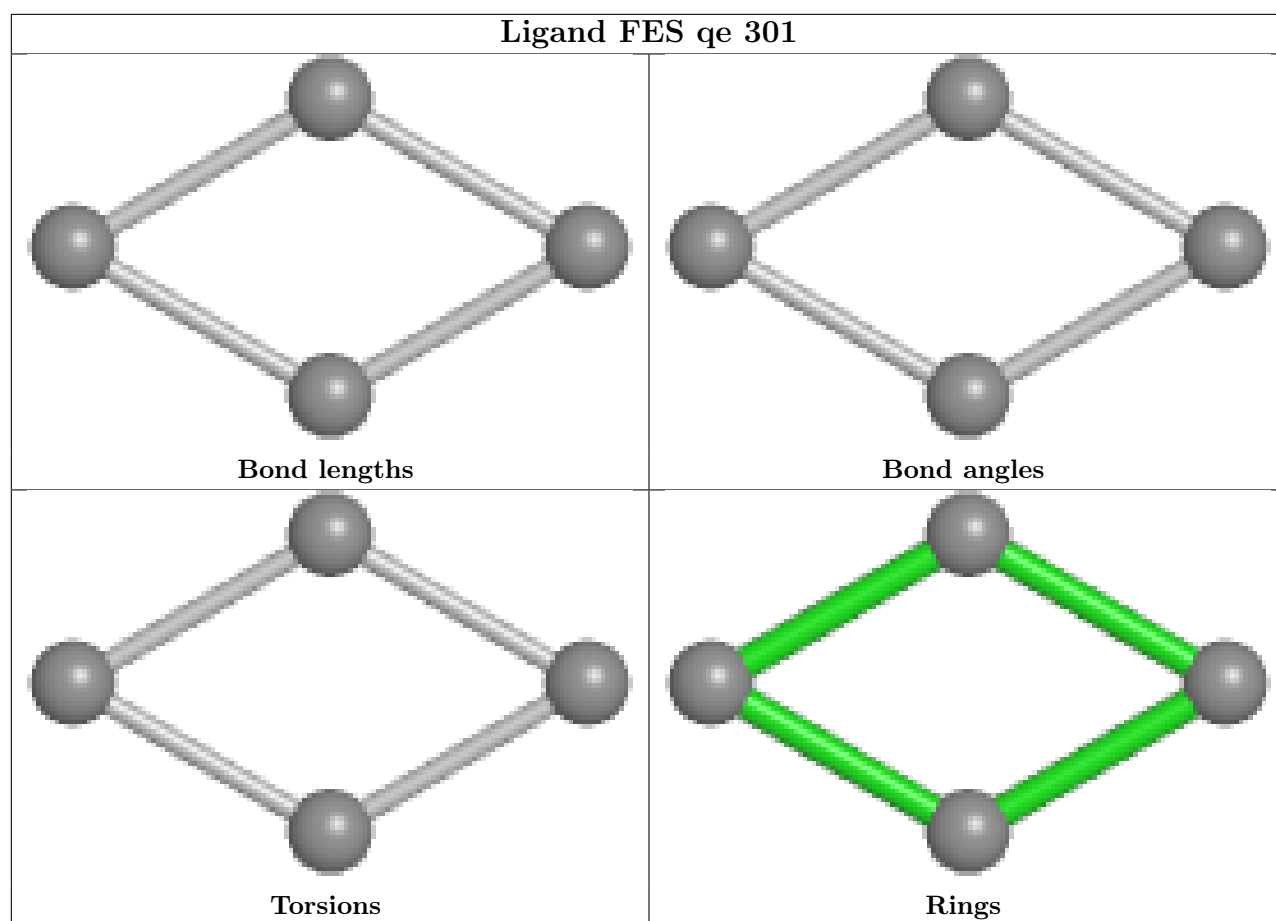


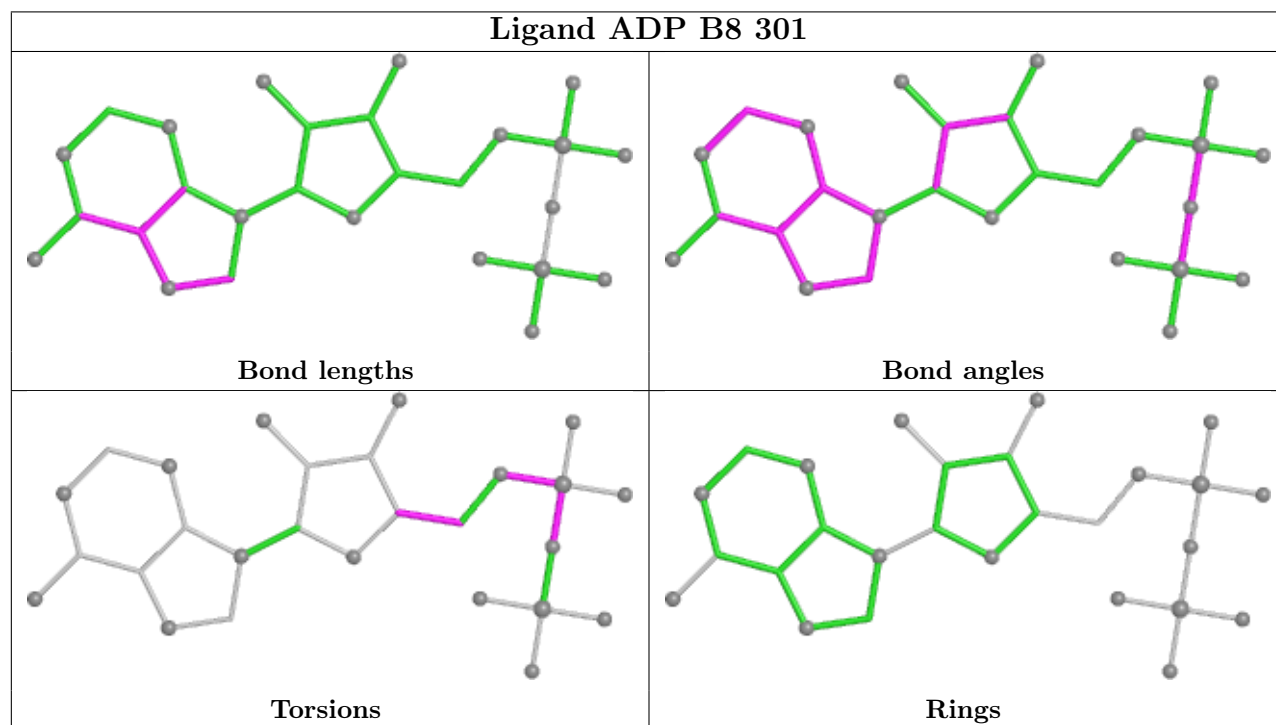
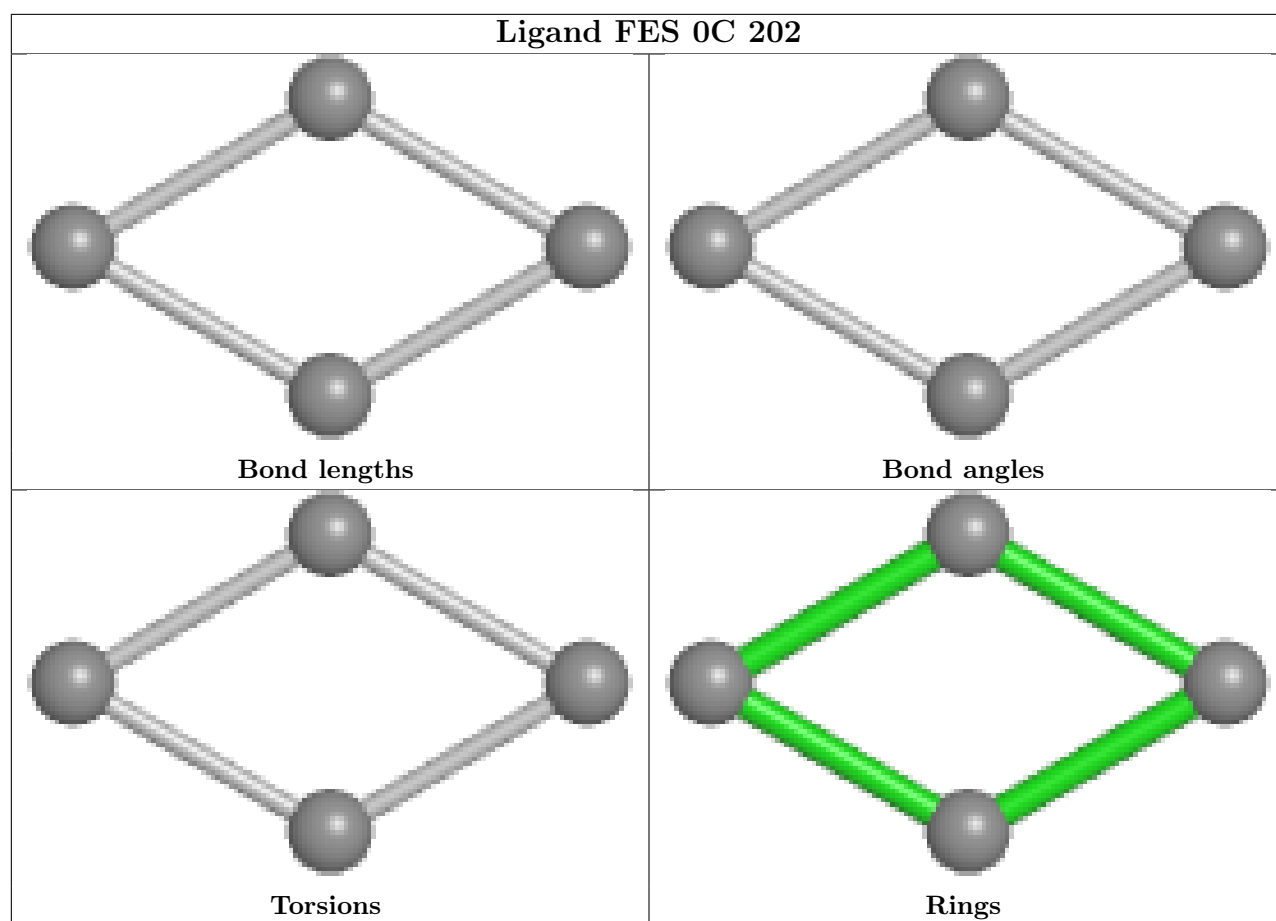
Ligand HEA c1 703

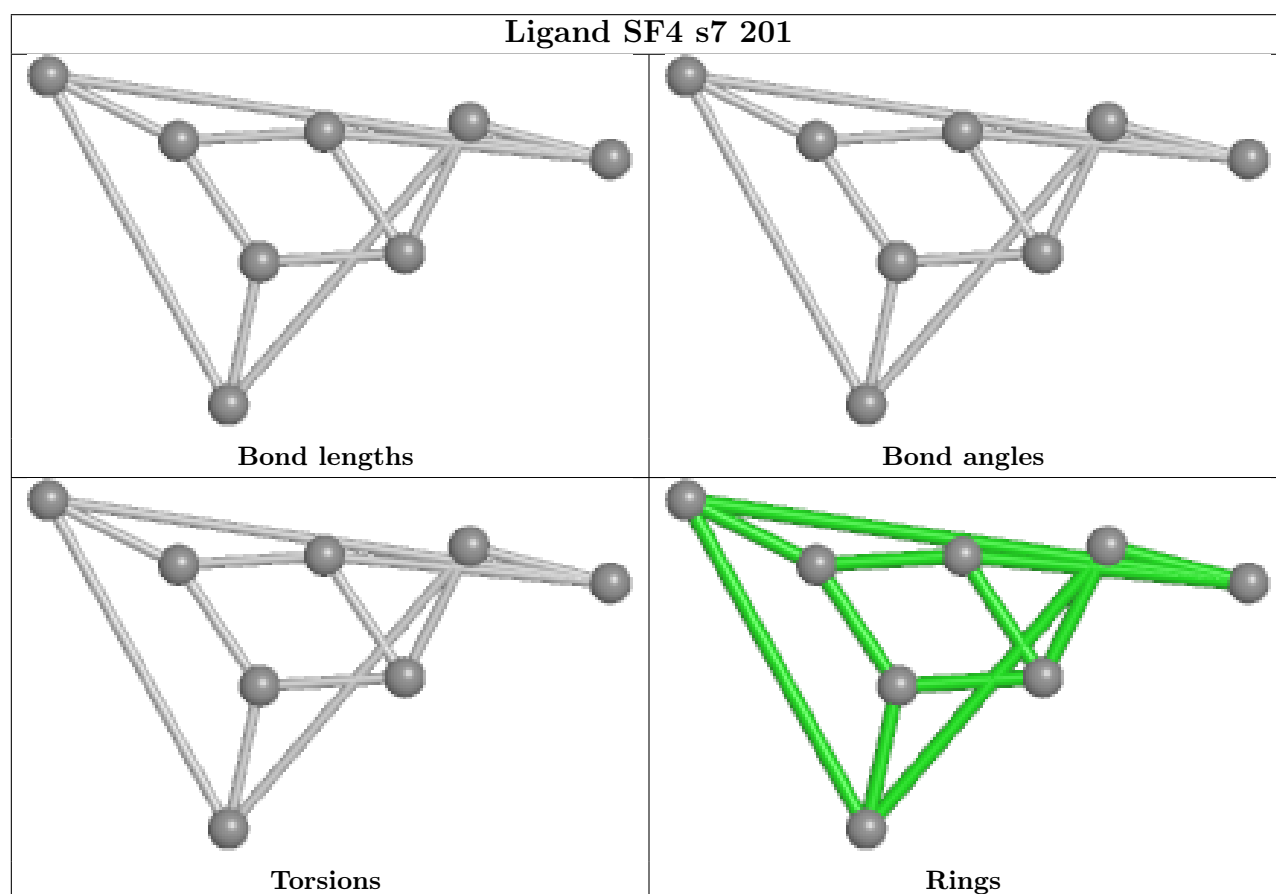
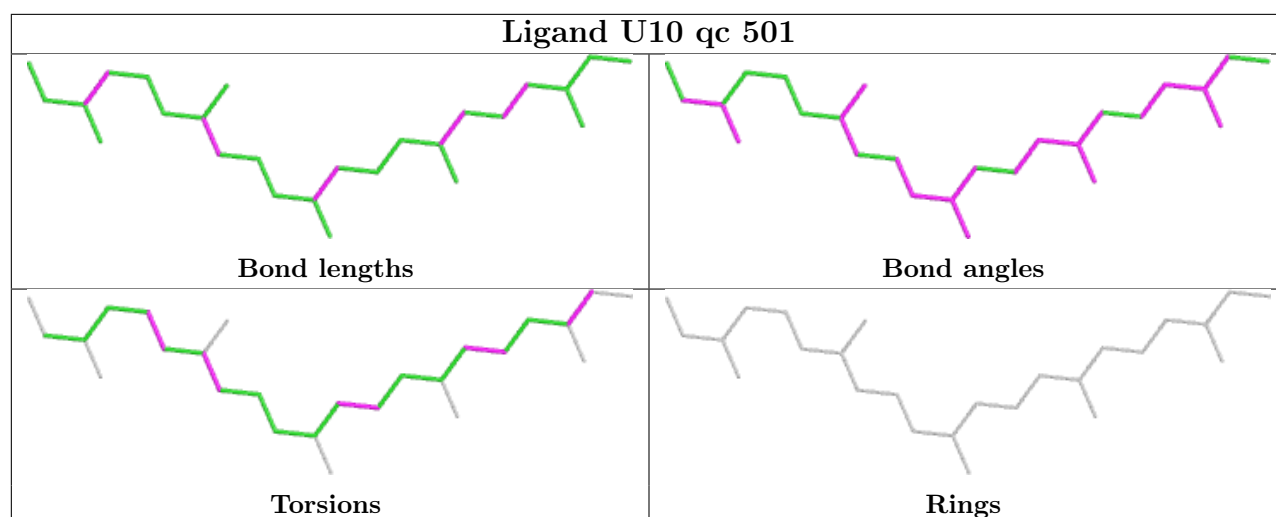


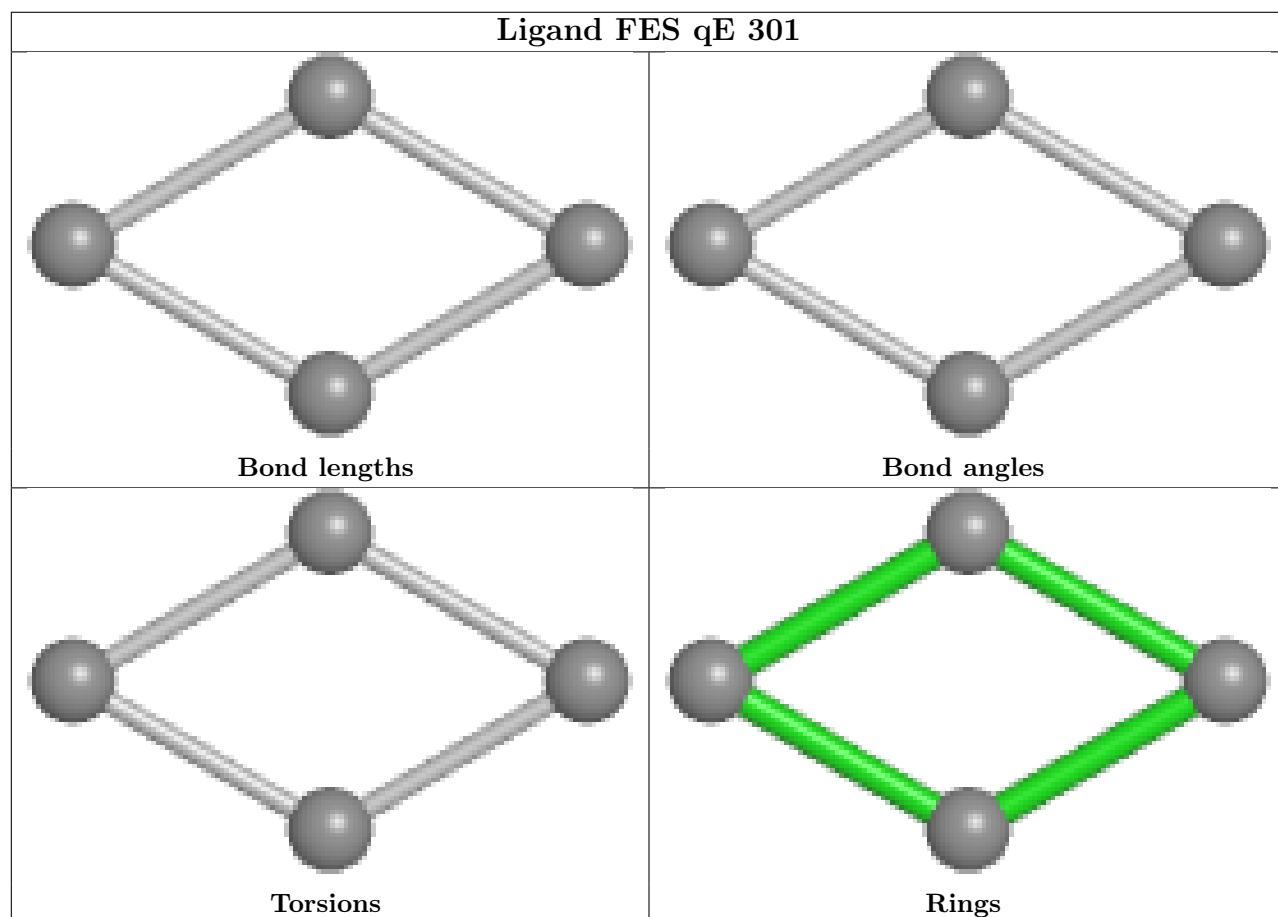
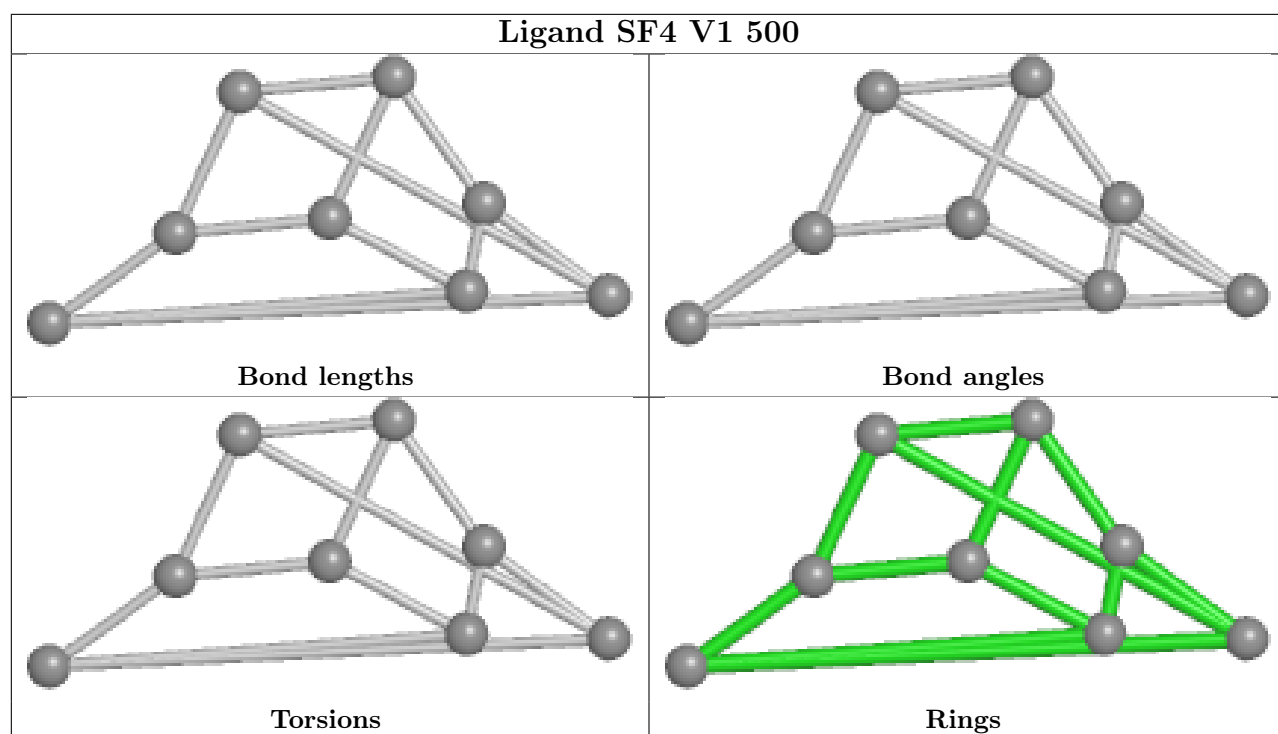


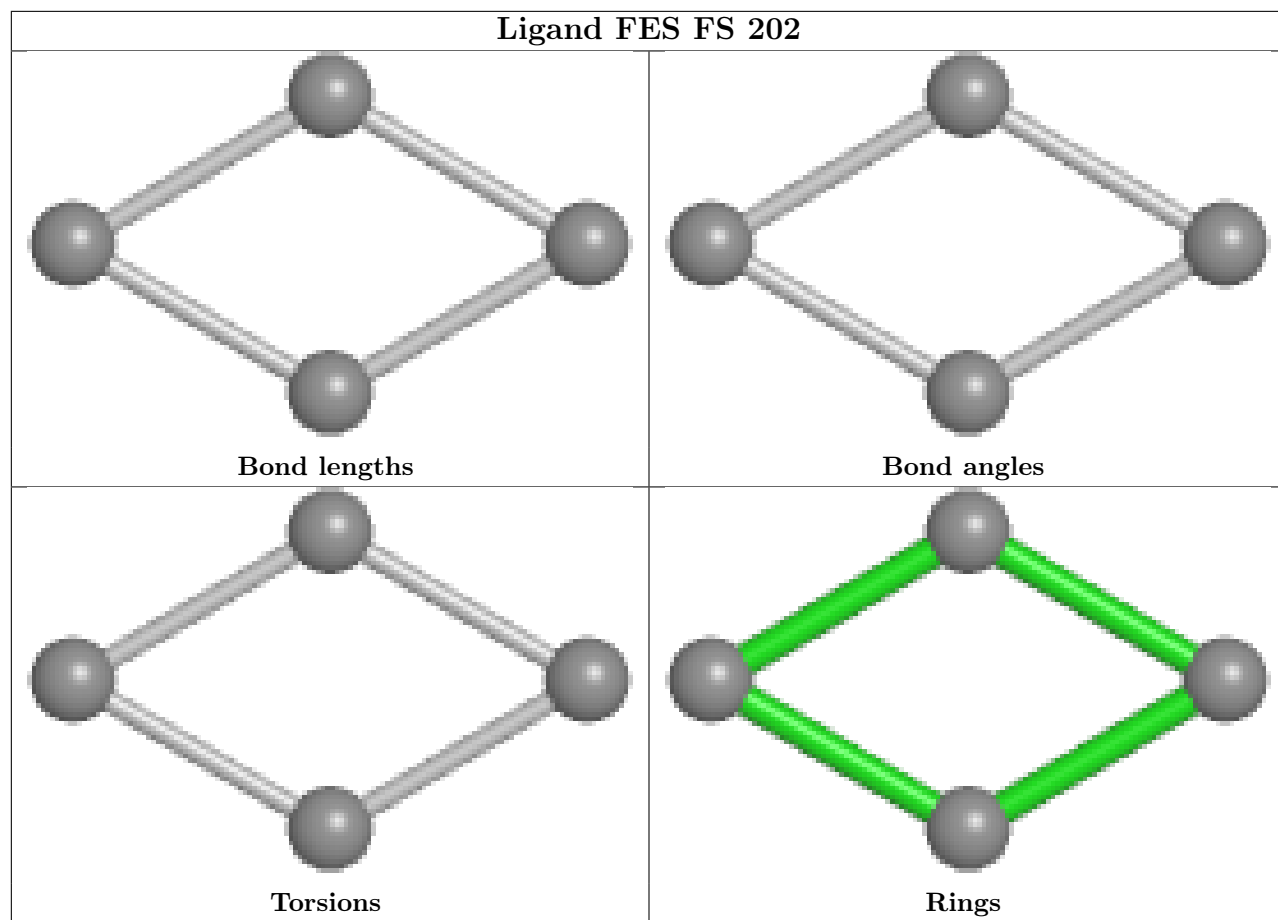


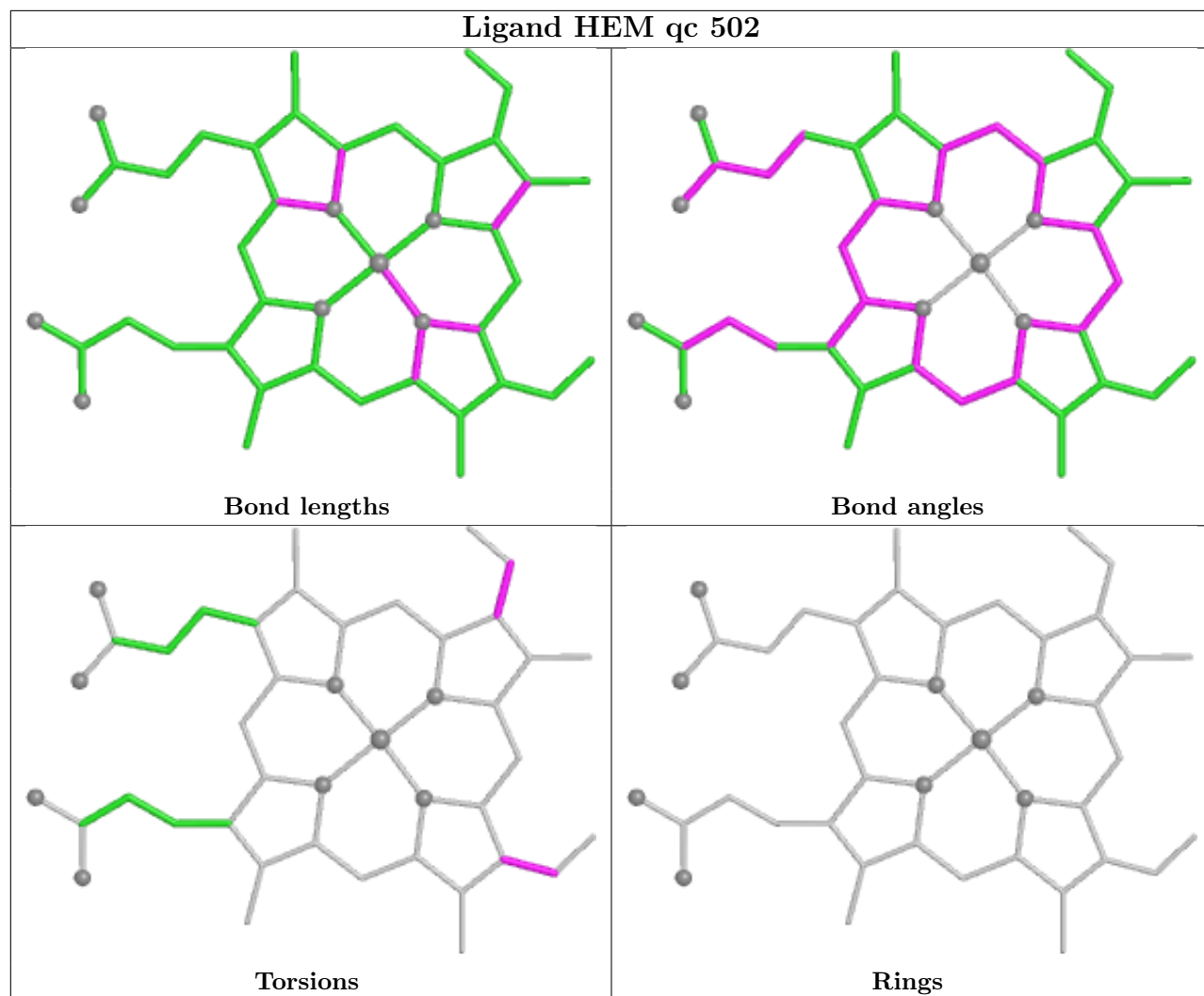


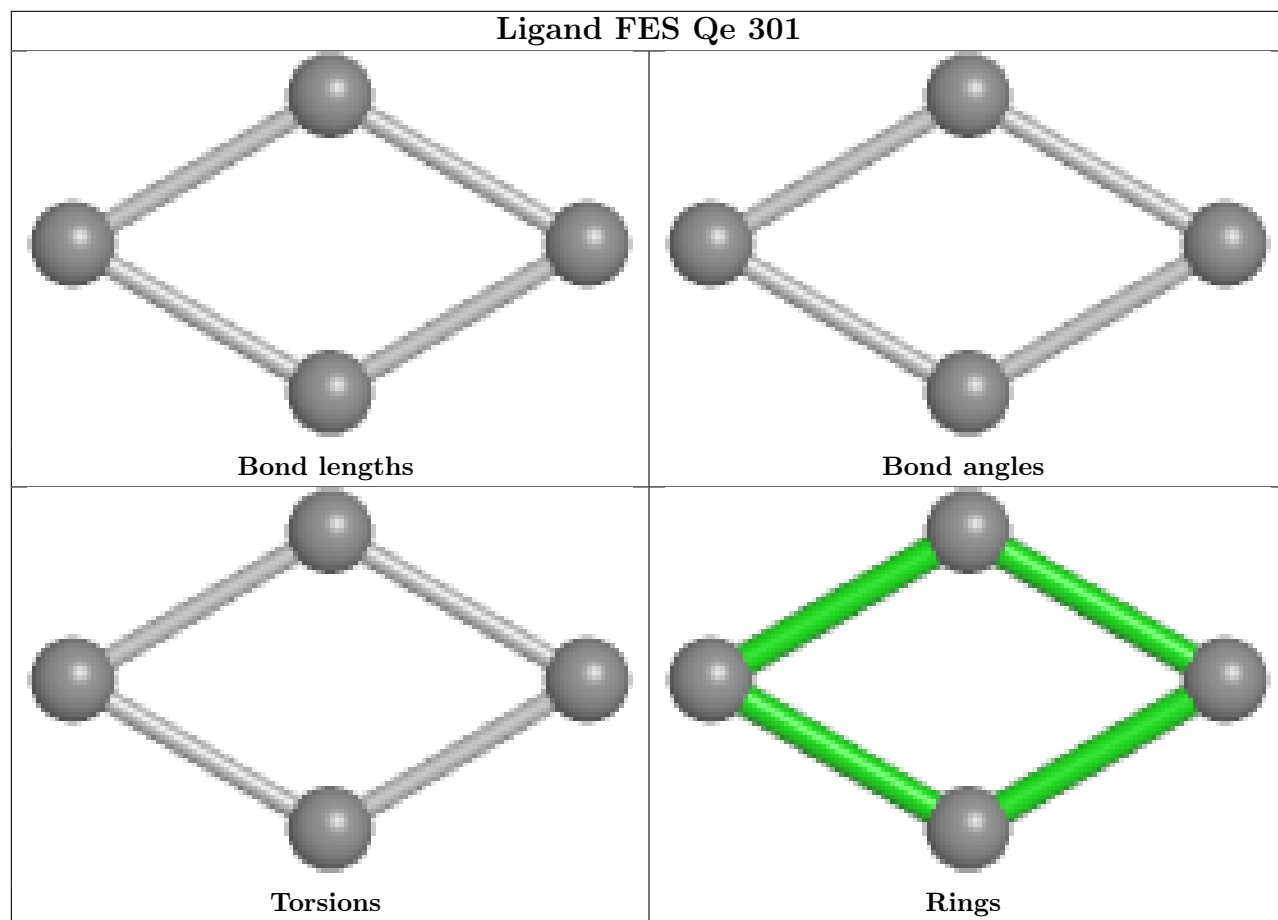




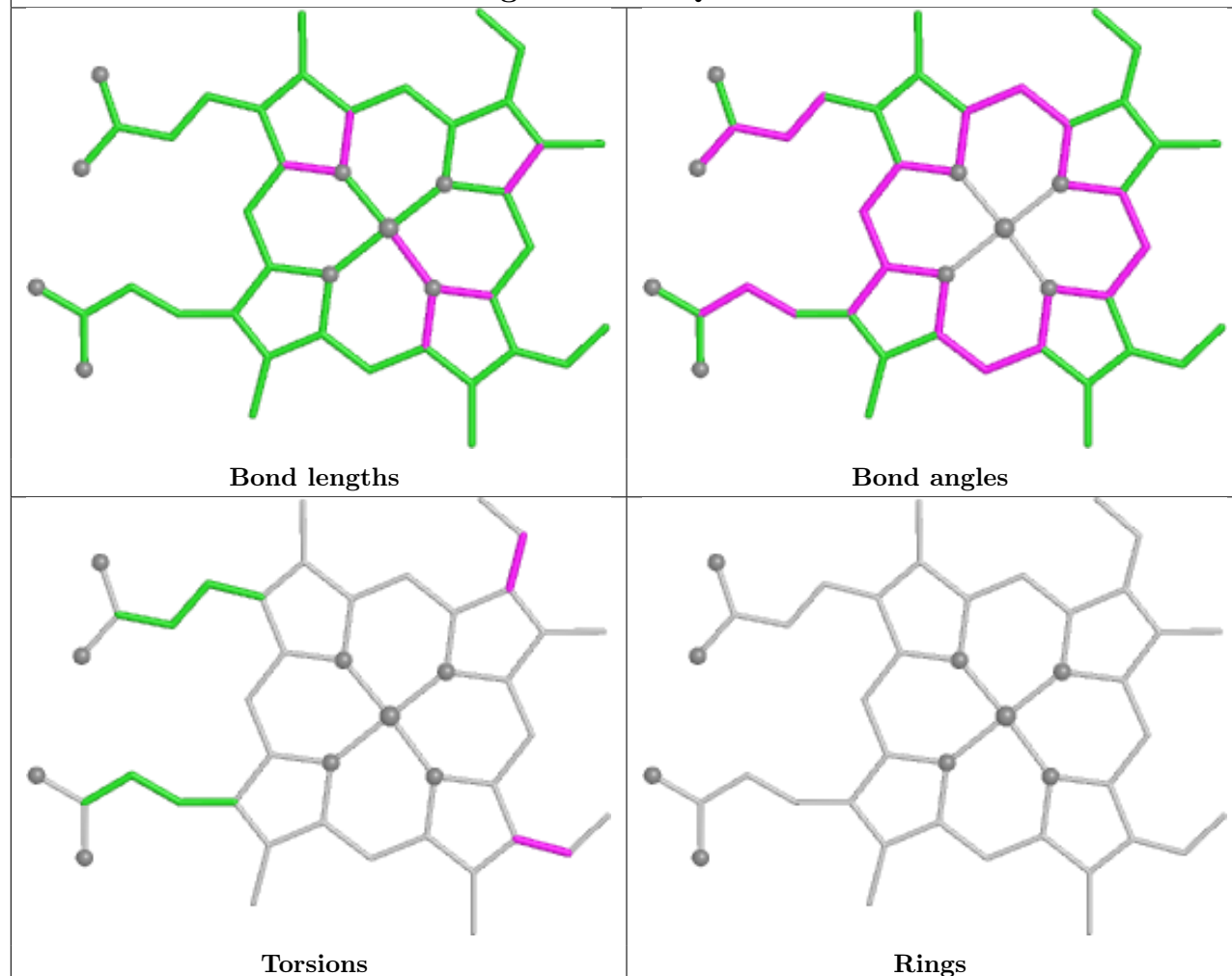




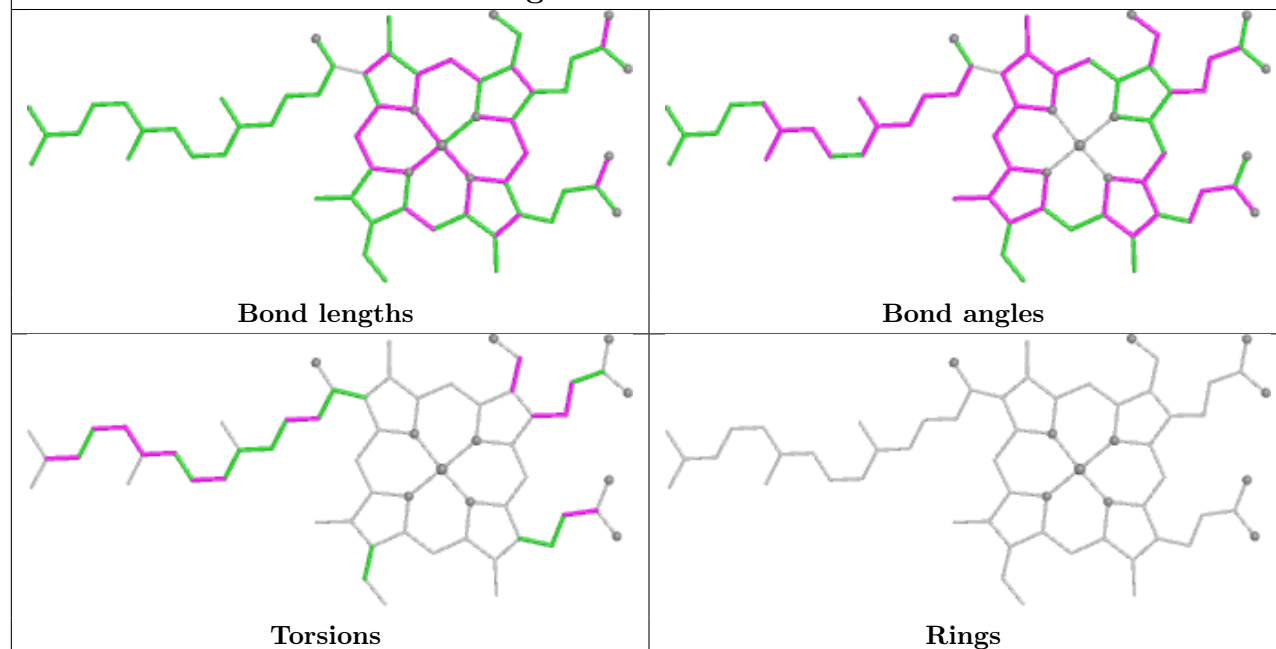


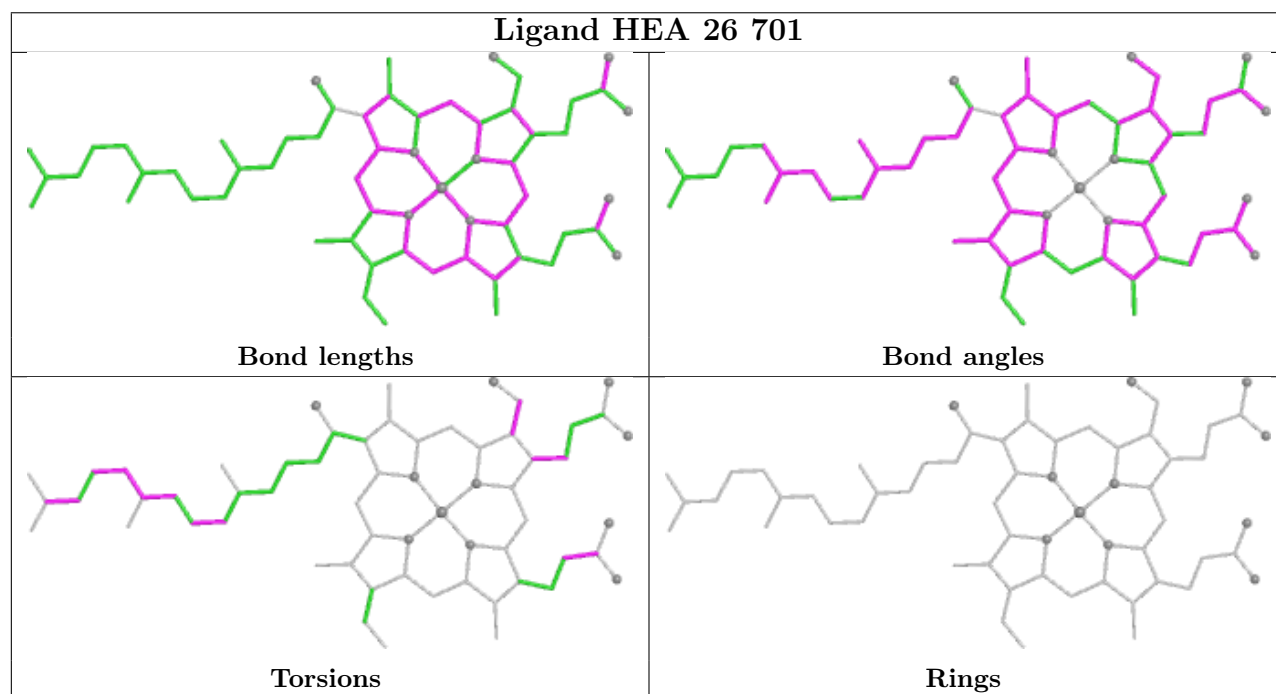
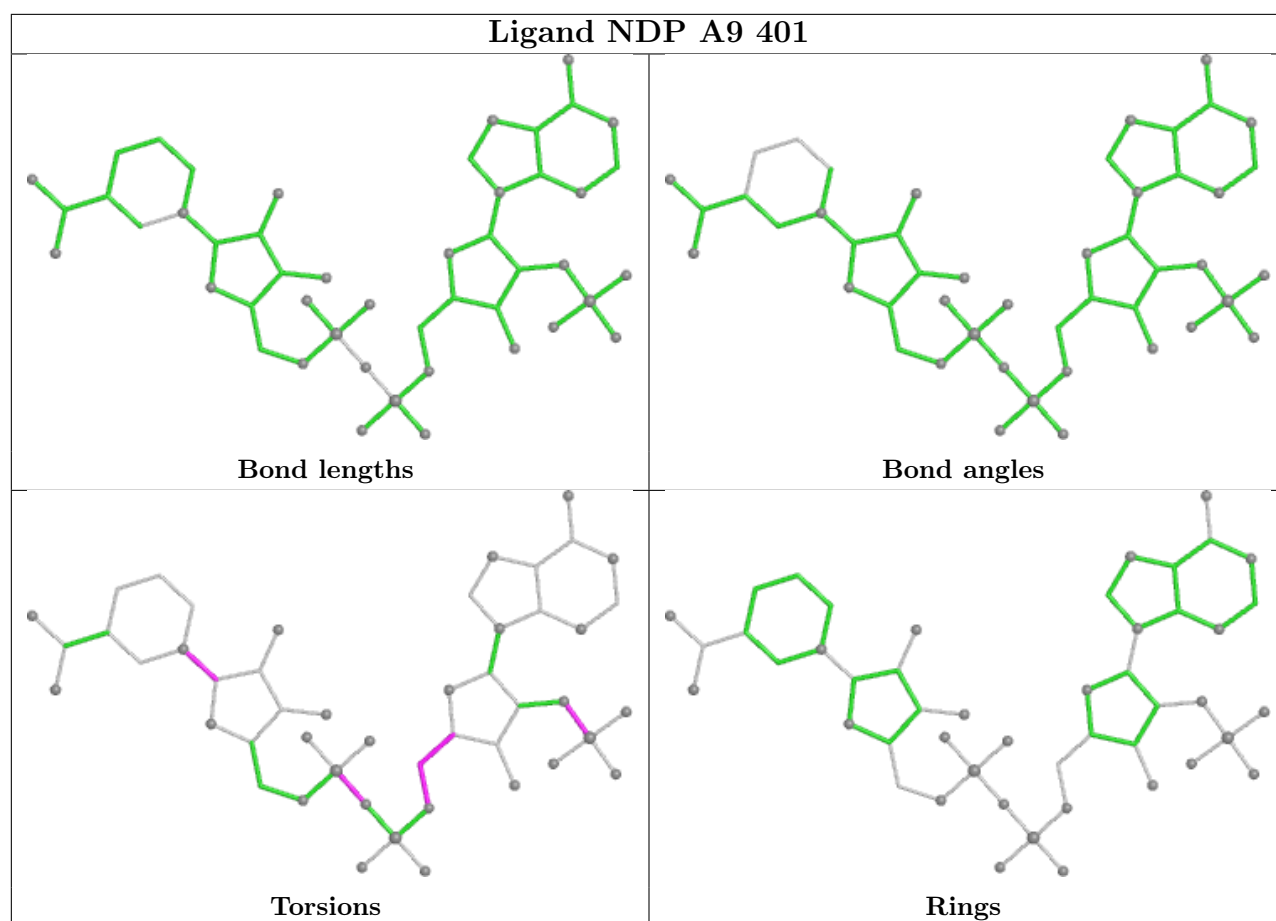


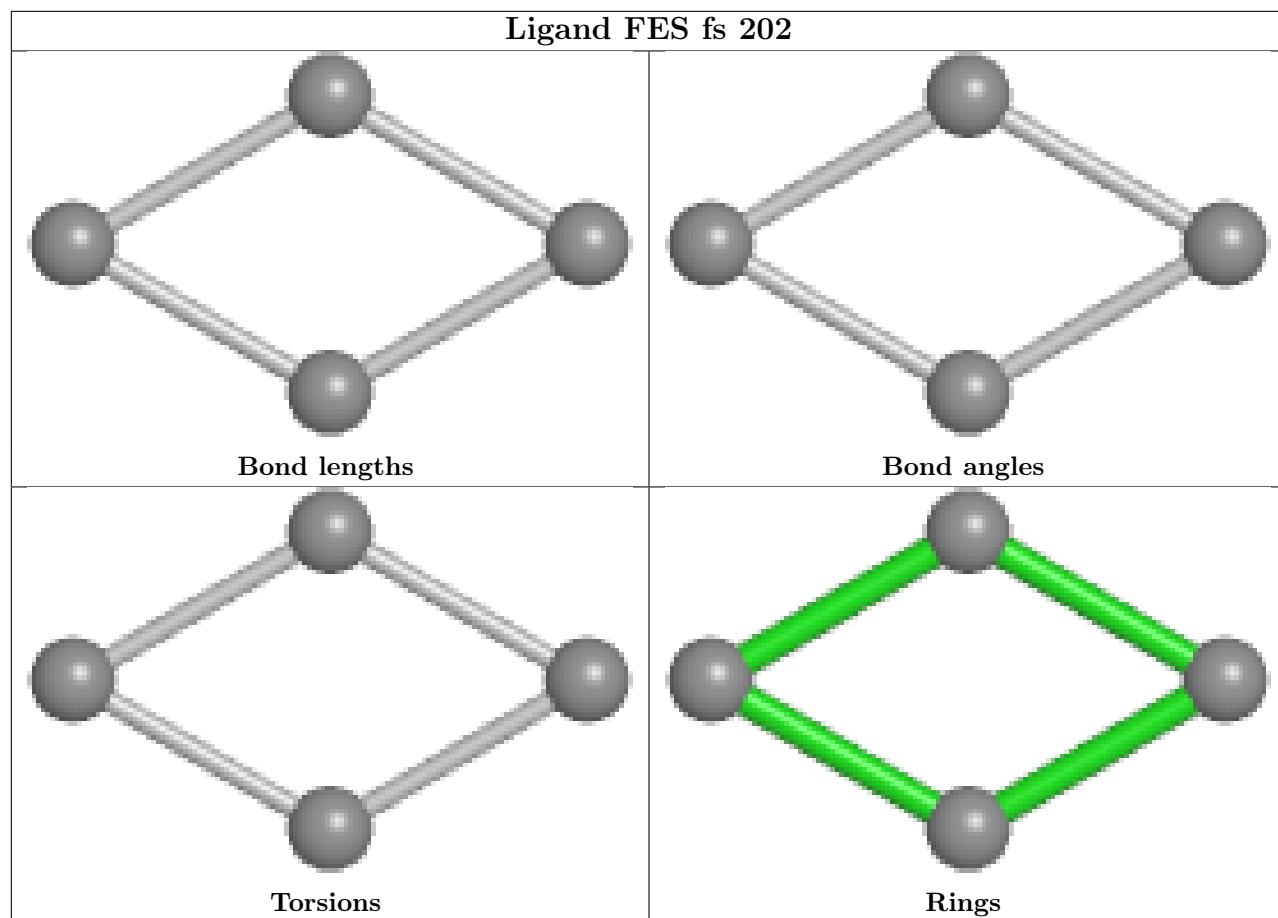
Ligand HEM Qc 502

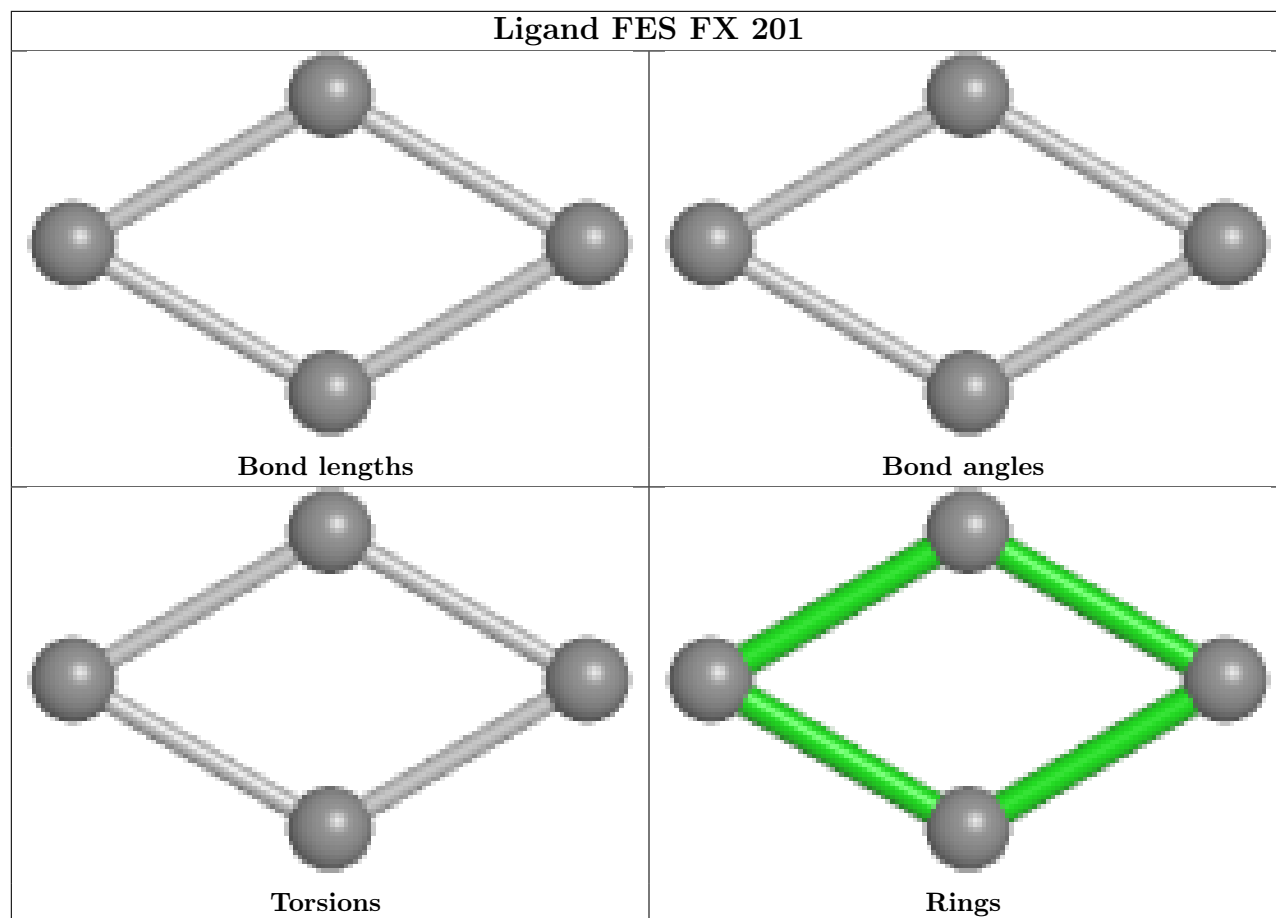


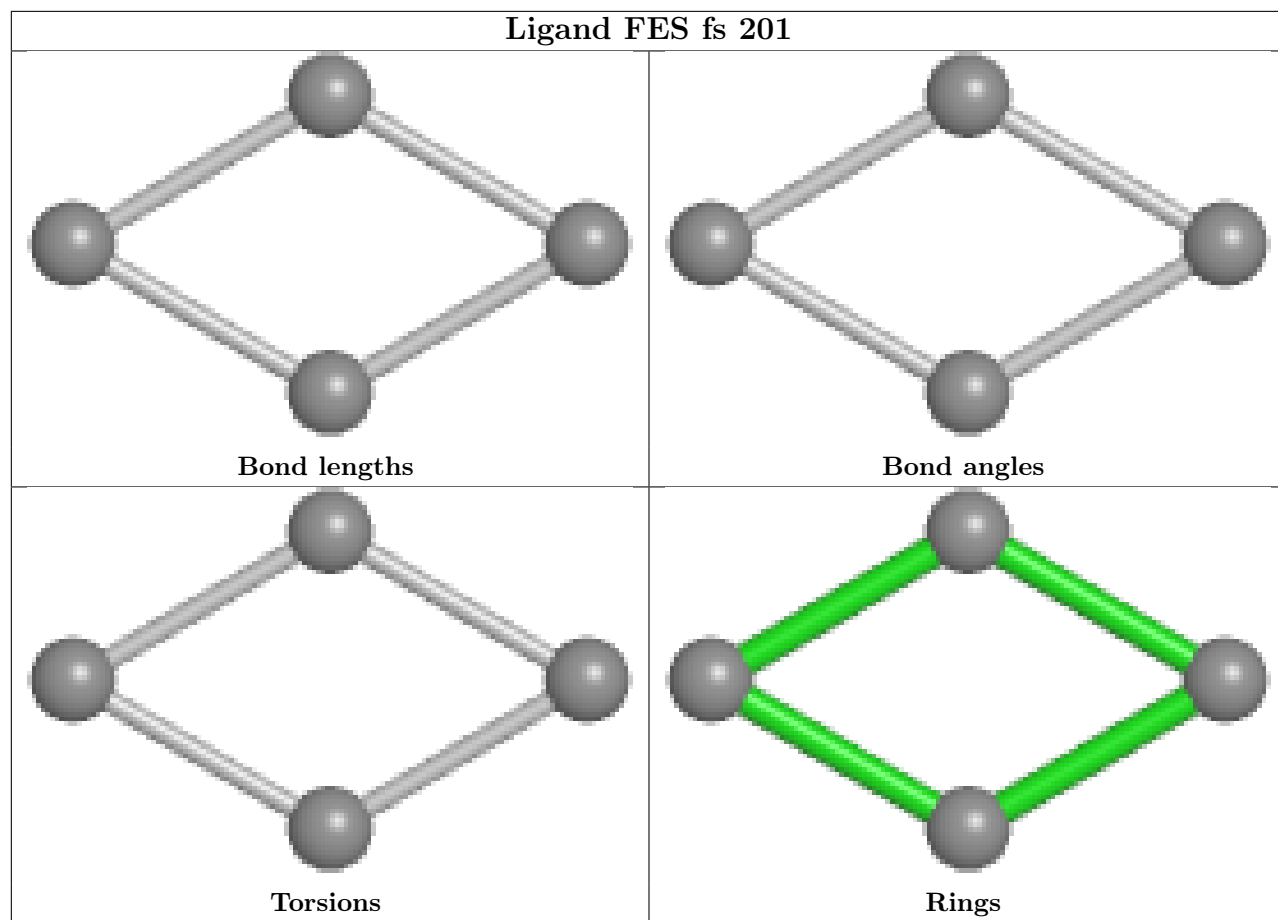
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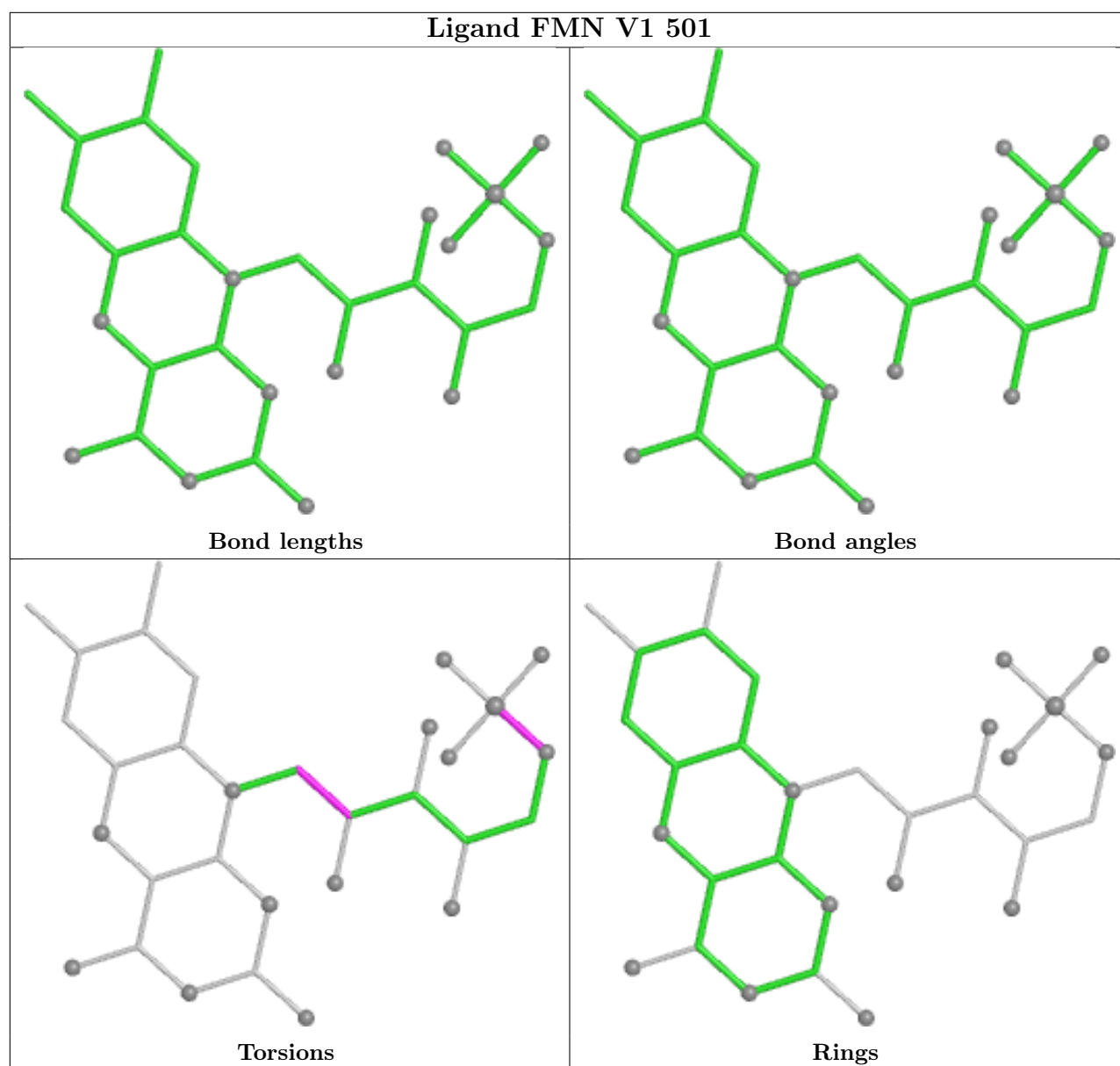


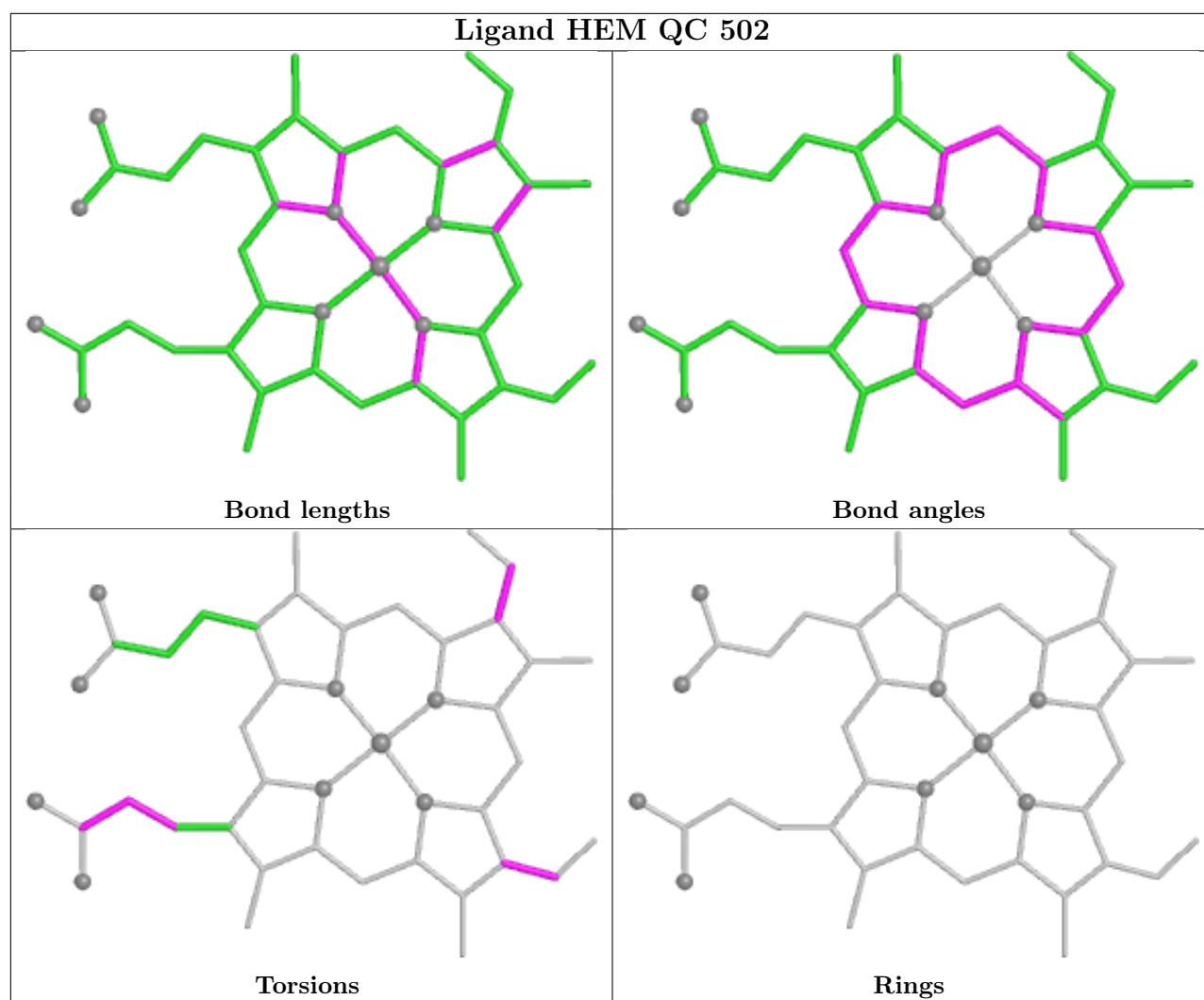


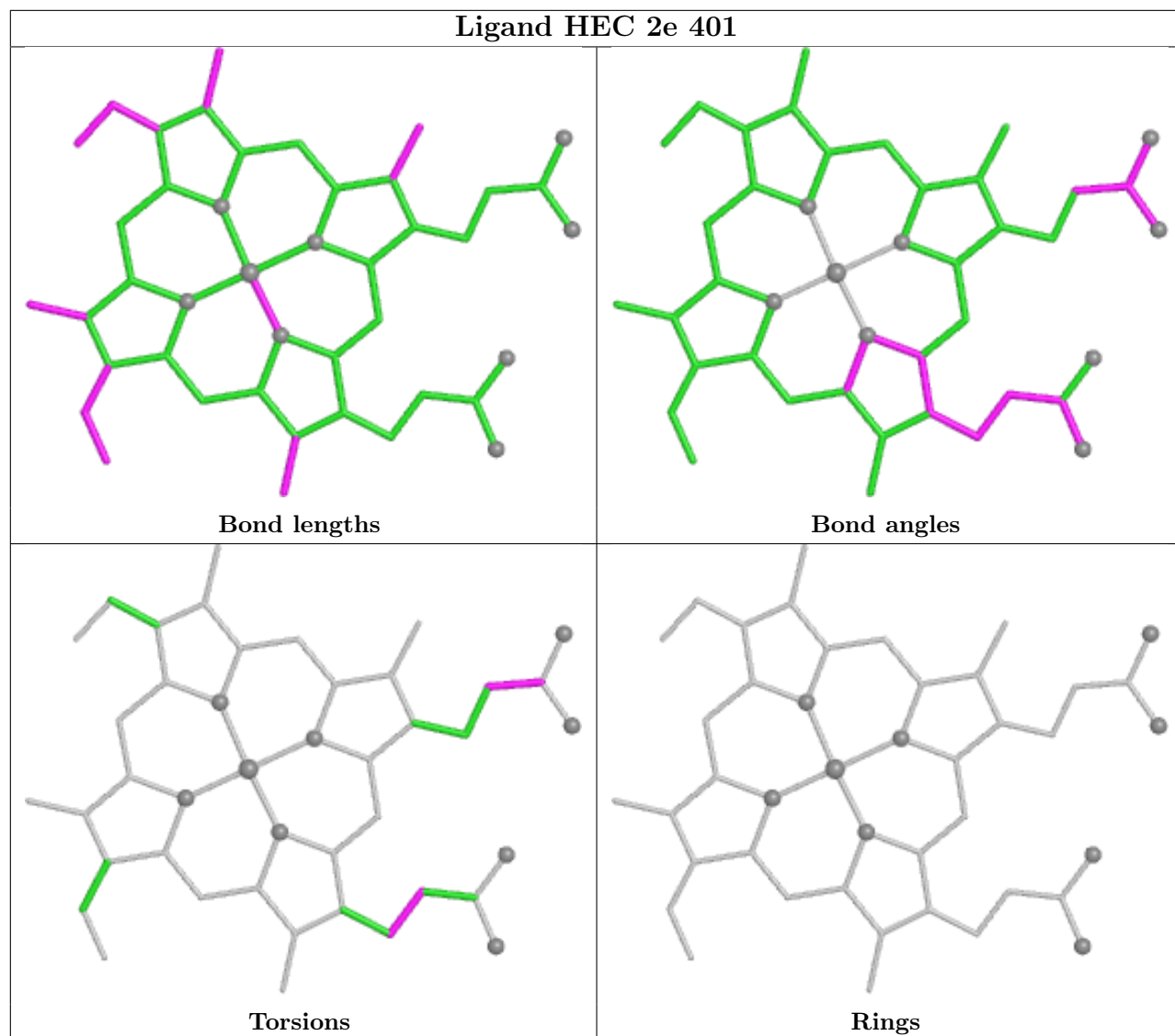


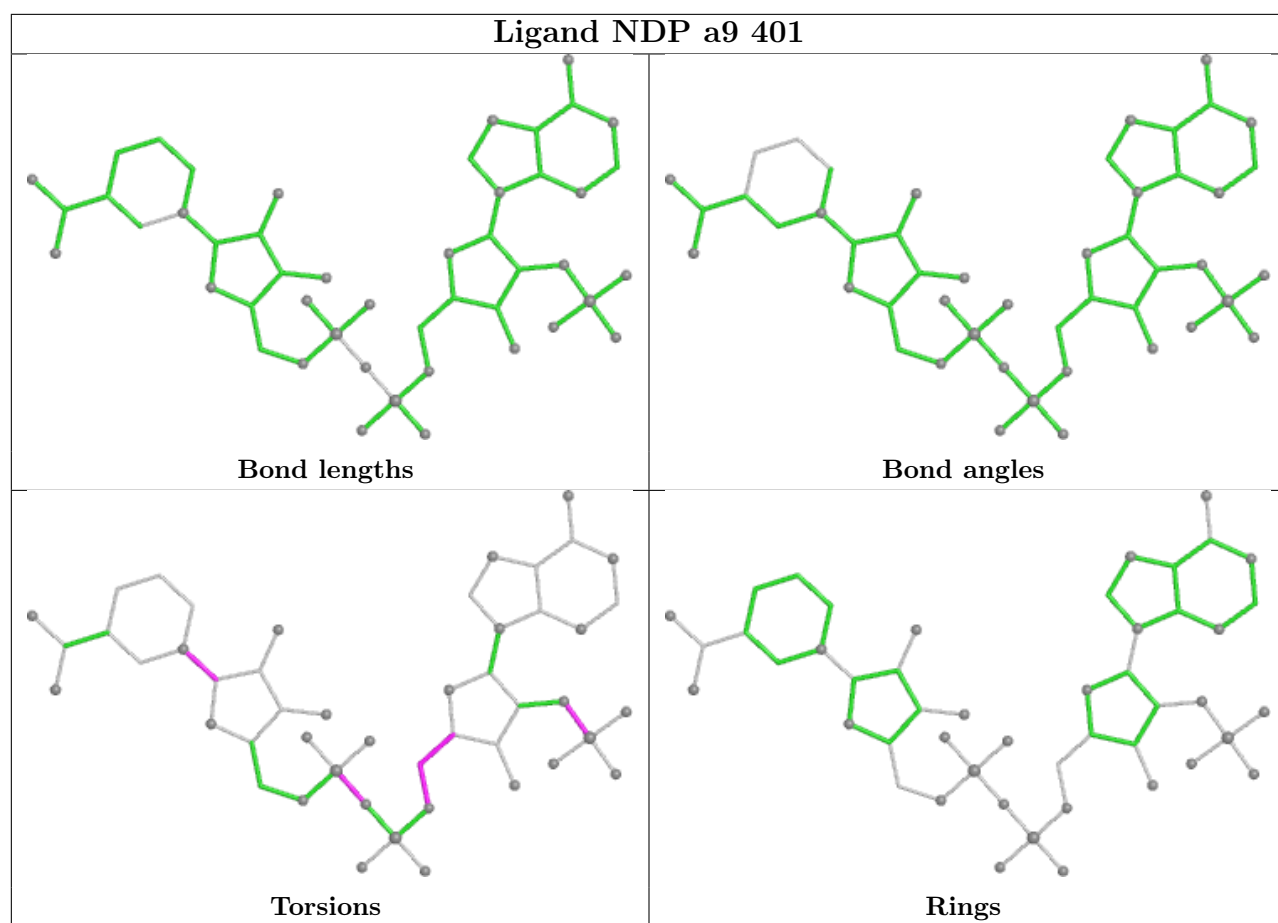


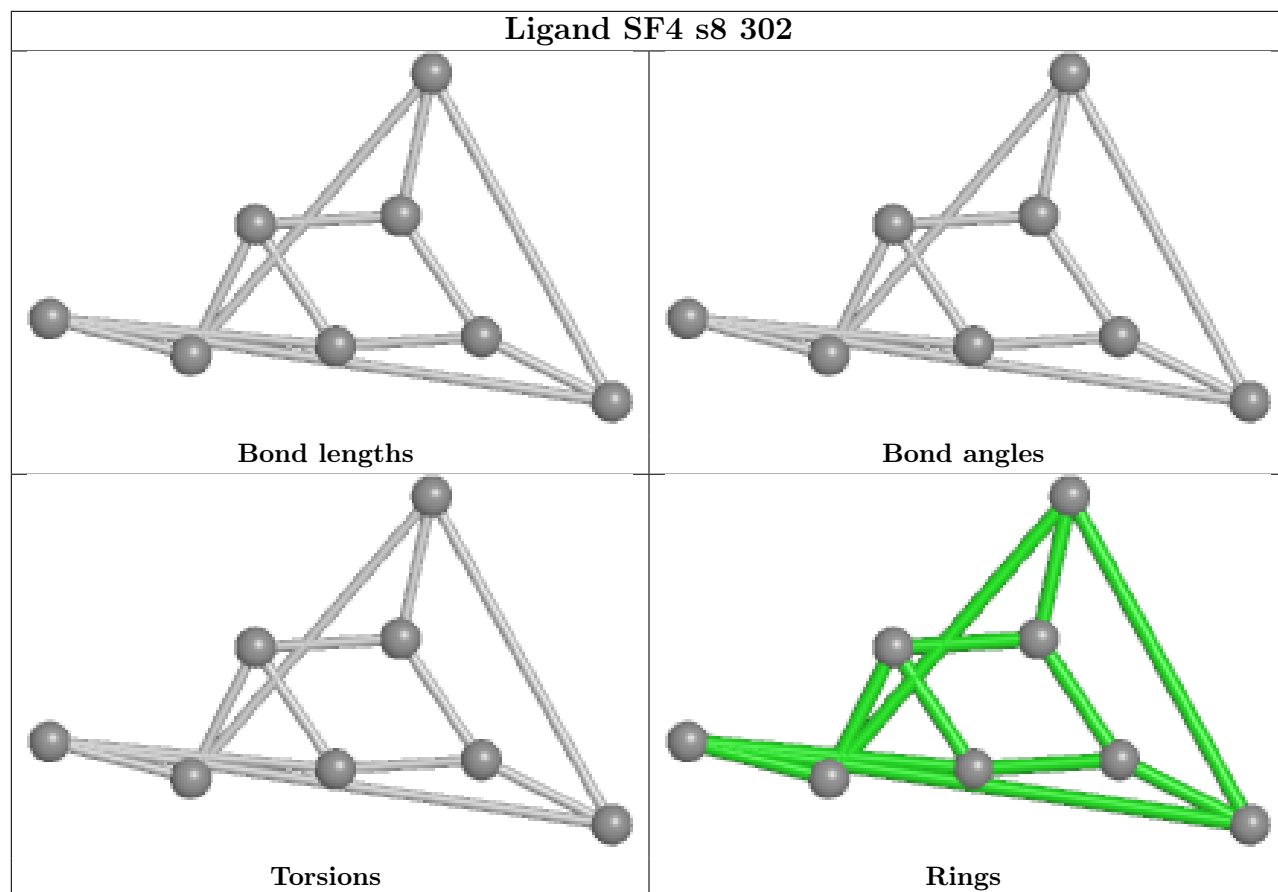


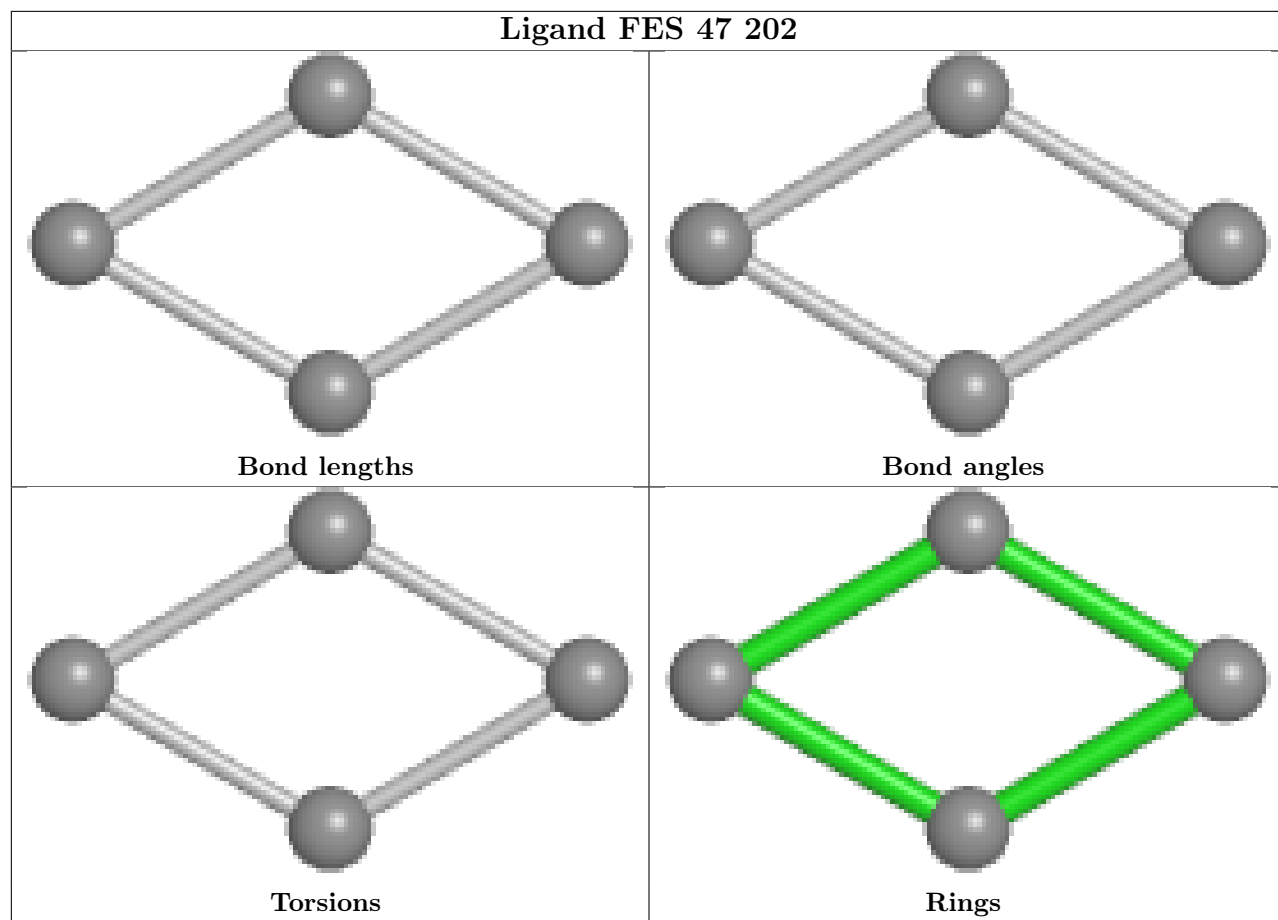


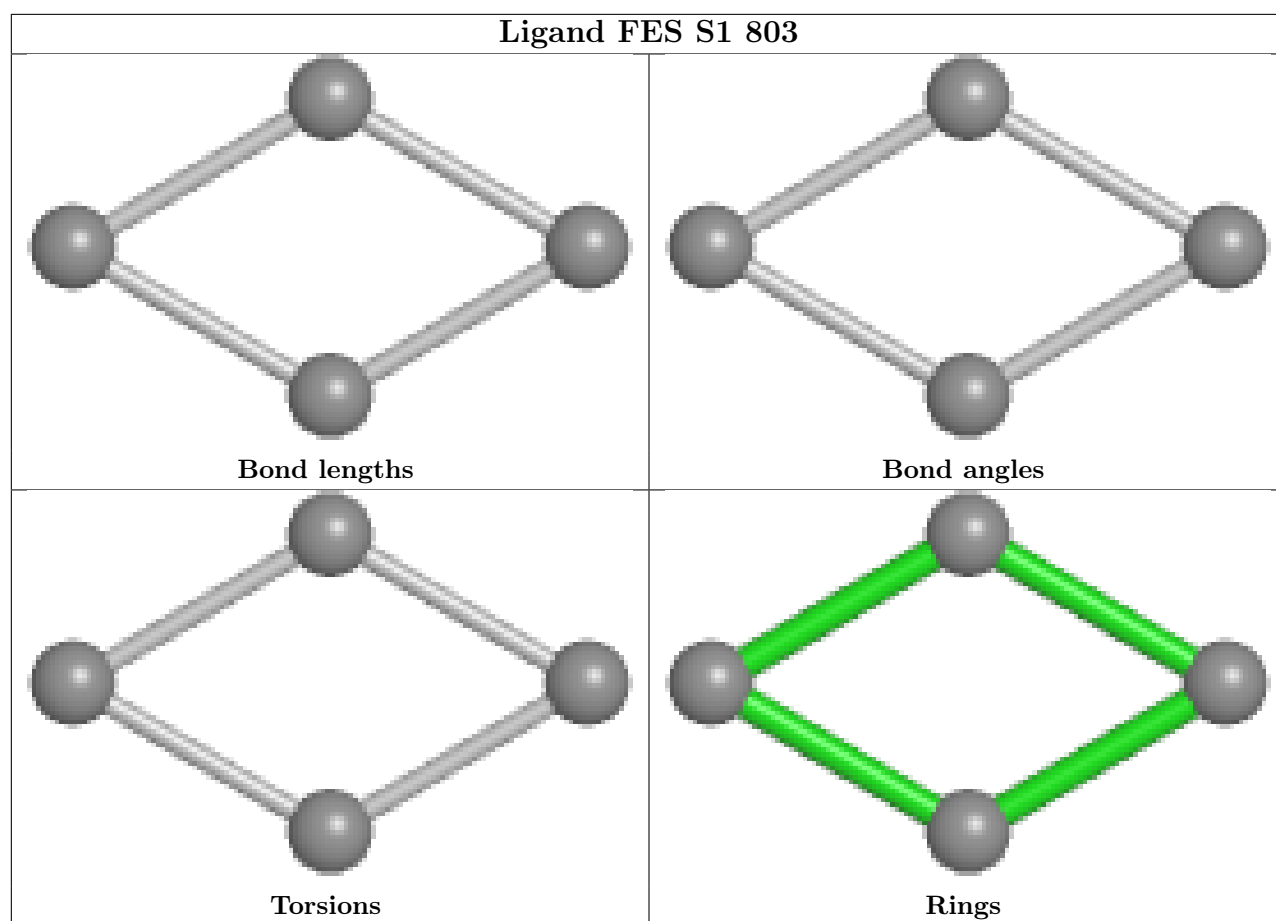




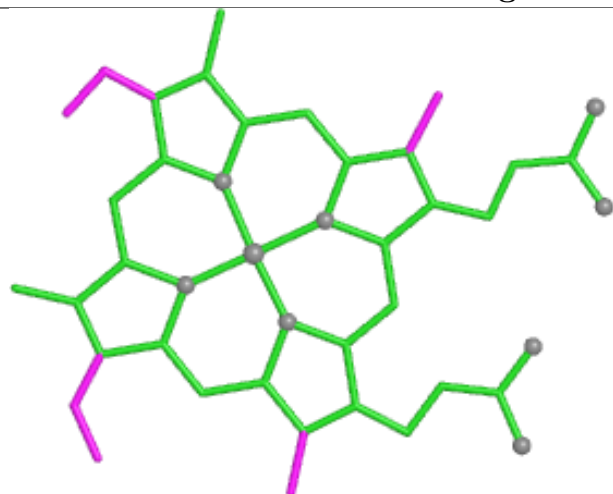




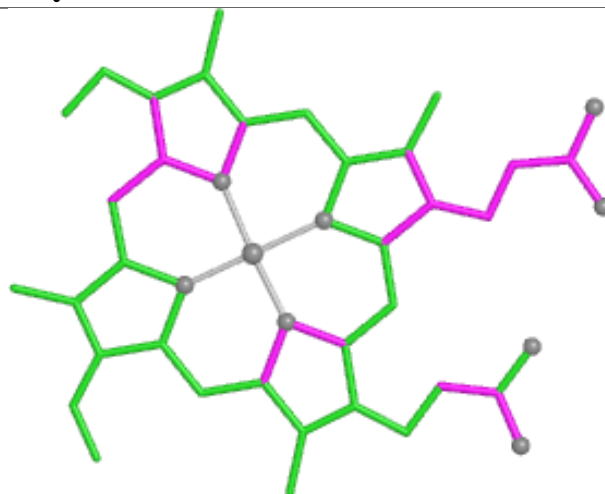




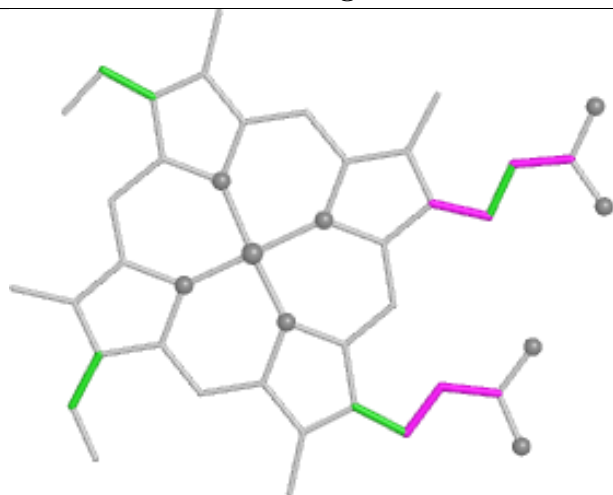
Ligand HEC QD 401



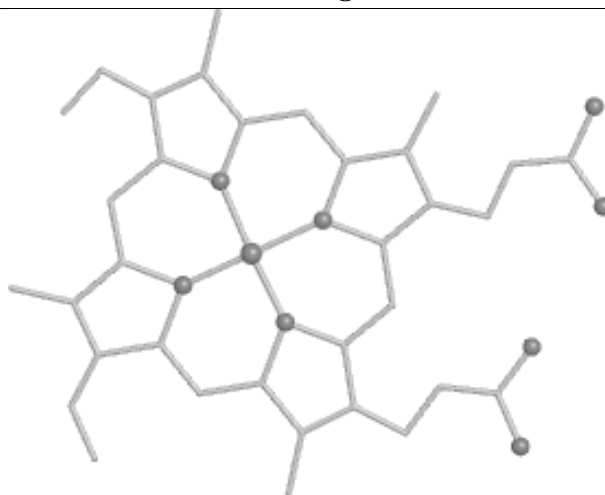
Bond lengths



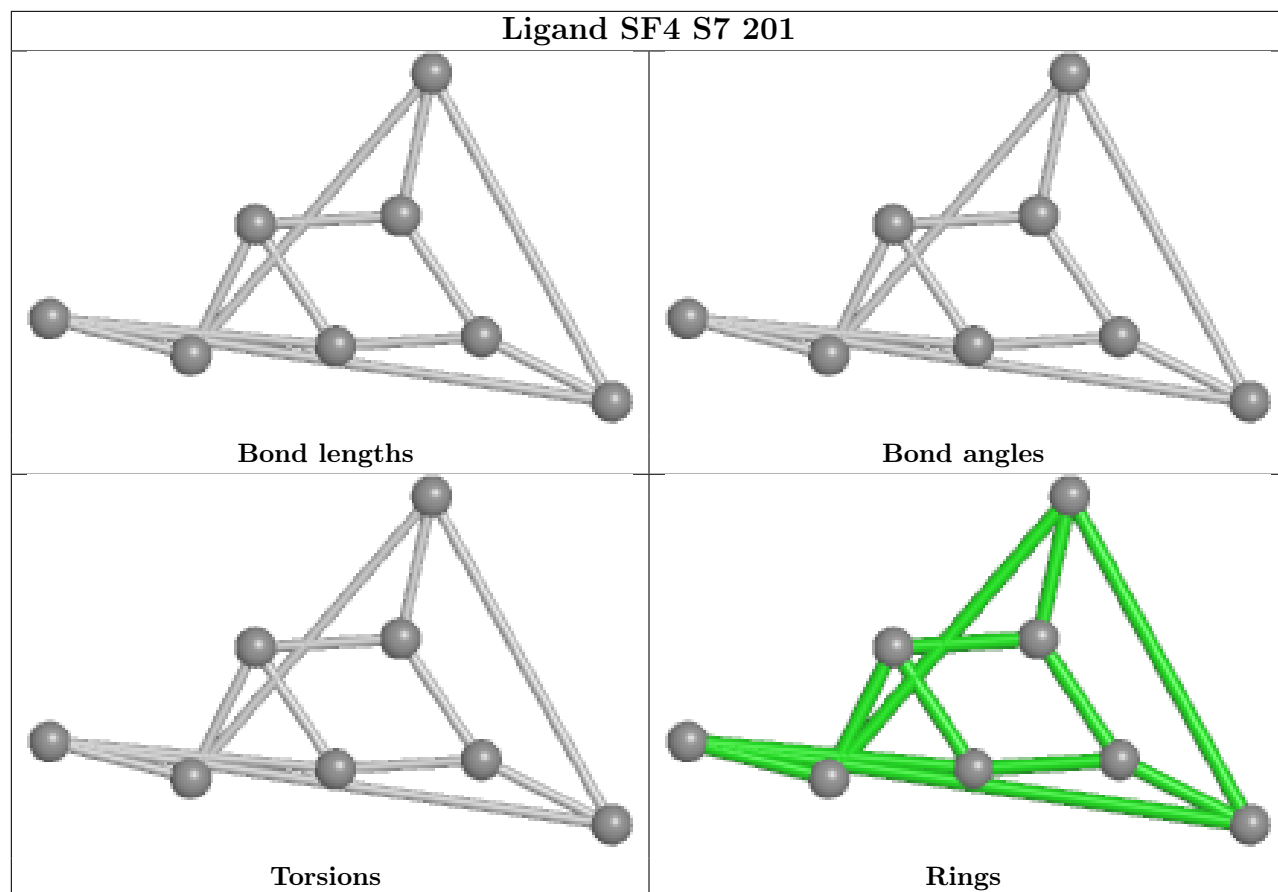
Bond angles

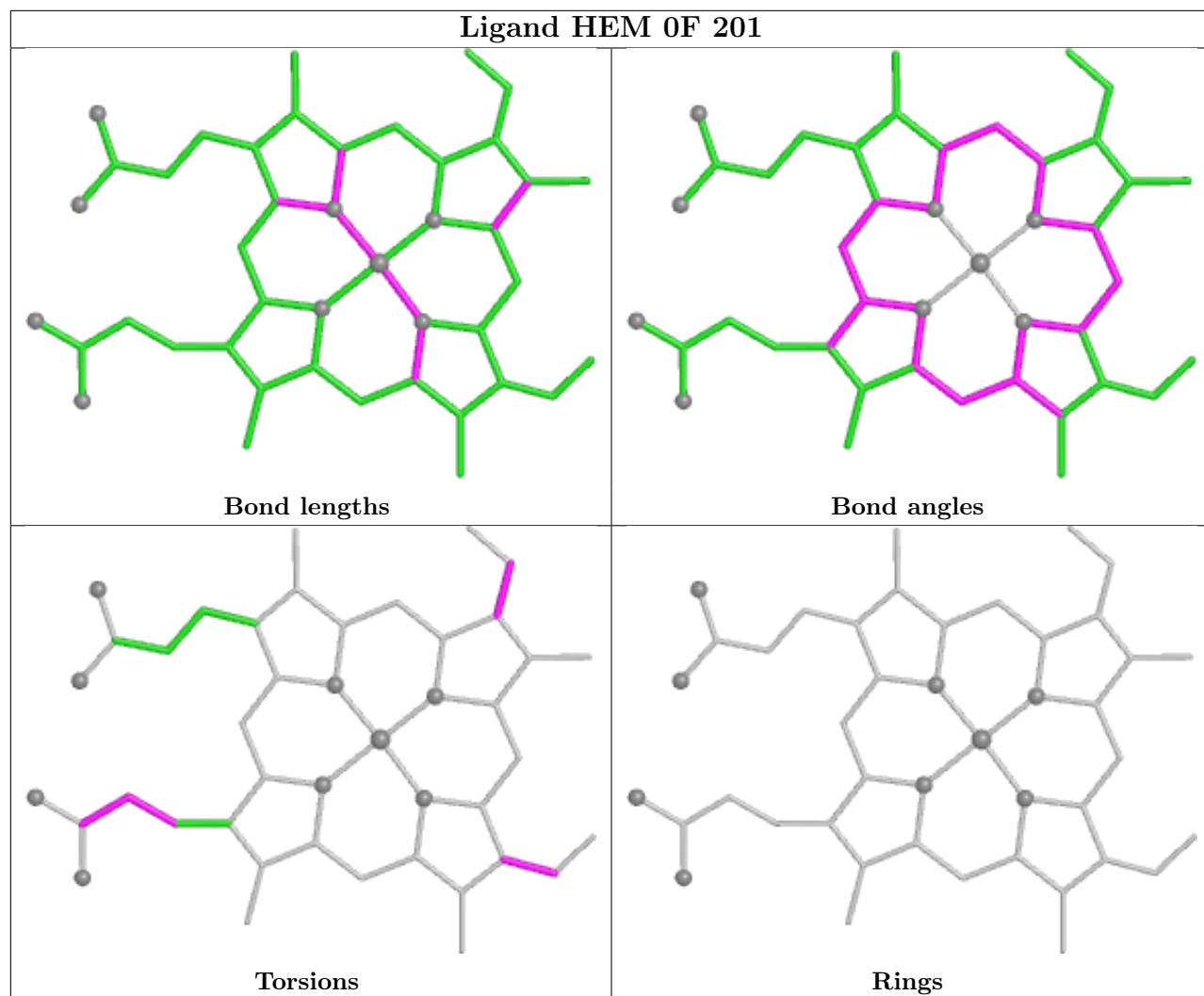


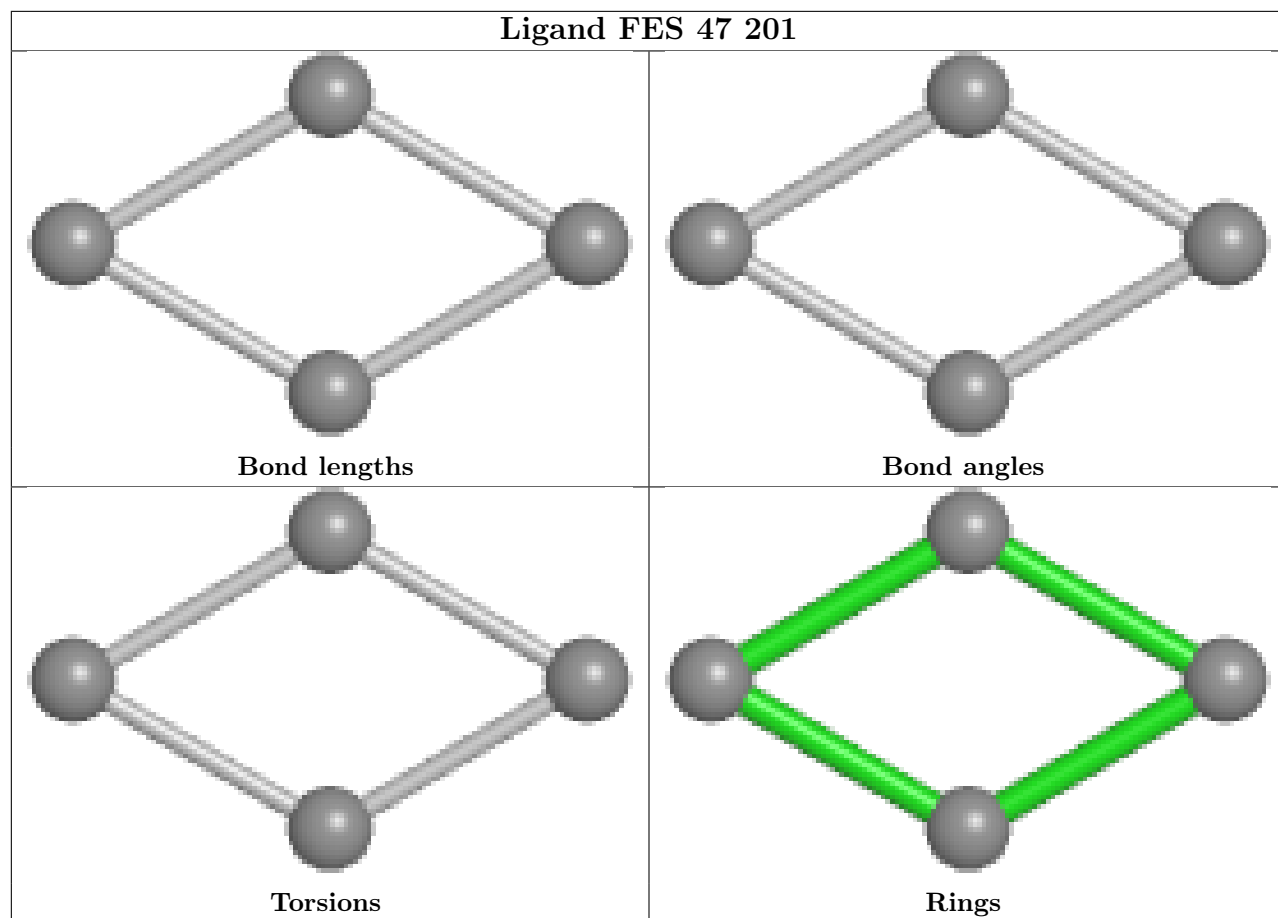
Torsions

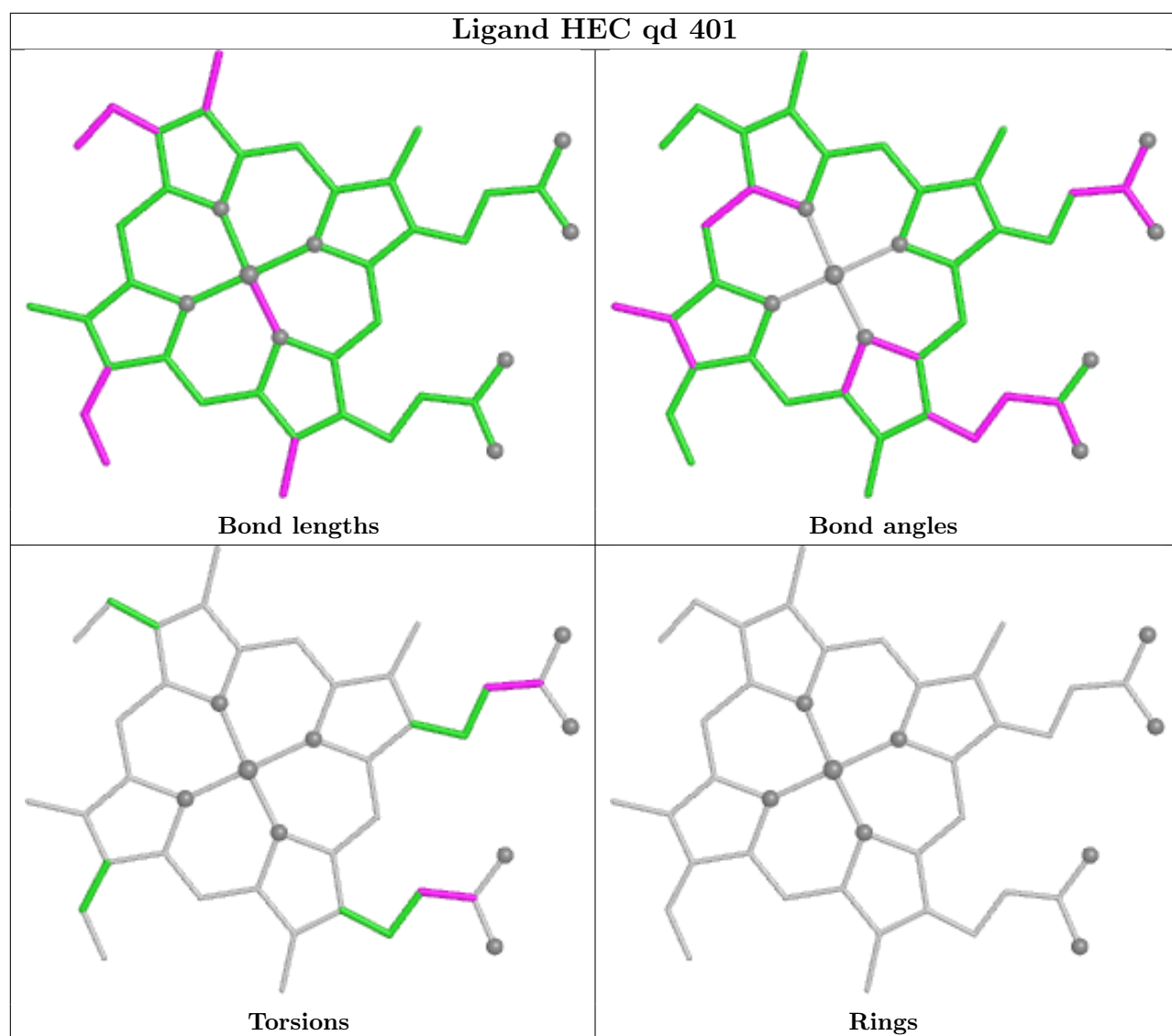


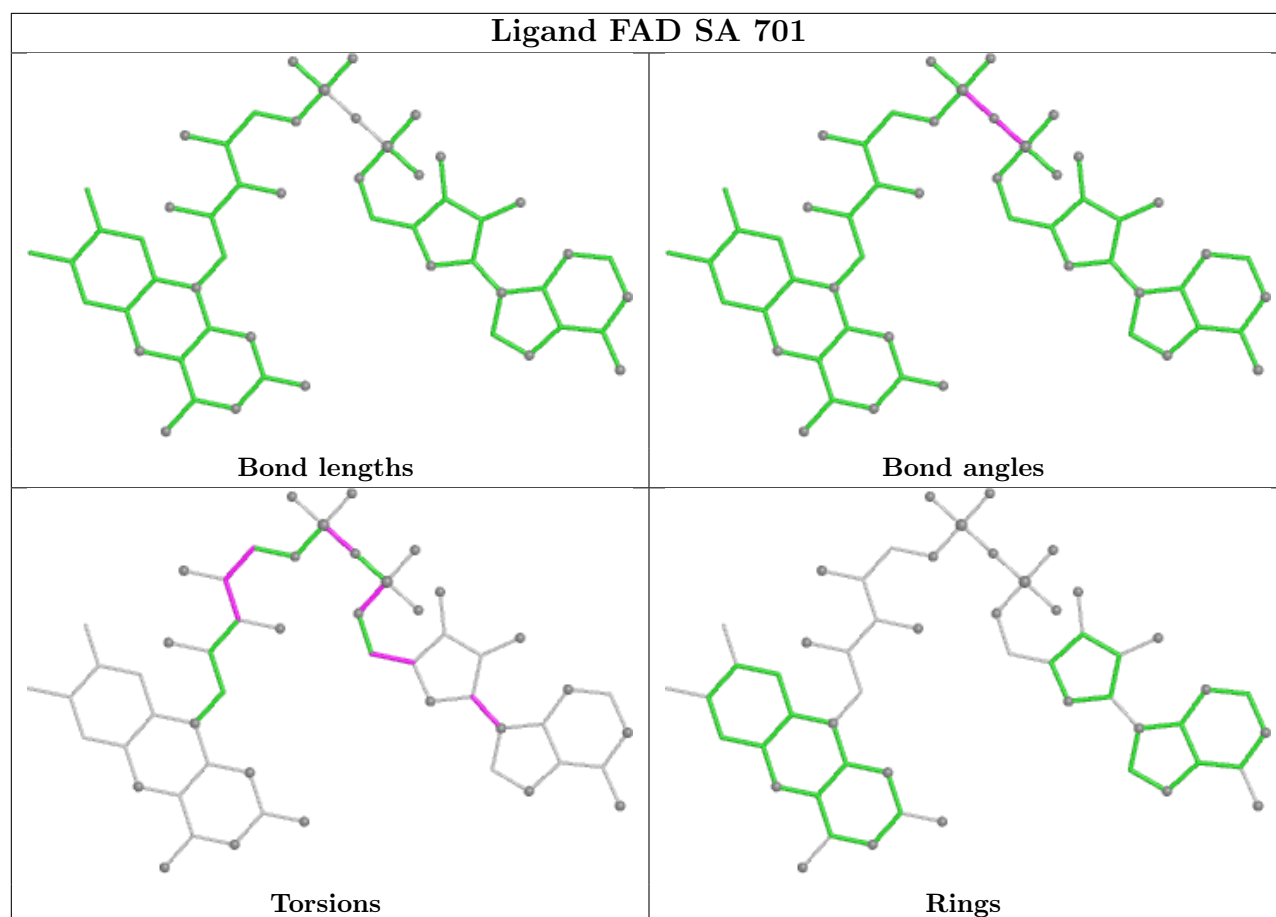
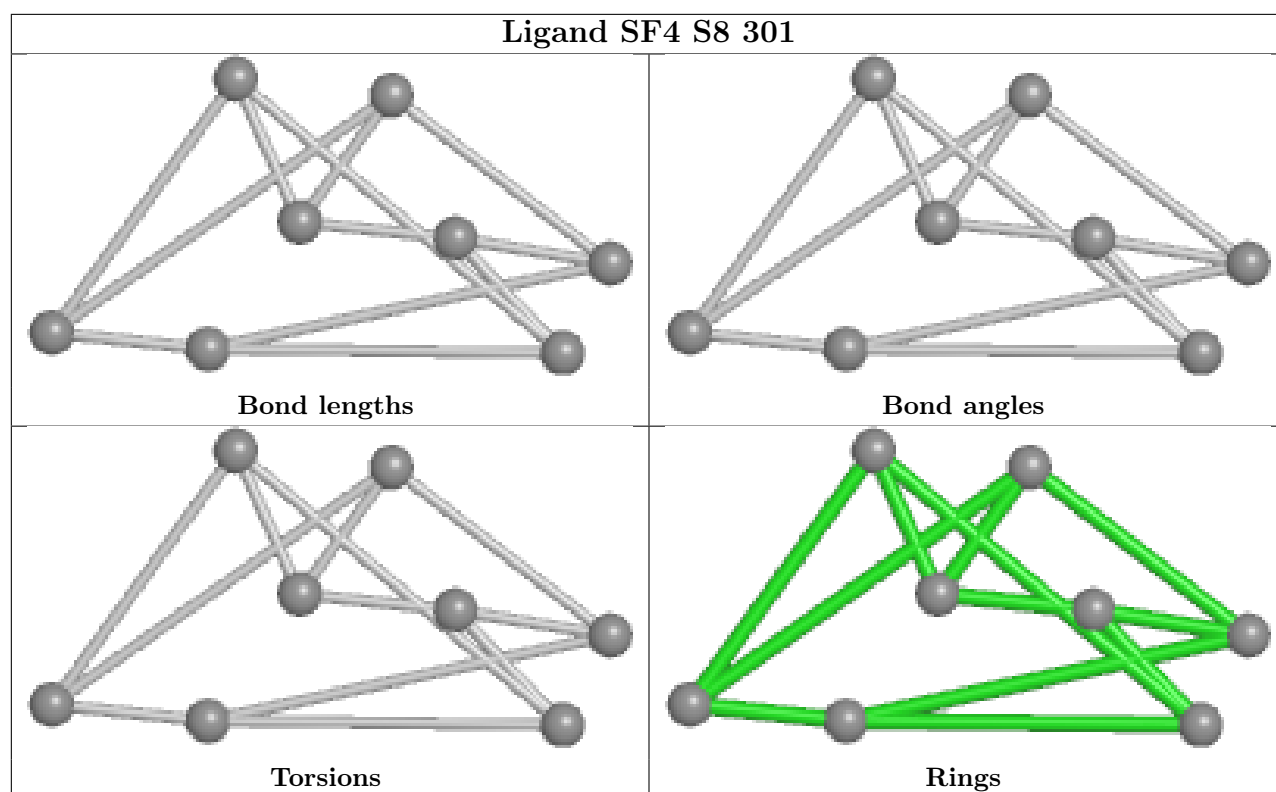
Rings

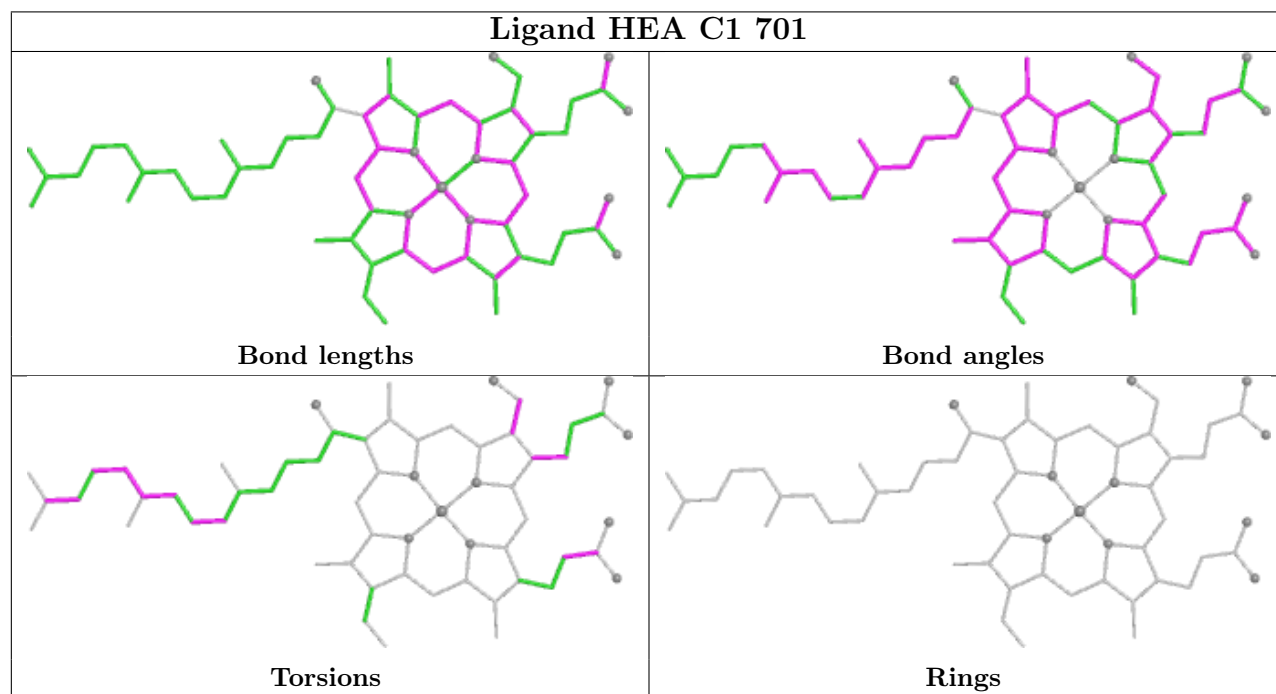
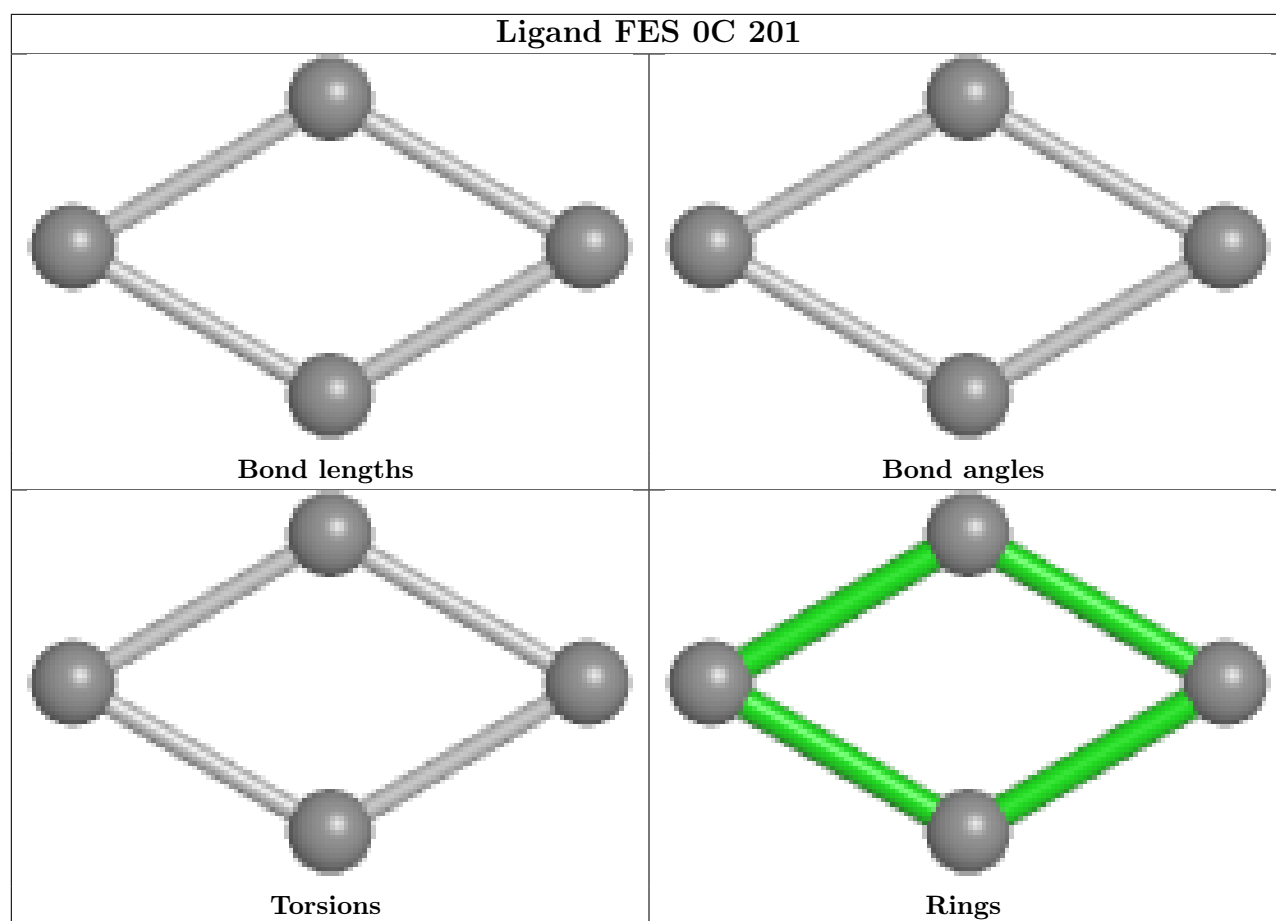


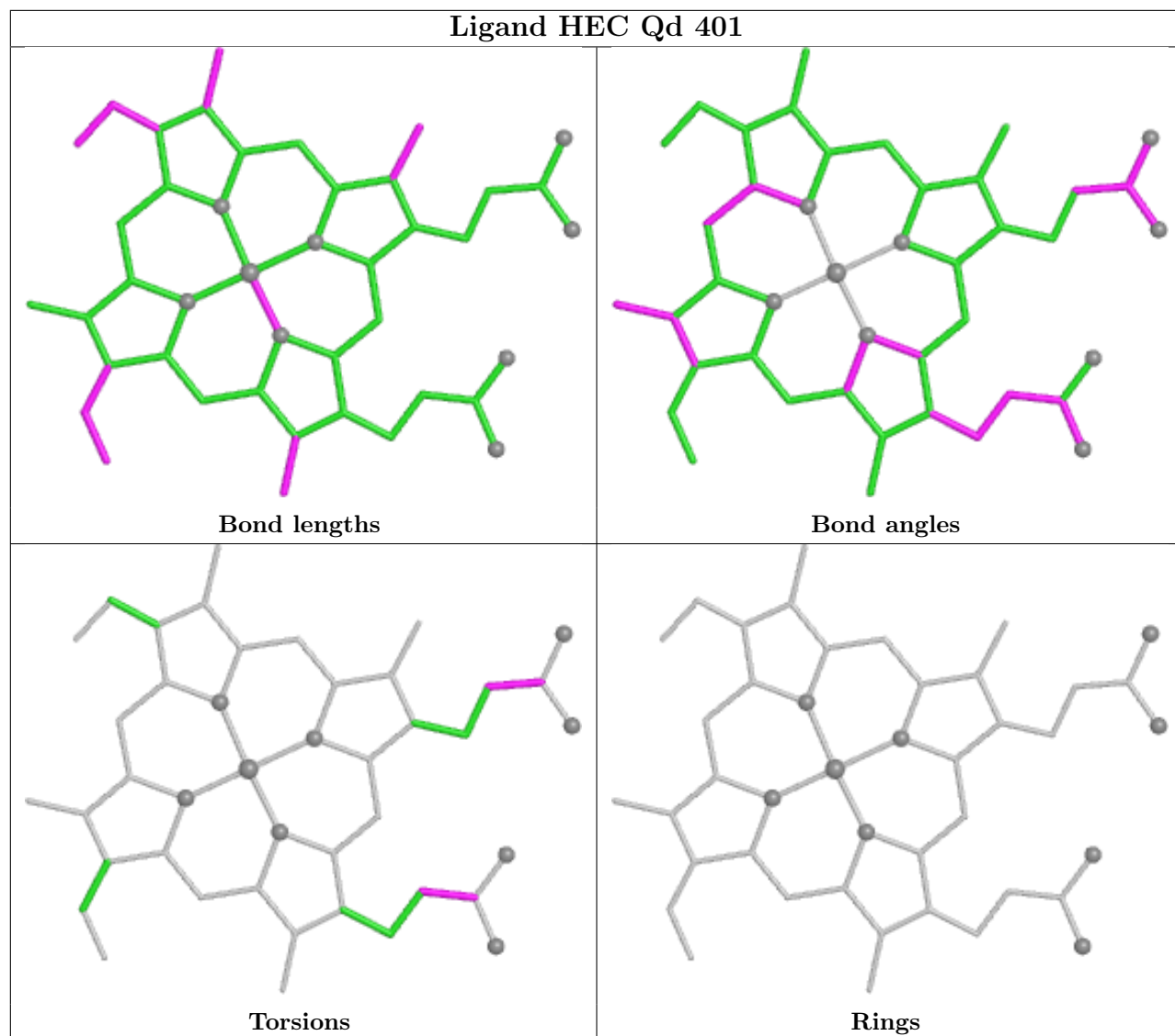


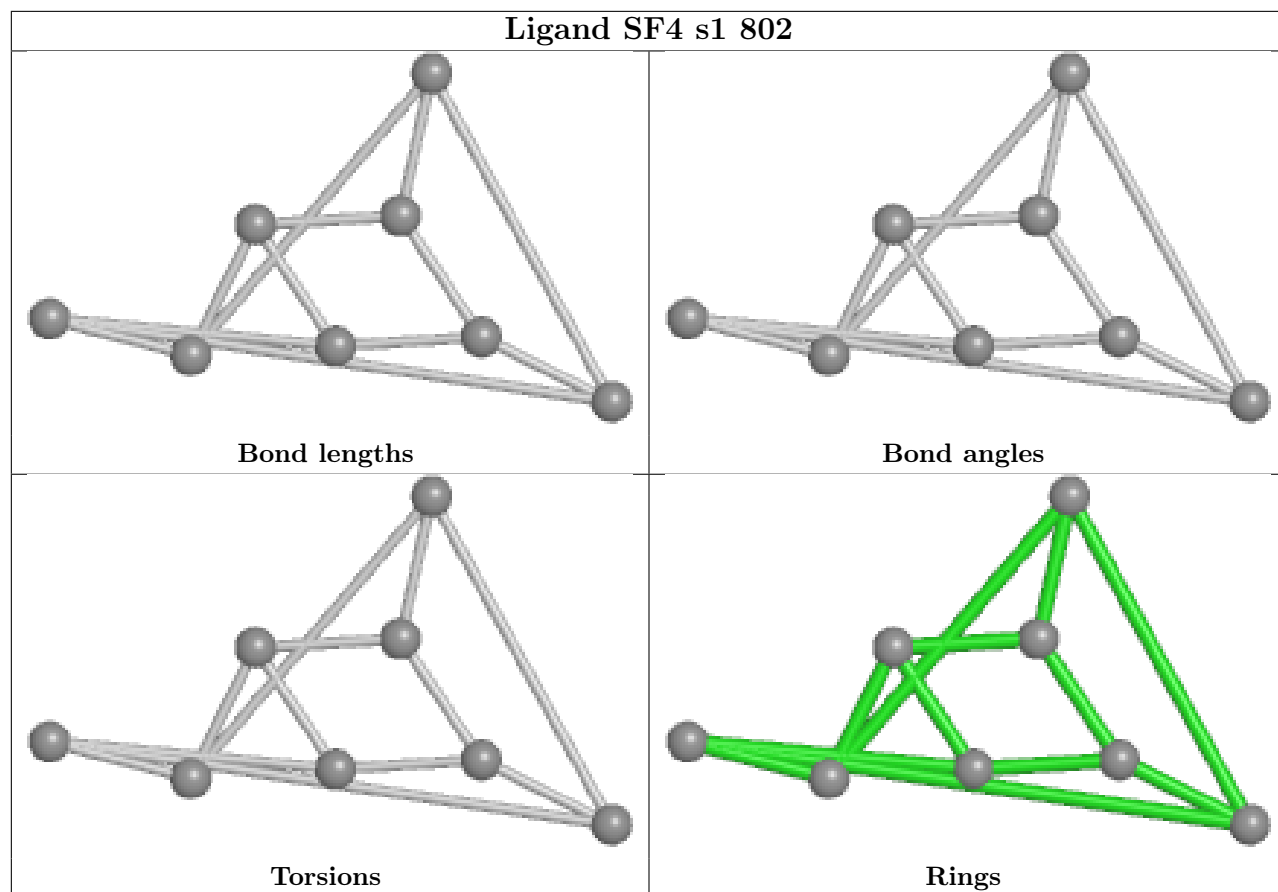


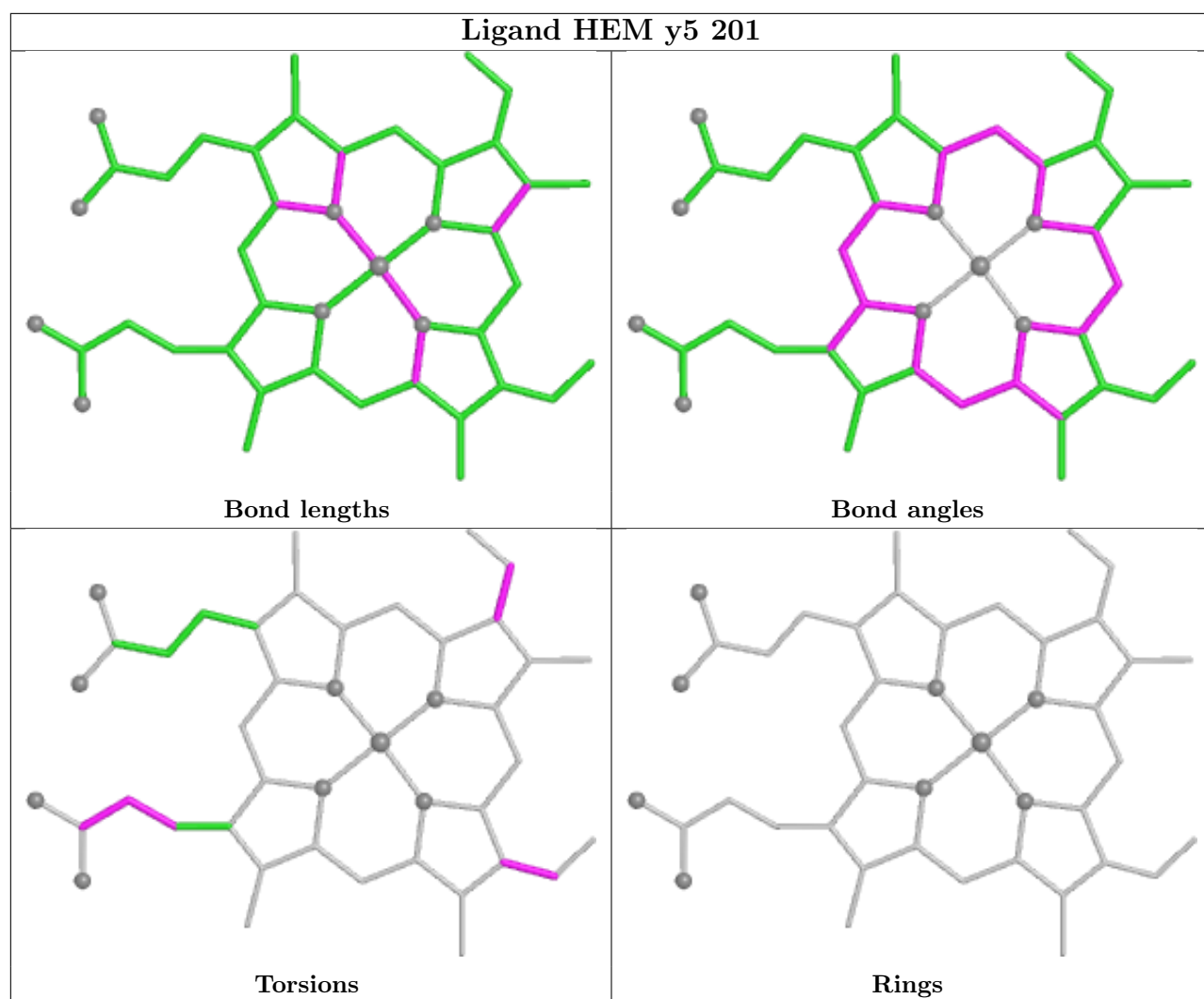


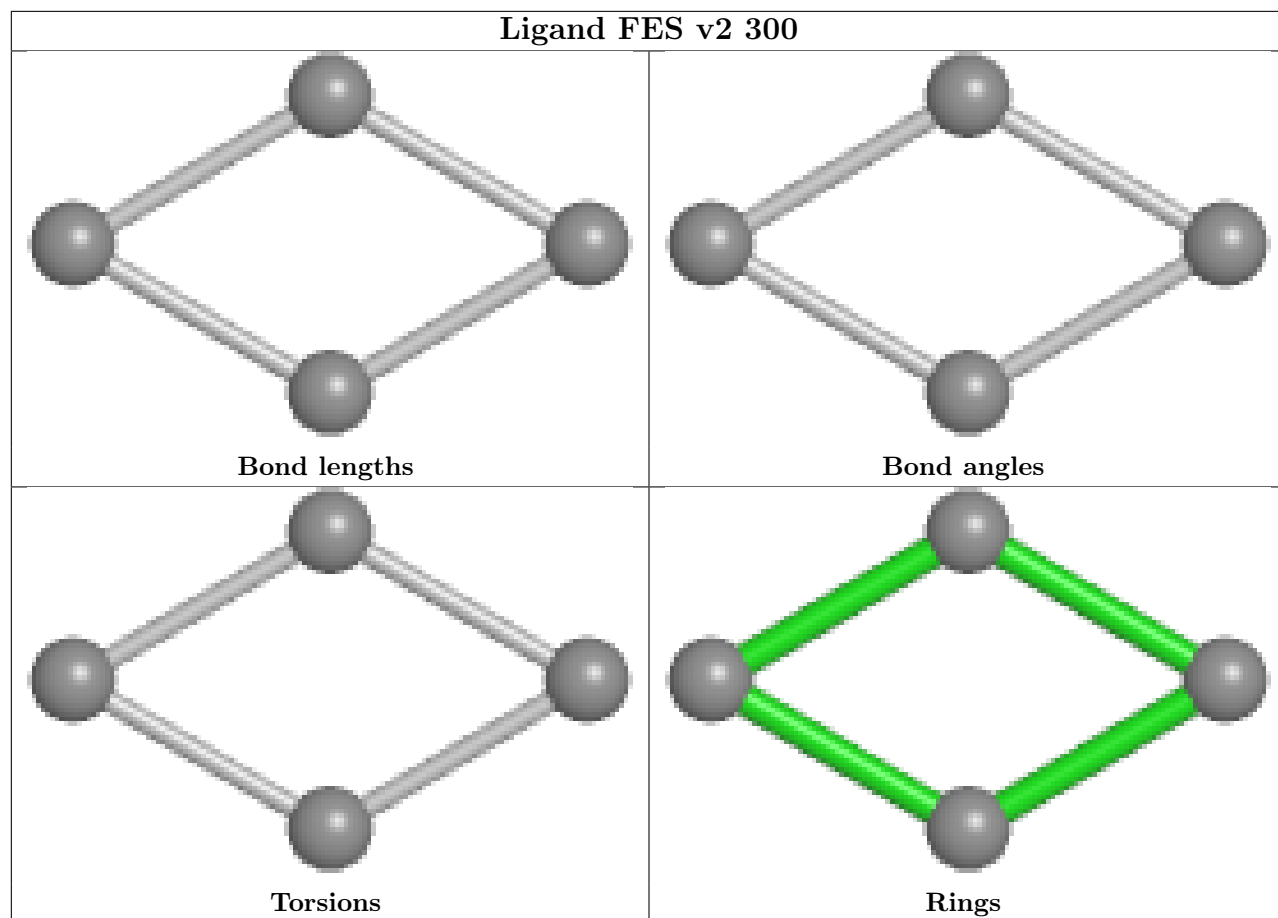


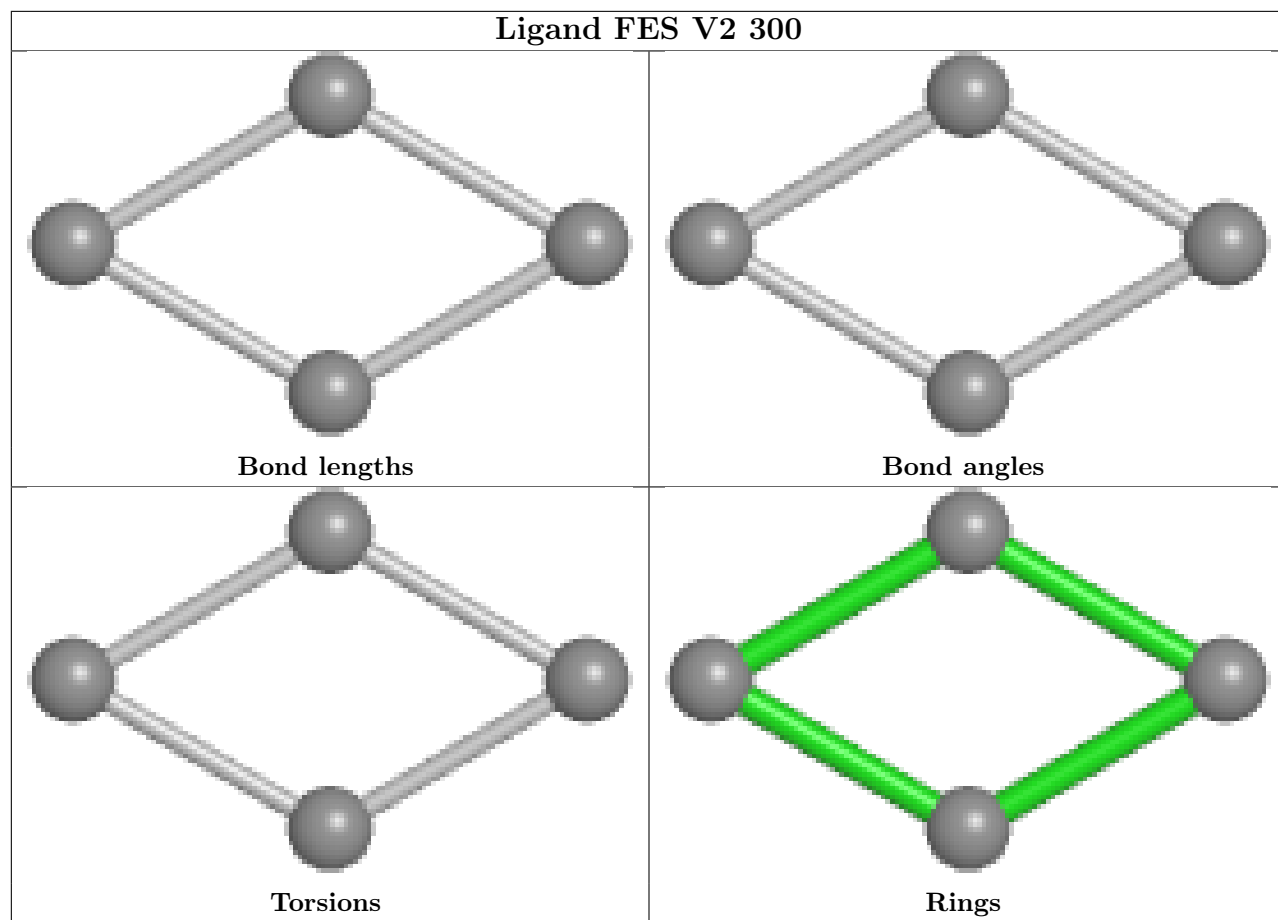




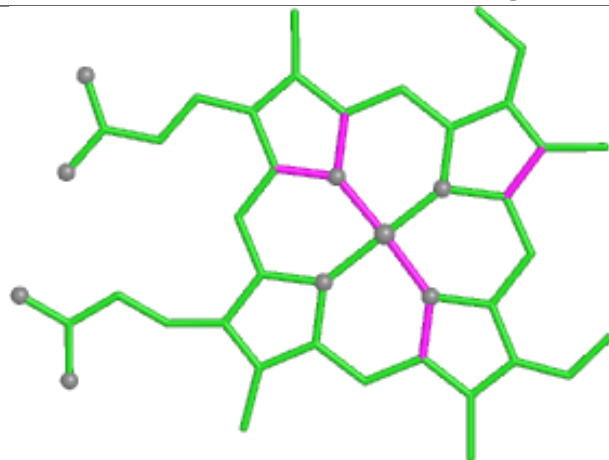




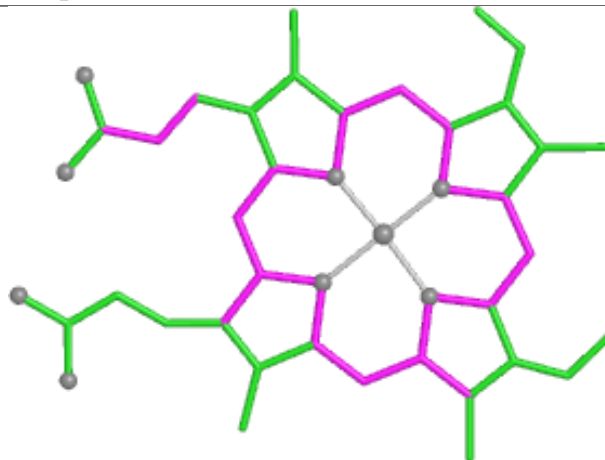




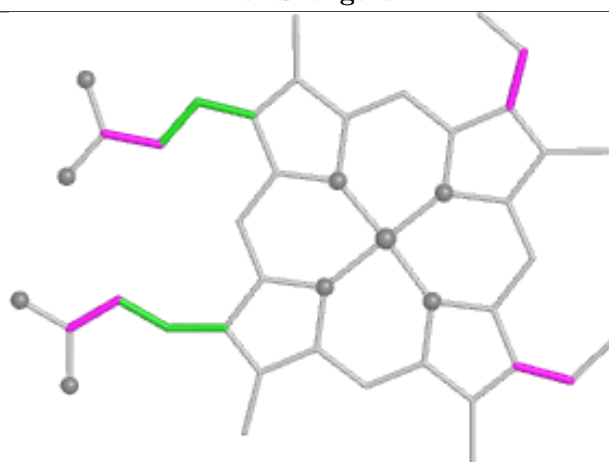
Ligand HEM qc 503



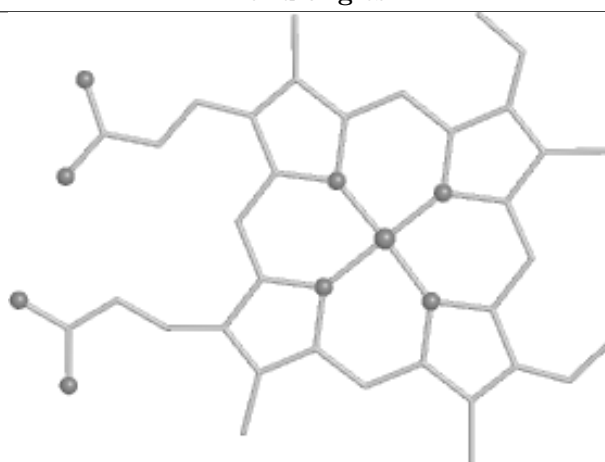
Bond lengths



Bond angles

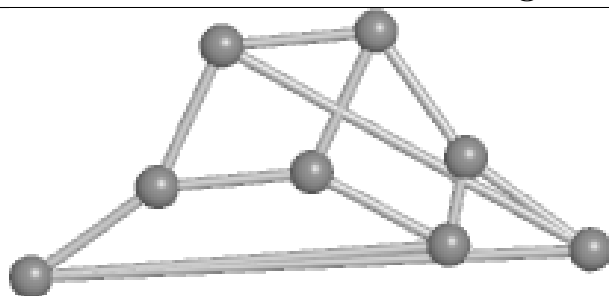


Torsions

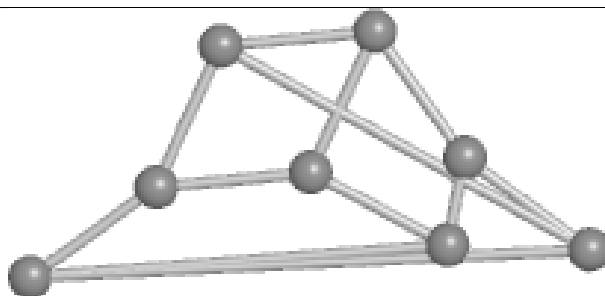


Rings

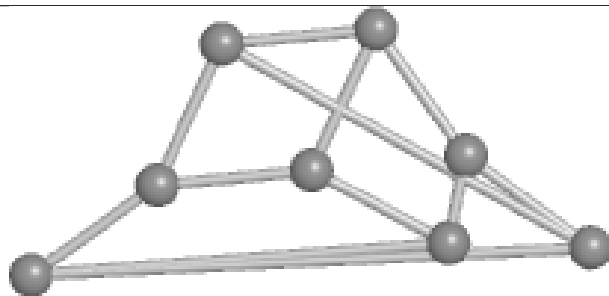
Ligand SF4 s8 301



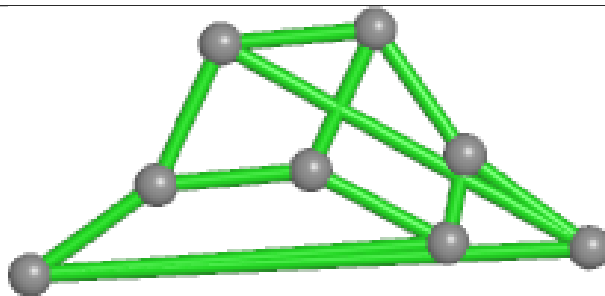
Bond lengths



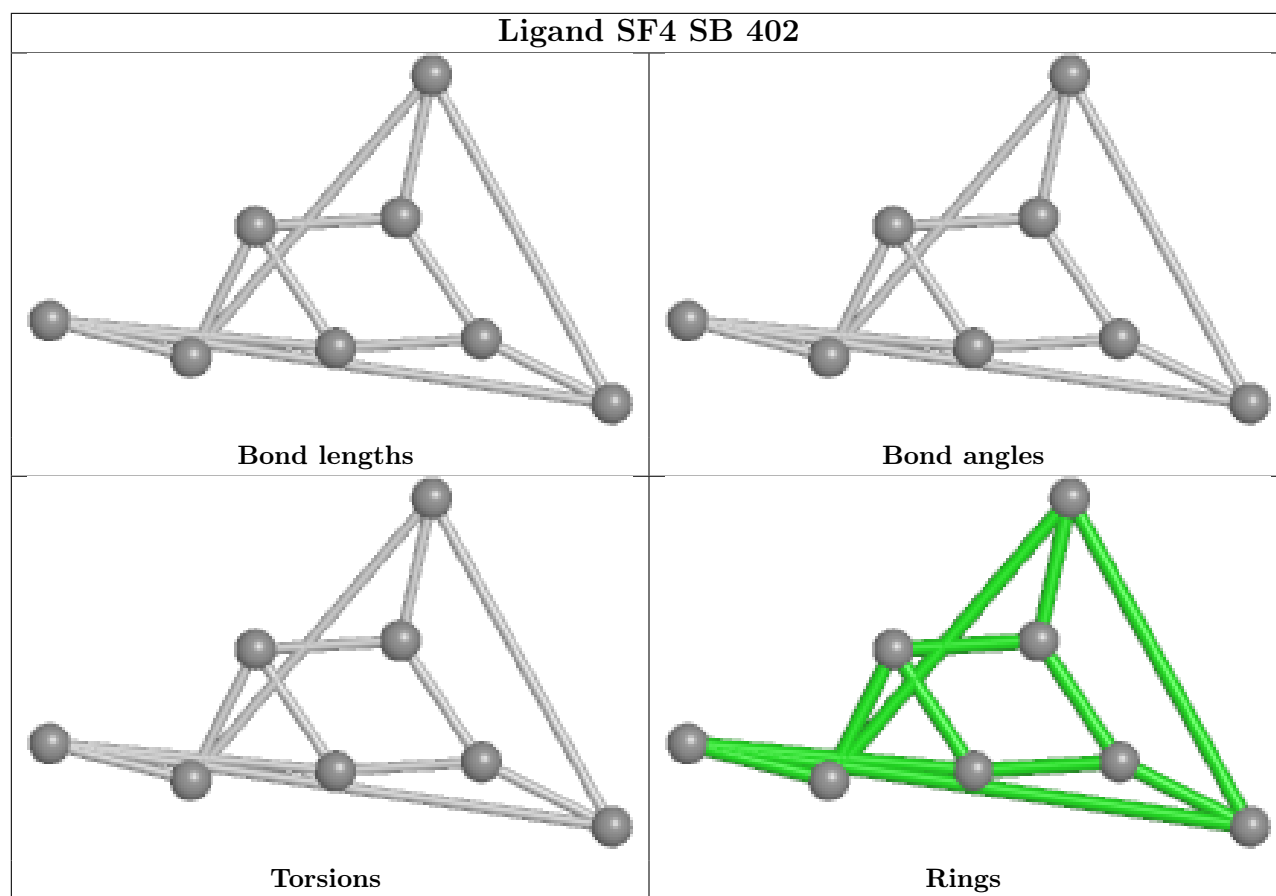
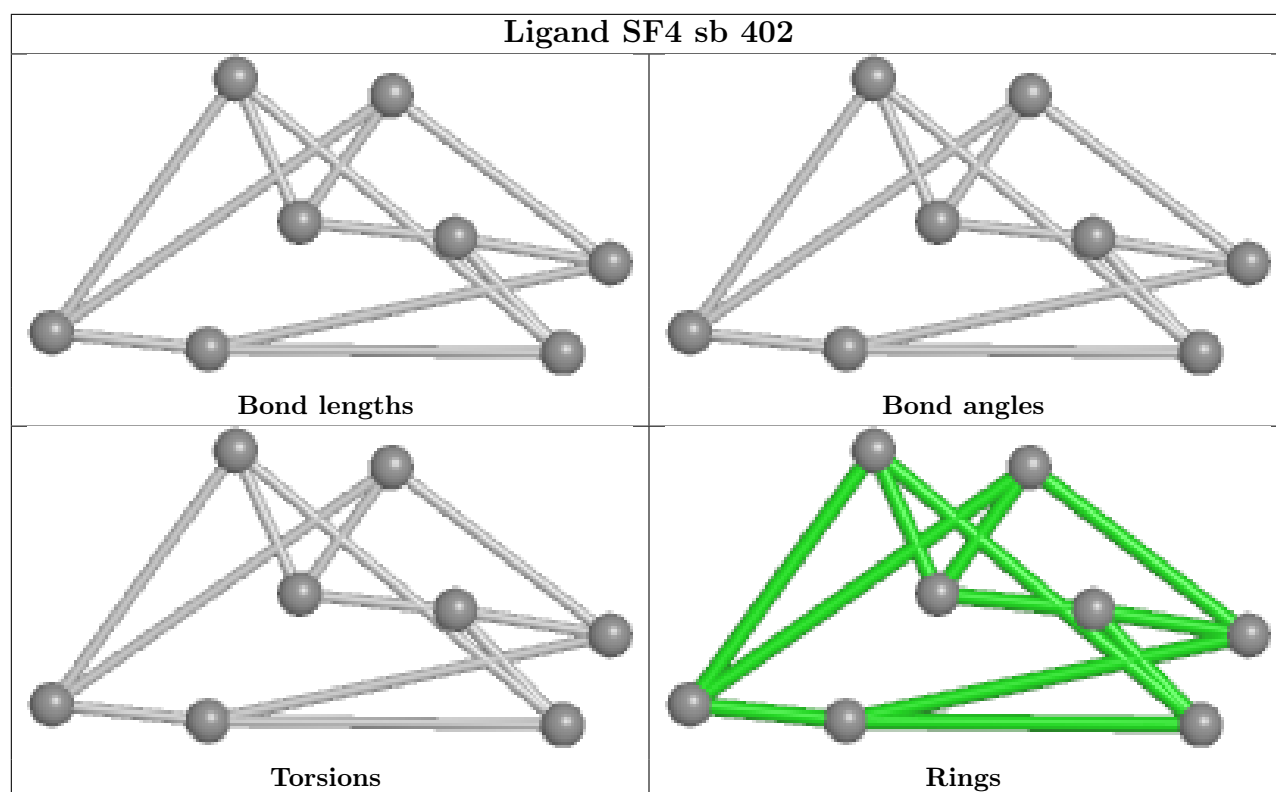
Bond angles

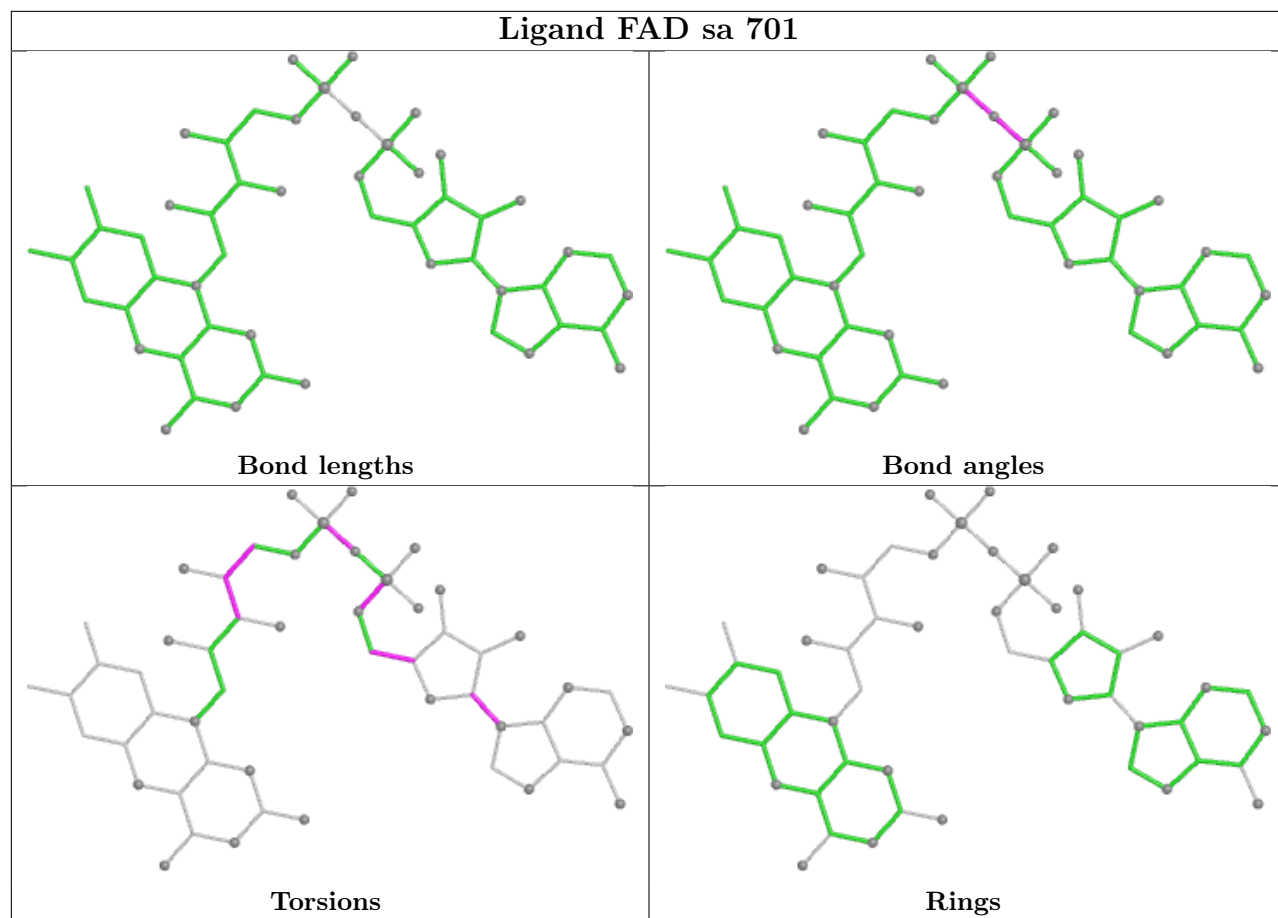


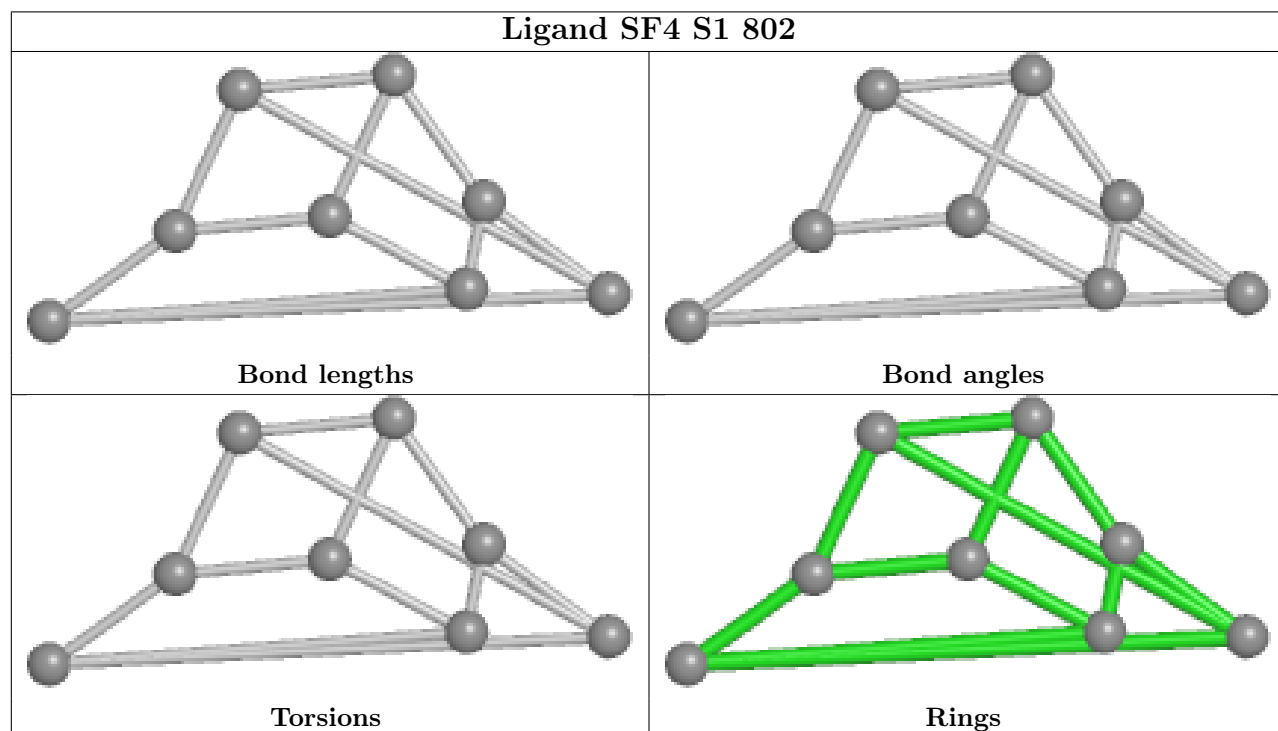
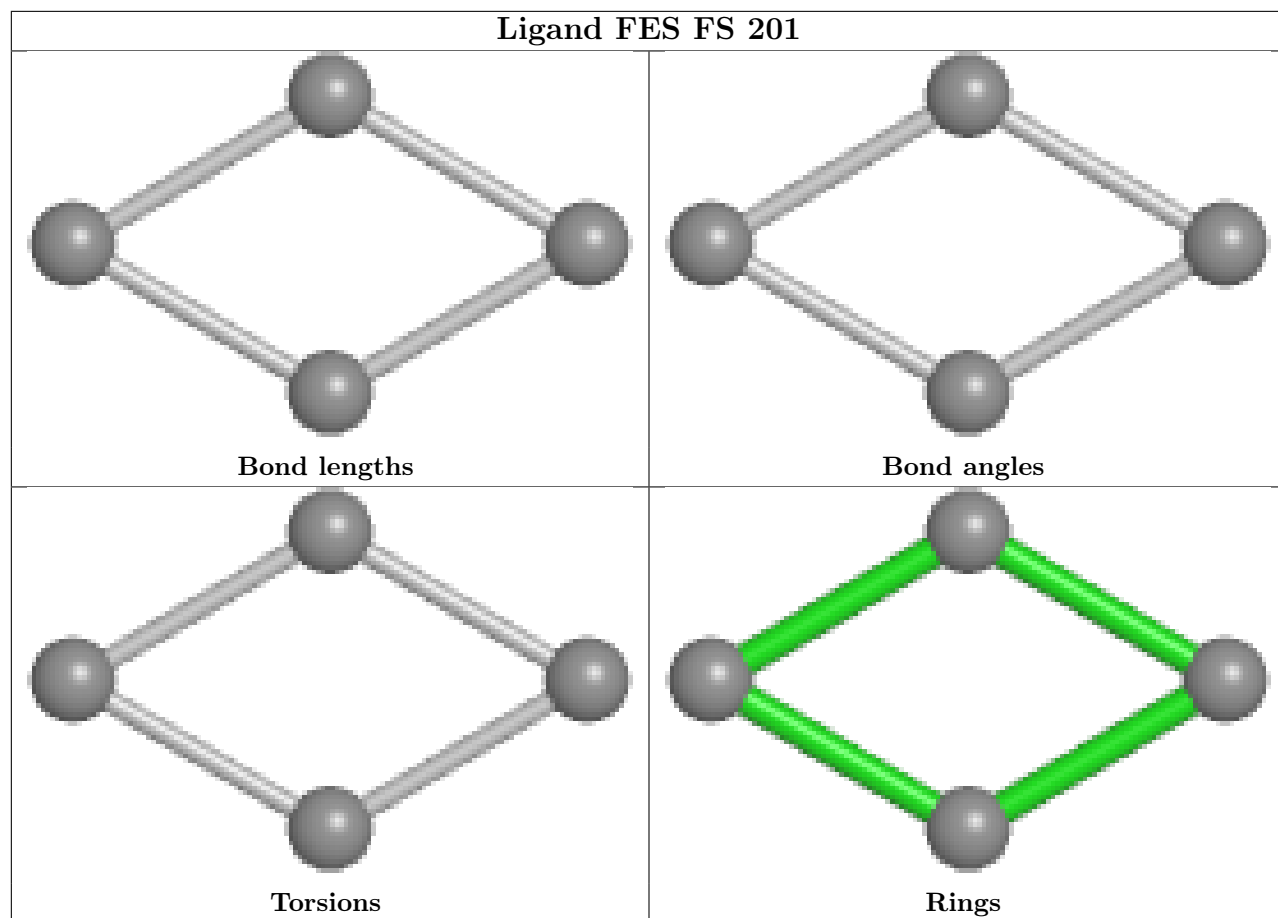
Torsions

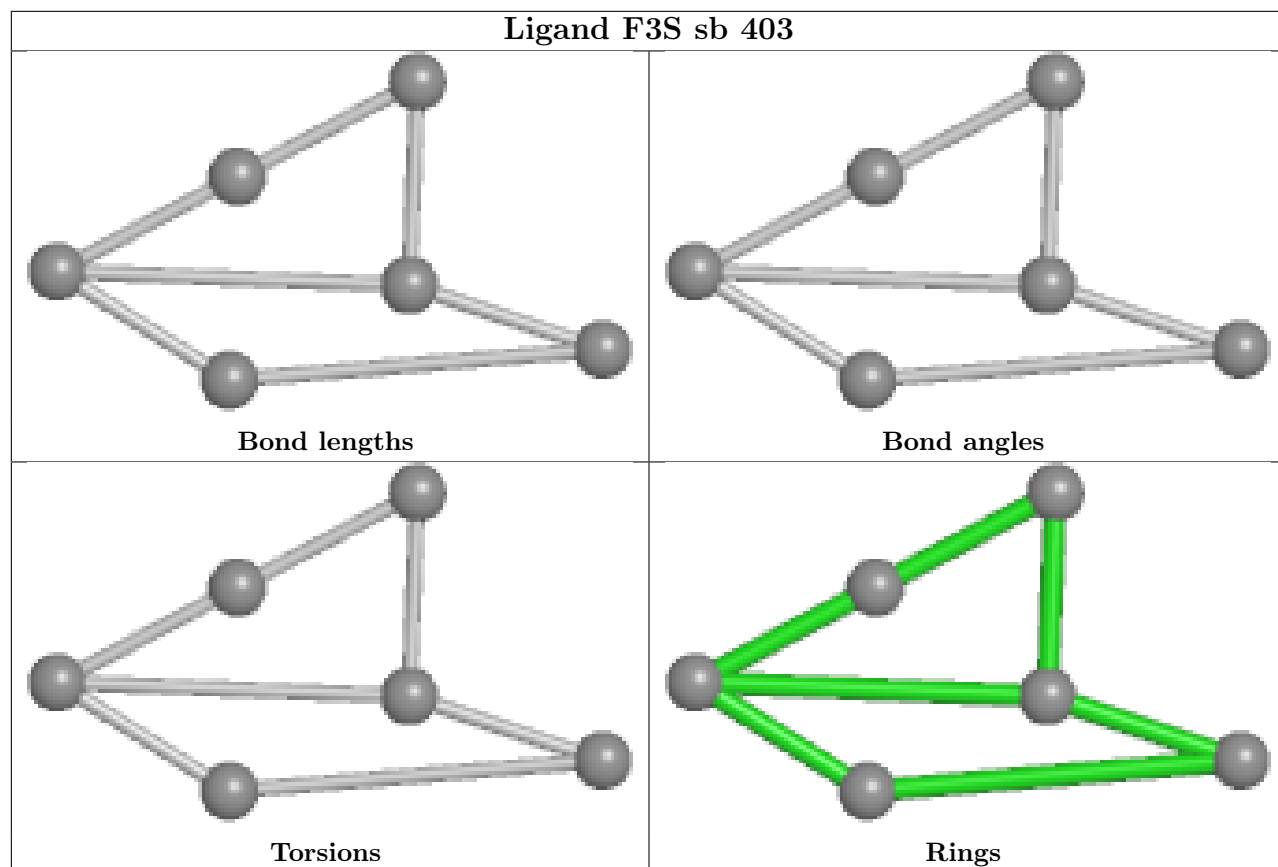


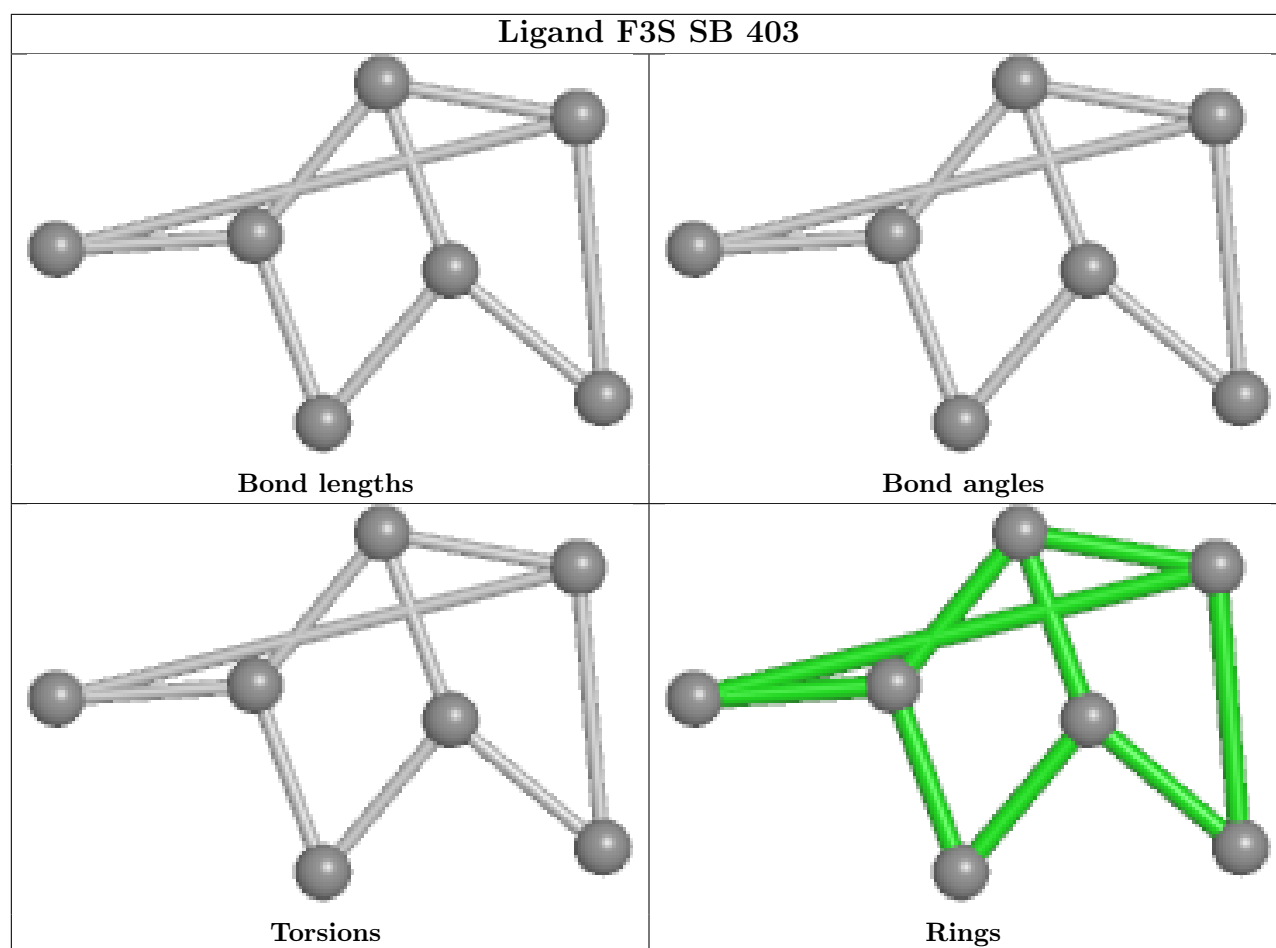
Rings

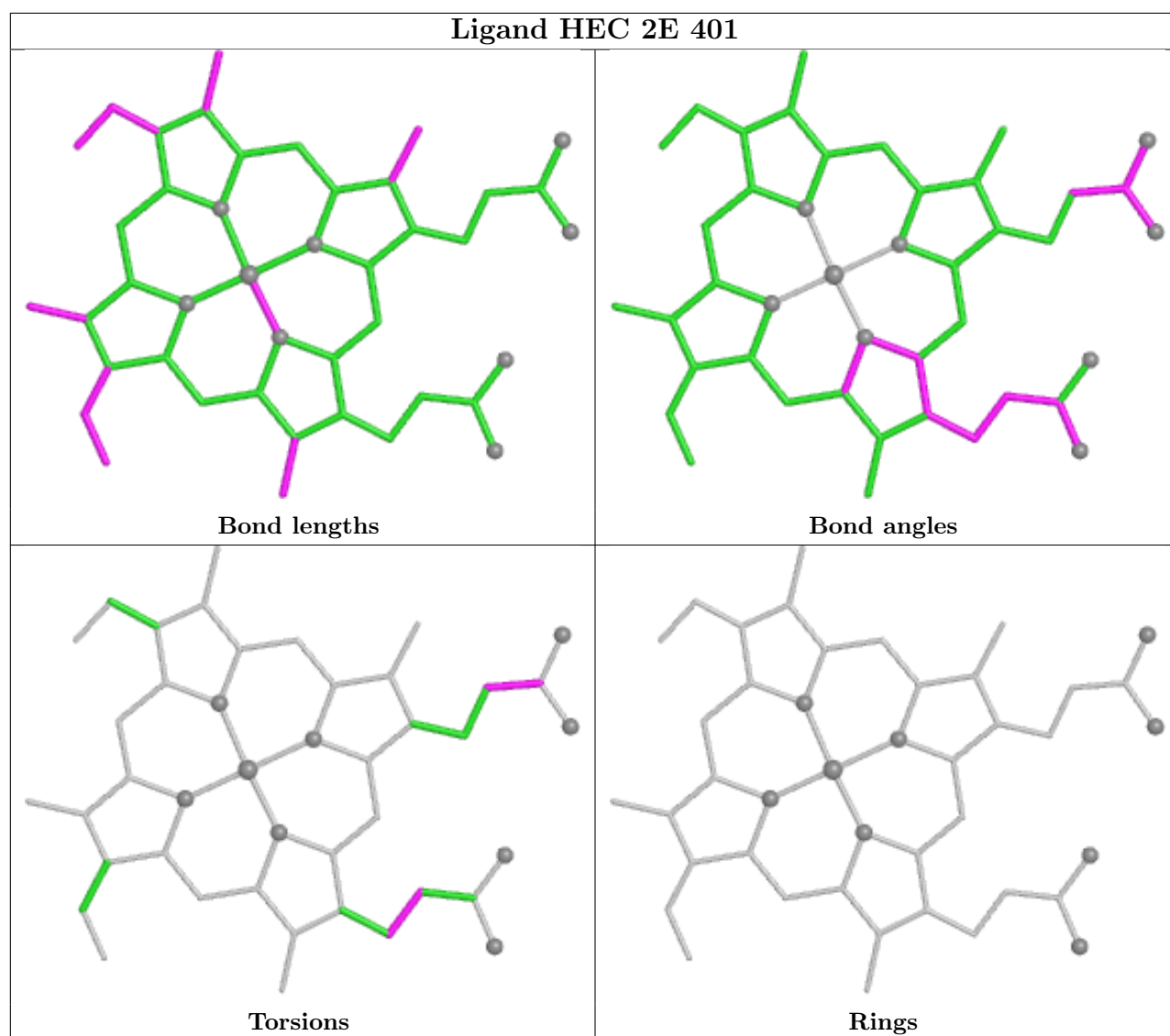


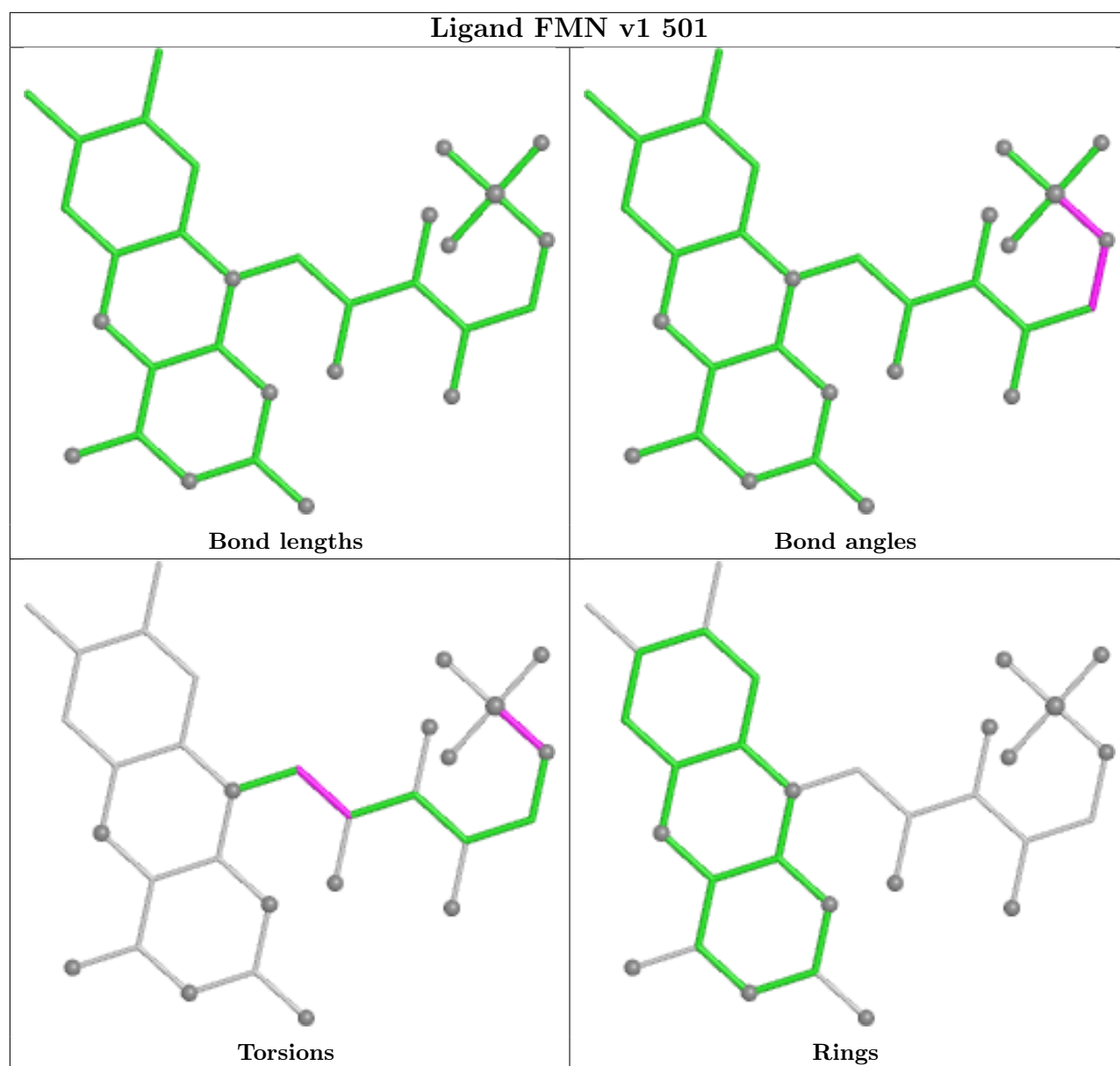












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

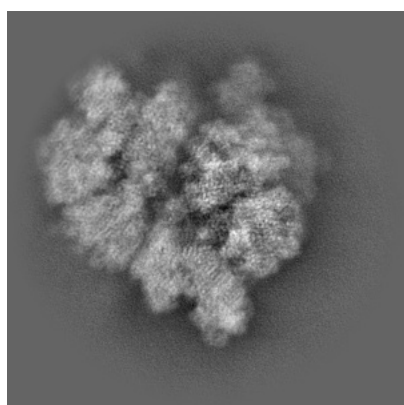
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34403. These allow visual inspection of the internal detail of the map and identification of artifacts.

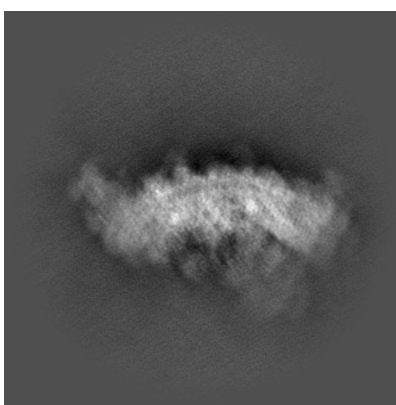
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

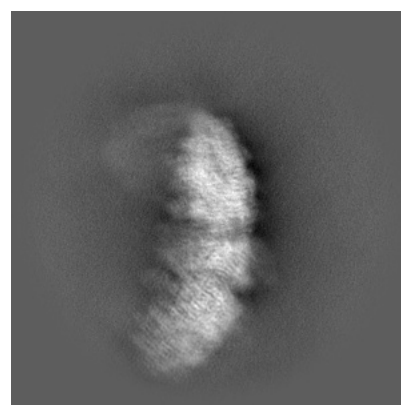
6.1.1 Primary map



X



Y

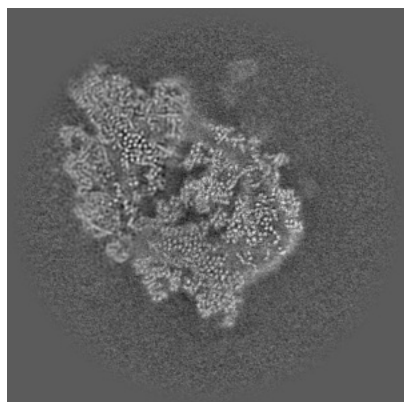


Z

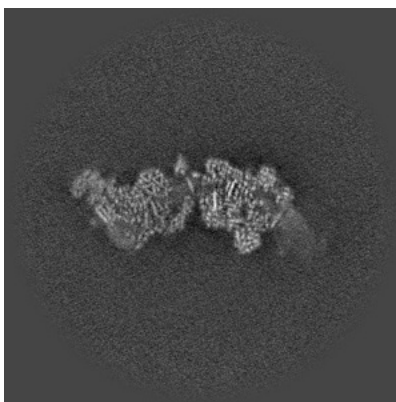
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

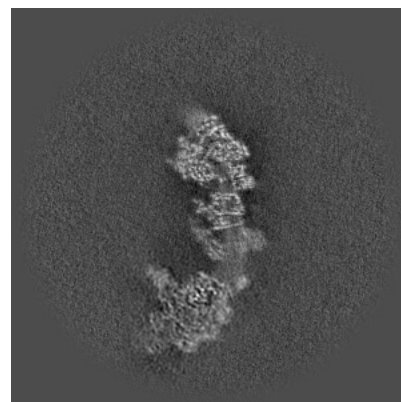
6.2.1 Primary map



X Index: 350



Y Index: 350

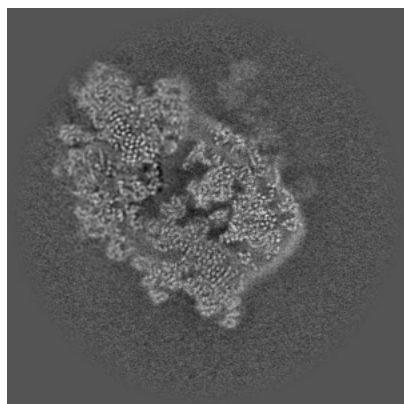


Z Index: 350

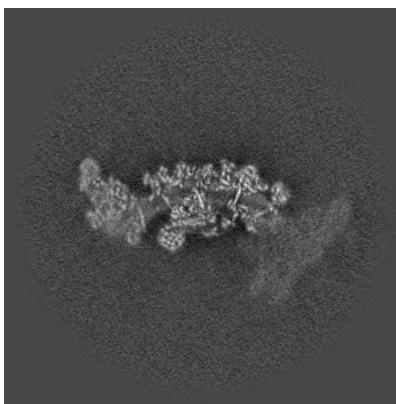
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

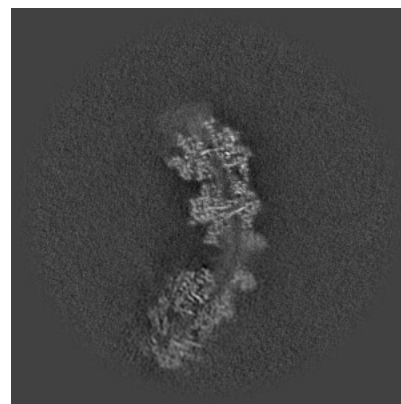
6.3.1 Primary map



X Index: 344



Y Index: 401

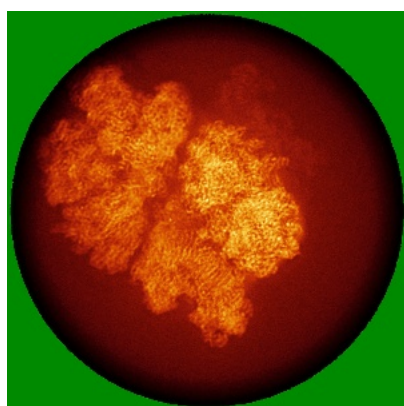


Z Index: 367

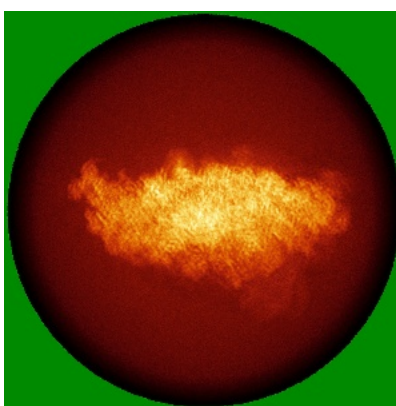
The images above show the largest variance slices of the map in three orthogonal directions.

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

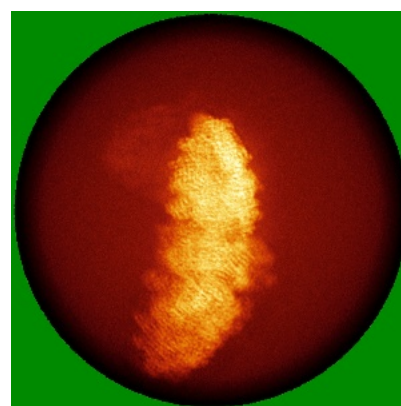
6.4.1 Primary map



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](#)

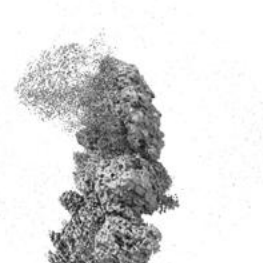
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

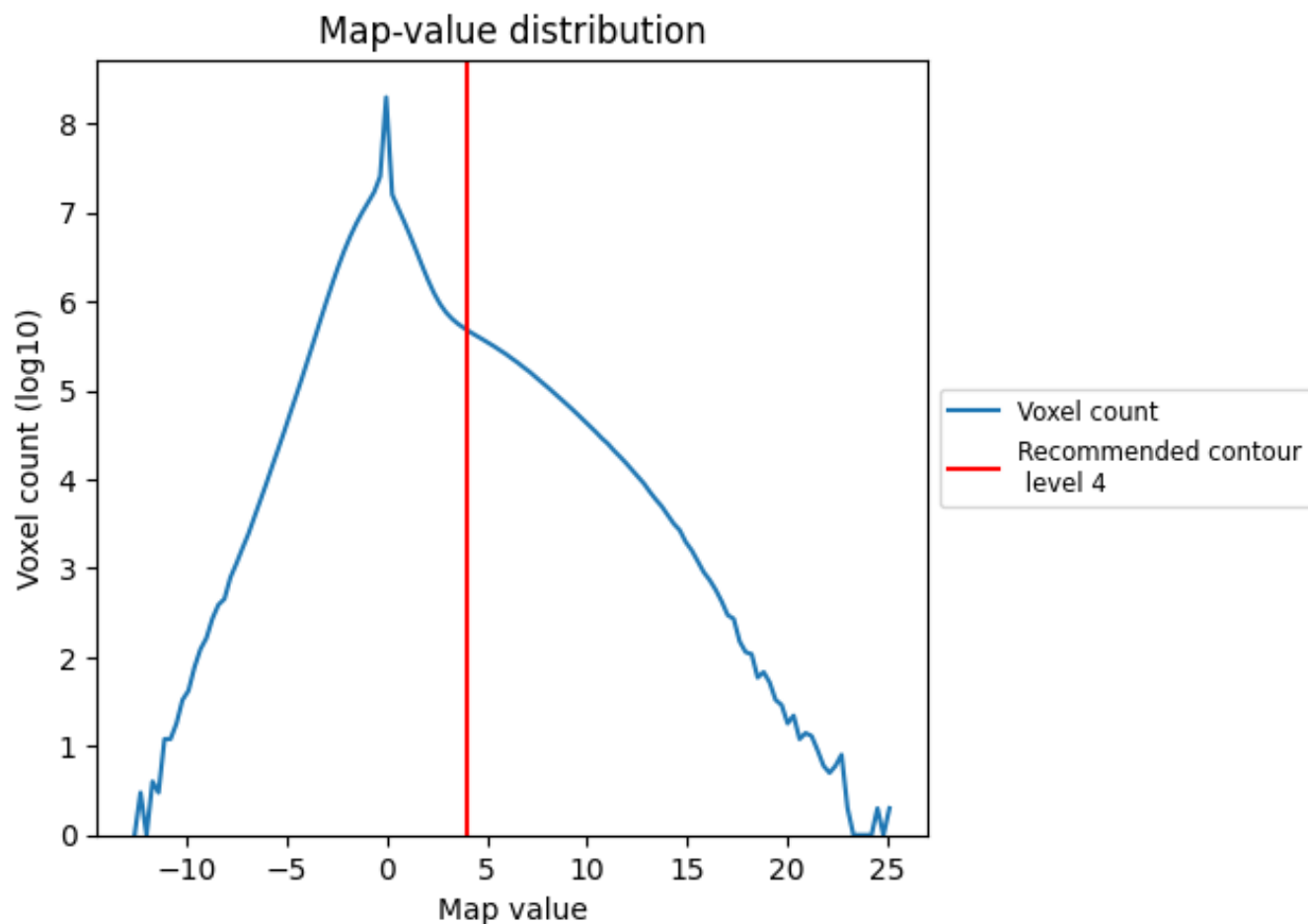
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

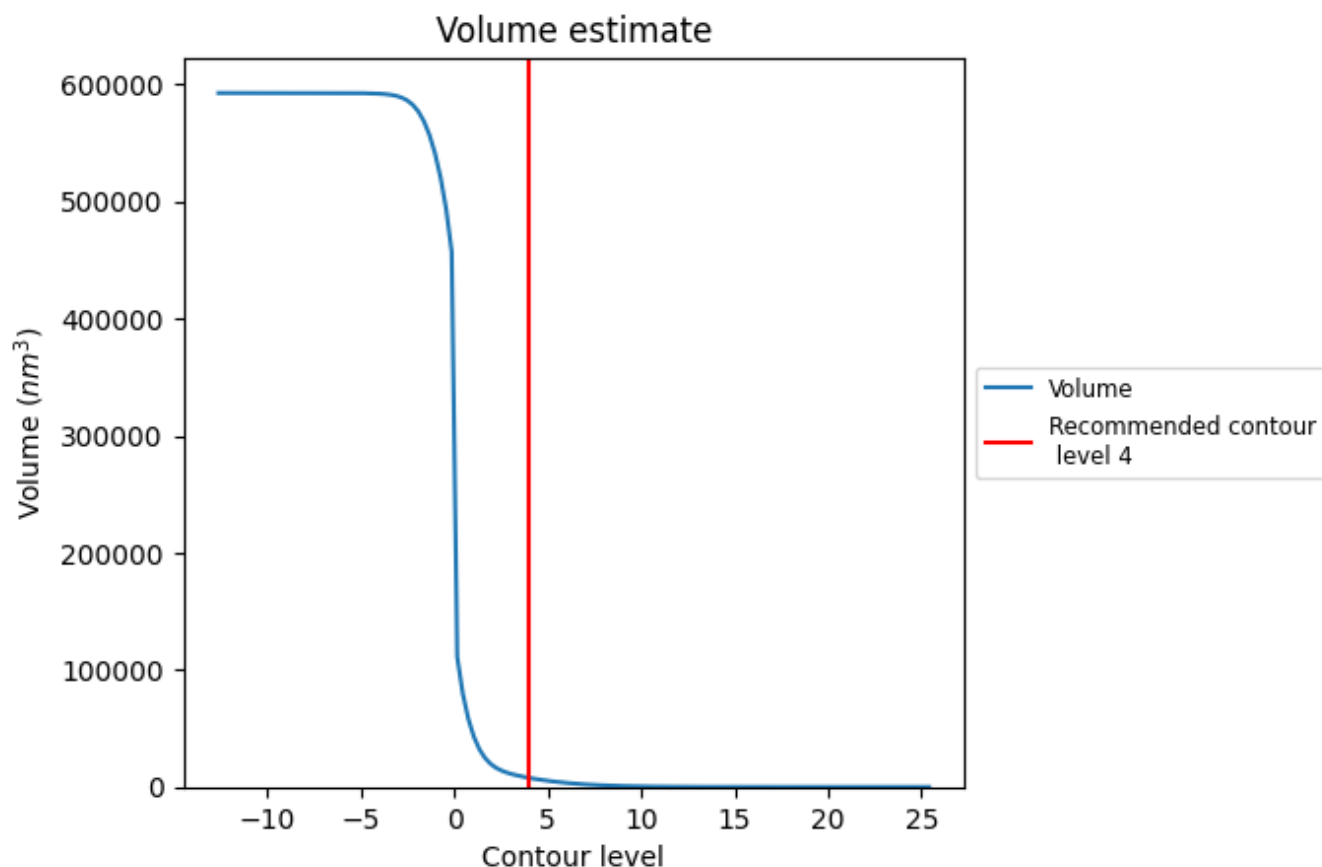
This section contains the results of statistical analysis of the map.

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.

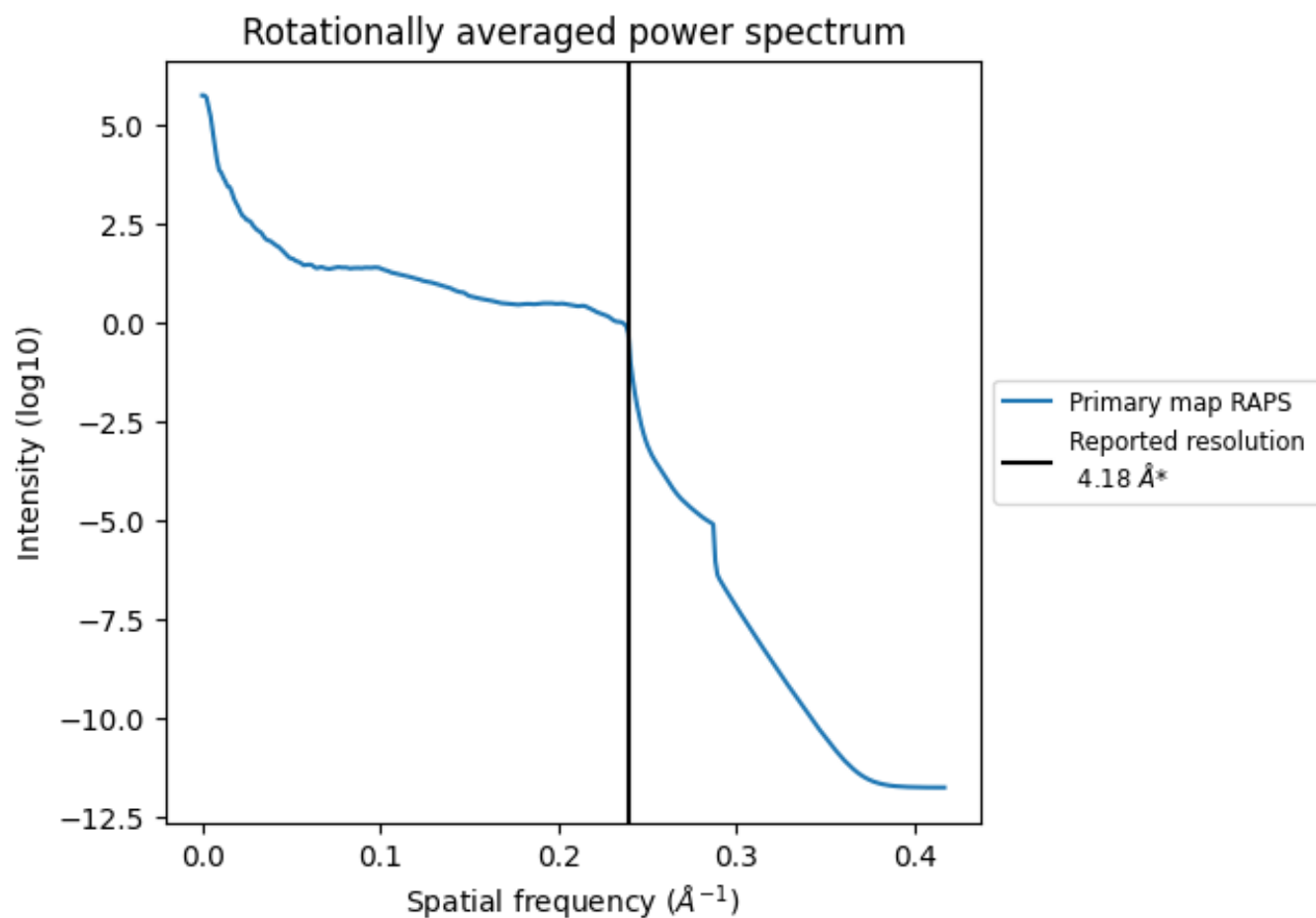
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7733 nm³; this corresponds to an approximate mass of 6985 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 0.239 Å⁻¹

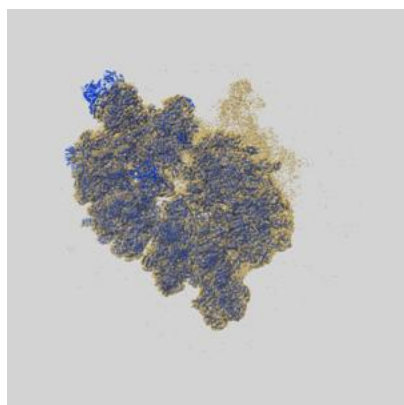
8 Fourier-Shell correlation

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

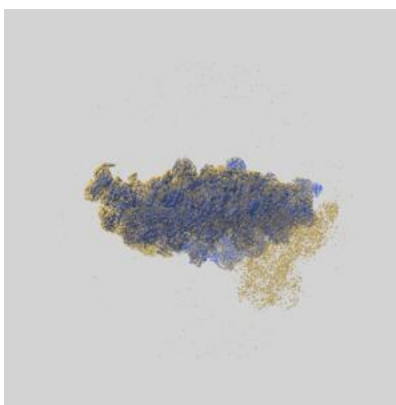
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34403 and PDB model 8GZU. Per-residue inclusion information can be found in section [3](#) on page [67](#).

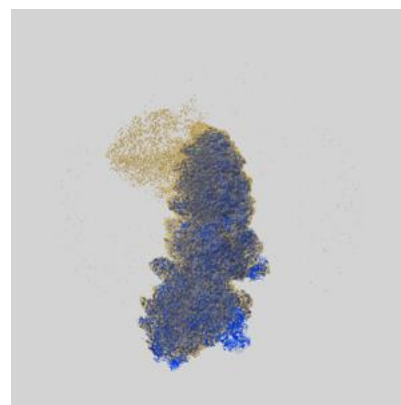
9.1 Map-model overlay [i](#)



X



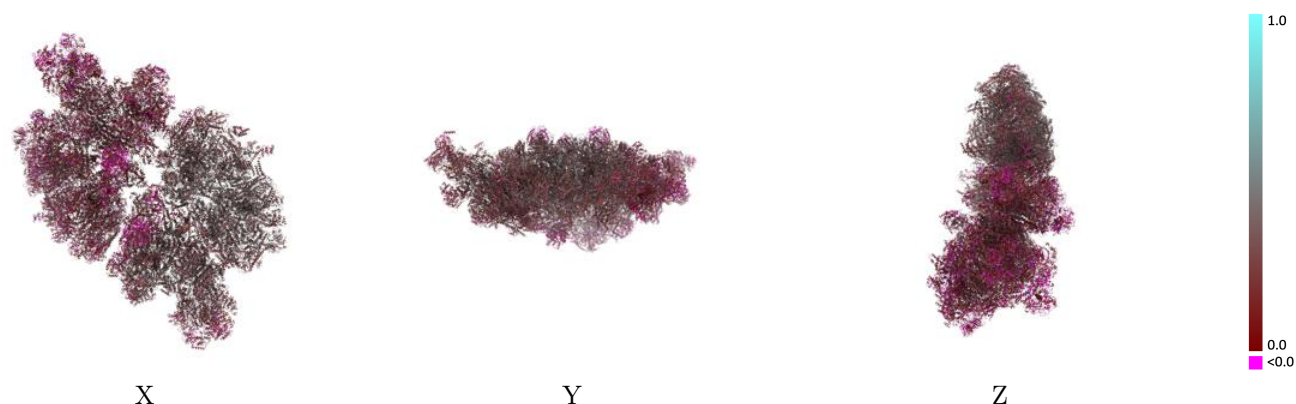
Y



Z

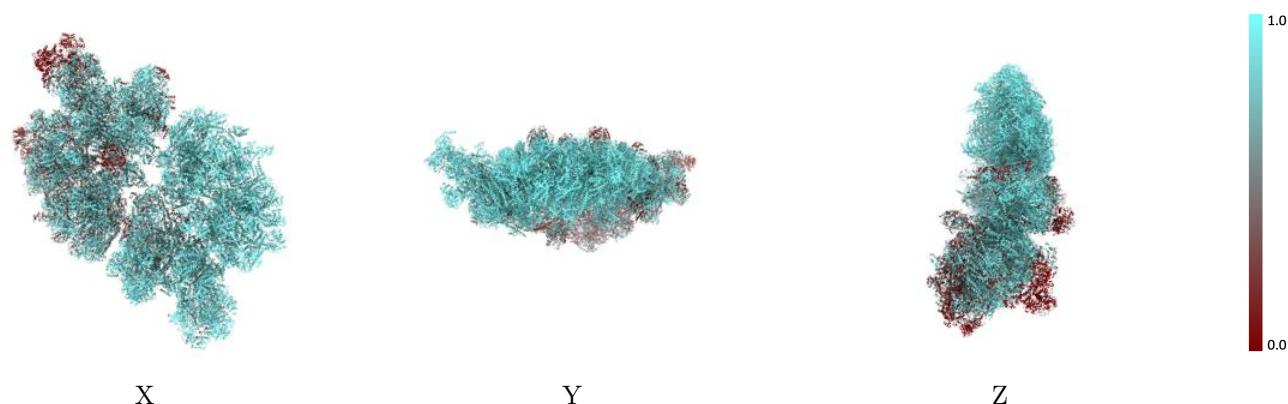
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



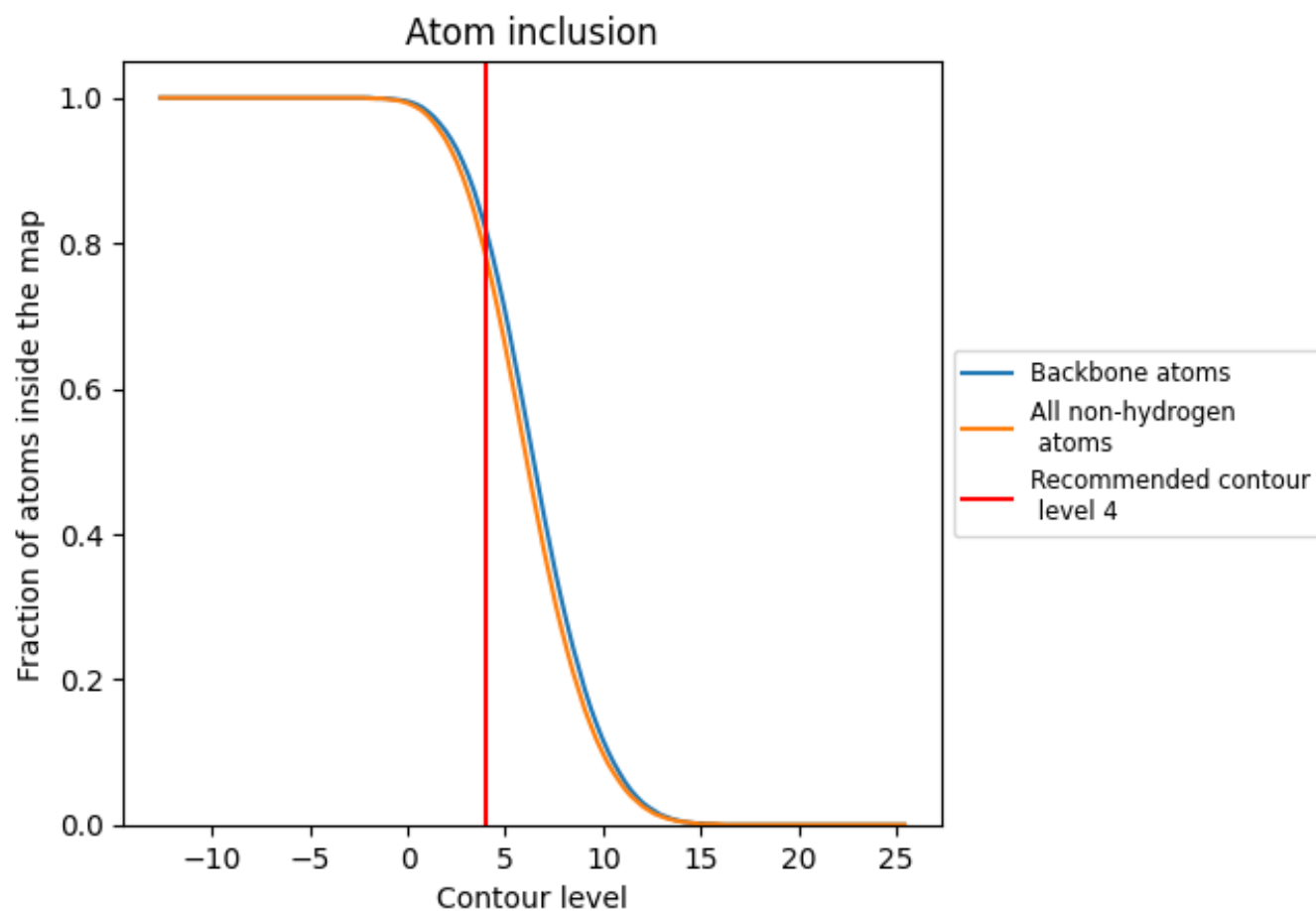
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.2530
00	 0.7960	 0.1970
01	 0.5440	 0.1470
02	 0.4120	 0.1360
03	 0.3770	 0.1520
04	 0.7010	 0.1980
05	 0.8910	 0.2120
06	 0.7960	 0.2040
07	 0.7370	 0.2230
08	 0.3420	 0.1910
09	 0.7060	 0.2120
0A	 0.6160	 0.1790
0B	 0.1520	 0.1330
0C	 0.7030	 0.1720
0D	 0.6720	 0.2060
0E	 0.7310	 0.1840
0F	 0.6880	 0.2100
0G	 0.6240	 0.1650
0H	 0.7720	 0.2630
0I	 0.5650	 0.1840
0J	 0.5770	 0.1810
10	 0.7310	 0.2270
11	 0.3140	 0.1880
12	 0.6560	 0.2270
13	 0.5870	 0.2150
14	 0.4180	 0.1990
15	 0.7310	 0.1710
16	 0.5840	 0.2140
17	 0.3090	 0.1690
18	 0.3340	 0.1840
19	 0.6290	 0.2330
1B	 0.9490	 0.3150
1T	 0.9430	 0.2970
1b	 0.7540	 0.2100
1t	 0.9690	 0.3020



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Chain	Atom inclusion	Q-score
20	 0.8420	 0.2370
21	 0.8530	 0.2010
22	 0.5870	 0.2420
23	 0.4980	 0.2060
24	 0.5070	 0.2120
25	 0.1380	 0.1900
26	 0.7100	 0.2290
27	 0.6100	 0.1960
28	 0.6810	 0.2100
29	 0.7220	 0.2020
2B	 0.8550	 0.3550
2E	 0.6230	 0.1370
2F	 0.7960	 0.3050
2G	 0.8680	 0.1890
2H	 0.6730	 0.3180
2I	 0.7570	 0.2970
2J	 0.8670	 0.2170
2K	 0.8550	 0.2910
2L	 0.8580	 0.3100
2M	 0.8030	 0.2720
2N	 0.6850	 0.2540
2O	 0.8190	 0.2750
2T	 0.9430	 0.2590
2b	 0.7870	 0.2480
2e	 0.7520	 0.1180
2f	 0.8150	 0.2280
2g	 0.8550	 0.1320
2h	 0.7650	 0.2390
2i	 0.7160	 0.2400
2j	 0.8850	 0.1760
2k	 0.8140	 0.2140
2l	 0.7610	 0.2430
2m	 0.8950	 0.2030
2n	 0.8480	 0.2050
2o	 0.9240	 0.1990
2t	 0.9710	 0.2620
30	 0.6490	 0.2300
31	 0.5480	 0.2070
32	 0.7500	 0.2280
33	 0.7340	 0.2210
34	 0.6720	 0.2130
35	 0.7220	 0.2050

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Chain	Atom inclusion	Q-score
36	 0.5870	 0.2240
37	 0.8170	 0.2280
38	 0.7880	 0.2070
39	 0.4530	 0.1870
3T	 0.9540	 0.2630
3t	 0.9900	 0.2980
40	 0.6990	 0.1910
41	 0.4110	 0.1540
42	 0.4600	 0.1410
43	 0.6700	 0.1470
44	 0.5920	 0.1190
45	 0.4480	 0.1000
46	 0.8240	 0.1670
47	 0.8600	 0.2030
48	 0.6800	 0.2160
49	 0.6830	 0.1960
4A	 0.9680	 0.3900
4L	 0.9030	 0.3650
4T	 0.9790	 0.3000
4a	 0.9820	 0.3890
4l	 0.8000	 0.2480
4t	 0.9930	 0.3190
50	 0.3780	 0.1890
51	 0.6910	 0.1960
52	 0.4260	 0.2080
53	 0.3170	 0.1740
54	 0.4000	 0.2400
55	 0.7410	 0.1920
56	 0.7610	 0.1780
57	 0.8430	 0.1660
58	 0.5510	 0.1670
59	 0.7840	 0.2080
5B	 0.8850	 0.3260
5T	 0.9770	 0.2620
5b	 0.8570	 0.2310
5t	 0.9810	 0.2840
60	 0.6850	 0.1860
61	 0.6730	 0.1770
62	 0.2730	 0.1160
63	 0.5890	 0.2310
64	 0.4550	 0.1820
65	 0.6160	 0.1690

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Chain	Atom inclusion	Q-score
66	 0.6180	 0.2250
67	 0.4700	 0.1790
68	 0.3910	 0.1410
69	 0.4650	 0.2030
6A	 0.9650	 0.3750
6B	 0.9540	 0.3750
6C	 0.9480	 0.3330
6L	 0.9790	 0.3210
6T	 0.9710	 0.2770
6a	 0.9620	 0.3730
6b	 0.9760	 0.3820
6c	 0.9780	 0.3270
6l	 0.9870	 0.3180
6t	 0.9740	 0.2930
70	 0.7720	 0.1700
71	 0.7350	 0.2340
72	 0.6720	 0.2410
73	 0.7530	 0.2250
74	 0.6470	 0.2310
75	 0.2680	 0.1540
76	 0.4240	 0.1560
77	 0.4790	 0.2130
78	 0.7720	 0.2070
79	 0.4160	 0.1780
7A	 0.9580	 0.3680
7C	 0.9400	 0.3800
7L	 0.9570	 0.3630
7a	 0.9790	 0.3730
7c	 0.9870	 0.3810
7l	 0.9800	 0.3490
80	 0.5060	 0.2520
81	 0.4630	 0.1770
82	 0.4180	 0.1450
83	 0.7050	 0.2100
84	 0.7470	 0.1800
85	 0.7390	 0.2220
86	 0.4900	 0.1810
87	 0.7230	 0.2220
88	 0.6530	 0.1510
89	 0.5300	 0.1770
90	 0.3840	 0.1430
91	 0.2540	 0.1150

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Chain	Atom inclusion	Q-score
92	 0.3560	 0.1420
93	 0.2080	 0.1630
94	 0.6070	 0.2080
95	 0.5900	 0.1980
96	 0.4540	 0.1690
97	 0.5350	 0.1550
98	 0.6000	 0.1670
99	 0.4720	 0.1350
A	 0.9780	 0.3750
A1	 0.9310	 0.3140
A2	 0.9610	 0.2560
A3	 0.9150	 0.3130
A5	 0.9180	 0.3280
A6	 0.9600	 0.3410
A7	 0.9460	 0.2930
A8	 0.9560	 0.2860
A9	 0.9540	 0.3280
AB	 0.8990	 0.3600
AC	 0.9690	 0.2940
AL	 0.9480	 0.2970
AM	 0.9240	 0.3160
AN	 0.8150	 0.3360
B	 0.8990	 0.2250
B2	 0.7880	 0.2450
B3	 0.8980	 0.2880
B4	 0.8130	 0.3230
B6	 0.8330	 0.3010
B7	 0.8440	 0.2550
B8	 0.8550	 0.3230
B9	 0.9110	 0.3220
BL	 0.7620	 0.3040
BM	 0.8150	 0.2880
BP	 0.9520	 0.2770
C	 0.9610	 0.2740
C1	 0.9430	 0.3560
C2	 0.9750	 0.3620
C3	 0.9570	 0.3200
C4	 0.8300	 0.2830
D	 0.8770	 0.2860
E	 0.9880	 0.3860
F	 0.9810	 0.3810
FS	 0.9860	 0.3910

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Chain	Atom inclusion	Q-score
FX	 0.9320	 0.3970
G	 0.9700	 0.4080
G1	 0.9420	 0.3610
G2	 0.9500	 0.3110
G3	 0.9530	 0.3190
H	 0.9220	 0.3380
I	 0.9590	 0.3690
J	 0.9550	 0.3050
J1	 0.9340	 0.3270
K	 0.9760	 0.3330
L	 0.9430	 0.3160
M	 0.9680	 0.3900
M1	 0.9490	 0.3310
M2	 0.9200	 0.2900
M3	 0.9380	 0.2800
N	 0.9330	 0.3250
N1	 0.8960	 0.3150
N2	 0.8920	 0.3420
N3	 0.8830	 0.3220
N4	 0.8410	 0.3260
N5	 0.8140	 0.2880
N6	 0.8810	 0.3270
O	 0.9770	 0.3220
P	 0.9790	 0.3020
P1	 0.9090	 0.2600
P2	 0.9370	 0.2110
Q	 0.9360	 0.3750
QA	 0.9710	 0.2900
QB	 0.9520	 0.3290
QC	 0.8670	 0.3180
QD	 0.8840	 0.3190
QE	 0.7750	 0.2820
QF	 0.8090	 0.3220
QG	 0.8940	 0.3130
QH	 0.9390	 0.3450
QI	 0.9260	 0.3420
QJ	 0.8810	 0.3380
QL	 0.8500	 0.2640
QM	 0.8240	 0.3240
Qa	 0.9460	 0.2730
Qb	 0.8490	 0.2580
Qc	 0.8680	 0.2930

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Chain	Atom inclusion	Q-score
Qd	 0.8800	 0.2800
Qe	 0.8320	 0.2450
Qf	 0.7030	 0.2440
Qg	 0.9140	 0.2940
Qh	 0.8680	 0.2860
Qi	 0.8890	 0.2780
Qj	 0.8010	 0.2900
Ql	 0.8690	 0.2920
Qm	 0.9060	 0.2680
R	 0.9590	 0.3500
S	 0.9890	 0.3360
S1	 0.8930	 0.2710
S2	 0.9290	 0.3410
S3	 0.9330	 0.3470
S4	 0.7990	 0.3110
S5	 0.7900	 0.3100
S6	 0.9690	 0.2540
S7	 0.9310	 0.3240
S8	 0.9380	 0.3160
SA	 0.5510	 0.1160
SB	 0.7800	 0.1770
SC	 0.7970	 0.2330
SD	 0.8680	 0.2320
T	 0.9390	 0.3830
T1	 0.9240	 0.2400
T2	 0.8210	 0.1990
T3	 0.8850	 0.1800
T4	 0.6570	 0.2210
T5	 0.7210	 0.2820
T6	 0.7420	 0.3080
T7	 0.9400	 0.2700
T8	 0.8140	 0.3070
T9	 0.7420	 0.2560
TA	 0.8850	 0.3240
TB	 0.8740	 0.3220
TC	 0.8890	 0.3230
TD	 0.9420	 0.2790
TE	 0.9230	 0.2880
TF	 0.9130	 0.2860
TG	 0.5500	 0.2700
TH	 0.8070	 0.2780
TX	 0.9360	 0.3620

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Chain	Atom inclusion	Q-score
U	 0.9430	 0.3410
U1	 0.9220	 0.3120
U2	 0.9060	 0.3790
V	 0.9530	 0.3620
V1	 0.8910	 0.2030
V2	 0.8820	 0.2110
VB	 0.9830	 0.3560
W	 0.9850	 0.3670
X	 0.9470	 0.3360
X1	 0.6840	 0.3000
Y	 0.9730	 0.3710
Y0	 0.9710	 0.4110
Y5	 0.9650	 0.3420
Y7	 0.9640	 0.3330
Z	 0.9250	 0.3670
Z1	 0.9140	 0.3480
a	 0.9900	 0.3890
a1	 0.7210	 0.1920
a2	 0.5960	 0.1670
a3	 0.7740	 0.1790
a5	 0.7210	 0.2070
a6	 0.7720	 0.2150
a7	 0.7230	 0.1930
a8	 0.6500	 0.1660
a9	 0.7640	 0.1700
ab	 0.8290	 0.2480
ac	 0.9550	 0.2160
al	 0.7780	 0.1600
am	 0.6750	 0.2030
an	 0.7080	 0.2240
b	 0.9610	 0.2900
b2	 0.8700	 0.1920
b3	 0.9150	 0.2270
b4	 0.8330	 0.2440
b6	 0.8710	 0.2280
b7	 0.8780	 0.2170
b8	 0.8470	 0.2290
b9	 0.8750	 0.2240
bl	 0.8190	 0.2440
bm	 0.8280	 0.2150
bp	 0.9920	 0.3370
c	 0.9680	 0.3010

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Chain	Atom inclusion	Q-score
c1	 0.9620	 0.3620
c2	 0.9800	 0.3630
c3	 0.9700	 0.3470
c4	 0.6920	 0.2280
d	 0.9590	 0.3030
e	 0.9730	 0.3890
f	 0.9950	 0.3870
fs	 0.9880	 0.3860
fx	 0.8680	 0.2390
g	 0.9810	 0.4200
g1	 0.8130	 0.1920
g2	 0.8730	 0.1970
g3	 0.8590	 0.2160
h	 0.9780	 0.3080
i	 0.9550	 0.3640
j	 0.9690	 0.3280
j1	 0.8080	 0.2230
k	 0.9890	 0.3700
l	 0.9490	 0.3410
m	 0.9790	 0.3980
m1	 0.9840	 0.3400
m2	 0.9900	 0.3160
m3	 0.9460	 0.3070
n	 0.9860	 0.3320
n1	 0.7330	 0.2160
n2	 0.8270	 0.2470
n3	 0.7370	 0.2120
n4	 0.8400	 0.2440
n5	 0.8220	 0.2360
n6	 0.7200	 0.2230
o	 0.9880	 0.3420
p	 0.9910	 0.3440
p1	 0.9070	 0.1860
p2	 0.8240	 0.1820
q	 0.9730	 0.3870
qA	 0.8550	 0.2060
qB	 0.8570	 0.2200
qC	 0.7790	 0.2090
qD	 0.8380	 0.2080
qE	 0.8410	 0.1880
qF	 0.8000	 0.2270
qG	 0.8110	 0.2070

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Chain	Atom inclusion	Q-score
qH	 0.8240	 0.1870
qI	 0.8840	 0.2610
qJ	 0.8630	 0.2280
qL	 0.8310	 0.2090
qM	 0.7290	 0.1390
qa	 0.8650	 0.1880
qb	 0.6150	 0.1290
qc	 0.8230	 0.2040
qd	 0.7400	 0.1800
qe	 0.6630	 0.1400
qf	 0.1010	 0.1100
qg	 0.7690	 0.1890
qh	 0.7170	 0.1700
qi	 0.6050	 0.1610
qj	 0.7700	 0.1950
ql	 0.8940	 0.2160
qm	 0.4710	 0.1100
r	 0.9410	 0.3500
s	 0.9450	 0.3580
s1	 0.4360	 0.1420
s2	 0.7190	 0.1790
s3	 0.7180	 0.1680
s4	 0.4320	 0.1650
s5	 0.5690	 0.1610
s6	 0.5200	 0.1240
s7	 0.7620	 0.1670
s8	 0.7400	 0.1570
sa	 0.1370	 0.0580
sb	 0.6150	 0.1080
sc	 0.8500	 0.1880
sd	 0.9090	 0.1990
t	 0.9610	 0.3930
t1	 0.6220	 0.1450
t2	 0.0530	 0.1350
t3	 0.7220	 0.1770
t4	 0.7840	 0.2030
t5	 0.8850	 0.2630
t6	 0.5870	 0.2000
t7	 0.6690	 0.1840
t8	 0.7400	 0.2300
t9	 0.6340	 0.2110
ta	 0.8090	 0.2360

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Chain	Atom inclusion	Q-score
tb	 0.8250	 0.2190
tc	 0.6550	 0.2200
td	 0.6880	 0.1670
te	 0.4400	 0.0920
tf	 0.3710	 0.1980
tg	 0.7370	 0.2420
th	 0.7760	 0.2550
tx	 0.8590	 0.2310
u	 0.9780	 0.3210
u1	 0.9000	 0.3360
u2	 0.8240	 0.3690
v	 0.9890	 0.3740
v1	 0.0340	 0.1160
v2	 0.0020	 0.1230
vb	 0.9810	 0.3850
w	 0.9770	 0.3680
x	 0.9850	 0.3490
x1	 0.6840	 0.1920
y	 0.9830	 0.3640
y0	 0.9780	 0.4330
y5	 0.8940	 0.3530
y7	 0.9830	 0.3440
z	 0.8440	 0.3580
z1	 0.9500	 0.3360