Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:26 PM JST

PDB ID	:	7DGQ
EMDB ID	:	EMD-30673
Title	:	Activity optimized supercomplex state1
Authors	:	Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on	:	2020-11-12
Resolution	:	5.00 Å(reported)

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

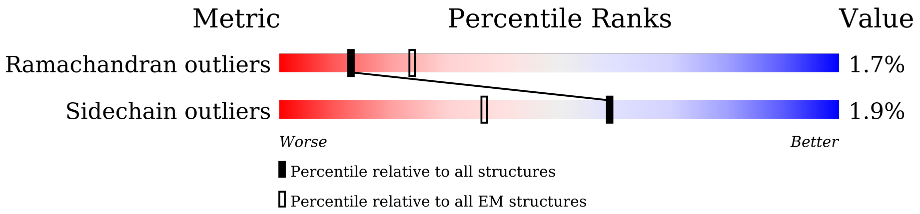
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

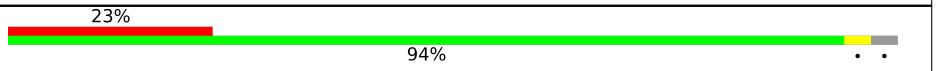
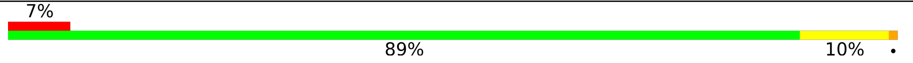
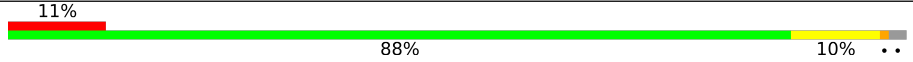
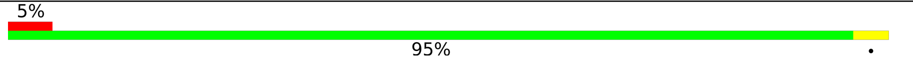
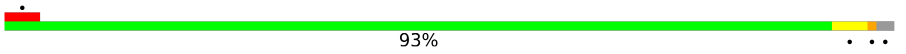
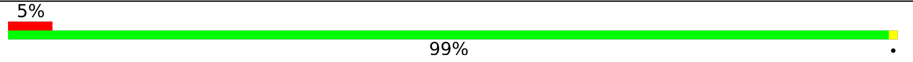
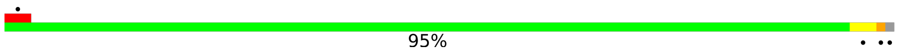
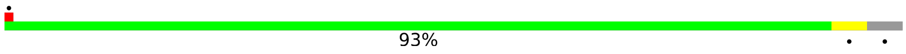
The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	3	115	
2	1	318	
3	9	217	
4	7	175	
5	4	459	
6	5	98	
7	6	606	
8	2	347	
9	8	444	

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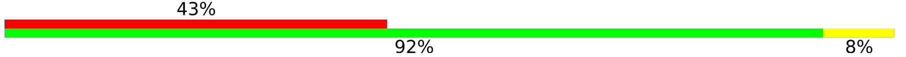
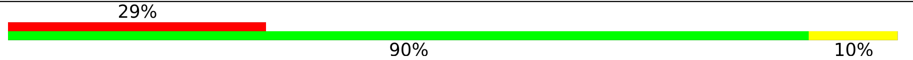
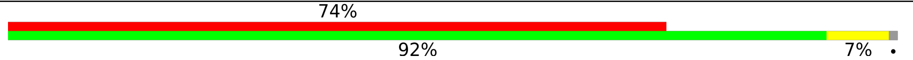
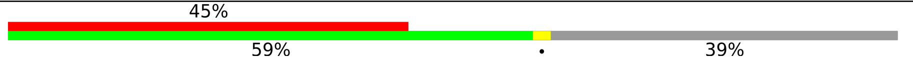
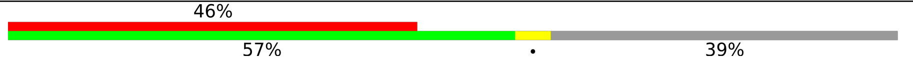
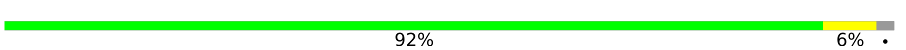
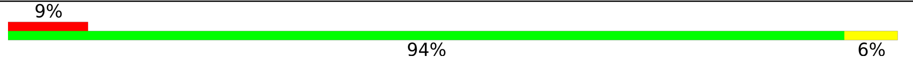
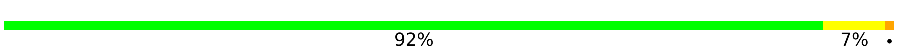
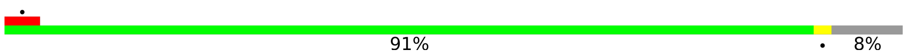
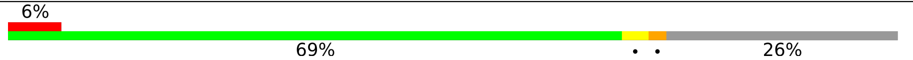
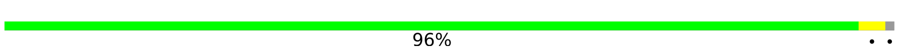
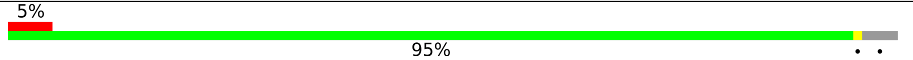
Mol	Chain	Length	Quality of chain
10	C3	514	 43% 92% 8%
11	C1	227	 29% 90% 10%
12	A9	261	 72% 90% 10%
13	A7	169	 72% 80% 5% 15%
14	B4	152	 71% 68% • 28%
15	A5	129	 64% 70% 5% • 24%
16	A6	97	 74% 64% 22% • 13%
17	C0	86	 58% 76% 12% 13%
18	C2	74	 74% 92% 7% •
19	B2	80	 64% 61% 6% • 30%
20	B3	80	 45% 59% • 39%
21	A0	63	 60% 71% • 25%
22	A8	70	 46% 57% • 39%
23	A	704	 92% 6% •
24	B	430	 9% 94% 6%
25	C	228	 89% • 9%
26	D	179	 • 78% 6% • 15%
27	E	176	 92% 7% •
28	F	75	 • 36% • 63%
29	G	133	 • 91% • 8%
30	H	105	 • 87% 5% 9%
31	I	96	 6% 69% • • 26%
32	J	70	 96% • •
33	K	98	 84% • 14%
34	L	83	 5% 95% • •

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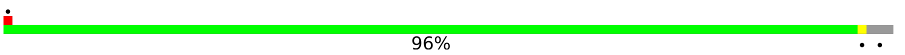
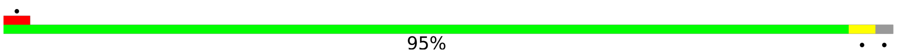
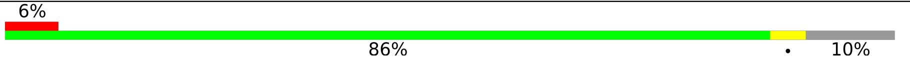
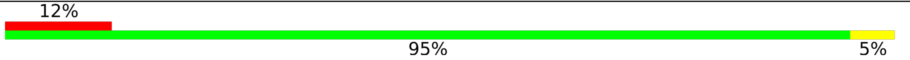
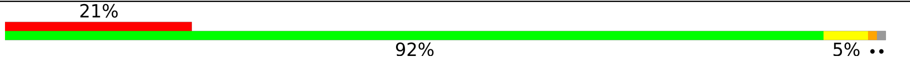
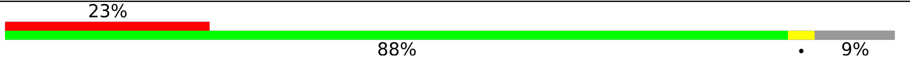
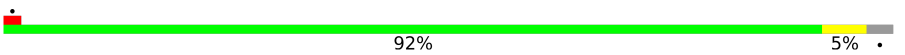
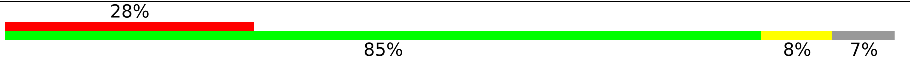
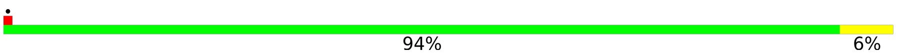
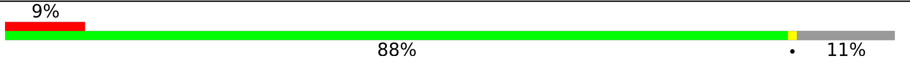
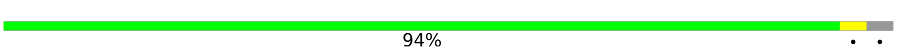
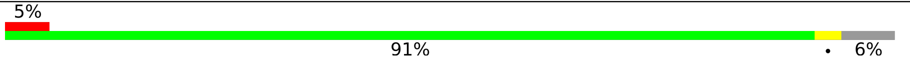
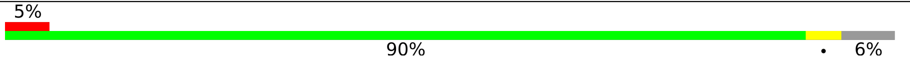
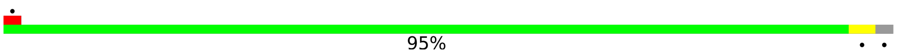
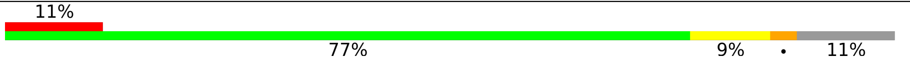
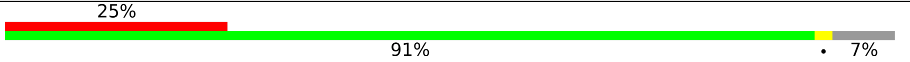
Mol	Chain	Length	Quality of chain
35	N	115	
36	O	127	
37	P	112	
38	Q	171	
39	R	345	
40	S	320	
41	T	140	
42	U	145	
43	V	143	
44	M	86	
44	W	86	
45	X	57	
46	Y	72	
47	Z	98	
48	a	128	
49	b	143	
50	c	128	
51	d	117	
52	f	178	
53	h	125	
54	i	49	
55	j	120	
56	g	176	
57	e	158	
58	k	480	

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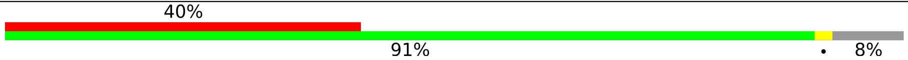
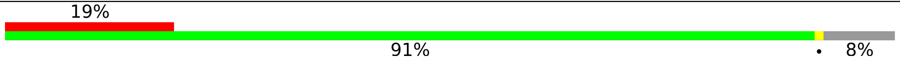
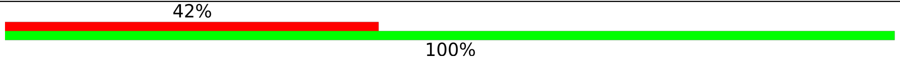
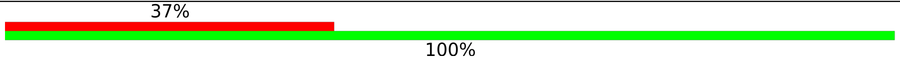
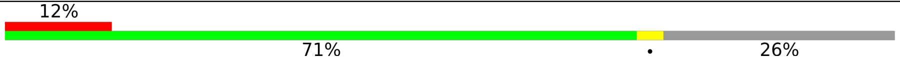
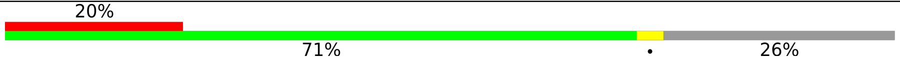
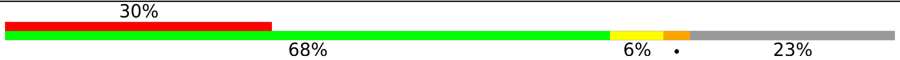
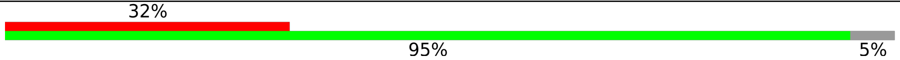
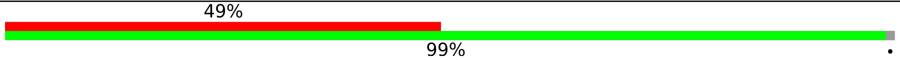
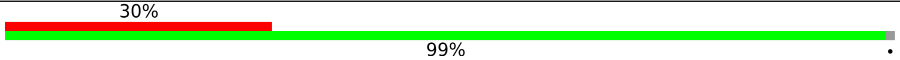
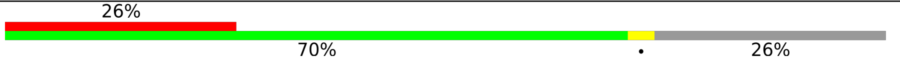
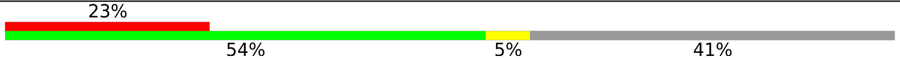
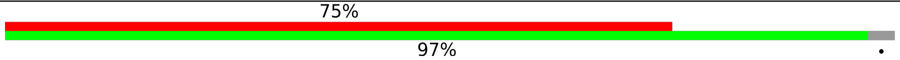
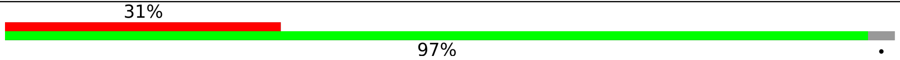
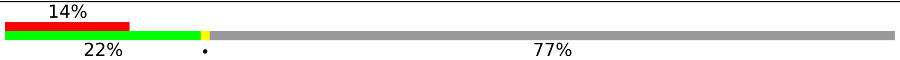
Mol	Chain	Length	Quality of chain
58	w	480	
59	l	453	
59	x	453	
60	m	379	
60	y	379	
61	o	325	
61	z	325	
62	A1	196	
62	p	196	
63	A2	111	
63	q	111	
64	A3	82	
64	r	82	
65	B7	91	
65	s	91	
66	A4	56	
66	t	56	
67	B6	64	
67	u	64	
68	B5	78	
68	v	78	

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
76	HEA	C3	602	X	-	-	-
76	HEA	C3	603	X	-	-	-

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 107321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	112	882	596	128	151	7	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	318	2503	1678	385	417	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	9	207	1579	1006	269	294	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	172	1235	835	181	211	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	458	3577	2382	561	599	35	1	0

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

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

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	606	4766	3172	732	820	42	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	2	344	2681	1779	413	449	40	0	0

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

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

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C3	514	4025	2690	623	677	35	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C1	227	1822	1184	281	339	18	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A9	261	2125	1421	338	353	13	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B4	109	878	558	150	168	2	0	0

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	A5	98	748	464	134	145	5	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	A6	84	671	431	129	110	1	0	0

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	C0	75	628	395	114	114	5	0	0

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	C2	73	598	388	107	99	4	0	0

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	B2	56	441	285	73	80	3	0	0

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	B3	49	384	250	65	67	2	0	0

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	A0	47	386	257	65	62	2	0	0

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	I	71	535	333	99	100	3	0	0

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

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

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

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	309	Total	C	N	O	S	0	0
			2349	1514	420	412	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	138	Total 923	C 584	N 162	O 171	S 6	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 44 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d	107	Total	C	N	O	S	0	0
			710	447	134	125	4		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	j	113	Total 892	C 587	N 149	O 153	S 3	0	0

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	k	446	Total 3454	C 2159	N 608	O 667	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	436	Total 3385	C 2117	N 599	O 649	S 20	0	0

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

- Molecule 60 is a protein called Cytochrome b.

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

- Molecule 61 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	p	151	Total 938	C 572	N 170	O 194	S 2	0	0
62	A1	188	Total 1117	C 679	N 207	O 229	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	q	106	Total 916	C 579	N 167	O 168	S 2	0	0
63	A2	106	Total 907	C 574	N 166	O 165	S 2	0	0

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	r	81	Total 682	C 441	N 128	O 112	S 1	0	0
64	A3	81	Total 676	C 438	N 125	O 112	S 1	0	0

- Molecule 65 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	s	67	Total 548	C 332	N 99	O 112	S 5	0	0
65	B7	69	Total 566	C 342	N 101	O 118	S 5	0	0

- Molecule 66 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	t	33	Total 262	C 174	N 46	O 42	0	0
66	A4	39	Total 318	C 212	N 56	O 50	0	0

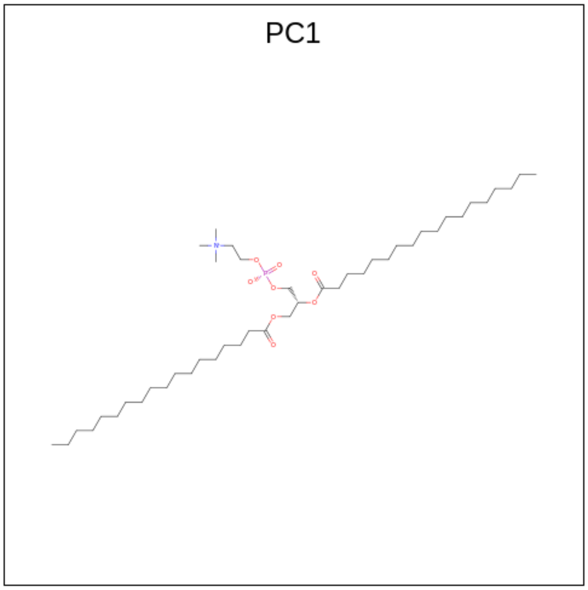
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	u	62	Total 511	C 335	N 89	O 87	0	0
67	B6	62	Total 511	C 335	N 89	O 87	0	0

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

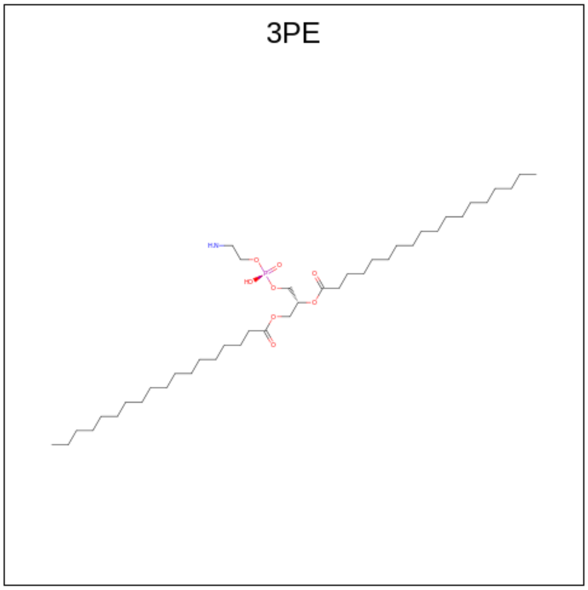
Mol	Chain	Residues	Atoms				AltConf	Trace
68	v	18	Total 114	C 70	N 22	O 22	0	0
68	B5	22	Total 148	C 91	N 30	O 27	0	0

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



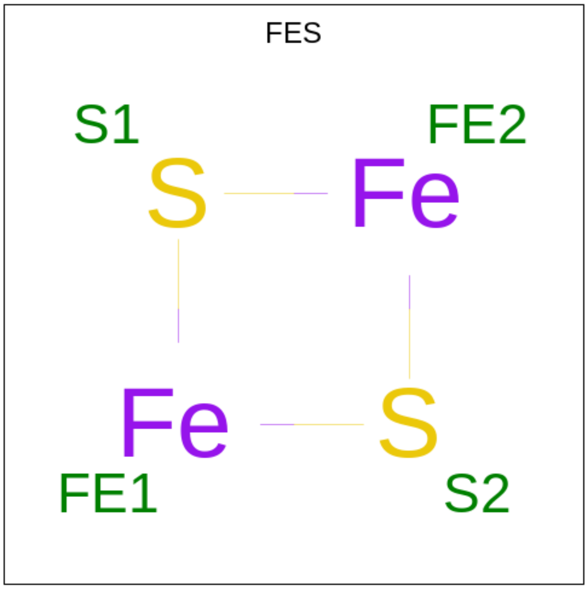
Mol	Chain	Residues	Atoms					AltConf
69	3	1	Total 47	C 37	N 1	O 8	P 1	0
69	2	1	Total 46	C 36	N 1	O 8	P 1	0
69	Q	1	Total 46	C 36	N 1	O 8	P 1	0
69	S	1	Total 47	C 37	N 1	O 8	P 1	0
69	j	1	Total 39	C 29	N 1	O 8	P 1	0

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



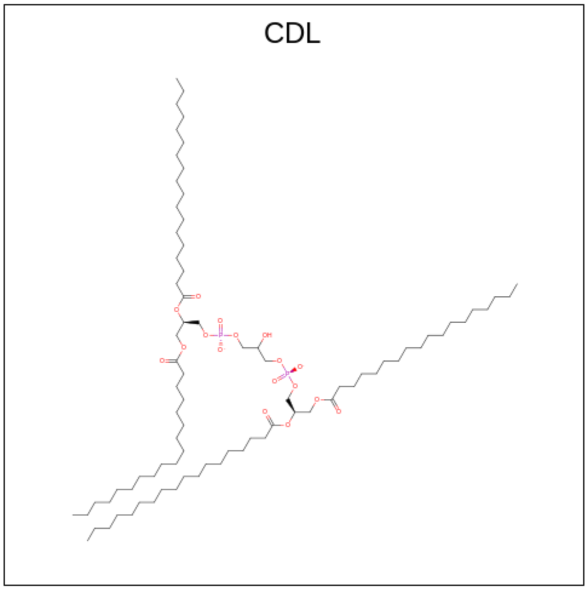
Mol	Chain	Residues	Atoms	AltConf
70	1	1	Total C N O P 51 41 1 8 1	0
70	4	1	Total C N O P 41 31 1 8 1	0
70	2	1	Total C N O P 41 31 1 8 1	0
70	B	1	Total C N O P 51 41 1 8 1	0
70	j	1	Total C N O P 46 36 1 8 1	0

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



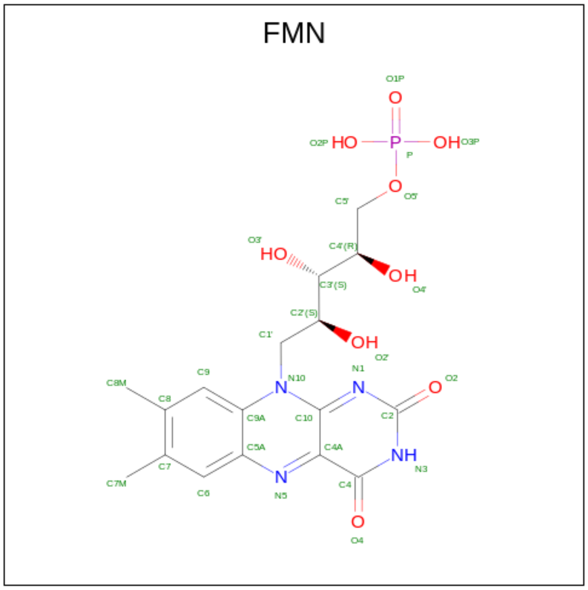
Mol	Chain	Residues	Atoms			AltConf
71	9	1	Total 4	Fe 2	S 2	0
71	A	1	Total 4	Fe 2	S 2	0
71	m	1	Total 4	Fe 2	S 2	0

- Molecule 72 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



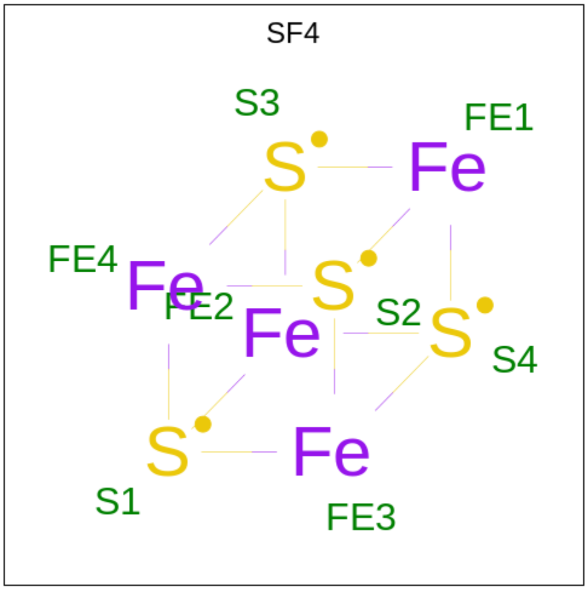
Mol	Chain	Residues	Atoms				AltConf
72	6	1	Total 64	C 45	O 17	P 2	0
72	J	1	Total 58	C 39	O 17	P 2	0
72	b	1	Total 82	C 63	O 17	P 2	0

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



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

- Molecule 74 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
74	8	1	Total Fe S 8 4 4	0
74	A	1	Total Fe S 16 8 8	0
74	A	1	Total Fe S 16 8 8	0

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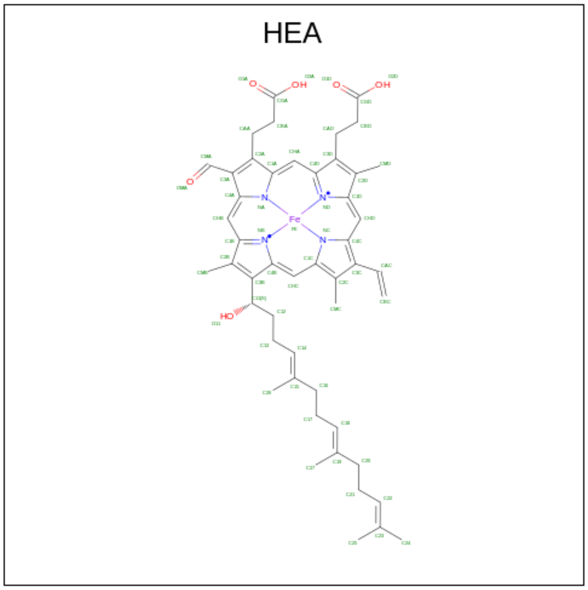
Mol	Chain	Residues	Atoms	AltConf
74	D	1	Total Fe S 8 4 4	0
74	E	1	Total Fe S 16 8 8	0
74	E	1	Total Fe S 16 8 8	0

- Molecule 75 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
75	C3	1	Total Cu 1 1	0
75	C1	2	Total Cu 2 2	0

- Molecule 76 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
76	C3	1	Total C Fe N O 120 98 2 8 12	0
76	C3	1	Total C Fe N O 120 98 2 8 12	0

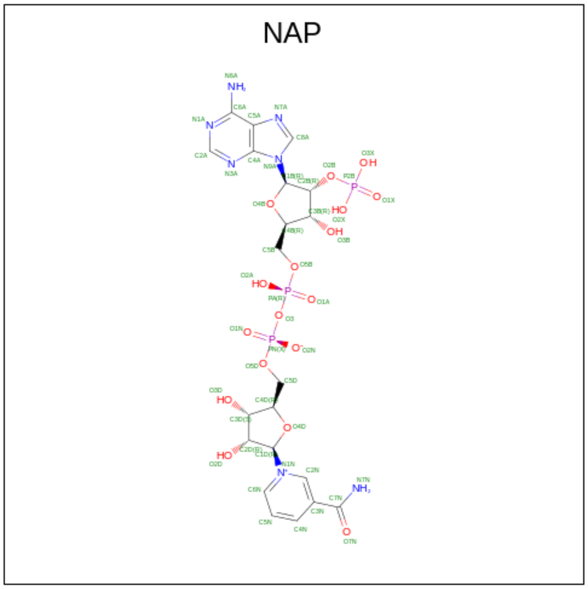
- Molecule 77 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
77	C1	1	1	1	0

- Molecule 78 is ZINC ION (three-letter code: ZN) (formula: Zn).

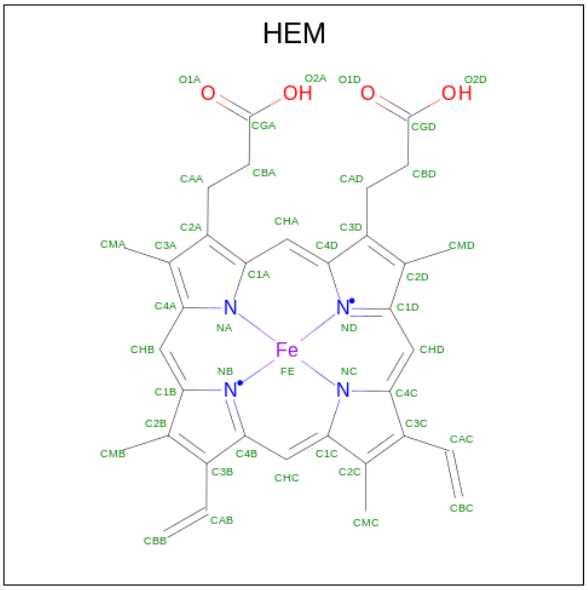
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
78	A5	1	1	1	0
78	I	1	1	1	0

- Molecule 79 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



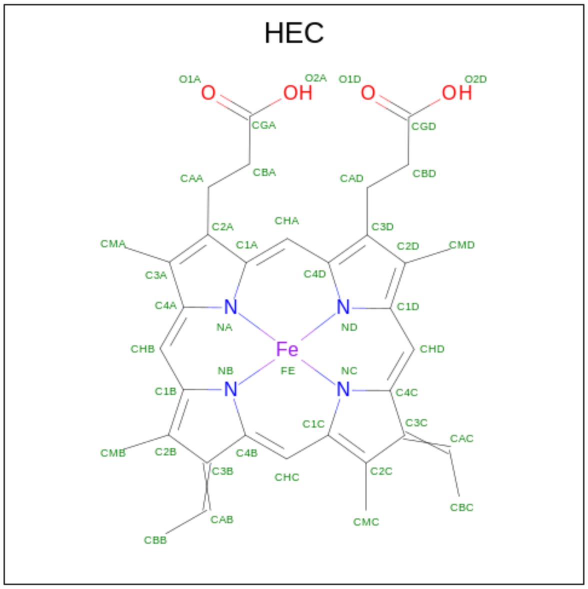
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
79	R	1	48	21	7	17	3	0

- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



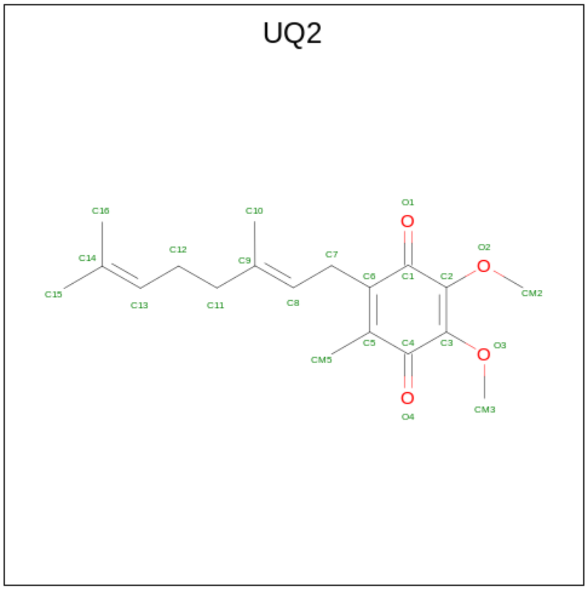
Mol	Chain	Residues	Atoms	AltConf
80	m	1	Total C Fe N O 86 68 2 8 8	0
80	m	1	Total C Fe N O 86 68 2 8 8	0
80	y	1	Total C Fe N O 86 68 2 8 8	0
80	y	1	Total C Fe N O 86 68 2 8 8	0

- Molecule 81 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 82 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



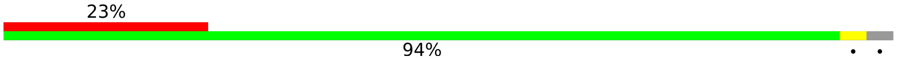
Mol	Chain	Residues	Atoms			AltConf
82	A2	1	Total 23	C 19	O 4	0

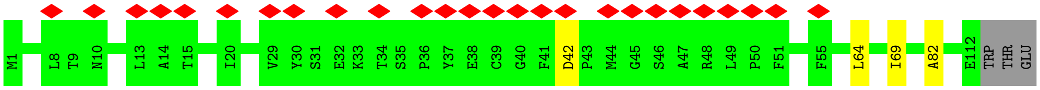
3 Residue-property plots ⓘ

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: NADH-ubiquinone oxidoreductase chain 3

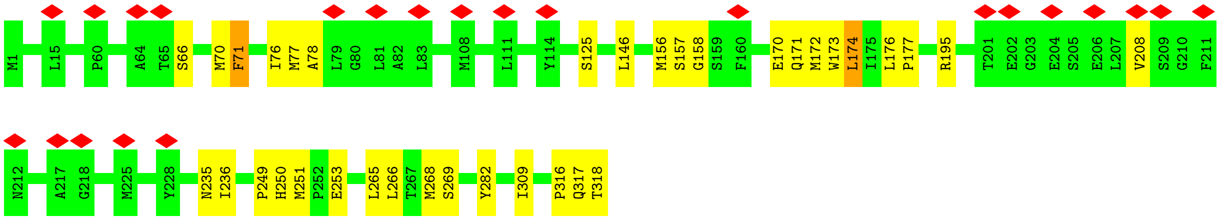
Chain 3:





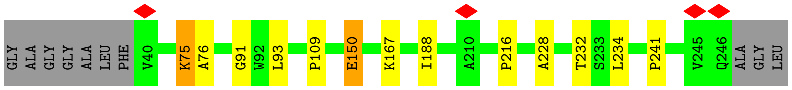
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



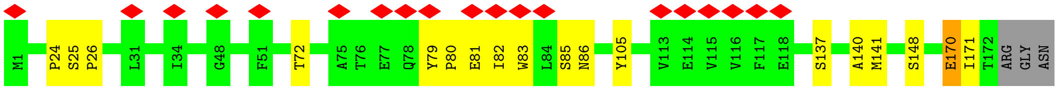
- Molecule 3: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 9:



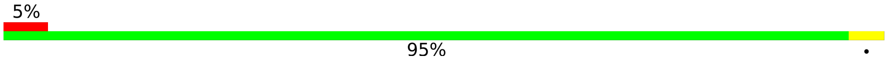
- Molecule 4: NADH-ubiquinone oxidoreductase chain 6

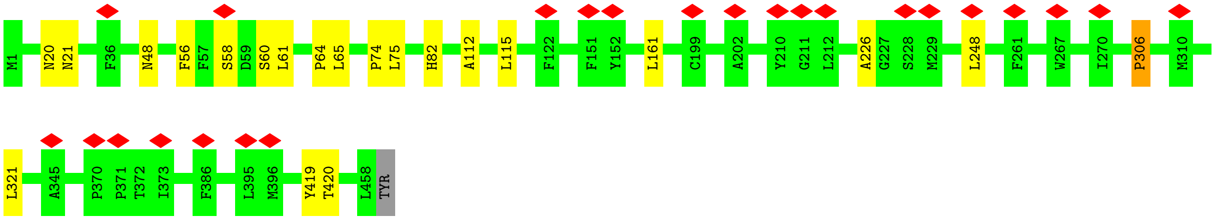
Chain 7:



- Molecule 5: NADH-ubiquinone oxidoreductase chain 4

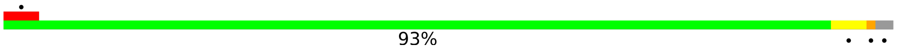
Chain 4:

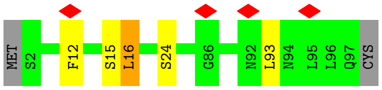




- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

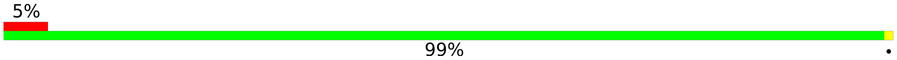
Chain 5:

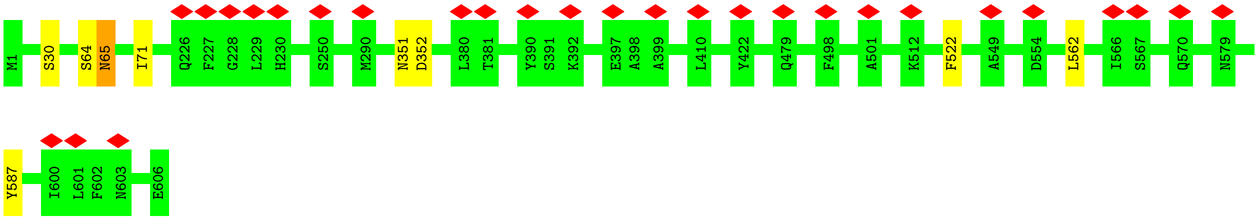




- Molecule 7: NADH-ubiquinone oxidoreductase chain 5

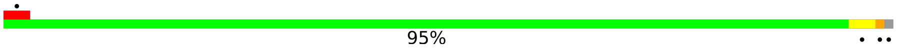
Chain 6:

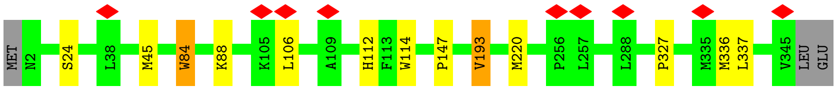




- Molecule 8: NADH-ubiquinone oxidoreductase chain 2

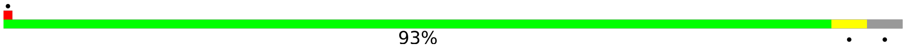
Chain 2:

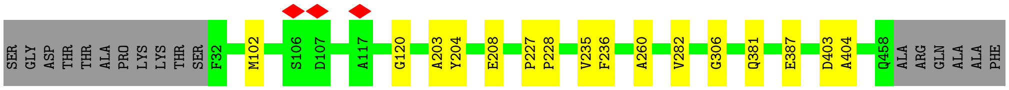




- Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

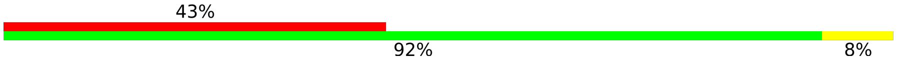
Chain 8:

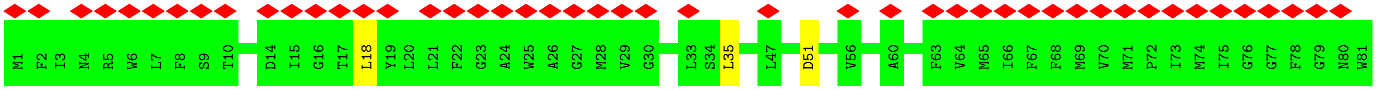


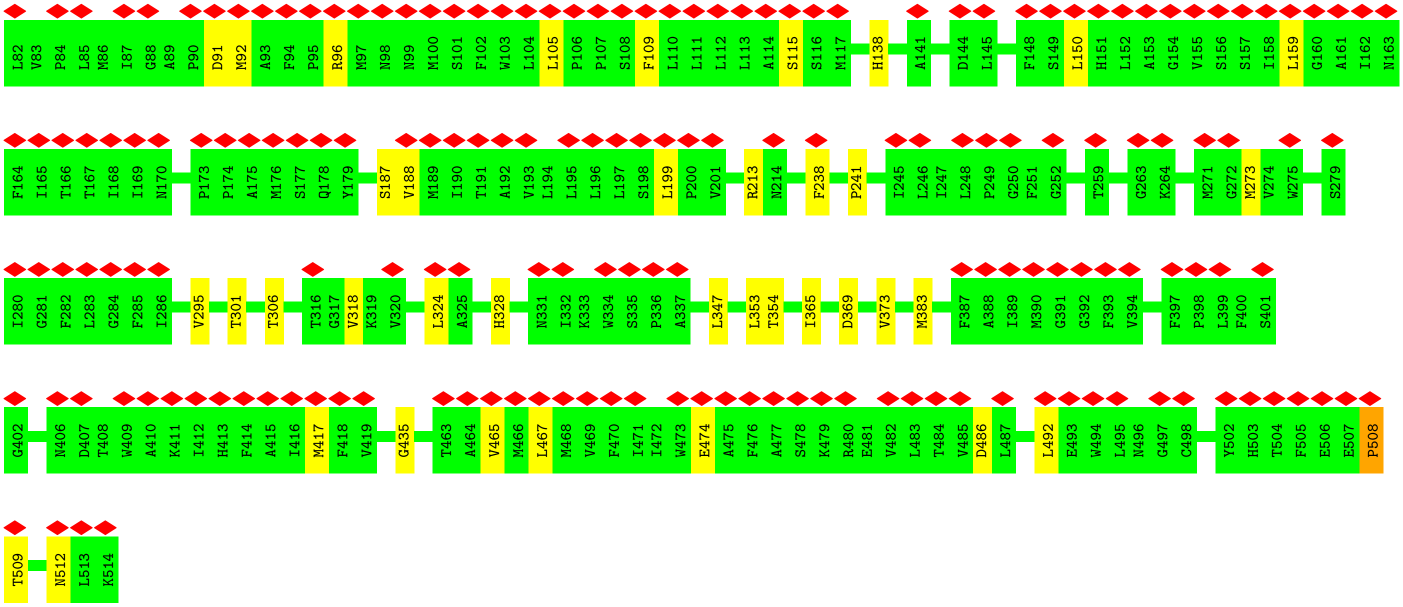


- Molecule 10: Cytochrome c oxidase subunit 1

Chain C3:

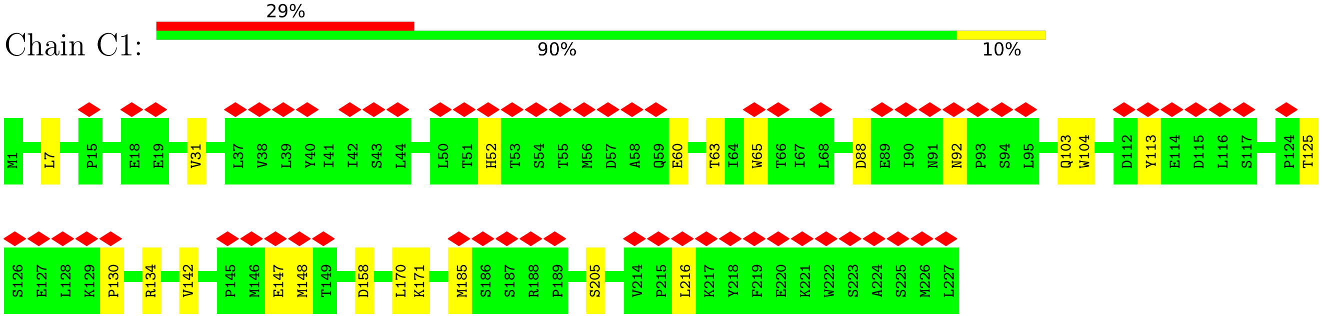






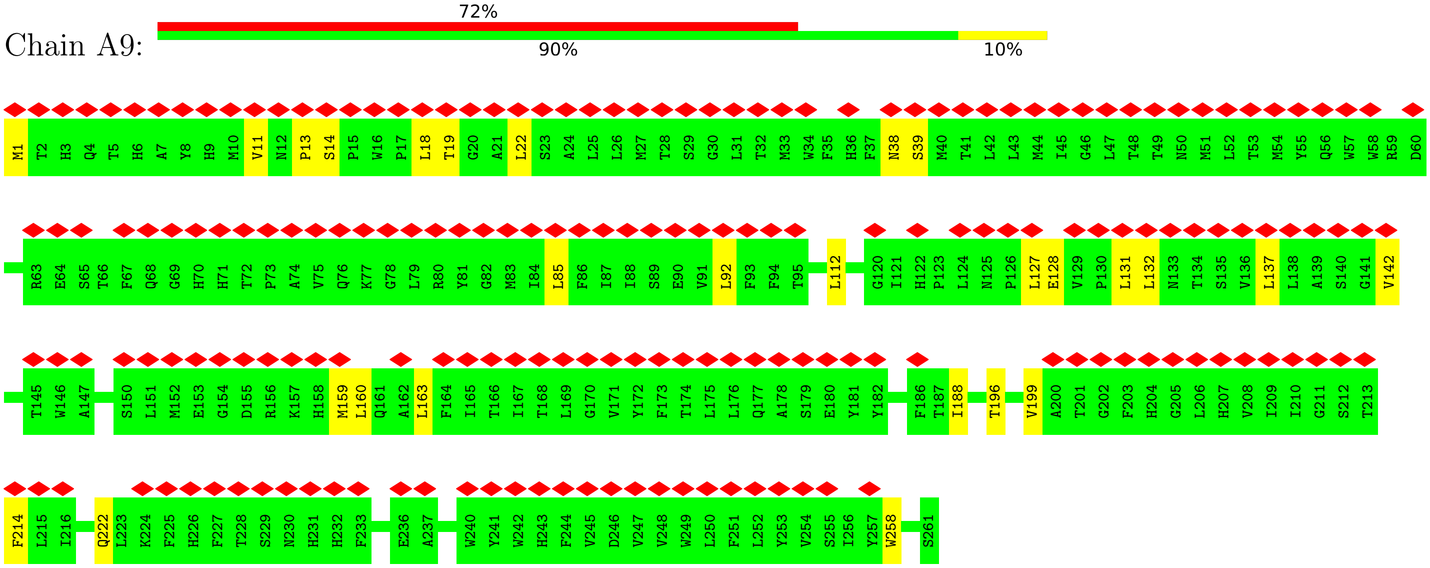
- Molecule 11: Cytochrome c oxidase subunit 2

Chain C1:



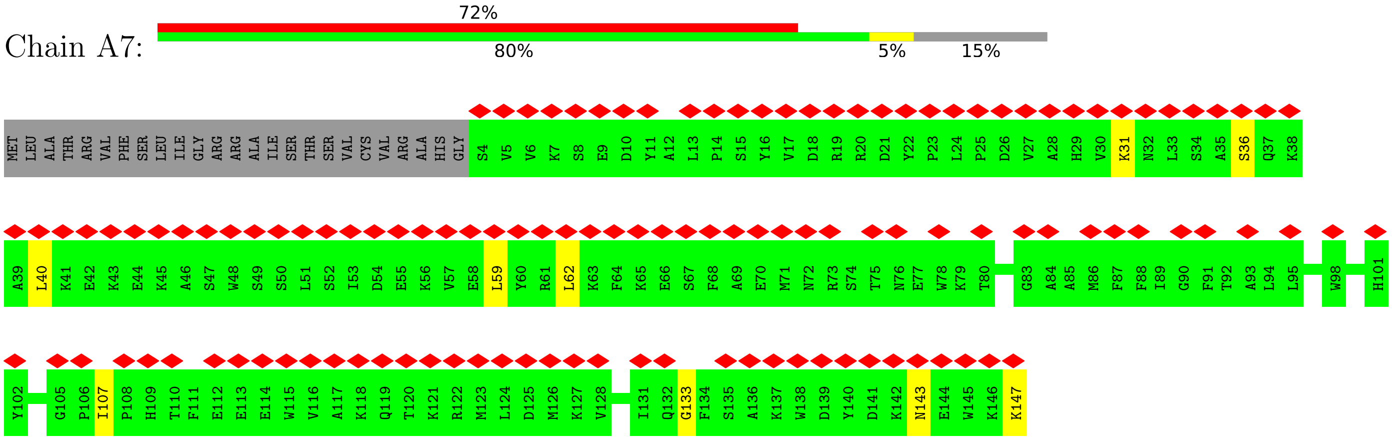
- Molecule 12: Cytochrome c oxidase subunit 3

Chain A9:



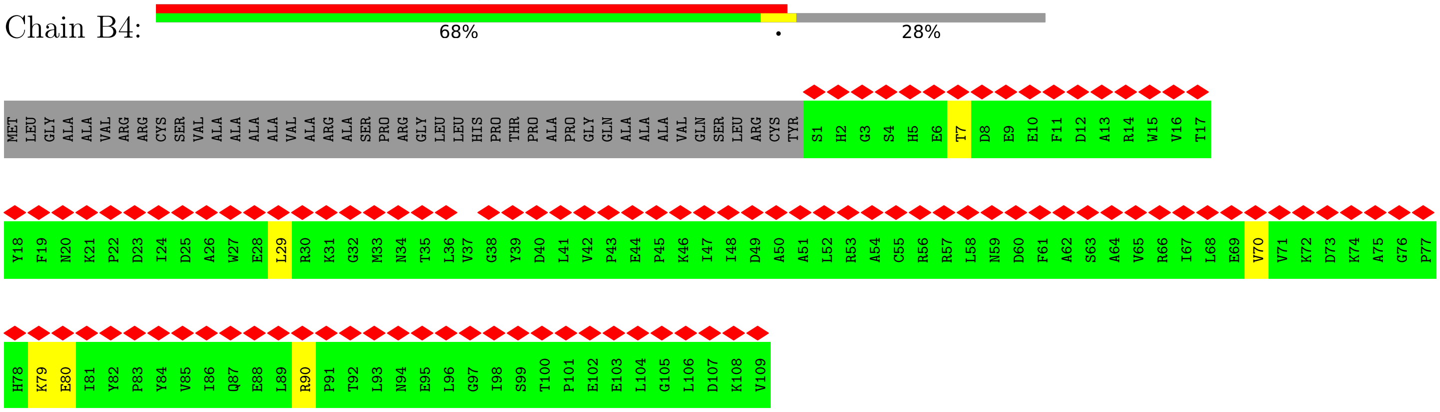
- Molecule 13: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain A7:



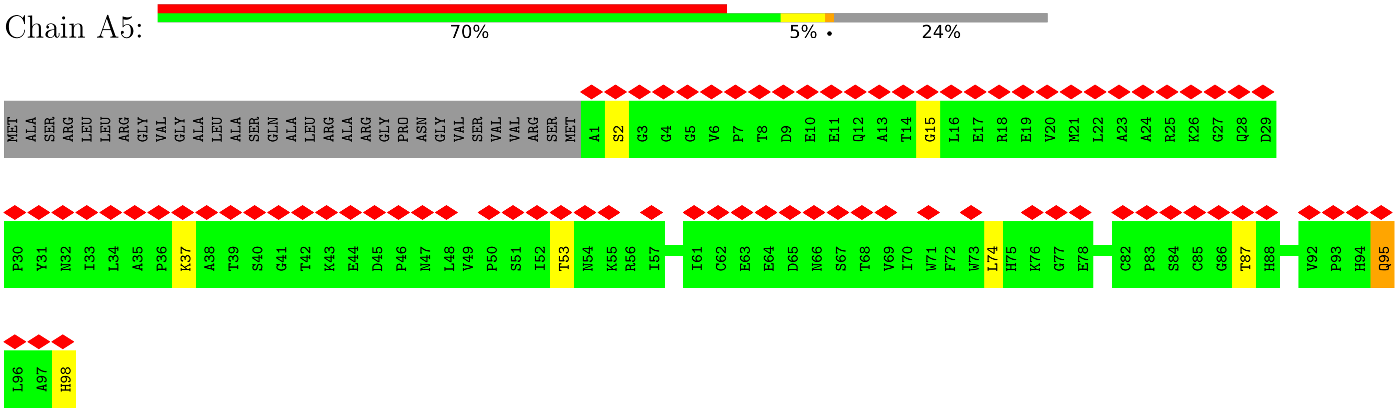
- Molecule 14: Cytochrome c oxidase subunit 5A, mitochondrial

Chain B4:



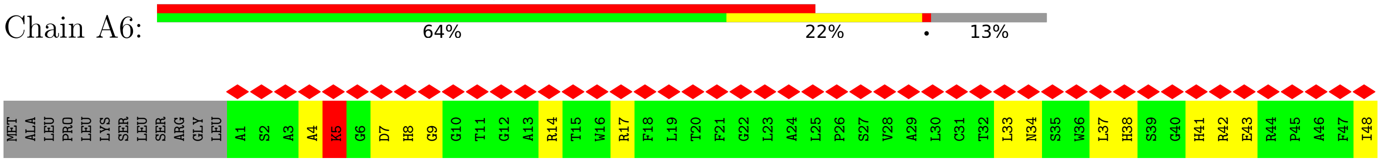
- Molecule 15: Cytochrome c oxidase subunit 5B, mitochondrial

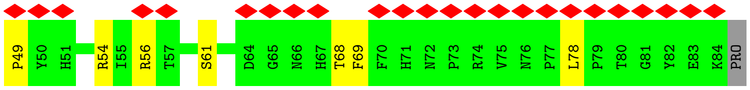
Chain A5:



- Molecule 16: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain A6:



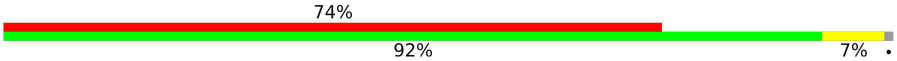


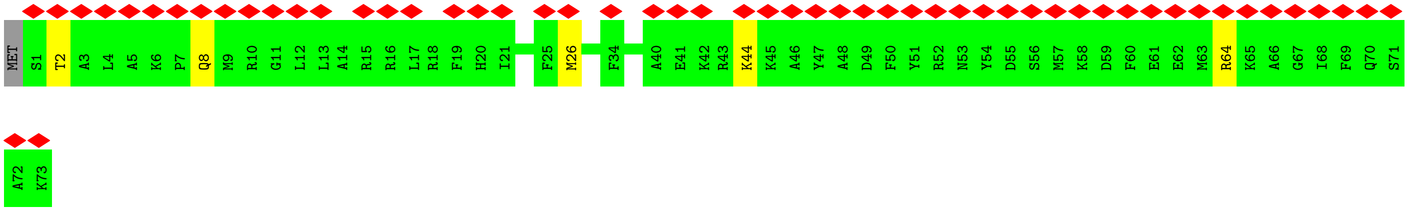
- Molecule 17: Cytochrome c oxidase subunit 6B1

Chain C0:

- Molecule 18: Cytochrome c oxidase subunit 6C

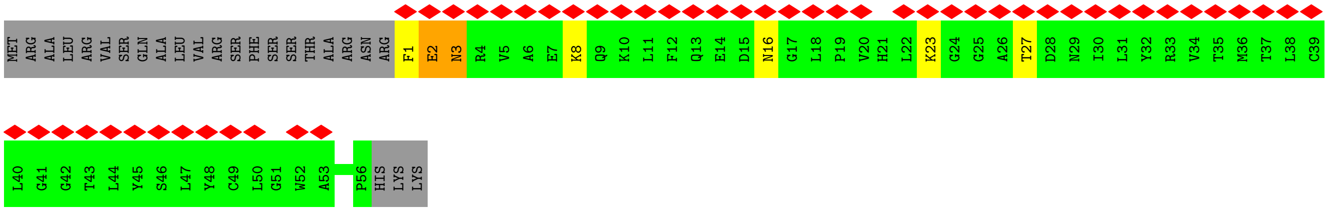
Chain C2:





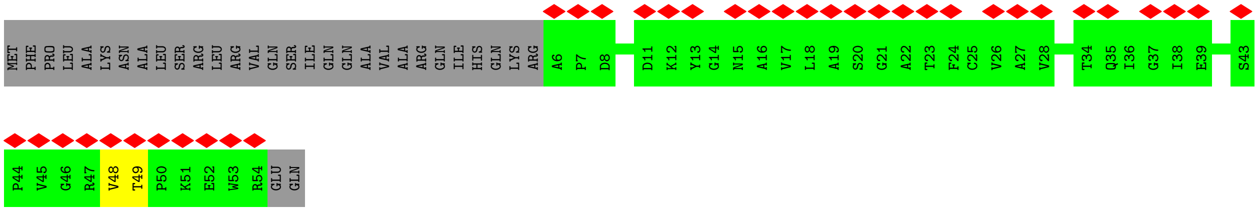
- Molecule 19: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain B2:



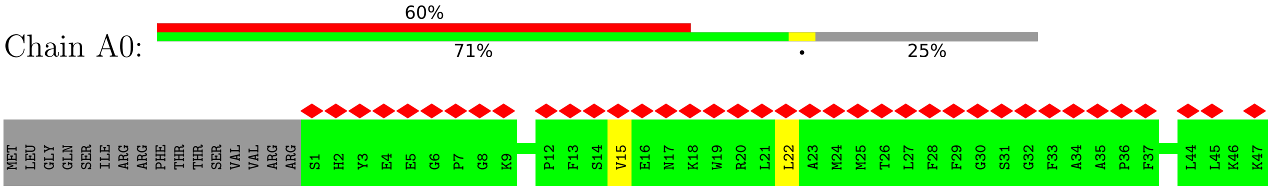
- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial

Chain B3:



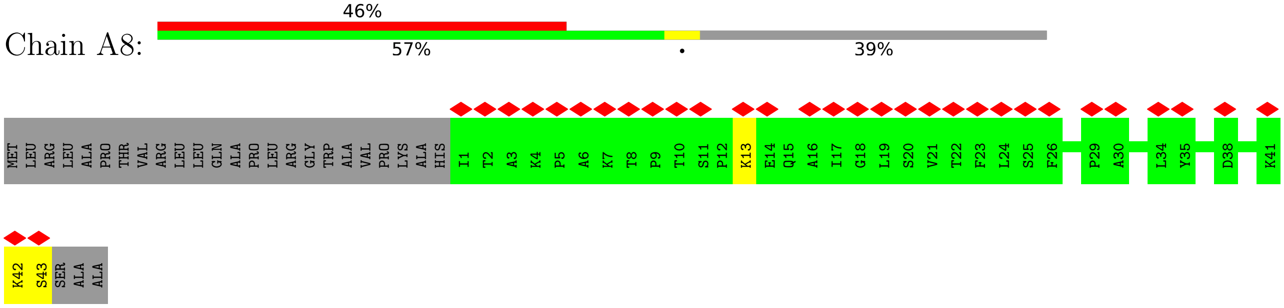
- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial

Chain A0:



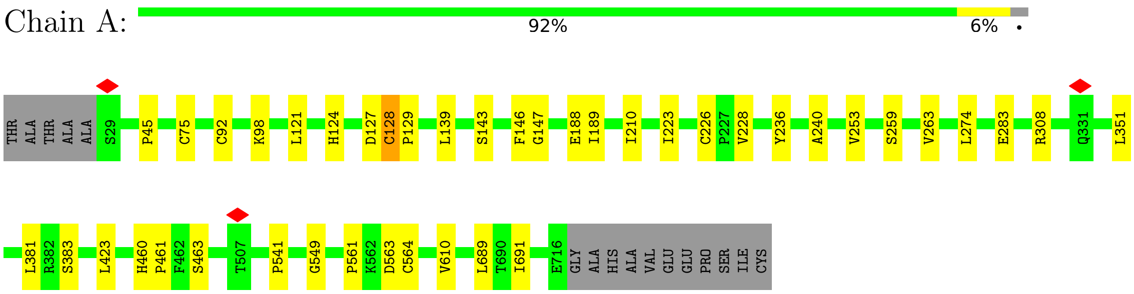
- Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial

Chain A8:



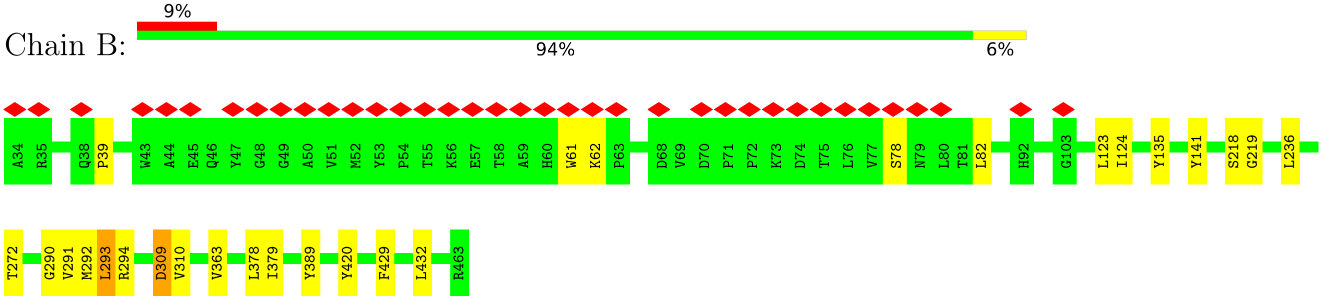
- Molecule 23: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A:



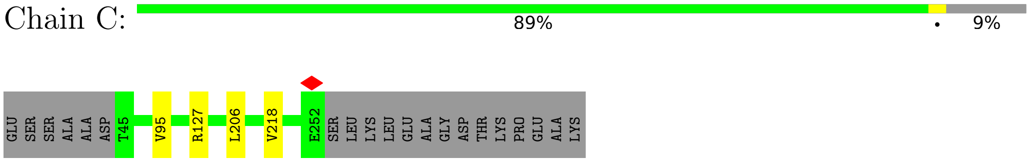
- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B:



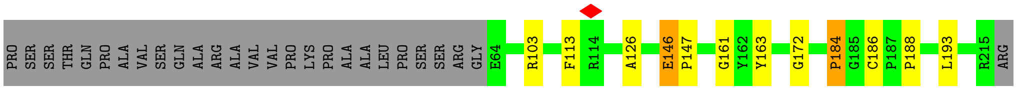
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



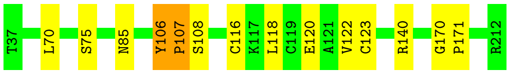
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D:



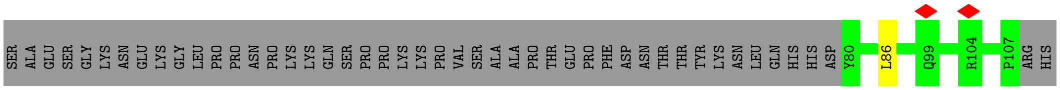
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E:



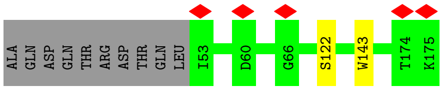
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:



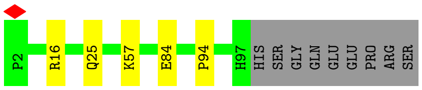
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G:



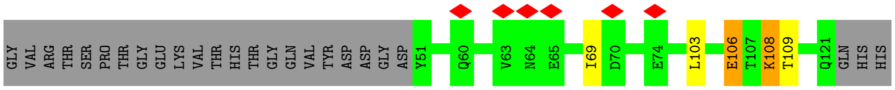
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain H:



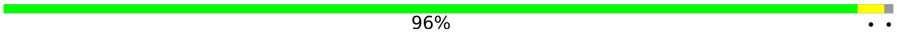
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain I:



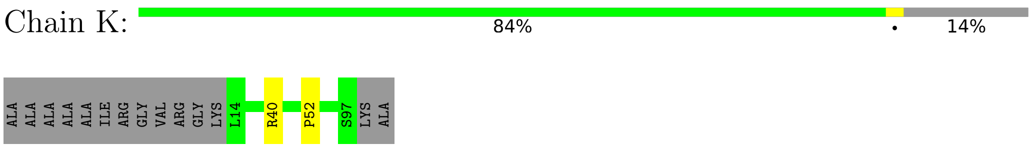
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain J:



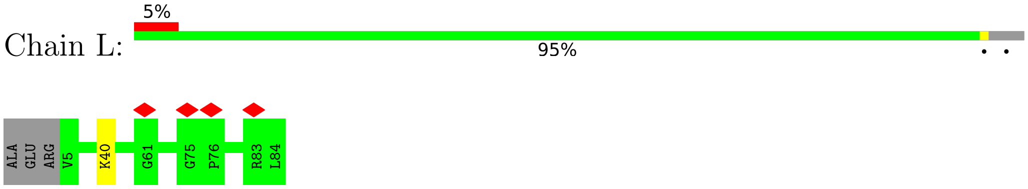
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain K:



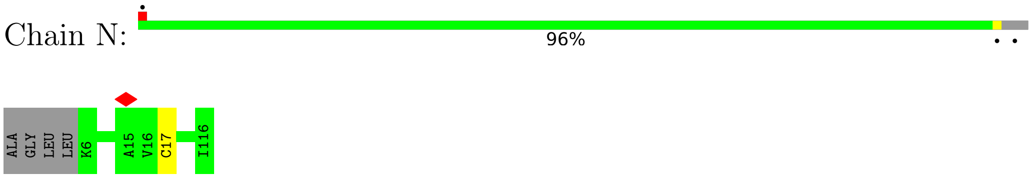
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain L:



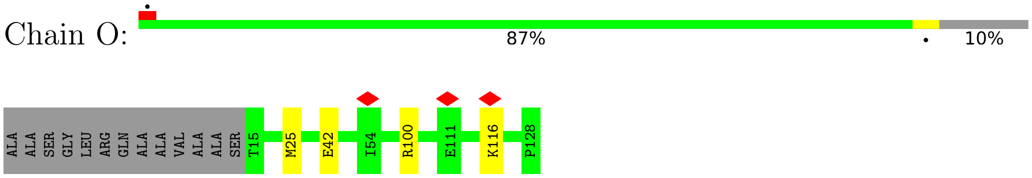
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N:



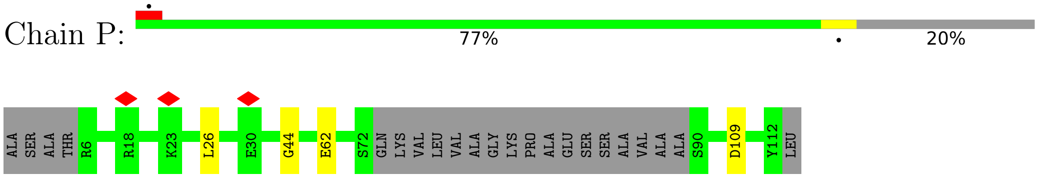
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O:



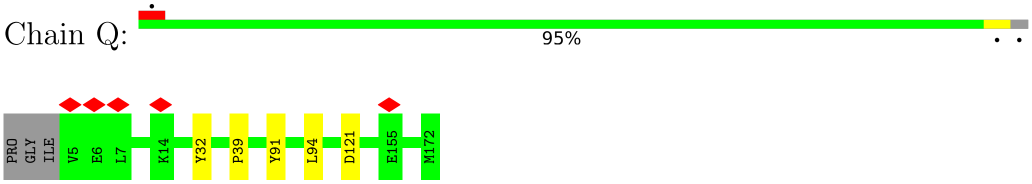
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P:



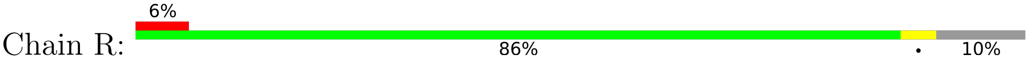
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

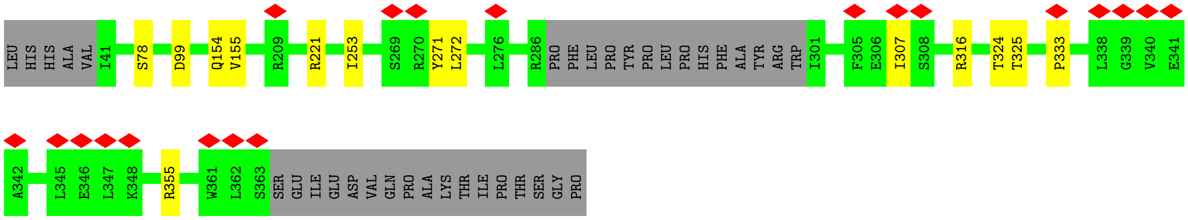
Chain Q:



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

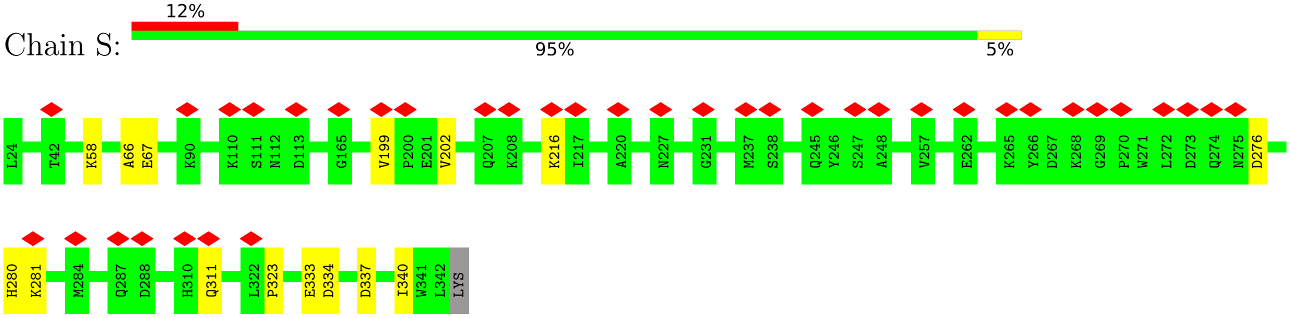
Chain R:





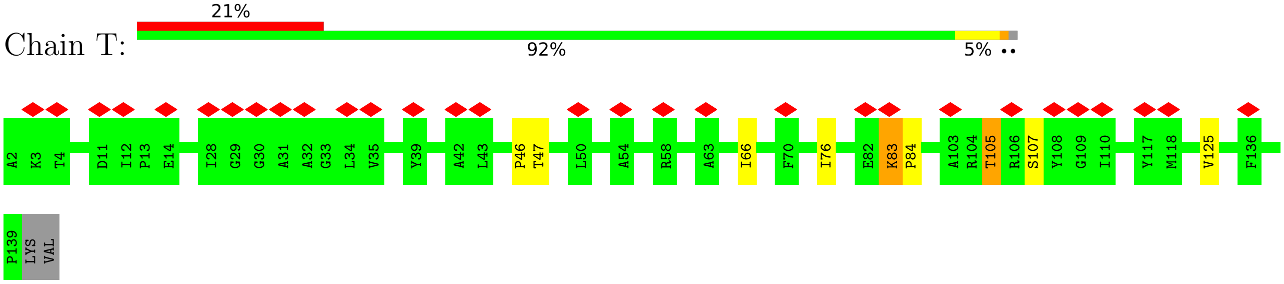
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain S:



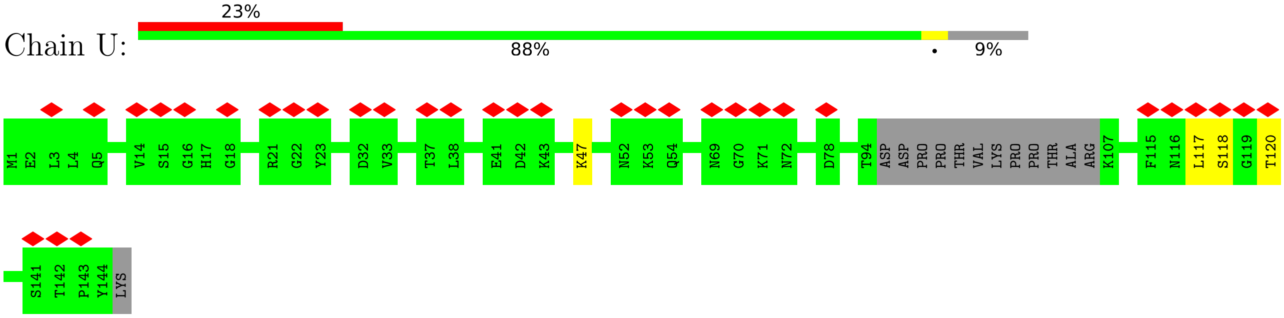
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T:



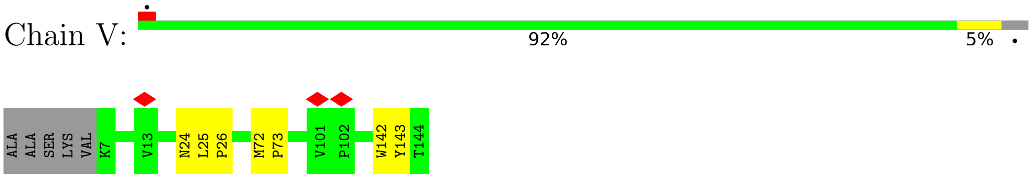
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain U:

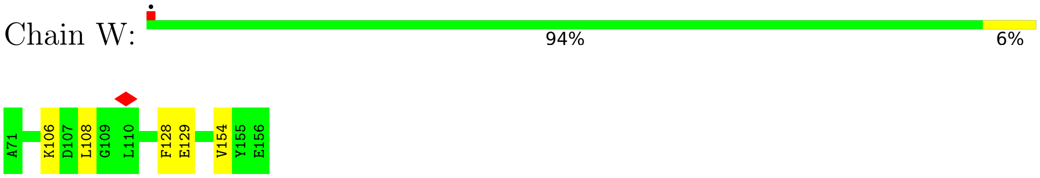


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

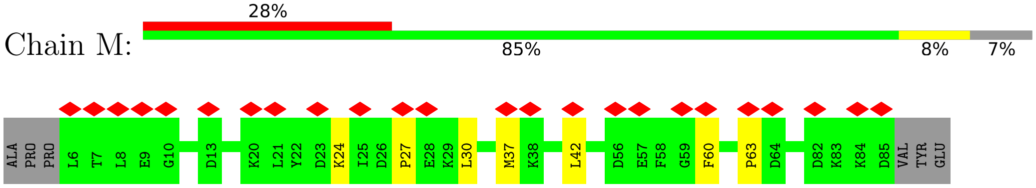
Chain V:



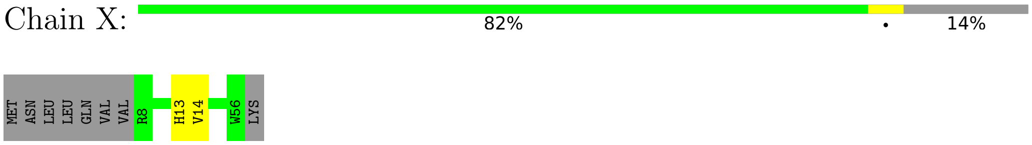
- Molecule 44: Acyl carrier protein, mitochondrial



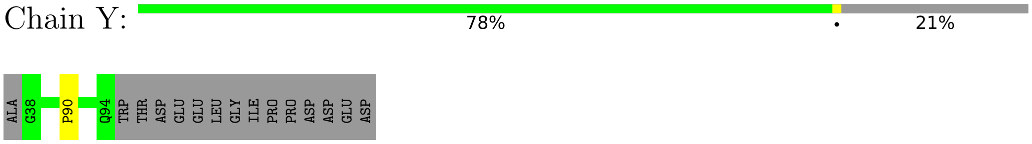
- Molecule 44: Acyl carrier protein, mitochondrial



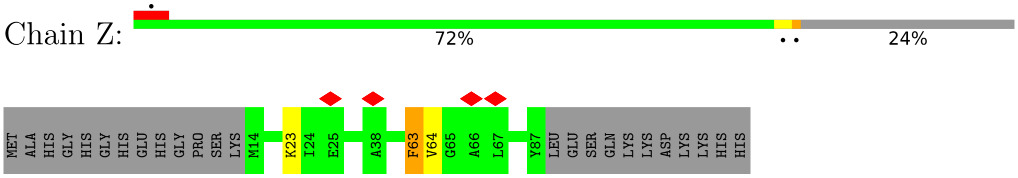
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



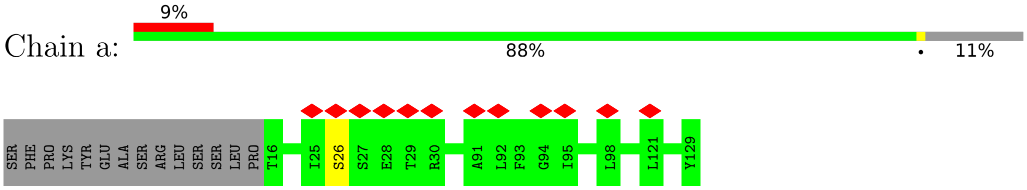
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



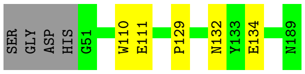
- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



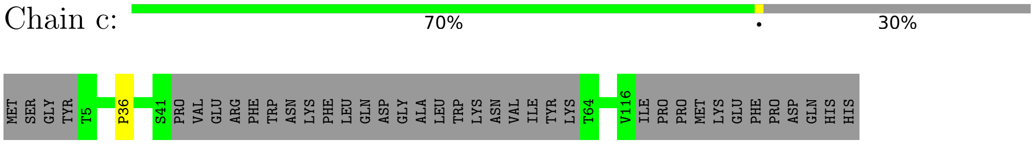
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



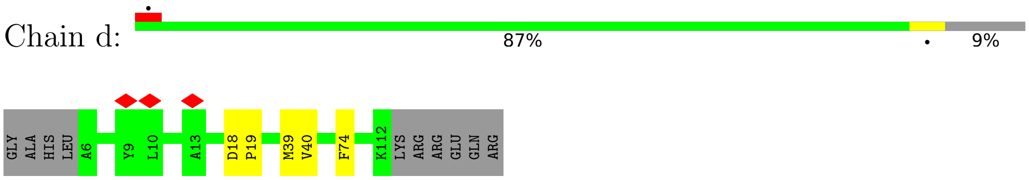
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



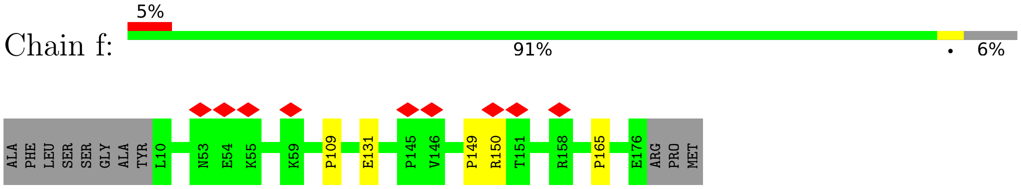
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



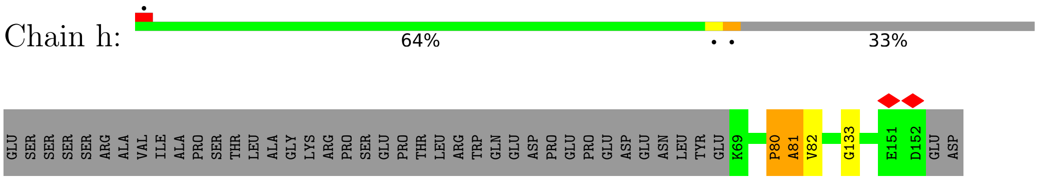
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



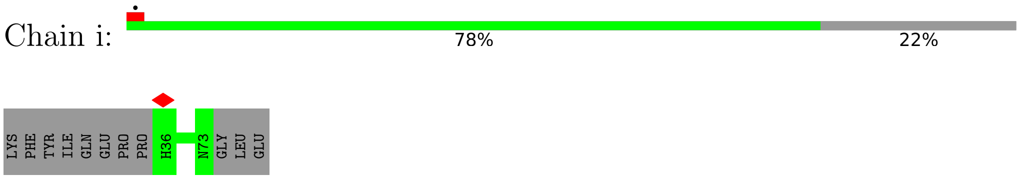
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



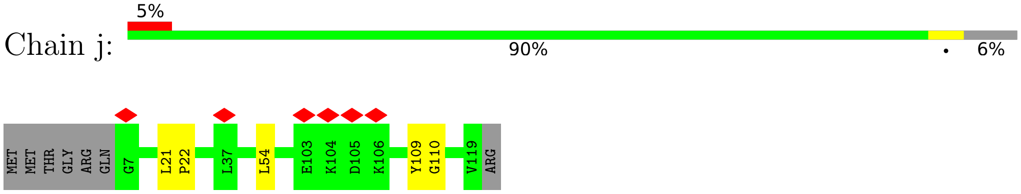
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



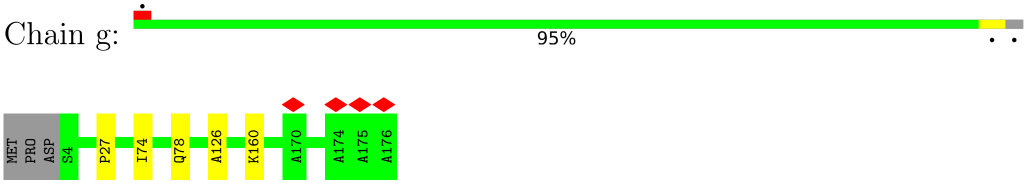
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



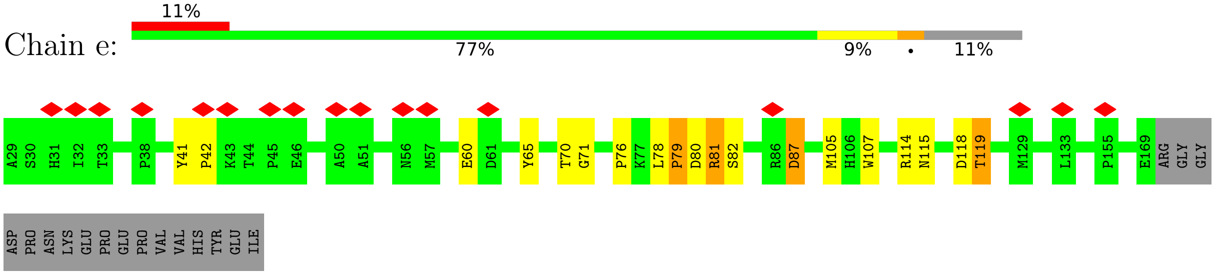
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2



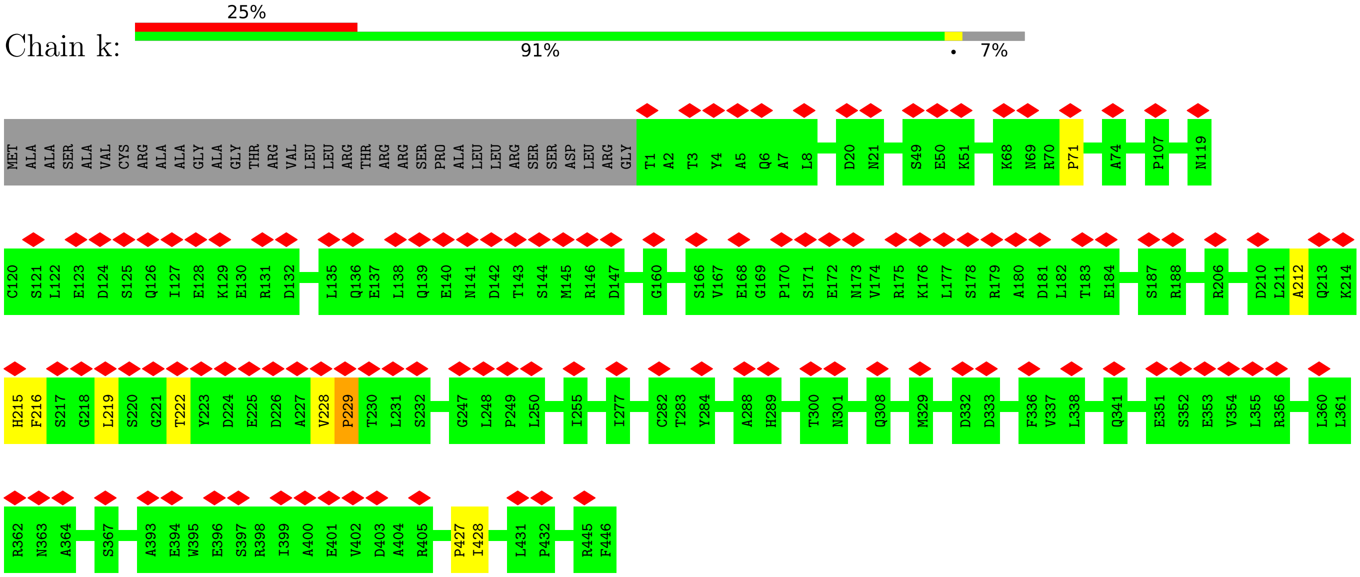
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



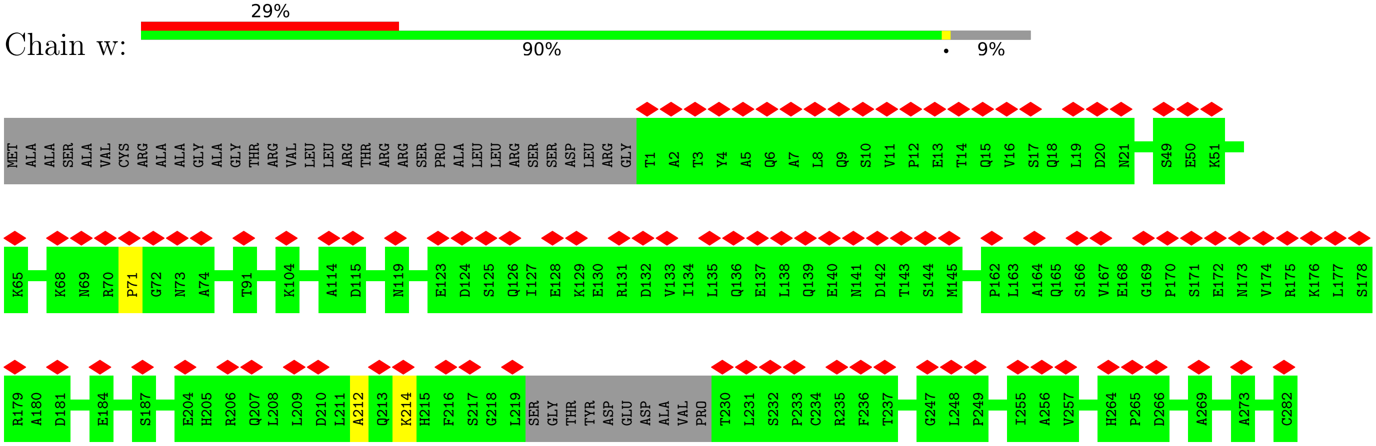
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

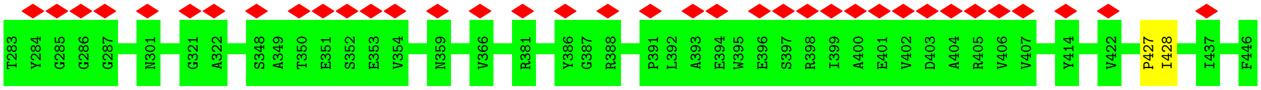


- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial



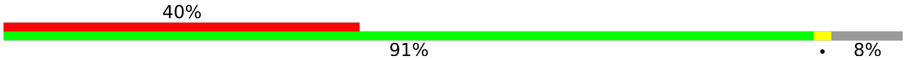
- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial

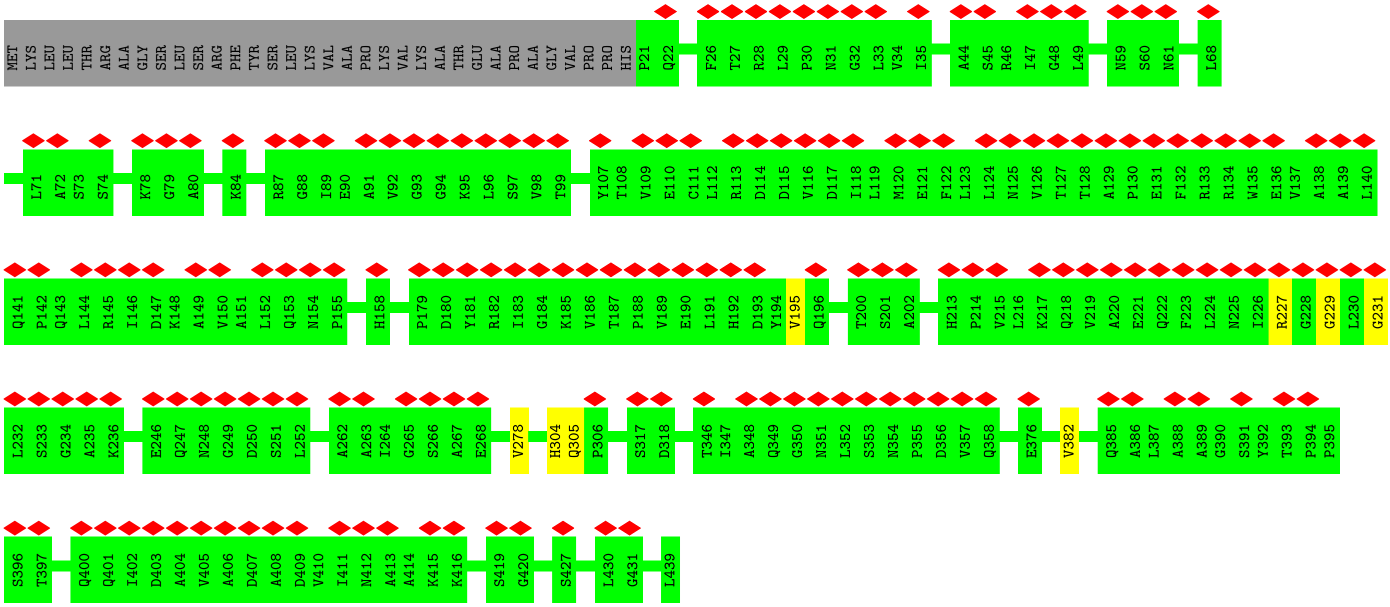




- Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

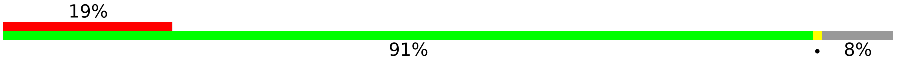
Chain l:

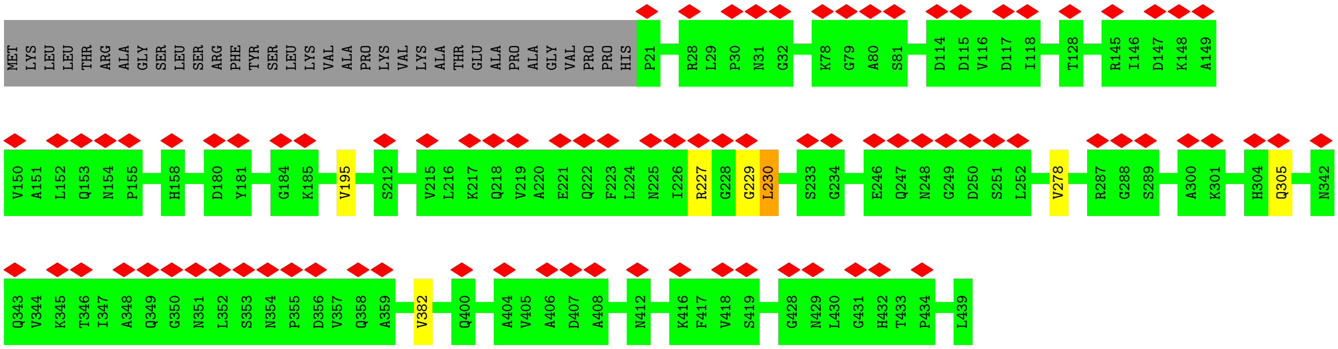




- Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

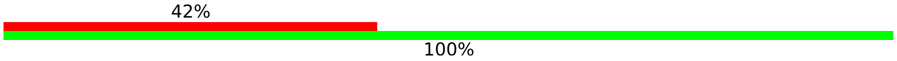
Chain x:

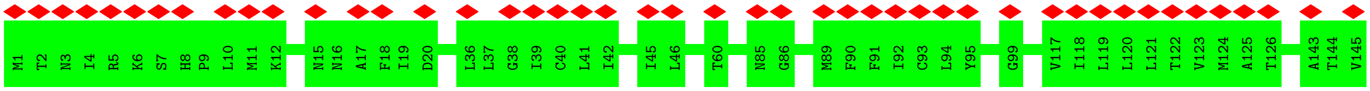


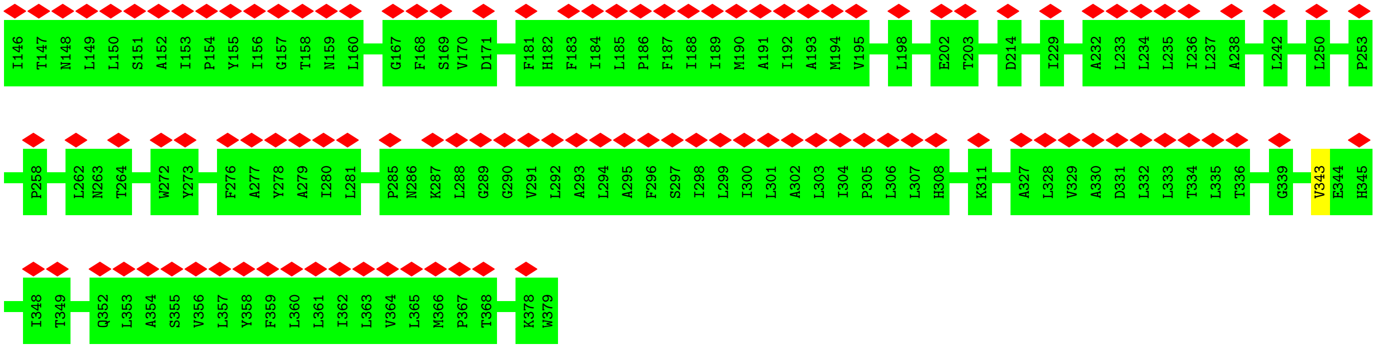


- Molecule 60: Cytochrome b

Chain m:

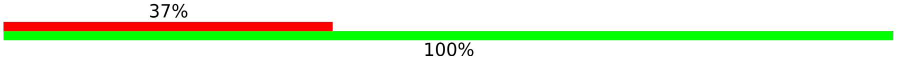


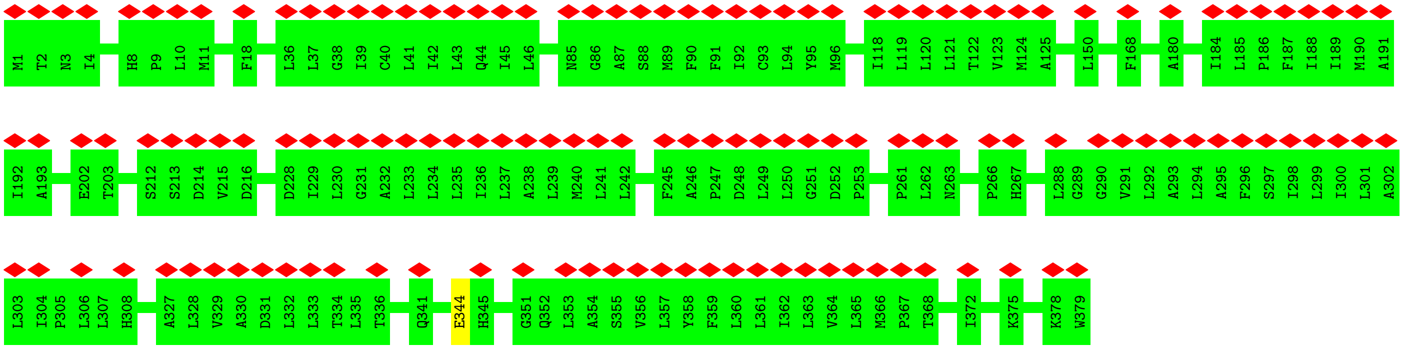




- Molecule 60: Cytochrome b

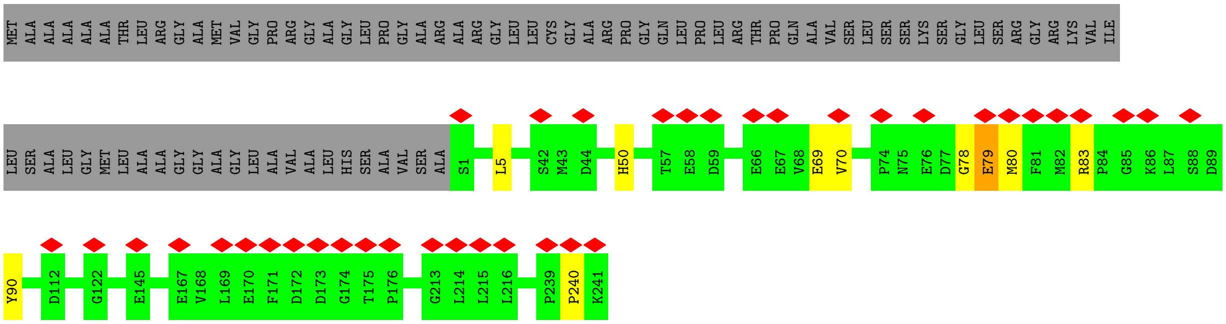
Chain y:





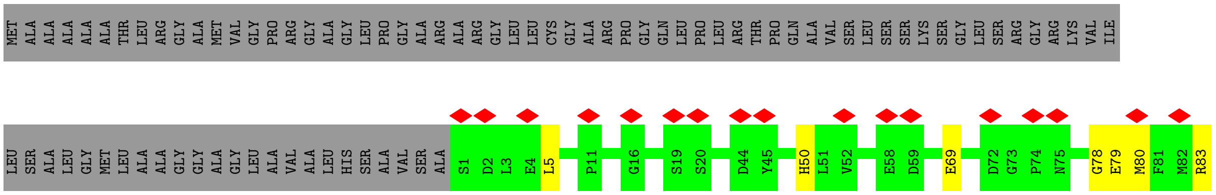
- Molecule 61: Cytochrome c1, heme protein, mitochondrial

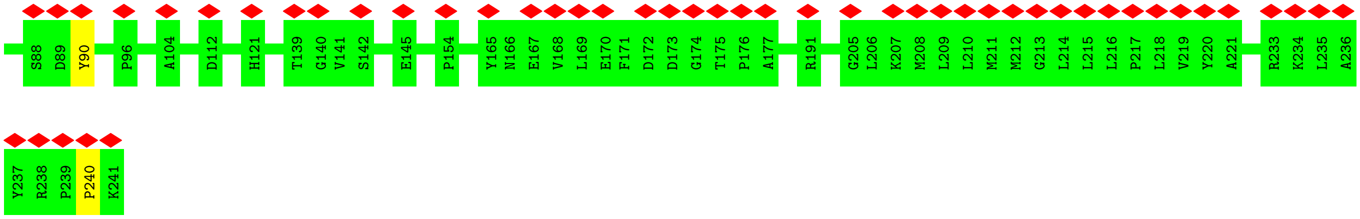
Chain o:



- Molecule 61: Cytochrome c1, heme protein, mitochondrial

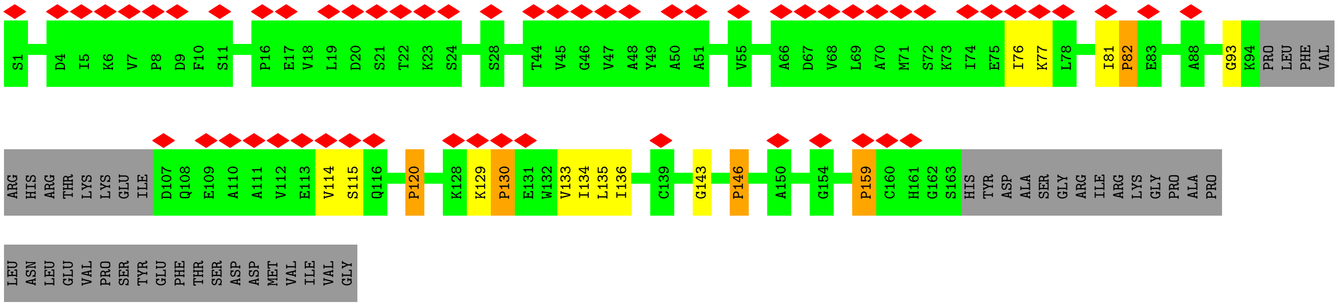
Chain z:





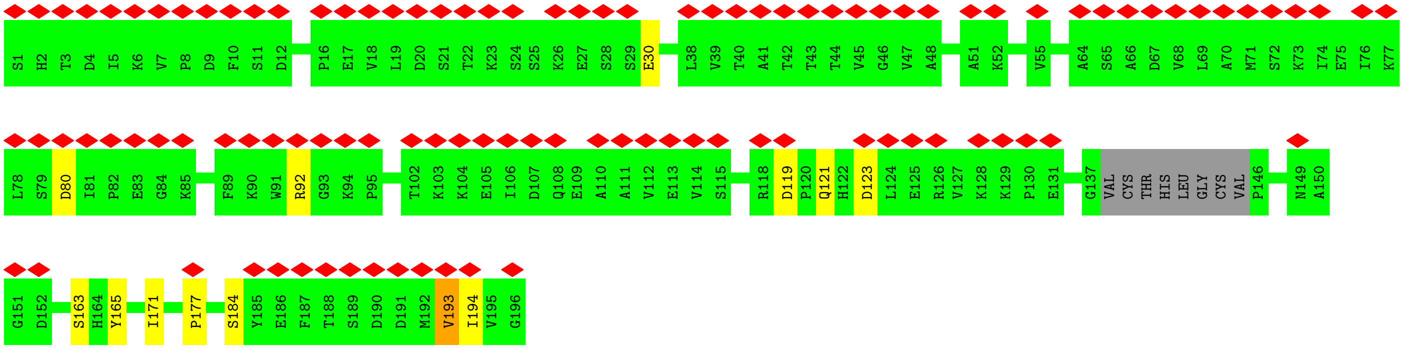
- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain p:



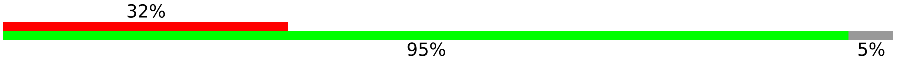
- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial

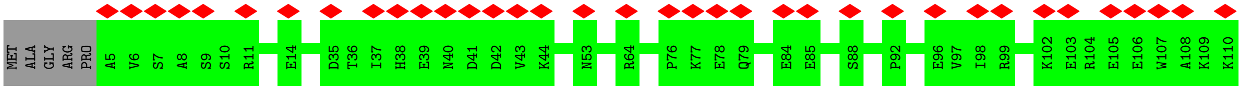
Chain A1:



- Molecule 63: Cytochrome b-c1 complex subunit 7

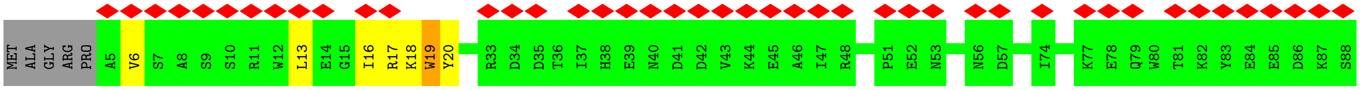
Chain q:

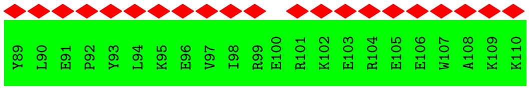




- Molecule 63: Cytochrome b-c1 complex subunit 7

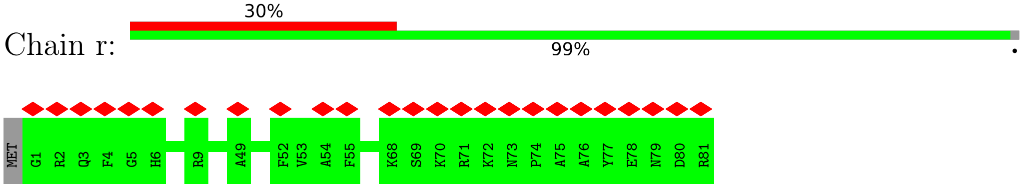
Chain A2:





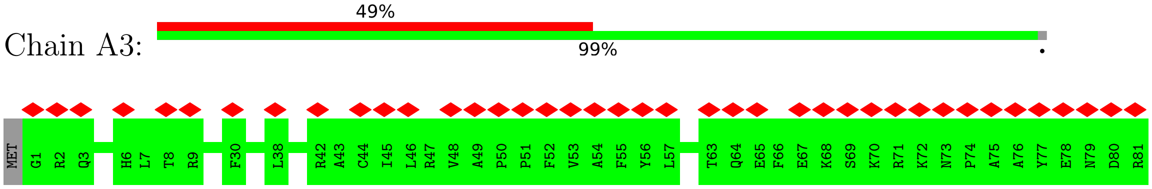
- Molecule 64: Cytochrome b-c1 complex subunit 8

Chain r:



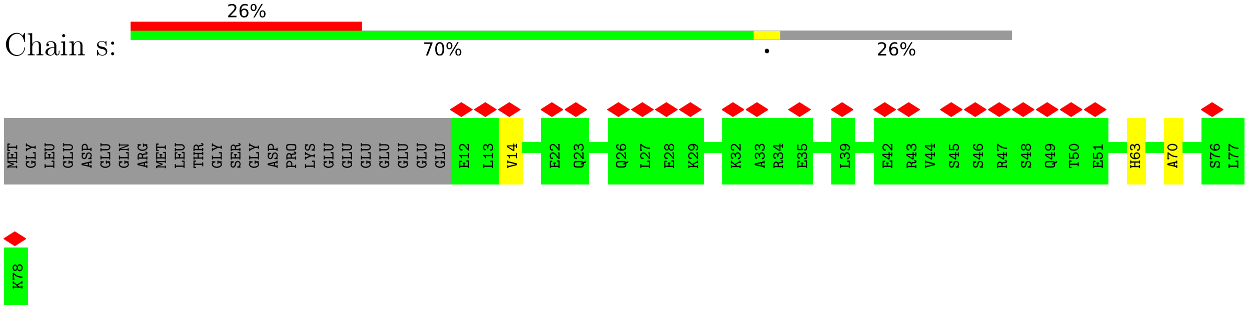
- Molecule 64: Cytochrome b-c1 complex subunit 8

Chain A3:



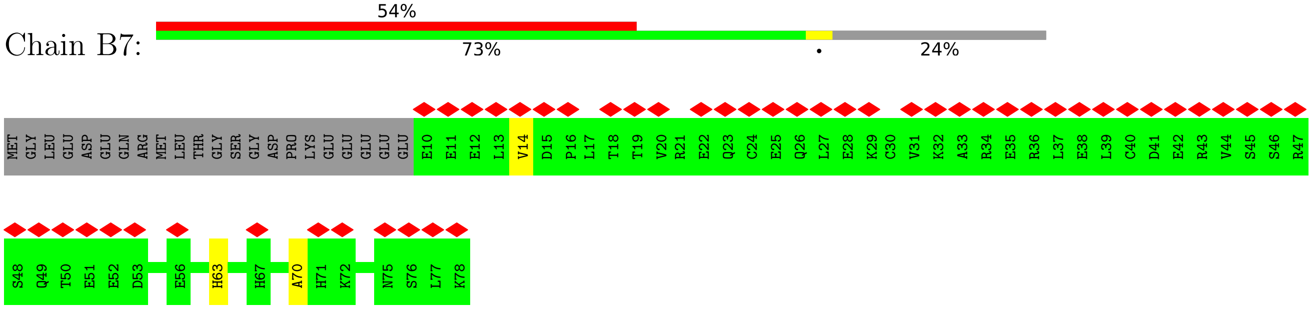
- Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain s:



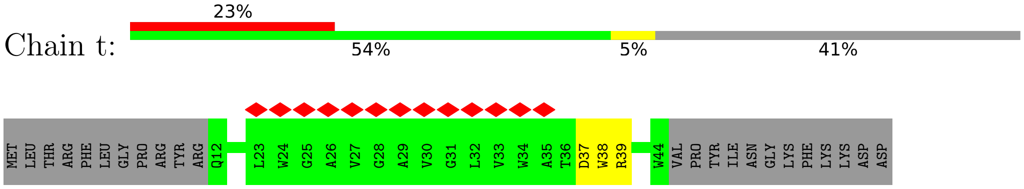
- Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain B7:



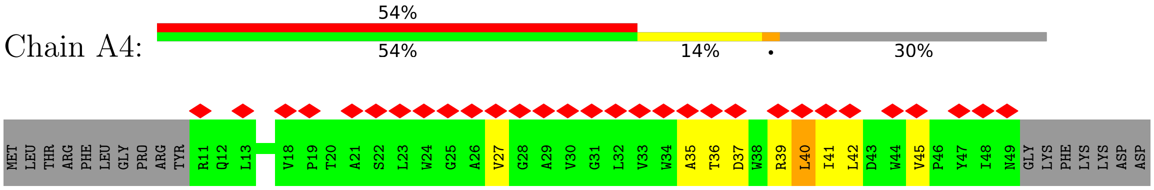
- Molecule 66: Cytochrome b-c1 complex subunit 10

Chain t:



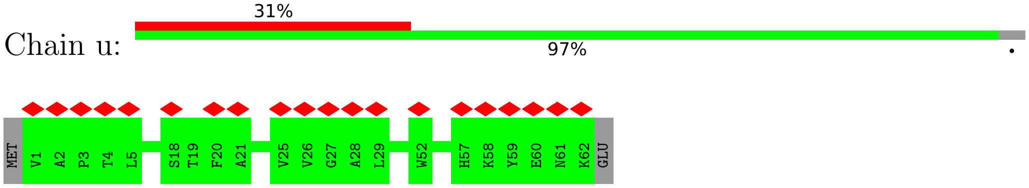
- Molecule 66: Cytochrome b-c1 complex subunit 10

Chain A4:



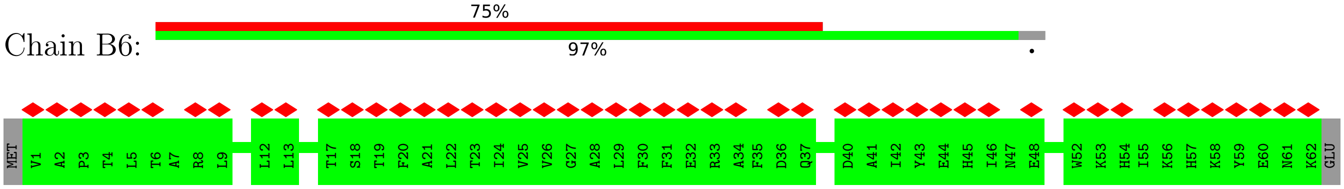
- Molecule 67: Cytochrome b-c1 complex subunit 9

Chain u:



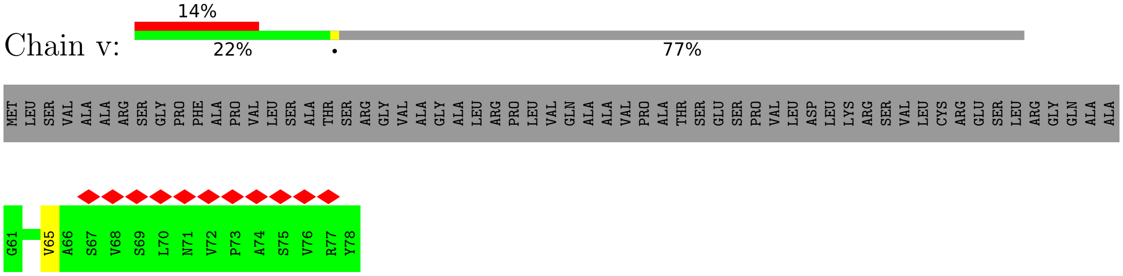
- Molecule 67: Cytochrome b-c1 complex subunit 9

Chain B6:



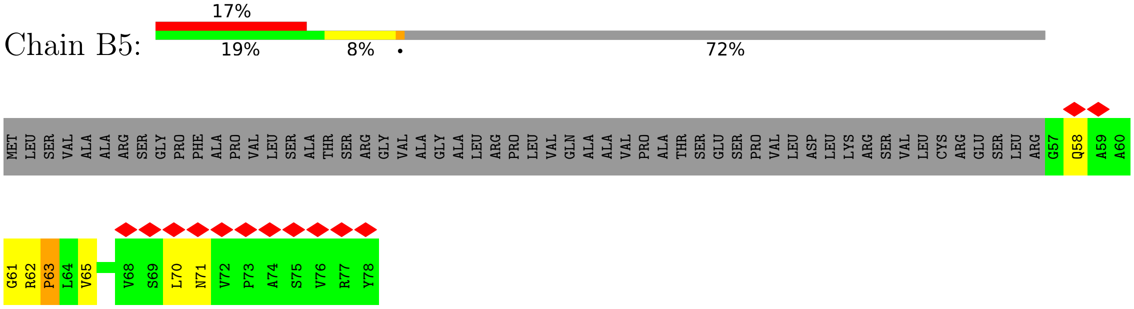
- Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain v:



- Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain B5:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.398	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, NAP, PC1, FMN, SF4, CU, HEM, FES, 3PE, CDL, ZN, UQ2, MG, HEA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	3	0.53	0/905	0.77	1/1237 (0.1%)
2	1	0.64	0/2575	0.83	3/3518 (0.1%)
3	9	0.50	0/1618	0.62	0/2207
4	7	0.61	0/1267	0.77	1/1731 (0.1%)
5	4	0.61	1/3674 (0.0%)	0.80	4/5020 (0.1%)
6	5	0.62	0/721	0.84	2/977 (0.2%)
7	6	0.46	0/4893	0.65	1/6661 (0.0%)
8	2	0.72	1/2749 (0.0%)	0.85	0/3744
9	8	0.50	0/3136	0.64	1/4258 (0.0%)
10	C3	0.60	0/4164	0.76	1/5688 (0.0%)
11	C1	0.57	0/1868	0.79	0/2544
12	A9	0.56	0/2212	0.68	0/3025
13	A7	0.57	0/1229	0.65	1/1658 (0.1%)
14	B4	0.50	0/898	0.66	0/1218
15	A5	0.56	0/765	0.81	0/1038
16	A6	0.54	0/698	0.73	1/950 (0.1%)
17	C0	0.55	0/648	0.73	0/877
18	C2	0.60	0/611	0.64	0/810
19	B2	0.61	0/451	0.72	0/610
20	B3	0.57	0/398	0.66	0/546
21	A0	0.63	0/399	0.62	0/534
22	A8	0.51	0/345	0.65	0/470
23	A	0.70	5/5304 (0.1%)	0.82	7/7193 (0.1%)
24	B	0.92	1/3512 (0.0%)	0.92	12/4763 (0.3%)
25	C	0.85	0/1777	0.79	1/2420 (0.0%)
26	D	0.98	2/1237 (0.2%)	0.88	2/1676 (0.1%)
27	E	0.96	4/1431 (0.3%)	0.98	7/1938 (0.4%)
28	F	0.33	0/191	0.82	0/262
29	G	0.78	0/1008	0.80	0/1363
30	H	0.55	0/800	0.73	0/1076
31	I	0.56	0/543	0.86	0/729
32	J	0.60	0/545	0.61	0/740

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	K	0.44	0/667	0.58	0/900
34	L	0.47	0/623	0.60	0/862
35	N	0.50	0/882	0.66	0/1203
36	O	0.54	0/948	0.67	0/1279
37	P	0.51	0/723	0.73	1/985 (0.1%)
38	Q	0.48	0/1381	0.66	0/1869
39	R	0.53	1/2407 (0.0%)	0.70	0/3269
40	S	0.39	0/2348	0.66	0/3198
41	T	0.51	0/938	0.61	0/1278
42	U	0.48	0/1053	0.72	1/1439 (0.1%)
43	V	0.58	1/1115 (0.1%)	0.67	0/1508
44	M	0.46	0/651	0.69	1/876 (0.1%)
44	W	0.39	0/624	0.58	0/847
45	X	0.37	0/383	0.57	0/523
46	Y	0.40	0/428	0.59	0/592
47	Z	0.38	0/506	0.57	0/688
48	a	0.50	0/878	0.60	0/1195
49	b	0.52	0/1058	0.68	0/1434
50	c	0.36	0/632	0.73	2/871 (0.2%)
51	d	0.51	1/726 (0.1%)	0.53	0/992
52	f	0.38	0/1191	0.55	0/1639
53	h	0.50	0/679	0.65	0/926
54	i	0.39	0/286	0.52	0/392
55	j	0.55	0/922	0.68	1/1254 (0.1%)
56	g	0.49	0/1380	0.61	1/1872 (0.1%)
57	e	0.38	0/888	0.72	1/1234 (0.1%)
58	k	0.48	0/3527	0.61	1/4787 (0.0%)
58	w	0.48	0/3455	0.59	0/4685
59	l	0.43	0/3192	0.57	0/4329
59	x	0.43	0/3198	0.58	1/4336 (0.0%)
60	m	0.56	0/3108	0.60	0/4252
60	y	0.56	0/3108	0.60	0/4252
61	o	0.51	0/1978	0.62	4/2684 (0.1%)
61	z	0.53	0/1965	0.61	2/2669 (0.1%)
62	A1	0.39	0/1124	0.69	0/1538
62	p	0.41	0/945	0.84	5/1288 (0.4%)
63	A2	0.48	0/926	0.54	0/1243
63	q	0.50	0/935	0.53	0/1253
64	A3	0.48	0/698	0.59	0/944
64	r	0.47	0/704	0.58	0/951
65	B7	0.43	0/571	0.64	0/765
65	s	0.43	0/553	0.63	0/741
66	A4	0.47	0/330	0.67	0/457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
66	t	0.42	0/272	0.52	0/377
67	B6	0.41	0/524	0.50	0/707
67	u	0.42	0/524	0.51	0/707
68	B5	0.45	0/149	1.11	1/203 (0.5%)
68	v	0.33	0/114	0.87	0/156
All	All	0.57	17/108789 (0.0%)	0.70	67/147930 (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
1	3	0	2
2	1	0	3
3	9	0	6
4	7	0	6
5	4	0	9
6	5	0	4
7	6	0	5
8	2	0	10
9	8	0	8
23	A	0	16
24	B	0	4
26	D	0	6
27	E	0	5
30	H	0	2
31	I	0	1
33	K	0	1
34	L	0	1
35	N	0	1
36	O	0	1
37	P	0	3
38	Q	0	2
39	R	0	8
40	S	0	4
41	T	0	2
42	U	0	3
43	V	0	3
44	M	0	3
44	W	0	2
47	Z	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	a	0	1
49	b	0	4
51	d	0	1
52	f	0	3
53	h	0	3
55	j	0	4
56	g	0	2
57	e	0	7
58	k	0	6
58	w	0	2
59	l	0	4
59	x	0	3
60	y	0	1
61	o	0	6
61	z	0	6
62	A1	0	8
62	p	0	5
68	B5	0	4
All	All	0	193

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	d	74	PHE	C-N	9.73	1.52	1.34
23	A	240	ALA	C-N	8.07	1.52	1.34
24	B	135	TYR	CE1-CZ	-7.42	1.28	1.38
43	V	25	LEU	C-N	-7.23	1.20	1.34
27	E	123	CYS	CB-SG	-6.97	1.70	1.82
39	R	307	ILE	C-N	6.95	1.50	1.34
27	E	116	CYS	CB-SG	-6.25	1.71	1.82
23	A	92	CYS	CB-SG	-5.94	1.72	1.81
8	2	193	VAL	CB-CG2	-5.58	1.41	1.52
26	D	163	TYR	CE2-CZ	-5.55	1.31	1.38
5	4	161	LEU	CA-C	-5.47	1.38	1.52
26	D	163	TYR	CD2-CE2	-5.30	1.31	1.39
27	E	122	VAL	CB-CG1	-5.29	1.41	1.52
23	A	226	CYS	CB-SG	-5.26	1.73	1.81
23	A	75	CYS	CB-SG	-5.26	1.73	1.81
27	E	120	GLU	CG-CD	-5.15	1.44	1.51
23	A	228	VAL	CB-CG1	-5.09	1.42	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	80	PRO	CA-N-CD	-8.63	99.42	111.50
27	E	140	ARG	CG-CD-NE	8.46	129.57	111.80
27	E	170	GLY	C-N-CD	-8.04	102.91	120.60
23	A	139	LEU	CA-CB-CG	-8.03	96.84	115.30
27	E	118	LEU	CB-CG-CD2	-7.90	97.57	111.00
50	c	36	PRO	C-N-CD	-7.74	103.57	120.60
23	A	121	LEU	CA-CB-CG	-7.67	97.66	115.30
23	A	610	VAL	C-N-CA	-7.31	103.44	121.70
62	p	146	PRO	N-CA-CB	7.20	111.94	103.30
24	B	363	VAL	C-N-CA	-6.67	105.03	121.70
24	B	123	LEU	CB-CG-CD1	-6.54	99.89	111.00
13	A7	133	GLY	N-CA-C	6.43	129.18	113.10
59	x	230	LEU	N-CA-C	6.38	128.22	111.00
62	p	159	PRO	N-CA-CB	6.32	110.88	103.30
62	p	82	PRO	N-CA-CB	6.30	110.87	103.30
27	E	70	LEU	CA-CB-CG	-6.25	100.93	115.30
24	B	379	ILE	CG1-CB-CG2	-6.23	97.70	111.40
24	B	420	TYR	N-CA-C	-6.15	94.38	111.00
24	B	309	ASP	N-CA-C	-6.14	94.42	111.00
24	B	82	LEU	CA-CB-CG	6.12	129.37	115.30
25	C	206	LEU	CB-CG-CD2	-6.10	100.62	111.00
24	B	218	SER	C-N-CA	-6.08	109.53	122.30
5	4	75	LEU	CB-CG-CD2	-6.06	100.69	111.00
24	B	293	LEU	N-CA-C	-6.06	94.64	111.00
44	M	42	LEU	CA-CB-CG	6.04	129.18	115.30
5	4	115	LEU	CA-CB-CG	-5.99	101.53	115.30
27	E	140	ARG	CA-CB-CG	5.97	126.54	113.40
1	3	64	LEU	CA-CB-CG	-5.97	101.57	115.30
27	E	140	ARG	CB-CG-CD	-5.89	96.28	111.60
24	B	123	LEU	CA-CB-CG	5.89	128.84	115.30
24	B	292	MET	C-N-CA	5.86	136.36	121.70
23	A	351	LEU	CA-CB-CG	-5.84	101.86	115.30
42	U	120	THR	C-N-CD	-5.81	107.82	120.60
68	B5	62	ARG	NE-CZ-NH1	-5.79	117.41	120.30
61	o	80	MET	CA-CB-CG	5.78	123.13	113.30
50	c	36	PRO	C-N-CA	5.71	145.99	122.00
2	1	146	LEU	CB-CG-CD1	-5.65	101.39	111.00
27	E	122	VAL	CB-CA-C	-5.61	100.74	111.40
24	B	378	LEU	CA-CB-CG	-5.61	102.40	115.30
62	p	120	PRO	N-CA-CB	5.60	110.02	103.30
7	6	562	LEU	CA-CB-CG	-5.58	102.47	115.30
58	k	215	HIS	C-N-CA	5.52	135.50	121.70
61	o	79	GLU	N-CA-C	5.48	125.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	16	LEU	CA-CB-CG	-5.46	102.75	115.30
23	A	381	LEU	CB-CG-CD2	-5.42	101.79	111.00
62	p	130	PRO	N-CA-CB	5.36	109.73	103.30
57	e	119	THR	N-CA-C	5.35	125.44	111.00
23	A	381	LEU	CA-CB-CG	5.31	127.52	115.30
5	4	248	LEU	CB-CG-CD1	-5.30	101.99	111.00
26	D	172	GLY	N-CA-C	5.29	126.32	113.10
61	z	90	TYR	C-N-CA	-5.25	108.56	121.70
16	A6	5	LYS	N-CA-C	5.22	125.09	111.00
55	j	22	PRO	C-N-CD	-5.21	109.13	120.60
24	B	124	ILE	CG1-CB-CG2	-5.21	99.93	111.40
2	1	158	GLY	N-CA-C	5.21	126.13	113.10
61	o	90	TYR	C-N-CA	-5.20	108.69	121.70
37	P	26	LEU	CA-CB-CG	5.19	127.24	115.30
23	A	423	LEU	CA-CB-CG	5.17	127.19	115.30
61	o	5	LEU	C-N-CA	-5.15	108.82	121.70
10	C3	435	GLY	N-CA-C	5.14	125.95	113.10
6	5	12	PHE	C-N-CA	-5.14	108.86	121.70
61	z	5	LEU	C-N-CA	-5.11	108.92	121.70
26	D	193	LEU	CA-CB-CG	-5.11	103.54	115.30
2	1	253	GLU	C-N-CA	-5.09	108.97	121.70
5	4	321	LEU	CA-CB-CG	-5.07	103.64	115.30
56	g	27	PRO	C-N-CA	-5.04	109.10	121.70
9	8	120	GLY	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (193) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	125	SER	Peptide
2	1	195	ARG	Peptide
2	1	66	SER	Mainchain
8	2	106	LEU	Peptide
8	2	112	HIS	Peptide
8	2	147	PRO	Peptide
8	2	193	VAL	Peptide
8	2	220	MET	Peptide
8	2	24	SER	Peptide
8	2	327	PRO	Peptide
8	2	336	MET	Peptide
8	2	337	LEU	Peptide
8	2	45	MET	Peptide

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Mol	Chain	Res	Type	Group
1	3	42	ASP	Peptide
1	3	69	ILE	Peptide
5	4	20	ASN	Peptide
5	4	226	ALA	Peptide
5	4	306	PRO	Peptide
5	4	419	TYR	Peptide
5	4	48	ASN	Peptide
5	4	56	PHE	Peptide
5	4	60	SER	Peptide
5	4	64	PRO	Peptide
5	4	74	PRO	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
6	5	93	LEU	Peptide
7	6	30	SER	Peptide
7	6	351	ASN	Peptide
7	6	522	PHE	Peptide
7	6	64	SER	Peptide
7	6	65	ASN	Peptide
4	7	137	SER	Peptide
4	7	170	GLU	Peptide
4	7	24	PRO	Peptide
4	7	25	SER	Peptide
4	7	26	PRO	Peptide
4	7	72	THR	Peptide
9	8	102	MET	Peptide
9	8	203	ALA	Peptide
9	8	204	TYR	Peptide
9	8	208	GLU	Peptide
9	8	228	PRO	Peptide
9	8	260	ALA	Peptide
9	8	306	GLY	Peptide
9	8	404	ALA	Peptide
3	9	109	PRO	Peptide
3	9	150	GLU	Peptide
3	9	167	LYS	Peptide
3	9	228	ALA	Peptide
3	9	75	LYS	Peptide
3	9	91	GLY	Peptide
23	A	124	HIS	Peptide
23	A	127	ASP	Peptide

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Mol	Chain	Res	Type	Group
23	A	128	CYS	Peptide
23	A	143	SER	Peptide
23	A	147	GLY	Peptide
23	A	236	TYR	Peptide
23	A	253	VAL	Peptide
23	A	259	SER	Peptide
23	A	274	LEU	Peptide
23	A	308	ARG	Peptide
23	A	460	HIS	Peptide
23	A	549	GLY	Peptide
23	A	564	CYS	Peptide
23	A	689	LEU	Peptide
23	A	691	ILE	Peptide
23	A	98	LYS	Peptide
62	A1	119	ASP	Peptide
62	A1	121	GLN	Peptide
62	A1	123	ASP	Peptide
62	A1	163	SER	Peptide
62	A1	165	TYR	Peptide
62	A1	177	PRO	Peptide
62	A1	184	SER	Peptide
62	A1	193	VAL	Peptide
24	B	219	GLY	Peptide
24	B	272	THR	Peptide
24	B	290	GLY	Peptide
24	B	309	ASP	Peptide
68	B5	58	GLN	Peptide
68	B5	61	GLY	Peptide
68	B5	63	PRO	Peptide
68	B5	71	ASN	Peptide
26	D	113	PHE	Peptide
26	D	126	ALA	Peptide
26	D	161	GLY	Peptide
26	D	184	PRO	Peptide
26	D	186	CYS	Peptide
26	D	188	PRO	Peptide
27	E	106	TYR	Peptide
27	E	107	PRO	Peptide
27	E	108	SER	Peptide
27	E	75	SER	Peptide
27	E	85	ASN	Peptide
30	H	84	GLU	Peptide

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Mol	Chain	Res	Type	Group
30	H	94	PRO	Peptide
31	I	69	ILE	Peptide
33	K	40	ARG	Peptide
34	L	40	LYS	Peptide
44	M	24	LYS	Peptide
44	M	37	MET	Peptide
44	M	63	PRO	Peptide
35	N	17	CYS	Peptide
36	O	42	GLU	Peptide
37	P	109	ASP	Peptide
37	P	44	GLY	Peptide
37	P	62	GLU	Peptide
38	Q	39	PRO	Peptide
38	Q	91	TYR	Peptide
39	R	154	GLN	Peptide
39	R	221	ARG	Peptide
39	R	253	ILE	Peptide
39	R	271	TYR	Peptide
39	R	324	THR	Peptide
39	R	333	PRO	Peptide
39	R	355	ARG	Peptide
39	R	78	SER	Peptide
40	S	311	GLN	Peptide
40	S	337	ASP	Peptide
40	S	66	ALA	Peptide
40	S	67	GLU	Peptide
41	T	105	THR	Peptide
41	T	83	LYS	Peptide
42	U	117	LEU	Peptide
42	U	118	SER	Peptide
42	U	47	LYS	Peptide
43	V	142	TRP	Peptide
43	V	24	ASN	Peptide
43	V	72	MET	Peptide
44	W	128	PHE	Peptide
44	W	154	VAL	Peptide
47	Z	23	LYS	Peptide
47	Z	63	PHE	Peptide
48	a	26	SER	Peptide
49	b	110	TRP	Peptide
49	b	129	PRO	Peptide
49	b	132	ASN	Peptide

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Mol	Chain	Res	Type	Group
49	b	134	GLU	Peptide
51	d	18	ASP	Peptide
57	e	107	TRP	Peptide
57	e	60	GLU	Peptide
57	e	65	TYR	Peptide
57	e	79	PRO	Peptide
57	e	80	ASP	Peptide
57	e	81	ARG	Peptide
57	e	87	ASP	Peptide
52	f	109	PRO	Peptide
52	f	131	GLU	Peptide
52	f	150	ARG	Peptide
56	g	160	LYS	Peptide
56	g	78	GLN	Peptide
53	h	133	GLY	Peptide
53	h	80	PRO	Peptide
53	h	81	ALA	Peptide
55	j	109	TYR	Peptide
55	j	110	GLY	Peptide
55	j	21	LEU	Peptide
55	j	54	LEU	Peptide
58	k	212	ALA	Peptide
58	k	216	PHE	Peptide
58	k	222	THR	Peptide
58	k	228	VAL	Peptide
58	k	229	PRO	Peptide
58	k	428	ILE	Peptide
59	l	227	ARG	Peptide
59	l	229	GLY	Mainchain
59	l	231	GLY	Peptide
59	l	304	HIS	Peptide
61	o	240	PRO	Peptide
61	o	50	HIS	Peptide
61	o	69	GLU	Mainchain
61	o	78	GLY	Peptide
61	o	79	GLU	Peptide
61	o	83	ARG	Peptide
62	p	133	VAL	Peptide
62	p	135	LEU	Peptide
62	p	143	GLY	Peptide
62	p	76	ILE	Peptide
62	p	77	LYS	Peptide

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Mol	Chain	Res	Type	Group
58	w	212	ALA	Peptide
58	w	428	ILE	Peptide
59	x	227	ARG	Peptide
59	x	229	GLY	Mainchain
59	x	230	LEU	Peptide
60	y	344	GLU	Peptide
61	z	240	PRO	Peptide
61	z	50	HIS	Peptide
61	z	69	GLU	Mainchain,Peptide
61	z	78	GLY	Peptide
61	z	83	ARG	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	17	56
2	1	316/318 (99%)	254 (80%)	49 (16%)	13 (4%)	3	25
3	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	29
4	7	170/175 (97%)	133 (78%)	27 (16%)	10 (6%)	1	19
5	4	457/459 (100%)	392 (86%)	57 (12%)	8 (2%)	8	41
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	6	604/606 (100%)	519 (86%)	82 (14%)	3 (0%)	29	68
8	2	342/347 (99%)	284 (83%)	56 (16%)	2 (1%)	25	65
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	9	44
10	C3	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C1	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
12	A9	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
13	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
14	B4	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
15	A5	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	3	25
16	A6	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	18
17	C0	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	11	46
18	C2	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
19	B2	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	3	27
20	B3	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
21	A0	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
22	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
23	A	686/704 (97%)	560 (82%)	112 (16%)	14 (2%)	7	39
24	B	428/430 (100%)	344 (80%)	77 (18%)	7 (2%)	9	44
25	C	206/228 (90%)	172 (84%)	32 (16%)	2 (1%)	15	54
26	D	150/179 (84%)	122 (81%)	24 (16%)	4 (3%)	5	33
27	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	9	43
28	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	3	26
29	G	121/133 (91%)	102 (84%)	18 (15%)	1 (1%)	19	60
30	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	4	30
31	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	24
32	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	4	31
33	K	82/98 (84%)	66 (80%)	15 (18%)	1 (1%)	13	50
34	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
35	N	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
36	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	5	33
37	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
38	Q	166/171 (97%)	115 (69%)	48 (29%)	3 (2%)	8	41
39	R	305/345 (88%)	240 (79%)	60 (20%)	5 (2%)	9	44
40	S	317/320 (99%)	239 (75%)	67 (21%)	11 (4%)	3	28
41	T	136/140 (97%)	115 (85%)	12 (9%)	9 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
43	V	136/143 (95%)	111 (82%)	22 (16%)	3 (2%)	6	37
44	M	78/86 (91%)	56 (72%)	19 (24%)	3 (4%)	3	26
44	W	84/86 (98%)	68 (81%)	15 (18%)	1 (1%)	13	50
45	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	24
46	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	8	41
47	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	5	32
48	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
49	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	22	62
50	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
51	d	105/117 (90%)	89 (85%)	13 (12%)	3 (3%)	4	31
52	f	165/178 (93%)	129 (78%)	34 (21%)	2 (1%)	13	50
53	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	3	27
54	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
55	j	111/120 (92%)	96 (86%)	15 (14%)	0	100	100
56	g	171/176 (97%)	142 (83%)	27 (16%)	2 (1%)	13	50
57	e	139/158 (88%)	80 (58%)	47 (34%)	12 (9%)	1	12
58	k	444/480 (92%)	405 (91%)	35 (8%)	4 (1%)	17	56
58	w	432/480 (90%)	400 (93%)	29 (7%)	3 (1%)	22	62
59	l	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	15	54
59	x	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	15	54
60	m	377/379 (100%)	341 (90%)	35 (9%)	1 (0%)	41	76
60	y	377/379 (100%)	341 (90%)	36 (10%)	0	100	100
61	o	239/325 (74%)	204 (85%)	34 (14%)	1 (0%)	34	72
61	z	239/325 (74%)	205 (86%)	32 (13%)	2 (1%)	19	60
62	A1	184/196 (94%)	137 (74%)	41 (22%)	6 (3%)	4	29
62	p	147/196 (75%)	100 (68%)	35 (24%)	12 (8%)	1	13
63	A2	104/111 (94%)	91 (88%)	8 (8%)	5 (5%)	2	23
63	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
64	A3	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
64	r	79/82 (96%)	72 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	B7	67/91 (74%)	57 (85%)	7 (10%)	3 (4%)	2	24
65	s	65/91 (71%)	55 (85%)	7 (11%)	3 (5%)	2	23
66	A4	37/56 (66%)	23 (62%)	8 (22%)	6 (16%)	0	3
66	t	31/56 (55%)	24 (77%)	7 (23%)	0	100	100
67	B6	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
67	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
68	B5	20/78 (26%)	10 (50%)	8 (40%)	2 (10%)	0	10
68	v	16/78 (20%)	8 (50%)	7 (44%)	1 (6%)	1	18
All	All	13628/15127 (90%)	11521 (84%)	1873 (14%)	234 (2%)	13	43

All (234) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	170	GLU
2	1	174	LEU
2	1	268	MET
4	7	79	TYR
4	7	82	ILE
4	7	85	SER
4	7	141	MET
4	7	171	ILE
8	2	84	TRP
10	C3	328	HIS
10	C3	508	PRO
15	A5	2	SER
15	A5	87	THR
15	A5	95	GLN
16	A6	4	ALA
16	A6	9	GLY
17	C0	46	LYS
19	B2	2	GLU
23	A	383	SER
23	A	461	PRO
23	A	463	SER
24	B	294	ARG
26	D	146	GLU
31	I	106	GLU
31	I	109	THR
40	S	199	VAL

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Mol	Chain	Res	Type
40	S	202	VAL
40	S	276	ASP
41	T	46	PRO
41	T	66	ILE
43	V	143	TYR
47	Z	63	PHE
47	Z	64	VAL
53	h	81	ALA
53	h	82	VAL
57	e	41	TYR
57	e	81	ARG
57	e	82	SER
57	e	115	ASN
62	p	82	PRO
62	p	120	PRO
62	p	129	LYS
62	p	146	PRO
62	p	159	PRO
65	s	14	VAL
61	z	79	GLU
61	z	80	MET
63	A2	17	ARG
63	A2	18	LYS
63	A2	19	TRP
63	A2	20	TYR
65	B7	14	VAL
66	A4	40	LEU
66	A4	41	ILE
66	A4	42	LEU
2	1	76	ILE
2	1	78	ALA
2	1	173	TRP
2	1	176	LEU
2	1	282	TYR
3	9	75	LYS
3	9	76	ALA
5	4	21	ASN
5	4	420	THR
8	2	88	LYS
16	A6	5	LYS
23	A	189	ILE
24	B	310	VAL

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Mol	Chain	Res	Type
26	D	147	PRO
26	D	184	PRO
30	H	16	ARG
36	O	100	ARG
39	R	155	VAL
39	R	272	LEU
40	S	58	LYS
45	X	14	VAL
57	e	71	GLY
62	p	130	PRO
68	v	65	VAL
58	w	214	LYS
62	A1	80	ASP
62	A1	92	ARG
68	B5	65	VAL
1	3	82	ALA
2	1	177	PRO
4	7	140	ALA
4	7	148	SER
4	7	170	GLU
5	4	61	LEU
5	4	65	LEU
7	6	352	ASP
9	8	235	VAL
9	8	403	ASP
11	C1	104	TRP
16	A6	61	SER
23	A	129	PRO
23	A	283	GLU
23	A	541	PRO
24	B	291	VAL
24	B	293	LEU
33	K	52	PRO
38	Q	94	LEU
38	Q	121	ASP
39	R	99	ASP
40	S	280	HIS
40	S	333	GLU
41	T	47	THR
44	W	129	GLU
56	g	74	ILE
56	g	126	ALA

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Mol	Chain	Res	Type
57	e	70	THR
59	l	305	GLN
62	p	81	ILE
2	1	71	PHE
4	7	81	GLU
10	C3	51	ASP
24	B	62	LYS
25	C	127	ARG
26	D	103	ARG
27	E	106	TYR
27	E	107	PRO
29	G	122	SER
30	H	57	LYS
31	I	108	LYS
36	O	25	MET
39	R	325	THR
40	S	216	LYS
40	S	281	LYS
41	T	105	THR
51	d	19	PRO
51	d	39	MET
52	f	165	PRO
57	e	42	PRO
57	e	76	PRO
44	M	30	LEU
44	M	60	PHE
58	k	219	LEU
58	k	427	PRO
62	p	115	SER
62	p	134	ILE
58	w	427	PRO
66	A4	36	THR
2	1	316	PRO
3	9	150	GLU
3	9	232	THR
3	9	234	LEU
5	4	58	SER
5	4	112	ALA
9	8	282	VAL
9	8	381	GLN
11	C1	103	GLN
19	B2	3	ASN

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Mol	Chain	Res	Type
23	A	188	GLU
23	A	563	ASP
24	B	78	SER
27	E	171	PRO
38	Q	32	TYR
39	R	316	ARG
40	S	334	ASP
41	T	107	SER
45	X	13	HIS
49	b	111	GLU
57	e	79	PRO
65	s	63	HIS
62	A1	30	GLU
62	A1	171	ILE
65	B7	63	HIS
4	7	105	TYR
5	4	82	HIS
7	6	65	ASN
9	8	227	PRO
9	8	236	PHE
9	8	387	GLU
10	C3	91	ASP
11	C1	158	ASP
16	A6	49	PRO
23	A	128	CYS
28	F	86	LEU
32	J	55	SER
36	O	116	LYS
52	f	149	PRO
57	e	105	MET
58	k	229	PRO
59	l	195	VAL
59	l	278	VAL
61	o	70	VAL
62	p	136	ILE
65	s	70	ALA
59	x	195	VAL
59	x	278	VAL
65	B7	70	ALA
66	A4	35	ALA
7	6	71	ILE
23	A	561	PRO

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Mol	Chain	Res	Type
24	B	39	PRO
32	J	57	VAL
43	V	26	PRO
51	d	40	VAL
62	A1	194	ILE
66	A4	27	VAL
2	1	249	PRO
41	T	83	LYS
41	T	84	PRO
43	V	73	PRO
53	h	80	PRO
59	l	382	VAL
59	x	305	GLN
59	x	382	VAL
2	1	208	VAL
15	A5	15	GLY
23	A	45	PRO
23	A	210	ILE
41	T	76	ILE
41	T	125	VAL
46	Y	90	PRO
3	9	241	PRO
5	4	306	PRO
23	A	263	VAL
25	C	218	VAL
30	H	25	GLN
58	k	71	PRO
62	p	93	GLY
62	p	114	VAL
58	w	71	PRO
62	A1	193	VAL
63	A2	6	VAL
3	9	216	PRO
40	S	340	ILE
57	e	78	LEU
57	e	87	ASP
44	M	27	PRO
60	m	343	VAL
68	B5	63	PRO
40	S	323	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	96/101 (95%)	96 (100%)	0	100	100
2	1	274/275 (100%)	256 (93%)	18 (7%)	16	43
3	9	170/183 (93%)	168 (99%)	2 (1%)	71	84
4	7	115/142 (81%)	113 (98%)	2 (2%)	60	78
5	4	389/413 (94%)	389 (100%)	0	100	100
6	5	80/86 (93%)	80 (100%)	0	100	100
7	6	524/534 (98%)	523 (100%)	1 (0%)	93	96
8	2	304/316 (96%)	302 (99%)	2 (1%)	84	90
9	8	270/353 (76%)	270 (100%)	0	100	100
10	C3	427/427 (100%)	389 (91%)	38 (9%)	9	33
11	C1	211/211 (100%)	191 (90%)	20 (10%)	8	29
12	A9	226/226 (100%)	199 (88%)	27 (12%)	5	22
13	A7	128/148 (86%)	120 (94%)	8 (6%)	18	44
14	B4	95/123 (77%)	89 (94%)	6 (6%)	18	44
15	A5	81/103 (79%)	76 (94%)	5 (6%)	18	45
16	A6	68/79 (86%)	50 (74%)	18 (26%)	0	4
17	C0	67/76 (88%)	58 (87%)	9 (13%)	4	19
18	C2	58/59 (98%)	53 (91%)	5 (9%)	10	35
19	B2	47/68 (69%)	40 (85%)	7 (15%)	3	16
20	B3	39/66 (59%)	37 (95%)	2 (5%)	24	50
21	A0	40/55 (73%)	38 (95%)	2 (5%)	24	50
22	A8	37/57 (65%)	34 (92%)	3 (8%)	11	37
23	A	560/588 (95%)	558 (100%)	2 (0%)	91	94
24	B	363/371 (98%)	357 (98%)	6 (2%)	60	78
25	C	188/204 (92%)	187 (100%)	1 (0%)	88	93
26	D	127/150 (85%)	126 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	E	148/151 (98%)	148 (100%)	0	100	100
28	F	14/69 (20%)	14 (100%)	0	100	100
29	G	106/119 (89%)	105 (99%)	1 (1%)	78	88
30	H	80/95 (84%)	80 (100%)	0	100	100
31	I	54/79 (68%)	51 (94%)	3 (6%)	21	48
32	J	50/59 (85%)	50 (100%)	0	100	100
33	K	67/81 (83%)	67 (100%)	0	100	100
34	L	63/71 (89%)	63 (100%)	0	100	100
35	N	88/101 (87%)	88 (100%)	0	100	100
36	O	95/113 (84%)	95 (100%)	0	100	100
37	P	73/96 (76%)	73 (100%)	0	100	100
38	Q	142/154 (92%)	142 (100%)	0	100	100
39	R	230/298 (77%)	230 (100%)	0	100	100
40	S	205/283 (72%)	205 (100%)	0	100	100
41	T	76/101 (75%)	76 (100%)	0	100	100
42	U	95/131 (72%)	95 (100%)	0	100	100
43	V	106/120 (88%)	106 (100%)	0	100	100
44	M	73/79 (92%)	73 (100%)	0	100	100
44	W	57/79 (72%)	55 (96%)	2 (4%)	36	59
45	X	32/54 (59%)	32 (100%)	0	100	100
46	Y	29/62 (47%)	29 (100%)	0	100	100
47	Z	28/76 (37%)	28 (100%)	0	100	100
48	a	70/114 (61%)	70 (100%)	0	100	100
49	b	85/124 (68%)	85 (100%)	0	100	100
50	c	45/122 (37%)	45 (100%)	0	100	100
51	d	43/107 (40%)	43 (100%)	0	100	100
52	f	80/160 (50%)	80 (100%)	0	100	100
53	h	63/112 (56%)	63 (100%)	0	100	100
54	i	23/45 (51%)	23 (100%)	0	100	100
55	j	88/106 (83%)	88 (100%)	0	100	100
56	g	130/157 (83%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	e	44/141 (31%)	41 (93%)	3 (7%)	16	42
58	k	369/394 (94%)	369 (100%)	0	100	100
58	w	362/394 (92%)	362 (100%)	0	100	100
59	l	327/355 (92%)	327 (100%)	0	100	100
59	x	328/355 (92%)	328 (100%)	0	100	100
60	m	327/327 (100%)	327 (100%)	0	100	100
60	y	327/327 (100%)	327 (100%)	0	100	100
61	o	206/257 (80%)	206 (100%)	0	100	100
61	z	202/257 (79%)	202 (100%)	0	100	100
62	A1	64/168 (38%)	64 (100%)	0	100	100
62	p	65/168 (39%)	65 (100%)	0	100	100
63	A2	93/99 (94%)	90 (97%)	3 (3%)	39	61
63	q	96/99 (97%)	96 (100%)	0	100	100
64	A3	70/72 (97%)	70 (100%)	0	100	100
64	r	71/72 (99%)	71 (100%)	0	100	100
65	B7	66/85 (78%)	66 (100%)	0	100	100
65	s	64/85 (75%)	64 (100%)	0	100	100
66	A4	31/46 (67%)	27 (87%)	4 (13%)	4	20
66	t	24/46 (52%)	21 (88%)	3 (12%)	4	21
67	B6	52/54 (96%)	52 (100%)	0	100	100
67	u	52/54 (96%)	52 (100%)	0	100	100
68	B5	15/60 (25%)	14 (93%)	1 (7%)	16	42
68	v	11/60 (18%)	11 (100%)	0	100	100
All	All	10788/12907 (84%)	10583 (98%)	205 (2%)	59	75

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	70	MET
2	1	71	PHE
2	1	77	MET
2	1	156	MET
2	1	157	SER
2	1	171	GLN

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Mol	Chain	Res	Type
2	1	172	MET
2	1	174	LEU
2	1	235	ASN
2	1	236	ILE
2	1	250	HIS
2	1	251	MET
2	1	265	LEU
2	1	266	LEU
2	1	269	SER
2	1	309	ILE
2	1	317	GLN
2	1	318	THR
3	9	93	LEU
3	9	188	ILE
4	7	83	TRP
4	7	86	ASN
7	6	587	TYR
8	2	84	TRP
8	2	114	TRP
10	C3	18	LEU
10	C3	35	LEU
10	C3	92	MET
10	C3	96	ARG
10	C3	105	LEU
10	C3	109	PHE
10	C3	115	SER
10	C3	138	HIS
10	C3	150	LEU
10	C3	159	LEU
10	C3	187	SER
10	C3	188	VAL
10	C3	199	LEU
10	C3	213	ARG
10	C3	238	PHE
10	C3	241	PRO
10	C3	273	MET
10	C3	295	VAL
10	C3	301	THR
10	C3	306	THR
10	C3	318	VAL
10	C3	324	LEU
10	C3	347	LEU

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Mol	Chain	Res	Type
10	C3	353	LEU
10	C3	354	THR
10	C3	365	ILE
10	C3	369	ASP
10	C3	373	VAL
10	C3	383	MET
10	C3	417	MET
10	C3	465	VAL
10	C3	467	LEU
10	C3	474	GLU
10	C3	486	ASP
10	C3	492	LEU
10	C3	508	PRO
10	C3	509	THR
10	C3	512	ASN
11	C1	7	LEU
11	C1	31	VAL
11	C1	52	HIS
11	C1	60	GLU
11	C1	63	THR
11	C1	65	TRP
11	C1	88	ASP
11	C1	92	ASN
11	C1	113	TYR
11	C1	125	THR
11	C1	130	PRO
11	C1	134	ARG
11	C1	142	VAL
11	C1	147	GLU
11	C1	148	MET
11	C1	170	LEU
11	C1	171	LYS
11	C1	185	MET
11	C1	205	SER
11	C1	216	LEU
12	A9	1	MET
12	A9	11	VAL
12	A9	13	PRO
12	A9	14	SER
12	A9	18	LEU
12	A9	19	THR
12	A9	22	LEU

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Mol	Chain	Res	Type
12	A9	38	ASN
12	A9	39	SER
12	A9	85	LEU
12	A9	92	LEU
12	A9	112	LEU
12	A9	127	LEU
12	A9	128	GLU
12	A9	131	LEU
12	A9	132	LEU
12	A9	137	LEU
12	A9	142	VAL
12	A9	159	MET
12	A9	160	LEU
12	A9	163	LEU
12	A9	188	ILE
12	A9	196	THR
12	A9	199	VAL
12	A9	214	PHE
12	A9	222	GLN
12	A9	258	TRP
13	A7	31	LYS
13	A7	36	SER
13	A7	40	LEU
13	A7	59	LEU
13	A7	62	LEU
13	A7	107	ILE
13	A7	143	ASN
13	A7	147	LYS
14	B4	7	THR
14	B4	29	LEU
14	B4	70	VAL
14	B4	79	LYS
14	B4	80	GLU
14	B4	90	ARG
15	A5	37	LYS
15	A5	53	THR
15	A5	74	LEU
15	A5	95	GLN
15	A5	98	HIS
16	A6	5	LYS
16	A6	7	ASP
16	A6	8	HIS

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Mol	Chain	Res	Type
16	A6	14	ARG
16	A6	17	ARG
16	A6	33	LEU
16	A6	34	ASN
16	A6	37	LEU
16	A6	38	HIS
16	A6	41	HIS
16	A6	42	ARG
16	A6	43	GLU
16	A6	48	ILE
16	A6	54	ARG
16	A6	56	ARG
16	A6	68	THR
16	A6	69	PHE
16	A6	78	LEU
17	C0	19	ARG
17	C0	24	ASN
17	C0	28	ASN
17	C0	29	CYS
17	C0	51	SER
17	C0	53	CYS
17	C0	57	ARG
17	C0	60	TYR
17	C0	75	ARG
18	C2	2	THR
18	C2	8	GLN
18	C2	26	MET
18	C2	44	LYS
18	C2	64	ARG
19	B2	1	PHE
19	B2	2	GLU
19	B2	3	ASN
19	B2	8	LYS
19	B2	16	ASN
19	B2	23	LYS
19	B2	27	THR
20	B3	48	VAL
20	B3	49	THR
21	A0	15	VAL
21	A0	22	LEU
22	A8	13	LYS
22	A8	42	LYS

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Mol	Chain	Res	Type
22	A8	43	SER
23	A	146	PHE
23	A	223	ILE
24	B	61	TRP
24	B	141	TYR
24	B	236	LEU
24	B	389	TYR
24	B	429	PHE
24	B	432	LEU
25	C	95	VAL
26	D	146	GLU
29	G	143	TRP
31	I	103	LEU
31	I	106	GLU
31	I	108	LYS
44	W	106	LYS
44	W	108	LEU
57	e	114	ARG
57	e	118	ASP
57	e	119	THR
66	t	37	ASP
66	t	38	TRP
66	t	39	ARG
63	A2	13	LEU
63	A2	16	ILE
63	A2	19	TRP
66	A4	37	ASP
66	A4	39	ARG
66	A4	40	LEU
66	A4	45	VAL
68	B5	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	5	ASN
2	1	169	GLN
2	1	171	GLN
2	1	230	ASN
2	1	287	HIS
2	1	317	GLN
3	9	87	GLN

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Mol	Chain	Res	Type
5	4	30	HIS
5	4	168	GLN
5	4	331	ASN
5	4	366	ASN
5	4	440	HIS
6	5	7	ASN
6	5	97	GLN
7	6	59	GLN
7	6	248	HIS
7	6	546	GLN
7	6	605	HIS
8	2	36	ASN
8	2	49	ASN
9	8	103	ASN
9	8	168	ASN
9	8	220	GLN
9	8	281	HIS
9	8	393	ASN
9	8	422	HIS
10	C3	11	ASN
10	C3	12	HIS
10	C3	43	GLN
10	C3	99	ASN
10	C3	170	ASN
10	C3	256	HIS
10	C3	360	ASN
10	C3	413	HIS
10	C3	512	ASN
11	C1	22	HIS
11	C1	103	GLN
11	C1	203	ASN
12	A9	6	HIS
12	A9	12	ASN
12	A9	133	ASN
12	A9	148	HIS
12	A9	207	HIS
12	A9	222	GLN
12	A9	232	HIS
13	A7	109	HIS
14	B4	34	ASN
15	A5	66	ASN
16	A6	52	HIS

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Mol	Chain	Res	Type
17	C0	23	GLN
17	C0	24	ASN
17	C0	25	GLN
17	C0	28	ASN
17	C0	37	HIS
19	B2	3	ASN
19	B2	16	ASN
20	B3	10	HIS
20	B3	15	ASN
20	B3	41	ASN
21	A0	42	HIS
22	A8	39	ASN
23	A	59	GLN
23	A	142	GLN
23	A	282	ASN
23	A	359	ASN
23	A	460	HIS
23	A	571	HIS
23	A	572	HIS
24	B	79	ASN
24	B	182	ASN
24	B	183	HIS
24	B	234	GLN
24	B	349	ASN
24	B	381	HIS
25	C	230	GLN
26	D	164	HIS
27	E	204	ASN
30	H	21	GLN
30	H	82	GLN
34	L	46	ASN
36	O	102	HIS
37	P	52	ASN
38	Q	35	GLN
38	Q	143	HIS
39	R	71	ASN
39	R	251	ASN
39	R	323	HIS
39	R	331	HIS
40	S	120	GLN
40	S	164	GLN
40	S	190	HIS

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Mol	Chain	Res	Type
42	U	123	GLN
43	V	76	GLN
44	W	115	GLN
45	X	13	HIS
46	Y	86	HIS
50	c	26	GLN
50	c	83	HIS
51	d	92	HIS
53	h	74	HIS
53	h	115	GLN
56	g	144	HIS
44	M	35	HIS
44	M	74	GLN
58	k	15	GLN
58	k	165	GLN
58	k	207	GLN
58	k	252	HIS
58	k	301	ASN
59	l	31	ASN
59	l	125	ASN
59	l	158	HIS
59	l	197	ASN
59	l	247	GLN
59	l	290	ASN
59	l	297	GLN
59	l	304	HIS
59	l	354	ASN
60	m	3	ASN
60	m	32	ASN
60	m	159	ASN
60	m	255	ASN
60	m	312	GLN
60	m	341	GLN
61	o	50	HIS
61	o	156	GLN
62	p	53	ASN
64	r	3	GLN
64	r	6	HIS
64	r	23	GLN
64	r	79	ASN
58	w	15	GLN
58	w	165	GLN

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Mol	Chain	Res	Type
58	w	207	GLN
58	w	252	HIS
58	w	323	HIS
59	x	31	ASN
59	x	125	ASN
59	x	156	GLN
59	x	158	HIS
59	x	197	ASN
59	x	247	GLN
59	x	290	ASN
59	x	297	GLN
59	x	304	HIS
59	x	354	ASN
60	y	3	ASN
60	y	32	ASN
60	y	255	ASN
60	y	312	GLN
60	y	341	GLN
61	z	50	HIS
61	z	75	ASN
64	A3	3	GLN
64	A3	23	GLN
64	A3	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
69	PC1	2	402	-	45,45,53	1.02	2 (4%)	51,53,61	0.99	2 (3%)
73	FMN	8	501	-	33,33,33	1.19	2 (6%)	48,50,50	1.62	12 (25%)
81	HEC	z	301	61	32,50,50	2.42	5 (15%)	24,82,82	1.79	6 (25%)
69	PC1	S	401	-	46,46,53	1.03	4 (8%)	52,54,61	1.07	2 (3%)
74	SF4	D	301	26	0,12,12	-	-	-		
70	3PE	2	401	-	40,40,50	0.93	3 (7%)	43,45,55	1.08	2 (4%)
74	SF4	A	802	-	0,12,12	-	-	-		
81	HEC	o	301	61	32,50,50	2.41	5 (15%)	24,82,82	1.80	6 (25%)
70	3PE	4	501	-	40,40,50	0.90	3 (7%)	43,45,55	1.38	2 (4%)
74	SF4	8	502	-	0,12,12	-	-	-		
76	HEA	C3	603	10	57,67,67	1.47	6 (10%)	61,103,103	1.45	11 (18%)
80	HEM	y	402	60	41,50,50	1.80	13 (31%)	45,82,82	1.29	5 (11%)
70	3PE	B	501	-	50,50,50	0.87	2 (4%)	53,55,55	1.34	4 (7%)
79	NAP	R	601	-	45,52,52	4.71	18 (40%)	56,80,80	1.90	7 (12%)
71	FES	m	403	-	0,4,4	-	-	-		
74	SF4	E	301	27	0,12,12	-	-	-		
70	3PE	j	202	-	45,45,50	0.89	3 (6%)	48,50,55	1.08	2 (4%)
76	HEA	C3	602	10	57,67,67	1.24	6 (10%)	61,103,103	1.47	12 (19%)
80	HEM	m	402	60	41,50,50	1.81	13 (31%)	45,82,82	1.29	5 (11%)
71	FES	9	301	-	0,4,4	-	-	-		
80	HEM	m	401	60	41,50,50	1.79	13 (31%)	45,82,82	1.60	6 (13%)
72	CDL	6	701	-	63,63,99	1.07	7 (11%)	69,75,111	1.26	4 (5%)
71	FES	A	803	23	0,4,4	-	-	-		
72	CDL	b	201	-	81,81,99	0.97	6 (7%)	87,93,111	1.15	4 (4%)
72	CDL	J	101	-	57,57,99	1.16	7 (12%)	63,69,111	1.19	5 (7%)
82	UQ2	A2	201	-	23,23,23	1.80	2 (8%)	28,31,31	1.44	5 (17%)
69	PC1	3	200	-	46,46,53	0.98	3 (6%)	52,54,61	1.08	2 (3%)
80	HEM	y	401	60	41,50,50	1.79	13 (31%)	45,82,82	1.59	6 (13%)
70	3PE	1	401	-	50,50,50	0.86	3 (6%)	53,55,55	1.13	2 (3%)
69	PC1	Q	201	-	45,45,53	1.06	3 (6%)	51,53,61	1.13	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
69	PC1	j	201	-	38,38,53	1.15	6 (15%)	44,46,61	1.06	2 (4%)
74	SF4	A	801	23	0,12,12	-	-	-		
74	SF4	E	302	27	0,12,12	-	-	-		

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
69	PC1	2	402	-	-	30/49/49/57	-
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
81	HEC	z	301	61	-	2/10/54/54	-
69	PC1	S	401	-	-	30/50/50/57	-
74	SF4	D	301	26	-	-	0/6/5/5
70	3PE	2	401	-	-	24/44/44/54	-
74	SF4	A	802	-	-	-	0/6/5/5
81	HEC	o	301	61	-	2/10/54/54	-
70	3PE	4	501	-	-	25/44/44/54	-
80	HEM	y	402	60	-	1/12/54/54	-
76	HEA	C3	603	10	3/3/7/16	5/32/76/76	-
74	SF4	8	502	-	-	-	0/6/5/5
70	3PE	B	501	-	-	28/54/54/54	-
79	NAP	R	601	-	-	14/31/67/67	0/5/5/5
71	FES	m	403	-	-	-	0/1/1/1
74	SF4	E	301	27	-	-	0/6/5/5
70	3PE	j	202	-	-	20/49/49/54	-
80	HEM	m	402	60	-	1/12/54/54	-
71	FES	9	301	-	-	-	0/1/1/1
74	SF4	E	302	27	-	-	0/6/5/5
80	HEM	m	401	60	-	3/12/54/54	-
72	CDL	6	701	-	-	34/74/74/110	-
71	FES	A	803	23	-	-	0/1/1/1
72	CDL	b	201	-	-	41/92/92/110	-
72	CDL	J	101	-	-	24/68/68/110	-
82	UQ2	A2	201	-	-	7/15/39/39	0/1/1/1
69	PC1	3	200	-	-	23/50/50/57	-
80	HEM	y	401	60	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	3PE	1	401	-	-	15/54/54/54	-
69	PC1	Q	201	-	-	23/49/49/57	-
69	PC1	j	201	-	-	21/42/42/57	-
74	SF4	A	801	23	-	-	0/6/5/5
76	HEA	C3	602	10	3/3/7/16	7/32/76/76	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	R	601	NAP	C2D-C1D	-15.67	1.30	1.53
79	R	601	NAP	O4D-C1D	15.35	1.62	1.41
79	R	601	NAP	O4B-C1B	14.97	1.62	1.41
81	z	301	HEC	C3C-C2C	-8.23	1.32	1.40
81	o	301	HEC	C3C-C2C	-8.10	1.32	1.40
82	A2	201	UQ2	C6-C5	7.64	1.49	1.35
81	z	301	HEC	C2B-C3B	-7.60	1.32	1.40
81	o	301	HEC	C2B-C3B	-7.56	1.32	1.40
79	R	601	NAP	O4D-C4D	-7.08	1.29	1.45
79	R	601	NAP	C7N-N7N	6.95	1.46	1.33
76	C3	603	HEA	C3A-C2A	-6.54	1.31	1.40
79	R	601	NAP	O4B-C4B	-6.13	1.31	1.45
80	m	401	HEM	C3C-C2C	-5.86	1.32	1.40
80	y	401	HEM	C3C-C2C	-5.85	1.32	1.40
80	m	402	HEM	C3C-C2C	-5.82	1.32	1.40
80	y	402	HEM	C3C-C2C	-5.76	1.32	1.40
81	o	301	HEC	C3D-C2D	4.91	1.52	1.37
81	z	301	HEC	C3D-C2D	4.87	1.52	1.37
79	R	601	NAP	C3N-C7N	4.71	1.57	1.50
79	R	601	NAP	O3D-C3D	-4.39	1.32	1.43
76	C3	603	HEA	C3A-CMA	-3.87	1.37	1.46
79	R	601	NAP	O7N-C7N	-3.68	1.17	1.24
79	R	601	NAP	O2D-C2D	3.59	1.51	1.43
80	m	401	HEM	FE-NB	-3.55	1.79	1.96
80	y	401	HEM	FE-NB	-3.51	1.79	1.96
76	C3	602	HEA	C3C-C2C	-3.21	1.35	1.40
82	A2	201	UQ2	C3-C2	3.15	1.49	1.36
80	m	402	HEM	FE-NB	-3.00	1.82	1.96
80	y	402	HEM	FE-NB	-3.00	1.82	1.96
69	Q	201	PC1	O21-C2	-2.98	1.39	1.46
79	R	601	NAP	C5A-C4A	-2.95	1.33	1.40
76	C3	602	HEA	C3A-CMA	-2.94	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	R	601	NAP	O3B-C3B	-2.93	1.36	1.43
70	B	501	3PE	O21-C2	-2.89	1.39	1.46
80	y	402	HEM	C4A-CHB	-2.82	1.33	1.41
80	m	402	HEM	C4A-CHB	-2.82	1.33	1.41
70	1	401	3PE	O21-C2	-2.81	1.39	1.46
80	y	401	HEM	C1B-NB	-2.78	1.35	1.40
76	C3	602	HEA	C4C-NC	2.77	1.41	1.36
72	6	701	CDL	OA6-CA4	-2.77	1.39	1.46
73	8	501	FMN	C4A-N5	2.76	1.36	1.30
80	y	402	HEM	C3C-CAC	2.75	1.53	1.47
80	y	402	HEM	C3D-C2D	-2.74	1.30	1.36
80	m	402	HEM	C3C-CAC	2.73	1.53	1.47
79	R	601	NAP	C6A-N6A	2.73	1.44	1.34
72	b	201	CDL	OB8-CB7	2.71	1.41	1.33
80	m	402	HEM	C3D-C2D	-2.71	1.30	1.36
72	J	101	CDL	OB6-CB4	-2.70	1.39	1.46
72	b	201	CDL	OA6-CA4	-2.67	1.39	1.46
70	j	202	3PE	O21-C2	-2.67	1.39	1.46
80	m	401	HEM	C1B-NB	-2.66	1.35	1.40
76	C3	603	HEA	C3C-C2C	-2.66	1.36	1.40
72	J	101	CDL	OA6-CA4	-2.65	1.40	1.46
80	m	402	HEM	C3B-C2B	-2.65	1.31	1.37
70	2	401	3PE	O21-C2	-2.61	1.40	1.46
80	y	402	HEM	C3B-C2B	-2.61	1.32	1.37
72	J	101	CDL	OA8-CA7	2.60	1.40	1.33
76	C3	603	HEA	C1D-C2D	2.59	1.49	1.44
76	C3	603	HEA	C1D-ND	-2.59	1.35	1.40
80	m	401	HEM	C1A-CHA	-2.56	1.33	1.41
80	y	401	HEM	C3D-C2D	-2.56	1.31	1.36
80	m	401	HEM	C3D-C2D	-2.55	1.31	1.36
70	B	501	3PE	O31-C3	-2.55	1.39	1.45
72	b	201	CDL	OB6-CB5	2.54	1.41	1.34
80	m	401	HEM	C3C-CAC	2.53	1.53	1.47
70	4	501	3PE	O31-C3	-2.53	1.39	1.45
80	y	401	HEM	C3C-CAC	2.52	1.53	1.47
80	y	401	HEM	C1A-CHA	-2.52	1.34	1.41
79	R	601	NAP	C4N-C3N	-2.51	1.35	1.39
69	2	402	PC1	O21-C21	2.51	1.41	1.34
69	Q	201	PC1	O31-C3	-2.51	1.39	1.45
69	3	200	PC1	O21-C2	-2.51	1.40	1.46
79	R	601	NAP	PA-O5B	2.51	1.69	1.59
69	S	401	PC1	O21-C2	-2.49	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	2	402	PC1	O31-C31	2.47	1.40	1.33
69	S	401	PC1	O31-C31	2.46	1.40	1.33
72	b	201	CDL	OA8-CA7	2.46	1.40	1.33
80	y	402	HEM	C2A-C3A	-2.46	1.30	1.37
69	j	201	PC1	O31-C31	2.45	1.40	1.33
80	m	402	HEM	C2A-C3A	-2.45	1.30	1.37
80	m	402	HEM	C1A-CHA	-2.44	1.34	1.41
80	y	402	HEM	C1A-CHA	-2.43	1.34	1.41
72	6	701	CDL	OA8-CA6	-2.42	1.39	1.45
80	m	402	HEM	CHD-C1D	-2.42	1.34	1.41
72	6	701	CDL	OB6-CB5	2.42	1.41	1.34
79	R	601	NAP	C5A-N7A	-2.41	1.31	1.39
72	6	701	CDL	OB8-CB6	-2.41	1.39	1.45
80	y	402	HEM	CHD-C1D	-2.41	1.34	1.41
80	m	401	HEM	C4A-CHB	-2.41	1.34	1.41
80	m	401	HEM	CAB-C3B	2.40	1.54	1.47
80	y	401	HEM	C4A-CHB	-2.40	1.34	1.41
80	m	402	HEM	C1B-NB	-2.39	1.36	1.40
80	y	402	HEM	C1B-NB	-2.38	1.36	1.40
70	2	401	3PE	O31-C31	2.38	1.40	1.33
80	y	401	HEM	CAB-C3B	2.38	1.53	1.47
80	y	401	HEM	CHC-C4B	-2.36	1.34	1.41
76	C3	603	HEA	CMD-C2D	2.35	1.55	1.50
80	m	401	HEM	CHC-C4B	-2.35	1.34	1.41
69	j	201	PC1	O21-C21	2.32	1.40	1.34
80	m	402	HEM	CAB-C3B	2.31	1.53	1.47
69	3	200	PC1	O31-C3	-2.31	1.39	1.45
70	1	401	3PE	O31-C31	2.30	1.40	1.33
80	y	402	HEM	CAB-C3B	2.30	1.53	1.47
70	j	202	3PE	O31-C31	2.30	1.40	1.33
72	J	101	CDL	OB8-CB7	2.29	1.40	1.33
69	j	201	PC1	O21-C2	-2.26	1.41	1.46
80	m	401	HEM	C3B-C2B	-2.25	1.32	1.37
80	m	401	HEM	C2A-C3A	-2.25	1.31	1.37
80	y	401	HEM	C2A-C3A	-2.23	1.31	1.37
70	1	401	3PE	O31-C3	-2.21	1.40	1.45
80	y	402	HEM	CHC-C4B	-2.21	1.34	1.41
80	y	401	HEM	C3B-C2B	-2.21	1.32	1.37
72	J	101	CDL	OB8-CB6	-2.19	1.40	1.45
80	m	402	HEM	CHC-C4B	-2.17	1.34	1.41
70	4	501	3PE	O21-C21	2.17	1.40	1.34
69	S	401	PC1	O31-C3	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	J	101	CDL	OA6-CA5	2.17	1.40	1.34
73	8	501	FMN	C4A-C10	-2.17	1.37	1.44
72	J	101	CDL	OB6-CB5	2.16	1.40	1.34
69	Q	201	PC1	O31-C31	2.16	1.39	1.33
80	y	402	HEM	C4D-ND	-2.15	1.36	1.40
72	6	701	CDL	OA8-CA7	2.15	1.39	1.33
69	j	201	PC1	O31-C3	-2.14	1.40	1.45
76	C3	602	HEA	C3A-C2A	-2.14	1.37	1.40
80	m	402	HEM	C4D-ND	-2.13	1.36	1.40
76	C3	602	HEA	C1C-NC	2.12	1.40	1.36
69	3	200	PC1	O21-C21	2.11	1.40	1.34
79	R	601	NAP	P2B-O2B	2.10	1.63	1.59
69	S	401	PC1	O21-C21	2.10	1.40	1.34
72	b	201	CDL	OA8-CA6	-2.10	1.40	1.45
81	z	301	HEC	C1D-CHD	-2.10	1.35	1.41
70	2	401	3PE	O31-C3	-2.09	1.40	1.45
76	C3	602	HEA	CHD-C1D	2.08	1.40	1.35
70	j	202	3PE	O31-C3	-2.07	1.40	1.45
72	b	201	CDL	OA6-CA5	2.07	1.40	1.34
69	j	201	PC1	C13-N	-2.07	1.44	1.50
81	z	301	HEC	C1B-CHB	-2.07	1.35	1.41
69	j	201	PC1	C12-N	-2.06	1.44	1.51
81	o	301	HEC	C1D-CHD	-2.05	1.35	1.41
79	R	601	NAP	C2A-N3A	2.05	1.35	1.32
80	y	401	HEM	C4D-ND	-2.04	1.36	1.40
81	o	301	HEC	C1C-CHC	-2.03	1.35	1.41
70	4	501	3PE	O21-C2	-2.03	1.41	1.46
80	m	401	HEM	CHD-C1D	-2.02	1.35	1.41
72	6	701	CDL	OA6-CA5	2.02	1.40	1.34
72	6	701	CDL	OB8-CB7	2.01	1.39	1.33
80	m	401	HEM	C4D-ND	-2.01	1.36	1.40
80	y	401	HEM	CHD-C1D	-2.01	1.35	1.41

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	R	601	NAP	C5A-C6A-N6A	7.65	131.97	120.35
79	R	601	NAP	N3A-C2A-N1A	-6.41	118.65	128.68
79	R	601	NAP	N6A-C6A-N1A	-5.96	106.19	118.57
80	m	401	HEM	C4B-CHC-C1C	-5.91	114.75	122.56
80	y	401	HEM	C4B-CHC-C1C	-5.87	114.81	122.56
70	B	501	3PE	O21-C21-C22	5.42	123.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	4	501	3PE	O21-C21-C22	5.11	122.51	111.50
72	6	701	CDL	OB6-CB5-C51	4.63	121.47	111.50
72	J	101	CDL	OA6-CA5-C11	4.43	121.06	111.50
69	S	401	PC1	O21-C21-C22	4.15	120.44	111.50
72	b	201	CDL	OA6-CA5-C11	4.12	120.39	111.50
72	6	701	CDL	OA6-CA5-C11	4.10	120.34	111.50
69	Q	201	PC1	O21-C21-C22	4.04	120.21	111.50
73	8	501	FMN	C4-N3-C2	-4.01	118.23	125.64
76	C3	602	HEA	C17-C18-C19	-3.98	118.09	127.66
79	R	601	NAP	C1B-N9A-C4A	-3.93	119.74	126.64
70	2	401	3PE	O21-C21-C22	3.83	119.76	111.50
72	b	201	CDL	OB6-CB5-C51	3.81	119.72	111.50
82	A2	201	UQ2	C7-C8-C9	-3.79	120.49	126.79
69	3	200	PC1	O21-C21-C22	3.74	119.56	111.50
80	y	402	HEM	CBA-CAA-C2A	-3.69	106.33	112.62
80	m	402	HEM	CBA-CAA-C2A	-3.68	106.35	112.62
70	j	202	3PE	O21-C21-C22	3.62	119.31	111.50
76	C3	603	HEA	C4A-CHB-C1B	3.57	127.27	122.56
81	o	301	HEC	CBD-CAD-C3D	-3.55	106.56	112.62
81	z	301	HEC	CBD-CAD-C3D	-3.55	106.56	112.62
70	1	401	3PE	O21-C21-C22	3.48	119.00	111.50
81	z	301	HEC	CMC-C2C-C1C	-3.48	123.12	128.46
81	o	301	HEC	CMC-C2C-C1C	-3.47	123.13	128.46
72	J	101	CDL	OB6-CB5-C51	3.46	118.96	111.50
69	2	402	PC1	O21-C21-C22	3.44	118.91	111.50
81	o	301	HEC	C1D-C2D-C3D	-3.41	104.62	107.00
69	j	201	PC1	O21-C21-C22	3.37	120.21	110.80
80	m	401	HEM	CAD-C3D-C4D	3.32	130.46	124.66
80	y	401	HEM	CAD-C3D-C4D	3.31	130.44	124.66
70	B	501	3PE	O31-C31-C32	3.27	122.17	111.91
81	z	301	HEC	C1D-C2D-C3D	-3.22	104.76	107.00
76	C3	602	HEA	C13-C14-C15	-3.18	120.00	127.66
80	y	401	HEM	CAD-CBD-CGD	-3.17	106.78	113.60
80	m	401	HEM	CAD-CBD-CGD	-3.16	106.81	113.60
73	8	501	FMN	C4A-C10-N1	-3.07	117.61	124.73
73	8	501	FMN	C5A-C9A-N10	3.07	121.12	117.95
72	b	201	CDL	OB8-CB7-C71	3.06	121.51	111.91
73	8	501	FMN	C4A-C10-N10	3.06	120.95	116.48
73	8	501	FMN	O4-C4-C4A	-3.03	118.57	126.60
70	1	401	3PE	O31-C31-C32	2.99	121.30	111.91
79	R	601	NAP	PN-O3-PA	-2.91	122.86	132.83
72	b	201	CDL	OA8-CA7-C31	2.89	120.96	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	Q	201	PC1	O31-C31-C32	2.88	120.94	111.91
72	J	101	CDL	OA8-CA7-C31	2.86	120.89	111.91
73	8	501	FMN	C4A-C4-N3	2.85	120.44	113.19
82	A2	201	UQ2	C10-C9-C11	2.85	120.06	115.27
76	C3	603	HEA	CBA-CAA-C2A	2.84	117.39	112.60
80	m	401	HEM	CBA-CAA-C2A	-2.83	107.79	112.62
80	y	401	HEM	CBA-CAA-C2A	-2.82	107.80	112.62
76	C3	602	HEA	C1B-C2B-C3B	2.81	110.16	106.80
72	6	701	CDL	OA8-CA7-C31	2.81	120.71	111.91
80	m	401	HEM	CAD-C3D-C2D	-2.80	122.66	127.88
80	y	401	HEM	CAD-C3D-C2D	-2.80	122.66	127.88
69	j	201	PC1	O31-C31-C32	2.78	120.64	111.91
69	S	401	PC1	O31-C31-C32	2.72	120.44	111.91
72	6	701	CDL	OB8-CB7-C71	2.71	120.41	111.91
72	J	101	CDL	OB8-CB7-C71	2.71	120.41	111.91
81	z	301	HEC	CAA-CBA-CGA	-2.70	106.20	113.76
82	A2	201	UQ2	CM5-C5-C6	-2.69	120.00	124.40
81	o	301	HEC	CAA-CBA-CGA	-2.68	106.24	113.76
73	8	501	FMN	C4-C4A-C10	2.67	121.28	116.79
70	2	401	3PE	O31-C31-C32	2.63	120.15	111.91
69	2	402	PC1	O31-C31-C32	2.62	120.14	111.91
70	j	202	3PE	O31-C31-C32	2.62	120.12	111.91
76	C3	603	HEA	CMD-C2D-C1D	2.58	128.96	125.04
80	y	402	HEM	CHC-C4B-NB	2.50	127.15	124.43
76	C3	603	HEA	C4D-CHA-C1A	2.49	125.85	122.56
80	m	402	HEM	CHC-C4B-NB	2.46	127.10	124.43
80	m	402	HEM	CMC-C2C-C3C	2.44	129.24	124.68
82	A2	201	UQ2	C16-C14-C15	2.44	119.99	114.60
80	y	402	HEM	CMC-C2C-C3C	2.43	129.22	124.68
70	4	501	3PE	C23-C22-C21	-2.42	104.81	113.62
76	C3	603	HEA	C1D-C2D-C3D	-2.41	104.42	106.96
76	C3	602	HEA	C17-C16-C15	-2.41	105.06	112.98
76	C3	603	HEA	CMC-C2C-C3C	2.40	129.17	124.68
76	C3	602	HEA	C20-C19-C18	2.37	125.92	121.12
76	C3	603	HEA	CMB-C2B-C3B	-2.36	125.83	130.34
80	m	402	HEM	CHB-C1B-NB	2.35	127.29	124.38
76	C3	602	HEA	C16-C17-C18	-2.35	104.16	111.88
80	y	402	HEM	CHB-C1B-NB	2.33	127.27	124.38
73	8	501	FMN	O2'-C2'-C3'	-2.33	103.44	109.10
76	C3	602	HEA	CAD-C3D-C4D	2.32	128.71	124.66
73	8	501	FMN	C10-N1-C2	2.31	121.53	116.90
76	C3	603	HEA	C13-C14-C15	-2.31	122.10	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	C3	603	HEA	C25-C23-C24	2.30	119.69	114.60
79	R	601	NAP	C2N-C3N-C4N	2.30	120.87	118.26
81	z	301	HEC	CMB-C2B-C1B	-2.28	124.96	128.46
81	o	301	HEC	CMB-C2B-C1B	-2.27	124.98	128.46
70	B	501	3PE	C23-C22-C21	-2.25	105.43	113.62
73	8	501	FMN	C4'-C3'-C2'	-2.23	108.72	113.36
70	B	501	3PE	O31-C31-O32	-2.22	117.98	123.59
72	J	101	CDL	CA4-OA6-CA5	-2.22	112.33	117.79
76	C3	603	HEA	C26-C15-C16	2.21	118.98	115.27
76	C3	602	HEA	C4A-CHB-C1B	2.19	125.44	122.56
76	C3	602	HEA	C12-C13-C14	-2.18	106.47	112.23
76	C3	602	HEA	C4B-C3B-C2B	-2.18	103.69	107.41
73	8	501	FMN	C9A-N10-C10	-2.16	117.41	120.77
82	A2	201	UQ2	C12-C13-C14	-2.14	120.45	127.75
73	8	501	FMN	C6-C5A-C9A	2.12	121.94	118.94
76	C3	602	HEA	C27-C19-C18	-2.08	118.34	123.68
80	m	401	HEM	CAA-CBA-CGA	-2.08	107.93	113.76
80	y	401	HEM	CAA-CBA-CGA	-2.07	107.94	113.76
79	R	601	NAP	O3B-C3B-C2B	-2.07	105.29	111.17
76	C3	602	HEA	C3C-C4C-NC	2.06	111.88	109.21
76	C3	603	HEA	CBD-CAD-C3D	2.06	118.35	112.63
80	m	402	HEM	CAA-CBA-CGA	-2.04	108.03	113.76
69	3	200	PC1	O31-C31-C32	2.04	118.30	111.91
81	o	301	HEC	CAD-CBD-CGD	-2.04	108.05	113.76
80	y	402	HEM	CAA-CBA-CGA	-2.03	108.06	113.76
81	z	301	HEC	CAD-CBD-CGD	-2.02	108.09	113.76

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
76	C3	602	HEA	NA
76	C3	602	HEA	ND
76	C3	602	HEA	NB
76	C3	603	HEA	NA
76	C3	603	HEA	ND
76	C3	603	HEA	NB

All (392) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	3	200	PC1	C22-C21-O21-C2
69	2	402	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
69	2	402	PC1	C1-O11-P-O14
69	Q	201	PC1	C11-O13-P-O12
69	Q	201	PC1	C1-O11-P-O12
69	Q	201	PC1	C1-O11-P-O13
69	Q	201	PC1	O13-C11-C12-N
69	Q	201	PC1	C22-C21-O21-C2
69	S	401	PC1	C11-O13-P-O12
69	S	401	PC1	C11-O13-P-O14
69	S	401	PC1	O13-C11-C12-N
69	j	201	PC1	C11-O13-P-O12
69	j	201	PC1	C1-O11-P-O13
69	j	201	PC1	O13-C11-C12-N
69	j	201	PC1	O22-C21-O21-C2
69	j	201	PC1	C22-C21-O21-C2
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	C22-C21-O21-C2
70	2	401	3PE	C11-O13-P-O12
70	2	401	3PE	C11-O13-P-O14
70	2	401	3PE	O13-C11-C12-N
70	2	401	3PE	C22-C21-O21-C2
70	B	501	3PE	C1-O11-P-O14
70	B	501	3PE	O22-C21-O21-C2
70	B	501	3PE	C22-C21-O21-C2
70	j	202	3PE	C11-O13-P-O12
70	j	202	3PE	C11-O13-P-O14
70	j	202	3PE	O13-C11-C12-N
72	6	701	CDL	CA3-OA5-PA1-OA4
72	6	701	CDL	CB2-OB2-PB2-OB3
72	6	701	CDL	CB2-OB2-PB2-OB4
72	6	701	CDL	CB3-OB5-PB2-OB3
72	J	101	CDL	CA2-OA2-PA1-OA3
72	J	101	CDL	CA2-OA2-PA1-OA5
72	J	101	CDL	C11-CA5-OA6-CA4
72	J	101	CDL	CB2-OB2-PB2-OB3
72	J	101	CDL	CB2-OB2-PB2-OB4
72	J	101	CDL	OB5-CB3-CB4-OB6
72	b	201	CDL	CA2-OA2-PA1-OA3
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	O4'-C4'-C5'-O5'
73	8	501	FMN	C5'-O5'-P-O1P
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
76	C3	602	HEA	C12-C11-C3B-C2B
79	R	601	NAP	C5B-O5B-PA-O2A
79	R	601	NAP	C5B-O5B-PA-O3
79	R	601	NAP	C1B-C2B-O2B-P2B
79	R	601	NAP	C5D-O5D-PN-O3
79	R	601	NAP	C5D-O5D-PN-O1N
79	R	601	NAP	C5D-O5D-PN-O2N
79	R	601	NAP	C2D-C1D-N1N-C2N
79	R	601	NAP	C2D-C1D-N1N-C6N
70	j	202	3PE	O32-C31-O31-C3
72	6	701	CDL	OA9-CA7-OA8-CA6
72	b	201	CDL	OA9-CA7-OA8-CA6
70	j	202	3PE	C32-C31-O31-C3
72	6	701	CDL	C31-CA7-OA8-CA6
72	b	201	CDL	OB9-CB7-OB8-CB6
69	3	200	PC1	O22-C21-O21-C2
69	2	402	PC1	O22-C21-O21-C2
69	Q	201	PC1	O22-C21-O21-C2
70	2	401	3PE	O22-C21-O21-C2
72	J	101	CDL	OA7-CA5-OA6-CA4
72	b	201	CDL	C31-CA7-OA8-CA6
72	J	101	CDL	OA9-CA7-OA8-CA6
72	J	101	CDL	C71-CB7-OB8-CB6
72	b	201	CDL	C71-CB7-OB8-CB6
80	m	401	HEM	C4D-C3D-CAD-CBD
80	y	401	HEM	C4D-C3D-CAD-CBD
70	4	501	3PE	O22-C21-O21-C2
72	J	101	CDL	OB9-CB7-OB8-CB6
70	2	401	3PE	C32-C31-O31-C3
69	2	402	PC1	C22-C21-O21-C2
79	R	601	NAP	O4D-C4D-C5D-O5D
72	J	101	CDL	C31-CA7-OA8-CA6
70	4	501	3PE	C2-C1-O11-P
69	2	402	PC1	C36-C37-C38-C39
82	A2	201	UQ2	C12-C11-C9-C10
82	A2	201	UQ2	C12-C11-C9-C8
69	2	402	PC1	C26-C27-C28-C29
70	2	401	3PE	O32-C31-O31-C3
76	C3	602	HEA	C15-C16-C17-C18
69	S	401	PC1	C23-C24-C25-C26
69	2	402	PC1	C32-C33-C34-C35
69	3	200	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	Q	201	PC1	C32-C31-O31-C3
69	j	201	PC1	C32-C31-O31-C3
69	3	200	PC1	C34-C35-C36-C37
72	b	201	CDL	C12-C13-C14-C15
80	m	401	HEM	C2D-C3D-CAD-CBD
80	y	401	HEM	C2D-C3D-CAD-CBD
69	S	401	PC1	C3B-C3C-C3D-C3E
69	2	402	PC1	C21-C22-C23-C24
69	j	201	PC1	O32-C31-O31-C3
69	3	200	PC1	C21-C22-C23-C24
70	4	501	3PE	C2B-C2C-C2D-C2E
69	Q	201	PC1	C21-C22-C23-C24
70	4	501	3PE	C31-C32-C33-C34
70	j	202	3PE	C31-C32-C33-C34
69	Q	201	PC1	O32-C31-O31-C3
72	6	701	CDL	C32-C33-C34-C35
72	J	101	CDL	CA7-C31-C32-C33
69	Q	201	PC1	C24-C25-C26-C27
69	3	200	PC1	O32-C31-O31-C3
70	1	401	3PE	C21-C22-C23-C24
70	2	401	3PE	C33-C34-C35-C36
70	4	501	3PE	C27-C28-C29-C2A
69	2	402	PC1	C1-O11-P-O13
69	S	401	PC1	C11-O13-P-O11
69	j	201	PC1	C11-O13-P-O11
70	4	501	3PE	C1-O11-P-O13
70	2	401	3PE	C11-O13-P-O11
70	B	501	3PE	C1-O11-P-O13
70	j	202	3PE	C11-O13-P-O11
72	6	701	CDL	CB2-OB2-PB2-OB5
72	6	701	CDL	CB3-OB5-PB2-OB2
72	J	101	CDL	CB2-OB2-PB2-OB5
72	b	201	CDL	CB2-OB2-PB2-OB5
72	6	701	CDL	OB7-CB5-OB6-CB4
69	S	401	PC1	C34-C35-C36-C37
69	S	401	PC1	C22-C21-O21-C2
72	6	701	CDL	C51-CB5-OB6-CB4
69	3	200	PC1	C3C-C3D-C3E-C3F
69	Q	201	PC1	C26-C27-C28-C29
69	S	401	PC1	C24-C25-C26-C27
70	4	501	3PE	C2E-C2F-C2G-C2H
70	2	401	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
70	B	501	3PE	C2B-C2C-C2D-C2E
72	b	201	CDL	C60-C61-C62-C63
69	3	200	PC1	C3B-C3C-C3D-C3E
69	j	201	PC1	C35-C36-C37-C38
69	j	201	PC1	C3B-C3C-C3D-C3E
70	B	501	3PE	C2A-C2B-C2C-C2D
69	S	401	PC1	O22-C21-O21-C2
70	2	401	3PE	C21-C22-C23-C24
72	b	201	CDL	O1-C1-CA2-OA2
72	J	101	CDL	C14-C15-C16-C17
72	b	201	CDL	C13-C14-C15-C16
69	j	201	PC1	C3D-C3E-C3F-C3G
72	b	201	CDL	C11-C12-C13-C14
69	2	402	PC1	C2C-C2D-C2E-C2F
69	S	401	PC1	C37-C38-C39-C3A
70	2	401	3PE	C32-C33-C34-C35
70	B	501	3PE	C37-C38-C39-C3A
70	B	501	3PE	C35-C36-C37-C38
70	4	501	3PE	C23-C24-C25-C26
70	j	202	3PE	C35-C36-C37-C38
69	2	402	PC1	C28-C29-C2A-C2B
70	B	501	3PE	C39-C3A-C3B-C3C
72	J	101	CDL	C15-C16-C17-C18
69	j	201	PC1	C33-C34-C35-C36
70	4	501	3PE	C2C-C2D-C2E-C2F
70	j	202	3PE	C22-C23-C24-C25
70	1	401	3PE	C24-C25-C26-C27
70	1	401	3PE	C2B-C2C-C2D-C2E
70	4	501	3PE	C2A-C2B-C2C-C2D
69	S	401	PC1	C32-C31-O31-C3
70	4	501	3PE	C32-C31-O31-C3
69	S	401	PC1	C35-C36-C37-C38
80	m	402	HEM	C2A-CAA-CBA-CGA
80	y	402	HEM	C2A-CAA-CBA-CGA
69	3	200	PC1	C3A-C3B-C3C-C3D
72	b	201	CDL	C81-C82-C83-C84
69	j	201	PC1	C31-C32-C33-C34
70	B	501	3PE	C28-C29-C2A-C2B
70	j	202	3PE	C28-C29-C2A-C2B
72	b	201	CDL	CA5-C11-C12-C13
69	3	200	PC1	C32-C33-C34-C35
70	B	501	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
69	3	200	PC1	C22-C23-C24-C25
69	Q	201	PC1	C33-C34-C35-C36
69	3	200	PC1	C11-C12-N-C13
69	2	402	PC1	C23-C24-C25-C26
72	6	701	CDL	C11-CA5-OA6-CA4
69	2	402	PC1	C22-C23-C24-C25
69	Q	201	PC1	C27-C28-C29-C2A
69	S	401	PC1	O32-C31-O31-C3
70	4	501	3PE	O32-C31-O31-C3
82	A2	201	UQ2	C3-C2-O2-CM2
70	4	501	3PE	C21-C22-C23-C24
72	6	701	CDL	C31-C32-C33-C34
72	J	101	CDL	CB5-C51-C52-C53
70	j	202	3PE	C22-C21-O21-C2
69	3	200	PC1	O11-C1-C2-O21
70	B	501	3PE	O11-C1-C2-O21
70	1	401	3PE	C23-C24-C25-C26
70	B	501	3PE	C23-C24-C25-C26
70	j	202	3PE	O22-C21-O21-C2
69	3	200	PC1	C11-C12-N-C14
69	3	200	PC1	C11-C12-N-C15
70	2	401	3PE	C23-C24-C25-C26
69	2	402	PC1	C25-C26-C27-C28
70	2	401	3PE	C25-C26-C27-C28
72	b	201	CDL	C31-C32-C33-C34
72	6	701	CDL	OA7-CA5-OA6-CA4
72	b	201	CDL	C51-CB5-OB6-CB4
70	1	401	3PE	C35-C36-C37-C38
69	2	402	PC1	C11-O13-P-O11
69	Q	201	PC1	C11-O13-P-O11
72	6	701	CDL	CA3-OA5-PA1-OA2
72	b	201	CDL	CA2-OA2-PA1-OA5
70	j	202	3PE	C2D-C2E-C2F-C2G
72	b	201	CDL	C76-C77-C78-C79
69	Q	201	PC1	C1-C2-C3-O31
70	1	401	3PE	C1-C2-C3-O31
70	j	202	3PE	C3A-C3B-C3C-C3D
72	6	701	CDL	C34-C35-C36-C37
70	B	501	3PE	C3B-C3C-C3D-C3E
69	Q	201	PC1	C2A-C2B-C2C-C2D
70	4	501	3PE	C35-C36-C37-C38
70	j	202	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
69	2	402	PC1	C24-C25-C26-C27
82	A2	201	UQ2	C1-C6-C7-C8
70	4	501	3PE	C33-C34-C35-C36
70	j	202	3PE	C36-C37-C38-C39
70	2	401	3PE	C3-C2-O21-C21
80	m	401	HEM	C3D-CAD-CBD-CGD
80	y	401	HEM	C3D-CAD-CBD-CGD
72	J	101	CDL	C51-C52-C53-C54
70	1	401	3PE	O21-C2-C3-O31
72	b	201	CDL	OB6-CB4-CB6-OB8
70	2	401	3PE	C2F-C2G-C2H-C2I
72	b	201	CDL	C59-C60-C61-C62
72	b	201	CDL	OB7-CB5-OB6-CB4
72	6	701	CDL	C72-C73-C74-C75
69	3	200	PC1	O11-C1-C2-C3
70	B	501	3PE	O11-C1-C2-C3
72	J	101	CDL	OB5-CB3-CB4-CB6
70	B	501	3PE	C38-C39-C3A-C3B
72	b	201	CDL	C57-C58-C59-C60
73	8	501	FMN	C2'-C1'-N10-C10
70	1	401	3PE	C27-C28-C29-C2A
69	3	200	PC1	C1-C2-C3-O31
70	2	401	3PE	C1-C2-C3-O31
70	B	501	3PE	C3C-C3D-C3E-C3F
72	6	701	CDL	CA5-C11-C12-C13
70	1	401	3PE	C34-C35-C36-C37
69	2	402	PC1	C39-C3A-C3B-C3C
69	S	401	PC1	C3C-C3D-C3E-C3F
70	1	401	3PE	C3E-C3F-C3G-C3H
72	J	101	CDL	OA5-CA3-CA4-OA6
69	3	200	PC1	O31-C31-C32-C33
70	1	401	3PE	C28-C29-C2A-C2B
72	6	701	CDL	C51-C52-C53-C54
69	3	200	PC1	O21-C2-C3-O31
69	S	401	PC1	O21-C2-C3-O31
70	2	401	3PE	O21-C2-C3-O31
72	b	201	CDL	OA6-CA4-CA6-OA8
72	b	201	CDL	OA7-CA5-OA6-CA4
69	2	402	PC1	C37-C38-C39-C3A
72	b	201	CDL	C11-CA5-OA6-CA4
70	1	401	3PE	C33-C34-C35-C36
79	R	601	NAP	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
69	S	401	PC1	O11-C1-C2-C3
70	2	401	3PE	O11-C1-C2-C3
69	Q	201	PC1	C2B-C2C-C2D-C2E
79	R	601	NAP	C3D-C4D-C5D-O5D
70	4	501	3PE	C24-C25-C26-C27
70	B	501	3PE	C3A-C3B-C3C-C3D
70	4	501	3PE	C1-C2-O21-C21
72	6	701	CDL	C71-C72-C73-C74
69	2	402	PC1	C32-C31-O31-C3
69	S	401	PC1	O11-C1-C2-O21
69	j	201	PC1	O11-C1-C2-O21
70	1	401	3PE	C38-C39-C3A-C3B
70	j	202	3PE	O21-C2-C3-O31
79	R	601	NAP	C2B-O2B-P2B-O3X
72	b	201	CDL	C34-C35-C36-C37
70	4	501	3PE	C11-O13-P-O11
69	Q	201	PC1	C2-C1-O11-P
72	6	701	CDL	C1-CA2-OA2-PA1
70	j	202	3PE	C2E-C2F-C2G-C2H
69	2	402	PC1	C11-O13-P-O12
69	Q	201	PC1	C11-O13-P-O14
69	Q	201	PC1	C1-O11-P-O14
69	j	201	PC1	C11-O13-P-O14
69	j	201	PC1	C1-O11-P-O12
70	4	501	3PE	C1-O11-P-O12
70	4	501	3PE	C1-O11-P-O14
70	B	501	3PE	C1-O11-P-O12
72	6	701	CDL	CA2-OA2-PA1-OA3
72	6	701	CDL	CA3-OA5-PA1-OA3
72	J	101	CDL	CA3-OA5-PA1-OA4
72	b	201	CDL	CA2-OA2-PA1-OA4
72	b	201	CDL	CB2-OB2-PB2-OB3
79	R	601	NAP	C5B-O5B-PA-O1A
72	b	201	CDL	OB5-CB3-CB4-CB6
69	2	402	PC1	C38-C39-C3A-C3B
69	j	201	PC1	C12-C11-O13-P
70	2	401	3PE	C12-C11-O13-P
73	8	501	FMN	C1'-C2'-C3'-O3'
69	3	200	PC1	C26-C27-C28-C29
70	2	401	3PE	O11-C1-C2-O21
70	B	501	3PE	C24-C25-C26-C27
70	2	401	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
69	3	200	PC1	O13-C11-C12-N
69	2	402	PC1	O13-C11-C12-N
69	S	401	PC1	C1-C2-C3-O31
69	S	401	PC1	C32-C33-C34-C35
72	b	201	CDL	CB3-CB4-CB6-OB8
69	Q	201	PC1	O21-C2-C3-O31
82	A2	201	UQ2	C5-C6-C7-C8
70	j	202	3PE	O21-C21-C22-C23
70	B	501	3PE	C2C-C2D-C2E-C2F
69	2	402	PC1	O32-C31-O31-C3
72	b	201	CDL	C63-C64-C65-C66
70	B	501	3PE	C29-C2A-C2B-C2C
72	b	201	CDL	C77-C78-C79-C80
72	J	101	CDL	OA5-CA3-CA4-CA6
69	j	201	PC1	C38-C39-C3A-C3B
69	S	401	PC1	C1-O11-P-O13
70	1	401	3PE	C1-O11-P-O13
72	J	101	CDL	CB3-OB5-PB2-OB2
69	j	201	PC1	C3F-C3G-C3H-C3I
72	6	701	CDL	CA4-CA3-OA5-PA1
69	2	402	PC1	C31-C32-C33-C34
70	B	501	3PE	C31-C32-C33-C34
72	6	701	CDL	OA6-CA4-CA6-OA8
72	b	201	CDL	CA2-C1-CB2-OB2
76	C3	602	HEA	CAD-CBD-CGD-O1D
69	2	402	PC1	C1-C2-O21-C21
72	6	701	CDL	CB3-CB4-OB6-CB5
72	b	201	CDL	CB3-CB4-OB6-CB5
69	Q	201	PC1	C38-C39-C3A-C3B
72	b	201	CDL	C71-C72-C73-C74
73	8	501	FMN	C3'-C4'-C5'-O5'
69	j	201	PC1	O11-C1-C2-C3
70	B	501	3PE	C26-C27-C28-C29
76	C3	603	HEA	CAD-CBD-CGD-O1D
72	6	701	CDL	O1-C1-CB2-OB2
76	C3	603	HEA	CAD-CBD-CGD-O2D
72	J	101	CDL	CA2-C1-CB2-OB2
72	b	201	CDL	CB2-C1-CA2-OA2
76	C3	602	HEA	CAA-CBA-CGA-O1A
76	C3	602	HEA	CAD-CBD-CGD-O2D
70	4	501	3PE	C22-C23-C24-C25
70	j	202	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
82	A2	201	UQ2	C4-C3-O3-CM3
69	S	401	PC1	C28-C29-C2A-C2B
69	2	402	PC1	C29-C2A-C2B-C2C
69	S	401	PC1	C21-C22-C23-C24
82	A2	201	UQ2	C9-C11-C12-C13
70	B	501	3PE	C32-C33-C34-C35
72	6	701	CDL	C72-C71-CB7-OB8
69	3	200	PC1	O32-C31-C32-C33
72	6	701	CDL	C15-C16-C17-C18
70	2	401	3PE	O31-C31-C32-C33
72	b	201	CDL	C12-C11-CA5-OA6
72	b	201	CDL	OB5-CB3-CB4-OB6
69	2	402	PC1	C2D-C2E-C2F-C2G
70	B	501	3PE	O31-C31-C32-C33
76	C3	603	HEA	CAA-CBA-CGA-O2A
72	6	701	CDL	CA7-C31-C32-C33
81	o	301	HEC	CAA-CBA-CGA-O1A
81	z	301	HEC	CAA-CBA-CGA-O1A
69	2	402	PC1	O31-C31-C32-C33
76	C3	603	HEA	CAA-CBA-CGA-O1A
79	R	601	NAP	O4B-C4B-C5B-O5B
70	1	401	3PE	C3C-C3D-C3E-C3F
72	6	701	CDL	CA3-CA4-CA6-OA8
72	b	201	CDL	CA3-CA4-CA6-OA8
69	S	401	PC1	C27-C28-C29-C2A
72	6	701	CDL	C72-C71-CB7-OB9
70	B	501	3PE	C25-C26-C27-C28
72	J	101	CDL	C55-C56-C57-C58
70	2	401	3PE	O32-C31-C32-C33
72	b	201	CDL	C12-C11-CA5-OA7
76	C3	602	HEA	CAA-CBA-CGA-O2A
69	2	402	PC1	C11-O13-P-O14
72	b	201	CDL	CB2-OB2-PB2-OB4
72	b	201	CDL	CB3-OB5-PB2-OB3
69	2	402	PC1	O32-C31-C32-C33
69	S	401	PC1	O31-C31-C32-C33
70	B	501	3PE	O32-C31-C32-C33
69	3	200	PC1	C38-C39-C3A-C3B
69	S	401	PC1	C12-C11-O13-P
69	S	401	PC1	C1-C2-O21-C21
70	4	501	3PE	C12-C11-O13-P
70	4	501	3PE	C26-C27-C28-C29

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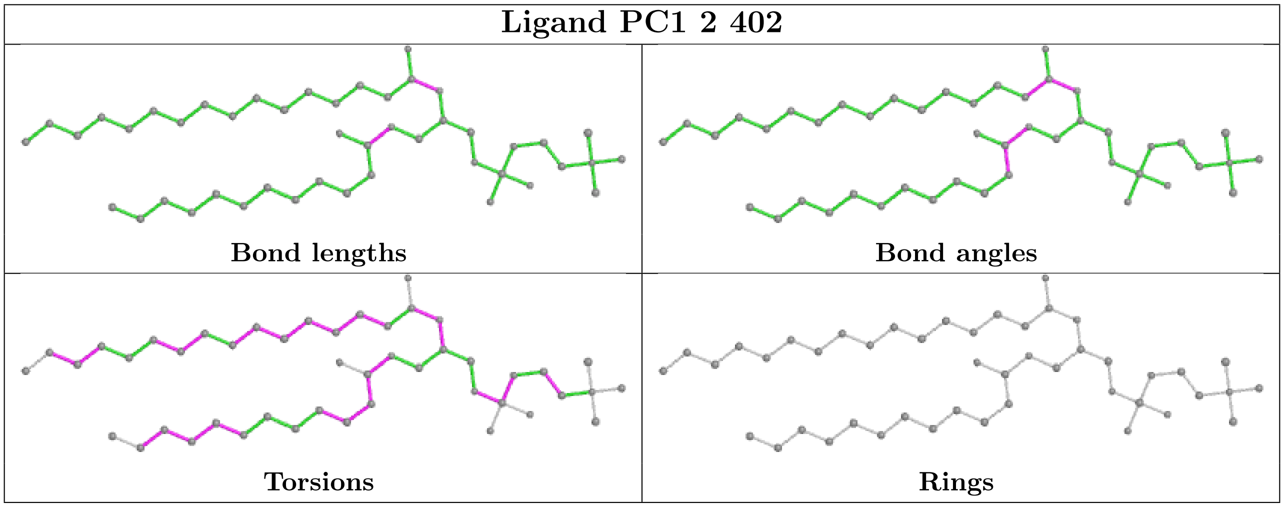
Mol	Chain	Res	Type	Atoms
69	S	401	PC1	C33-C34-C35-C36
69	j	201	PC1	C36-C37-C38-C39
81	o	301	HEC	CAA-CBA-CGA-O2A
81	z	301	HEC	CAA-CBA-CGA-O2A
76	C3	603	HEA	C26-C15-C16-C17
73	8	501	FMN	N10-C1'-C2'-O2'
76	C3	602	HEA	O11-C11-C3B-C2B
72	6	701	CDL	C32-C31-CA7-OA8
69	S	401	PC1	O32-C31-C32-C33
69	Q	201	PC1	O31-C31-C32-C33
72	6	701	CDL	C74-C75-C76-C77
69	S	401	PC1	C11-C12-N-C13

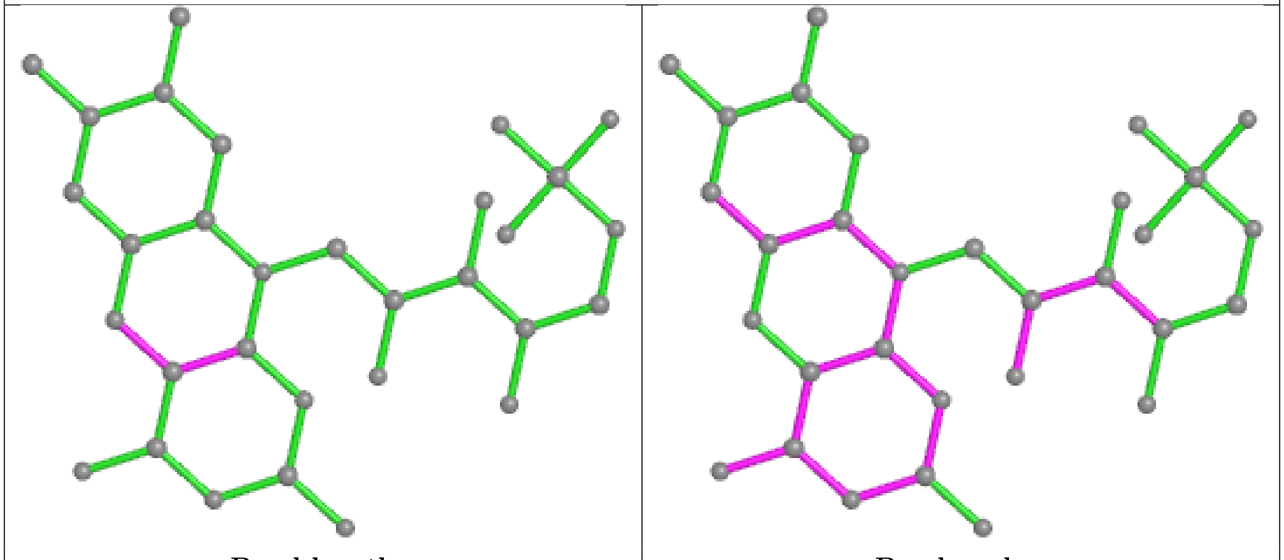
There are no ring outliers.

No monomer is involved in short contacts.

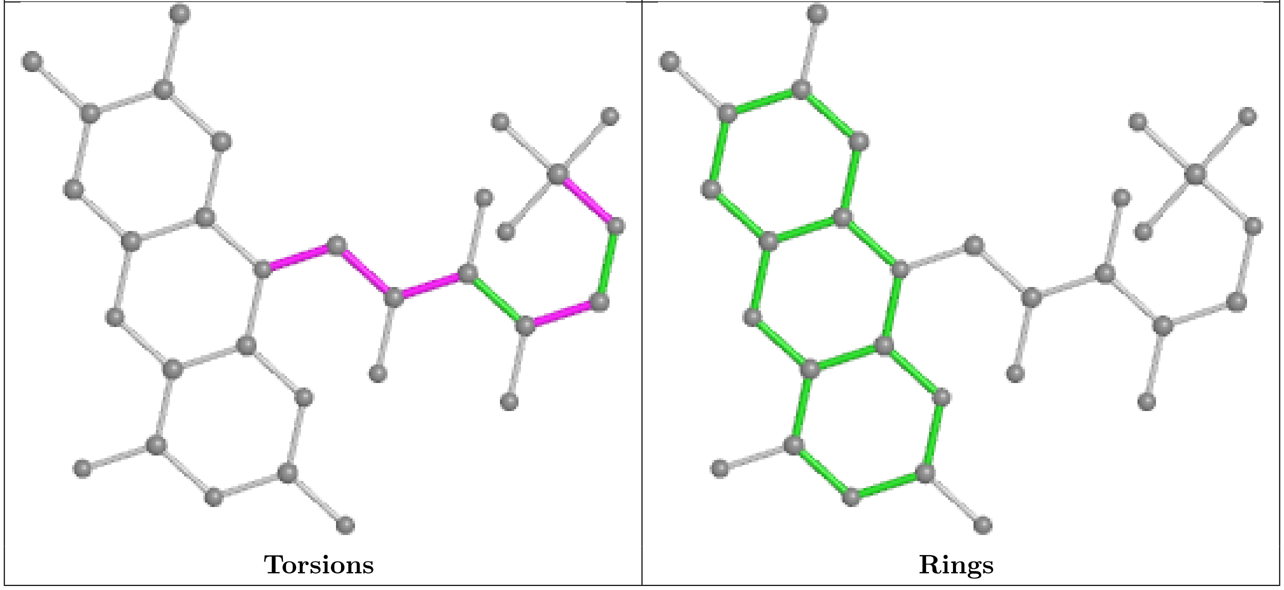
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand FMN 8 501

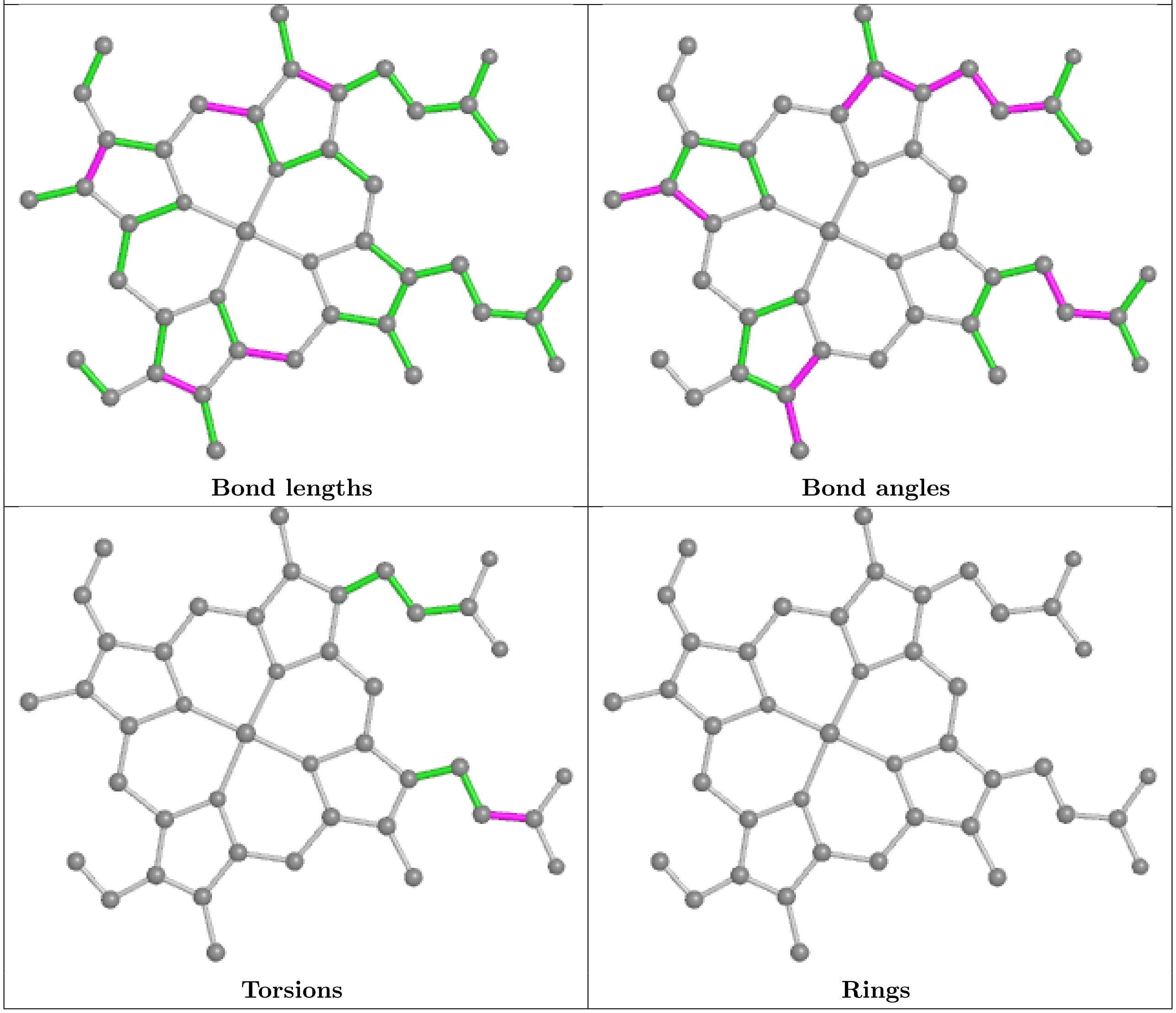


Bond lengths **Bond angles**



Torsions **Rings**

Ligand HEC z 301



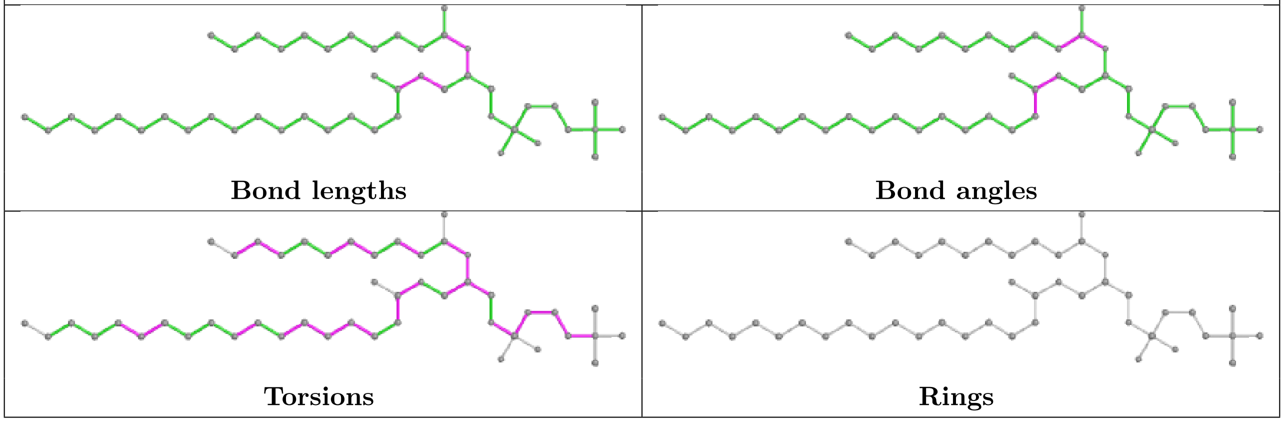
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 S 401



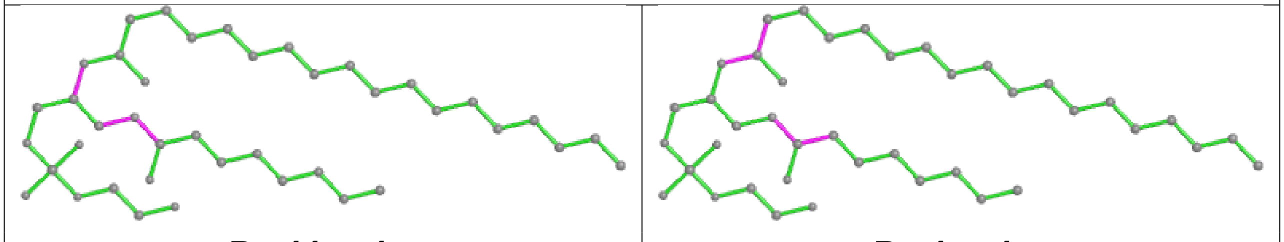
Bond lengths

Bond angles

Torsions

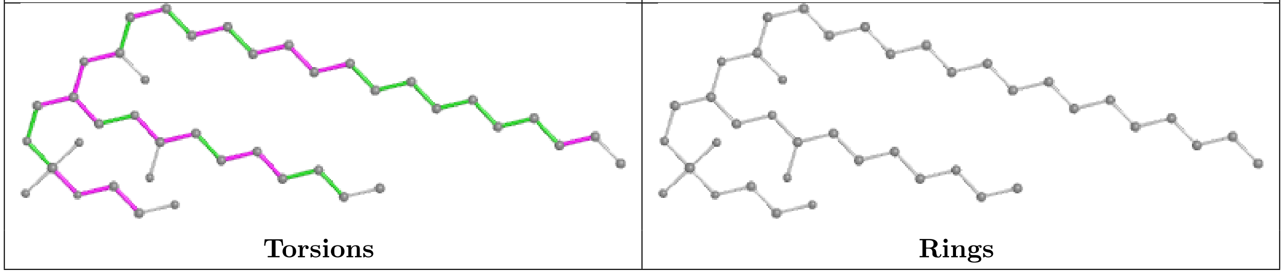
Rings

Ligand 3PE 2 401



Bond lengths

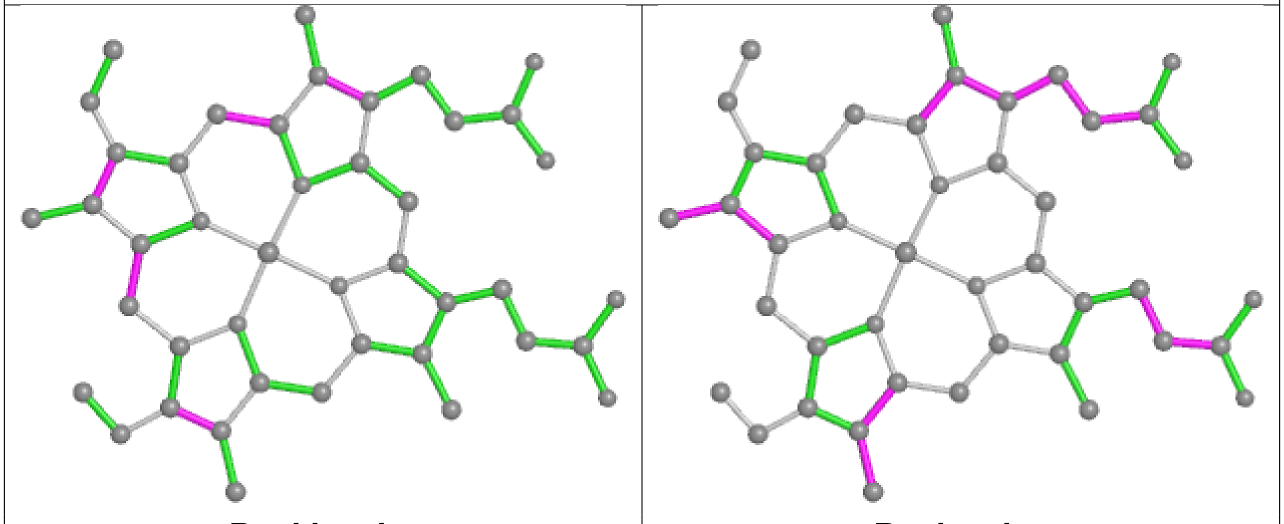
Bond angles



Torsions

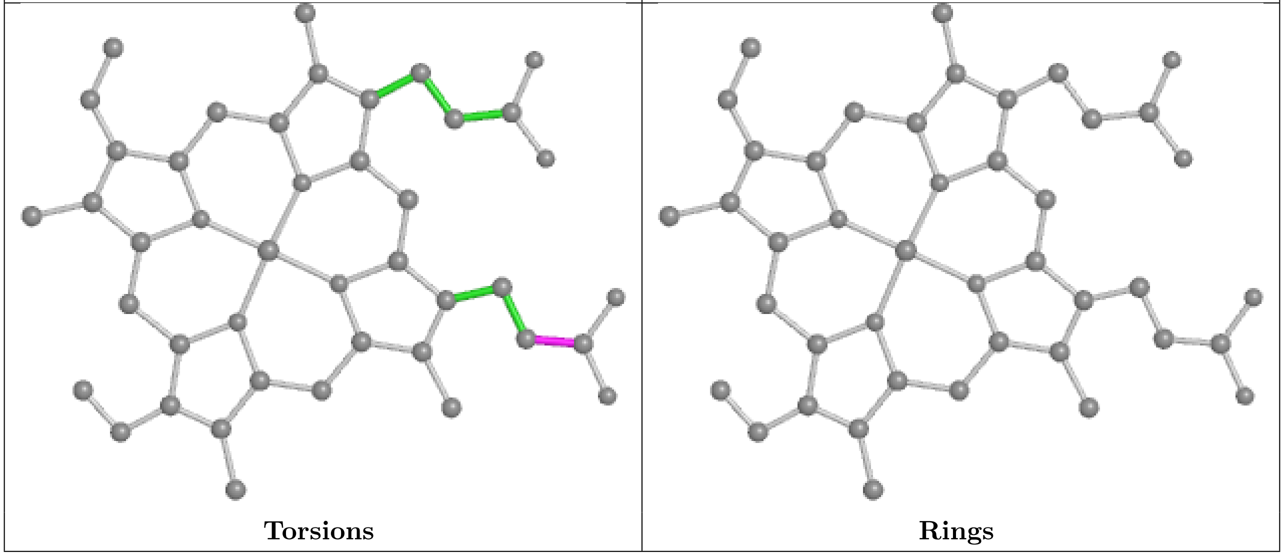
Rings

Ligand HEC o 301



Bond lengths

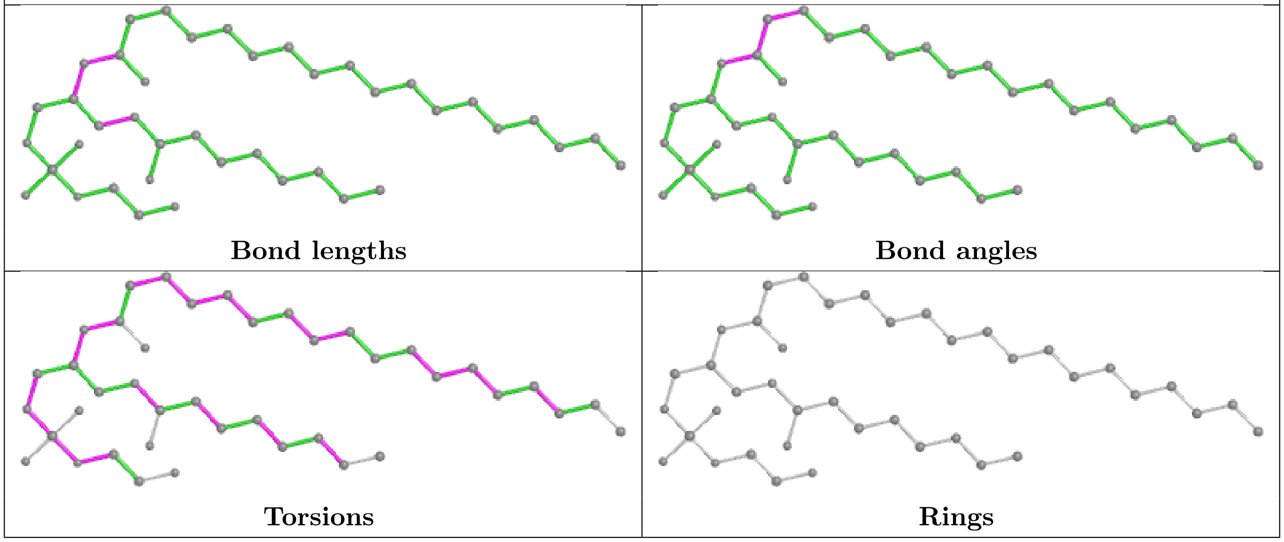
Bond angles



Torsions

Rings

Ligand 3PE 4 501



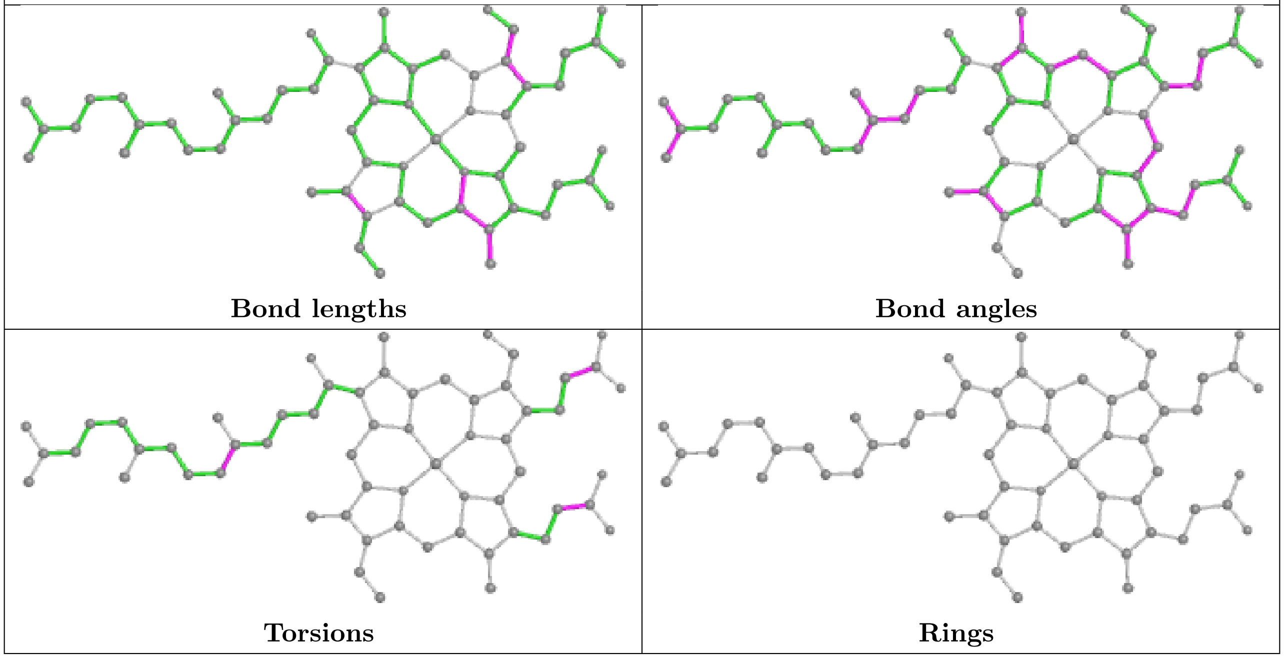
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA C3 603



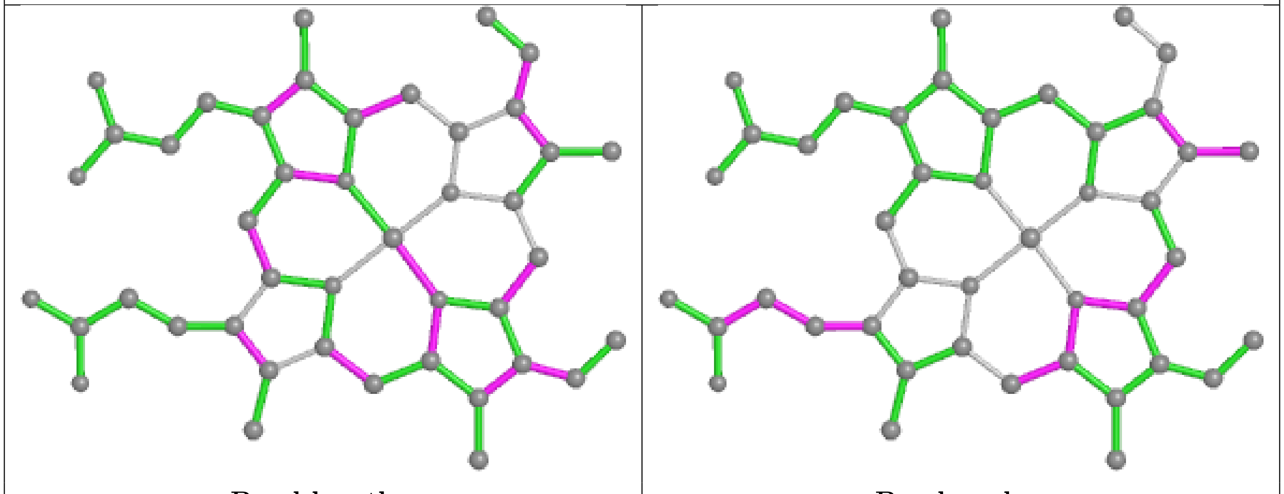
Bond lengths

Bond angles

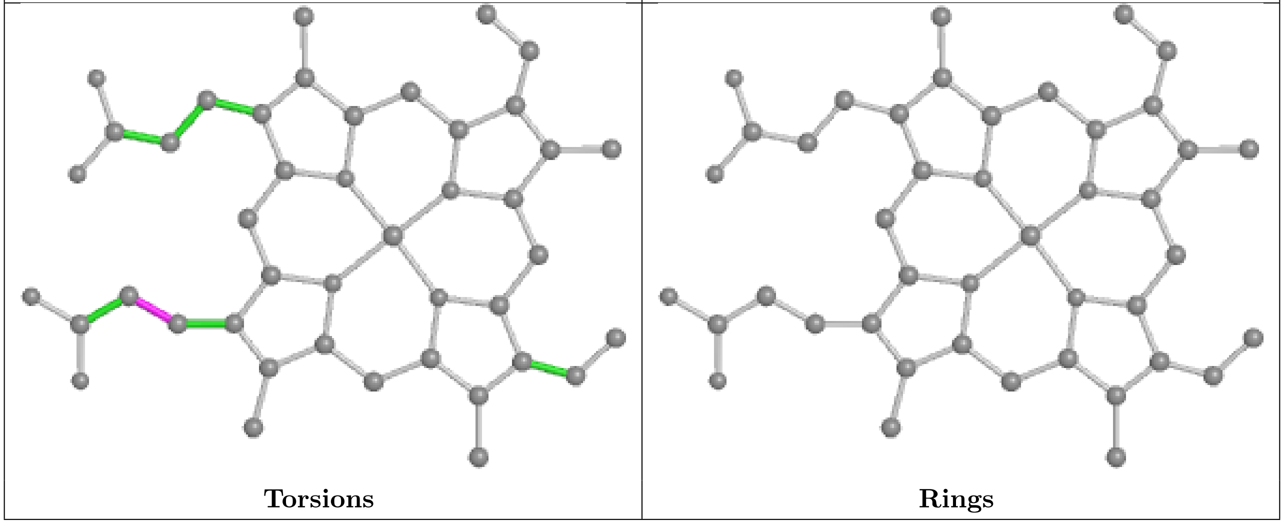
Torsions

Rings

Ligand HEM y 402

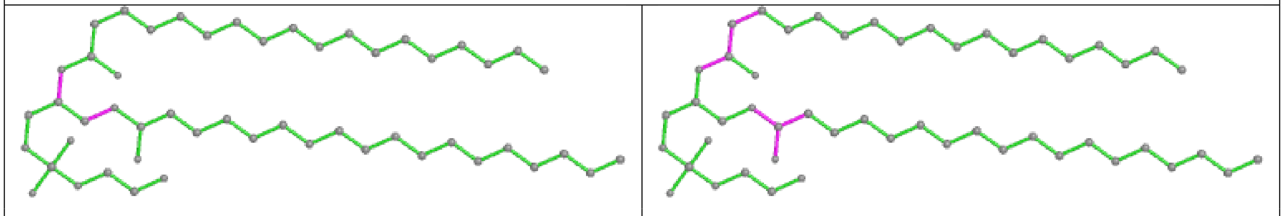


Bond lengths Bond angles

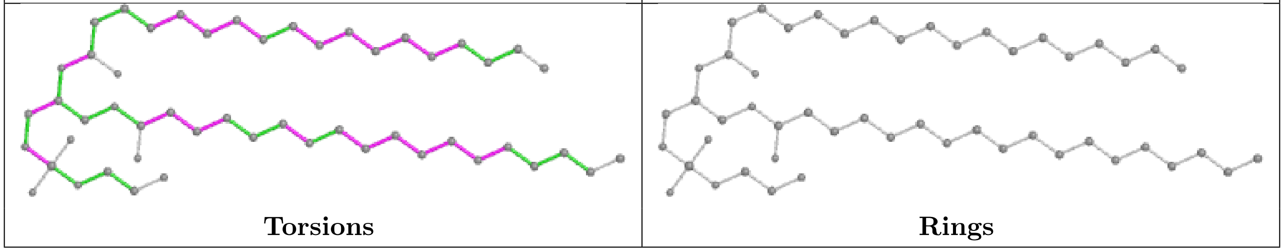


Torsions Rings

Ligand 3PE B 501

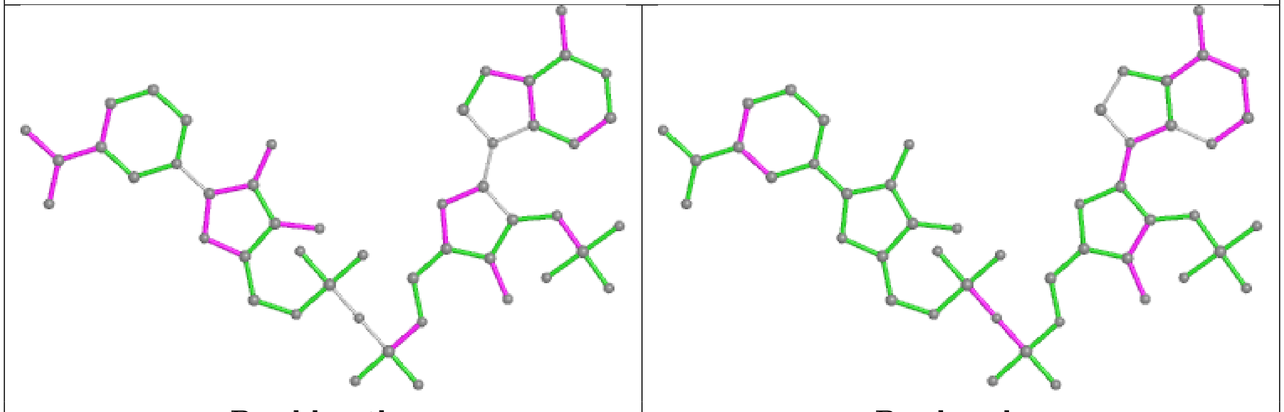


Bond lengths Bond angles



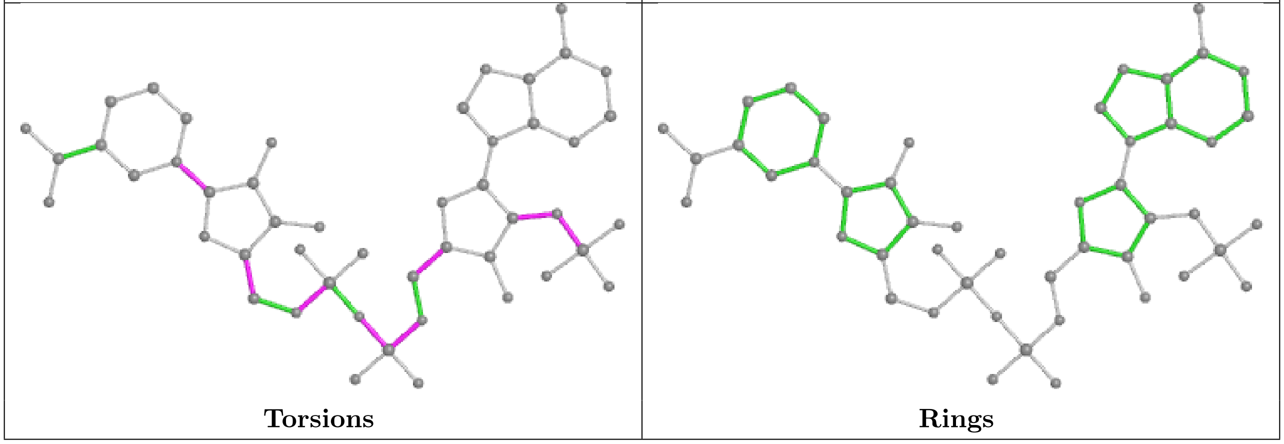
Torsions Rings

Ligand NAP R 601



Bond lengths

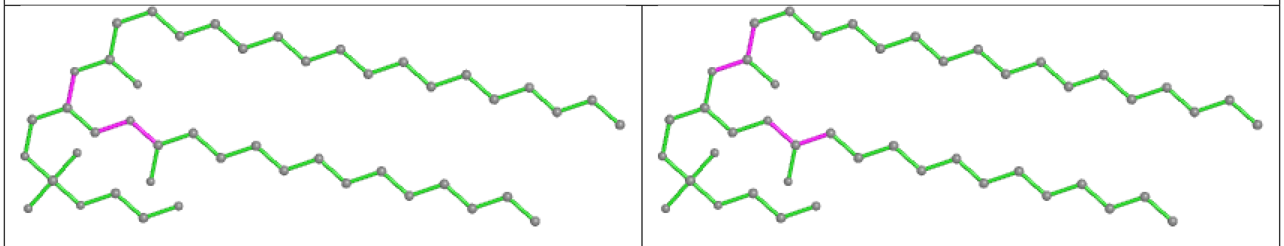
Bond angles



Torsions

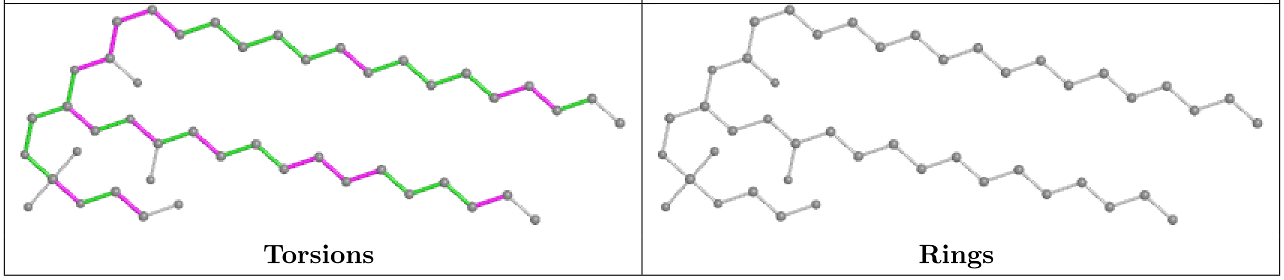
Rings

Ligand 3PE j 202



Bond lengths

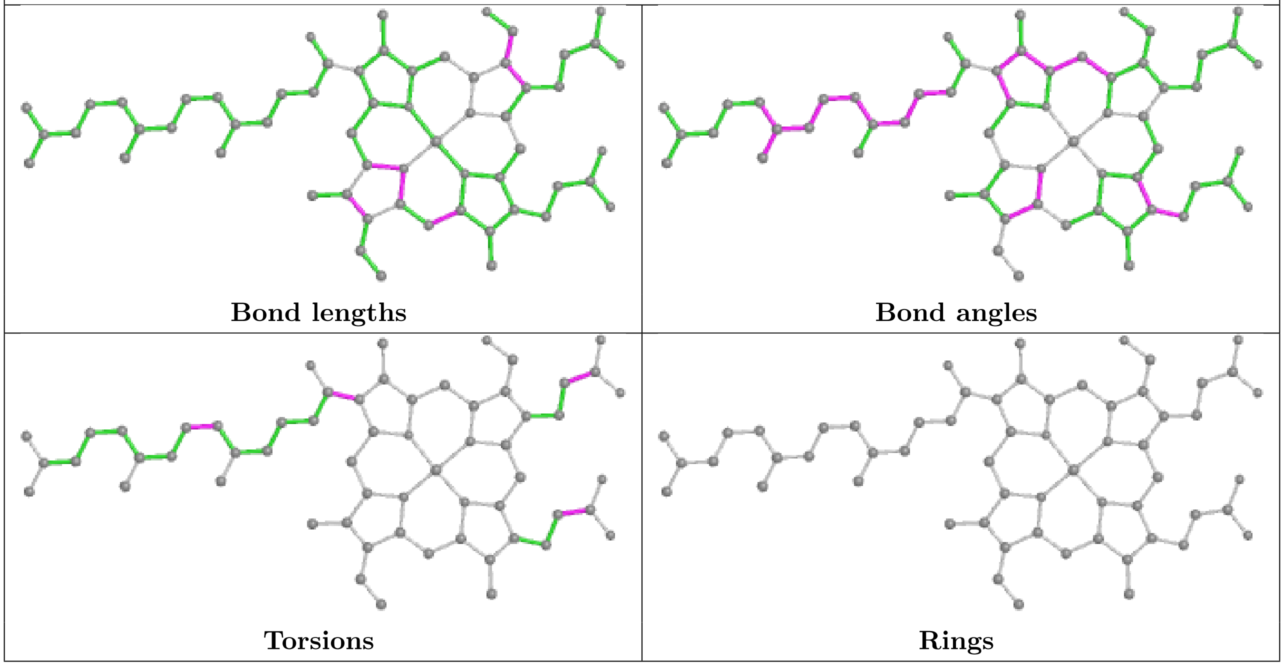
Bond angles



Torsions

Rings

Ligand HEA C3 602



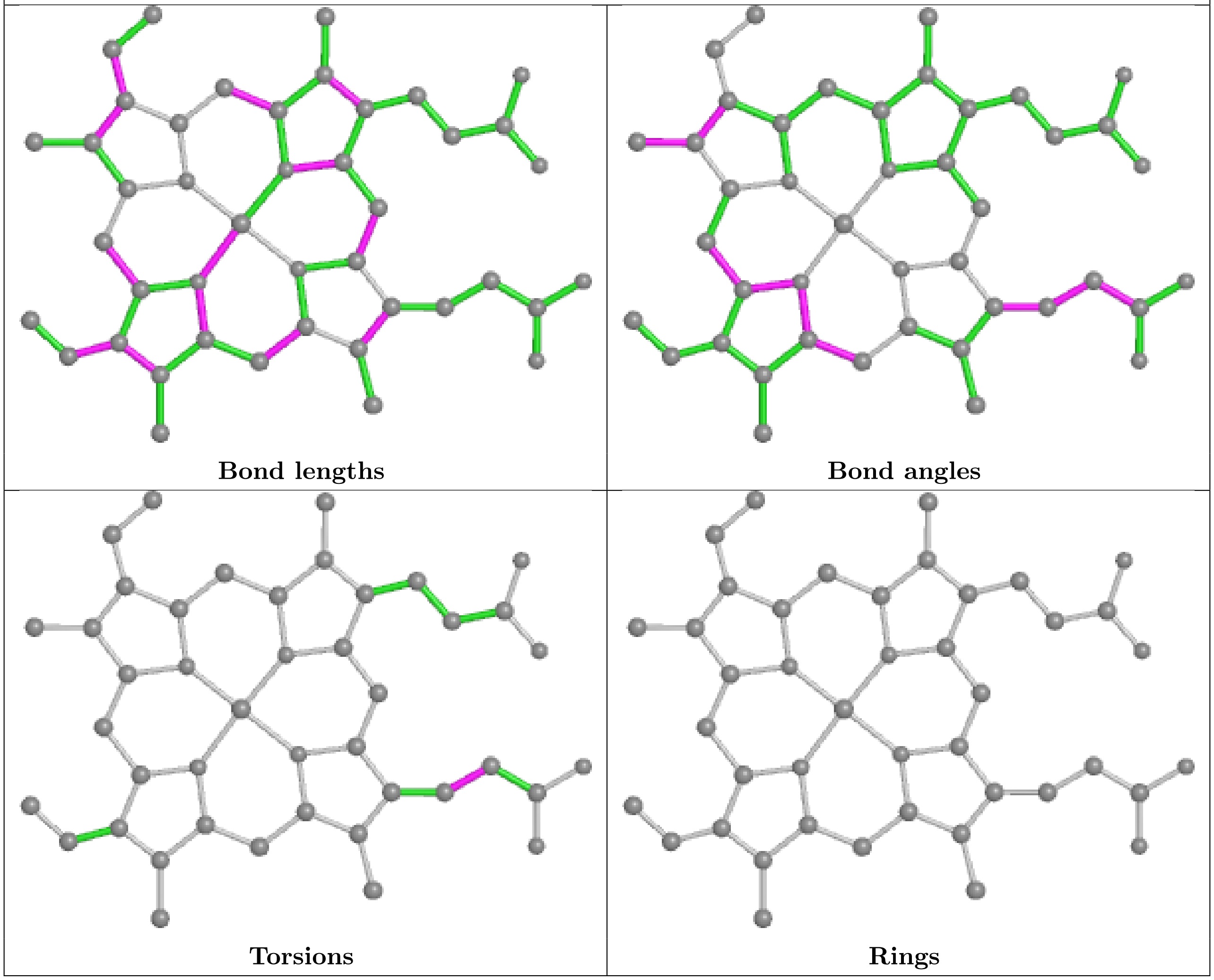
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM m 402



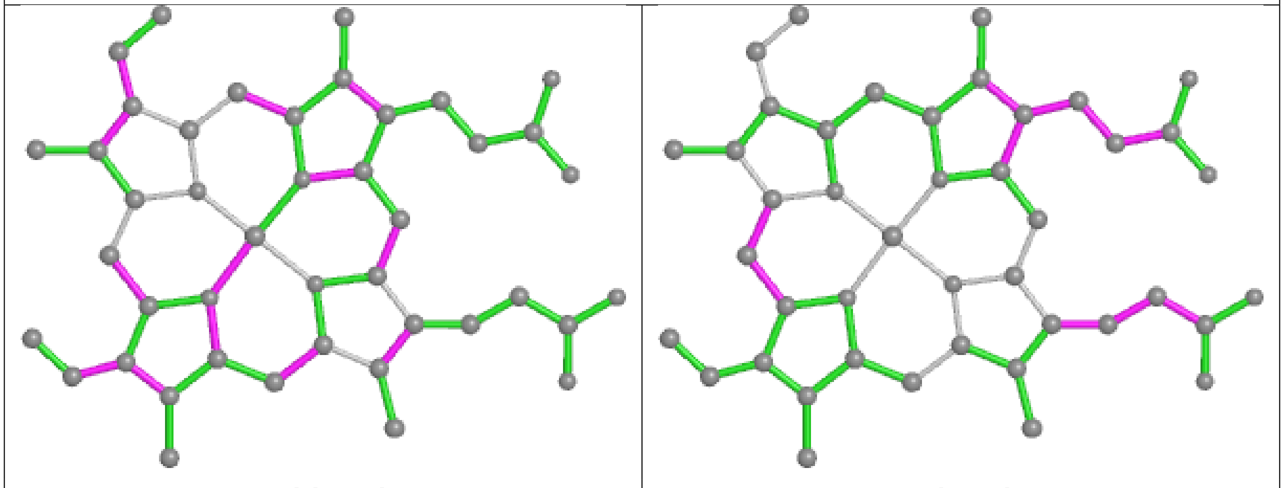
Bond lengths

Bond angles

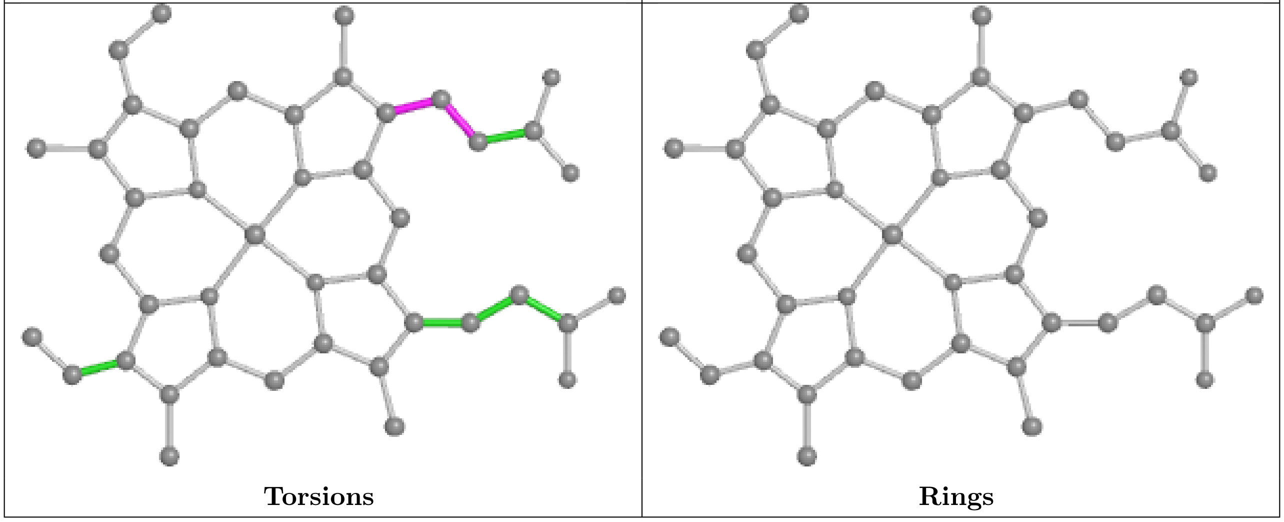
Torsions

Rings

Ligand HEM m 401

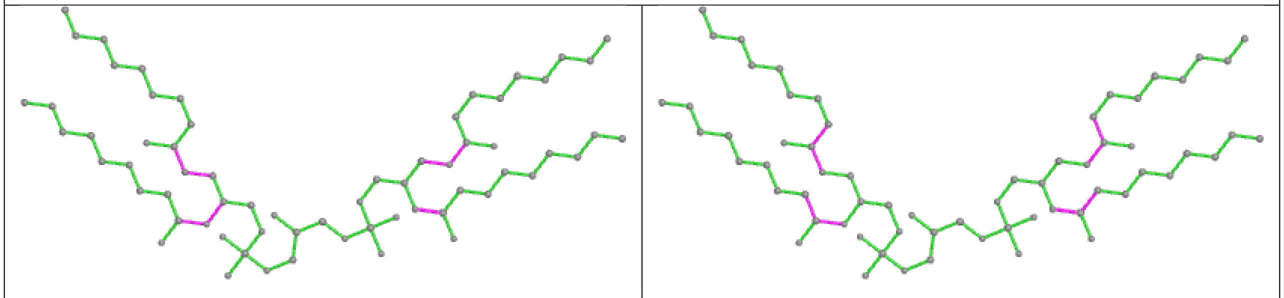


Bond lengths Bond angles

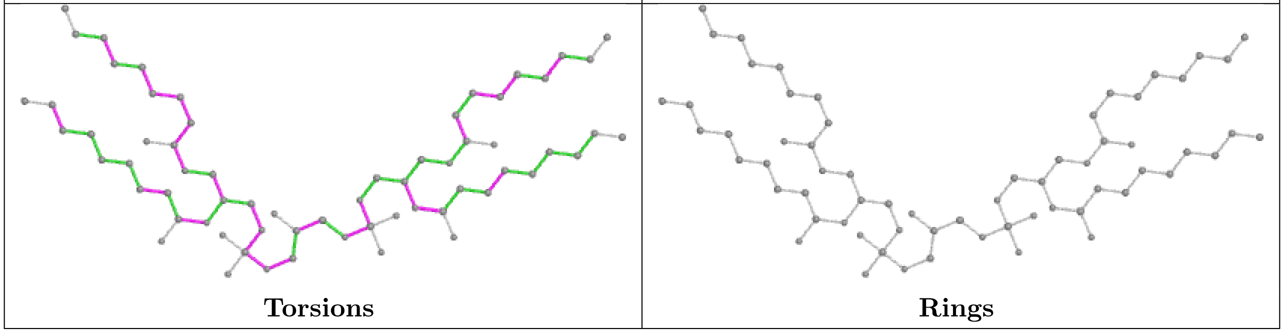


Torsions Rings

Ligand CDL 6 701

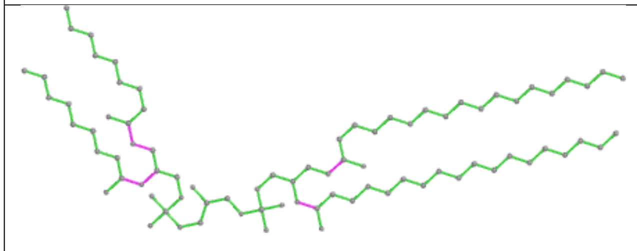


Bond lengths Bond angles

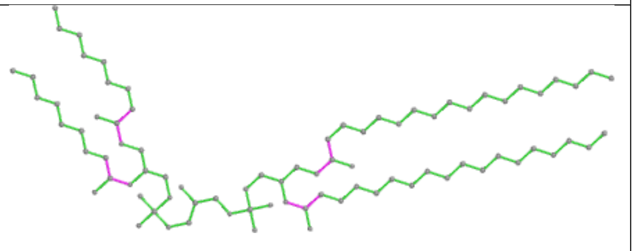


Torsions Rings

Ligand CDL b 201



Bond lengths



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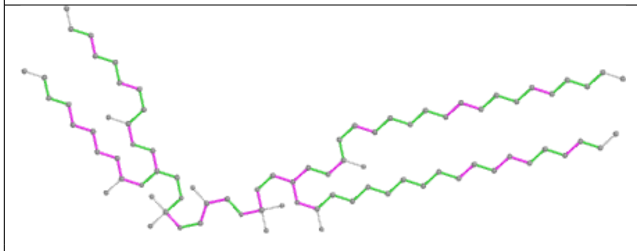
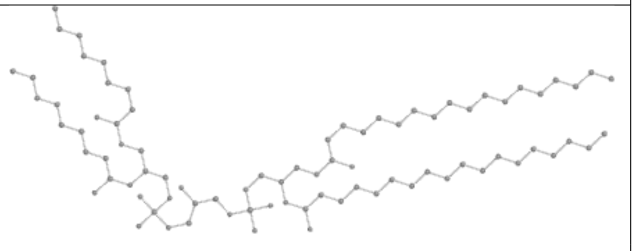
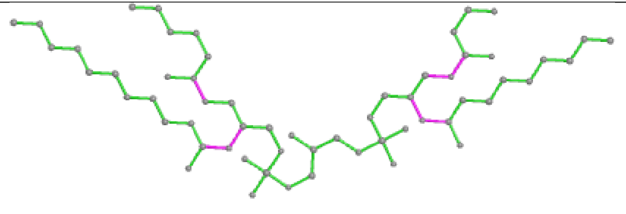


Torsions



Rings

Ligand CDL J 101



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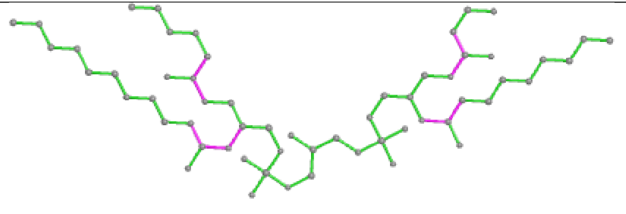

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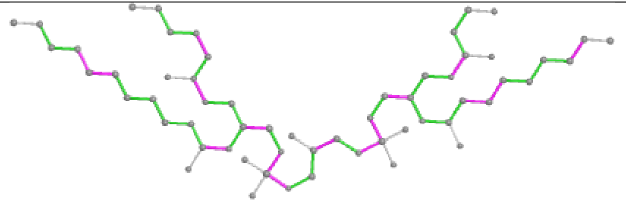
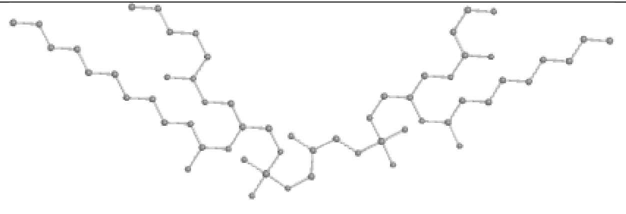
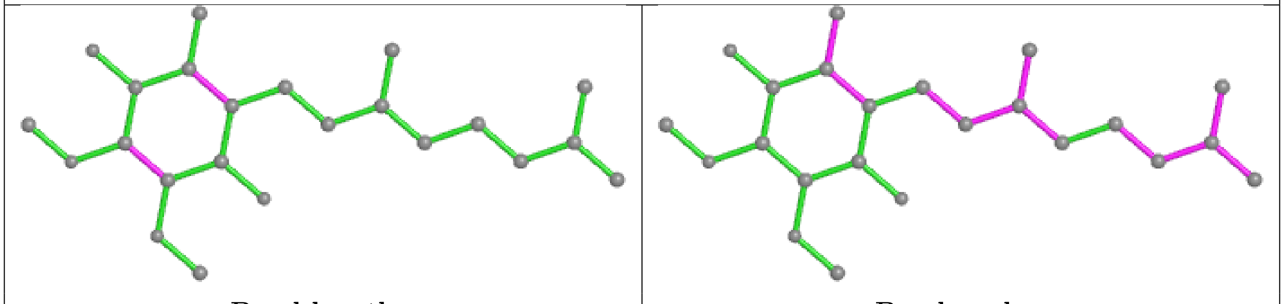


Torsions



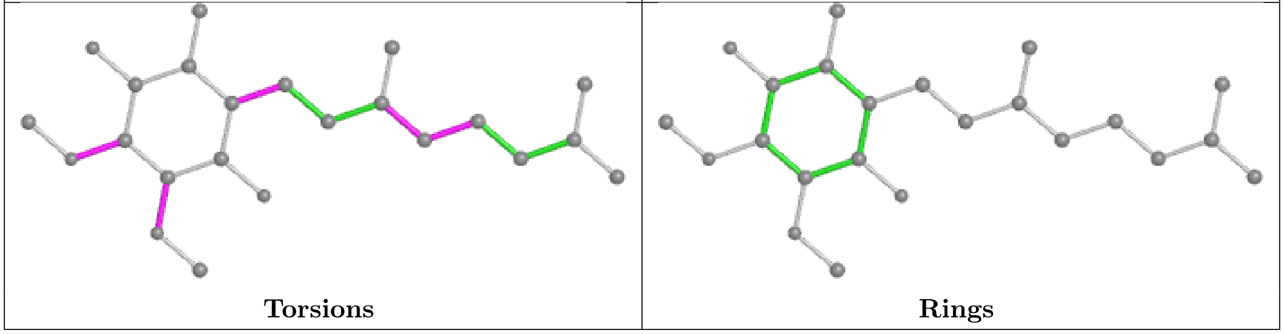
Rings

Ligand UQ2 A2 201



Bond lengths

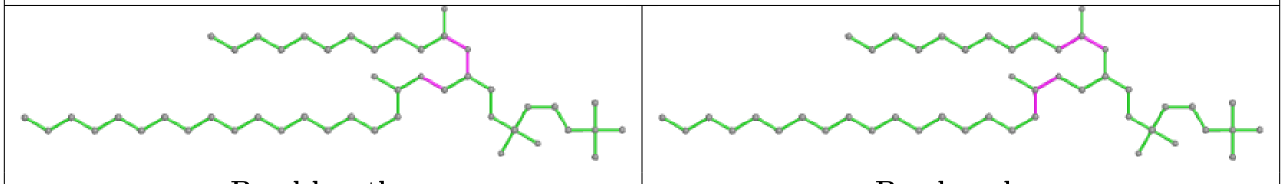
Bond angles



Torsions

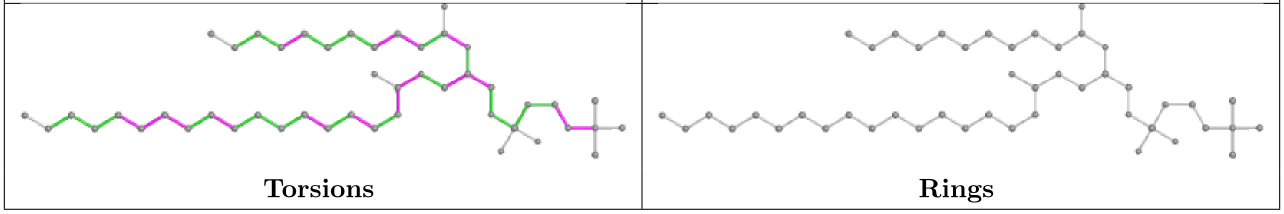
Rings

Ligand PC1 3 200



Bond lengths

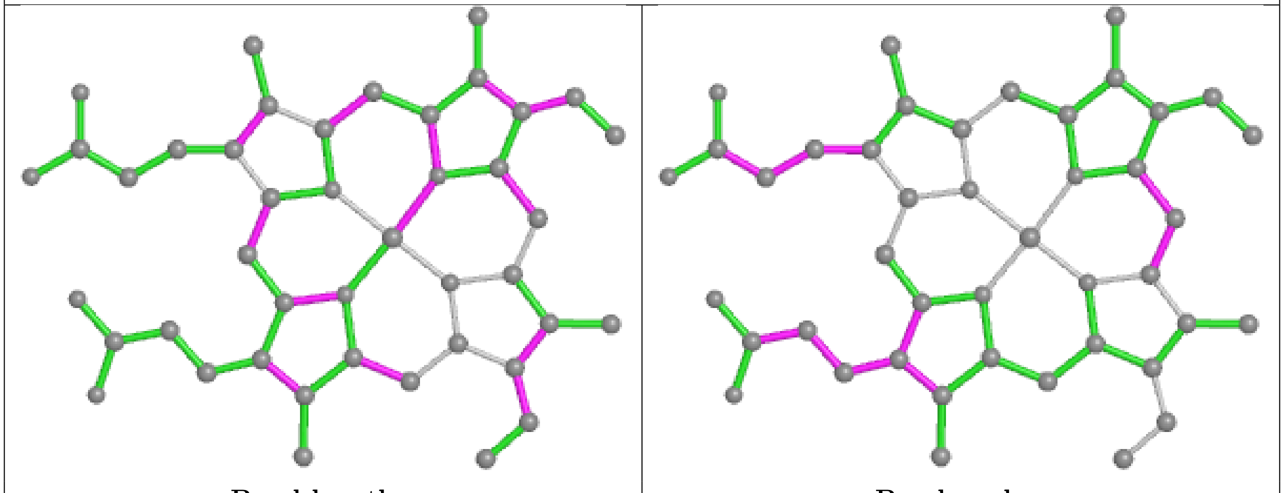
Bond angles



Torsions

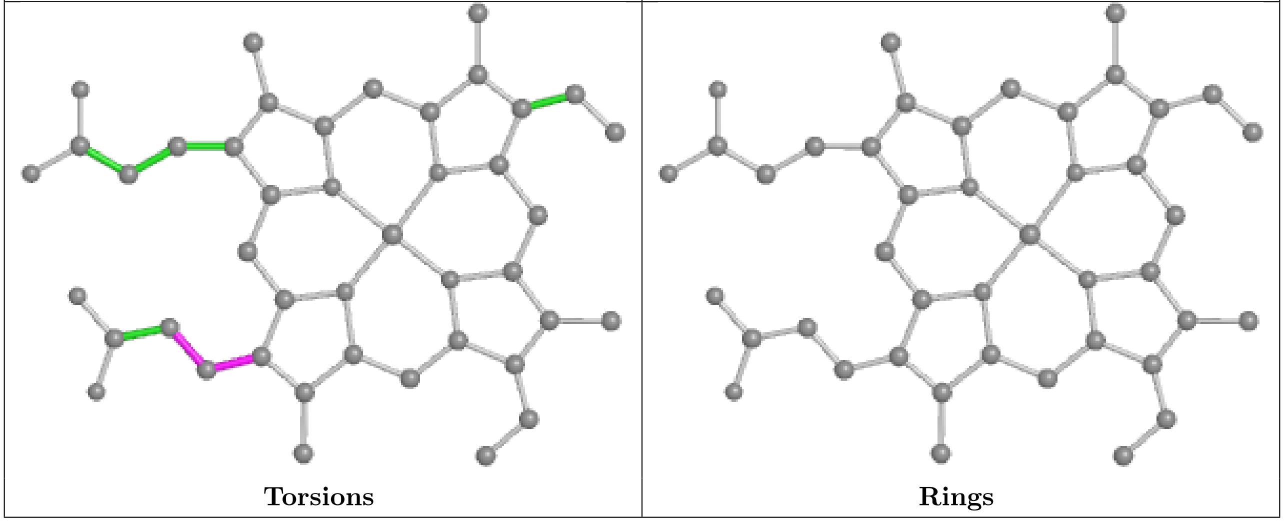
Rings

Ligand HEM y 401



Bond lengths

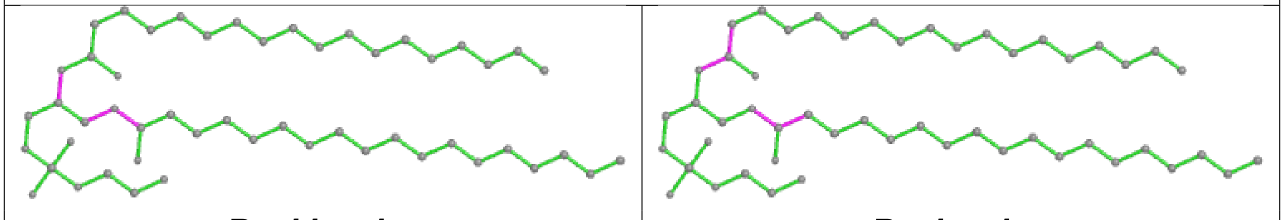
Bond angles



Torsions

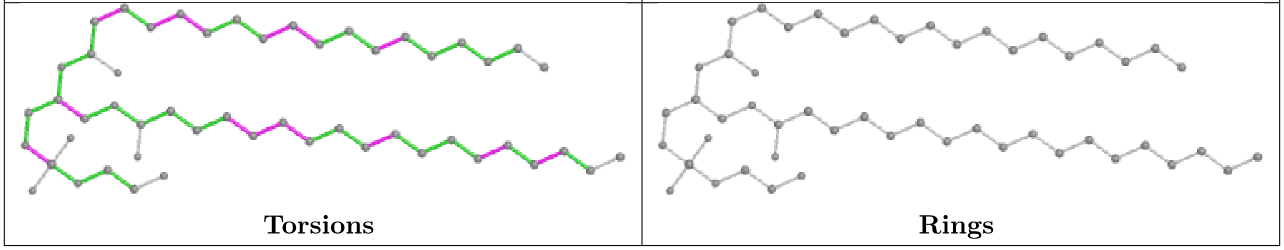
Rings

Ligand 3PE 1 401



Bond lengths

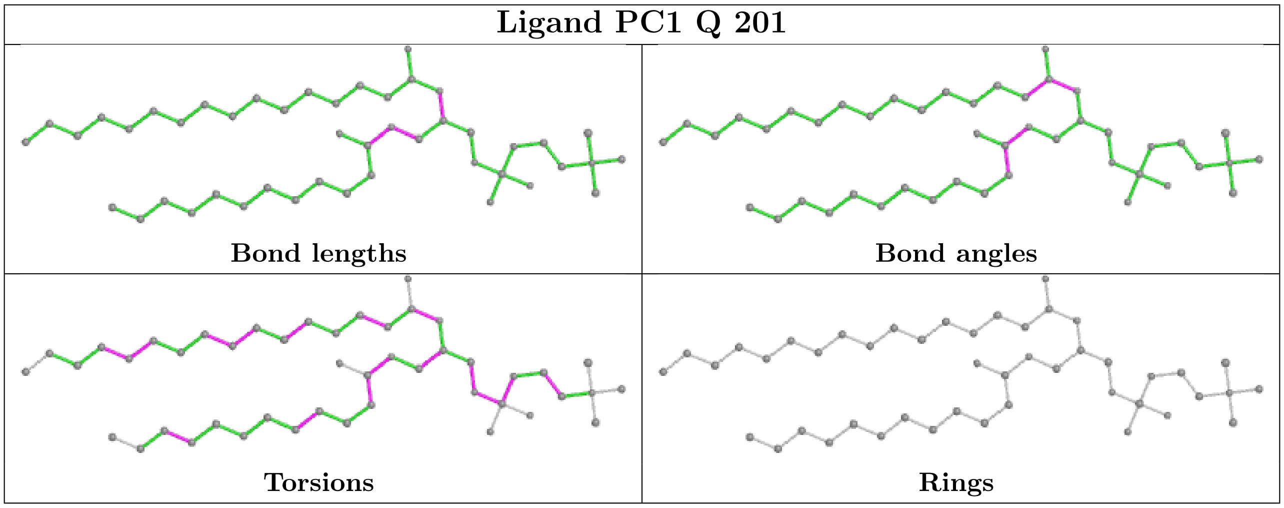
Bond angles



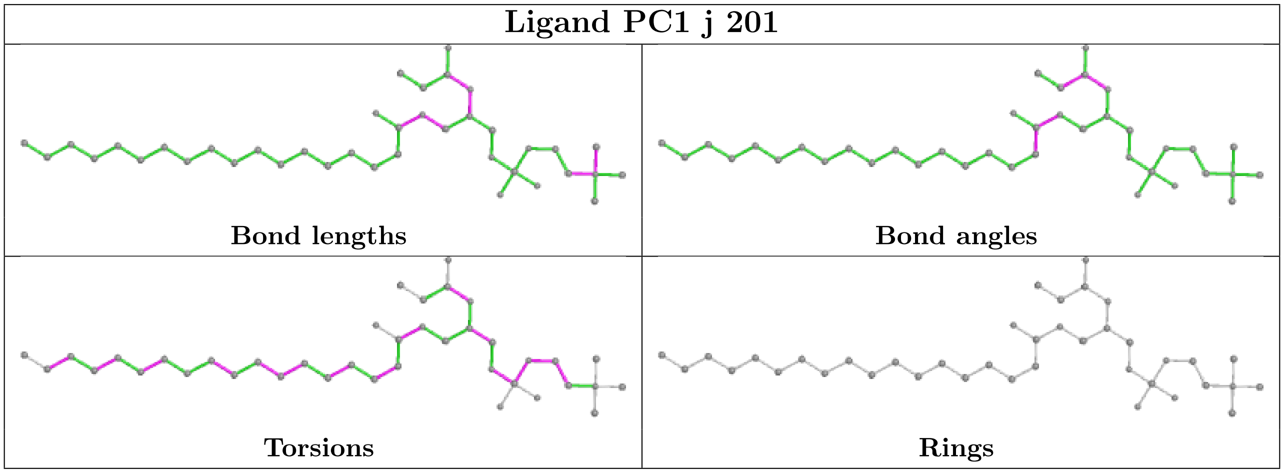
Torsions

Rings

Ligand PC1 Q 201



Ligand PC1 j 201



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

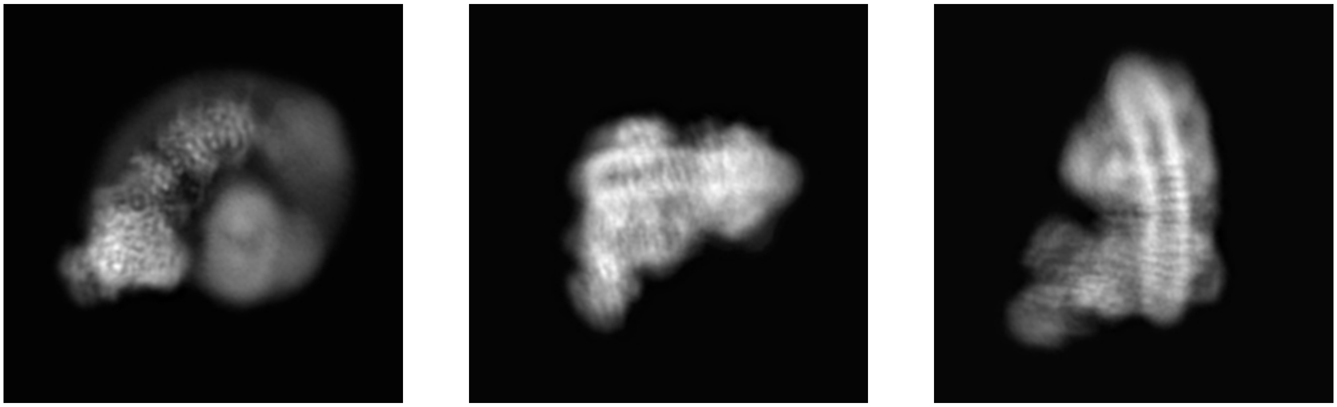
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30673. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map

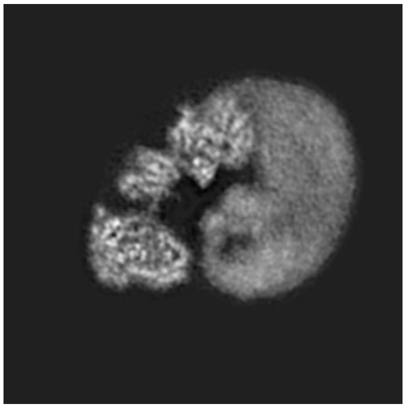


X Y Z

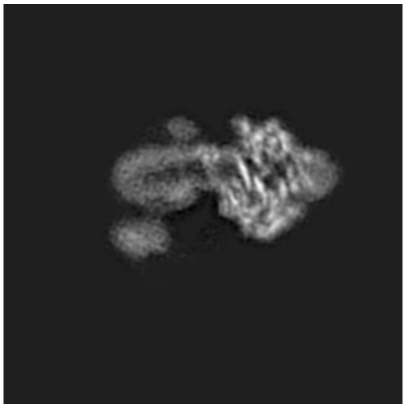
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

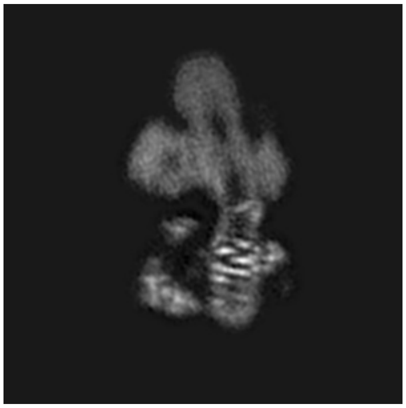
6.2.1 Primary map



X Index: 140



Y Index: 140

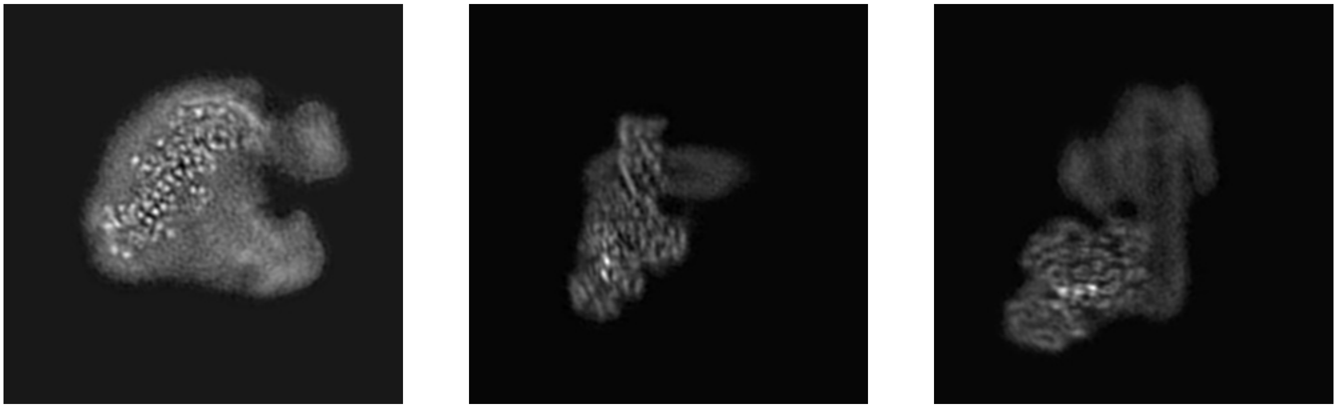


Z Index: 140

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

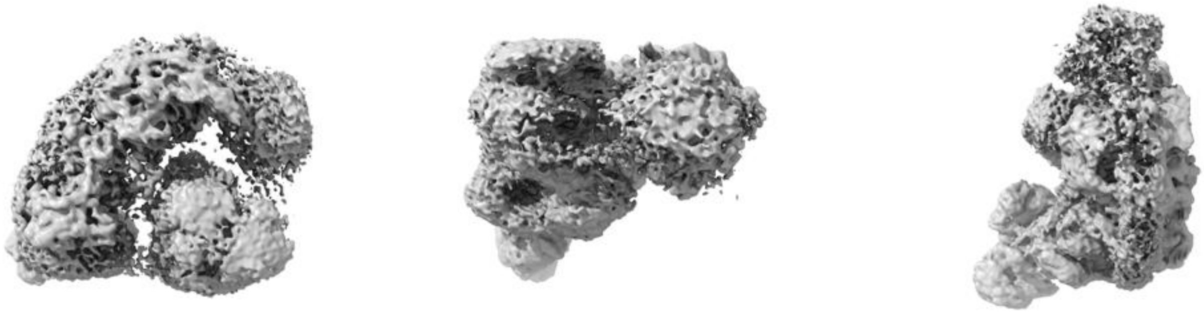


X Index: 173 Y Index: 78 Z Index: 95

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

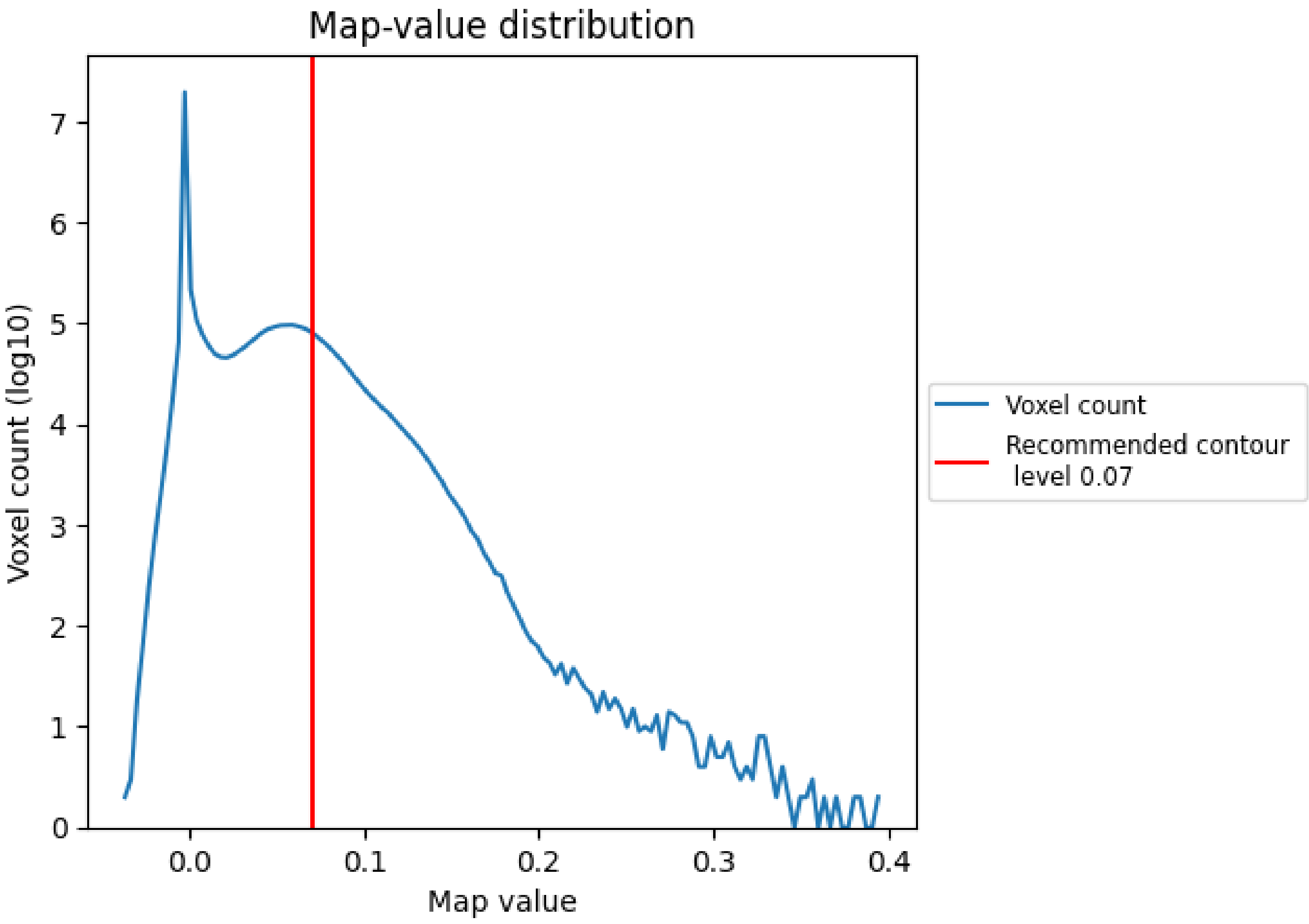
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

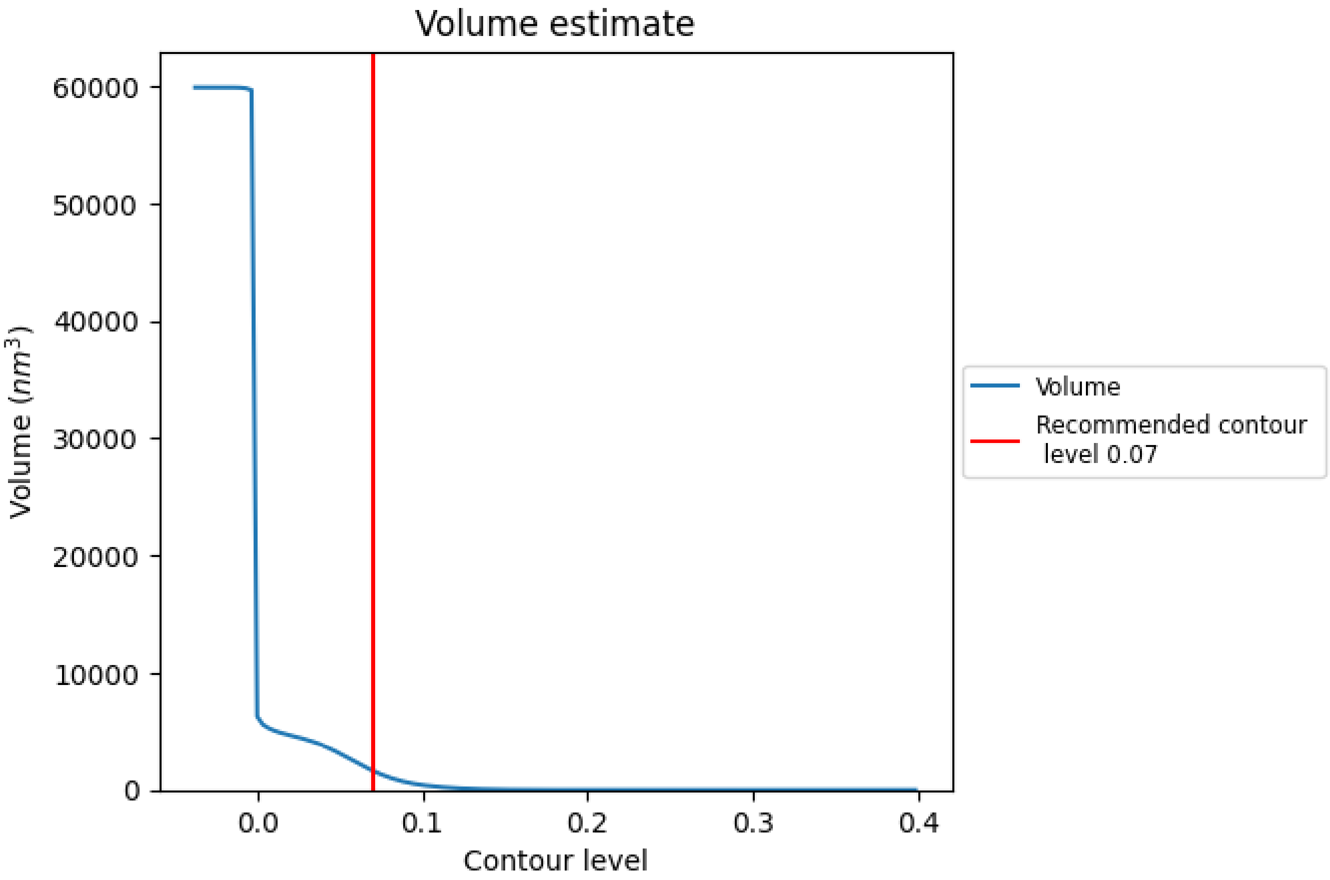
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

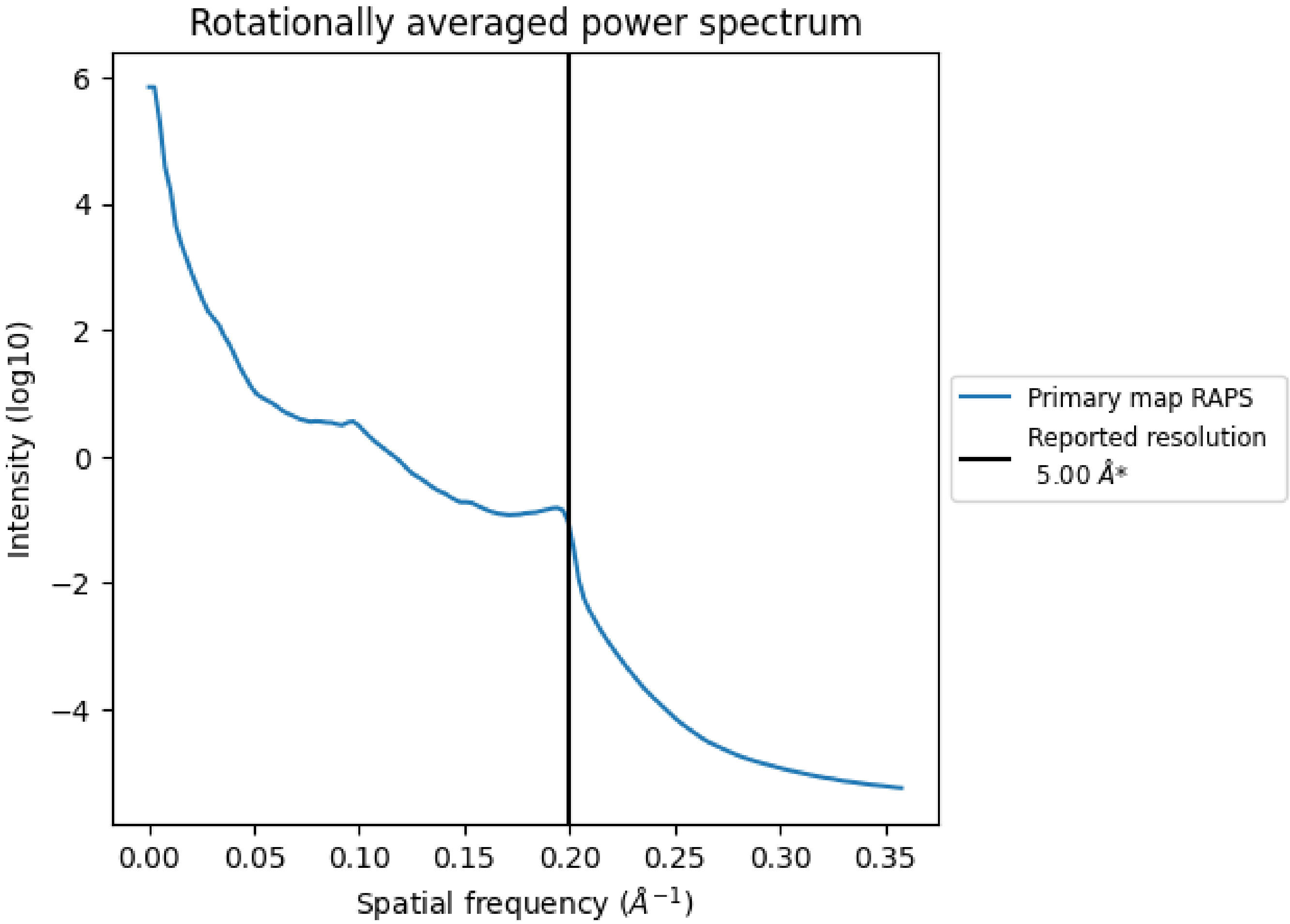
7.2 Volume estimate (i)



The volume at the recommended contour level is 1648 nm^3; this corresponds to an approximate mass of 1489 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 0.200 Å^{-1}

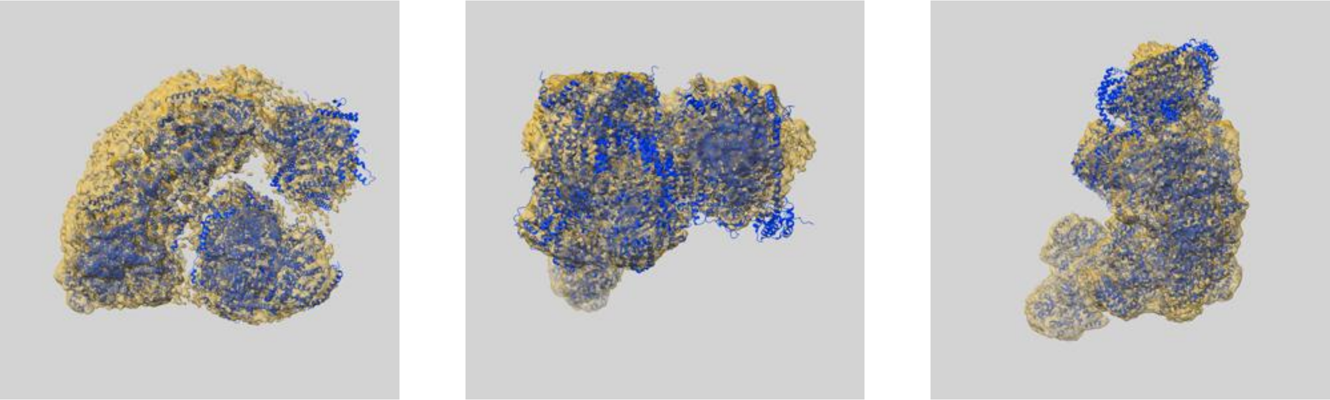
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30673 and PDB model 7DGQ. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay



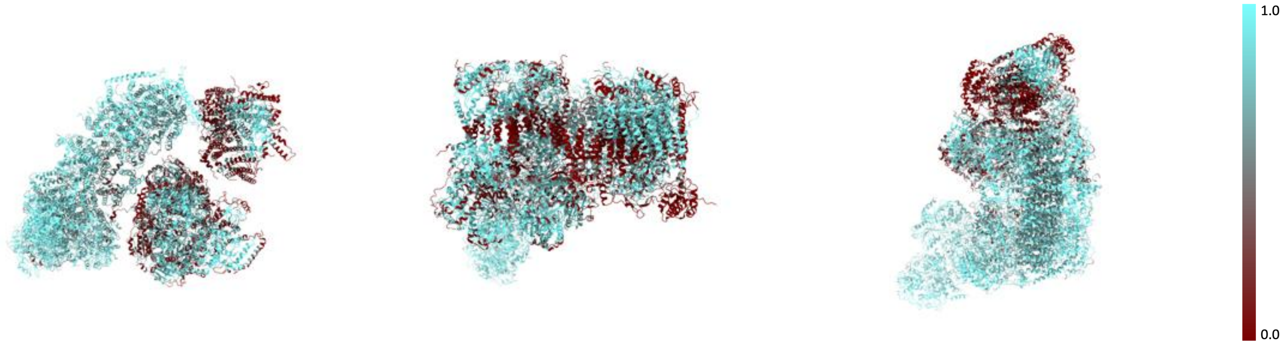
X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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 ⓘ

This section was not generated.

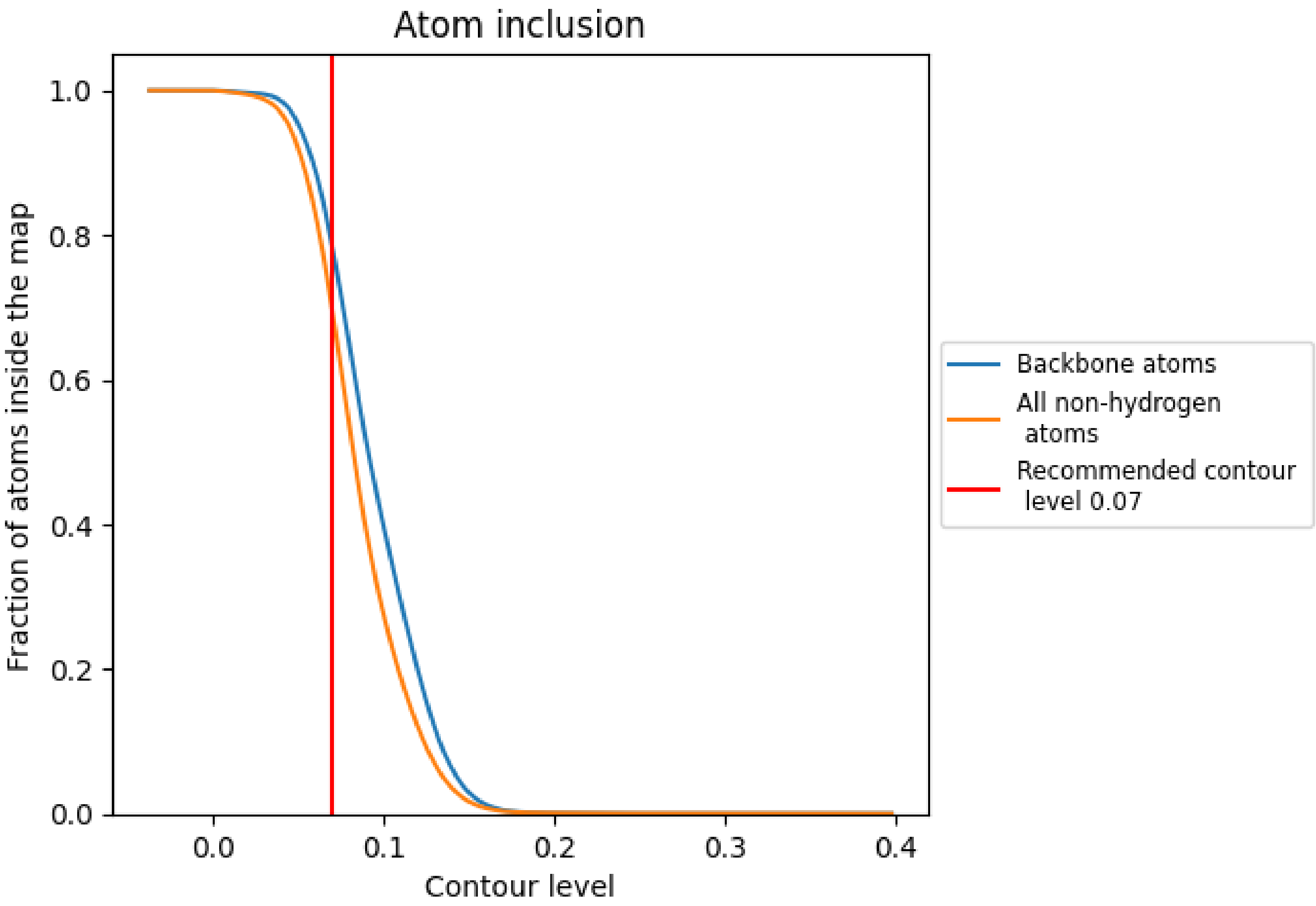
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6936
1	0.7226
2	0.7404
3	0.5620
4	0.7336
5	0.7100
6	0.7258
7	0.6964
8	0.9592
9	0.9320
A	0.9352
A0	0.2079
A1	0.4260
A2	0.3527
A3	0.4264
A4	0.2549
A5	0.1520
A6	0.1564
A7	0.1288
A8	0.2349
A9	0.2672
B	0.8152
B2	0.1039
B3	0.2533
B4	0.0245
B5	0.3056
B6	0.1844
B7	0.2870
C	0.9059
C0	0.3152
C1	0.6678
C2	0.2379
C3	0.5321
D	0.8569
E	0.9311

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Chain	Atom inclusion
F	▬ 0.9011
G	▬ 0.8669
H	▬ 0.8867
I	▬ 0.7859
J	▬ 0.8706
K	▬ 0.9184
L	▬ 0.8311
M	▬ 0.5950
N	▬ 0.9197
O	▬ 0.8256
P	▬ 0.8649
Q	▬ 0.8940
R	▬ 0.8114
S	▬ 0.8080
T	▬ 0.6509
U	▬ 0.7062
V	▬ 0.8730
W	▬ 0.9363
X	▬ 0.8607
Y	▬ 0.9553
Z	▬ 0.8574
a	▬ 0.7881
b	▬ 0.8673
c	▬ 0.9454
d	▬ 0.9698
e	▬ 0.8136
f	▬ 0.8951
g	▬ 0.9179
h	▬ 0.8656
i	▬ 0.8938
j	▬ 0.8153
k	▬ 0.6736
l	▬ 0.5389
m	▬ 0.5362
o	▬ 0.7827
p	▬ 0.5511
q	▬ 0.6247
r	▬ 0.6616
s	▬ 0.5896
t	▬ 0.5810
u	▬ 0.6012
v	▬ 0.3036

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Chain	**Atom inclusion**
w	▬ 0.5845
x	▬ 0.7487
y	▬ 0.5750
z	▬ 0.6911