WORLDWIDE PDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 08:27 PM JST

PDB ID : 7DGR
EMDB ID : EMD-30674
Title : Activity optimized supercomplex state2
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 : 4.60 Å(reported)

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

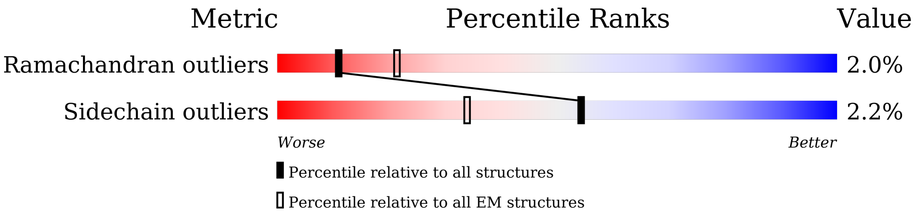
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

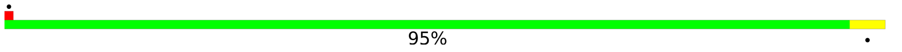
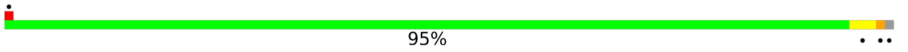
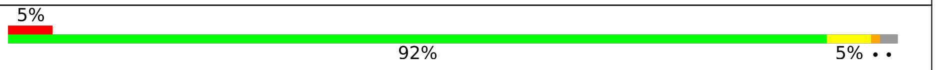
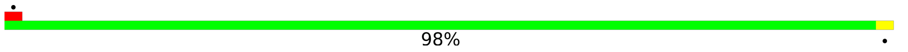
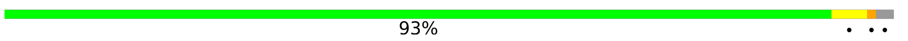
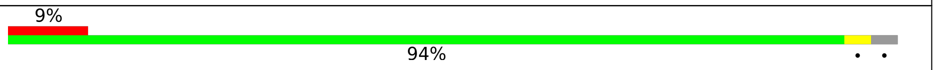
The reported resolution of this entry is 4.60 Å.

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

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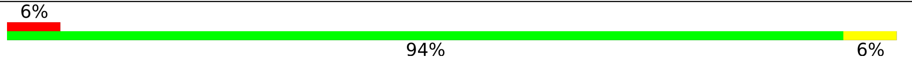
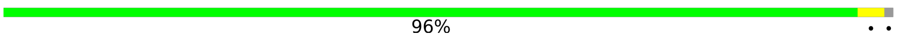
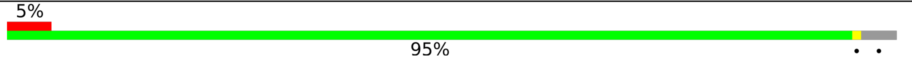
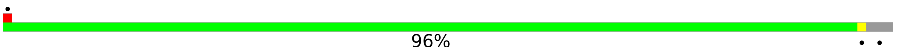
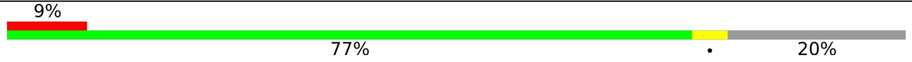
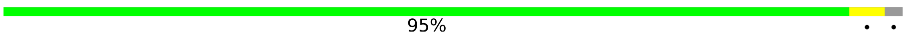
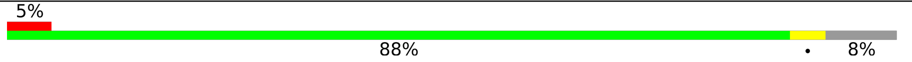
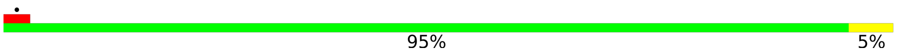
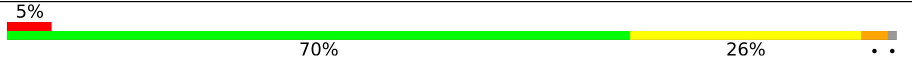
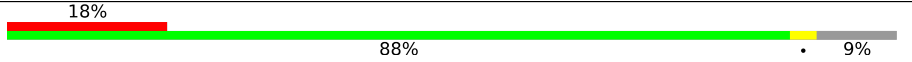
Mol	Chain	Length	Quality of chain
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	

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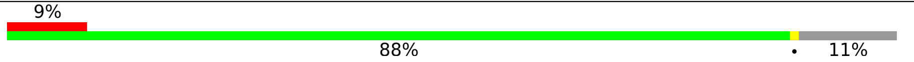
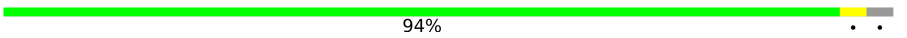
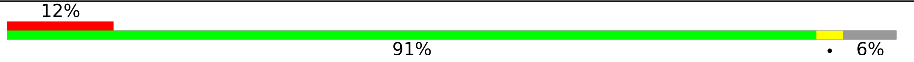
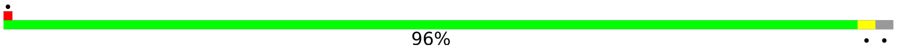
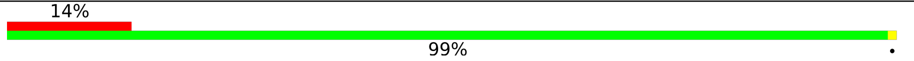
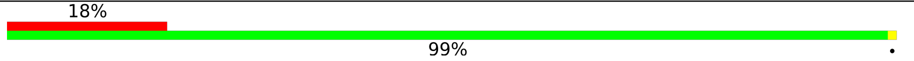
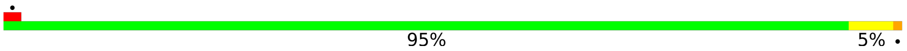
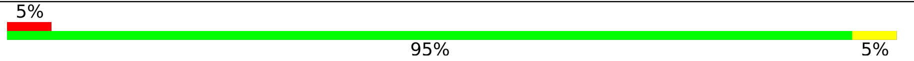
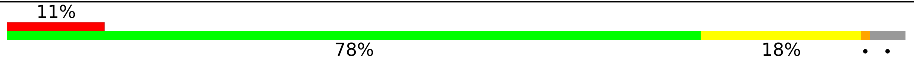
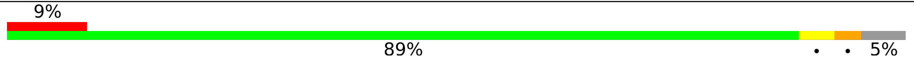
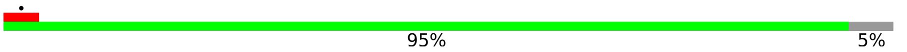
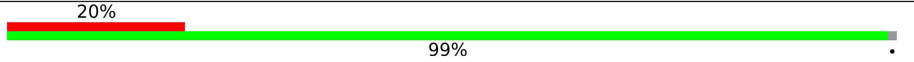
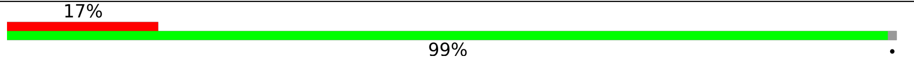
Mol	Chain	Length	Quality of chain
34	Z	98	
35	a	128	
36	b	143	
37	c	128	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	241	
48	z	241	
49	A0	196	
49	p	196	
50	A1	111	
50	q	111	
51	A2	82	
51	r	82	

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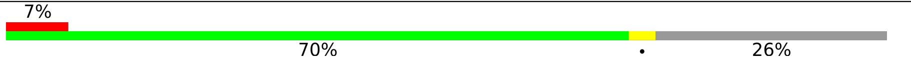
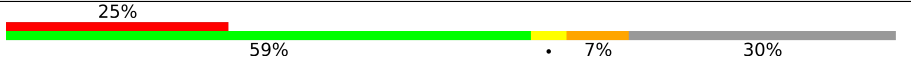
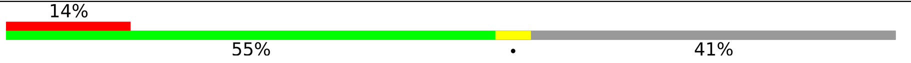
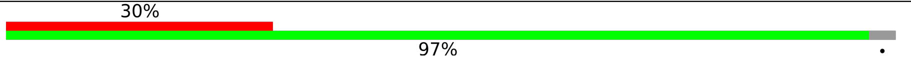
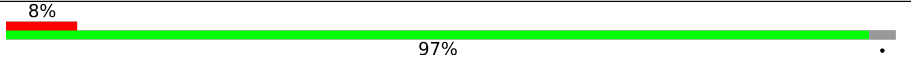
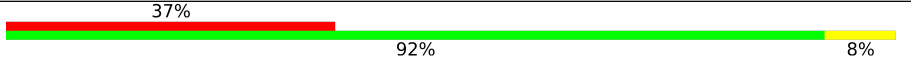
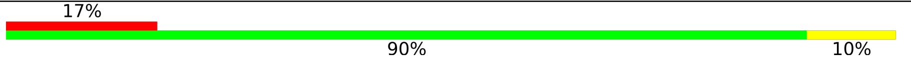
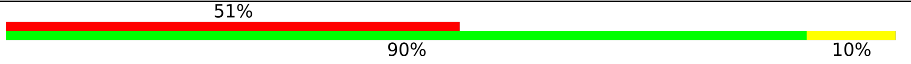
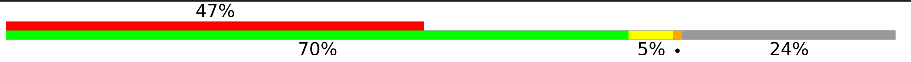
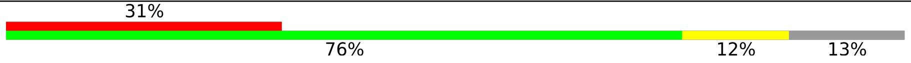
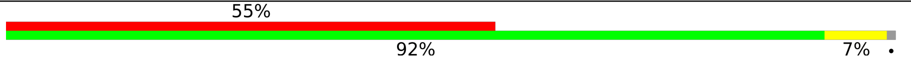
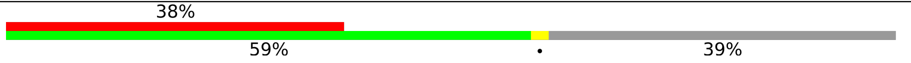
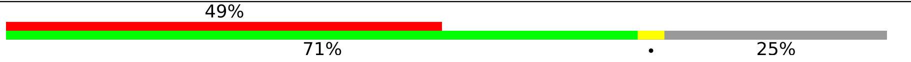
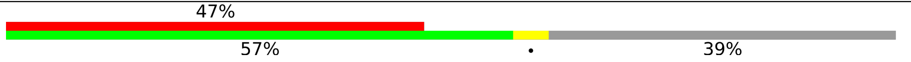
Mol	Chain	Length	Quality of chain
52	B3	91	
52	s	91	
53	A3	56	
53	t	56	
54	B2	64	
54	u	64	
55	B1	78	
55	v	78	
56	A9	514	
57	C4	227	
58	C2	261	
59	A7	169	
60	C0	152	
61	A6	129	
62	A4	97	
63	A5	86	
64	B4	74	
65	C3	80	
66	B0	80	
67	C1	63	
68	A8	70	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
79	HEA	A9	601	X	-	-	-
79	HEA	A9	602	X	-	-	-

2 Entry composition ⓘ

There are 81 unique types of molecules in this entry. The entry contains 107305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9	207	1578	1006	269	293	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	458	3577	2382	561	599	35	1	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	344	2681	1779	413	449	40	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	1239	838	182	211	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	606	4766	3172	732	820	42	0	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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	3	112	879	593	128	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1	318	2503	1678	385	417	23	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 NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	71	Total 533	C 332	N 99	O 99	S 3	0	0

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

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	319	2407	1548	431	425	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	138	923	586	163	168	6	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 31 is a protein called Acyl carrier protein, mitochondrial.

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

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

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

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

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	107	Total	C	N	O	S	0	0
			713	448	134	127	4		

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

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	113	Total	C	N	O	S	0	0
			883	580	149	151	3		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	446	Total 3454	C 2159	N 608	O 667	S 20	0	0
45	w	436	Total 3385	C 2117	N 599	O 649	S 20	0	0

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

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

- Molecule 47 is a protein called Cytochrome b.

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

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

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

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	151	Total 938	C 572	N 170	O 194	S 2	0	0
49	A0	188	Total 1117	C 679	N 207	O 229	S 2	0	0

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	106	Total 916	C 579	N 167	O 168	S 2	0	0
50	A1	106	Total 916	C 579	N 167	O 168	S 2	0	0

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	81	Total 682	C 441	N 128	O 112	S 1	0	0
51	A2	81	Total 676	C 438	N 125	O 112	S 1	0	0

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	67	Total 548	C 332	N 99	O 112	S 5	0	0
52	B3	69	Total 566	C 342	N 101	O 118	S 5	0	0

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	33	Total 262	C 174	N 46	O 42	0	0
53	A3	39	Total 318	C 212	N 56	O 50	0	0

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	u	62	Total 511	C 335	N 89	O 87	0	0
54	B2	62	Total 511	C 335	N 89	O 87	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
55	v	18	Total 114	C 70	N 22	O 22	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	B1	22	148	91	30	27	0	0

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	A9	514	4025	2690	623	677	35	0	0

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	C4	227	1822	1184	281	339	18	0	0

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	C2	261	2124	1420	338	353	13	0	0

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	C0	109	878	558	150	168	2	0	0

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	A6	98	748	464	134	145	5	0	0

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	A4	84	671	431	129	110	1	0	0

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	A5	75	628	395	114	114	5	0	0

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	B4	73	598	388	107	99	4	0	0

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	C3	56	441	285	73	80	3	0	0

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	B0	49	384	250	65	67	2	0	0

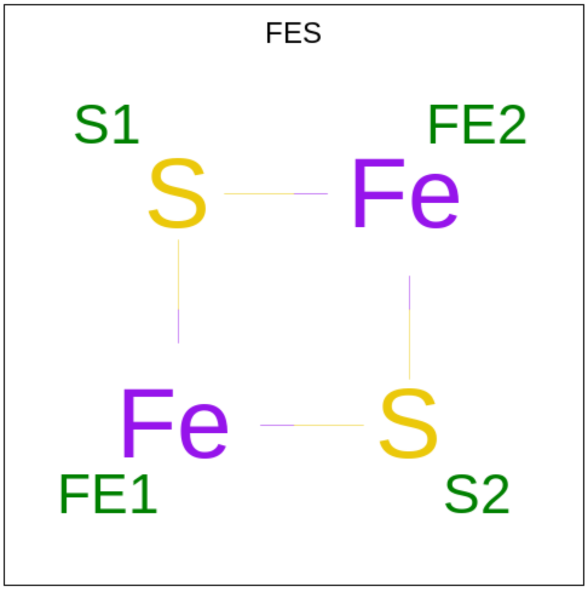
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	C1	47	386	257	65	62	2	0	0

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

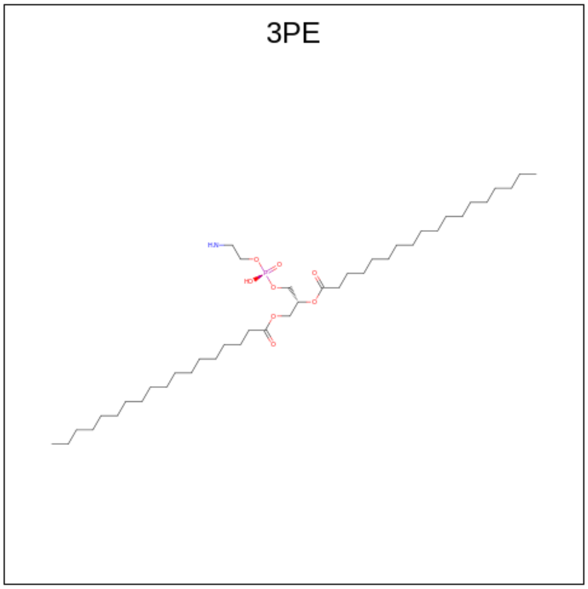
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	A8	43	335	223	53	59	0	0

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



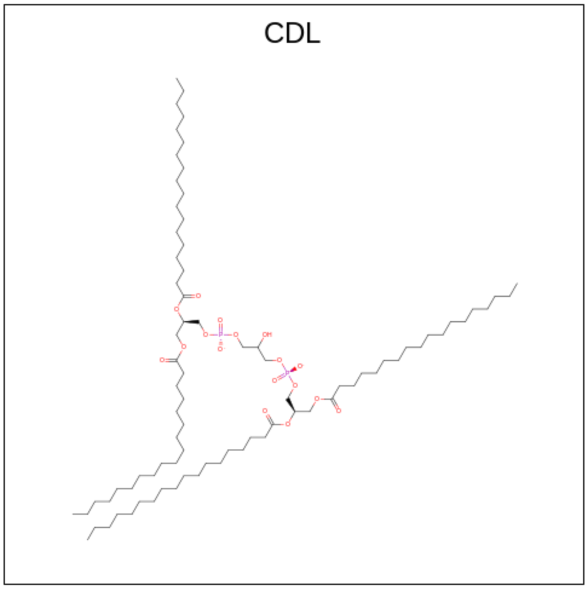
Mol	Chain	Residues	Atoms	AltConf
69	9	1	Total Fe S 4 2 2	0
69	A	1	Total Fe S 4 2 2	0
69	m	1	Total Fe S 4 2 2	0

- 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).



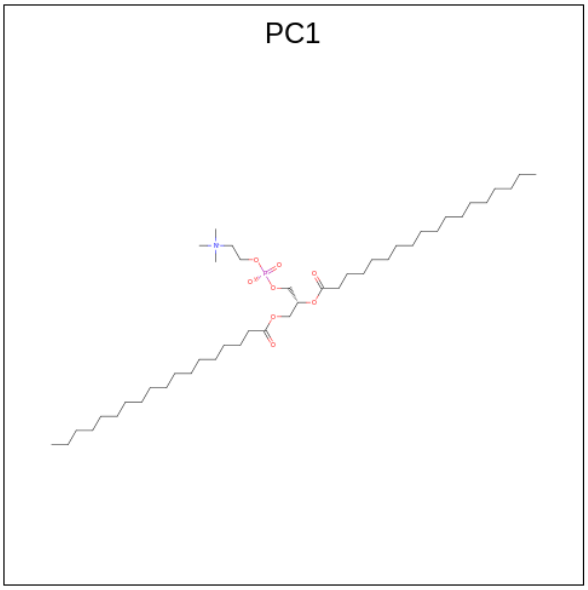
Mol	Chain	Residues	Atoms					AltConf
70	4	1	Total 82	C 62	N 2	O 16	P 2	0
70	4	1	Total 82	C 62	N 2	O 16	P 2	0
70	2	1	Total 46	C 36	N 1	O 8	P 1	0
70	B	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 71 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



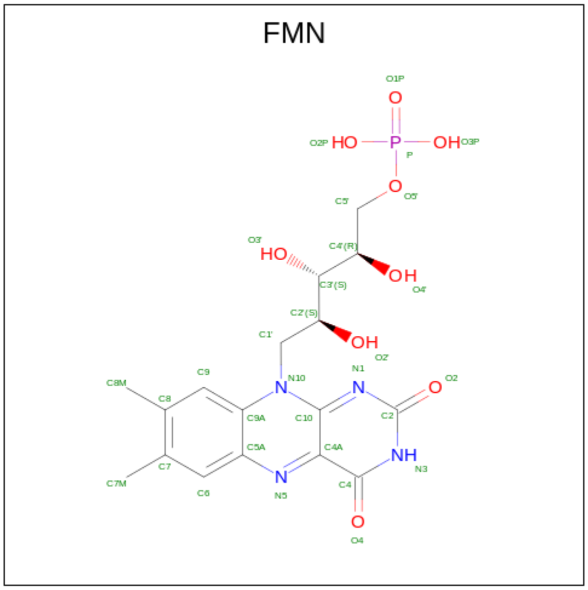
Mol	Chain	Residues	Atoms				AltConf
71	4	1	Total 82	C 63	O 17	P 2	0
71	6	1	Total 64	C 45	O 17	P 2	0
71	J	1	Total 58	C 39	O 17	P 2	0

- Molecule 72 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).



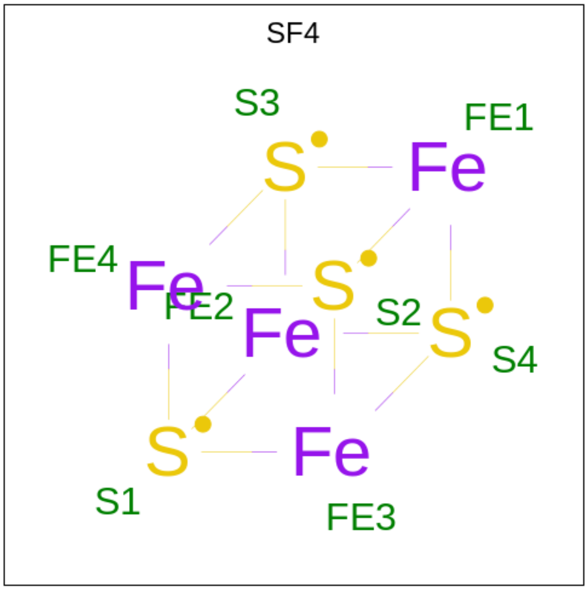
Mol	Chain	Residues	Atoms	AltConf
72	4	1	Total C N O P 46 36 1 8 1	0
72	2	1	Total C N O P 46 36 1 8 1	0
72	L	1	Total C N O P 47 37 1 8 1	0
72	S	1	Total C N O P 47 37 1 8 1	0
72	j	1	Total C N O P 39 29 1 8 1	0

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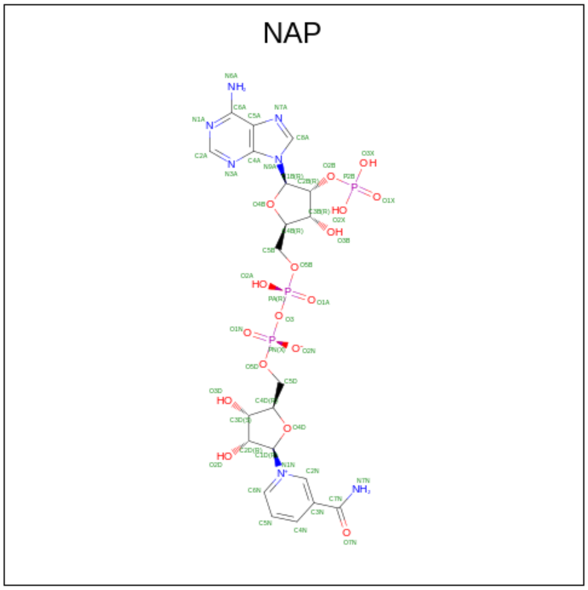
Mol	Chain	Residues	Atoms	AltConf
74	D	1	Total Fe S 8 4 4	0
74	E	1	Total Fe S 16 8 8	0
74	E	1	Total Fe S 16 8 8	0

- Molecule 75 is ZINC ION (three-letter code: ZN) (formula: Zn).

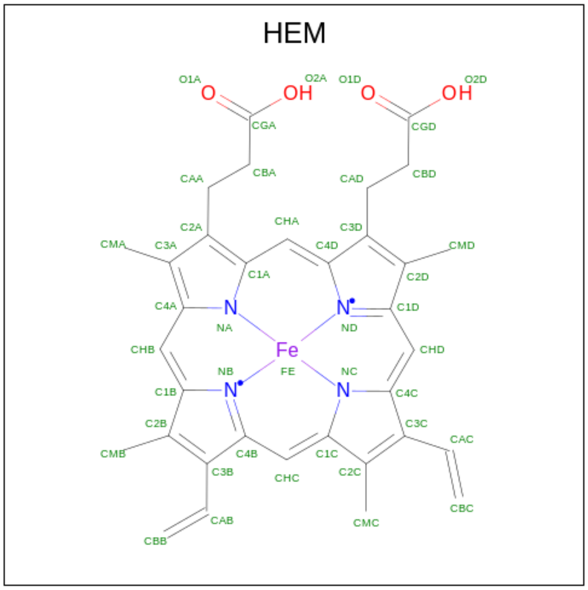
Mol	Chain	Residues	Atoms	AltConf
75	I	1	Total Zn 1 1	0
75	A6	1	Total Zn 1 1	0

- Molecule 76 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



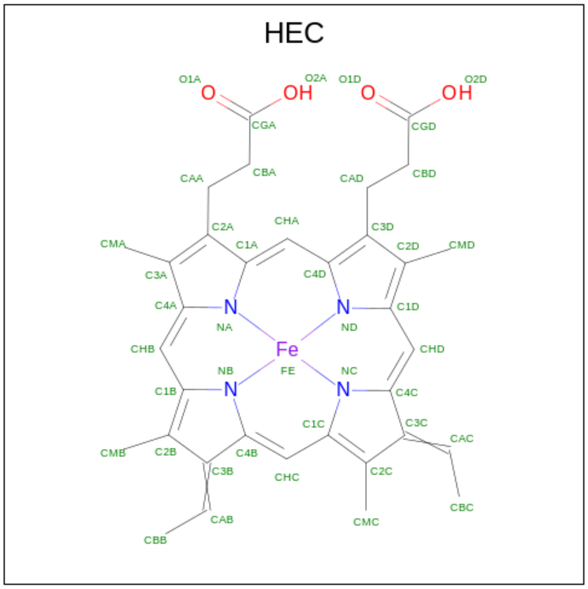
Mol	Chain	Residues	Atoms	AltConf
76	R	1	Total C N O P 48 21 7 17 3	0

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



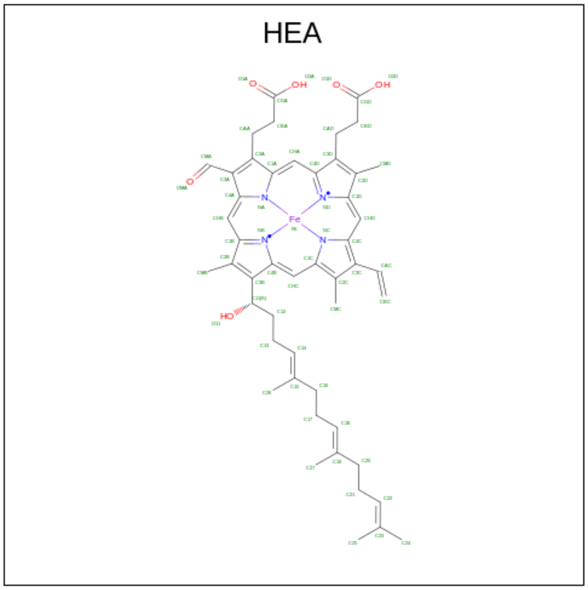
Mol	Chain	Residues	Atoms	AltConf
77	m	1	Total C Fe N O 86 68 2 8 8	0
77	m	1	Total C Fe N O 86 68 2 8 8	0
77	y	1	Total C Fe N O 86 68 2 8 8	0
77	y	1	Total C Fe N O 86 68 2 8 8	0

- Molecule 78 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
78	o	1	Total 43	C 34	Fe 1	N 4	O 4	0
78	z	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 79 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
79	A9	1	Total 120	C 98	Fe 2	N 8	O 12	0
79	A9	1	Total 120	C 98	Fe 2	N 8	O 12	0

- Molecule 80 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	A9	1	Total 1	Cu 1	0
80	C4	2	Total 2	Cu 2	0

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

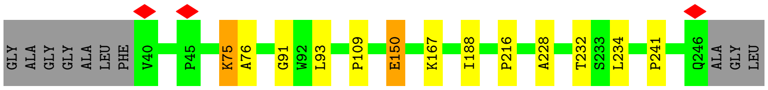
Mol	Chain	Residues	Atoms		AltConf
81	A9	1	Total 1	Mg 1	0

3 Residue-property plots

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

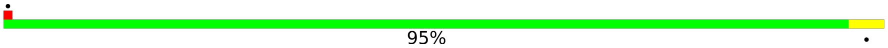
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

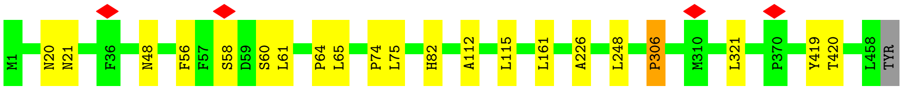
Chain 9:



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

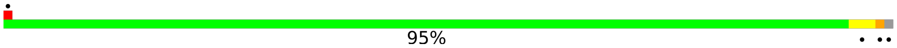
Chain 4:

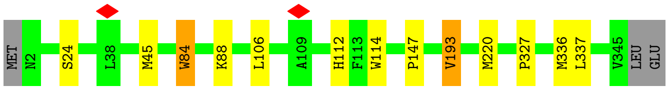




- Molecule 3: NADH-ubiquinone oxidoreductase chain 2

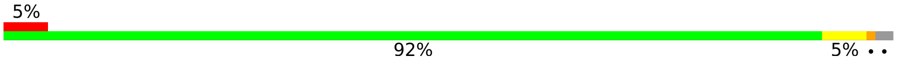
Chain 2:

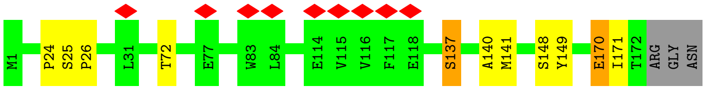




- Molecule 4: NADH-ubiquinone oxidoreductase chain 6

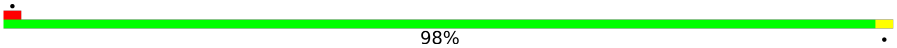
Chain 7:

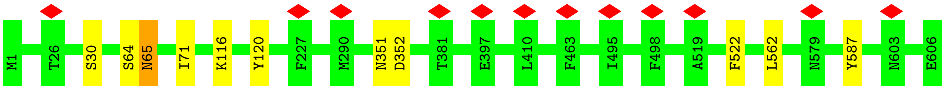




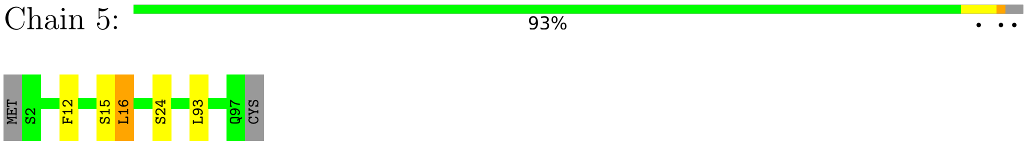
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5

Chain 6:

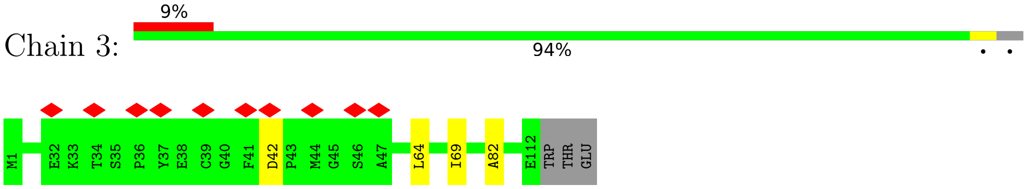




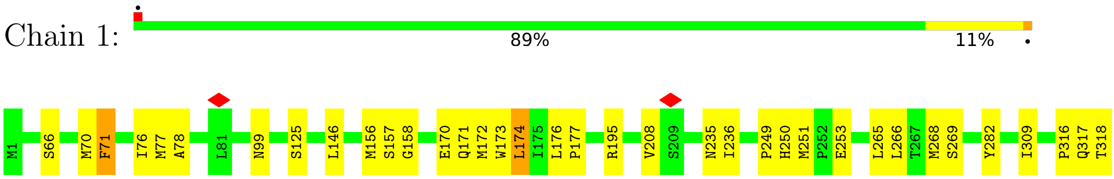
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L



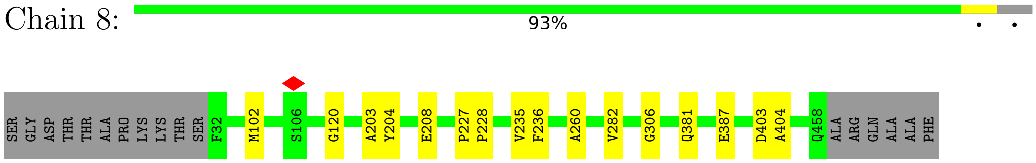
- Molecule 7: NADH-ubiquinone oxidoreductase chain 3



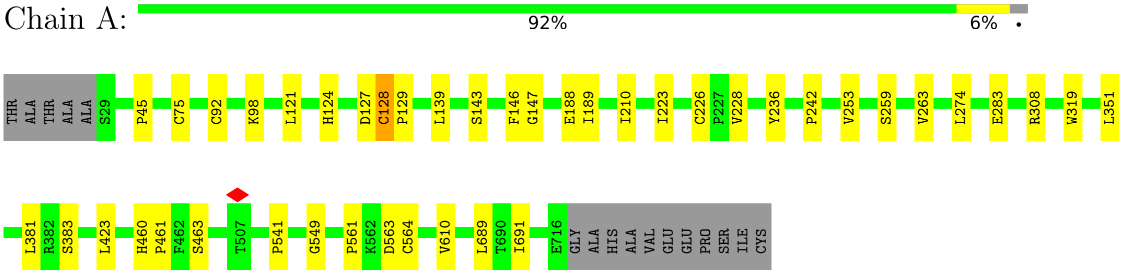
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



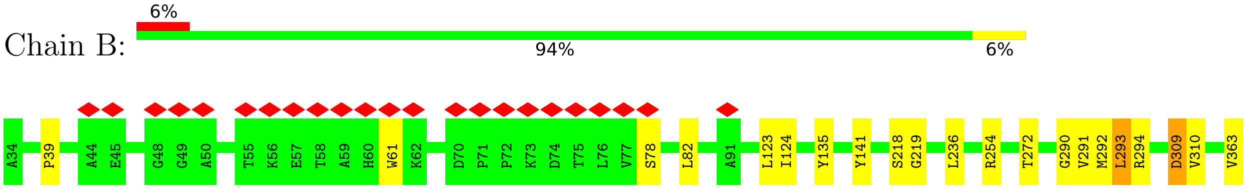
- Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

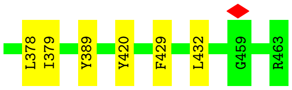


- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



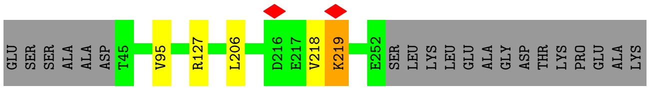
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





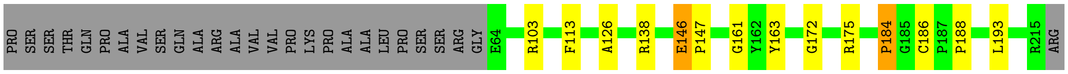
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



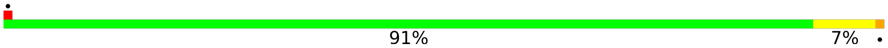
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

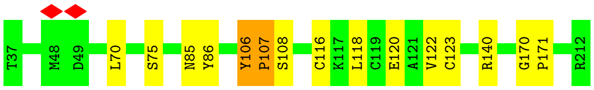
Chain D:



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

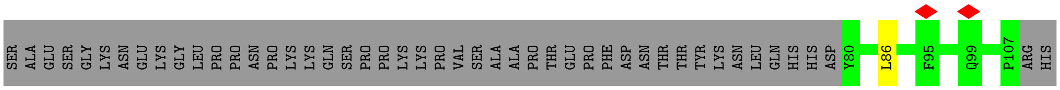
Chain E:





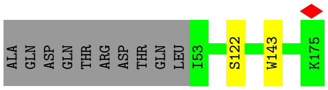
- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:



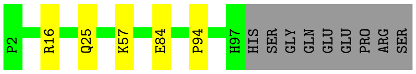
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G:



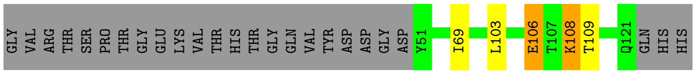
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain H:



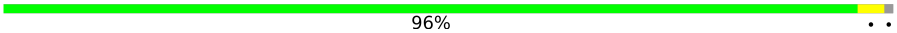
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain I:



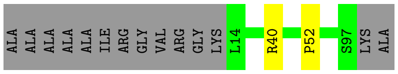
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain J:



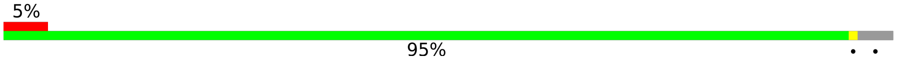
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

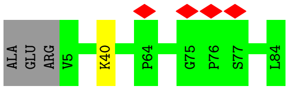
Chain K:



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

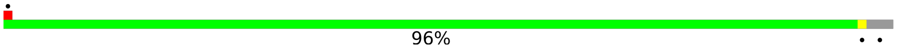
Chain L:

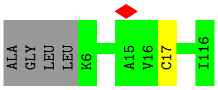




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

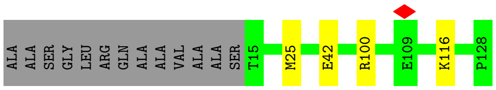
Chain N:





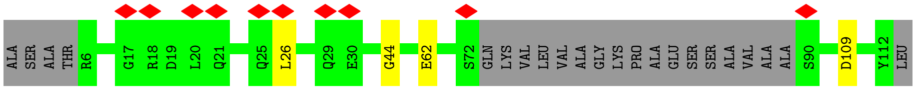
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O:

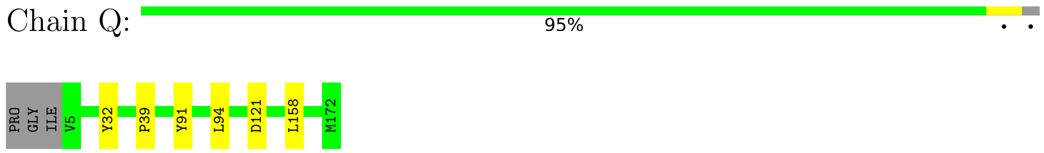


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

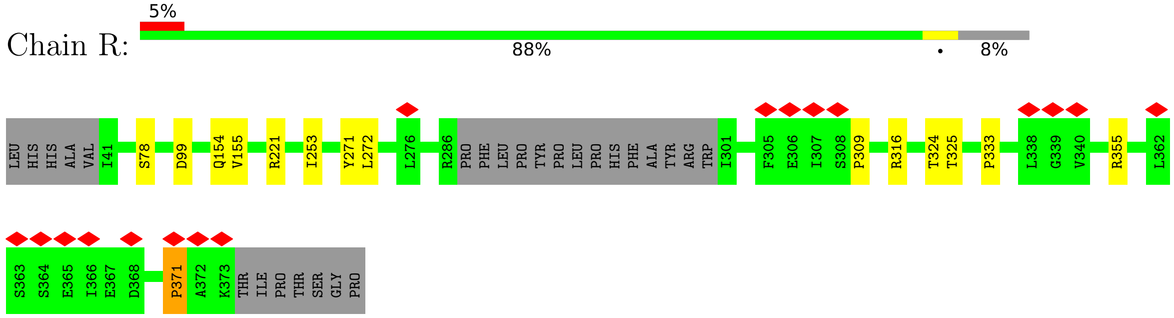
Chain P:



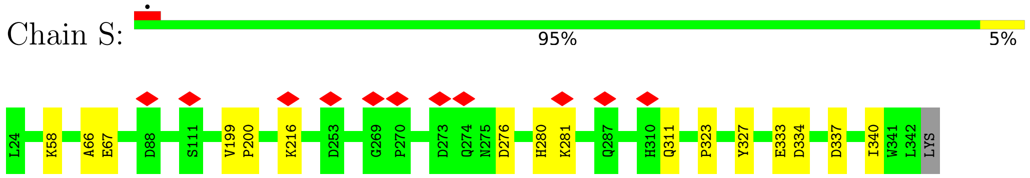
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



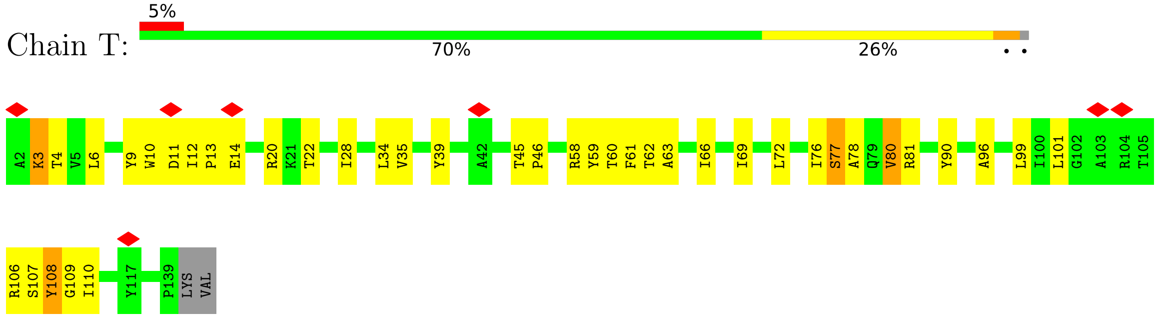
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



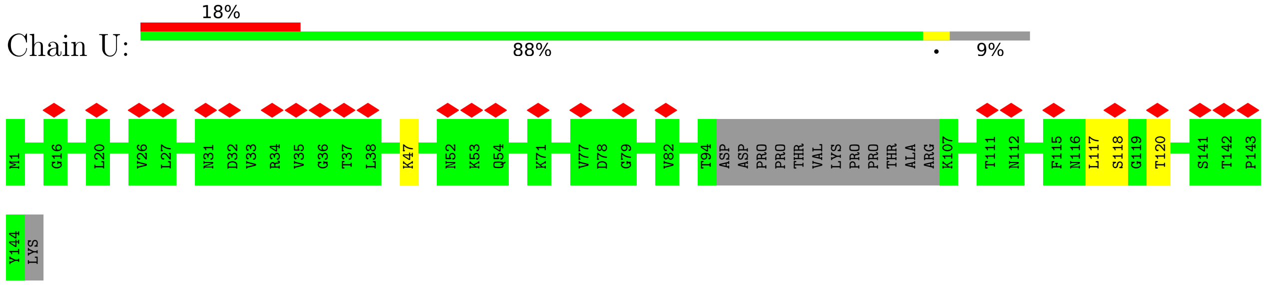
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



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

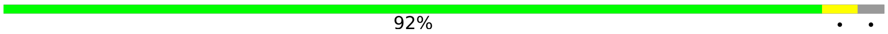


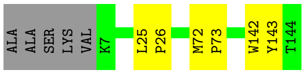
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

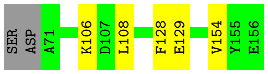
Chain V:





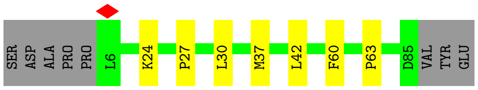
• Molecule 31: Acyl carrier protein, mitochondrial

Chain W:



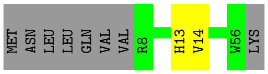
• Molecule 31: Acyl carrier protein, mitochondrial

Chain M:



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

Chain X:

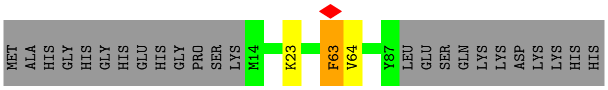


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:

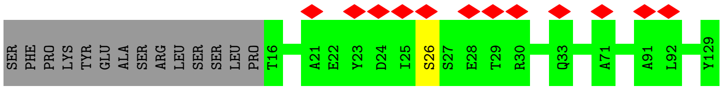
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:

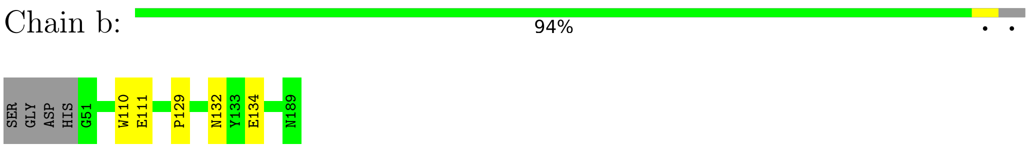


• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

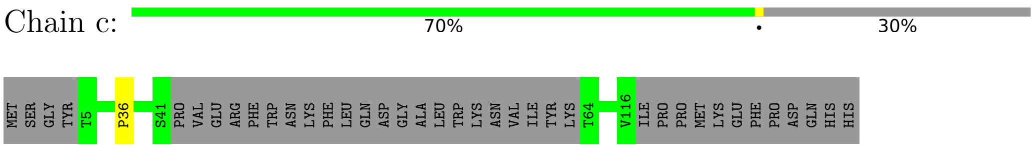
Chain a:



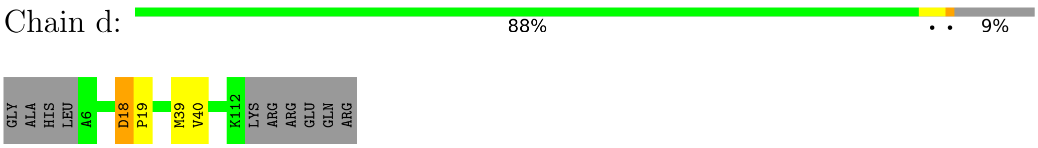
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



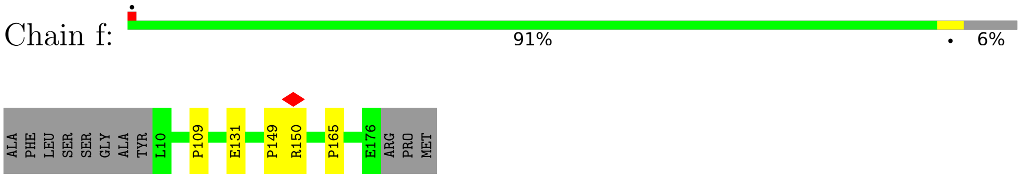
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



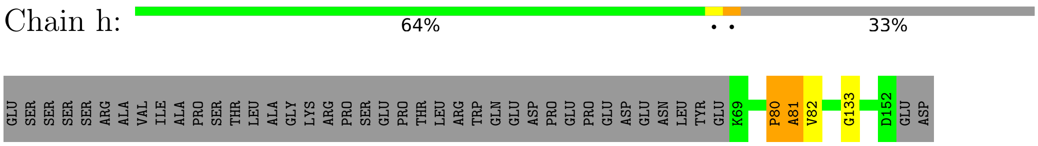
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



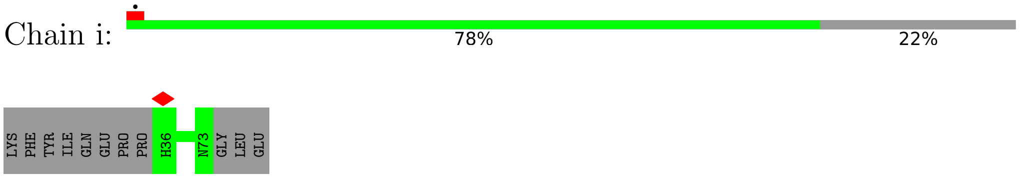
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



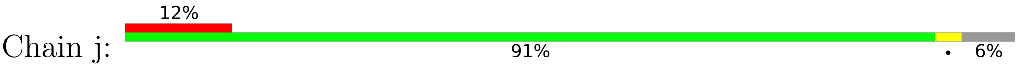
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

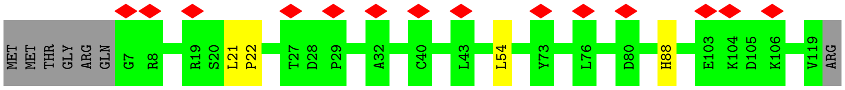


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



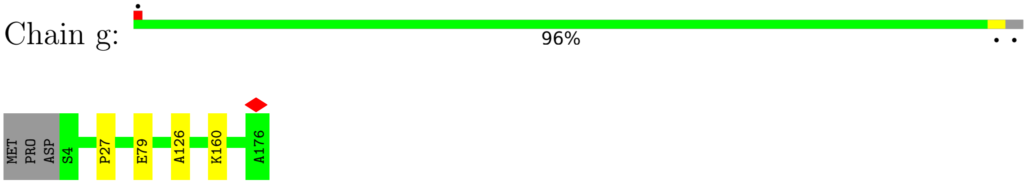
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C2





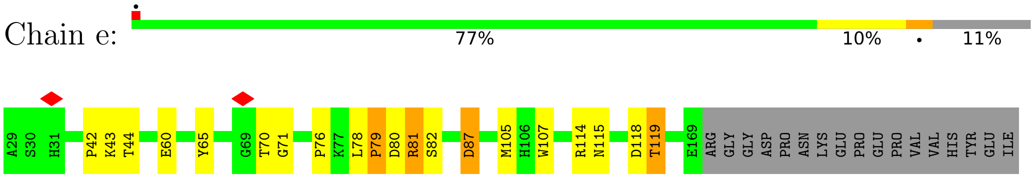
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain g:



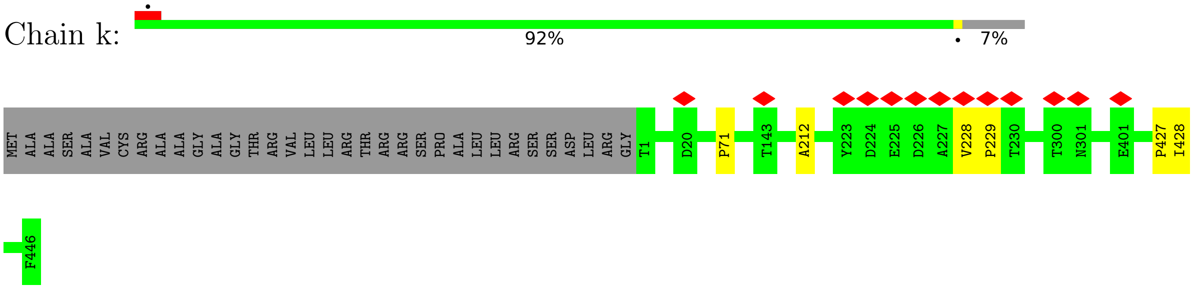
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain e:



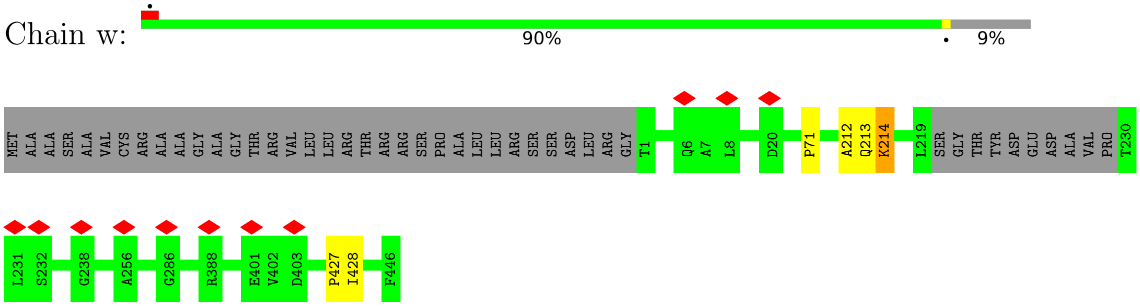
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain k:



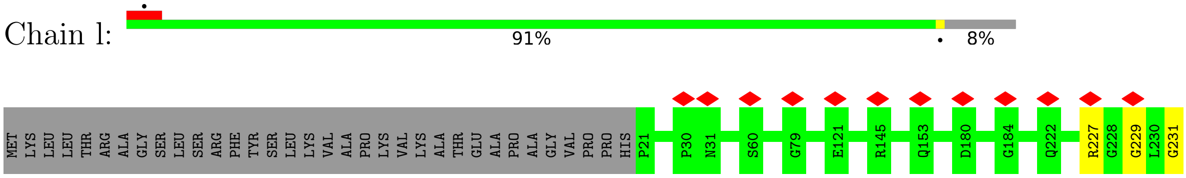
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

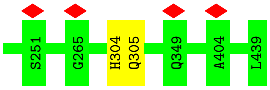
Chain w:



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

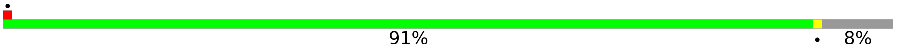
Chain l:

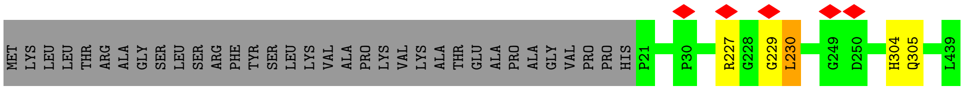




- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

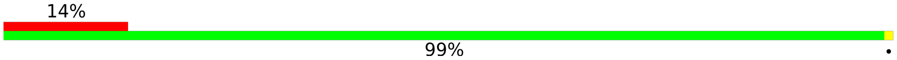
Chain x:

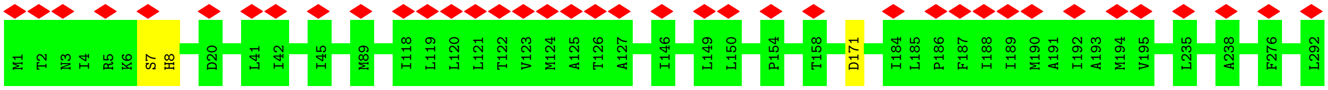


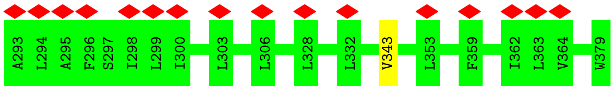


- Molecule 47: Cytochrome b

Chain m:

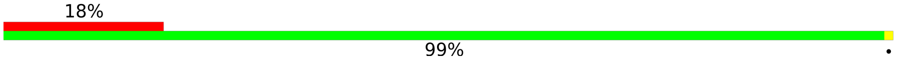


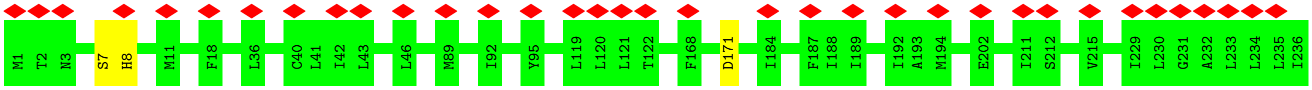


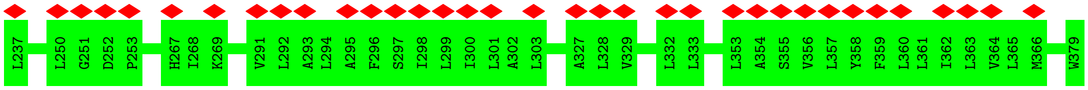


- Molecule 47: Cytochrome b

Chain y:

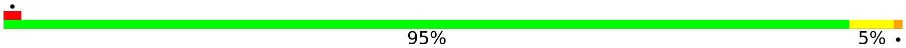


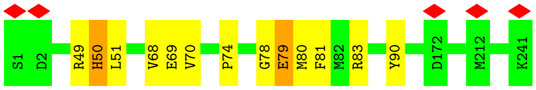




- Molecule 48: Cytochrome c1, heme protein, mitochondrial

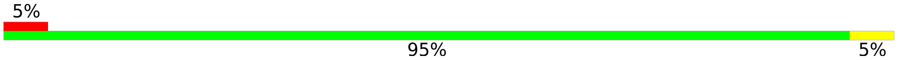
Chain o:

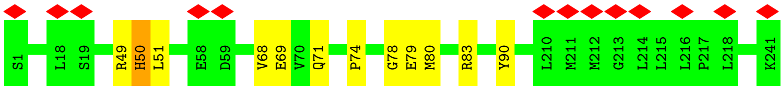




- Molecule 48: Cytochrome c1, heme protein, mitochondrial

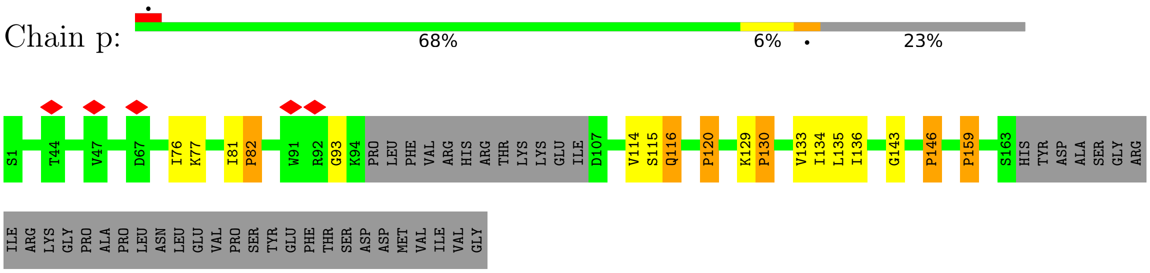
Chain z:





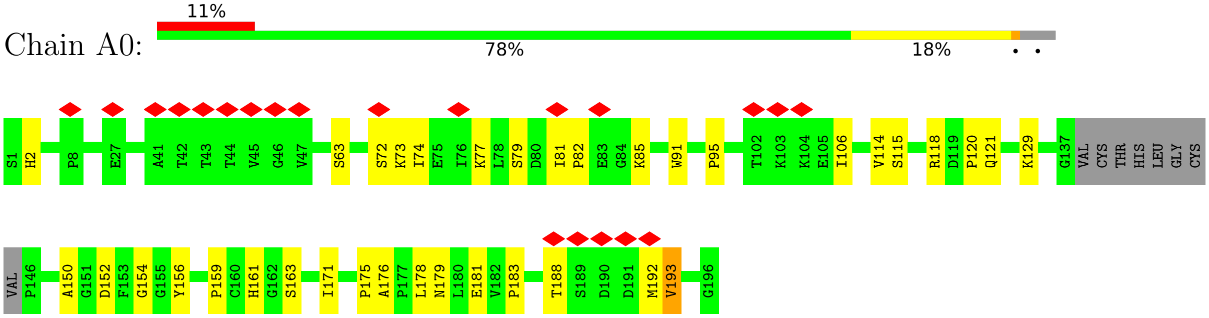
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain p:



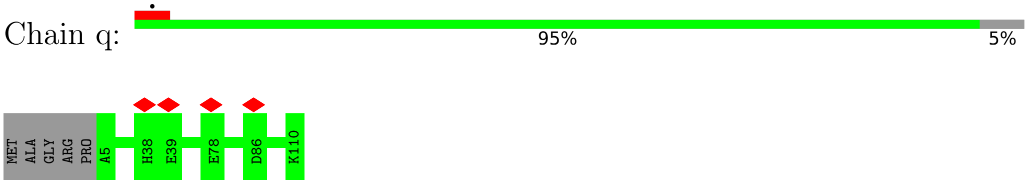
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain A0:



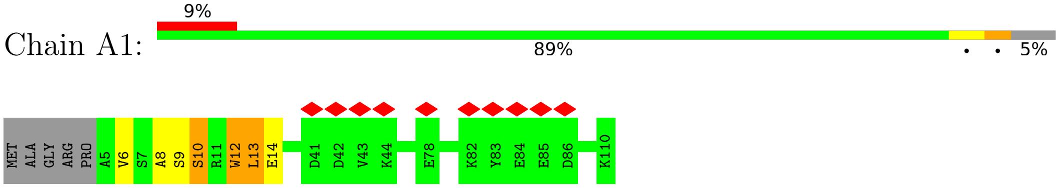
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain q:



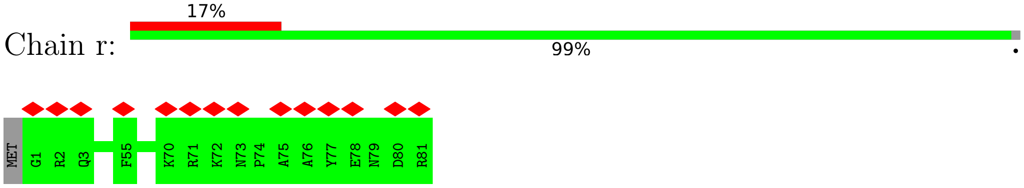
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain A1:



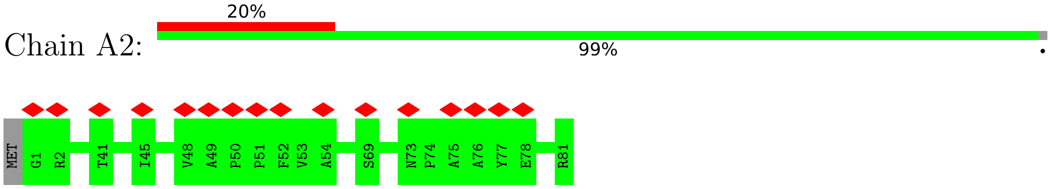
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain r:



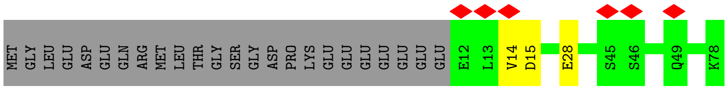
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain A2:



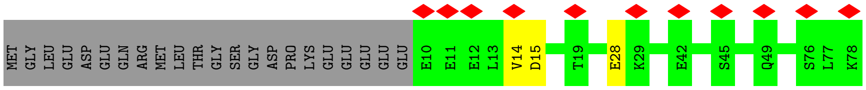
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain s:



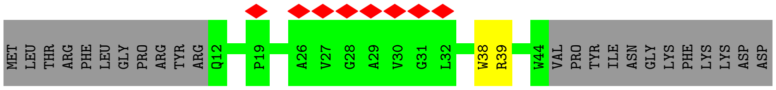
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain B3:



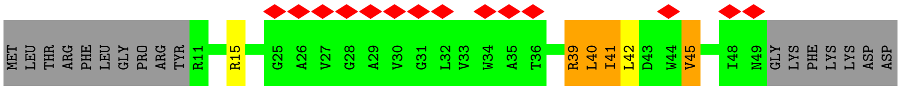
- Molecule 53: Cytochrome b-c1 complex subunit 10

Chain t:



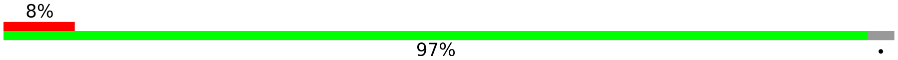
- Molecule 53: Cytochrome b-c1 complex subunit 10

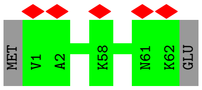
Chain A3:



- Molecule 54: Cytochrome b-c1 complex subunit 9

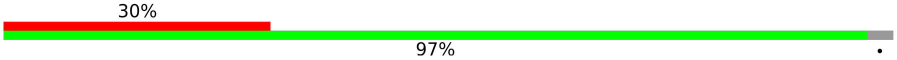
Chain u:

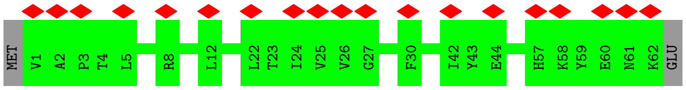




- Molecule 54: Cytochrome b-c1 complex subunit 9

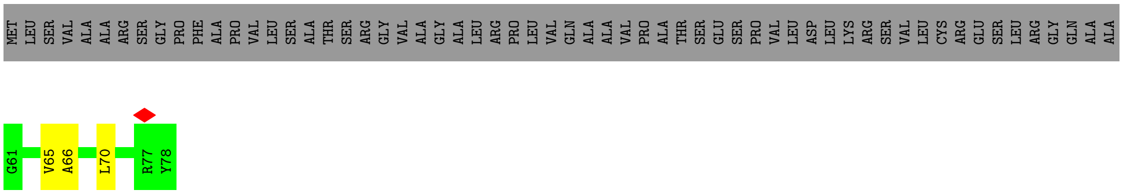
Chain B2:





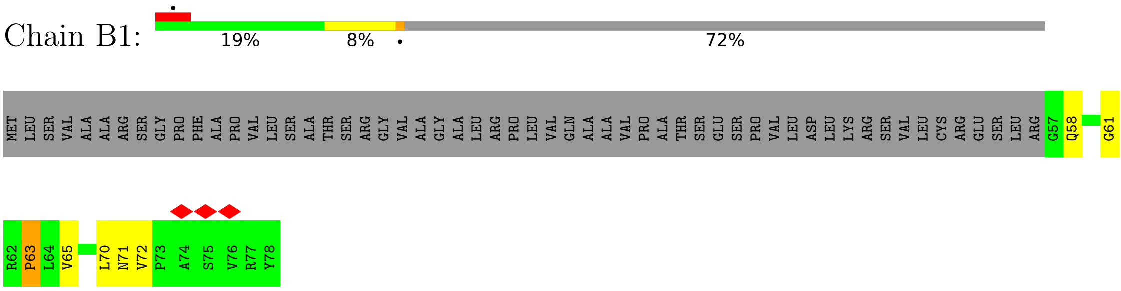
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain v:



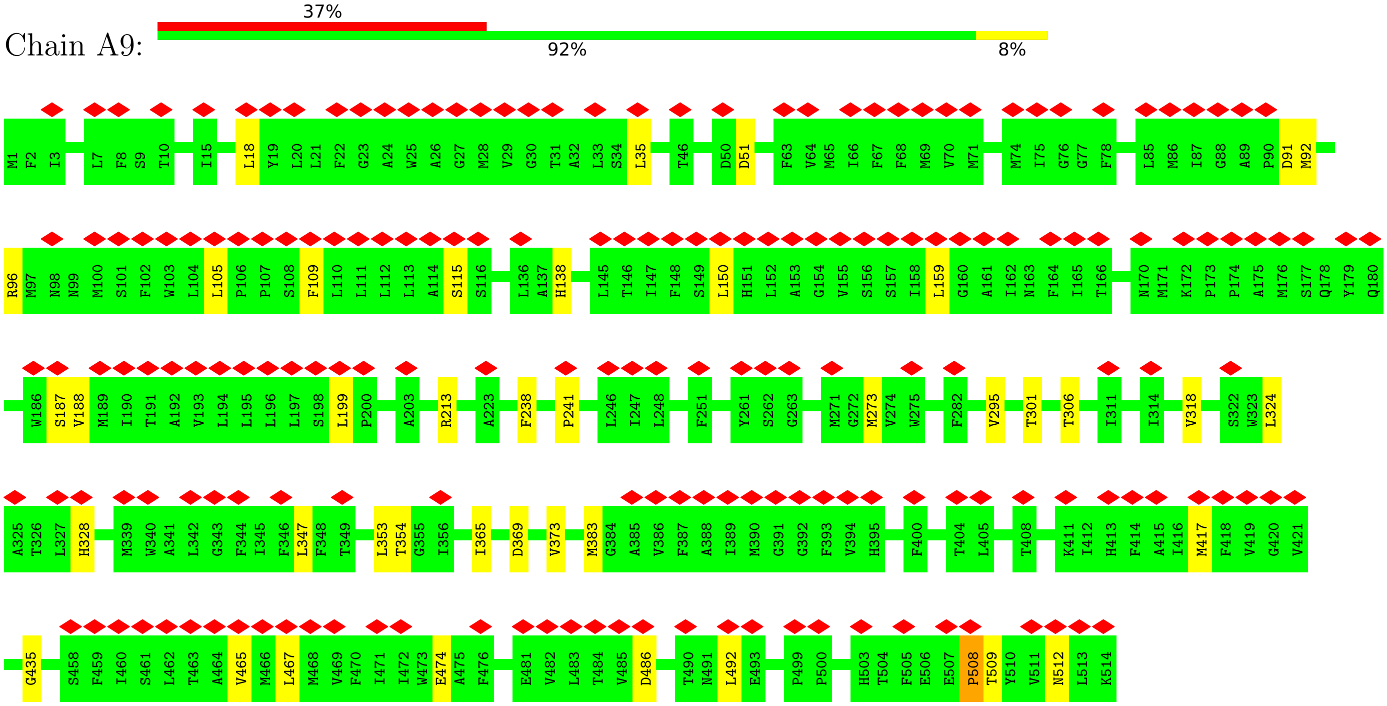
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain B1:



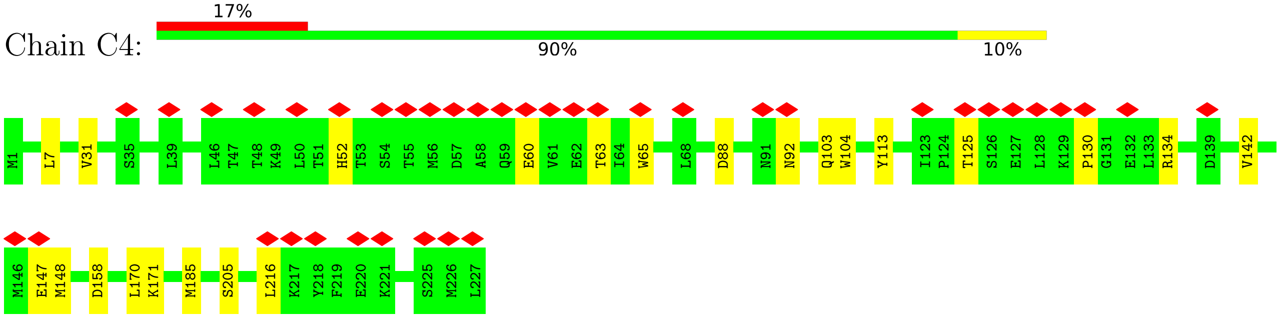
- Molecule 56: Cytochrome c oxidase subunit 1

Chain A9:



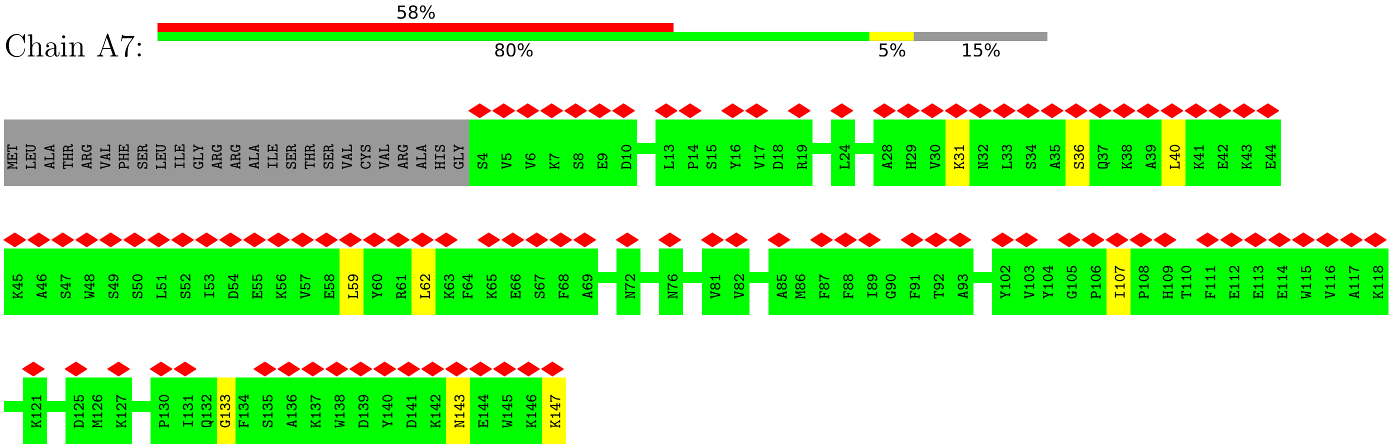
- Molecule 57: Cytochrome c oxidase subunit 2

Chain C4:



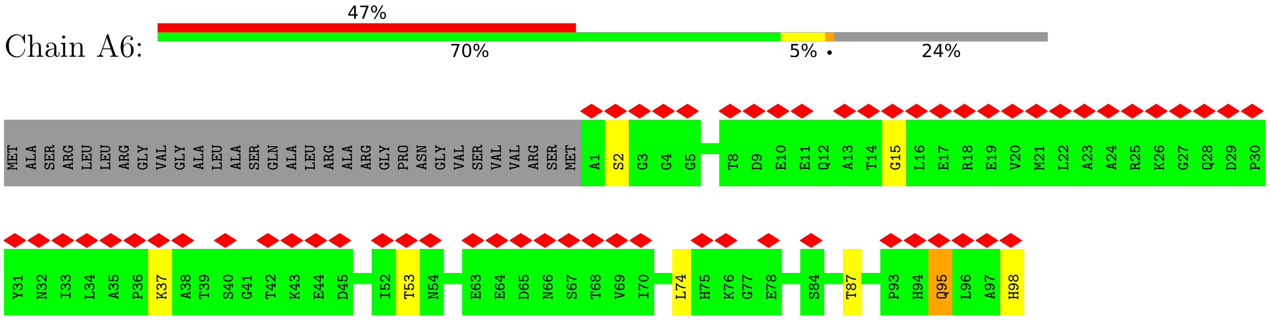
- Molecule 58: Cytochrome c oxidase subunit 3

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

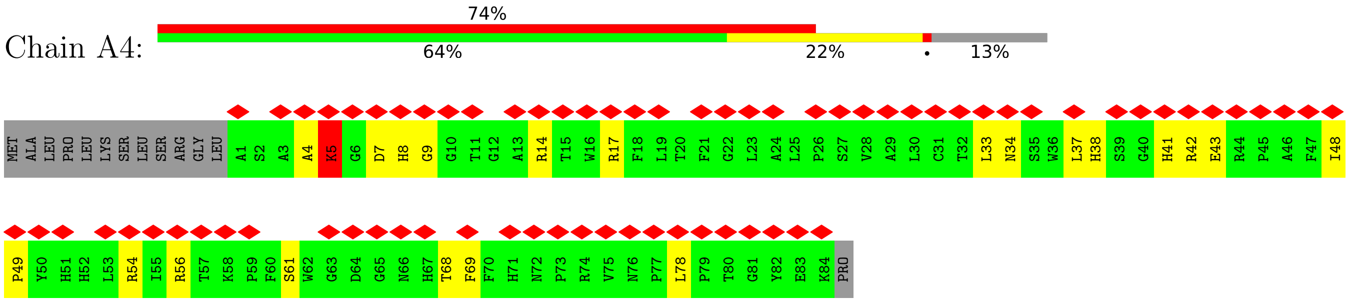


- Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

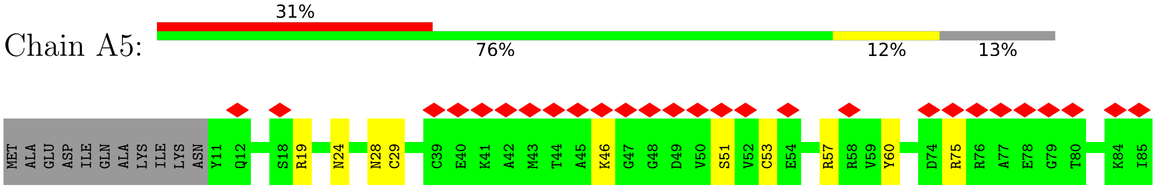
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial



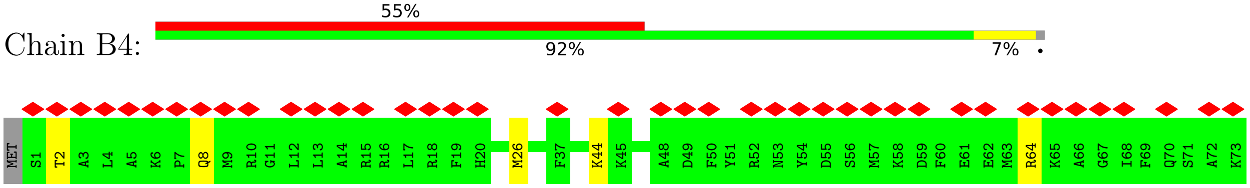
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial



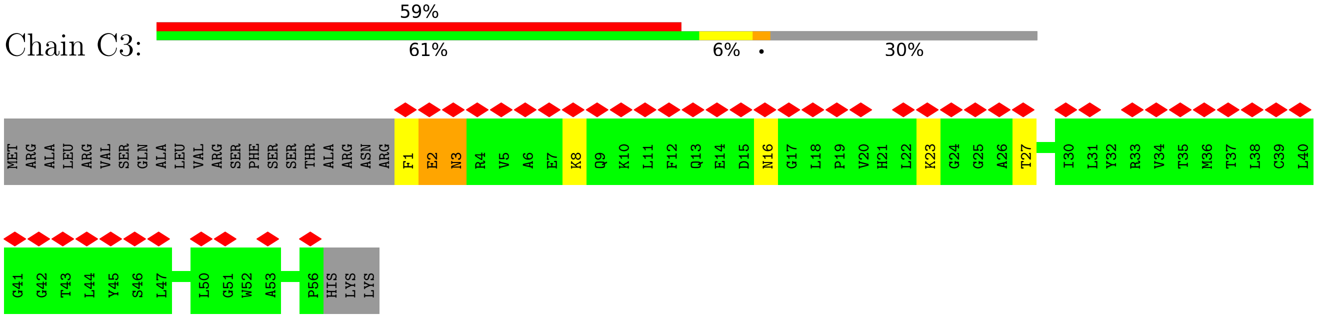
- Molecule 63: Cytochrome c oxidase subunit 6B1



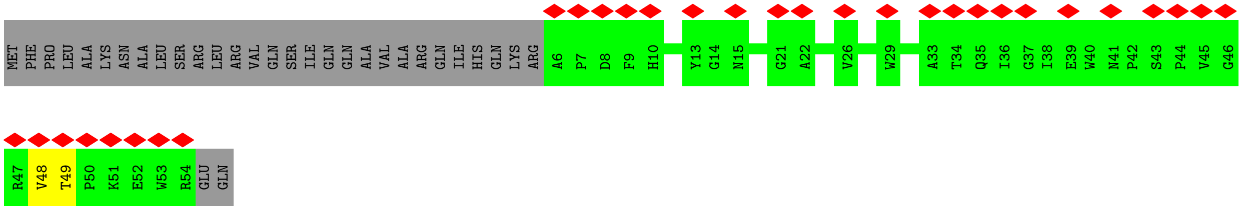
- Molecule 64: Cytochrome c oxidase subunit 6C



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

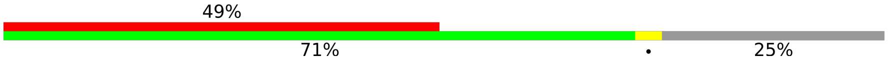


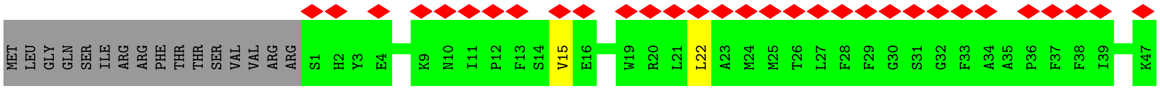
- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial

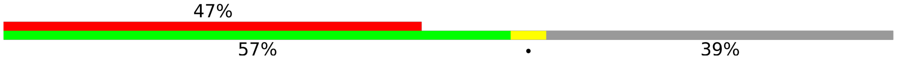
Chain C1:

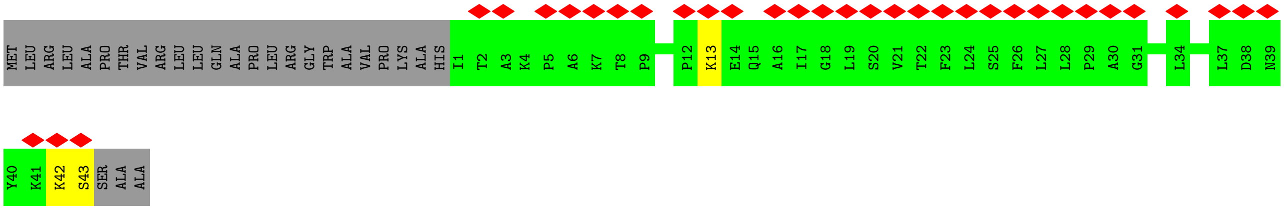




- Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial

Chain A8:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57806	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	0.509	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	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: HEM, 3PE, HEC, ZN, NAP, SF4, CU, FMN, FES, CDL, HEA, MG, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	9	0.50	0/1617	0.62	0/2206
2	4	0.61	1/3674 (0.0%)	0.80	4/5020 (0.1%)
3	2	0.72	1/2749 (0.0%)	0.85	0/3744
4	7	0.61	0/1271	0.74	0/1735
5	6	0.46	0/4893	0.65	1/6661 (0.0%)
6	5	0.63	0/721	0.84	2/977 (0.2%)
7	3	0.53	0/902	0.76	1/1233 (0.1%)
8	1	0.64	0/2575	0.83	3/3518 (0.1%)
9	8	0.50	0/3136	0.64	1/4258 (0.0%)
10	A	0.69	4/5304 (0.1%)	0.82	7/7193 (0.1%)
11	B	0.92	1/3512 (0.0%)	0.92	12/4763 (0.3%)
12	C	0.84	0/1777	0.78	1/2420 (0.0%)
13	D	0.95	2/1237 (0.2%)	0.87	2/1676 (0.1%)
14	E	0.96	4/1431 (0.3%)	0.98	8/1938 (0.4%)
15	F	0.33	0/191	0.82	0/262
16	G	0.78	0/1008	0.80	0/1363
17	H	0.55	0/800	0.73	0/1076
18	I	0.56	0/541	0.85	0/726
19	J	0.60	0/545	0.61	0/740
20	K	0.44	0/667	0.58	0/900
21	L	0.47	0/623	0.60	0/862
22	N	0.50	0/882	0.66	0/1203
23	O	0.54	0/948	0.67	0/1279
24	P	0.51	0/723	0.73	1/985 (0.1%)
25	Q	0.48	0/1381	0.66	0/1869
26	R	0.50	0/2465	0.69	0/3349
27	S	0.38	0/2348	0.71	1/3198 (0.0%)
28	T	0.42	0/938	0.65	0/1278
29	U	0.48	0/1053	0.72	1/1439 (0.1%)
30	V	0.53	0/1115	0.67	0/1508
31	M	0.46	0/651	0.69	1/876 (0.1%)
31	W	0.39	0/624	0.59	0/847

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	X	0.37	0/383	0.56	0/523
33	Y	0.40	0/428	0.59	0/592
34	Z	0.38	0/506	0.57	0/688
35	a	0.50	0/878	0.60	0/1195
36	b	0.52	0/1058	0.68	0/1434
37	c	0.36	0/632	0.74	2/871 (0.2%)
38	d	0.36	0/729	0.56	1/996 (0.1%)
39	f	0.38	0/1191	0.55	0/1639
40	h	0.50	0/679	0.65	0/926
41	i	0.38	0/286	0.52	0/392
42	j	0.55	0/912	0.67	1/1240 (0.1%)
43	g	0.48	0/1380	0.59	1/1872 (0.1%)
44	e	0.38	0/888	0.73	1/1234 (0.1%)
45	k	0.50	0/3527	0.60	0/4787
45	w	0.50	0/3455	0.59	0/4685
46	l	0.45	0/3192	0.55	0/4329
46	x	0.45	0/3198	0.56	2/4336 (0.0%)
47	m	0.60	0/3108	0.60	0/4252
47	y	0.60	0/3108	0.60	0/4252
48	o	0.52	0/1978	0.63	3/2684 (0.1%)
48	z	0.53	0/1965	0.62	1/2669 (0.0%)
49	A0	0.39	0/1124	0.62	0/1538
49	p	0.46	0/945	0.88	5/1288 (0.4%)
50	A1	0.53	0/935	0.53	0/1253
50	q	0.51	0/935	0.55	0/1253
51	A2	0.49	0/698	0.53	0/944
51	r	0.49	0/704	0.53	0/951
52	B3	0.36	0/571	0.59	1/765 (0.1%)
52	s	0.37	0/553	0.58	1/741 (0.1%)
53	A3	0.47	0/330	0.70	1/457 (0.2%)
53	t	0.36	0/272	0.50	0/377
54	B2	0.42	0/524	0.48	0/707
54	u	0.42	0/524	0.48	0/707
55	B1	0.50	0/149	0.95	0/203
55	v	0.44	0/114	0.94	1/156 (0.6%)
56	A9	0.60	0/4164	0.76	1/5688 (0.0%)
57	C4	0.57	0/1868	0.79	0/2544
58	C2	0.56	0/2211	0.68	0/3023
59	A7	0.57	0/1229	0.65	1/1658 (0.1%)
60	C0	0.50	0/898	0.66	0/1218
61	A6	0.56	0/765	0.81	0/1038
62	A4	0.54	0/698	0.73	1/950 (0.1%)
63	A5	0.55	0/648	0.73	0/877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
64	B4	0.60	0/611	0.64	0/810
65	C3	0.61	0/451	0.72	0/610
66	B0	0.57	0/398	0.66	0/546
67	C1	0.63	0/399	0.62	0/534
68	A8	0.51	0/345	0.65	0/470
All	All	0.57	13/108846 (0.0%)	0.70	70/148004 (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	9	0	6
2	4	0	9
3	2	0	10
4	7	0	6
5	6	0	5
6	5	0	4
7	3	0	2
8	1	0	3
9	8	0	8
10	A	0	16
11	B	0	4
13	D	0	6
14	E	0	5
17	H	0	2
18	I	0	1
20	K	0	1
21	L	0	1
22	N	0	1
23	O	0	1
24	P	0	3
25	Q	0	2
26	R	0	9
27	S	0	4
29	U	0	3
30	V	0	2
31	M	0	3
31	W	0	2
34	Z	0	2
35	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	b	0	4
38	d	0	1
39	f	0	3
40	h	0	3
42	j	0	2
43	g	0	1
44	e	0	7
45	k	0	3
45	w	0	4
46	l	0	5
46	x	0	3
47	m	0	4
47	y	0	3
48	o	0	7
48	z	0	7
49	A0	0	3
49	p	0	6
53	A3	0	1
55	B1	0	5
All	All	0	194

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	135	TYR	CE1-CZ	-7.40	1.28	1.38
14	E	123	CYS	CB-SG	-6.99	1.70	1.82
14	E	116	CYS	CB-SG	-6.28	1.71	1.82
10	A	92	CYS	CB-SG	-5.91	1.72	1.81
3	2	193	VAL	CB-CG2	-5.57	1.41	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	199	VAL	C-N-CD	-15.74	85.97	120.60
14	E	140	ARG	CG-CD-NE	8.45	129.55	111.80
10	A	139	LEU	CA-CB-CG	-8.02	96.85	115.30
14	E	118	LEU	CB-CG-CD2	-7.90	97.57	111.00
37	c	36	PRO	C-N-CD	-7.73	103.60	120.60

There are no chirality outliers.

5 of 194 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	9	109	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	75	LYS	Peptide
1	9	91	GLY	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	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	29
2	4	457/459 (100%)	393 (86%)	56 (12%)	8 (2%)	8	42
3	2	342/347 (99%)	283 (83%)	57 (17%)	2 (1%)	25	65
4	7	170/175 (97%)	138 (81%)	25 (15%)	7 (4%)	3	25
5	6	604/606 (100%)	517 (86%)	84 (14%)	3 (0%)	29	68
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	17	56
8	1	316/318 (99%)	255 (81%)	48 (15%)	13 (4%)	3	25
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	9	45
10	A	686/704 (97%)	559 (82%)	112 (16%)	15 (2%)	6	37
11	B	428/430 (100%)	343 (80%)	79 (18%)	6 (1%)	11	47
12	C	206/228 (90%)	173 (84%)	30 (15%)	3 (2%)	10	46
13	D	150/179 (84%)	121 (81%)	25 (17%)	4 (3%)	5	34
14	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	9	43
15	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	G	121/133 (91%)	101 (84%)	19 (16%)	1 (1%)	19	60
17	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	4	30
18	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	25
19	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	4	31
20	K	82/98 (84%)	65 (79%)	16 (20%)	1 (1%)	13	50
21	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
22	N	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
23	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	5	34
24	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
25	Q	166/171 (97%)	112 (68%)	51 (31%)	3 (2%)	8	42
26	R	315/345 (91%)	243 (77%)	65 (21%)	7 (2%)	6	37
27	S	317/320 (99%)	240 (76%)	67 (21%)	10 (3%)	4	30
28	T	136/140 (97%)	102 (75%)	15 (11%)	19 (14%)	0	4
29	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
30	V	136/143 (95%)	110 (81%)	22 (16%)	4 (3%)	4	32
31	M	78/88 (89%)	56 (72%)	19 (24%)	3 (4%)	3	27
31	W	84/88 (96%)	68 (81%)	15 (18%)	1 (1%)	13	50
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	25
33	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	8	42
34	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	5	33
35	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
36	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	22	62
37	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
38	d	105/117 (90%)	87 (83%)	15 (14%)	3 (3%)	4	32
39	f	165/178 (93%)	130 (79%)	33 (20%)	2 (1%)	13	50
40	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	3	27
41	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
42	j	111/120 (92%)	94 (85%)	17 (15%)	0	100	100
43	g	171/176 (97%)	141 (82%)	29 (17%)	1 (1%)	25	65
44	e	139/158 (88%)	81 (58%)	45 (32%)	13 (9%)	0	12
45	k	444/480 (92%)	407 (92%)	34 (8%)	3 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	w	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	22	62
46	l	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	47	81
46	x	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	47	81
47	m	377/379 (100%)	348 (92%)	29 (8%)	0	100	100
47	y	377/379 (100%)	349 (93%)	28 (7%)	0	100	100
48	o	239/241 (99%)	213 (89%)	21 (9%)	5 (2%)	7	38
48	z	239/241 (99%)	213 (89%)	20 (8%)	6 (2%)	5	35
49	A0	184/196 (94%)	105 (57%)	48 (26%)	31 (17%)	0	3
49	p	147/196 (75%)	101 (69%)	33 (22%)	13 (9%)	1	12
50	A1	104/111 (94%)	91 (88%)	7 (7%)	6 (6%)	1	20
50	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
51	A2	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
51	r	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
52	B3	67/91 (74%)	59 (88%)	6 (9%)	2 (3%)	4	31
52	s	65/91 (71%)	58 (89%)	5 (8%)	2 (3%)	4	31
53	A3	37/56 (66%)	23 (62%)	10 (27%)	4 (11%)	0	8
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	4	30
54	B2	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
54	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
55	B1	20/78 (26%)	10 (50%)	7 (35%)	3 (15%)	0	4
55	v	16/78 (20%)	8 (50%)	6 (38%)	2 (12%)	0	5
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
57	C4	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
58	C2	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	C0	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	A6	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	3	25
62	A4	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	19
63	A5	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	11	47
64	B4	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	C3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	C1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13638/14963 (91%)	11529 (84%)	1839 (14%)	270 (2%)	11	40

5 of 270 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	84	TRP
4	7	141	MET
4	7	171	ILE
8	1	170	GLU
8	1	174	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	169/183 (92%)	167 (99%)	2 (1%)	71	84
2	4	389/413 (94%)	389 (100%)	0	100	100
3	2	304/316 (96%)	302 (99%)	2 (1%)	84	90
4	7	116/142 (82%)	116 (100%)	0	100	100
5	6	524/534 (98%)	521 (99%)	3 (1%)	86	92
6	5	80/86 (93%)	80 (100%)	0	100	100
7	3	95/101 (94%)	95 (100%)	0	100	100
8	1	274/275 (100%)	255 (93%)	19 (7%)	15	42
9	8	270/353 (76%)	270 (100%)	0	100	100
10	A	560/588 (95%)	557 (100%)	3 (0%)	88	93
11	B	363/371 (98%)	356 (98%)	7 (2%)	57	75
12	C	188/204 (92%)	186 (99%)	2 (1%)	73	85
13	D	127/150 (85%)	124 (98%)	3 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	E	148/151 (98%)	148 (100%)	0	100	100
15	F	14/69 (20%)	14 (100%)	0	100	100
16	G	106/119 (89%)	105 (99%)	1 (1%)	78	87
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	53/79 (67%)	50 (94%)	3 (6%)	20	47
19	J	50/59 (85%)	50 (100%)	0	100	100
20	K	67/81 (83%)	67 (100%)	0	100	100
21	L	63/71 (89%)	63 (100%)	0	100	100
22	N	88/101 (87%)	88 (100%)	0	100	100
23	O	95/113 (84%)	95 (100%)	0	100	100
24	P	73/96 (76%)	73 (100%)	0	100	100
25	Q	142/154 (92%)	141 (99%)	1 (1%)	84	90
26	R	232/298 (78%)	232 (100%)	0	100	100
27	S	205/283 (72%)	204 (100%)	1 (0%)	88	93
28	T	73/101 (72%)	48 (66%)	25 (34%)	0	1
29	U	95/131 (72%)	95 (100%)	0	100	100
30	V	106/120 (88%)	106 (100%)	0	100	100
31	M	73/81 (90%)	73 (100%)	0	100	100
31	W	57/81 (70%)	55 (96%)	2 (4%)	36	60
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/76 (37%)	28 (100%)	0	100	100
35	a	70/114 (61%)	70 (100%)	0	100	100
36	b	85/124 (68%)	85 (100%)	0	100	100
37	c	45/122 (37%)	45 (100%)	0	100	100
38	d	44/107 (41%)	44 (100%)	0	100	100
39	f	80/160 (50%)	80 (100%)	0	100	100
40	h	63/112 (56%)	63 (100%)	0	100	100
41	i	23/45 (51%)	23 (100%)	0	100	100
42	j	86/106 (81%)	85 (99%)	1 (1%)	71	84
43	g	130/157 (83%)	129 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	e	44/141 (31%)	41 (93%)	3 (7%)	16	42
45	k	369/394 (94%)	369 (100%)	0	100	100
45	w	362/394 (92%)	362 (100%)	0	100	100
46	l	327/355 (92%)	327 (100%)	0	100	100
46	x	328/355 (92%)	328 (100%)	0	100	100
47	m	327/327 (100%)	327 (100%)	0	100	100
47	y	327/327 (100%)	327 (100%)	0	100	100
48	o	206/206 (100%)	206 (100%)	0	100	100
48	z	202/206 (98%)	202 (100%)	0	100	100
49	A0	64/168 (38%)	61 (95%)	3 (5%)	26	52
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	92 (96%)	4 (4%)	30	55
50	q	96/99 (97%)	96 (100%)	0	100	100
51	A2	70/72 (97%)	70 (100%)	0	100	100
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B3	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	31/46 (67%)	27 (87%)	4 (13%)	4	20
53	t	24/46 (52%)	23 (96%)	1 (4%)	30	55
54	B2	52/54 (96%)	52 (100%)	0	100	100
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B1	15/60 (25%)	15 (100%)	0	100	100
55	v	11/60 (18%)	11 (100%)	0	100	100
56	A9	427/427 (100%)	389 (91%)	38 (9%)	9	33
57	C4	211/211 (100%)	191 (90%)	20 (10%)	8	29
58	C2	226/226 (100%)	199 (88%)	27 (12%)	5	22
59	A7	128/148 (86%)	120 (94%)	8 (6%)	18	44
60	C0	95/123 (77%)	89 (94%)	6 (6%)	18	44
61	A6	81/103 (79%)	76 (94%)	5 (6%)	18	45
62	A4	68/79 (86%)	50 (74%)	18 (26%)	0	4
63	A5	67/76 (88%)	58 (87%)	9 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	B4	58/59 (98%)	53 (91%)	5 (9%)	10	35
65	C3	47/68 (69%)	40 (85%)	7 (15%)	3	16
66	B0	39/66 (59%)	37 (95%)	2 (5%)	24	50
67	C1	40/55 (73%)	38 (95%)	2 (5%)	24	51
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	37
All	All	10787/12809 (84%)	10546 (98%)	241 (2%)	54	71

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	A9	354	THR
63	A5	75	ARG
57	C4	148	MET
63	A5	57	ARG
67	C1	15	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
56	A9	43	GLN
66	B0	10	HIS
56	A9	360	ASN
58	C2	222	GLN
21	L	71	GLN

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 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
78	HEC	z	301	48	32,50,50	2.50	5 (15%)	24,82,82	1.62	6 (25%)
71	CDL	6	701	-	63,63,99	1.08	7 (11%)	69,75,111	1.26	4 (5%)
74	SF4	A	801	10	0,12,12	-	-	-		
70	3PE	B	501	-	50,50,50	0.87	2 (4%)	53,55,55	1.34	4 (7%)
78	HEC	o	301	48	32,50,50	2.51	5 (15%)	24,82,82	1.61	6 (25%)
77	HEM	m	401	47	41,50,50	1.73	10 (24%)	45,82,82	1.45	5 (11%)
79	HEA	A9	602	56	57,67,67	1.48	6 (10%)	61,103,103	1.45	11 (18%)
69	FES	m	403	-	0,4,4	-	-	-		
72	PC1	L	200	-	46,46,53	0.98	3 (6%)	52,54,61	1.08	2 (3%)
73	FMN	8	501	-	33,33,33	1.19	2 (6%)	48,50,50	1.62	12 (25%)
72	PC1	S	401	27	46,46,53	1.03	4 (8%)	52,54,61	1.07	2 (3%)
72	PC1	4	504	-	45,45,53	1.05	3 (6%)	51,53,61	1.13	2 (3%)
76	NAP	R	601	-	45,52,52	4.72	18 (40%)	56,80,80	1.90	7 (12%)
77	HEM	y	401	47	41,50,50	1.73	11 (26%)	45,82,82	1.45	5 (11%)
79	HEA	A9	601	56	57,67,67	1.24	6 (10%)	61,103,103	1.47	12 (19%)
72	PC1	j	201	-	38,38,53	1.15	6 (15%)	44,46,61	1.06	2 (4%)
70	3PE	4	503	-	40,40,50	0.90	3 (7%)	43,45,55	1.38	2 (4%)
74	SF4	D	301	13	0,12,12	-	-	-		
74	SF4	A	802	-	0,12,12	-	-	-		
77	HEM	m	402	47	41,50,50	1.75	12 (29%)	45,82,82	1.29	4 (8%)
77	HEM	y	402	47	41,50,50	1.74	12 (29%)	45,82,82	1.28	4 (8%)
71	CDL	J	101	-	57,57,99	1.16	7 (12%)	63,69,111	1.19	5 (7%)
69	FES	9	301	1	0,4,4	-	-	-		
72	PC1	2	402	-	45,45,53	1.02	2 (4%)	51,53,61	0.99	2 (3%)
74	SF4	E	302	14	0,12,12	-	-	-		
70	3PE	2	401	-	45,45,50	0.89	3 (6%)	48,50,55	1.08	2 (4%)
74	SF4	8	502	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
70	3PE	4	501	-	40,40,50	1.03	2 (5%)	43,45,55	1.10	3 (6%)
69	FES	A	803	10	0,4,4	-	-	-		
71	CDL	4	502	-	81,81,99	0.98	6 (7%)	87,93,111	1.15	4 (4%)
74	SF4	E	301	14	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
78	HEC	z	301	48	-	5/10/54/54	-
71	CDL	6	701	-	-	34/74/74/110	-
74	SF4	A	801	10	-	-	0/6/5/5
70	3PE	B	501	-	-	28/54/54/54	-
78	HEC	o	301	48	-	5/10/54/54	-
77	HEM	m	401	47	-	4/12/54/54	-
79	HEA	A9	602	56	3/3/7/16	5/32/76/76	-
72	PC1	L	200	-	-	23/50/50/57	-
69	FES	m	403	-	-	-	0/1/1/1
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
72	PC1	S	401	27	-	30/50/50/57	-
72	PC1	4	504	-	-	23/49/49/57	-
76	NAP	R	601	-	-	14/31/67/67	0/5/5/5
77	HEM	y	401	47	-	4/12/54/54	-
79	HEA	A9	601	56	3/3/7/16	7/32/76/76	-
72	PC1	j	201	-	-	21/42/42/57	-
70	3PE	4	503	-	-	25/44/44/54	-
74	SF4	D	301	13	-	-	0/6/5/5
74	SF4	A	802	-	-	-	0/6/5/5
77	HEM	m	402	47	-	2/12/54/54	-
77	HEM	y	402	47	-	2/12/54/54	-
71	CDL	J	101	-	-	24/68/68/110	-
69	FES	9	301	1	-	-	0/1/1/1
72	PC1	2	402	-	-	30/49/49/57	-
74	SF4	E	302	14	-	-	0/6/5/5
70	3PE	2	401	-	-	20/49/49/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	SF4	8	502	-	-	-	0/6/5/5
70	3PE	4	501	-	-	29/44/44/54	-
69	FES	A	803	10	-	-	0/1/1/1
71	CDL	4	502	-	-	41/92/92/110	-
74	SF4	E	301	14	-	-	0/6/5/5

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	C2D-C1D	-15.67	1.30	1.53
76	R	601	NAP	O4D-C1D	15.38	1.62	1.41
76	R	601	NAP	O4B-C1B	15.02	1.62	1.41
78	z	301	HEC	C3C-C2C	-8.60	1.31	1.40
78	o	301	HEC	C3C-C2C	-8.54	1.31	1.40

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	R	601	NAP	C5A-C6A-N6A	7.64	131.96	120.35
76	R	601	NAP	N3A-C2A-N1A	-6.43	118.62	128.68
76	R	601	NAP	N6A-C6A-N1A	-5.97	106.17	118.57
70	B	501	3PE	O21-C21-C22	5.41	123.16	111.50
70	4	503	3PE	O21-C21-C22	5.12	122.53	111.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	A9	601	HEA	NB
79	A9	601	HEA	NA
79	A9	601	HEA	ND
79	A9	602	HEA	NB
79	A9	602	HEA	NA

5 of 385 torsion outliers are listed below:

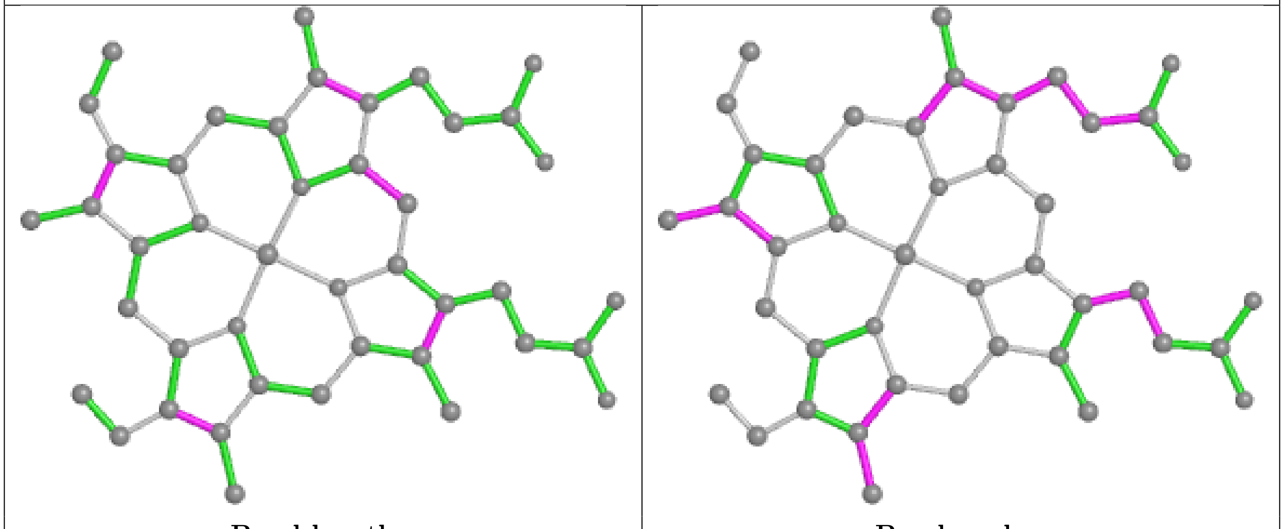
Mol	Chain	Res	Type	Atoms
70	4	501	3PE	C11-O13-P-O11
70	4	501	3PE	C11-O13-P-O12
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	O13-C11-C12-N
70	4	501	3PE	C22-C21-O21-C2

There are no ring outliers.

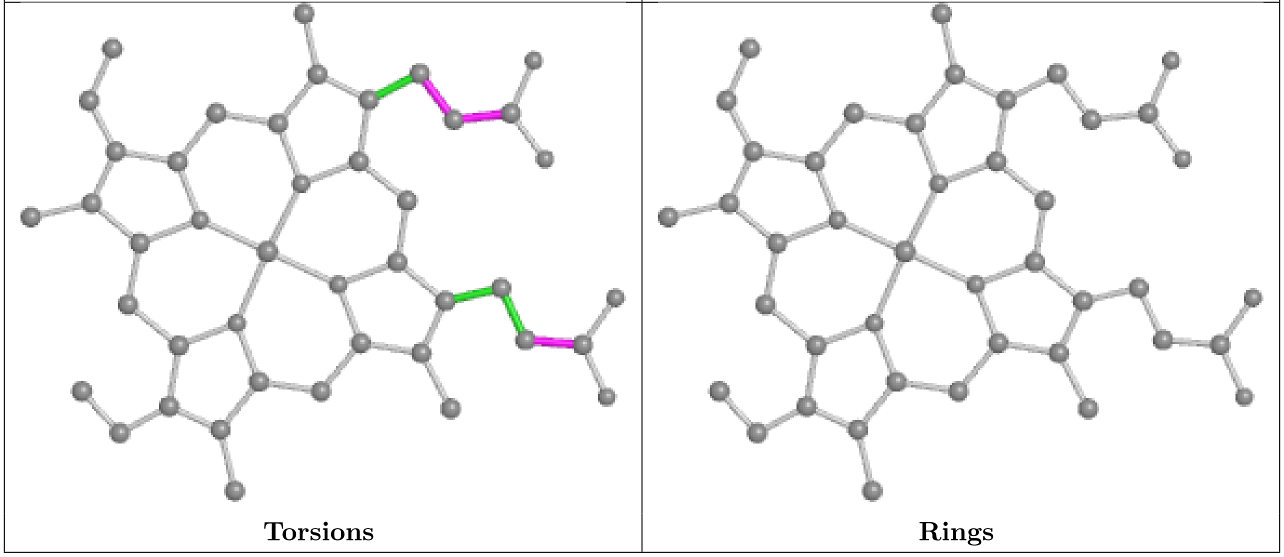
No monomer is involved in short contacts.

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 HEC z 301

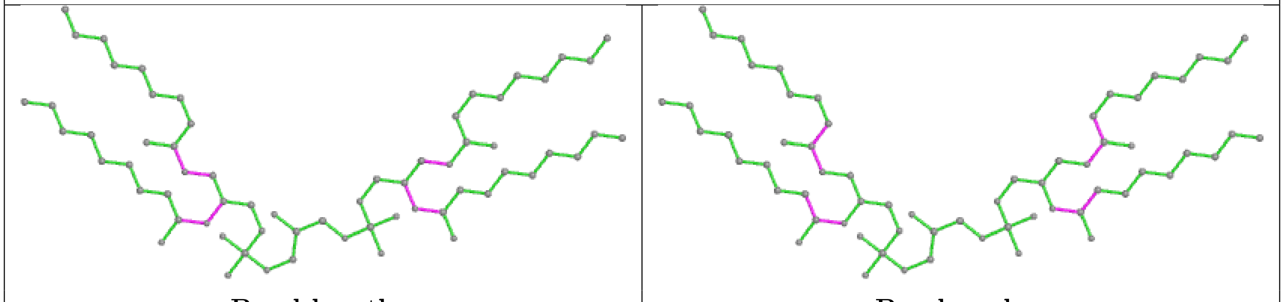


Bond lengths **Bond angles**

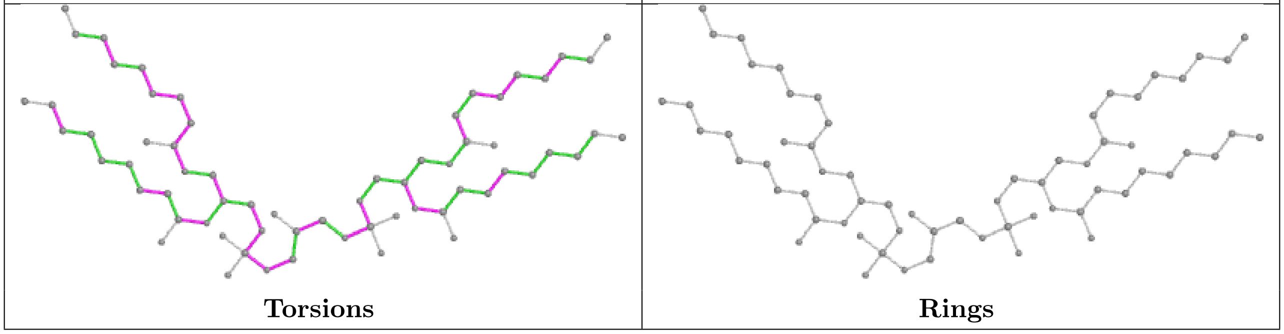


Torsions **Rings**

Ligand CDL 6 701

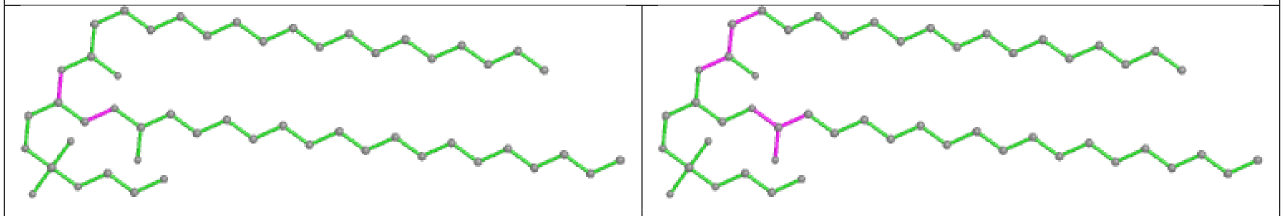


Bond lengths Bond angles

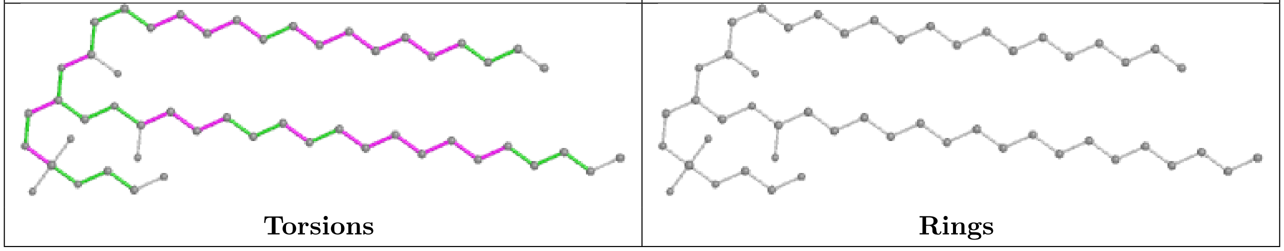


Torsions Rings

Ligand 3PE B 501

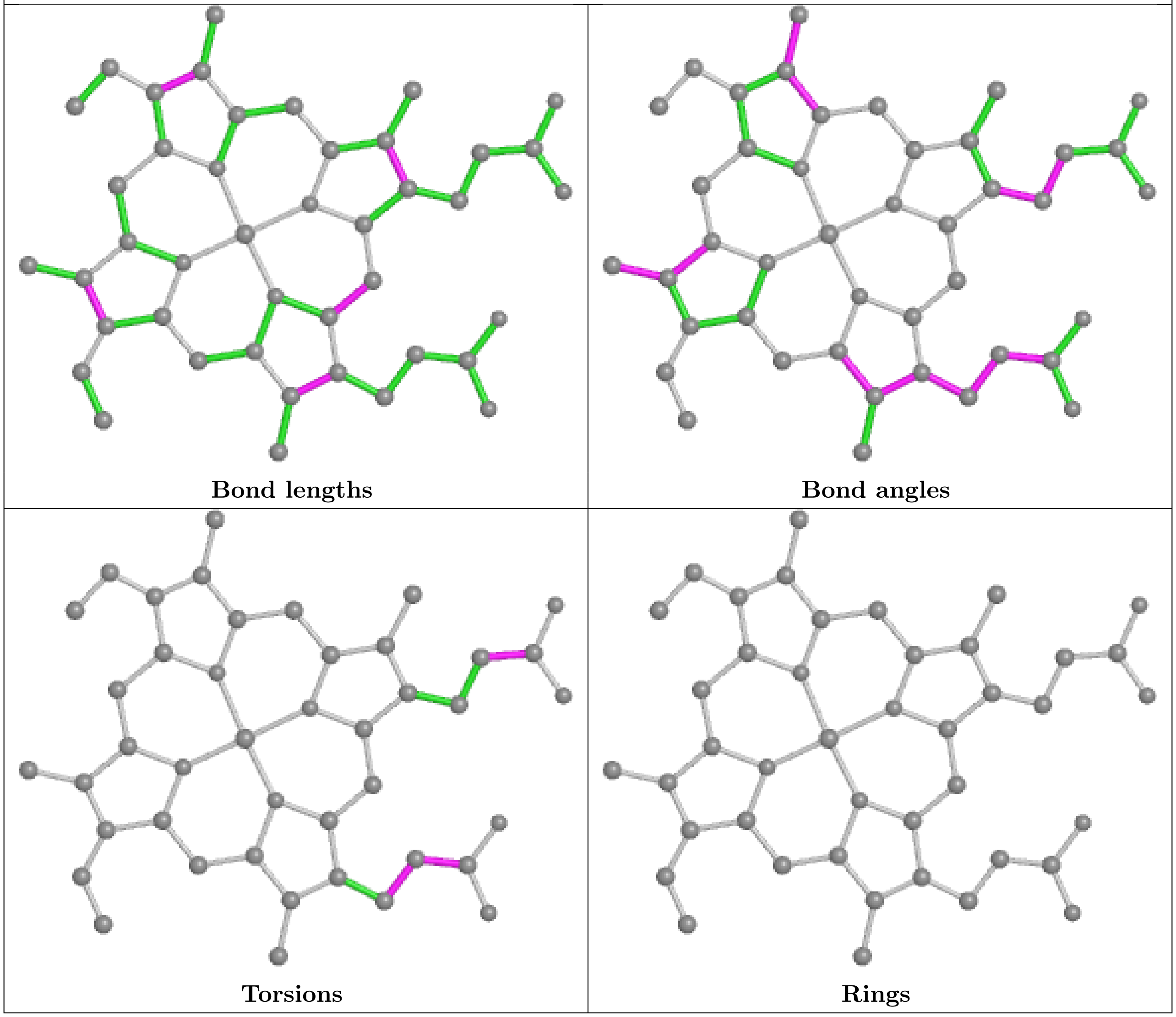


Bond lengths Bond angles

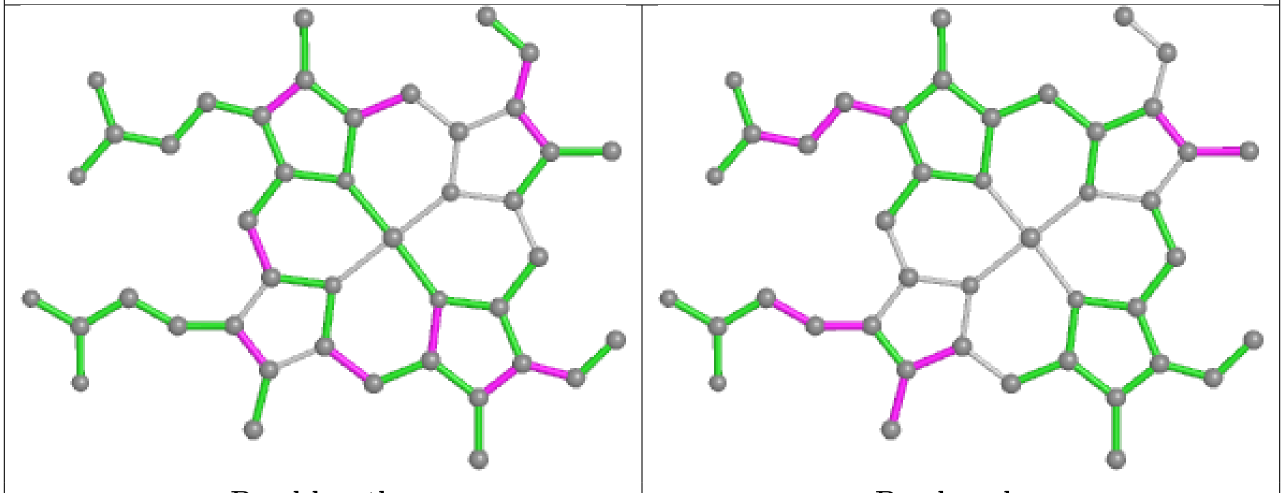


Torsions Rings

Ligand HEC o 301

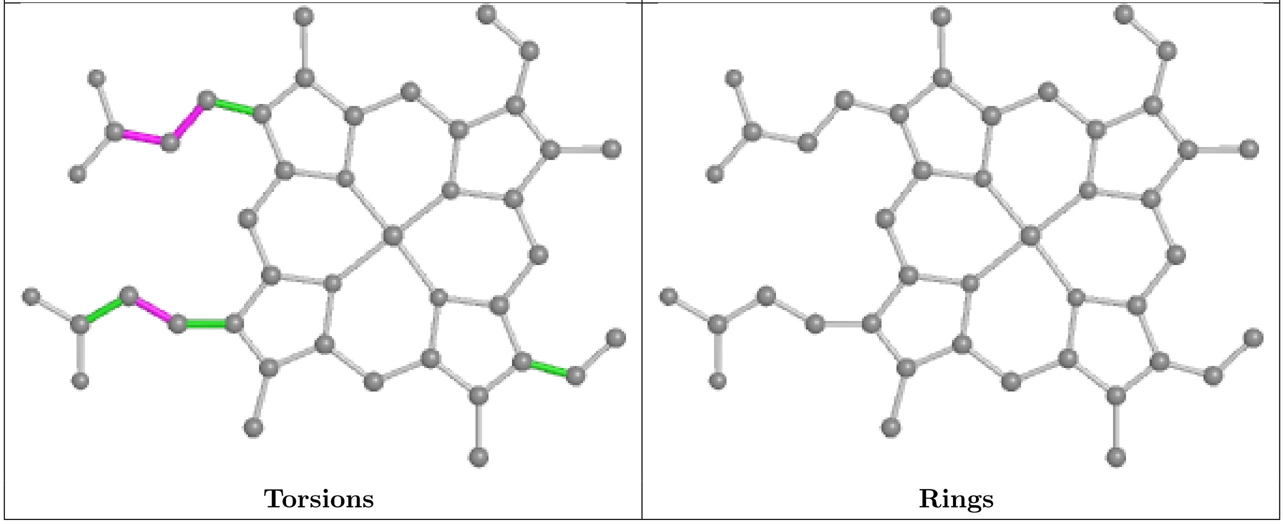


Ligand HEM m 401



Bond lengths

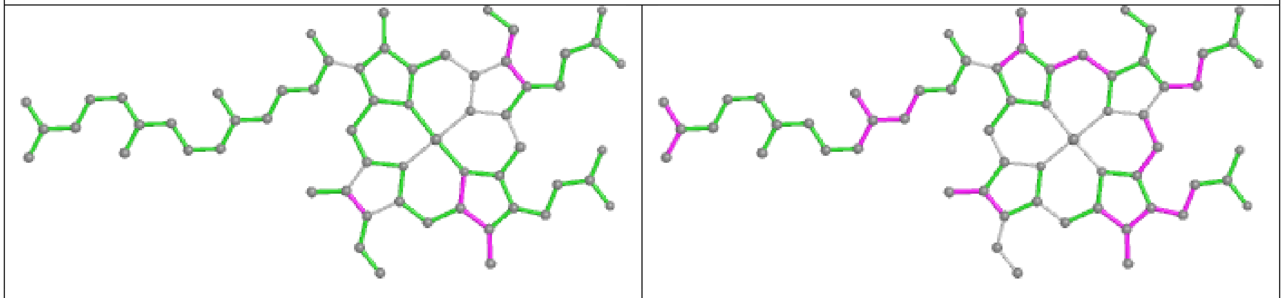
Bond angles



Torsions

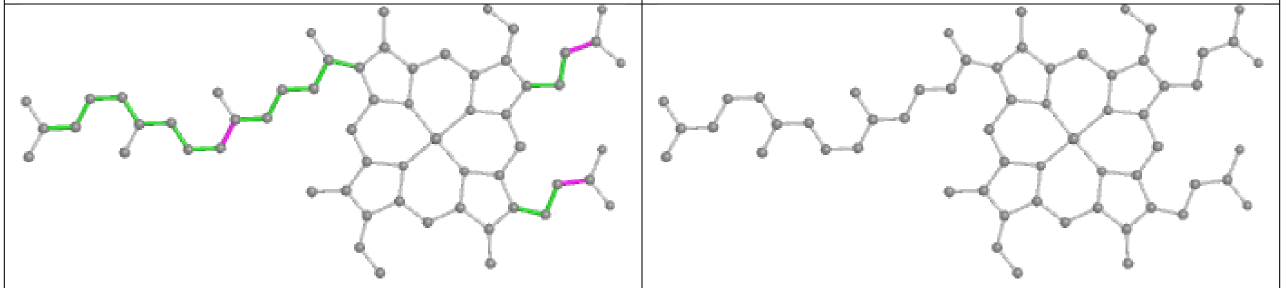
Rings

Ligand HEA A9 602



Bond lengths

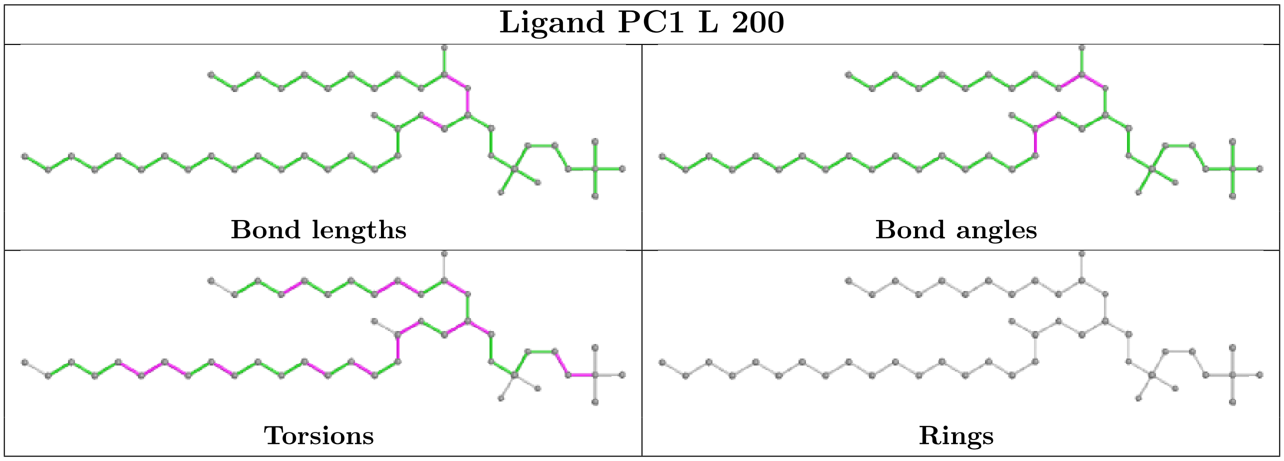
Bond angles



Torsions

Rings

Ligand PC1 L 200



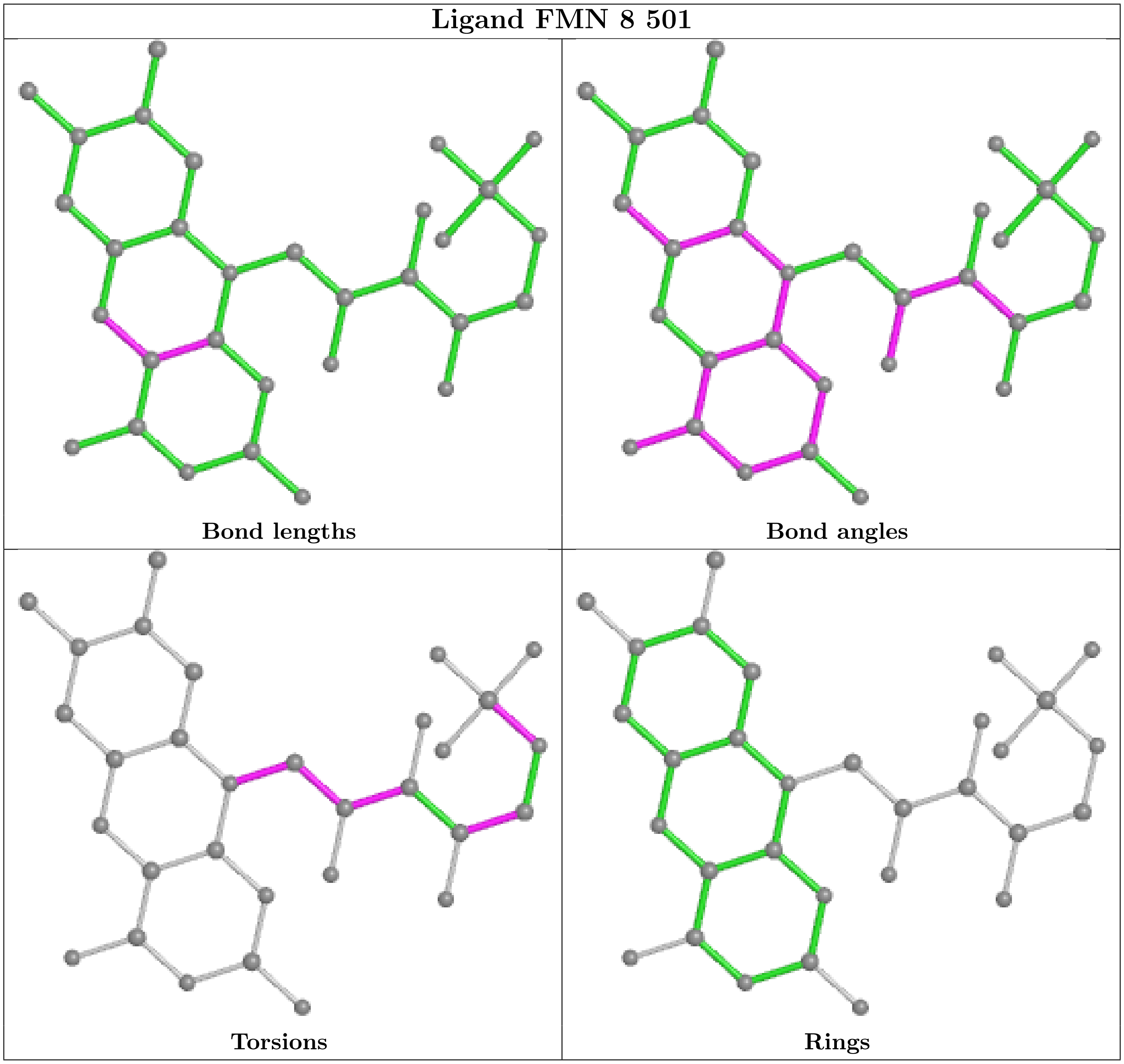
Bond lengths

Bond angles

Torsions

Rings

Ligand FMN 8 501



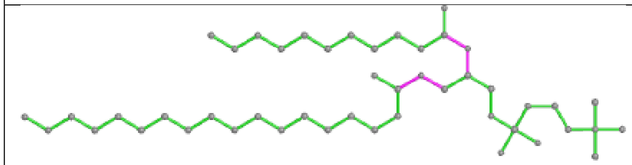
Bond lengths

Bond angles

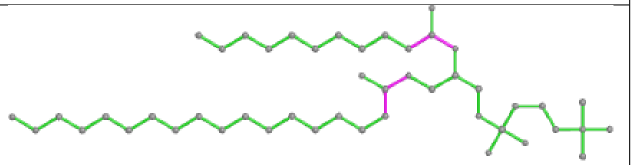
Torsions

Rings

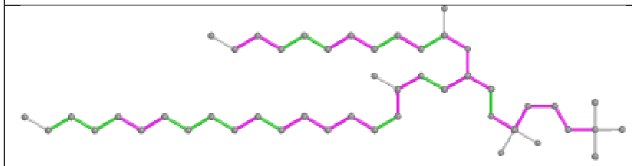
Ligand PC1 S 401



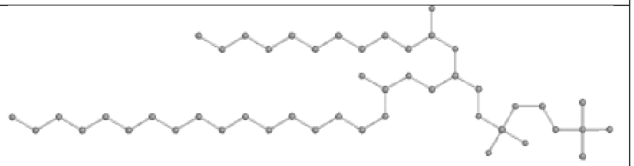
Bond lengths



Bond angles

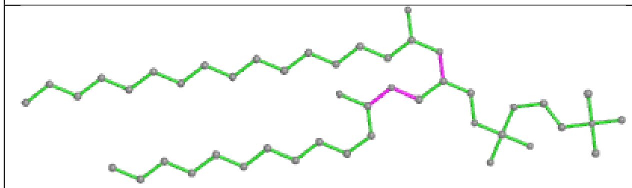


Torsions

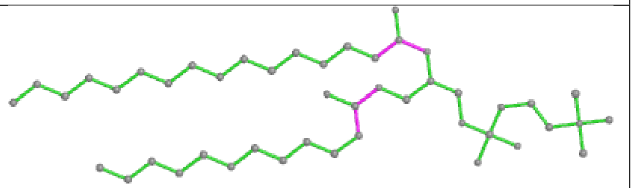


Rings

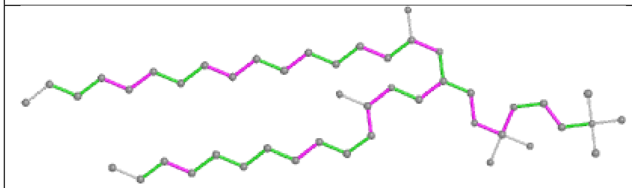
Ligand PC1 4 504



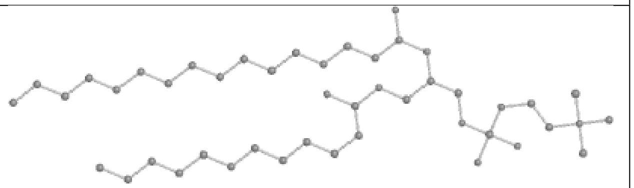
Bond lengths



Bond angles

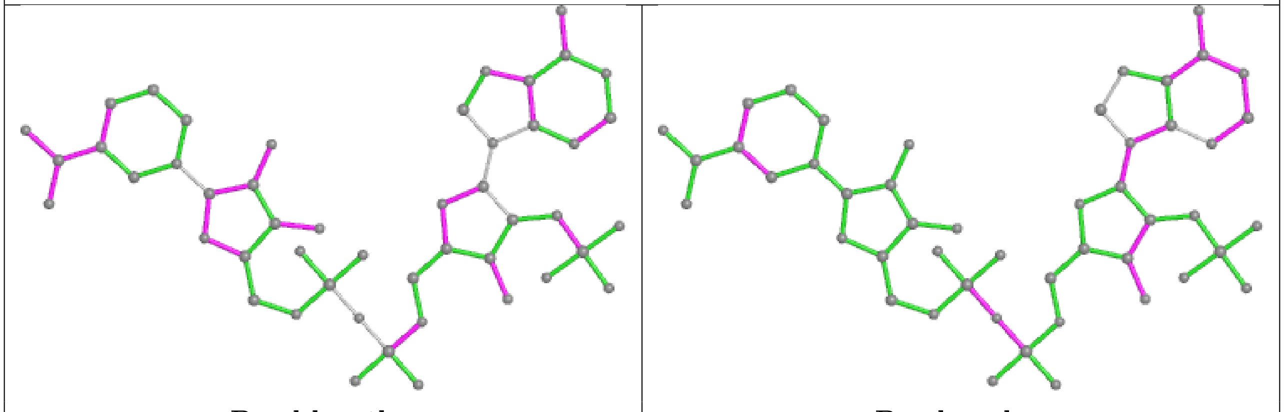


Torsions



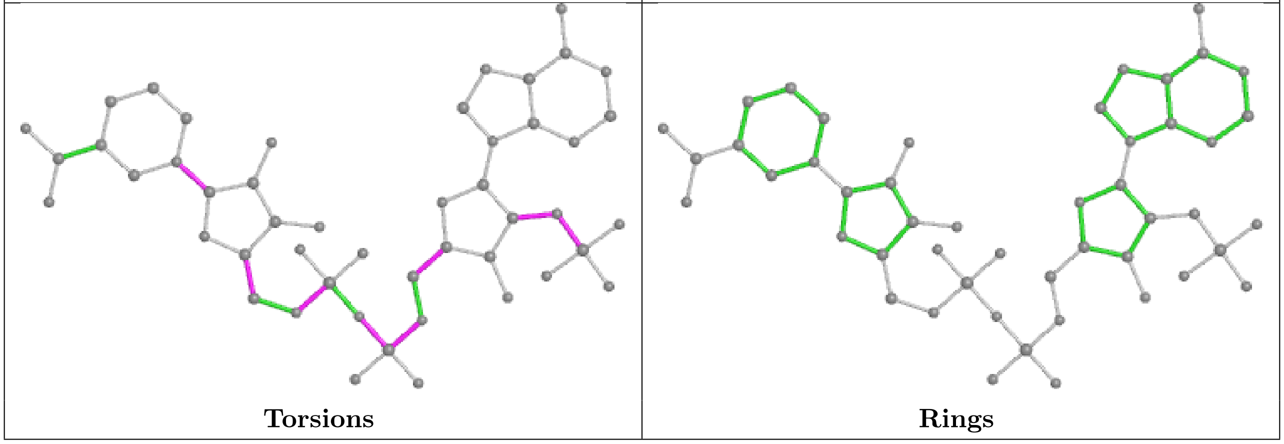
Rings

Ligand NAP R 601



Bond lengths

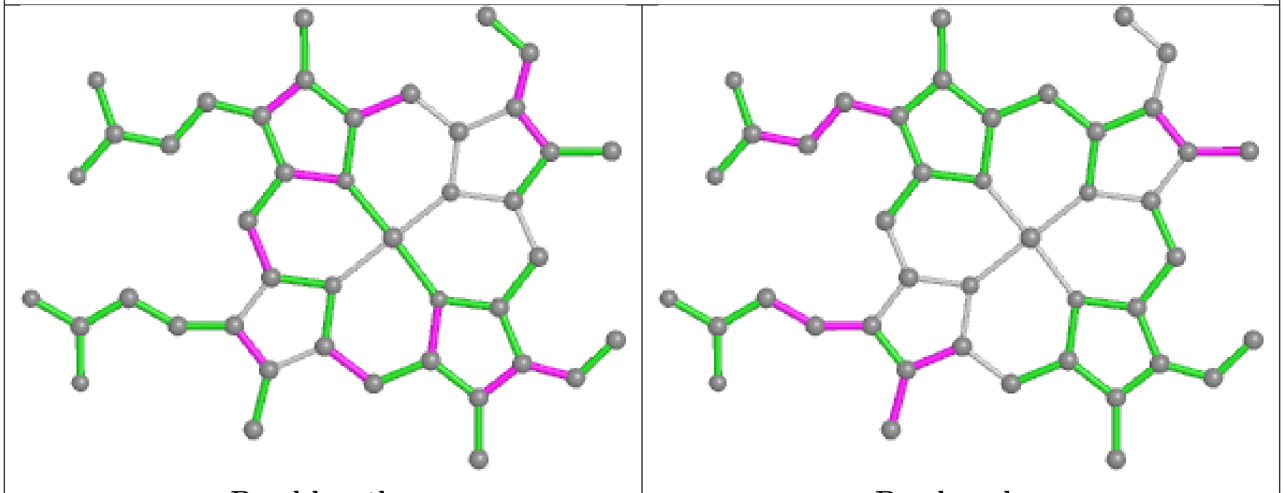
Bond angles



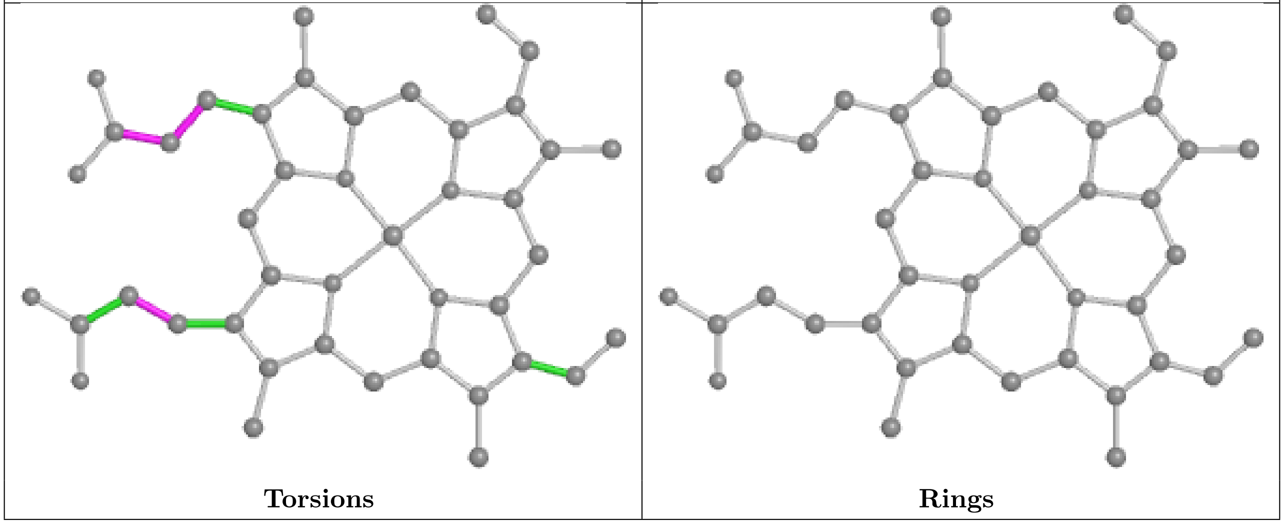
Torsions

Rings

Ligand HEM y 401

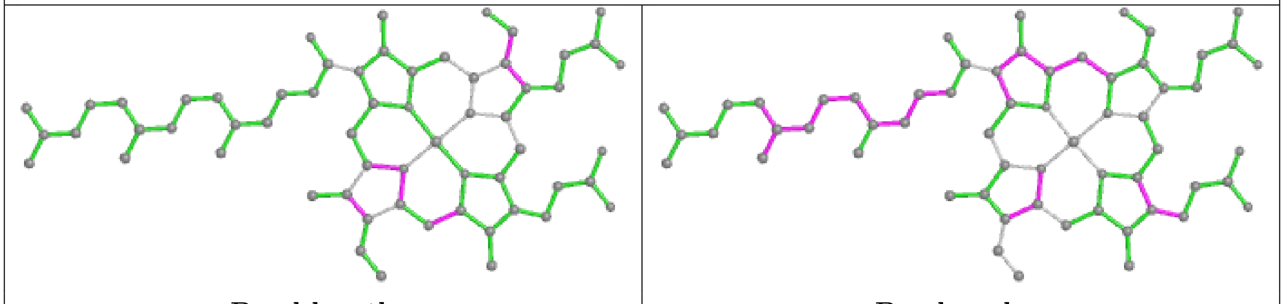


Bond lengths | Bond angles

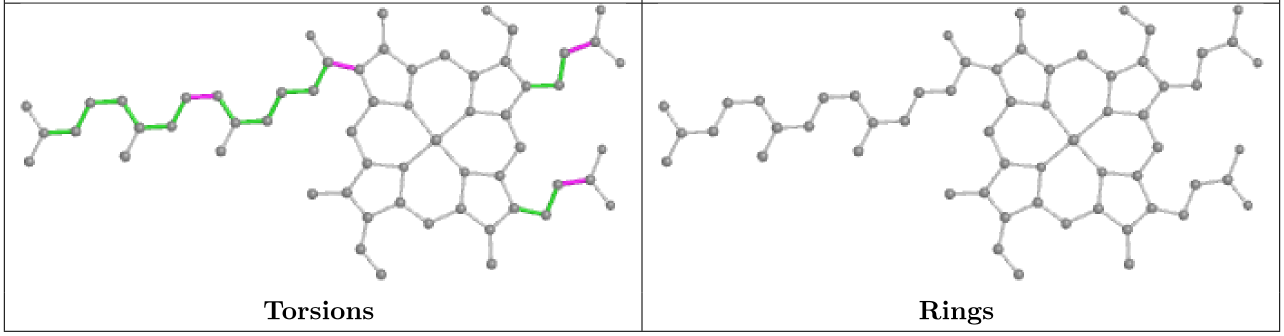


Torsions | Rings

Ligand HEA A9 601

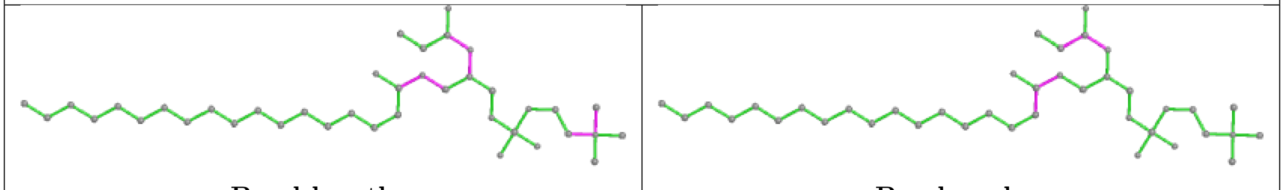


Bond lengths | Bond angles



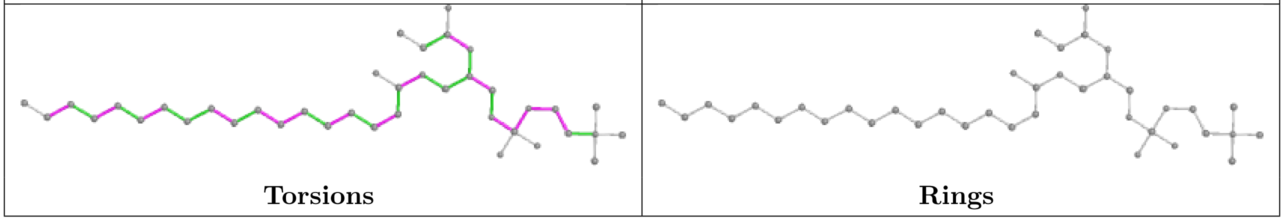
Torsions | Rings

Ligand PC1 j 201



Bond lengths

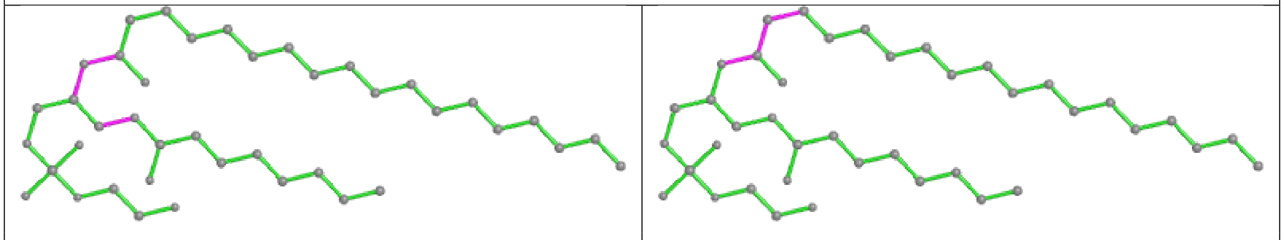
Bond angles



Torsions

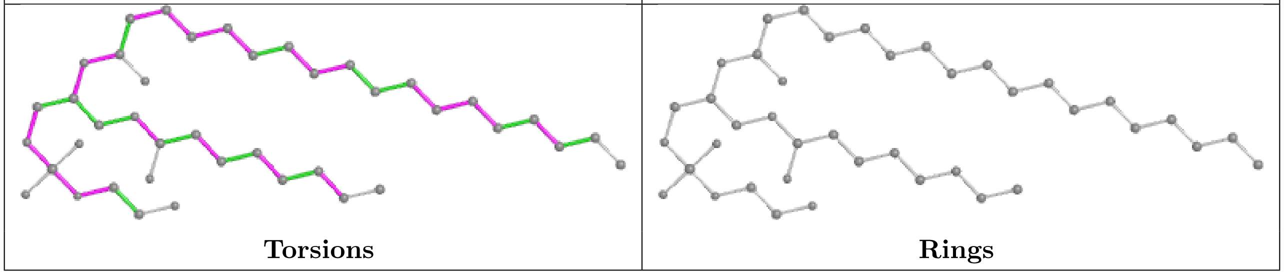
Rings

Ligand 3PE 4 503



Bond lengths

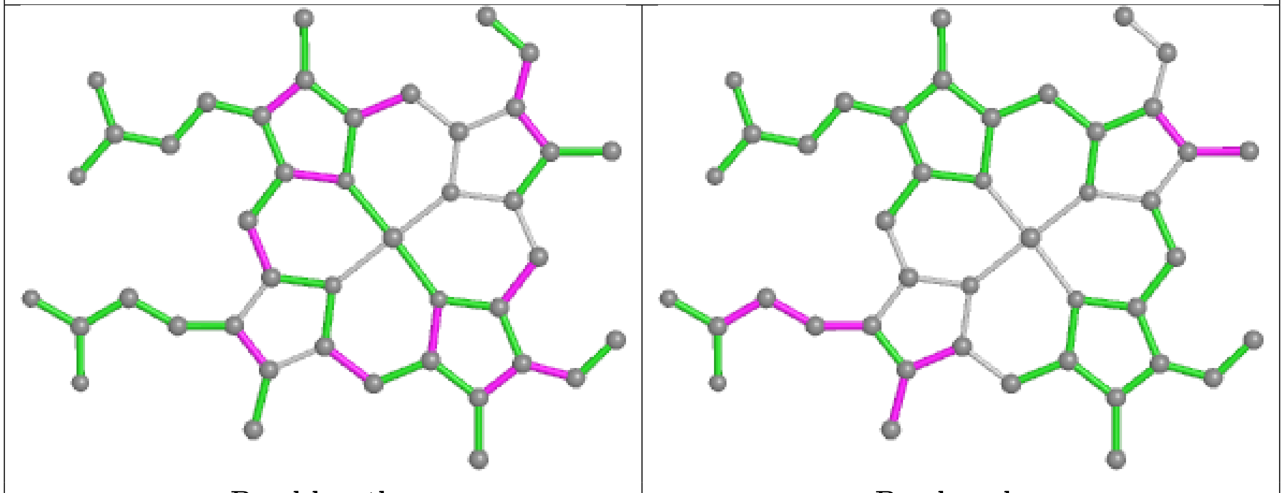
Bond angles



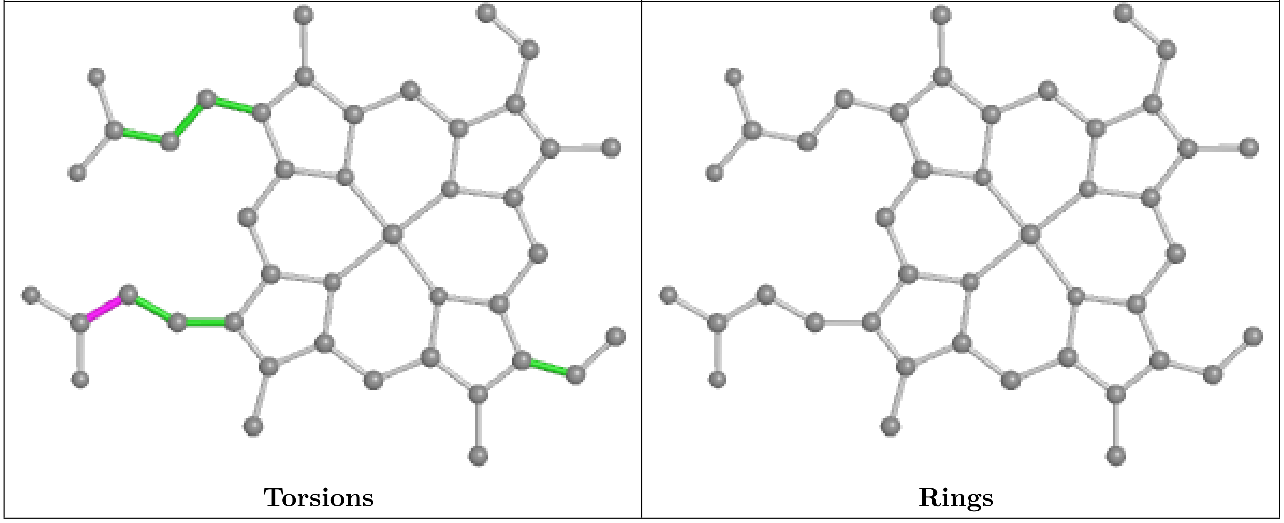
Torsions

Rings

Ligand HEM m 402

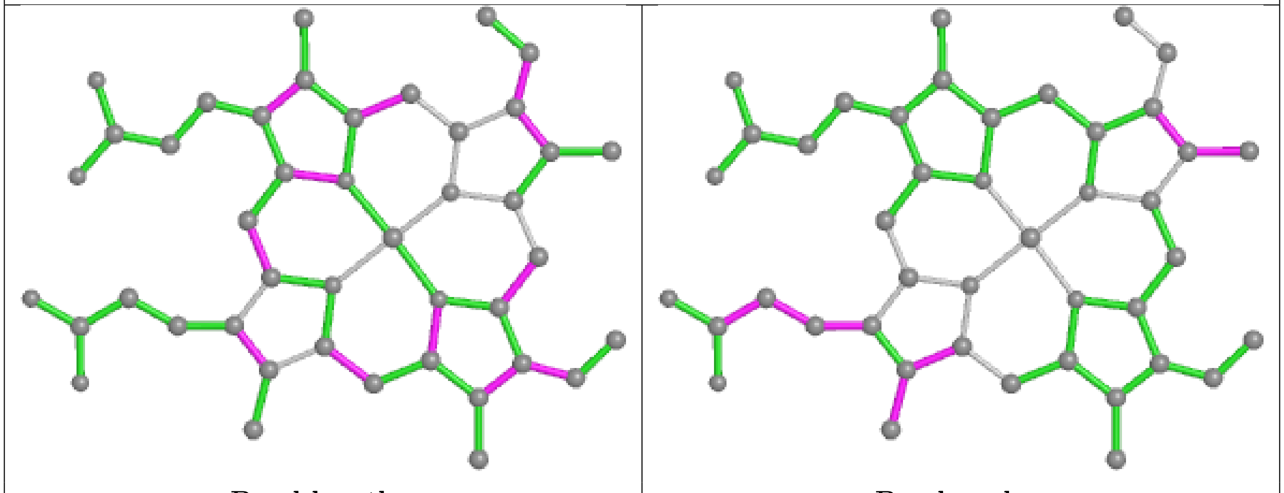


Bond lengths **Bond angles**

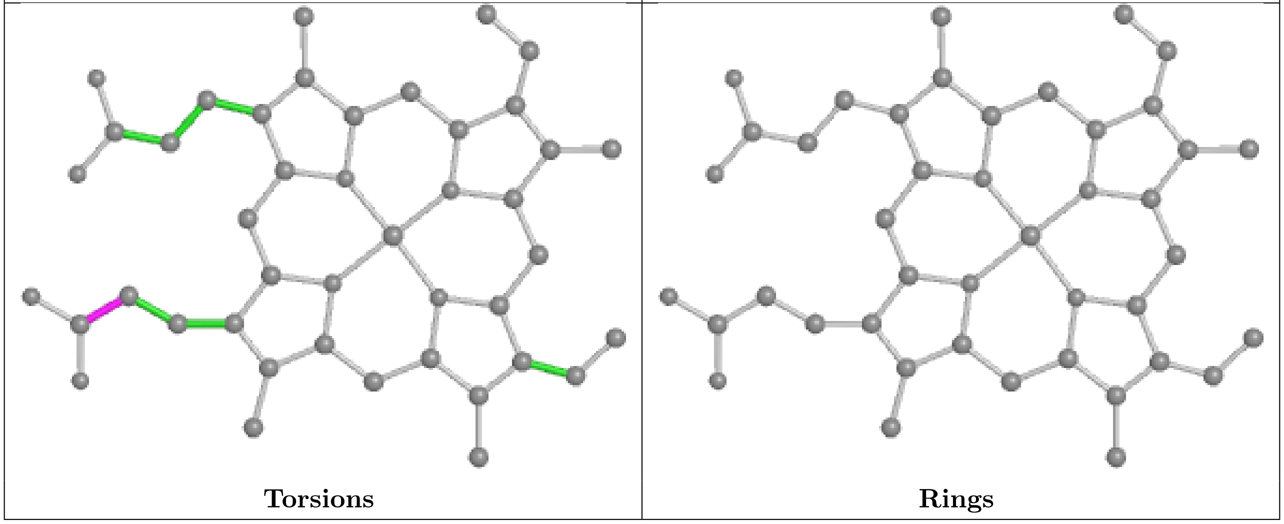


Torsions **Rings**

Ligand HEM y 402

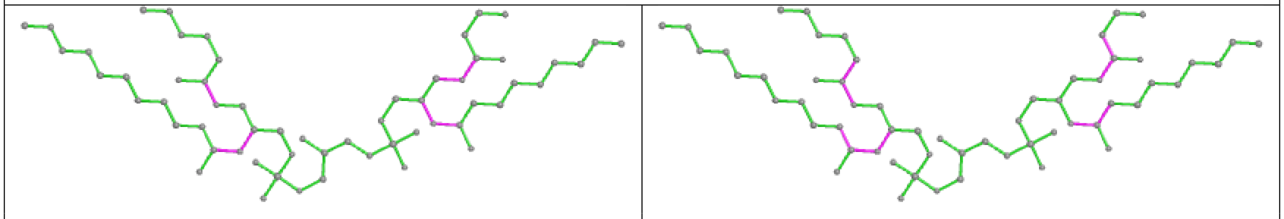


Bond lengths Bond angles

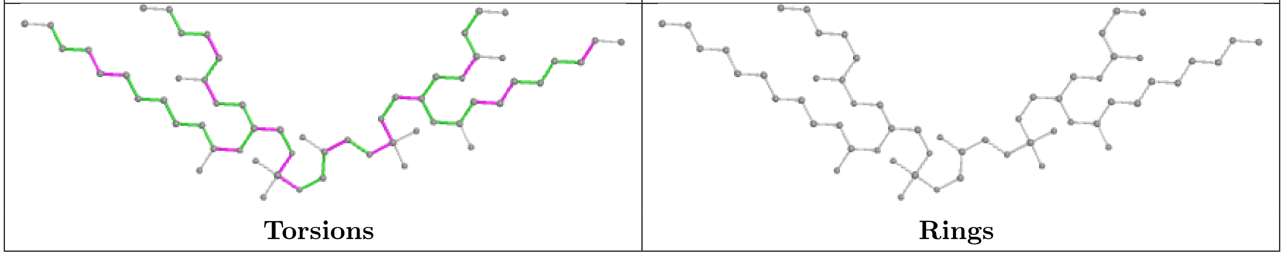


Torsions Rings

Ligand CDL J 101

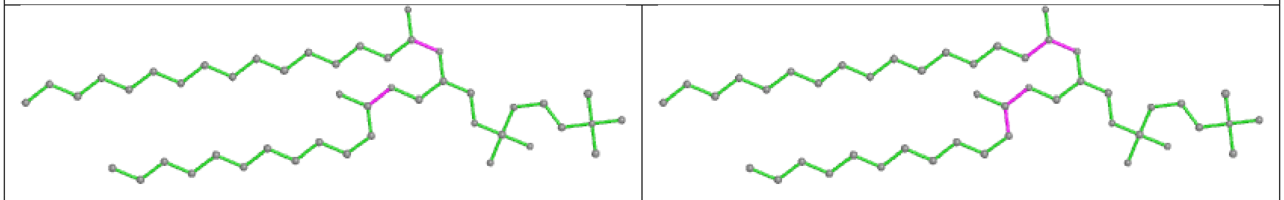


Bond lengths Bond angles

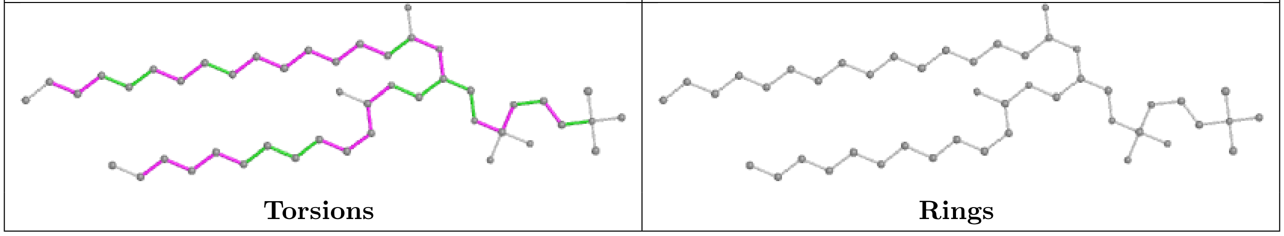


Torsions Rings

Ligand PC1 2 402

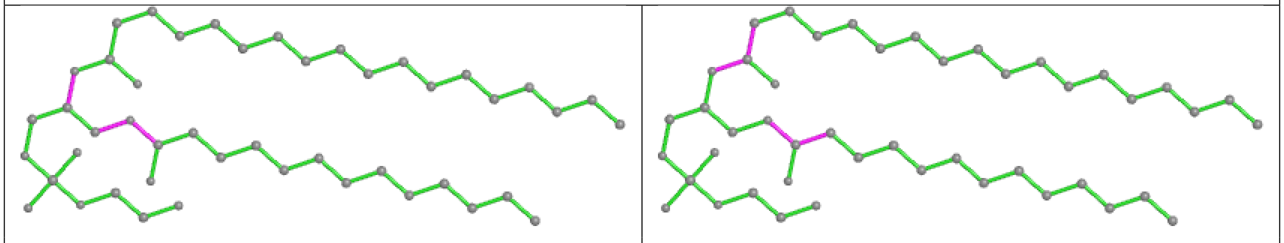


Bond lengths Bond angles

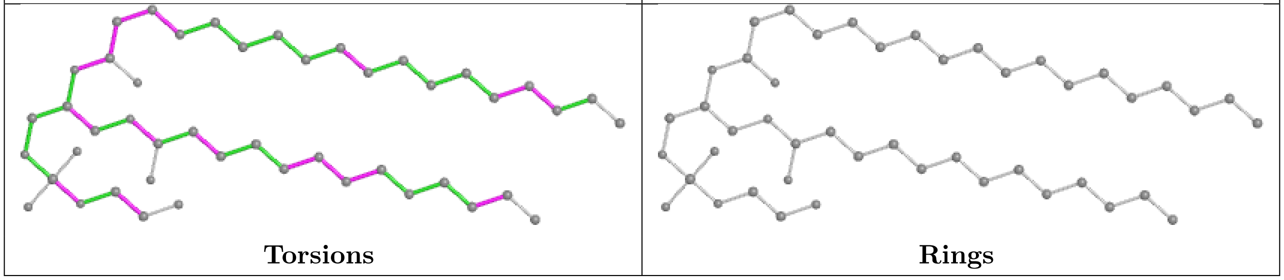


Torsions Rings

Ligand 3PE 2 401

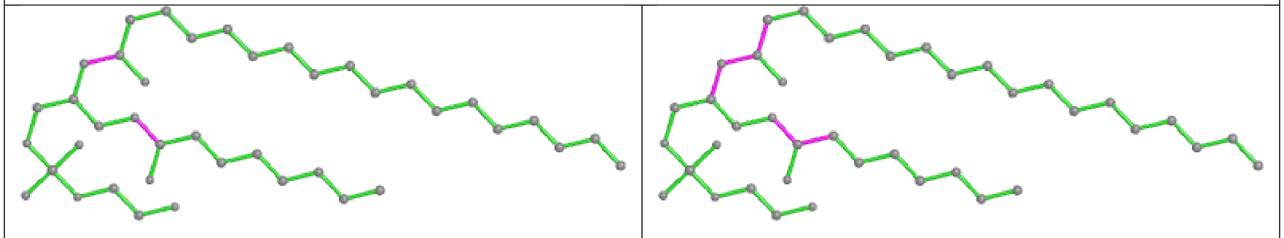


Bond lengths Bond angles

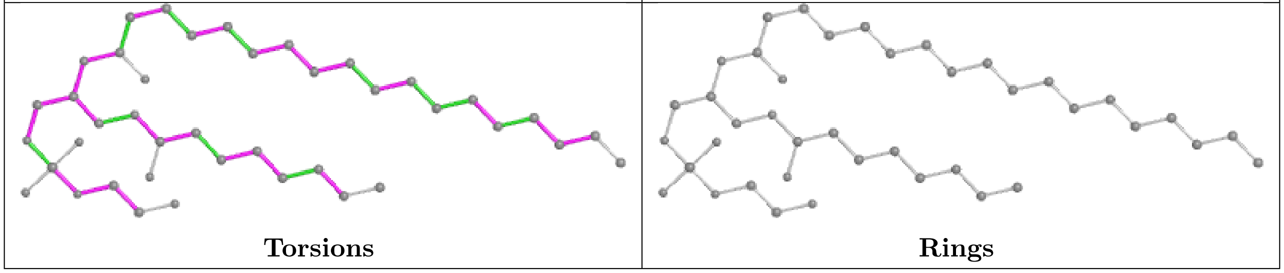


Torsions Rings

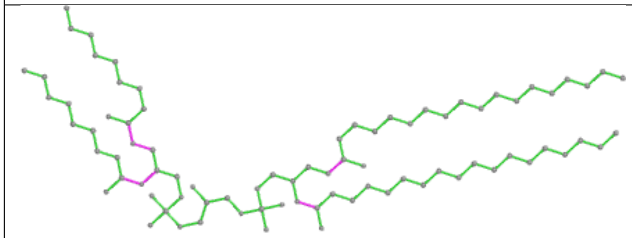
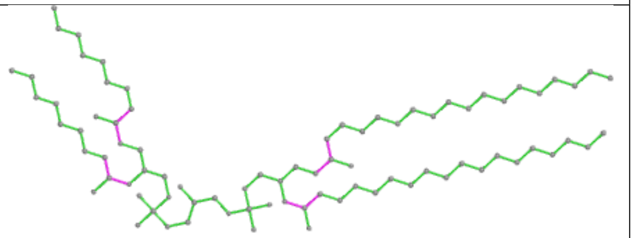
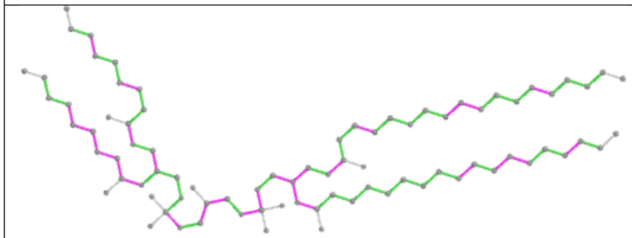
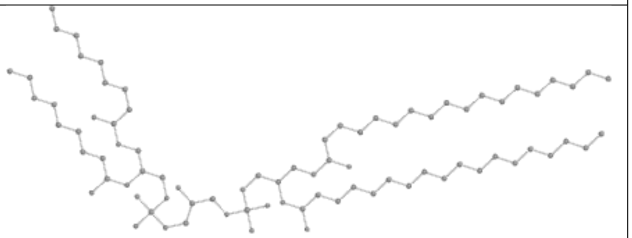
Ligand 3PE 4 501



Bond lengths Bond angles



Torsions Rings

Ligand CDL 4 502	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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.

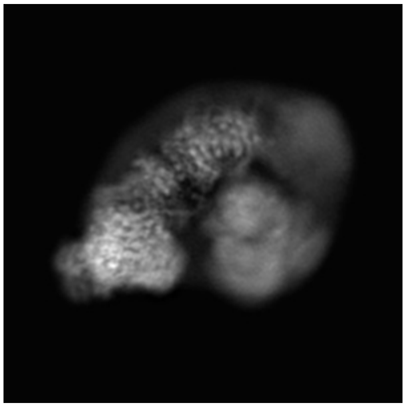
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30674. These allow visual inspection of the internal detail of the map and identification of artifacts.

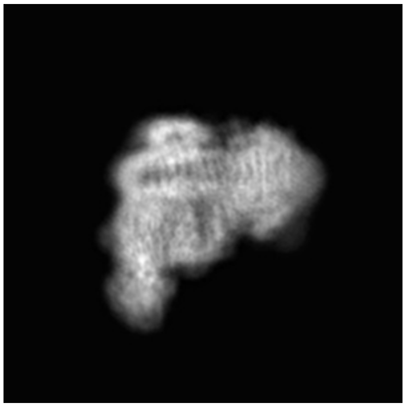
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

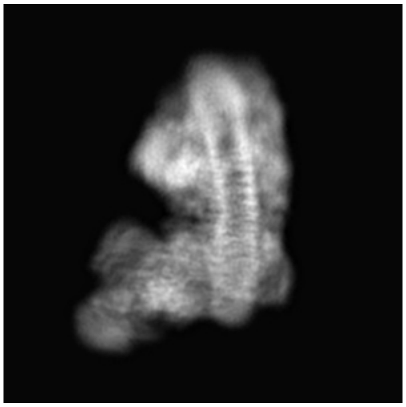
6.1.1 Primary map



X



Y

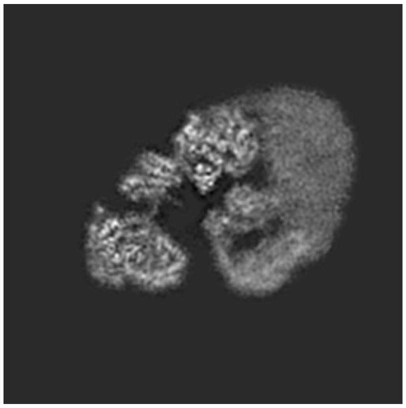


Z

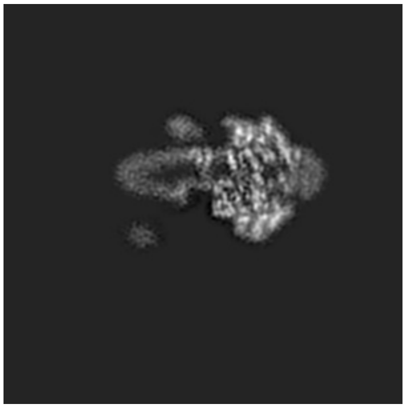
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

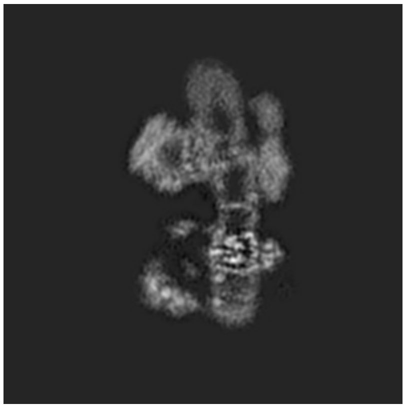
6.2.1 Primary map



X Index: 140



Y Index: 140

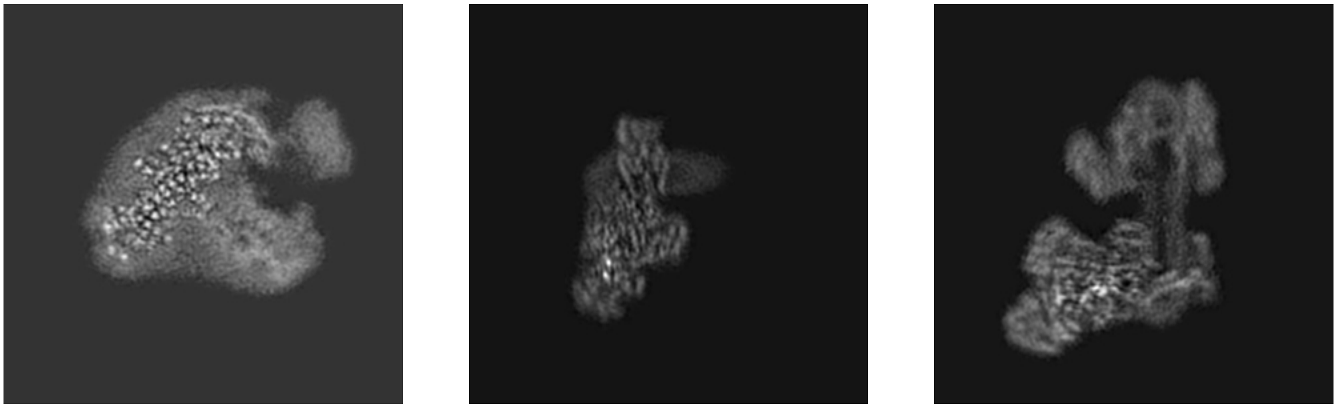


Z Index: 140

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: 75 Z Index: 103

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

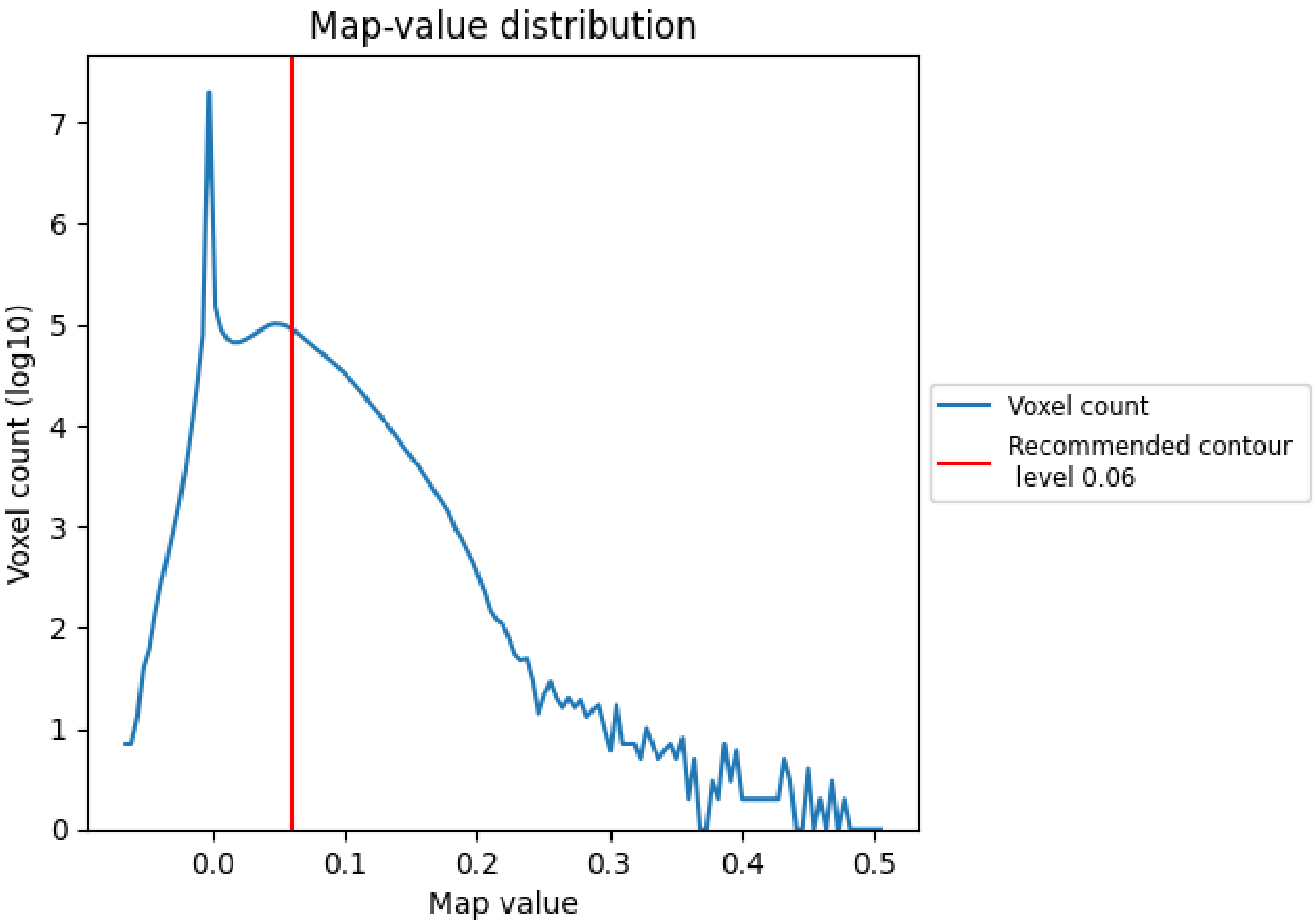
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

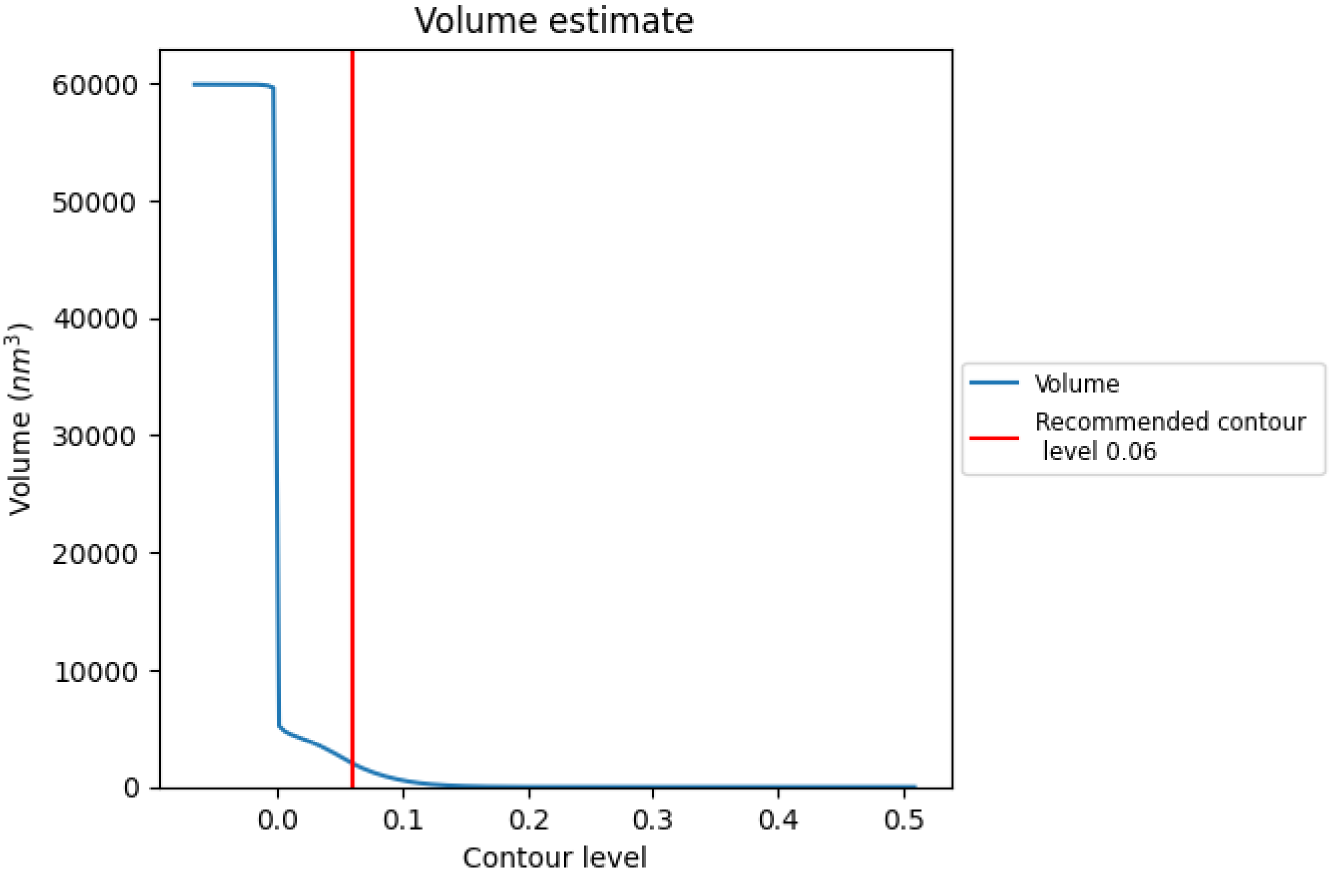
This section contains the results of statistical analysis of the map.

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.

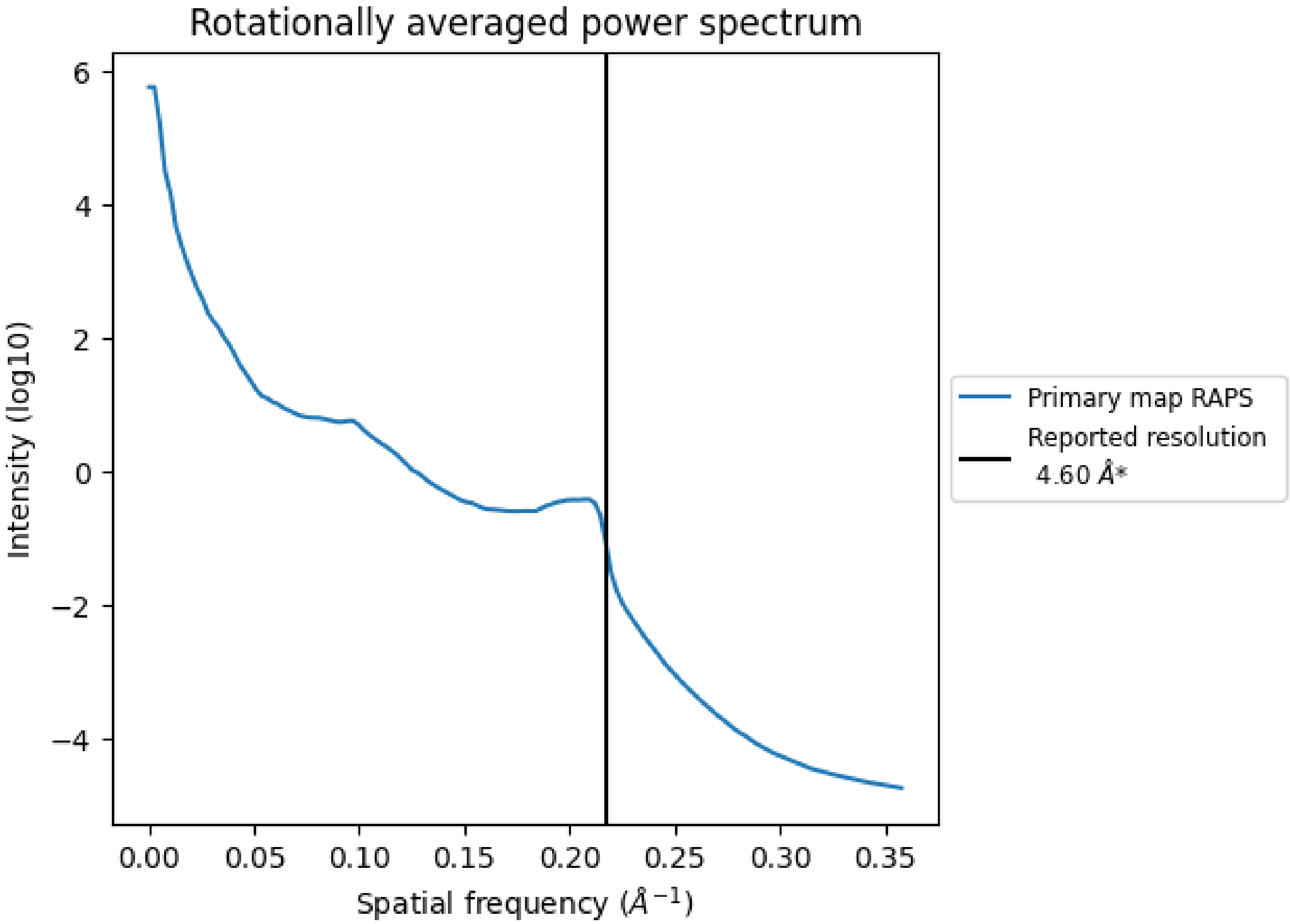
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2007 nm^3; this corresponds to an approximate mass of 1813 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 0.217 $Å^{-1}$

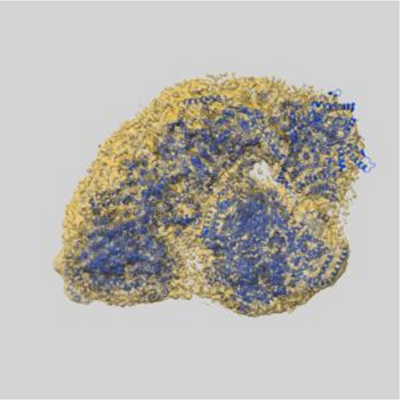
8 Fourier-Shell correlation ⓘ

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

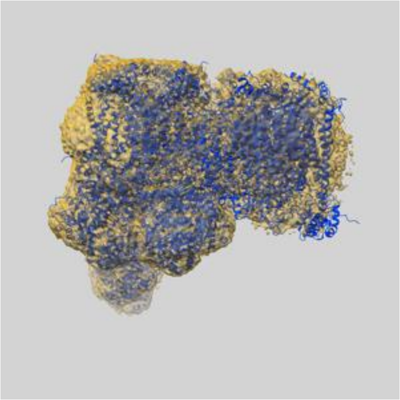
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-30674 and PDB model 7DGR. Per-residue inclusion information can be found in section 3 on page 24.

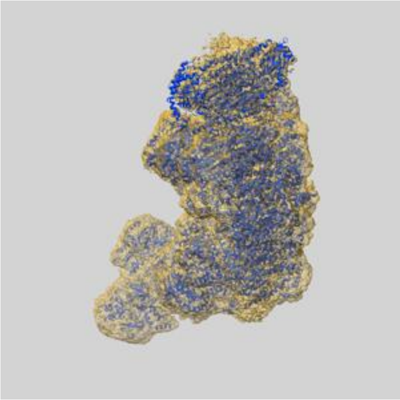
9.1 Map-model overlay ⓘ



X



Y



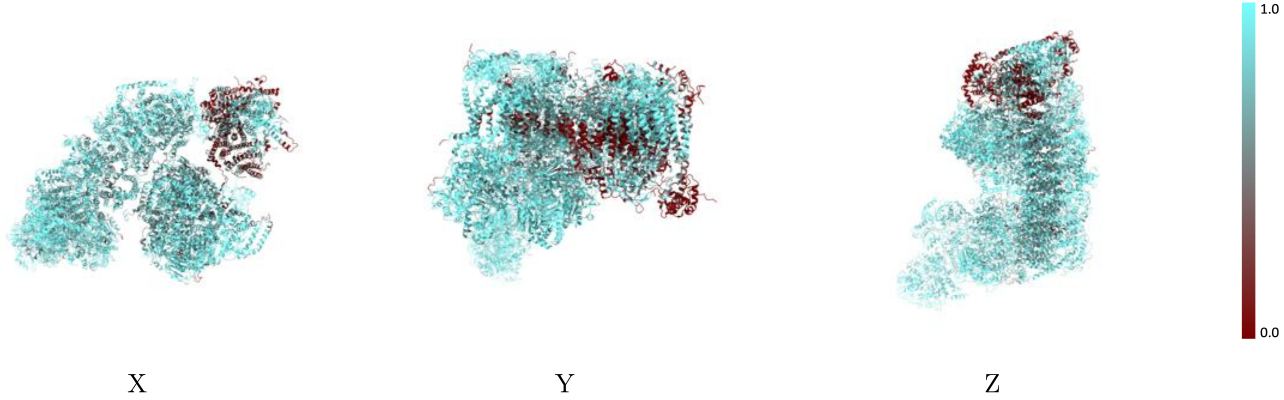
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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 ⓘ

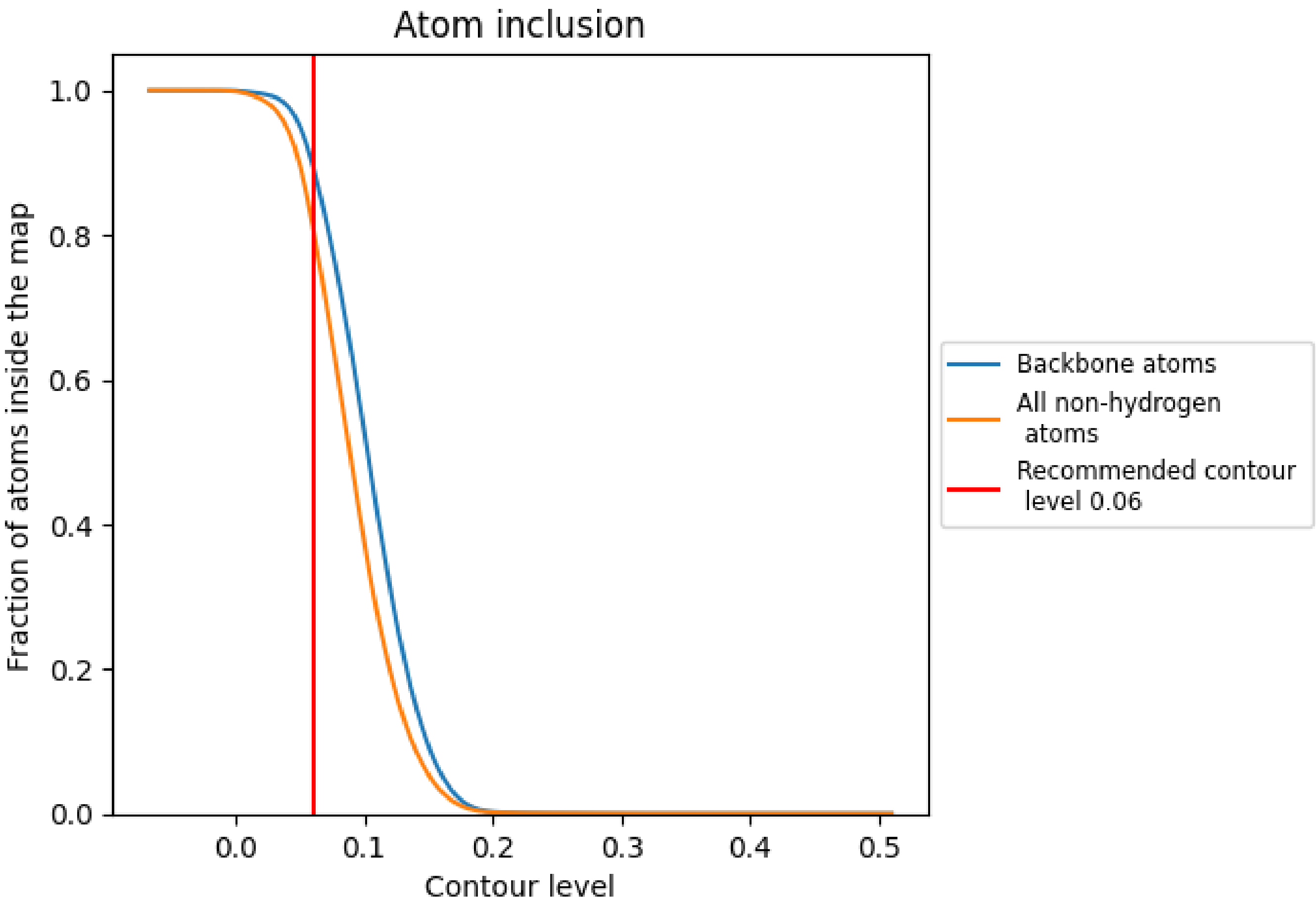
This section was not generated.

9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8142
1	0.8293
2	0.8068
3	0.7049
4	0.7842
5	0.7907
6	0.7761
7	0.7749
8	0.9829
9	0.9634
A	0.9669
A0	0.7870
A1	0.7438
A2	0.6871
A3	0.6471
A4	0.1933
A5	0.5644
A6	0.3284
A7	0.2773
A8	0.2681
A9	0.5823
B	0.8676
B0	0.3547
B1	0.8125
B2	0.5711
B3	0.7509
B4	0.3914
C	0.9196
C0	0.1480
C1	0.3263
C2	0.4266
C3	0.1824
C4	0.7762
D	0.9029
E	0.9122

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Chain	Atom inclusion
F	0.9121
G	0.9283
H	0.9526
I	0.8983
J	0.9353
K	0.9733
L	0.8103
M	0.8681
N	0.9162
O	0.8667
P	0.8341
Q	0.9566
R	0.8841
S	0.9044
T	0.8077
U	0.6761
V	0.9460
W	0.9804
X	0.8989
Y	0.9504
Z	0.9277
a	0.7954
b	0.9462
c	0.9536
d	0.9771
e	0.9168
f	0.9647
g	0.9346
h	0.9234
i	0.9231
j	0.7833
k	0.9267
l	0.9113
m	0.7760
o	0.9361
p	0.8967
q	0.8844
r	0.7957
s	0.8787
t	0.7312
u	0.8397
v	0.8393

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Chain	**Atom inclusion**
w	🟦 0.8908
x	🟦 0.9434
y	🟦 0.7238
z	🟦 0.8809