Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:27 PM JST

PDB ID	:	7DGS
EMDB ID	:	EMD-30675
Title	:	Activity optimized supercomplex state3
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	:	7.80 Å(reported)

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

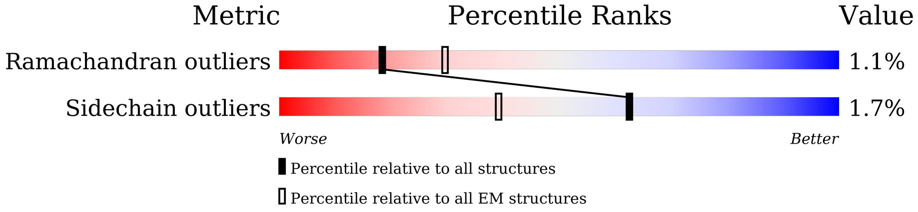
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

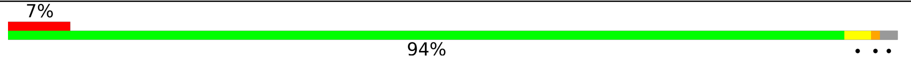
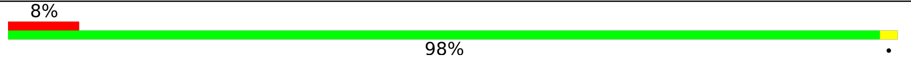
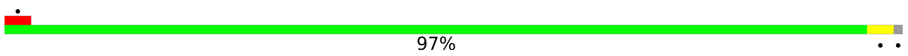
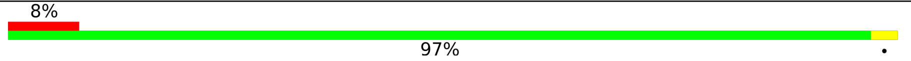
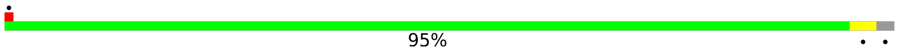
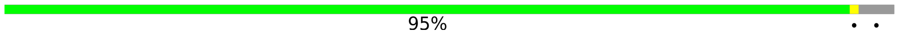
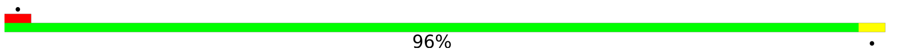
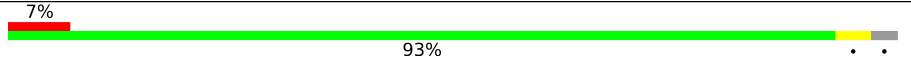
The reported resolution of this entry is 7.80 Å.

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

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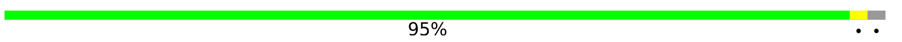
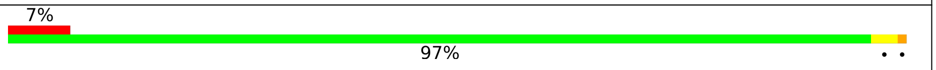
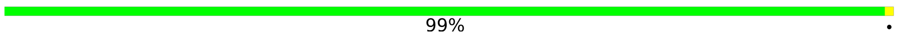
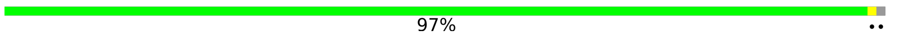
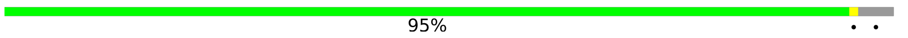
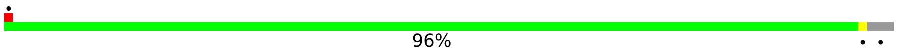
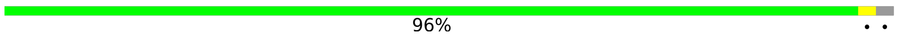
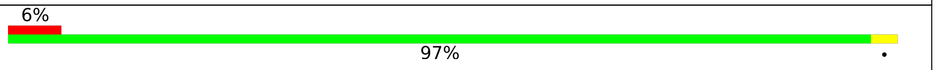
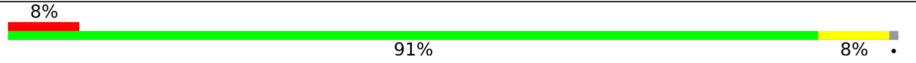
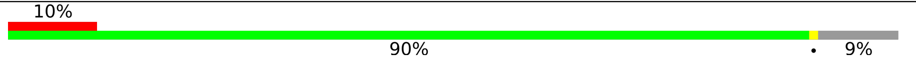
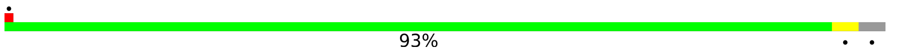
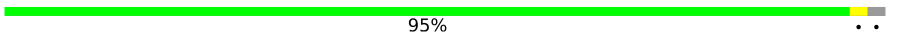
Mol	Chain	Length	Quality of chain
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	

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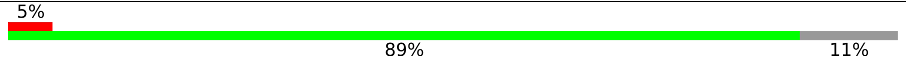
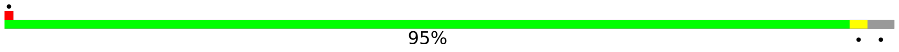
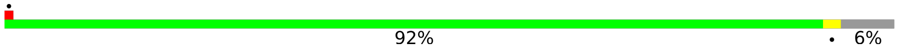
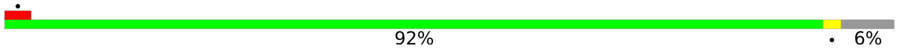
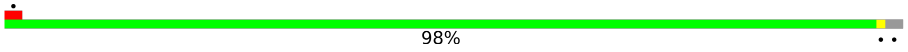
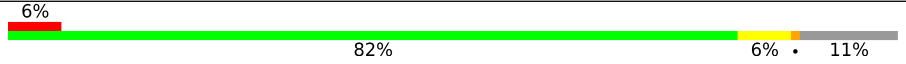
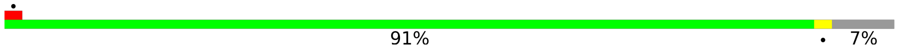
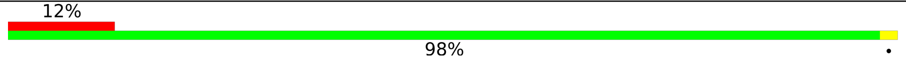
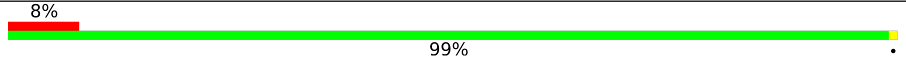
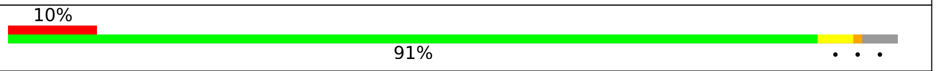
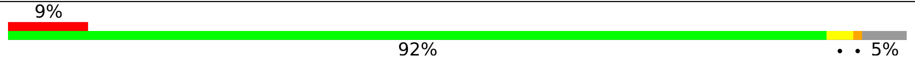
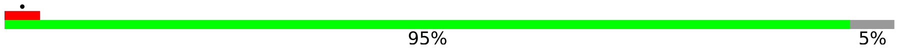
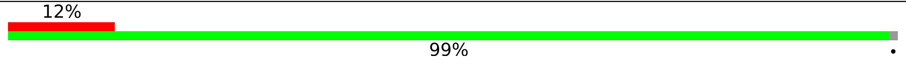
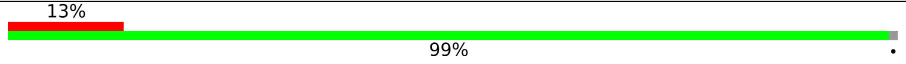
Mol	Chain	Length	Quality of chain
34	Z	97	
35	a	128	
36	b	143	
37	c	127	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	325	
48	z	325	
49	A0	196	
49	p	196	
50	A1	111	
50	q	111	
51	A2	82	
51	r	82	

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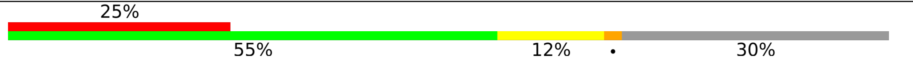
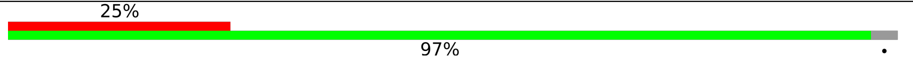
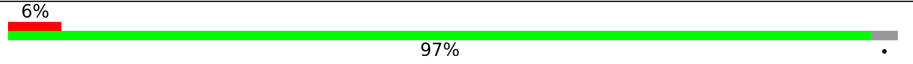
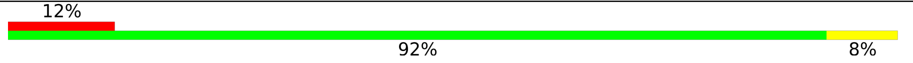
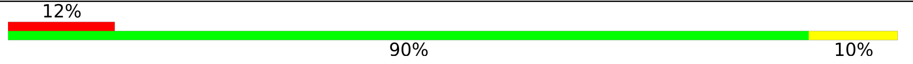
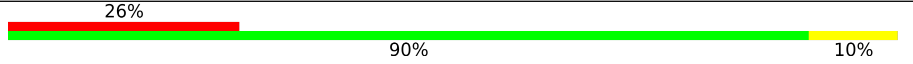
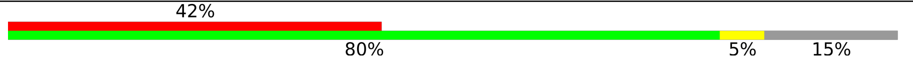
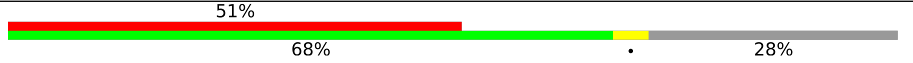
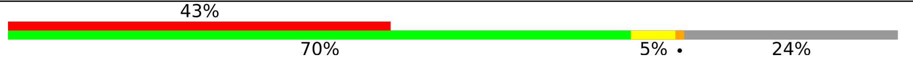
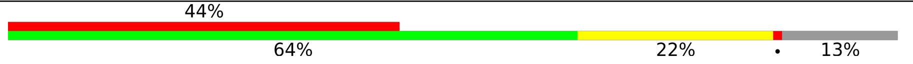
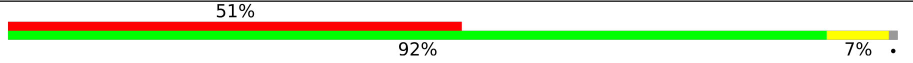
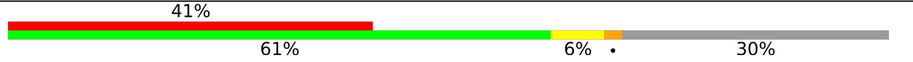
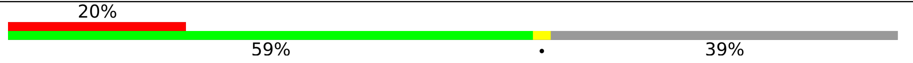
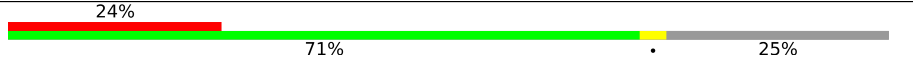
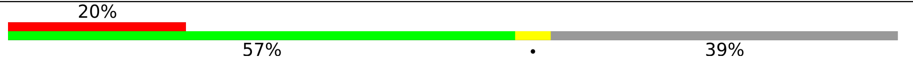
Mol	Chain	Length	Quality of chain
52	B5	91	
52	s	91	
53	A3	56	
53	t	56	
54	B4	64	
54	u	64	
55	B3	78	
55	v	78	
56	A9	514	
57	B9	227	
58	B7	261	
59	A7	169	
60	A6	152	
61	B2	129	
62	A4	97	
63	A5	86	
64	B6	74	
65	B8	80	
66	B0	80	
67	B1	63	
68	A8	70	

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 106778 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	1534	978	261	285	10	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	7	172	1186	798	179	202	7	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	606	4765	3172	732	819	42	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	344	2582	1707	404	437	34	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	458	3447	2293	548	574	32	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	96	697	454	109	124	10	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	427	Total 2965	C 1864	N 552	O 534	S 15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	317	Total 2499	C 1676	N 384	O 416	S 23	0	0

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	112	Total 862	C 580	N 127	O 150	S 5	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	688	Total 5179	C 3252	N 914	O 977	S 36	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	430	Total 3416	C 2179	N 589	O 623	S 25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	208	Total 1705	C 1102	N 294	O 306	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	152	1200	769	209	208	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	176	1388	874	239	264	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	F	28	183	116	32	35	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	123	981	619	177	182	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	I	71	530	331	99	97	3	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	K	84	Total 652	C 409	N 125	O 118	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	90	Total 698	C 442	N 128	O 126	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	168	Total 1345	C 851	N 242	O 243	S 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	2297	1455	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	922	584	161	171	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
			Total	C	N	O	S		
38	d	107	708	445	134	125	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
50	q	106	916	579	167	168	2	0	0
50	A1	106	916	579	167	168	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s	67	548	332	99	112	5	0	0
52	B5	69	566	342	101	118	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	t	33	262	174	46	42	0	0
53	A3	39	304	202	55	47	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	u	62	511	335	89	87	0	0
54	B4	62	511	335	89	87	0	0

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

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	B3	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	B9	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	B7	261	2125	1421	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	A6	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	B2	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
62	A4	84	Total 671	C 431	N 129	O 110	S 1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	B6	73	Total 598	C 388	N 107	O 99	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	B8	56	Total 441	C 285	N 73	O 80	S 3	0	0

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

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

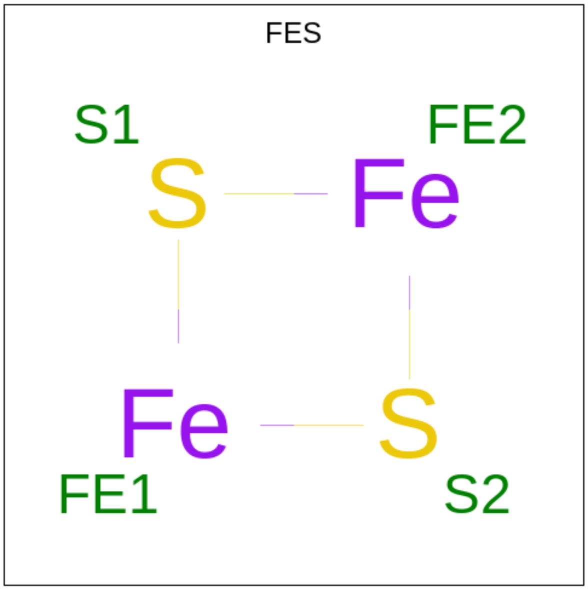
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	B1	47	Total 386	C 257	N 65	O 62	S 2	0	0

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

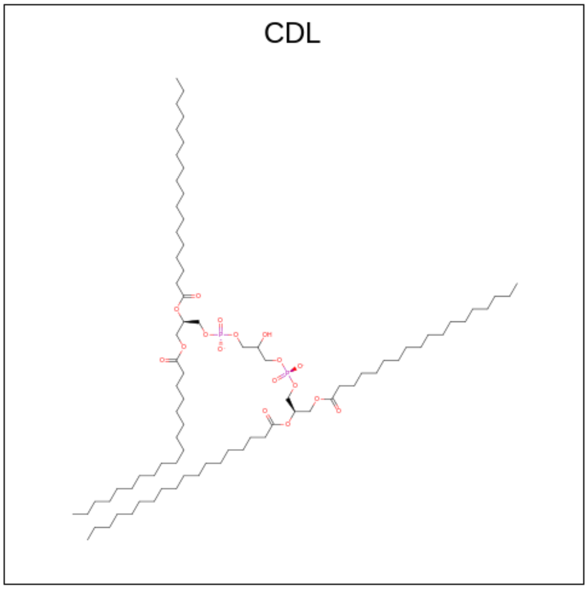
Mol	Chain	Residues	Atoms				AltConf	Trace
68	A8	43	Total 335	C 223	N 53	O 59	0	0

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



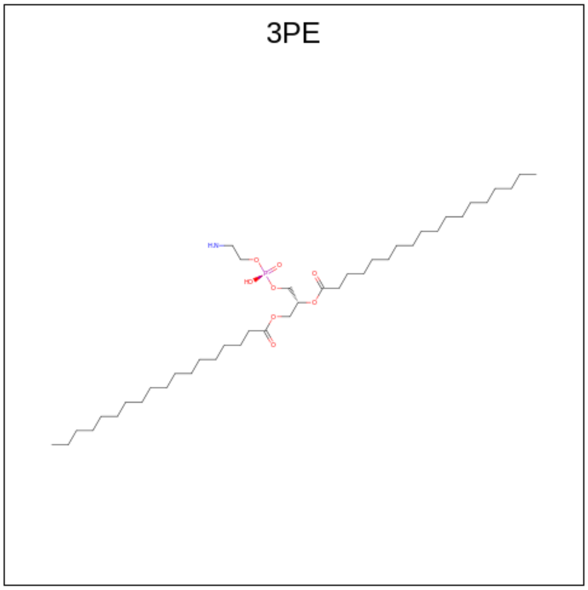
Mol	Chain	Residues	Atoms	AltConf
69	9	1	Total Fe S 4 2 2	0
69	A	1	Total Fe S 4 2 2	0
69	m	1	Total Fe S 4 2 2	0

- Molecule 70 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



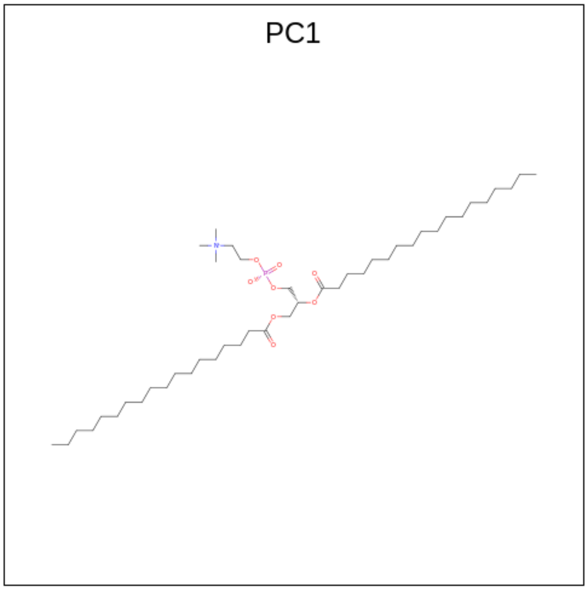
Mol	Chain	Residues	Atoms				AltConf
70	6	1	Total 64	C 45	O 17	P 2	0
70	4	1	Total 82	C 63	O 17	P 2	0
70	J	1	Total 58	C 39	O 17	P 2	0

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



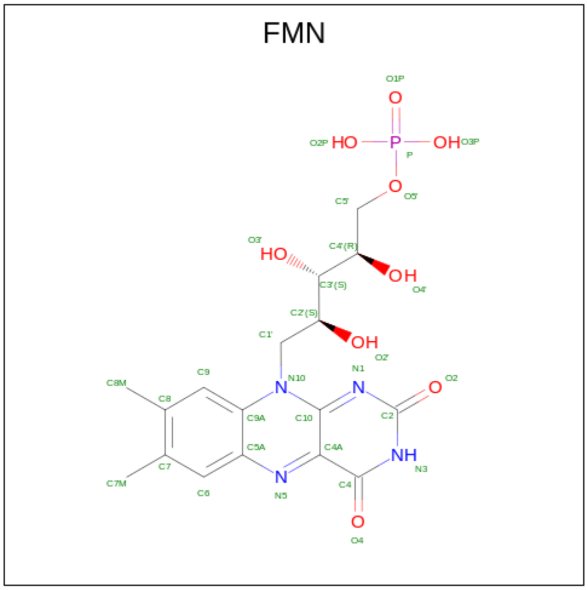
Mol	Chain	Residues	Atoms					AltConf
71	2	1	Total 41	C 31	N 1	O 8	P 1	0
71	4	1	Total 41	C 31	N 1	O 8	P 1	0
71	B	1	Total 51	C 41	N 1	O 8	P 1	0
71	V	1	Total 51	C 41	N 1	O 8	P 1	0
71	j	1	Total 46	C 36	N 1	O 8	P 1	0

- 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).



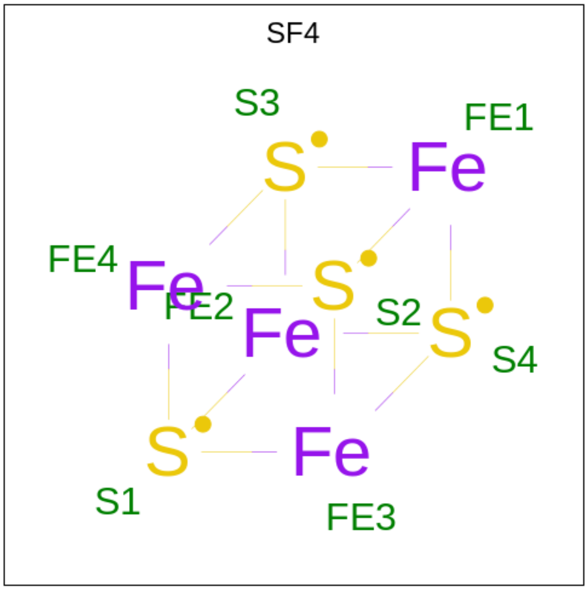
Mol	Chain	Residues	Atoms					AltConf
72	2	1	Total 46	C 36	N 1	O 8	P 1	0
72	L	1	Total 47	C 37	N 1	O 8	P 1	0
72	Q	1	Total 46	C 36	N 1	O 8	P 1	0
72	S	1	Total 47	C 37	N 1	O 8	P 1	0
72	j	1	Total 39	C 29	N 1	O 8	P 1	0

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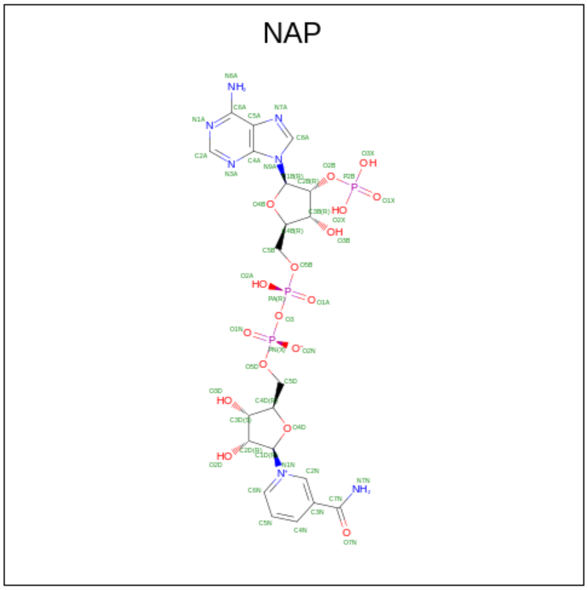
Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total 8	Fe 4	S 4	0
74	E	1	Total 16	Fe 8	S 8	0
74	E	1	Total 16	Fe 8	S 8	0

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

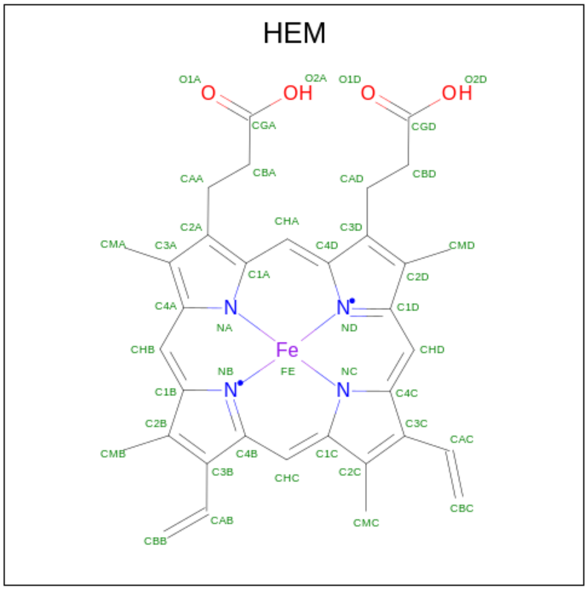
Mol	Chain	Residues	Atoms		AltConf
75	I	1	Total 1	Zn 1	0
75	B2	1	Total 1	Zn 1	0

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



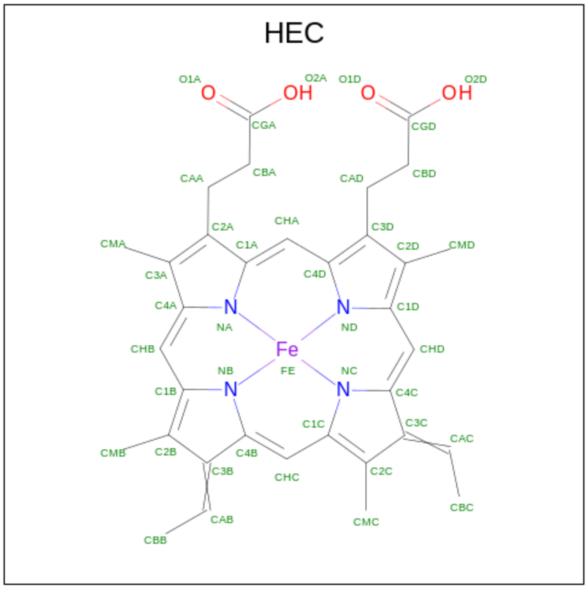
Mol	Chain	Residues	Atoms					AltConf
76	R	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



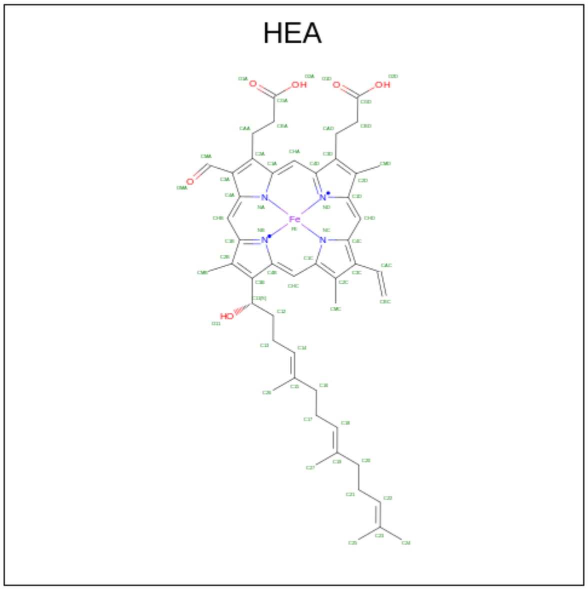
Mol	Chain	Residues	Atoms	AltConf
77	m	1	Total C Fe N O 86 68 2 8 8	0
77	m	1	Total C Fe N O 86 68 2 8 8	0
77	y	1	Total C Fe N O 86 68 2 8 8	0
77	y	1	Total C Fe N O 86 68 2 8 8	0

- 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	B9	2	Total 2	Cu 2	0

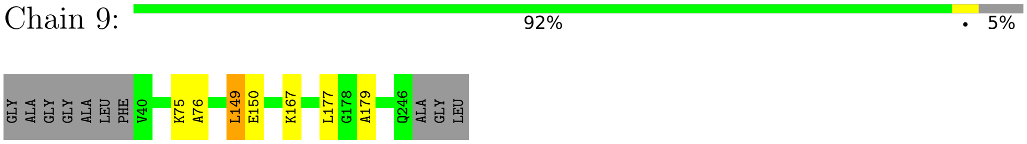
- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

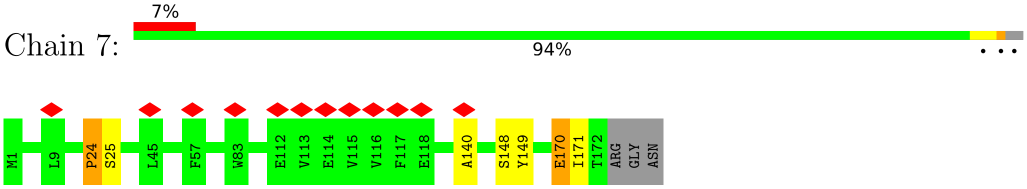
3 Residue-property plots ⓘ

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.

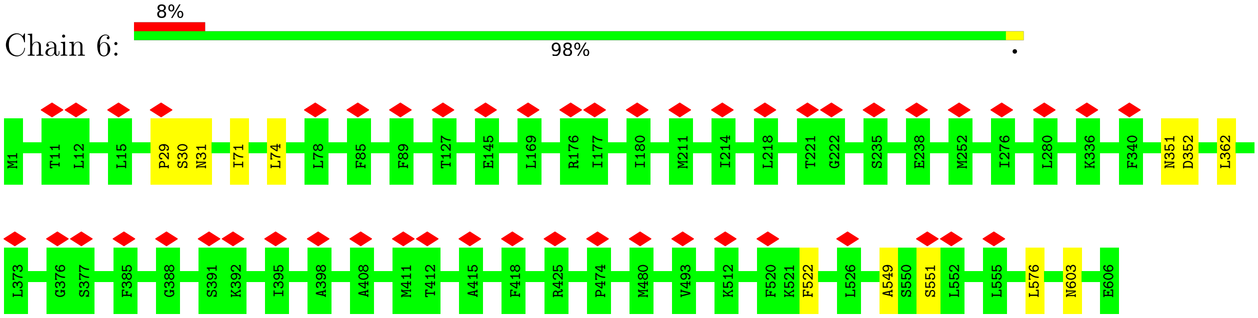
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



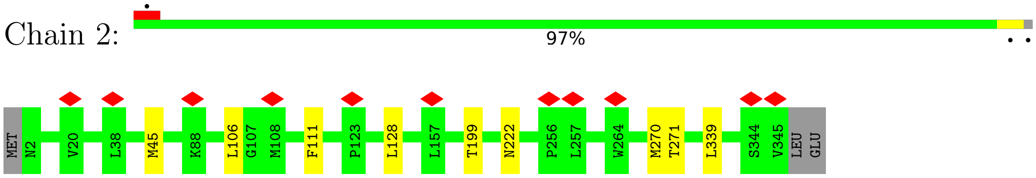
- Molecule 2: NADH-ubiquinone oxidoreductase chain 6



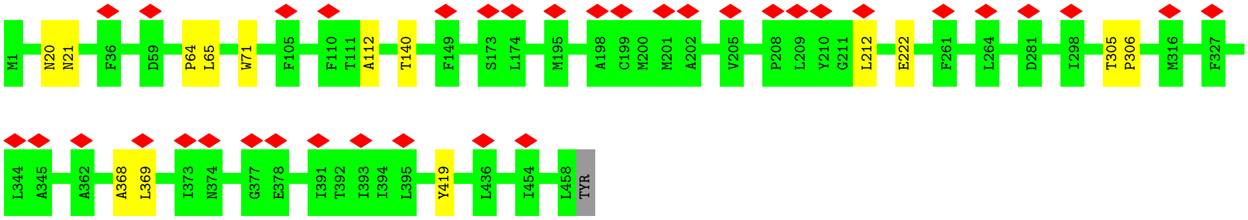
- Molecule 3: NADH-ubiquinone oxidoreductase chain 5



- Molecule 4: NADH-ubiquinone oxidoreductase chain 2

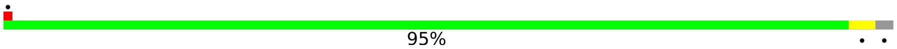


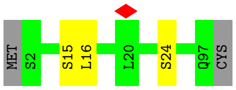
- Molecule 5: NADH-ubiquinone oxidoreductase chain 4



- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

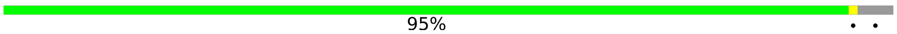
Chain 5:

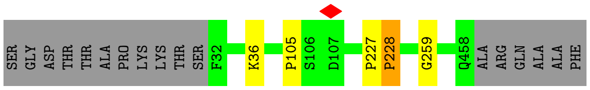




- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

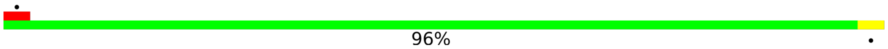
Chain 8:

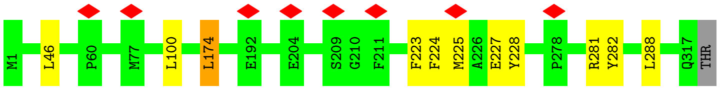




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

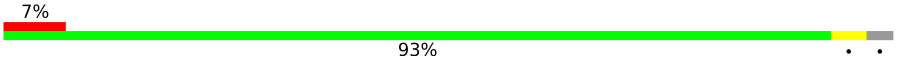
Chain 1:

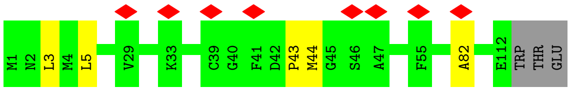




- Molecule 9: NADH-ubiquinone oxidoreductase chain 3

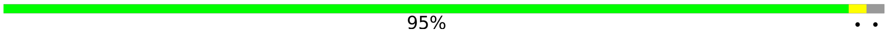
Chain 3:

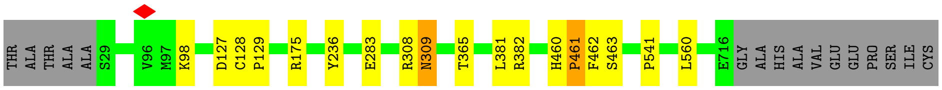




- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

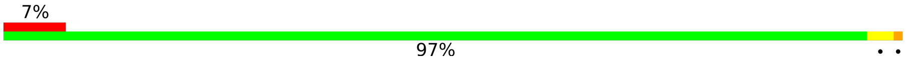
Chain A:

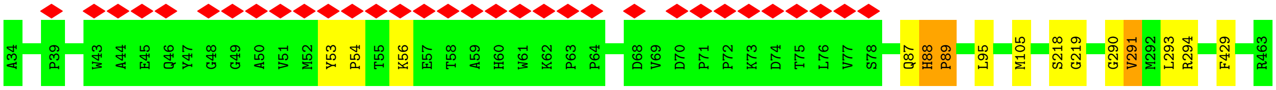




- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

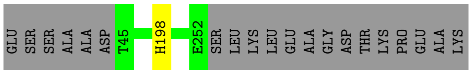
Chain B:





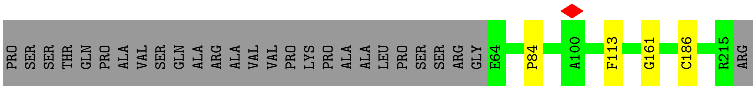
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



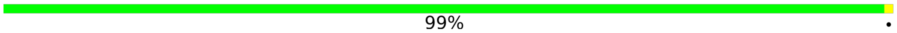
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

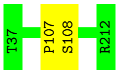
Chain D:



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

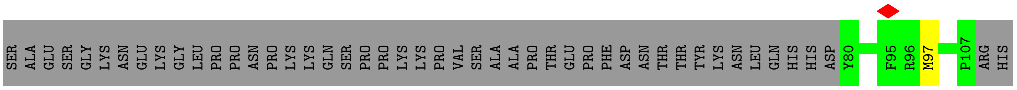
Chain E:





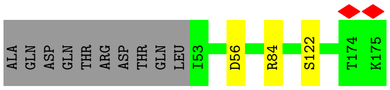
- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:



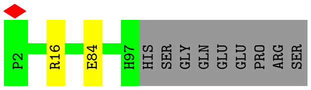
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G:

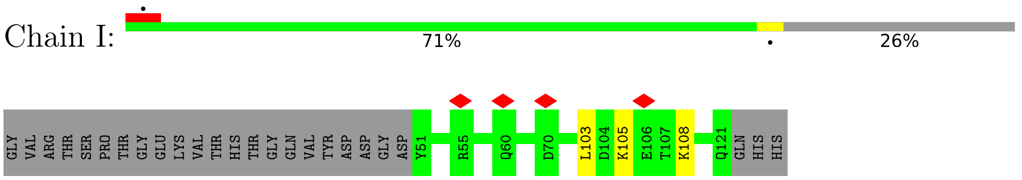


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

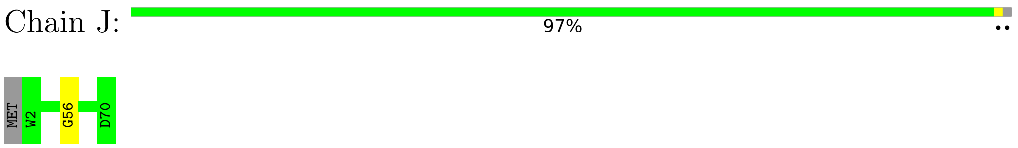
Chain H:



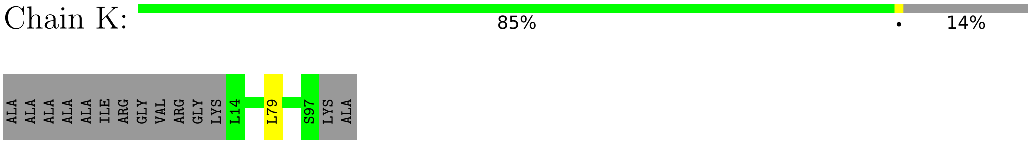
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



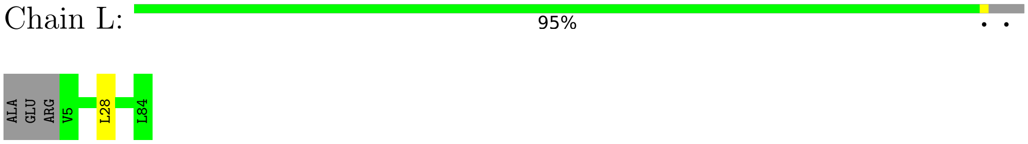
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



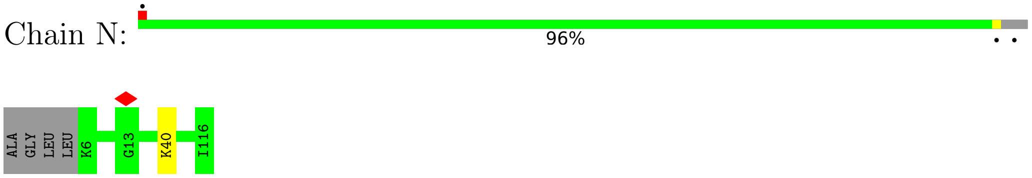
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



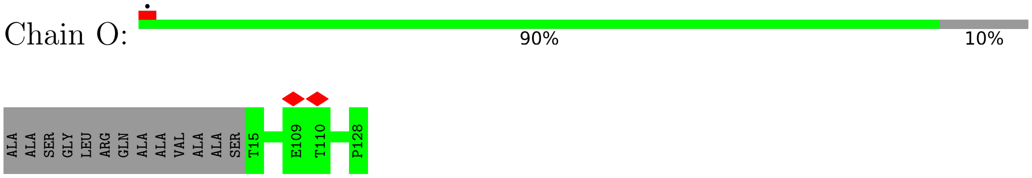
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



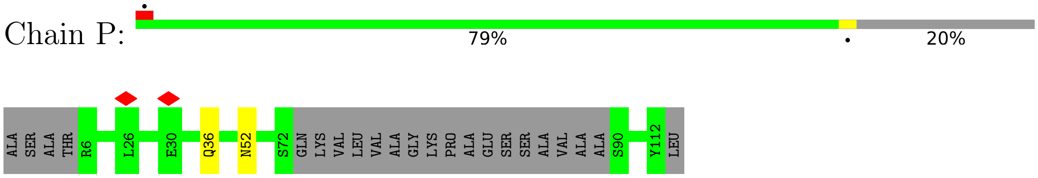
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



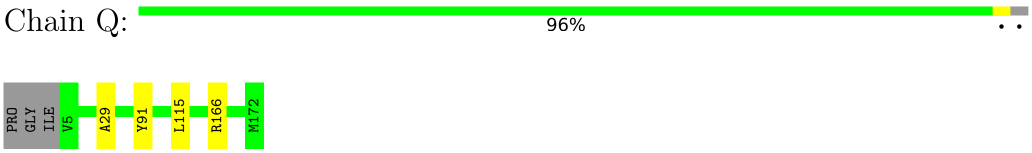
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



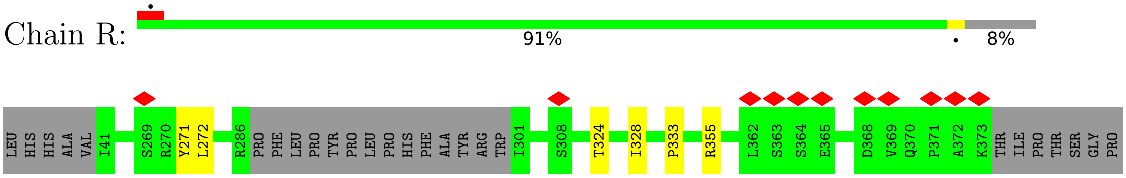
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



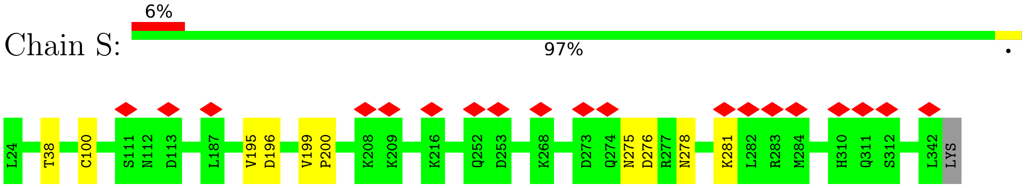
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



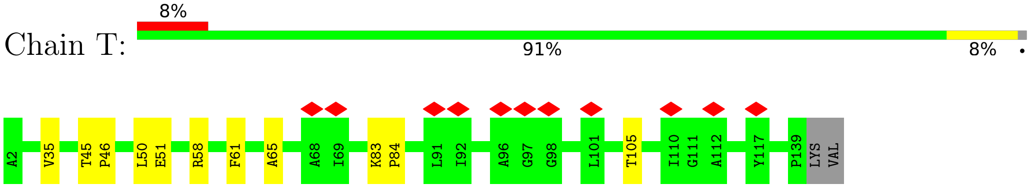
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



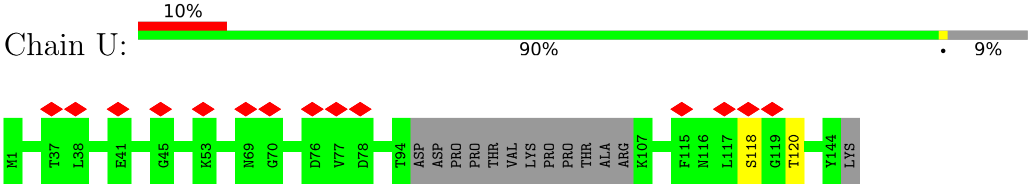
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



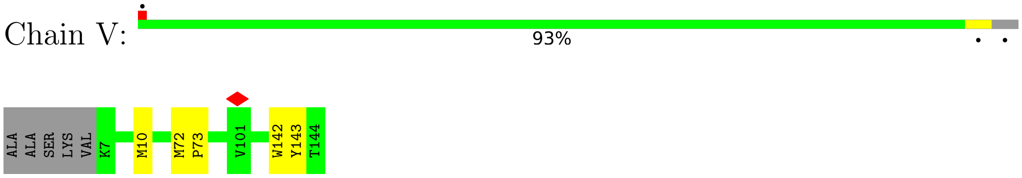
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



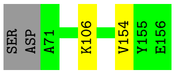
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

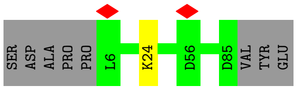


- Molecule 31: Acyl carrier protein, mitochondrial



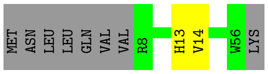
- Molecule 31: Acyl carrier protein, mitochondrial

Chain M:



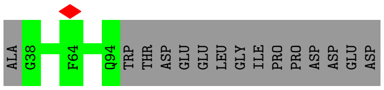
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain X:



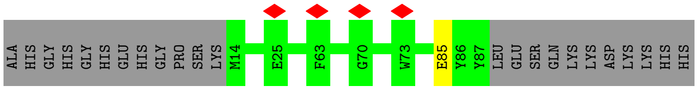
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



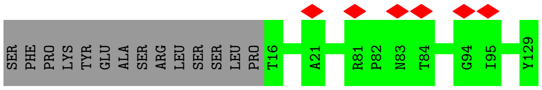
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



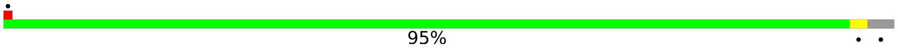
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

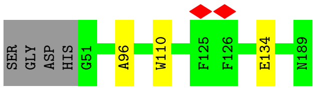
Chain a:



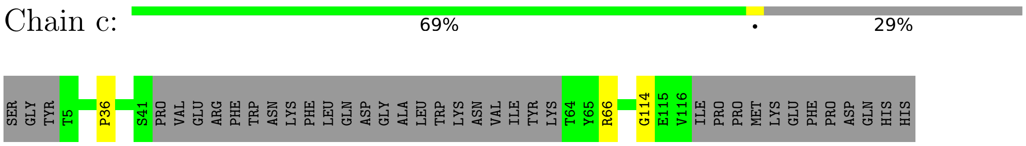
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain b:

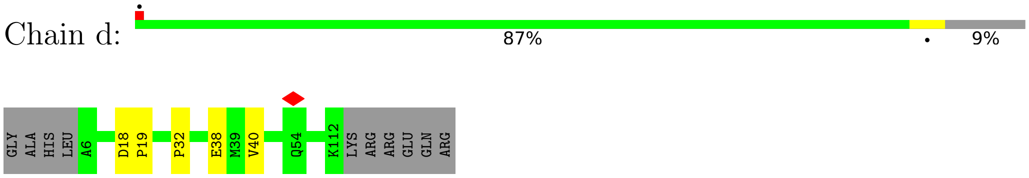




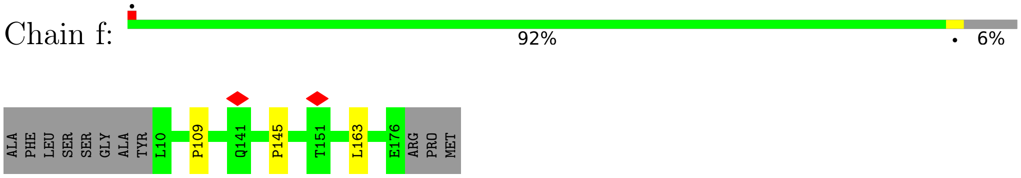
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



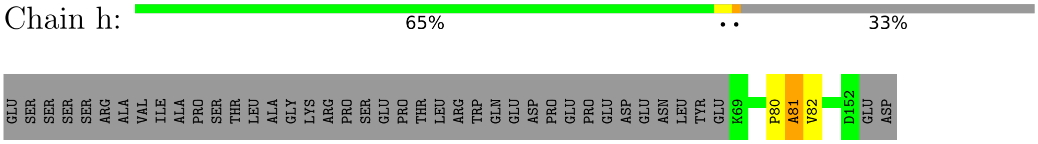
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



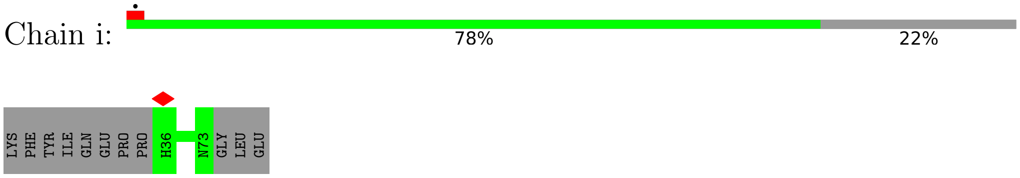
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



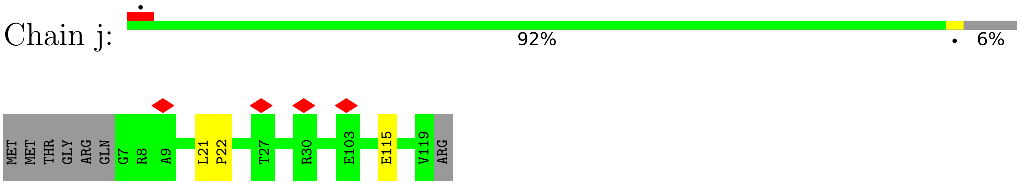
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



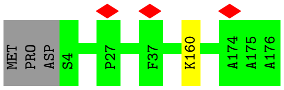
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

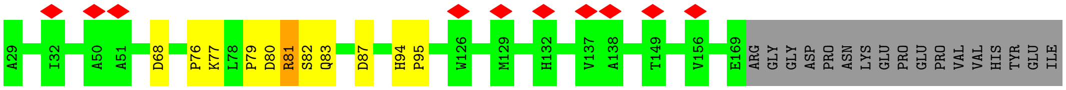


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



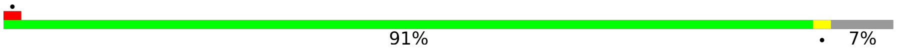
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

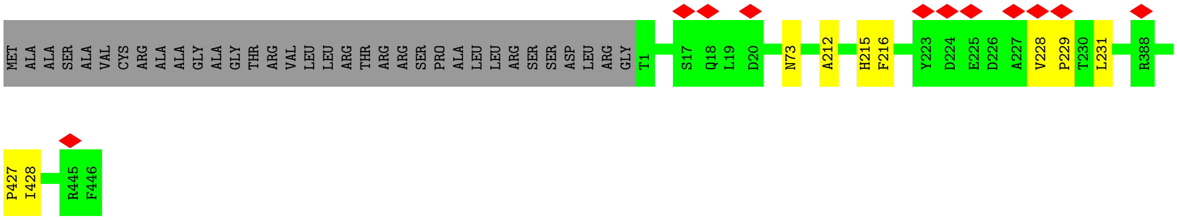
Chain e:



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

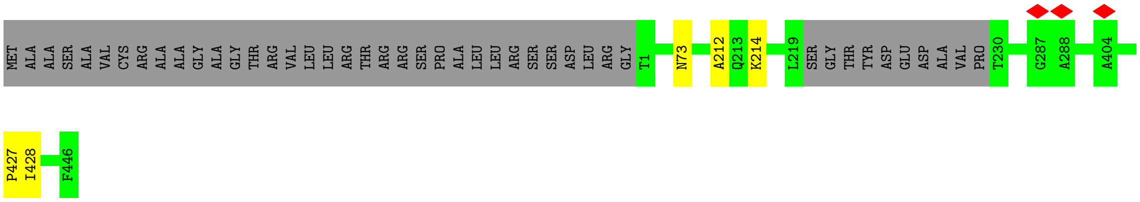
Chain k:





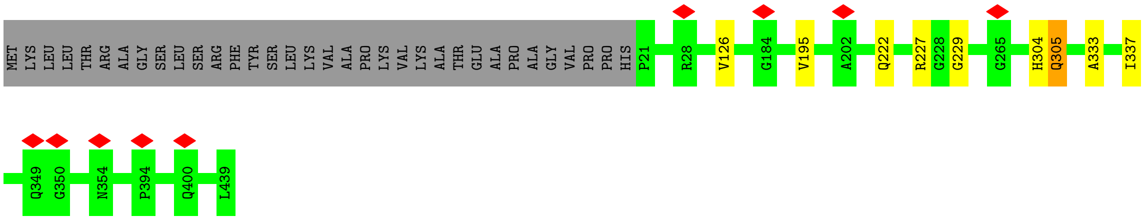
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain w:



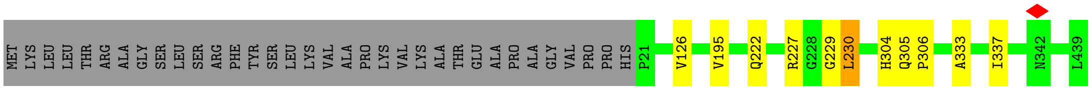
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain l:

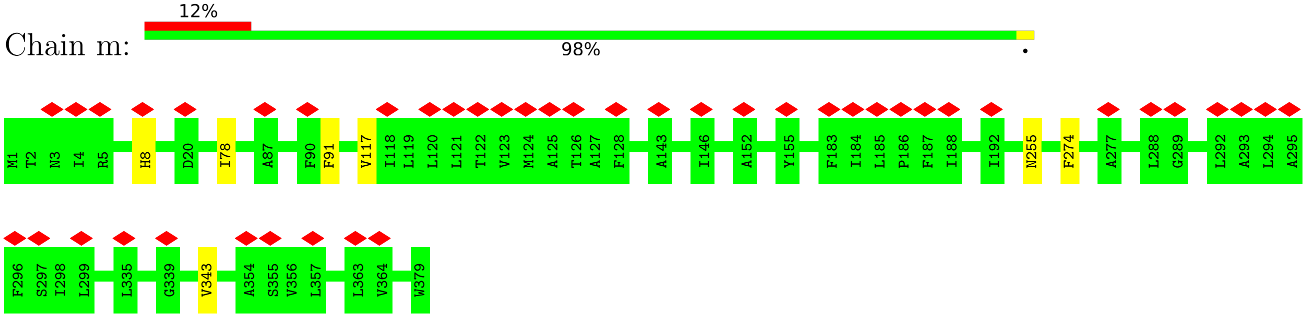


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

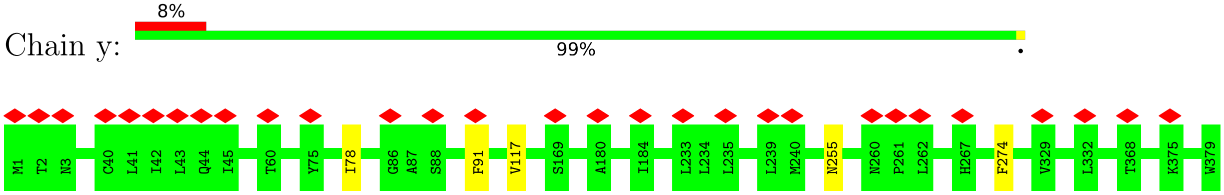
Chain x:



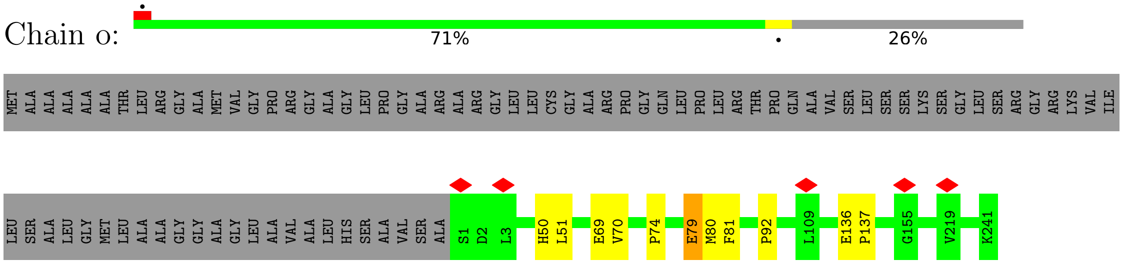
- Molecule 47: Cytochrome b



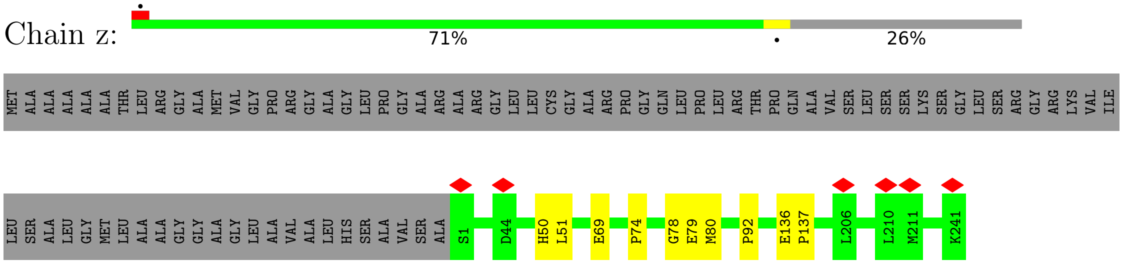
- Molecule 47: Cytochrome b



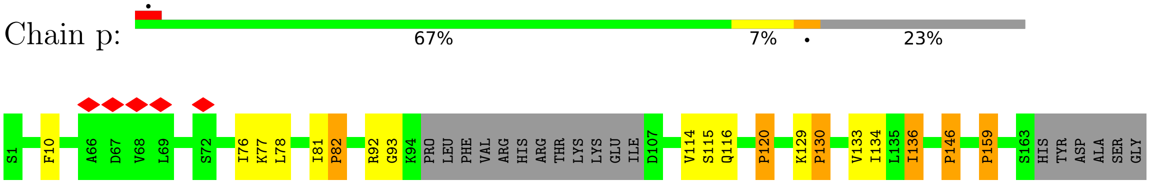
- Molecule 48: Cytochrome c1, heme protein, mitochondrial



- Molecule 48: Cytochrome c1, heme protein, mitochondrial

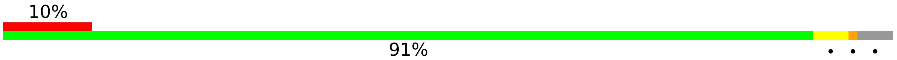


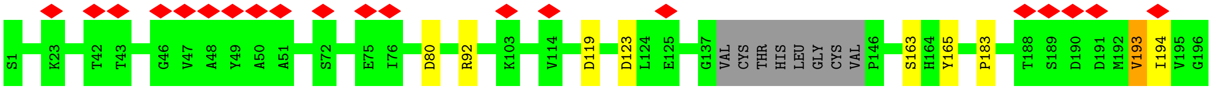
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

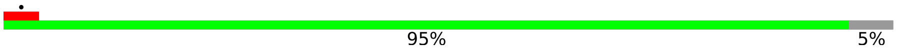
Chain A0:

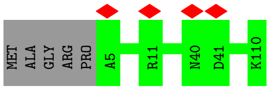




- Molecule 50: Cytochrome b-c1 complex subunit 7

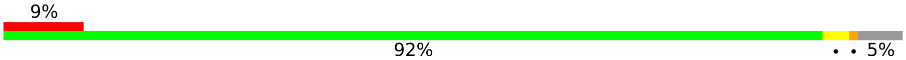
Chain q:

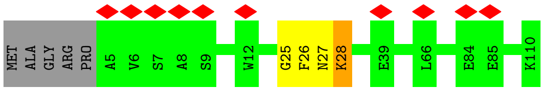




- Molecule 50: Cytochrome b-c1 complex subunit 7

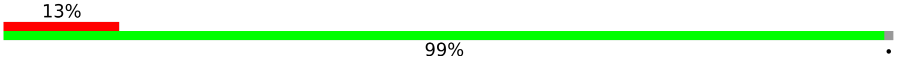
Chain A1:

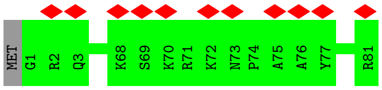




- Molecule 51: Cytochrome b-c1 complex subunit 8

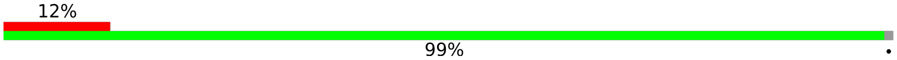
Chain r:

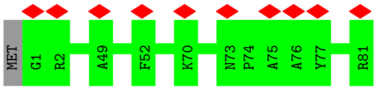




- Molecule 51: Cytochrome b-c1 complex subunit 8

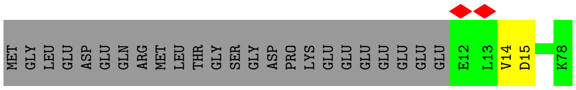
Chain A2:



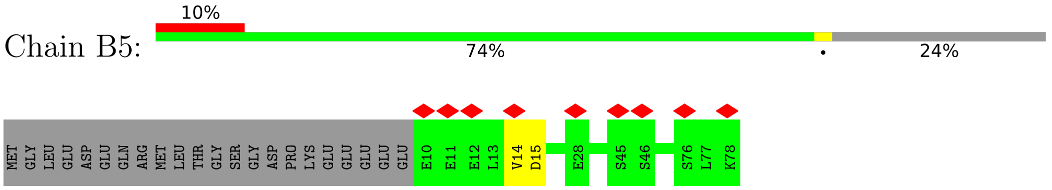


- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

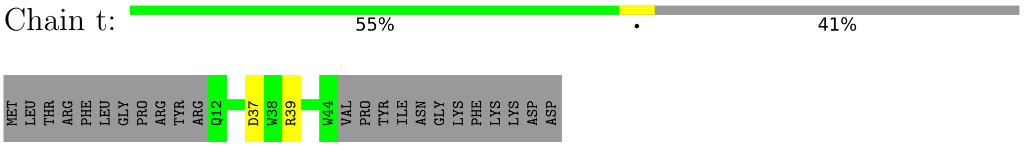
Chain s:



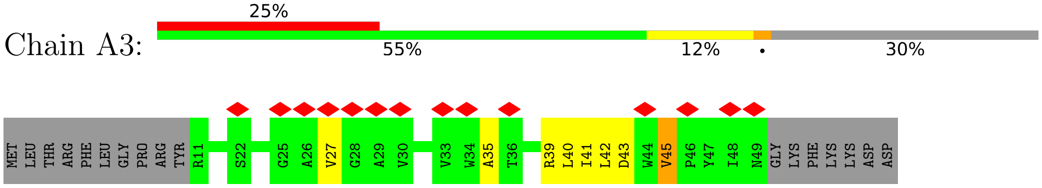
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



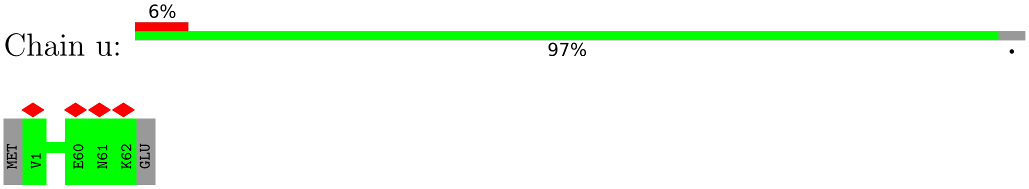
- Molecule 53: Cytochrome b-c1 complex subunit 10



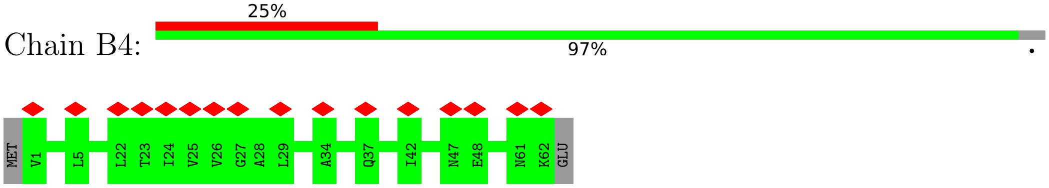
- Molecule 53: Cytochrome b-c1 complex subunit 10



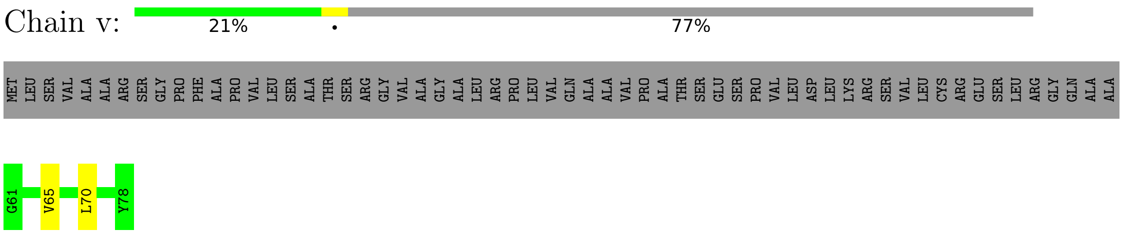
- Molecule 54: Cytochrome b-c1 complex subunit 9



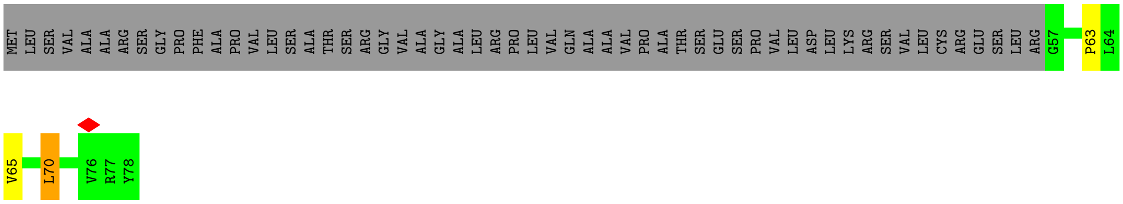
- Molecule 54: Cytochrome b-c1 complex subunit 9



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

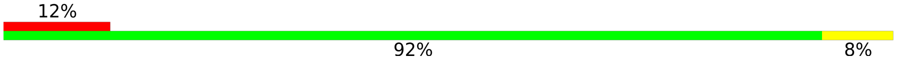


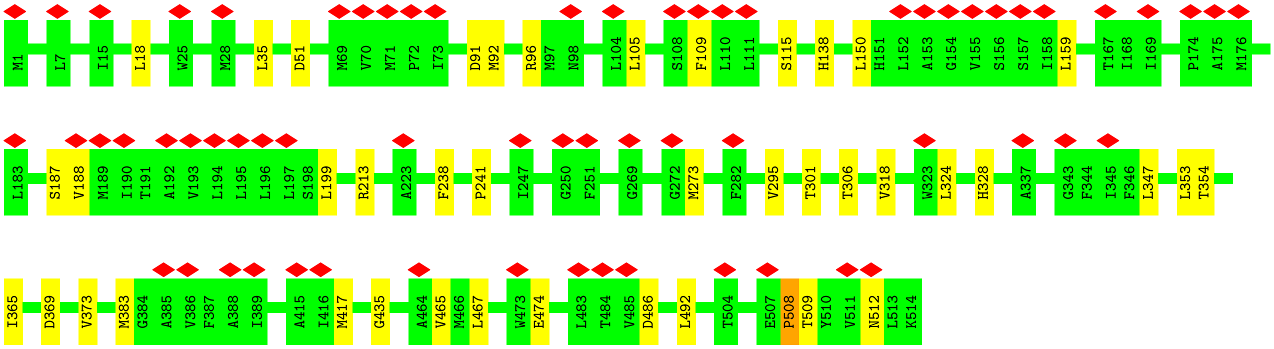
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 56: Cytochrome c oxidase subunit 1

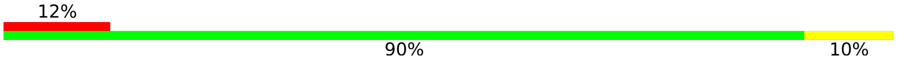
Chain A9:

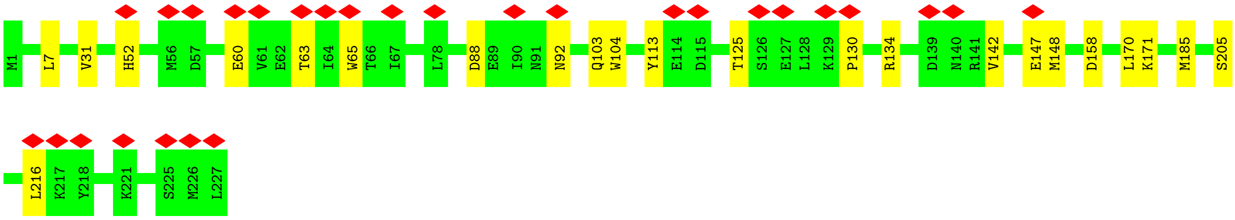




- Molecule 57: Cytochrome c oxidase subunit 2

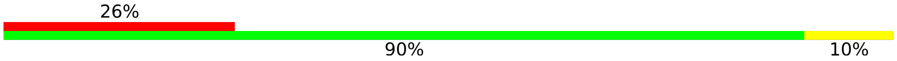
Chain B9:

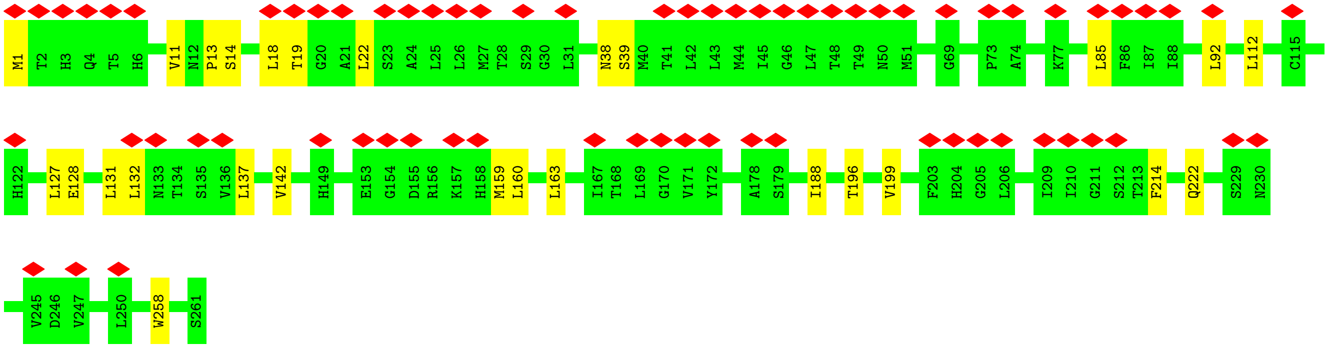




- Molecule 58: Cytochrome c oxidase subunit 3

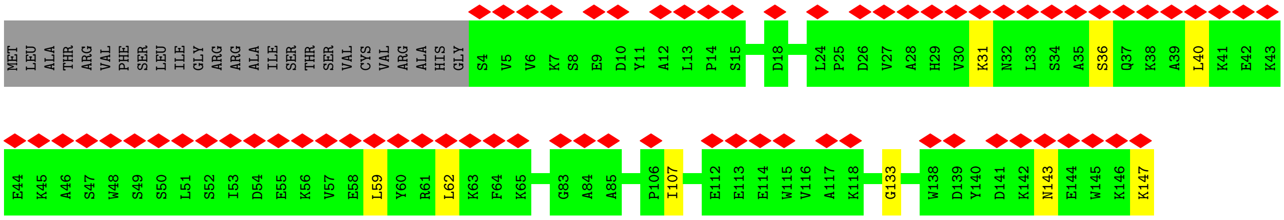
Chain B7:





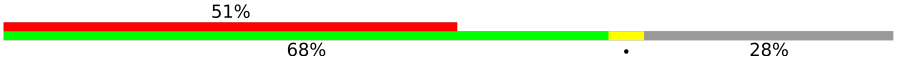
- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

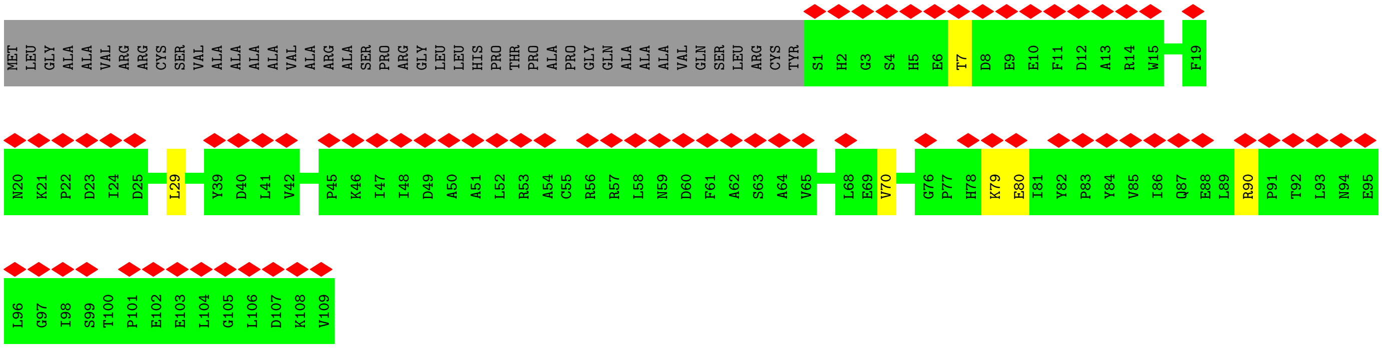
Chain A7:



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

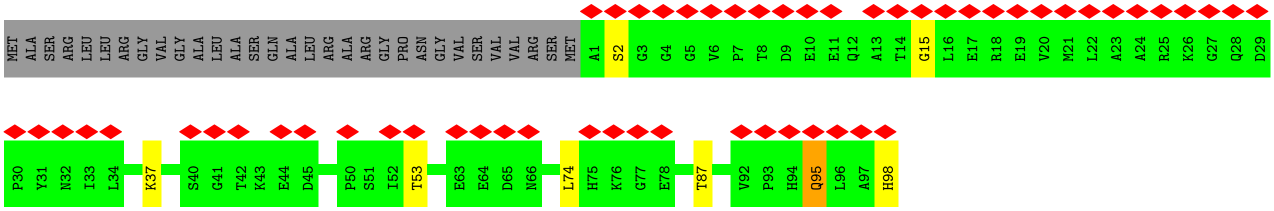
Chain A6:





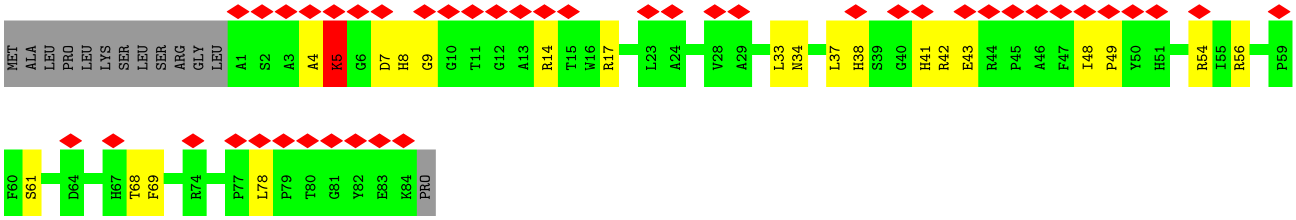
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial

Chain B2:



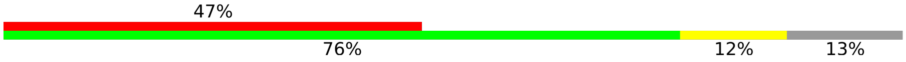
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial

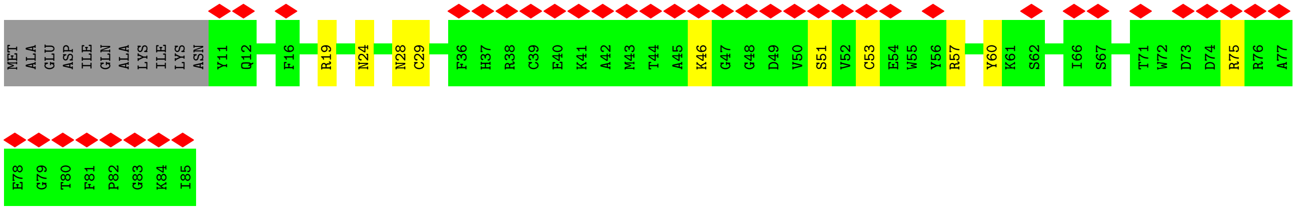
Chain A4:



- Molecule 63: Cytochrome c oxidase subunit 6B1

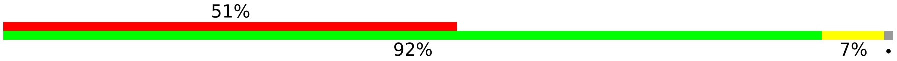
Chain A5:

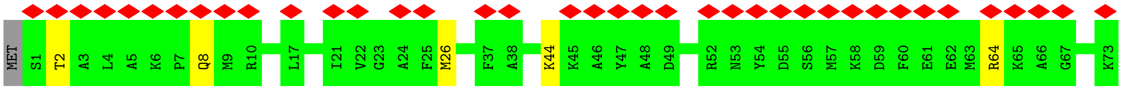




- Molecule 64: Cytochrome c oxidase subunit 6C

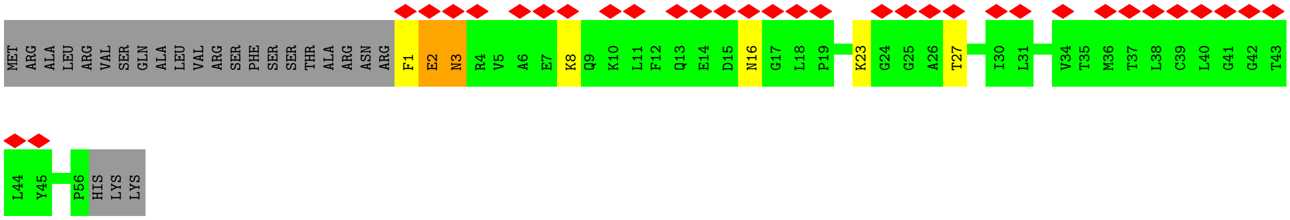
Chain B6:





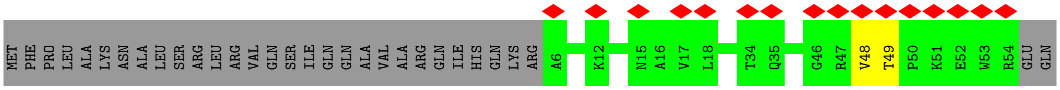
- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain B8:



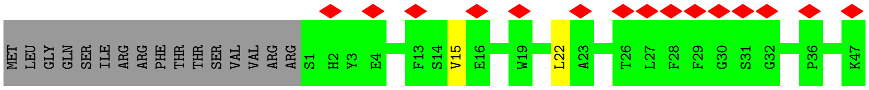
- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial

Chain B0:



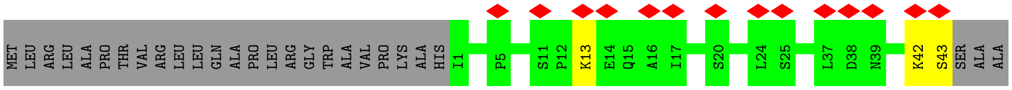
- Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial

Chain B1:



- 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	24810	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	0.368	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/1571	0.66	2/2149 (0.1%)
2	7	0.37	0/1213	0.68	0/1659
3	6	0.33	0/4892	0.64	3/6660 (0.0%)
4	2	0.43	0/2646	0.71	0/3618
5	4	0.40	0/3538	0.74	2/4845 (0.0%)
6	5	0.37	0/706	0.70	0/960
7	8	0.36	0/3035	0.60	3/4130 (0.1%)
8	1	0.41	0/2571	0.72	4/3512 (0.1%)
9	3	0.37	0/885	0.70	2/1213 (0.2%)
10	A	0.40	0/5265	0.66	3/7147 (0.0%)
11	B	0.50	0/3505	0.72	3/4752 (0.1%)
12	C	0.44	0/1756	0.65	0/2394
13	D	0.52	0/1231	0.67	0/1669
14	E	0.52	0/1418	0.68	0/1922
15	F	0.36	0/188	1.00	1/259 (0.4%)
16	G	0.42	0/1004	0.70	1/1359 (0.1%)
17	H	0.36	0/800	0.62	0/1076
18	I	0.38	0/538	0.65	0/722
19	J	0.34	0/545	0.52	0/740
20	K	0.30	0/663	0.63	1/896 (0.1%)
21	L	0.34	0/623	0.66	1/862 (0.1%)
22	N	0.31	0/882	0.60	0/1203
23	O	0.34	0/948	0.58	0/1279
24	P	0.34	0/719	0.68	0/981
25	Q	0.32	0/1381	0.63	0/1869
26	R	0.33	0/2465	0.67	0/3349
27	S	0.33	0/2345	0.66	1/3193 (0.0%)
28	T	0.34	0/938	0.64	0/1279
29	U	0.32	0/1053	0.65	1/1439 (0.1%)
30	V	0.36	0/1115	0.62	0/1508
31	M	0.30	0/651	0.65	0/876
31	W	0.28	0/624	0.66	0/847

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	X	0.32	0/383	0.65	0/523
33	Y	0.31	0/428	0.49	0/592
34	Z	0.37	0/506	0.71	1/688 (0.1%)
35	a	0.32	0/878	0.62	0/1195
36	b	0.33	0/1058	0.63	0/1434
37	c	0.33	0/632	0.75	4/871 (0.5%)
38	d	0.30	0/724	0.55	0/989
39	f	0.29	0/1191	0.56	1/1639 (0.1%)
40	h	0.38	0/679	0.64	0/926
41	i	0.27	0/286	0.45	0/392
42	j	0.37	0/922	0.70	1/1254 (0.1%)
43	g	0.31	0/1380	0.57	0/1872
44	e	0.30	0/888	0.70	0/1234
45	k	0.47	0/3527	0.62	2/4787 (0.0%)
45	w	0.46	0/3455	0.60	0/4685
46	l	0.43	0/3192	0.58	1/4329 (0.0%)
46	x	0.43	0/3198	0.59	2/4336 (0.0%)
47	m	0.58	0/3108	0.61	1/4252 (0.0%)
47	y	0.58	0/3108	0.61	1/4252 (0.0%)
48	o	0.54	1/1978 (0.1%)	0.64	2/2684 (0.1%)
48	z	0.54	1/1965 (0.1%)	0.62	0/2669
49	A0	0.39	0/1124	0.66	0/1538
49	p	0.45	0/945	0.85	5/1288 (0.4%)
50	A1	0.56	0/935	0.59	0/1253
50	q	0.57	0/935	0.56	0/1253
51	A2	0.47	0/698	0.57	0/944
51	r	0.47	0/704	0.56	0/951
52	B5	0.39	0/571	0.62	1/765 (0.1%)
52	s	0.40	0/553	0.63	1/741 (0.1%)
53	A3	0.47	0/314	0.63	0/434
53	t	0.32	0/272	0.50	0/377
54	B4	0.44	0/524	0.51	0/707
54	u	0.44	0/524	0.51	0/707
55	B3	0.42	0/149	1.04	0/203
55	v	0.38	0/114	0.88	1/156 (0.6%)
56	A9	0.60	0/4164	0.76	1/5688 (0.0%)
57	B9	0.58	0/1868	0.79	0/2544
58	B7	0.56	0/2212	0.68	0/3025
59	A7	0.57	0/1229	0.65	1/1658 (0.1%)
60	A6	0.50	0/898	0.66	0/1218
61	B2	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	B6	0.60	0/611	0.65	0/810
65	B8	0.61	0/451	0.72	0/610
66	B0	0.58	0/398	0.66	0/546
67	B1	0.63	0/399	0.62	0/534
68	A8	0.51	0/345	0.65	0/470
All	All	0.44	2/108248 (0.0%)	0.66	55/147255 (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	4
2	7	0	5
3	6	0	6
4	2	0	9
5	4	0	6
6	5	0	3
7	8	0	1
8	1	0	1
10	A	0	12
11	B	0	6
12	C	0	1
13	D	0	4
14	E	0	1
17	H	0	1
22	N	0	1
24	P	0	2
25	Q	0	1
26	R	0	4
27	S	0	4
28	T	0	2
29	U	0	1
30	V	0	3
31	M	0	1
31	W	0	1
36	b	0	3
38	d	0	1
39	f	0	1
40	h	0	2
42	j	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	g	0	1
44	e	0	5
45	k	0	6
45	w	0	3
46	l	0	3
46	x	0	3
47	m	0	4
47	y	0	2
48	o	0	4
48	z	0	4
49	A0	0	6
49	p	0	6
53	A3	0	1
55	B3	0	1
All	All	0	138

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	z	92	PRO	C-N	-5.38	1.21	1.34
48	o	92	PRO	C-N	-5.35	1.21	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	231	LEU	CB-CG-CD1	-7.72	97.88	111.00
49	p	146	PRO	N-CA-CB	7.18	111.92	103.30
5	4	212	LEU	CA-CB-CG	7.00	131.41	115.30
48	o	80	MET	CA-CB-CG	6.93	125.08	113.30
37	c	36	PRO	C-N-CD	-6.84	105.55	120.60
11	B	53	TYR	C-N-CD	-6.45	106.42	120.60
3	6	362	LEU	CA-CB-CG	6.44	130.11	115.30
8	1	100	LEU	CA-CB-CG	6.43	130.10	115.30
59	A7	133	GLY	N-CA-C	6.43	129.18	113.10
46	x	230	LEU	N-CA-C	6.35	128.14	111.00
8	1	174	LEU	CA-CB-CG	6.24	129.64	115.30
39	f	163	LEU	C-N-CA	6.17	147.91	122.00
10	A	560	LEU	CA-CB-CG	5.96	129.02	115.30
8	1	46	LEU	CA-CB-CG	5.92	128.92	115.30
7	8	228	PRO	C-N-CA	5.89	136.43	121.70
42	j	22	PRO	C-N-CD	-5.81	107.81	120.60
1	9	177	LEU	CA-CB-CG	5.81	128.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	x	304	HIS	C-N-CA	5.79	136.18	121.70
49	p	159	PRO	N-CA-CB	5.77	110.23	103.30
49	p	82	PRO	N-CA-CB	5.71	110.15	103.30
15	F	97	MET	C-N-CD	-5.67	108.12	120.60
9	3	3	LEU	C-N-CA	5.56	135.59	121.70
1	9	149	LEU	CA-CB-CG	5.54	128.03	115.30
47	m	78	ILE	CG1-CB-CG2	-5.53	99.22	111.40
49	p	120	PRO	N-CA-CB	5.53	109.93	103.30
9	3	5	LEU	CA-CB-CG	5.52	128.00	115.30
37	c	66	ARG	C-N-CA	5.52	135.50	121.70
29	U	120	THR	C-N-CD	-5.52	108.47	120.60
49	p	130	PRO	N-CA-CB	5.51	109.91	103.30
47	y	78	ILE	CG1-CB-CG2	-5.50	99.29	111.40
11	B	95	LEU	CA-CB-CG	5.40	127.71	115.30
37	c	36	PRO	C-N-CA	5.38	144.61	122.00
46	l	305	GLN	N-CA-C	5.35	125.45	111.00
48	o	79	GLU	N-CA-C	5.33	125.38	111.00
45	k	215	HIS	C-N-CA	5.32	135.00	121.70
3	6	74	LEU	CA-CB-CG	5.30	127.48	115.30
7	8	36	LYS	C-N-CA	5.28	134.91	121.70
52	B5	15	ASP	CB-CG-OD1	5.23	123.01	118.30
20	K	79	LEU	CA-CB-CG	5.23	127.33	115.30
62	A4	5	LYS	N-CA-C	5.22	125.10	111.00
27	S	196	ASP	CB-CG-OD2	5.21	122.98	118.30
52	s	15	ASP	CB-CG-OD1	5.20	122.98	118.30
7	8	259	GLY	C-N-CA	5.20	134.70	121.70
34	Z	85	GLU	C-N-CA	5.20	134.69	121.70
10	A	461	PRO	C-N-CA	5.17	134.63	121.70
10	A	381	LEU	CA-CB-CG	5.16	127.16	115.30
56	A9	435	GLY	N-CA-C	5.15	125.97	113.10
21	L	28	LEU	CA-CB-CG	5.13	127.10	115.30
37	c	114	GLY	C-N-CA	5.13	134.53	121.70
8	1	288	LEU	CA-CB-CG	5.13	127.10	115.30
16	G	56	ASP	CB-CG-OD1	5.12	122.90	118.30
11	B	293	LEU	N-CA-C	-5.07	97.31	111.00
5	4	65	LEU	CA-CB-CG	5.06	126.94	115.30
3	6	576	LEU	CB-CG-CD1	-5.04	102.43	111.00
55	v	70	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (138) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	281	ARG	Peptide
4	2	106	LEU	Peptide
4	2	111	PHE	Peptide
4	2	128	LEU	Peptide
4	2	199	THR	Peptide
4	2	222	ASN	Peptide
4	2	270	MET	Peptide
4	2	271	THR	Peptide
4	2	339	LEU	Peptide
4	2	45	MET	Peptide
5	4	140	THR	Peptide
5	4	222	GLU	Peptide
5	4	306	PRO	Peptide
5	4	368	ALA	Peptide
5	4	369	LEU	Peptide
5	4	71	TRP	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
3	6	29	PRO	Peptide
3	6	351	ASN	Peptide
3	6	352	ASP	Peptide
3	6	522	PHE	Peptide
3	6	549	ALA	Peptide
3	6	71	ILE	Peptide
2	7	140	ALA	Peptide
2	7	148	SER	Peptide
2	7	170	GLU	Peptide
2	7	24	PRO	Peptide
2	7	25	SER	Peptide
7	8	228	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	179	ALA	Peptide
1	9	75	LYS	Peptide
10	A	127	ASP	Peptide
10	A	128	CYS	Peptide
10	A	175	ARG	Peptide
10	A	236	TYR	Peptide
10	A	283	GLU	Peptide
10	A	308	ARG	Peptide
10	A	309	ASN	Peptide
10	A	382	ARG	Peptide

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Mol	Chain	Res	Type	Group
10	A	460	HIS	Peptide
10	A	461	PRO	Peptide
10	A	462	PHE	Peptide
10	A	98	LYS	Peptide
49	A0	119	ASP	Peptide
49	A0	123	ASP	Peptide
49	A0	163	SER	Peptide
49	A0	165	TYR	Peptide
49	A0	183	PRO	Peptide
49	A0	193	VAL	Peptide
53	A3	45	VAL	Peptide
11	B	218	SER	Peptide
11	B	290	GLY	Peptide
11	B	291	VAL	Peptide
11	B	87	GLN	Peptide
11	B	88	HIS	Peptide
11	B	89	PRO	Peptide
55	B3	70	LEU	Peptide
12	C	198	HIS	Peptide
13	D	113	PHE	Peptide
13	D	161	GLY	Peptide
13	D	186	CYS	Peptide
13	D	84	PRO	Peptide
14	E	107	PRO	Peptide
17	H	84	GLU	Peptide
31	M	24	LYS	Peptide
22	N	40	LYS	Peptide
24	P	36	GLN	Peptide
24	P	52	ASN	Peptide
25	Q	91	TYR	Peptide
26	R	271	TYR	Peptide
26	R	324	THR	Peptide
26	R	333	PRO	Peptide
26	R	355	ARG	Peptide
27	S	100	CYS	Peptide
27	S	275	ASN	Peptide
27	S	278	ASN	Peptide
27	S	38	THR	Peptide
28	T	105	THR	Peptide
28	T	83	LYS	Peptide
29	U	118	SER	Peptide
30	V	10	MET	Peptide

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Mol	Chain	Res	Type	Group
30	V	142	TRP	Peptide
30	V	72	MET	Peptide
31	W	154	VAL	Peptide
36	b	110	TRP	Peptide
36	b	134	GLU	Peptide
36	b	96	ALA	Peptide
38	d	18	ASP	Peptide
44	e	77	LYS	Peptide
44	e	79	PRO	Peptide
44	e	81	ARG	Peptide
44	e	87	ASP	Peptide
44	e	94	HIS	Peptide
39	f	109	PRO	Peptide
43	g	160	LYS	Peptide
40	h	80	PRO	Peptide
40	h	81	ALA	Peptide
42	j	115	GLU	Peptide
42	j	21	LEU	Peptide
45	k	212	ALA	Peptide
45	k	216	PHE	Peptide
45	k	228	VAL	Peptide
45	k	229	PRO	Peptide
45	k	428	ILE	Peptide
45	k	73	ASN	Peptide
46	l	227	ARG	Peptide
46	l	229	GLY	Mainchain
46	l	304	HIS	Peptide
47	m	255	ASN	Peptide
47	m	274	PHE	Peptide
47	m	343	VAL	Mainchain
47	m	8	HIS	Peptide
48	o	50	HIS	Peptide
48	o	69	GLU	Mainchain
48	o	79	GLU	Peptide
48	o	81	PHE	Peptide
49	p	10	PHE	Peptide
49	p	133	VAL	Peptide
49	p	136	ILE	Peptide
49	p	76	ILE	Peptide
49	p	77	LYS	Peptide
49	p	78	LEU	Peptide
45	w	212	ALA	Peptide

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Mol	Chain	Res	Type	Group
45	w	428	ILE	Peptide
45	w	73	ASN	Peptide
46	x	227	ARG	Peptide
46	x	229	GLY	Mainchain
46	x	230	LEU	Peptide
47	y	255	ASN	Peptide
47	y	274	PHE	Peptide
48	z	50	HIS	Peptide
48	z	69	GLU	Peptide,Mainchain
48	z	78	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%)	166 (81%)	38 (18%)	1 (0%)	29	69
2	7	170/175 (97%)	135 (79%)	31 (18%)	4 (2%)	6	33
3	6	604/606 (100%)	518 (86%)	82 (14%)	4 (1%)	22	63
4	2	342/347 (99%)	298 (87%)	44 (13%)	0	100	100
5	4	457/459 (100%)	374 (82%)	77 (17%)	6 (1%)	12	48
6	5	94/98 (96%)	80 (85%)	14 (15%)	0	100	100
7	8	425/444 (96%)	343 (81%)	80 (19%)	2 (0%)	29	69
8	1	315/318 (99%)	270 (86%)	43 (14%)	2 (1%)	25	66
9	3	110/115 (96%)	92 (84%)	16 (14%)	2 (2%)	8	40
10	A	686/704 (97%)	563 (82%)	118 (17%)	5 (1%)	22	63
11	B	428/430 (100%)	357 (83%)	64 (15%)	7 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	C	206/228 (90%)	175 (85%)	31 (15%)	0	100	100
13	D	150/179 (84%)	133 (89%)	17 (11%)	0	100	100
14	E	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	25	66
15	F	26/75 (35%)	17 (65%)	9 (35%)	0	100	100
16	G	121/133 (91%)	99 (82%)	20 (16%)	2 (2%)	9	42
17	H	94/105 (90%)	74 (79%)	19 (20%)	1 (1%)	14	52
18	I	69/96 (72%)	57 (83%)	11 (16%)	1 (1%)	11	46
19	J	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	10	46
20	K	82/98 (84%)	62 (76%)	20 (24%)	0	100	100
21	L	78/83 (94%)	68 (87%)	10 (13%)	0	100	100
22	N	109/115 (95%)	91 (84%)	18 (16%)	0	100	100
23	O	112/127 (88%)	98 (88%)	14 (12%)	0	100	100
24	P	86/112 (77%)	66 (77%)	20 (23%)	0	100	100
25	Q	166/171 (97%)	117 (70%)	47 (28%)	2 (1%)	13	50
26	R	315/345 (91%)	249 (79%)	64 (20%)	2 (1%)	25	66
27	S	317/320 (99%)	249 (78%)	64 (20%)	4 (1%)	12	48
28	T	136/140 (97%)	112 (82%)	16 (12%)	8 (6%)	1	17
29	U	128/145 (88%)	101 (79%)	27 (21%)	0	100	100
30	V	136/143 (95%)	119 (88%)	15 (11%)	2 (2%)	10	46
31	M	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
31	W	84/88 (96%)	66 (79%)	18 (21%)	0	100	100
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	22
33	Y	55/72 (76%)	44 (80%)	11 (20%)	0	100	100
34	Z	72/97 (74%)	49 (68%)	23 (32%)	0	100	100
35	a	112/128 (88%)	87 (78%)	25 (22%)	0	100	100
36	b	137/143 (96%)	118 (86%)	19 (14%)	0	100	100
37	c	86/127 (68%)	67 (78%)	19 (22%)	0	100	100
38	d	105/117 (90%)	77 (73%)	24 (23%)	4 (4%)	3	24
39	f	165/178 (93%)	126 (76%)	38 (23%)	1 (1%)	25	66
40	h	82/125 (66%)	57 (70%)	23 (28%)	2 (2%)	6	33
41	i	36/49 (74%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	j	111/120 (92%)	95 (86%)	16 (14%)	0	100	100
43	g	171/176 (97%)	143 (84%)	28 (16%)	0	100	100
44	e	139/158 (88%)	80 (58%)	52 (37%)	7 (5%)	2	20
45	k	444/480 (92%)	401 (90%)	42 (10%)	1 (0%)	47	81
45	w	432/480 (90%)	397 (92%)	33 (8%)	2 (0%)	29	69
46	l	417/453 (92%)	380 (91%)	31 (7%)	6 (1%)	11	46
46	x	417/453 (92%)	379 (91%)	31 (7%)	7 (2%)	9	42
47	m	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	41	77
47	y	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	41	77
48	o	239/325 (74%)	211 (88%)	24 (10%)	4 (2%)	9	42
48	z	239/325 (74%)	211 (88%)	23 (10%)	5 (2%)	7	36
49	A0	184/196 (94%)	135 (73%)	45 (24%)	4 (2%)	6	35
49	p	147/196 (75%)	93 (63%)	40 (27%)	14 (10%)	0	10
50	A1	104/111 (94%)	94 (90%)	7 (7%)	3 (3%)	4	29
50	q	104/111 (94%)	98 (94%)	6 (6%)	0	100	100
51	A2	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
51	r	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
52	B5	67/91 (74%)	57 (85%)	9 (13%)	1 (2%)	10	46
52	s	65/91 (71%)	55 (85%)	9 (14%)	1 (2%)	10	46
53	A3	37/56 (66%)	26 (70%)	7 (19%)	4 (11%)	0	8
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	4	26
54	B4	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
54	u	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
55	B3	20/78 (26%)	9 (45%)	9 (45%)	2 (10%)	0	9
55	v	16/78 (20%)	7 (44%)	8 (50%)	1 (6%)	1	17
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
57	B9	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
58	B7	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	A6	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	B2	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	A4	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	17
63	A5	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	11	46
64	B6	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	B8	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	3	24
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	B1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13637/15129 (90%)	11563 (85%)	1924 (14%)	150 (1%)	18	52

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	7	171	ILE
9	3	43	PRO
10	A	463	SER
11	B	54	PRO
11	B	56	LYS
11	B	294	ARG
27	S	200	PRO
27	S	276	ASP
28	T	35	VAL
28	T	46	PRO
28	T	51	GLU
38	d	40	VAL
40	h	81	ALA
40	h	82	VAL
44	e	81	ARG
44	e	82	SER
49	p	82	PRO
49	p	120	PRO
49	p	129	LYS
49	p	146	PRO
49	p	159	PRO
52	s	14	VAL
48	z	80	MET
50	A1	25	GLY
50	A1	27	ASN
50	A1	28	LYS
52	B5	14	VAL
53	A3	35	ALA

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Mol	Chain	Res	Type
53	A3	43	ASP
56	A9	328	HIS
56	A9	508	PRO
61	B2	2	SER
61	B2	87	THR
61	B2	95	GLN
62	A4	4	ALA
62	A4	9	GLY
63	A5	46	LYS
65	B8	2	GLU
3	6	31	ASN
3	6	603	ASN
5	4	20	ASN
5	4	419	TYR
8	1	282	TYR
10	A	365	THR
16	G	122	SER
18	I	105	LYS
26	R	272	LEU
28	T	65	ALA
30	V	143	TYR
32	X	14	VAL
49	p	130	PRO
53	t	37	ASP
55	v	65	VAL
48	z	79	GLU
49	A0	80	ASP
49	A0	92	ARG
53	A3	42	LEU
55	B3	65	VAL
62	A4	5	LYS
1	9	76	ALA
2	7	149	TYR
5	4	21	ASN
10	A	129	PRO
10	A	309	ASN
10	A	541	PRO
17	H	16	ARG
38	d	19	PRO
44	e	68	ASP
44	e	76	PRO
46	l	305	GLN

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Mol	Chain	Res	Type
49	p	81	ILE
45	w	214	LYS
46	x	305	GLN
57	B9	104	TRP
62	A4	61	SER
2	7	170	GLU
3	6	551	SER
5	4	64	PRO
5	4	112	ALA
8	1	174	LEU
9	3	82	ALA
11	B	291	VAL
14	E	108	SER
27	S	199	VAL
28	T	50	LEU
28	T	58	ARG
38	d	38	GLU
44	e	80	ASP
44	e	83	GLN
45	k	427	PRO
49	p	115	SER
49	p	116	GLN
49	p	134	ILE
49	p	136	ILE
45	w	427	PRO
49	A0	193	VAL
56	A9	51	ASP
3	6	30	SER
11	B	89	PRO
11	B	219	GLY
25	Q	29	ALA
25	Q	166	ARG
44	e	95	PRO
48	o	51	LEU
49	p	92	ARG
48	z	51	LEU
57	B9	103	GLN
65	B8	3	ASN
7	8	227	PRO
11	B	88	HIS
16	G	84	ARG
27	S	281	LYS

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Mol	Chain	Res	Type
32	X	13	HIS
46	l	222	GLN
46	l	333	ALA
46	x	222	GLN
46	x	333	ALA
56	A9	91	ASP
57	B9	158	ASP
62	A4	49	PRO
48	o	70	VAL
48	o	74	PRO
48	z	74	PRO
39	f	145	PRO
46	l	126	VAL
46	l	195	VAL
47	m	117	VAL
49	p	93	GLY
46	x	126	VAL
46	x	195	VAL
47	y	117	VAL
49	A0	194	ILE
2	7	24	PRO
5	4	305	THR
7	8	105	PRO
46	l	337	ILE
46	x	337	ILE
53	A3	27	VAL
61	B2	15	GLY
19	J	56	GLY
28	T	84	PRO
48	o	137	PRO
49	p	114	VAL
46	x	306	PRO
48	z	137	PRO
55	B3	63	PRO
26	R	328	ILE
28	T	45	THR
30	V	73	PRO
38	d	32	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	159/183 (87%)	158 (99%)	1 (1%)	86	92
2	7	104/142 (73%)	104 (100%)	0	100	100
3	6	523/534 (98%)	523 (100%)	0	100	100
4	2	274/316 (87%)	274 (100%)	0	100	100
5	4	351/413 (85%)	351 (100%)	0	100	100
6	5	75/86 (87%)	75 (100%)	0	100	100
7	8	236/353 (67%)	236 (100%)	0	100	100
8	1	273/275 (99%)	268 (98%)	5 (2%)	59	77
9	3	89/101 (88%)	88 (99%)	1 (1%)	73	84
10	A	550/588 (94%)	550 (100%)	0	100	100
11	B	362/371 (98%)	360 (99%)	2 (1%)	86	92
12	C	183/204 (90%)	183 (100%)	0	100	100
13	D	126/150 (84%)	126 (100%)	0	100	100
14	E	145/151 (96%)	145 (100%)	0	100	100
15	F	13/69 (19%)	13 (100%)	0	100	100
16	G	105/119 (88%)	105 (100%)	0	100	100
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	52/79 (66%)	50 (96%)	2 (4%)	33	57
19	J	50/59 (85%)	50 (100%)	0	100	100
20	K	66/81 (82%)	66 (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	72/96 (75%)	72 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	S	204/283 (72%)	203 (100%)	1 (0%)	88	93
28	T	75/101 (74%)	74 (99%)	1 (1%)	69	81
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%)	56 (98%)	1 (2%)	59	77
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/75 (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	45/121 (37%)	45 (100%)	0	100	100
38	d	42/107 (39%)	42 (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	88/106 (83%)	88 (100%)	0	100	100
43	g	130/157 (83%)	130 (100%)	0	100	100
44	e	44/141 (31%)	44 (100%)	0	100	100
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%)	326 (100%)	1 (0%)	92	95
47	y	327/327 (100%)	326 (100%)	1 (0%)	92	95
48	o	206/257 (80%)	205 (100%)	1 (0%)	88	93
48	z	202/257 (79%)	201 (100%)	1 (0%)	88	93
49	A0	64/168 (38%)	64 (100%)	0	100	100
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	94 (98%)	2 (2%)	53	72
50	q	96/99 (97%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	A2	70/72 (97%)	70 (100%)	0	100	100
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B5	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	28/46 (61%)	24 (86%)	4 (14%)	3	16
53	t	24/46 (52%)	23 (96%)	1 (4%)	30	54
54	B4	52/54 (96%)	52 (100%)	0	100	100
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B3	15/60 (25%)	14 (93%)	1 (7%)	16	41
55	v	11/60 (18%)	11 (100%)	0	100	100
56	A9	427/427 (100%)	389 (91%)	38 (9%)	9	30
57	B9	211/211 (100%)	191 (90%)	20 (10%)	8	27
58	B7	226/226 (100%)	199 (88%)	27 (12%)	5	20
59	A7	128/148 (86%)	120 (94%)	8 (6%)	18	43
60	A6	95/123 (77%)	89 (94%)	6 (6%)	18	43
61	B2	81/103 (79%)	76 (94%)	5 (6%)	18	43
62	A4	68/79 (86%)	50 (74%)	18 (26%)	0	3
63	A5	67/76 (88%)	58 (87%)	9 (13%)	4	17
64	B6	58/59 (98%)	53 (91%)	5 (9%)	10	32
65	B8	47/68 (69%)	40 (85%)	7 (15%)	3	15
66	B0	39/66 (59%)	37 (95%)	2 (5%)	24	48
67	B1	40/55 (73%)	38 (95%)	2 (5%)	24	49
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	35
All	All	10623/12909 (82%)	10446 (98%)	177 (2%)	62	78

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9	149	LEU
8	1	223	PHE
8	1	224	PHE
8	1	225	MET
8	1	227	GLU
8	1	228	TYR

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Mol	Chain	Res	Type
9	3	44	MET
11	B	105	MET
11	B	429	PHE
18	I	103	LEU
18	I	108	LYS
25	Q	115	LEU
27	S	195	VAL
28	T	61	PHE
31	W	106	LYS
47	m	91	PHE
48	o	136	GLU
53	t	39	ARG
47	y	91	PHE
48	z	136	GLU
50	A1	26	PHE
50	A1	28	LYS
53	A3	39	ARG
53	A3	40	LEU
53	A3	41	ILE
53	A3	45	VAL
55	B3	70	LEU
56	A9	18	LEU
56	A9	35	LEU
56	A9	92	MET
56	A9	96	ARG
56	A9	105	LEU
56	A9	109	PHE
56	A9	115	SER
56	A9	138	HIS
56	A9	150	LEU
56	A9	159	LEU
56	A9	187	SER
56	A9	188	VAL
56	A9	199	LEU
56	A9	213	ARG
56	A9	238	PHE
56	A9	241	PRO
56	A9	273	MET
56	A9	295	VAL
56	A9	301	THR
56	A9	306	THR
56	A9	318	VAL

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Mol	Chain	Res	Type
56	A9	324	LEU
56	A9	347	LEU
56	A9	353	LEU
56	A9	354	THR
56	A9	365	ILE
56	A9	369	ASP
56	A9	373	VAL
56	A9	383	MET
56	A9	417	MET
56	A9	465	VAL
56	A9	467	LEU
56	A9	474	GLU
56	A9	486	ASP
56	A9	492	LEU
56	A9	508	PRO
56	A9	509	THR
56	A9	512	ASN
57	B9	7	LEU
57	B9	31	VAL
57	B9	52	HIS
57	B9	60	GLU
57	B9	63	THR
57	B9	65	TRP
57	B9	88	ASP
57	B9	92	ASN
57	B9	113	TYR
57	B9	125	THR
57	B9	130	PRO
57	B9	134	ARG
57	B9	142	VAL
57	B9	147	GLU
57	B9	148	MET
57	B9	170	LEU
57	B9	171	LYS
57	B9	185	MET
57	B9	205	SER
57	B9	216	LEU
58	B7	1	MET
58	B7	11	VAL
58	B7	13	PRO
58	B7	14	SER
58	B7	18	LEU

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Mol	Chain	Res	Type
58	B7	19	THR
58	B7	22	LEU
58	B7	38	ASN
58	B7	39	SER
58	B7	85	LEU
58	B7	92	LEU
58	B7	112	LEU
58	B7	127	LEU
58	B7	128	GLU
58	B7	131	LEU
58	B7	132	LEU
58	B7	137	LEU
58	B7	142	VAL
58	B7	159	MET
58	B7	160	LEU
58	B7	163	LEU
58	B7	188	ILE
58	B7	196	THR
58	B7	199	VAL
58	B7	214	PHE
58	B7	222	GLN
58	B7	258	TRP
59	A7	31	LYS
59	A7	36	SER
59	A7	40	LEU
59	A7	59	LEU
59	A7	62	LEU
59	A7	107	ILE
59	A7	143	ASN
59	A7	147	LYS
60	A6	7	THR
60	A6	29	LEU
60	A6	70	VAL
60	A6	79	LYS
60	A6	80	GLU
60	A6	90	ARG
61	B2	37	LYS
61	B2	53	THR
61	B2	74	LEU
61	B2	95	GLN
61	B2	98	HIS
62	A4	5	LYS

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Mol	Chain	Res	Type
62	A4	7	ASP
62	A4	8	HIS
62	A4	14	ARG
62	A4	17	ARG
62	A4	33	LEU
62	A4	34	ASN
62	A4	37	LEU
62	A4	38	HIS
62	A4	41	HIS
62	A4	42	ARG
62	A4	43	GLU
62	A4	48	ILE
62	A4	54	ARG
62	A4	56	ARG
62	A4	68	THR
62	A4	69	PHE
62	A4	78	LEU
63	A5	19	ARG
63	A5	24	ASN
63	A5	28	ASN
63	A5	29	CYS
63	A5	51	SER
63	A5	53	CYS
63	A5	57	ARG
63	A5	60	TYR
63	A5	75	ARG
64	B6	2	THR
64	B6	8	GLN
64	B6	26	MET
64	B6	44	LYS
64	B6	64	ARG
65	B8	1	PHE
65	B8	2	GLU
65	B8	3	ASN
65	B8	8	LYS
65	B8	16	ASN
65	B8	23	LYS
65	B8	27	THR
66	B0	48	VAL
66	B0	49	THR
67	B1	15	VAL
67	B1	22	LEU

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Mol	Chain	Res	Type
68	A8	13	LYS
68	A8	42	LYS
68	A8	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	9	90	ASN
1	9	189	ASN
2	7	46	ASN
3	6	226	GLN
3	6	270	ASN
3	6	332	HIS
3	6	405	ASN
3	6	479	GLN
3	6	546	GLN
4	2	49	ASN
5	4	26	ASN
5	4	168	GLN
5	4	374	ASN
6	5	7	ASN
7	8	281	HIS
7	8	422	HIS
8	1	5	ASN
8	1	124	ASN
8	1	284	GLN
8	1	292	ASN
8	1	317	GLN
9	3	10	ASN
10	A	142	GLN
10	A	309	ASN
10	A	359	ASN
10	A	571	HIS
11	B	112	HIS
11	B	182	ASN
11	B	250	ASN
12	C	249	GLN
13	D	98	HIS
13	D	158	ASN
14	E	192	ASN
14	E	204	ASN
17	H	82	GLN

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Mol	Chain	Res	Type
18	I	118	GLN
21	L	46	ASN
22	N	83	GLN
22	N	111	GLN
26	R	43	HIS
26	R	171	ASN
26	R	251	ASN
26	R	323	HIS
26	R	331	HIS
28	T	89	ASN
29	U	31	ASN
31	W	115	GLN
32	X	13	HIS
37	c	14	GLN
39	f	139	GLN
41	i	62	HIS
42	j	88	HIS
31	M	74	GLN
45	k	15	GLN
45	k	85	HIS
45	k	118	GLN
45	k	207	GLN
45	k	243	HIS
45	k	252	HIS
45	k	363	ASN
46	l	162	ASN
46	l	254	HIS
46	l	277	HIS
46	l	304	HIS
46	l	354	ASN
47	m	3	ASN
47	m	32	ASN
47	m	255	ASN
47	m	308	HIS
47	m	312	GLN
48	o	105	ASN
49	p	53	ASN
51	r	12	HIS
51	r	23	GLN
51	r	79	ASN
52	s	71	HIS
45	w	15	GLN

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Mol	Chain	Res	Type
45	w	21	ASN
45	w	85	HIS
45	w	159	GLN
45	w	207	GLN
45	w	252	HIS
45	w	363	ASN
46	x	162	ASN
46	x	254	HIS
46	x	277	HIS
46	x	304	HIS
46	x	354	ASN
47	y	3	ASN
47	y	32	ASN
47	y	255	ASN
47	y	308	HIS
47	y	312	GLN
47	y	374	ASN
48	z	75	ASN
48	z	105	ASN
49	A0	57	GLN
51	A2	12	HIS
51	A2	79	ASN
52	B5	71	HIS
56	A9	11	ASN
56	A9	12	HIS
56	A9	43	GLN
56	A9	99	ASN
56	A9	170	ASN
56	A9	256	HIS
56	A9	360	ASN
56	A9	413	HIS
56	A9	512	ASN
57	B9	103	GLN
57	B9	203	ASN
58	B7	6	HIS
58	B7	12	ASN
58	B7	133	ASN
58	B7	148	HIS
58	B7	158	HIS
58	B7	207	HIS
58	B7	222	GLN
58	B7	232	HIS

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Mol	Chain	Res	Type
59	A7	109	HIS
60	A6	34	ASN
61	B2	66	ASN
62	A4	52	HIS
63	A5	23	GLN
63	A5	24	ASN
63	A5	25	GLN
63	A5	28	ASN
63	A5	37	HIS
64	B6	53	ASN
65	B8	3	ASN
65	B8	16	ASN
66	B0	10	HIS
66	B0	15	ASN
66	B0	41	ASN
67	B1	42	HIS
68	A8	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
69	FES	9	301	-	0,4,4	-	-	-		
69	FES	A	803	-	0,4,4	-	-	-		
71	3PE	4	502	-	40,40,50	0.93	3 (7%)	43,45,55	1.37	3 (6%)
79	HEA	A9	602	56	57,67,67	1.47	6 (10%)	61,103,103	1.45	11 (18%)
70	CDL	4	501	-	81,81,99	0.97	6 (7%)	87,93,111	1.10	5 (5%)
71	3PE	V	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
72	PC1	S	401	-	46,46,53	0.99	4 (8%)	52,54,61	0.99	2 (3%)
78	HEC	o	301	48	32,50,50	2.46	6 (18%)	24,82,82	1.67	7 (29%)
74	SF4	D	301	-	0,12,12	-	-	-		
72	PC1	L	200	-	46,46,53	1.02	4 (8%)	52,54,61	1.06	2 (3%)
74	SF4	E	301	-	0,12,12	-	-	-		
72	PC1	Q	201	-	45,45,53	1.00	4 (8%)	51,53,61	1.07	2 (3%)
71	3PE	2	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.18	2 (4%)
77	HEM	m	402	47	41,50,50	1.93	12 (29%)	45,82,82	1.50	7 (15%)
77	HEM	y	402	47	41,50,50	1.91	12 (29%)	45,82,82	1.50	7 (15%)
72	PC1	j	201	-	38,38,53	1.12	4 (10%)	44,46,61	1.10	2 (4%)
72	PC1	2	402	-	45,45,53	1.00	3 (6%)	51,53,61	1.03	2 (3%)
74	SF4	A	801	-	0,12,12	-	-	-		
79	HEA	A9	601	56	57,67,67	1.24	6 (10%)	61,103,103	1.47	12 (19%)
71	3PE	B	501	11	50,50,50	0.85	4 (8%)	53,55,55	1.12	2 (3%)
74	SF4	A	802	-	0,12,12	-	-	-		
78	HEC	z	301	48	32,50,50	2.45	6 (18%)	24,82,82	1.67	7 (29%)
69	FES	m	403	-	0,4,4	-	-	-		
74	SF4	8	502	-	0,12,12	-	-	-		
77	HEM	m	401	47	41,50,50	1.80	11 (26%)	45,82,82	1.88	10 (22%)
74	SF4	E	302	-	0,12,12	-	-	-		
71	3PE	j	202	-	45,45,50	0.91	4 (8%)	48,50,55	1.05	2 (4%)
77	HEM	y	401	47	41,50,50	1.79	11 (26%)	45,82,82	1.88	10 (22%)
73	FMN	8	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.62	11 (22%)
76	NAP	R	601	-	45,52,52	4.64	20 (44%)	56,80,80	1.79	7 (12%)
70	CDL	6	701	-	63,63,99	1.07	7 (11%)	69,75,111	1.28	4 (5%)
70	CDL	J	101	-	57,57,99	1.14	7 (12%)	63,69,111	1.19	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	FES	9	301	-	-	-	0/1/1/1
69	FES	A	803	-	-	-	0/1/1/1
71	3PE	4	502	-	-	24/44/44/54	-
79	HEA	A9	602	56	3/3/7/16	5/32/76/76	-
70	CDL	4	501	-	-	39/92/92/110	-
71	3PE	V	201	-	-	21/54/54/54	-
72	PC1	S	401	-	-	32/50/50/57	-
78	HEC	o	301	48	-	3/10/54/54	-
74	SF4	D	301	-	-	-	0/6/5/5
72	PC1	L	200	-	-	23/50/50/57	-
74	SF4	E	301	-	-	-	0/6/5/5
72	PC1	Q	201	-	-	20/49/49/57	-
71	3PE	2	401	-	-	21/44/44/54	-
77	HEM	m	402	47	-	2/12/54/54	-
77	HEM	y	402	47	-	2/12/54/54	-
72	PC1	j	201	-	-	23/42/42/57	-
72	PC1	2	402	-	-	20/49/49/57	-
74	SF4	A	801	-	-	-	0/6/5/5
79	HEA	A9	601	56	3/3/7/16	7/32/76/76	-
71	3PE	B	501	11	-	26/54/54/54	-
78	HEC	z	301	48	-	3/10/54/54	-
74	SF4	A	802	-	-	-	0/6/5/5
69	FES	m	403	-	-	-	0/1/1/1
77	HEM	m	401	47	-	4/12/54/54	-
74	SF4	8	502	-	-	-	0/6/5/5
74	SF4	E	302	-	-	-	0/6/5/5
71	3PE	j	202	-	-	24/49/49/54	-
77	HEM	y	401	47	-	4/12/54/54	-
73	FMN	8	501	-	-	10/18/18/18	0/3/3/3
76	NAP	R	601	-	-	15/31/67/67	0/5/5/5
70	CDL	6	701	-	-	42/74/74/110	-
70	CDL	J	101	-	-	31/68/68/110	-

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	O4D-C1D	16.09	1.63	1.41
76	R	601	NAP	O4B-C1B	14.68	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	C2D-C1D	-14.41	1.31	1.53
78	o	301	HEC	C2B-C3B	-8.31	1.32	1.40
78	z	301	HEC	C2B-C3B	-8.22	1.32	1.40
78	o	301	HEC	C3C-C2C	-7.99	1.32	1.40
78	z	301	HEC	C3C-C2C	-7.91	1.32	1.40
76	R	601	NAP	C7N-N7N	6.91	1.46	1.33
76	R	601	NAP	O4D-C4D	-6.70	1.30	1.45
77	m	402	HEM	C3C-C2C	-6.58	1.31	1.40
79	A9	602	HEA	C3A-C2A	-6.55	1.31	1.40
77	y	402	HEM	C3C-C2C	-6.52	1.31	1.40
76	R	601	NAP	O4B-C4B	-5.84	1.31	1.45
77	m	401	HEM	C3C-C2C	-5.84	1.32	1.40
77	y	401	HEM	C3C-C2C	-5.84	1.32	1.40
76	R	601	NAP	C3N-C7N	5.43	1.58	1.50
78	z	301	HEC	C3D-C2D	4.63	1.51	1.37
78	o	301	HEC	C3D-C2D	4.59	1.51	1.37
76	R	601	NAP	O3D-C3D	-4.25	1.33	1.43
79	A9	602	HEA	C3A-CMA	-3.85	1.37	1.46
76	R	601	NAP	O2D-C2D	3.80	1.51	1.43
77	y	402	HEM	FE-NB	-3.71	1.78	1.96
77	m	402	HEM	FE-NB	-3.70	1.78	1.96
76	R	601	NAP	O7N-C7N	-3.47	1.17	1.24
73	8	501	FMN	C4A-N5	3.40	1.37	1.30
79	A9	601	HEA	C3C-C2C	-3.23	1.35	1.40
77	m	402	HEM	C4A-CHB	-3.04	1.32	1.41
77	y	402	HEM	C4A-CHB	-3.00	1.32	1.41
77	m	401	HEM	CHD-C1D	-2.97	1.32	1.41
77	y	401	HEM	CHD-C1D	-2.97	1.32	1.41
77	m	402	HEM	C3B-C2B	-2.93	1.31	1.37
77	y	402	HEM	C3B-C2B	-2.93	1.31	1.37
79	A9	601	HEA	C3A-CMA	-2.93	1.39	1.46
76	R	601	NAP	C6A-N6A	2.92	1.44	1.34
77	m	401	HEM	C3C-CAC	2.84	1.53	1.47
70	4	501	CDL	OB6-CB5	2.81	1.42	1.34
77	y	401	HEM	C3C-CAC	2.81	1.53	1.47
77	m	401	HEM	C3D-C2D	-2.79	1.30	1.36
79	A9	601	HEA	C4C-NC	2.77	1.41	1.36
77	m	402	HEM	C3D-C2D	-2.76	1.30	1.36
77	y	401	HEM	C3D-C2D	-2.75	1.30	1.36
77	y	402	HEM	C3D-C2D	-2.72	1.30	1.36
77	m	402	HEM	C3C-CAC	2.70	1.53	1.47
76	R	601	NAP	O3B-C3B	-2.70	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	401	HEM	C1A-CHA	-2.67	1.33	1.41
77	m	401	HEM	C1A-CHA	-2.66	1.33	1.41
70	6	701	CDL	OA6-CA4	-2.65	1.40	1.46
77	y	402	HEM	C3C-CAC	2.65	1.53	1.47
76	R	601	NAP	C2A-N3A	2.63	1.36	1.32
71	V	201	3PE	O21-C2	-2.63	1.40	1.46
77	y	401	HEM	CHC-C4B	-2.62	1.33	1.41
79	A9	602	HEA	C1D-ND	-2.62	1.35	1.40
77	y	402	HEM	CHC-C4B	-2.61	1.33	1.41
77	m	401	HEM	CHC-C4B	-2.61	1.33	1.41
77	m	402	HEM	CHC-C4B	-2.61	1.33	1.41
79	A9	602	HEA	C1D-C2D	2.61	1.49	1.44
79	A9	602	HEA	C3C-C2C	-2.59	1.36	1.40
72	Q	201	PC1	O21-C2	-2.59	1.40	1.46
78	z	301	HEC	C4D-CHA	-2.58	1.33	1.41
72	S	401	PC1	O21-C2	-2.57	1.40	1.46
70	4	501	CDL	OB8-CB7	2.57	1.40	1.33
78	o	301	HEC	C4D-CHA	-2.57	1.33	1.41
71	j	202	3PE	O21-C2	-2.56	1.40	1.46
77	y	402	HEM	CHD-C1D	-2.54	1.33	1.41
70	6	701	CDL	OB6-CB5	2.54	1.41	1.34
77	m	402	HEM	CHD-C1D	-2.53	1.33	1.41
77	m	401	HEM	C1B-NB	-2.51	1.36	1.40
70	J	101	CDL	OB8-CB7	2.51	1.40	1.33
70	4	501	CDL	OA6-CA4	-2.50	1.40	1.46
70	4	501	CDL	OA8-CA7	2.49	1.40	1.33
77	y	401	HEM	C1B-NB	-2.47	1.36	1.40
70	J	101	CDL	OB6-CB4	-2.47	1.40	1.46
72	j	201	PC1	O21-C2	-2.47	1.40	1.46
70	J	101	CDL	OA6-CA4	-2.45	1.40	1.46
71	4	502	3PE	O21-C21	2.44	1.41	1.34
72	2	402	PC1	O21-C21	2.43	1.41	1.34
76	R	601	NAP	PA-O5B	2.43	1.69	1.59
71	j	202	3PE	O31-C31	2.41	1.40	1.33
71	V	201	3PE	O31-C31	2.40	1.40	1.33
70	J	101	CDL	OA8-CA7	2.40	1.40	1.33
71	4	502	3PE	O31-C3	-2.39	1.39	1.45
71	B	501	3PE	O21-C2	-2.39	1.40	1.46
77	m	402	HEM	C1B-NB	-2.38	1.36	1.40
72	L	200	PC1	O31-C31	2.38	1.40	1.33
77	m	402	HEM	C2A-C3A	-2.37	1.30	1.37
76	R	601	NAP	C5A-N7A	-2.37	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	402	HEM	C1B-NB	-2.36	1.36	1.40
77	y	402	HEM	C2A-C3A	-2.36	1.30	1.37
73	8	501	FMN	C10-N1	2.36	1.38	1.33
79	A9	602	HEA	CMD-C2D	2.34	1.55	1.50
71	2	401	3PE	O21-C21	2.34	1.40	1.34
72	j	201	PC1	O31-C31	2.34	1.40	1.33
70	6	701	CDL	OA8-CA6	-2.33	1.39	1.45
76	R	601	NAP	C5A-C4A	-2.33	1.34	1.40
77	m	401	HEM	C4A-CHB	-2.32	1.34	1.41
72	L	200	PC1	O21-C2	-2.32	1.40	1.46
77	m	401	HEM	C2A-C3A	-2.32	1.30	1.37
72	2	402	PC1	O31-C31	2.32	1.40	1.33
72	L	200	PC1	O31-C3	-2.32	1.39	1.45
72	S	401	PC1	O31-C31	2.32	1.40	1.33
71	2	401	3PE	O31-C3	-2.32	1.39	1.45
77	y	401	HEM	C2A-C3A	-2.31	1.30	1.37
77	m	401	HEM	CAB-C3B	2.31	1.53	1.47
71	B	501	3PE	O31-C3	-2.30	1.39	1.45
77	y	401	HEM	CAB-C3B	2.30	1.53	1.47
77	y	401	HEM	C4A-CHB	-2.29	1.34	1.41
70	6	701	CDL	OB8-CB7	2.28	1.40	1.33
72	Q	201	PC1	O31-C3	-2.28	1.40	1.45
71	V	201	3PE	O31-C3	-2.27	1.40	1.45
72	j	201	PC1	O21-C21	2.26	1.40	1.34
70	6	701	CDL	OA8-CA7	2.26	1.39	1.33
72	j	201	PC1	O31-C3	-2.26	1.40	1.45
76	R	601	NAP	P2B-O2B	2.26	1.63	1.59
71	2	401	3PE	O31-C31	2.23	1.39	1.33
72	S	401	PC1	O21-C21	2.22	1.40	1.34
76	R	601	NAP	C4N-C3N	-2.21	1.35	1.39
71	B	501	3PE	O21-C21	2.19	1.40	1.34
70	J	101	CDL	OB6-CB5	2.19	1.40	1.34
72	L	200	PC1	O21-C21	2.17	1.40	1.34
77	y	402	HEM	CAB-C3B	2.17	1.53	1.47
71	j	202	3PE	O31-C3	-2.16	1.40	1.45
70	6	701	CDL	OA6-CA5	2.15	1.40	1.34
79	A9	601	HEA	C3A-C2A	-2.15	1.37	1.40
77	m	402	HEM	CAB-C3B	2.14	1.53	1.47
71	4	502	3PE	O31-C31	2.14	1.39	1.33
71	B	501	3PE	O31-C31	2.13	1.39	1.33
70	J	101	CDL	OB8-CB6	-2.13	1.40	1.45
77	y	401	HEM	C3B-C2B	-2.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	m	401	HEM	C3B-C2B	-2.13	1.33	1.37
78	o	301	HEC	C1B-CHB	-2.13	1.35	1.41
78	z	301	HEC	C1B-CHB	-2.12	1.35	1.41
70	6	701	CDL	OB8-CB6	-2.12	1.40	1.45
79	A9	601	HEA	CHD-C1D	2.11	1.40	1.35
79	A9	601	HEA	C1C-NC	2.11	1.40	1.36
71	2	401	3PE	O21-C2	-2.09	1.41	1.46
70	J	101	CDL	OA6-CA5	2.08	1.40	1.34
78	z	301	HEC	C1D-CHD	-2.08	1.35	1.41
70	4	501	CDL	OA6-CA5	2.08	1.40	1.34
72	2	402	PC1	O31-C3	-2.07	1.40	1.45
70	4	501	CDL	OA8-CA6	-2.07	1.40	1.45
76	R	601	NAP	PN-O5D	2.07	1.67	1.59
77	m	402	HEM	C4D-ND	-2.06	1.36	1.40
78	o	301	HEC	C1D-CHD	-2.06	1.35	1.41
72	S	401	PC1	O31-C3	-2.05	1.40	1.45
77	y	402	HEM	C4D-ND	-2.05	1.36	1.40
71	V	201	3PE	O21-C21	2.04	1.40	1.34
72	Q	201	PC1	O31-C31	2.04	1.39	1.33
72	Q	201	PC1	O21-C21	2.02	1.40	1.34
71	j	202	3PE	O21-C21	2.02	1.40	1.34
76	R	601	NAP	O2B-C2B	2.01	1.51	1.44

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	R	601	NAP	C5A-C6A-N6A	7.27	131.40	120.35
77	y	401	HEM	C4B-CHC-C1C	-6.74	113.67	122.56
77	m	401	HEM	C4B-CHC-C1C	-6.69	113.72	122.56
76	R	601	NAP	N3A-C2A-N1A	-6.07	119.19	128.68
76	R	601	NAP	N6A-C6A-N1A	-5.18	107.81	118.57
71	4	502	3PE	O21-C21-C22	4.88	122.03	111.50
77	m	402	HEM	C4C-CHD-C1D	-4.64	116.44	122.56
72	L	200	PC1	O21-C21-C22	4.60	121.42	111.50
77	y	402	HEM	C4C-CHD-C1D	-4.56	116.54	122.56
71	B	501	3PE	O21-C21-C22	4.52	121.24	111.50
71	2	401	3PE	O21-C21-C22	4.38	120.94	111.50
70	4	501	CDL	OA6-CA5-C11	4.31	120.79	111.50
70	6	701	CDL	OB6-CB5-C51	4.26	120.67	111.50
70	J	101	CDL	OA6-CA5-C11	4.20	120.56	111.50
71	V	201	3PE	O21-C21-C22	4.17	120.48	111.50
70	J	101	CDL	OB6-CB5-C51	4.09	120.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	6	701	CDL	OA6-CA5-C11	3.97	120.06	111.50
79	A9	601	HEA	C17-C18-C19	-3.97	118.11	127.66
72	2	402	PC1	O21-C21-C22	3.93	119.97	111.50
77	y	401	HEM	CAD-CBD-CGD	-3.92	105.17	113.60
77	m	401	HEM	CAD-CBD-CGD	-3.91	105.18	113.60
73	8	501	FMN	C4-N3-C2	-3.86	118.52	125.64
73	8	501	FMN	C4A-C10-N1	-3.84	115.82	124.73
77	m	401	HEM	CBA-CAA-C2A	-3.84	106.07	112.62
72	S	401	PC1	O21-C21-C22	3.83	119.75	111.50
71	j	202	3PE	O21-C21-C22	3.82	119.74	111.50
72	Q	201	PC1	O21-C21-C22	3.82	119.74	111.50
77	y	401	HEM	CBA-CAA-C2A	-3.82	106.11	112.62
77	y	401	HEM	CMC-C2C-C3C	3.76	131.71	124.68
77	m	401	HEM	CMC-C2C-C3C	3.76	131.71	124.68
79	A9	602	HEA	C4A-CHB-C1B	3.58	127.29	122.56
72	j	201	PC1	O21-C21-C22	3.56	120.72	110.80
76	R	601	NAP	C1B-N9A-C4A	-3.50	120.49	126.64
78	z	301	HEC	C1D-C2D-C3D	-3.41	104.63	107.00
77	y	402	HEM	CMC-C2C-C3C	3.37	130.99	124.68
77	m	402	HEM	CMC-C2C-C3C	3.33	130.92	124.68
78	o	301	HEC	C1D-C2D-C3D	-3.32	104.68	107.00
77	m	402	HEM	CHC-C4B-NB	3.29	128.01	124.43
70	6	701	CDL	OA8-CA7-C31	3.27	122.16	111.91
73	8	501	FMN	C10-N1-C2	3.23	123.37	116.90
70	4	501	CDL	CB4-OB6-CB5	3.21	125.69	117.79
77	y	402	HEM	CHC-C4B-NB	3.21	127.92	124.43
79	A9	601	HEA	C13-C14-C15	-3.18	120.01	127.66
77	m	401	HEM	CAD-C3D-C4D	3.16	130.18	124.66
77	y	401	HEM	CAD-C3D-C4D	3.15	130.17	124.66
70	4	501	CDL	OB6-CB5-C51	3.04	118.06	111.50
73	8	501	FMN	C1'-N10-C9A	-3.03	115.47	120.51
73	8	501	FMN	C4A-C4-N3	2.98	120.75	113.19
77	m	402	HEM	CAA-CBA-CGA	-2.89	105.66	113.76
77	y	402	HEM	CAA-CBA-CGA	-2.88	105.68	113.76
76	R	601	NAP	PN-O3-PA	-2.87	122.97	132.83
72	j	201	PC1	O31-C31-C32	2.87	120.90	111.91
70	4	501	CDL	OA8-CA7-C31	2.85	120.85	111.91
79	A9	602	HEA	CBA-CAA-C2A	2.84	117.40	112.60
73	8	501	FMN	C4-C4A-C10	2.80	121.50	116.79
73	8	501	FMN	C5A-C9A-N10	2.80	120.85	117.95
70	J	101	CDL	OA8-CA7-C31	2.79	120.67	111.91
78	o	301	HEC	CAA-CBA-CGA	-2.79	105.94	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	y	402	HEM	CBA-CAA-C2A	-2.79	107.87	112.62
79	A9	601	HEA	C1B-C2B-C3B	2.78	110.12	106.80
78	z	301	HEC	CAA-CBA-CGA	-2.78	105.97	113.76
71	2	401	3PE	O31-C31-C32	2.76	120.58	111.91
77	m	402	HEM	CBA-CAA-C2A	-2.76	107.91	112.62
70	6	701	CDL	OB8-CB7-C71	2.75	120.55	111.91
73	8	501	FMN	O4-C4-C4A	-2.71	119.41	126.60
78	z	301	HEC	CBA-CAA-C2A	-2.71	108.04	112.60
77	m	402	HEM	CBD-CAD-C3D	-2.70	105.13	112.63
78	o	301	HEC	CBA-CAA-C2A	-2.69	108.06	112.60
78	o	301	HEC	CMB-C2B-C1B	-2.69	124.34	128.46
77	y	402	HEM	CBD-CAD-C3D	-2.68	105.19	112.63
78	z	301	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
77	y	401	HEM	CAD-C3D-C2D	-2.66	122.92	127.88
70	J	101	CDL	OB8-CB7-C71	2.66	120.26	111.91
78	z	301	HEC	CMC-C2C-C1C	-2.64	124.40	128.46
78	o	301	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
72	S	401	PC1	O31-C31-C32	2.63	120.16	111.91
77	y	401	HEM	C4C-CHD-C1D	-2.63	119.09	122.56
71	4	502	3PE	O31-C31-C32	2.63	120.15	111.91
77	m	401	HEM	C4C-CHD-C1D	-2.62	119.10	122.56
73	8	501	FMN	C4A-C10-N10	2.62	120.31	116.48
72	L	200	PC1	O31-C31-C32	2.61	120.08	111.91
77	m	401	HEM	CAD-C3D-C2D	-2.61	123.03	127.88
79	A9	602	HEA	CMD-C2D-C1D	2.58	128.97	125.04
77	y	401	HEM	CAA-CBA-CGA	-2.58	106.52	113.76
77	m	401	HEM	CAA-CBA-CGA	-2.57	106.55	113.76
72	2	402	PC1	O31-C31-C32	2.55	119.91	111.91
78	o	301	HEC	CAD-CBD-CGD	-2.55	106.62	113.76
71	B	501	3PE	O31-C31-C32	2.54	119.89	111.91
78	z	301	HEC	CAD-CBD-CGD	-2.52	106.70	113.76
78	o	301	HEC	CBD-CAD-C3D	-2.51	108.33	112.62
77	m	402	HEM	CHC-C4B-C3B	-2.50	120.75	124.57
79	A9	602	HEA	C4D-CHA-C1A	2.48	125.83	122.56
71	V	201	3PE	O31-C31-C32	2.48	119.68	111.91
78	z	301	HEC	CBD-CAD-C3D	-2.47	108.41	112.62
77	y	402	HEM	CHC-C4B-C3B	-2.46	120.81	124.57
79	A9	602	HEA	C1D-C2D-C3D	-2.44	104.39	106.96
76	R	601	NAP	C3D-C2D-C1D	2.43	104.64	100.98
79	A9	601	HEA	C17-C16-C15	-2.40	105.08	112.98
71	j	202	3PE	O31-C31-C32	2.40	119.43	111.91
79	A9	602	HEA	CMC-C2C-C3C	2.40	129.16	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	4	501	CDL	OB8-CB7-C71	2.39	119.41	111.91
79	A9	601	HEA	C20-C19-C18	2.38	125.93	121.12
79	A9	602	HEA	CMB-C2B-C3B	-2.35	125.87	130.34
79	A9	601	HEA	C16-C17-C18	-2.34	104.18	111.88
79	A9	602	HEA	C13-C14-C15	-2.32	122.07	127.66
79	A9	601	HEA	CAD-C3D-C4D	2.30	128.68	124.66
73	8	501	FMN	C5'-C4'-C3'	-2.30	107.77	112.20
79	A9	602	HEA	C25-C23-C24	2.28	119.65	114.60
77	m	401	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
77	y	401	HEM	CMA-C3A-C4A	-2.26	124.99	128.46
72	Q	201	PC1	O31-C31-C32	2.25	118.97	111.91
79	A9	602	HEA	C26-C15-C16	2.22	119.00	115.27
79	A9	601	HEA	C12-C13-C14	-2.18	106.48	112.23
79	A9	601	HEA	C4A-CHB-C1B	2.16	125.41	122.56
79	A9	601	HEA	C4B-C3B-C2B	-2.15	103.74	107.41
77	m	401	HEM	CHA-C4D-ND	-2.14	121.73	124.38
71	4	502	3PE	C2-O21-C21	2.14	123.06	117.79
77	y	401	HEM	CHA-C4D-ND	-2.12	121.76	124.38
79	A9	601	HEA	C27-C19-C18	-2.10	118.28	123.68
73	8	501	FMN	C9A-C5A-N5	-2.06	120.19	122.43
79	A9	601	HEA	C3C-C4C-NC	2.06	111.87	109.21
76	R	601	NAP	C6N-N1N-C2N	-2.04	120.11	121.97
79	A9	602	HEA	CBD-CAD-C3D	2.04	118.29	112.63

All (6) chirality outliers are listed below:

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

All (401) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	6	701	CDL	CB2-C1-CA2-OA2
70	6	701	CDL	CA3-OA5-PA1-OA2
70	6	701	CDL	CA3-OA5-PA1-OA3
70	6	701	CDL	CA3-OA5-PA1-OA4
70	6	701	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
70	6	701	CDL	CB2-OB2-PB2-OB4
70	6	701	CDL	CB2-OB2-PB2-OB5
70	6	701	CDL	C51-CB5-OB6-CB4
70	4	501	CDL	C1-CA2-OA2-PA1
70	4	501	CDL	CA2-OA2-PA1-OA4
70	J	101	CDL	CB2-C1-CA2-OA2
70	J	101	CDL	CA2-OA2-PA1-OA3
70	J	101	CDL	CA2-OA2-PA1-OA5
70	J	101	CDL	OA7-CA5-OA6-CA4
71	2	401	3PE	C11-O13-P-O12
71	2	401	3PE	C11-O13-P-O14
71	2	401	3PE	C22-C21-O21-C2
71	4	502	3PE	C1-O11-P-O12
71	4	502	3PE	C1-O11-P-O13
71	4	502	3PE	C1-O11-P-O14
71	4	502	3PE	C22-C21-O21-C2
71	B	501	3PE	C1-O11-P-O12
71	B	501	3PE	C1-O11-P-O13
71	B	501	3PE	C1-O11-P-O14
71	B	501	3PE	O13-C11-C12-N
71	B	501	3PE	O22-C21-O21-C2
71	B	501	3PE	C22-C21-O21-C2
71	V	201	3PE	C1-O11-P-O12
71	V	201	3PE	C1-O11-P-O14
71	V	201	3PE	O21-C2-C3-O31
71	j	202	3PE	C1-O11-P-O12
71	j	202	3PE	C1-O11-P-O14
71	j	202	3PE	C11-O13-P-O12
72	2	402	PC1	O13-C11-C12-N
72	L	200	PC1	C11-O13-P-O14
72	L	200	PC1	C1-O11-P-O12
72	L	200	PC1	C1-O11-P-O14
72	L	200	PC1	O13-C11-C12-N
72	Q	201	PC1	C1-O11-P-O12
72	Q	201	PC1	C1-O11-P-O14
72	Q	201	PC1	C1-O11-P-O13
72	Q	201	PC1	O22-C21-O21-C2
72	S	401	PC1	C11-O13-P-O12
72	S	401	PC1	C1-O11-P-O14
72	S	401	PC1	O13-C11-C12-N
72	j	201	PC1	C11-O13-P-O12
72	j	201	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
72	j	201	PC1	C1-O11-P-O14
72	j	201	PC1	C22-C21-O21-C2
73	8	501	FMN	C2'-C1'-N10-C10
73	8	501	FMN	N10-C1'-C2'-O2'
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	C1'-C2'-C3'-O3'
73	8	501	FMN	C1'-C2'-C3'-C4'
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P
76	R	601	NAP	C5B-O5B-PA-O1A
76	R	601	NAP	C5B-O5B-PA-O2A
76	R	601	NAP	C1B-C2B-O2B-P2B
76	R	601	NAP	C5D-O5D-PN-O1N
76	R	601	NAP	C5D-O5D-PN-O2N
76	R	601	NAP	C2D-C1D-N1N-C2N
76	R	601	NAP	C2D-C1D-N1N-C6N
77	m	401	HEM	C2A-CAA-CBA-CGA
77	y	401	HEM	C2A-CAA-CBA-CGA
79	A9	601	HEA	C12-C11-C3B-C2B
70	6	701	CDL	OA9-CA7-OA8-CA6
70	4	501	CDL	OB9-CB7-OB8-CB6
71	j	202	3PE	O32-C31-O31-C3
70	6	701	CDL	OB7-CB5-OB6-CB4
71	2	401	3PE	O22-C21-O21-C2
72	j	201	PC1	O22-C21-O21-C2
70	6	701	CDL	C31-CA7-OA8-CA6
70	4	501	CDL	C71-CB7-OB8-CB6
71	j	202	3PE	C32-C31-O31-C3
70	J	101	CDL	C11-CA5-OA6-CA4
72	Q	201	PC1	C22-C21-O21-C2
70	J	101	CDL	C31-CA7-OA8-CA6
70	J	101	CDL	C71-CB7-OB8-CB6
71	4	502	3PE	C32-C31-O31-C3
72	S	401	PC1	C32-C31-O31-C3
71	4	502	3PE	O22-C21-O21-C2
72	2	402	PC1	O22-C21-O21-C2
70	J	101	CDL	OB9-CB7-OB8-CB6
72	S	401	PC1	O32-C31-O31-C3
72	j	201	PC1	O32-C31-O31-C3
70	6	701	CDL	O1-C1-CA2-OA2
70	J	101	CDL	O1-C1-CA2-OA2
72	2	402	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
73	8	501	FMN	O2'-C2'-C3'-O3'
76	R	601	NAP	O4B-C4B-C5B-O5B
76	R	601	NAP	O4D-C4D-C5D-O5D
72	j	201	PC1	C32-C31-O31-C3
70	J	101	CDL	OA9-CA7-OA8-CA6
71	4	502	3PE	O32-C31-O31-C3
79	A9	601	HEA	C15-C16-C17-C18
71	2	401	3PE	C32-C31-O31-C3
70	J	101	CDL	CA2-C1-CB2-OB2
72	L	200	PC1	C32-C31-O31-C3
72	2	402	PC1	C22-C23-C24-C25
72	L	200	PC1	C31-C32-C33-C34
71	B	501	3PE	O11-C1-C2-O21
72	2	402	PC1	C21-C22-C23-C24
71	2	401	3PE	O32-C31-O31-C3
70	4	501	CDL	C11-CA5-OA6-CA4
70	6	701	CDL	CA7-C31-C32-C33
72	2	402	PC1	C31-C32-C33-C34
78	o	301	HEC	C2A-CAA-CBA-CGA
78	z	301	HEC	C2A-CAA-CBA-CGA
70	6	701	CDL	CB5-C51-C52-C53
72	L	200	PC1	O32-C31-O31-C3
70	6	701	CDL	CA5-C11-C12-C13
70	4	501	CDL	CA5-C11-C12-C13
73	8	501	FMN	O2'-C2'-C3'-C4'
72	Q	201	PC1	C31-C32-C33-C34
72	j	201	PC1	C31-C32-C33-C34
70	J	101	CDL	O1-C1-CB2-OB2
70	4	501	CDL	OA7-CA5-OA6-CA4
70	6	701	CDL	CA4-CA6-OA8-CA7
70	6	701	CDL	CB3-OB5-PB2-OB2
70	4	501	CDL	CA2-OA2-PA1-OA5
71	2	401	3PE	C11-O13-P-O11
71	V	201	3PE	C1-O11-P-O13
71	j	202	3PE	C1-O11-P-O13
72	L	200	PC1	C11-O13-P-O11
72	L	200	PC1	C1-O11-P-O13
72	S	401	PC1	C11-O13-P-O11
72	S	401	PC1	C1-O11-P-O13
72	j	201	PC1	C11-O13-P-O11
72	S	401	PC1	C23-C24-C25-C26
71	2	401	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
71	B	501	3PE	C32-C33-C34-C35
72	S	401	PC1	C3E-C3F-C3G-C3H
71	2	401	3PE	C3-C2-O21-C21
70	6	701	CDL	C52-C53-C54-C55
70	J	101	CDL	C54-C55-C56-C57
71	j	202	3PE	C38-C39-C3A-C3B
77	m	401	HEM	C3D-CAD-CBD-CGD
77	y	401	HEM	C3D-CAD-CBD-CGD
72	S	401	PC1	C31-C32-C33-C34
72	j	201	PC1	C36-C37-C38-C39
70	6	701	CDL	C14-C15-C16-C17
71	B	501	3PE	C2D-C2E-C2F-C2G
70	4	501	CDL	CA7-C31-C32-C33
70	4	501	CDL	C62-C63-C64-C65
72	L	200	PC1	C34-C35-C36-C37
72	L	200	PC1	C39-C3A-C3B-C3C
72	j	201	PC1	C3B-C3C-C3D-C3E
70	4	501	CDL	C77-C78-C79-C80
70	J	101	CDL	C15-C16-C17-C18
71	4	502	3PE	C28-C29-C2A-C2B
70	4	501	CDL	C78-C79-C80-C81
71	4	502	3PE	C32-C33-C34-C35
71	j	202	3PE	C22-C23-C24-C25
72	2	402	PC1	C27-C28-C29-C2A
70	6	701	CDL	C51-C52-C53-C54
70	6	701	CDL	C72-C73-C74-C75
71	B	501	3PE	C2C-C2D-C2E-C2F
71	j	202	3PE	O13-C11-C12-N
71	2	401	3PE	C26-C27-C28-C29
71	B	501	3PE	C31-C32-C33-C34
72	Q	201	PC1	C2B-C2C-C2D-C2E
70	J	101	CDL	C53-C54-C55-C56
71	B	501	3PE	C33-C34-C35-C36
72	S	401	PC1	C25-C26-C27-C28
72	S	401	PC1	C32-C33-C34-C35
70	4	501	CDL	C54-C55-C56-C57
77	m	401	HEM	C4D-C3D-CAD-CBD
77	y	401	HEM	C4D-C3D-CAD-CBD
71	4	502	3PE	C31-C32-C33-C34
71	V	201	3PE	C32-C33-C34-C35
71	j	202	3PE	C22-C21-O21-C2
70	4	501	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
71	B	501	3PE	C26-C27-C28-C29
71	j	202	3PE	C33-C34-C35-C36
71	4	502	3PE	C24-C25-C26-C27
72	j	201	PC1	C32-C33-C34-C35
70	4	501	CDL	CA2-C1-CB2-OB2
71	j	202	3PE	C24-C25-C26-C27
71	j	202	3PE	C36-C37-C38-C39
70	4	501	CDL	C13-C14-C15-C16
71	2	401	3PE	C25-C26-C27-C28
71	V	201	3PE	C26-C27-C28-C29
72	2	402	PC1	C37-C38-C39-C3A
71	V	201	3PE	C2A-C2B-C2C-C2D
71	j	202	3PE	O22-C21-O21-C2
71	B	501	3PE	C21-C22-C23-C24
70	6	701	CDL	C74-C75-C76-C77
71	V	201	3PE	C36-C37-C38-C39
72	2	402	PC1	C34-C35-C36-C37
71	j	202	3PE	C21-C22-C23-C24
72	L	200	PC1	C27-C28-C29-C2A
72	S	401	PC1	C39-C3A-C3B-C3C
71	V	201	3PE	C2E-C2F-C2G-C2H
72	L	200	PC1	C25-C26-C27-C28
70	J	101	CDL	CA7-C31-C32-C33
71	B	501	3PE	C35-C36-C37-C38
72	L	200	PC1	C3C-C3D-C3E-C3F
72	S	401	PC1	C24-C25-C26-C27
71	4	502	3PE	C2E-C2F-C2G-C2H
71	B	501	3PE	C23-C24-C25-C26
70	4	501	CDL	C80-C81-C82-C83
71	B	501	3PE	C34-C35-C36-C37
70	4	501	CDL	OA6-CA4-CA6-OA8
71	V	201	3PE	C2B-C2C-C2D-C2E
72	S	401	PC1	C22-C23-C24-C25
70	4	501	CDL	C73-C74-C75-C76
77	m	401	HEM	C2D-C3D-CAD-CBD
77	y	401	HEM	C2D-C3D-CAD-CBD
70	6	701	CDL	C33-C34-C35-C36
70	6	701	CDL	C53-C54-C55-C56
70	4	501	CDL	C74-C75-C76-C77
71	j	202	3PE	C11-O13-P-O11
70	6	701	CDL	OB5-CB3-CB4-CB6
71	B	501	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
70	4	501	CDL	C34-C35-C36-C37
71	j	202	3PE	C26-C27-C28-C29
71	j	202	3PE	C27-C28-C29-C2A
72	S	401	PC1	C21-C22-C23-C24
71	4	502	3PE	C21-C22-C23-C24
72	L	200	PC1	C26-C27-C28-C29
71	j	202	3PE	C23-C24-C25-C26
76	R	601	NAP	C3B-C4B-C5B-O5B
70	6	701	CDL	C13-C14-C15-C16
70	4	501	CDL	C52-C53-C54-C55
70	4	501	CDL	C84-C85-C86-C87
73	8	501	FMN	C5'-O5'-P-O1P
70	4	501	CDL	O1-C1-CB2-OB2
72	L	200	PC1	O21-C2-C3-O31
72	S	401	PC1	O21-C2-C3-O31
71	4	502	3PE	C35-C36-C37-C38
71	B	501	3PE	C3E-C3F-C3G-C3H
72	2	402	PC1	C35-C36-C37-C38
71	j	202	3PE	C2C-C2D-C2E-C2F
71	2	401	3PE	C28-C29-C2A-C2B
70	4	501	CDL	C15-C16-C17-C18
72	S	401	PC1	C3F-C3G-C3H-C3I
72	2	402	PC1	O11-C1-C2-C3
72	L	200	PC1	O11-C1-C2-C3
71	j	202	3PE	C2A-C2B-C2C-C2D
71	V	201	3PE	C38-C39-C3A-C3B
70	6	701	CDL	C31-C32-C33-C34
72	Q	201	PC1	C21-C22-C23-C24
72	Q	201	PC1	C2A-C2B-C2C-C2D
70	4	501	CDL	CA3-CA4-CA6-OA8
70	J	101	CDL	CA3-CA4-CA6-OA8
71	2	401	3PE	C1-C2-C3-O31
71	V	201	3PE	C1-C2-C3-O31
72	j	201	PC1	C1-C2-C3-O31
72	S	401	PC1	C3D-C3E-C3F-C3G
71	4	502	3PE	C23-C24-C25-C26
71	4	502	3PE	C2C-C2D-C2E-C2F
70	6	701	CDL	OB5-CB3-CB4-OB6
71	2	401	3PE	O11-C1-C2-O21
72	L	200	PC1	O11-C1-C2-O21
72	L	200	PC1	C35-C36-C37-C38
70	4	501	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
70	J	101	CDL	OA6-CA4-CA6-OA8
70	J	101	CDL	C12-C13-C14-C15
71	4	502	3PE	C2-C1-O11-P
71	V	201	3PE	O21-C21-C22-C23
76	R	601	NAP	PN-O3-PA-O5B
76	R	601	NAP	PA-O3-PN-O5D
70	J	101	CDL	C16-C17-C18-C19
70	4	501	CDL	OA5-CA3-CA4-CA6
70	4	501	CDL	OB5-CB3-CB4-CB6
72	S	401	PC1	O11-C1-C2-C3
71	V	201	3PE	C3F-C3G-C3H-C3I
72	2	402	PC1	C32-C31-O31-C3
72	j	201	PC1	C35-C36-C37-C38
72	2	402	PC1	C3-C2-O21-C21
70	J	101	CDL	C11-C12-C13-C14
70	6	701	CDL	C1-CA2-OA2-PA1
71	B	501	3PE	C2-C1-O11-P
72	Q	201	PC1	C1-C2-C3-O31
72	2	402	PC1	O11-C1-C2-O21
72	S	401	PC1	O11-C1-C2-O21
70	4	501	CDL	OB6-CB4-CB6-OB8
72	Q	201	PC1	O21-C2-C3-O31
72	j	201	PC1	O21-C2-C3-O31
76	R	601	NAP	C5B-O5B-PA-O3
76	R	601	NAP	C2B-O2B-P2B-O3X
70	J	101	CDL	CB7-C71-C72-C73
72	Q	201	PC1	C32-C33-C34-C35
72	j	201	PC1	C1-O11-P-O13
70	J	101	CDL	C31-C32-C33-C34
72	2	402	PC1	O32-C31-O31-C3
70	6	701	CDL	CB3-OB5-PB2-OB3
70	6	701	CDL	CB3-OB5-PB2-OB4
71	j	202	3PE	C11-O13-P-O14
72	L	200	PC1	C11-O13-P-O12
72	S	401	PC1	C11-O13-P-O14
72	S	401	PC1	C1-O11-P-O12
70	J	101	CDL	OB5-CB3-CB4-CB6
71	2	401	3PE	O11-C1-C2-C3
71	4	502	3PE	O11-C1-C2-C3
72	2	402	PC1	C33-C34-C35-C36
70	4	501	CDL	OA5-CA3-CA4-OA6
71	B	501	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
72	Q	201	PC1	C35-C36-C37-C38
71	V	201	3PE	C23-C24-C25-C26
71	V	201	3PE	C2C-C2D-C2E-C2F
70	4	501	CDL	CB3-CB4-CB6-OB8
72	Q	201	PC1	O13-C11-C12-N
72	j	201	PC1	O13-C11-C12-N
78	o	301	HEC	C1A-C2A-CAA-CBA
78	o	301	HEC	C3A-C2A-CAA-CBA
78	z	301	HEC	C1A-C2A-CAA-CBA
78	z	301	HEC	C3A-C2A-CAA-CBA
71	2	401	3PE	O21-C2-C3-O31
70	4	501	CDL	C14-C15-C16-C17
71	V	201	3PE	C2-C1-O11-P
70	6	701	CDL	CB3-CB4-OB6-CB5
70	6	701	CDL	CA4-CA3-OA5-PA1
72	Q	201	PC1	C2-C1-O11-P
72	S	401	PC1	C2-C1-O11-P
70	4	501	CDL	C35-C36-C37-C38
71	4	502	3PE	C34-C35-C36-C37
70	J	101	CDL	CB2-OB2-PB2-OB5
71	4	502	3PE	C11-O13-P-O11
71	V	201	3PE	C11-O13-P-O11
72	2	402	PC1	C1-O11-P-O13
72	L	200	PC1	C1-C2-C3-O31
72	S	401	PC1	C1-C2-C3-O31
71	2	401	3PE	C33-C34-C35-C36
70	4	501	CDL	CA4-CA3-OA5-PA1
70	6	701	CDL	OA7-CA5-OA6-CA4
70	6	701	CDL	C71-CB7-OB8-CB6
71	B	501	3PE	C38-C39-C3A-C3B
71	B	501	3PE	C37-C38-C39-C3A
71	4	502	3PE	O13-C11-C12-N
71	B	501	3PE	C36-C37-C38-C39
70	6	701	CDL	OB9-CB7-OB8-CB6
71	V	201	3PE	C3E-C3F-C3G-C3H
72	j	201	PC1	C3A-C3B-C3C-C3D
72	2	402	PC1	O21-C21-C22-C23
72	2	402	PC1	C28-C29-C2A-C2B
77	m	402	HEM	CAA-CBA-CGA-O1A
77	y	402	HEM	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O1D
72	j	201	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
70	4	501	CDL	CB3-CB4-OB6-CB5
71	4	502	3PE	C1-C2-O21-C21
77	m	402	HEM	CAA-CBA-CGA-O2A
77	y	402	HEM	CAA-CBA-CGA-O2A
70	6	701	CDL	CB4-CB3-OB5-PB2
71	j	202	3PE	C39-C3A-C3B-C3C
70	6	701	CDL	C11-CA5-OA6-CA4
79	A9	602	HEA	CAD-CBD-CGD-O1D
72	L	200	PC1	C32-C33-C34-C35
72	2	402	PC1	C38-C39-C3A-C3B
70	J	101	CDL	OB7-CB5-OB6-CB4
79	A9	602	HEA	CAD-CBD-CGD-O2D
72	L	200	PC1	C22-C23-C24-C25
79	A9	601	HEA	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O2D
70	4	501	CDL	C71-C72-C73-C74
72	S	401	PC1	C34-C35-C36-C37
70	J	101	CDL	C14-C15-C16-C17
71	2	401	3PE	C29-C2A-C2B-C2C
71	2	401	3PE	C21-C22-C23-C24
70	4	501	CDL	C52-C51-CB5-OB6
72	Q	201	PC1	O21-C21-C22-C23
72	Q	201	PC1	C26-C27-C28-C29
79	A9	602	HEA	CAA-CBA-CGA-O2A
72	S	401	PC1	C38-C39-C3A-C3B
70	6	701	CDL	C12-C11-CA5-OA6
70	6	701	CDL	OB6-CB4-CB6-OB8
79	A9	602	HEA	CAA-CBA-CGA-O1A
72	S	401	PC1	O31-C31-C32-C33
72	j	201	PC1	O31-C31-C32-C33
76	R	601	NAP	C5D-O5D-PN-O3
70	J	101	CDL	C51-CB5-OB6-CB4
72	S	401	PC1	O21-C21-C22-C23
71	4	502	3PE	C2D-C2E-C2F-C2G
70	4	501	CDL	C52-C51-CB5-OB7
72	Q	201	PC1	O22-C21-C22-C23
70	J	101	CDL	CB3-CB4-CB6-OB8
72	S	401	PC1	O32-C31-C32-C33
79	A9	601	HEA	CAA-CBA-CGA-O2A
71	4	502	3PE	C11-O13-P-O14
71	V	201	3PE	C11-O13-P-O14
72	Q	201	PC1	C11-O13-P-O14

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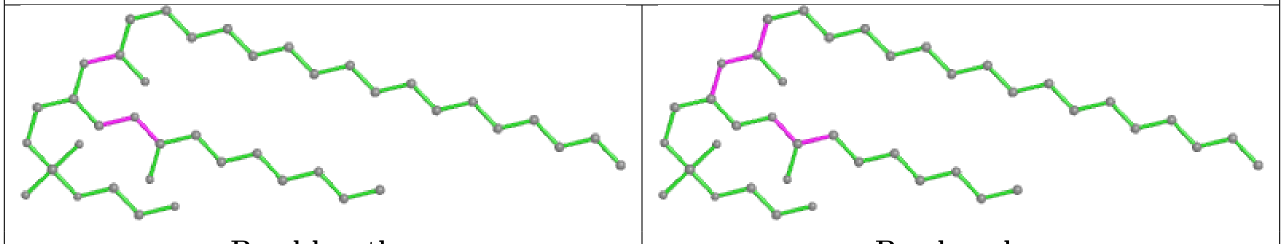
Mol	Chain	Res	Type	Atoms
70	6	701	CDL	C12-C11-CA5-OA7
72	j	201	PC1	O32-C31-C32-C33
72	S	401	PC1	C27-C28-C29-C2A
70	6	701	CDL	C52-C51-CB5-OB6
70	J	101	CDL	C13-C14-C15-C16
71	V	201	3PE	O22-C21-C22-C23
72	j	201	PC1	C12-C11-O13-P
70	J	101	CDL	C12-C11-CA5-OA6
71	B	501	3PE	O31-C31-C32-C33
72	Q	201	PC1	C22-C23-C24-C25
79	A9	602	HEA	C26-C15-C16-C17
72	j	201	PC1	O11-C1-C2-O21
79	A9	601	HEA	O11-C11-C3B-C2B
71	2	401	3PE	O31-C31-C32-C33
71	j	202	3PE	O21-C21-C22-C23
72	S	401	PC1	O22-C21-C22-C23
71	B	501	3PE	O32-C31-C32-C33
71	2	401	3PE	O32-C31-C32-C33

There are no ring outliers.

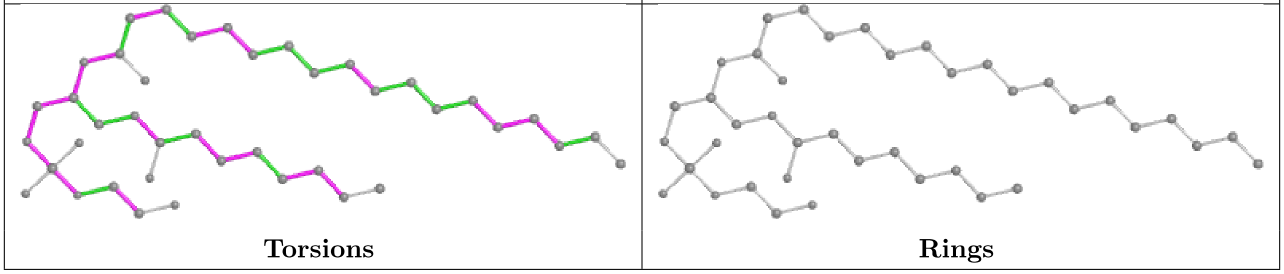
No monomer is involved in short contacts.

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 3PE 4 502

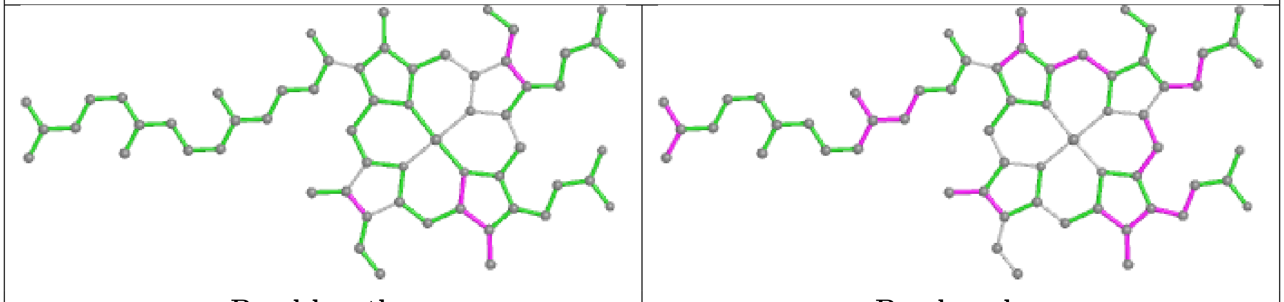


Bond lengths Bond angles

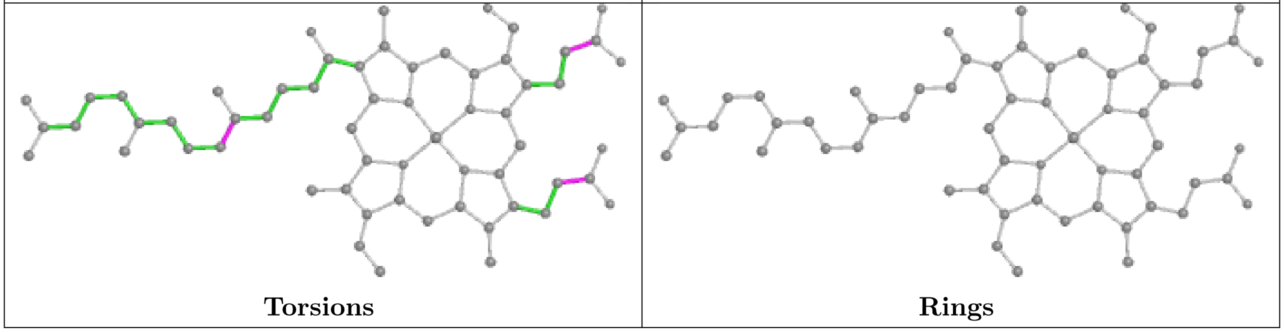


Torsions Rings

Ligand HEA A9 602

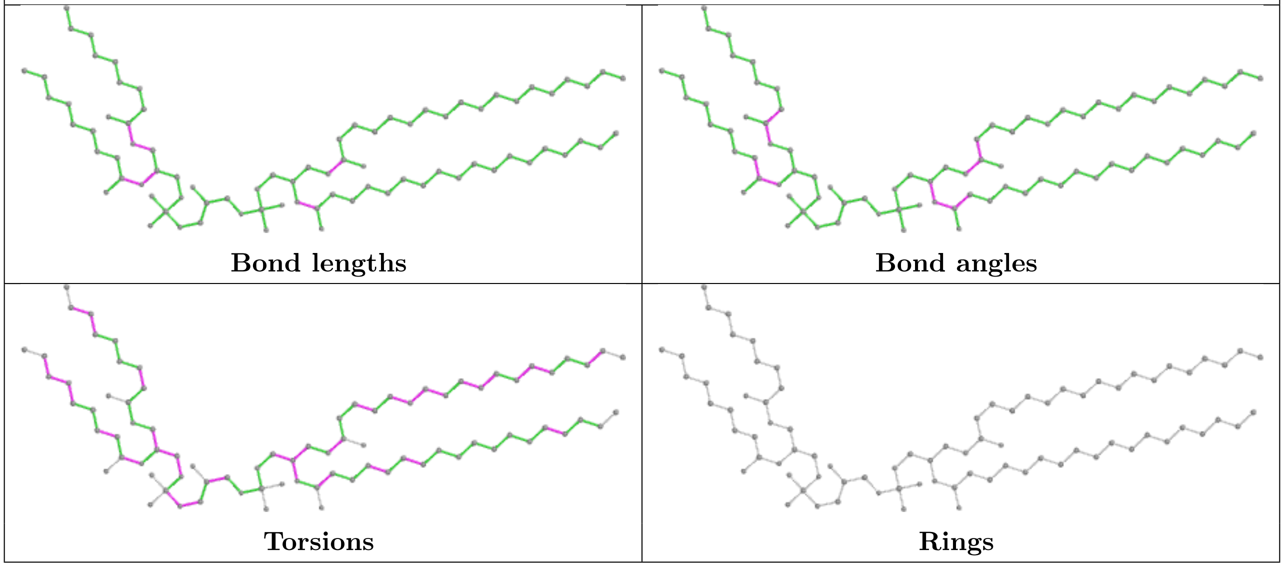


Bond lengths Bond angles



Torsions Rings

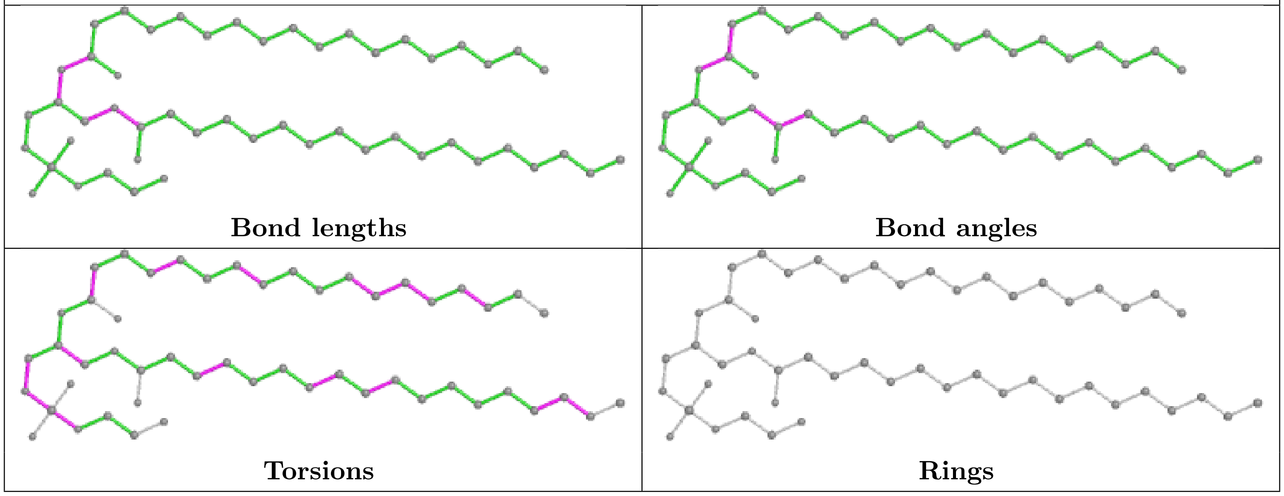
Ligand CDL 4 501



Bond lengths Bond angles

Torsions Rings

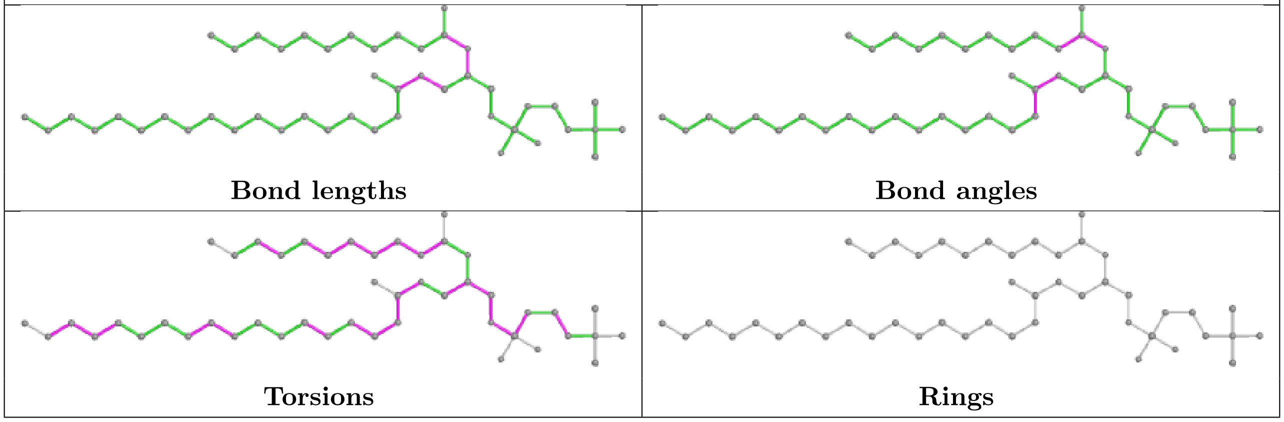
Ligand 3PE V 201



Bond lengths Bond angles

Torsions Rings

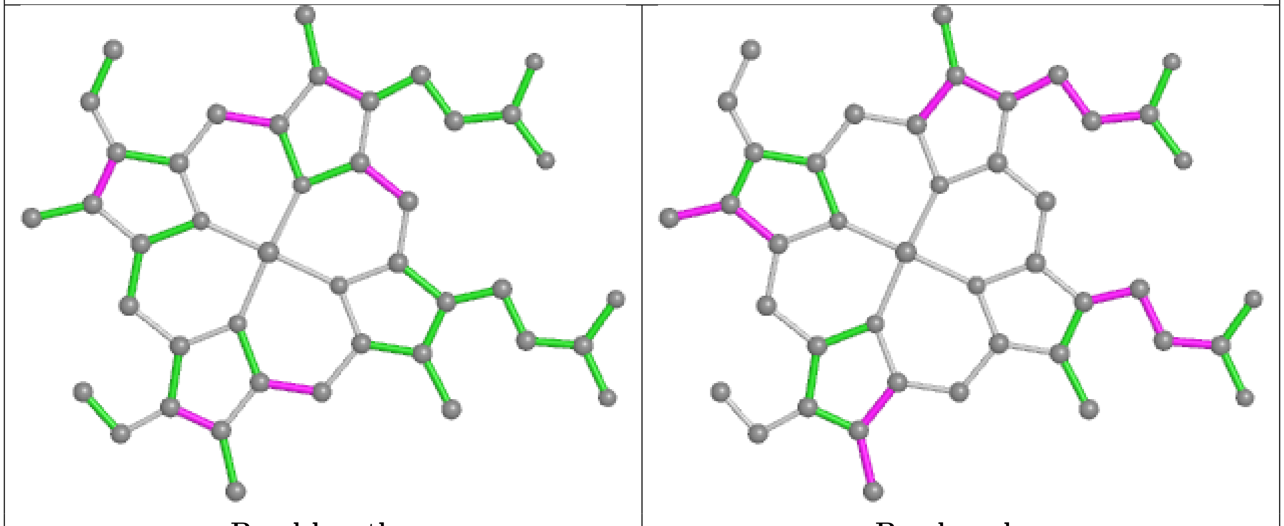
Ligand PC1 S 401



Bond lengths Bond angles

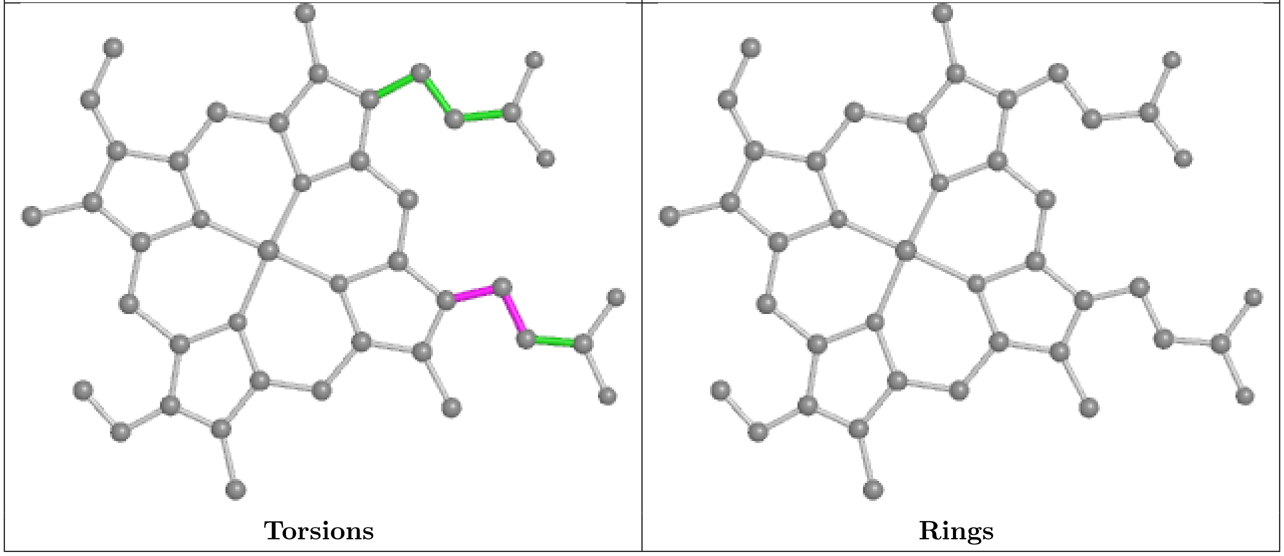
Torsions Rings

Ligand HEC o 301



Bond lengths

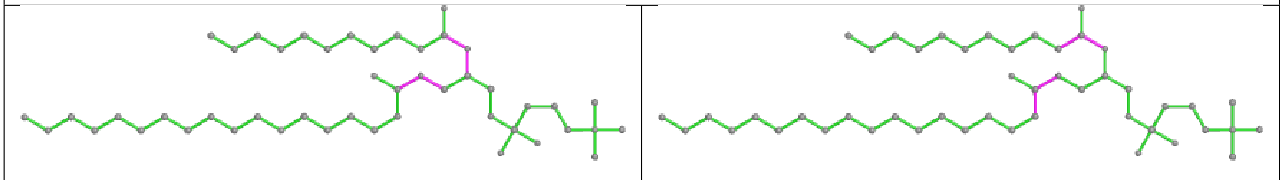
Bond angles



Torsions

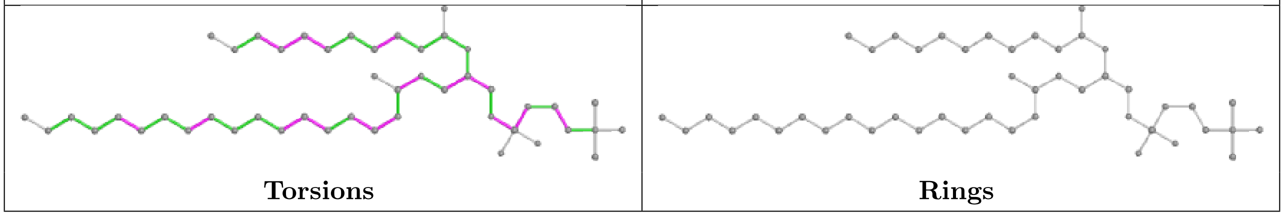
Rings

Ligand PC1 L 200



Bond lengths

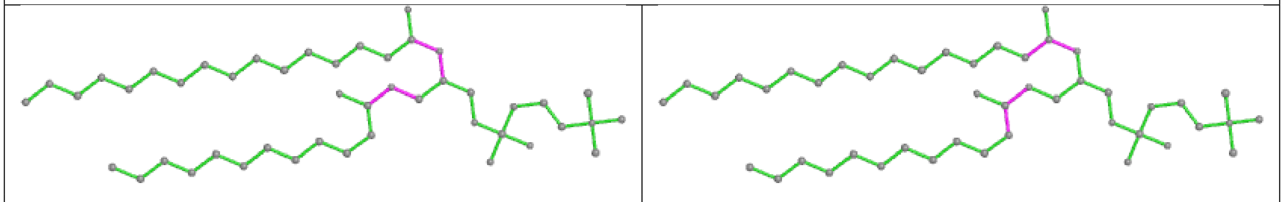
Bond angles



Torsions

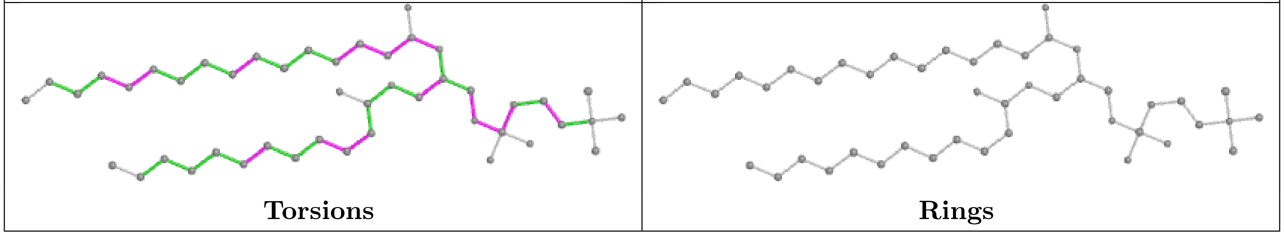
Rings

Ligand PC1 Q 201



Bond lengths

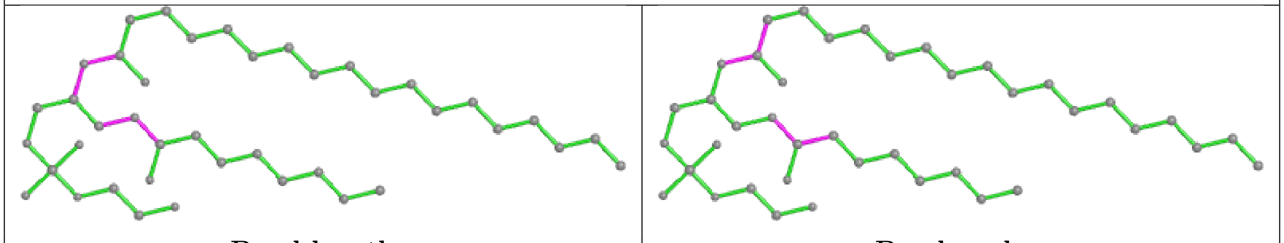
Bond angles



Torsions

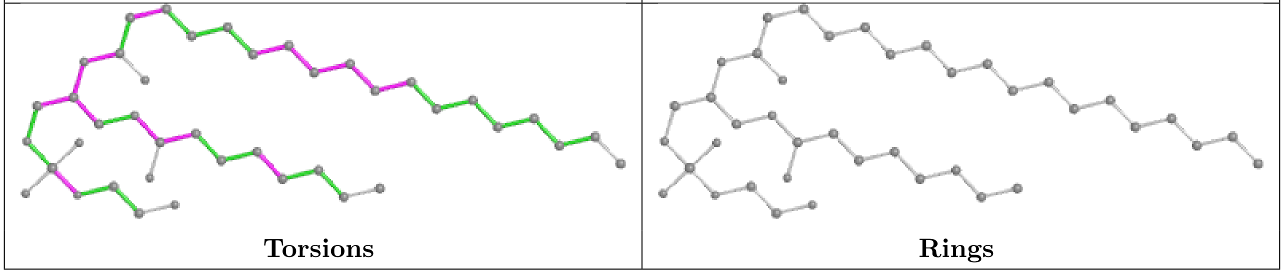
Rings

Ligand 3PE 2 401



Bond lengths

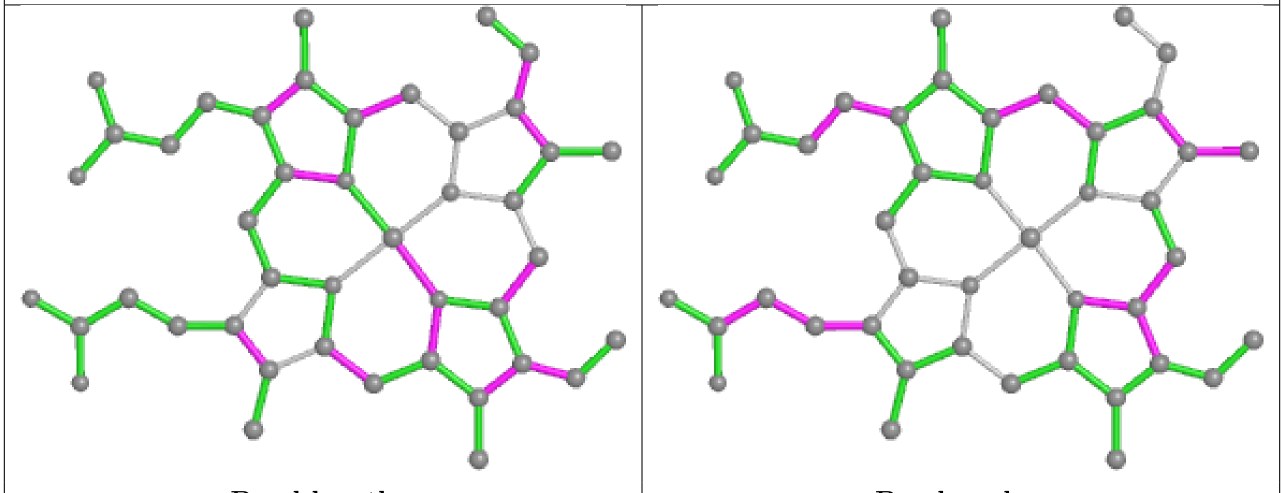
Bond angles



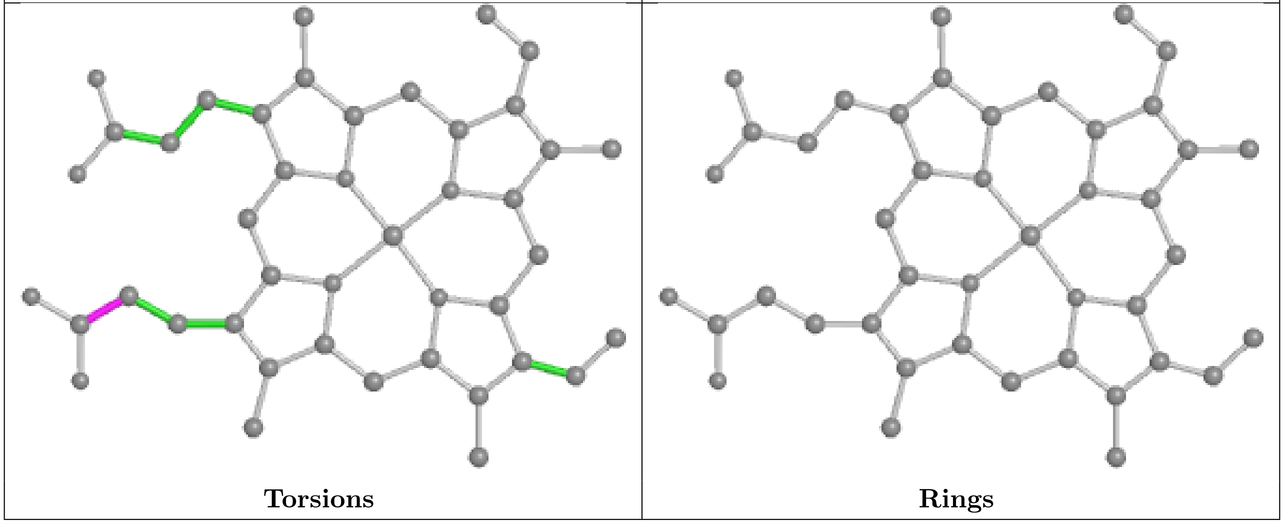
Torsions

Rings

Ligand HEM m 402

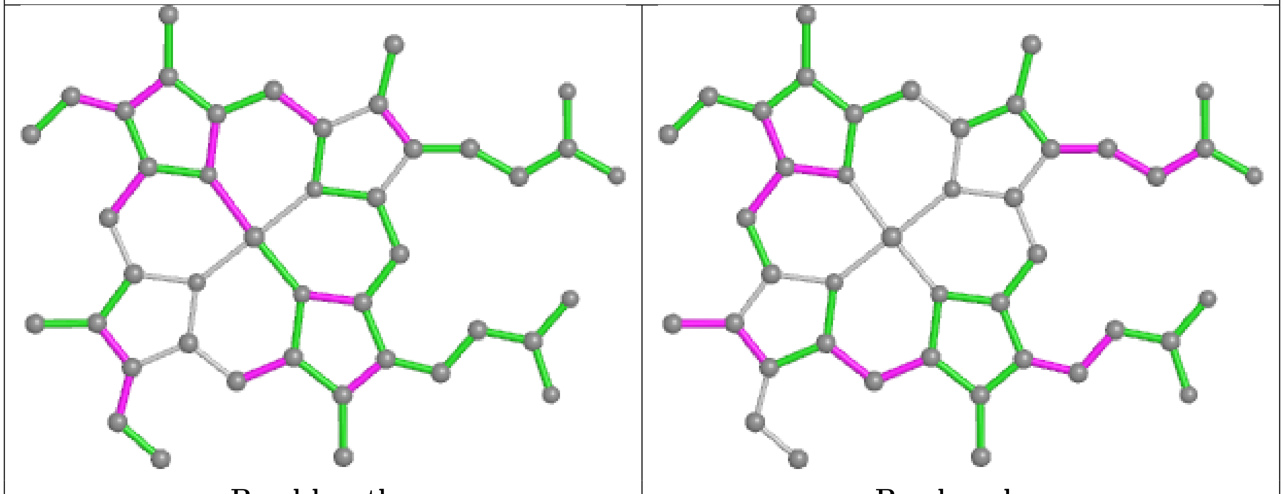


Bond lengths **Bond angles**



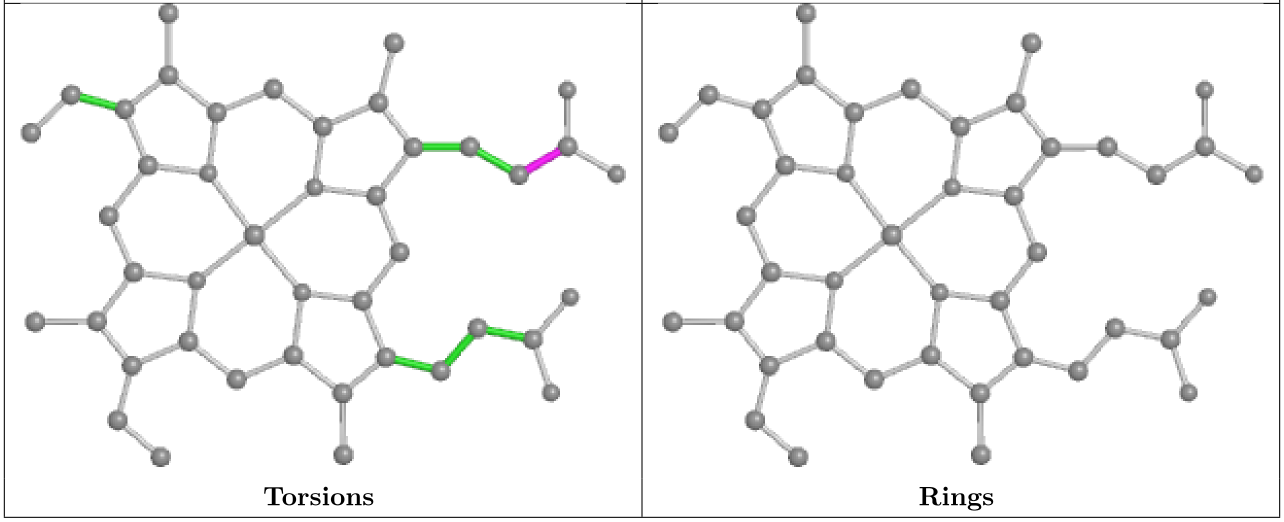
Torsions **Rings**

Ligand HEM y 402



Bond lengths

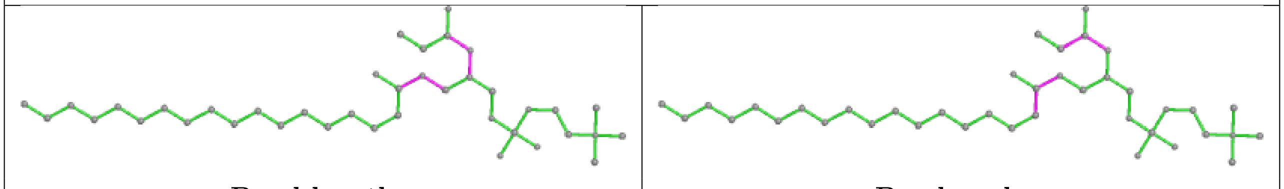
Bond angles



Torsions

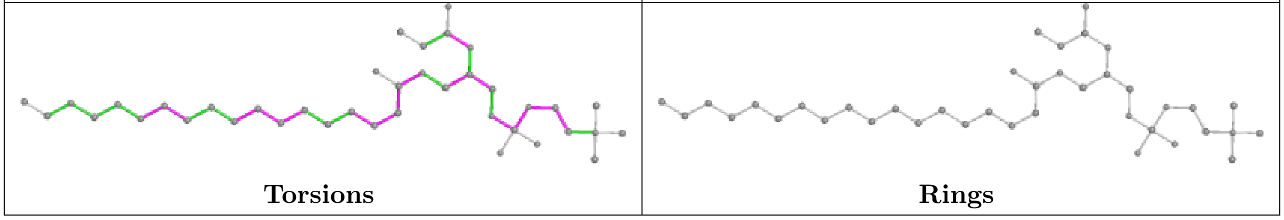
Rings

Ligand PC1 j 201



Bond lengths

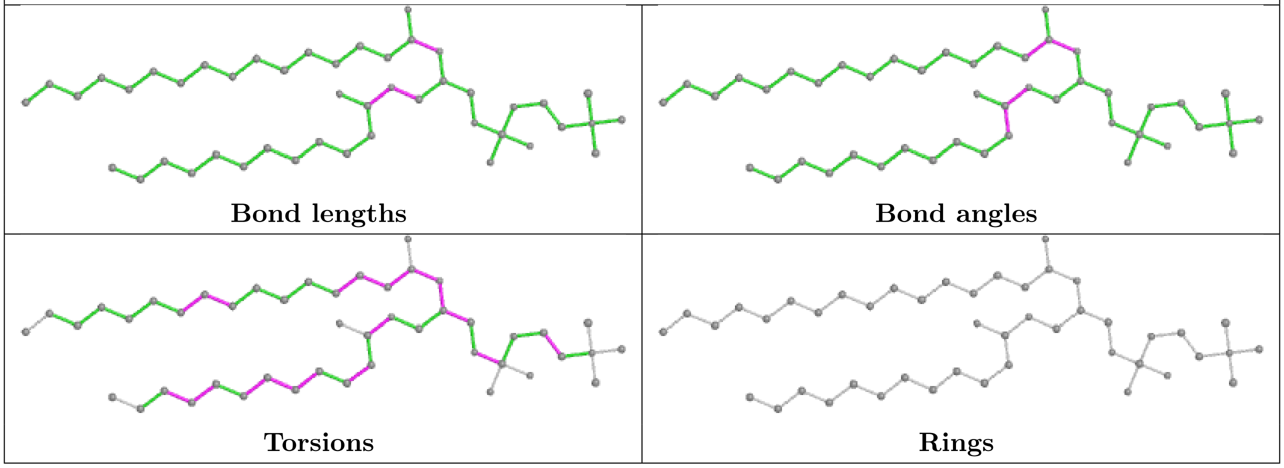
Bond angles



Torsions

Rings

Ligand PC1 2 402



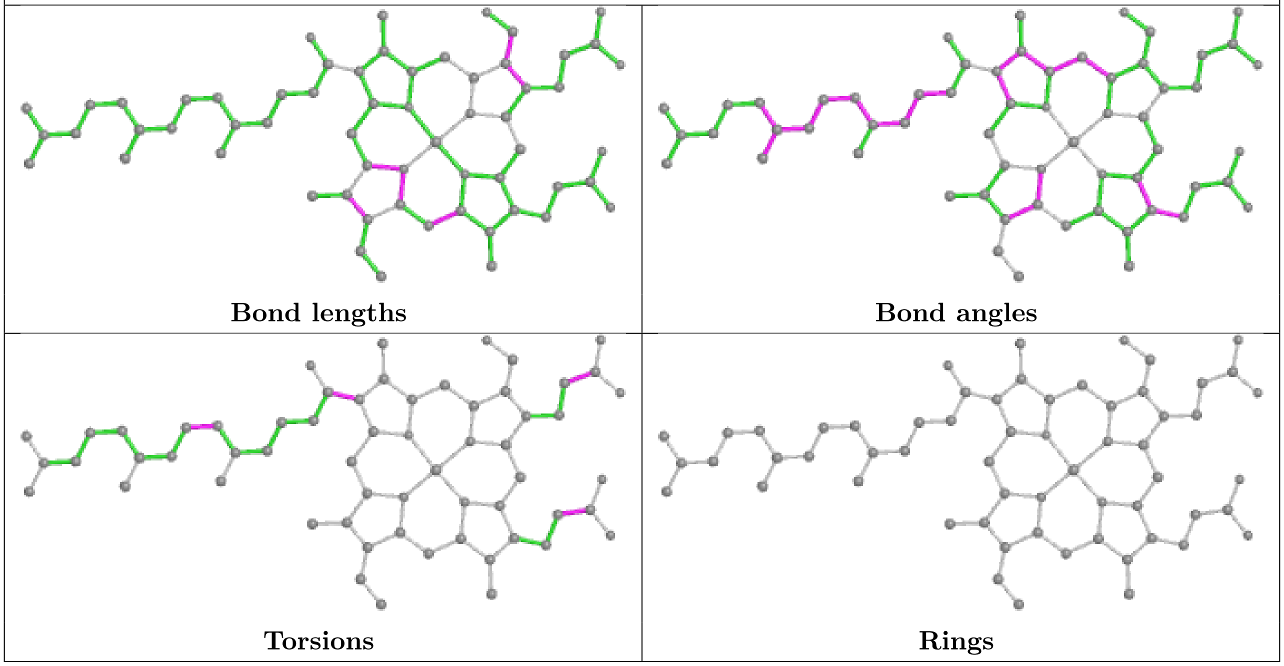
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA A9 601



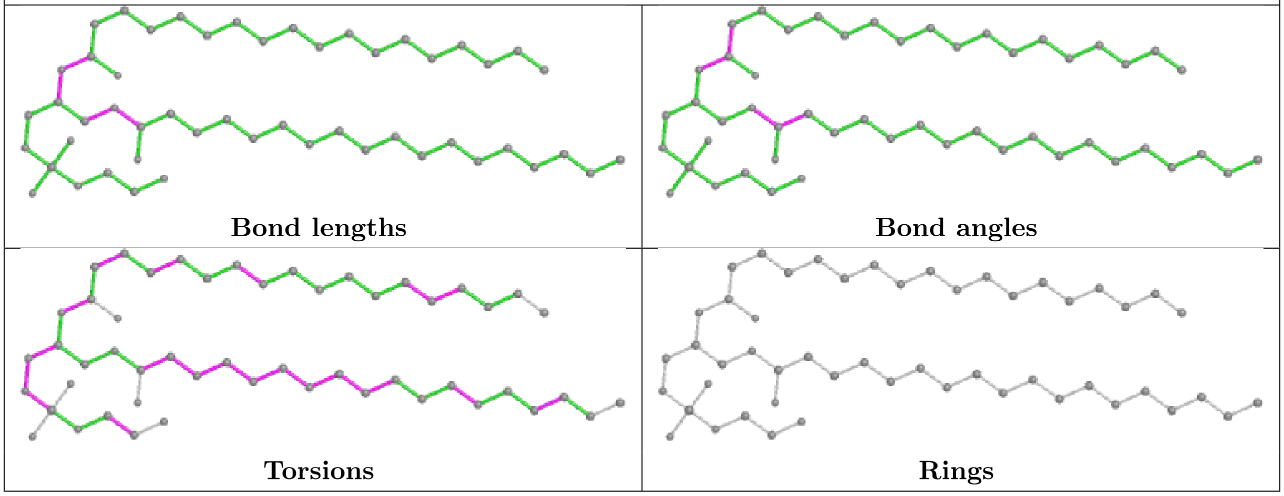
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE B 501



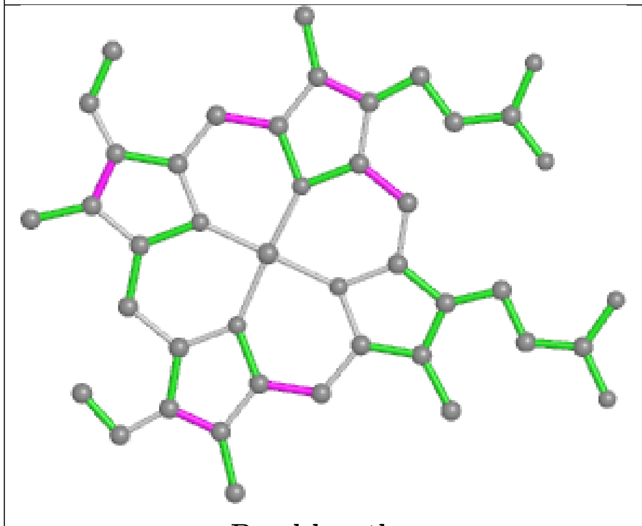
Bond lengths

Bond angles

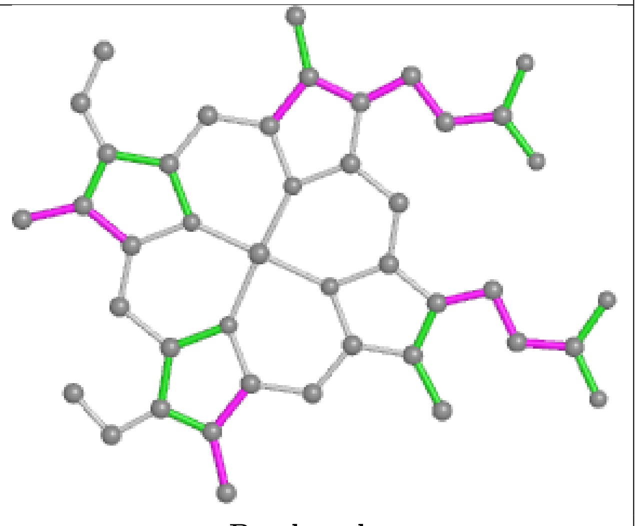
Torsions

Rings

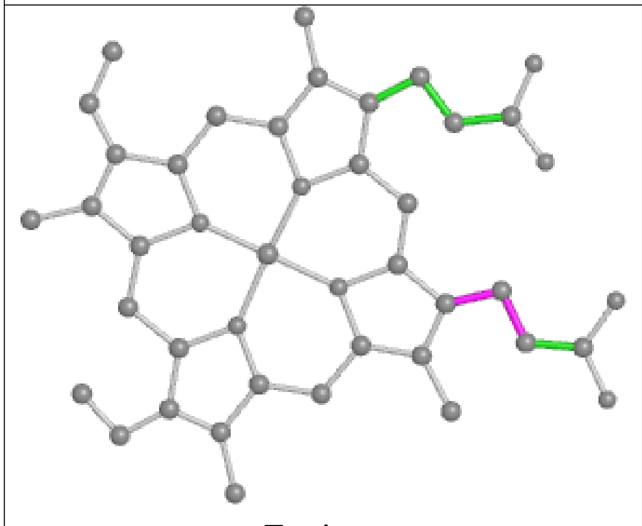
Ligand HEC z 301



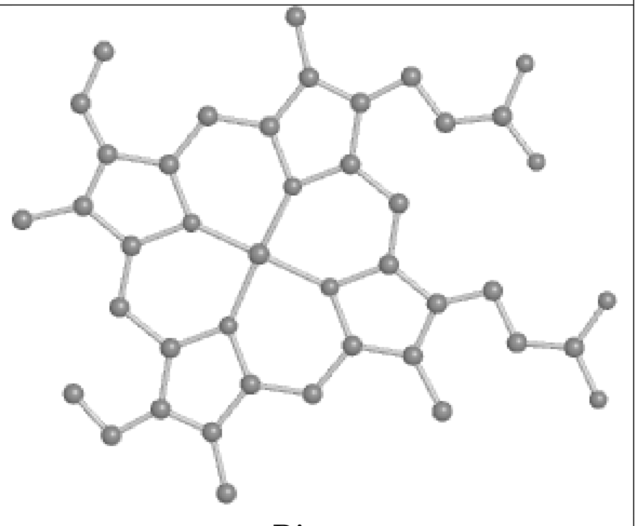
Bond lengths



Bond angles

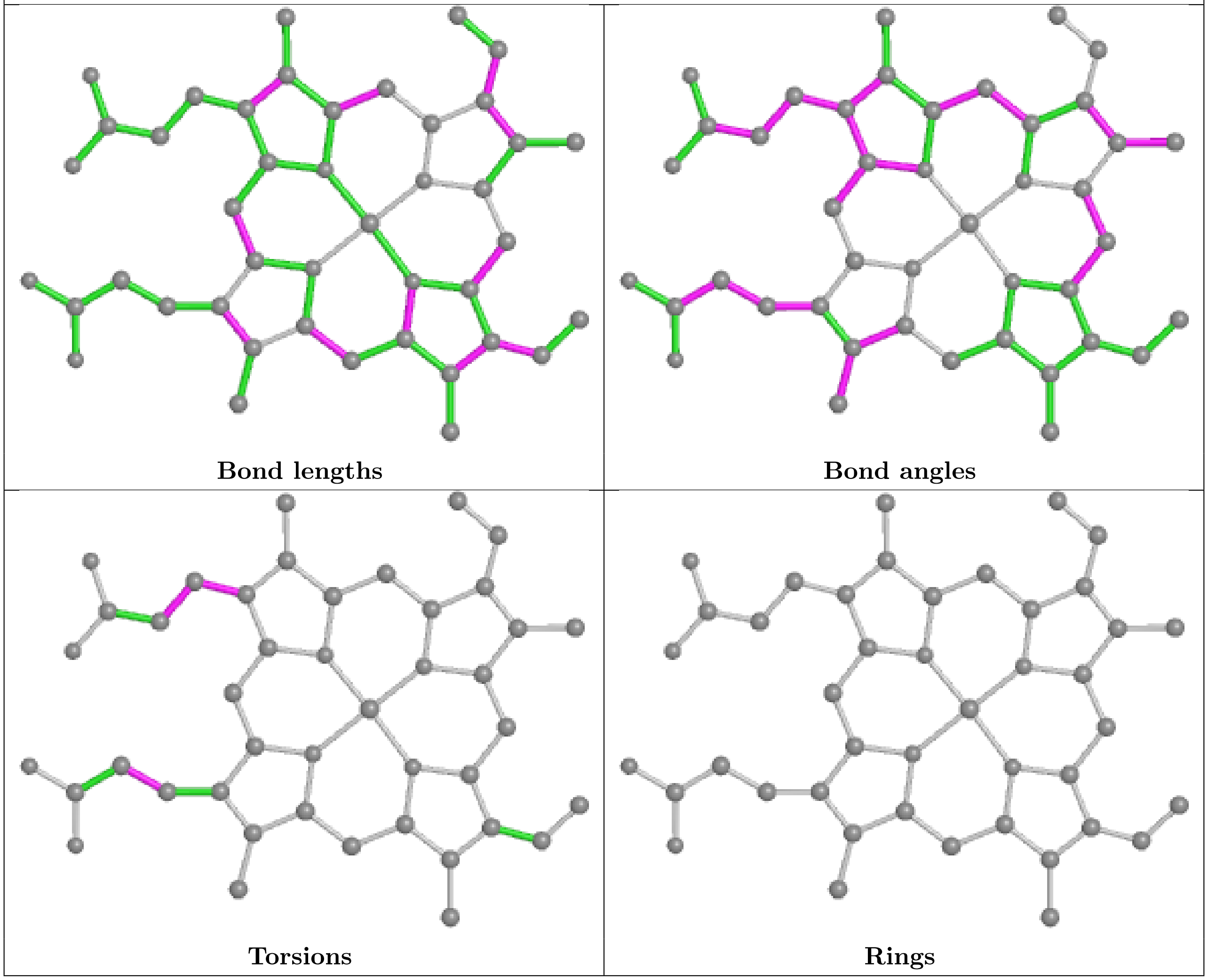


Torsions



Rings

Ligand HEM m 401



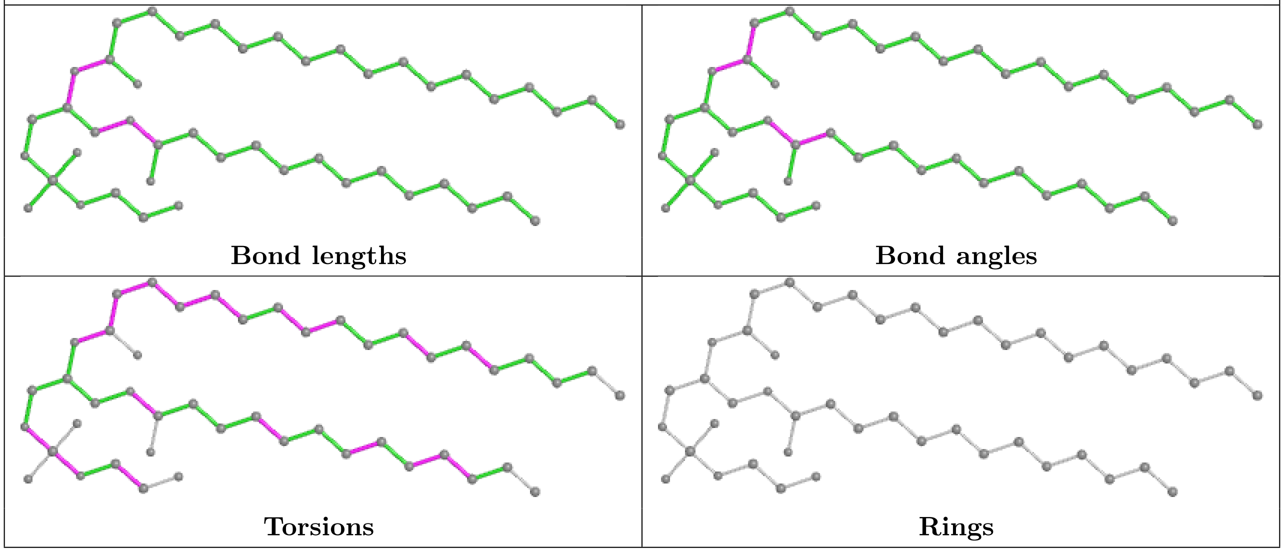
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE j 202



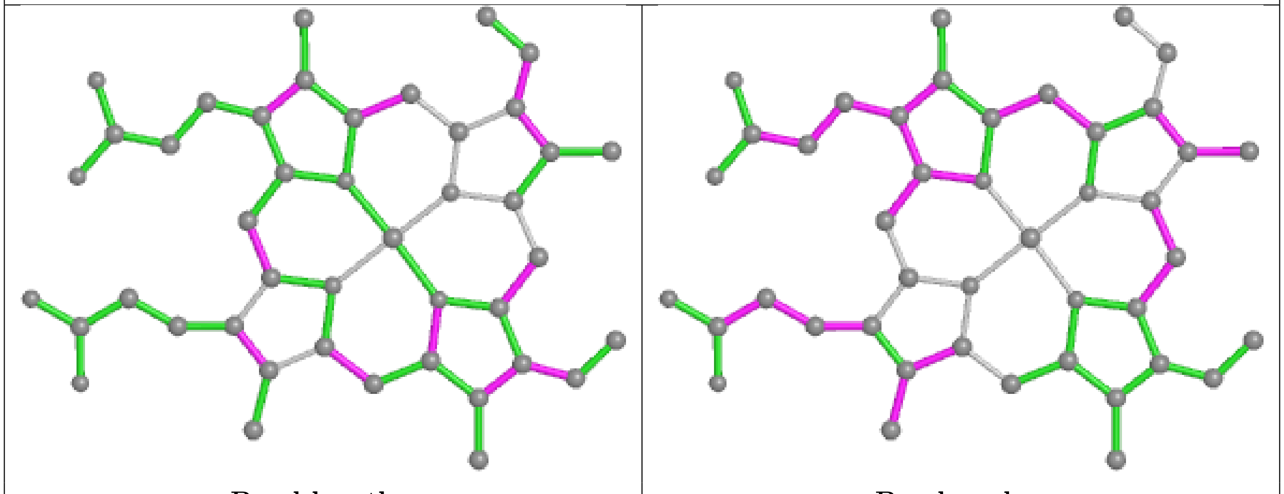
Bond lengths

Bond angles

Torsions

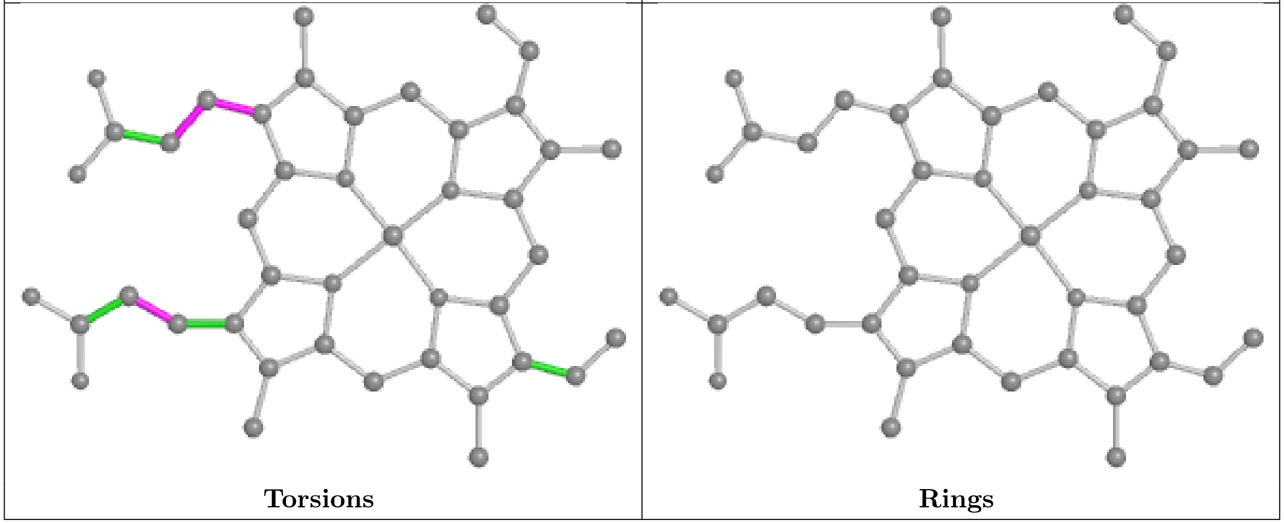
Rings

Ligand HEM y 401



Bond lengths

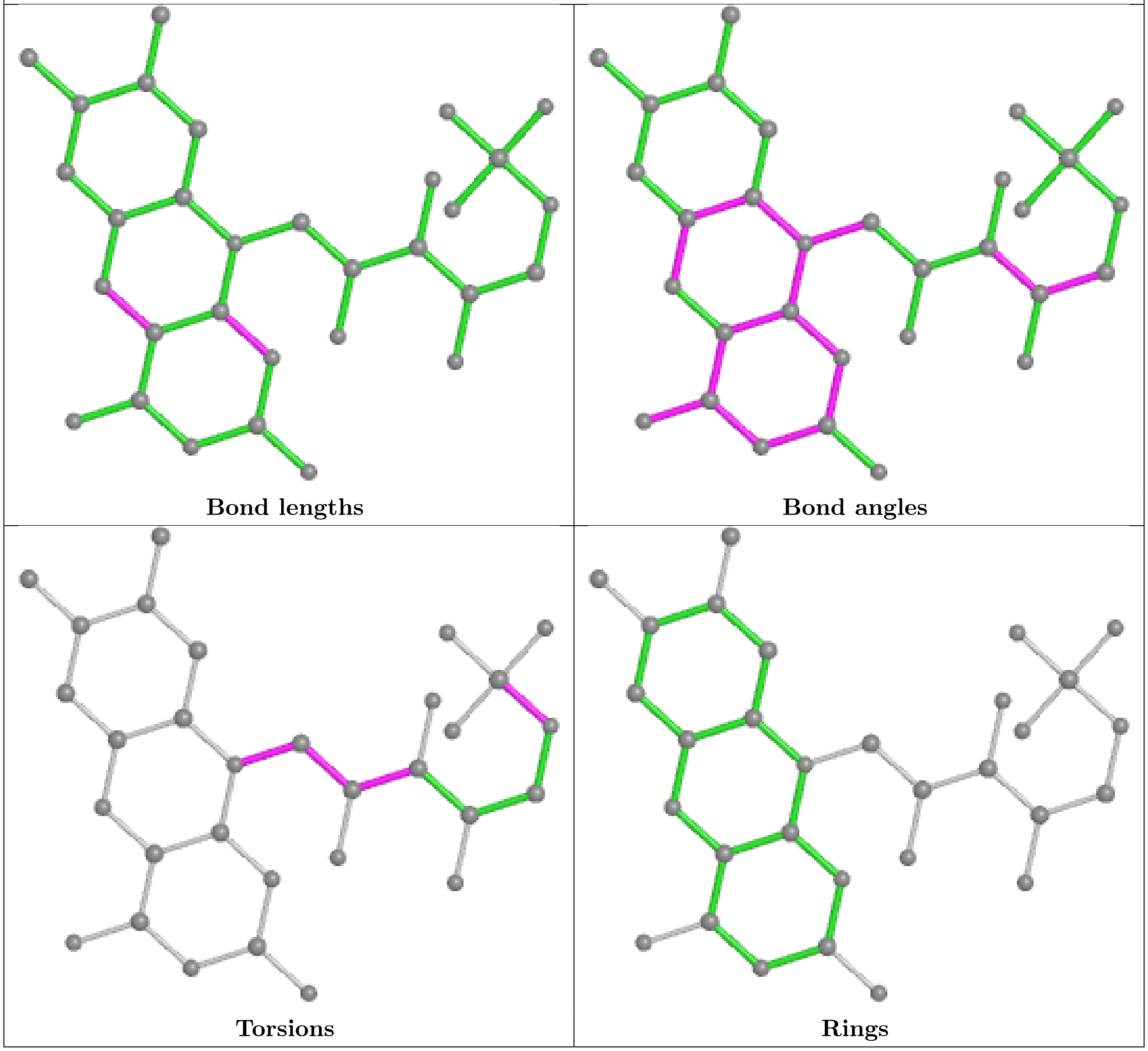
Bond angles



Torsions

Rings

Ligand FMN 8 501



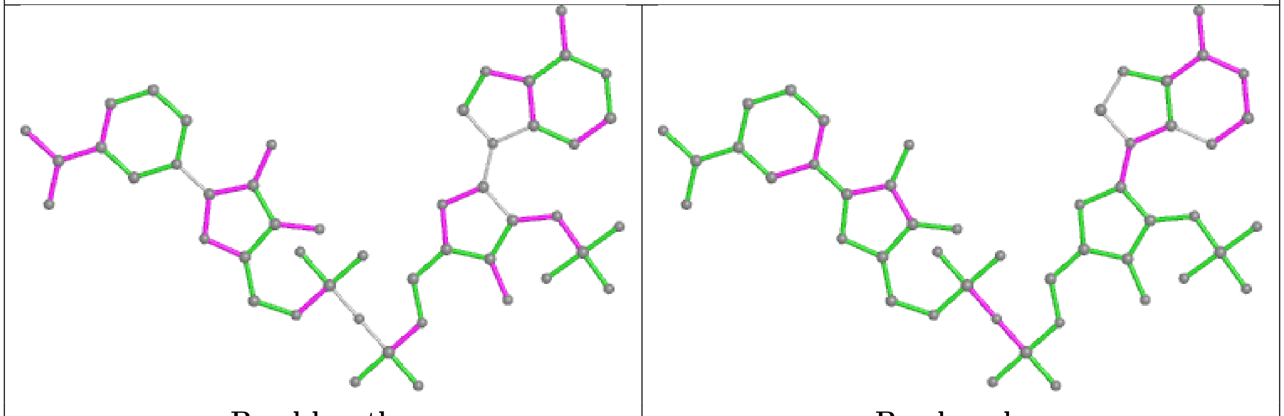
Bond lengths

Bond angles

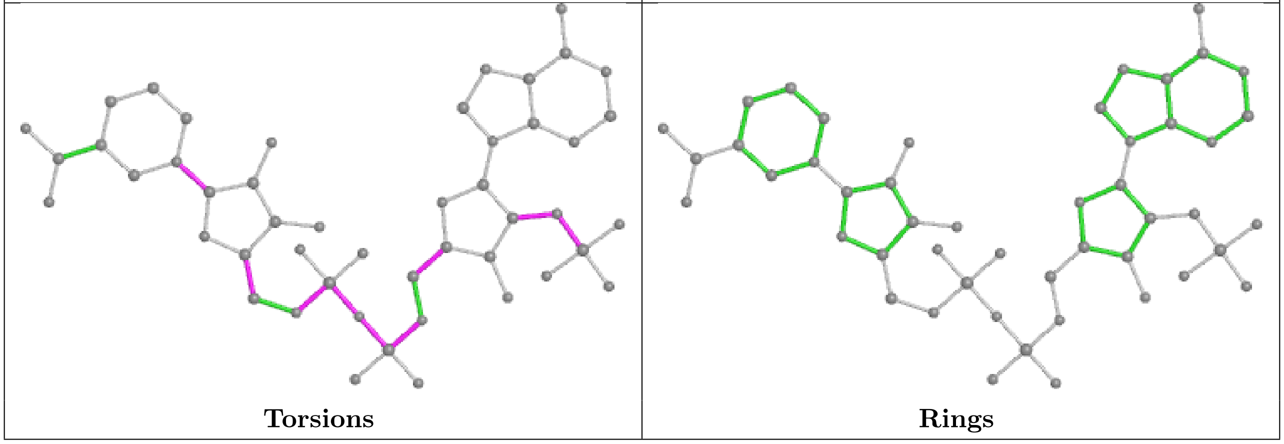
Torsions

Rings

Ligand NAP R 601

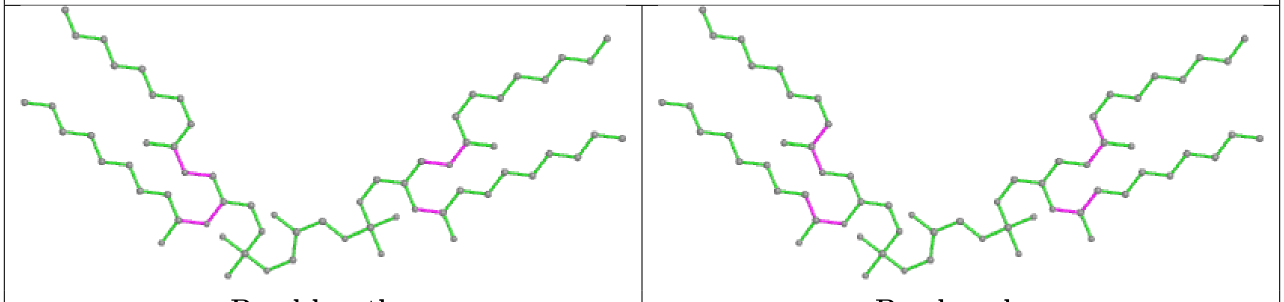


Bond lengths **Bond angles**

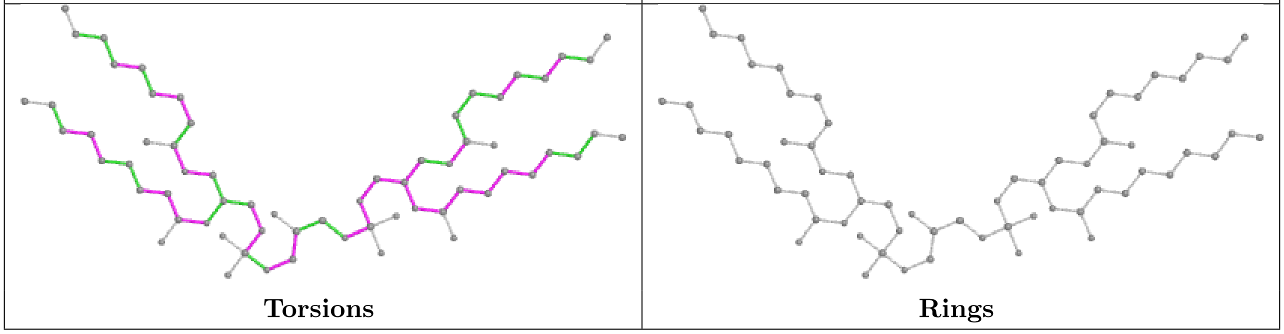


Torsions **Rings**

Ligand CDL 6 701

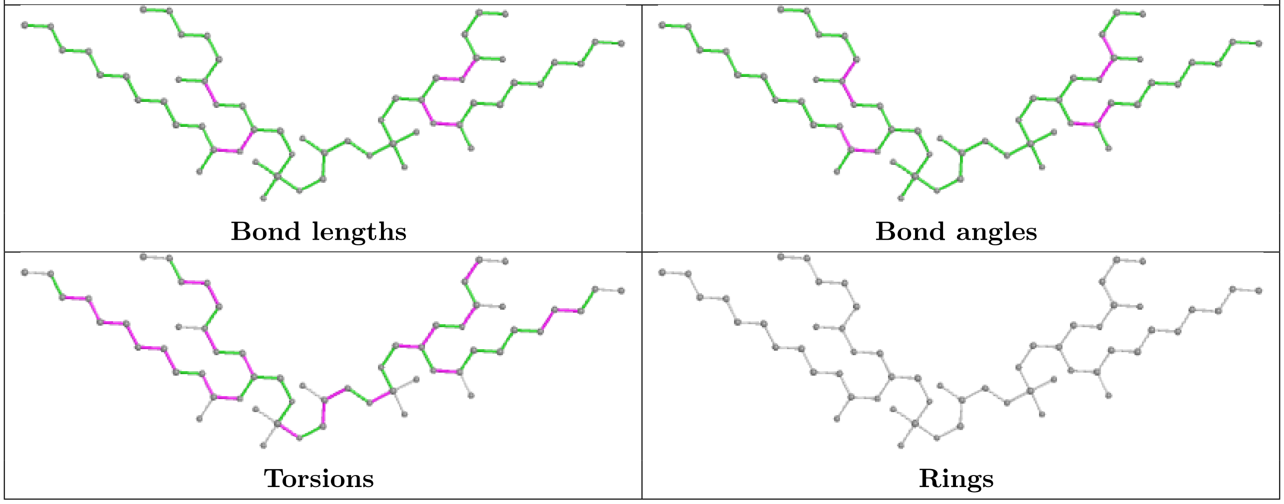


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CDL J 101



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.

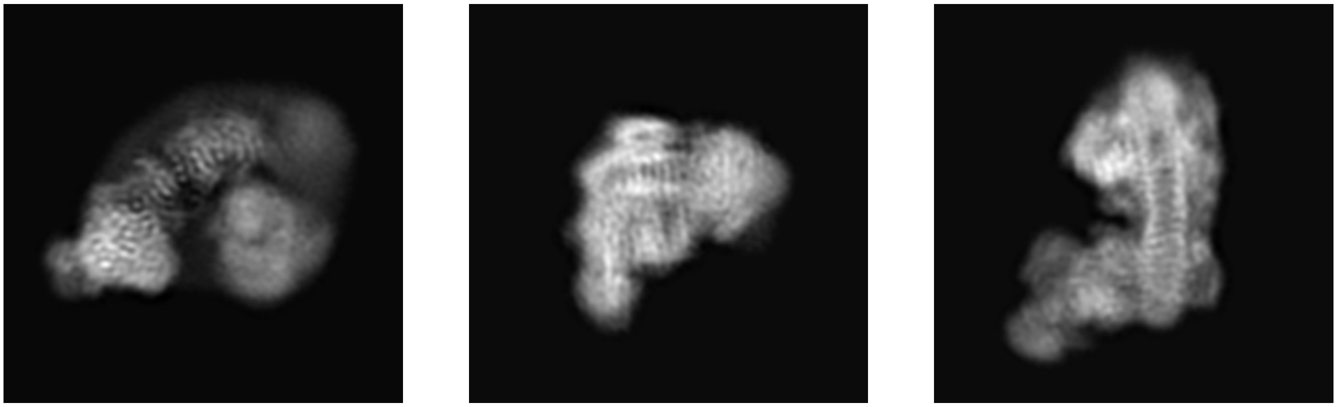
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30675. 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

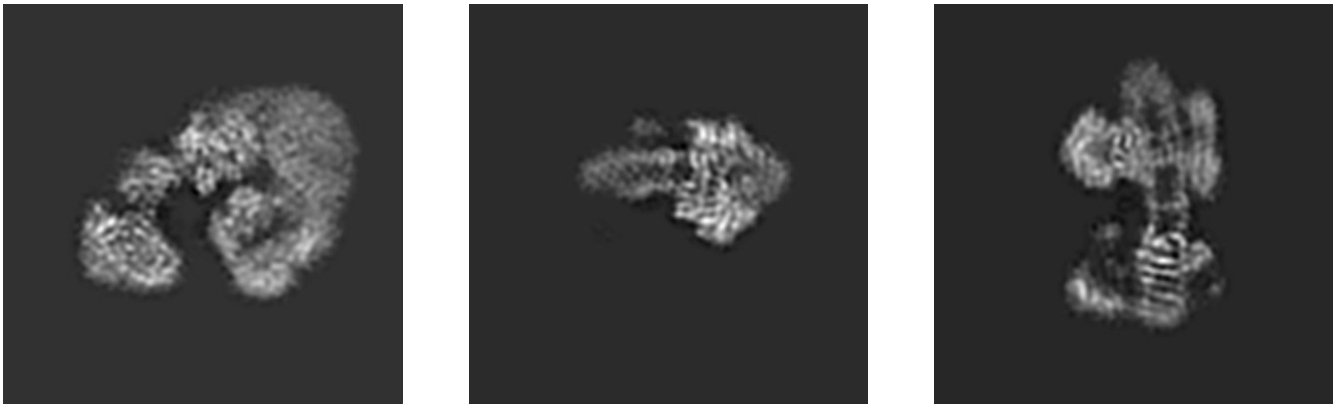


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

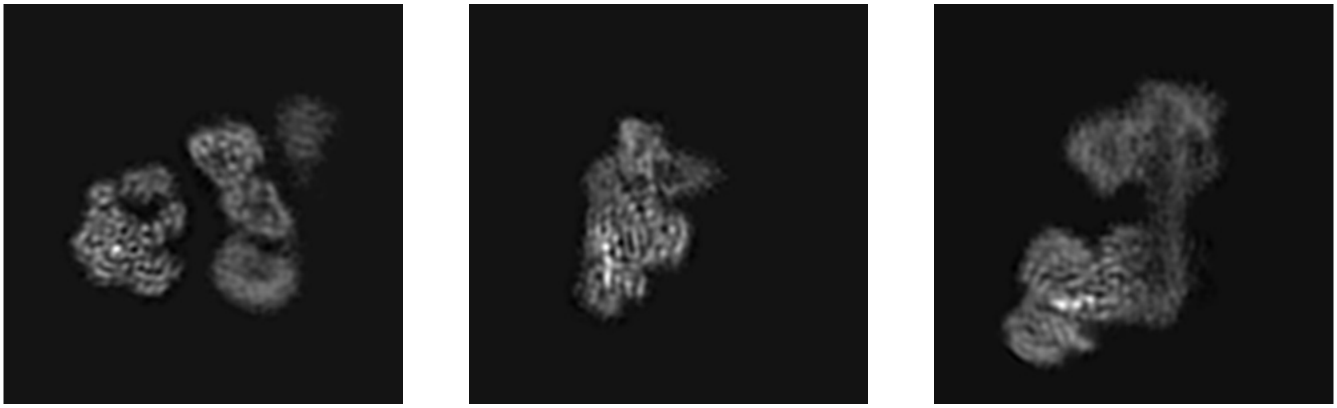


X Index: 140 Y Index: 140 Z Index: 140

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

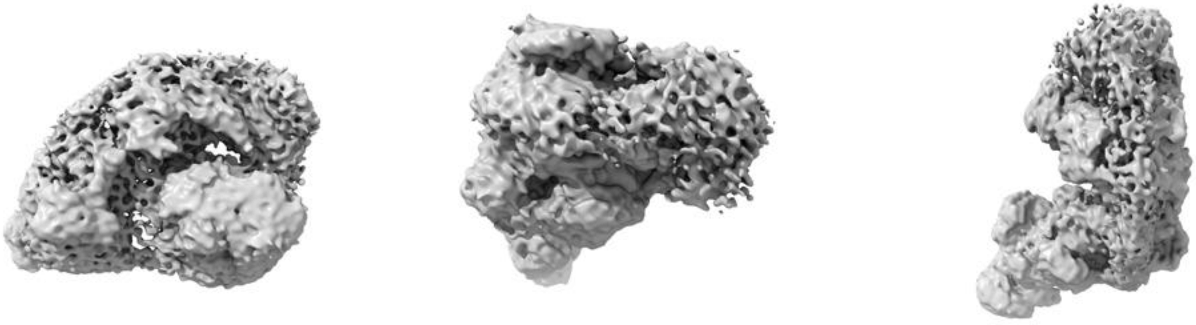


X Index: 123 Y Index: 71 Z Index: 97

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

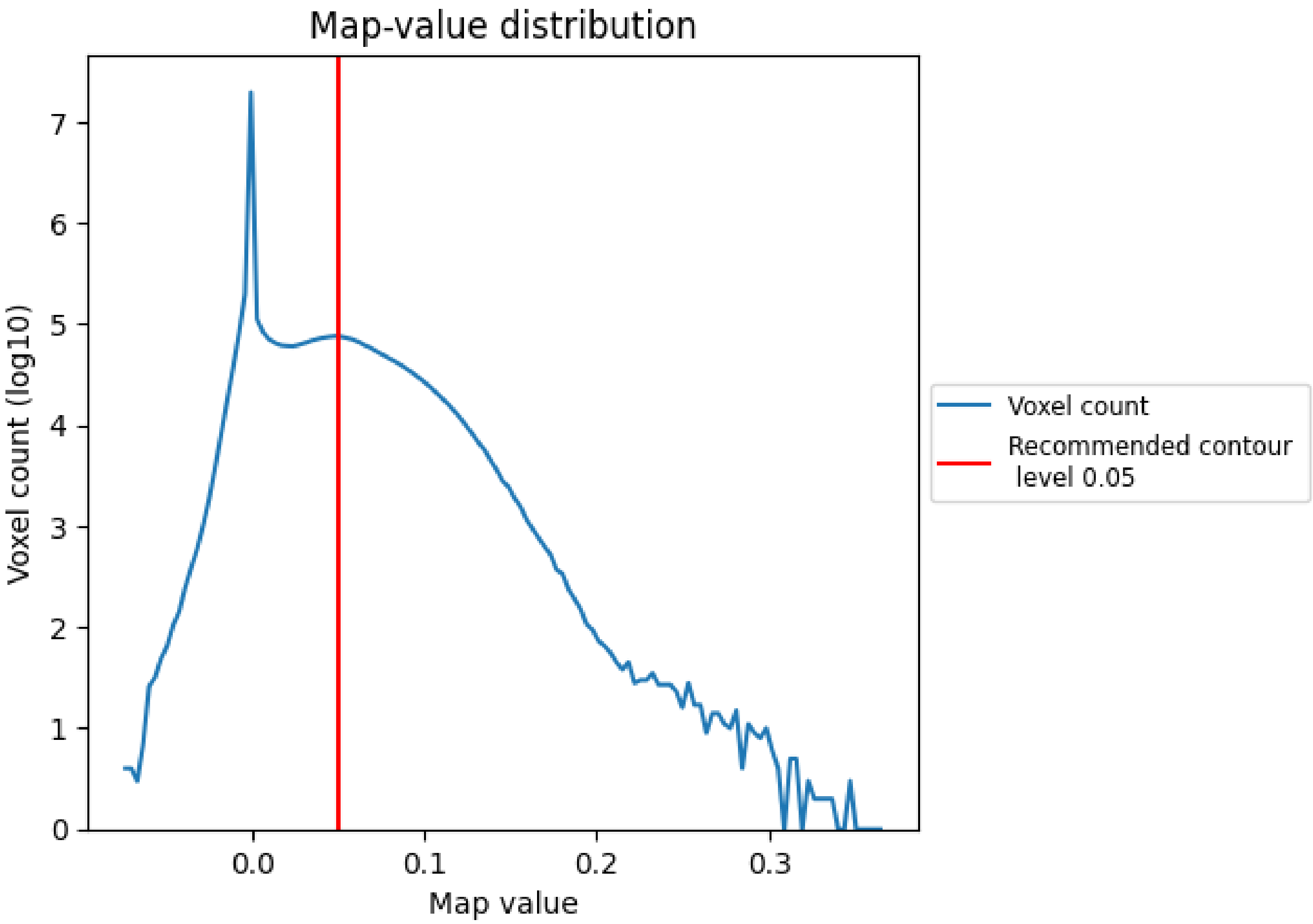
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

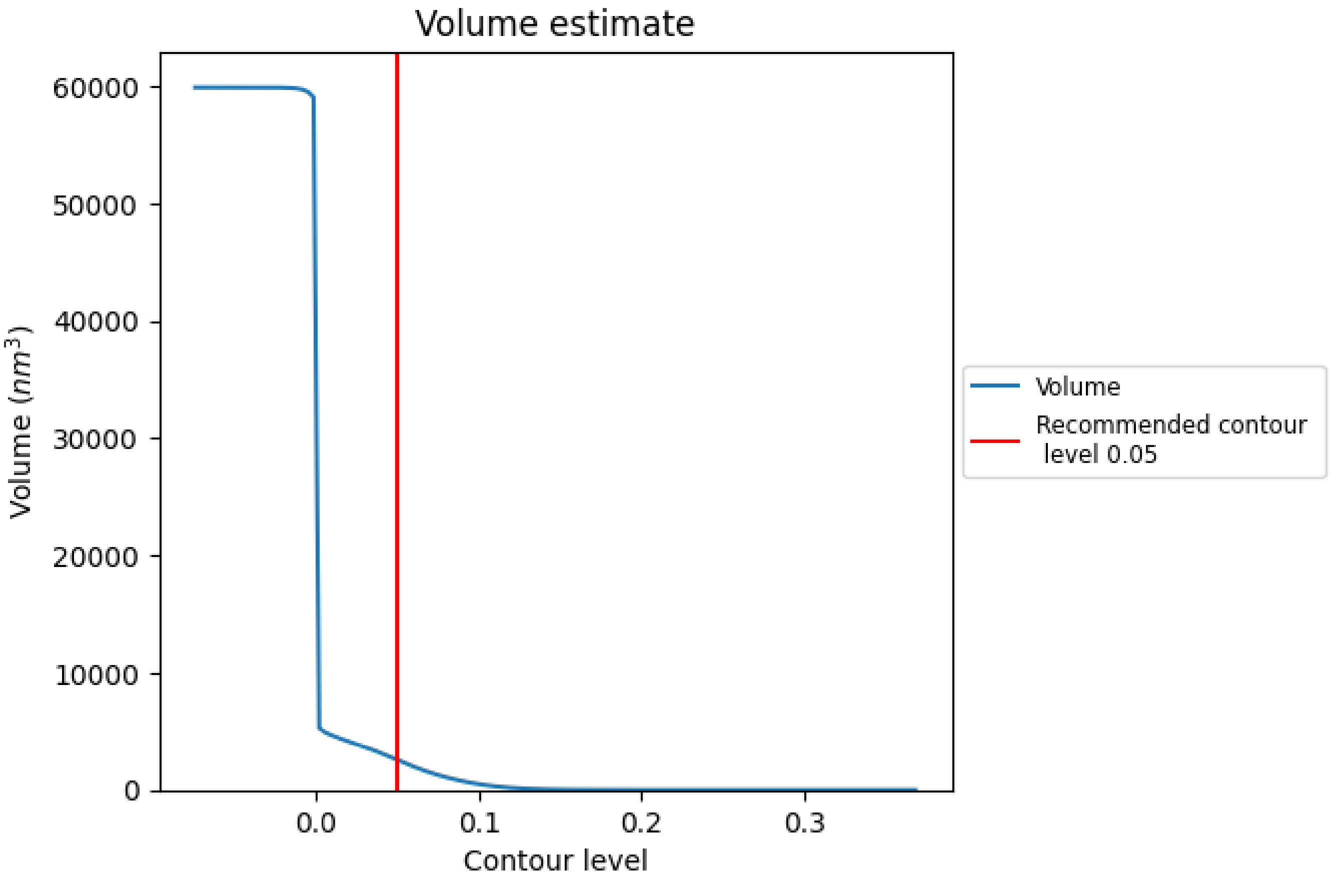
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

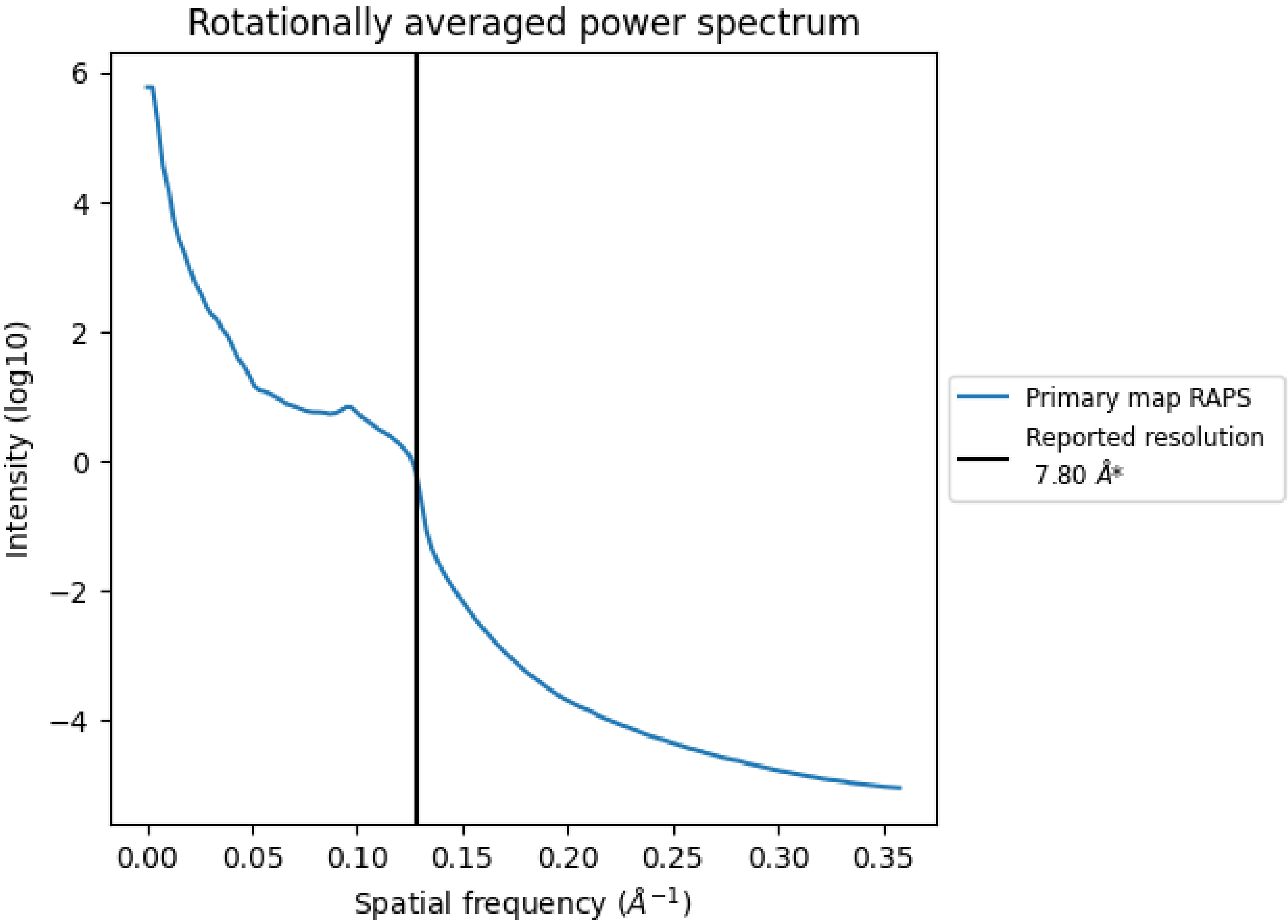
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2566 nm^3; this corresponds to an approximate mass of 2318 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 0.128 Å^{-1}

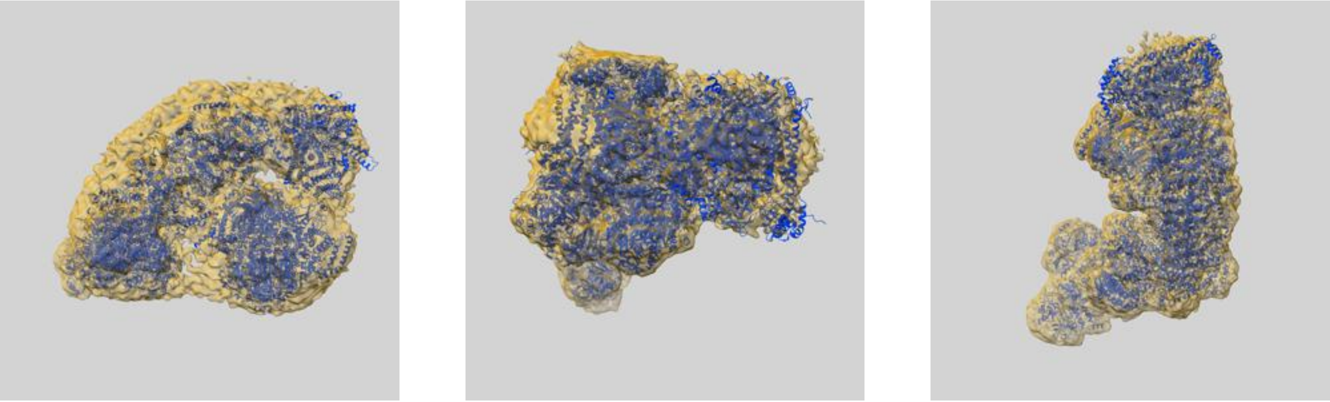
8 Fourier-Shell correlation ⓘ

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-30675 and PDB model 7DGS. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay ⓘ

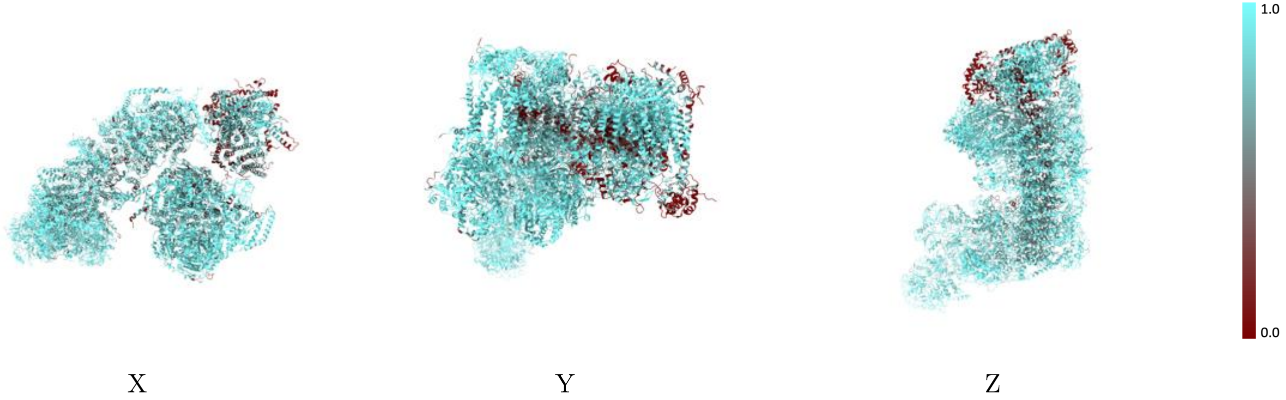

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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 ⓘ

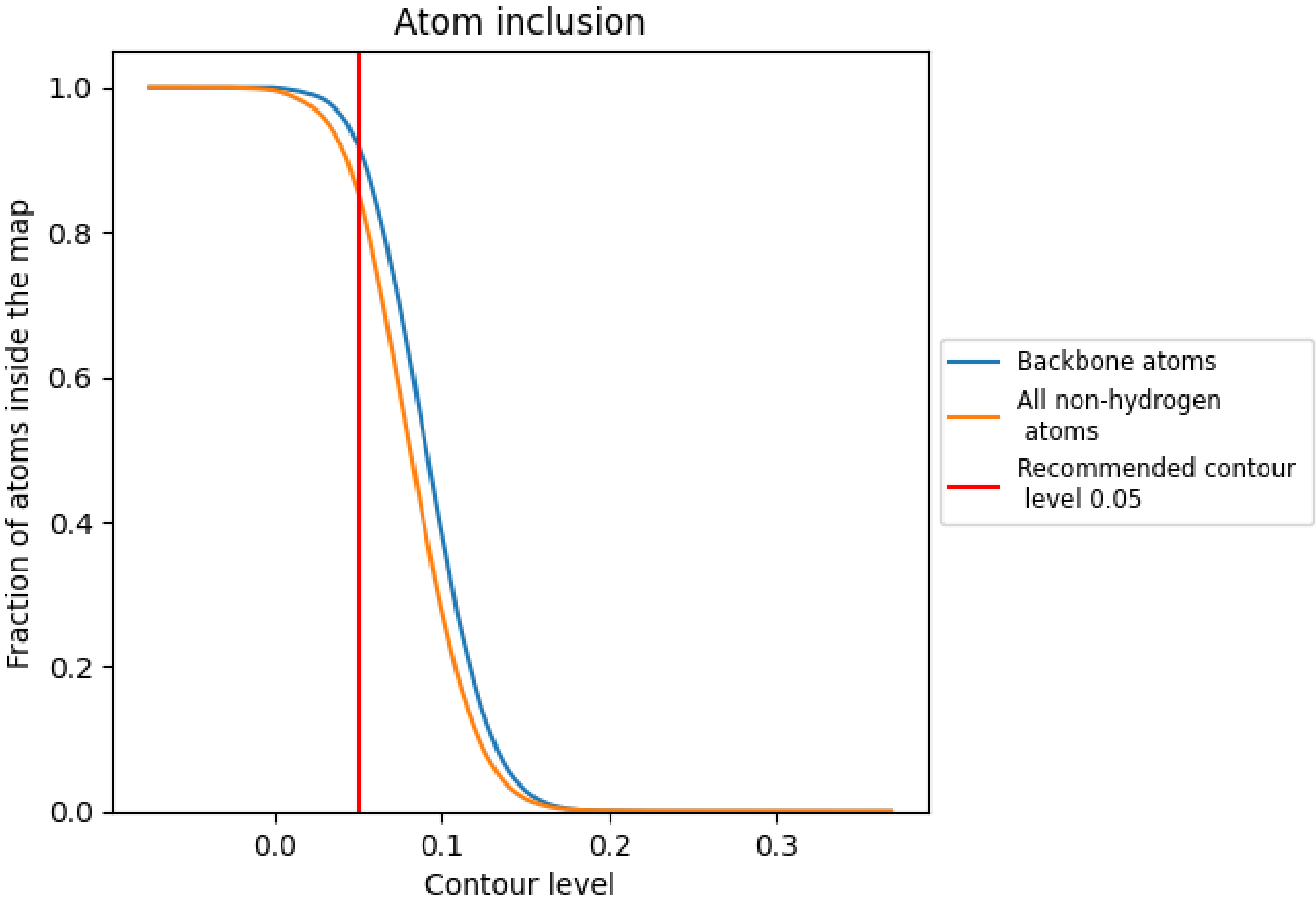
This section was not generated.

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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	■ 0.8552
1	■ 0.8100
2	■ 0.7716
3	■ 0.7319
4	■ 0.7440
5	■ 0.7717
6	■ 0.7792
7	■ 0.7819
8	■ 0.9884
9	■ 0.9756
A	■ 0.9755
A0	■ 0.8538
A1	■ 0.8095
A2	■ 0.8052
A3	■ 0.6246
A4	■ 0.4463
A5	■ 0.4851
A6	■ 0.2506
A7	■ 0.4573
A8	■ 0.5753
A9	■ 0.8317
B	■ 0.8541
B0	■ 0.6293
B1	■ 0.6553
B2	■ 0.3772
B3	■ 0.8958
B4	■ 0.6473
B5	■ 0.7726
B6	■ 0.4397
B7	■ 0.7017
B8	■ 0.3880
B9	■ 0.8096
C	■ 0.9518
D	■ 0.9060
E	■ 0.9598

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Chain	Atom inclusion
F	0.9441
G	0.9301
H	0.9117
I	0.8938
J	0.9703
K	0.9526
L	0.8871
M	0.8885
N	0.9823
O	0.9178
P	0.9365
Q	0.9257
R	0.9260
S	0.8463
T	0.7905
U	0.8581
V	0.9375
W	0.9542
X	0.9098
Y	0.9479
Z	0.9091
a	0.8208
b	0.9362
c	0.9470
d	0.9798
e	0.8617
f	0.9383
g	0.9551
h	0.8891
i	0.9194
j	0.8489
k	0.9556
l	0.9550
m	0.8255
o	0.9471
p	0.9451
q	0.9286
r	0.8369
s	0.9123
t	0.9091
u	0.9018
v	0.9464

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Chain	Atom inclusion
w	▬ 0.9538
x	▬ 0.9822
y	▬ 0.8197
z	▬ 0.9157