wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 12:23 pm BST

PDB ID	:	6QC3
EMDB ID	:	EMD-4495
Title	:	Ovine respiratory supercomplex I+III2 open class 1
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-26
Resolution	:	4.20 Å(reported)
Based on initial model	:	1PPJ

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

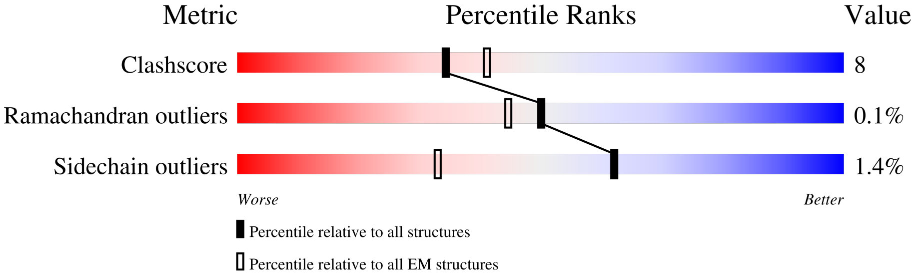
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

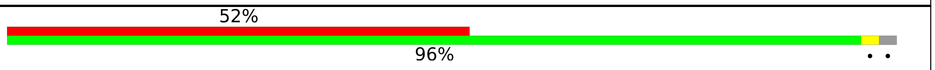
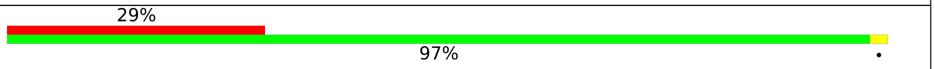
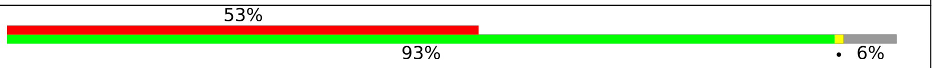
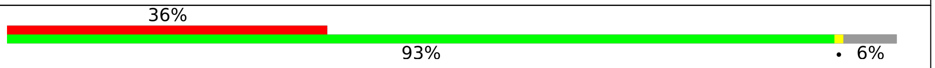
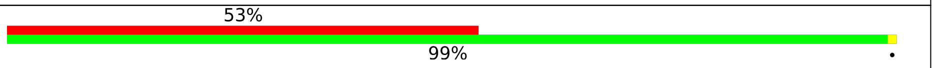
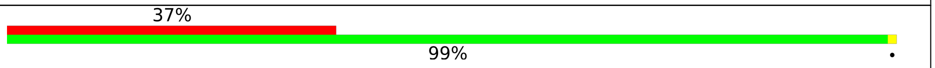
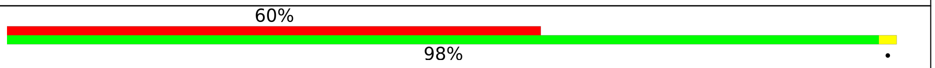
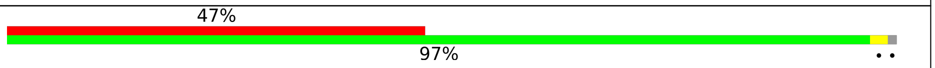
The reported resolution of this entry is 4.20 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	a1	446	
1	a3	446	
2	a2	439	
2	a4	439	
3	b1	379	
3	b2	379	
4	c1	240	
4	c2	240	

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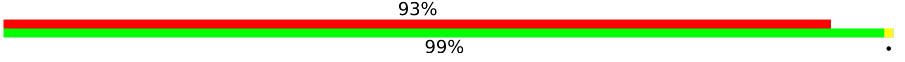
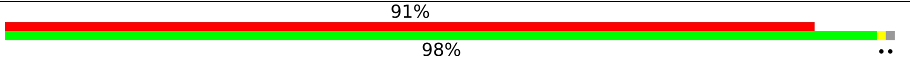
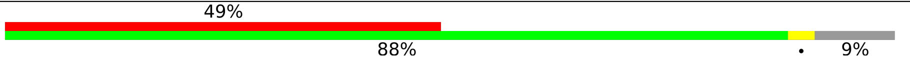
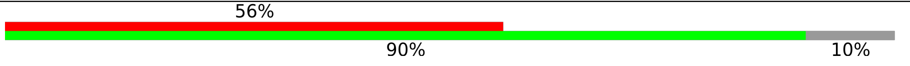
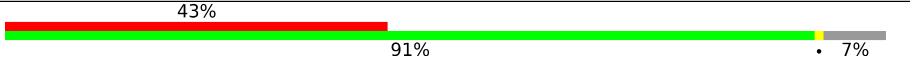
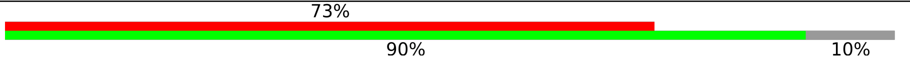
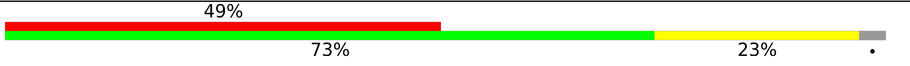
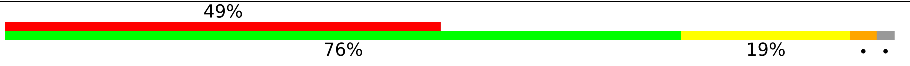
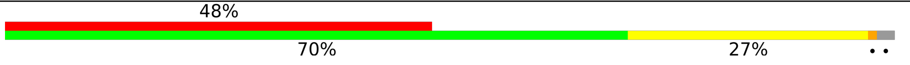
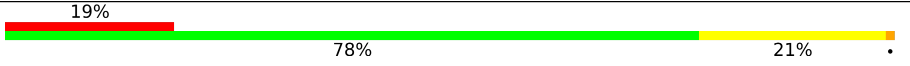
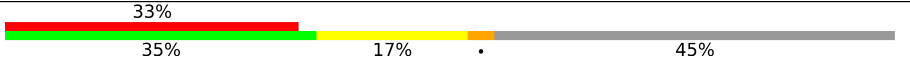
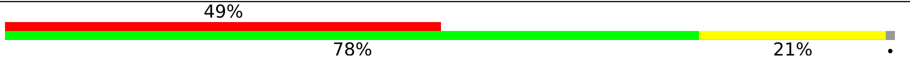
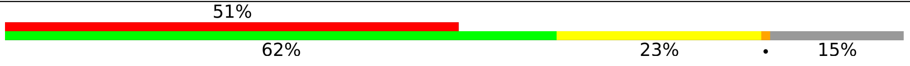
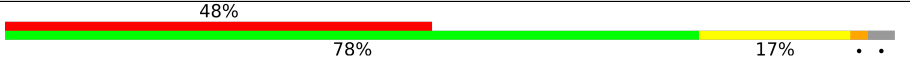
Mol	Chain	Length	Quality of chain
5	f1	196	
5	f2	196	
6	d1	110	
6	d2	110	
7	q1	81	
7	q2	81	
8	h1	78	
8	h2	78	
9	x1	26	
9	x2	26	
10	i1	63	
10	i2	63	
11	V1	445	
12	V2	217	
13	S1	704	
14	S2	430	
15	S3	228	
16	S7	179	
17	S8	176	
18	V3	75	
19	S6	96	
20	S4	133	
21	A9	338	
22	A2	98	
23	A5	115	

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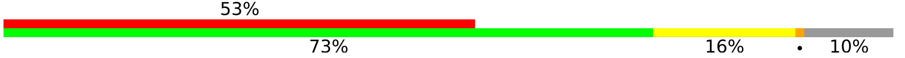
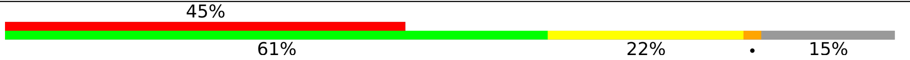
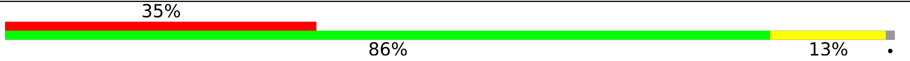
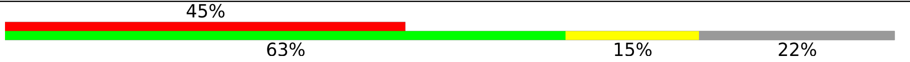
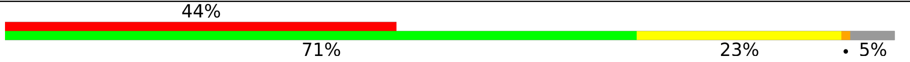
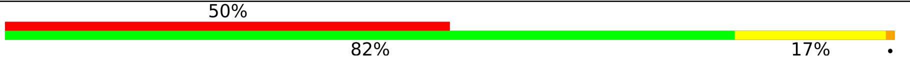
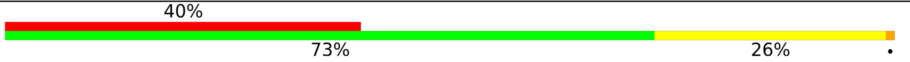
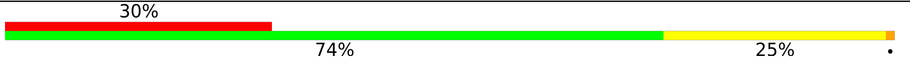
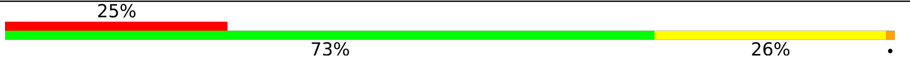
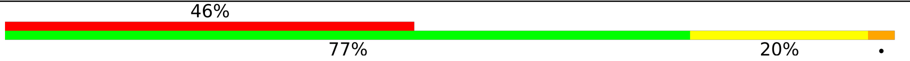
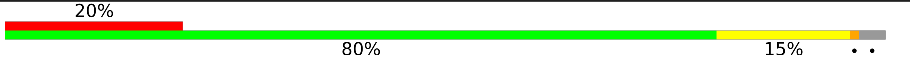
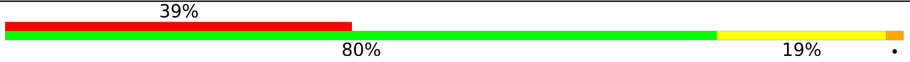
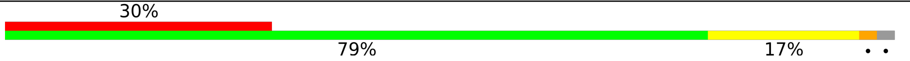
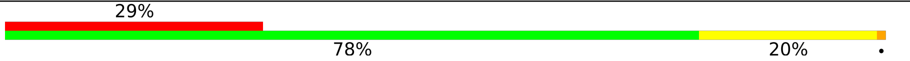
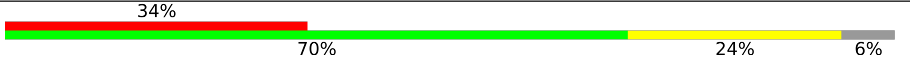
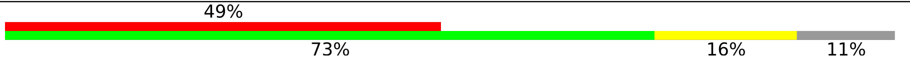
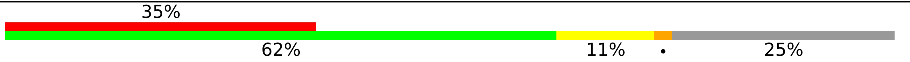
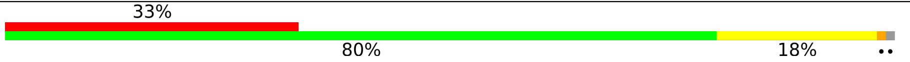
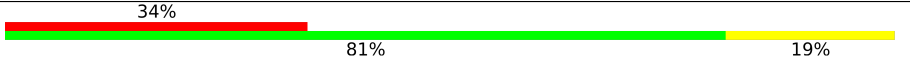
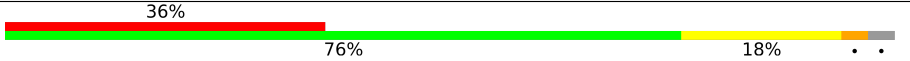
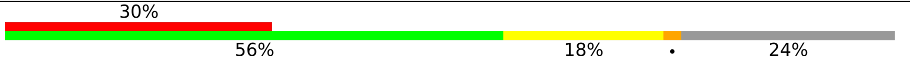
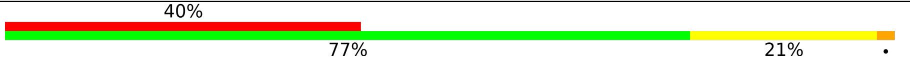
Mol	Chain	Length	Quality of chain
24	A6	127	
25	A7	112	
26	AL	145	
27	AA	88	
27	AB	88	
28	D3	115	
29	D1	318	
30	D6	175	
31	4L	98	
32	D5	606	
33	D4	459	
34	D2	347	
35	AK	140	
36	B5	143	
37	A8	171	
38	BJ	175	
39	AJ	320	
40	S5	105	
41	A3	83	
42	B3	97	
43	C2	120	
44	B4	128	
45	AM	143	
46	B6	127	
47	B7	119	

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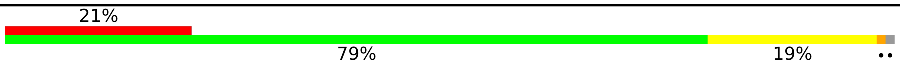
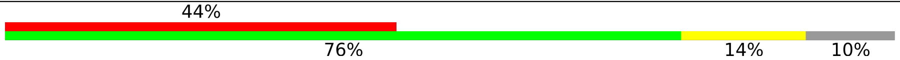
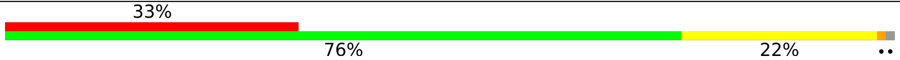
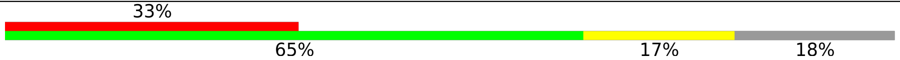
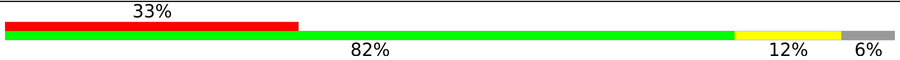
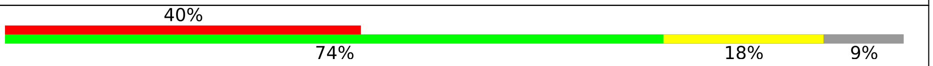
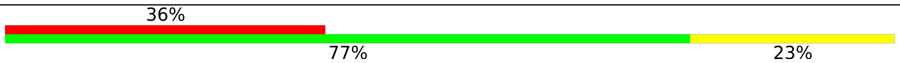
Mol	Chain	Length	Quality of chain
48	B9	178	
49	B2	72	
50	B8	158	
51	BK	125	
52	C1	49	
53	B1	57	
54	A1	70	

2 Entry composition ⓘ

There are 65 unique types of molecules in this entry. The entry contains 96897 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 UQCRC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a1	439	Total	C	N	O	S	0	0
			3409	2132	603	654	20		
1	a3	444	Total	C	N	O	S	0	0
			3447	2153	608	666	20		

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a2	414	Total	C	N	O	S	0	0
			3126	1963	554	601	8		
2	a4	413	Total	C	N	O	S	0	0
			3122	1961	553	600	8		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b1	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		
3	b2	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c1	239	Total	C	N	O	S	0	0
			1909	1219	330	345	15		
4	c2	238	Total	C	N	O	S	0	0
			1903	1216	329	343	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f1	196	1520	958	263	291	8	0	0
5	f2	195	1514	955	262	289	8	0	0

- Molecule 6 is a protein called UQCRB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	d1	100	886	566	159	159	2	0	0
6	d2	101	888	566	159	161	2	0	0

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	q1	73	618	404	116	97	1	0	0
7	q2	75	631	413	118	99	1	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h1	65	532	324	96	107	5	0	0
8	h2	65	532	324	96	107	5	0	0

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	x1	23	114	68	23	23	0	0
9	x2	26	130	78	26	26	0	0

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	i1	55	459	303	80	76	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	i2	57	473	312	82	79	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	V1	430	3312	2086	593	613	20	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	V2	212	1647	1052	277	308	10	0	0

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S1	688	5275	3301	922	1011	41	0	0

- Molecule 14 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S2	424	3414	2180	584	625	25	0	0

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S3	208	1726	1112	296	315	3	0	0

- Molecule 16 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S7	156	1247	795	225	213	14	0	0

- Molecule 17 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S8	176	1414	889	243	270	12	0	0

- Molecule 18 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	V3	41	345	215	63	66	1	0	0

- Molecule 19 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S6	95	737	451	139	144	3	0	0

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S4	126	1024	646	182	193	3	0	0

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	A9	287	2293	1464	419	405	5	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	A2	82	665	419	124	120	2	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	A5	111	901	583	151	165	2	0	0

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	A6	114	969	619	180	166	4	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	A7	95	757	473	144	137	3	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	AL	144	1201	773	215	209	4	0	0

- Molecule 27 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	AA	80	645	416	96	128	5	0	0
			Total	C	N	O	S		
27	AB	87	702	451	103	143	5	0	0

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	D3	90	728	500	103	120	5	0	0

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	D1	303	2415	1633	368	395	19	0	0

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	D6	171	1308	878	187	230	13	0	0

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	4L	98	748	489	112	132	15	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	D5	606	4805	3187	746	828	44	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	D4	459	3646	2428	571	607	40	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	D2	347	2724	1808	416	460	40	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AK	140	1025	654	175	190	6	0	0

- Molecule 36 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B5	139	1156	761	194	199	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	A8	171	1404	889	253	252	10	0	0

- Molecule 38 is a protein called MT-ND5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BJ	171	Total 1441	C 905	N 266	O 262	S 8	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AJ	319	Total 2583	C 1653	N 430	O 490	S 10	0	0

- Molecule 40 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S5	99	Total 822	C 520	N 154	O 142	S 6	0	0

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A3	74	Total 582	C 379	N 96	O 105	S 2	0	0

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B3	73	Total 578	C 378	N 100	O 98	S 2	0	0

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	C2	119	Total 997	C 647	N 174	O 172	S 4	0	0

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	B4	128	Total 1059	C 675	N 189	O 194	S 1	0	0

- Molecule 45 is a protein called MT-ND1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AM	139	1143	733	200	201	9	0	0

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	B6	96	815	536	139	139	1	0	0

- Molecule 47 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	B7	119	1026	641	196	181	8	0	0

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	B9	176	1515	970	278	261	6	0	0

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	B2	65	563	372	93	97	1	0	0

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	B8	157	1324	855	217	243	9	0	0

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BK	102	853	547	141	161	4	0	0

- Molecule 52 is a protein called NDUFB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	C1	46	391	258	67	66	0	0

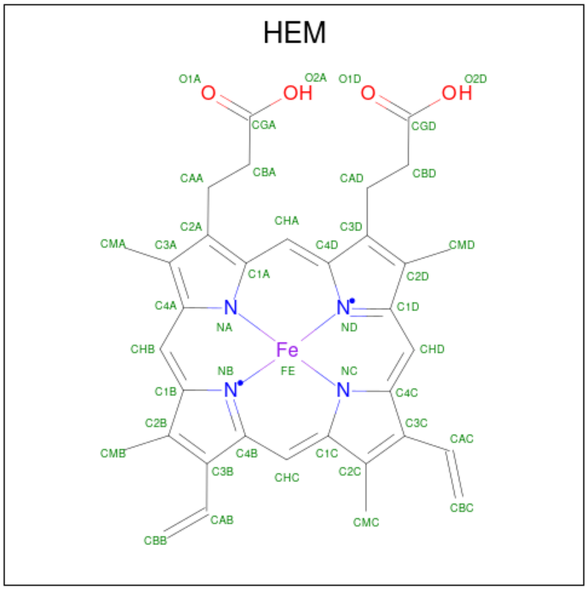
- Molecule 53 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	B1	52	449	296	79	74	0	0

- Molecule 54 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	A1	70	577	369	106	97	5	0	0

- Molecule 55 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
55	b1	1	43	34	1	4	4	0
55	b1	1	43	34	1	4	4	0
55	b2	1	43	34	1	4	4	0

Continued on next page...

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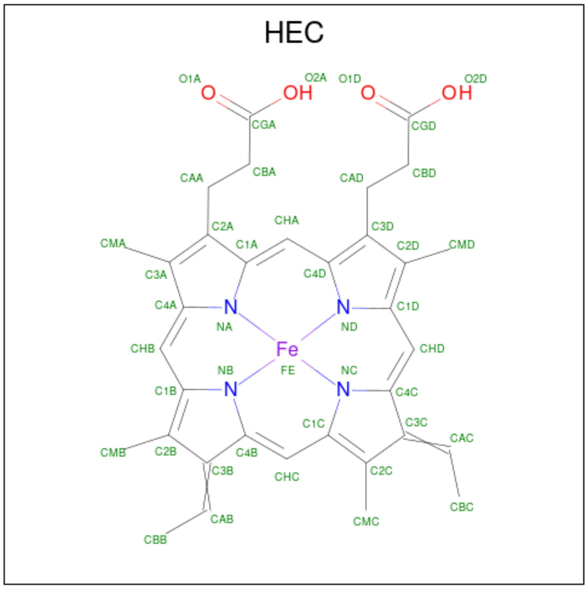
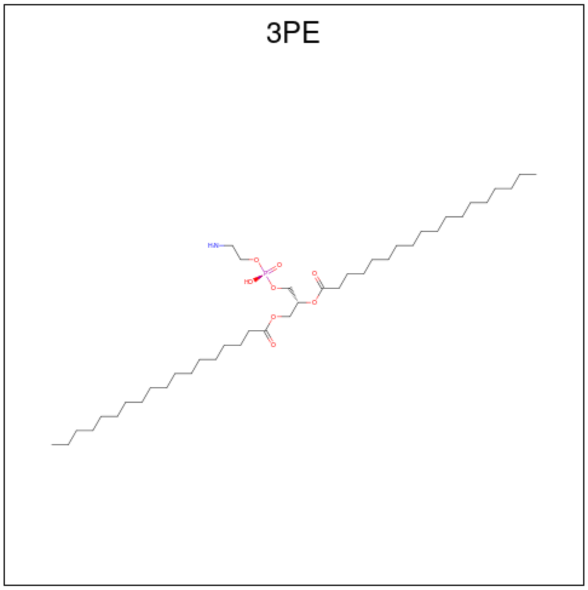
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
55	b2	1	43	34	1	4	4	0

- Molecule 56 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



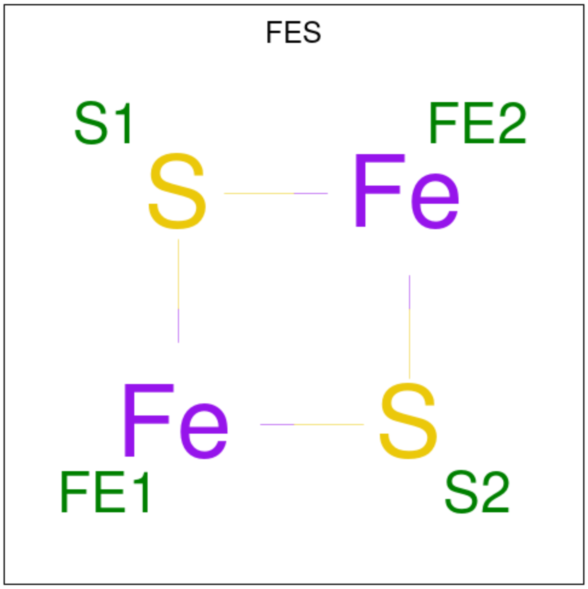
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
56	c1	1	43	34	1	4	4	0
56	c2	1	43	34	1	4	4	0

- Molecule 57 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



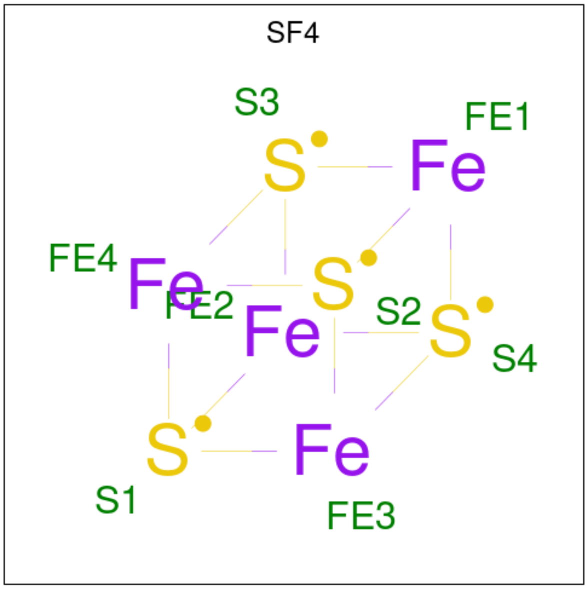
Mol	Chain	Residues	Atoms	AltConf
57	c1	1	Total C N O P 13 5 1 6 1	0
57	f2	1	Total C N O P 23 13 1 8 1	0
57	D1	1	Total C N O P 26 16 1 8 1	0
57	D5	1	Total C N O P 38 28 1 8 1	0
57	D4	1	Total C N O P 40 30 1 8 1	0

- Molecule 58 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



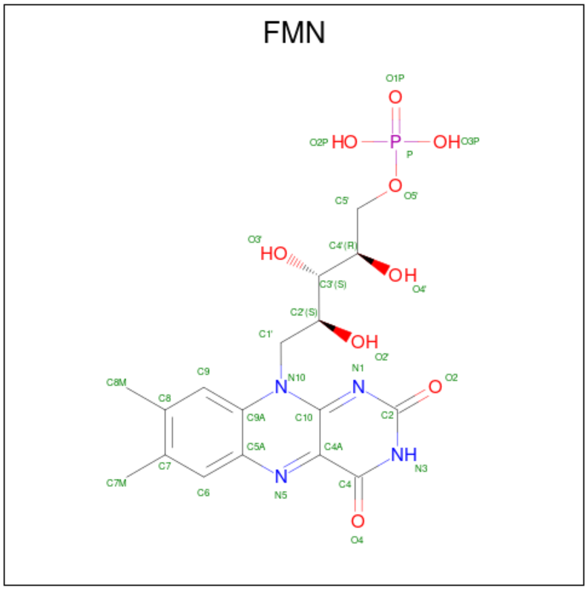
Mol	Chain	Residues	Atoms	AltConf
58	f1	1	Total Fe S 4 2 2	0
58	f2	1	Total Fe S 4 2 2	0
58	V2	1	Total Fe S 4 2 2	0
58	S1	1	Total Fe S 4 2 2	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
59	V1	1	Total Fe S 8 4 4	0
59	S1	1	Total Fe S 8 4 4	0
59	S1	1	Total Fe S 8 4 4	0
59	S7	1	Total Fe S 8 4 4	0
59	S8	1	Total Fe S 8 4 4	0
59	S8	1	Total Fe S 8 4 4	0

- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

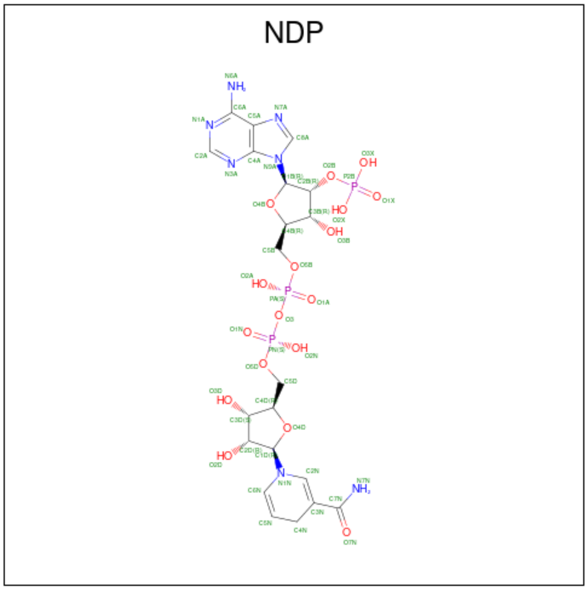


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	V1	1	31	17	4	9	1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

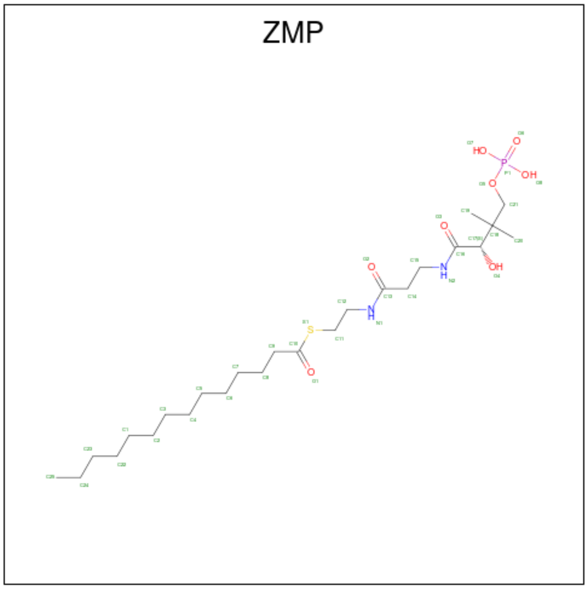
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	S6	1	1	1	0

- Molecule 62 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_{7}O_{17}P_{3}$).



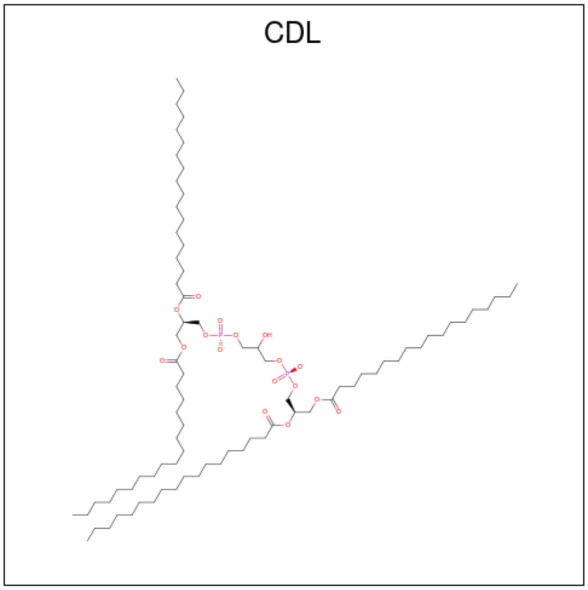
Mol	Chain	Residues	Atoms					AltConf
62	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 63 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



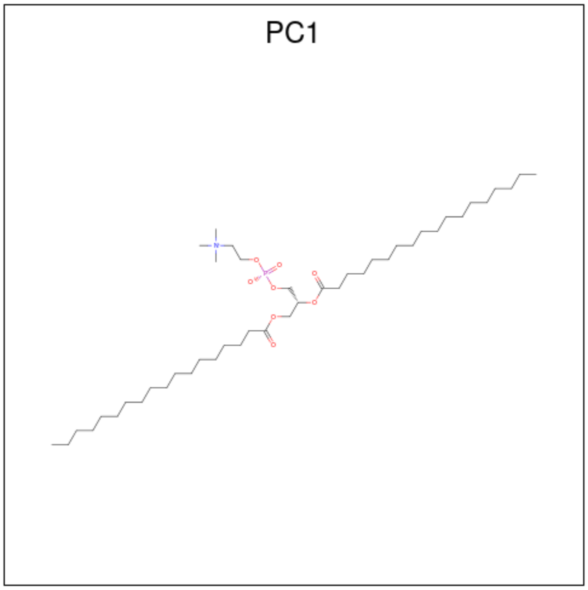
Mol	Chain	Residues	Atoms						AltConf
63	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
63	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 64 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
64	D5	1	60	41	17	2	0

- Molecule 65 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



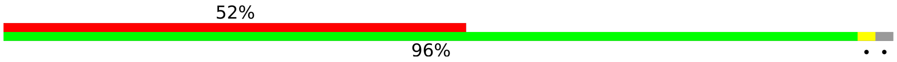
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	AK	1	28	18	1	8	1	0

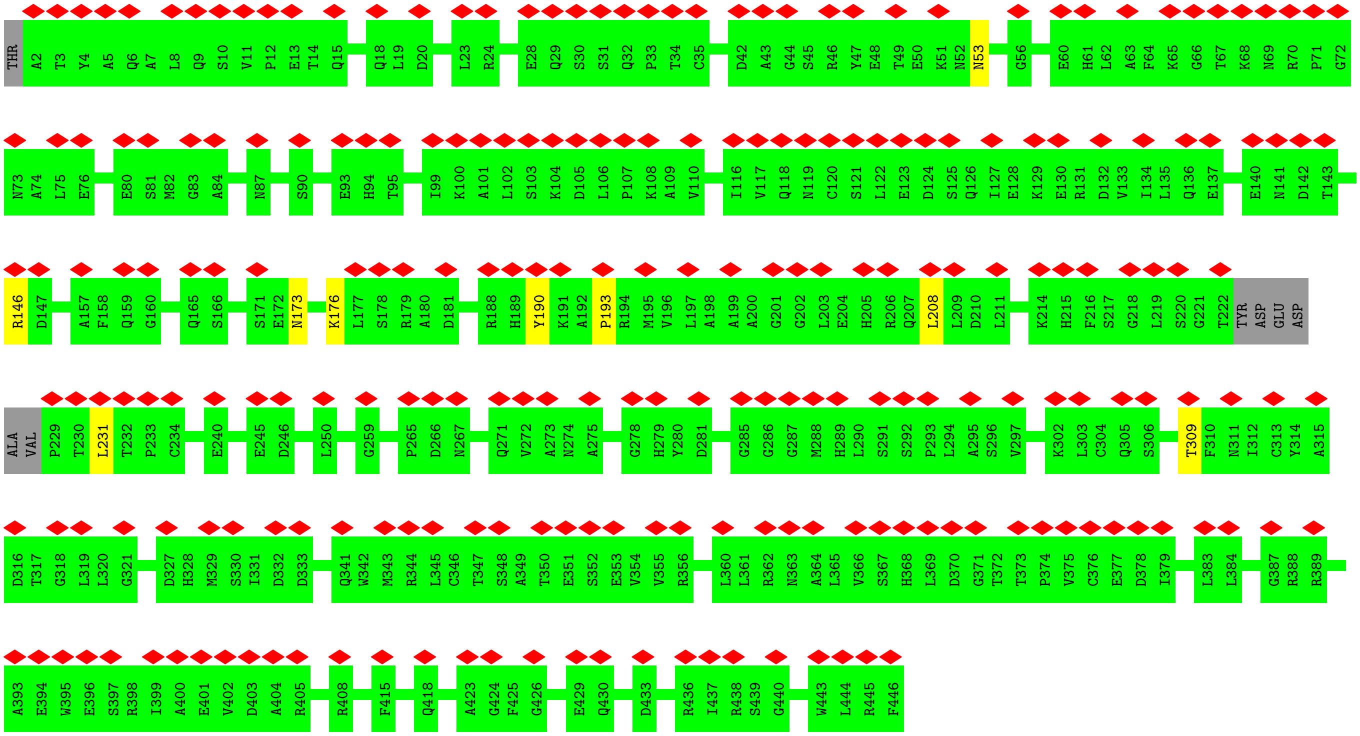
3 Residue-property plots ⓘ

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: UQCRC1

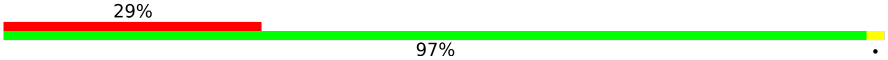
Chain a1:

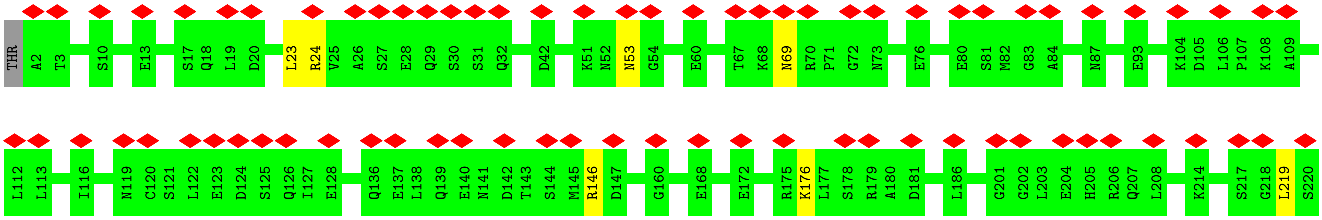


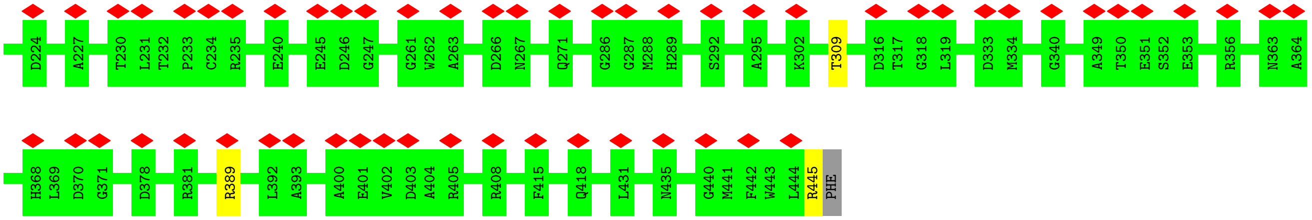


- Molecule 1: UQCRC1

Chain a3:

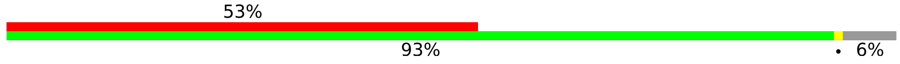


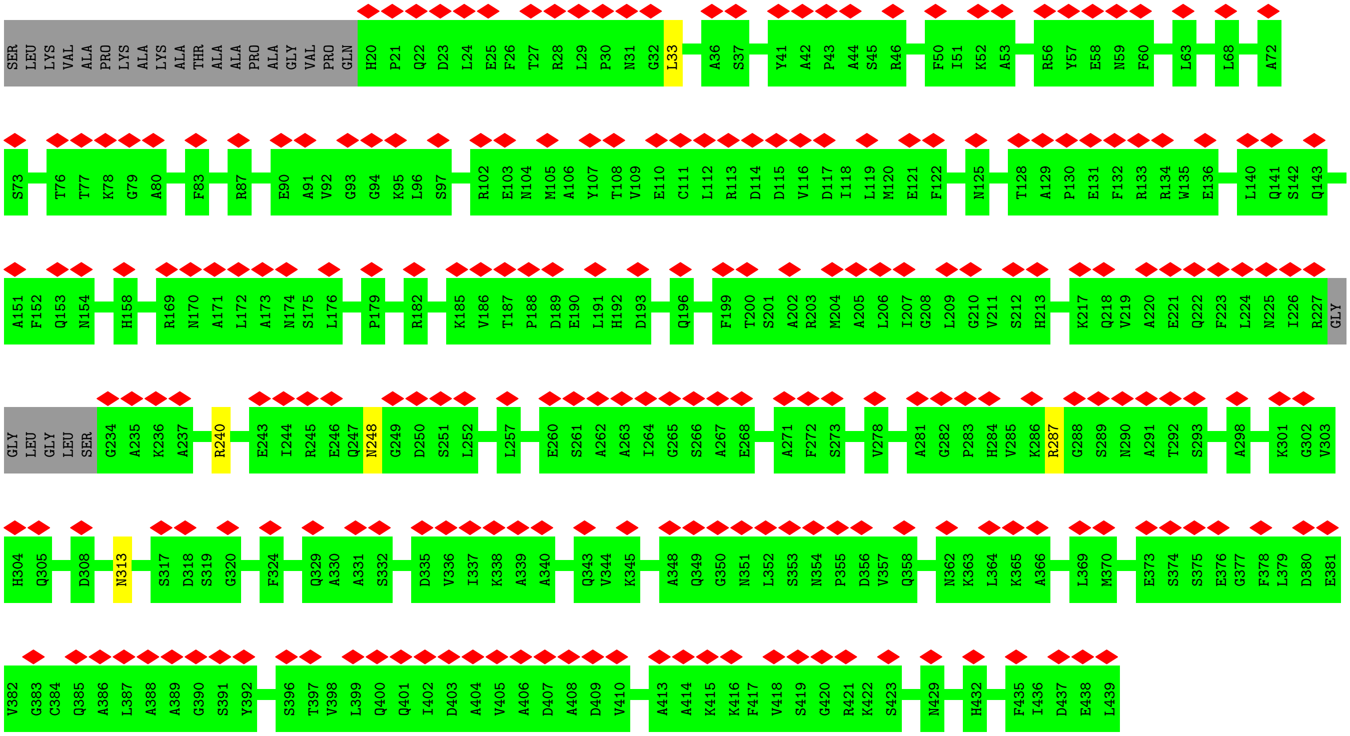




- Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

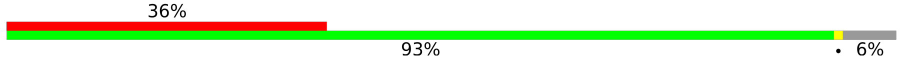
Chain a2:

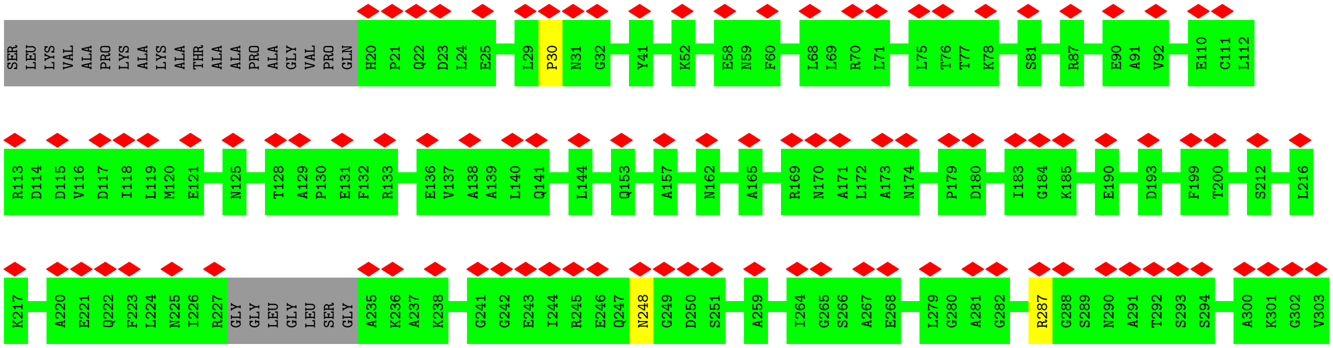


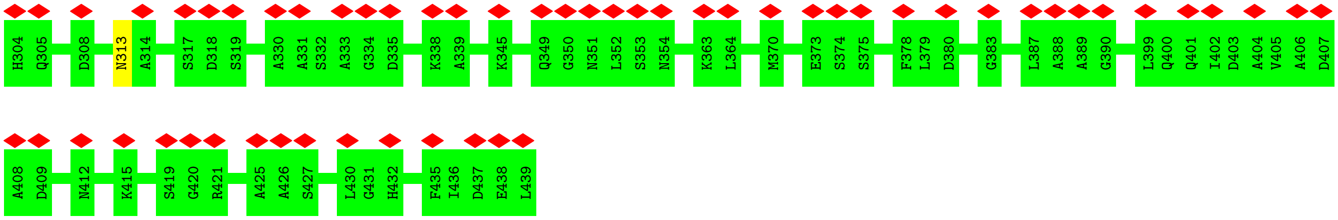


- Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

Chain a4:

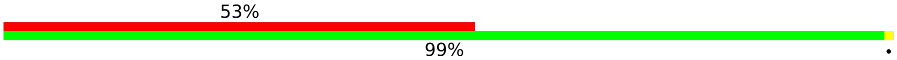


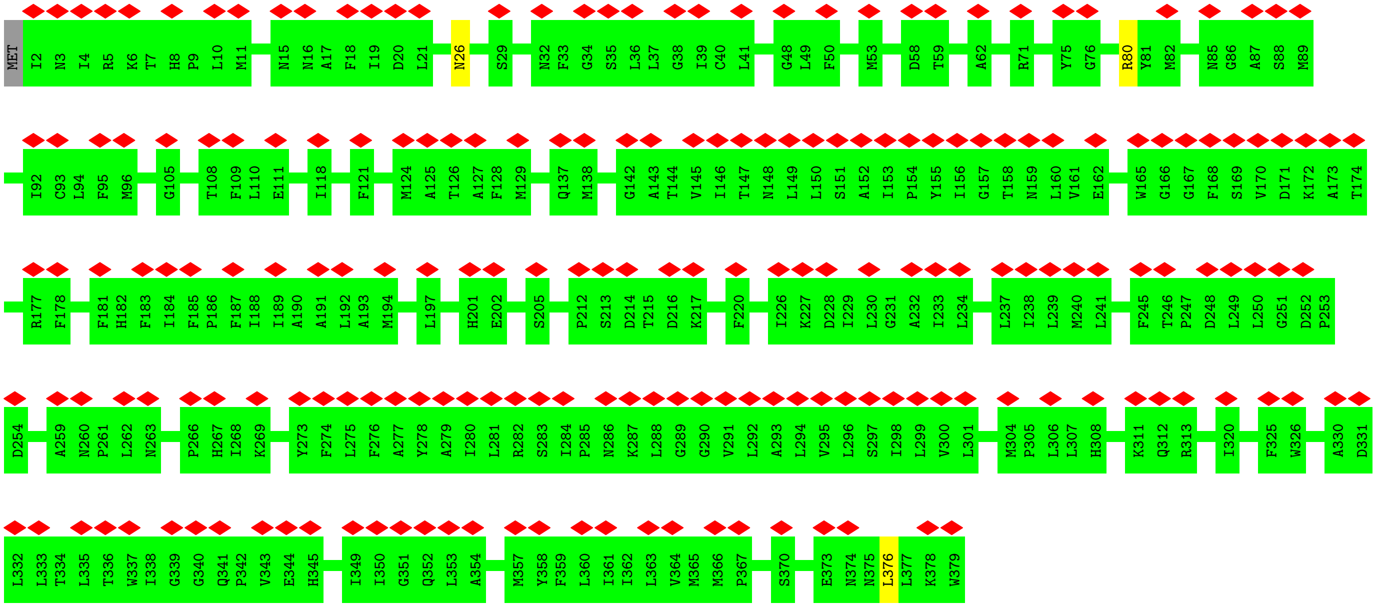




- Molecule 3: Cytochrome b

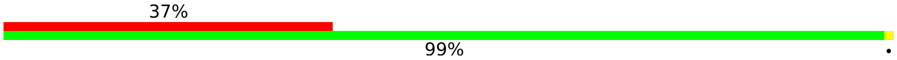
Chain b1:

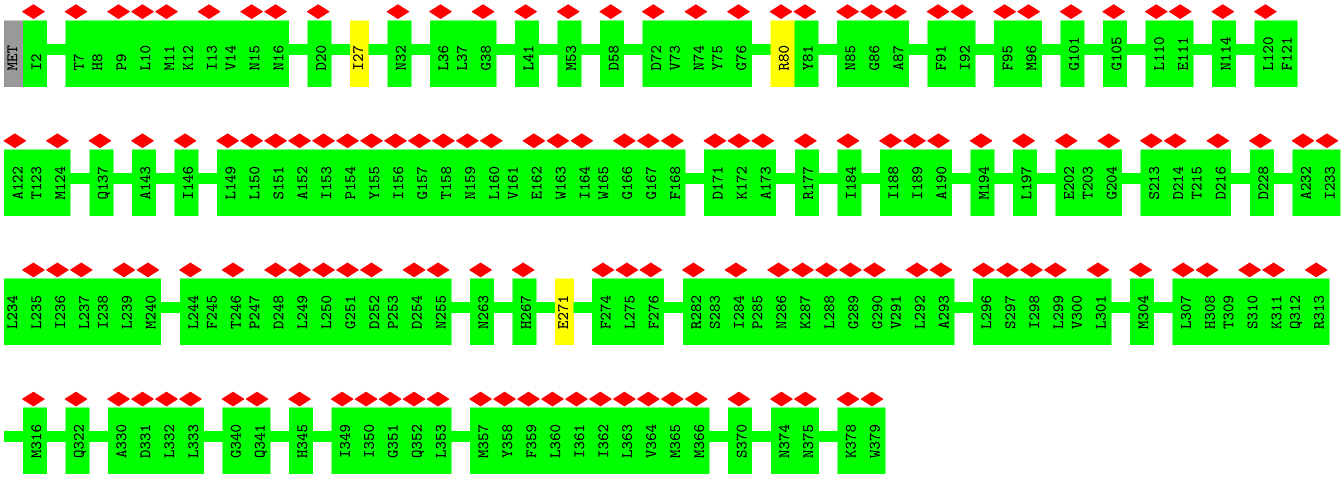




- Molecule 3: Cytochrome b

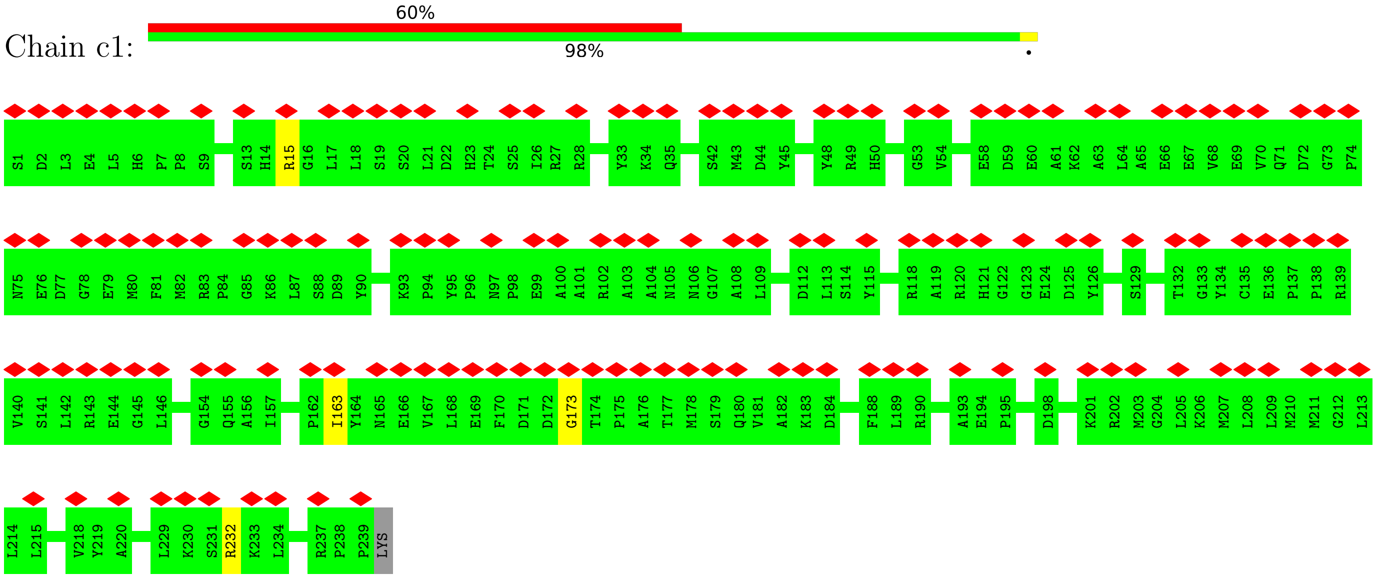
Chain b2:





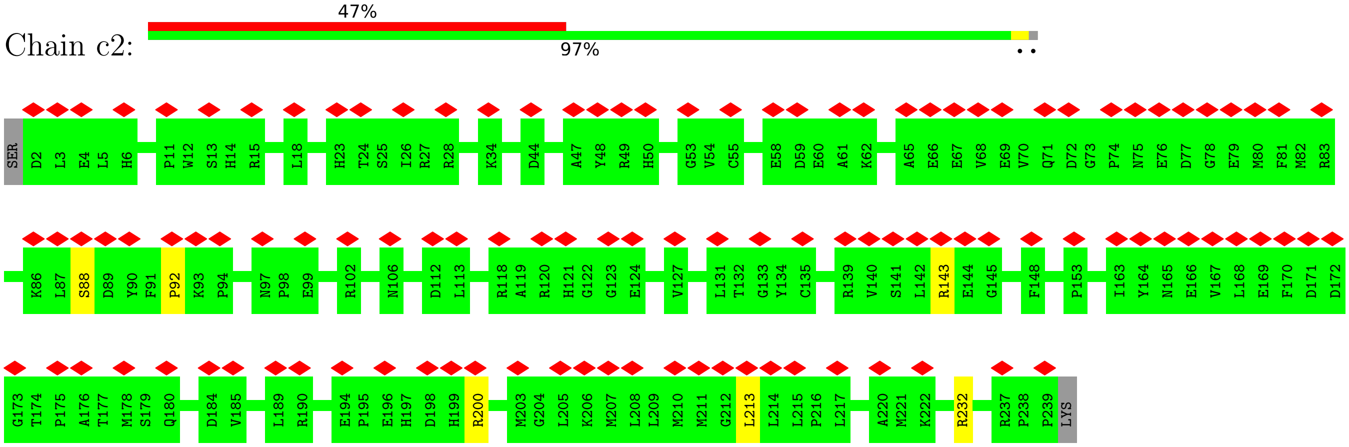
- Molecule 4: Cytochrome c1

Chain c1:



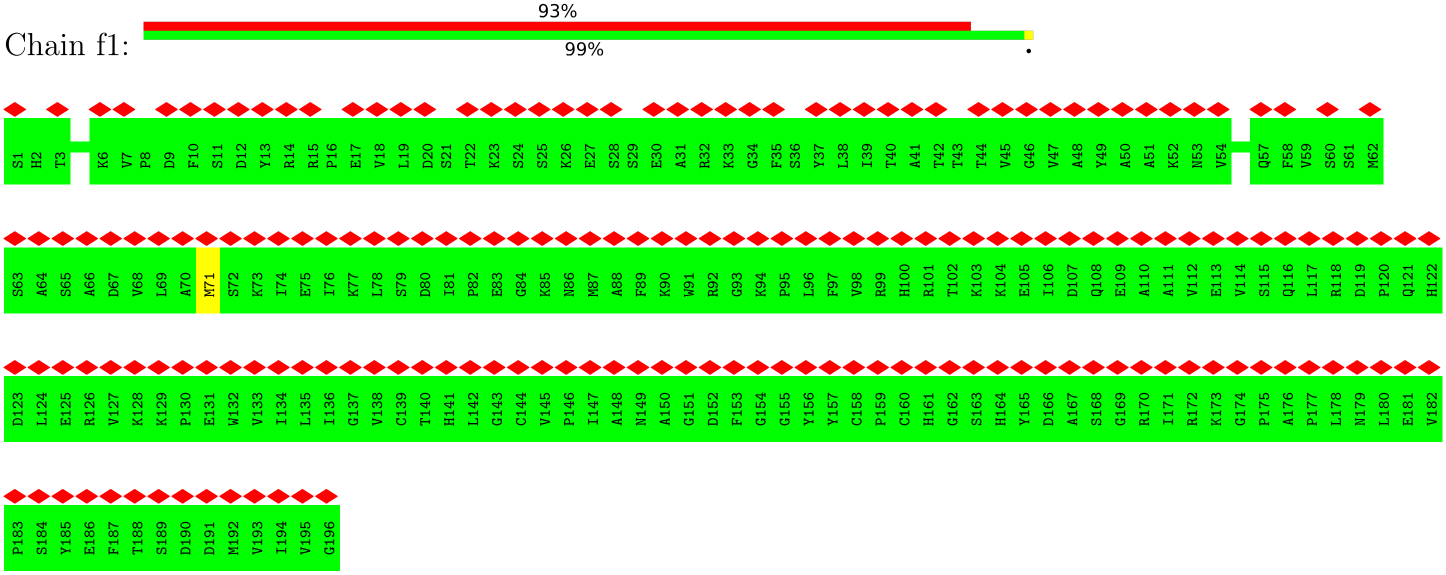
- Molecule 4: Cytochrome c1

Chain c2:



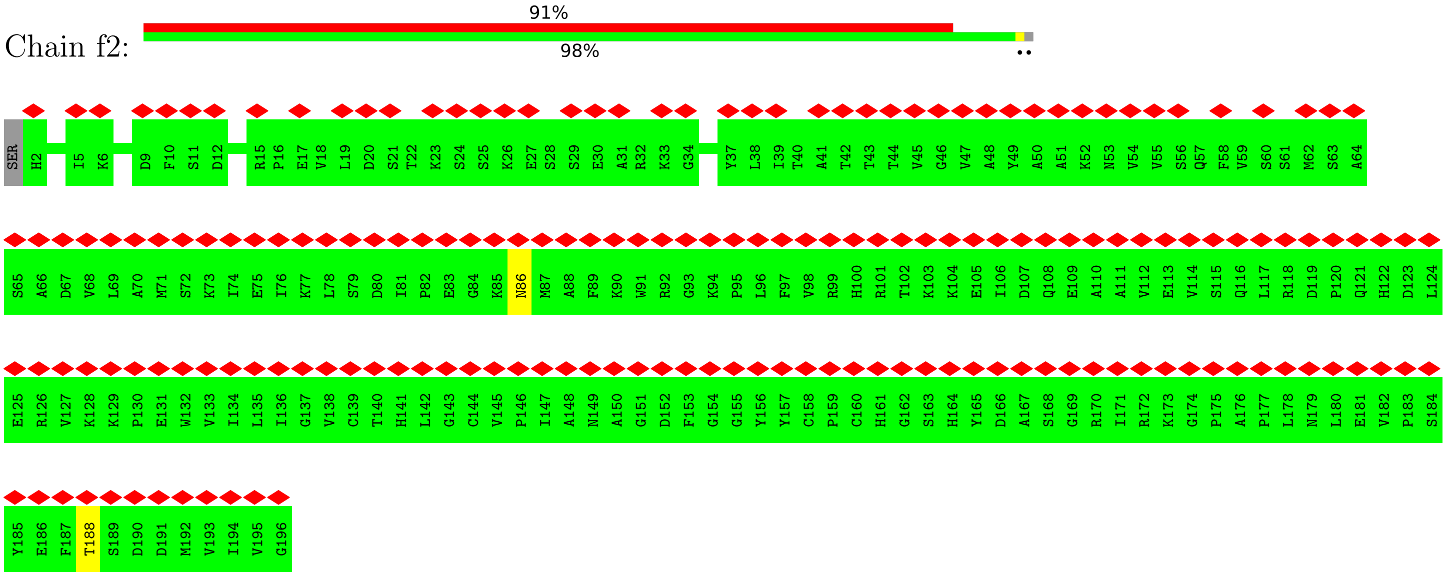
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain f1:



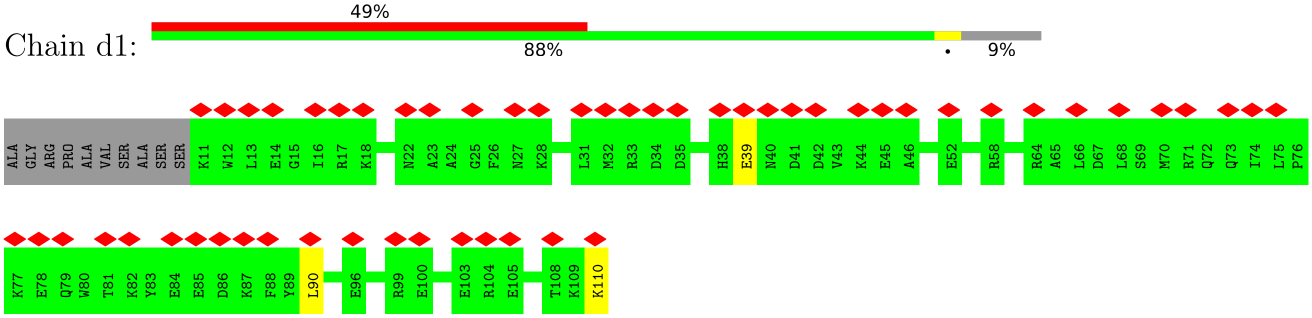
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain f2:



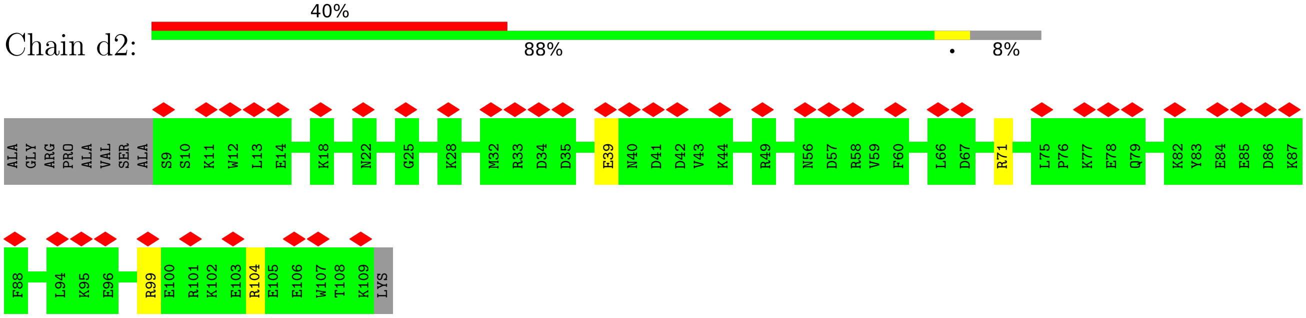
- Molecule 6: UQCRB

Chain d1:



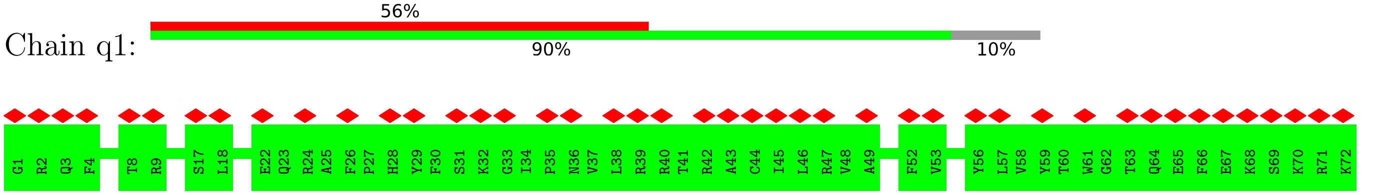
- Molecule 6: UQCRB

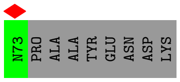
Chain d2:



- Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

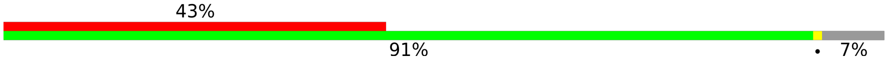
Chain q1:

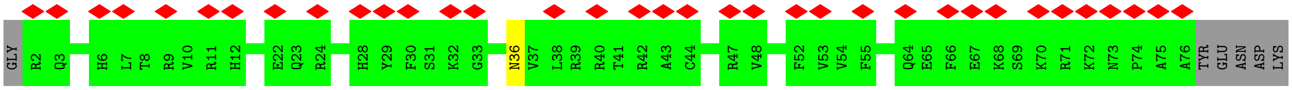




- Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

Chain q2:



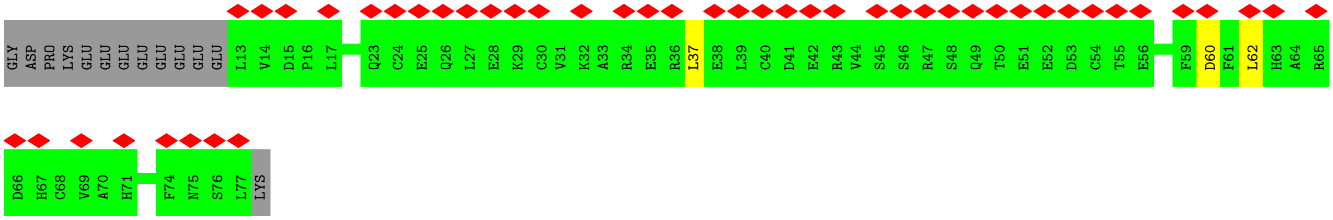


- Molecule 8: Cytochrome b-c1 complex subunit 6

Chain h1:

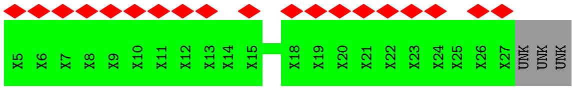
- Molecule 8: Cytochrome b-c1 complex subunit 6

Chain h2:



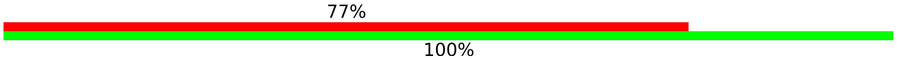
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

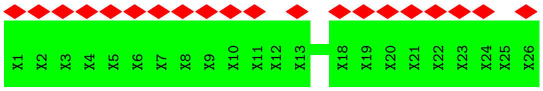
Chain x1:



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

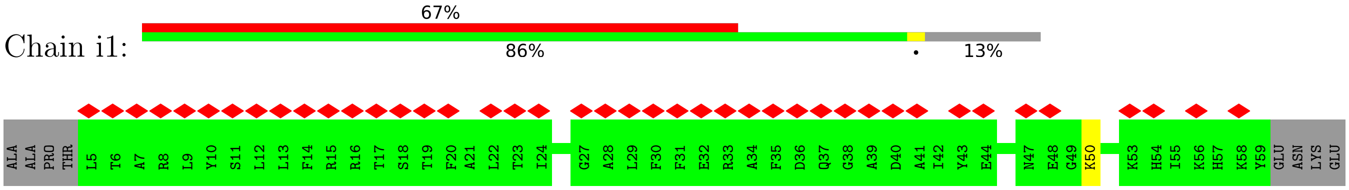
Chain x2:





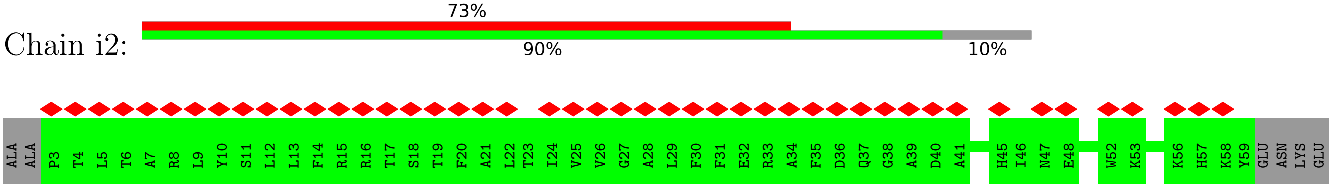
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

Chain i1:



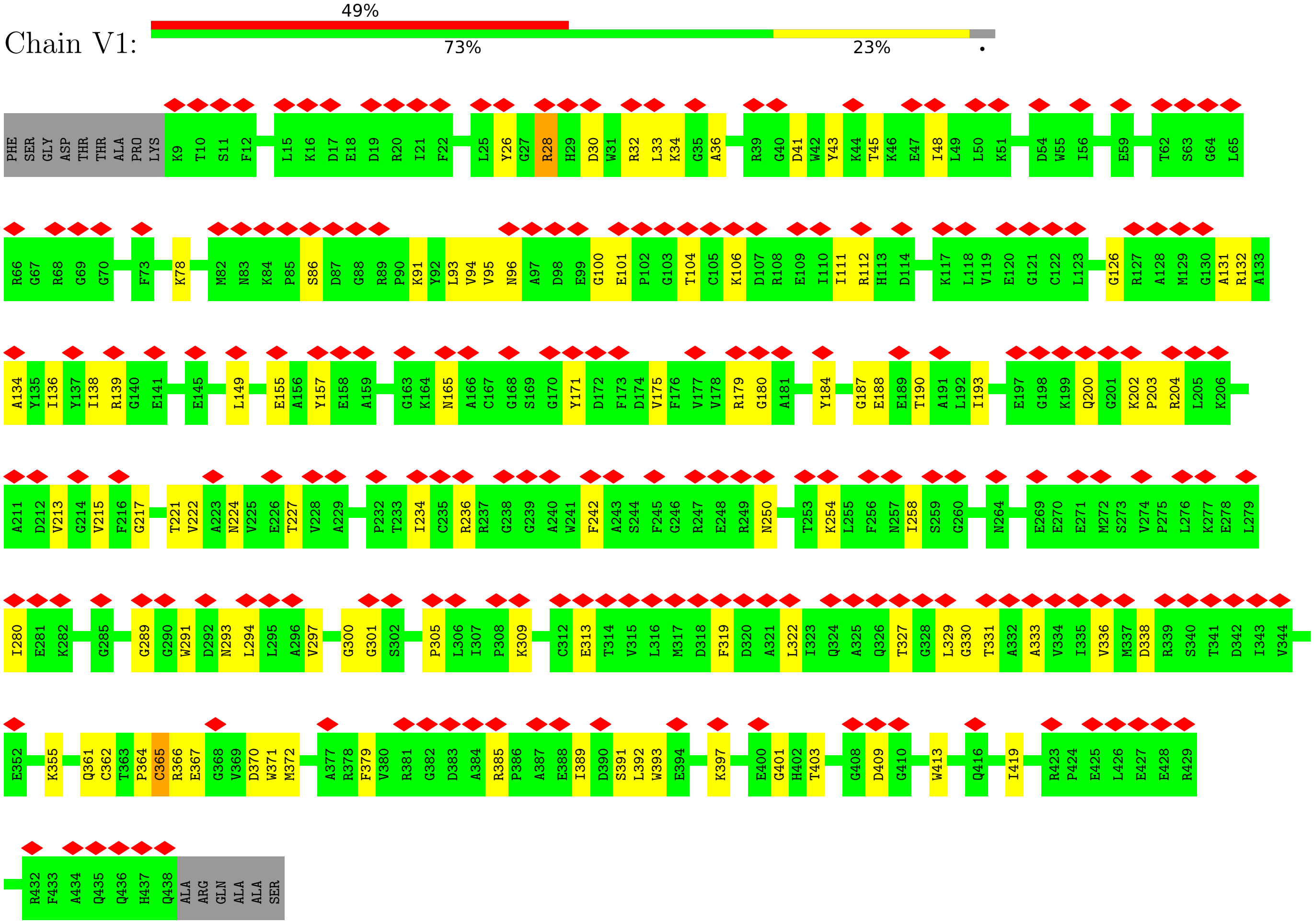
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

Chain i2:



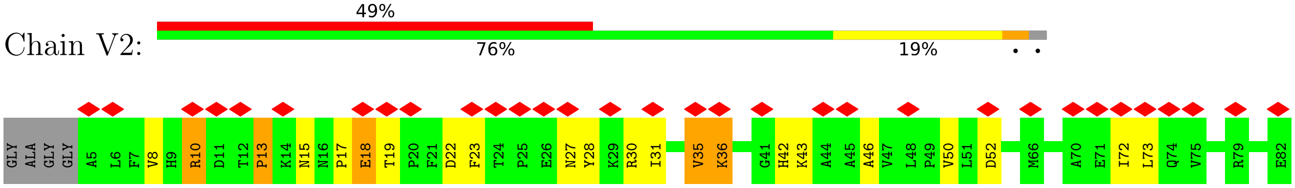
- Molecule 11: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

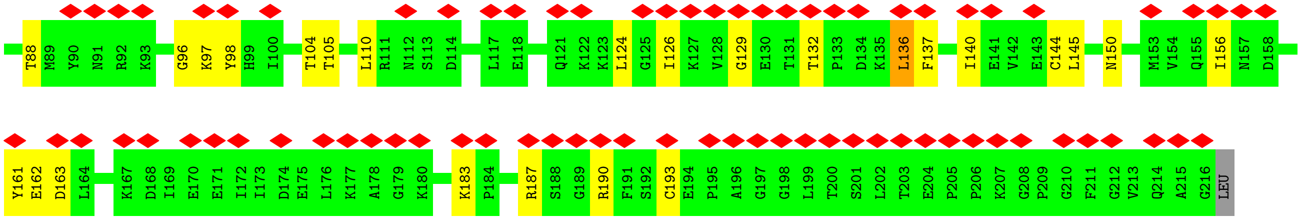
Chain V1:



- Molecule 12: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

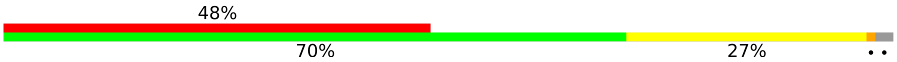
Chain V2:

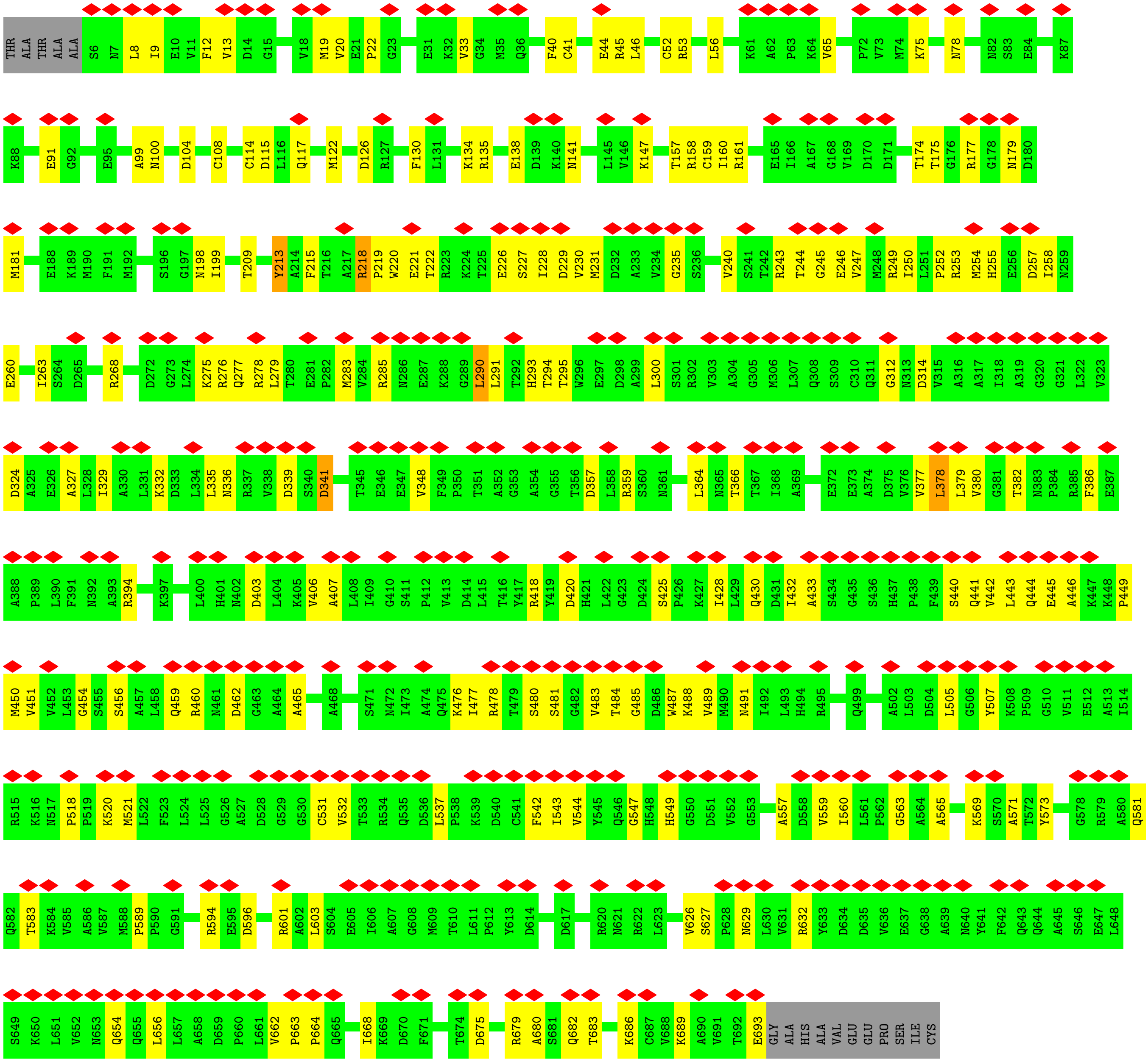




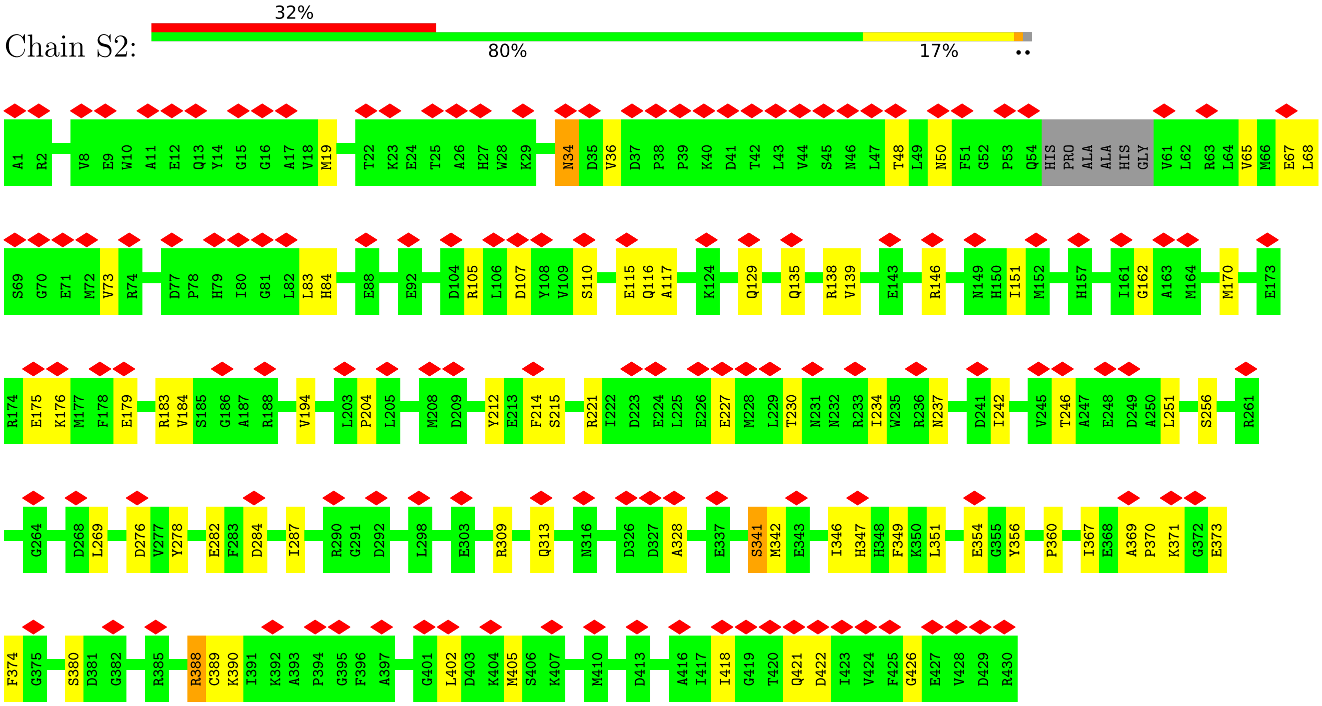
- Molecule 13: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1:

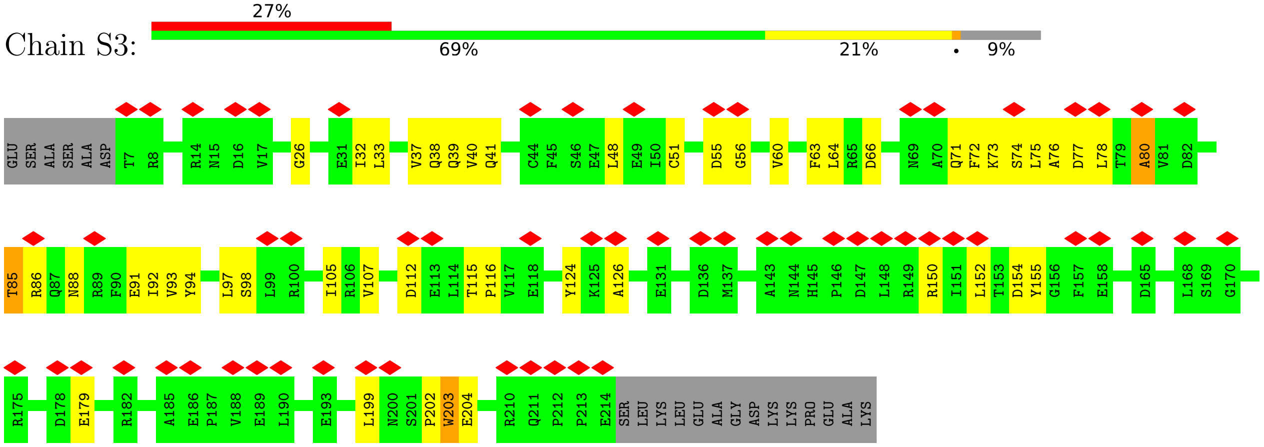




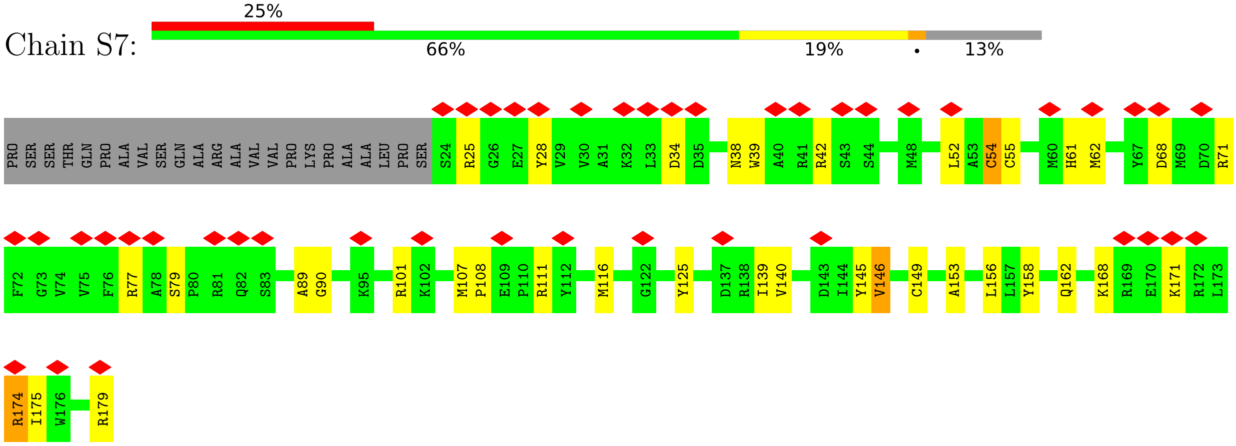
- Molecule 14: NDUFB11



- Molecule 15: NADH:ubiquinone oxidoreductase core subunit S3

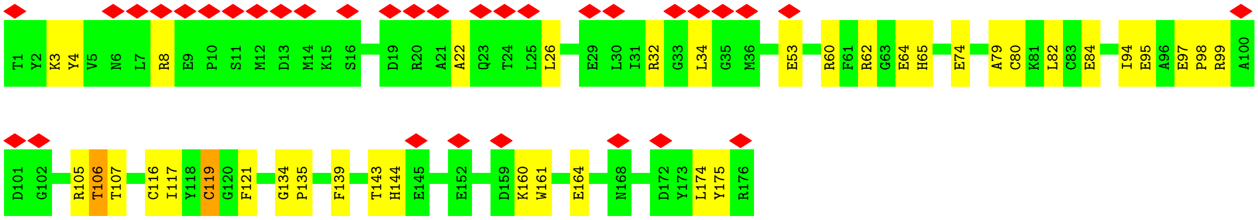


- Molecule 16: NDUFB1



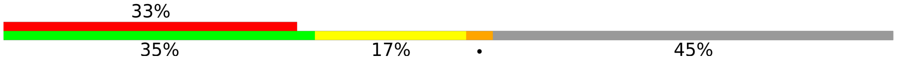
- Molecule 17: NDUFA1

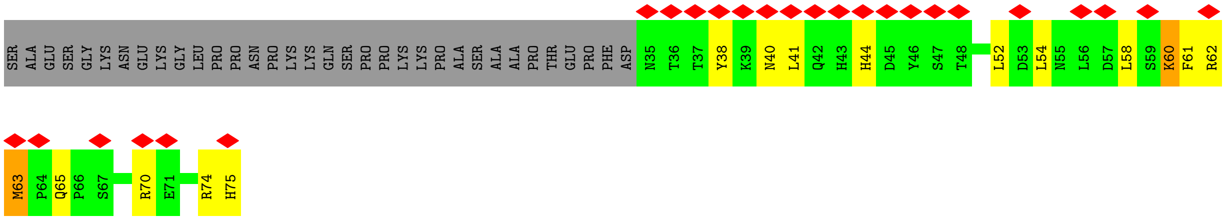
Chain S8:



- Molecule 18: NDUFV3

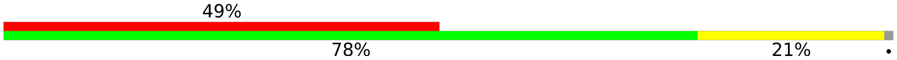
Chain V3:

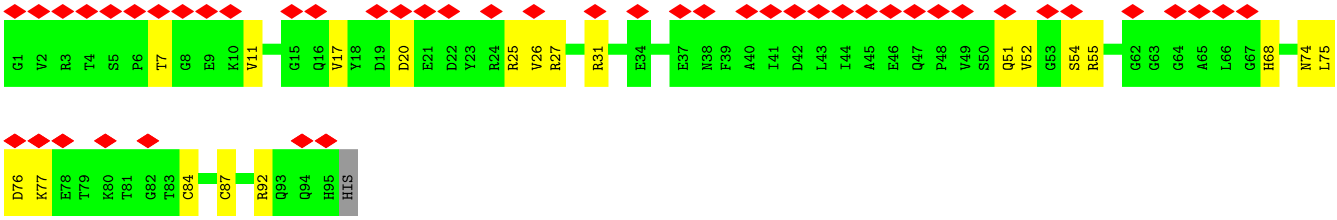




- Molecule 19: NDUFB6

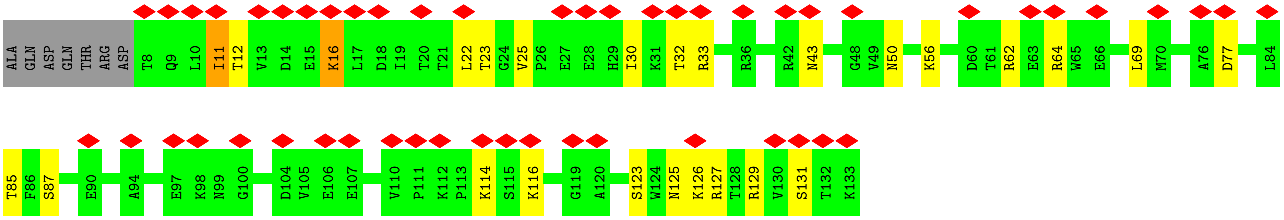
Chain S6:





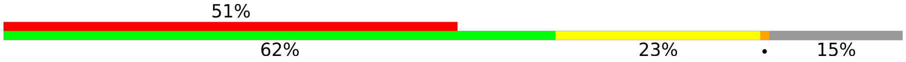
- Molecule 20: NADH:ubiquinone oxidoreductase subunit S4

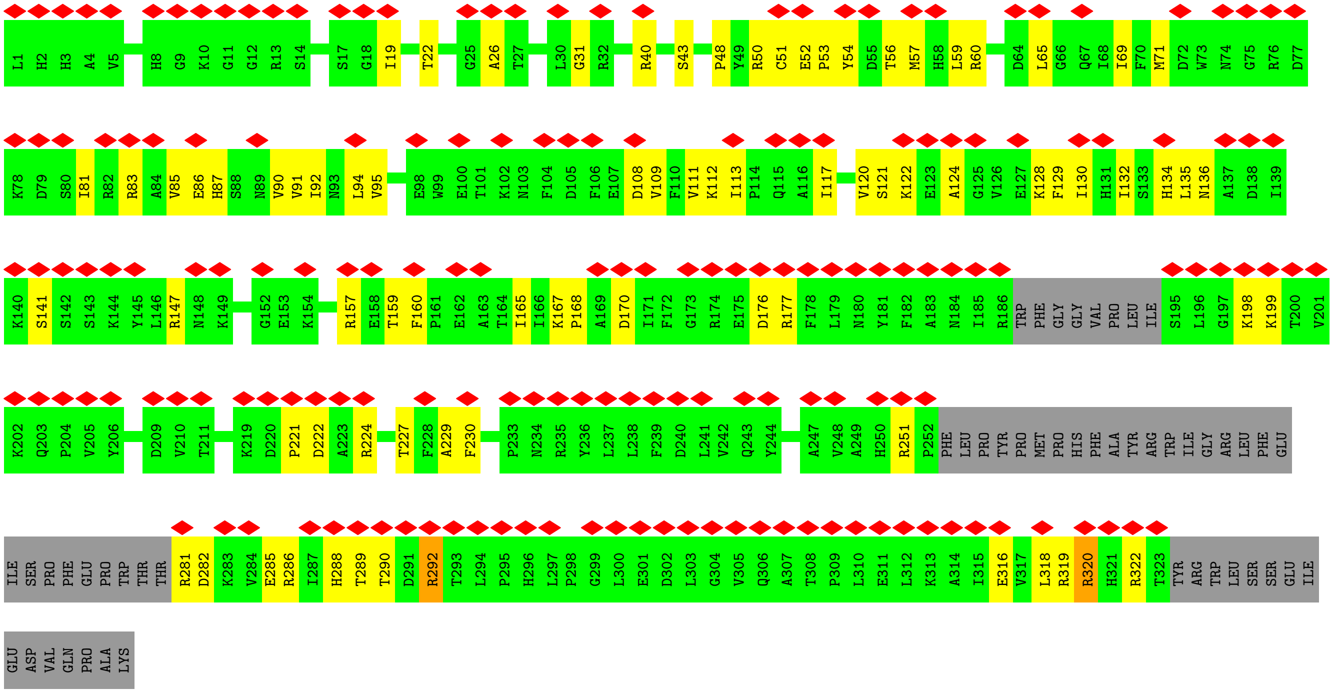
Chain S4:



- Molecule 21: NADH:ubiquinone oxidoreductase subunit A9

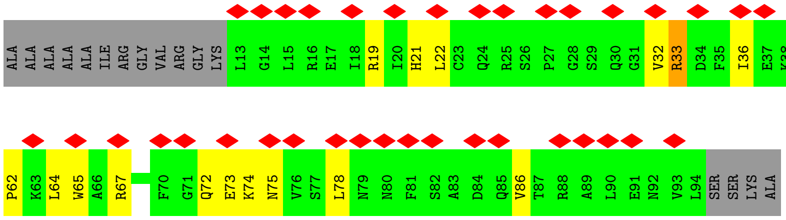
Chain A9:





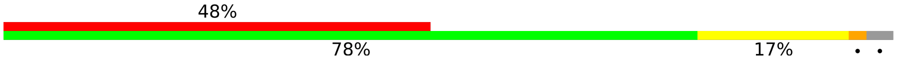
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

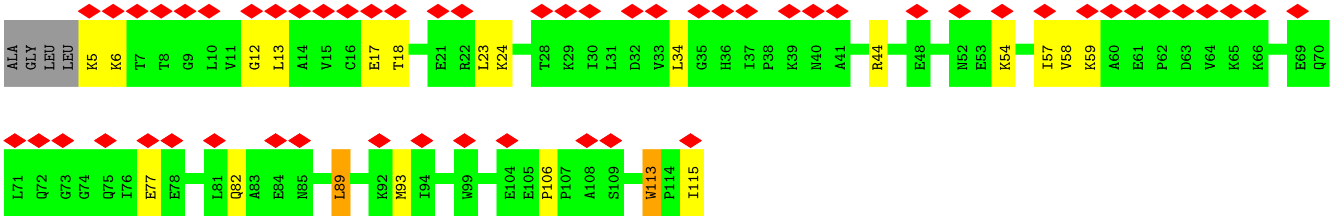
Chain A2:



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

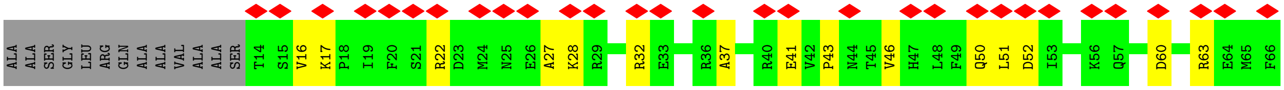
Chain A5:

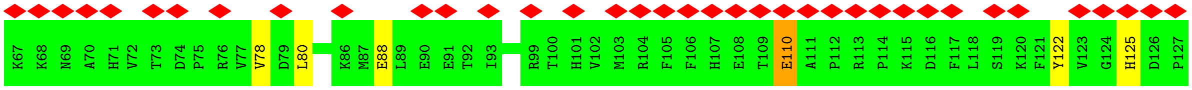




- Molecule 24: NADH:ubiquinone oxidoreductase subunit A6

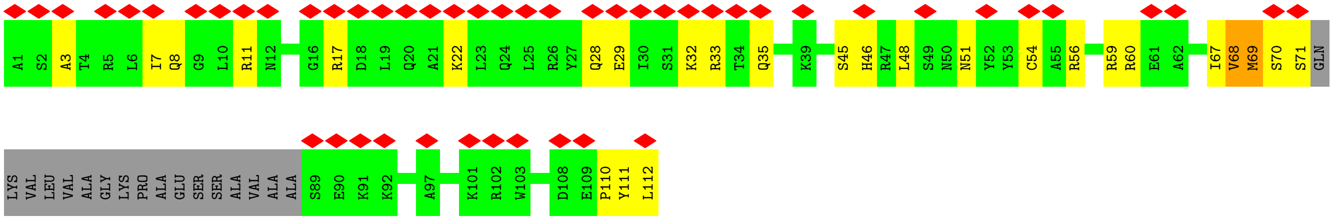
Chain A6:





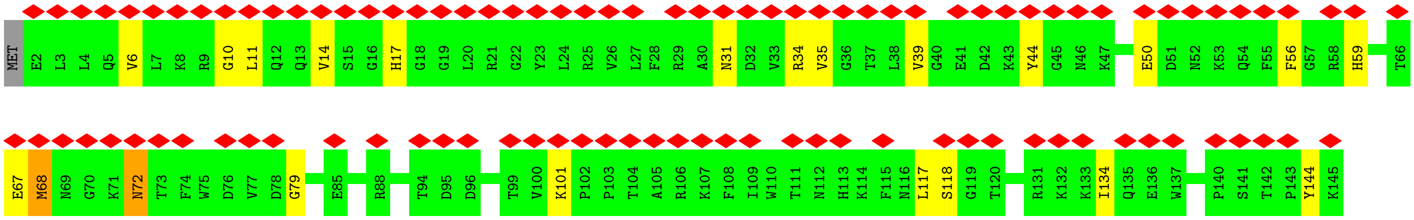
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7:



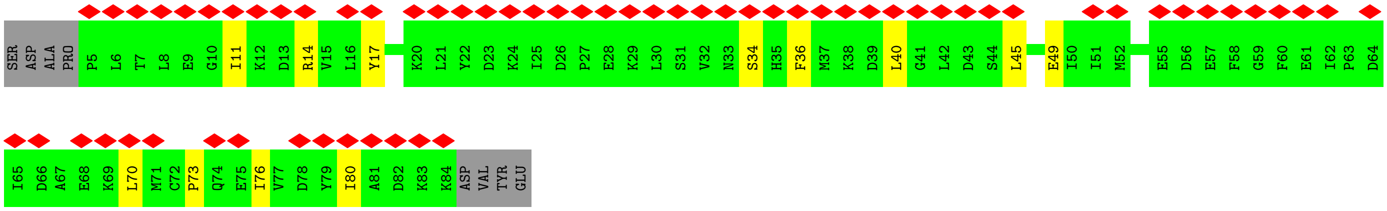
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:



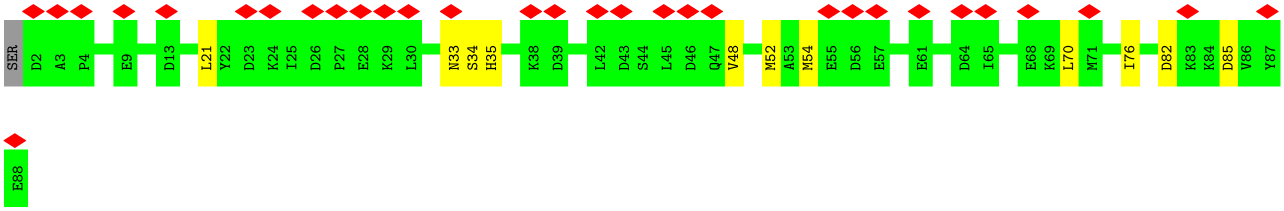
- Molecule 27: Acyl carrier protein

Chain AA:



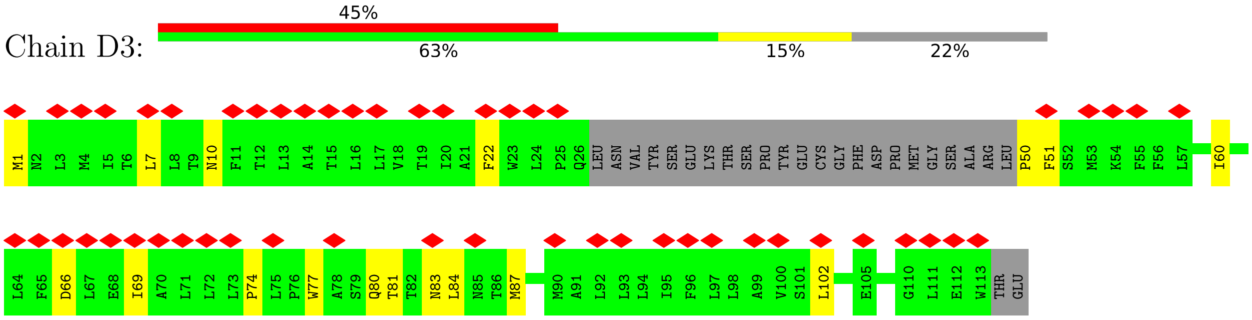
- Molecule 27: Acyl carrier protein

Chain AB:



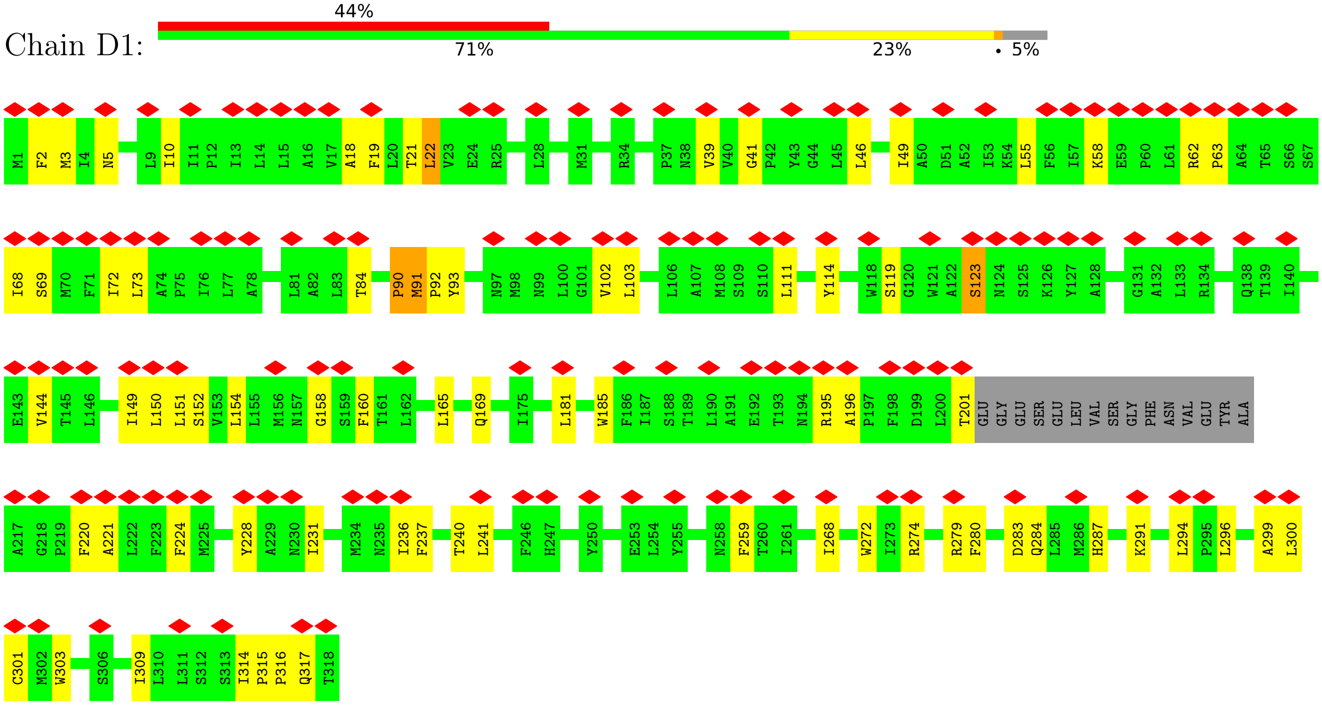
- Molecule 28: NADH-ubiquinone oxidoreductase chain 3

Chain D3:



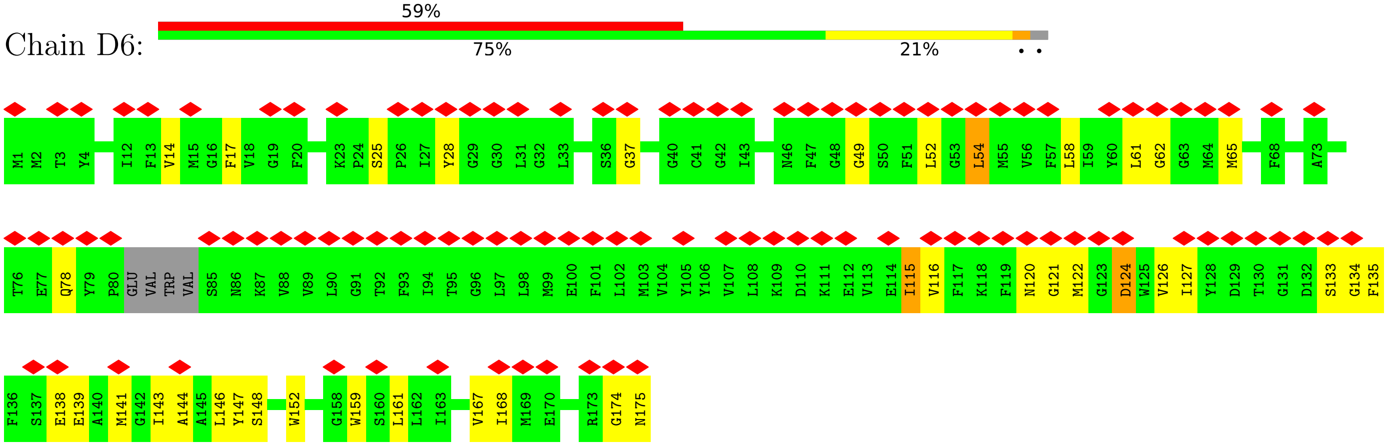
- Molecule 29: NADH-ubiquinone oxidoreductase chain 1

Chain D1:



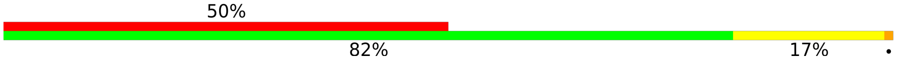
- Molecule 30: NADH-ubiquinone oxidoreductase chain 6

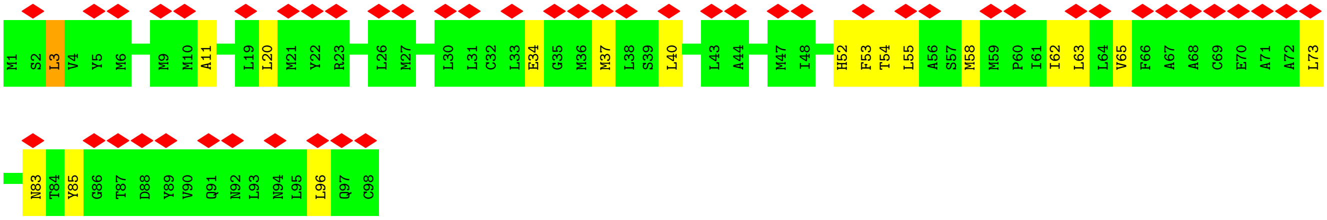
Chain D6:



- Molecule 31: NADH-ubiquinone oxidoreductase chain 4L

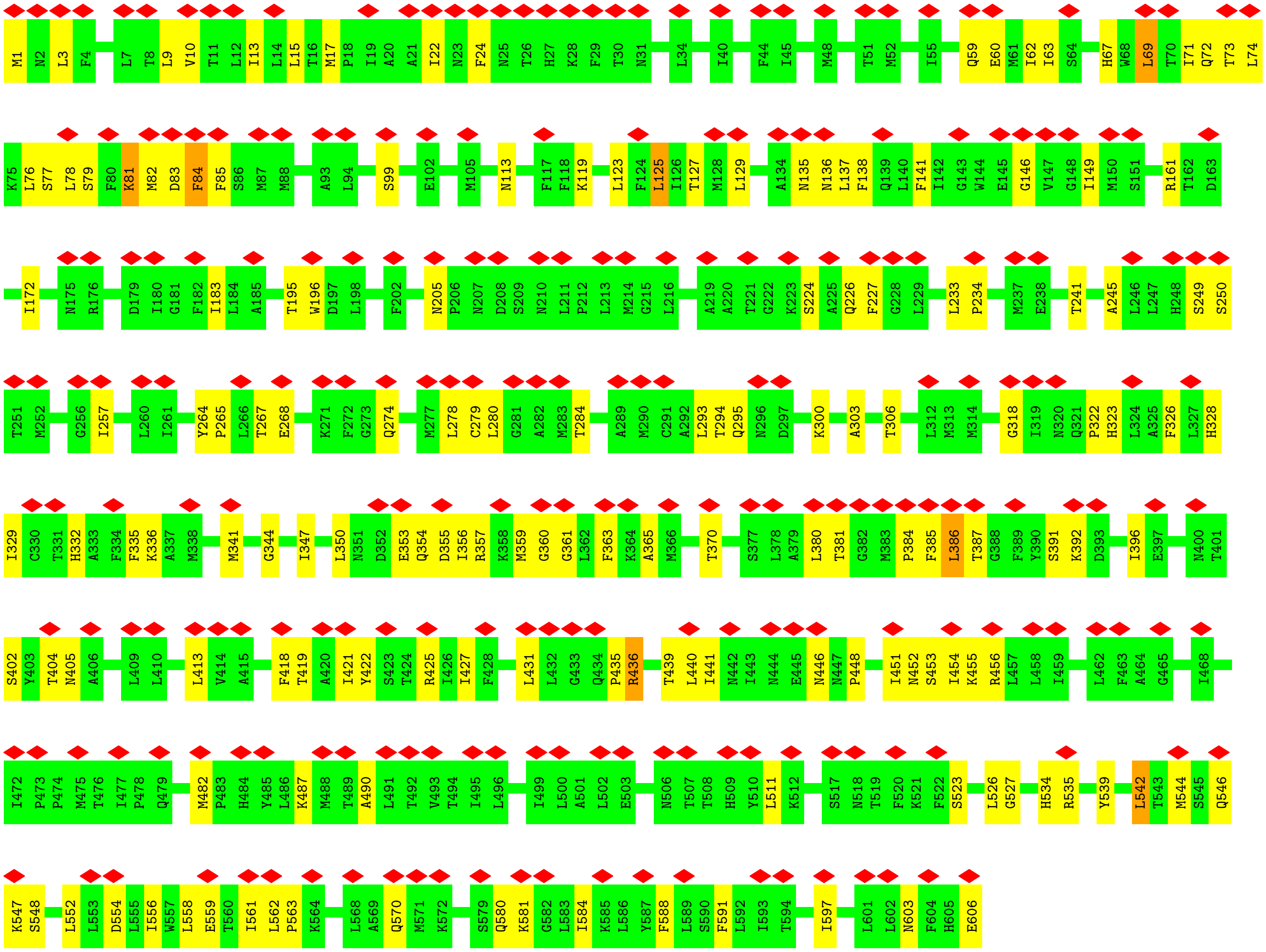
Chain 4L:





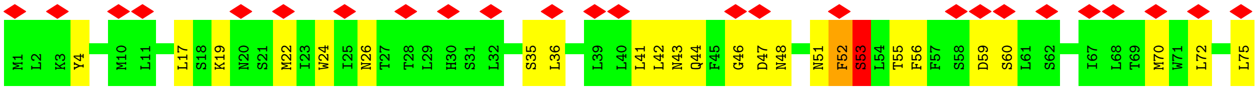
- Molecule 32: NADH-ubiquinone oxidoreductase chain 5

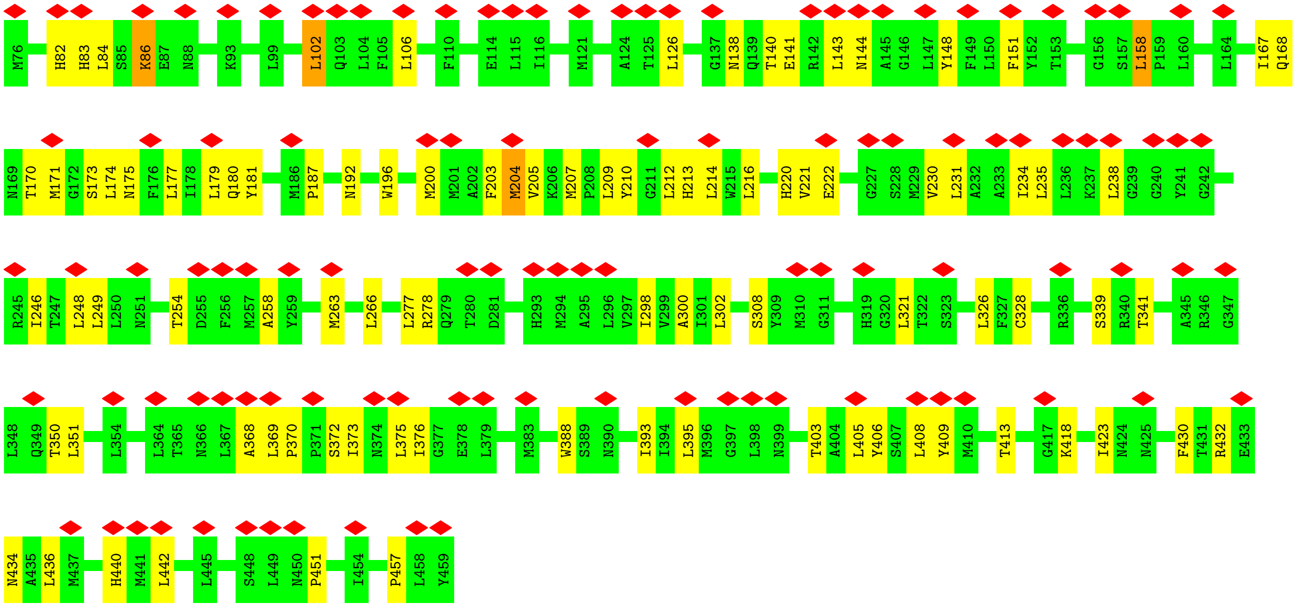
Chain D5:



- Molecule 33: NADH-ubiquinone oxidoreductase chain 4

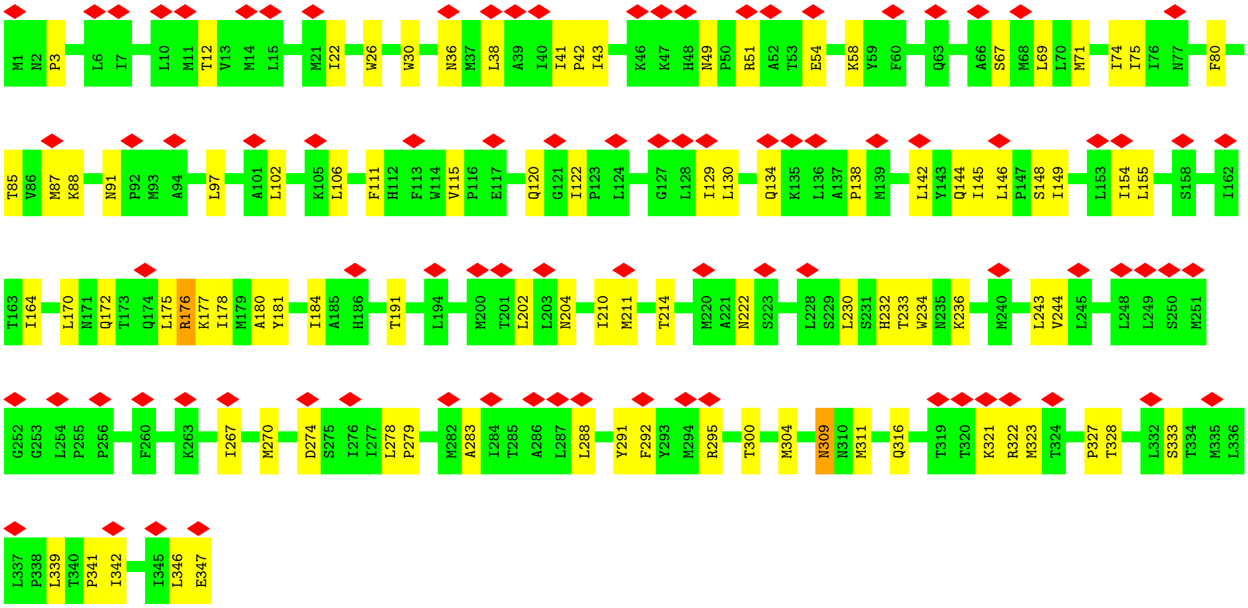
Chain D4:





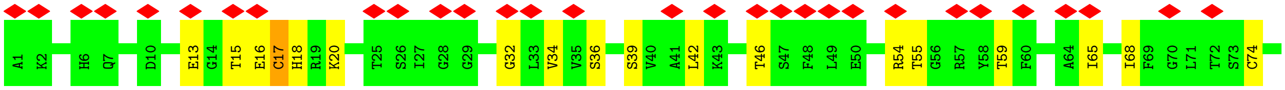
- Molecule 34: NADH-ubiquinone oxidoreductase chain 2

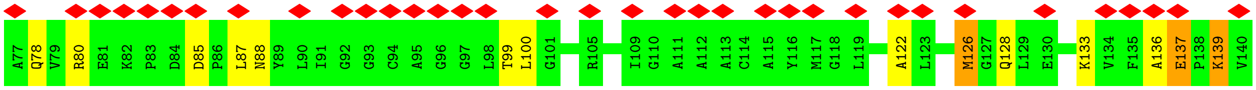
Chain D2:



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

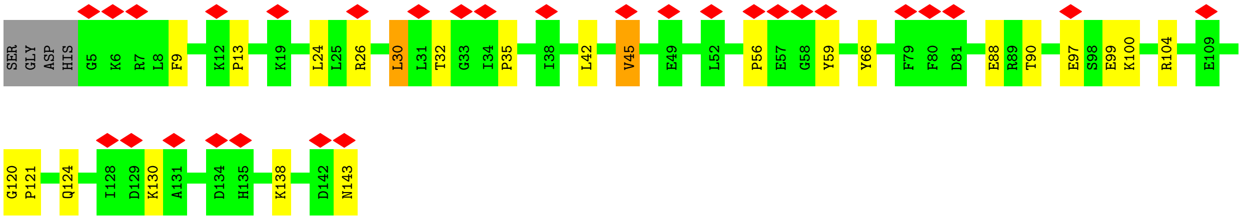
Chain AK:





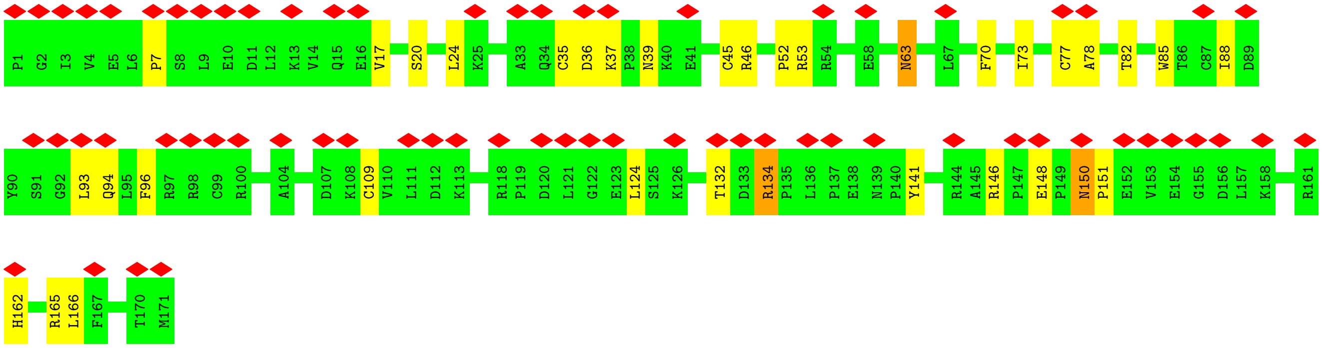
- Molecule 36: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



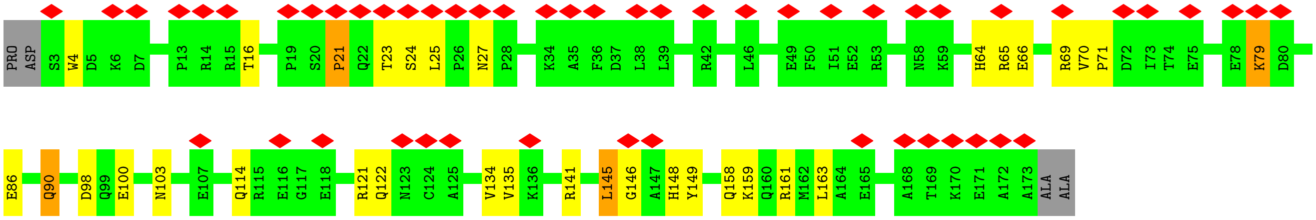
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



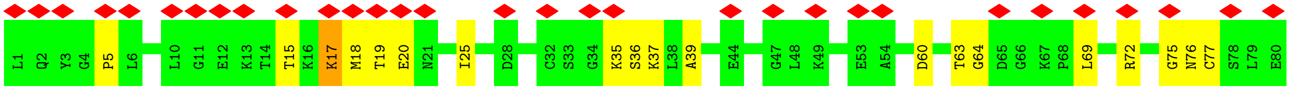
- Molecule 38: MT-ND5

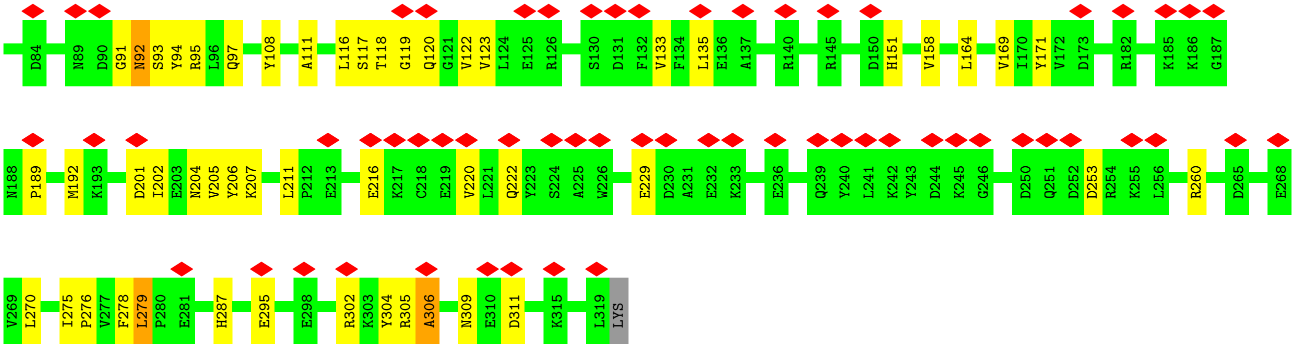
Chain BJ:



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

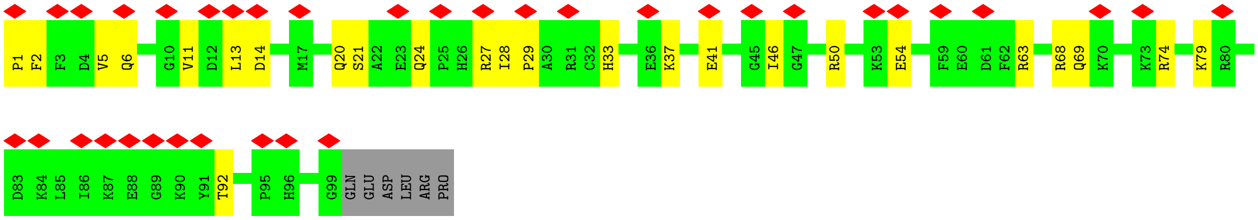
Chain AJ:





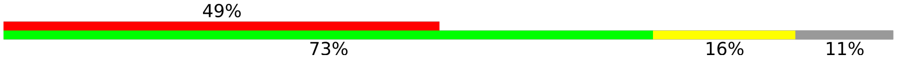
- Molecule 40: NADH:ubiquinone oxidoreductase subunit S5

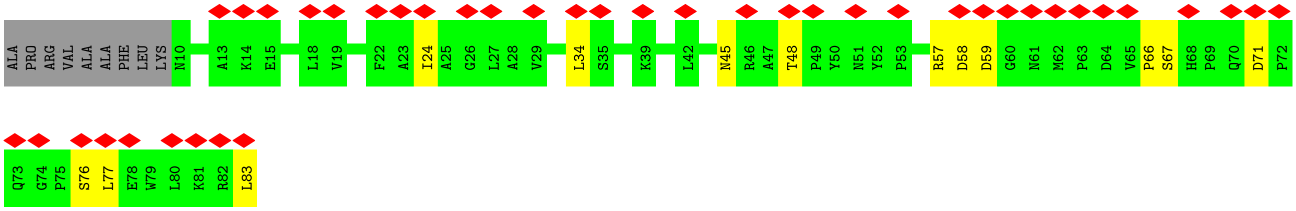
Chain S5:



- Molecule 41: NADH:ubiquinone oxidoreductase subunit A3

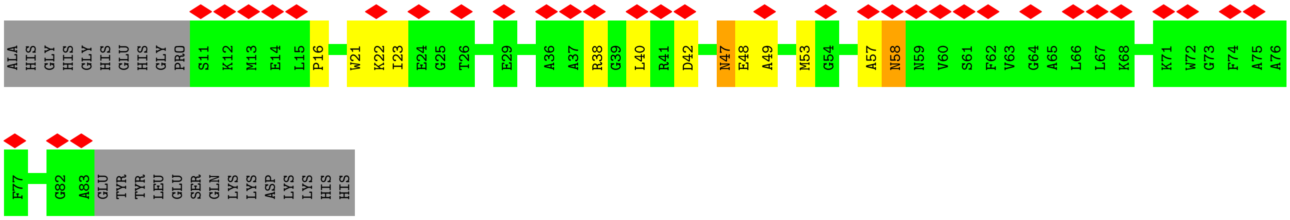
Chain A3:





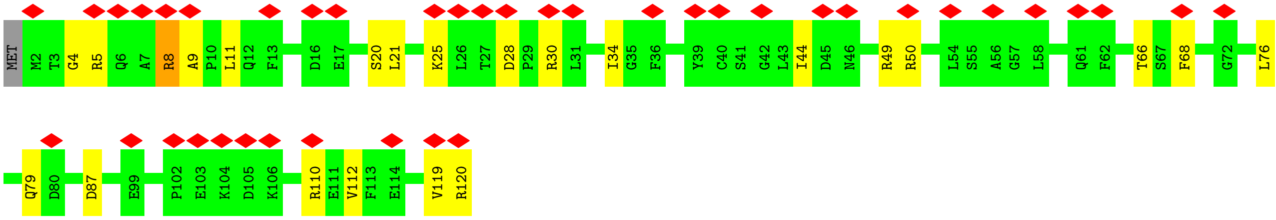
- Molecule 42: NADH:ubiquinone oxidoreductase subunit B3

Chain B3:



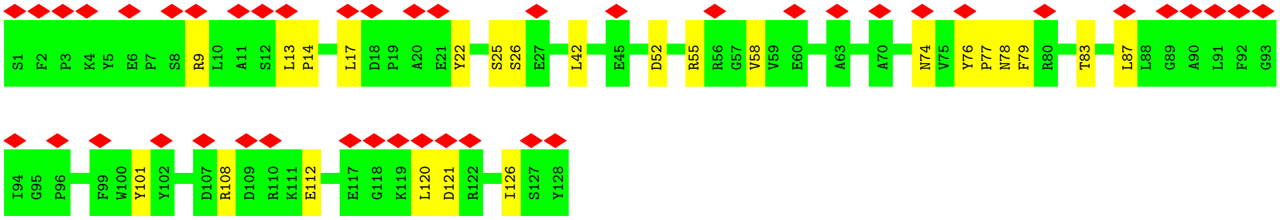
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:



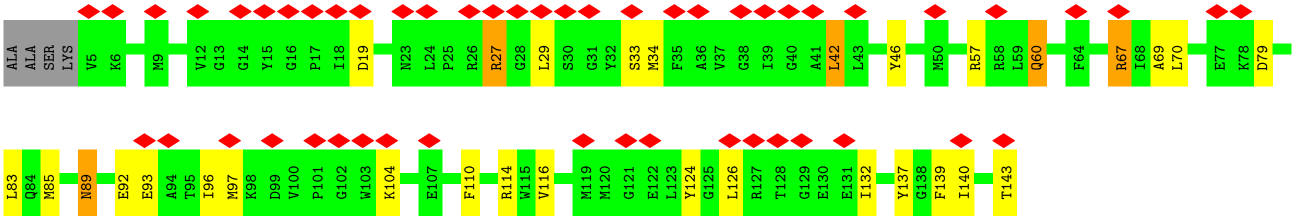
- Molecule 44: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



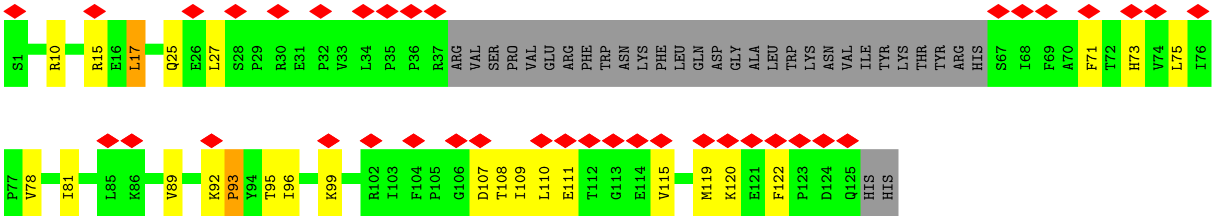
- Molecule 45: MT-ND1

Chain AM:



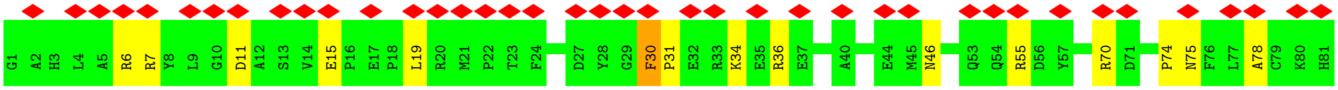
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

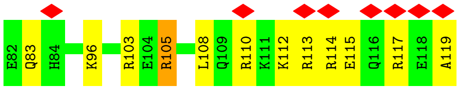
Chain B6:



- Molecule 47: NADH:ubiquinone oxidoreductase subunit B7

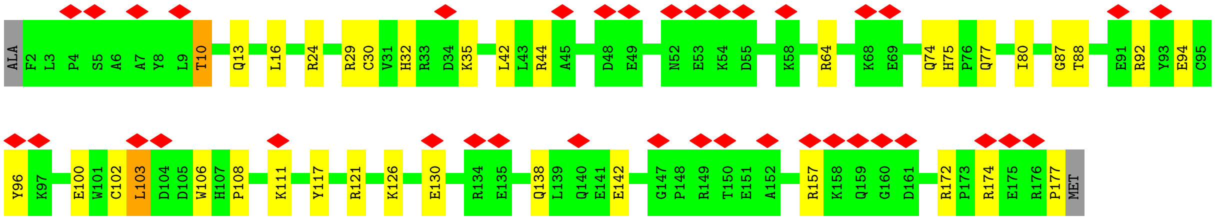
Chain B7:





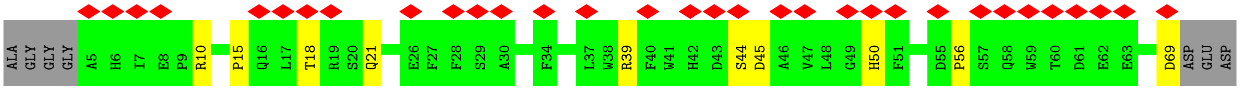
- Molecule 48: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:



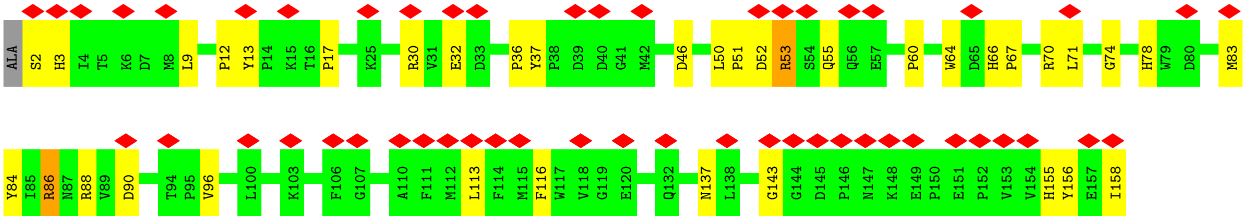
- Molecule 49: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:



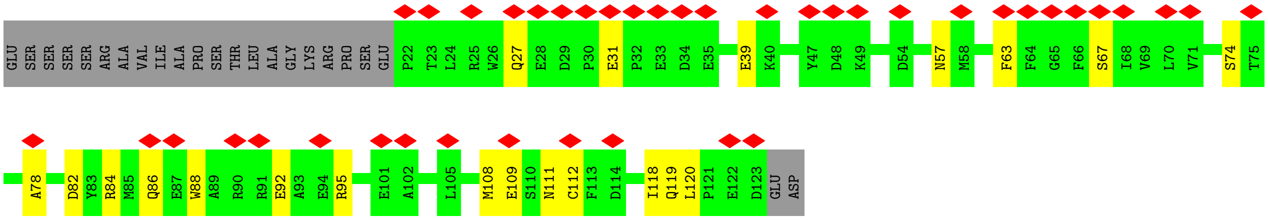
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



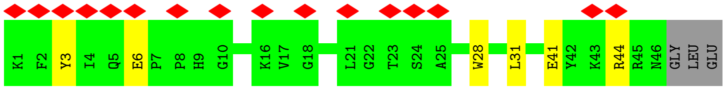
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BK:



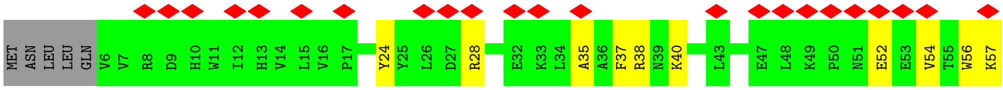
- Molecule 52: NDUFB4

Chain C1:



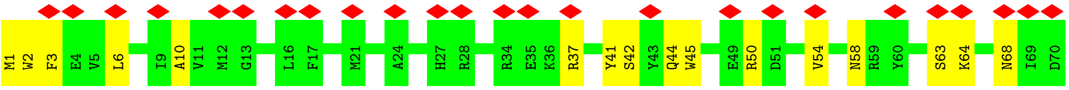
- Molecule 53: NDUFA13

Chain B1:



- Molecule 54: NDUFA1

Chain A1:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.179	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	a1	0.43	0/3479	0.64	1/4719 (0.0%)
1	a3	0.49	0/3518	0.66	2/4776 (0.0%)
2	a2	0.39	0/3183	0.60	0/4313
2	a4	0.43	0/3179	0.62	0/4308
3	b1	0.47	0/3119	0.63	0/4268
3	b2	0.52	0/3119	0.65	0/4268
4	c1	0.43	0/1968	0.61	0/2672
4	c2	0.45	0/1962	0.64	1/2664 (0.0%)
5	f1	0.35	0/1554	0.57	0/2101
5	f2	0.36	0/1548	0.58	0/2093
6	d1	0.44	0/906	0.60	1/1213 (0.1%)
6	d2	0.46	0/908	0.60	0/1218
7	q1	0.42	0/638	0.60	0/862
7	q2	0.53	0/652	0.64	0/883
8	h1	0.38	0/538	0.69	0/723
8	h2	0.39	0/538	0.77	2/723 (0.3%)
10	i1	0.37	0/471	0.58	0/634
10	i2	0.39	0/486	0.56	0/655
11	V1	0.45	0/3386	0.65	0/4575
12	V2	0.45	0/1687	0.76	2/2295 (0.1%)
13	S1	0.47	0/5362	0.69	1/7266 (0.0%)
14	S2	0.58	0/3502	0.72	1/4744 (0.0%)
15	S3	0.56	1/1776 (0.1%)	0.67	0/2417
16	S7	0.59	0/1278	0.70	0/1728
17	S8	0.68	1/1445 (0.1%)	0.73	0/1956
18	V3	0.39	0/355	0.73	1/480 (0.2%)
19	S6	0.47	0/749	0.63	0/1009
20	S4	0.46	0/1047	0.64	0/1415
21	A9	0.43	0/2343	0.71	3/3164 (0.1%)
22	A2	0.35	0/676	0.65	0/911
23	A5	0.41	0/921	0.71	1/1249 (0.1%)
24	A6	0.44	0/993	0.61	1/1336 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
25	A7	0.42	0/775	0.70	0/1048
26	AL	0.46	0/1242	0.69	0/1688
27	AA	0.35	0/655	0.71	0/881
27	AB	0.52	0/714	0.71	0/963
28	D3	0.47	0/747	0.79	0/1022
29	D1	0.57	0/2487	0.80	2/3401 (0.1%)
30	D6	0.50	0/1339	0.73	1/1810 (0.1%)
31	4L	0.52	0/758	0.84	0/1024
32	D5	0.52	0/4933	0.81	9/6710 (0.1%)
33	D4	0.58	1/3740 (0.0%)	0.81	6/5095 (0.1%)
34	D2	0.56	0/2788	0.77	1/3795 (0.0%)
35	AK	0.45	0/1046	0.74	3/1419 (0.2%)
36	B5	0.52	0/1189	0.64	1/1607 (0.1%)
37	A8	0.47	0/1441	0.72	0/1942
38	BJ	0.52	0/1475	0.65	2/1989 (0.1%)
39	AJ	0.53	0/2644	0.72	5/3579 (0.1%)
40	S5	0.50	0/843	0.71	0/1128
41	A3	0.43	0/602	0.75	2/828 (0.2%)
42	B3	0.50	0/595	0.73	0/803
43	C2	0.51	0/1028	0.72	1/1388 (0.1%)
44	B4	0.51	0/1085	0.71	1/1467 (0.1%)
45	AM	0.46	0/1172	0.72	2/1579 (0.1%)
46	B6	0.48	0/841	0.79	1/1144 (0.1%)
47	B7	0.47	0/1051	0.69	1/1408 (0.1%)
48	B9	0.57	0/1568	0.68	1/2123 (0.0%)
49	B2	0.46	0/590	0.68	1/810 (0.1%)
50	B8	0.59	0/1379	0.77	1/1884 (0.1%)
51	BK	0.55	0/880	0.72	0/1196
52	C1	0.43	0/404	0.62	1/548 (0.2%)
53	B1	0.45	0/462	0.66	0/624
54	A1	0.45	0/592	0.65	0/795
All	All	0.49	3/98351 (0.0%)	0.69	59/133336 (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	a1	0	3
1	a3	0	1
2	a4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	b2	0	1
4	c1	0	1
4	c2	0	2
5	f2	0	1
6	d1	0	1
6	d2	0	1
11	V1	0	2
12	V2	0	4
13	S1	0	6
14	S2	0	4
15	S3	0	3
17	S8	0	1
18	V3	0	2
20	S4	0	2
22	A2	0	1
23	A5	0	2
25	A7	0	2
29	D1	0	3
30	D6	0	2
32	D5	0	4
33	D4	0	4
34	D2	0	1
35	AK	0	3
37	A8	0	2
38	BJ	0	2
39	AJ	0	3
40	S5	0	1
41	A3	0	1
42	B3	0	3
43	C2	0	1
44	B4	0	1
46	B6	0	1
47	B7	0	1
49	B2	0	1
50	B8	0	3
51	BK	0	1
52	C1	0	1
53	B1	0	1
54	A1	0	1
All	All	0	82

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	S8	119	CYS	CB-SG	-7.33	1.69	1.82
33	D4	24	TRP	CB-CG	-5.45	1.40	1.50
15	S3	203	TRP	CB-CG	-5.43	1.40	1.50

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A9	222	ASP	CB-CG-OD1	8.72	126.15	118.30
32	D5	69	LEU	CA-CB-CG	8.24	134.25	115.30
12	V2	23	PHE	C-N-CA	7.83	141.29	121.70
8	h2	60	ASP	CB-CG-OD1	7.03	124.63	118.30
41	A3	34	LEU	CA-CB-CG	6.96	131.31	115.30

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a1	190	TYR	Peptide
1	a1	193	PRO	Peptide
1	a1	309	THR	Peptide
4	c1	173	GLY	Peptide
6	d1	39	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a1	3409	0	3322	0	0
1	a3	3447	0	3350	0	0
2	a2	3126	0	3093	0	0
2	a4	3122	0	3090	0	0
3	b1	3019	0	3082	0	0
3	b2	3019	0	3082	0	0
4	c1	1909	0	1858	0	0
4	c2	1903	0	1850	0	0
5	f1	1520	0	1505	0	0
5	f2	1514	0	1497	0	0
6	d1	886	0	883	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	d2	888	0	880	0	0
7	q1	618	0	628	0	0
7	q2	631	0	639	0	0
8	h1	532	0	509	0	0
8	h2	532	0	509	0	0
9	x1	114	0	28	0	0
9	x2	130	0	33	0	0
10	i1	459	0	462	0	0
10	i2	473	0	477	0	0
11	V1	3312	0	3266	67	0
12	V2	1647	0	1657	33	0
13	S1	5275	0	5300	138	0
14	S2	3414	0	3360	54	0
15	S3	1726	0	1676	39	0
16	S7	1247	0	1256	24	0
17	S8	1414	0	1370	33	0
18	V3	345	0	323	9	0
19	S6	737	0	710	14	0
20	S4	1024	0	1023	24	0
21	A9	2293	0	2326	53	0
22	A2	665	0	678	16	0
23	A5	901	0	936	12	0
24	A6	969	0	980	20	0
25	A7	757	0	771	22	0
26	AL	1201	0	1170	13	0
27	AA	645	0	649	7	0
27	AB	702	0	692	8	0
28	D3	728	0	773	17	0
29	D1	2415	0	2542	52	0
30	D6	1308	0	1329	33	0
31	4L	748	0	794	17	0
32	D5	4805	0	4950	108	0
33	D4	3646	0	3850	78	0
34	D2	2724	0	2930	70	0
35	AK	1025	0	1033	19	0
36	B5	1156	0	1177	20	0
37	A8	1404	0	1384	26	0
38	BJ	1441	0	1417	24	0
39	AJ	2583	0	2547	39	0
40	S5	822	0	820	23	0
41	A3	582	0	583	8	0
42	B3	578	0	570	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	C2	997	0	983	20	0
44	B4	1059	0	1062	16	0
45	AM	1143	0	1137	24	0
46	B6	815	0	837	21	0
47	B7	1026	0	995	21	0
48	B9	1515	0	1469	25	0
49	B2	563	0	509	9	0
50	B8	1324	0	1219	27	0
51	BK	853	0	800	19	0
52	C1	391	0	391	4	0
53	B1	449	0	453	5	0
54	A1	577	0	570	11	0
55	b1	86	0	60	0	0
55	b2	86	0	60	0	0
56	c1	43	0	30	0	0
56	c2	43	0	30	0	0
57	D1	26	0	26	1	0
57	D4	40	0	54	3	0
57	D5	38	0	50	2	0
57	c1	13	0	12	0	0
57	f2	23	0	20	0	0
58	S1	4	0	0	0	0
58	V2	4	0	0	1	0
58	f1	4	0	0	0	0
58	f2	4	0	0	0	0
59	S1	16	0	0	1	0
59	S7	8	0	0	1	0
59	S8	16	0	0	1	0
59	V1	8	0	0	1	0
60	V1	31	0	19	3	0
61	S6	1	0	0	0	0
62	A9	48	0	26	3	0
63	AA	34	0	40	0	0
63	AB	31	0	34	1	0
64	D5	60	0	64	4	0
65	AK	28	0	30	0	0
All	All	96897	0	96599	1074	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1074 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S3:80:ALA:HA	15:S3:91:GLU:O	1.15	1.24
13:S1:449:PRO:O	13:S1:489:VAL:HA	1.60	1.02
15:S3:80:ALA:CA	15:S3:91:GLU:O	2.11	0.98
15:S3:38:GLN:HA	25:A7:70:SER:O	1.64	0.97
33:D4:52:PHE:O	33:D4:56:PHE:HB2	1.73	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a1	435/446 (98%)	391 (90%)	44 (10%)	0	100	100
1	a3	442/446 (99%)	400 (90%)	42 (10%)	0	100	100
2	a2	410/439 (93%)	367 (90%)	43 (10%)	0	100	100
2	a4	409/439 (93%)	369 (90%)	40 (10%)	0	100	100
3	b1	376/379 (99%)	351 (93%)	25 (7%)	0	100	100
3	b2	376/379 (99%)	349 (93%)	27 (7%)	0	100	100
4	c1	237/240 (99%)	195 (82%)	42 (18%)	0	100	100
4	c2	236/240 (98%)	202 (86%)	34 (14%)	0	100	100
5	f1	194/196 (99%)	179 (92%)	15 (8%)	0	100	100
5	f2	193/196 (98%)	168 (87%)	25 (13%)	0	100	100
6	d1	98/110 (89%)	93 (95%)	5 (5%)	0	100	100
6	d2	99/110 (90%)	96 (97%)	3 (3%)	0	100	100
7	q1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
7	q2	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
8	h1	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
8	h2	63/78 (81%)	56 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
11	V1	428/445 (96%)	380 (89%)	48 (11%)	0	100	100
12	V2	210/217 (97%)	165 (79%)	45 (21%)	0	100	100
13	S1	686/704 (97%)	595 (87%)	90 (13%)	1 (0%)	48	82
14	S2	420/430 (98%)	373 (89%)	47 (11%)	0	100	100
15	S3	206/228 (90%)	176 (85%)	30 (15%)	0	100	100
16	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	22	59
17	S8	174/176 (99%)	155 (89%)	19 (11%)	0	100	100
18	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
19	S6	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
21	A9	281/338 (83%)	245 (87%)	36 (13%)	0	100	100
22	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
23	A5	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
24	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
25	A7	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	12	46
26	AL	142/145 (98%)	111 (78%)	31 (22%)	0	100	100
27	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
27	AB	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
28	D3	86/115 (75%)	83 (96%)	3 (4%)	0	100	100
29	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	37	71
30	D6	167/175 (95%)	144 (86%)	23 (14%)	0	100	100
31	4L	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	13	48
32	D5	604/606 (100%)	524 (87%)	78 (13%)	2 (0%)	37	71
33	D4	457/459 (100%)	411 (90%)	44 (10%)	2 (0%)	30	67
34	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
35	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
36	B5	137/143 (96%)	120 (88%)	17 (12%)	0	100	100
37	A8	169/171 (99%)	138 (82%)	31 (18%)	0	100	100
38	BJ	169/175 (97%)	150 (89%)	18 (11%)	1 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AJ	317/320 (99%)	270 (85%)	46 (14%)	1 (0%)	37	71
40	S5	97/105 (92%)	82 (84%)	15 (16%)	0	100	100
41	A3	72/83 (87%)	58 (81%)	14 (19%)	0	100	100
42	B3	71/97 (73%)	59 (83%)	12 (17%)	0	100	100
43	C2	117/120 (98%)	100 (86%)	17 (14%)	0	100	100
44	B4	126/128 (98%)	112 (89%)	14 (11%)	0	100	100
45	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
46	B6	92/127 (72%)	79 (86%)	12 (13%)	1 (1%)	12	46
47	B7	117/119 (98%)	97 (83%)	19 (16%)	1 (1%)	14	50
48	B9	174/178 (98%)	144 (83%)	29 (17%)	1 (1%)	22	59
49	B2	63/72 (88%)	51 (81%)	12 (19%)	0	100	100
50	B8	155/158 (98%)	115 (74%)	38 (24%)	2 (1%)	10	42
51	BK	100/125 (80%)	83 (83%)	17 (17%)	0	100	100
52	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
53	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
54	A1	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
All	All	11862/12556 (94%)	10455 (88%)	1391 (12%)	16 (0%)	50	82

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	D5	84	PHE
33	D4	53	SER
16	S7	54	CYS
25	A7	69	MET
32	D5	527	GLY

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	a1	366/372 (98%)	361 (99%)	5 (1%)	62	75
1	a3	370/372 (100%)	363 (98%)	7 (2%)	52	69
2	a2	326/341 (96%)	321 (98%)	5 (2%)	60	74
2	a4	326/341 (96%)	323 (99%)	3 (1%)	75	83
3	b1	330/331 (100%)	327 (99%)	3 (1%)	75	83
3	b2	330/331 (100%)	328 (99%)	2 (1%)	84	88
4	c1	205/206 (100%)	202 (98%)	3 (2%)	60	74
4	c2	204/206 (99%)	201 (98%)	3 (2%)	60	74
5	f1	168/168 (100%)	167 (99%)	1 (1%)	84	88
5	f2	167/168 (99%)	166 (99%)	1 (1%)	84	88
6	d1	93/99 (94%)	92 (99%)	1 (1%)	70	79
6	d2	94/99 (95%)	91 (97%)	3 (3%)	34	55
7	q1	66/72 (92%)	66 (100%)	0	100	100
7	q2	67/72 (93%)	66 (98%)	1 (2%)	60	74
8	h1	62/74 (84%)	61 (98%)	1 (2%)	58	73
8	h2	62/74 (84%)	61 (98%)	1 (2%)	58	73
10	i1	46/52 (88%)	45 (98%)	1 (2%)	47	65
10	i2	48/52 (92%)	48 (100%)	0	100	100
11	V1	344/354 (97%)	341 (99%)	3 (1%)	75	83
12	V2	182/183 (100%)	178 (98%)	4 (2%)	47	65
13	S1	578/588 (98%)	574 (99%)	4 (1%)	81	86
14	S2	368/371 (99%)	363 (99%)	5 (1%)	62	75
15	S3	189/204 (93%)	188 (100%)	1 (0%)	86	90
16	S7	132/150 (88%)	129 (98%)	3 (2%)	45	64
17	S8	151/151 (100%)	150 (99%)	1 (1%)	81	86
18	V3	40/68 (59%)	37 (92%)	3 (8%)	11	33
19	S6	79/80 (99%)	78 (99%)	1 (1%)	65	76
20	S4	113/119 (95%)	112 (99%)	1 (1%)	75	83
21	A9	246/292 (84%)	242 (98%)	4 (2%)	58	73
22	A2	73/81 (90%)	72 (99%)	1 (1%)	62	75
23	A5	99/101 (98%)	99 (100%)	0	100	100
24	A6	107/113 (95%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	A7	83/94 (88%)	82 (99%)	1 (1%)	67	78
26	AL	130/131 (99%)	126 (97%)	4 (3%)	35	56
27	AA	74/81 (91%)	73 (99%)	1 (1%)	62	75
27	AB	80/81 (99%)	78 (98%)	2 (2%)	42	62
28	D3	81/103 (79%)	80 (99%)	1 (1%)	67	78
29	D1	266/278 (96%)	262 (98%)	4 (2%)	60	74
30	D6	140/144 (97%)	139 (99%)	1 (1%)	81	86
31	4L	87/87 (100%)	85 (98%)	2 (2%)	45	64
32	D5	539/539 (100%)	532 (99%)	7 (1%)	65	76
33	D4	412/412 (100%)	406 (98%)	6 (2%)	60	74
34	D2	315/315 (100%)	310 (98%)	5 (2%)	58	73
35	AK	101/101 (100%)	99 (98%)	2 (2%)	50	68
36	B5	122/125 (98%)	119 (98%)	3 (2%)	42	62
37	A8	154/154 (100%)	150 (97%)	4 (3%)	41	61
38	BJ	155/157 (99%)	151 (97%)	4 (3%)	41	61
39	AJ	283/284 (100%)	281 (99%)	2 (1%)	81	86
40	S5	88/94 (94%)	88 (100%)	0	100	100
41	A3	65/71 (92%)	65 (100%)	0	100	100
42	B3	55/75 (73%)	53 (96%)	2 (4%)	30	52
43	C2	106/107 (99%)	106 (100%)	0	100	100
44	B4	114/114 (100%)	113 (99%)	1 (1%)	75	83
45	AM	119/121 (98%)	114 (96%)	5 (4%)	25	48
46	B6	92/121 (76%)	90 (98%)	2 (2%)	47	65
47	B7	108/108 (100%)	104 (96%)	4 (4%)	29	51
48	B9	159/160 (99%)	156 (98%)	3 (2%)	52	69
49	B2	59/62 (95%)	59 (100%)	0	100	100
50	B8	142/142 (100%)	139 (98%)	3 (2%)	48	66
51	BK	93/112 (83%)	91 (98%)	2 (2%)	47	65
52	C1	42/44 (96%)	42 (100%)	0	100	100
53	B1	48/53 (91%)	48 (100%)	0	100	100
54	A1	59/59 (100%)	56 (95%)	3 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10402/10814 (96%)	10256 (99%)	146 (1%)	62 75

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BJ	79	LYS
54	A1	50	ARG
39	AJ	17	LYS
46	B6	89	VAL
13	S1	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
34	D2	174	GLN
48	B9	13	GLN
27	AB	33	ASN
39	AJ	251	GLN
54	A1	27	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	#$\|Z\| > 2$
63	ZMP	AA	101	27	27,33,36	0.59	0	32,40,45	1.07	2 (6%)
64	CDL	D5	901	-	59,59,99	0.40	0	65,71,111	0.56	1 (1%)
60	FMN	V1	501	-	33,33,33	0.44	0	48,50,50	0.43	0
57	3PE	f2	201	-	22,22,50	0.44	0	25,27,55	0.46	0
59	SF4	S8	202	17	0,12,12	-	-	-		
59	SF4	S1	801	13	0,12,12	-	-	-		
65	PC1	AK	201	-	27,27,53	0.41	0	33,35,61	0.39	0
59	SF4	S7	300	16	0,12,12	-	-	-		
57	3PE	D5	902	-	37,37,50	0.36	0	40,42,55	0.41	0
62	NDP	A9	401	-	45,52,52	0.66	2 (4%)	53,80,80	0.75	2 (3%)
59	SF4	S8	201	17	0,12,12	-	-	-		
57	3PE	D1	501	-	25,25,50	0.40	0	28,30,55	0.46	0
57	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.39	0
58	FES	f1	501	5	0,4,4	-	-	-		
55	HEM	b2	402	3	41,50,50	1.58	6 (14%)	45,82,82	1.86	10 (22%)
55	HEM	b1	402	3	41,50,50	1.54	6 (14%)	45,82,82	2.03	10 (22%)
57	3PE	c1	502	-	12,12,50	0.62	0	13,15,55	0.64	0
55	HEM	b1	401	3	41,50,50	1.41	4 (9%)	45,82,82	1.93	12 (26%)
58	FES	V2	300	12	0,4,4	-	-	-		
55	HEM	b2	401	3	41,50,50	1.46	5 (12%)	45,82,82	1.93	14 (31%)
58	FES	S1	803	13	0,4,4	-	-	-		
59	SF4	V1	500	11	0,12,12	-	-	-		
63	ZMP	AB	101	27	24,30,36	0.69	0	29,37,45	1.45	4 (13%)
58	FES	f2	202	5	0,4,4	-	-	-		
56	HEC	c1	501	4	32,50,50	2.10	4 (12%)	24,82,82	2.65	12 (50%)
56	HEC	c2	501	4	32,50,50	2.26	5 (15%)	24,82,82	2.43	11 (45%)
59	SF4	S1	802	13	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	ZMP	AA	101	27	-	17/38/40/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	CDL	D5	901	-	-	15/70/70/110	-
60	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
57	3PE	f2	201	-	-	7/26/26/54	-
59	SF4	S8	202	17	-	-	0/6/5/5
65	PC1	AK	201	-	-	9/31/31/57	-
59	SF4	S1	801	13	-	-	0/6/5/5
59	SF4	S7	300	16	-	-	0/6/5/5
62	NDP	A9	401	-	-	11/30/77/77	0/5/5/5
57	3PE	D5	902	-	-	12/41/41/54	-
59	SF4	S8	201	17	-	-	0/6/5/5
57	3PE	D1	501	-	-	12/28/28/54	-
57	3PE	D4	501	-	-	7/43/43/54	-
59	SF4	S1	802	13	-	-	0/6/5/5
58	FES	f1	501	5	-	-	0/1/1/1
55	HEM	b2	402	3	-	4/12/54/54	-
55	HEM	b1	402	3	-	8/12/54/54	-
57	3PE	c1	502	-	-	7/13/13/54	-
58	FES	V2	300	12	-	-	0/1/1/1
55	HEM	b2	401	3	-	3/12/54/54	-
58	FES	S1	803	13	-	-	0/1/1/1
63	ZMP	AB	101	27	-	16/35/37/43	-
59	SF4	V1	500	11	-	-	0/6/5/5
58	FES	f2	202	5	-	-	0/1/1/1
56	HEC	c1	501	4	-	4/10/54/54	-
56	HEC	c2	501	4	-	3/10/54/54	-
55	HEM	b1	401	3	-	7/12/54/54	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c2	501	HEC	C3C-C2C	-7.75	1.32	1.40
56	c2	501	HEC	C2B-C3B	-7.04	1.33	1.40
56	c1	501	HEC	C3C-C2C	-6.95	1.33	1.40
56	c1	501	HEC	C2B-C3B	-6.67	1.33	1.40
55	b1	401	HEM	C4D-ND	-4.56	1.32	1.40

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	b1	402	HEM	CHC-C4B-NB	6.31	131.28	124.43
55	b1	401	HEM	CHC-C4B-NB	6.19	131.16	124.43
55	b2	401	HEM	CHC-C4B-NB	6.07	131.03	124.43
55	b2	402	HEM	CHC-C4B-NB	5.44	130.34	124.43
56	c1	501	HEC	CMD-C2D-C1D	-5.26	120.38	128.46

There are no chirality outliers.

5 of 149 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	b1	401	HEM	C2B-C3B-CAB-CBB
55	b1	401	HEM	C4B-C3B-CAB-CBB
55	b1	402	HEM	C2B-C3B-CAB-CBB
55	b1	402	HEM	C4B-C3B-CAB-CBB
55	b2	401	HEM	C2A-CAA-CBA-CGA

There are no ring outliers.

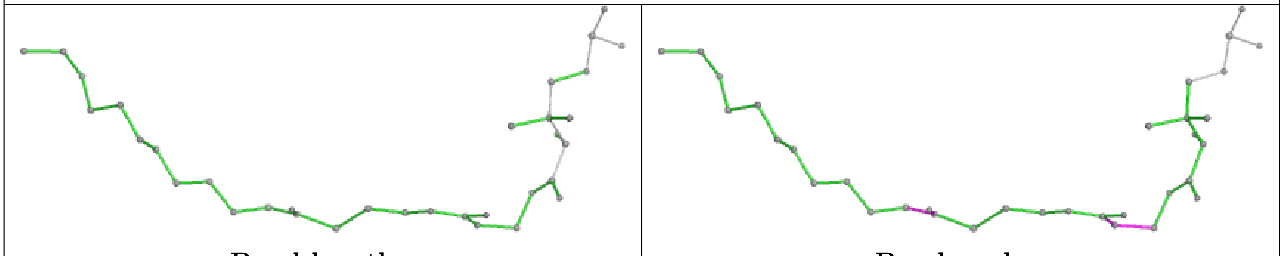
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	D5	901	CDL	4	0
60	V1	501	FMN	3	0
59	S8	202	SF4	1	0
59	S1	801	SF4	1	0
59	S7	300	SF4	1	0
57	D5	902	3PE	2	0
62	A9	401	NDP	3	0
57	D1	501	3PE	1	0
57	D4	501	3PE	3	0
58	V2	300	FES	1	0
59	V1	500	SF4	1	0
63	AB	101	ZMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

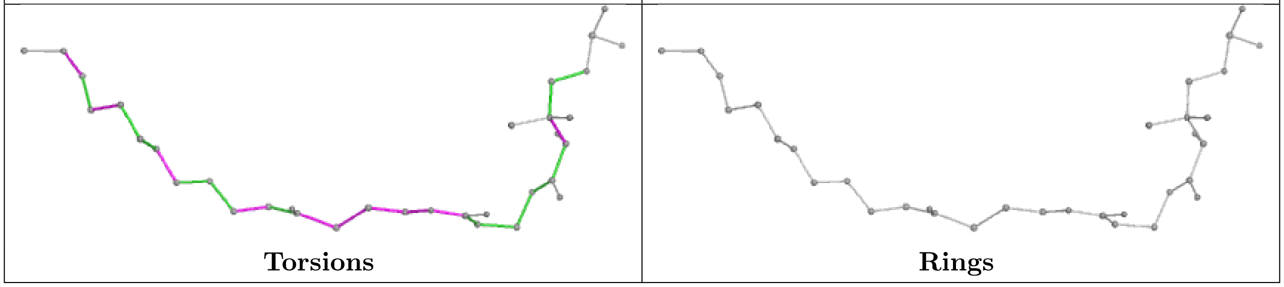
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ZMP AA 101



Bond lengths

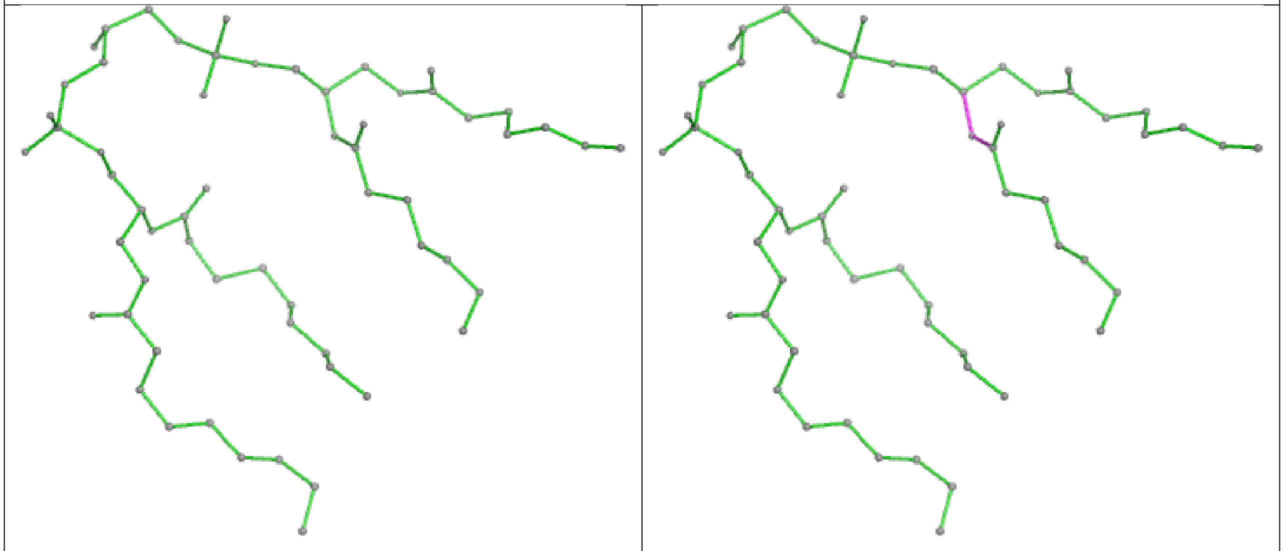
Bond angles



Torsions

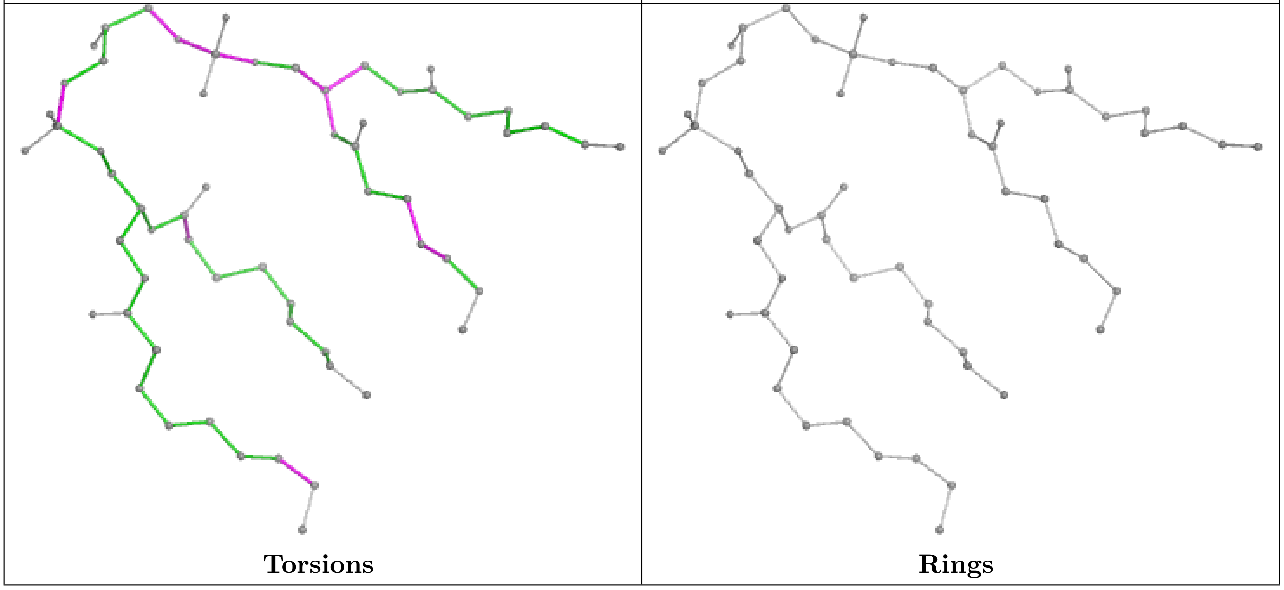
Rings

Ligand CDL D5 901



Bond lengths

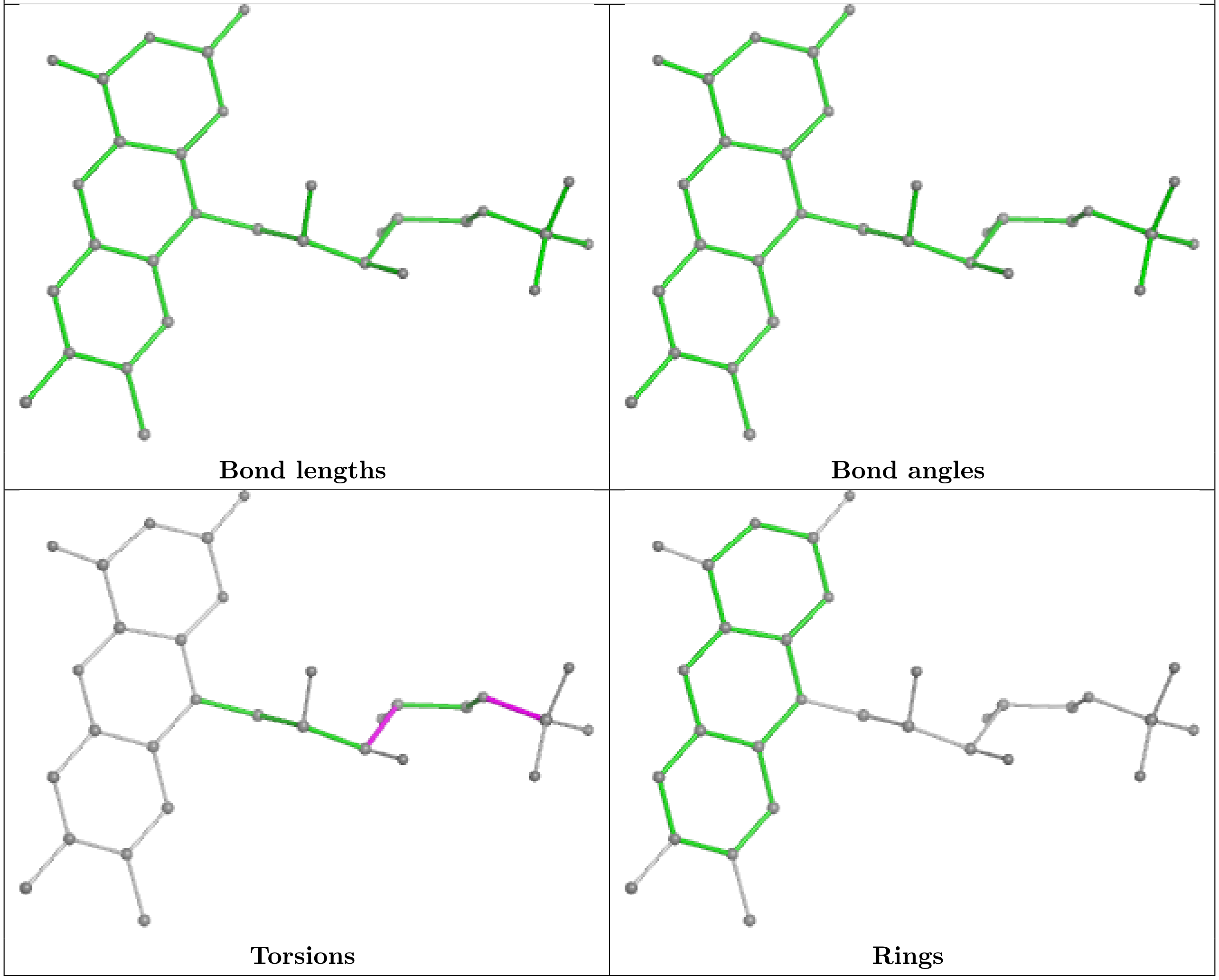
Bond angles



Torsions

Rings

Ligand FMN V1 501



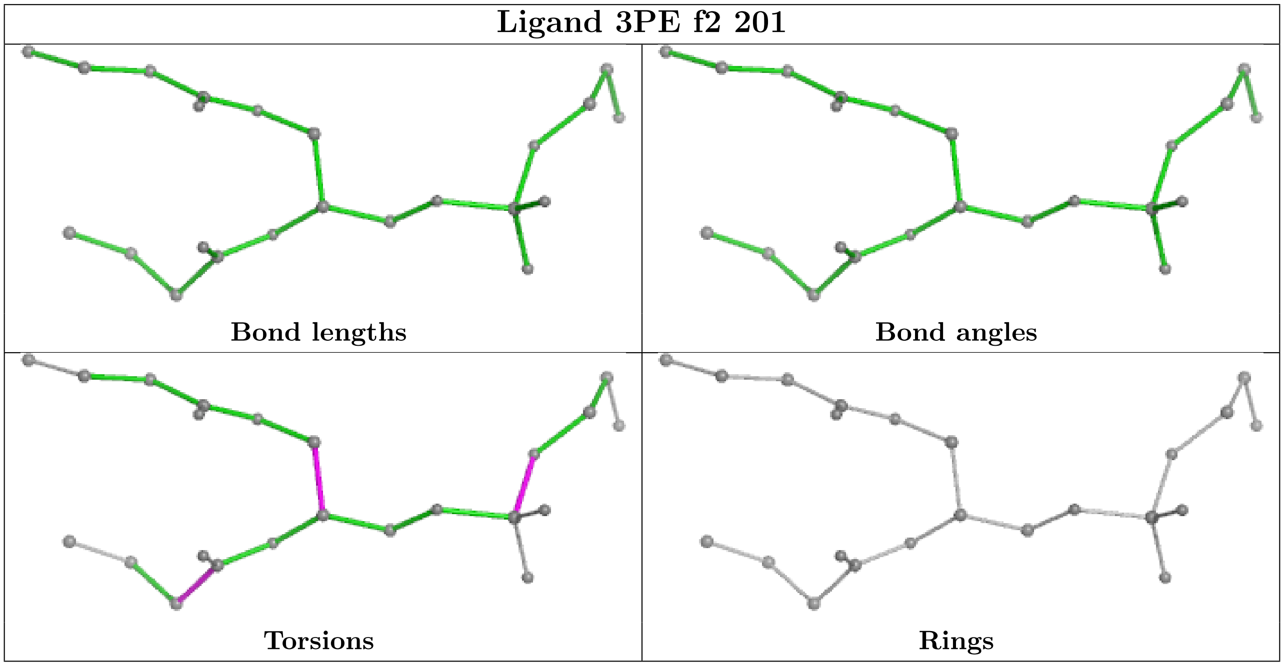
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE f2 201



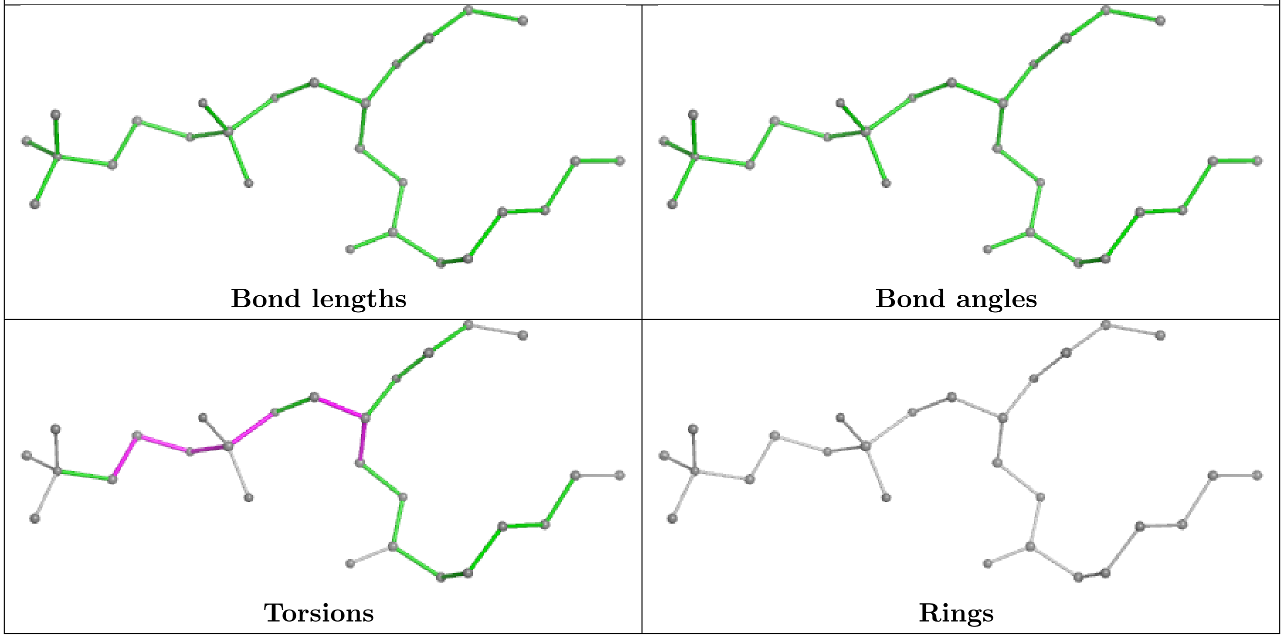
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 AK 201



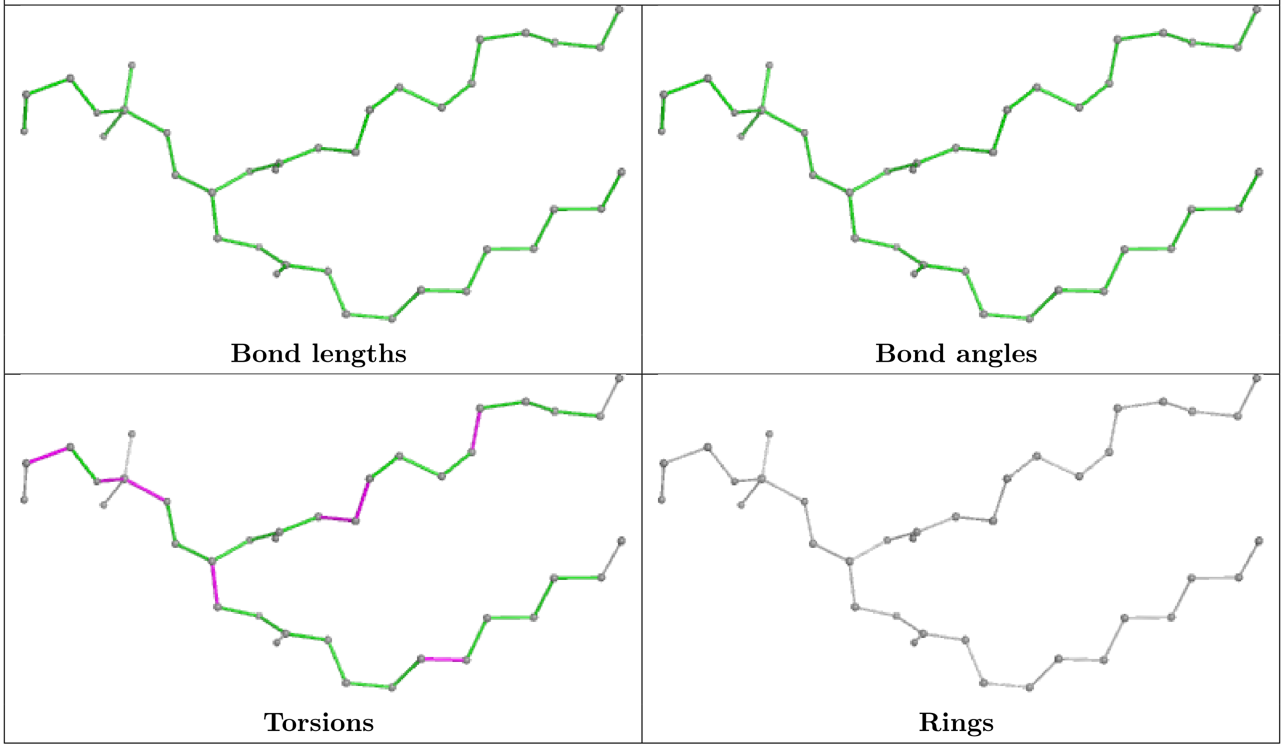
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE D5 902



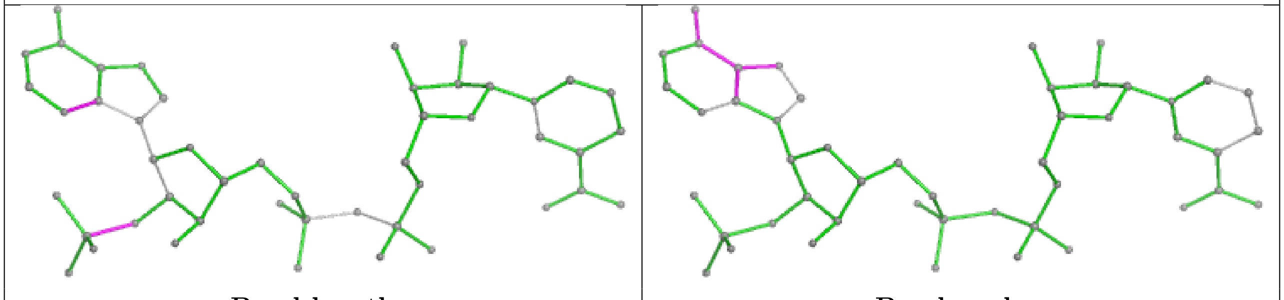
Bond lengths

Bond angles

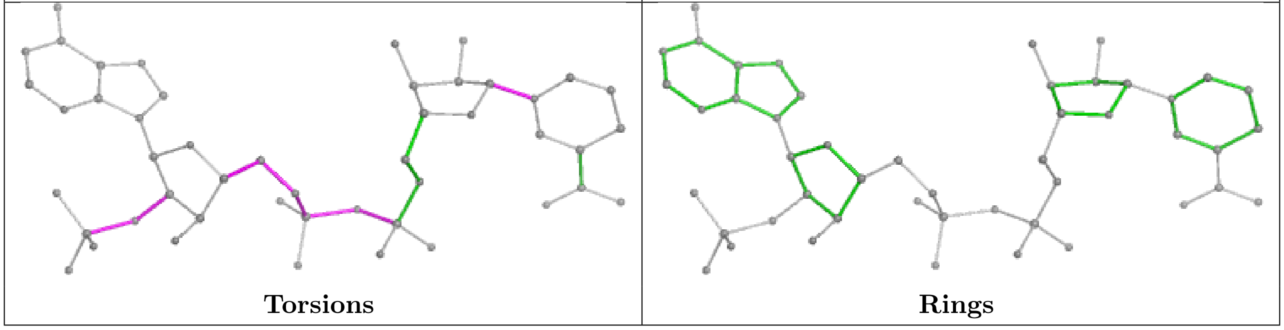
Torsions

Rings

Ligand NDP A9 401

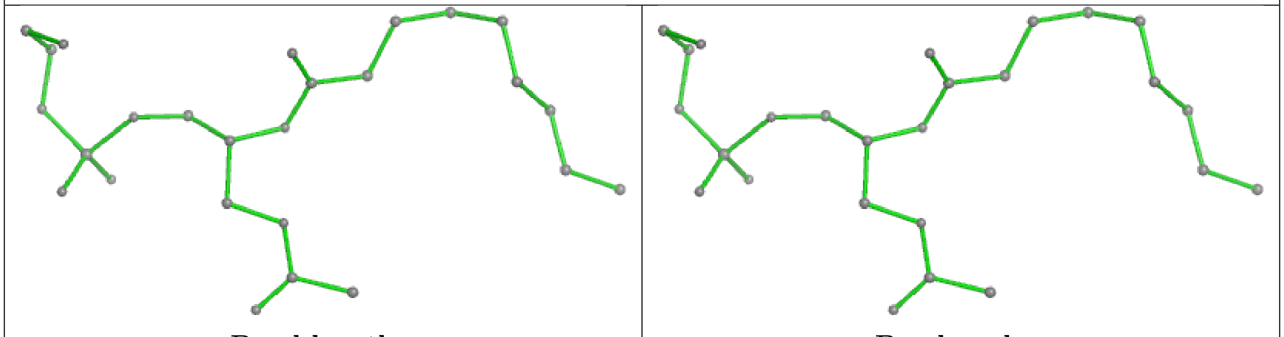


Bond lengths Bond angles

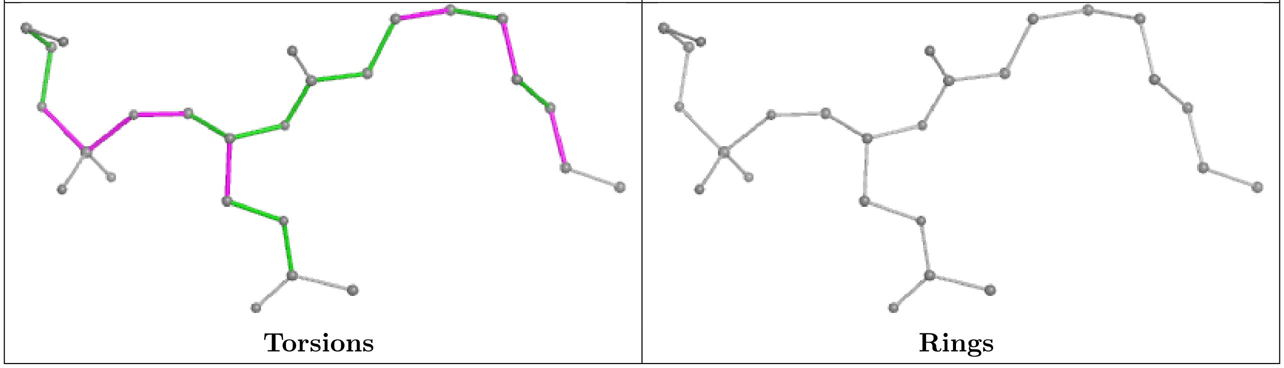


Torsions Rings

Ligand 3PE D1 501

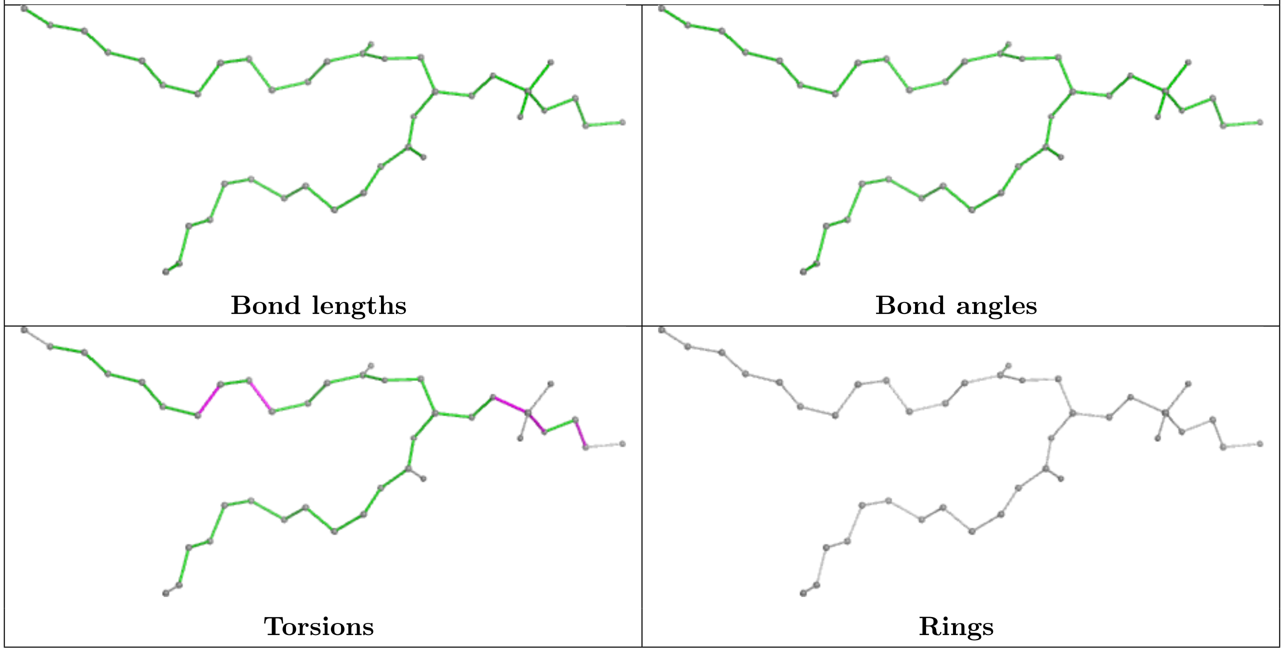


Bond lengths Bond angles

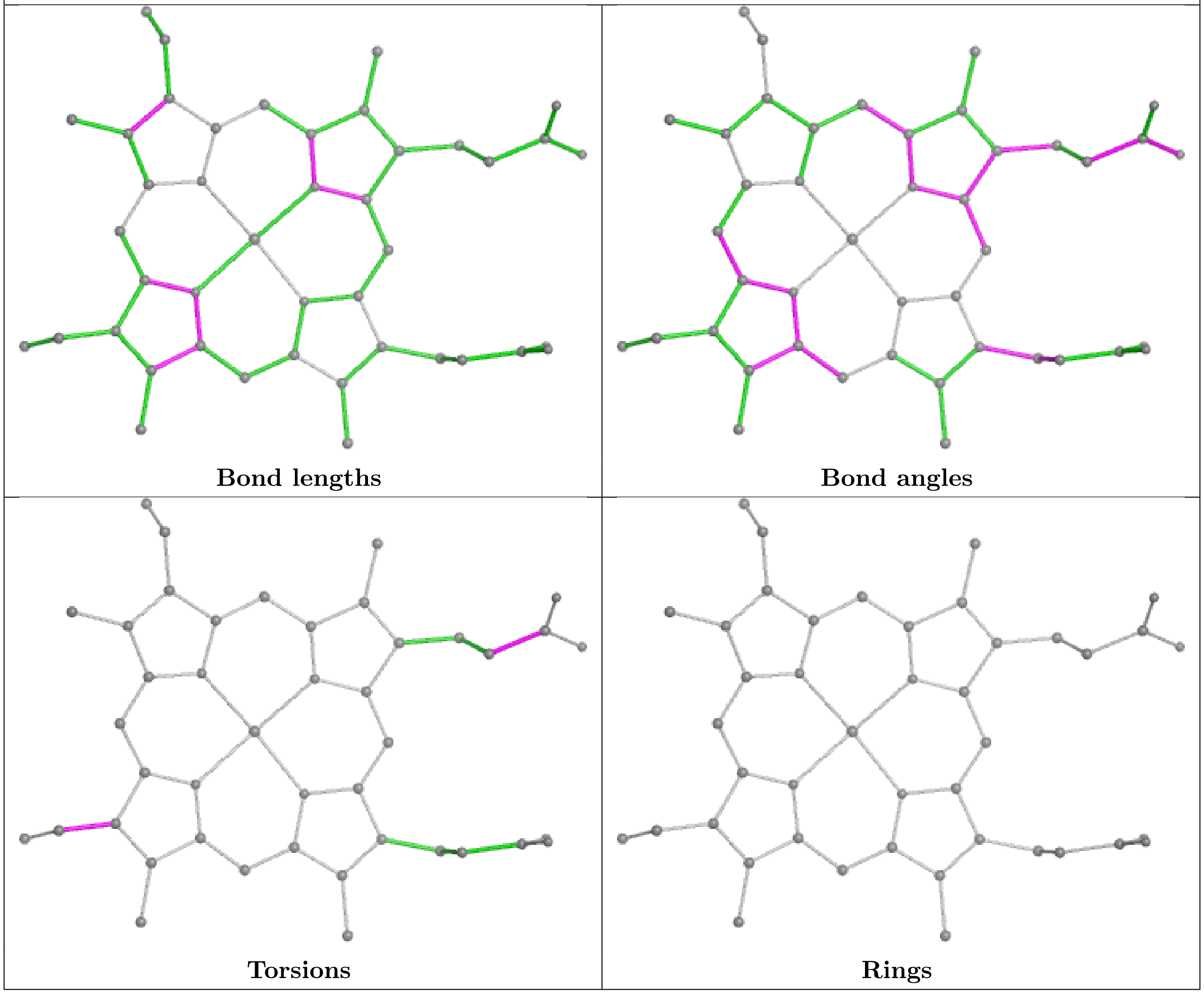


Torsions Rings

Ligand 3PE D4 501



Ligand HEM b2 402



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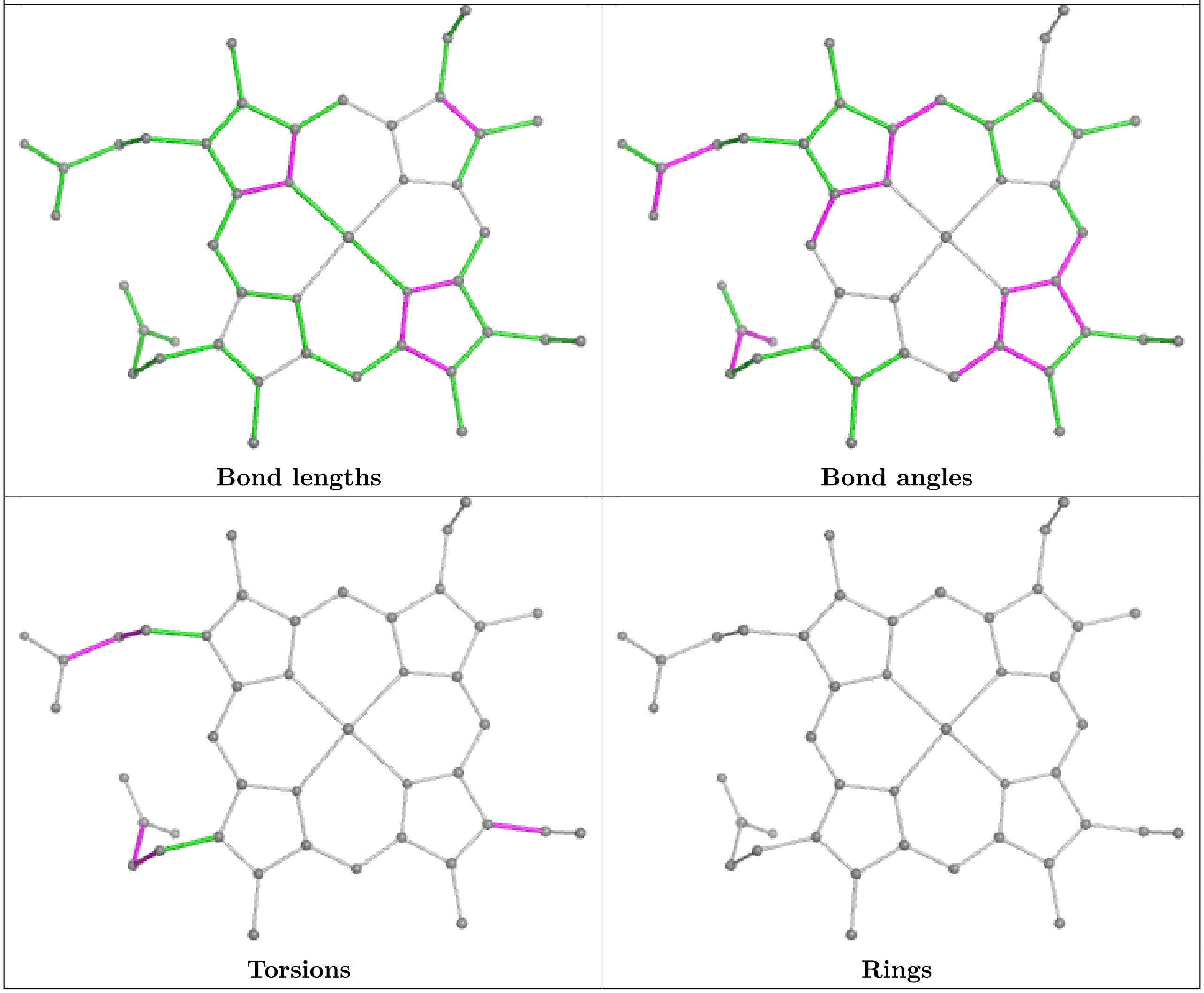


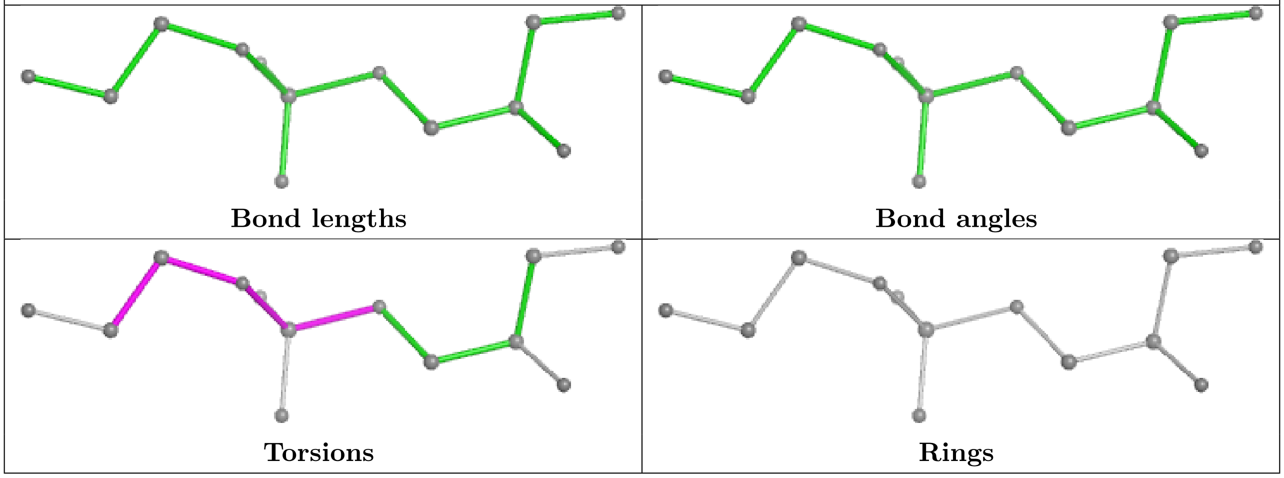
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE c1 502



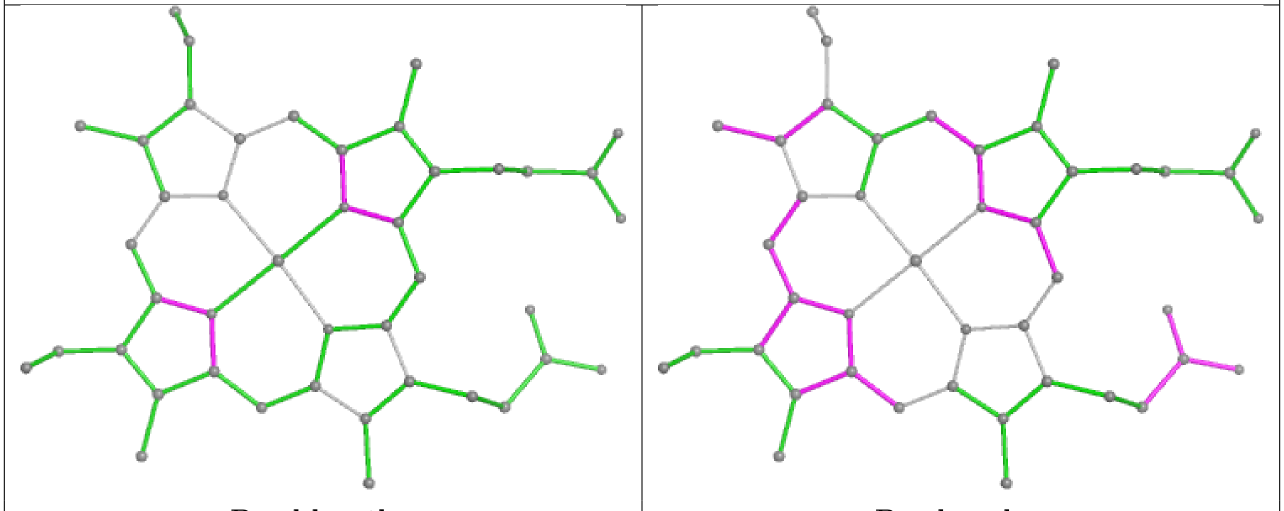
Bond lengths

Bond angles

Torsions

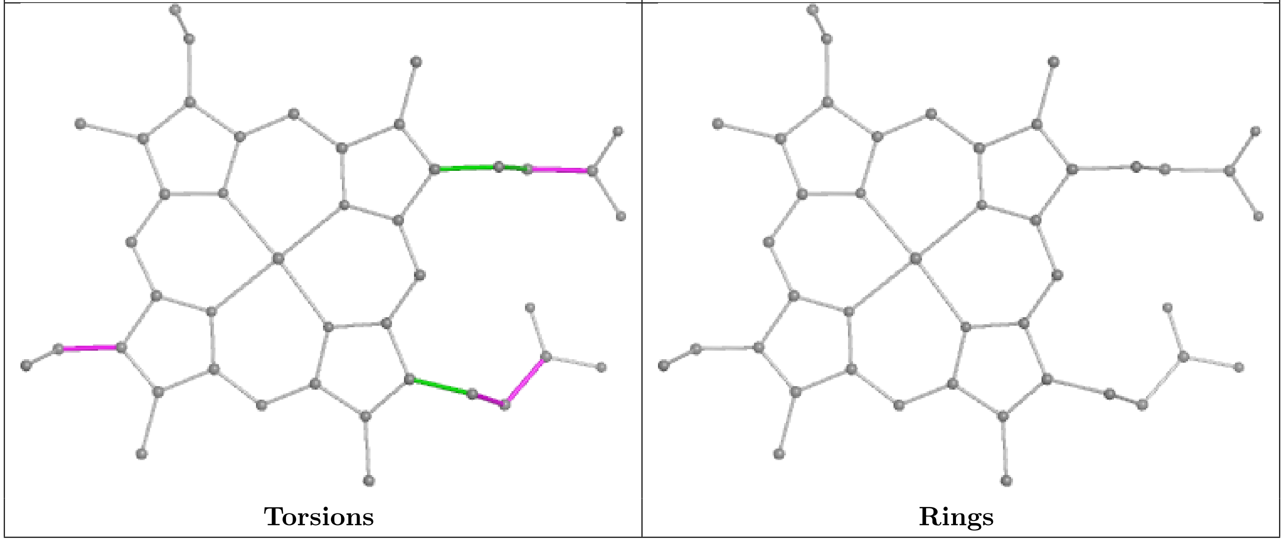
Rings

Ligand HEM b1 401



Bond lengths

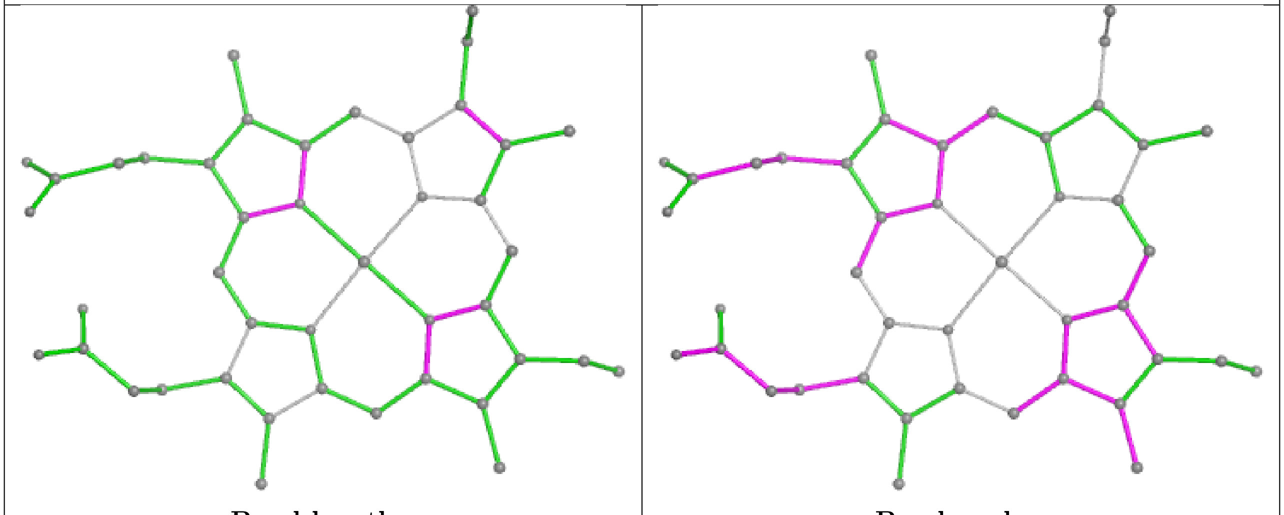
Bond angles



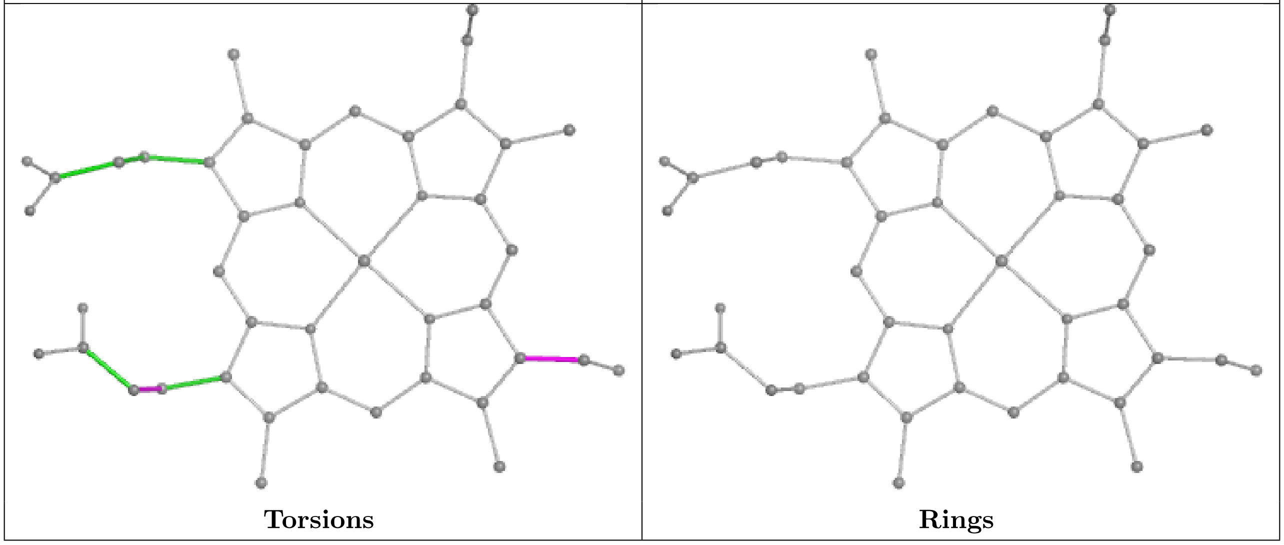
Torsions

Rings

Ligand HEM b2 401

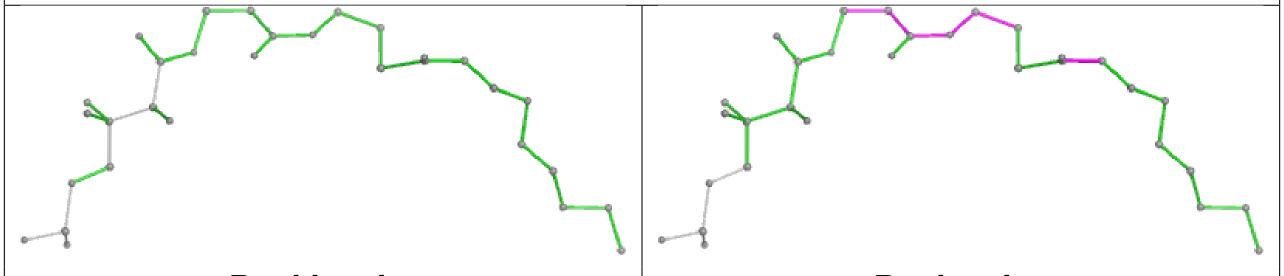


Bond lengths Bond angles

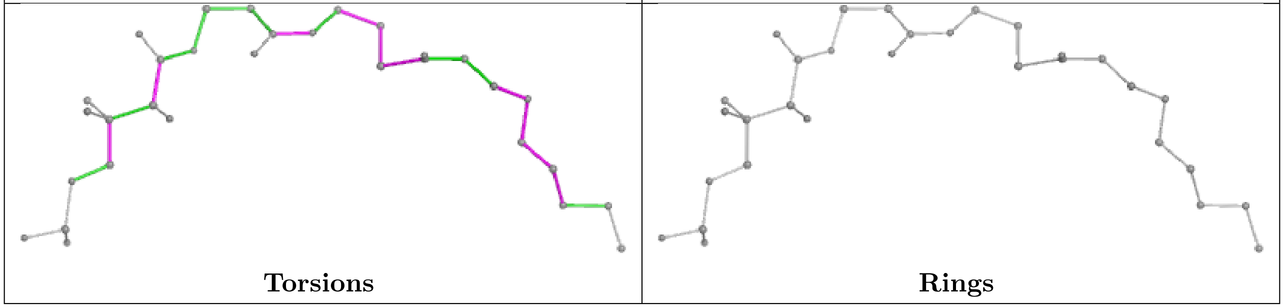


Torsions Rings

Ligand ZMP AB 101

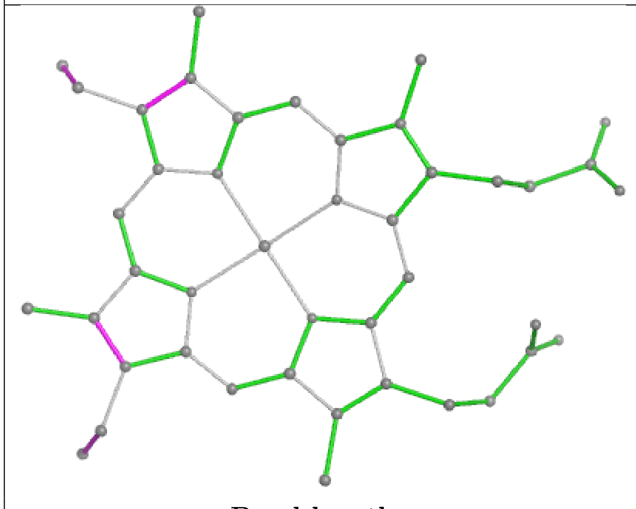


Bond lengths Bond angles

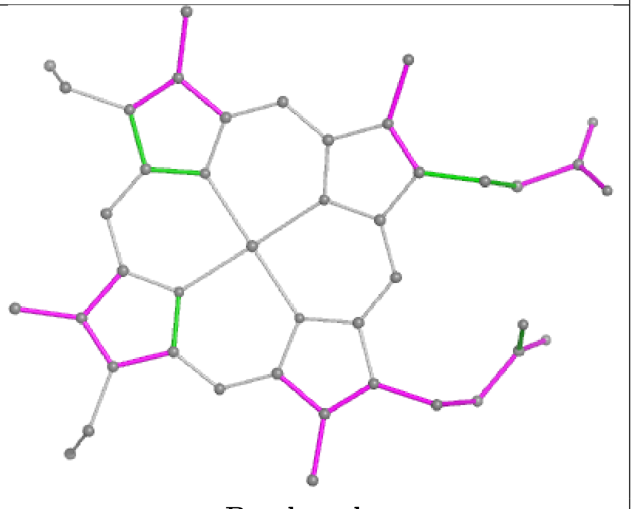


Torsions Rings

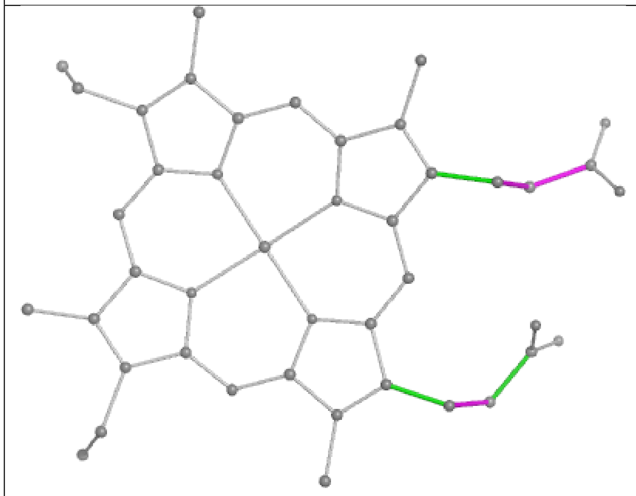
Ligand HEC c1 501



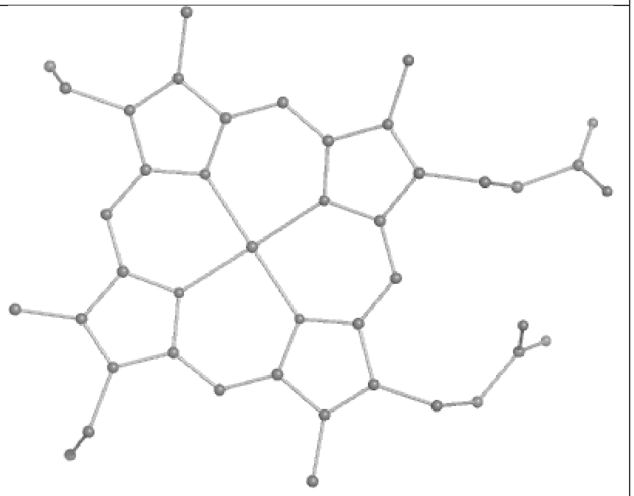
Bond lengths



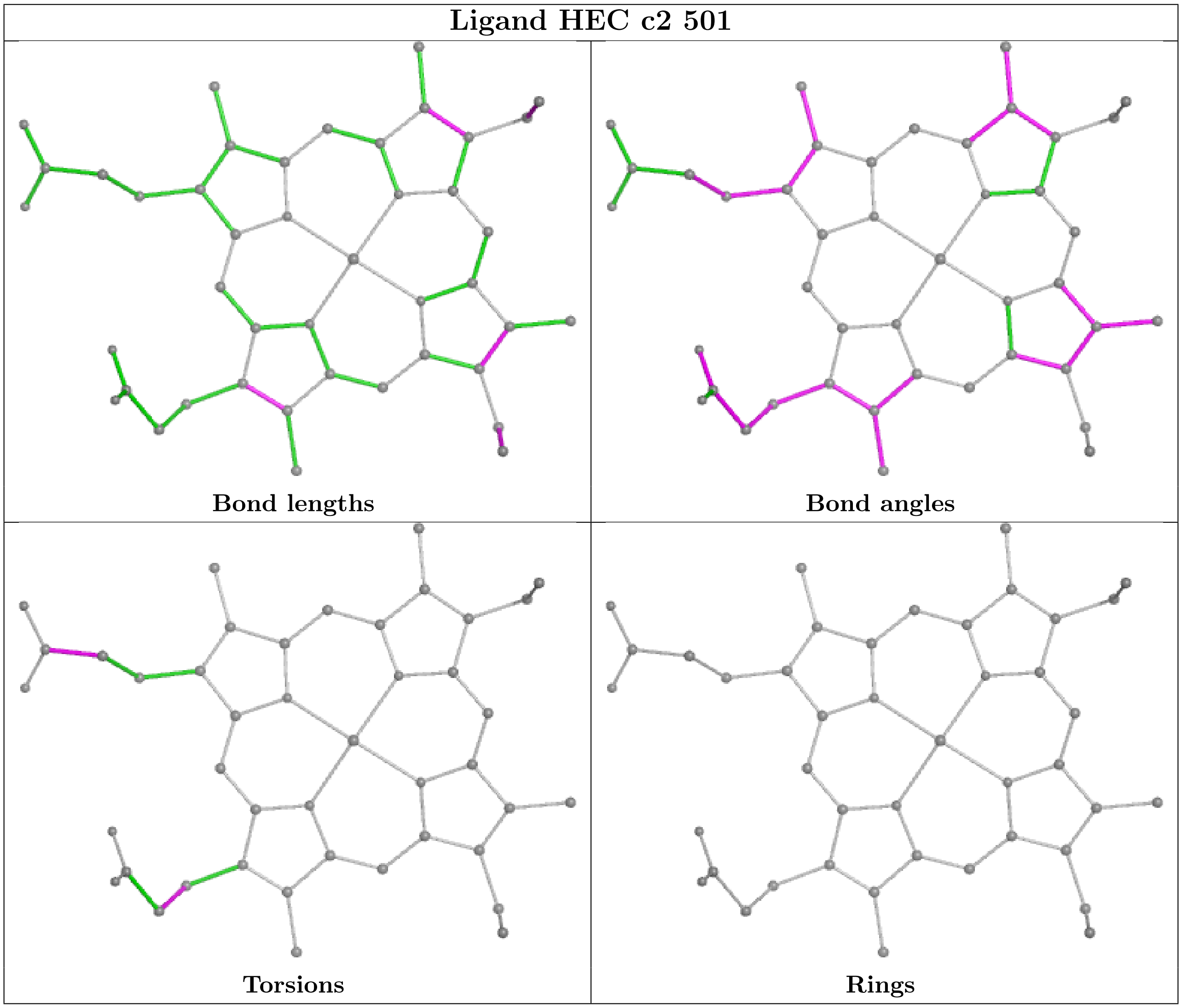
Bond angles



Torsions



Rings



Ligand HEC c2 501

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.

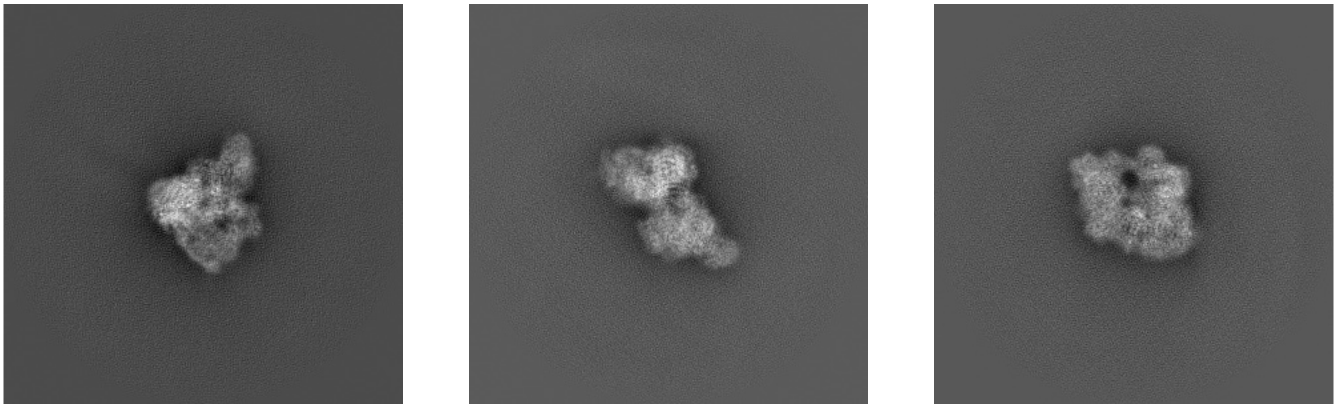
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4495. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

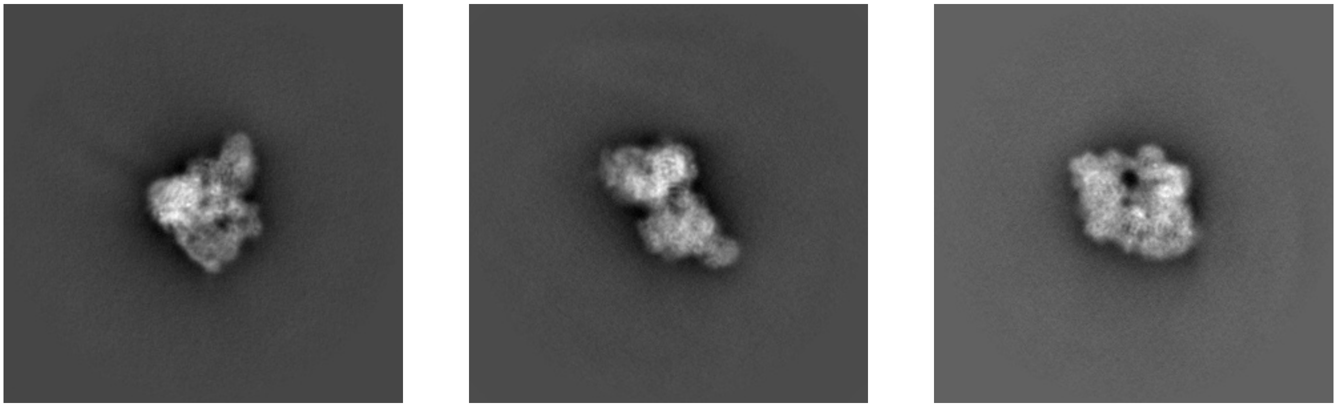
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

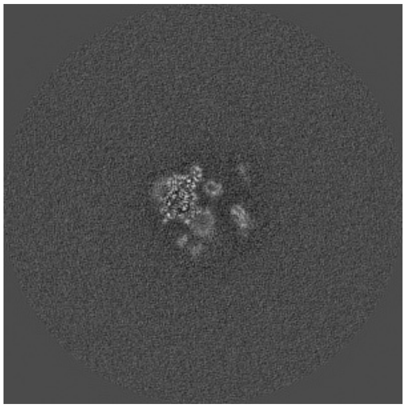


X Y Z

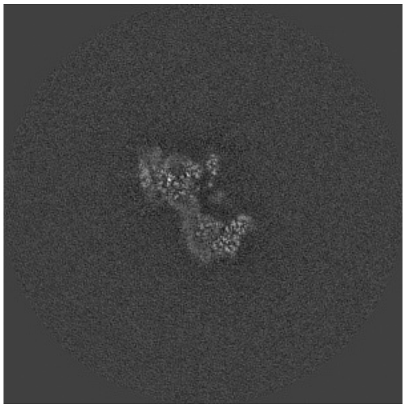
The images above show the map projected in three orthogonal directions.

6.2 Central slices

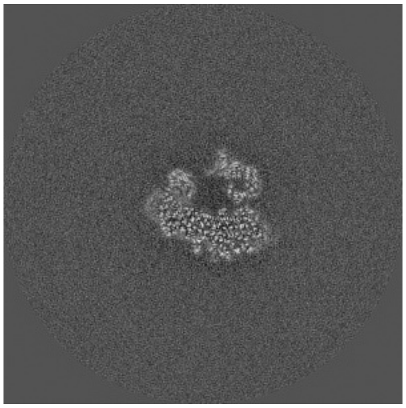
6.2.1 Primary map



X Index: 256

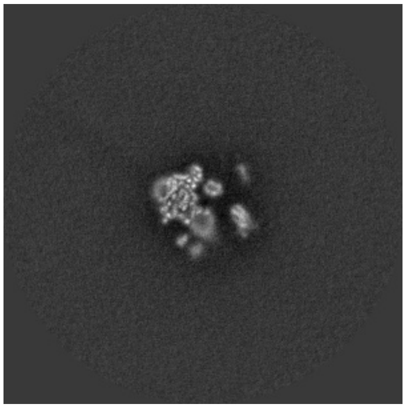


Y Index: 256

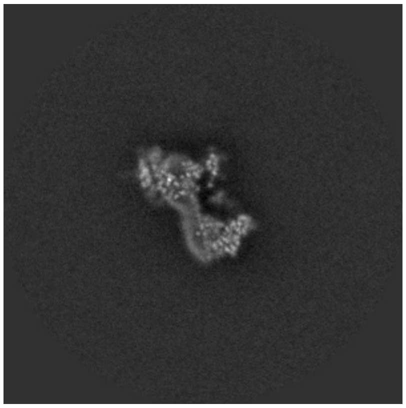


Z Index: 256

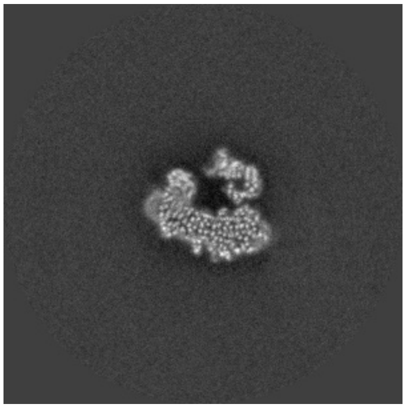
6.2.2 Raw map



X Index: 256



Y Index: 256

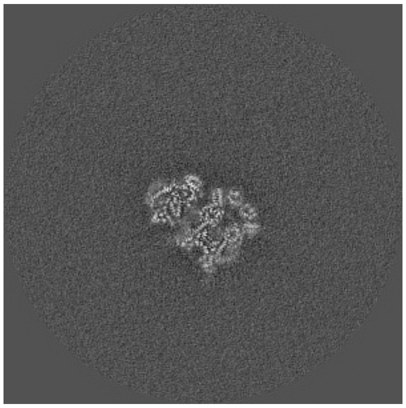


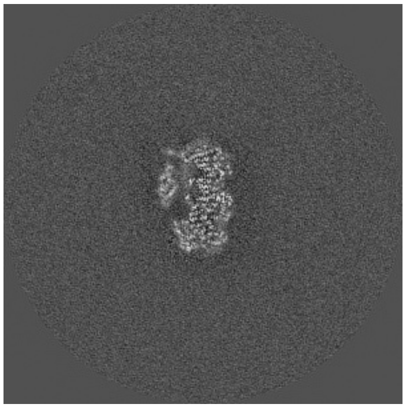
Z Index: 256

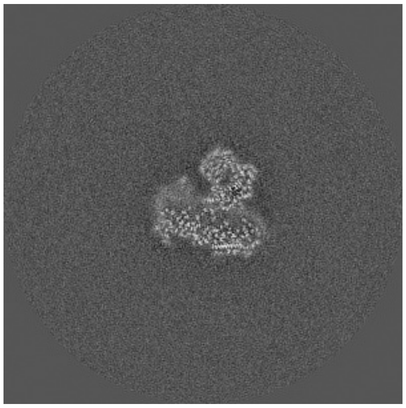
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

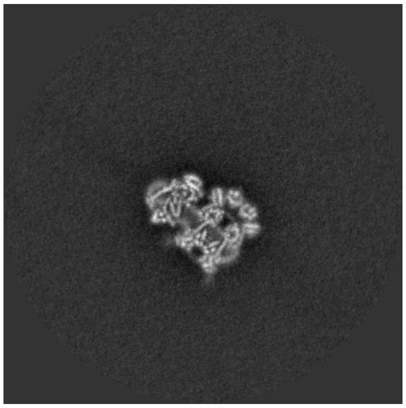
6.3.1 Primary map

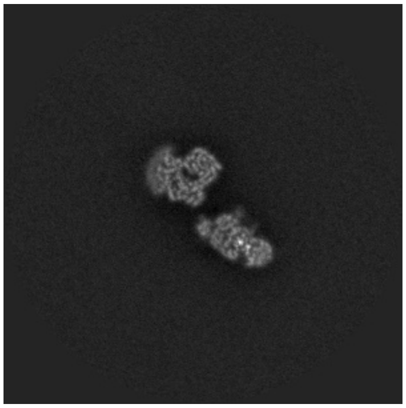

X Index: 290

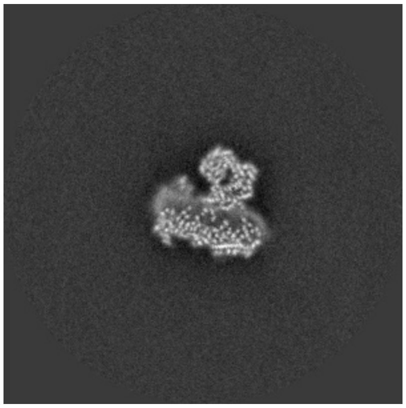

Y Index: 229


Z Index: 243

6.3.2 Raw map


X Index: 290

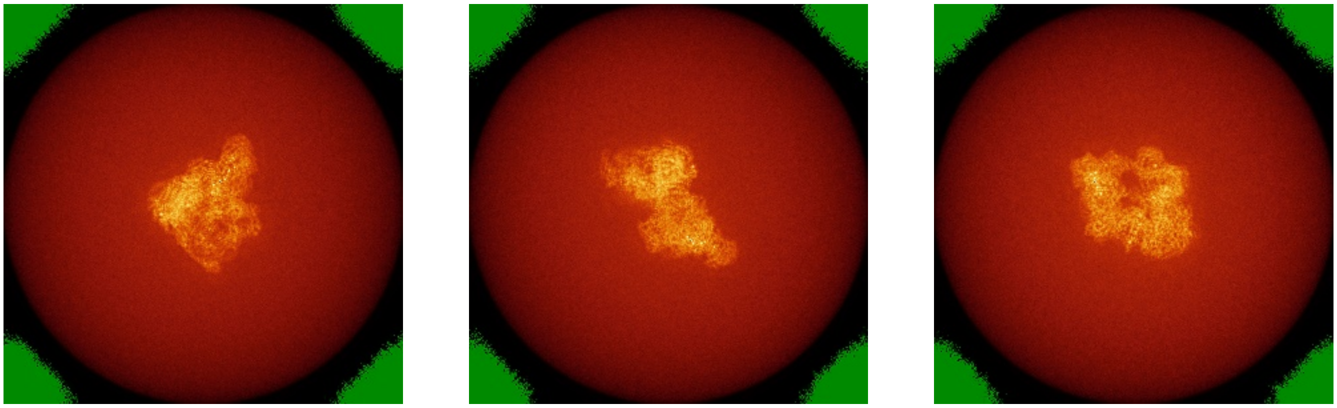

Y Index: 295


Z Index: 243

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

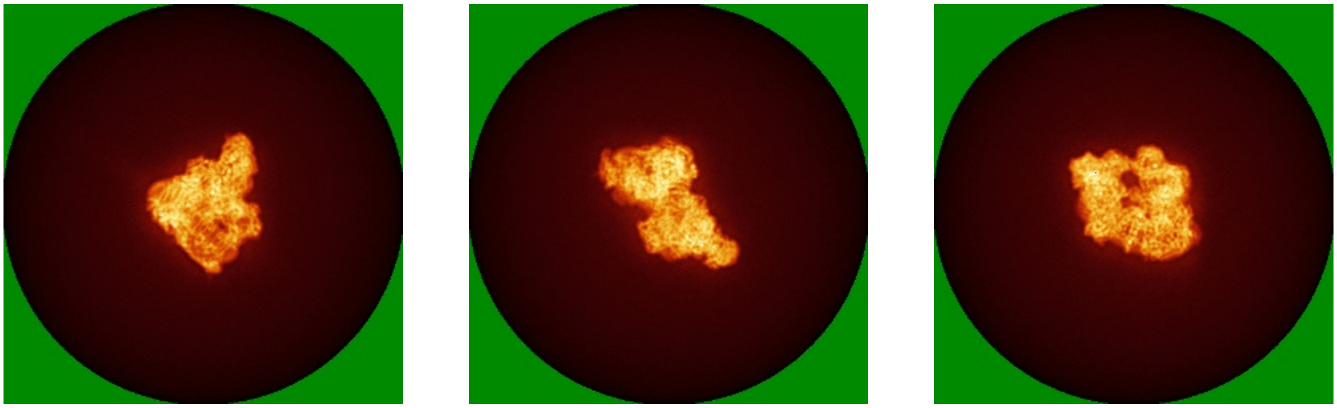
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

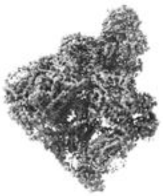


X Y Z

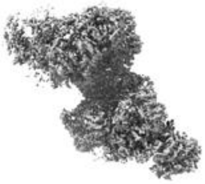
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

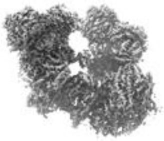
6.5.1 Primary map



X



Y

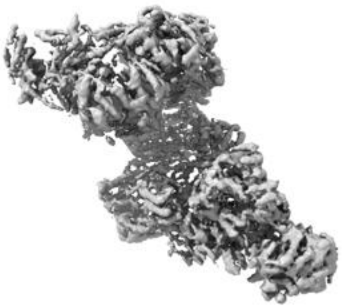


Z

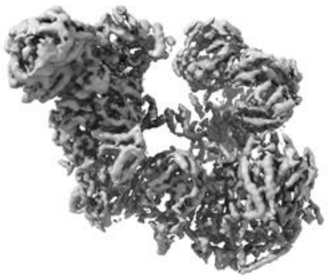
The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

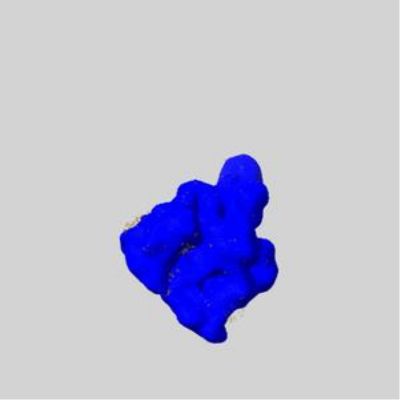
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

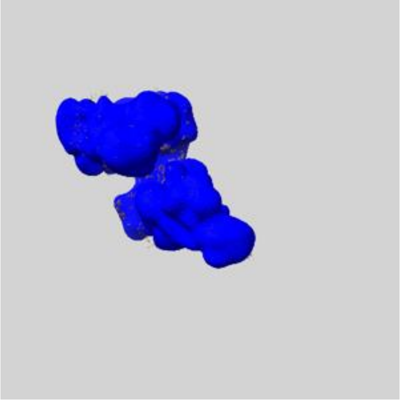
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

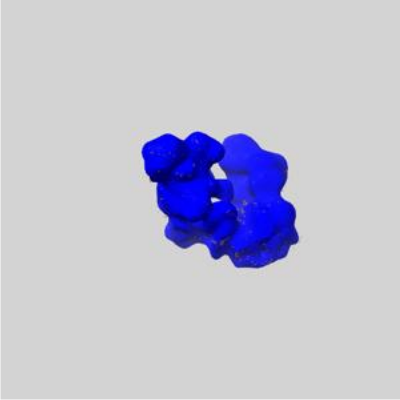
6.6.1 emd_4495_msk_1.map



X



Y

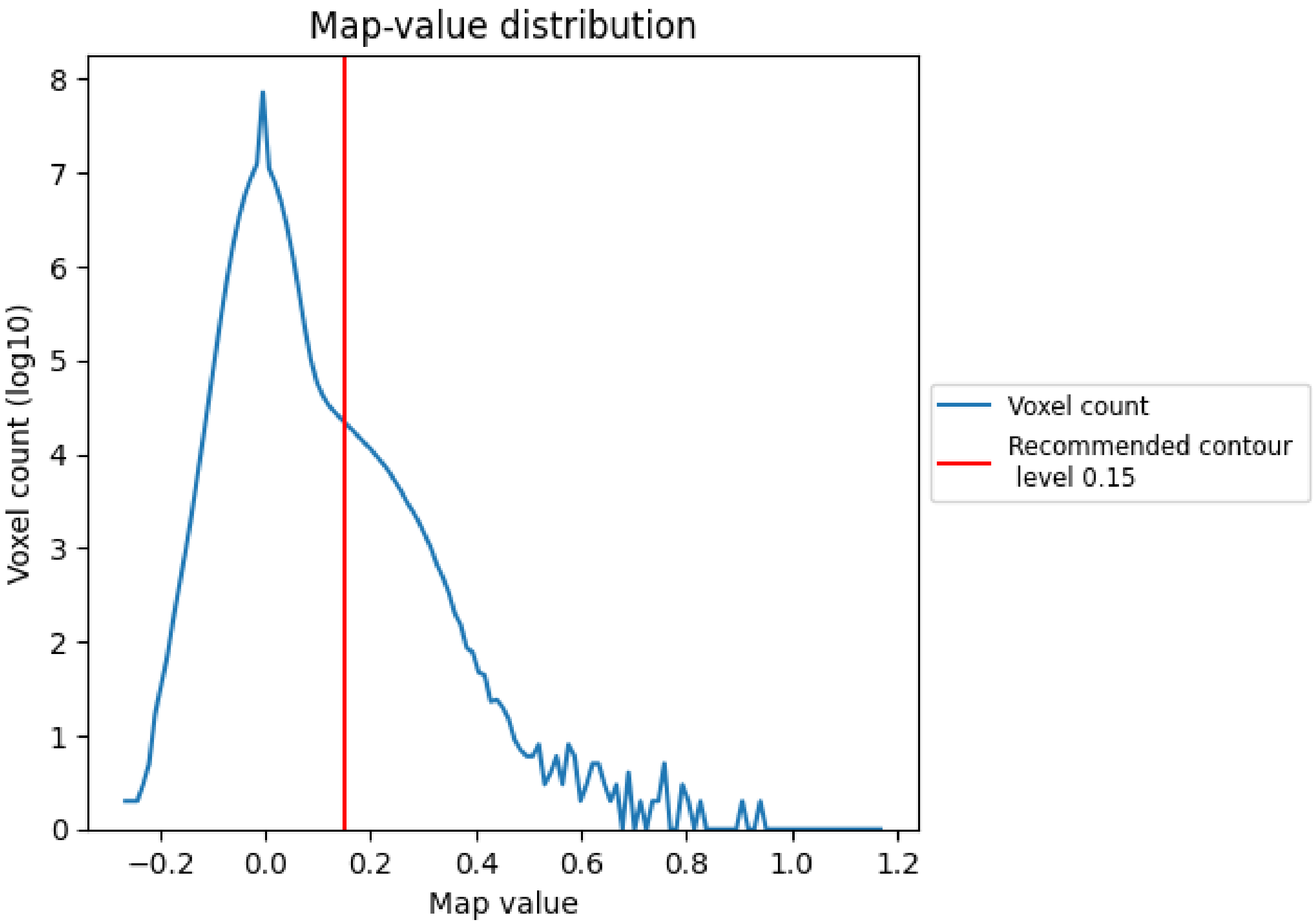


Z

7 Map analysis ⓘ

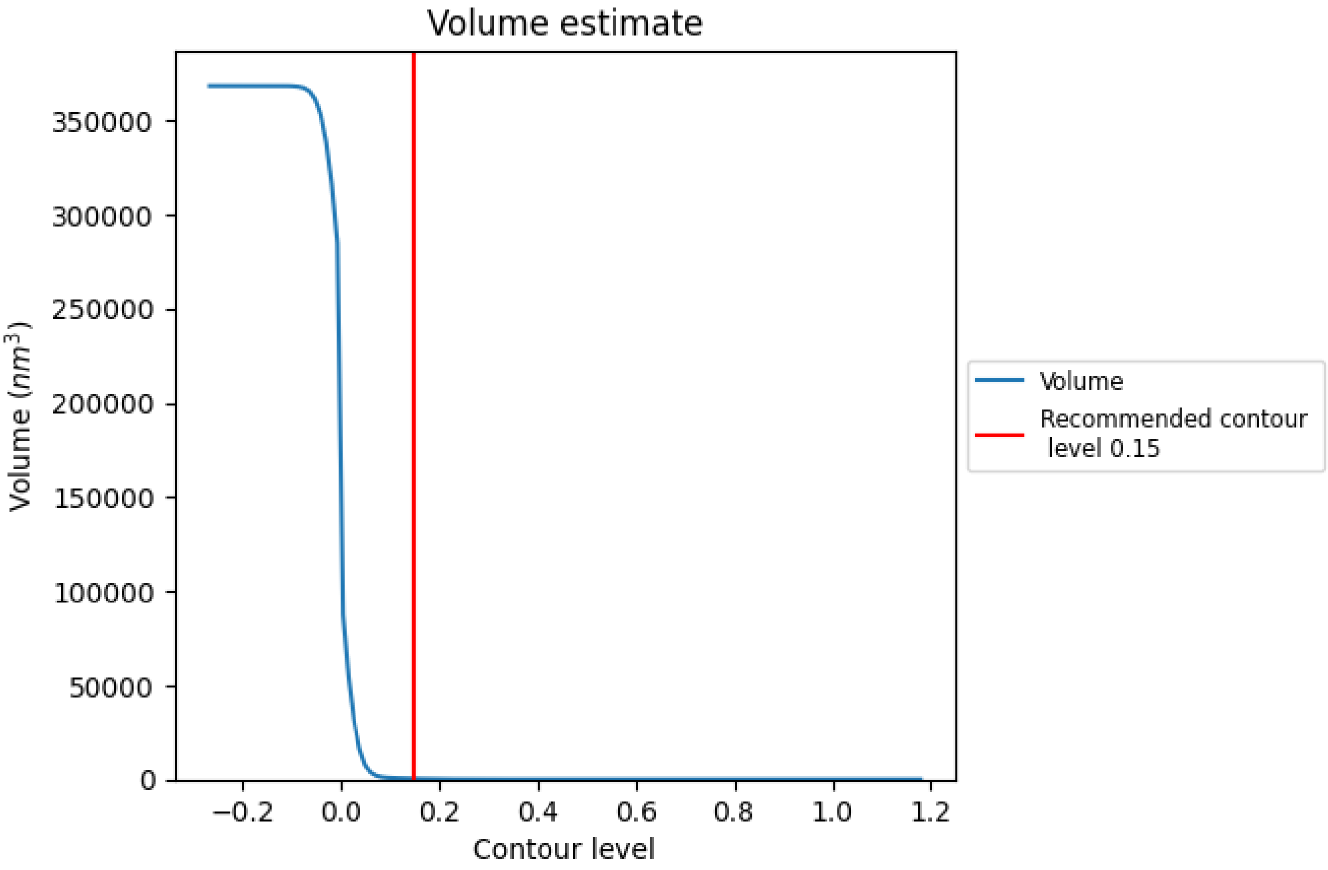
This section contains the results of statistical analysis of the map.

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.

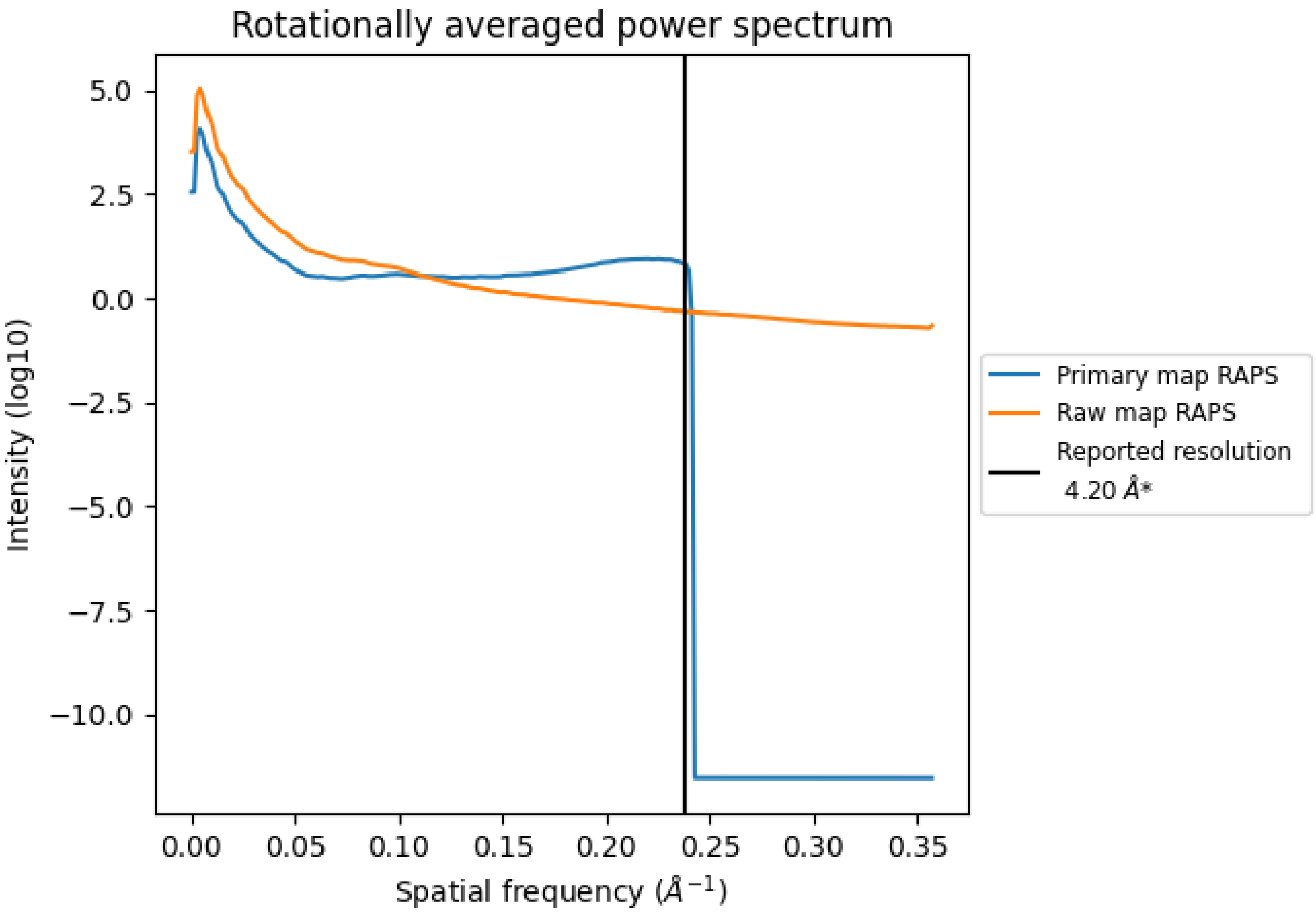
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 330 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 ⓘ

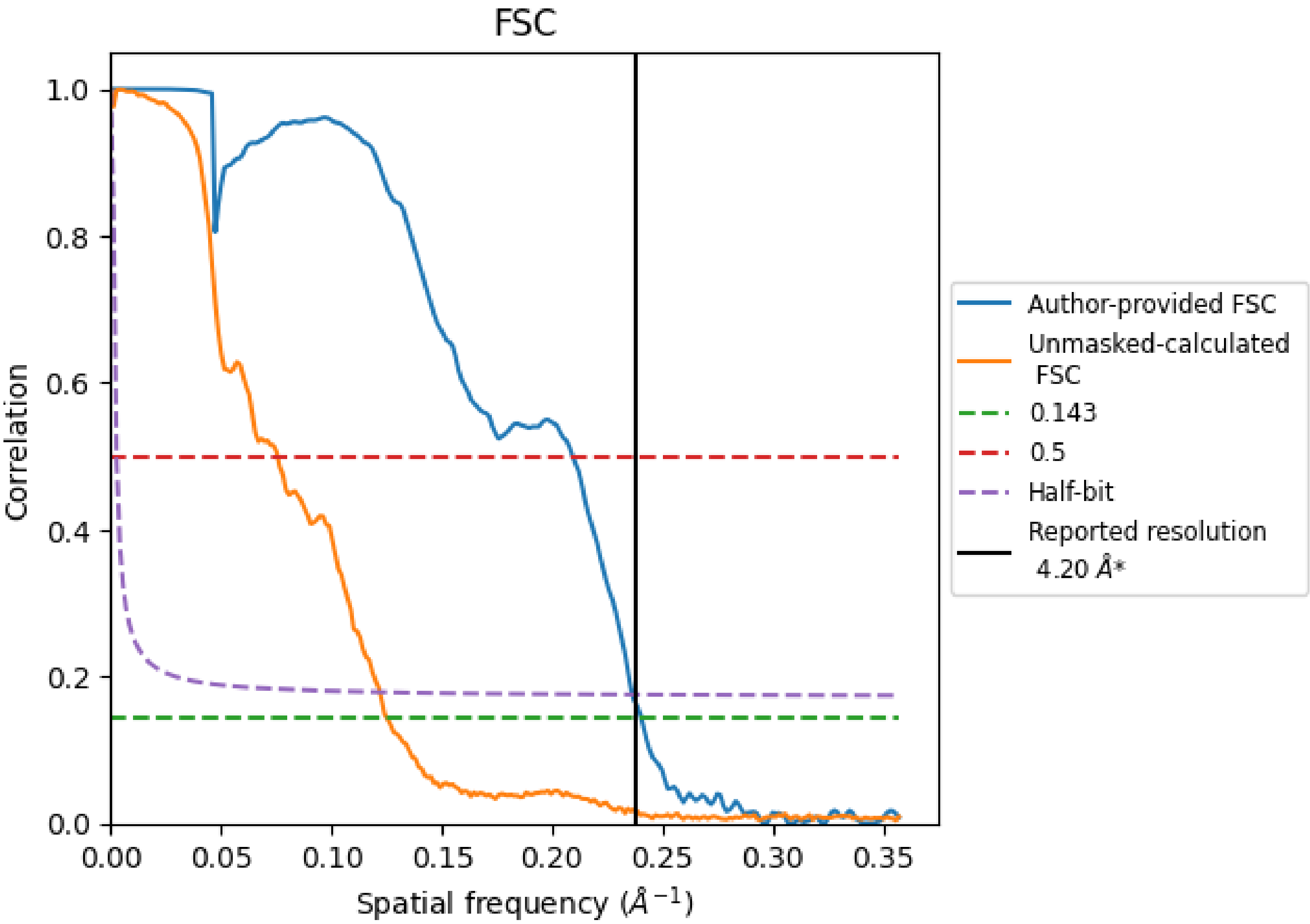


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

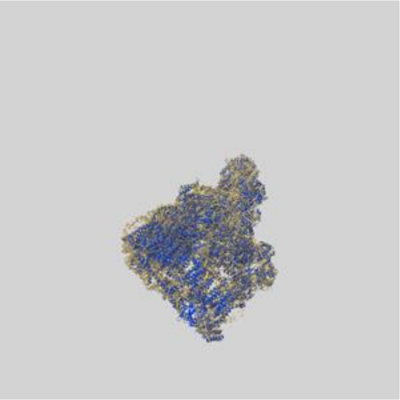
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	4.78	4.23
Unmasked-calculated*	7.99	13.21	8.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 4.2 by more than 10 %

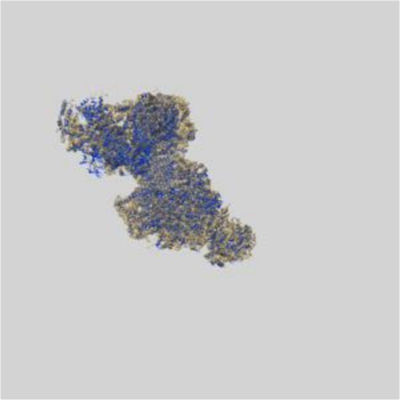
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4495 and PDB model 6QC3. Per-residue inclusion information can be found in section 3 on page 21.

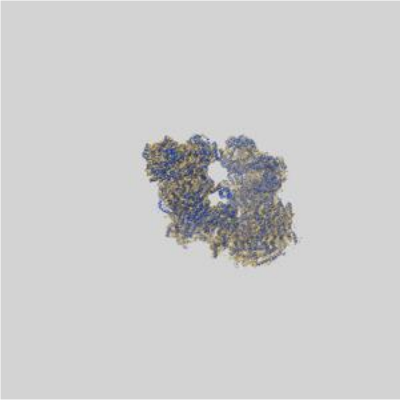
9.1 Map-model overlay



X



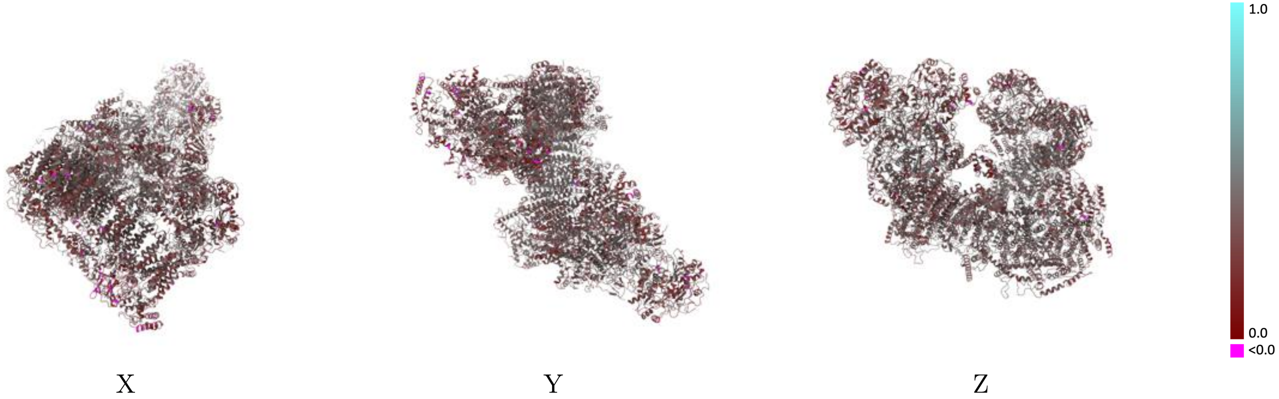
Y



Z

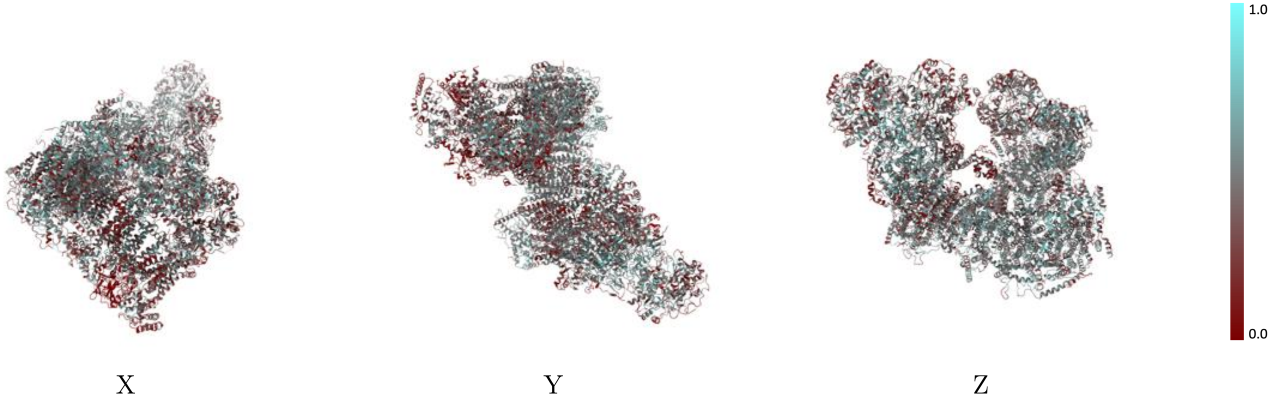
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



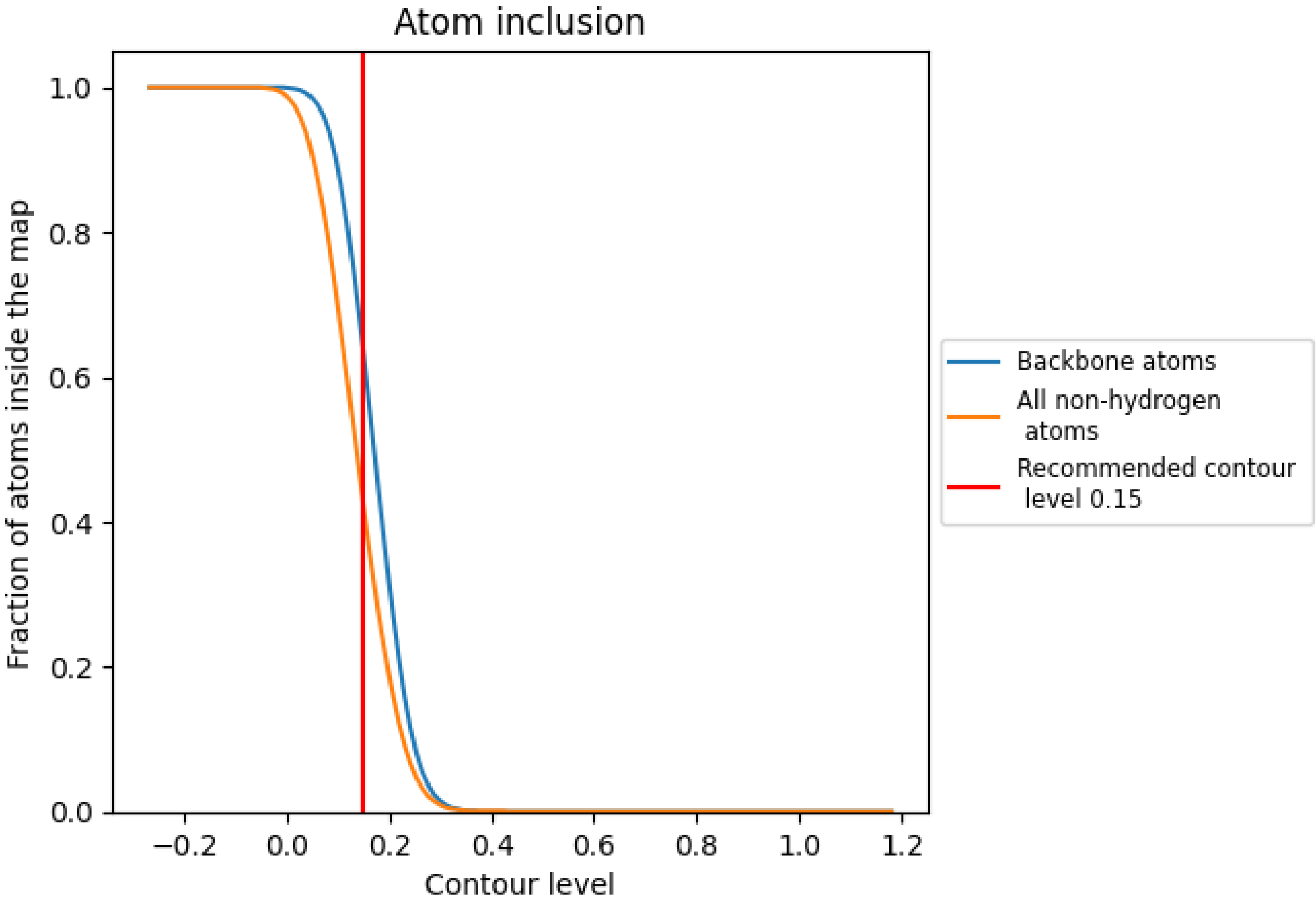
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 42% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4230	0.3540
4L	0.4160	0.3700
A1	0.4660	0.3710
A2	0.3140	0.2760
A3	0.4170	0.3490
A5	0.4010	0.3400
A6	0.3640	0.3520
A7	0.3320	0.3480
A8	0.4610	0.3420
A9	0.3330	0.3300
AA	0.1990	0.2840
AB	0.4620	0.3350
AJ	0.4950	0.3710
AK	0.4050	0.3780
AL	0.3000	0.3580
AM	0.4660	0.3500
B1	0.4060	0.3760
B2	0.4230	0.3280
B3	0.4400	0.3180
B4	0.4940	0.3850
B5	0.5330	0.3720
B6	0.4530	0.3460
B7	0.4400	0.3040
B8	0.5030	0.3840
B9	0.5660	0.3800
BJ	0.5100	0.3570
BK	0.4560	0.3700
C1	0.4580	0.3520
C2	0.4930	0.3920
D1	0.4210	0.3780
D2	0.4970	0.3980
D3	0.3680	0.3780
D4	0.4860	0.3970
D5	0.4420	0.3640
D6	0.3330	0.3560

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Chain	Atom inclusion	Q-score
S1	0.4170	0.3430
S2	0.4960	0.3800
S3	0.5020	0.3990
S4	0.4440	0.3890
S5	0.4780	0.3540
S6	0.4160	0.3720
S7	0.5130	0.3790
S8	0.5730	0.3970
V1	0.4180	0.3130
V2	0.3950	0.3090
V3	0.3420	0.3270
a1	0.3890	0.3280
a2	0.3650	0.3260
a3	0.5050	0.3810
a4	0.4610	0.3530
b1	0.3900	0.3570
b2	0.4720	0.3910
c1	0.3560	0.3280
c2	0.4320	0.3670
d1	0.4020	0.3300
d2	0.4360	0.3630
f1	0.0800	0.2870
f2	0.0910	0.2590
h1	0.2130	0.2530
h2	0.2900	0.2710
i1	0.2600	0.2770
i2	0.2410	0.2970
q1	0.3400	0.3290
q2	0.4310	0.3880
x1	0.2720	0.3730
x2	0.2770	0.4020