



wwPDB EM Validation Summary Report ⓘ

Jun 30, 2025 – 09:06 AM EDT

PDB ID : 9CE2 / pdb_00009ce2
EMDB ID : EMD-45490
Title : Respiratory supercomplex I+III₂+IV open state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-06-25
Resolution : 3.41 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

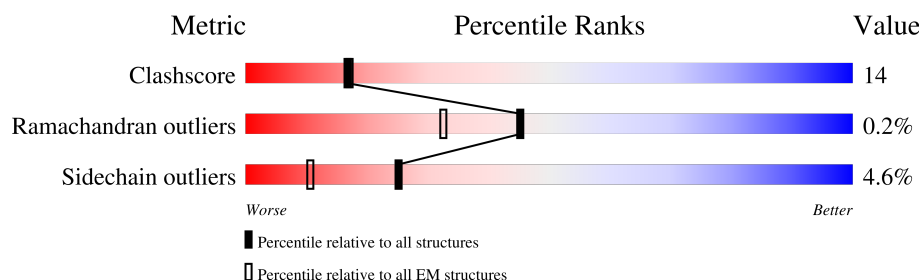
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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.














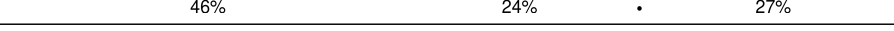



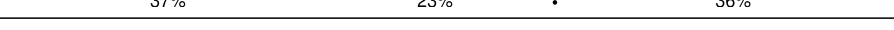
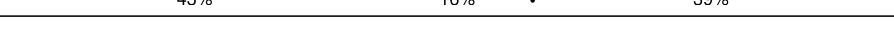


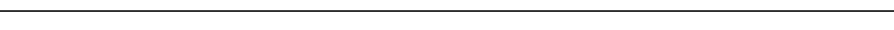

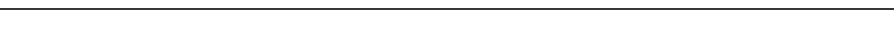
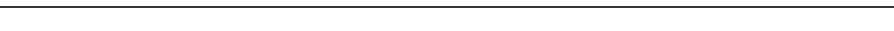


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	91	
1	Ab	91	
2	1	64	
2	Ac	64	
3	2	299	
3	4	299	
3	Ae	299	
3	Af	299	











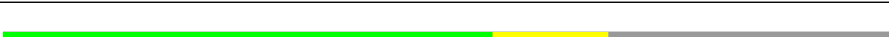


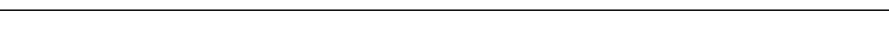
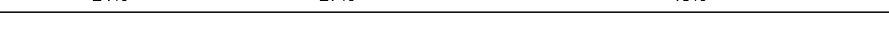
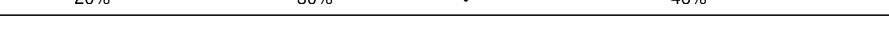



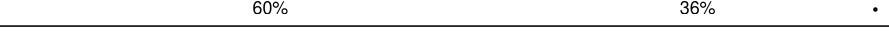
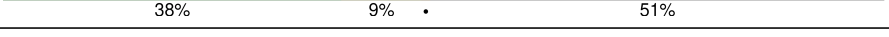




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Mol	Chain	Length	Quality of chain
4	3	56	
4	Ad	56	
5	6	453	
5	v	453	
6	7	379	
6	w	379	
7	8	326	
7	x	326	
8	9	111	
8	y	111	
9	A	75	
10	a	189	
11	b	128	
12	c	186	
13	d	176	
14	e	154	
15	f	76	
16	g	122	
17	h	106	
18	i	347	
19	j	115	
20	k	98	
21	m	175	
22	n	58	
23	o	129	


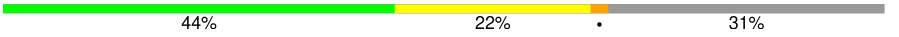





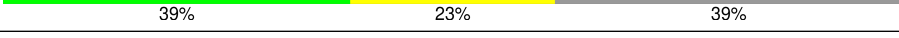

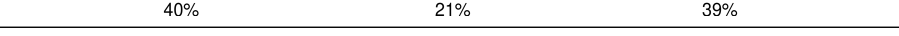

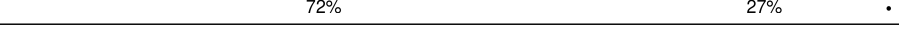

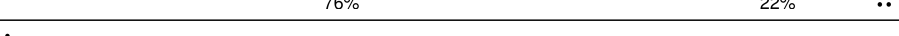


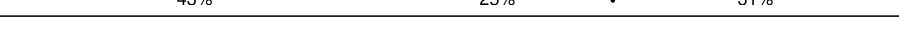

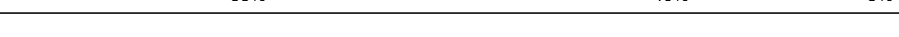



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Mol	Chain	Length	Quality of chain
24	p	221	
25	q	459	
26	r	318	
27	B	464	
28	C	469	
29	D	264	
30	E	249	
31	F	123	
32	H	212	
33	I	263	
34	J	175	
35	K	145	
36	N	116	
37	O	156	
37	X	156	
38	P	99	
39	Q	154	
40	R	110	
41	S	70	
42	T	169	
43	U	357	
44	V	141	
45	W	144	
46	Y	105	
47	Z	114	

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Mol	Chain	Length	Quality of chain
48	l	606	
49	s	249	
50	t	137	
51	5	480	
51	u	480	
52	Aa	82	
52	z	82	
53	Ag	70	
54	Ah	80	
55	Ai	80	
56	Aj	63	
57	Ak	514	
58	Al	228	
59	Am	261	
60	An	169	
61	Ao	152	
62	Ap	129	
63	Aq	97	
64	Ar	86	
65	G	727	
66	L	372	
67	M	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
68	FES	2	301	-	-	X	-
68	FES	G	803	-	-	X	-
72	SF4	B	502	-	-	X	-
72	SF4	G	802	-	-	X	-
72	SF4	H	301	-	-	X	-
72	SF4	H	302	-	-	X	-
72	SF4	I	201	-	-	X	-

2 Entry composition

There are 75 unique types of molecules in this entry. The entry contains 111989 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 Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			561	341	101	114	5		
1	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	60	Total	C	N	O	0	0
			493	322	87	84		
2	Ac	59	Total	C	N	O	0	0
			485	318	85	82		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	195	Total	C	N	O	S	0	0
			1513	953	264	289	7		
3	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
3	Ae	39	Total	C	N	O	S	0	0
			275	172	53	47	3		
3	Af	33	Total	C	N	O	S	0	0
			223	141	39	41	2		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		
4	Ad	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
5	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 6 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
6	w	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 7 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	239	Total	C	N	O	S	0	0
			1906	1217	328	345	16		
7	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
8	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	63	Total	C	N	O	S	0	0
			510	335	88	85	2		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	105	Total	C	N	O	S	0	0
			871	570	155	145	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	152	Total	C	N	O	S	0	0
			1278	829	205	236	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	169	Total	C	N	O	S	0	0
			1420	892	256	264	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	99	Total	C	N	O	S	0	0
			822	527	136	155	4		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	f	46	Total	C	N	O	0	0
			385	256	64	65		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	347	Total	C	N	O	S	0	0
			2711	1782	420	463	46		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	91	Total	C	N	O	S	0	0
			721	492	106	120	3		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	161	Total	C	N	O	S	0	0
			1227	826	174	216	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	53	Total	C	N	O	S	0	0
			452	293	83	75	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	q	459	Total	C	N	O	S	0	0
			3630	2410	572	609	39		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	r	308	Total	C	N	O	S	0	0
			2435	1633	375	406	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	430	Total	C	N	O	S	0	0
			3458	2210	594	630	24		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	208	Total	C	N	O	S	0	0
			1732	1121	297	312	2		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	95	Total	C	N	O	S	0	0
			738	450	139	146	3		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	118	Total	C	N	O	S	0	0
			962	608	173	178	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	144	Total	C	N	O	S	0	0
			1203	769	217	212	5		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 37 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
37	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	83	Total	C	N	O	S	0	0
			669	419	125	123	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	112	Total	C	N	O	S	0	0
			954	610	176	163	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	82	Total	C	N	O	S	0	0
			638	414	109	114	1		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	318	Total	C	N	O	S	0	0
			2562	1630	435	487	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	W	140	Total	C	N	O	S	0	0
			1162	749	201	203	9		

- Molecule 46 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	60	Total	C	N	O	S	0	0
			524	347	87	89	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	78	Total	C	N	O	S	0	0
			626	410	105	110	1		

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	602	Total	C	N	O	S	0	0
			4773	3166	739	818	50		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	119	Total	C	N	O	S	0	0
			970	609	177	175	9		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
51	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
52	Aa	78	Total	C	N	O	S	0	0
			662	432	121	107	2		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Ag	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ah	56	Total	C	N	O	S	0	0
			437	281	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ai	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Aj	46	Total	C	N	O	S	0	0
			377	251	63	61	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ak	513	Total	C	N	O	S	0	0
			4002	2680	617	673	32		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Al	222	Total	C	N	O	S	0	0
			1785	1166	275	327	17		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Am	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	An	138	Total	C	N	O	S	0	0
			1154	752	189	209	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ao	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ap	89	Total	C	N	O	S	0	0
			689	429	121	133	6		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aq	73	Total	C	N	O	S	0	0
			606	392	116	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ar	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

- Molecule 65 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	G	684	Total	C	N	O	S	0	0
			5260	3298	917	1006	39		

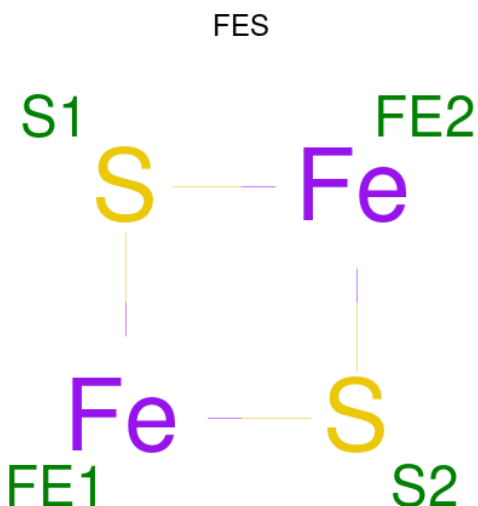
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	L	314	Total	C	N	O	S	0	0
			2493	1605	437	442	9		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

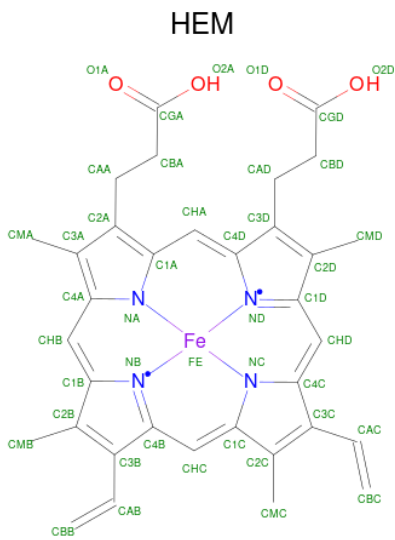
Mol	Chain	Residues	Atoms					AltConf	Trace
67	M	96	Total	C	N	O	S	0	0
			769	485	146	135	3		

- Molecule 68 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



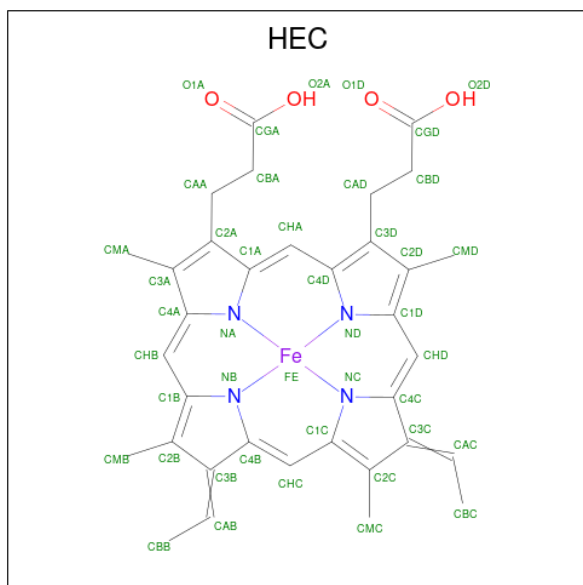
Mol	Chain	Residues	Atoms			AltConf
68	2	1	Total 4	Fe 2	S 2	0
68	4	1	Total 4	Fe 2	S 2	0
68	E	1	Total 4	Fe 2	S 2	0
68	G	1	Total 4	Fe 2	S 2	0

- Molecule 69 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



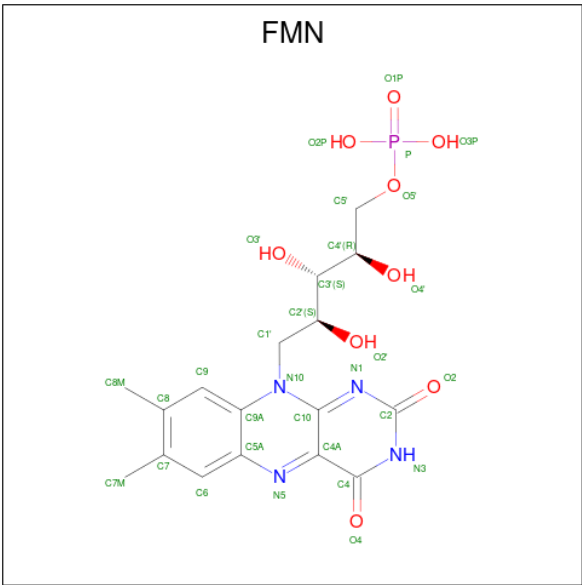
Mol	Chain	Residues	Atoms					AltConf
69	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



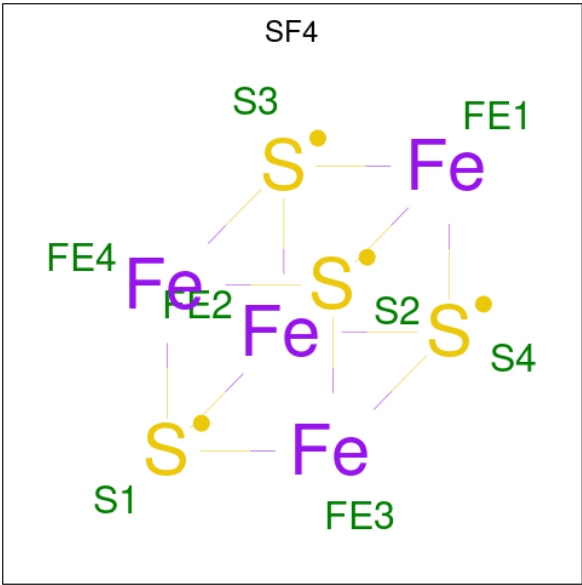
Mol	Chain	Residues	Atoms					AltConf
70	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 72 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



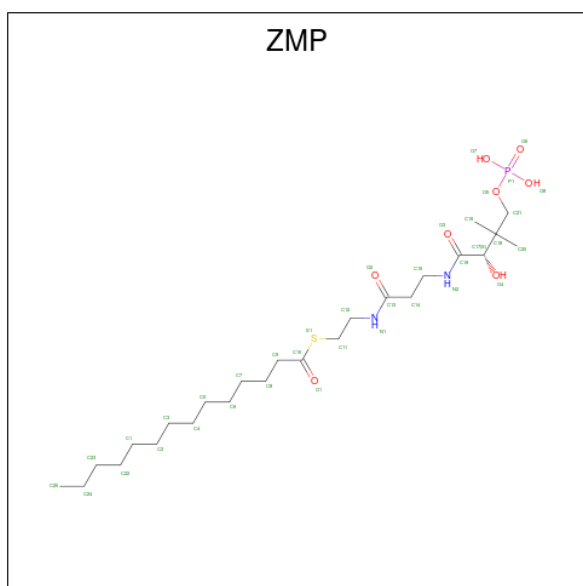
Mol	Chain	Residues	Atoms			AltConf
72	B	1	Total	Fe	S	0
			8	4	4	
72	H	1	Total	Fe	S	0
			8	4	4	
72	H	1	Total	Fe	S	0
			8	4	4	

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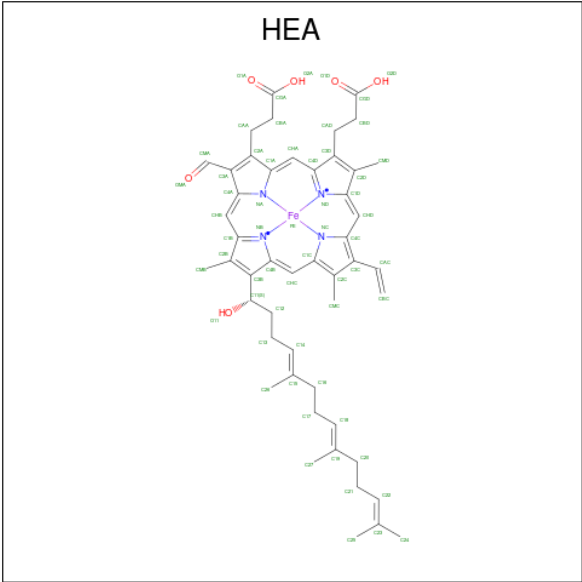
Mol	Chain	Residues	Atoms			AltConf
72	I	1	Total	Fe	S	0
			8	4	4	
72	G	1	Total	Fe	S	0
			8	4	4	
72	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 73 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl} amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



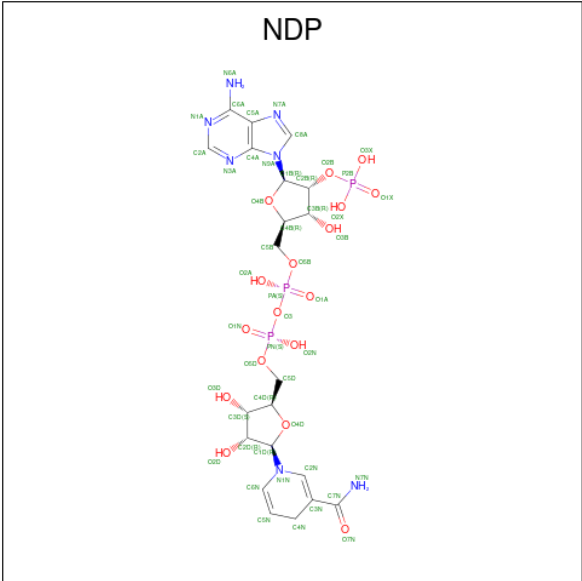
Mol	Chain	Residues	Atoms						AltConf
73	Q	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

- Molecule 74 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
74	Ak	1	Total 60	C 49	Fe 1	N 4	O 6	0
74	Ak	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 75 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

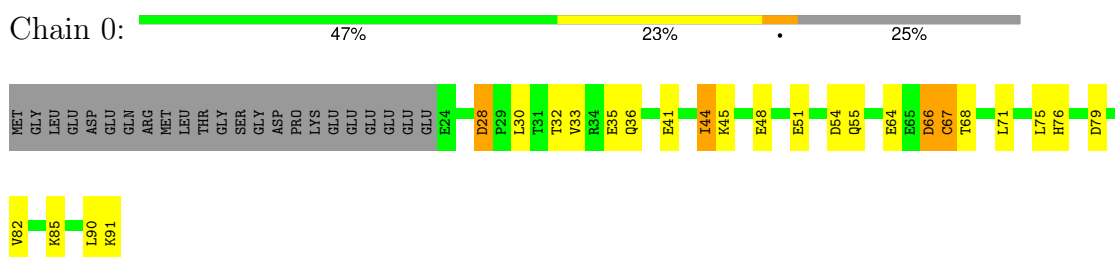


Mol	Chain	Residues	Atoms					AltConf
75	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

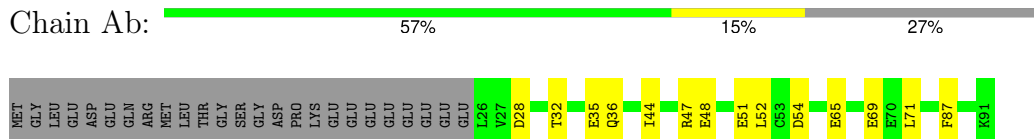
3 Residue-property plots

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.

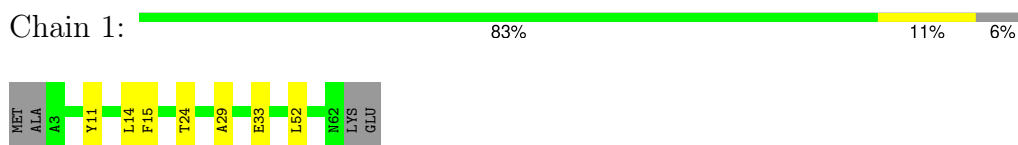
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



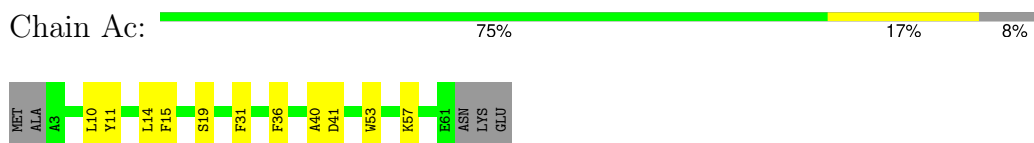
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



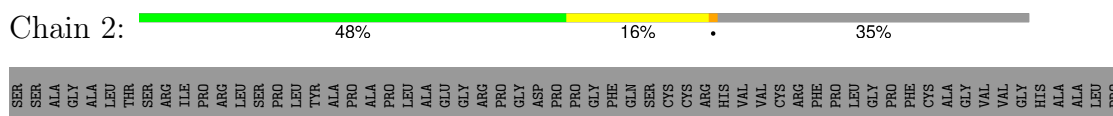
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

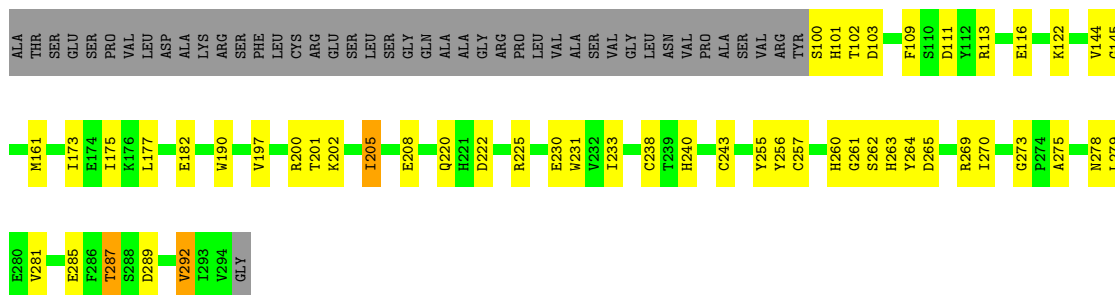


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

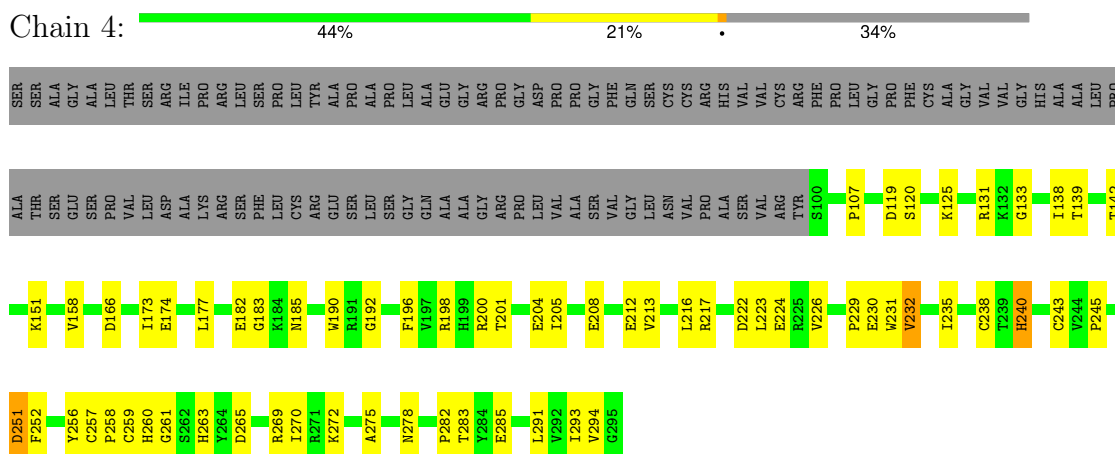


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

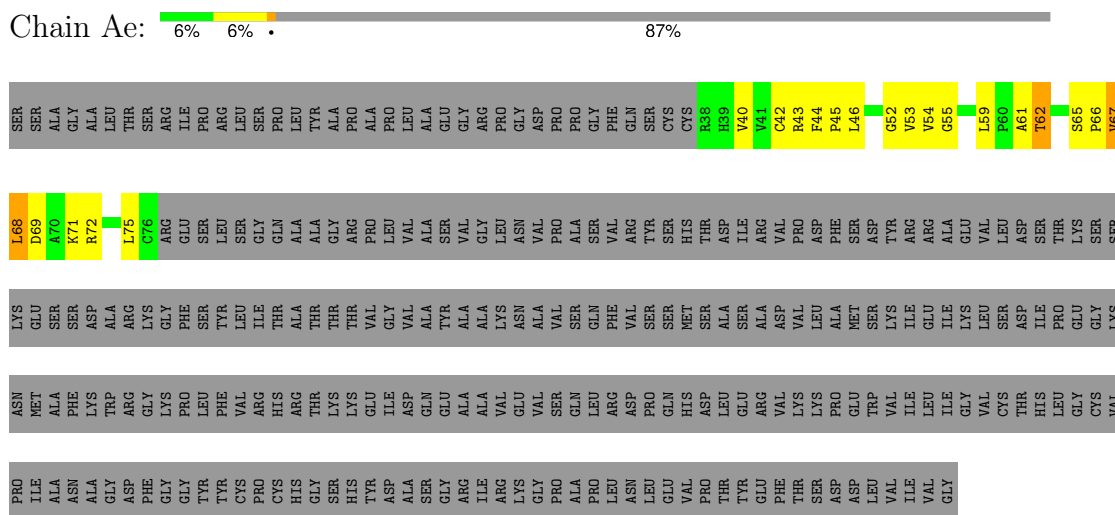




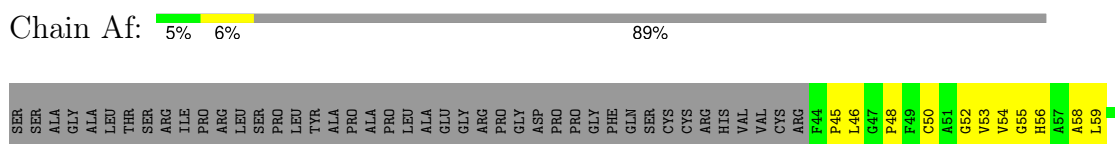
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

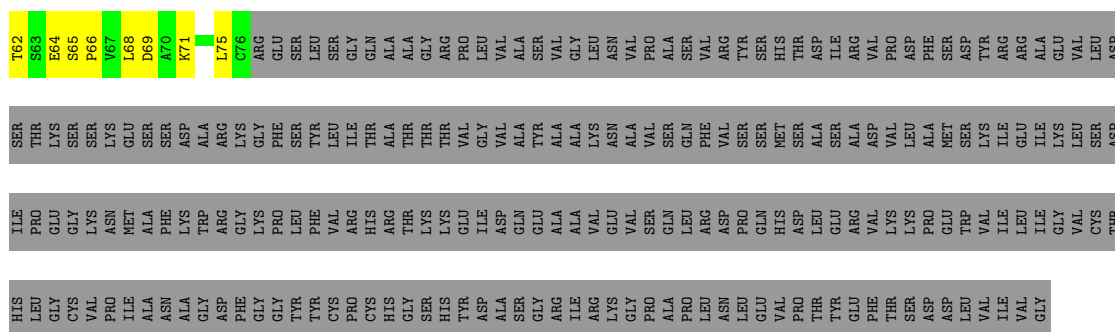


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

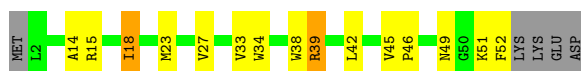


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1





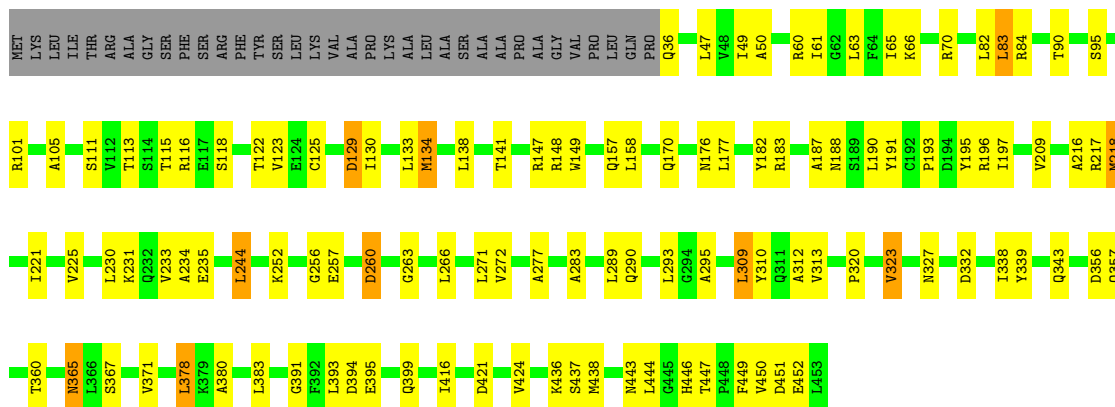
- Molecule 4: Cytochrome b-c1 complex subunit 10



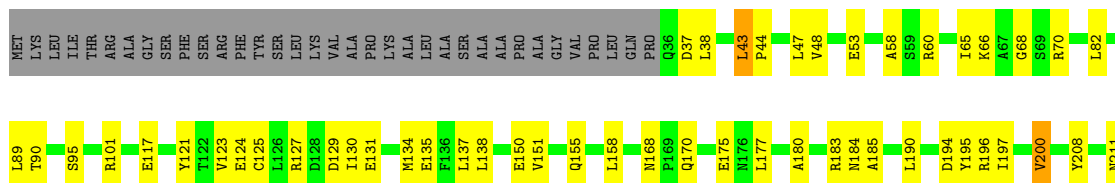
- Molecule 4: Cytochrome b-c1 complex subunit 10



- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

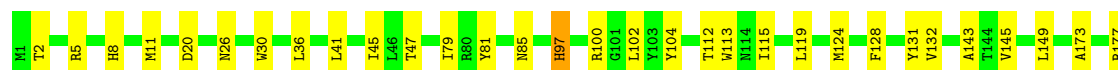
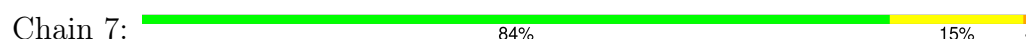


- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

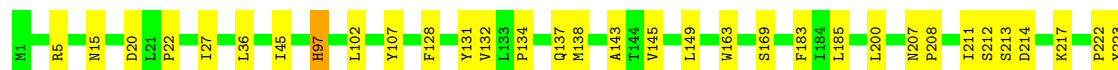
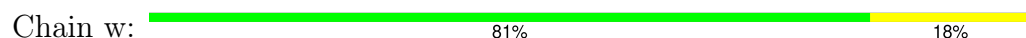




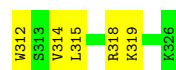
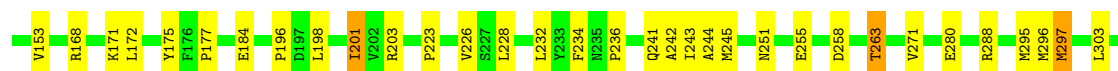
- Molecule 6: Cytochrome b



- Molecule 6: Cytochrome b

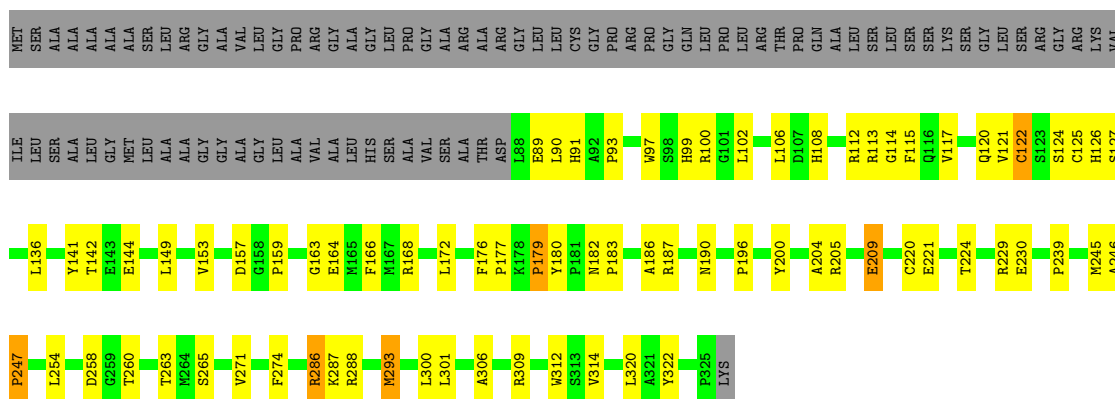


- Molecule 7: Cytochrome c1

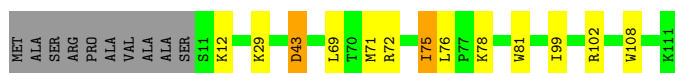
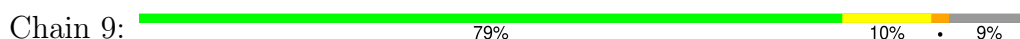


- Molecule 7: Cytochrome c1

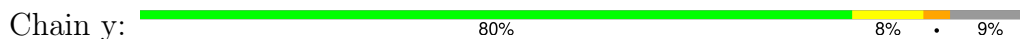




- Molecule 8: Cytochrome b-c1 complex subunit 7



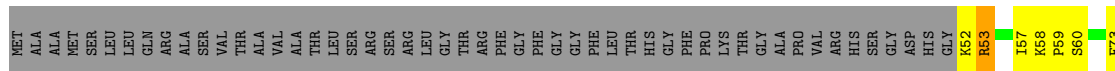
- Molecule 8: Cytochrome b-c1 complex subunit 7



- Molecule 9: Cytochrome c oxidase subunit 6C

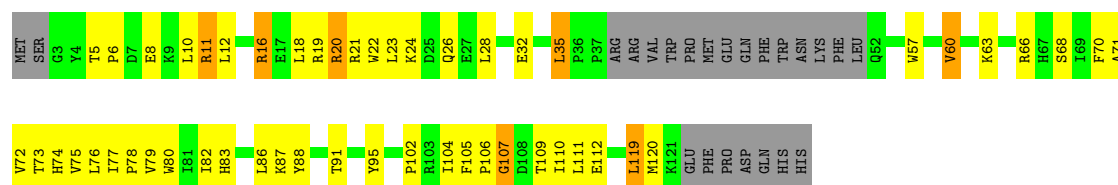


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



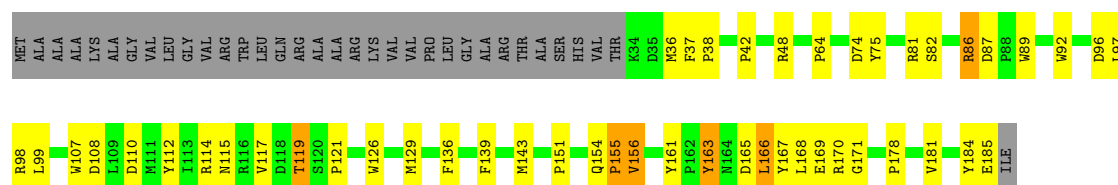
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 



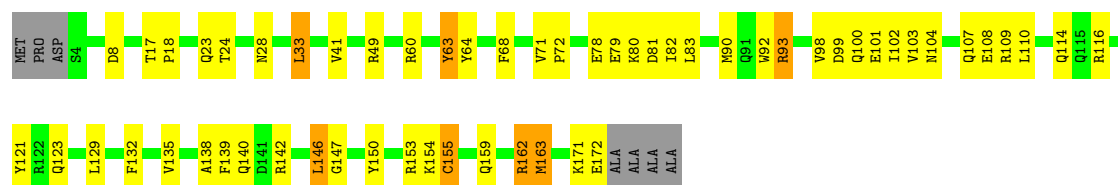
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



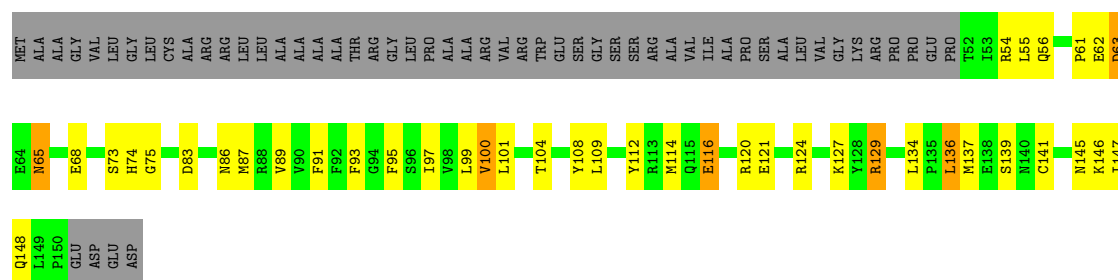
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



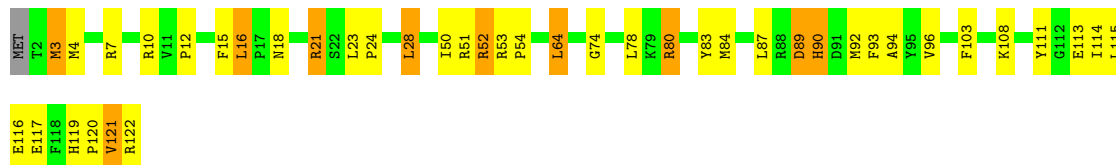
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



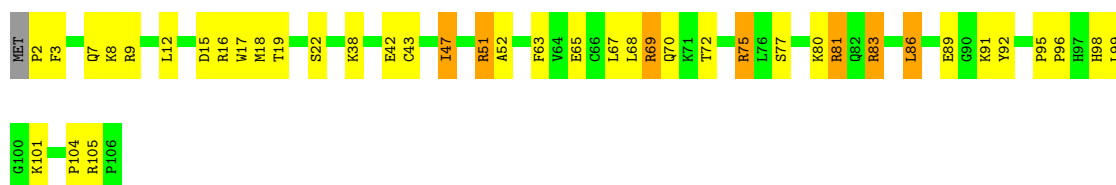
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



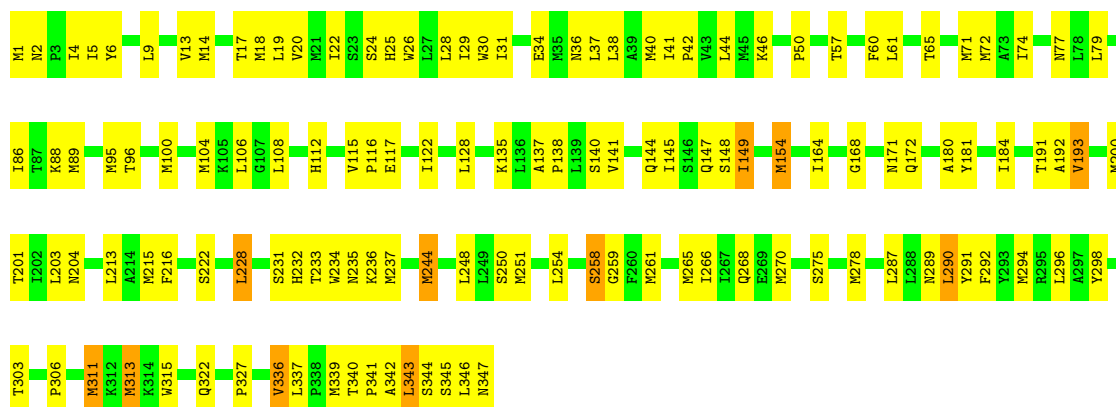
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



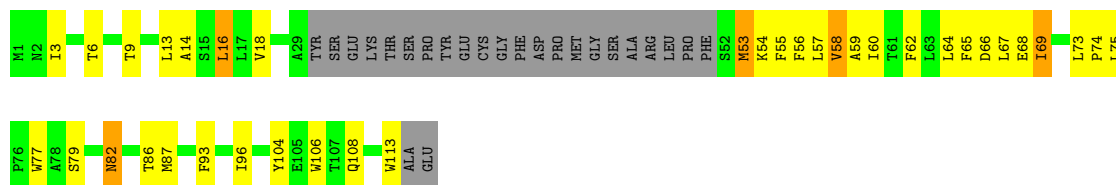
- Molecule 18: NADH-ubiquinone oxidoreductase chain 2

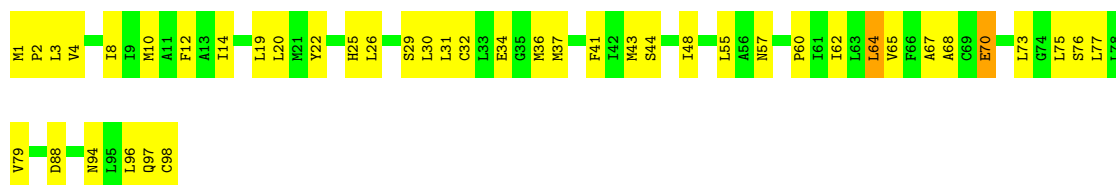
Chain i: 



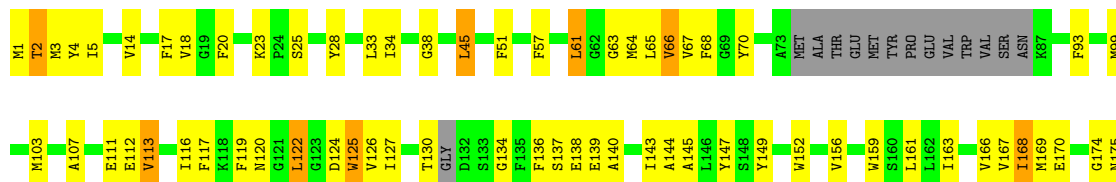
- Molecule 19: NADH-ubiquinone oxidoreductase chain 3

Chain j: 





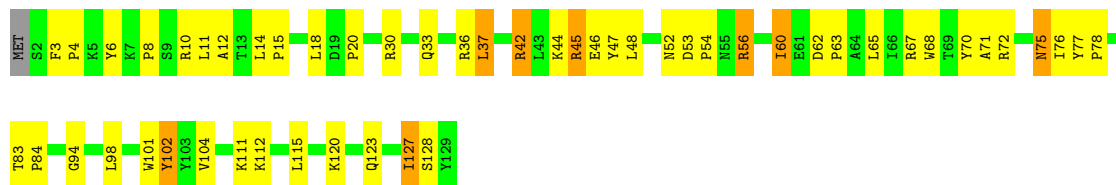
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6



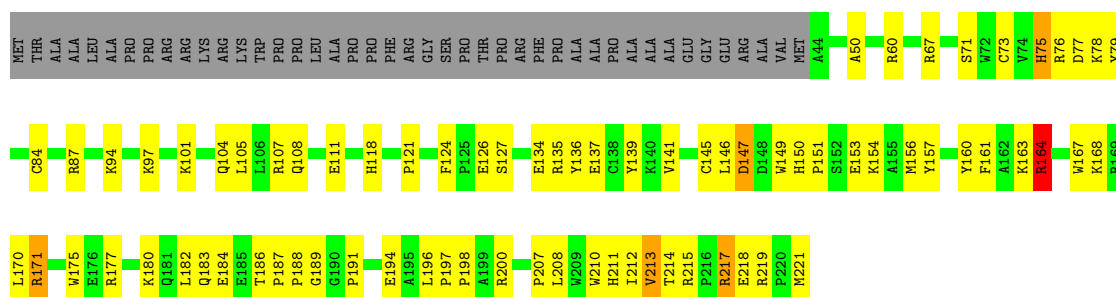
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

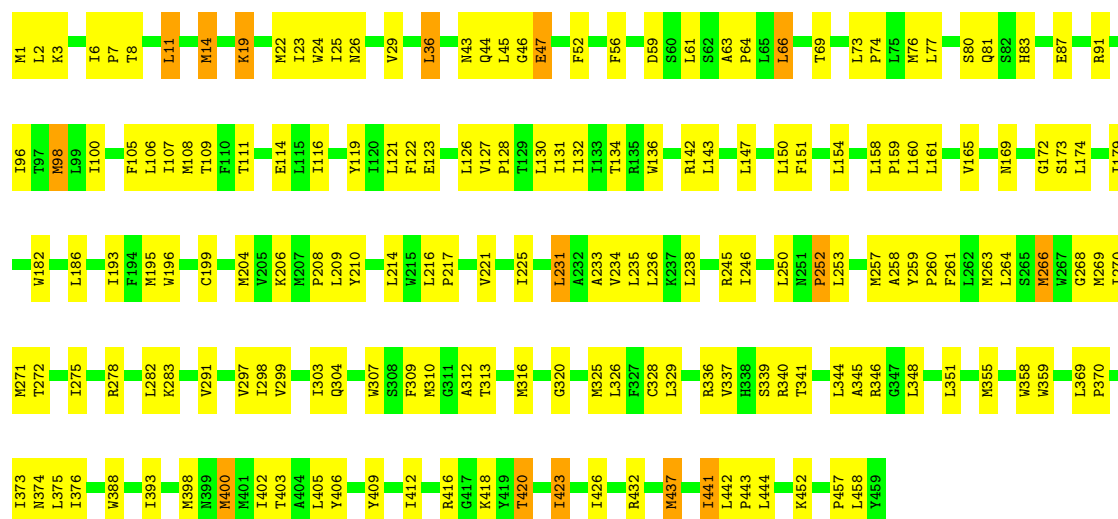


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



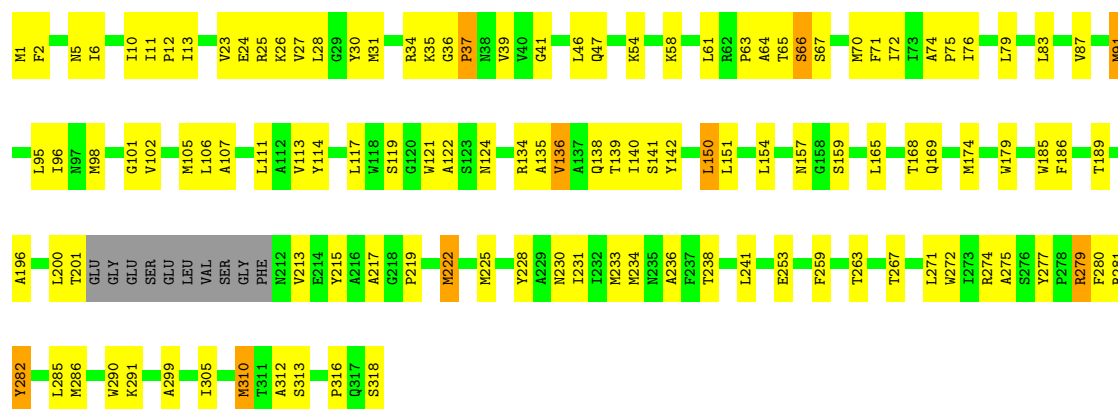
• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain q:  61% 36%



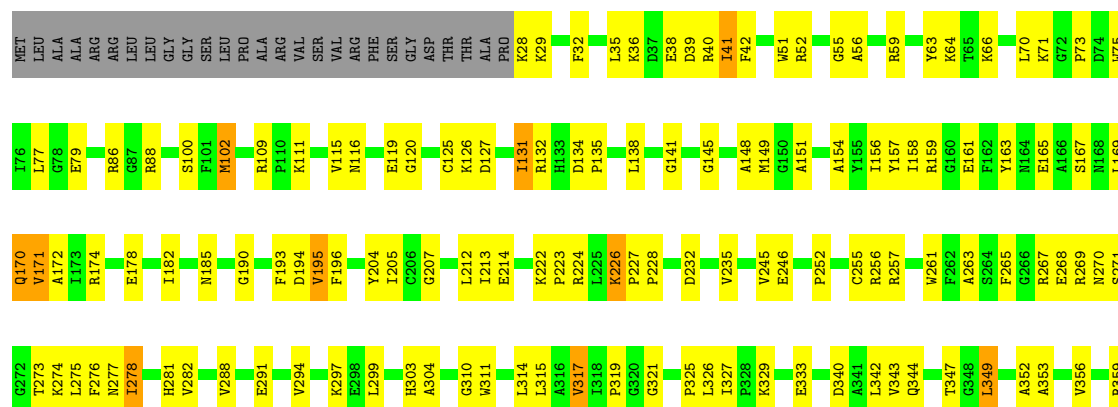
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain r:  59% 35%



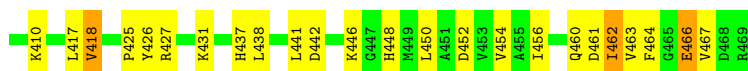
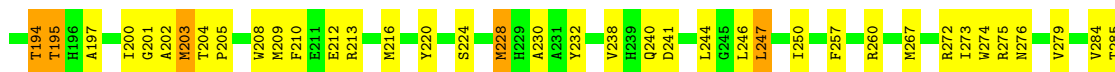
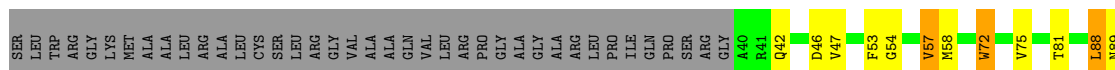
• Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:  58% 32% 7%

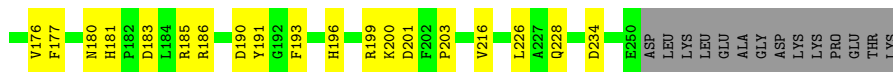
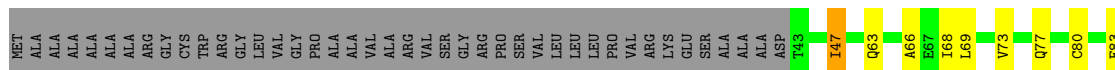




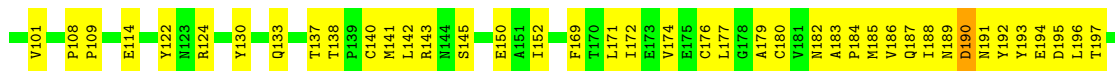
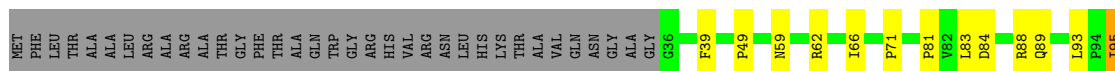
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

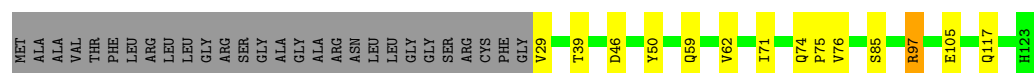


- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



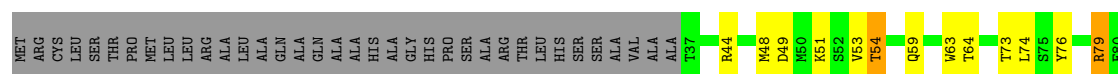
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 




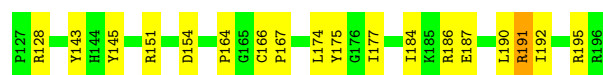
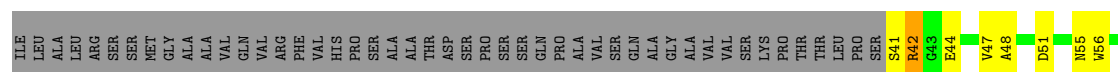
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain H: 



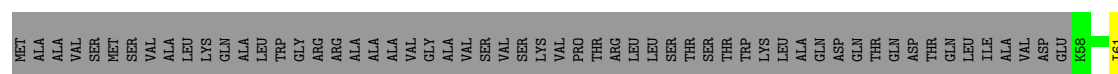
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain I: 




- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain J: 



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain K: 



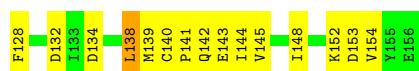
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain N: 72% 24% . .



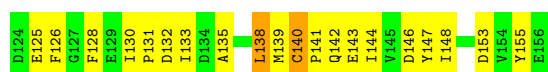
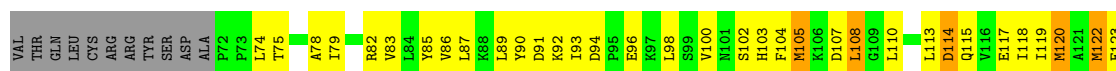
- Molecule 37: Acyl carrier protein

Chain O: 24% 27% . 46%



- Molecule 37: Acyl carrier protein

Chain X: 20% 30% . 46%



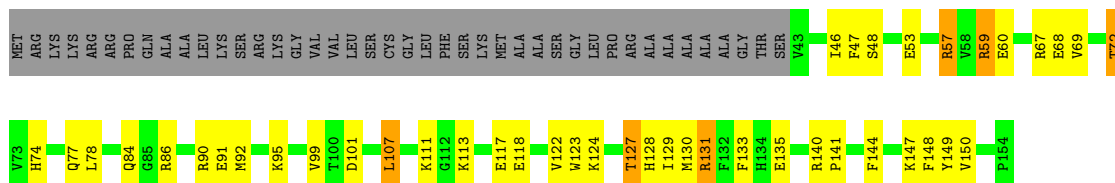
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 56% 28% 16%



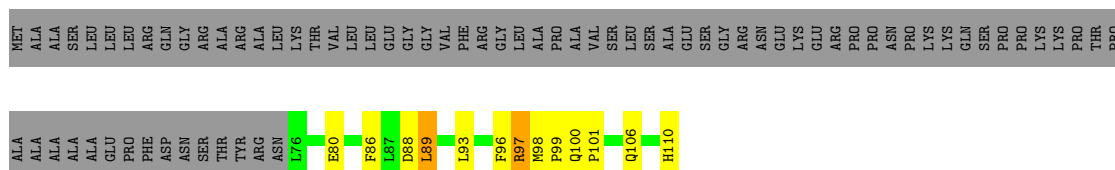
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 44% 25% . 27%



- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R: 20% 10% 68%



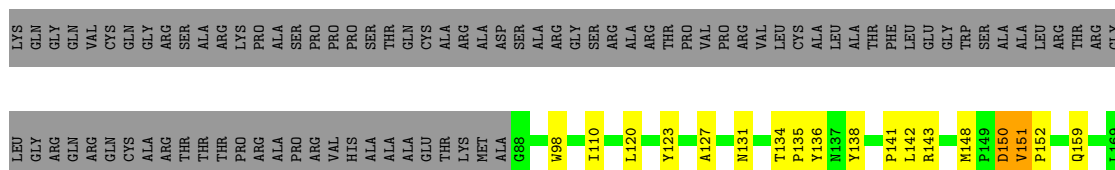
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 60% 36%



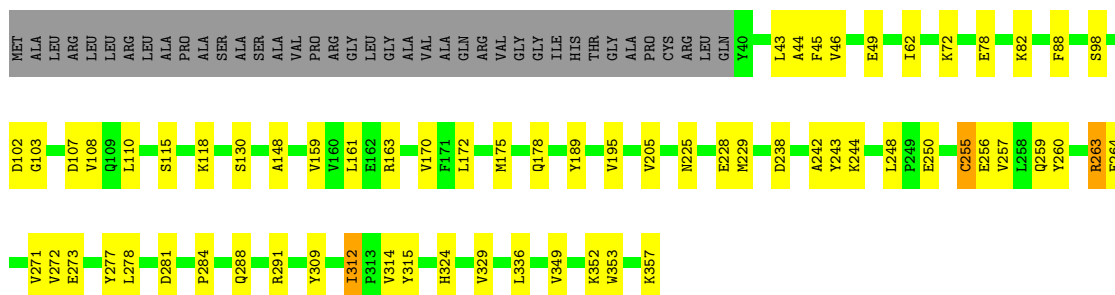
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T: 38% 9% 51%



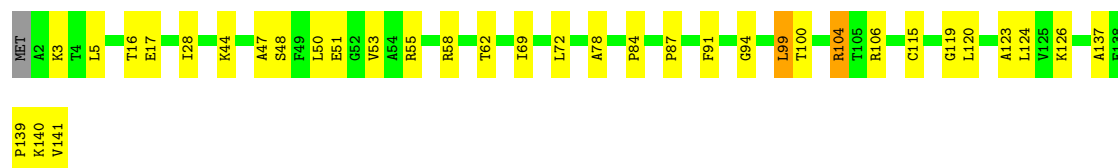
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U: 71% 18% 11%



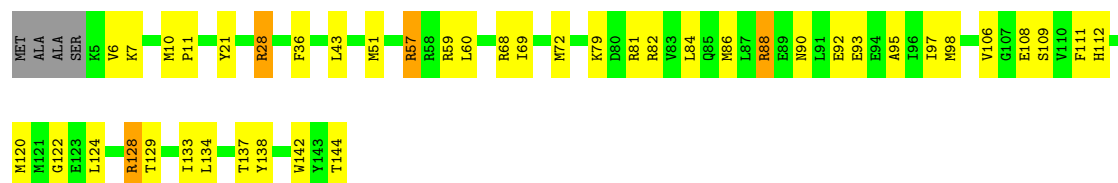
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 74% 23%



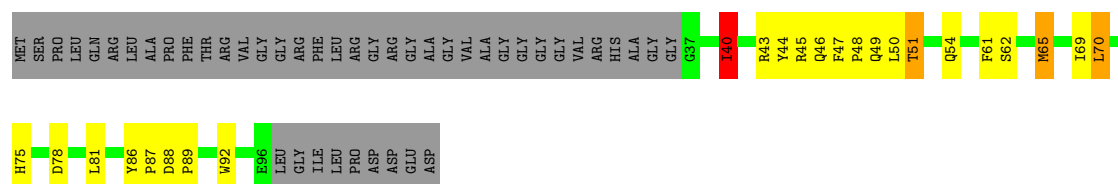
- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

Chain W: 67% 27%



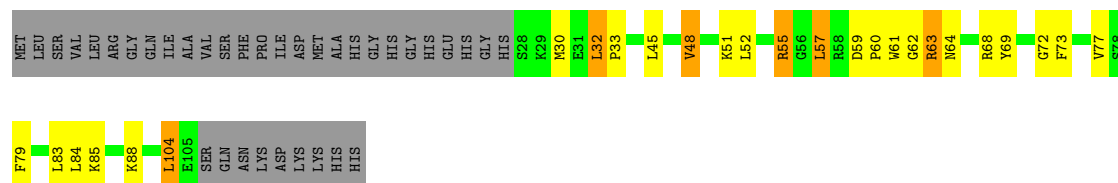
- Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 34% 19% 43%



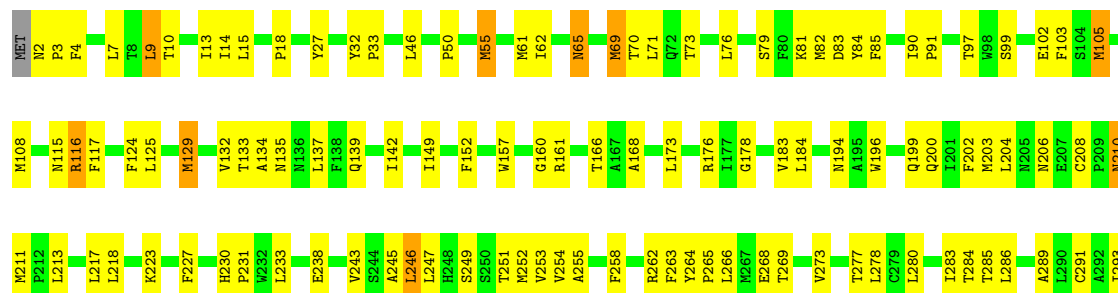
- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

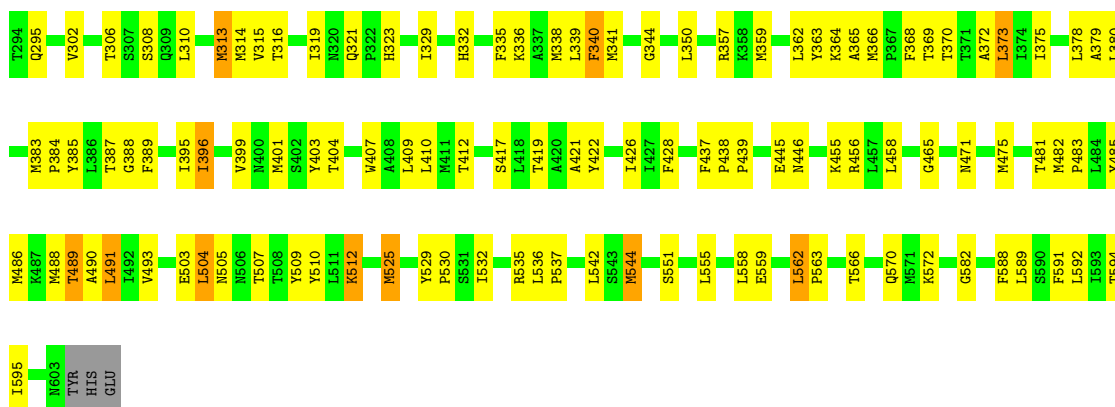
Chain Z: 46% 18% 5% 32%



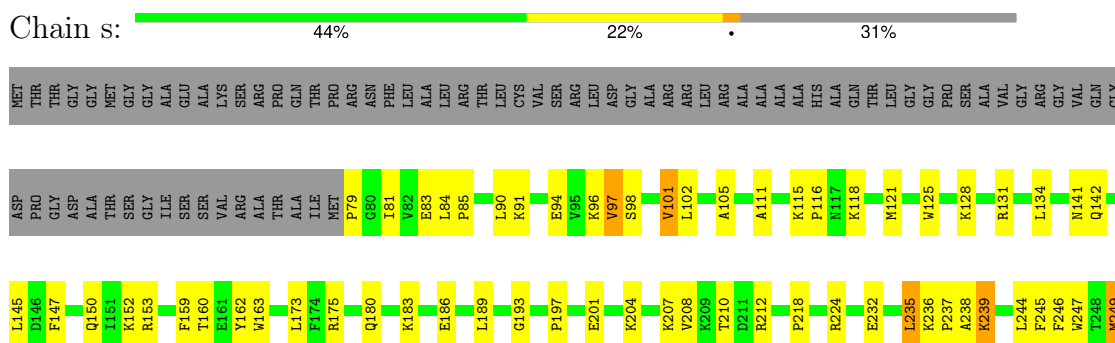
- Molecule 48: NADH-ubiquinone oxidoreductase chain 5

Chain I: 62% 34%

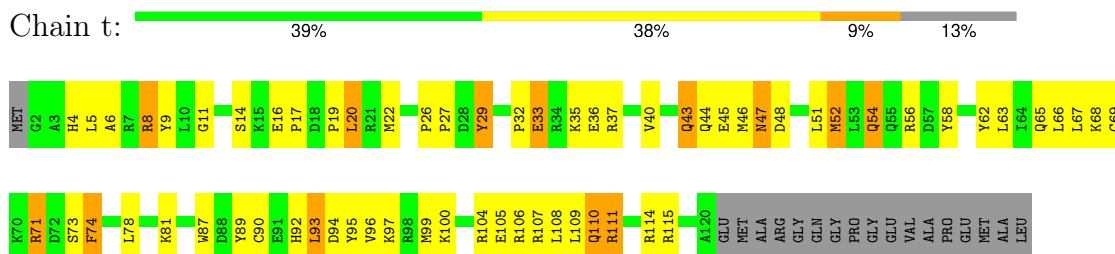




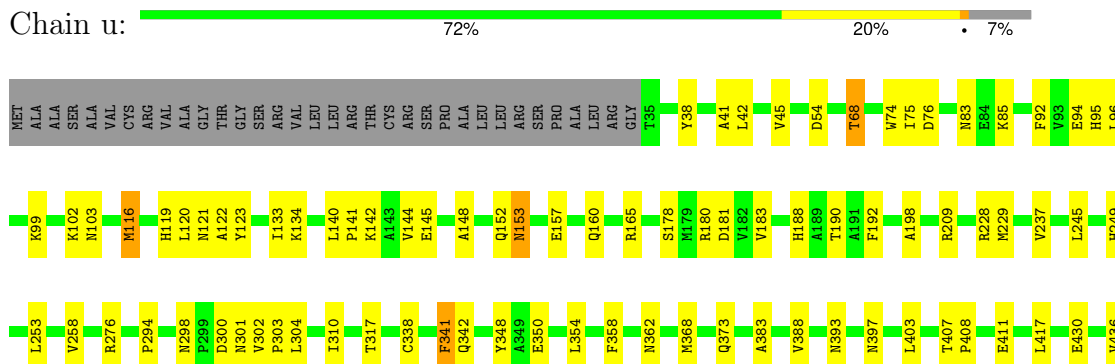
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



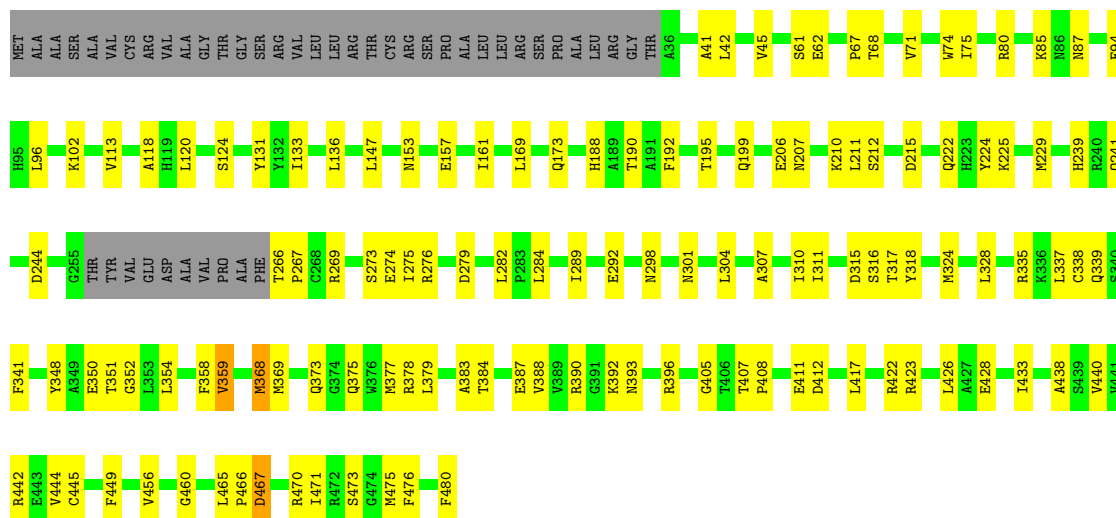
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial





- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 5: 64% 26% 9%



- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain z: 62% 29% 5%



- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain Aa: 74% 18% 5%



- Molecule 53: Cytochrome c oxidase subunit 8

Chain Ag: 39% 23% 39%



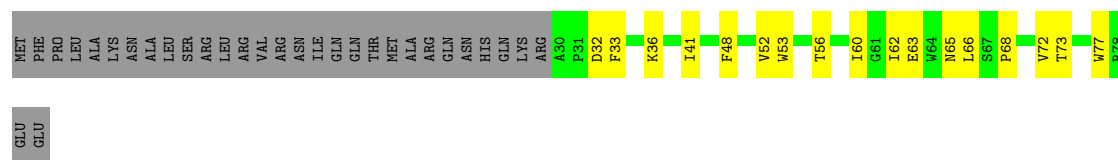
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain Ah: 50% 18% 30%



- Molecule 55: Cytochrome c oxidase subunit 7B

Chain Ai: 



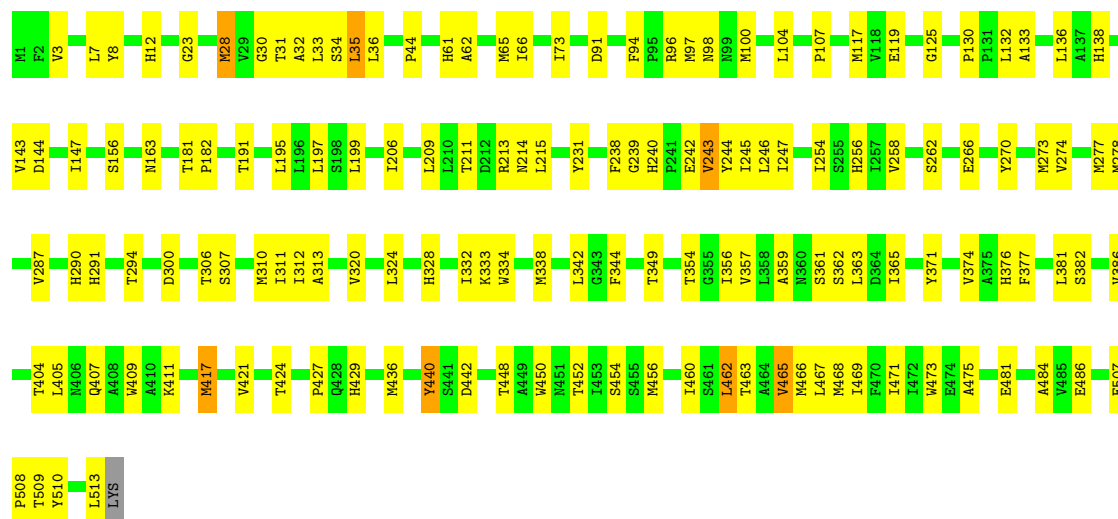
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Aj: 



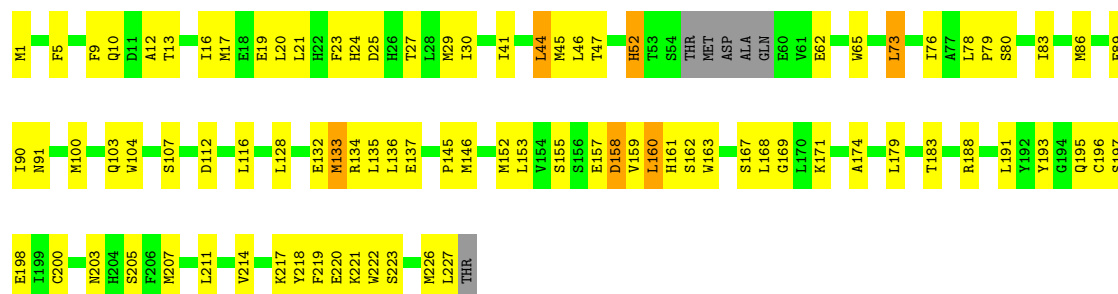
- Molecule 57: Cytochrome c oxidase subunit 1

Chain Ak: 

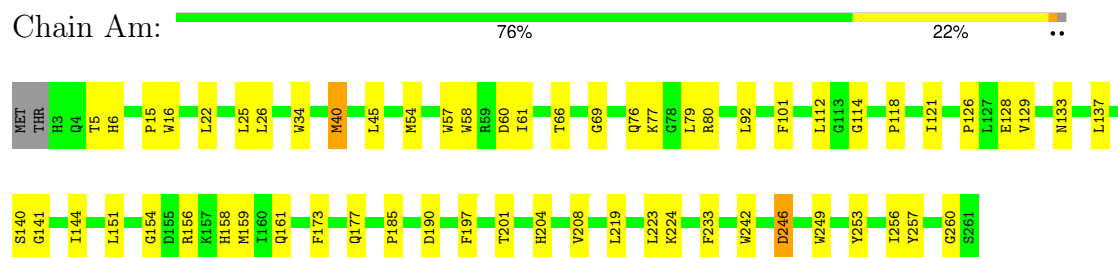


- Molecule 58: Cytochrome c oxidase subunit 2

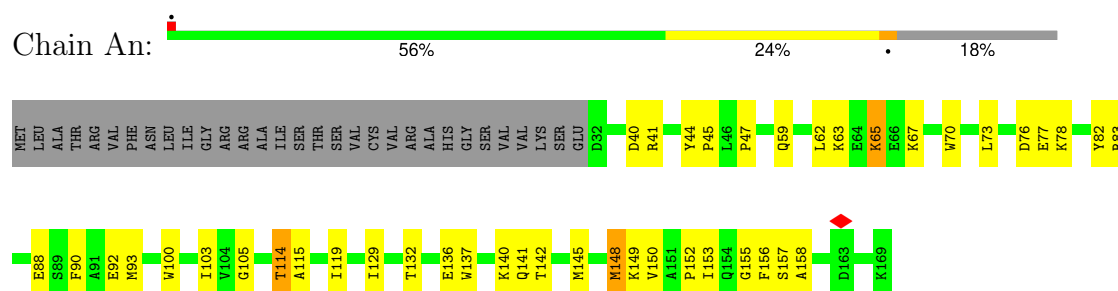
Chain Al: 



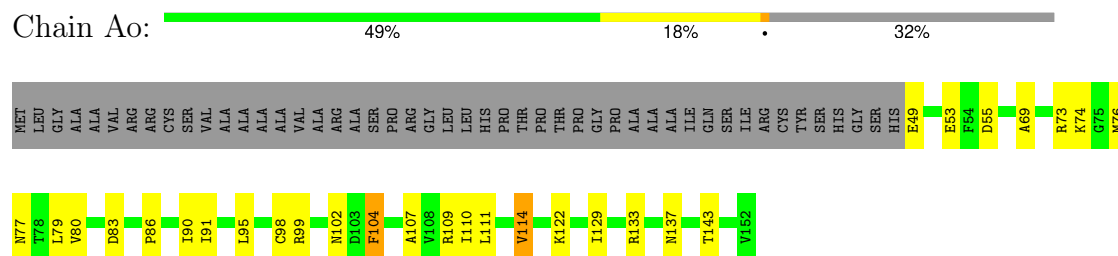
- Molecule 59: Cytochrome c oxidase subunit 3



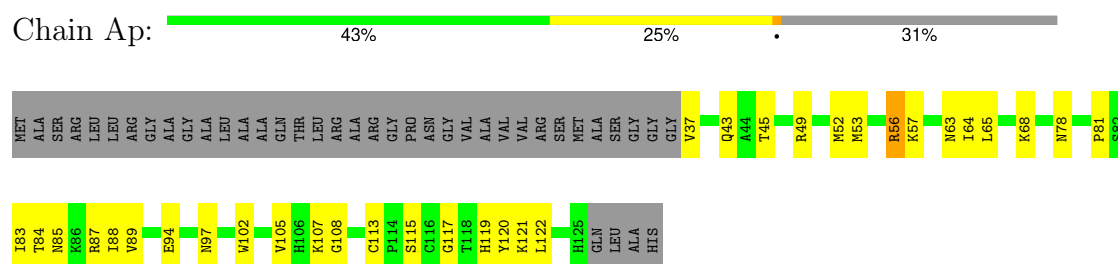
- Molecule 60: Cytochrome c oxidase subunit 4



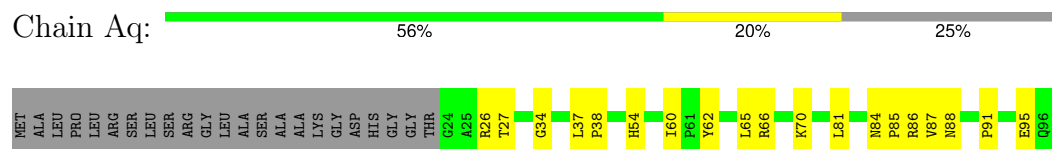
- Molecule 61: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 62: Cytochrome c oxidase subunit 5B, mitochondrial

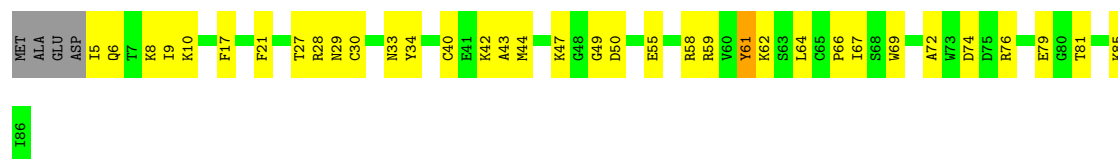


- Molecule 63: Cytochrome c oxidase subunit 6A2



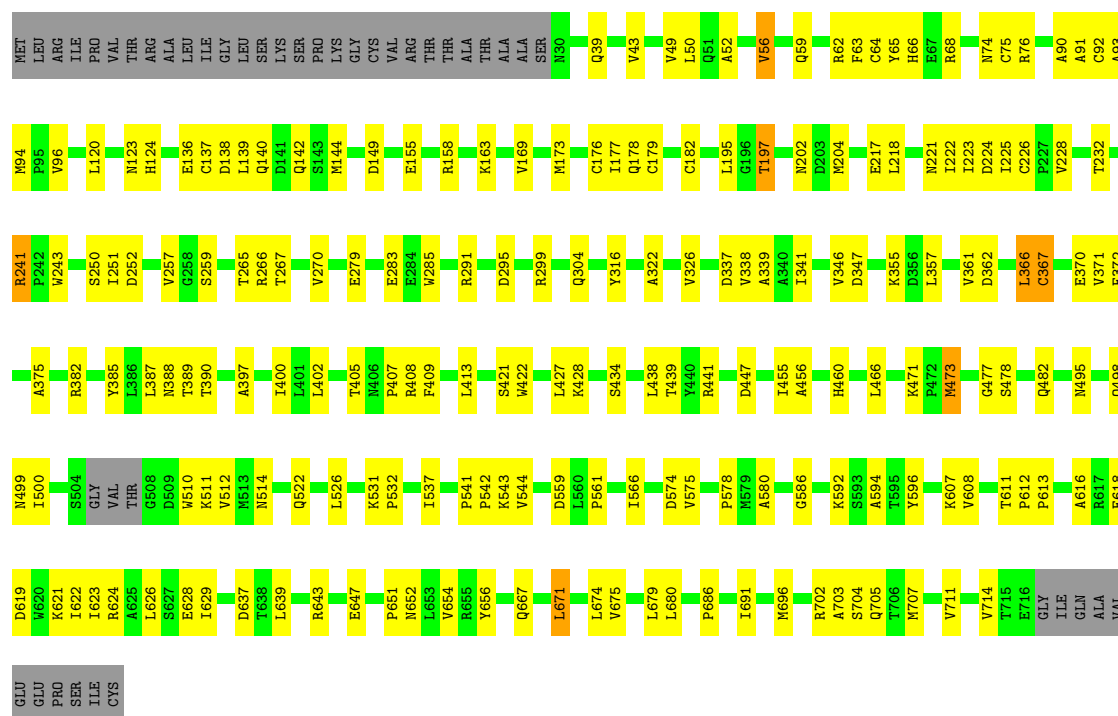
- Molecule 64: Cytochrome c oxidase subunit





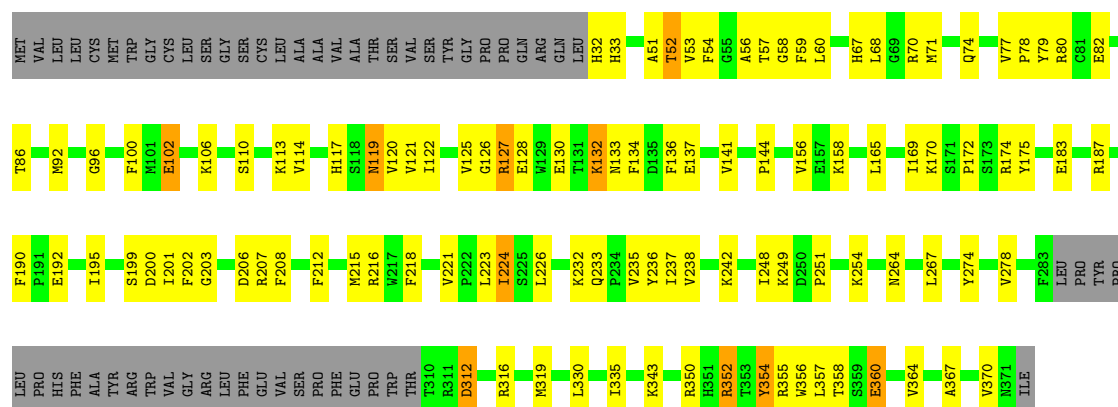
- Molecule 65: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 68% 26% • 6%



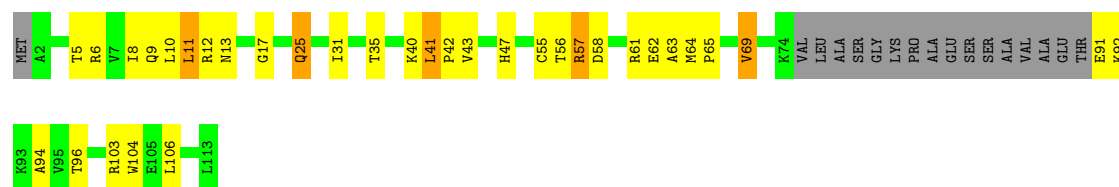
- Molecule 66: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 55% 26% • 16%



- Molecule 67: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Response	Percentage
Yes	55%
No	26%
Don't know	1%
No opinion	15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.151	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.36	0/567	0.51	0/759
1	Ab	0.16	0/549	0.32	0/735
2	1	0.13	0/506	0.24	0/683
2	Ac	0.14	0/498	0.29	0/672
3	2	0.15	0/1546	0.31	0/2093
3	4	0.17	0/1551	0.34	1/2098 (0.0%)
3	Ae	0.23	0/281	0.60	0/383
3	Af	0.27	0/228	0.57	0/312
4	3	0.13	0/433	0.29	0/593
4	Ad	0.11	0/437	0.27	0/598
5	6	0.15	0/3192	0.30	0/4322
5	v	0.15	0/3192	0.31	0/4322
6	7	0.16	0/3123	0.31	0/4269
6	w	0.16	0/3123	0.29	0/4269
7	8	0.14	0/1964	0.32	0/2663
7	x	0.92	0/1954	1.12	0/2652
8	9	0.11	0/913	0.24	0/1223
8	y	0.12	0/913	0.23	0/1223
9	A	0.65	0/522	0.85	0/697
10	a	0.88	0/1184	1.16	0/1603
11	b	0.90	0/896	1.08	0/1219
12	c	0.86	0/1332	1.09	0/1821
13	d	0.89	0/1452	1.16	0/1958
14	e	0.88	0/845	1.14	0/1149
15	f	0.86	0/398	1.15	0/540
16	g	0.89	0/1031	1.14	0/1394
17	h	0.89	0/889	1.18	1/1190 (0.1%)
18	i	0.21	0/2774	0.35	0/3768
19	j	0.61	0/737	0.79	0/1009
20	k	0.22	0/759	0.37	0/1029
21	m	0.90	0/1256	1.20	1/1696 (0.1%)
22	n	0.88	0/464	1.12	0/627

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	o	0.87	0/1092	1.15	0/1481
24	p	0.79	0/1590	0.99	0/2155
25	q	0.91	0/3721	1.16	0/5073
26	r	0.61	0/2506	0.82	1/3427 (0.0%)
27	B	0.93	0/3393	1.17	1/4584 (0.0%)
28	C	0.37	0/3551	0.53	0/4813
29	D	0.19	0/1783	0.38	0/2428
30	E	0.24	0/1698	0.44	0/2311
31	F	0.36	0/752	0.48	0/1013
32	H	0.89	0/1443	1.15	0/1952
33	I	0.88	0/1279	1.12	0/1730
34	J	0.13	0/985	0.27	0/1329
35	K	0.46	0/1244	0.55	0/1693
36	N	0.28	0/929	0.39	0/1258
37	O	0.91	0/701	1.19	0/946
37	X	0.90	0/701	1.21	0/946
38	P	0.15	0/680	0.36	0/916
39	Q	0.52	0/978	0.74	0/1317
40	R	0.35	0/304	0.43	0/410
41	S	0.89	0/577	1.14	1/777 (0.1%)
42	T	0.13	0/659	0.28	0/905
43	U	0.23	0/2622	0.38	0/3552
44	V	0.90	0/1042	1.25	0/1411
45	W	0.88	0/1193	1.16	0/1609
46	Y	0.73	0/549	0.95	0/752
47	Z	0.88	0/645	1.12	0/872
48	l	0.91	0/4902	1.17	0/6669
49	s	0.90	0/1436	1.11	0/1938
50	t	0.89	0/994	1.16	0/1339
51	5	0.13	0/3442	0.28	0/4667
51	u	0.13	0/3531	0.29	0/4793
52	Aa	0.15	0/684	0.32	0/926
52	z	0.89	0/688	1.14	0/931
53	Ag	0.17	0/349	0.38	0/477
54	Ah	0.44	0/446	0.59	0/605
55	Ai	0.14	0/396	0.34	0/543
56	Aj	0.15	0/390	0.31	0/525
57	Ak	0.27	0/4142	0.43	1/5664 (0.0%)
58	Al	0.38	0/1831	0.55	0/2496
59	Am	0.30	0/2179	0.43	0/2981
60	An	0.12	0/1188	0.27	0/1605
61	Ao	0.33	0/860	0.48	0/1167
62	Ap	0.28	0/704	0.44	0/956

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	Aq	0.22	0/633	0.37	0/866
64	Ar	0.15	0/704	0.32	0/951
65	G	0.29	0/5347	0.41	0/7243
66	L	0.51	0/2554	0.66	0/3455
67	M	0.97	0/787	1.10	0/1064
All	All	0.57	0/114313	0.75	7/155090 (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
7	x	0	5
9	A	0	2
10	a	0	5
11	b	0	4
12	c	0	3
13	d	0	5
14	e	0	2
16	g	0	4
17	h	0	6
22	n	0	2
23	o	0	1
24	p	0	3
25	q	0	4
26	r	0	3
27	B	0	7
31	F	0	1
32	H	0	4
33	I	0	5
35	K	0	2
39	Q	0	3
40	R	0	1
41	S	0	2
44	V	0	1
45	W	0	4
47	Z	0	2
48	l	0	3
49	s	0	1
50	t	0	4
52	z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	Ah	0	1
66	L	0	4
67	M	0	4
All	All	0	99

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	280	PHE	CB-CA-C	-6.87	105.82	114.40
27	B	310	GLY	CA-C-O	-5.75	118.26	122.23
41	S	57	VAL	N-CA-C	-5.47	107.15	112.29
17	h	47	ILE	N-CA-C	-5.37	107.74	112.90
21	m	116	ILE	N-CA-C	-5.14	106.90	113.22

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	10	ARG	Sidechain
9	A	18	ARG	Sidechain
10	a	119	ARG	Sidechain
10	a	150	ARG	Sidechain
10	a	53	ARG	Sidechain

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	0	561	0	542	19	0
1	Ab	543	0	530	7	0
2	1	493	0	491	5	0
2	Ac	485	0	485	9	0
3	2	1513	0	1497	41	0
3	4	1518	0	1498	47	0
3	Ae	275	0	276	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Af	223	0	220	20	0
4	3	417	0	414	10	0
4	Ad	421	0	418	9	0
5	6	3140	0	3121	83	0
5	v	3140	0	3121	79	0
6	7	3025	0	3090	41	0
6	w	3025	0	3090	62	0
7	8	1906	0	1857	38	0
7	x	1896	0	1843	70	0
8	9	893	0	888	11	0
8	y	893	0	888	11	0
9	A	510	0	511	16	0
10	a	1151	0	1164	57	0
11	b	871	0	899	50	0
12	c	1278	0	1169	67	0
13	d	1420	0	1384	70	0
14	e	822	0	778	41	0
15	f	385	0	381	14	0
16	g	1000	0	994	46	0
17	h	867	0	871	36	0
18	i	2711	0	2874	118	0
19	j	721	0	768	62	0
20	k	748	0	799	56	0
21	m	1227	0	1236	75	0
22	n	452	0	449	27	0
23	o	1062	0	1072	58	0
24	p	1534	0	1470	79	0
25	q	3630	0	3837	151	0
26	r	2435	0	2543	121	0
27	B	3318	0	3283	121	0
28	C	3458	0	3394	126	0
29	D	1732	0	1682	54	0
30	E	1658	0	1664	46	0
31	F	738	0	701	10	0
32	H	1412	0	1369	62	0
33	I	1248	0	1257	69	0
34	J	962	0	962	20	0
35	K	1203	0	1161	26	0
36	N	910	0	950	21	0
37	O	689	0	687	42	0
37	X	689	0	687	70	0
38	P	669	0	677	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Q	954	0	960	33	0
40	R	295	0	279	26	0
41	S	562	0	557	29	0
42	T	638	0	637	16	0
43	U	2562	0	2508	47	0
44	V	1021	0	1027	23	0
45	W	1162	0	1156	48	0
46	Y	524	0	469	25	0
47	Z	626	0	607	41	0
48	l	4773	0	4912	174	0
49	s	1398	0	1378	56	0
50	t	970	0	898	55	0
51	5	3374	0	3272	86	0
51	u	3459	0	3350	59	0
52	Aa	662	0	660	12	0
52	z	666	0	663	27	0
53	Ag	338	0	342	11	0
54	Ah	437	0	436	17	0
55	Ai	383	0	366	13	0
56	Aj	377	0	372	9	0
57	Ak	4002	0	3971	122	0
58	Al	1785	0	1800	79	0
59	Am	2096	0	2027	46	0
60	An	1154	0	1137	36	0
61	Ao	842	0	838	17	0
62	Ap	689	0	676	26	0
63	Aq	606	0	575	13	0
64	Ar	684	0	647	23	0
65	G	5260	0	5296	140	0
66	L	2493	0	2512	69	0
67	M	769	0	797	24	0
68	2	4	0	0	6	0
68	4	4	0	0	1	0
68	E	4	0	0	0	0
68	G	4	0	0	8	0
69	7	86	0	60	12	0
69	w	86	0	60	8	0
70	8	43	0	31	3	0
70	x	43	0	31	13	0
71	B	31	0	19	0	0
72	B	8	0	0	6	0
72	G	16	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	H	16	0	0	12	0
72	I	8	0	0	11	0
73	Q	30	0	30	1	0
74	Ak	120	0	108	20	0
75	L	48	0	26	6	0
All	All	111989	0	111432	3057	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 14.

The worst 5 of 3057 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)
65:G:75:CYS:SG	68:G:803:FES:FE2	1.25	1.29
30:E:176:CYS:SG	30:E:180:CYS:SG	2.37	1.22
33:I:71:CYS:SG	72:I:201:SF4:FE1	1.32	1.20
67:M:43:VAL:HB	67:M:47:HIS:ND1	1.65	1.12
65:G:179:CYS:SG	72:G:802:SF4:FE1	1.42	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	0	66/91 (72%)	63 (96%)	2 (3%)	1 (2%)	8	31
1	Ab	64/91 (70%)	62 (97%)	2 (3%)	0	100	100
2	1	58/64 (91%)	58 (100%)	0	0	100	100
2	Ac	57/64 (89%)	57 (100%)	0	0	100	100
3	2	193/299 (64%)	186 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4	194/299 (65%)	189 (97%)	5 (3%)	0	100	100
3	Ae	37/299 (12%)	26 (70%)	11 (30%)	0	100	100
3	Af	31/299 (10%)	20 (64%)	11 (36%)	0	100	100
4	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
4	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
5	6	416/453 (92%)	402 (97%)	14 (3%)	0	100	100
5	v	416/453 (92%)	407 (98%)	9 (2%)	0	100	100
6	7	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
6	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
7	8	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
7	x	236/326 (72%)	223 (94%)	11 (5%)	2 (1%)	16	45
8	9	99/111 (89%)	99 (100%)	0	0	100	100
8	y	99/111 (89%)	99 (100%)	0	0	100	100
9	A	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
10	a	136/189 (72%)	128 (94%)	8 (6%)	0	100	100
11	b	101/128 (79%)	87 (86%)	12 (12%)	2 (2%)	6	25
12	c	150/186 (81%)	139 (93%)	9 (6%)	2 (1%)	10	34
13	d	167/176 (95%)	160 (96%)	7 (4%)	0	100	100
14	e	97/154 (63%)	88 (91%)	9 (9%)	0	100	100
15	f	44/76 (58%)	41 (93%)	3 (7%)	0	100	100
16	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
17	h	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
18	i	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
19	j	87/115 (76%)	85 (98%)	2 (2%)	0	100	100
20	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
21	m	155/175 (89%)	142 (92%)	10 (6%)	3 (2%)	6	26
22	n	51/58 (88%)	43 (84%)	8 (16%)	0	100	100
23	o	126/129 (98%)	120 (95%)	5 (4%)	1 (1%)	16	45
24	p	176/221 (80%)	168 (96%)	6 (3%)	2 (1%)	12	38
25	q	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
26	r	304/318 (96%)	290 (95%)	12 (4%)	2 (1%)	19	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	B	429/464 (92%)	405 (94%)	24 (6%)	0	100	100
28	C	428/469 (91%)	403 (94%)	24 (6%)	1 (0%)	44	73
29	D	206/264 (78%)	180 (87%)	25 (12%)	1 (0%)	25	55
30	E	212/249 (85%)	201 (95%)	11 (5%)	0	100	100
31	F	93/123 (76%)	88 (95%)	5 (5%)	0	100	100
32	H	174/212 (82%)	168 (97%)	6 (3%)	0	100	100
33	I	154/263 (59%)	144 (94%)	9 (6%)	1 (1%)	22	51
34	J	116/175 (66%)	116 (100%)	0	0	100	100
35	K	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
36	N	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
37	O	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
37	X	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
38	P	81/99 (82%)	73 (90%)	8 (10%)	0	100	100
39	Q	110/154 (71%)	106 (96%)	3 (3%)	1 (1%)	14	43
40	R	33/110 (30%)	33 (100%)	0	0	100	100
41	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
42	T	80/169 (47%)	76 (95%)	4 (5%)	0	100	100
43	U	316/357 (88%)	308 (98%)	7 (2%)	1 (0%)	37	67
44	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
45	W	138/144 (96%)	134 (97%)	4 (3%)	0	100	100
46	Y	58/105 (55%)	52 (90%)	4 (7%)	2 (3%)	3	17
47	Z	76/114 (67%)	72 (95%)	4 (5%)	0	100	100
48	l	600/606 (99%)	567 (94%)	29 (5%)	4 (1%)	19	48
49	s	169/249 (68%)	153 (90%)	14 (8%)	2 (1%)	11	36
50	t	117/137 (85%)	107 (92%)	9 (8%)	1 (1%)	14	43
51	5	431/480 (90%)	415 (96%)	16 (4%)	0	100	100
51	u	444/480 (92%)	432 (97%)	12 (3%)	0	100	100
52	Aa	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
52	z	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
53	Ag	41/70 (59%)	41 (100%)	0	0	100	100
54	Ah	54/80 (68%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Ai	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
56	Aj	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
57	Ak	511/514 (99%)	498 (98%)	13 (2%)	0	100	100
58	Al	218/228 (96%)	212 (97%)	4 (2%)	2 (1%)	14	43
59	Am	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
60	An	136/169 (80%)	132 (97%)	4 (3%)	0	100	100
61	Ao	102/152 (67%)	100 (98%)	2 (2%)	0	100	100
62	Ap	87/129 (67%)	85 (98%)	2 (2%)	0	100	100
63	Aq	71/97 (73%)	66 (93%)	5 (7%)	0	100	100
64	Ar	80/86 (93%)	80 (100%)	0	0	100	100
65	G	680/727 (94%)	658 (97%)	21 (3%)	1 (0%)	48	78
66	L	310/372 (83%)	291 (94%)	18 (6%)	1 (0%)	37	67
67	M	92/113 (81%)	85 (92%)	6 (6%)	1 (1%)	12	38
All	All	13802/16800 (82%)	13230 (96%)	538 (4%)	34 (0%)	45	73

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	Y	40	ILE
7	x	179	PRO
66	L	224	ILE
1	0	67	CYS
48	l	562	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	65/85 (76%)	59 (91%)	6 (9%)	7	26
1	Ab	63/85 (74%)	57 (90%)	6 (10%)	7	25
2	1	49/52 (94%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ac	48/52 (92%)	48 (100%)	0	100	100
3	2	166/245 (68%)	161 (97%)	5 (3%)	36	61
3	4	166/245 (68%)	157 (95%)	9 (5%)	18	44
3	Ae	29/245 (12%)	26 (90%)	3 (10%)	6	22
3	Af	23/245 (9%)	23 (100%)	0	100	100
4	3	40/46 (87%)	37 (92%)	3 (8%)	11	35
4	Ad	41/46 (89%)	39 (95%)	2 (5%)	21	47
5	6	329/355 (93%)	315 (96%)	14 (4%)	25	50
5	v	329/355 (93%)	317 (96%)	12 (4%)	30	55
6	7	332/332 (100%)	328 (99%)	4 (1%)	67	79
6	w	332/332 (100%)	325 (98%)	7 (2%)	48	69
7	8	204/259 (79%)	197 (97%)	7 (3%)	32	57
7	x	203/259 (78%)	195 (96%)	8 (4%)	27	53
8	9	93/99 (94%)	91 (98%)	2 (2%)	47	68
8	y	93/99 (94%)	89 (96%)	4 (4%)	25	50
9	A	49/61 (80%)	47 (96%)	2 (4%)	26	51
10	a	121/158 (77%)	119 (98%)	2 (2%)	56	74
11	b	95/121 (78%)	87 (92%)	8 (8%)	9	29
12	c	136/160 (85%)	130 (96%)	6 (4%)	24	50
13	d	152/156 (97%)	143 (94%)	9 (6%)	16	41
14	e	90/129 (70%)	81 (90%)	9 (10%)	6	23
15	f	41/66 (62%)	39 (95%)	2 (5%)	21	47
16	g	108/109 (99%)	98 (91%)	10 (9%)	7	25
17	h	93/94 (99%)	88 (95%)	5 (5%)	18	44
18	i	311/311 (100%)	296 (95%)	15 (5%)	21	48
19	j	78/100 (78%)	68 (87%)	10 (13%)	3	14
20	k	85/85 (100%)	79 (93%)	6 (7%)	12	37
21	m	129/141 (92%)	118 (92%)	11 (8%)	8	29
22	n	49/55 (89%)	46 (94%)	3 (6%)	15	40
23	o	113/114 (99%)	105 (93%)	8 (7%)	12	37
24	p	159/190 (84%)	152 (96%)	7 (4%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	q	409/409 (100%)	386 (94%)	23 (6%)	17	43
26	r	267/275 (97%)	254 (95%)	13 (5%)	21	47
27	B	345/368 (94%)	327 (95%)	18 (5%)	19	45
28	C	371/398 (93%)	349 (94%)	22 (6%)	16	41
29	D	188/228 (82%)	181 (96%)	7 (4%)	29	54
30	E	183/207 (88%)	177 (97%)	6 (3%)	33	58
31	F	79/97 (81%)	77 (98%)	2 (2%)	42	65
32	H	151/176 (86%)	141 (93%)	10 (7%)	14	38
33	I	132/217 (61%)	124 (94%)	8 (6%)	15	40
34	J	107/152 (70%)	105 (98%)	2 (2%)	52	71
35	K	130/131 (99%)	126 (97%)	4 (3%)	35	60
36	N	99/101 (98%)	93 (94%)	6 (6%)	15	40
37	O	79/132 (60%)	71 (90%)	8 (10%)	6	22
37	X	79/132 (60%)	70 (89%)	9 (11%)	4	17
38	P	74/82 (90%)	70 (95%)	4 (5%)	18	44
39	Q	105/134 (78%)	100 (95%)	5 (5%)	21	48
40	R	34/92 (37%)	33 (97%)	1 (3%)	37	61
41	S	58/58 (100%)	56 (97%)	2 (3%)	32	57
42	T	69/134 (52%)	66 (96%)	3 (4%)	25	50
43	U	278/307 (91%)	269 (97%)	9 (3%)	34	59
44	V	101/102 (99%)	99 (98%)	2 (2%)	50	70
45	W	122/124 (98%)	119 (98%)	3 (2%)	42	65
46	Y	54/84 (64%)	46 (85%)	8 (15%)	2	10
47	Z	60/90 (67%)	54 (90%)	6 (10%)	6	23
48	l	535/540 (99%)	502 (94%)	33 (6%)	15	40
49	s	153/206 (74%)	145 (95%)	8 (5%)	19	45
50	t	97/120 (81%)	83 (86%)	14 (14%)	2	10
51	5	363/397 (91%)	357 (98%)	6 (2%)	56	74
51	u	372/397 (94%)	359 (96%)	13 (4%)	31	56
52	Aa	70/73 (96%)	64 (91%)	6 (9%)	8	28
52	z	70/73 (96%)	65 (93%)	5 (7%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Ag	37/57 (65%)	37 (100%)	0	100	100
54	Ah	47/68 (69%)	45 (96%)	2 (4%)	25	50
55	Ai	38/66 (58%)	36 (95%)	2 (5%)	19	44
56	Aj	39/55 (71%)	38 (97%)	1 (3%)	41	64
57	Ak	422/425 (99%)	405 (96%)	17 (4%)	27	52
58	Al	206/212 (97%)	199 (97%)	7 (3%)	32	57
59	Am	223/225 (99%)	220 (99%)	3 (1%)	65	78
60	An	123/149 (83%)	117 (95%)	6 (5%)	21	47
61	Ao	91/124 (73%)	86 (94%)	5 (6%)	18	43
62	Ap	77/101 (76%)	75 (97%)	2 (3%)	41	64
63	Aq	64/80 (80%)	63 (98%)	1 (2%)	58	75
64	Ar	73/76 (96%)	68 (93%)	5 (7%)	13	38
65	G	576/610 (94%)	561 (97%)	15 (3%)	41	64
66	L	268/320 (84%)	254 (95%)	14 (5%)	19	45
67	M	85/98 (87%)	78 (92%)	7 (8%)	9	31
All	All	12017/14188 (85%)	11459 (95%)	558 (5%)	25	49

5 of 558 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	Ah	49	ASP
57	Ak	300	ASP
54	Ah	32	ILE
65	G	137	CYS
26	r	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 214 such sidechains are listed below:

Mol	Chain	Res	Type
37	O	142	GLN
49	s	141	ASN
65	G	59	GLN
39	Q	96	ASN
48	l	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
72	SF4	H	302	-	0,12,12	-	-	-		
72	SF4	I	201	33	0,12,12	-	-	-		
74	HEA	Ak	602	57	58,67,67	2.18	19 (32%)	63,103,103	2.44	29 (46%)
68	FES	2	301	3	0,4,4	-	-	-		
69	HEM	7	402	-	42,50,50	1.32	6 (14%)	46,82,82	1.77	9 (19%)
75	NDP	L	401	-	47,52,52	0.65	0	61,80,80	0.92	2 (3%)
68	FES	E	301	30	0,4,4	-	-	-		
73	ZMP	Q	201	-	27,29,36	0.32	0	34,38,45	1.20	1 (2%)
74	HEA	Ak	601	57	58,67,67	2.33	22 (37%)	63,103,103	2.43	26 (41%)
70	HEC	8	401	7	32,50,50	1.99	3 (9%)	30,82,82	2.34	7 (23%)
72	SF4	G	802	-	0,12,12	-	-	-		
68	FES	G	803	65	0,4,4	-	-	-		
69	HEM	w	402	6	42,50,50	1.46	4 (9%)	46,82,82	1.18	3 (6%)
69	HEM	7	401	6	42,50,50	1.54	4 (9%)	46,82,82	1.41	5 (10%)
68	FES	4	301	3	0,4,4	-	-	-		
72	SF4	B	502	27	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	HEC	x	401	7	32,50,50	1.94	3 (9%)	30,82,82	2.23	7 (23%)
72	SF4	G	801	65	0,12,12	-	-	-		
72	SF4	H	301	-	0,12,12	-	-	-		
69	HEM	w	401	-	42,50,50	1.44	4 (9%)	46,82,82	1.34	5 (10%)
71	FMN	B	501	-	33,33,33	0.61	0	48,50,50	0.64	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	SF4	H	302	-	-	-	0/6/5/5
72	SF4	I	201	33	-	-	0/6/5/5
74	HEA	Ak	602	57	-	4/32/76/76	-
68	FES	2	301	3	-	-	0/1/1/1
69	HEM	7	402	-	-	4/12/54/54	-
75	NDP	L	401	-	-	7/30/77/77	0/5/5/5
68	FES	E	301	30	-	-	0/1/1/1
73	ZMP	Q	201	-	-	8/36/36/43	-
74	HEA	Ak	601	57	-	10/32/76/76	-
70	HEC	8	401	7	-	0/10/54/54	-
72	SF4	G	802	-	-	-	0/6/5/5
69	HEM	w	402	6	-	3/12/54/54	-
68	FES	G	803	65	-	-	0/1/1/1
69	HEM	7	401	6	-	7/12/54/54	-
68	FES	4	301	3	-	-	0/1/1/1
72	SF4	B	502	27	-	-	0/6/5/5
70	HEC	x	401	7	-	5/10/54/54	-
72	SF4	G	801	65	-	-	0/6/5/5
72	SF4	H	301	-	-	-	0/6/5/5
69	HEM	w	401	-	-	3/12/54/54	-
71	FMN	B	501	-	-	2/18/18/18	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Ak	601	HEA	C3A-C2A	6.08	1.48	1.40
74	Ak	601	HEA	C3B-C2B	5.69	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Ak	601	HEA	CHD-C1D	5.68	1.48	1.34
70	8	401	HEC	C3D-C2D	5.50	1.54	1.37
70	8	401	HEC	C2B-C3B	-5.48	1.34	1.40

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	8	401	HEC	CBB-CAB-C3B	-8.25	108.18	127.49
74	Ak	601	HEA	CHA-C4D-ND	-6.98	116.93	124.44
74	Ak	602	HEA	C3D-C4D-ND	6.78	116.90	110.35
70	x	401	HEC	CBC-CAC-C3C	-6.42	112.47	127.49
73	Q	201	ZMP	C11-S1-C10	6.15	120.03	101.84

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	7	402	HEM	C1A-C2A-CAA-CBA
69	7	402	HEM	C3A-C2A-CAA-CBA
69	7	402	HEM	C2B-C3B-CAB-CBB
70	x	401	HEC	C1A-C2A-CAA-CBA
70	x	401	HEC	C3A-C2A-CAA-CBA

There are no ring outliers.

19 monomers are involved in 119 short contacts:

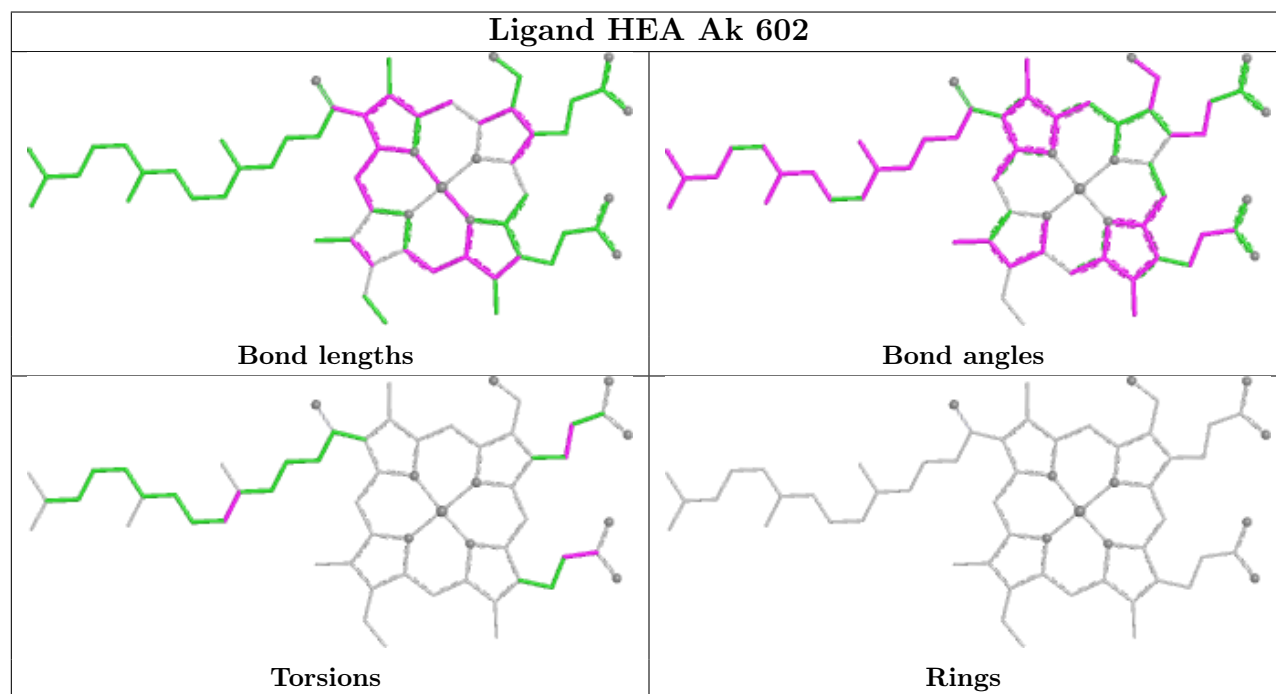
Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	H	302	SF4	8	0
72	I	201	SF4	11	0
74	Ak	602	HEA	6	0
68	2	301	FES	6	0
69	7	402	HEM	6	0
75	L	401	NDP	6	0
73	Q	201	ZMP	1	0
74	Ak	601	HEA	14	0
70	8	401	HEC	3	0
72	G	802	SF4	11	0
68	G	803	FES	8	0
69	w	402	HEM	4	0
69	7	401	HEM	6	0
68	4	301	FES	1	0

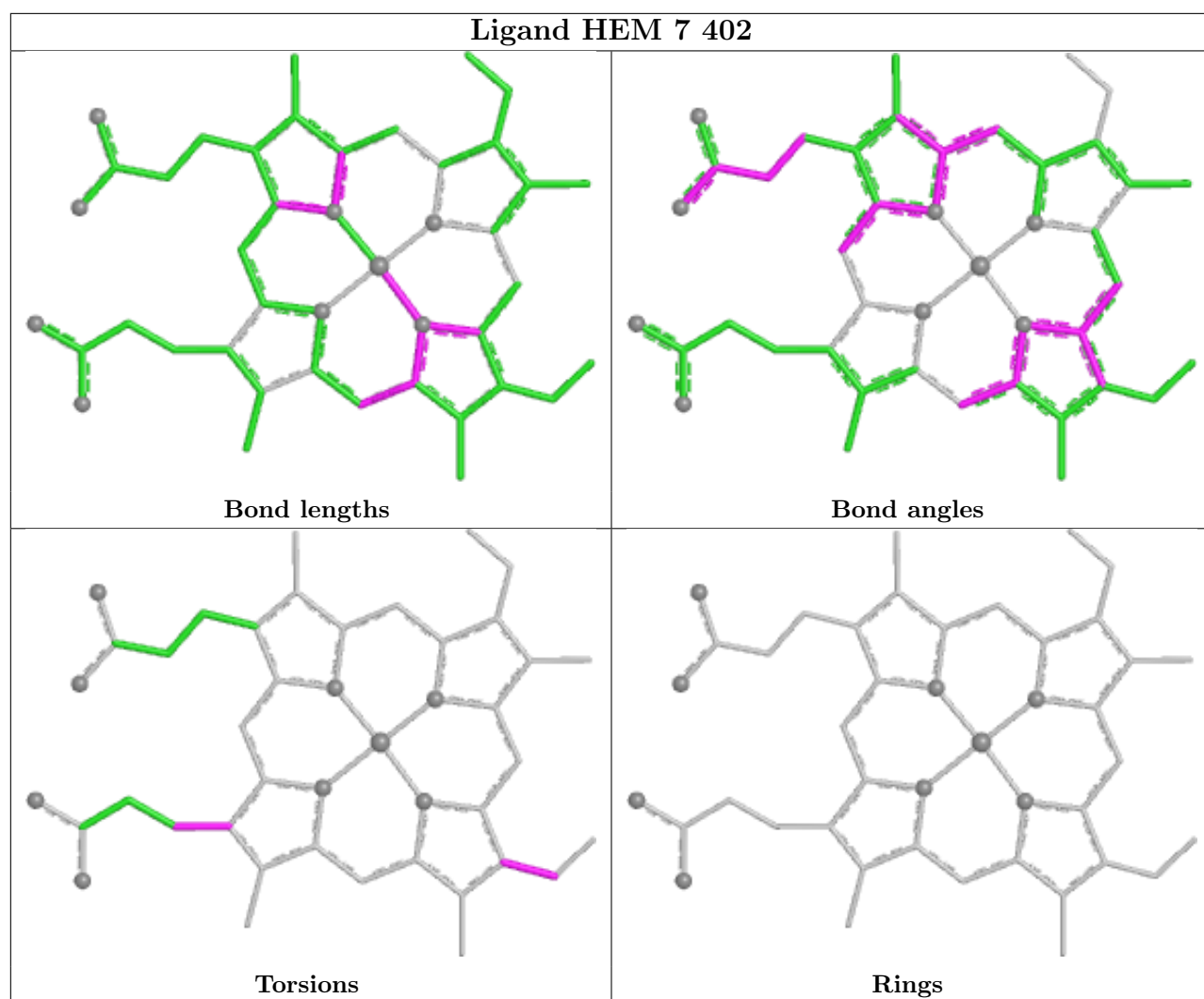
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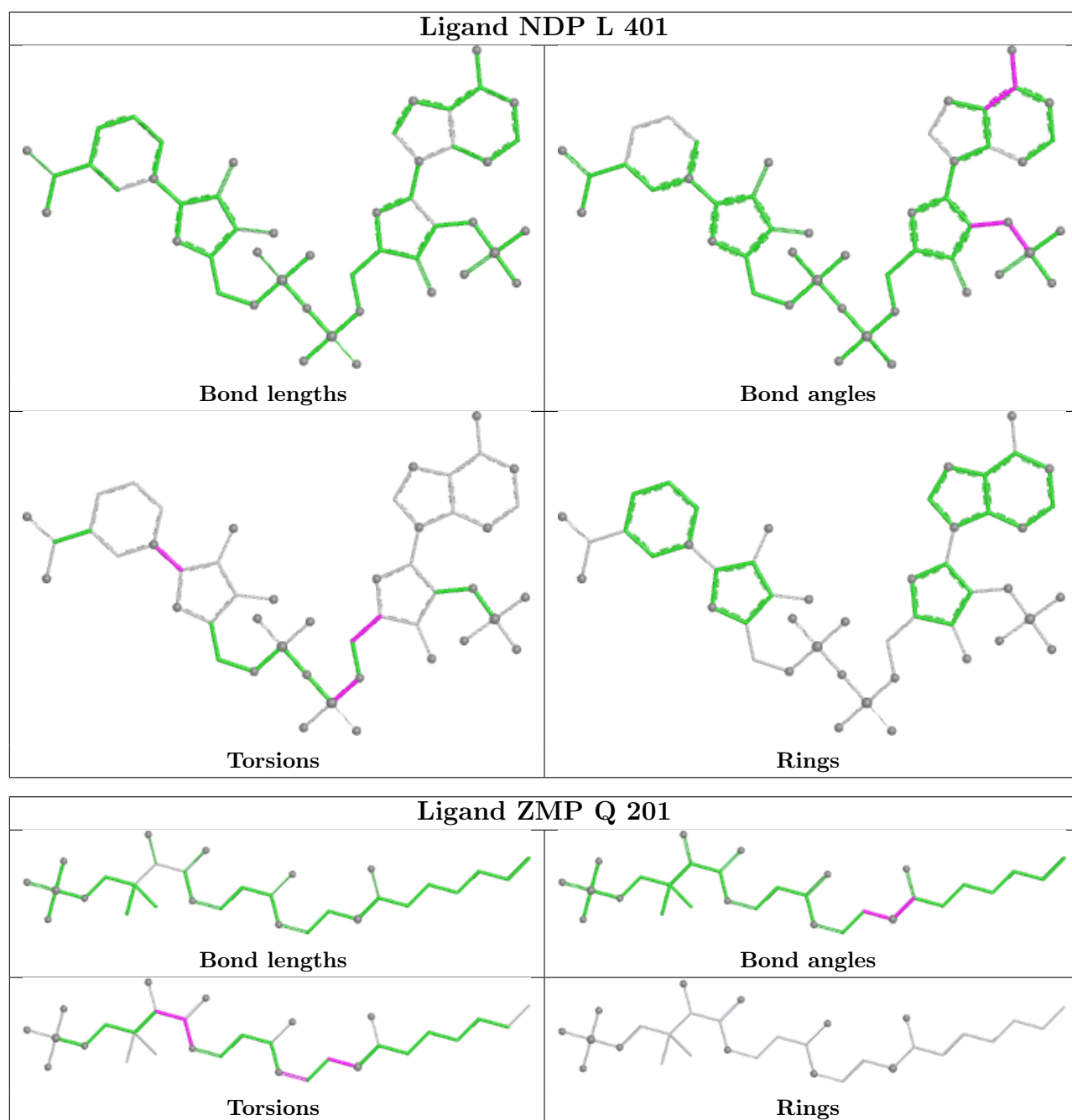
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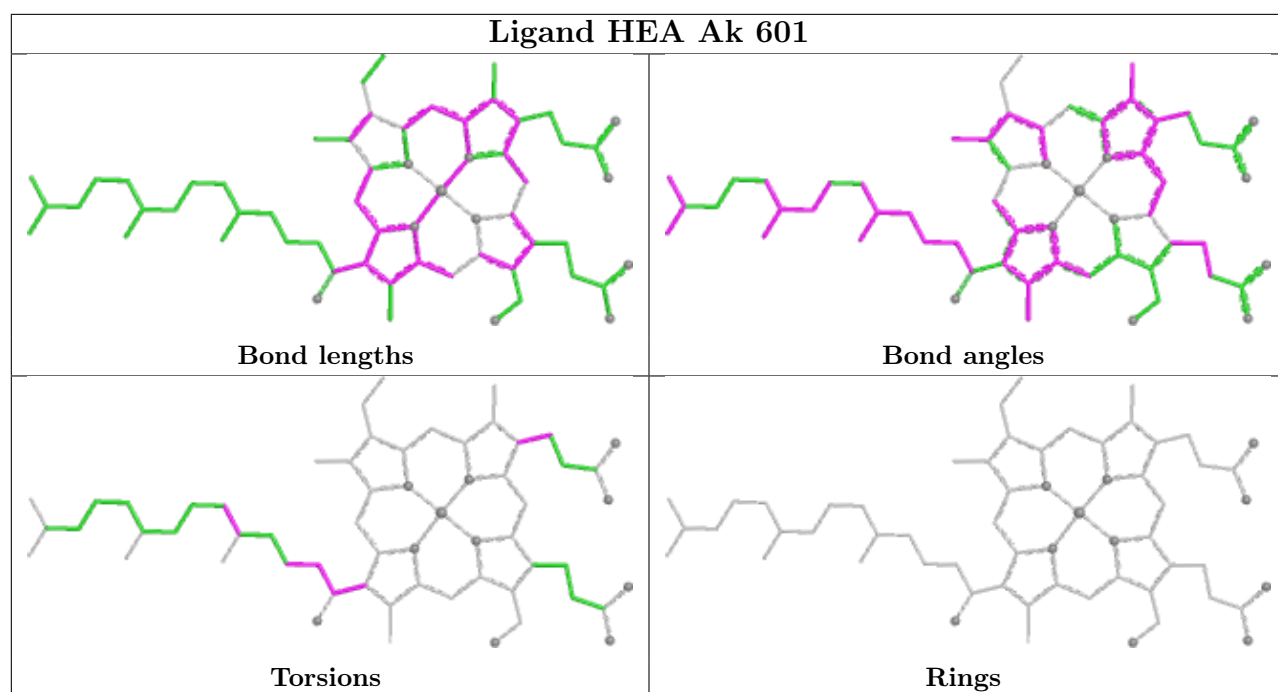
Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	B	502	SF4	6	0
70	x	401	HEC	13	0
72	G	801	SF4	1	0
72	H	301	SF4	4	0
69	w	401	HEM	4	0

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

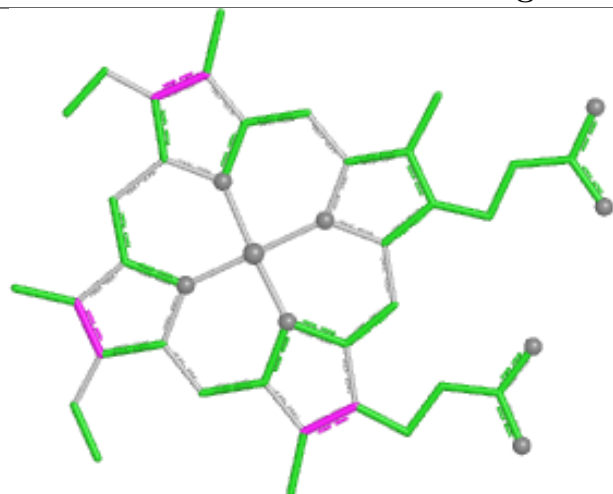




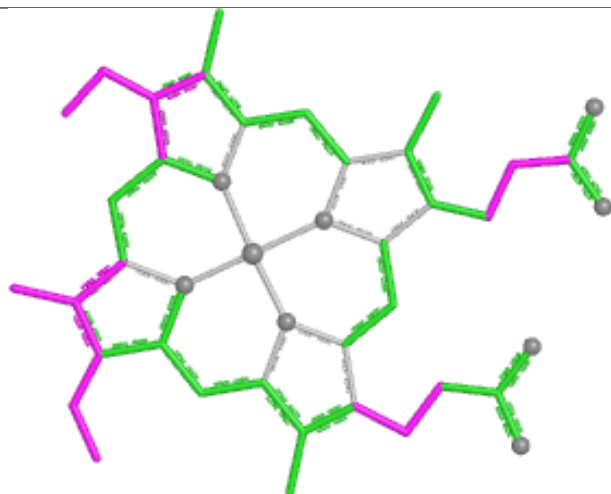




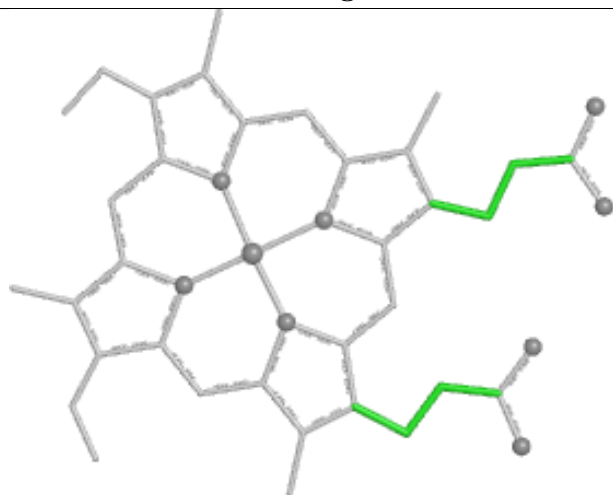
Ligand HEC 8 401



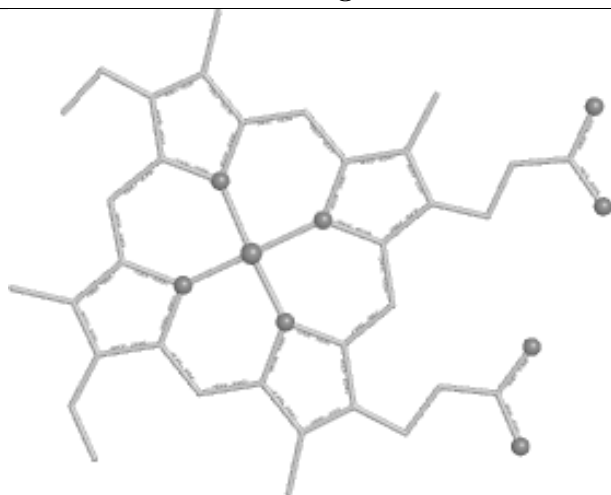
Bond lengths



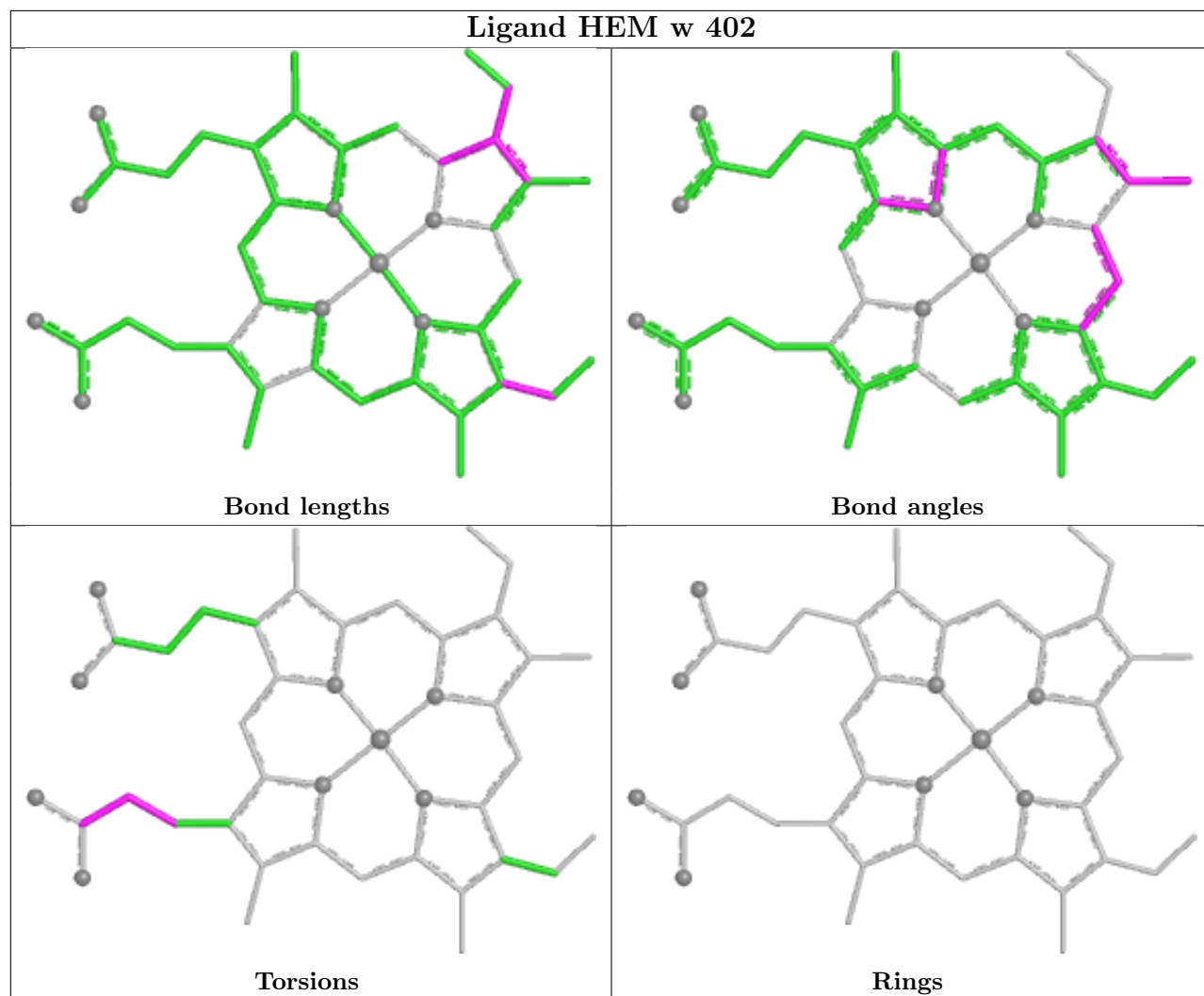
Bond angles

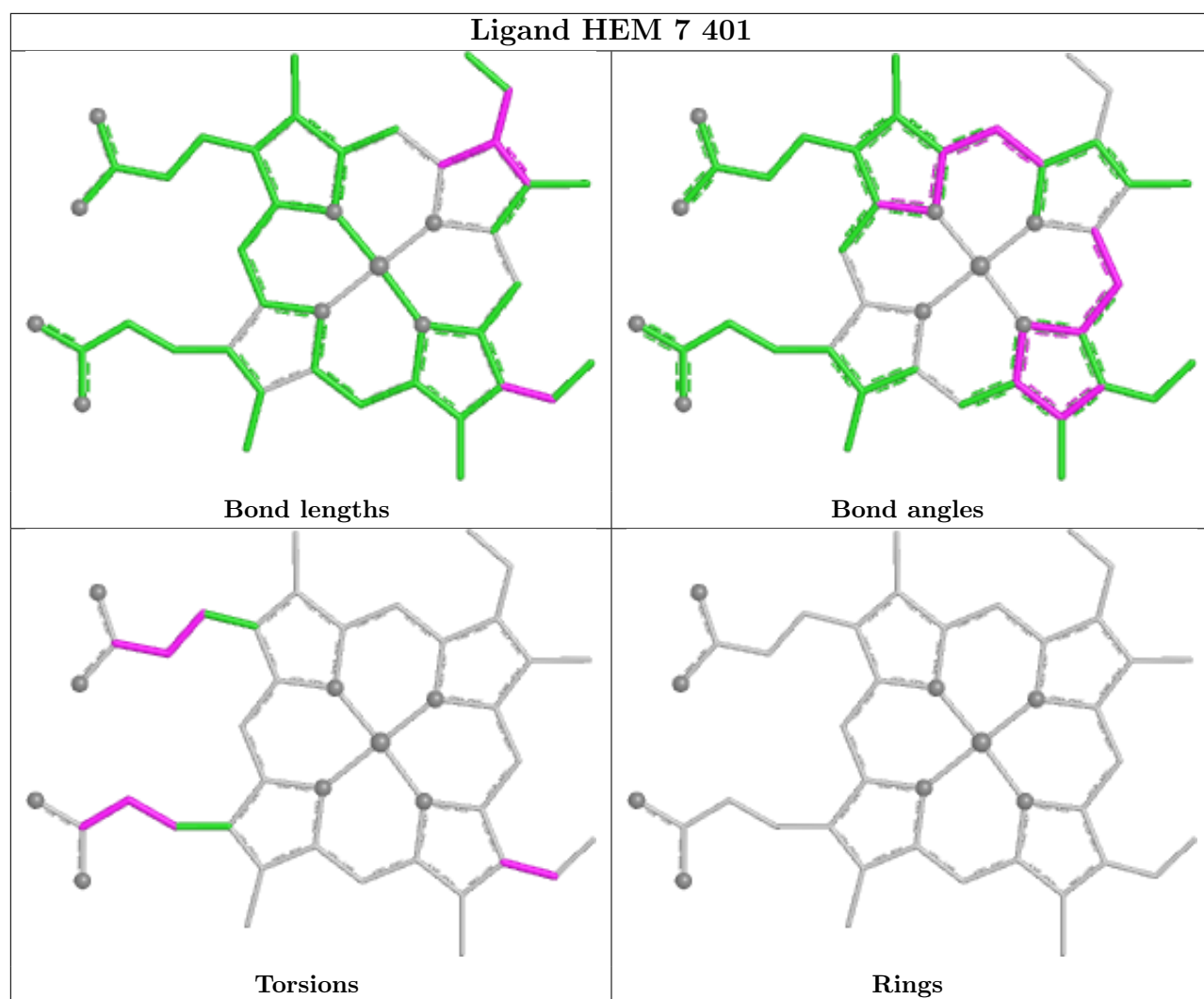


Torsions

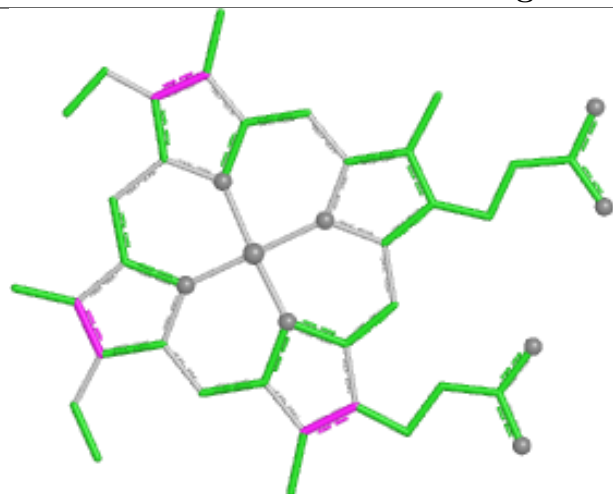


Rings

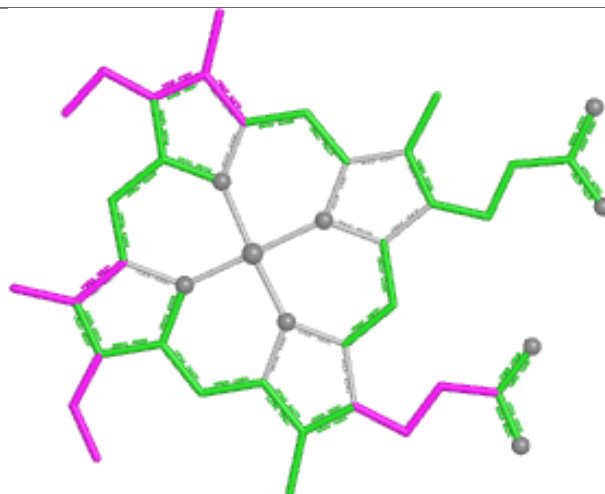




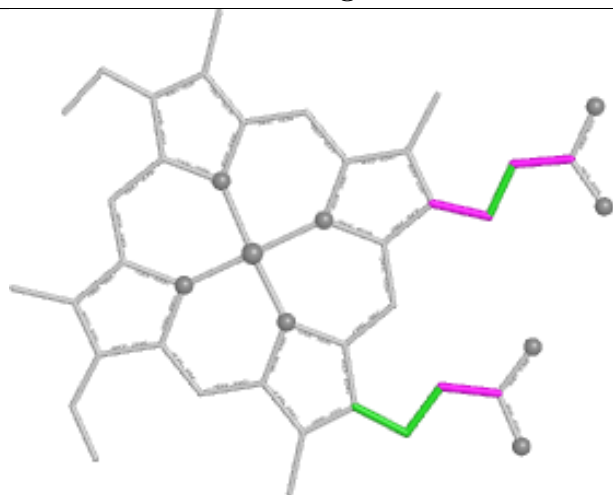
Ligand HEC x 401



Bond lengths



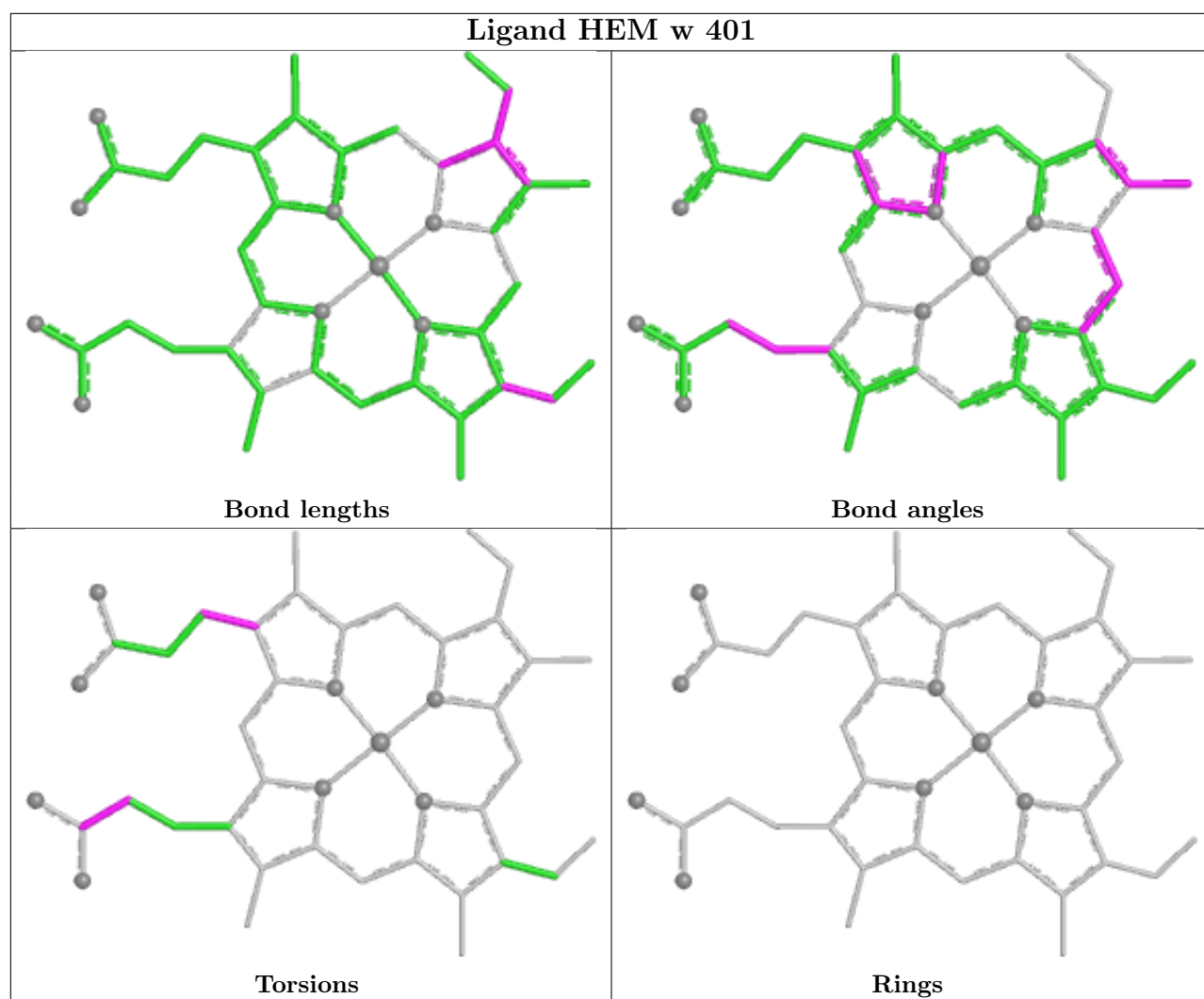
Bond angles

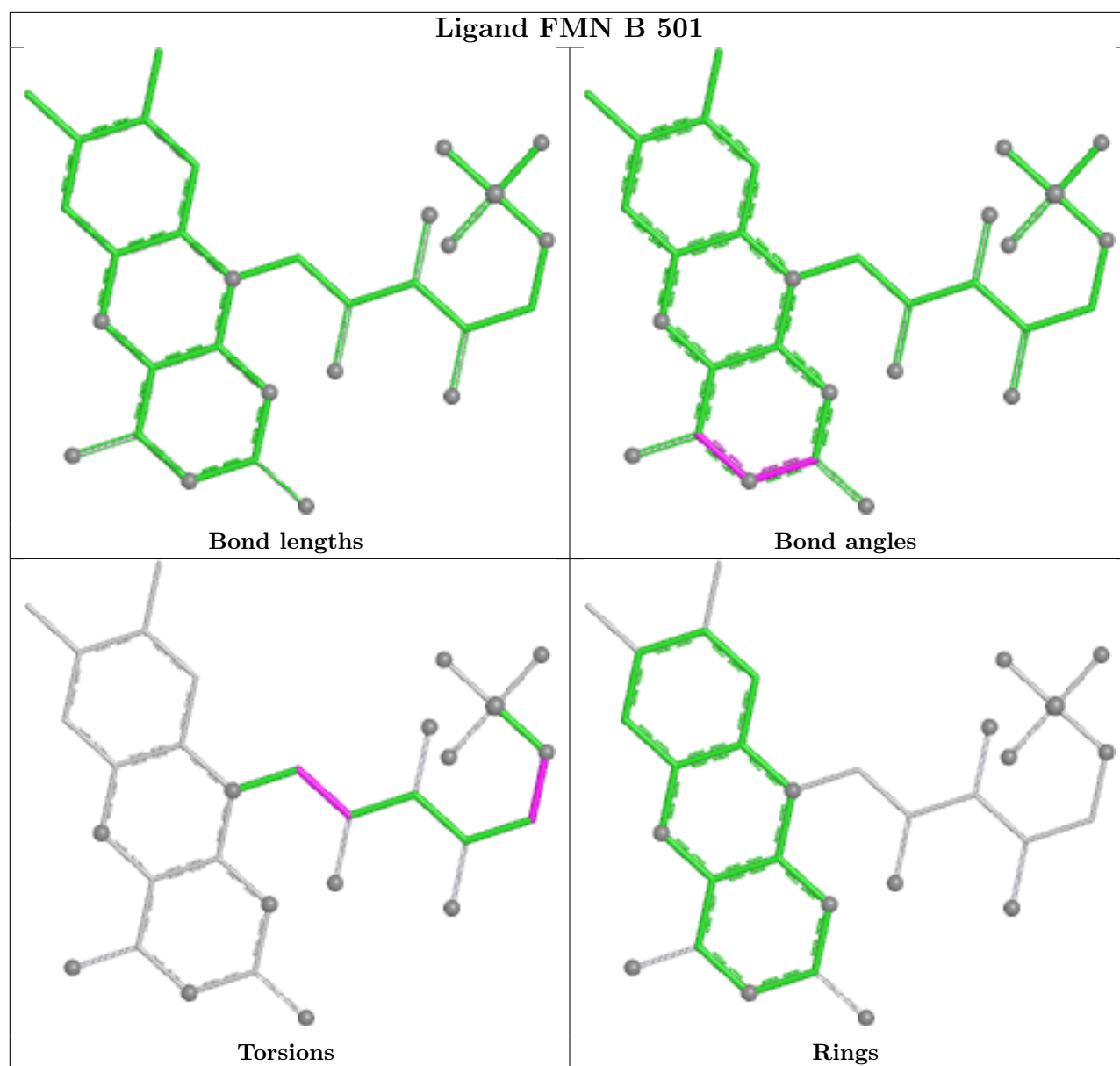


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

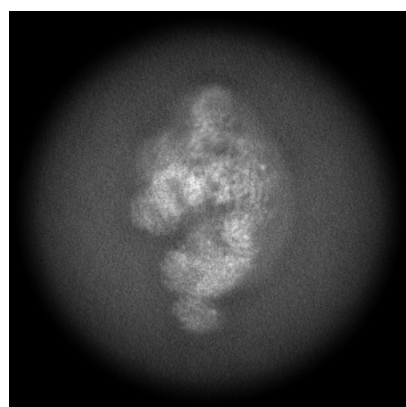
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45490. These allow visual inspection of the internal detail of the map and identification of artifacts.

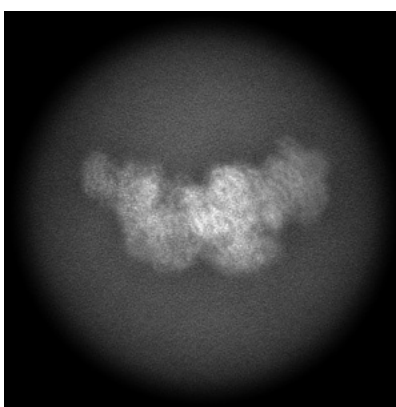
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

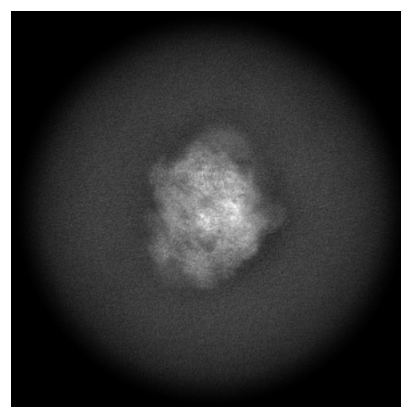
6.1.1 Primary map



X



Y

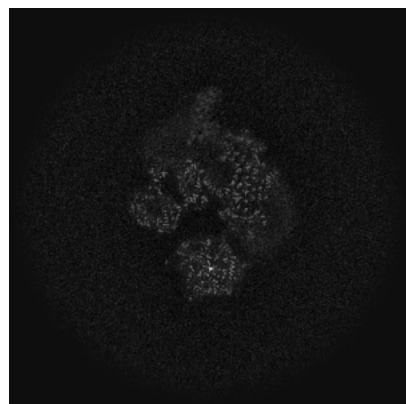


Z

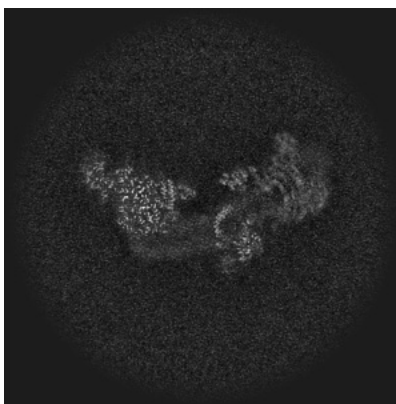
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

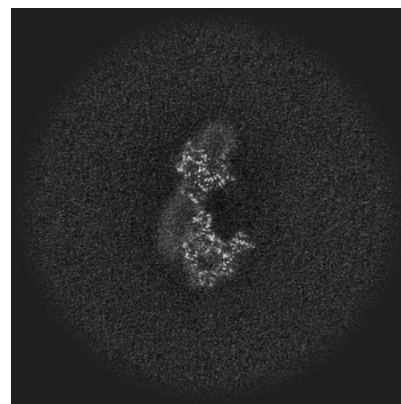
6.2.1 Primary map



X Index: 256



Y Index: 256

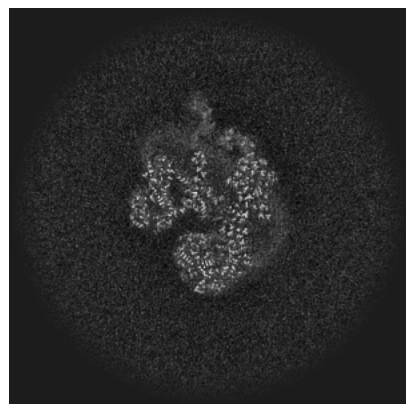


Z Index: 256

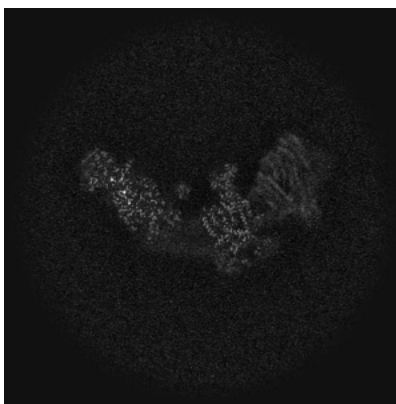
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

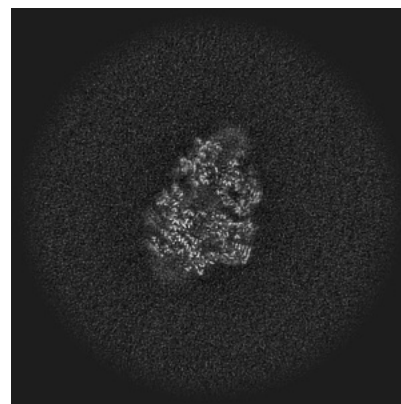
6.3.1 Primary map



X Index: 244



Y Index: 242

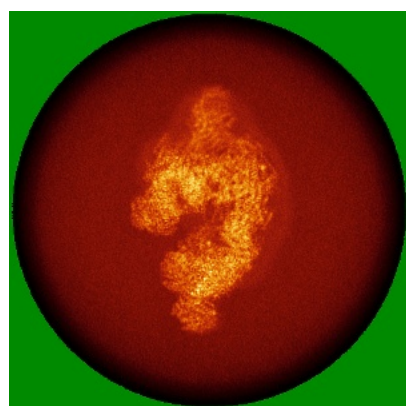


Z Index: 298

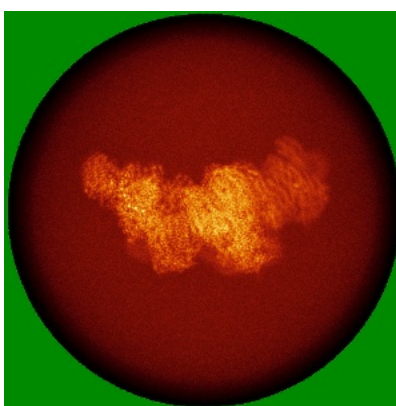
The images above show the largest variance slices of the map in three orthogonal directions.

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

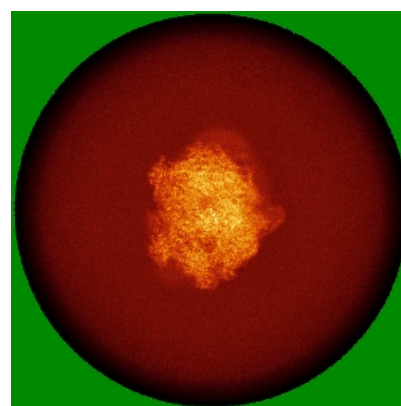
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

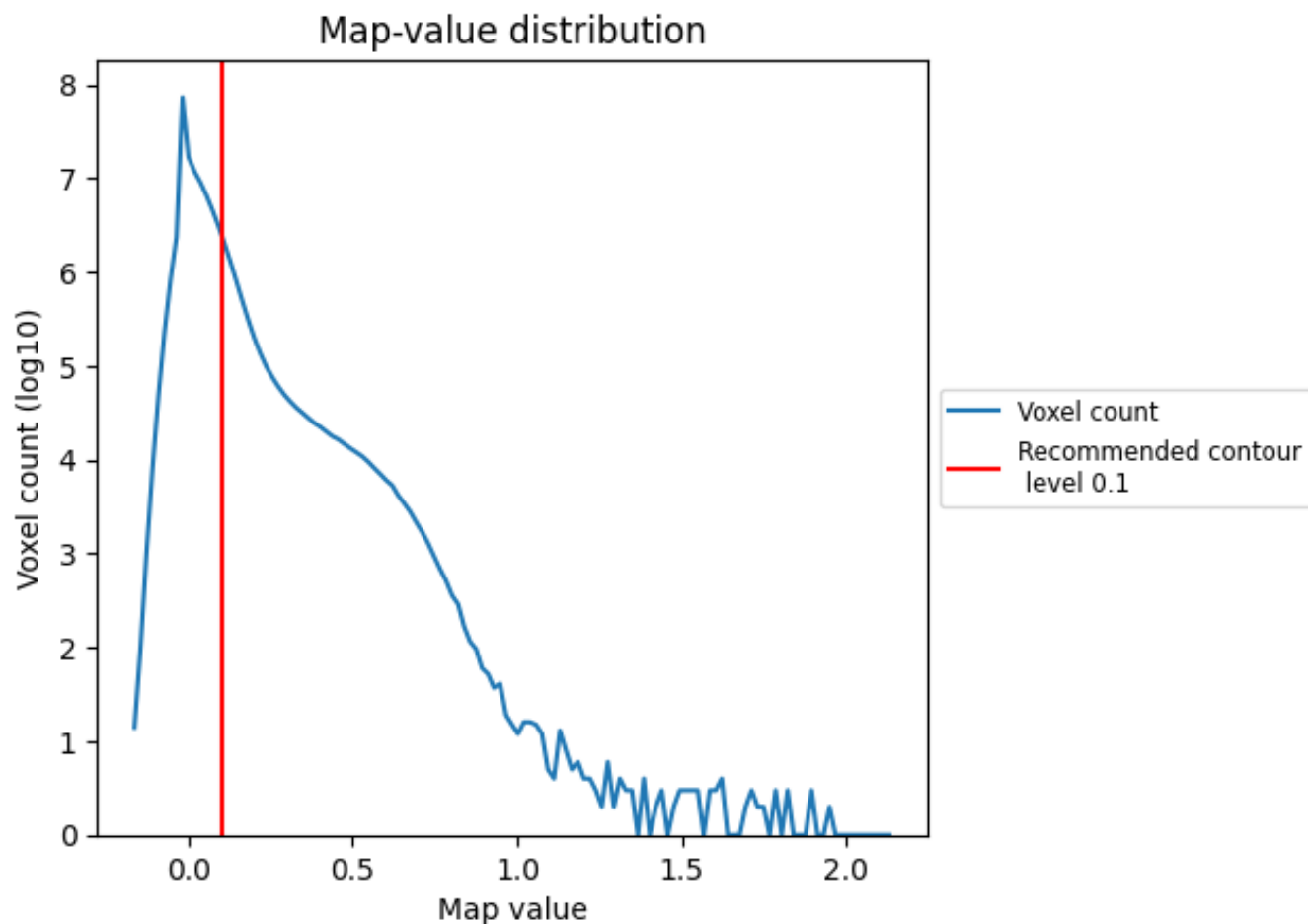
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

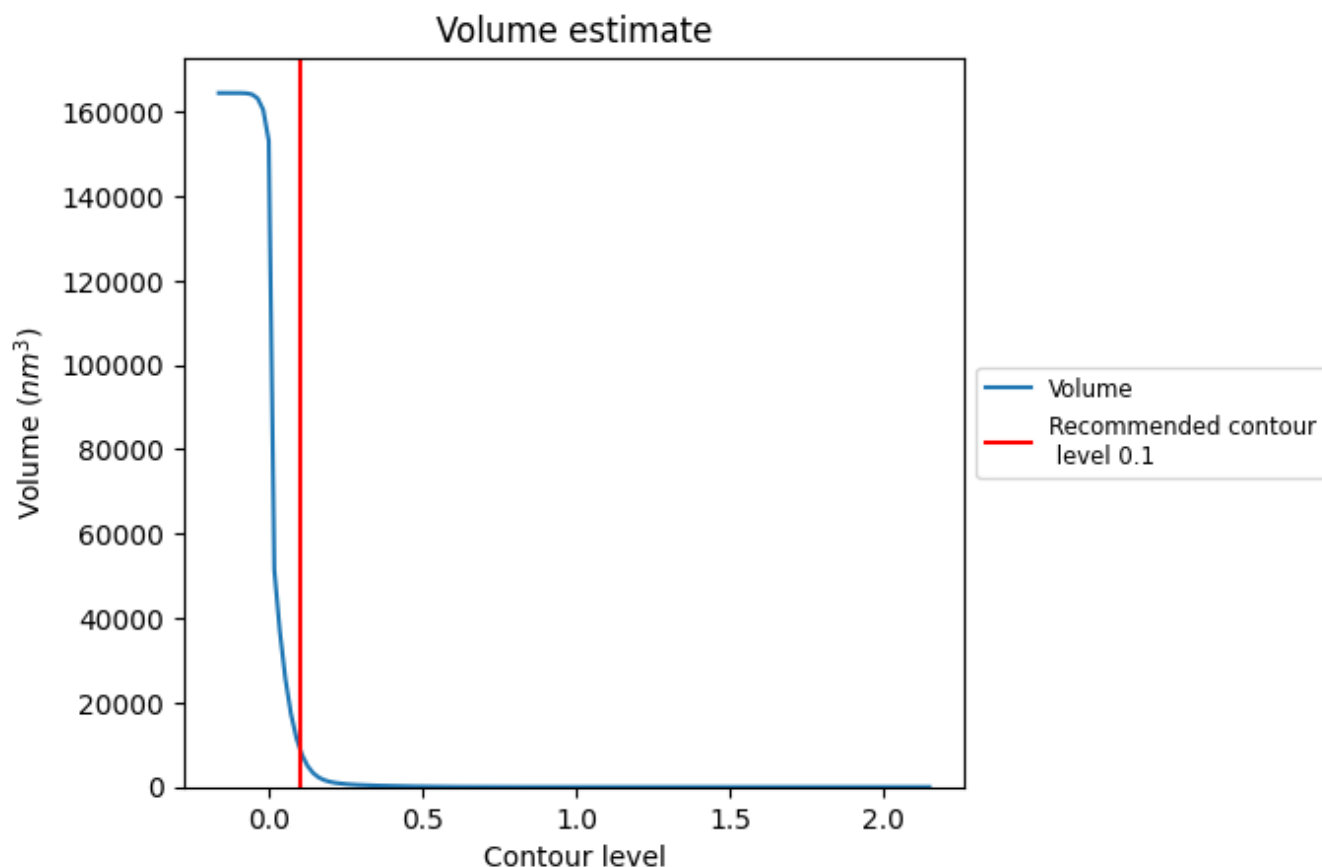
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

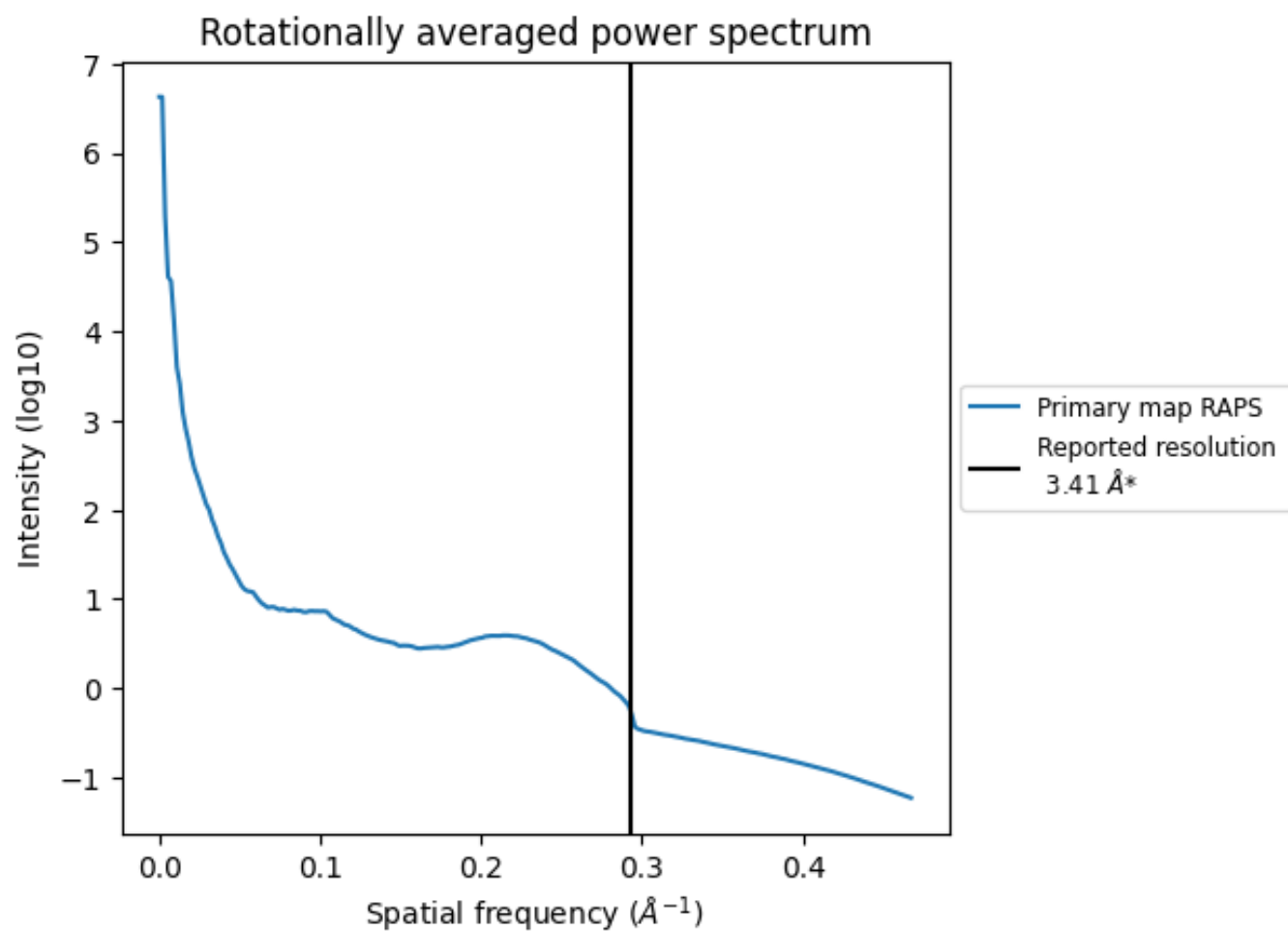
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9143 nm^3 ; this corresponds to an approximate mass of 8259 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 0.293 Å⁻¹

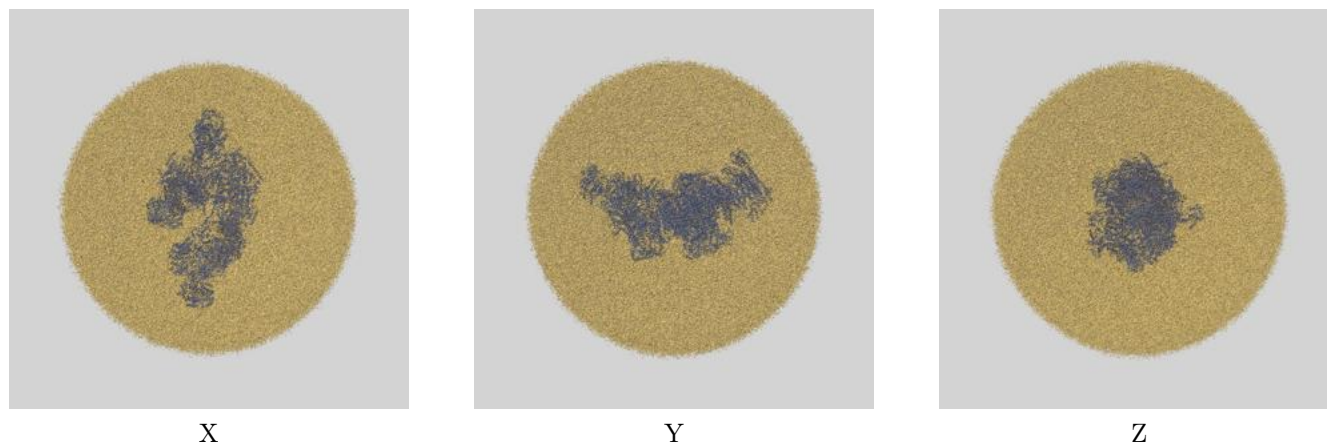
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

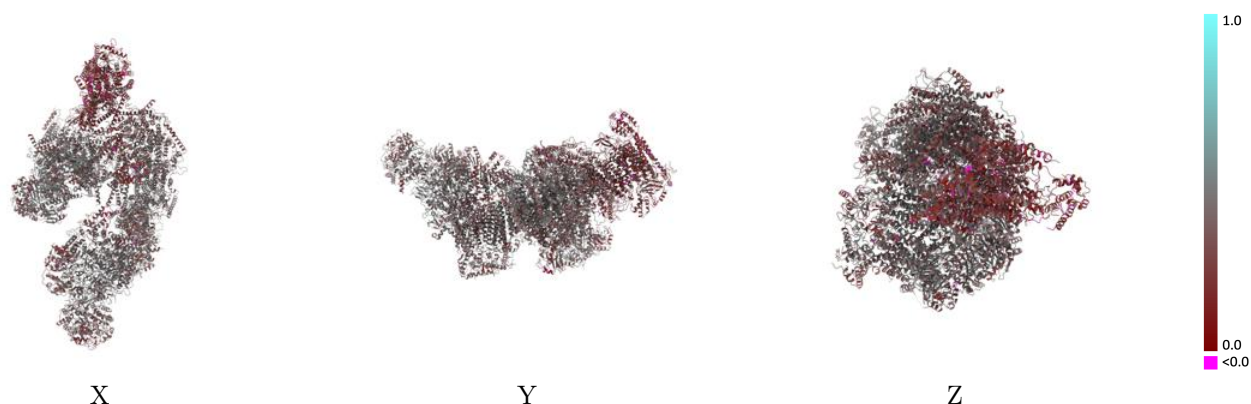
This section contains information regarding the fit between EMDB map EMD-45490 and PDB model 9CE2. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



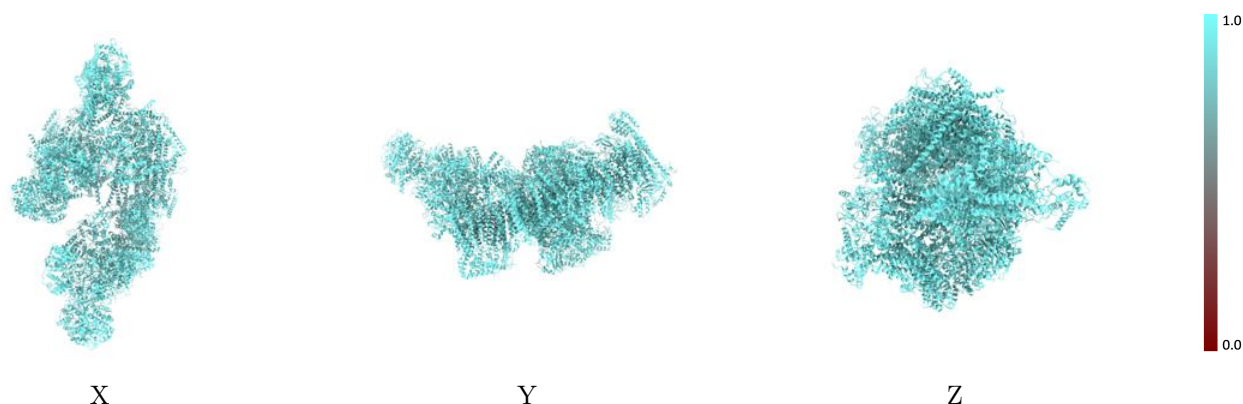
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



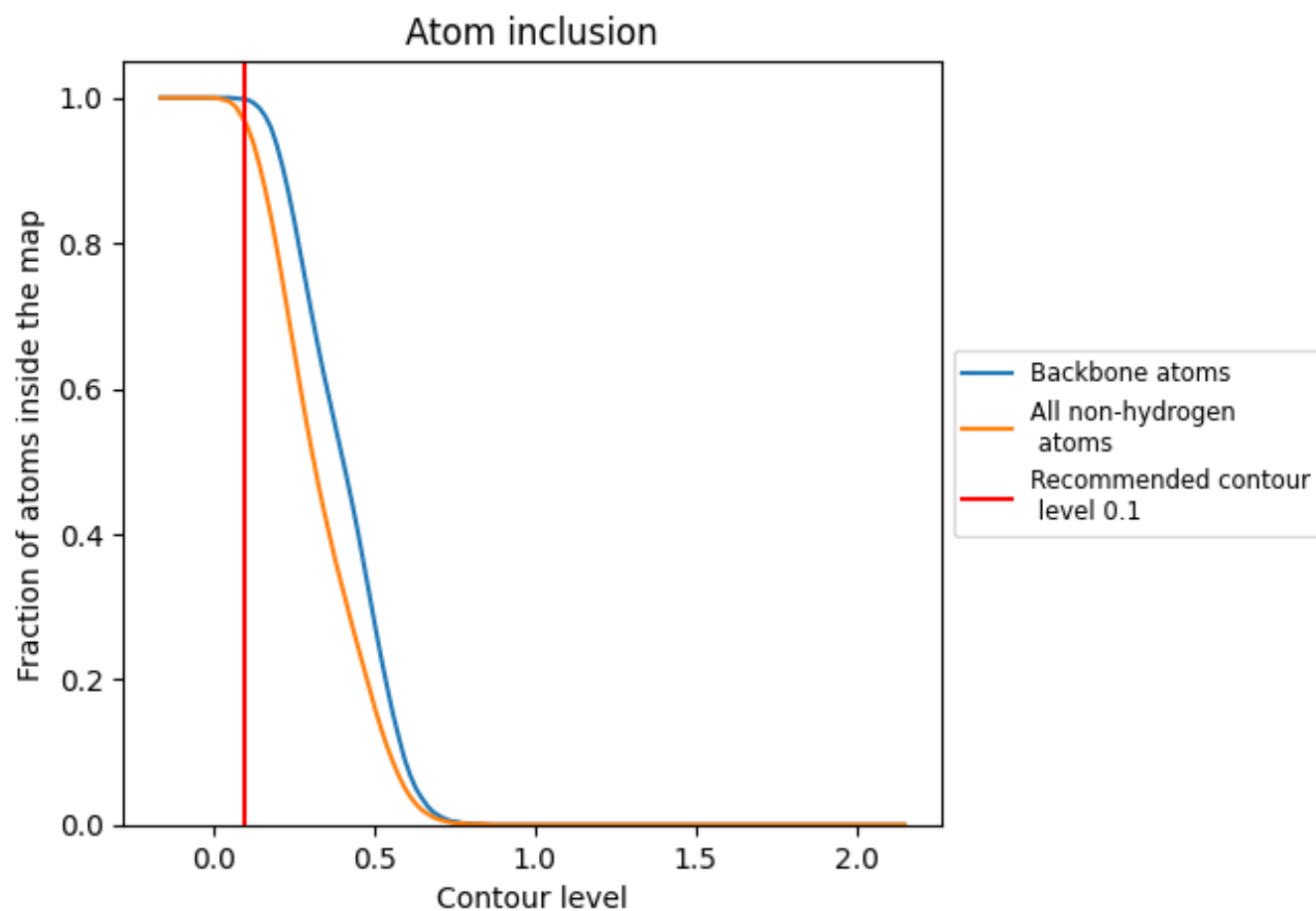
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.3770
0	 0.9580	 0.3210
1	 0.9880	 0.4190
2	 0.9480	 0.3390
3	 0.9830	 0.4170
4	 0.9590	 0.3310
5	 0.9820	 0.4210
6	 0.9770	 0.4170
7	 0.9740	 0.4400
8	 0.9780	 0.4210
9	 0.9540	 0.4050
A	 0.9700	 0.2370
Aa	 0.9720	 0.4120
Ab	 0.9510	 0.3380
Ac	 0.9830	 0.4040
Ad	 0.9750	 0.3950
Ae	 0.9180	 0.2260
Af	 0.8820	 0.2710
Ag	 0.9460	 0.2220
Ah	 0.9350	 0.2430
Ai	 0.9680	 0.2280
Aj	 0.9220	 0.2560
Ak	 0.9440	 0.2680
Al	 0.9660	 0.2470
Am	 0.9390	 0.2380
An	 0.9460	 0.2120
Ao	 0.9560	 0.1840
Ap	 0.9350	 0.2120
Aq	 0.9660	 0.1860
Ar	 0.9640	 0.2260
B	 0.9770	 0.3840
C	 0.9780	 0.4220
D	 0.9840	 0.4420
E	 0.9510	 0.3710
F	 0.9460	 0.4210











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Chain	Atom inclusion	Q-score
G	 0.9710	 0.4010
H	 0.9890	 0.4510
I	 0.9790	 0.4330
J	 0.9750	 0.4320
K	 0.9750	 0.4330
L	 0.9540	 0.3780
M	 0.9810	 0.4200
N	 0.9750	 0.3920
O	 0.9330	 0.2770
P	 0.9630	 0.3300
Q	 0.9670	 0.3860
R	 0.9480	 0.3290
S	 0.9910	 0.4140
T	 0.9760	 0.3900
U	 0.9570	 0.3770
V	 0.9700	 0.3820
W	 0.9790	 0.4080
X	 0.9580	 0.3020
Y	 0.9650	 0.3100
Z	 0.9460	 0.3060
a	 0.9760	 0.4160
b	 0.9750	 0.3310
c	 0.9610	 0.3670
d	 0.9720	 0.3620
e	 0.9550	 0.3670
f	 0.9810	 0.3730
g	 0.9620	 0.3970
h	 0.9550	 0.3850
i	 0.9740	 0.4390
j	 0.9270	 0.3790
k	 0.9680	 0.4130
l	 0.9590	 0.3940
m	 0.9420	 0.3540
n	 0.9500	 0.3750
o	 0.9500	 0.3380
p	 0.9650	 0.2680
q	 0.9680	 0.4410
r	 0.9630	 0.3960
s	 0.9740	 0.4030
t	 0.9780	 0.2980
u	 0.9730	 0.4200
v	 0.9770	 0.4190

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Chain	Atom inclusion	Q-score
w	 0.9830	 0.4390
x	 0.9790	 0.4240
y	 0.9690	 0.4150
z	 0.9780	 0.4120