



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 9BUH / pdb_00009buh
EMDB ID : EMD-44908
Title : Cryo-EM structure of respiratory supercomplex I III IV
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-17
Resolution : 2.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

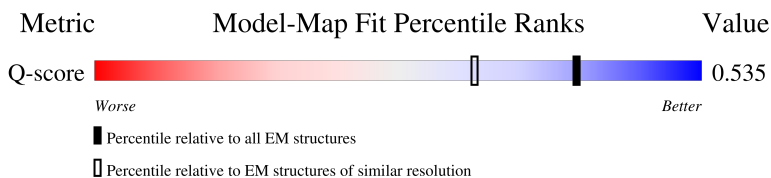
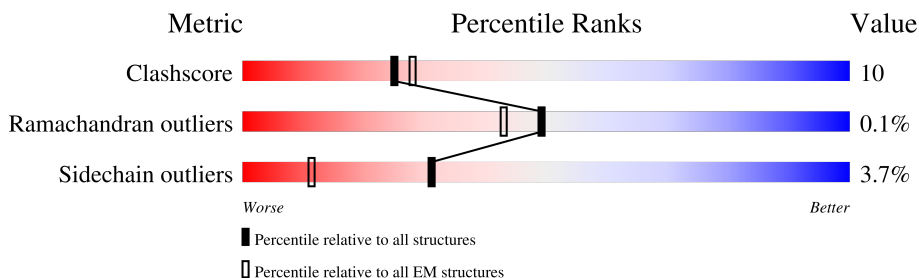
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



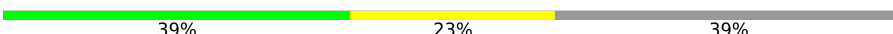
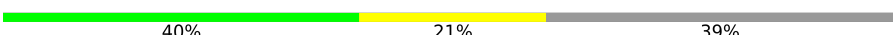
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A	74	
2	t	137	
3	F	123	
4	K	145	

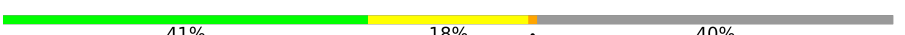
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Mol	Chain	Length	Quality of chain
5	U	357	
6	Z	114	
7	a	189	
8	i	347	
9	m	175	
10	p	221	
11	q	459	
12	Aa	82	
12	z	82	
13	0	91	
13	Ab	91	
14	1	64	
14	Ac	64	
15	3	56	
15	Ad	56	
16	Ag	70	
17	Ah	80	
18	Ai	80	
19	Aj	63	
20	Ak	514	
21	Al	228	
22	Am	261	
23	An	169	
24	Ao	152	
25	Ap	129	

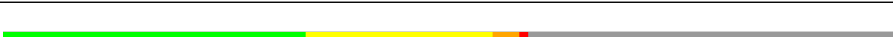
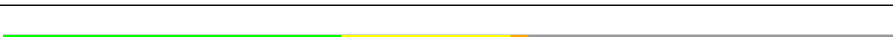
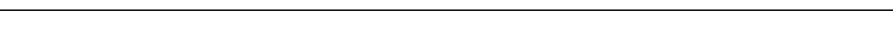
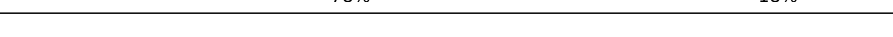
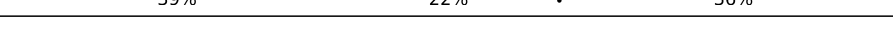
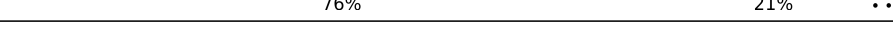
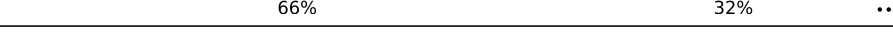
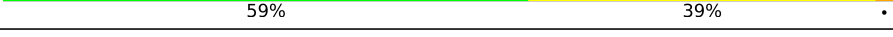
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Mol	Chain	Length	Quality of chain
26	Aq	97	
27	Ar	86	
28	2	299	
28	4	299	
28	Ae	299	
28	Af	299	
29	5	480	
29	u	480	
30	6	453	
30	v	453	
31	7	379	
31	w	379	
32	8	326	
32	x	326	
33	9	111	
33	y	111	
34	B	464	
35	C	469	
36	D	264	
37	E	249	
38	G	727	
39	H	212	
40	I	258	
41	J	175	
42	L	372	

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Mol	Chain	Length	Quality of chain
43	M	113	
44	N	116	
45	O	156	
45	X	156	
46	P	99	
47	Q	154	
48	S	70	
49	T	169	
50	V	141	
51	W	144	
52	Y	105	
53	b	188	
54	c	186	
55	d	176	
56	e	154	
57	f	76	
58	g	122	
59	h	106	
60	j	115	
61	k	98	
62	l	606	
63	n	58	
64	o	129	
65	r	318	
66	s	249	

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Mol	Chain	Length	Quality of chain
67	R	110	

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
69	FES	2	301	-	-	X	-
73	SF4	B	502	-	-	X	-
73	SF4	G	802	-	-	X	-

2 Entry composition

There are 75 unique types of molecules in this entry. The entry contains 112807 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 c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	70	Total	C	N	O	S	0	0
			575	375	103	93	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	t	119	Total	C	N	O	S	0	0
			991	619	186	177	9		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

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

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

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

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

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

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	175	Total	C	N	O	S	0	0
			1338	897	190	238	13		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 12 is a protein called Cytochrome b-c1 complex subunit 8.

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

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		
13	0	68	Total	C	N	O	S	0	0
			561	341	101	114	5		

- Molecule 14 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Ac	59	Total	C	N	O	0	0
			485	318	85	82		
14	1	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 15 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ad	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
15	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 8.

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 7B.

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

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

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ak	513	Total	C	N	O	S	0	0
			4014	2686	623	673	32		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 22 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 23 is a protein called Cytochrome c oxidase subunit 4.

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

- Molecule 24 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 25 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ap	91	Total	C	N	O	S	0	0
			697	433	123	135	6		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 6A2.

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

- Molecule 27 is a protein called Cytochrome c oxidase subunit.

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

- Molecule 28 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	195	Total	C	N	O	S	0	0
			1513	953	264	289	7		
28	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
28	Ae	39	Total	C	N	O	S	0	0
			275	172	53	47	3		
28	Af	33	Total	C	N	O	S	0	0
			223	141	39	41	2		

- Molecule 29 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		
29	u	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 30 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
30	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 31 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

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

- Molecule 32 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	239	Total	C	N	O	S	0	0
			1906	1217	328	345	16		
32	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

- Molecule 33 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	9	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
33	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L	340	Total	C	N	O	S	0	0
			2735	1771	479	476	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	96	Total	C	N	O	S	0	0
			773	487	146	137	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5 isoform X1.

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

- Molecule 45 is a protein called Acyl carrier protein.

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

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 1.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 51 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

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

- Molecule 52 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Y	62	Total	C	N	O	S	0	0
			536	355	89	91	1		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	b	110	Total	C	N	O	S	0	0
			915	598	161	155	1		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	c	153	Total	C	N	O	S	0	0
			1291	838	208	237	8		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	e	99	Total	C	N	O	S	0	0
			826	530	137	155	4		

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 60 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	j	114	Total	C	N	O	S	0	0
			899	606	133	155	5		

- Molecule 61 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 62 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	l	602	Total	C	N	O	S	0	0
			4777	3169	740	818	50		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 65 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

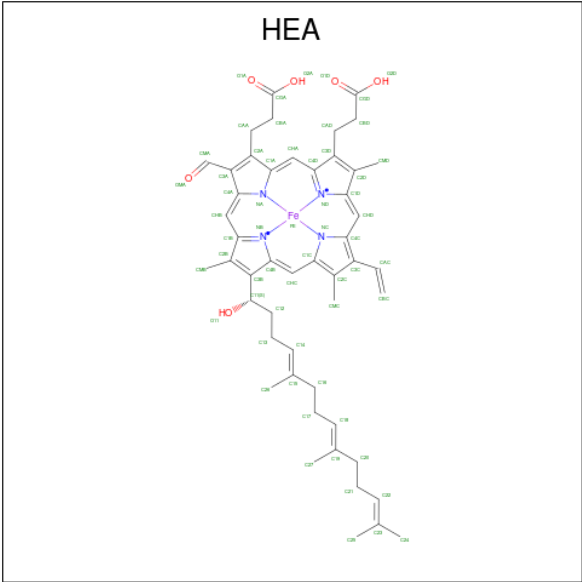
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

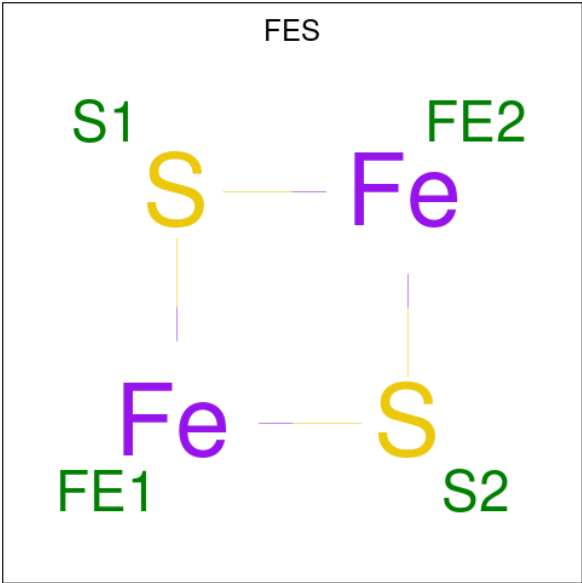
Mol	Chain	Residues	Atoms					AltConf	Trace
67	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

- Molecule 68 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



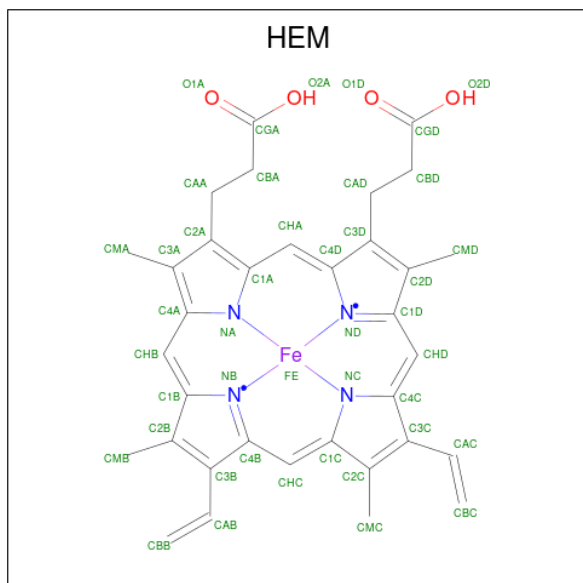
Mol	Chain	Residues	Atoms			AltConf
69	2	1	Total	Fe	S	0
			4	2	2	
69	4	1	Total	Fe	S	0
			4	2	2	

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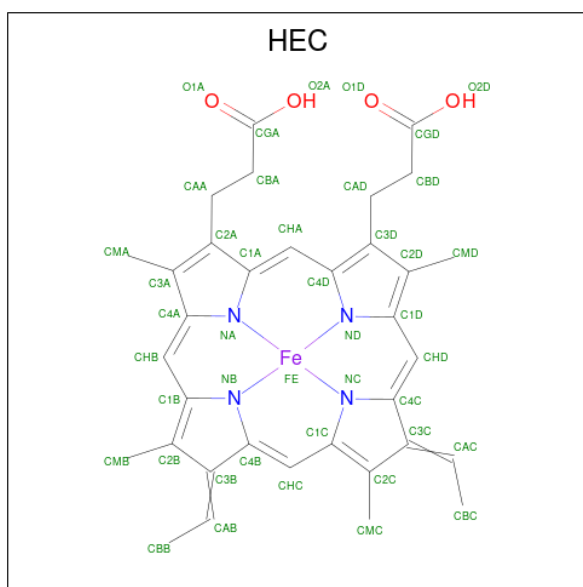
Mol	Chain	Residues	Atoms			AltConf
69	E	1	Total	Fe	S	0
			4	2	2	
69	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 70 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



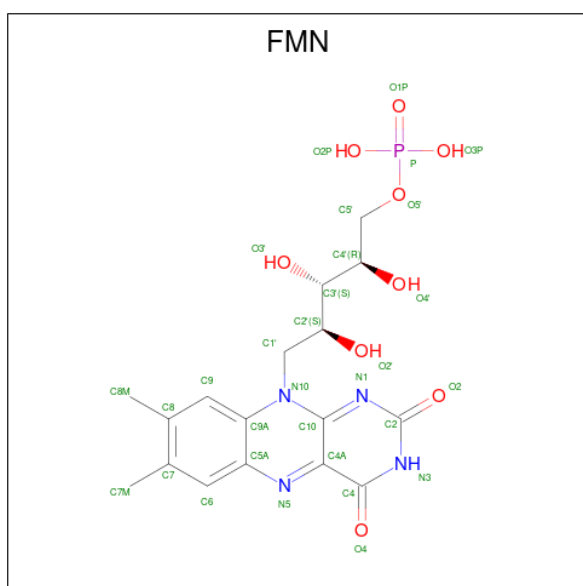
Mol	Chain	Residues	Atoms					AltConf
70	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



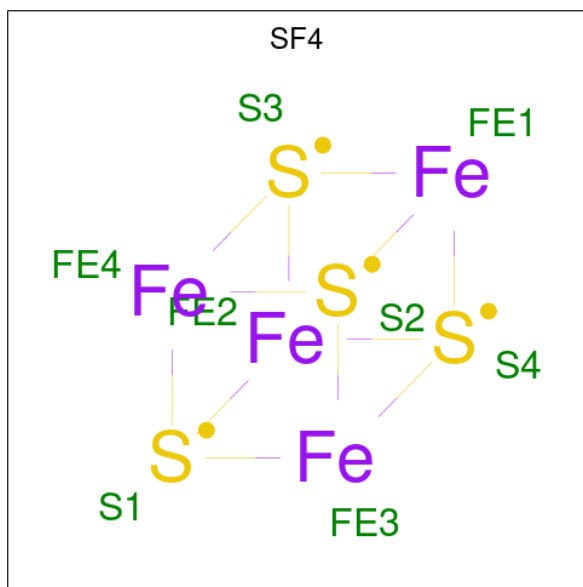
Mol	Chain	Residues	Atoms					AltConf
71	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
71	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 72 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



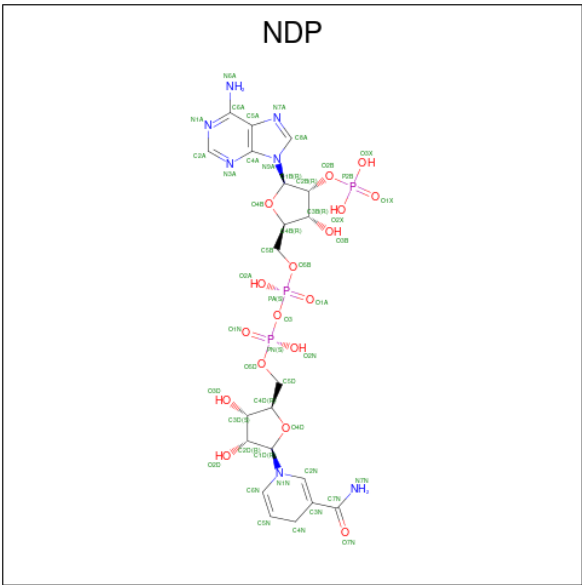
Mol	Chain	Residues	Atoms					AltConf
72	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 73 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



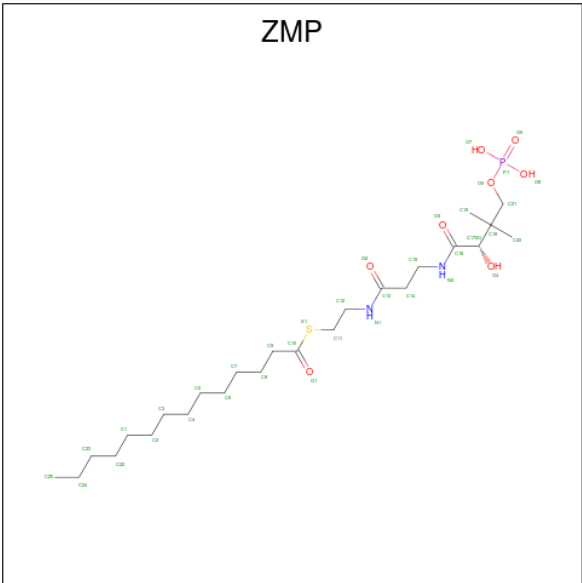
Mol	Chain	Residues	Atoms			AltConf
73	B	1	Total	Fe	S	0
			8	4	4	
73	G	1	Total	Fe	S	0
			8	4	4	
73	G	1	Total	Fe	S	0
			8	4	4	
73	H	1	Total	Fe	S	0
			8	4	4	
73	H	1	Total	Fe	S	0
			8	4	4	
73	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 74 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
74	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

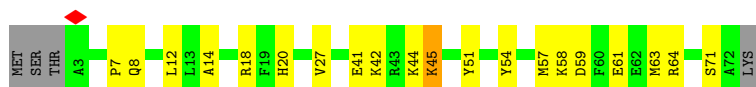


3 Residue-property plots [i](#)

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.

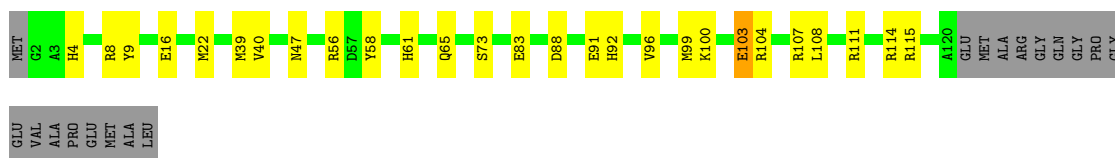
- Molecule 1: Cytochrome c oxidase subunit 6C

Chain A: 



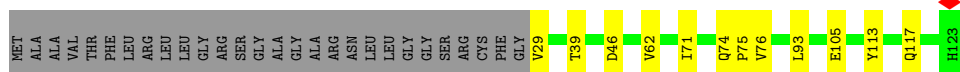
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t: 



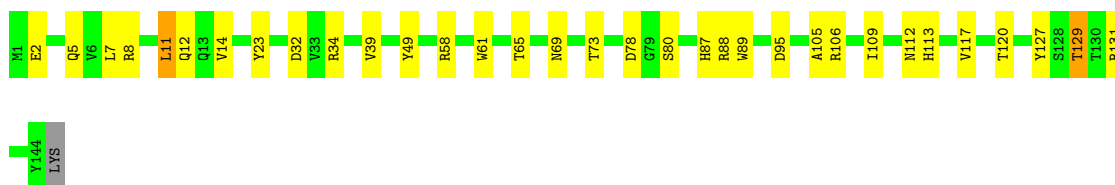
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain K: 



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

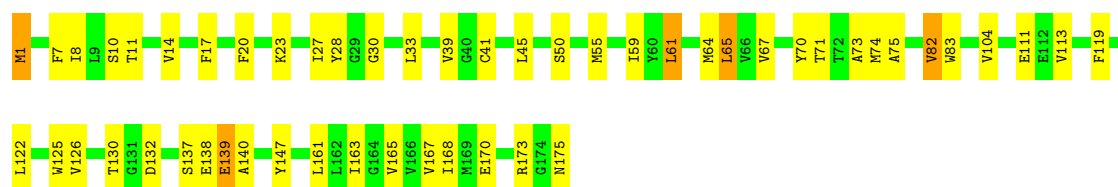
V271	D102	ME1
V272	D107	LEU
L278	V108	ARG
D281	Q109	LEU
P284	L110	LEU
Q288	S115	ARG
L307	K118	ALA
R308	S130	ALA
Y309	L143	ALA
T310	A148	ALA
T311	V159	PR0
T312	V160	ARG
P313	L161	GLY
V314	E162	GLY
P317	R163	ALA
H324	V170	VAL
V329	F171	ALA
L336	L172	GLN
D348	M175	ARG
V349	Q178	VAL
K352	Y189	GLY
W353	V205	GLY
L354	V205	ILE
W355	N225	HIS
L356	E228	THR
R357	M229	GLY
	D238	ALA
	A242	PR0
	Y243	CYS
	K244	ARG
	L248	LEU
	P249	LEU
	E250	GLN
	C255	Y40
	E256	L43
	V257	A44
	L258	E49
	Q259	T56
	Y260	S59
	R263	I62
	E264	K72
		E78
		K82
		F88

- | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|------|
| SER | GLN | ASN | LYS | ASP | LYS | LYS | HIS | HIS |
| MET | LEU | VAL | LEU | ARG | GLY | GLN | ILE | ALA |
| | | | | | | VAL | SER | PHE |
| | | | | | | PRO | ILE | ASP |
| | | | | | | ASP | MET | ALA |
| | | | | | | HIS | GLY | HIS |
| | | | | | | GLY | GLY | HIS |
| | | | | | | GLU | HIS | GLY |
| | | | | | | HIS | HIS | HIS |
| | | | | | | S28 | K29 | N30 |
| | | | | | | E31 | Y35 | T47 |
| | | | | | | | | V48 |
| | | | | | | | | Q49 |
| | | | | | | | | E50 |
| | | | | | | | | R51 |
| | | | | | | | | L52 |
| | | | | | | | | L57 |
| | | | | | | | | R63 |
| | | | | | | | | N64 |
| | | | | | | | | E65 |
| | | | | | | | | A66 |
| | | | | | | | | D67 |
| | | | | | | | | R68 |
| | | | | | | | | Y69 |
| | | | | | | | | K88 |
| | | | | | | | | V98 |
| | | | | | | | | E101 |
| | | | | | | | | Y102 |
| | | | | | | | | L104 |
| | | | | | | | | F105 |

- | | | | | | |
|-----|-----|-----|-----|-----|-----|
| V82 | A83 | I84 | V91 | I101 | K130 | K131 | N132 | V133 | E134 | I139 | K146 | A147 | R150 | W168 | V169 | Q170 | I174 | D175 | K176 | I179 | K184 | T185 | P187 | D188 | M189 | |
| ALA | ALA | ALA | SER | LEU | GLN | ARG | ALA | SER | VAL | THR | ALA | VAL | ALA | THR | THR | LEU | SER | ARG | ARG | GLY | THR | PHE | PHE | GLY | GLY | GLY | PHE | LEU | THR | HIS | GLY | PHE | PRO | LYS | THR | GLY | ALA | PRO | VAL | ARG | HIS | SER | SER | ASP | GLY | HIS | GLY | K52 | R53 | P59 | F67 | T80 | R81 |

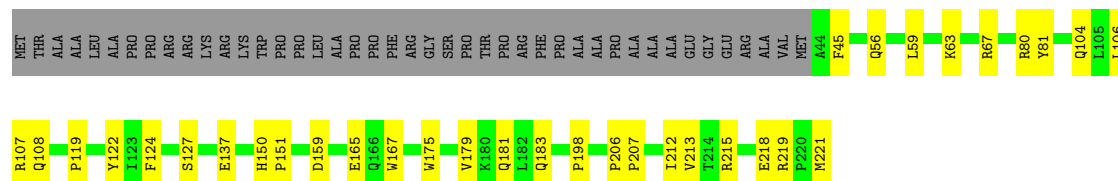
- | | | | |
|------|------|------|------|
| L337 | S222 | M104 | M1 |
| P338 | L228 | K105 | Y6 |
| M339 | S231 | G107 | L9 |
| T340 | H232 | L108 | |
| P341 | T233 | H112 | T12 |
| A342 | P234 | V115 | V13 |
| L343 | M235 | P116 | M14 |
| S344 | K236 | E117 | T17 |
| S345 | M237 | I122 | M18 |
| L346 | M244 | L128 | L19 |
| N347 | L248 | K135 | V20 |
| | L249 | L136 | |
| | S250 | A137 | W26 |
| | M251 | P138 | L28 |
| | S258 | V141 | I29 |
| | G259 | I145 | W30 |
| | F260 | S148 | I31 |
| | M261 | I149 | E34 |
| | M265 | M154 | M35 |
| | I266 | L155 | N36 |
| | Q268 | I164 | L37 |
| | E269 | G168 | L38 |
| | M270 | Q172 | A39 |
| | M278 | L175 | M40 |
| | M282 | A180 | I41 |
| | N289 | I184 | P42 |
| | L290 | T191 | V43 |
| | Y291 | A192 | L44 |
| | Y292 | V193 | M45 |
| | Y293 | L200 | K46 |
| | M294 | I201 | |
| | R295 | L203 | T57 |
| | L296 | N204 | F60 |
| | | I209 | L61 |
| | N310 | L213 | T65 |
| | M311 | A214 | M71 |
| | K312 | M215 | I74 |
| | M313 | F316 | |
| | K314 | | W77 |
| | W315 | | L78 |
| | Q316 | | L79 |
| | F317 | | I86 |
| | | | T87 |
| | L325 | | K88 |
| | M329 | | M89 |
| | | | |
| | | | M95 |
| | | | T96 |
| | | | |
| | | | M100 |

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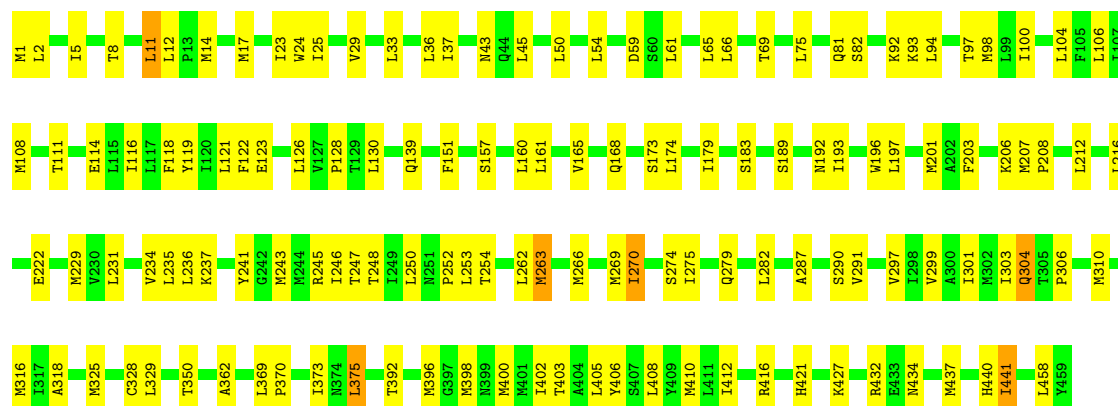
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 65% 15% 19%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4

Chain q: 70% 29%



- Molecule 12: Cytochrome b-c1 complex subunit 8

Chain Aa: 74% 18% 5%



- Molecule 12: Cytochrome b-c1 complex subunit 8

Chain z: 79% 16%



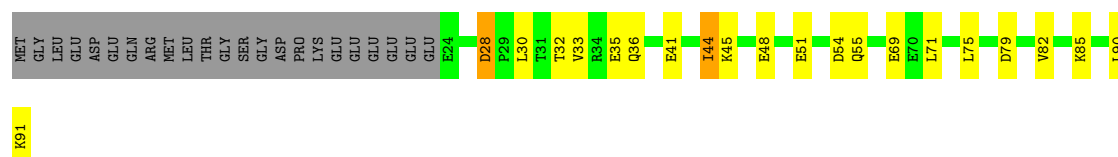
- Molecule 13: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ab: 



- Molecule 13: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 0: 



- Molecule 14: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain Ac: 



- Molecule 14: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 1: 



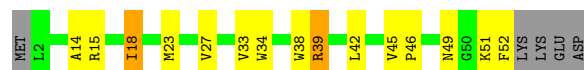
- Molecule 15: Cytochrome b-c1 complex subunit 10

Chain Ad: 

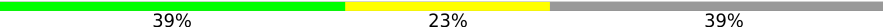


- Molecule 15: Cytochrome b-c1 complex subunit 10

Chain 3: 



- Molecule 16: Cytochrome c oxidase subunit 8

Chain Ag: 

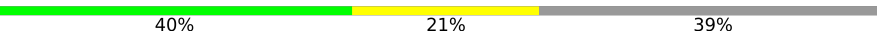


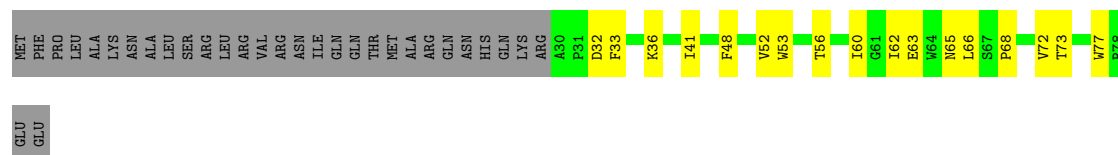
- Molecule 17: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain Ah: 



- Molecule 18: Cytochrome c oxidase subunit 7B

Chain Ai: 



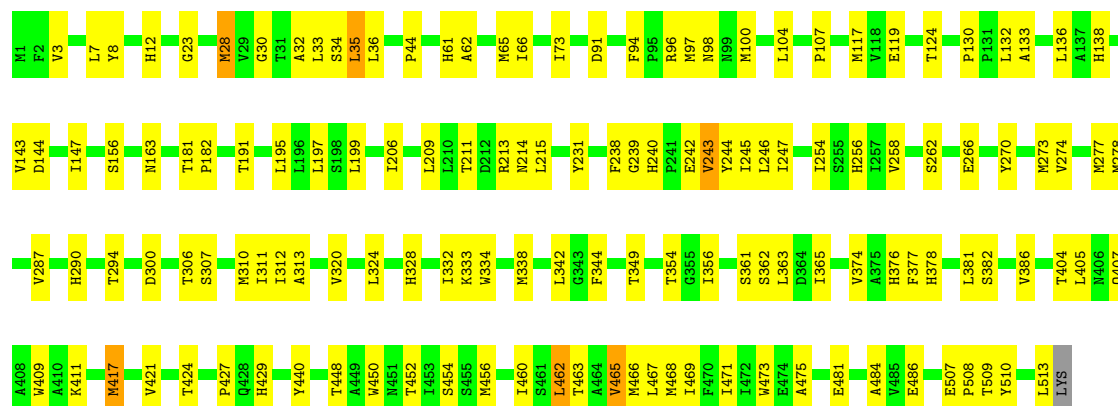
- Molecule 19: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Aj: 



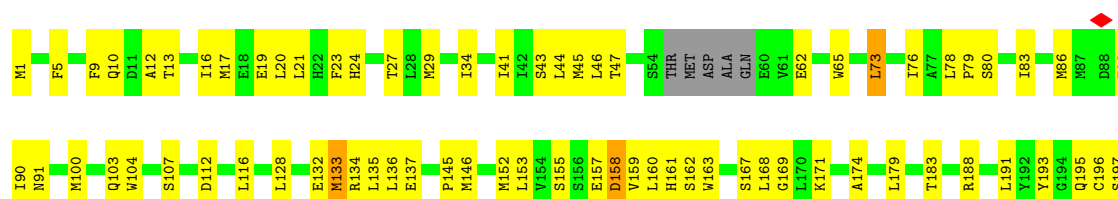
- Molecule 20: Cytochrome c oxidase subunit 1

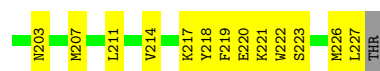
Chain Ak: 



- Molecule 21: Cytochrome c oxidase subunit 2

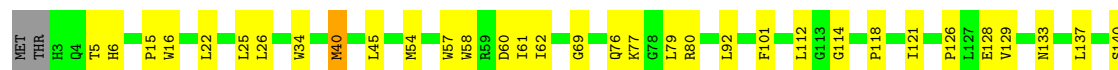
Chain Al: 





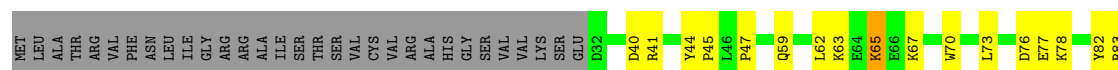
• Molecule 22: Cytochrome c oxidase subunit 3

Chain Am: 77% 21% ..



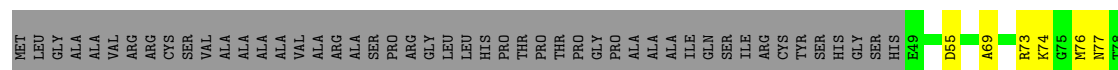
• Molecule 23: Cytochrome c oxidase subunit 4

Chain An: 56% 24% • 18%



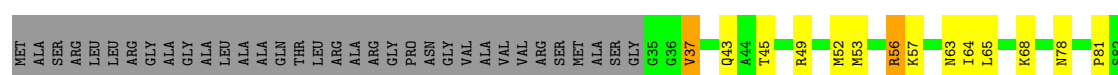
• Molecule 24: Cytochrome c oxidase subunit 5A, mitochondrial

Chain Ao: 50% 17% • 32%



• Molecule 25: Cytochrome c oxidase subunit 5B, mitochondrial

Chain Ap: 45% 24% • 29%



• Molecule 26: Cytochrome c oxidase subunit 6A2

Chain Aq: 57% 19% 25%



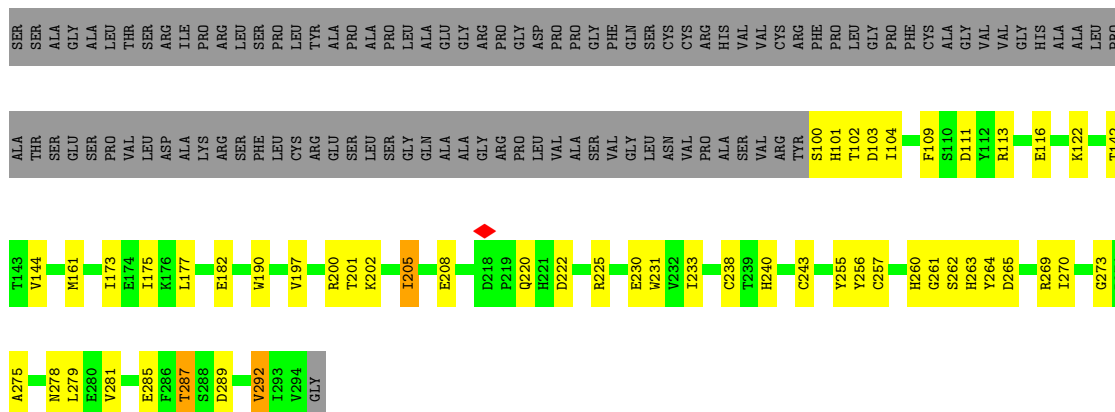
- Molecule 27: Cytochrome c oxidase subunit

Chain Ar: 55% 40% 5%



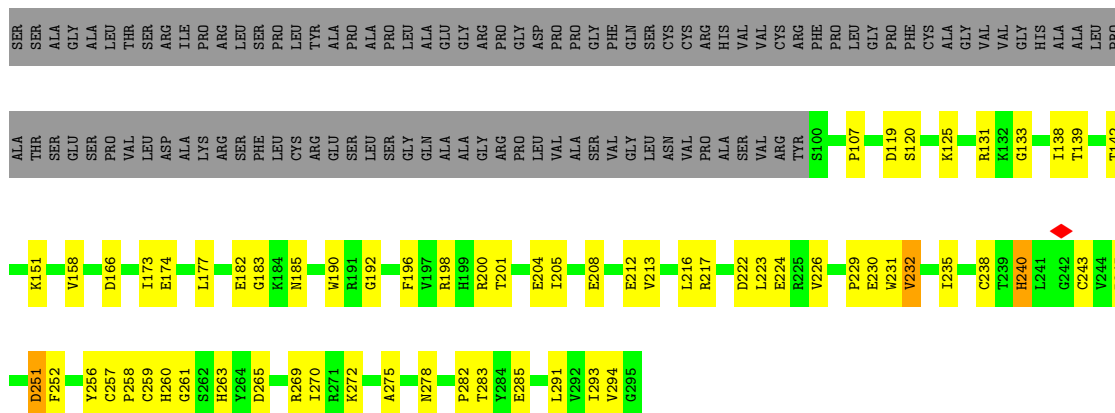
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 2: 47% 17% 35%



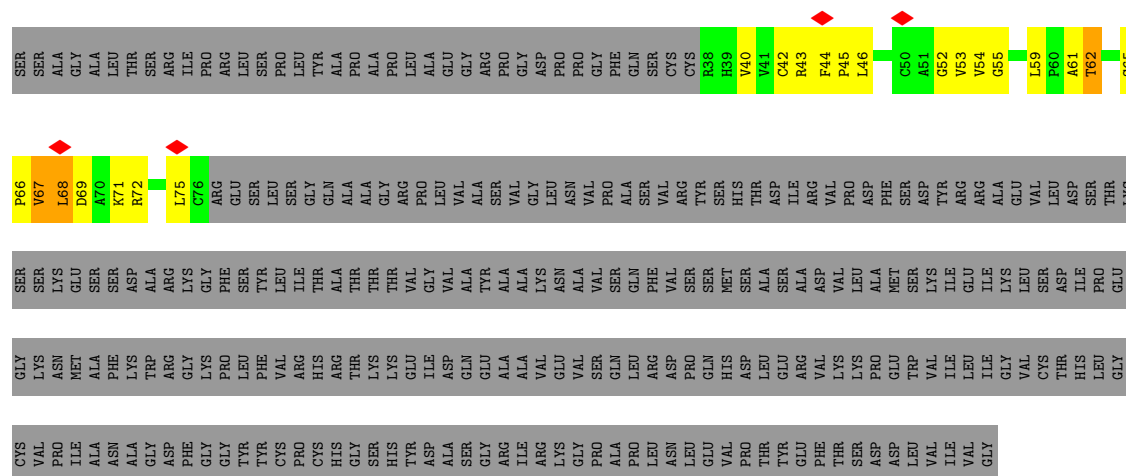
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 4: 44% 21% 34%



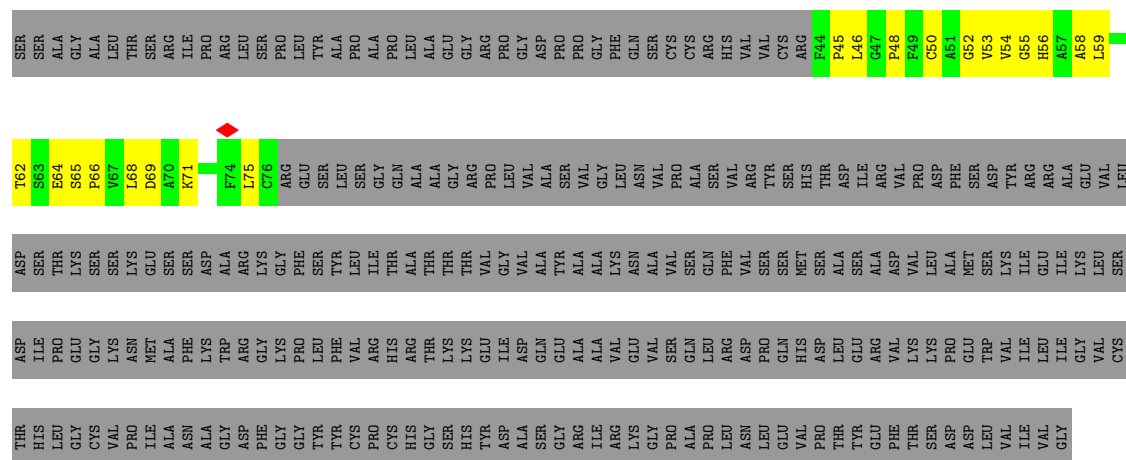
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Ae: 6% 6% 87%



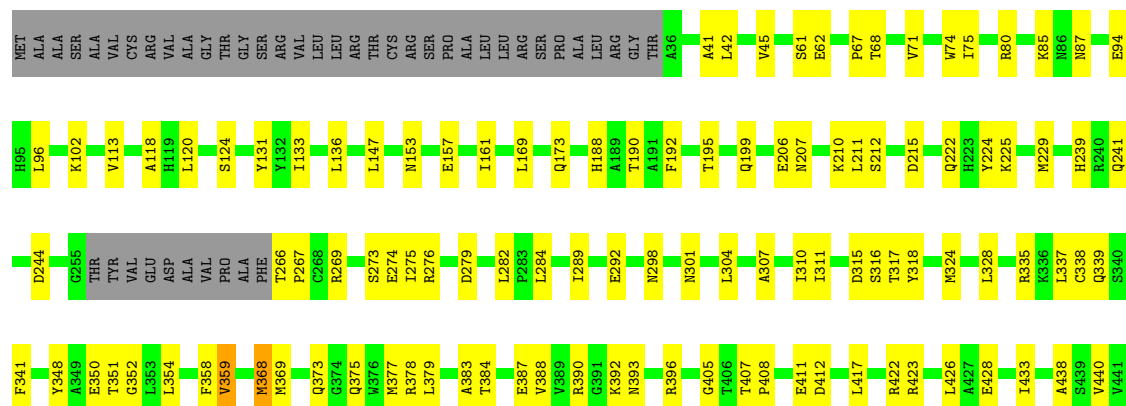
- Molecule 28: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Af: 5% 6% 89%



- Molecule 29: Cytochrome b-c1 complex subunit 1, mitochondrial

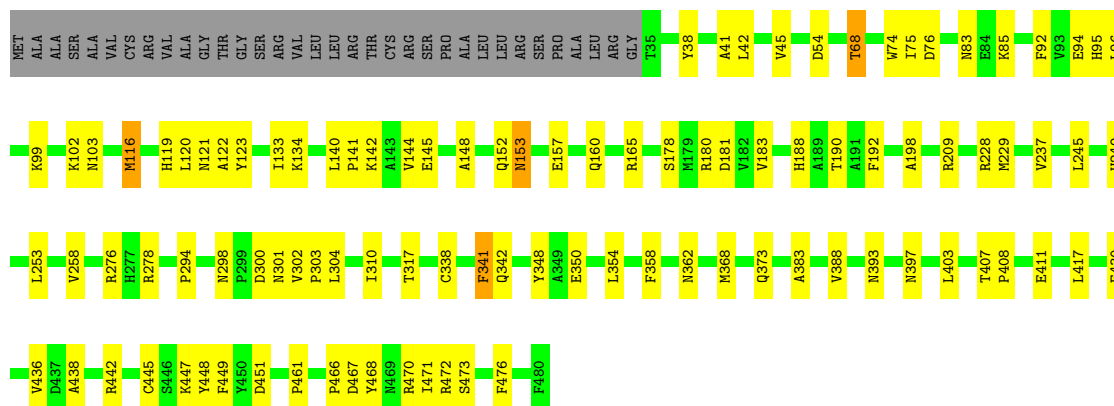
Chain 5: 64% 26% 9%





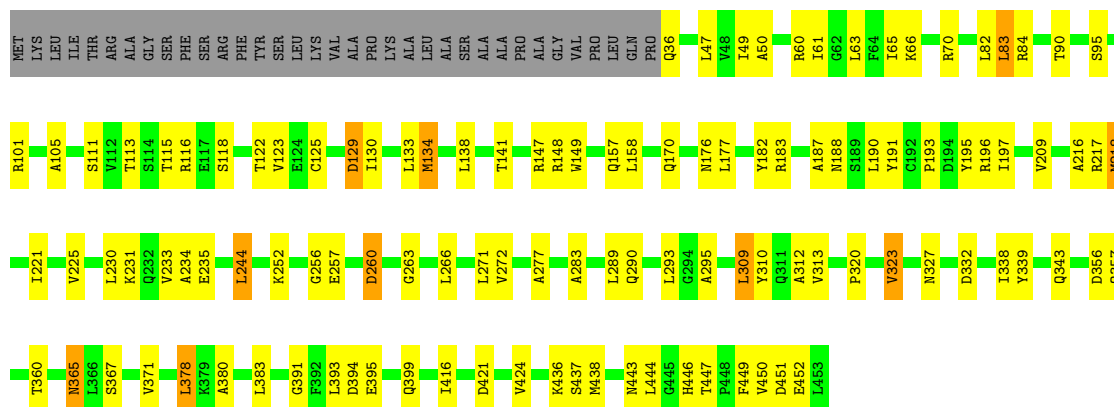
- Molecule 29: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain u: 72% 20% 7%



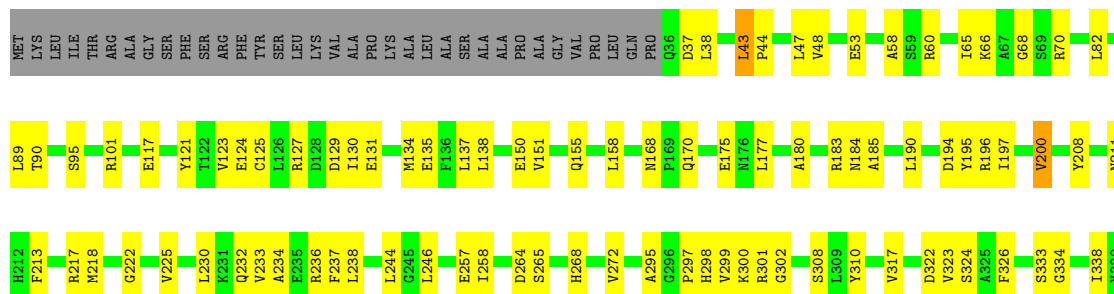
- Molecule 30: Cytochrome b-c1 complex subunit 2, mitochondrial

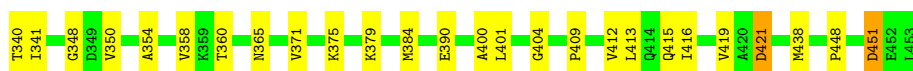
Chain 6: 67% 23% 8%



- Molecule 30: Cytochrome b-c1 complex subunit 2, mitochondrial

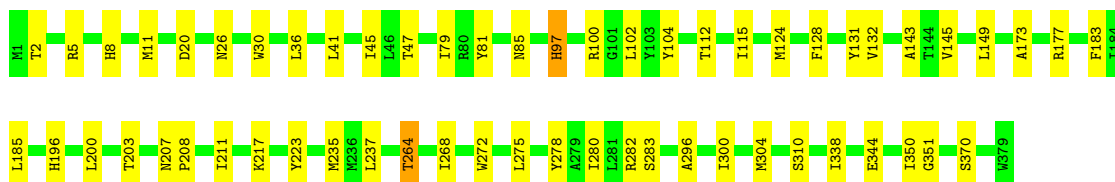
Chain v: 67% 24% 8%





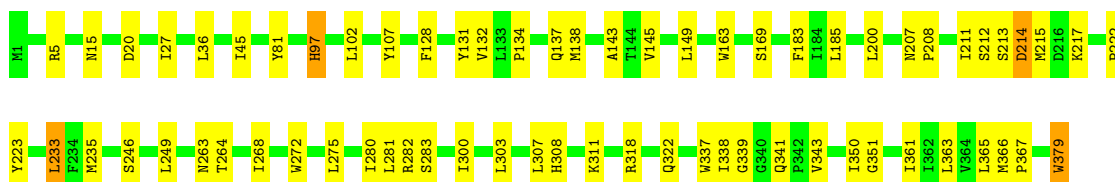
• Molecule 31: Cytochrome b

Chain 7: 85% 15%



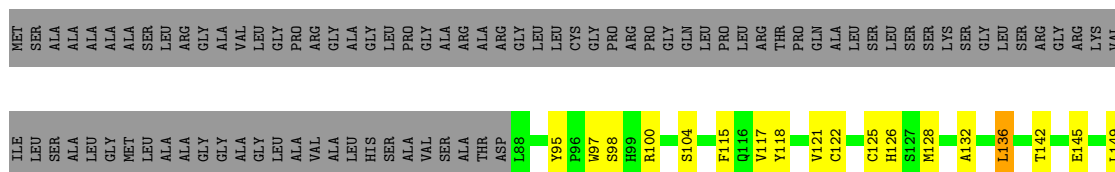
• Molecule 31: Cytochrome b

Chain w: 82% 17%



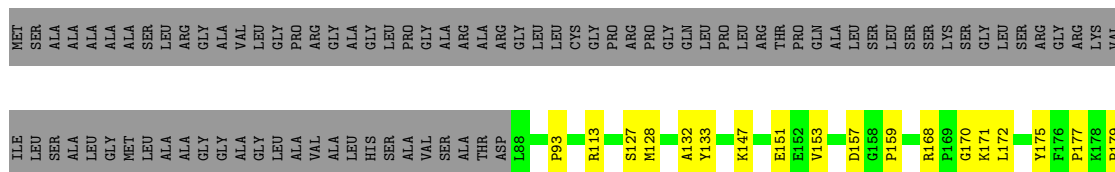
• Molecule 32: Cytochrome c1

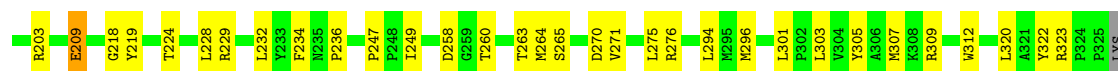
Chain 8: 56% 16% 27%



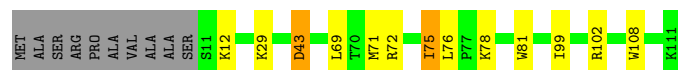
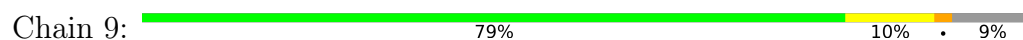
• Molecule 32: Cytochrome c1

Chain x: 58% 15% 27%

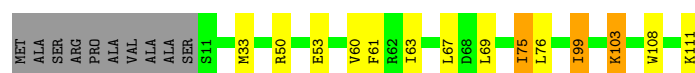
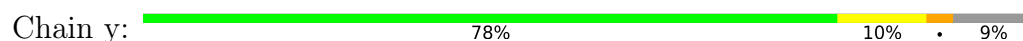




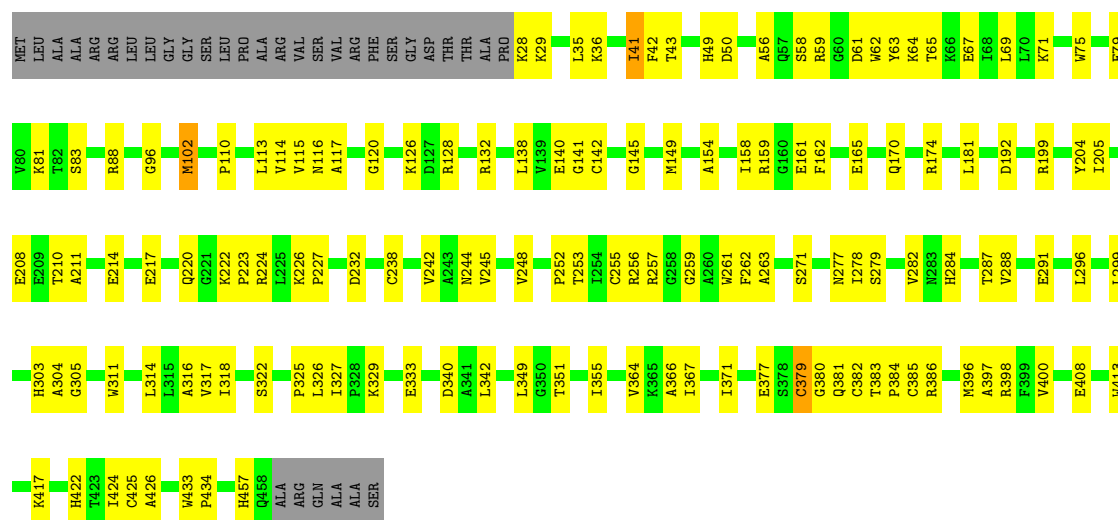
• Molecule 33: Cytochrome b-c1 complex subunit 7



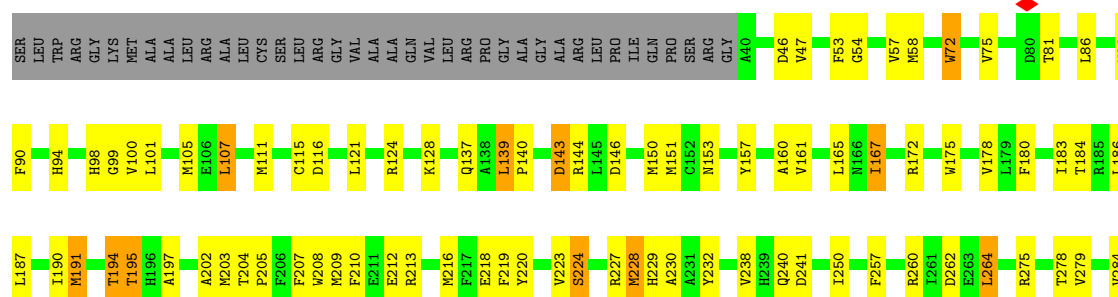
• Molecule 33: Cytochrome b-c1 complex subunit 7

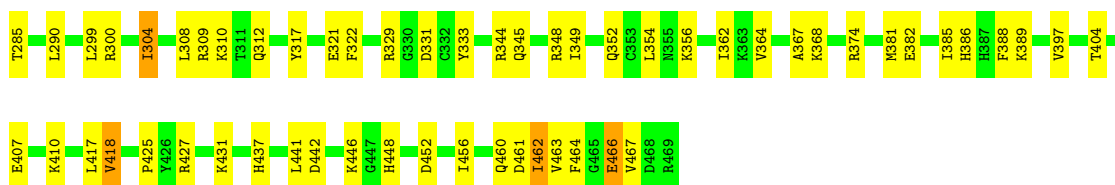


• Molecule 34: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

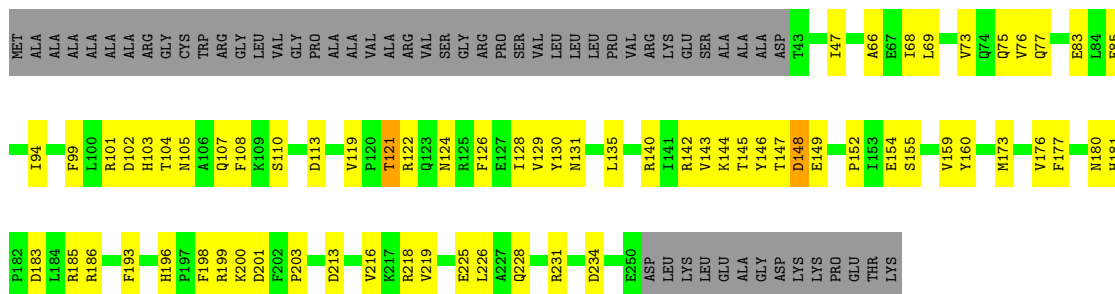


• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

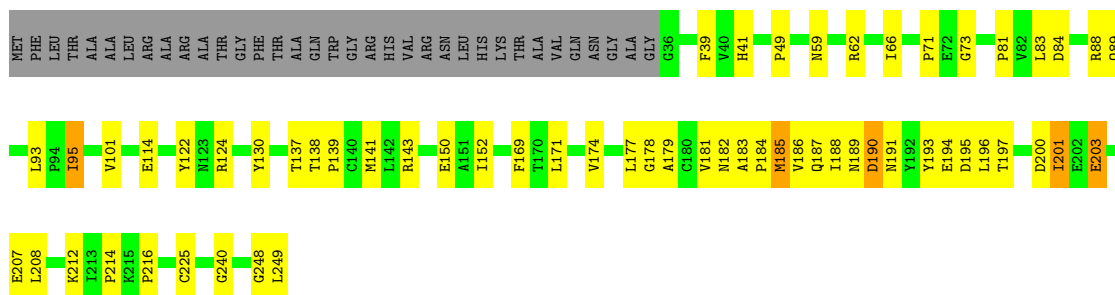




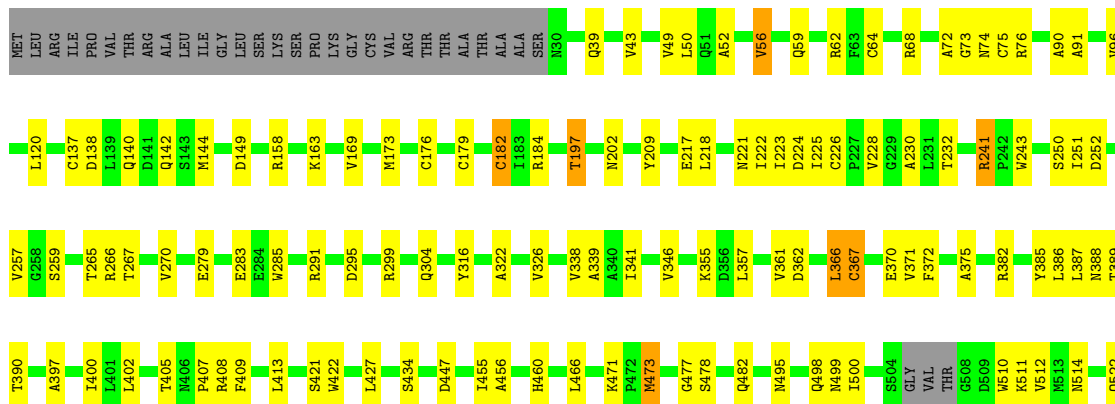
- Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

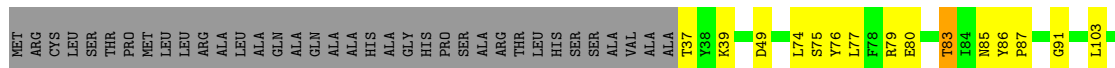


- Molecule 38: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

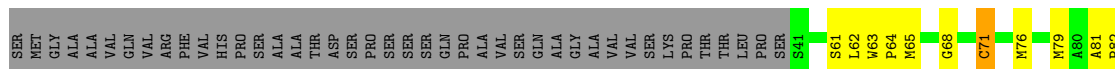




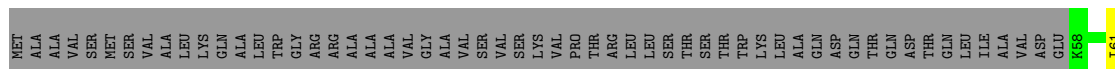
- Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



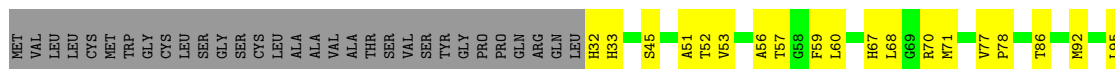
- Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

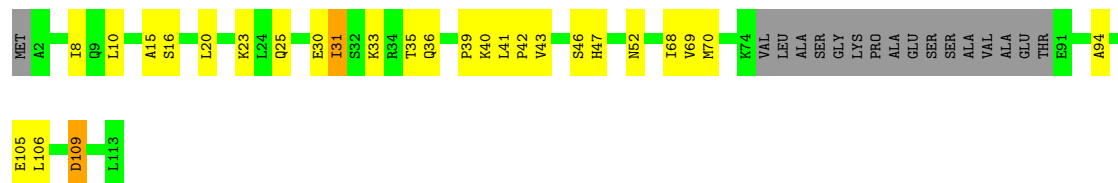


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial





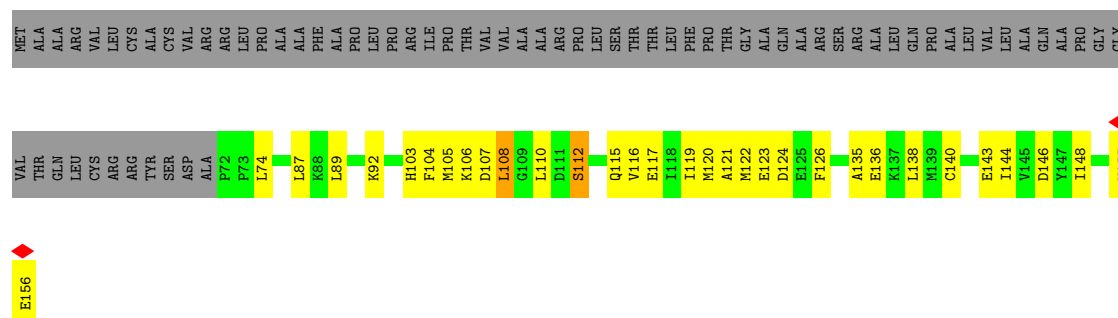
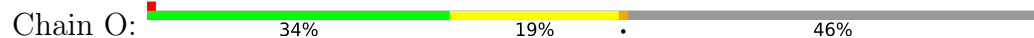
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



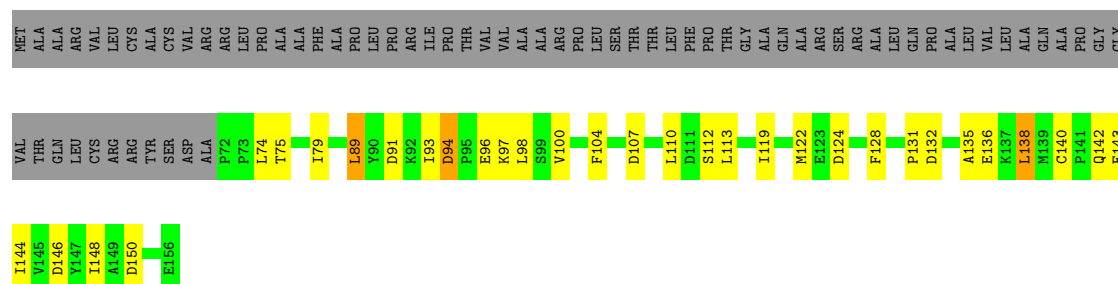
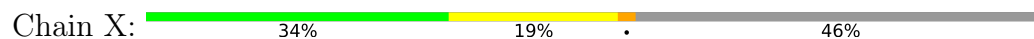
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



- Molecule 45: Acyl carrier protein

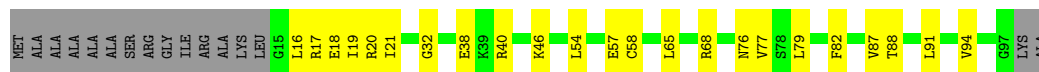


- Molecule 45: Acyl carrier protein



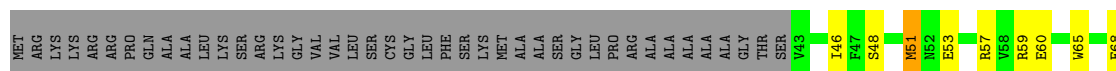
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P:  61% 23% 16%



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q:  53% 18% 27%



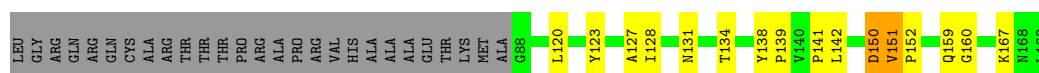
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  71% 27% 2%



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T:  39% 8% 51%



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  89% 10% 1%



- Molecule 51: NADH:ubiquinone oxidoreductase subunit A13

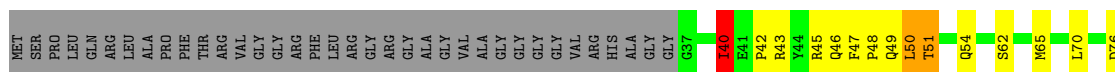
Chain W:  73% 24% 3%





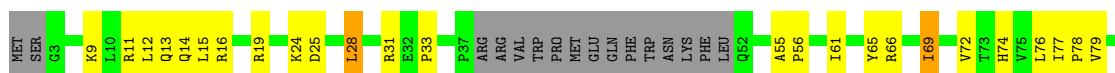
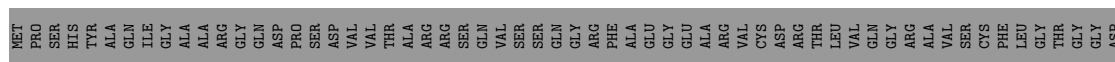
- Molecule 52: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 34% 21% 41%



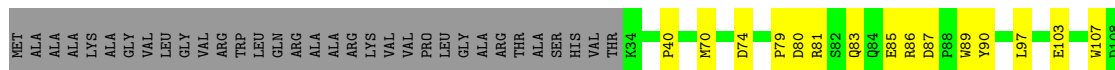
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 38% 19% 41%



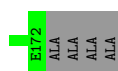
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 61% 20% 18%

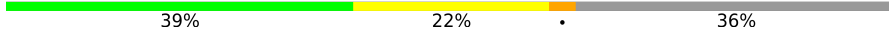


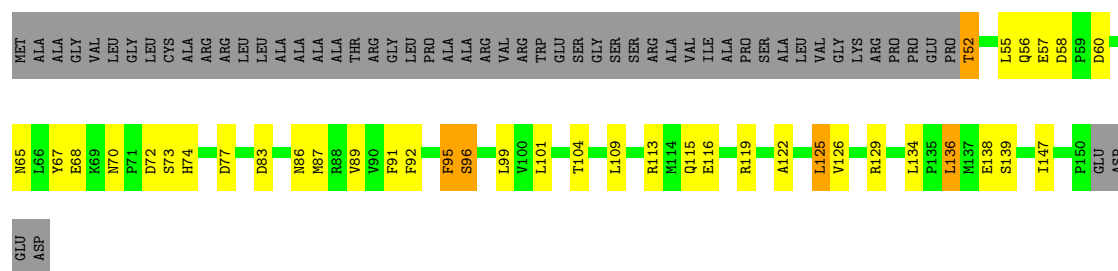
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 78% 18% 4%



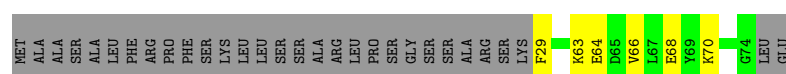
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



- Molecule 57: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



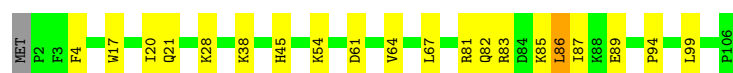
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



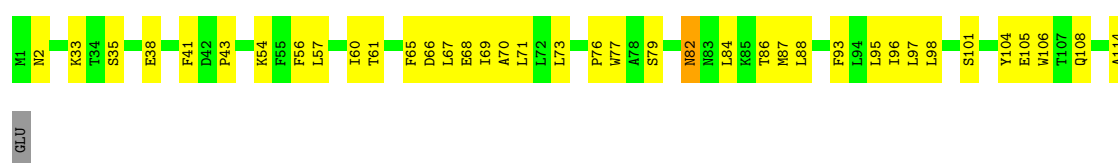
- Molecule 59: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



- Molecule 60: NADH-ubiquinone oxidoreductase chain 3

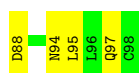
Chain j: 



- Molecule 61: NADH-ubiquinone oxidoreductase chain 4L

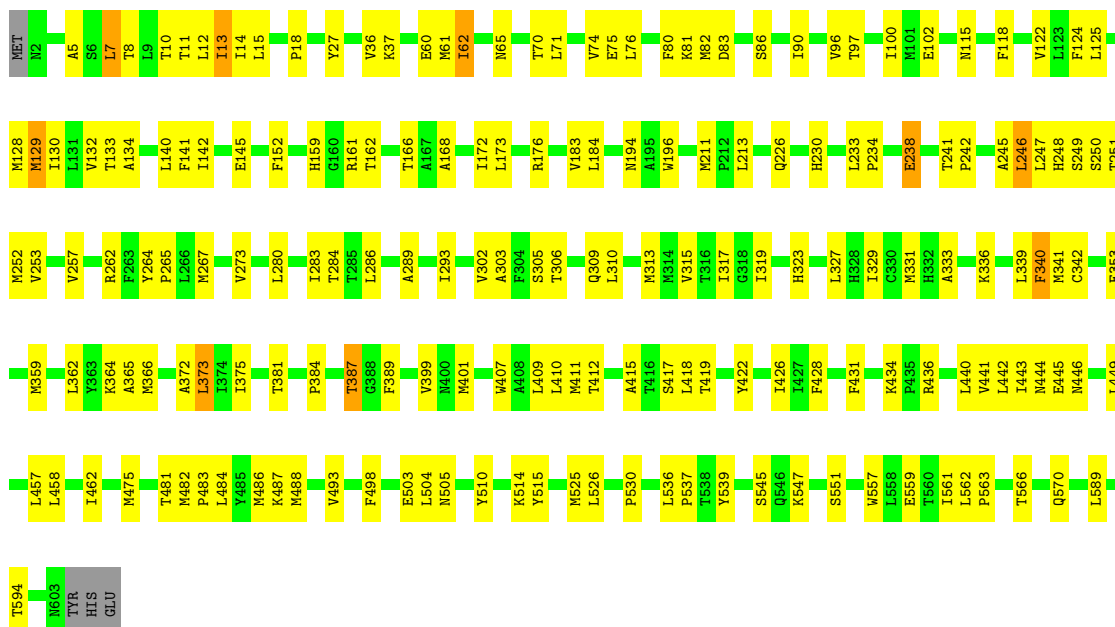
Chain k: 





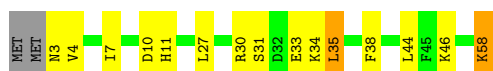
• Molecule 62: NADH-ubiquinone oxidoreductase chain 5

Chain l: 69% 29% ..



• Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 71% 22% . .



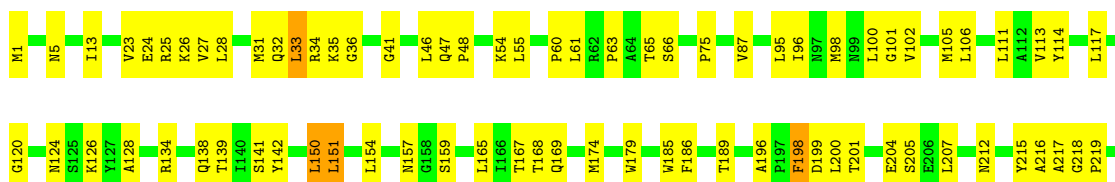
• Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 80% 19% .



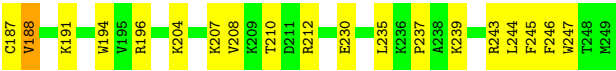
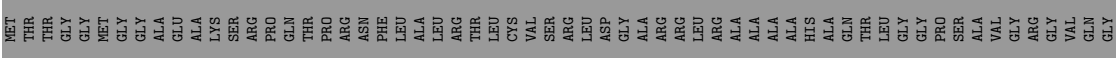
• Molecule 65: NADH-ubiquinone oxidoreductase chain 1

Chain r: 64% 34% .

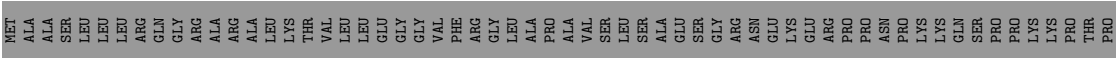




• Molecule 66: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



• Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54742	Depositor
Resolution determination method	OTHER	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	2.129	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	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: FMN, HEC, ZMP, NDP, HEM, HEA, FES, SF4

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	A	0.12	0/588	0.27	0/781
2	t	0.13	0/1015	0.28	0/1364
3	F	0.12	0/752	0.26	0/1013
4	K	0.11	0/1244	0.24	0/1693
5	U	0.11	0/2622	0.26	0/3552
6	Z	0.12	0/645	0.26	0/872
7	a	0.13	0/1184	0.27	0/1603
8	i	0.17	0/2774	0.32	0/3768
9	m	0.25	0/1373	0.42	0/1860
10	p	0.12	0/1590	0.27	0/2155
11	q	0.15	0/3721	0.30	0/5073
12	Aa	0.15	0/684	0.32	0/926
12	z	0.14	0/688	0.30	0/931
13	0	0.16	0/567	0.35	0/759
13	Ab	0.16	0/549	0.32	0/735
14	1	0.13	0/506	0.24	0/683
14	Ac	0.14	0/498	0.29	0/672
15	3	0.13	0/433	0.29	0/593
15	Ad	0.11	0/437	0.27	0/598
16	Ag	0.17	0/349	0.38	0/477
17	Ah	0.14	0/446	0.27	0/605
18	Ai	0.14	0/396	0.34	0/543
19	Aj	0.15	0/390	0.31	0/525
20	Ak	0.16	0/4154	0.32	0/5678
21	Al	0.22	0/1831	0.42	0/2496
22	Am	0.14	0/2179	0.27	0/2981
23	An	0.12	0/1188	0.27	0/1605
24	Ao	0.15	0/860	0.30	0/1167
25	Ap	0.14	0/712	0.33	0/966
26	Aq	0.14	0/633	0.27	0/866
27	Ar	0.15	0/704	0.32	0/951
28	2	0.15	0/1546	0.31	0/2093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	4	0.17	0/1551	0.34	1/2098 (0.0%)
28	Ae	0.23	0/281	0.60	0/383
28	Af	0.27	0/228	0.57	0/312
29	5	0.13	0/3442	0.28	0/4667
29	u	0.13	0/3531	0.29	0/4793
30	6	0.15	0/3192	0.30	0/4322
30	v	0.15	0/3192	0.31	0/4322
31	7	0.16	0/3123	0.31	0/4269
31	w	0.16	0/3123	0.29	0/4269
32	8	0.14	0/1964	0.32	0/2663
32	x	0.14	0/1954	0.28	0/2652
33	9	0.11	0/913	0.24	0/1223
33	y	0.12	0/913	0.23	0/1223
34	B	0.14	0/3393	0.31	0/4584
35	C	0.17	0/3551	0.34	0/4813
36	D	0.15	0/1783	0.35	0/2428
37	E	0.18	0/1698	0.38	0/2311
38	G	0.13	0/5347	0.28	0/7243
39	H	0.16	0/1443	0.32	0/1952
40	I	0.17	0/1279	0.32	0/1730
41	J	0.13	0/985	0.27	0/1329
42	L	0.13	0/2812	0.28	0/3812
43	M	0.11	0/791	0.28	0/1069
44	N	0.15	0/929	0.29	0/1258
45	O	0.13	0/701	0.34	0/946
45	X	0.15	0/701	0.34	0/946
46	P	0.15	0/680	0.36	0/916
47	Q	0.13	0/978	0.28	0/1317
48	S	0.15	0/577	0.30	0/777
49	T	0.12	0/659	0.28	0/905
50	V	0.12	0/1042	0.28	0/1411
51	W	0.23	1/1193 (0.1%)	0.31	1/1609 (0.1%)
52	Y	0.20	0/561	0.42	0/768
53	b	0.14	0/942	0.35	0/1282
54	c	0.13	0/1346	0.28	0/1840
55	d	0.13	0/1452	0.29	0/1958
56	e	0.42	2/849 (0.2%)	0.43	1/1153 (0.1%)
57	f	0.11	0/398	0.22	0/540
58	g	0.13	0/1031	0.30	0/1394
59	h	0.12	0/889	0.27	0/1190
60	j	0.17	0/923	0.34	0/1263
61	k	0.15	0/759	0.30	0/1029
62	l	0.15	0/4906	0.34	0/6673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	n	0.15	0/491	0.36	0/663
64	o	0.13	0/1092	0.28	0/1481
65	r	0.25	0/2581	0.42	0/3529
66	s	0.13	0/1436	0.32	0/1938
67	R	0.13	0/304	0.25	0/410
All	All	0.16	3/115167 (0.0%)	0.31	3/156247 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	e	95	PHE	C-N	9.73	1.47	1.34
51	W	11	PRO	CA-C	6.43	1.55	1.51
56	e	96	SER	C-N	-5.39	1.27	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	W	11	PRO	O-C-N	5.27	123.73	121.31
56	e	95	PHE	O-C-N	5.16	129.26	122.30
28	4	258	PRO	N-CA-C	-5.13	107.45	113.86

There are no chirality outliers.

There are no planarity outliers.

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	A	575	0	584	17	0
2	t	991	0	933	26	0
3	F	738	0	701	7	0
4	K	1203	0	1161	25	0
5	U	2562	0	2508	36	0
6	Z	626	0	607	11	0
7	a	1151	0	1164	24	0
8	i	2711	0	2874	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	m	1338	0	1338	49	0
10	p	1534	0	1470	29	0
11	q	3630	0	3837	97	0
12	Aa	662	0	660	12	0
12	z	666	0	663	13	0
13	0	561	0	542	15	0
13	Ab	543	0	530	7	0
14	1	493	0	491	5	0
14	Ac	485	0	485	9	0
15	3	417	0	414	10	0
15	Ad	421	0	418	9	0
16	Ag	338	0	342	11	0
17	Ah	437	0	436	7	0
18	Ai	383	0	366	13	0
19	Aj	377	0	372	9	0
20	Ak	4014	0	3993	111	0
21	Al	1785	0	1800	74	0
22	Am	2096	0	2027	46	0
23	An	1154	0	1137	36	0
24	Ao	842	0	838	17	0
25	Ap	697	0	682	25	0
26	Aq	606	0	575	12	0
27	Ar	684	0	647	23	0
28	2	1513	0	1497	42	0
28	4	1518	0	1498	47	0
28	Ae	275	0	276	29	0
28	Af	223	0	220	20	0
29	5	3374	0	3272	86	0
29	u	3459	0	3350	60	0
30	6	3140	0	3121	83	0
30	v	3140	0	3121	79	0
31	7	3025	0	3090	39	0
31	w	3025	0	3090	49	0
32	8	1906	0	1857	37	0
32	x	1896	0	1843	33	0
33	9	893	0	888	11	0
33	y	893	0	888	13	0
34	B	3318	0	3281	102	0
35	C	3458	0	3394	116	0
36	D	1732	0	1682	53	0
37	E	1658	0	1662	44	0
38	G	5260	0	5291	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	H	1412	0	1364	46	0
40	I	1248	0	1254	38	0
41	J	962	0	962	19	0
42	L	2735	0	2751	59	0
43	M	773	0	801	21	0
44	N	910	0	950	17	0
45	O	689	0	687	23	0
45	X	689	0	687	24	0
46	P	669	0	677	15	0
47	Q	954	0	960	18	0
48	S	562	0	557	21	0
49	T	638	0	637	15	0
50	V	1021	0	1027	7	0
51	W	1162	0	1156	30	0
52	Y	536	0	483	22	0
53	b	915	0	933	30	0
54	c	1291	0	1185	34	0
55	d	1420	0	1386	26	0
56	e	826	0	789	34	0
57	f	385	0	381	6	0
58	g	1000	0	994	29	0
59	h	867	0	871	17	0
60	j	899	0	931	35	0
61	k	748	0	799	38	0
62	l	4777	0	4923	126	0
63	n	479	0	486	12	0
64	o	1062	0	1072	20	0
65	r	2508	0	2607	91	0
66	s	1398	0	1378	35	0
67	R	295	0	279	11	0
68	Ak	120	0	108	13	0
69	2	4	0	0	6	0
69	4	4	0	0	1	0
69	E	4	0	0	0	0
69	G	4	0	0	1	0
70	7	86	0	60	12	0
70	w	86	0	60	8	0
71	8	43	0	31	3	0
71	x	43	0	30	2	0
72	B	31	0	19	1	0
73	B	8	0	0	2	0
73	G	16	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	H	16	0	0	1	0
73	I	8	0	0	1	0
74	L	48	0	26	3	0
75	Q	30	0	30	1	0
All	All	112807	0	112247	2364	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 10.

The worst 5 of 2364 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)
38:G:179:CYS:SG	73:G:802:SF4:FE1	1.15	1.36
38:G:226:CYS:SG	73:G:802:SF4:FE3	1.17	1.35
38:G:182:CYS:SG	73:G:802:SF4:FE2	1.25	1.28
38:G:176:CYS:SG	73:G:802:SF4:FE4	1.30	1.22
35:C:275:ARG:O	35:C:279:VAL:HB	1.60	1.01

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	A	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
2	t	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
3	F	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
4	K	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
5	U	316/357 (88%)	308 (98%)	7 (2%)	1 (0%)	36	66
6	Z	76/114 (67%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
8	i	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
9	m	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	51
10	p	176/221 (80%)	173 (98%)	3 (2%)	0	100	100
11	q	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
12	Aa	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
12	z	77/82 (94%)	77 (100%)	0	0	100	100
13	0	66/91 (72%)	64 (97%)	2 (3%)	0	100	100
13	Ab	64/91 (70%)	62 (97%)	2 (3%)	0	100	100
14	1	58/64 (91%)	58 (100%)	0	0	100	100
14	Ac	57/64 (89%)	57 (100%)	0	0	100	100
15	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
15	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
16	Ag	41/70 (59%)	41 (100%)	0	0	100	100
17	Ah	54/80 (68%)	54 (100%)	0	0	100	100
18	Ai	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
19	Aj	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
20	Ak	511/514 (99%)	498 (98%)	13 (2%)	0	100	100
21	Al	218/228 (96%)	211 (97%)	6 (3%)	1 (0%)	24	55
22	Am	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
23	An	136/169 (80%)	132 (97%)	4 (3%)	0	100	100
24	Ao	102/152 (67%)	100 (98%)	2 (2%)	0	100	100
25	Ap	89/129 (69%)	86 (97%)	3 (3%)	0	100	100
26	Aq	71/97 (73%)	66 (93%)	5 (7%)	0	100	100
27	Ar	80/86 (93%)	80 (100%)	0	0	100	100
28	2	193/299 (64%)	186 (96%)	7 (4%)	0	100	100
28	4	194/299 (65%)	189 (97%)	5 (3%)	0	100	100
28	Ae	37/299 (12%)	26 (70%)	11 (30%)	0	100	100
28	Af	31/299 (10%)	20 (64%)	11 (36%)	0	100	100
29	5	431/480 (90%)	415 (96%)	16 (4%)	0	100	100
29	u	444/480 (92%)	432 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	6	416/453 (92%)	402 (97%)	14 (3%)	0	100	100
30	v	416/453 (92%)	407 (98%)	9 (2%)	0	100	100
31	7	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
31	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
32	8	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
32	x	236/326 (72%)	229 (97%)	7 (3%)	0	100	100
33	9	99/111 (89%)	99 (100%)	0	0	100	100
33	y	99/111 (89%)	99 (100%)	0	0	100	100
34	B	429/464 (92%)	414 (96%)	14 (3%)	1 (0%)	43	72
35	C	428/469 (91%)	407 (95%)	21 (5%)	0	100	100
36	D	206/264 (78%)	180 (87%)	25 (12%)	1 (0%)	24	55
37	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
38	G	680/727 (94%)	662 (97%)	18 (3%)	0	100	100
39	H	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
40	I	154/258 (60%)	146 (95%)	8 (5%)	0	100	100
41	J	116/175 (66%)	116 (100%)	0	0	100	100
42	L	338/372 (91%)	326 (96%)	12 (4%)	0	100	100
43	M	92/113 (81%)	86 (94%)	6 (6%)	0	100	100
44	N	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
45	O	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
45	X	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
46	P	81/99 (82%)	73 (90%)	8 (10%)	0	100	100
47	Q	110/154 (71%)	107 (97%)	2 (2%)	1 (1%)	14	41
48	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
49	T	80/169 (47%)	76 (95%)	4 (5%)	0	100	100
50	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
51	W	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
52	Y	60/105 (57%)	54 (90%)	4 (7%)	2 (3%)	3	11
53	b	106/188 (56%)	99 (93%)	7 (7%)	0	100	100
54	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
55	d	167/176 (95%)	166 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	e	97/154 (63%)	91 (94%)	6 (6%)	0	100	100
57	f	44/76 (58%)	43 (98%)	1 (2%)	0	100	100
58	g	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
59	h	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
60	j	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
61	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
62	l	600/606 (99%)	576 (96%)	24 (4%)	0	100	100
63	n	54/58 (93%)	48 (89%)	6 (11%)	0	100	100
64	o	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
65	r	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
66	s	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
67	R	33/110 (30%)	33 (100%)	0	0	100	100
All	All	13905/16854 (82%)	13458 (97%)	439 (3%)	8 (0%)	49	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	Y	40	ILE
9	m	138	GLU
34	B	316	ALA
5	U	255	CYS
21	Al	158	ASP

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	A	55/59 (93%)	53 (96%)	2 (4%)	31	66
2	t	101/120 (84%)	96 (95%)	5 (5%)	22	54
3	F	79/97 (81%)	77 (98%)	2 (2%)	42	76
4	K	130/131 (99%)	127 (98%)	3 (2%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	U	278/307 (91%)	269 (97%)	9 (3%)	34	70
6	Z	60/90 (67%)	53 (88%)	7 (12%)	5	18
7	a	121/158 (77%)	120 (99%)	1 (1%)	73	90
8	i	311/311 (100%)	297 (96%)	14 (4%)	24	58
9	m	141/141 (100%)	132 (94%)	9 (6%)	16	44
10	p	159/190 (84%)	157 (99%)	2 (1%)	61	86
11	q	409/409 (100%)	398 (97%)	11 (3%)	39	74
12	Aa	70/73 (96%)	64 (91%)	6 (9%)	10	31
12	z	70/73 (96%)	68 (97%)	2 (3%)	37	73
13	0	65/85 (76%)	60 (92%)	5 (8%)	12	36
13	Ab	63/85 (74%)	57 (90%)	6 (10%)	8	26
14	1	49/52 (94%)	49 (100%)	0	100	100
14	Ac	48/52 (92%)	48 (100%)	0	100	100
15	3	40/46 (87%)	37 (92%)	3 (8%)	12	37
15	Ad	41/46 (89%)	39 (95%)	2 (5%)	22	55
16	Ag	37/57 (65%)	37 (100%)	0	100	100
17	Ah	47/68 (69%)	44 (94%)	3 (6%)	16	44
18	Ai	38/66 (58%)	36 (95%)	2 (5%)	20	52
19	Aj	39/55 (71%)	38 (97%)	1 (3%)	40	75
20	Ak	424/425 (100%)	408 (96%)	16 (4%)	29	64
21	Al	206/212 (97%)	201 (98%)	5 (2%)	43	77
22	Am	223/225 (99%)	220 (99%)	3 (1%)	61	86
23	An	123/149 (83%)	117 (95%)	6 (5%)	22	55
24	Ao	91/124 (73%)	85 (93%)	6 (7%)	15	43
25	Ap	77/101 (76%)	74 (96%)	3 (4%)	28	64
26	Aq	64/80 (80%)	63 (98%)	1 (2%)	55	83
27	Ar	73/76 (96%)	68 (93%)	5 (7%)	14	42
28	2	166/245 (68%)	161 (97%)	5 (3%)	36	72
28	4	166/245 (68%)	157 (95%)	9 (5%)	20	51
28	Ae	29/245 (12%)	26 (90%)	3 (10%)	7	23
28	Af	23/245 (9%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	5	363/397 (91%)	357 (98%)	6 (2%)	53	83
29	u	372/397 (94%)	359 (96%)	13 (4%)	32	67
30	6	329/355 (93%)	315 (96%)	14 (4%)	26	60
30	v	329/355 (93%)	317 (96%)	12 (4%)	31	66
31	7	332/332 (100%)	328 (99%)	4 (1%)	63	87
31	w	332/332 (100%)	325 (98%)	7 (2%)	47	79
32	8	204/259 (79%)	197 (97%)	7 (3%)	32	68
32	x	203/259 (78%)	196 (97%)	7 (3%)	32	68
33	9	93/99 (94%)	91 (98%)	2 (2%)	45	78
33	y	93/99 (94%)	89 (96%)	4 (4%)	26	60
34	B	345/368 (94%)	335 (97%)	10 (3%)	37	73
35	C	371/398 (93%)	349 (94%)	22 (6%)	18	48
36	D	188/228 (82%)	181 (96%)	7 (4%)	30	65
37	E	183/207 (88%)	176 (96%)	7 (4%)	29	64
38	G	576/610 (94%)	559 (97%)	17 (3%)	36	72
39	H	151/176 (86%)	142 (94%)	9 (6%)	17	47
40	I	132/212 (62%)	129 (98%)	3 (2%)	44	78
41	J	107/152 (70%)	105 (98%)	2 (2%)	50	81
42	L	294/320 (92%)	279 (95%)	15 (5%)	21	54
43	M	86/98 (88%)	79 (92%)	7 (8%)	11	33
44	N	99/101 (98%)	93 (94%)	6 (6%)	17	46
45	O	79/132 (60%)	73 (92%)	6 (8%)	12	36
45	X	79/132 (60%)	73 (92%)	6 (8%)	12	36
46	P	74/82 (90%)	70 (95%)	4 (5%)	20	51
47	Q	105/134 (78%)	99 (94%)	6 (6%)	18	49
48	S	58/58 (100%)	57 (98%)	1 (2%)	53	83
49	T	69/134 (52%)	66 (96%)	3 (4%)	26	60
50	V	101/102 (99%)	100 (99%)	1 (1%)	68	88
51	W	122/124 (98%)	120 (98%)	2 (2%)	55	83
52	Y	55/84 (66%)	44 (80%)	11 (20%)	1	4
53	b	100/166 (60%)	93 (93%)	7 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	c	138/160 (86%)	135 (98%)	3 (2%)	45	78
55	d	152/156 (97%)	148 (97%)	4 (3%)	40	75
56	e	91/129 (70%)	83 (91%)	8 (9%)	9	29
57	f	41/66 (62%)	41 (100%)	0	100	100
58	g	108/109 (99%)	104 (96%)	4 (4%)	30	65
59	h	93/94 (99%)	91 (98%)	2 (2%)	45	78
60	j	97/100 (97%)	94 (97%)	3 (3%)	35	70
61	k	85/85 (100%)	80 (94%)	5 (6%)	18	48
62	l	536/540 (99%)	518 (97%)	18 (3%)	32	68
63	n	53/55 (96%)	48 (91%)	5 (9%)	8	27
64	o	113/114 (99%)	111 (98%)	2 (2%)	51	82
65	r	275/275 (100%)	265 (96%)	10 (4%)	31	66
66	s	153/206 (74%)	149 (97%)	4 (3%)	40	75
67	R	34/92 (37%)	33 (97%)	1 (3%)	37	73
All	All	12109/14226 (85%)	11655 (96%)	454 (4%)	31	65

5 of 454 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	G	56	VAL
12	z	16	THR
44	N	19	THR
33	y	33	MET
29	u	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
42	L	149	GLN
59	h	7	GLN
44	N	50	GLN
51	W	76	GLN
62	l	446	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	$\# Z > 2$
73	SF4	B	502	34	0,12,12	-	-	-		
73	SF4	G	801	38	0,12,12	-	-	-		
73	SF4	G	802	-	0,12,12	-	-	-		
68	HEA	Ak	602	20	67,67,67	1.20	6 (8%)	81,103,103	1.55	19 (23%)
68	HEA	Ak	601	20	67,67,67	1.22	7 (10%)	81,103,103	1.57	18 (22%)
69	FES	G	803	38	0,4,4	-	-	-		
71	HEC	8	401	32	46,50,50	1.80	3 (6%)	58,82,82	1.91	7 (12%)
70	HEM	w	401	-	50,50,50	1.33	6 (12%)	67,82,82	1.10	3 (4%)
73	SF4	I	201	40	0,12,12	-	-	-		
70	HEM	7	402	-	50,50,50	1.34	6 (12%)	67,82,82	1.09	5 (7%)
73	SF4	H	301	39	0,12,12	-	-	-		
71	HEC	x	401	32	46,50,50	1.81	3 (6%)	58,82,82	1.75	7 (12%)
72	FMN	B	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.28	8 (16%)
69	FES	E	301	37	0,4,4	-	-	-		
75	ZMP	Q	201	-	27,29,36	1.80	6 (22%)	34,38,45	1.77	7 (20%)
73	SF4	H	302	39	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	NDP	L	401	-	51,52,52	0.49	0	71,80,80	0.77	1 (1%)
70	HEM	w	402	31	50,50,50	1.45	6 (12%)	67,82,82	0.96	1 (1%)
69	FES	4	301	28	0,4,4	-	-	-	-	-
70	HEM	7	401	31	50,50,50	1.46	6 (12%)	67,82,82	1.19	3 (4%)
69	FES	2	301	28	0,4,4	-	-	-	-	-

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
73	SF4	B	502	34	-	-	0/6/5/5
73	SF4	G	801	38	-	-	0/6/5/5
73	SF4	G	802	-	-	-	0/6/5/5
68	HEA	Ak	602	20	-	8/36/76/76	-
68	HEA	Ak	601	20	-	14/36/76/76	-
69	FES	G	803	38	-	-	0/1/1/1
71	HEC	8	401	32	-	4/14/54/54	-
70	HEM	w	401	-	-	3/14/54/54	-
70	HEM	7	402	-	-	4/14/54/54	-
73	SF4	I	201	40	-	-	0/6/5/5
73	SF4	H	301	39	-	-	0/6/5/5
71	HEC	x	401	32	-	9/14/54/54	-
72	FMN	B	501	-	-	6/18/18/18	0/3/3/3
69	FES	E	301	37	-	-	0/1/1/1
75	ZMP	Q	201	-	-	13/36/36/43	-
73	SF4	H	302	39	-	-	0/6/5/5
74	NDP	L	401	-	-	8/34/77/77	0/5/5/5
70	HEM	w	402	31	-	3/14/54/54	-
69	FES	4	301	28	-	-	0/1/1/1
70	HEM	7	401	31	-	8/14/54/54	-
69	FES	2	301	28	-	-	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	x	401	HEC	CAC-C3C	6.30	1.55	1.35
71	8	401	HEC	CAC-C3C	6.25	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	x	401	HEC	CAB-C3B	6.23	1.55	1.35
71	8	401	HEC	CAB-C3B	5.87	1.54	1.35
71	8	401	HEC	C3D-C2D	5.78	1.54	1.38

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	8	401	HEC	CBB-CAB-C3B	-9.63	108.18	127.43
71	x	401	HEC	CBC-CAC-C3C	-7.49	112.47	127.43
71	x	401	HEC	CBB-CAB-C3B	-6.07	115.30	127.43
71	8	401	HEC	CBC-CAC-C3C	-6.04	115.37	127.43
75	Q	201	ZMP	C9-C10-S1	5.52	119.98	113.40

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	Ak	601	HEA	C1A-C2A-CAA-CBA
68	Ak	601	HEA	C2A-C3A-CMA-OMA
68	Ak	601	HEA	C2C-C3C-CAC-CBC
68	Ak	601	HEA	C4C-C3C-CAC-CBC
68	Ak	602	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

19 monomers are involved in 73 short contacts:

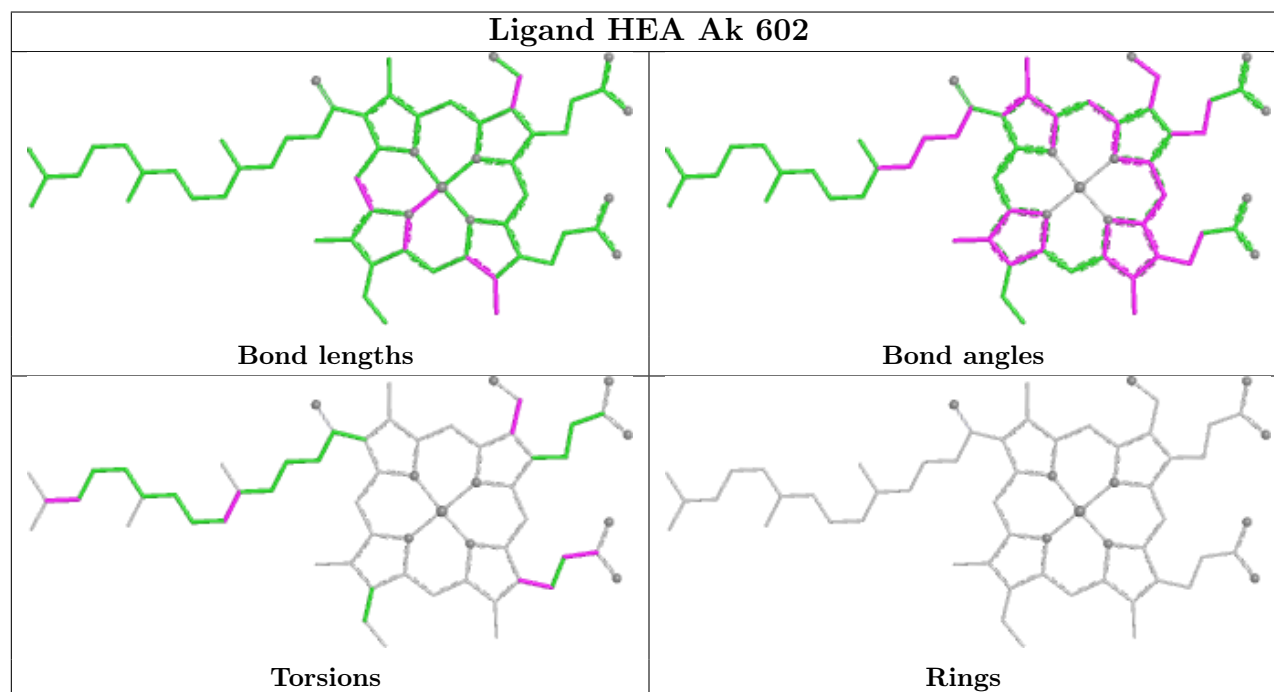
Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	B	502	SF4	2	0
73	G	801	SF4	1	0
73	G	802	SF4	17	0
68	Ak	602	HEA	4	0
68	Ak	601	HEA	9	0
69	G	803	FES	1	0
71	8	401	HEC	3	0
70	w	401	HEM	4	0
73	I	201	SF4	1	0
70	7	402	HEM	6	0
71	x	401	HEC	2	0
72	B	501	FMN	1	0
75	Q	201	ZMP	1	0
73	H	302	SF4	1	0

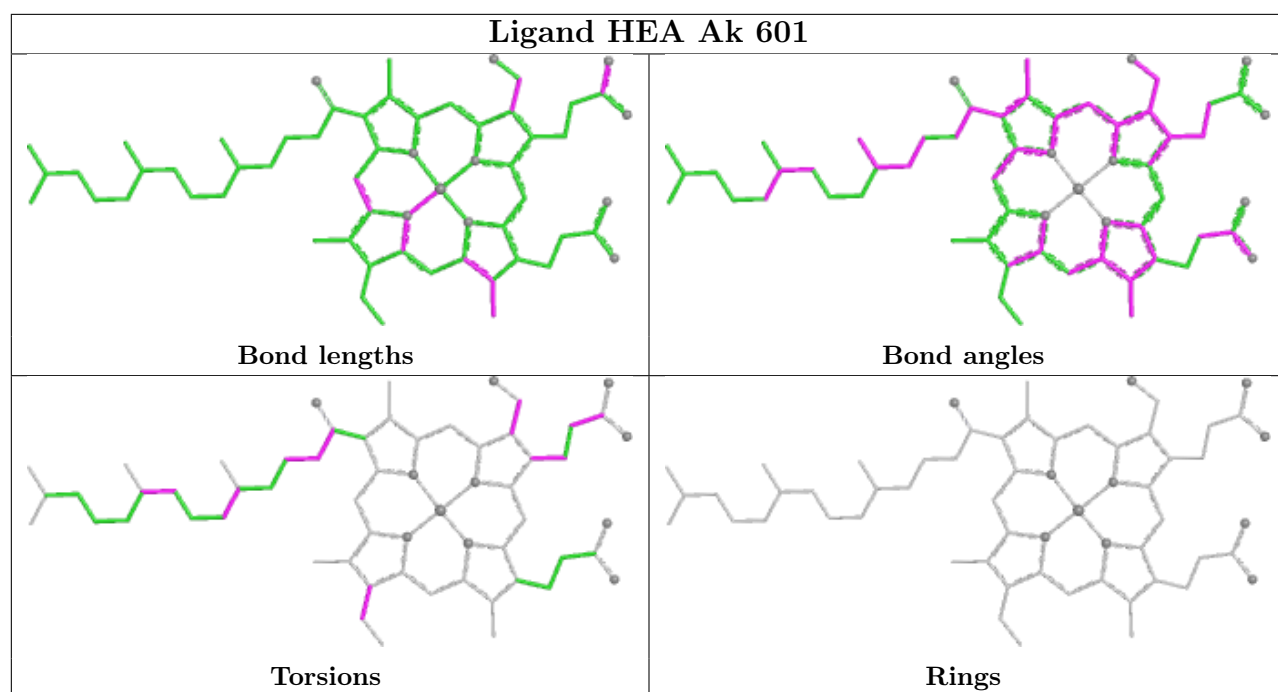
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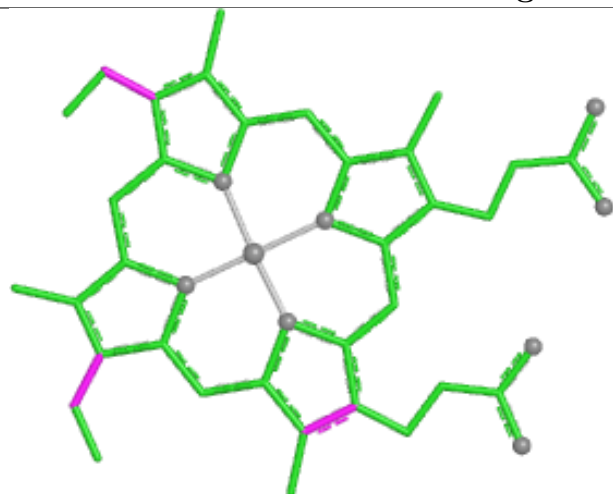
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L	401	NDP	3	0
70	w	402	HEM	4	0
69	4	301	FES	1	0
70	7	401	HEM	6	0
69	2	301	FES	6	0

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.

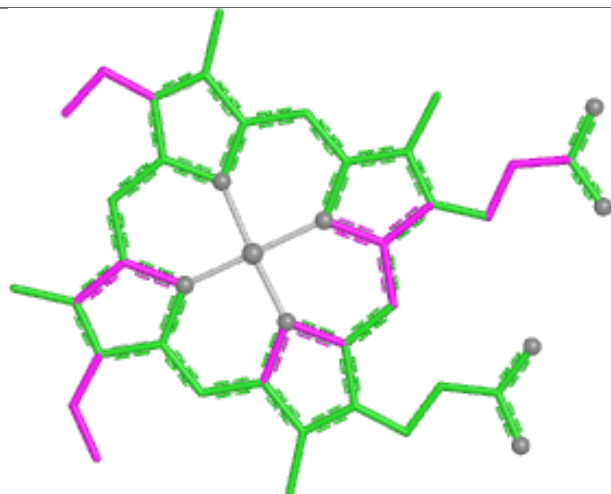




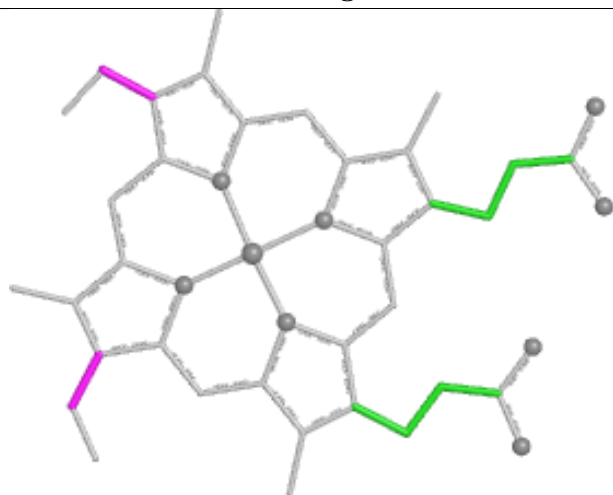
Ligand HEC 8 401



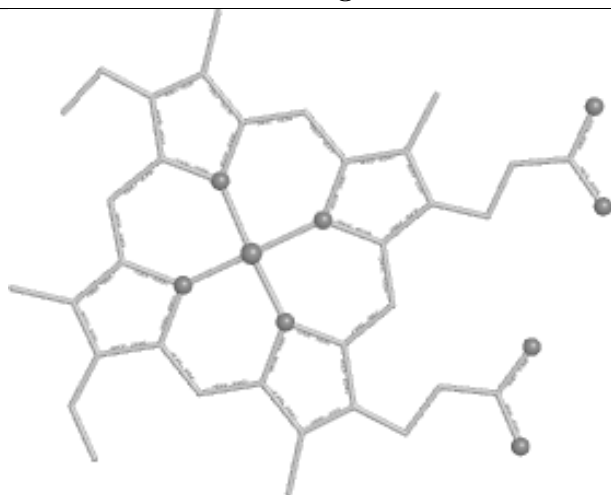
Bond lengths



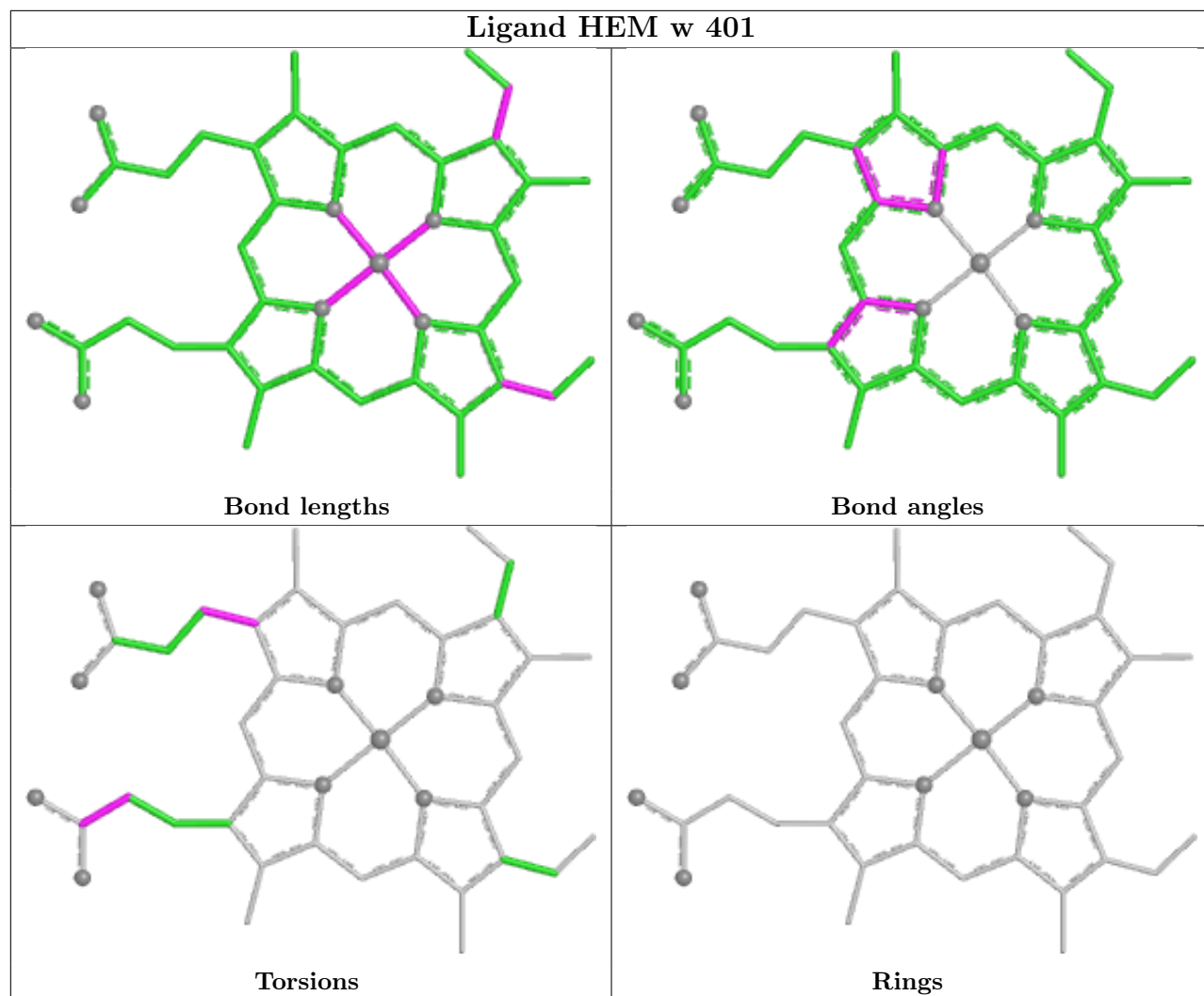
Bond angles

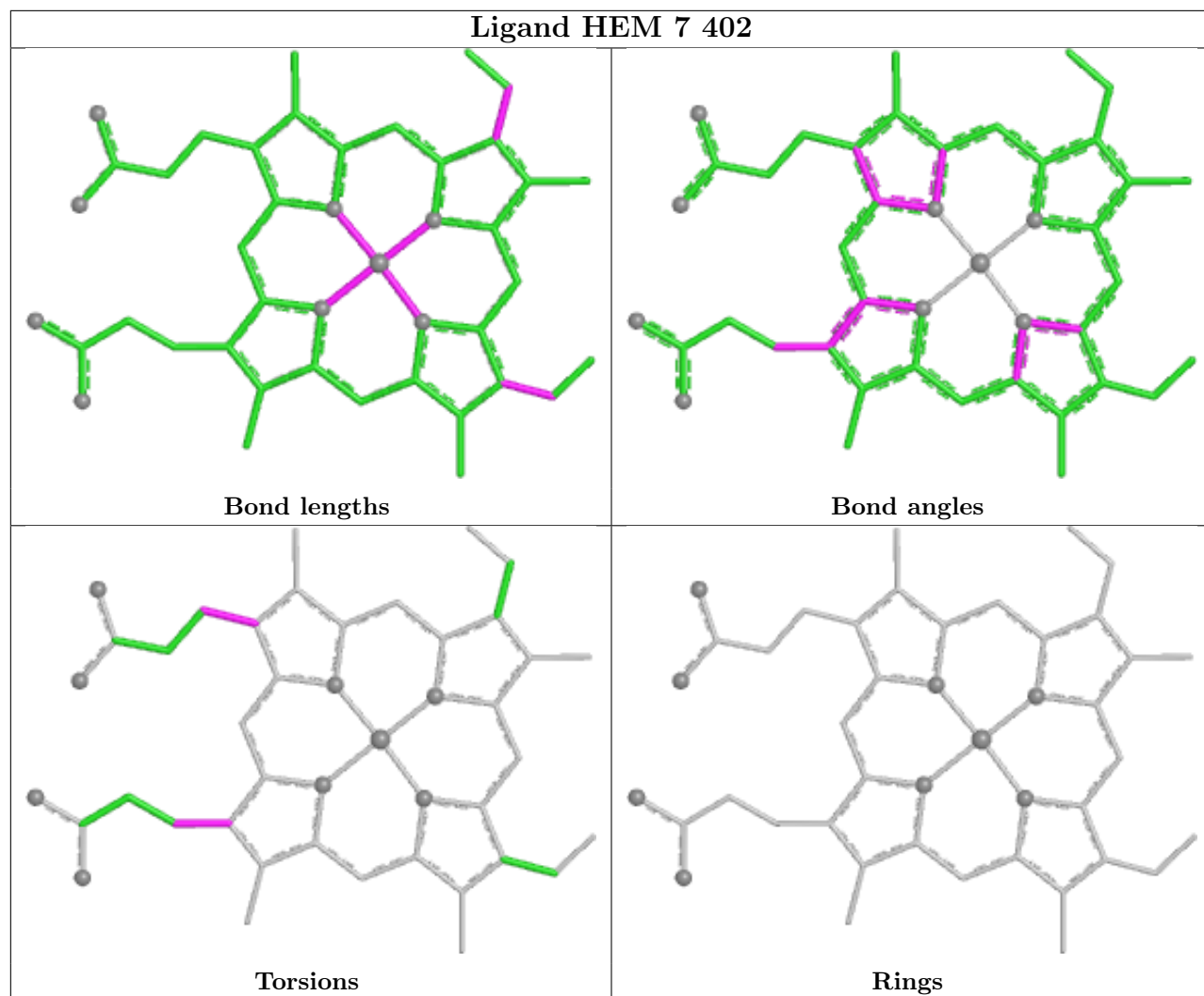


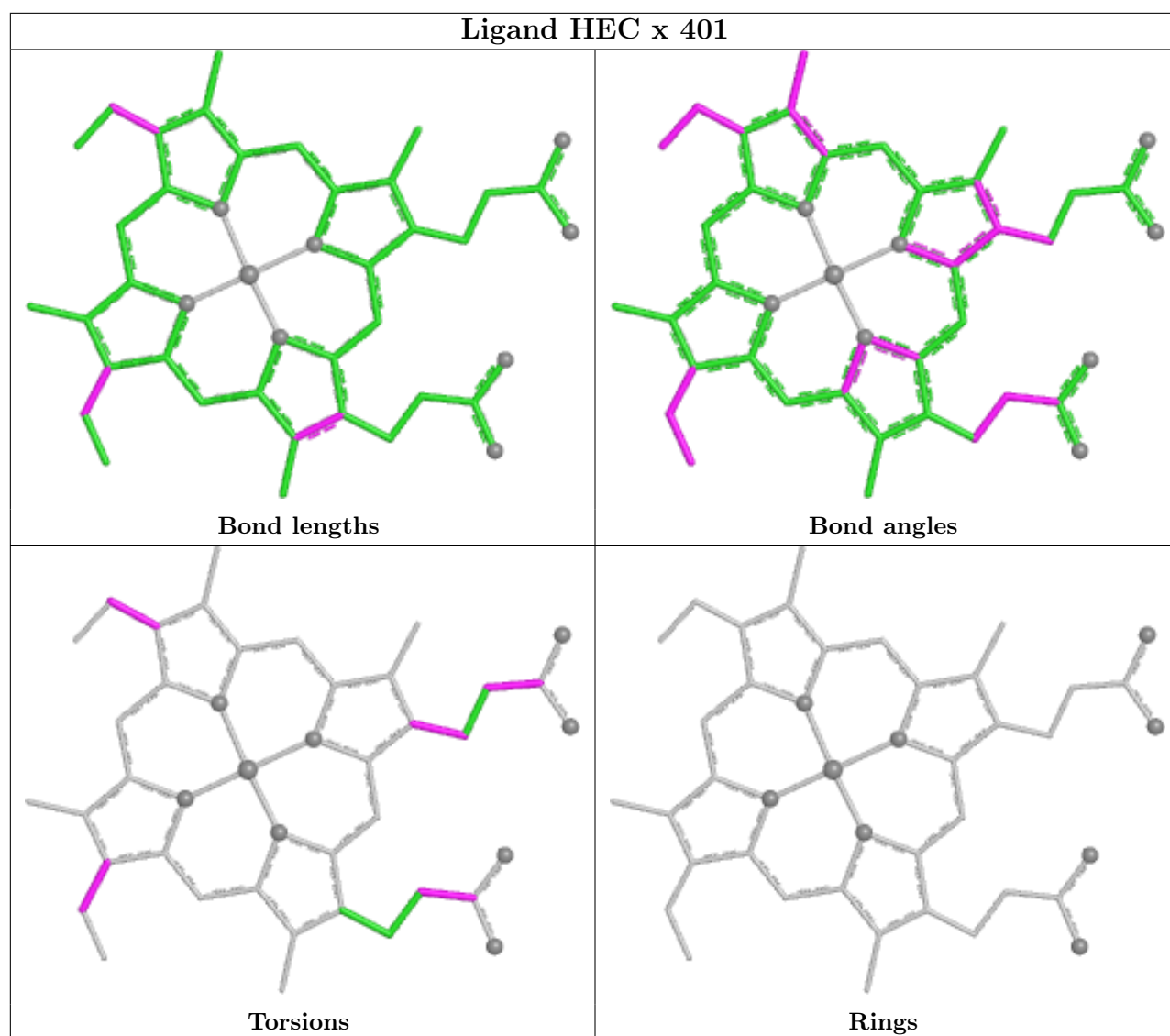
Torsions

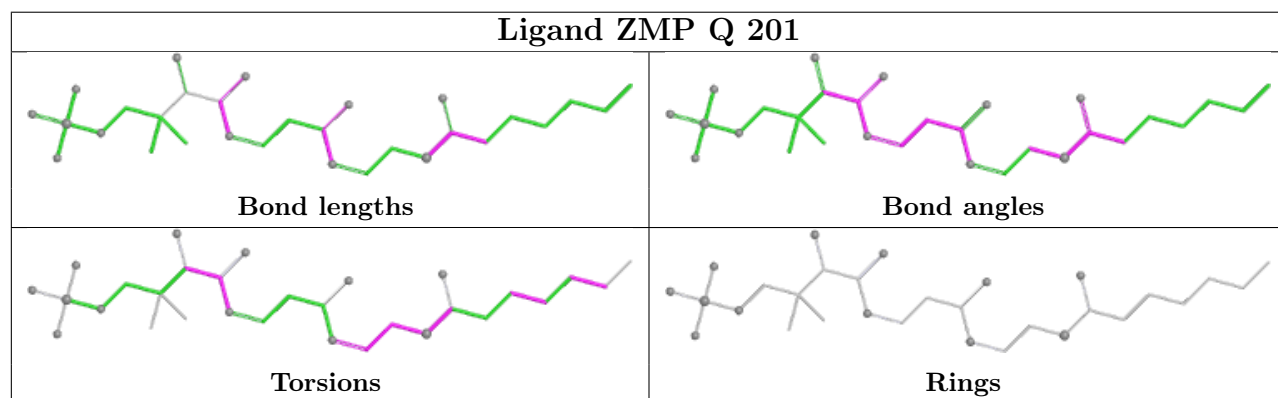
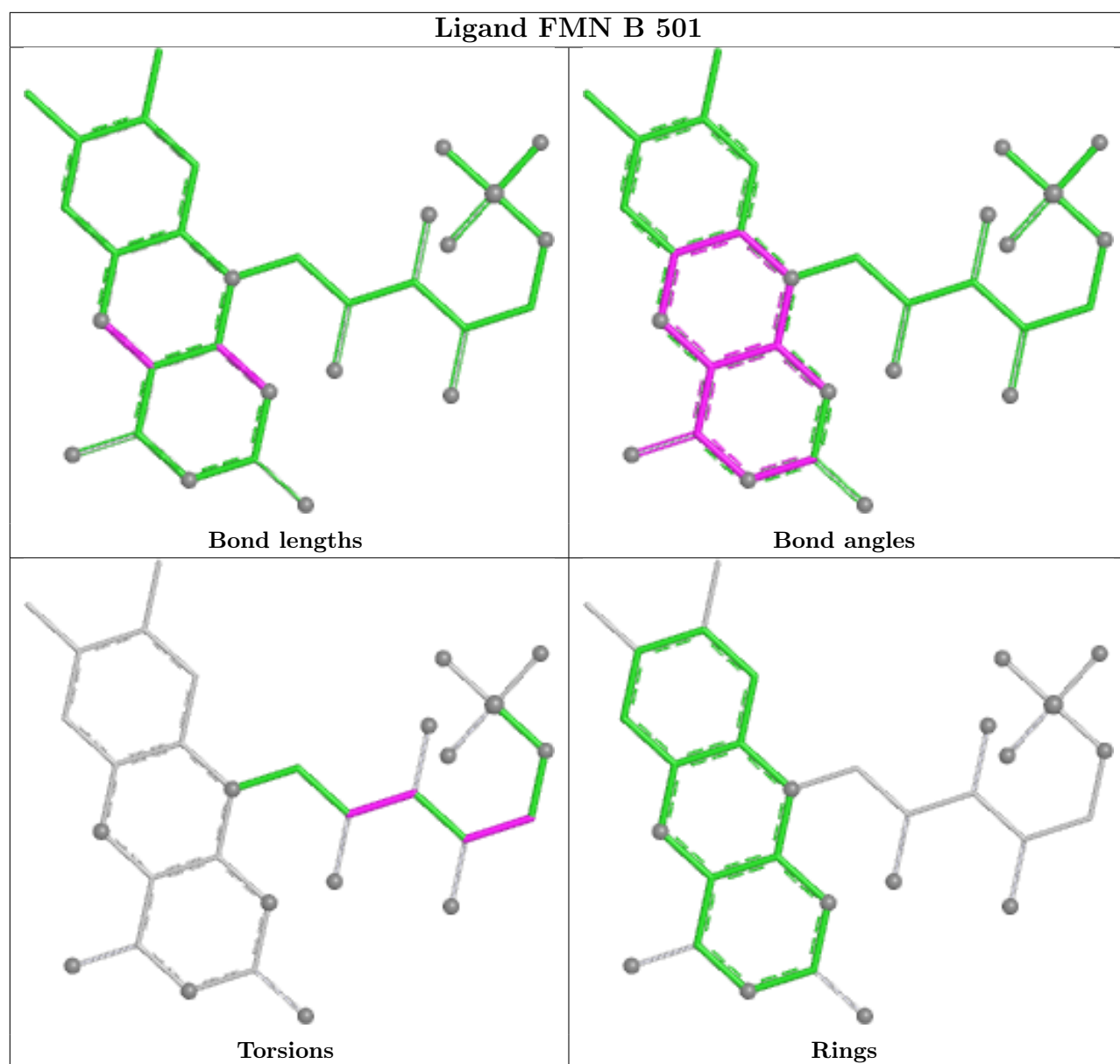


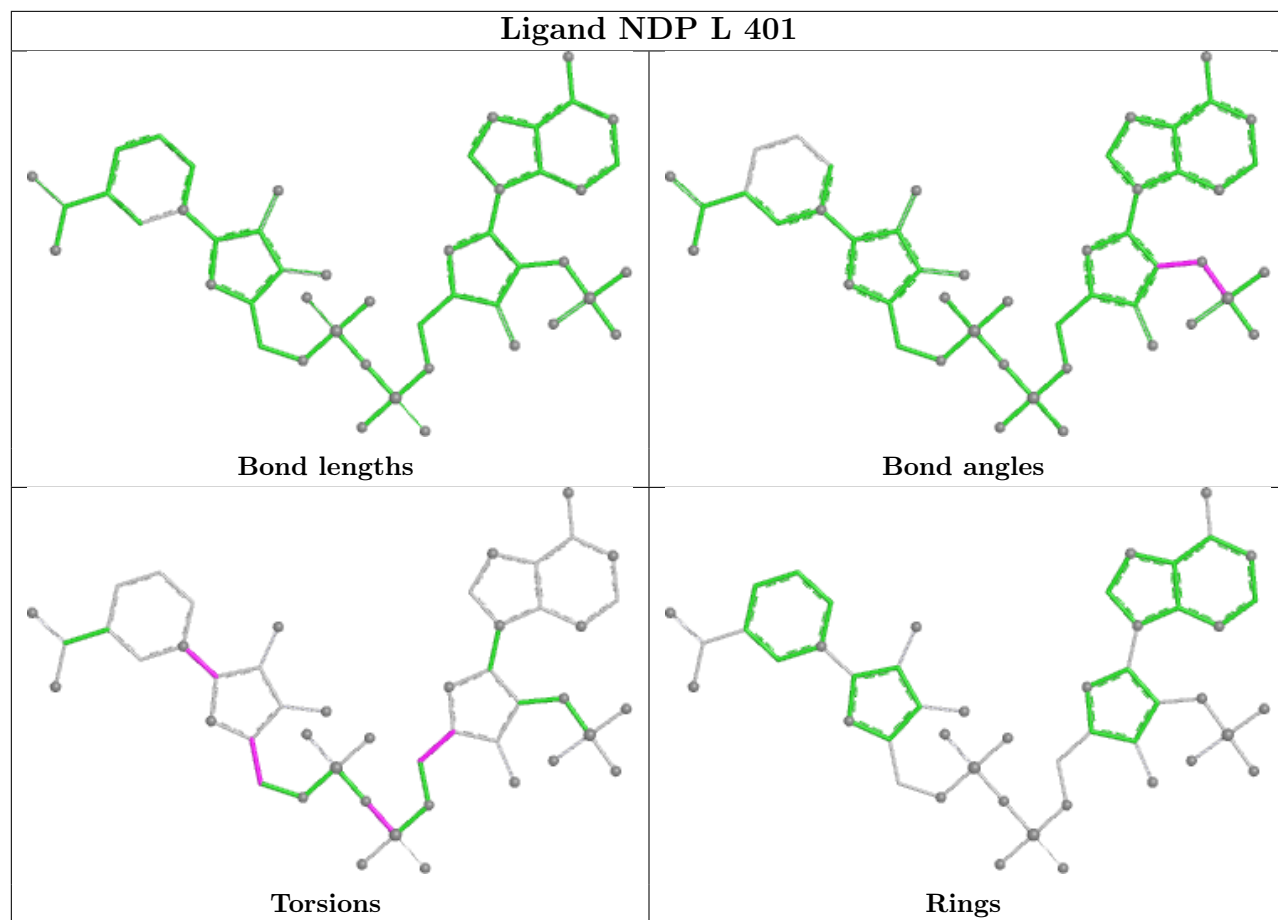
Rings

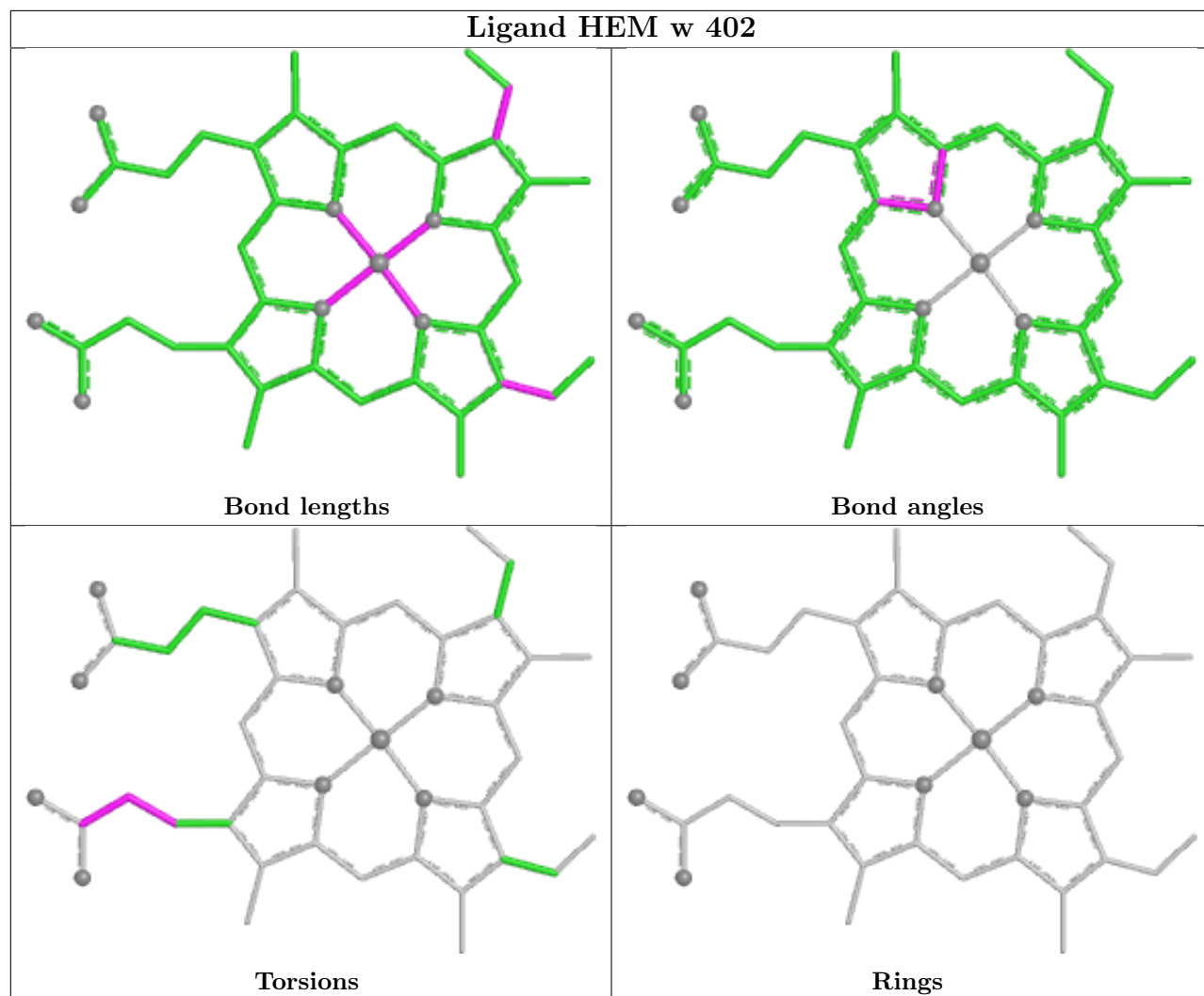


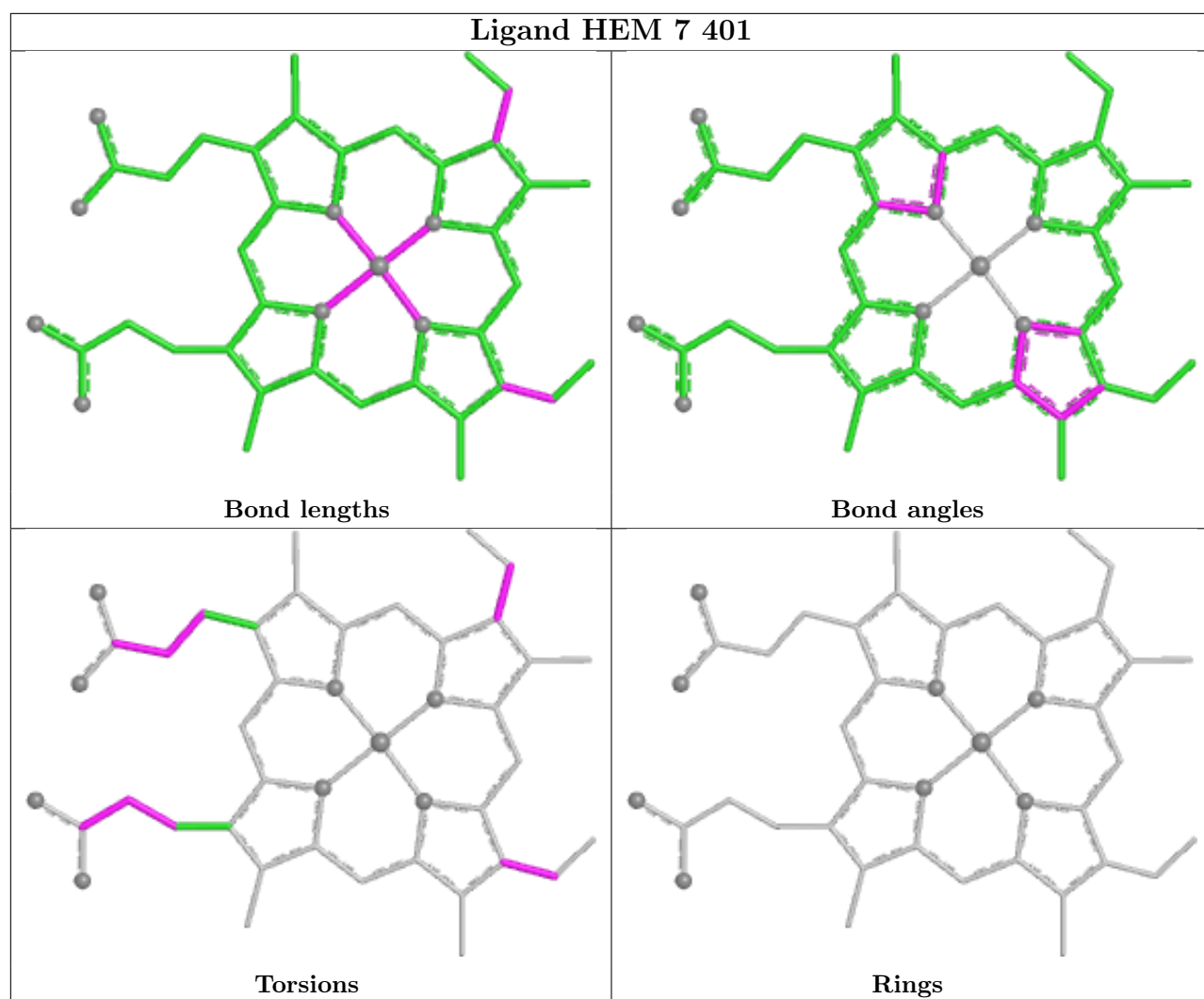












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

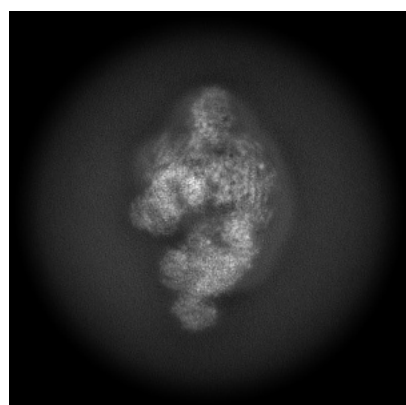
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44908. These allow visual inspection of the internal detail of the map and identification of artifacts.

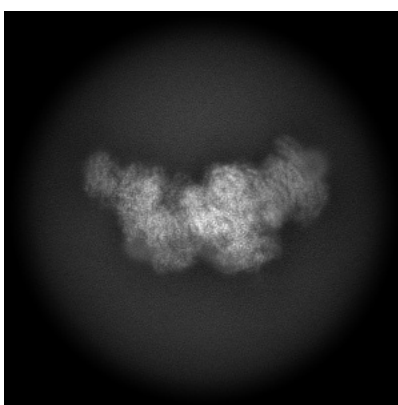
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

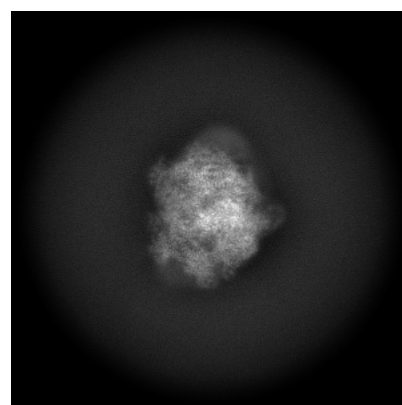
6.1.1 Primary map



X



Y

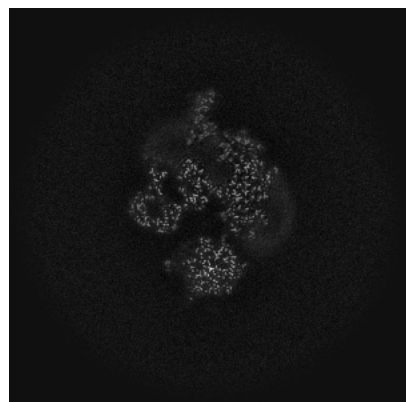


Z

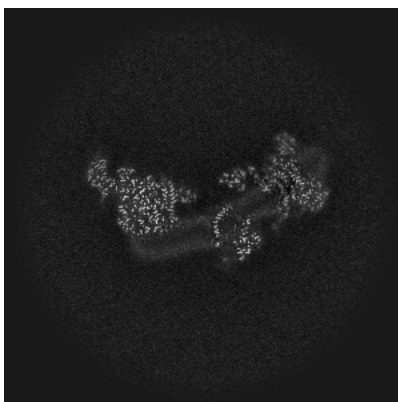
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

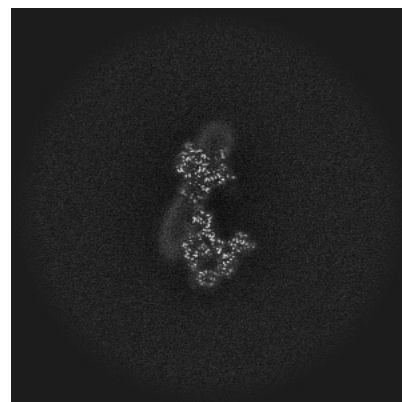
6.2.1 Primary map



X Index: 256



Y Index: 256

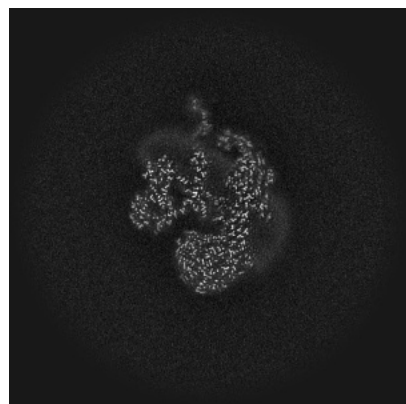


Z Index: 256

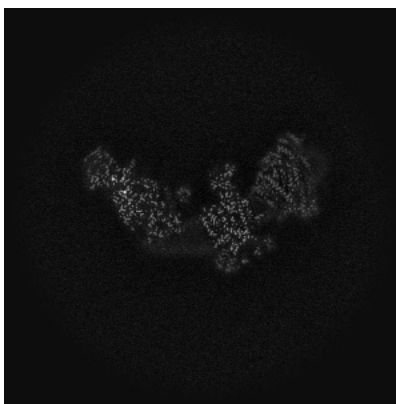
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

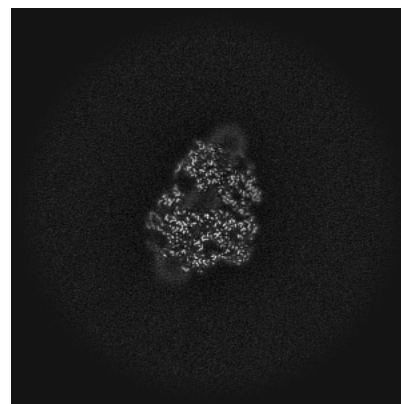
6.3.1 Primary map



X Index: 244



Y Index: 242

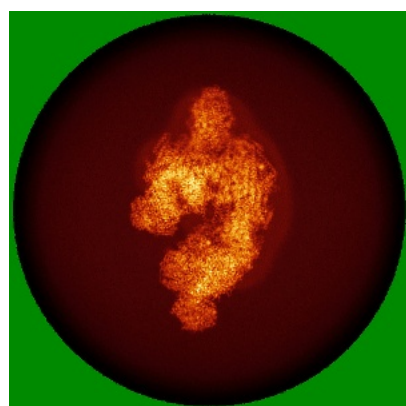


Z Index: 294

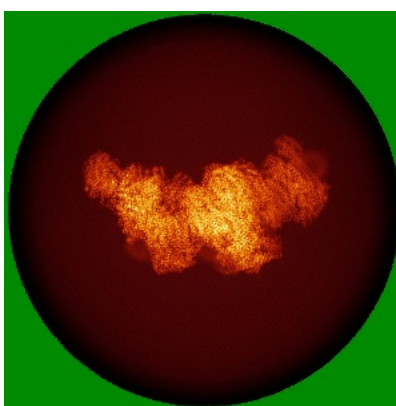
The images above show the largest variance slices of the map in three orthogonal directions.

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

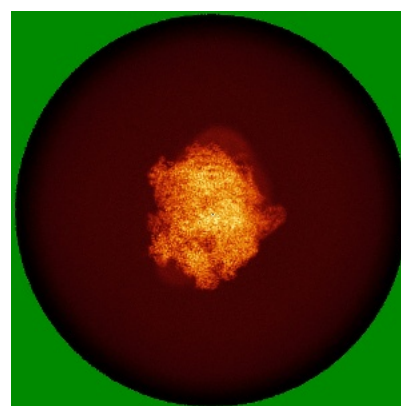
6.4.1 Primary map



X



Y

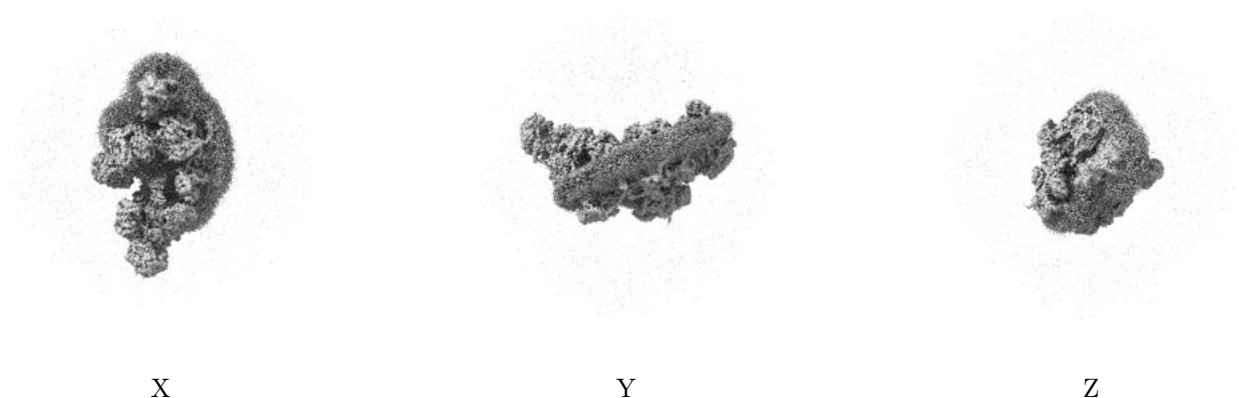


Z

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



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.

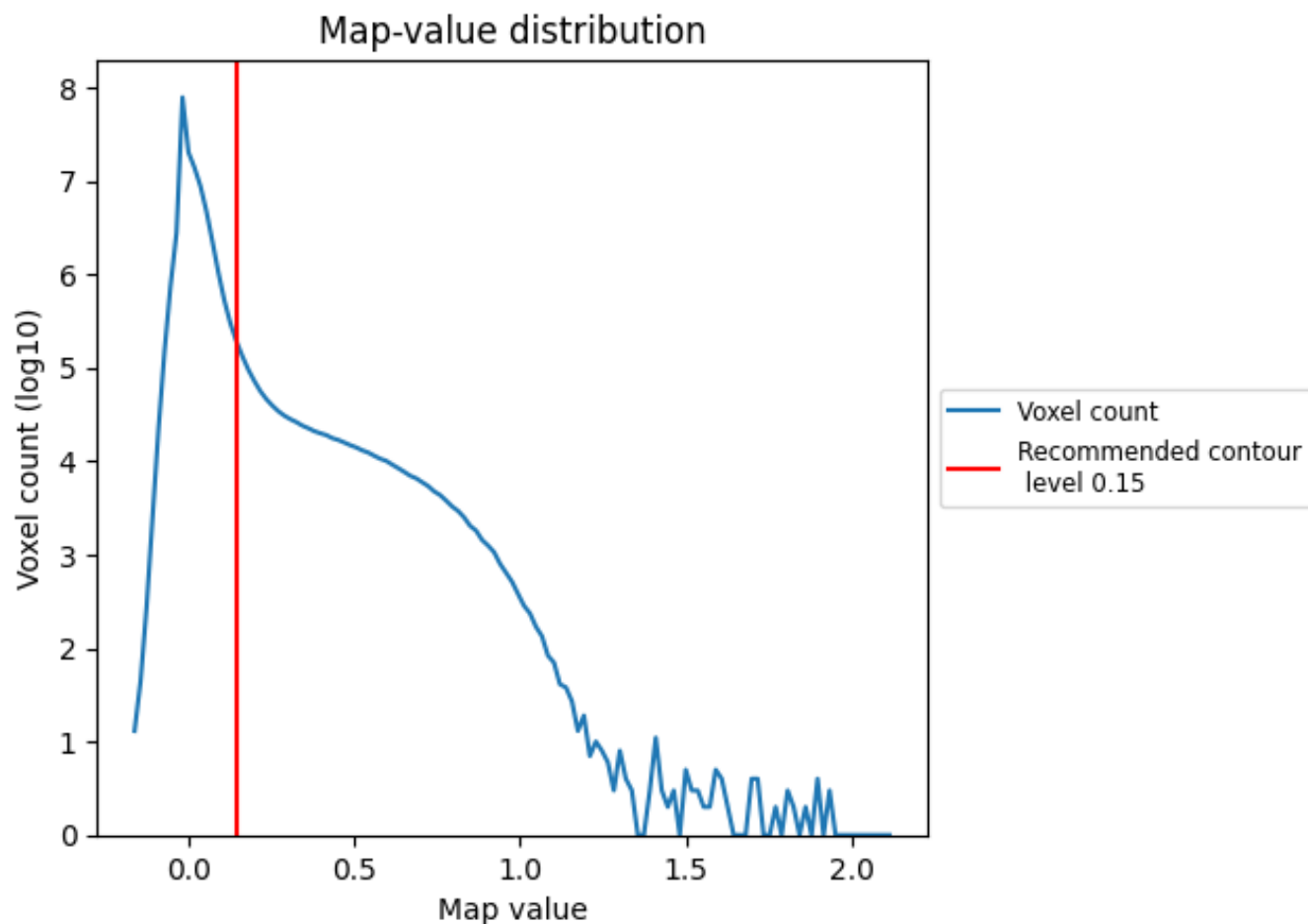
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

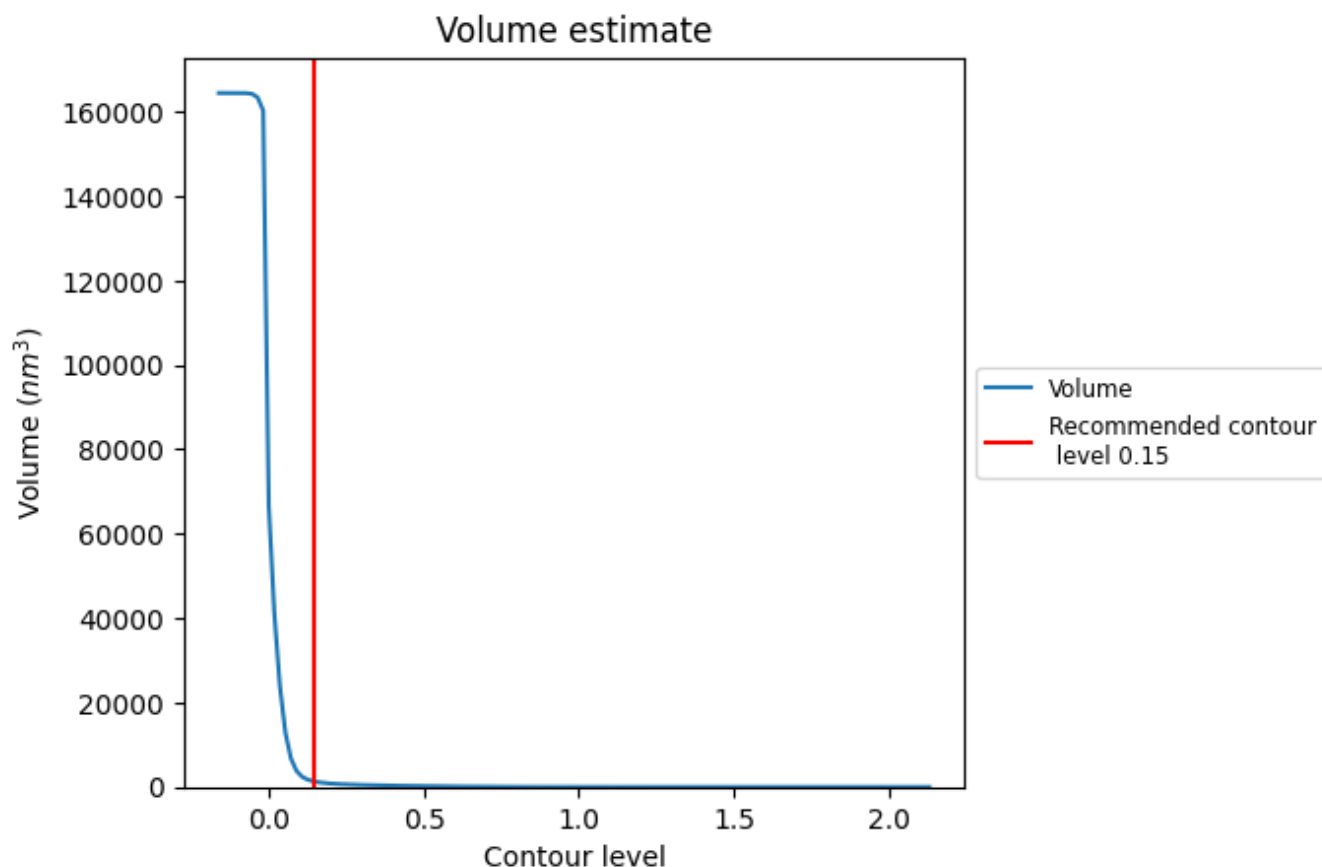
This section contains the results of statistical analysis of the map.

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.

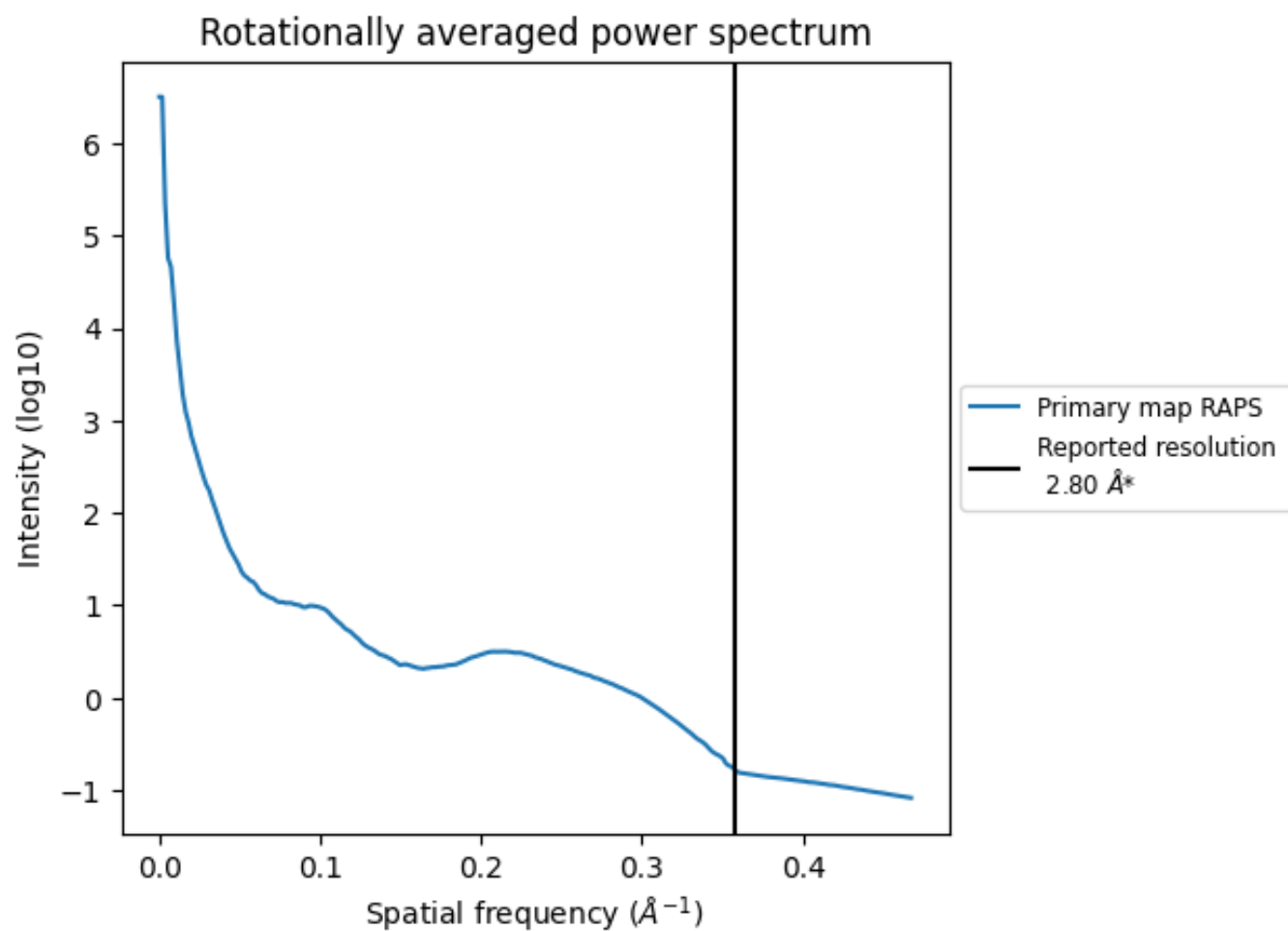
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1279 nm³; this corresponds to an approximate mass of 1155 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 0.357 Å⁻¹

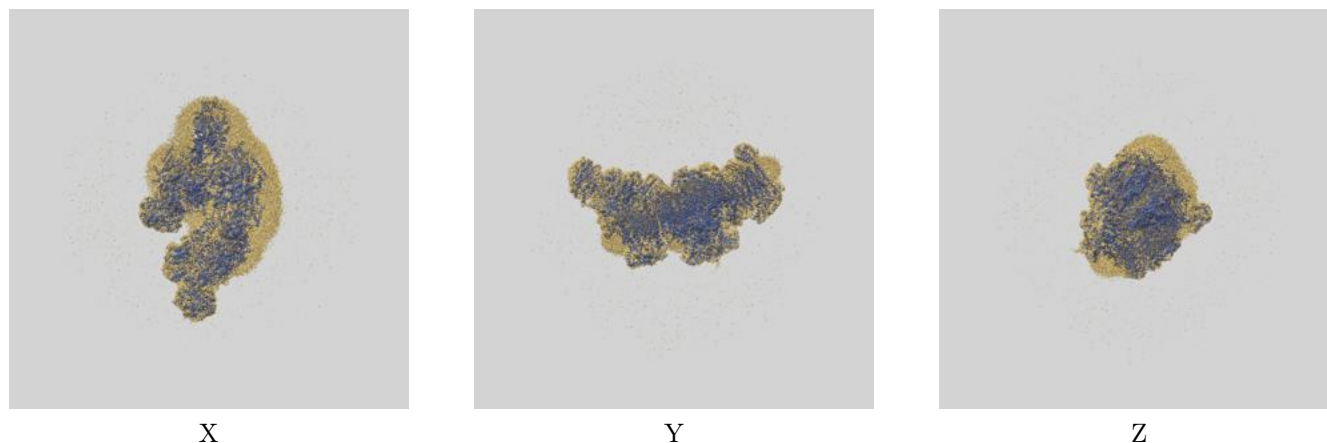
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

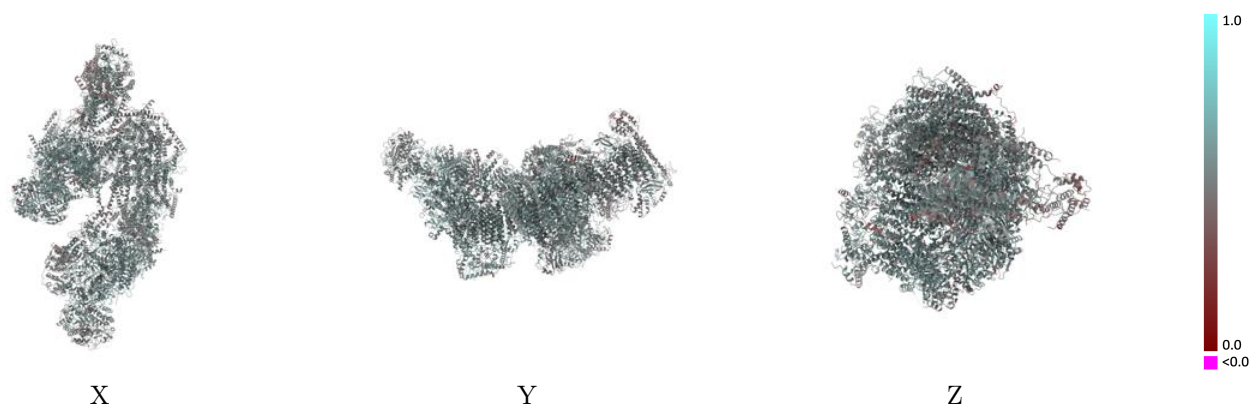
This section contains information regarding the fit between EMDB map EMD-44908 and PDB model 9BUH. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



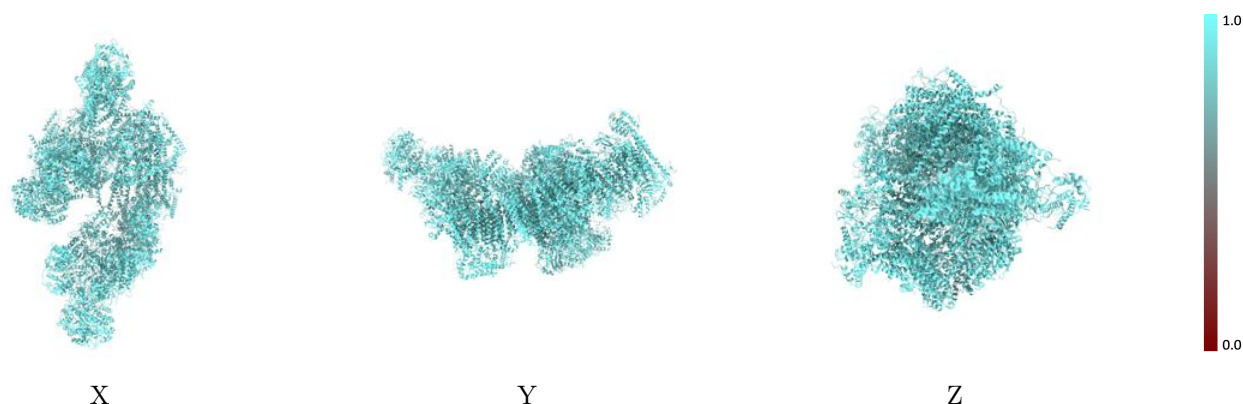
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



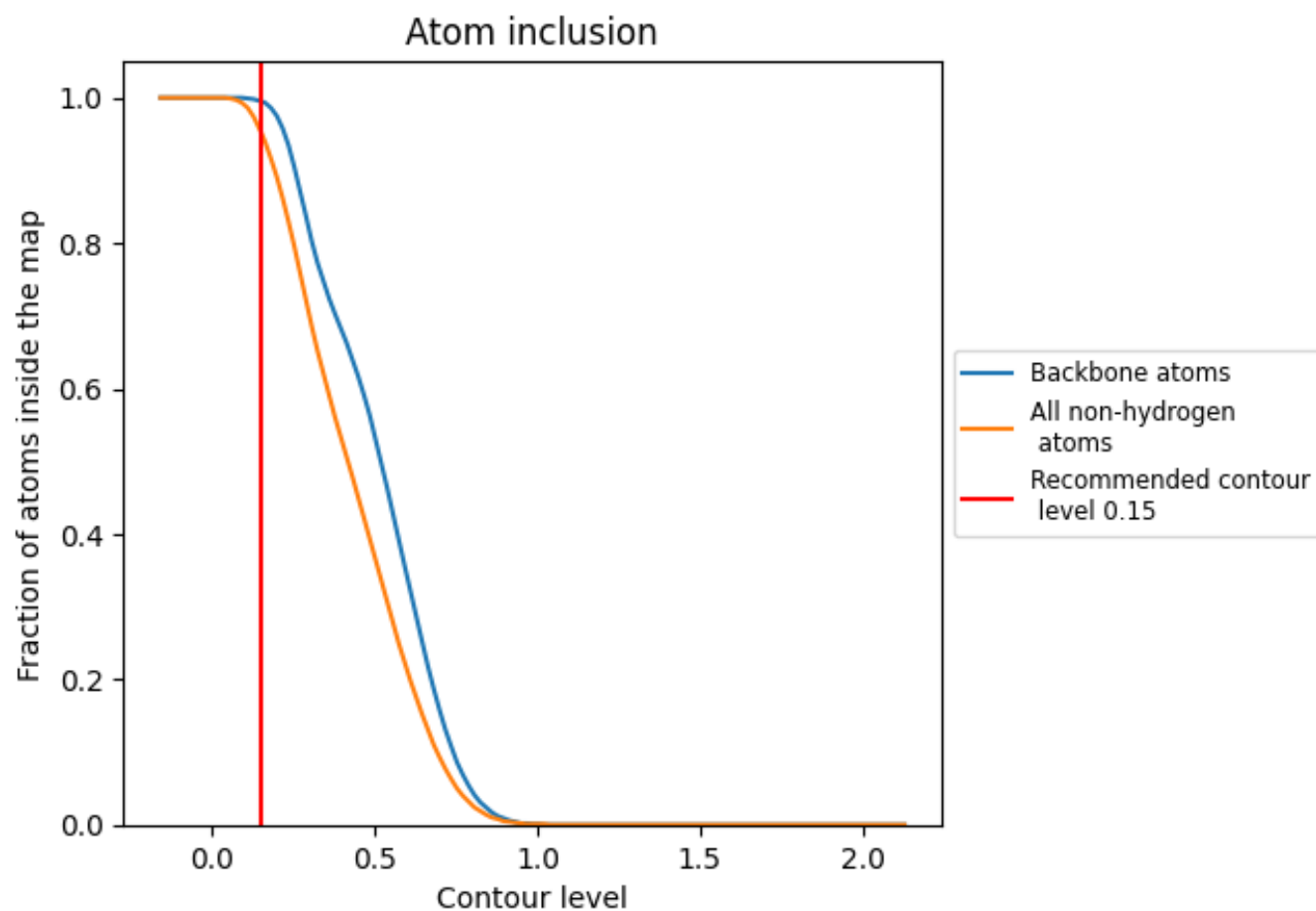
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 95% 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	 0.9520	 0.5350
0	 0.9050	 0.4930
1	 0.9650	 0.5750
2	 0.9080	 0.5020
3	 0.9780	 0.5580
4	 0.9180	 0.5050
5	 0.9630	 0.5490
6	 0.9590	 0.5460
7	 0.9760	 0.5700
8	 0.9670	 0.5530
9	 0.9560	 0.5590
A	 0.9050	 0.4660
Aa	 0.9730	 0.5540
Ab	 0.9190	 0.4880
Ac	 0.9730	 0.5590
Ad	 0.9830	 0.5520
Ae	 0.7100	 0.3260
Af	 0.7830	 0.3660
Ag	 0.9150	 0.4820
Ah	 0.8900	 0.4840
Ai	 0.9390	 0.4870
Aj	 0.9600	 0.5290
Ak	 0.9700	 0.5390
Al	 0.9400	 0.5120
Am	 0.9500	 0.5190
An	 0.9120	 0.4770
Ao	 0.9100	 0.4400
Ap	 0.8920	 0.4840
Aq	 0.9060	 0.4700
Ar	 0.9490	 0.4840
B	 0.9530	 0.5140
C	 0.9680	 0.5630
D	 0.9730	 0.5600
E	 0.9340	 0.5110
F	 0.9390	 0.5560



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Chain	Atom inclusion	Q-score
G	 0.9520	 0.5360
H	 0.9810	 0.5700
I	 0.9860	 0.5720
J	 0.9560	 0.5620
K	 0.9670	 0.5670
L	 0.9540	 0.5430
M	 0.9750	 0.5630
N	 0.9500	 0.5430
O	 0.8520	 0.4460
P	 0.9310	 0.4760
Q	 0.9420	 0.5520
R	 0.9340	 0.5100
S	 0.9780	 0.5550
T	 0.9570	 0.5290
U	 0.9330	 0.5160
V	 0.9530	 0.5250
W	 0.9520	 0.5340
X	 0.9190	 0.4910
Y	 0.9080	 0.4650
Z	 0.9180	 0.4880
a	 0.9580	 0.5520
b	 0.9490	 0.4760
c	 0.9360	 0.5310
d	 0.9420	 0.5190
e	 0.9340	 0.5100
f	 0.9360	 0.5100
g	 0.9650	 0.5430
h	 0.9430	 0.5370
i	 0.9750	 0.5590
j	 0.9640	 0.5550
k	 0.9720	 0.5600
l	 0.9480	 0.5320
m	 0.9320	 0.5240
n	 0.9270	 0.5020
o	 0.9250	 0.5250
p	 0.9490	 0.5300
q	 0.9750	 0.5560
r	 0.9710	 0.5550
s	 0.9440	 0.5290
t	 0.9320	 0.4760
u	 0.9630	 0.5590
v	 0.9640	 0.5500

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Chain	Atom inclusion	Q-score
w	 0.9810	 0.5730
x	 0.9720	 0.5650
y	 0.9380	 0.5590
z	 0.9720	 0.5640