



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 04:16 PM EDT

PDB ID : 9CDN / pdb\_00009cdn  
EMDB ID : EMD-45479  
Title : Respiratory supercomplex I+III2 open state  
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.  
Deposited on : 2024-06-25  
Resolution : 3.47 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
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) : 2.45.1

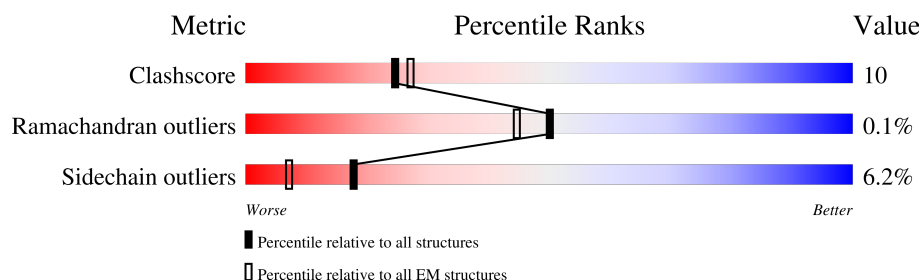
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.47 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.











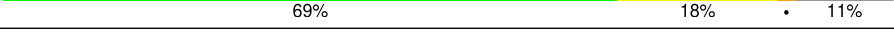

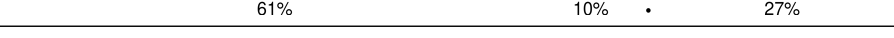
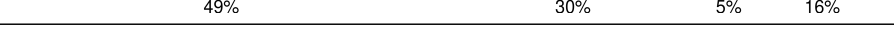

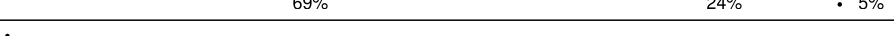
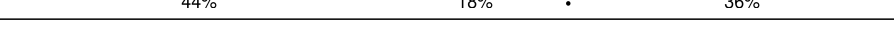
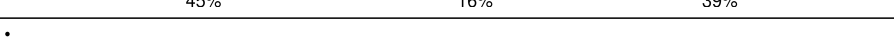
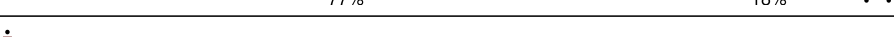

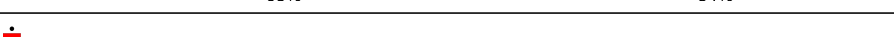






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	







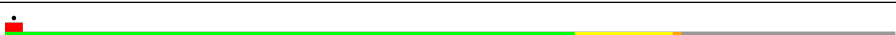
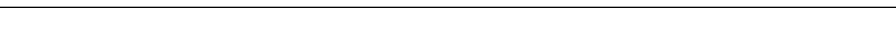
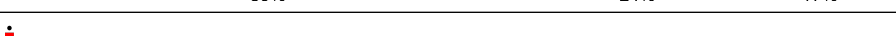
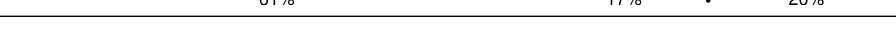
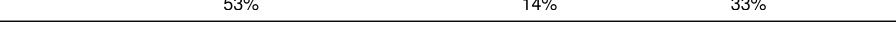
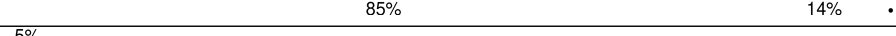



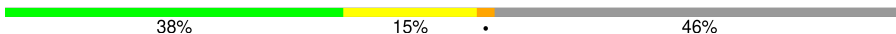









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Mol	Chain	Length	Quality of chain
4	3	56	
4	Ad	56	
5	6	453	
5	v	453	
6	7	379	
6	w	379	
7	8	326	
7	x	326	
8	9	111	
8	y	111	
9	a	189	
10	b	128	
11	c	186	
12	d	176	
13	e	154	
14	f	76	
15	g	122	
16	h	106	
17	i	347	
18	j	115	
19	k	98	
20	m	175	
21	n	58	
22	o	129	
23	p	221	









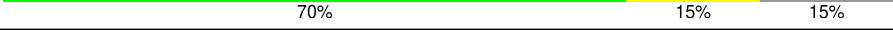
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Mol	Chain	Length	Quality of chain
24	q	459	
25	r	318	
26	B	464	
27	C	469	
28	D	264	
29	E	249	
30	F	123	
31	H	212	
32	I	196	
33	J	175	
34	K	145	
35	L	372	
36	N	116	
37	O	156	
37	X	156	
38	P	99	
39	Q	154	
40	R	110	
41	S	70	
42	T	169	
43	U	357	
44	V	141	
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	G	727	
54	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
55	FES	2	301	-	-	X	-
55	FES	4	301	-	-	X	-
59	SF4	H	301	-	-	X	-
59	SF4	H	302	-	-	X	-

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 98319 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
			557	338	100	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
			1509	951	264	287	7		
3	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
3	Ae	23	Total	C	N	O	S	0	0
			143	89	25	28	1		
3	Af	29	Total	C	N	O	S	0	0
			191	118	35	37	1		

- 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	238	Total	C	N	O	S	0	0
			1896	1211	326	343	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	99	Total	C	N	O	S	0	0
			878	563	154	159	2		
8	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	108	Total	C	N	O	0	0
			900	591	156	153		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	168	Total	C	N	O	S	0	0
			1417	890	258	261	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	46	Total	C	N	O	0	0
			391	259	67	65		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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



- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	100	Total	C	N	O	S	0	0
			793	537	116	135	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	175	Total	C	N	O	S	0	0
			1309	873	189	235	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	56	Total	C	N	O	S	0	0
			475	308	87	79	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	o	128	Total	C	N	O	0	0
			1058	688	181	189		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	430	Total	C	N	O	S	0	0
			3454	2207	593	630	24		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	94	Total	C	N	O	S	0	0
			727	444	136	144	3		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	117	Total	C	N	O	S	0	0
			953	602	171	177	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	340	Total	C	N	O	S	0	0
			2702	1745	473	475	9		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 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	84	Total	C	N	O	S	0	0
			680	440	100	135	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 subunit 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 subunit 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 subunit 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 subunit 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 subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	318	Total	C	N	O	S	0	0
			2574	1638	437	489	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	139	Total	C	N	O	S	0	0
			1016	648	173	189	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	62	Total	C	N	O	S	0	0
			531	352	88	90	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	603	Total	C	N	O	S	0	0
			4785	3174	741	819	51		

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

unit 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
			1019	635	195	180	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 NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

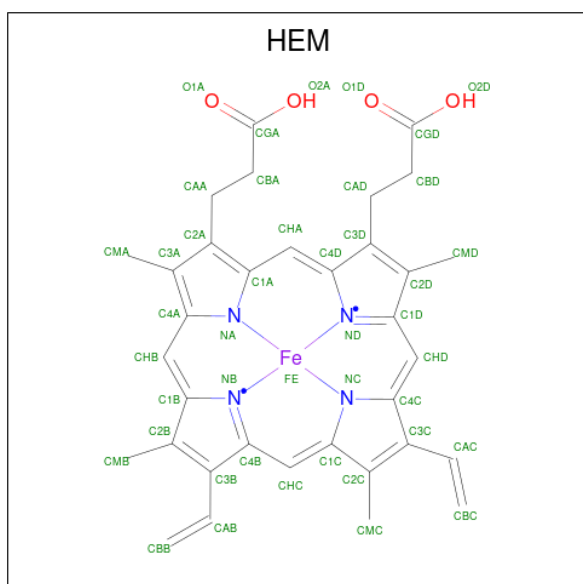
Mol	Chain	Residues	Atoms					AltConf	Trace
54	M	96	Total	C	N	O	S	0	0
			773	487	146	137	3		

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



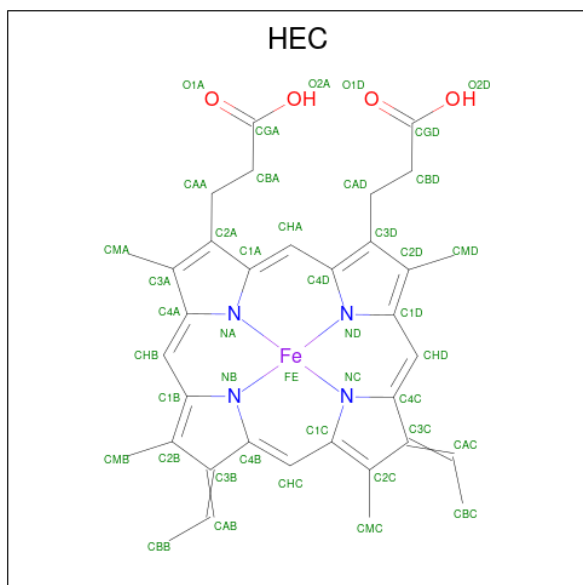
Mol	Chain	Residues	Atoms			AltConf
55	2	1	Total	Fe	S	0
			4	2	2	
55	4	1	Total	Fe	S	0
			4	2	2	
55	E	1	Total	Fe	S	0
			4	2	2	
55	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 56 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
56	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

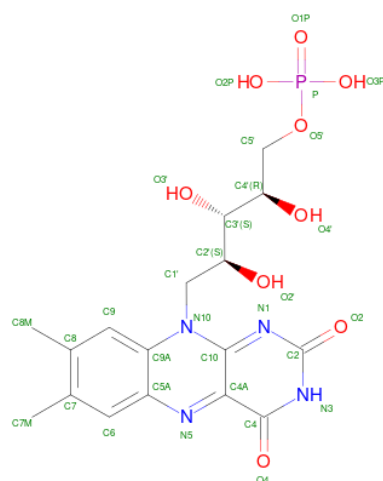
- Molecule 57 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
57	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
57	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

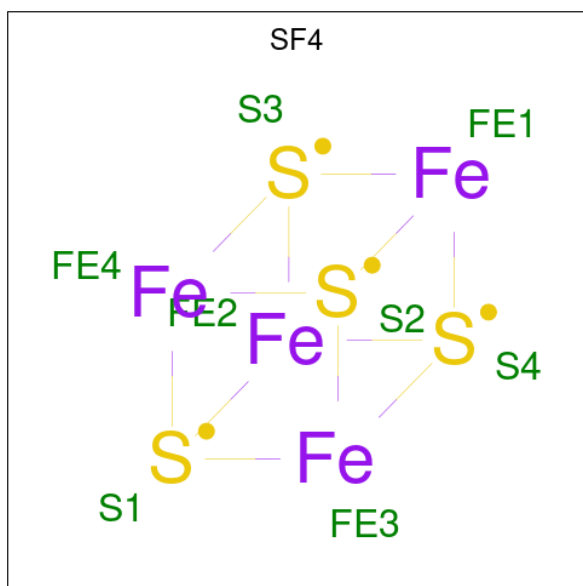
- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).





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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



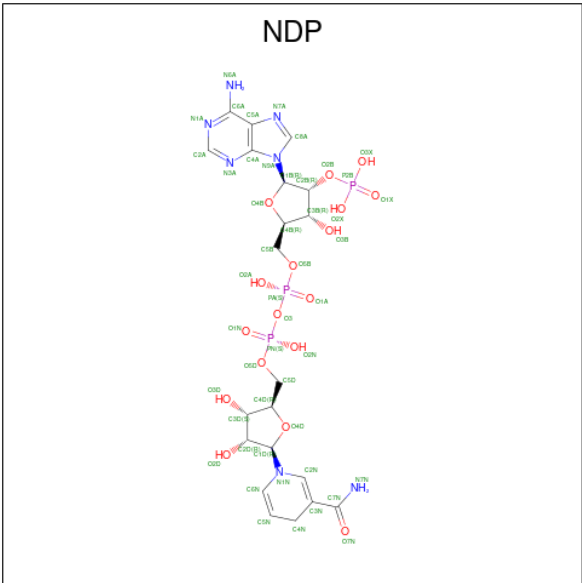
Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total 8	Fe 4	S 4	0
59	H	1	Total 8	Fe 4	S 4	0
59	H	1	Total 8	Fe 4	S 4	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 60 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



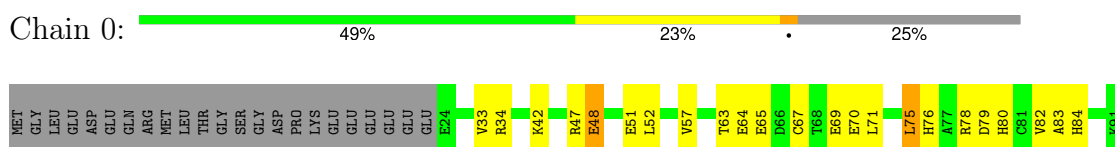


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
61	Q	1	30	18	2	8	1	1	0

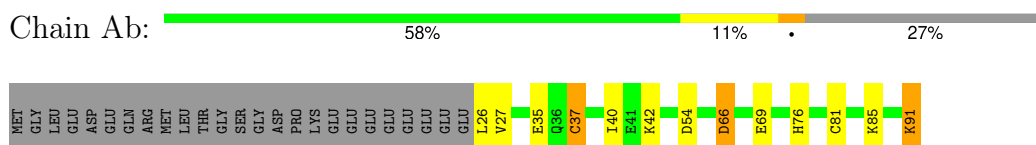
### 3 Residue-property plots

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

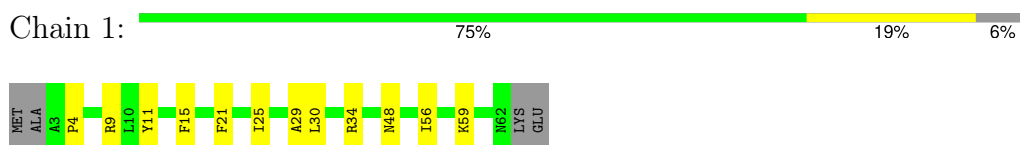
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



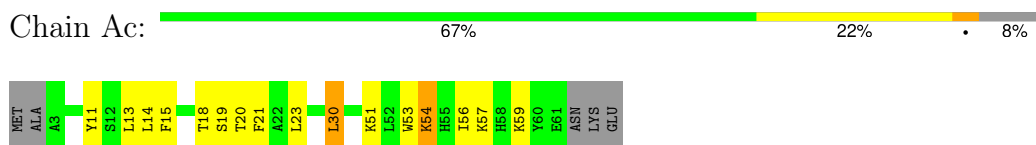
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



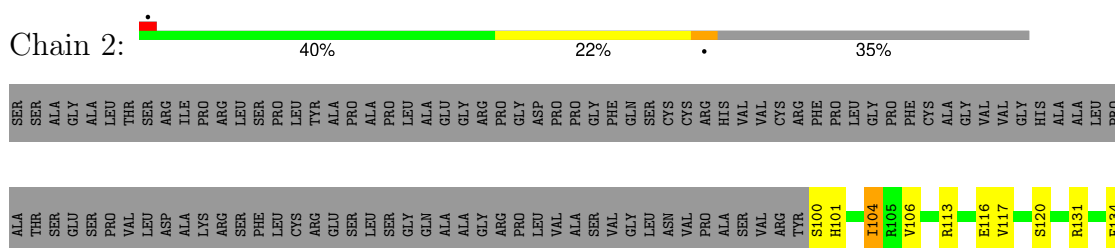
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

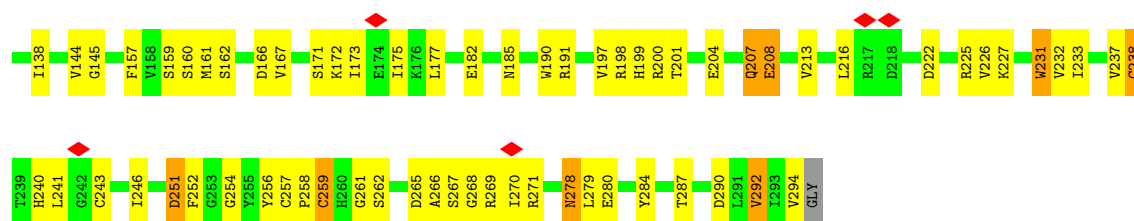


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



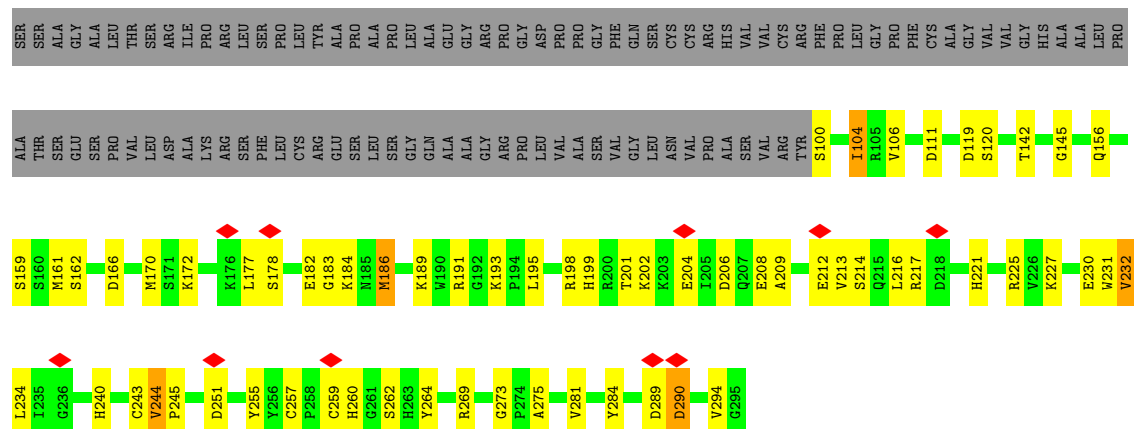
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1





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

Chain 4: 44% 20% 34%



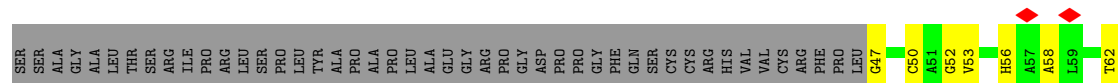
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

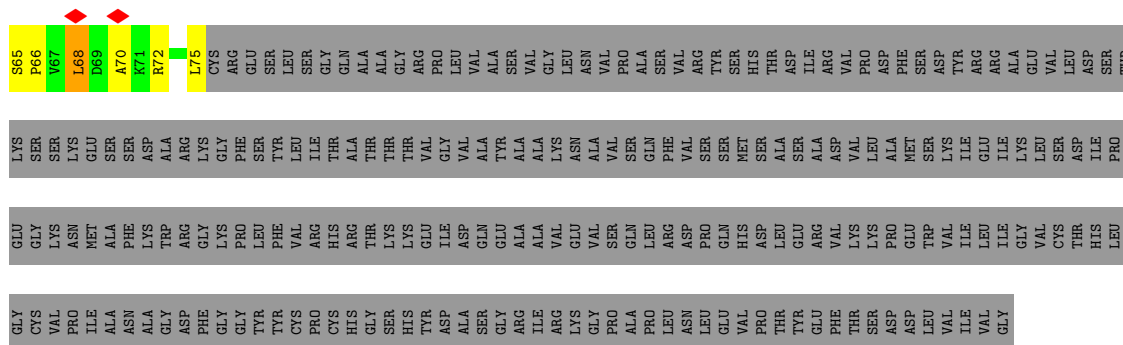
Chain Ae: 92%



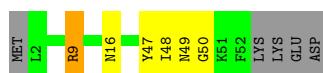
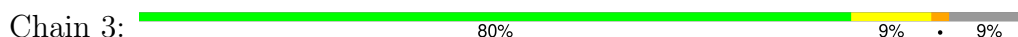
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Af: 5% 90%

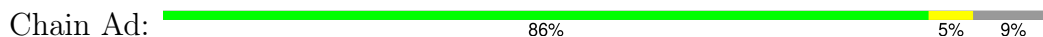




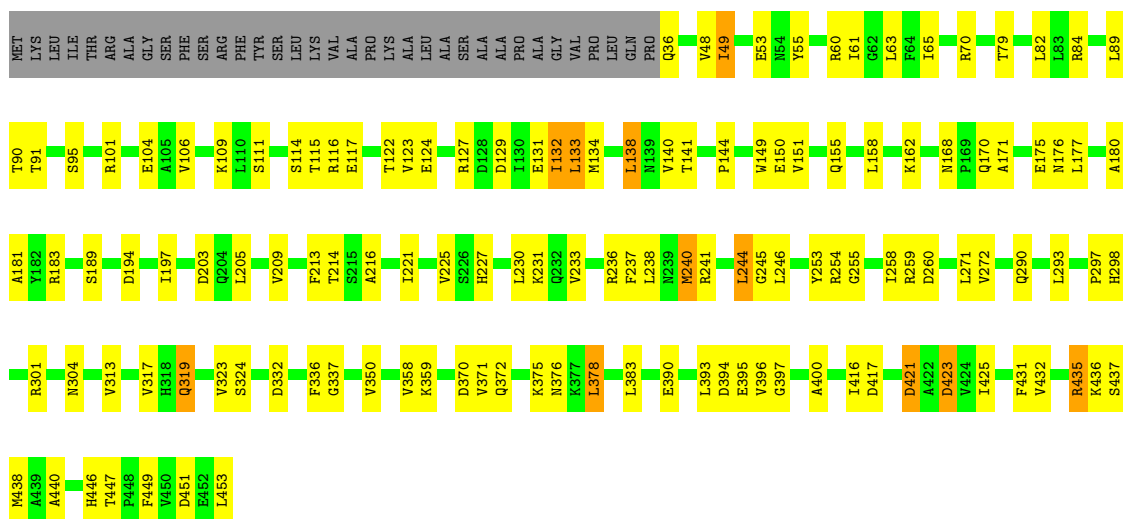
- Molecule 4: Cytochrome b-c1 complex subunit 10



- Molecule 4: Cytochrome b-c1 complex subunit 10

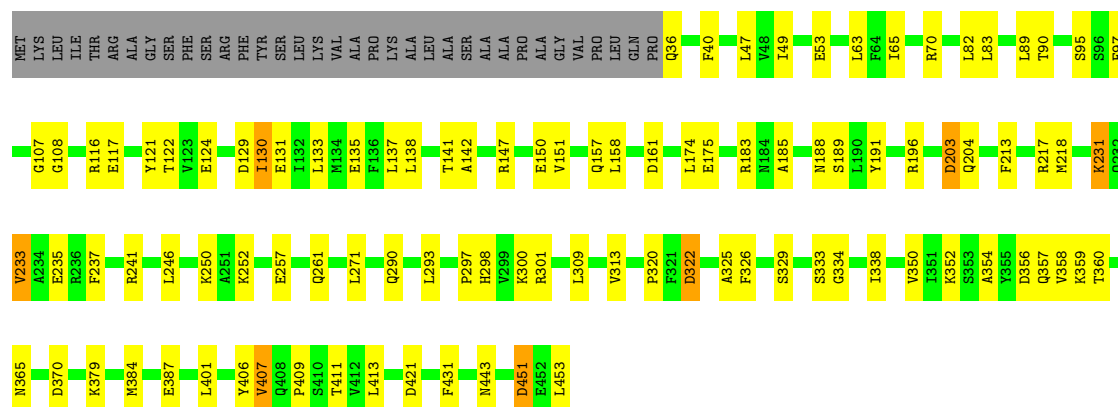


- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



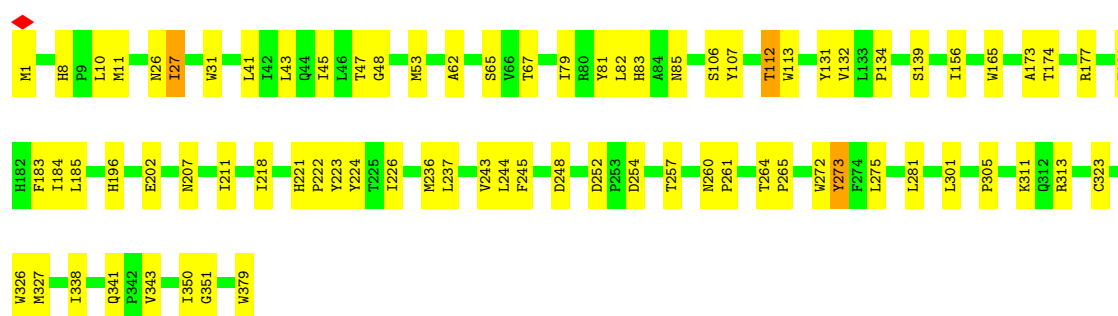
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial





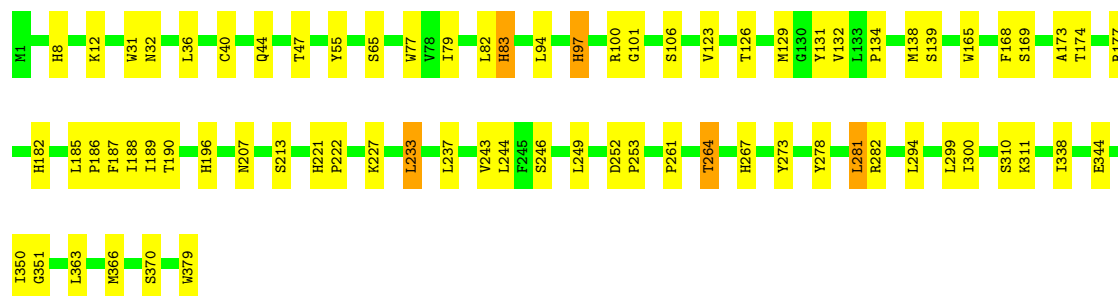
### • Molecule 6: Cytochrome b

Chain 7: 79% 20%



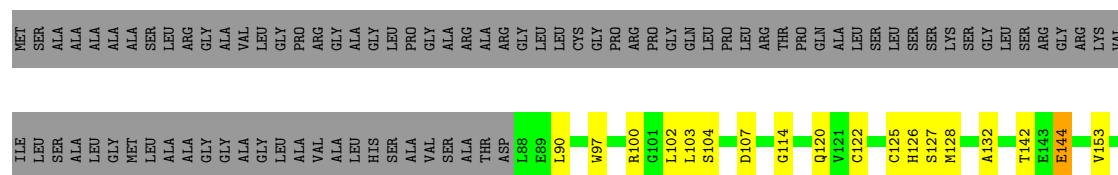
### • Molecule 6: Cytochrome b

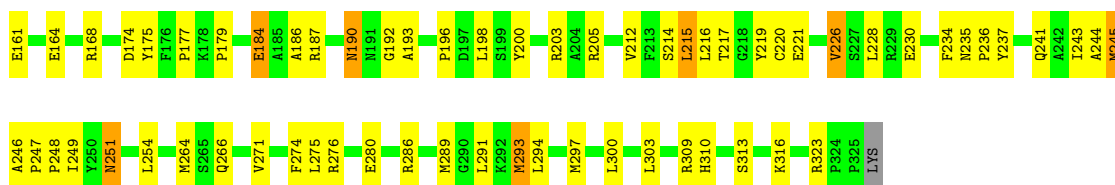
Chain w: 80% 18%



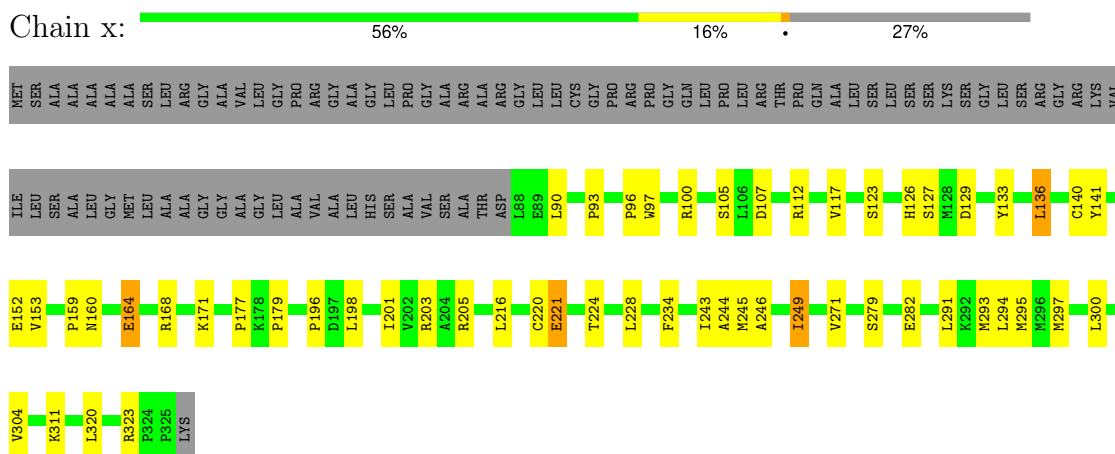
### • Molecule 7: Cytochrome c1

Chain 8: 48% 22% 27%

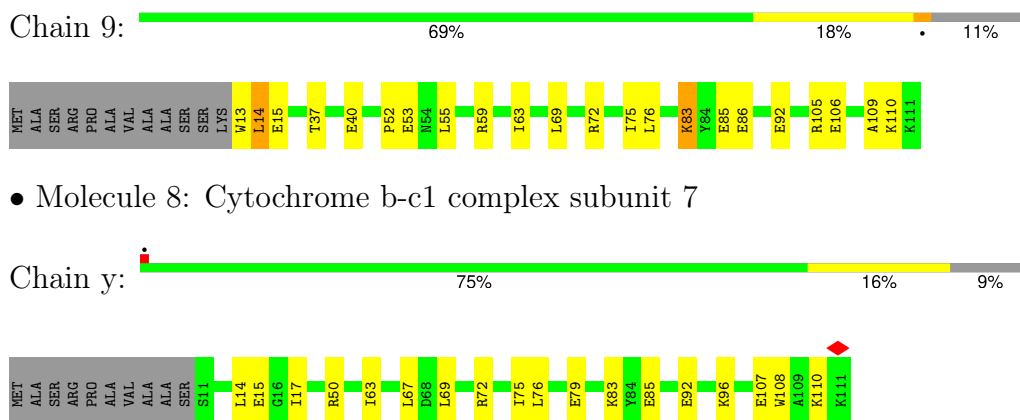




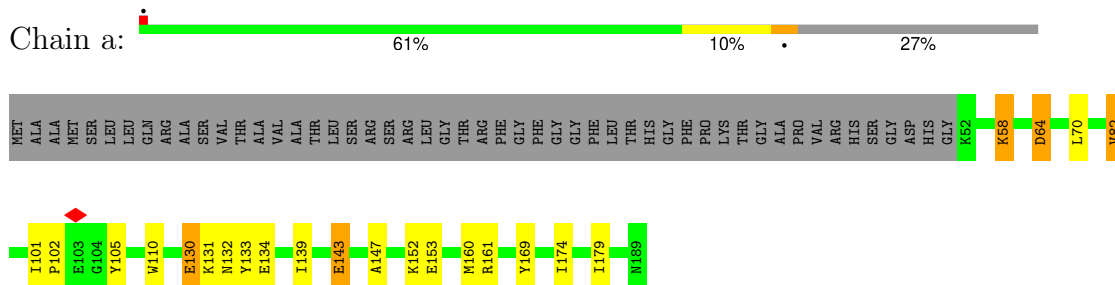
- Molecule 7: Cytochrome c1



- Molecule 8: Cytochrome b-c1 complex subunit 7

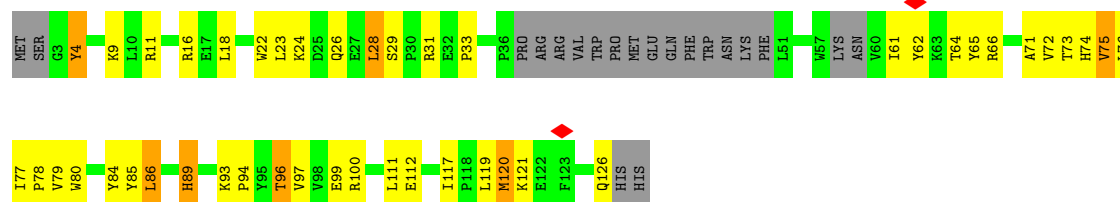


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

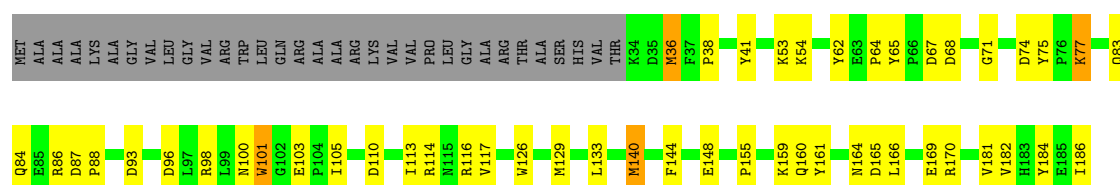


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

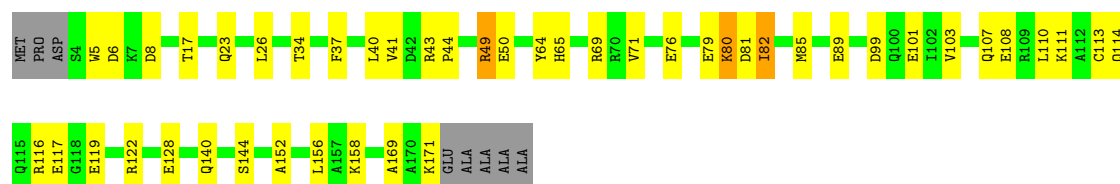




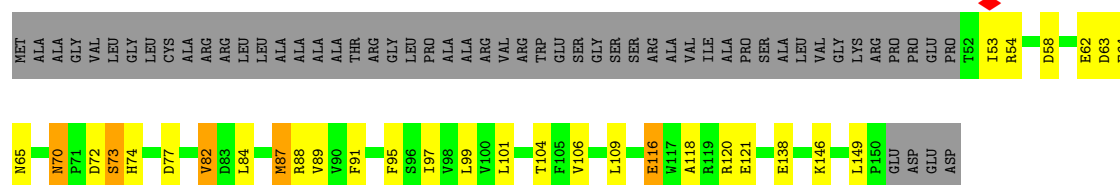
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



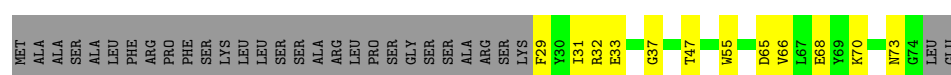
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

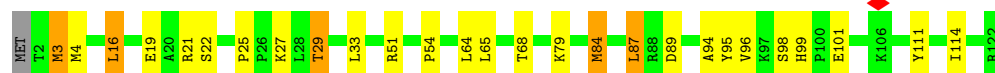


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  77% 18%



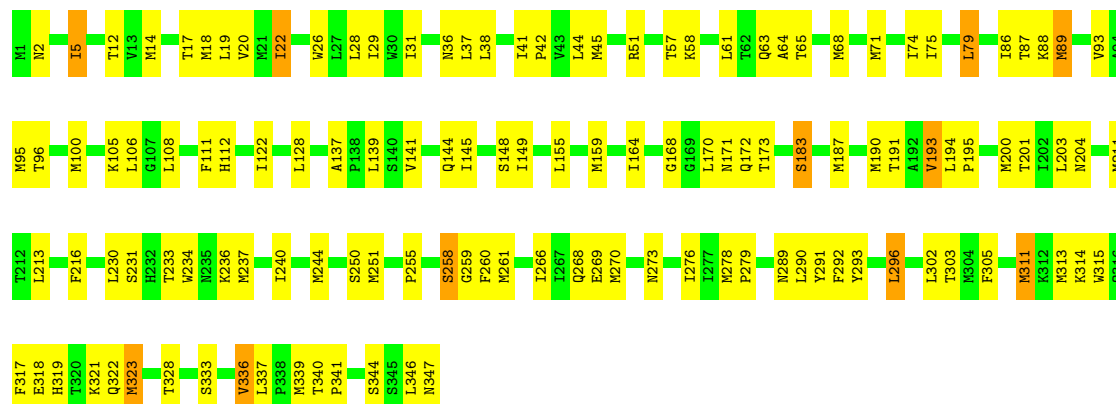
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  78% 19%



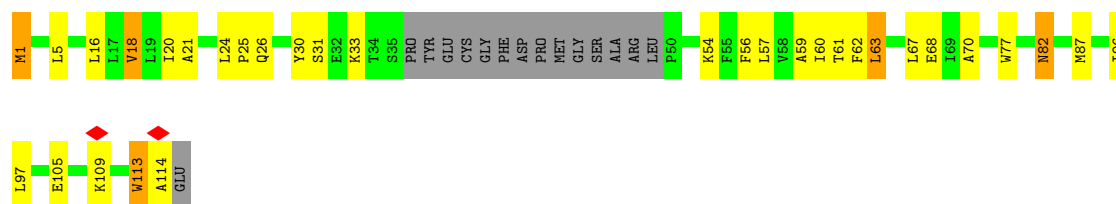
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i:  63% 34%



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:  59% 23% 13%

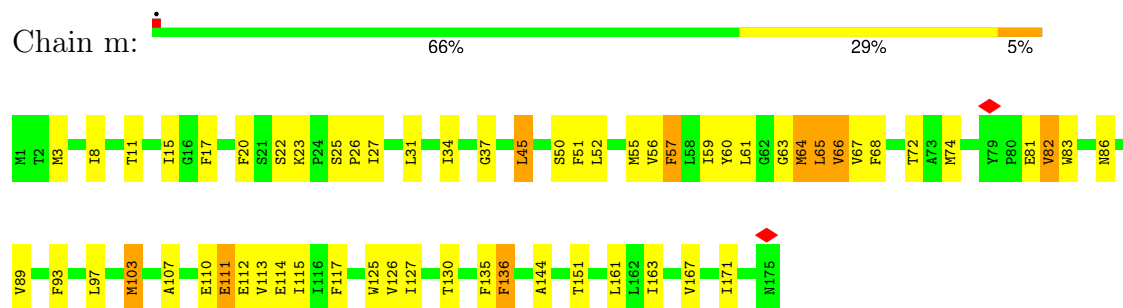


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

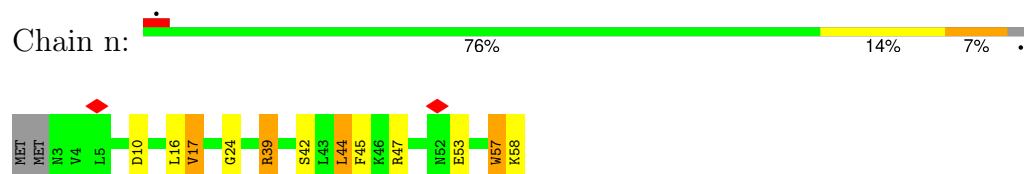
Chain k:  66% 32%



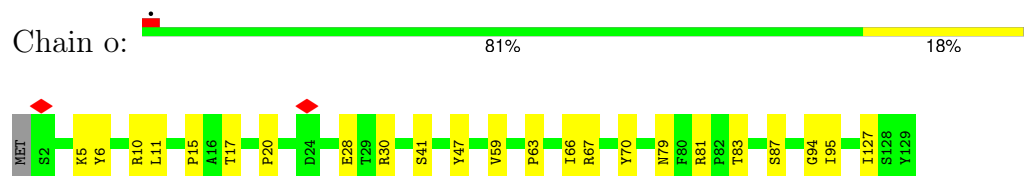
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



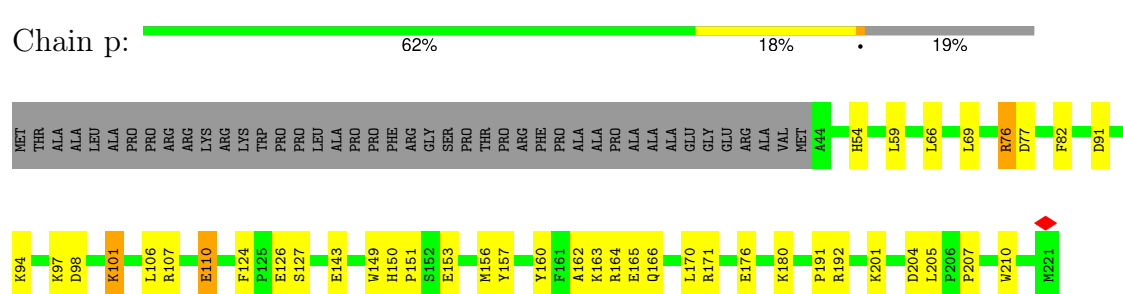
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



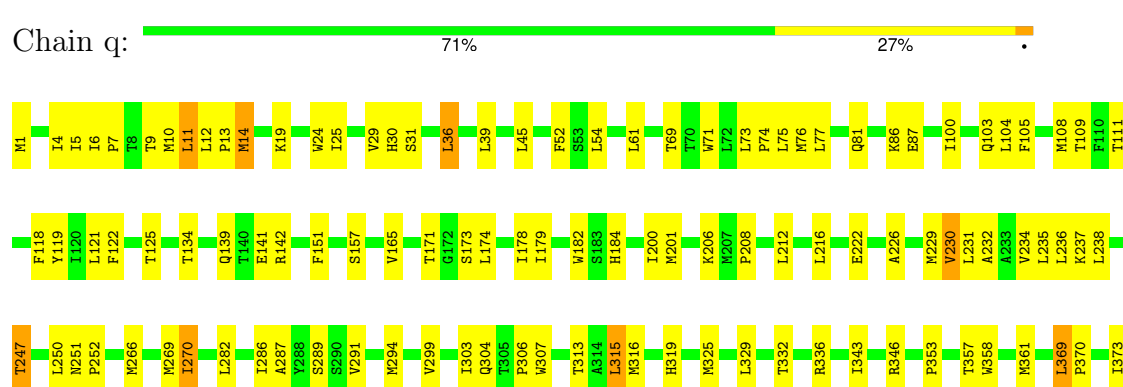
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

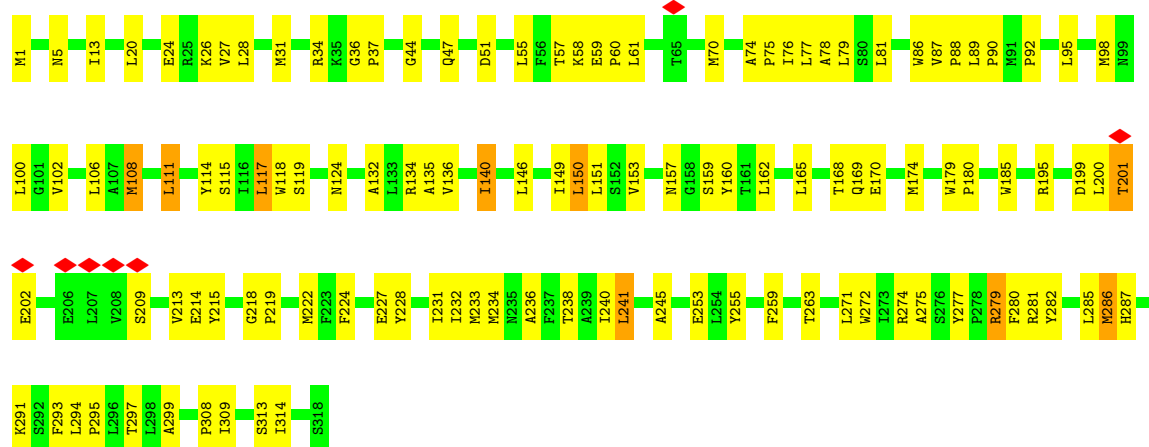


- Molecule 24: NADH-ubiquinone oxidoreductase chain 4

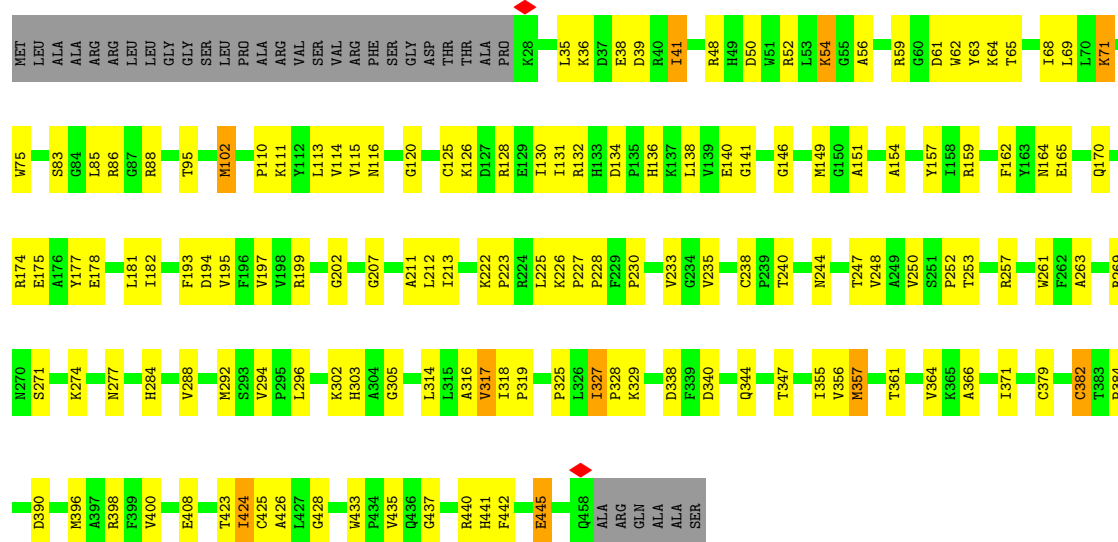




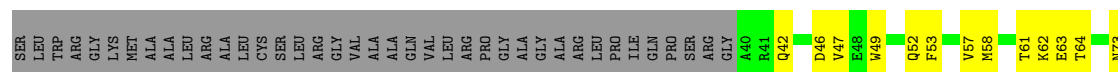
• Molecule 25: NADH-ubiquinone oxidoreductase chain 1

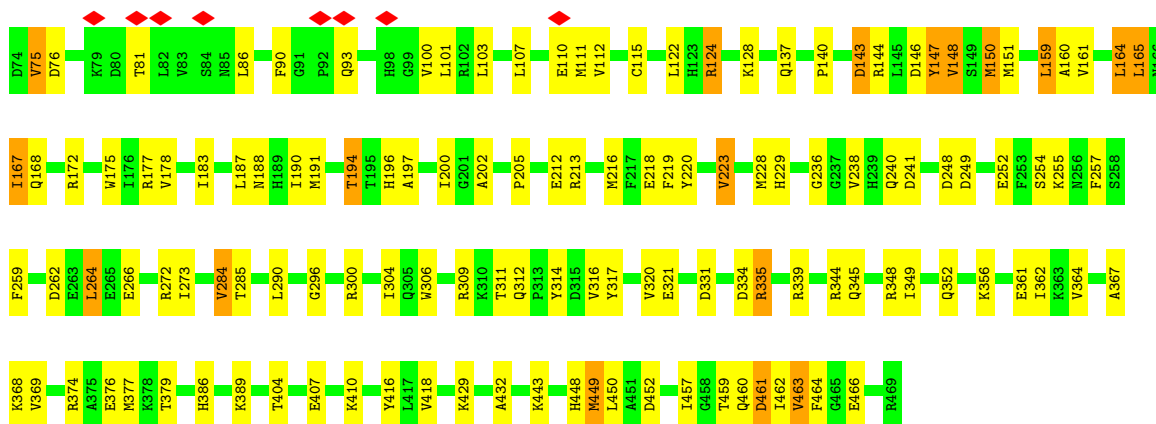


• Molecule 26: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



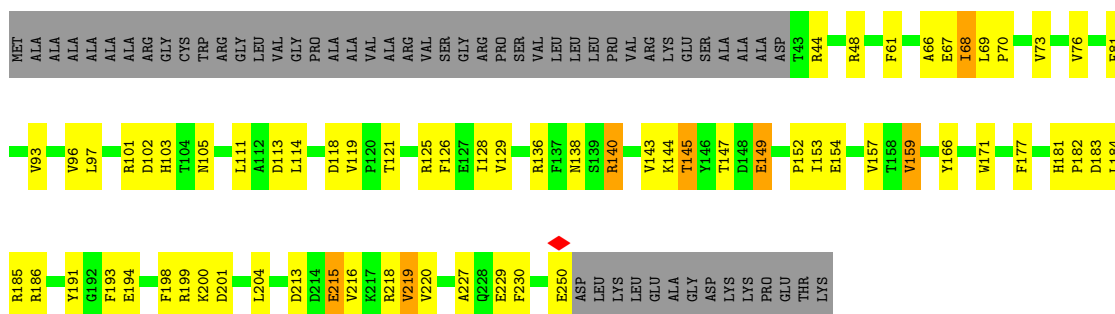
• Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





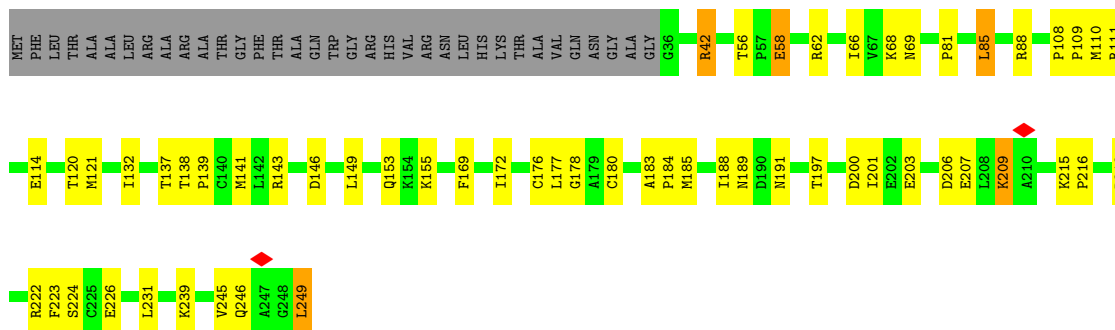
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain D: 53% 23% 21%



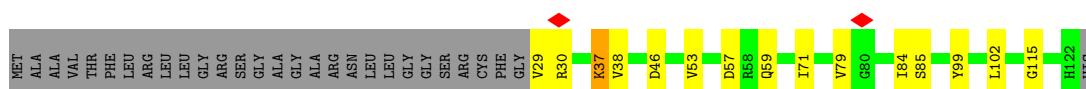
- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 63% 21% 14%



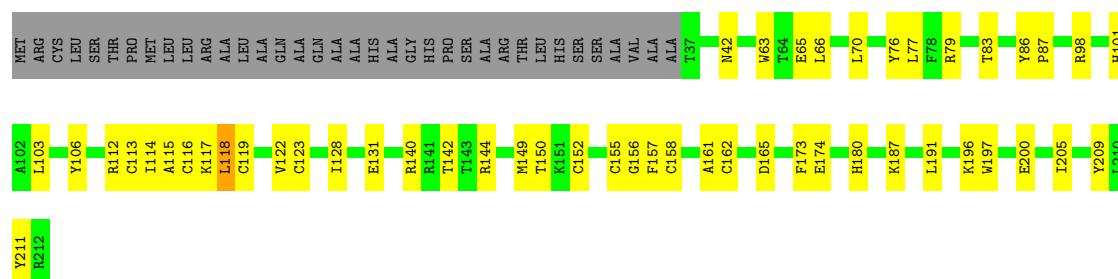
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 64% 11% 24%



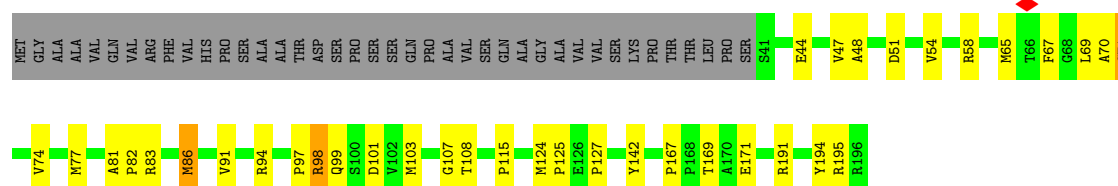
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain H: 



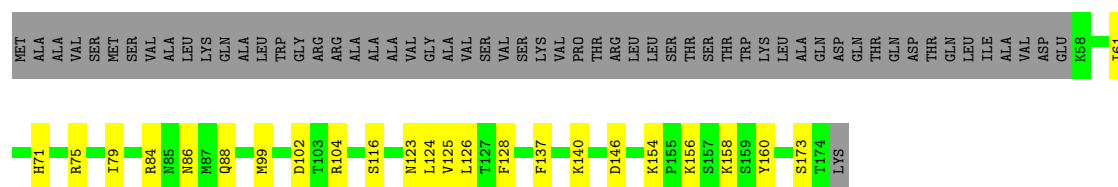
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain I: 




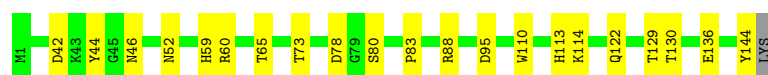
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain J: 



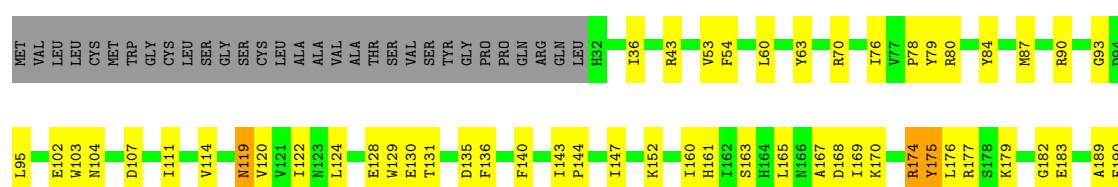
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

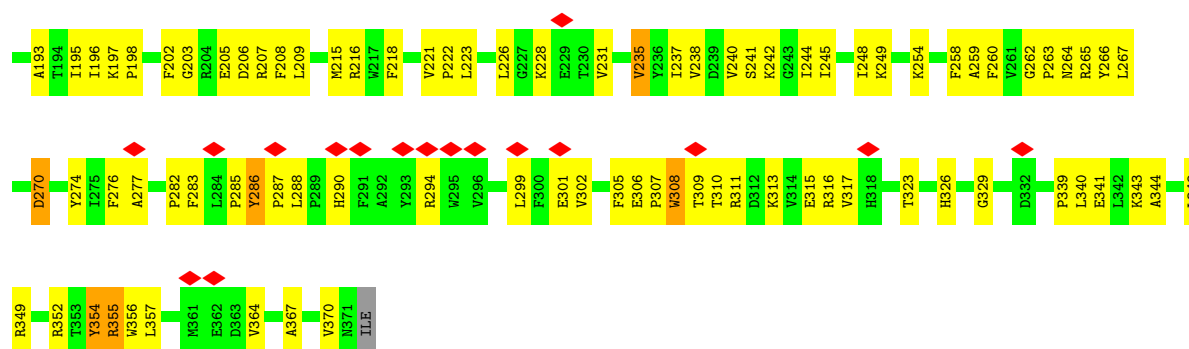
Chain K: 



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 





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

Chain N: 76% 19%



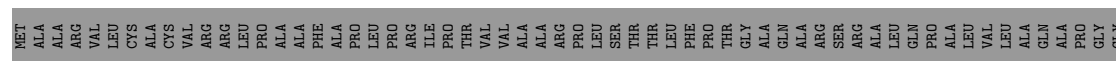
- Molecule 37: Acyl carrier protein

Chain O: 33% 17% 46%



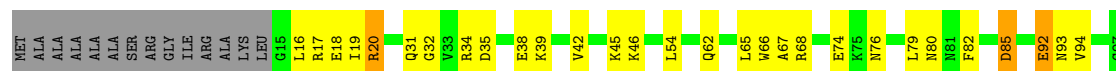
- Molecule 37: Acyl carrier protein

Chain X: 38% 15% 46%



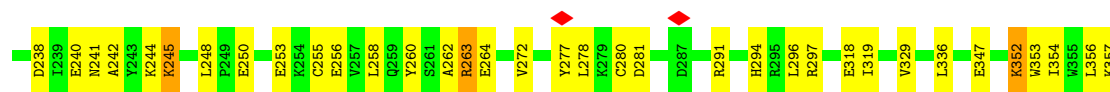
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 55% 26% 16%









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

Chain V: 80% 16% . .



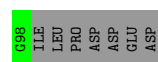
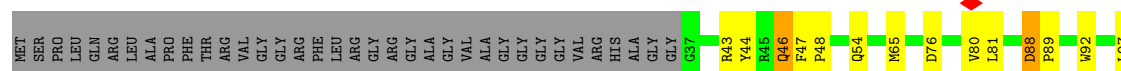
- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

Chain W: 73% 24% . .



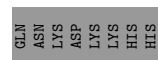
- Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 46% 11% 41% .



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

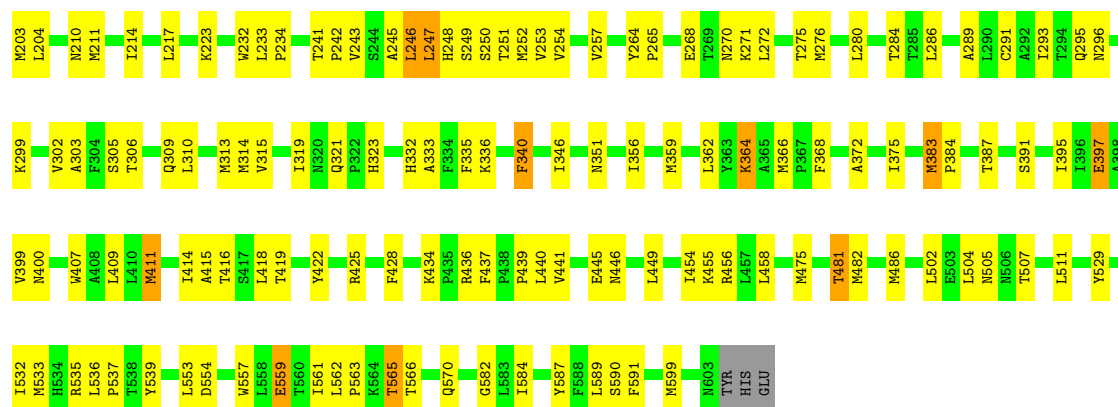
Chain Z: 54% 13% 32% .



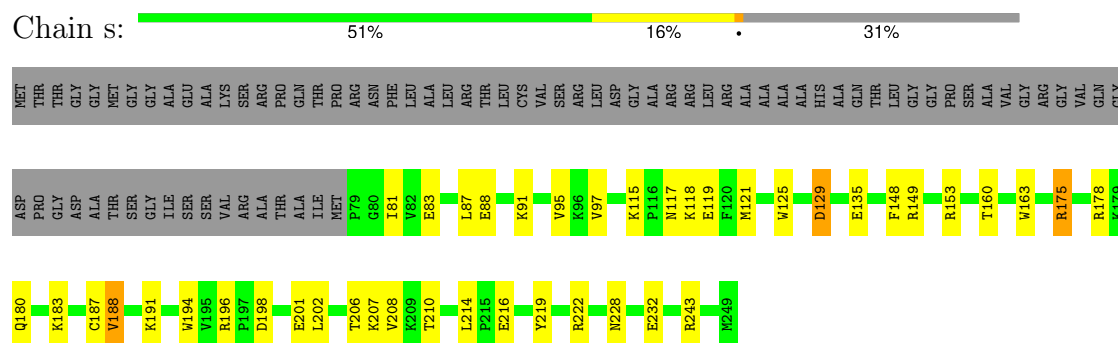
- Molecule 48: NADH-ubiquinone oxidoreductase chain 5

Chain I: 66% 31% .

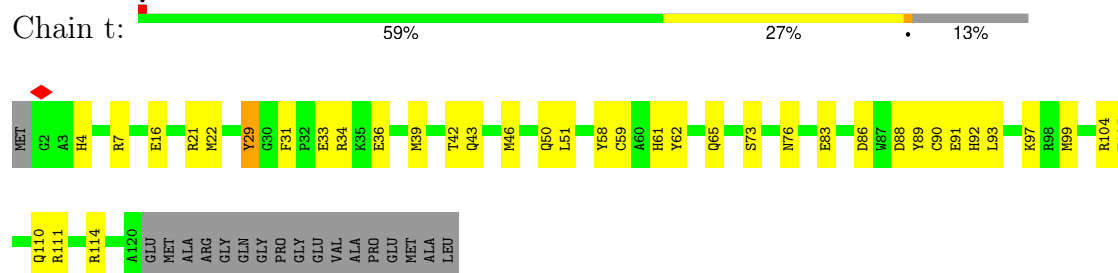




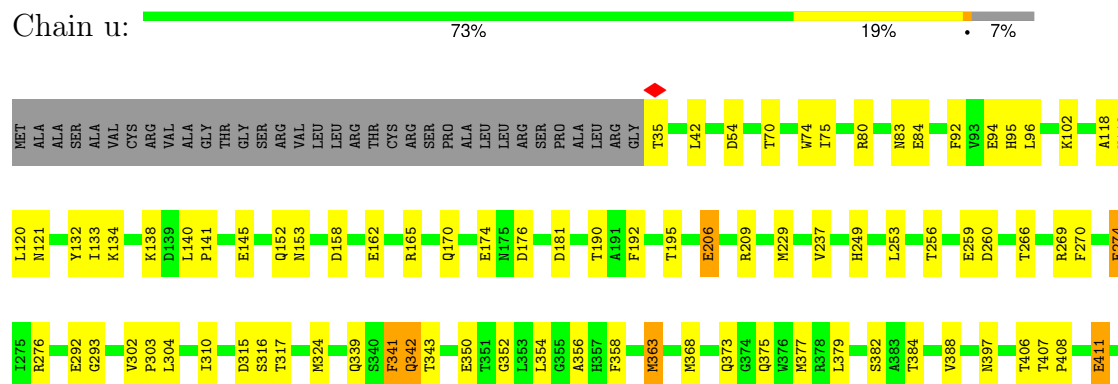
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



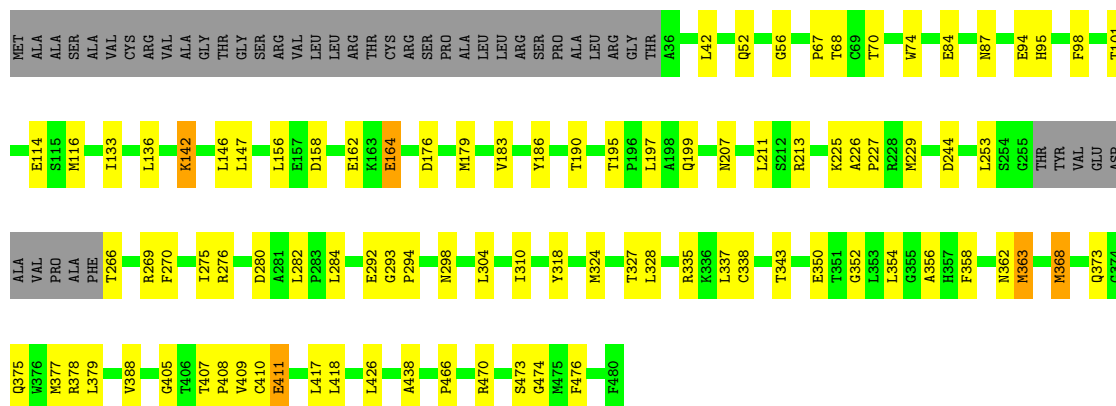
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial





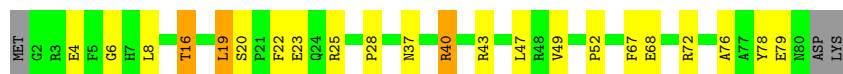
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 5: 71% 18% 9%



- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain z: 70% 23% 7%



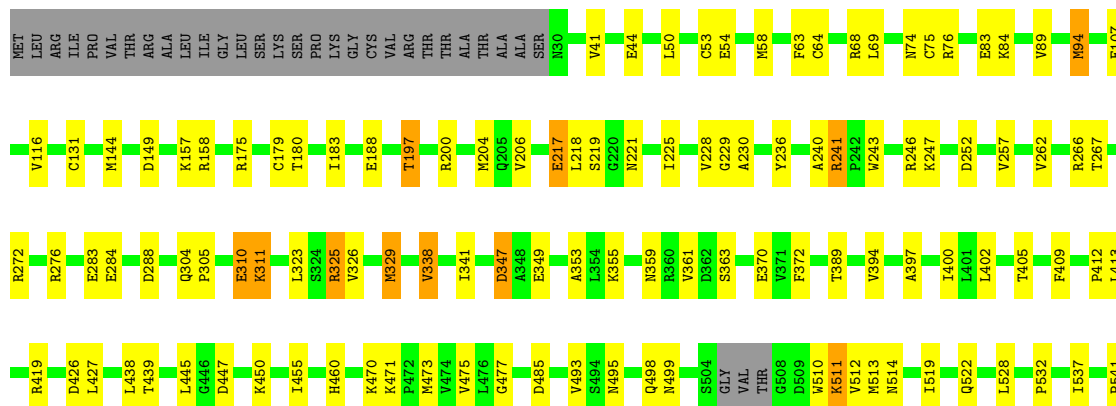
- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain Aa: 71% 23% 6%



- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 73% 19% 8%





- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11787	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	1.793	Depositor
Minimum map value	-0.229	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.036	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: FES, SF4, HEC, NDP, HEM, FMN, ZMP

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	0.17	0/563	0.32	0/755
1	Ab	0.17	0/549	0.27	0/735
2	1	0.20	0/506	0.30	0/683
2	Ac	0.15	0/498	0.23	0/672
3	2	0.19	0/1542	0.35	0/2088
3	4	0.39	1/1551 (0.1%)	0.48	0/2098
3	Ae	0.28	0/147	0.64	0/203
3	Af	0.25	0/194	0.55	0/265
4	3	0.23	0/433	0.42	0/593
4	Ad	0.14	0/437	0.22	0/598
5	6	0.20	0/3192	0.32	0/4322
5	v	0.17	0/3192	0.29	0/4322
6	7	0.25	0/3123	0.37	0/4269
6	w	0.28	0/3123	0.41	0/4269
7	8	0.50	0/1954	0.64	0/2652
7	x	0.18	0/1954	0.27	0/2652
8	9	0.17	0/898	0.29	0/1204
8	y	0.17	0/913	0.27	0/1223
9	a	0.27	0/1184	0.36	0/1603
10	b	0.38	0/927	0.55	0/1264
11	c	0.18	0/1346	0.30	0/1840
12	d	0.23	0/1449	0.35	0/1953
13	e	0.18	0/849	0.36	0/1153
14	f	0.22	0/404	0.34	0/547
15	g	0.26	0/1031	0.37	0/1394
16	h	0.17	0/889	0.27	0/1190
17	i	0.21	0/2774	0.33	0/3768
18	j	0.42	0/811	0.62	0/1107
19	k	0.38	0/759	0.57	0/1029
20	m	0.56	0/1340	0.75	0/1816
21	n	0.16	0/487	0.32	0/659
22	o	0.17	0/1088	0.31	0/1477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
23	p	0.21	0/1590	0.36	0/2155
24	q	0.21	0/3721	0.33	0/5073
25	r	0.45	0/2581	0.61	0/3529
26	B	0.15	0/3393	0.32	0/4584
27	C	0.30	0/3547	0.46	1/4809 (0.0%)
28	D	0.18	0/1783	0.32	0/2428
29	E	0.15	0/1698	0.32	0/2311
30	F	0.14	0/740	0.26	0/998
31	H	0.42	0/1443	0.56	0/1952
32	I	0.22	0/1279	0.35	0/1730
33	J	0.14	0/976	0.26	0/1318
34	K	0.14	0/1244	0.23	0/1693
35	L	0.21	0/2774	0.38	0/3761
36	N	0.15	0/929	0.28	0/1258
37	O	0.14	0/692	0.37	0/934
37	X	0.12	0/701	0.29	0/946
38	P	0.12	0/680	0.28	0/916
39	Q	0.16	0/978	0.30	0/1317
40	R	0.11	0/304	0.25	0/410
41	S	0.18	0/577	0.32	0/777
42	T	0.15	0/659	0.26	0/905
43	U	0.38	0/2634	0.51	0/3565
44	V	0.16	0/1037	0.30	0/1404
45	W	0.20	0/1193	0.32	0/1609
46	Y	0.16	0/555	0.30	0/760
47	Z	0.12	0/645	0.23	0/872
48	l	0.19	0/4914	0.34	0/6683
49	s	0.16	0/1436	0.32	0/1938
50	t	0.28	0/1043	0.40	0/1396
51	5	0.18	0/3442	0.30	0/4667
51	u	0.17	0/3531	0.29	0/4793
52	Aa	0.16	0/684	0.29	0/926
52	z	0.17	0/688	0.33	0/931
53	G	0.15	0/5347	0.30	0/7243
54	M	0.14	0/791	0.29	0/1069
All	All	0.25	1/100336 (0.0%)	0.38	1/136063 (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	8	0	1
25	r	0	1
27	C	0	2
32	I	0	1
43	U	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	244	VAL	N-CA	5.10	1.49	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	110	GLU	N-CA-C	-6.42	103.98	113.61

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	8	205	ARG	Sidechain
27	C	335	ARG	Sidechain
27	C	339	ARG	Sidechain
32	I	98	ARG	Sidechain
25	r	279	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	557	0	529	18	0
1	Ab	543	0	528	6	0
2	1	493	0	491	9	0
2	Ac	485	0	485	10	0
3	2	1509	0	1492	56	0
3	4	1518	0	1499	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ae	143	0	134	10	0
3	Af	191	0	188	8	0
4	3	417	0	414	7	0
4	Ad	421	0	418	4	0
5	6	3140	0	3121	87	0
5	v	3140	0	3121	60	0
6	7	3025	0	3090	55	0
6	w	3025	0	3090	57	0
7	8	1896	0	1844	74	0
7	x	1896	0	1843	38	0
8	9	878	0	870	11	0
8	y	893	0	888	7	0
9	a	1151	0	1164	25	0
10	b	900	0	903	44	0
11	c	1291	0	1185	36	0
12	d	1417	0	1393	35	0
13	e	826	0	789	18	0
14	f	391	0	392	12	0
15	g	1000	0	994	23	0
16	h	867	0	871	18	0
17	i	2711	0	2874	94	0
18	j	793	0	842	27	0
19	k	748	0	799	37	0
20	m	1309	0	1305	70	0
21	n	475	0	475	11	0
22	o	1058	0	1061	19	0
23	p	1534	0	1470	27	0
24	q	3630	0	3837	97	0
25	r	2508	0	2607	91	0
26	B	3318	0	3282	105	0
27	C	3454	0	3383	94	0
28	D	1732	0	1682	47	0
29	E	1658	0	1662	48	0
30	F	727	0	694	7	0
31	H	1412	0	1368	42	0
32	I	1248	0	1254	29	0
33	J	953	0	949	18	0
34	K	1203	0	1161	13	0
35	L	2702	0	2713	89	0
36	N	910	0	950	15	0
37	O	680	0	681	24	0
37	X	689	0	687	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	P	669	0	677	24	0
39	Q	954	0	960	27	0
40	R	295	0	279	14	0
41	S	562	0	557	8	0
42	T	638	0	637	6	0
43	U	2574	0	2532	52	0
44	V	1016	0	1022	19	0
45	W	1162	0	1156	27	0
46	Y	531	0	480	11	0
47	Z	626	0	607	11	0
48	l	4785	0	4935	147	0
49	s	1398	0	1374	31	0
50	t	1019	0	987	22	0
51	5	3374	0	3272	57	0
51	u	3459	0	3350	57	0
52	Aa	662	0	660	14	0
52	z	666	0	663	15	0
53	G	5260	0	5287	92	0
54	M	773	0	801	11	0
55	2	4	0	0	3	0
55	4	4	0	0	3	0
55	E	4	0	0	1	0
55	G	4	0	0	0	0
56	7	86	0	60	14	0
56	w	86	0	60	16	0
57	8	43	0	31	18	0
57	x	43	0	30	4	0
58	B	31	0	19	1	0
59	B	8	0	0	1	0
59	G	16	0	0	1	0
59	H	16	0	0	11	0
59	I	8	0	0	1	0
60	L	48	0	26	1	0
61	Q	30	0	30	3	0
All	All	98319	0	97964	2035	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 2035 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)
7:8:122:CYS:SG	57:8:401:HEC:CAB	2.22	1.28
31:H:116:CYS:SG	59:H:302:SF4:FE1	1.44	1.07
7:8:122:CYS:SG	57:8:401:HEC:C3B	2.43	1.06
31:H:162:CYS:SG	59:H:302:SF4:FE4	1.59	0.94
31:H:113:CYS:SG	59:H:302:SF4:FE3	1.61	0.92

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%)	64 (97%)	2 (3%)	0	100	100
1	Ab	64/91 (70%)	64 (100%)	0	0	100	100
2	1	58/64 (91%)	58 (100%)	0	0	100	100
2	Ac	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
3	2	193/299 (64%)	188 (97%)	5 (3%)	0	100	100
3	4	194/299 (65%)	184 (95%)	9 (5%)	1 (0%)	25	59
3	Ae	21/299 (7%)	13 (62%)	7 (33%)	1 (5%)	2	17
3	Af	27/299 (9%)	20 (74%)	7 (26%)	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%)	412 (99%)	4 (1%)	0	100	100
5	v	416/453 (92%)	412 (99%)	4 (1%)	0	100	100
6	7	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
6	w	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
7	8	236/326 (72%)	227 (96%)	8 (3%)	1 (0%)	30	64
7	x	236/326 (72%)	231 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	9	97/111 (87%)	97 (100%)	0	0	100	100
8	y	99/111 (89%)	99 (100%)	0	0	100	100
9	a	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
10	b	102/128 (80%)	93 (91%)	8 (8%)	1 (1%)	13	46
11	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
12	d	166/176 (94%)	165 (99%)	0	1 (1%)	22	55
13	e	97/154 (63%)	90 (93%)	7 (7%)	0	100	100
14	f	44/76 (58%)	44 (100%)	0	0	100	100
15	g	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
16	h	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
17	i	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
18	j	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
19	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
20	m	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	22	55
21	n	54/58 (93%)	49 (91%)	5 (9%)	0	100	100
22	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
23	p	176/221 (80%)	175 (99%)	1 (1%)	0	100	100
24	q	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
25	r	316/318 (99%)	298 (94%)	17 (5%)	1 (0%)	37	69
26	B	429/464 (92%)	418 (97%)	11 (3%)	0	100	100
27	C	428/469 (91%)	411 (96%)	16 (4%)	1 (0%)	44	76
28	D	206/264 (78%)	197 (96%)	9 (4%)	0	100	100
29	E	212/249 (85%)	204 (96%)	8 (4%)	0	100	100
30	F	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
31	H	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
32	I	154/196 (79%)	151 (98%)	3 (2%)	0	100	100
33	J	115/175 (66%)	115 (100%)	0	0	100	100
34	K	142/145 (98%)	142 (100%)	0	0	100	100
35	L	338/372 (91%)	324 (96%)	14 (4%)	0	100	100
36	N	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
37	O	82/156 (53%)	79 (96%)	2 (2%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	X	83/156 (53%)	80 (96%)	3 (4%)	0	100	100
38	P	81/99 (82%)	80 (99%)	1 (1%)	0	100	100
39	Q	110/154 (71%)	108 (98%)	2 (2%)	0	100	100
40	R	33/110 (30%)	33 (100%)	0	0	100	100
41	S	68/70 (97%)	68 (100%)	0	0	100	100
42	T	80/169 (47%)	78 (98%)	2 (2%)	0	100	100
43	U	316/357 (88%)	307 (97%)	9 (3%)	0	100	100
44	V	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
45	W	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
46	Y	60/105 (57%)	55 (92%)	5 (8%)	0	100	100
47	Z	76/114 (67%)	76 (100%)	0	0	100	100
48	l	601/606 (99%)	578 (96%)	23 (4%)	0	100	100
49	s	169/249 (68%)	167 (99%)	2 (1%)	0	100	100
50	t	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
51	5	431/480 (90%)	423 (98%)	8 (2%)	0	100	100
51	u	444/480 (92%)	437 (98%)	7 (2%)	0	100	100
52	Aa	76/82 (93%)	76 (100%)	0	0	100	100
52	z	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
53	G	680/727 (94%)	668 (98%)	12 (2%)	0	100	100
54	M	92/113 (81%)	89 (97%)	3 (3%)	0	100	100
All	All	12140/14729 (82%)	11826 (97%)	305 (2%)	9 (0%)	50	79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	b	120	MET
25	r	201	THR
27	C	461	ASP
3	Ae	50	CYS
12	d	80	LYS

### 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	64/85 (75%)	59 (92%)	5 (8%)	10	34
1	Ab	63/85 (74%)	53 (84%)	10 (16%)	2	12
2	1	49/52 (94%)	49 (100%)	0	100	100
2	Ac	48/52 (92%)	44 (92%)	4 (8%)	9	32
3	2	165/245 (67%)	152 (92%)	13 (8%)	10	34
3	4	166/245 (68%)	155 (93%)	11 (7%)	14	41
3	Ae	14/245 (6%)	12 (86%)	2 (14%)	2	16
3	Af	19/245 (8%)	15 (79%)	4 (21%)	1	5
4	3	40/46 (87%)	39 (98%)	1 (2%)	42	68
4	Ad	41/46 (89%)	40 (98%)	1 (2%)	44	68
5	6	329/355 (93%)	310 (94%)	19 (6%)	17	44
5	v	329/355 (93%)	308 (94%)	21 (6%)	14	42
6	7	332/332 (100%)	318 (96%)	14 (4%)	25	54
6	w	332/332 (100%)	323 (97%)	9 (3%)	40	65
7	8	203/259 (78%)	189 (93%)	14 (7%)	13	39
7	x	203/259 (78%)	194 (96%)	9 (4%)	24	54
8	9	91/99 (92%)	82 (90%)	9 (10%)	6	26
8	y	93/99 (94%)	87 (94%)	6 (6%)	14	41
9	a	121/158 (77%)	115 (95%)	6 (5%)	20	49
10	b	97/121 (80%)	87 (90%)	10 (10%)	6	26
11	c	138/160 (86%)	130 (94%)	8 (6%)	17	44
12	d	152/156 (97%)	142 (93%)	10 (7%)	14	41
13	e	91/129 (70%)	74 (81%)	17 (19%)	1	7
14	f	42/66 (64%)	42 (100%)	0	100	100
15	g	108/109 (99%)	100 (93%)	8 (7%)	11	36
16	h	93/94 (99%)	88 (95%)	5 (5%)	18	46
17	i	311/311 (100%)	287 (92%)	24 (8%)	10	35
18	j	87/100 (87%)	76 (87%)	11 (13%)	3	19
19	k	85/85 (100%)	80 (94%)	5 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	m	136/141 (96%)	125 (92%)	11 (8%)	9	34
21	n	52/55 (94%)	48 (92%)	4 (8%)	10	35
22	o	112/114 (98%)	109 (97%)	3 (3%)	40	65
23	p	159/190 (84%)	149 (94%)	10 (6%)	15	43
24	q	409/409 (100%)	391 (96%)	18 (4%)	24	54
25	r	275/275 (100%)	257 (94%)	18 (6%)	14	41
26	B	345/368 (94%)	330 (96%)	15 (4%)	25	54
27	C	370/398 (93%)	332 (90%)	38 (10%)	6	26
28	D	188/228 (82%)	169 (90%)	19 (10%)	6	26
29	E	183/207 (88%)	174 (95%)	9 (5%)	21	50
30	F	78/97 (80%)	72 (92%)	6 (8%)	10	35
31	H	151/176 (86%)	144 (95%)	7 (5%)	23	52
32	I	132/163 (81%)	128 (97%)	4 (3%)	36	63
33	J	106/152 (70%)	102 (96%)	4 (4%)	28	57
34	K	130/131 (99%)	126 (97%)	4 (3%)	35	63
35	L	289/320 (90%)	269 (93%)	20 (7%)	13	39
36	N	99/101 (98%)	94 (95%)	5 (5%)	20	49
37	O	78/132 (59%)	69 (88%)	9 (12%)	4	22
37	X	79/132 (60%)	74 (94%)	5 (6%)	15	43
38	P	74/82 (90%)	69 (93%)	5 (7%)	13	40
39	Q	105/134 (78%)	100 (95%)	5 (5%)	21	51
40	R	34/92 (37%)	32 (94%)	2 (6%)	16	44
41	S	58/58 (100%)	57 (98%)	1 (2%)	56	75
42	T	69/134 (52%)	64 (93%)	5 (7%)	12	38
43	U	281/307 (92%)	266 (95%)	15 (5%)	19	47
44	V	101/102 (99%)	95 (94%)	6 (6%)	16	44
45	W	122/124 (98%)	117 (96%)	5 (4%)	26	55
46	Y	54/84 (64%)	48 (89%)	6 (11%)	5	23
47	Z	60/90 (67%)	56 (93%)	4 (7%)	13	41
48	l	537/540 (99%)	503 (94%)	34 (6%)	15	43
49	s	153/206 (74%)	144 (94%)	9 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	t	107/120 (89%)	97 (91%)	10 (9%)	7	29
51	5	363/397 (91%)	349 (96%)	14 (4%)	27	57
51	u	372/397 (94%)	353 (95%)	19 (5%)	20	49
52	Aa	70/73 (96%)	65 (93%)	5 (7%)	12	38
52	z	70/73 (96%)	65 (93%)	5 (7%)	12	38
53	G	576/610 (94%)	539 (94%)	37 (6%)	14	42
54	M	86/98 (88%)	80 (93%)	6 (7%)	12	39
All	All	10569/12435 (85%)	9911 (94%)	658 (6%)	18	43

5 of 658 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	l	246	LEU
52	z	47	LEU
48	l	411	MET
48	l	169	LEU
51	u	368	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
48	l	65	ASN
6	w	196	HIS
48	l	309	GLN
50	t	82	HIS
51	5	119	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

19 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
56	HEM	w	401	-	42,50,50	1.46	4 (9%)	46,82,82	1.28	4 (8%)
55	FES	E	301	29	0,4,4	-	-	-	-	-
58	FMN	B	501	-	33,33,33	1.11	3 (9%)	48,50,50	1.23	8 (16%)
56	HEM	7	401	6	42,50,50	1.35	7 (16%)	46,82,82	1.83	10 (21%)
59	SF4	H	302	31	0,12,12	-	-	-	-	-
59	SF4	B	502	26	0,12,12	-	-	-	-	-
59	SF4	G	801	53	0,12,12	-	-	-	-	-
59	SF4	G	802	53	0,12,12	-	-	-	-	-
61	ZMP	Q	201	-	27,29,36	1.86	5 (18%)	34,38,45	1.74	8 (23%)
59	SF4	I	201	32	0,12,12	-	-	-	-	-
57	HEC	8	401	7	32,50,50	2.63	12 (37%)	30,82,82	1.99	7 (23%)
59	SF4	H	301	31	0,12,12	-	-	-	-	-
55	FES	G	803	53	0,4,4	-	-	-	-	-
55	FES	4	301	3	0,4,4	-	-	-	-	-
55	FES	2	301	3	0,4,4	-	-	-	-	-
56	HEM	w	402	6	42,50,50	1.46	5 (11%)	46,82,82	1.17	2 (4%)
56	HEM	7	402	-	42,50,50	1.50	4 (9%)	46,82,82	1.24	7 (15%)
60	NDP	L	401	-	47,52,52	0.64	0	61,80,80	0.99	3 (4%)
57	HEC	x	401	7	32,50,50	2.14	3 (9%)	30,82,82	2.37	7 (23%)

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
56	HEM	w	401	-	-	0/12/54/54	-
55	FES	E	301	29	-	-	0/1/1/1
58	FMN	B	501	-	-	0/18/18/18	0/3/3/3
56	HEM	7	401	6	-	4/12/54/54	-
59	SF4	H	302	31	-	-	0/6/5/5
59	SF4	B	502	26	-	-	0/6/5/5
59	SF4	G	801	53	-	-	0/6/5/5
59	SF4	G	802	53	-	-	0/6/5/5
61	ZMP	Q	201	-	-	11/36/36/43	-
59	SF4	I	201	32	-	-	0/6/5/5
57	HEC	8	401	7	-	7/10/54/54	-
59	SF4	H	301	31	-	-	0/6/5/5
55	FES	G	803	53	-	-	0/1/1/1
55	FES	4	301	3	-	-	0/1/1/1
55	FES	2	301	3	-	-	0/1/1/1
56	HEM	w	402	6	-	1/12/54/54	-
56	HEM	7	402	-	-	6/12/54/54	-
60	NDP	L	401	-	-	4/30/77/77	0/5/5/5
57	HEC	x	401	7	-	4/10/54/54	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	8	401	HEC	C3C-C2C	7.58	1.49	1.40
57	8	401	HEC	C2B-C3B	7.09	1.48	1.40
57	x	401	HEC	C3C-C2C	-6.59	1.33	1.40
57	x	401	HEC	C2B-C3B	-5.63	1.34	1.40
61	Q	201	ZMP	C13-N1	5.36	1.46	1.33

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	401	HEC	CBC-CAC-C3C	-8.47	107.66	127.49
57	8	401	HEC	CMB-C2B-C3B	5.84	132.69	125.82
57	x	401	HEC	CBB-CAB-C3B	-5.49	114.65	127.49
60	L	401	NDP	P2B-O2B-C2B	-5.38	109.06	123.43
57	8	401	HEC	C1D-C2D-C3D	-5.06	103.48	107.00

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

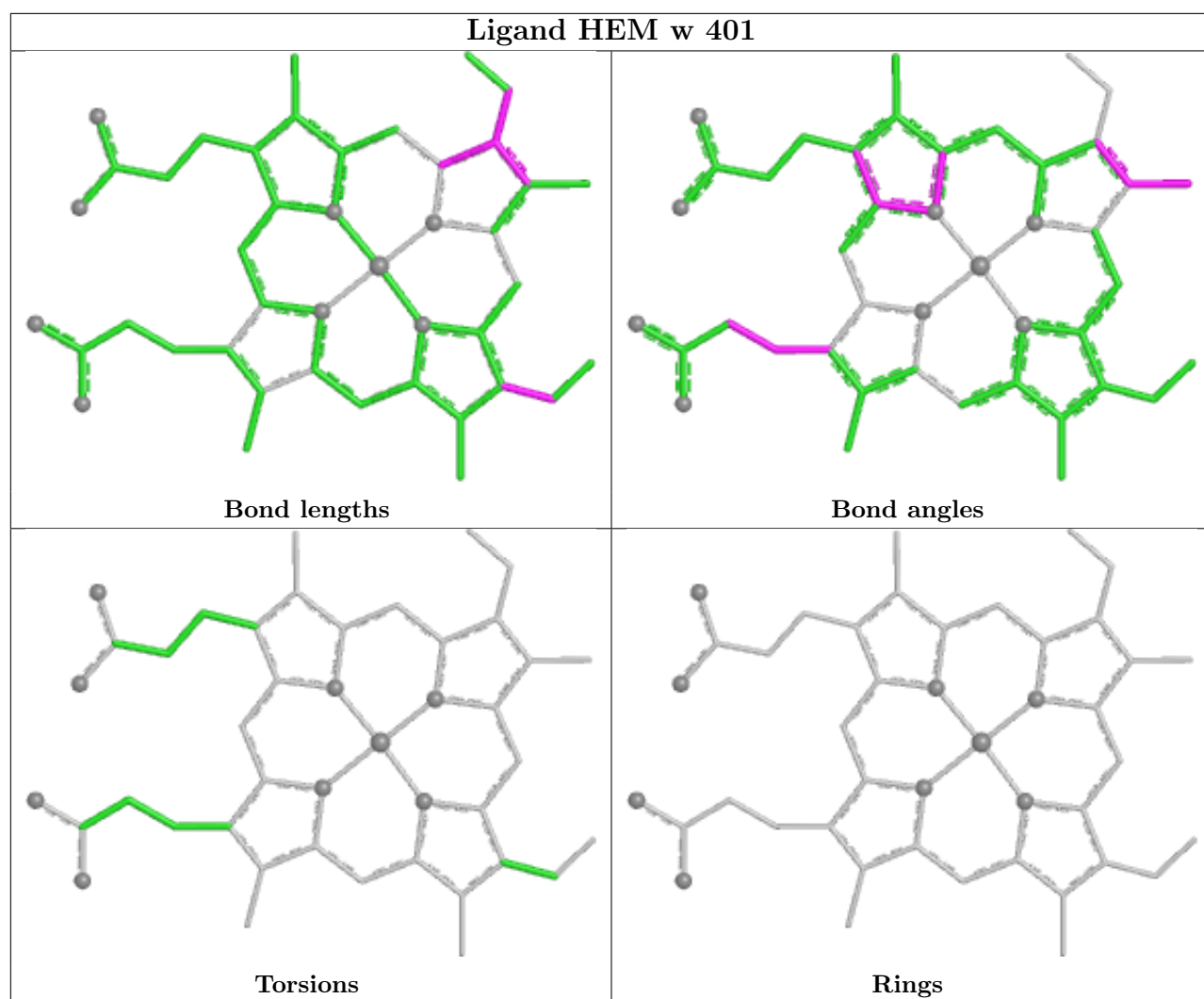
Mol	Chain	Res	Type	Atoms
56	7	402	HEM	C1A-C2A-CAA-CBA
56	7	402	HEM	C3A-C2A-CAA-CBA
57	8	401	HEC	C2D-C3D-CAD-CBD
57	8	401	HEC	C4D-C3D-CAD-CBD
61	Q	201	ZMP	C17-C16-N2-C15

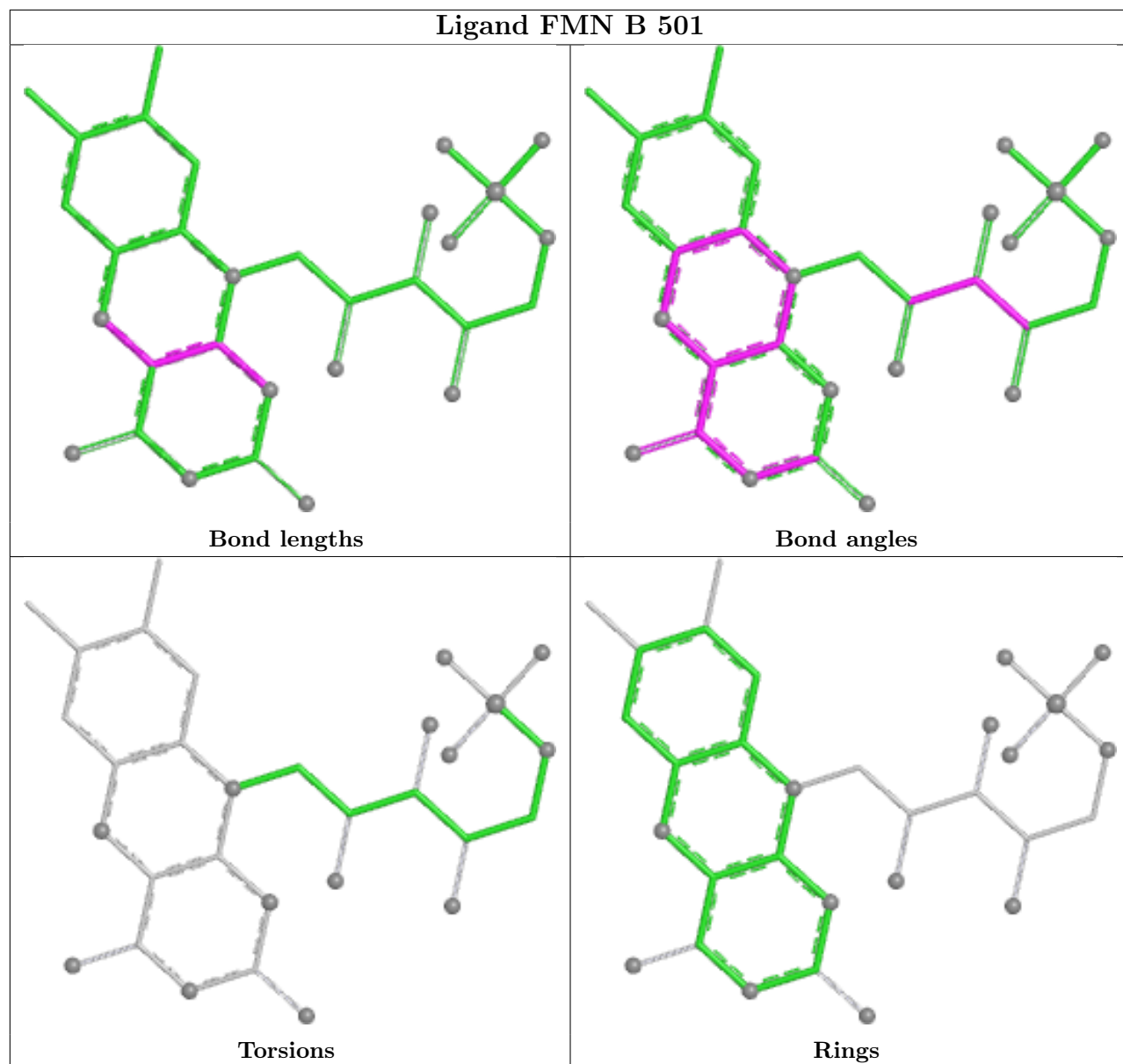
There are no ring outliers.

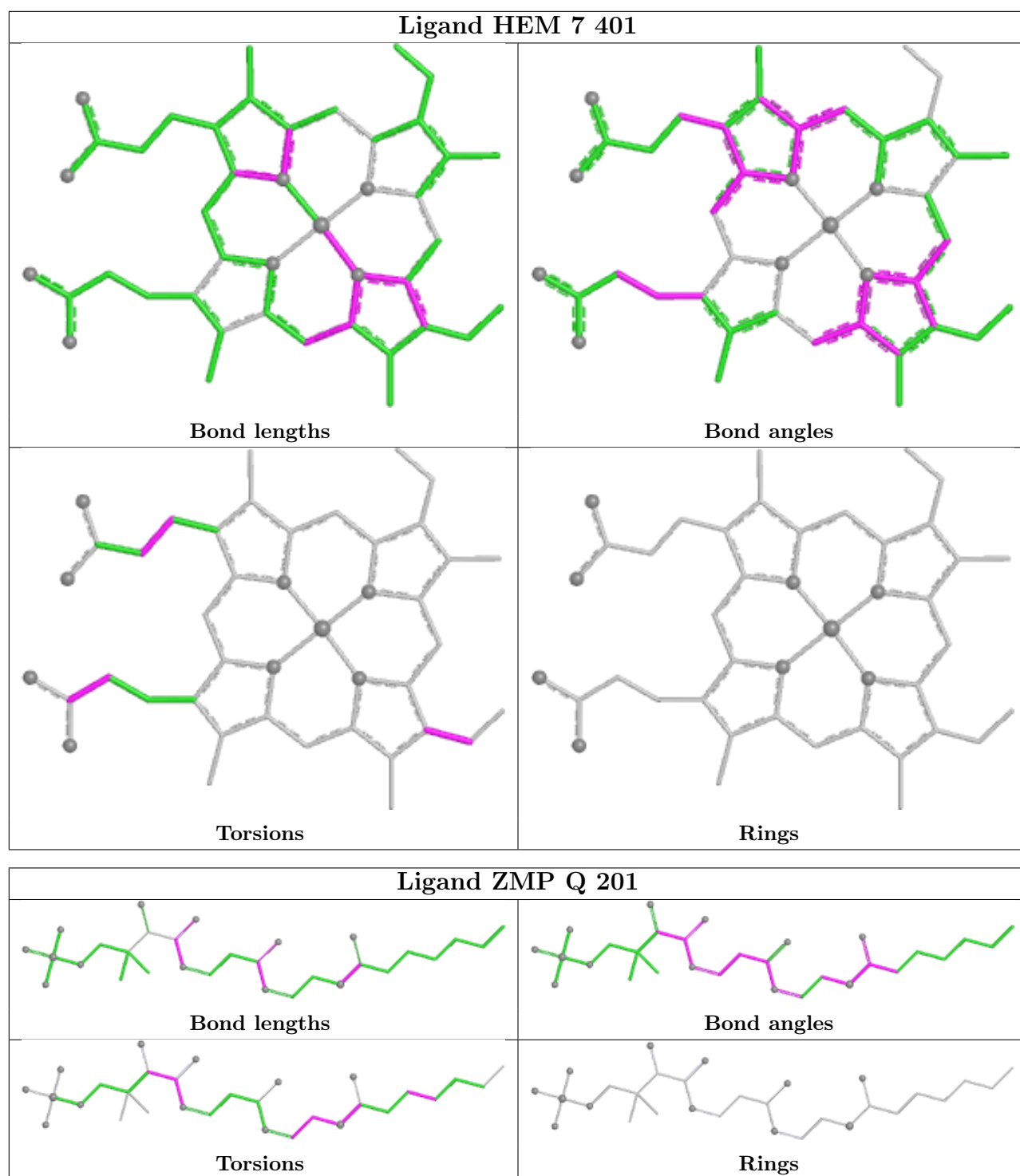
17 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	w	401	HEM	9	0
55	E	301	FES	1	0
58	B	501	FMN	1	0
56	7	401	HEM	7	0
59	H	302	SF4	9	0
59	B	502	SF4	1	0
59	G	801	SF4	1	0
61	Q	201	ZMP	3	0
59	I	201	SF4	1	0
57	8	401	HEC	18	0
59	H	301	SF4	2	0
55	4	301	FES	3	0
55	2	301	FES	3	0
56	w	402	HEM	7	0
56	7	402	HEM	7	0
60	L	401	NDP	1	0
57	x	401	HEC	4	0

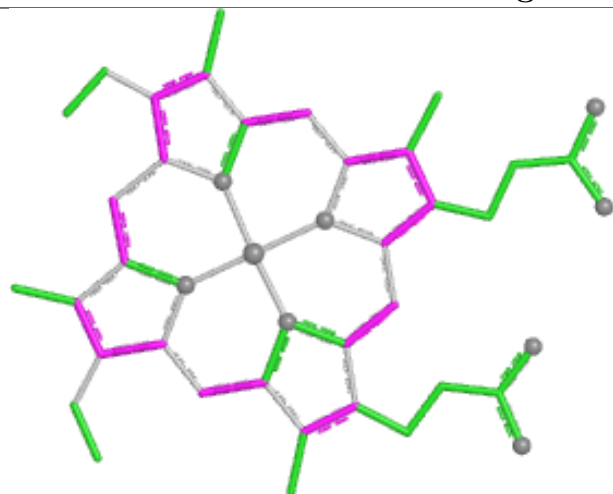
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



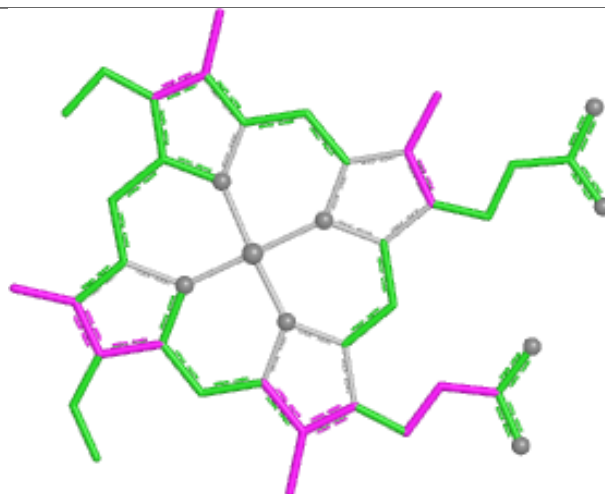




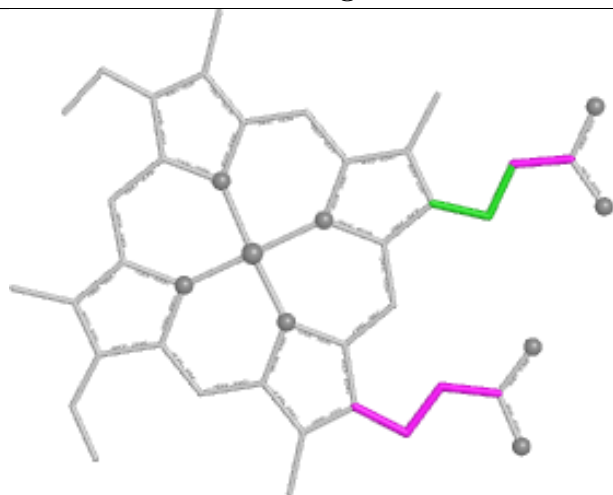
## Ligand HEC 8 401



Bond lengths



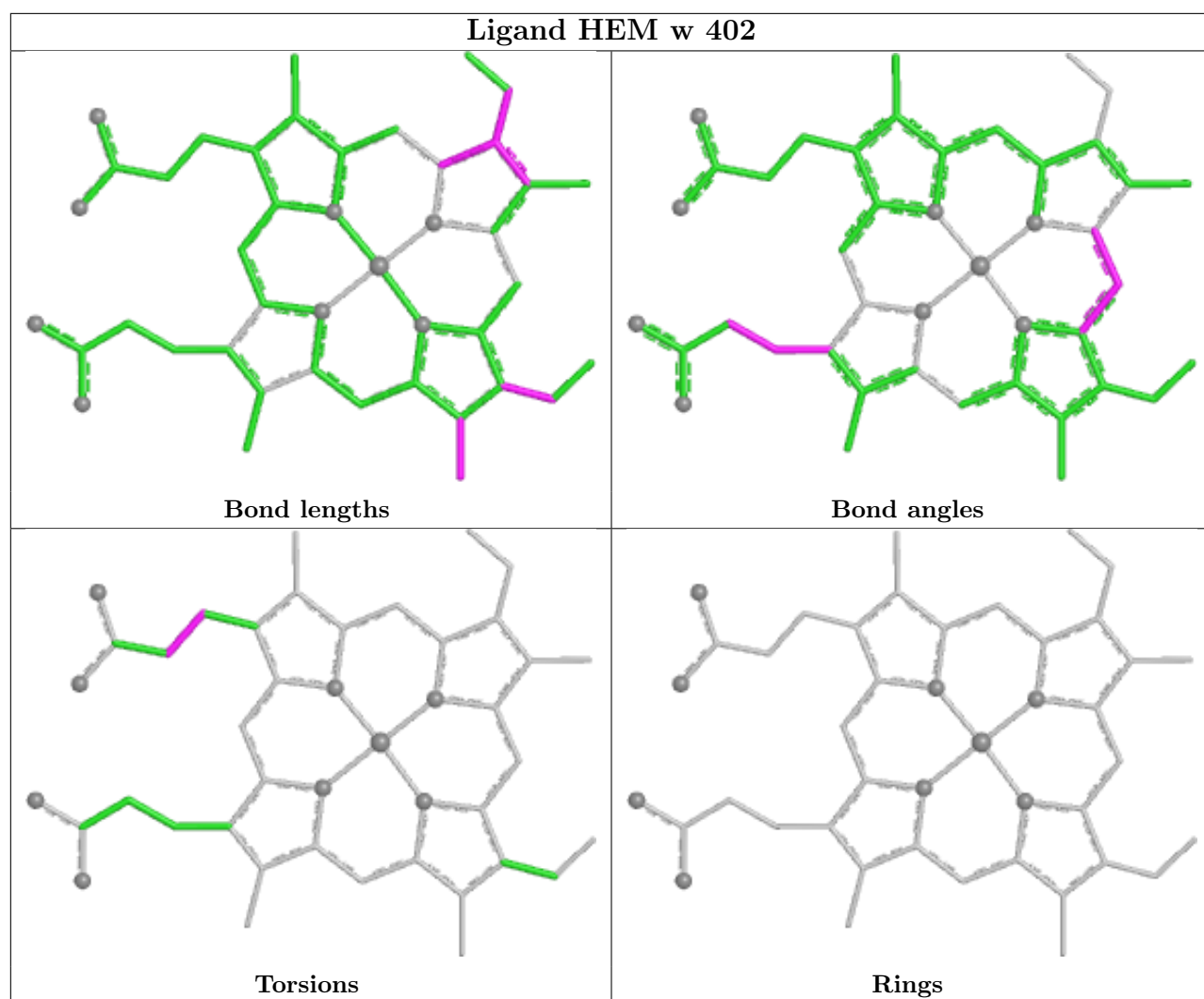
Bond angles



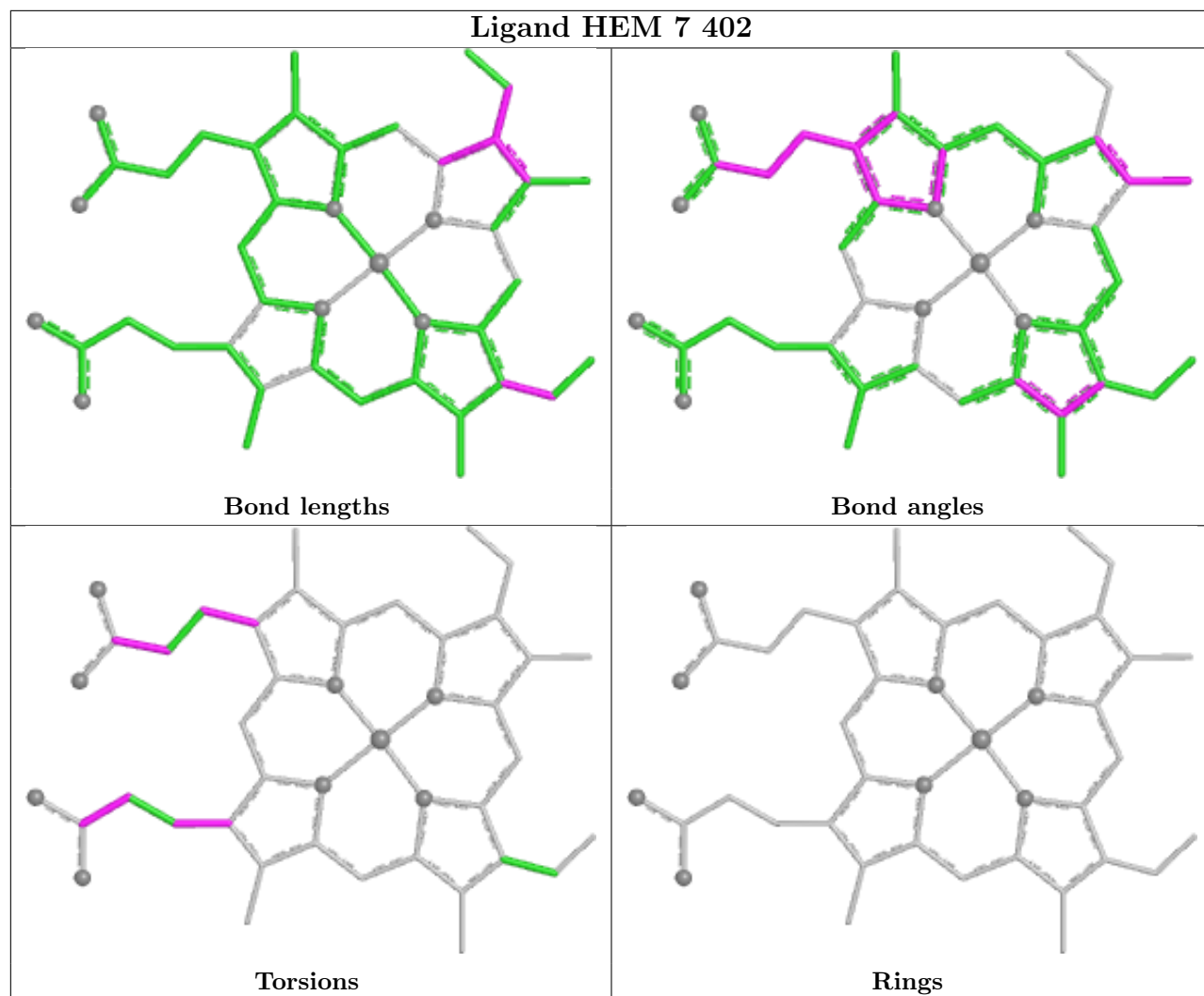
Torsions

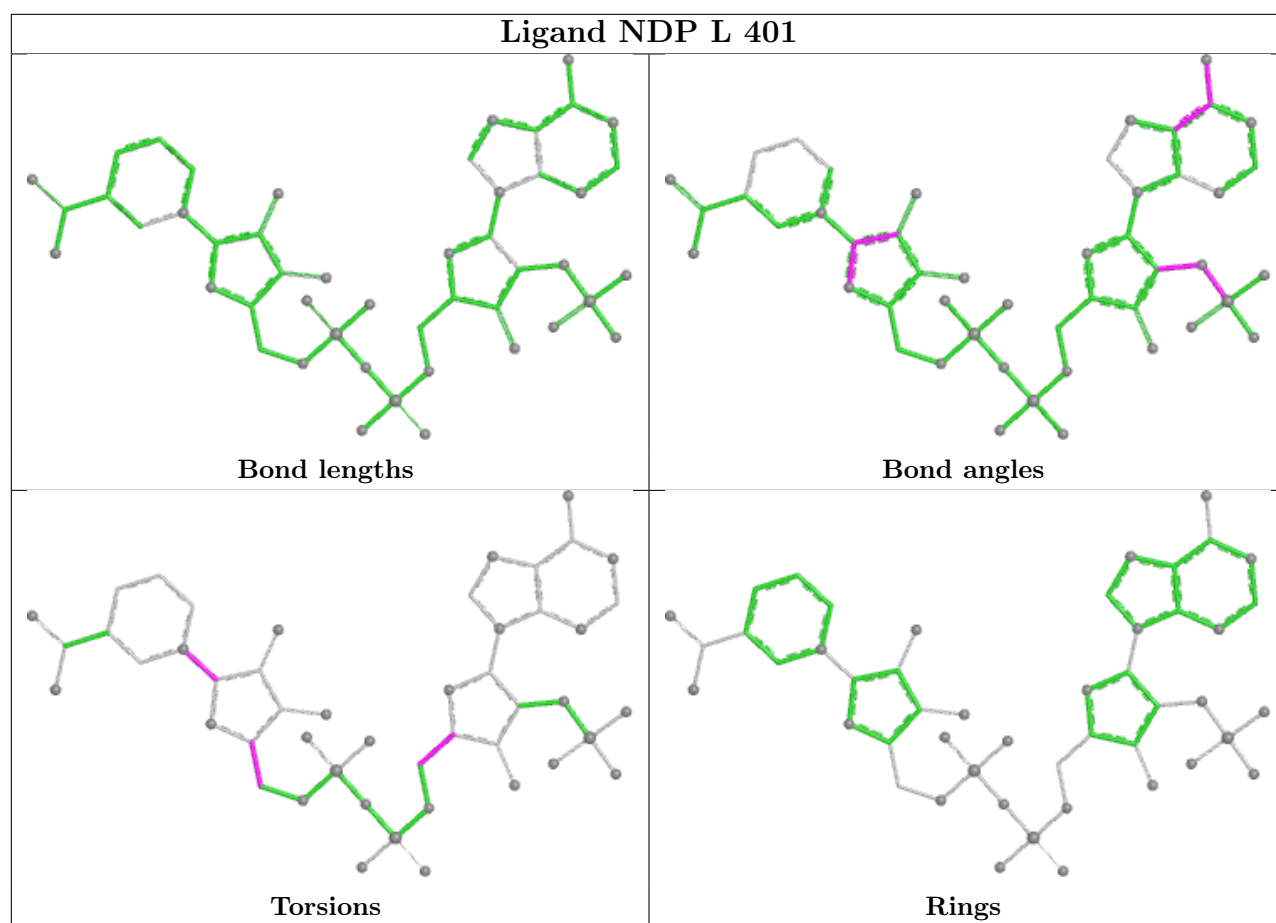


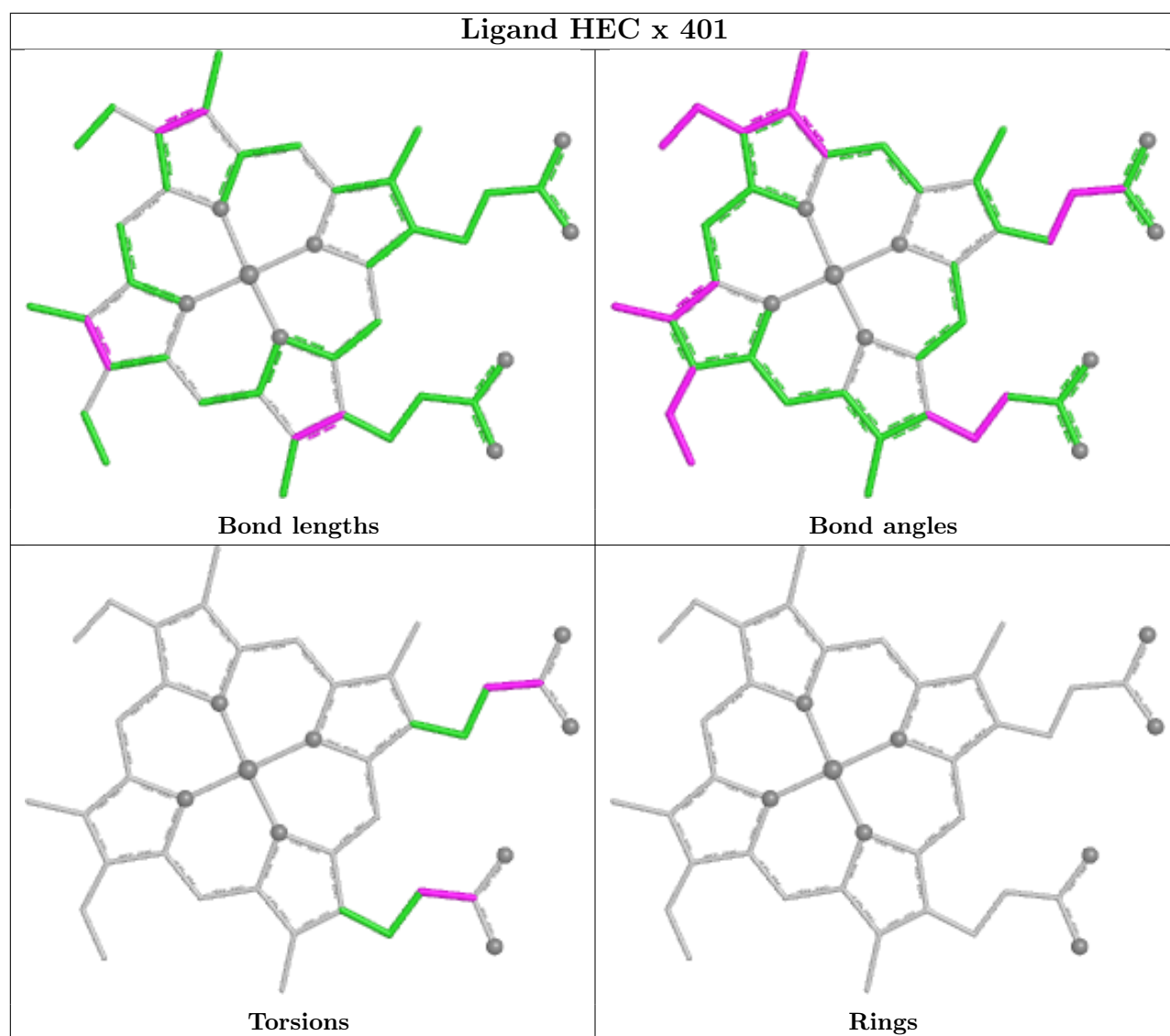
Rings











## 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.

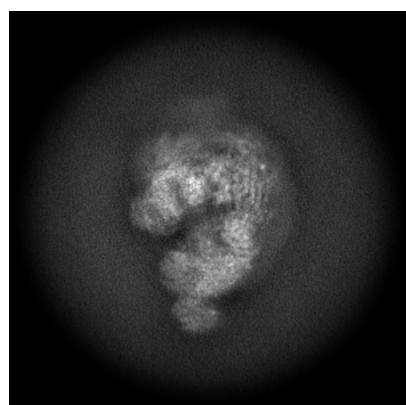
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45479. These allow visual inspection of the internal detail of the map and identification of artifacts.

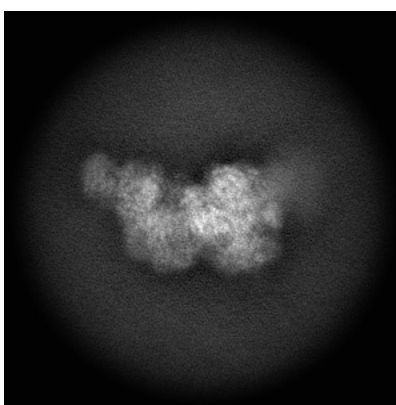
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

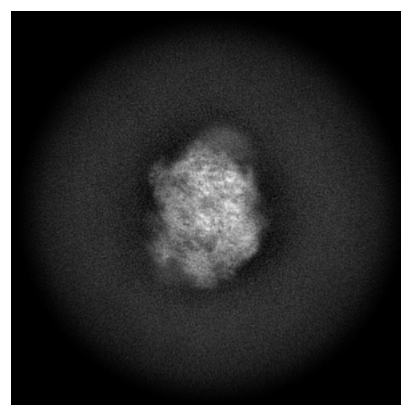
#### 6.1.1 Primary map



X



Y

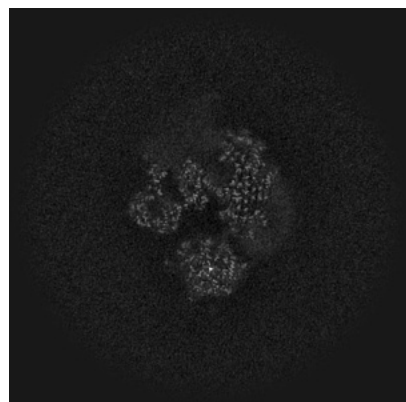


Z

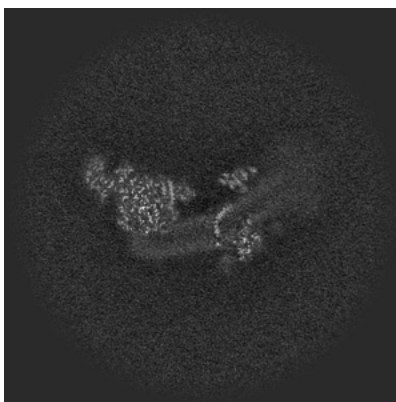
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

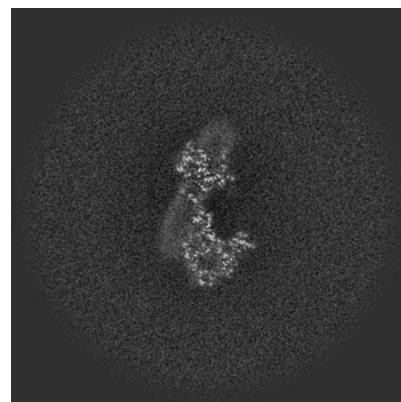
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

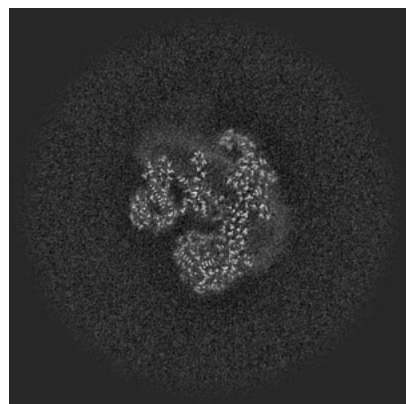


Z Index: 256

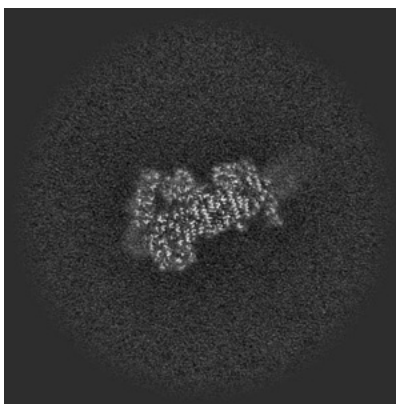
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

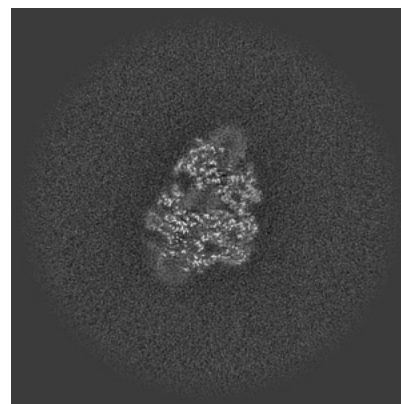
### 6.3.1 Primary map



X Index: 244



Y Index: 291

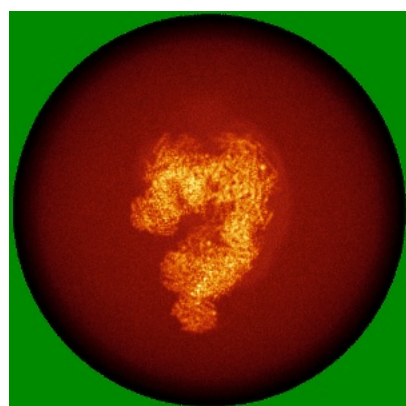


Z Index: 294

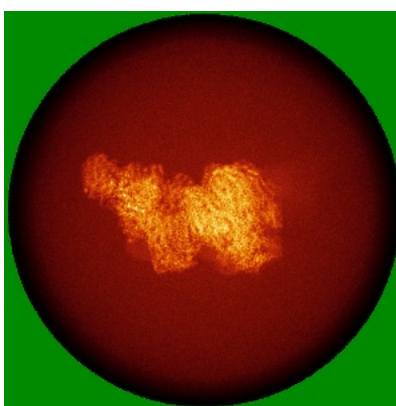
The images above show the largest variance slices of the map in three orthogonal directions.

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

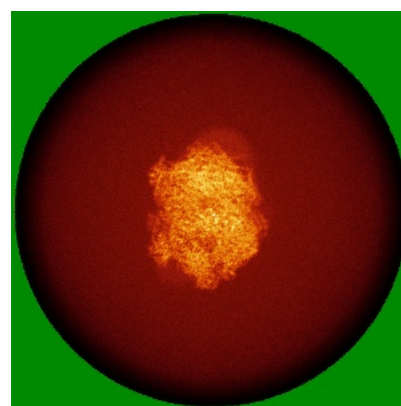
### 6.4.1 Primary map



X



Y



Z

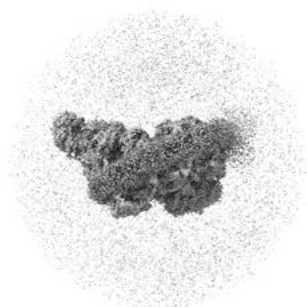
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

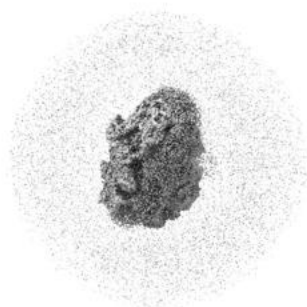
### 6.5.1 Primary map



X



Y



Z

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

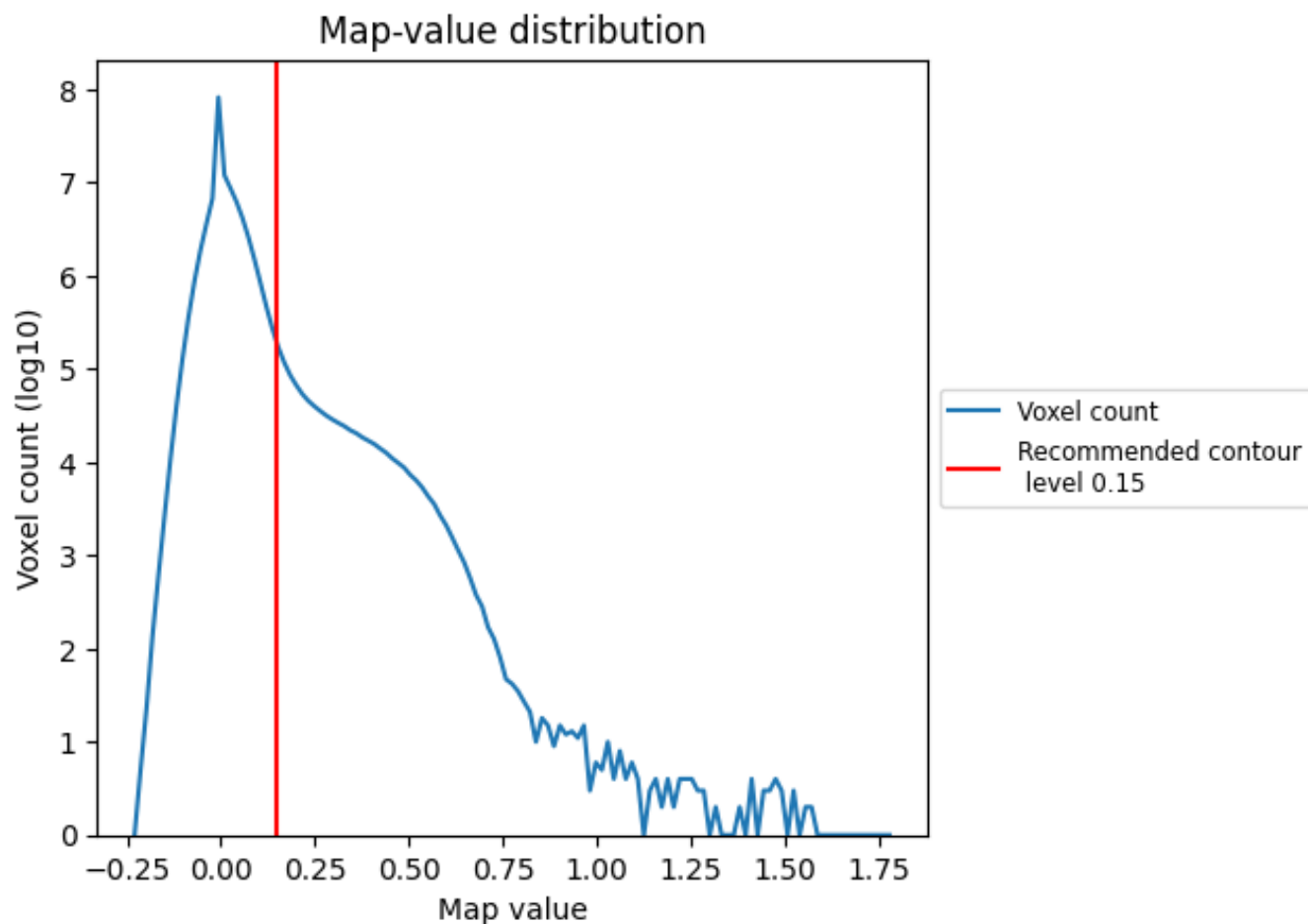
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

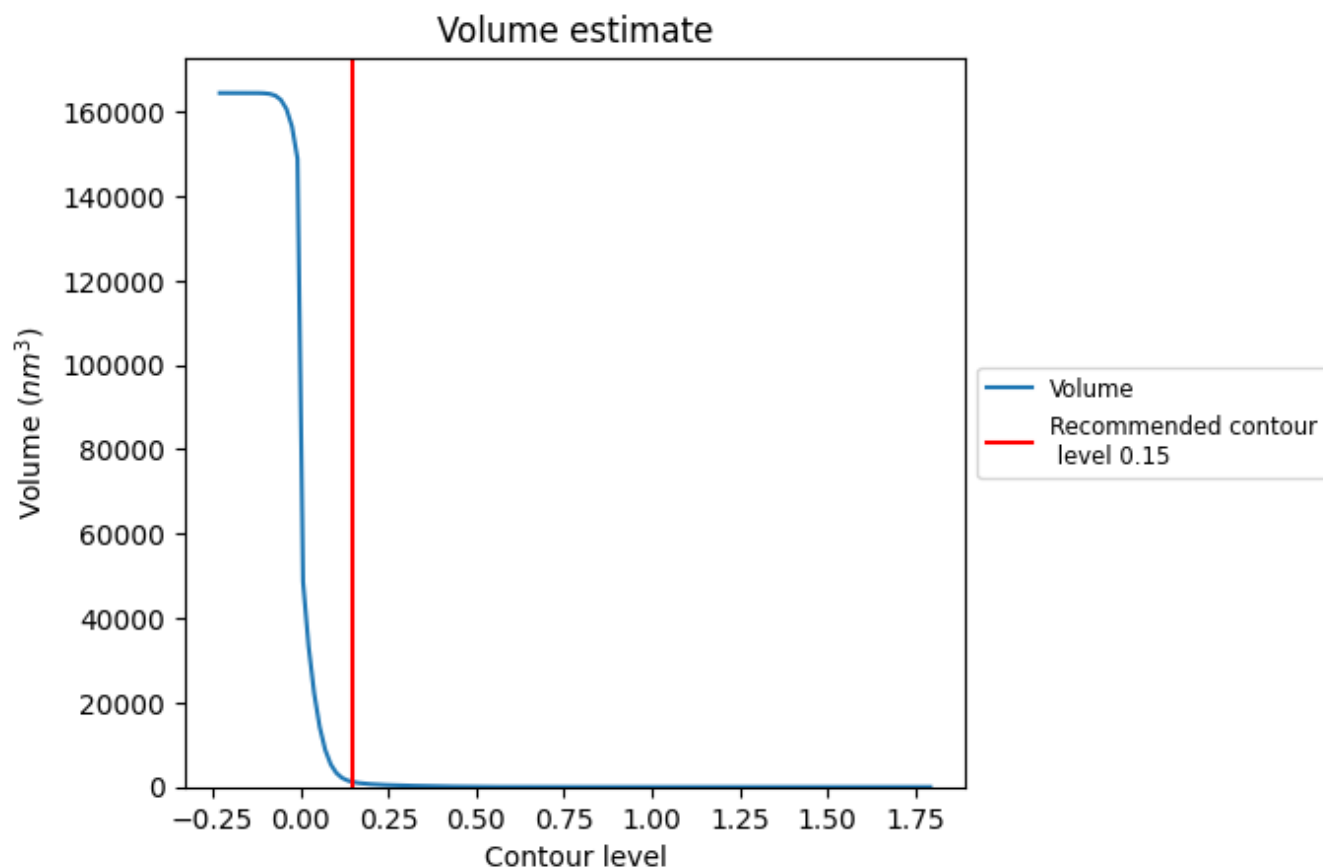
This section contains the results of statistical analysis of the map.

### 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](#)

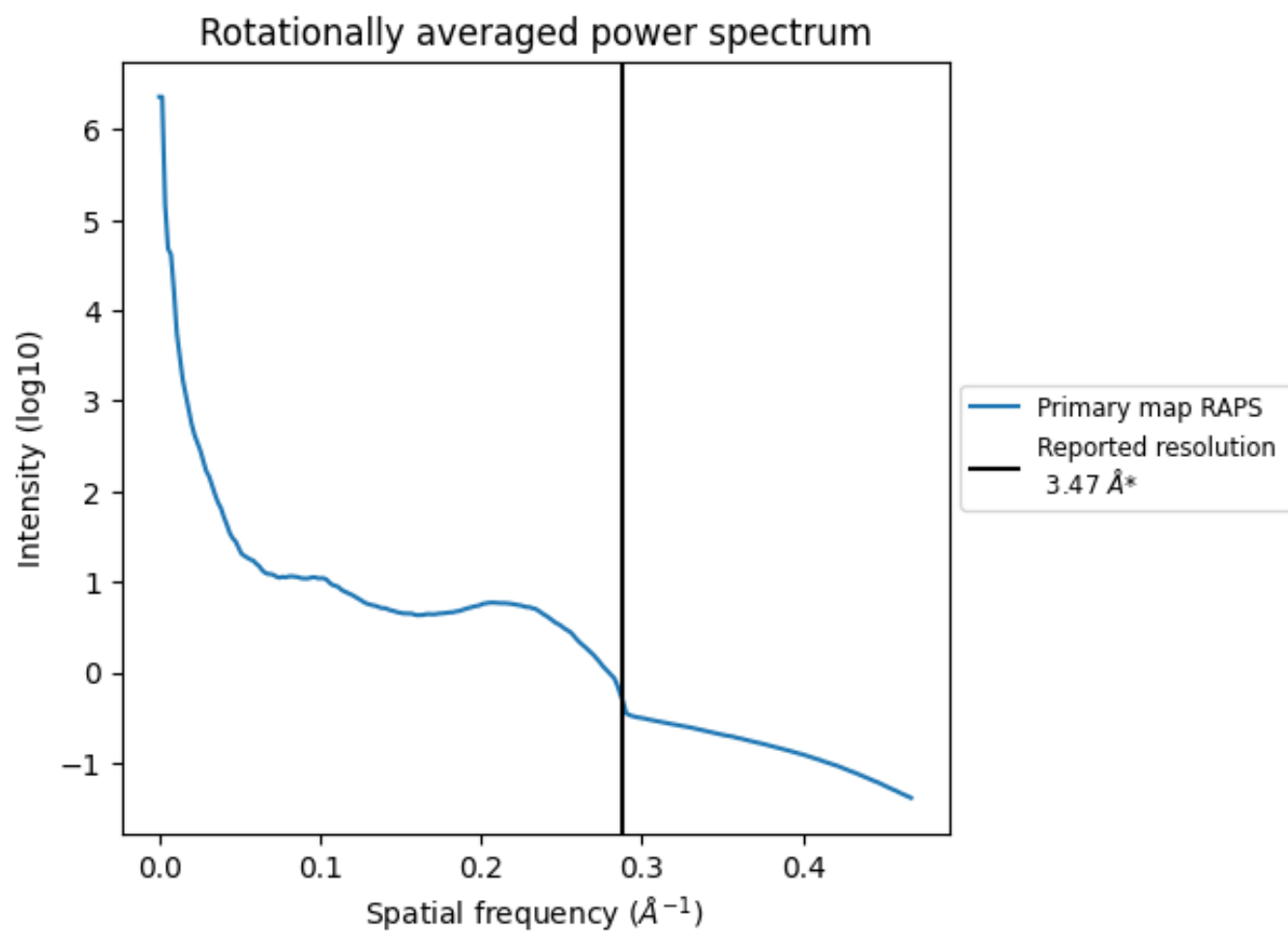


The volume at the recommended contour level is 1168 nm<sup>3</sup>; this corresponds to an approximate mass of 1055 kDa.

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 0.288 Å<sup>-1</sup>

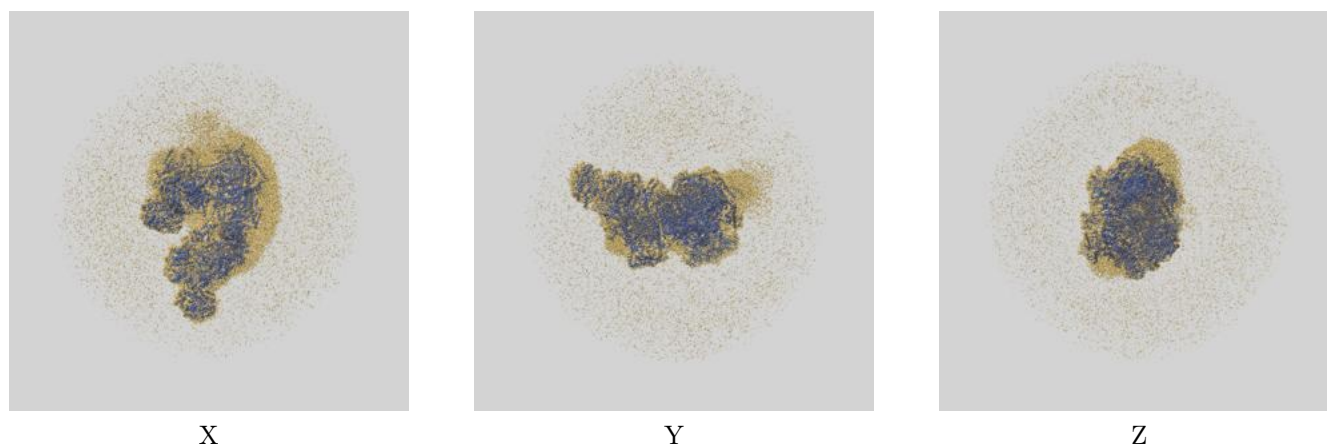
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

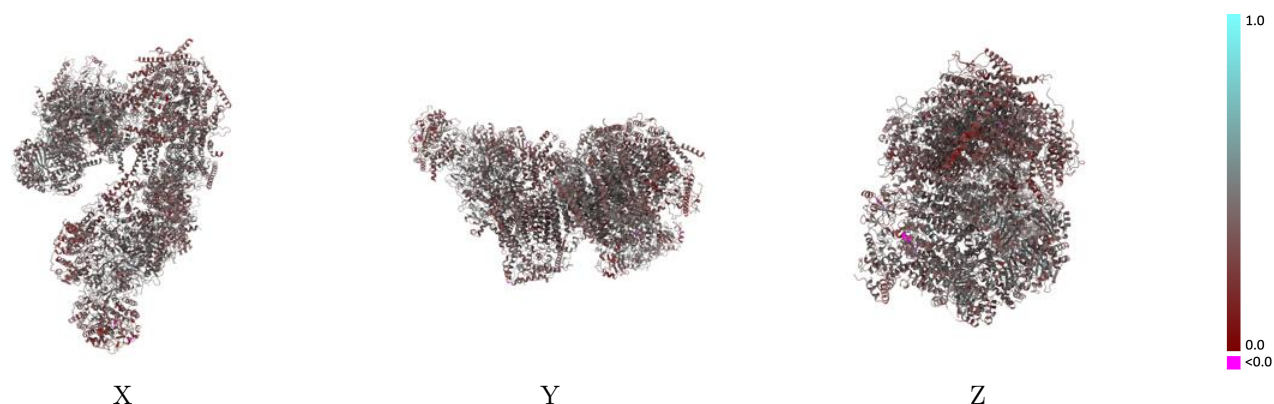
This section contains information regarding the fit between EMDB map EMD-45479 and PDB model 9CDN. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



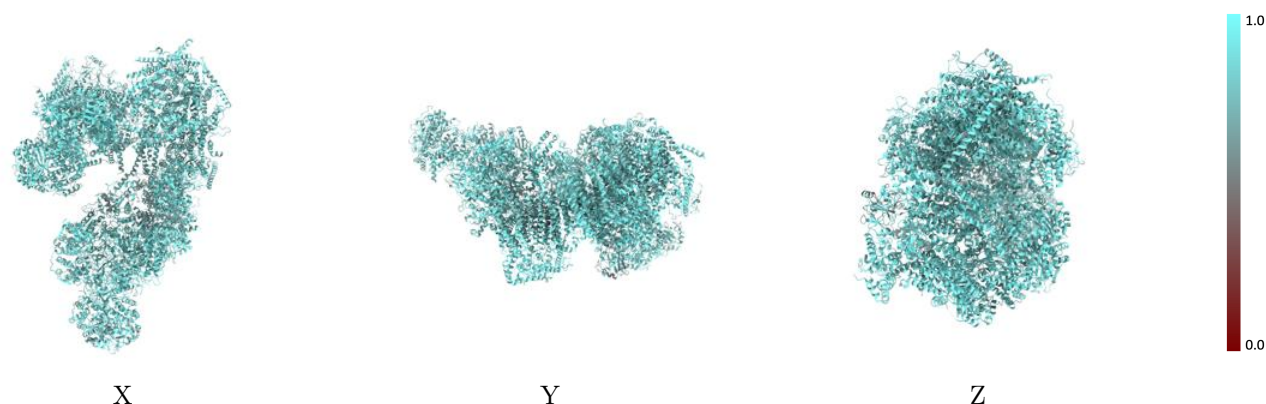
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



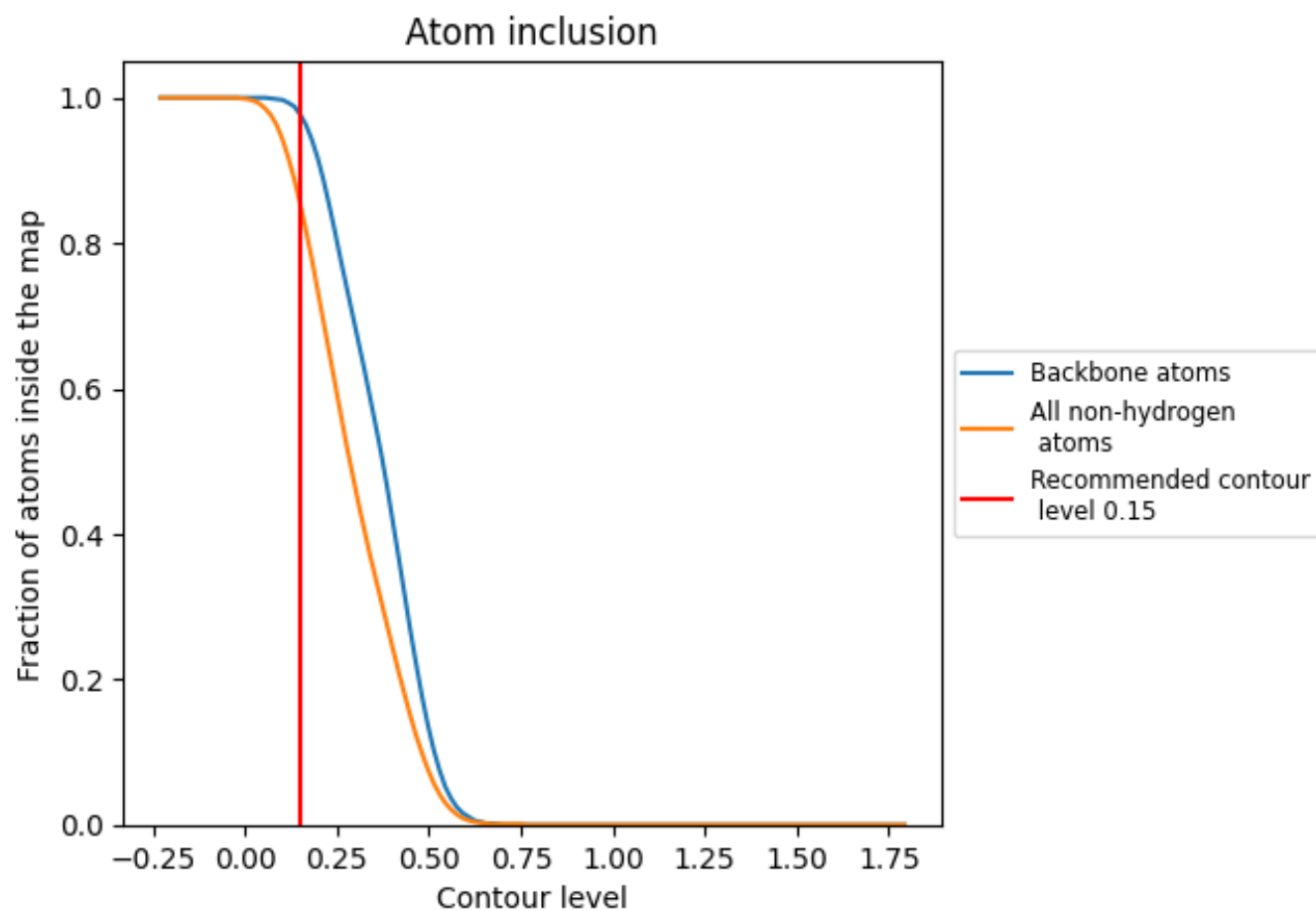
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 98% of all backbone atoms, 85% 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	 0.8540	 0.3920
0	 0.8330	 0.3460
1	 0.8810	 0.3980
2	 0.7930	 0.3530
3	 0.8900	 0.4090
4	 0.7490	 0.3420
5	 0.8900	 0.4250
6	 0.8730	 0.4220
7	 0.8850	 0.4340
8	 0.8860	 0.4220
9	 0.8750	 0.4170
Aa	 0.8720	 0.4260
Ab	 0.8290	 0.3390
Ac	 0.8250	 0.3840
Ad	 0.8590	 0.4140
Ae	 0.7060	 0.2910
Af	 0.7040	 0.3210
B	 0.8240	 0.3410
C	 0.8710	 0.4090
D	 0.8850	 0.4230
E	 0.8250	 0.3620
F	 0.8160	 0.4170
G	 0.8470	 0.3850
H	 0.8980	 0.4290
I	 0.8800	 0.4120
J	 0.8540	 0.4240
K	 0.8360	 0.4160
L	 0.7840	 0.3420
M	 0.8600	 0.4160
N	 0.8510	 0.3720
O	 0.7540	 0.2820
P	 0.7980	 0.3090
Q	 0.8090	 0.3610
R	 0.7730	 0.3480
S	 0.8940	 0.4280



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Chain	Atom inclusion	Q-score
T	 0.8770	 0.4100
U	 0.8420	 0.3610
V	 0.8460	 0.3630
W	 0.8790	 0.3790
X	 0.8240	 0.3320
Y	 0.8510	 0.3340
Z	 0.8440	 0.3300
a	 0.8690	 0.3640
b	 0.8480	 0.3240
c	 0.8770	 0.3890
d	 0.8670	 0.3560
e	 0.8120	 0.3640
f	 0.8000	 0.3520
g	 0.8910	 0.4140
h	 0.8690	 0.4010
i	 0.8750	 0.4290
j	 0.7880	 0.3740
k	 0.8420	 0.3990
l	 0.8400	 0.3940
m	 0.7880	 0.3420
n	 0.8150	 0.3460
o	 0.8250	 0.3500
p	 0.8710	 0.3620
q	 0.8620	 0.4250
r	 0.8290	 0.3930
s	 0.8710	 0.3890
t	 0.8560	 0.2930
u	 0.8910	 0.4220
v	 0.8890	 0.4220
w	 0.8890	 0.4370
x	 0.9040	 0.4310
y	 0.8850	 0.4220
z	 0.9100	 0.4220