



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:47 PM UTC

PDB ID : 5XTD / pdb_00005xtd
EMDB ID : EMD-6773
Title : Cryo-EM structure of human respiratory complex I
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.70 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:

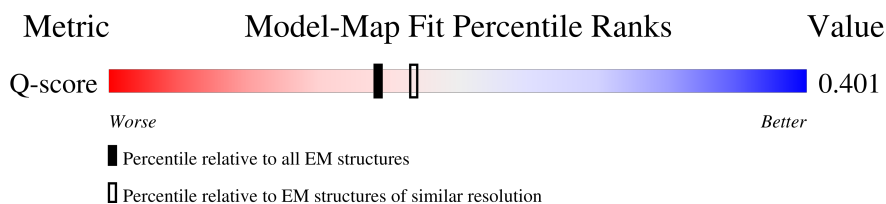
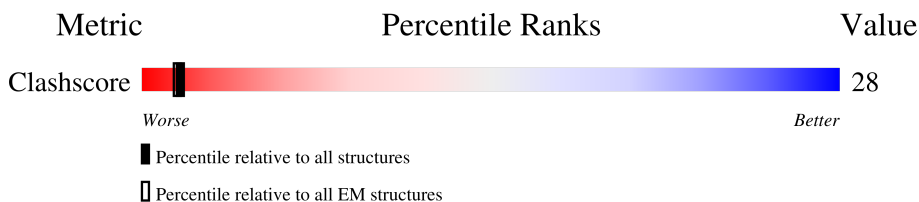
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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


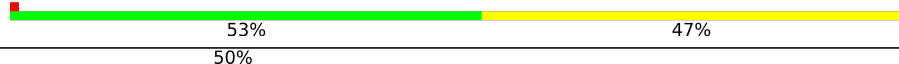


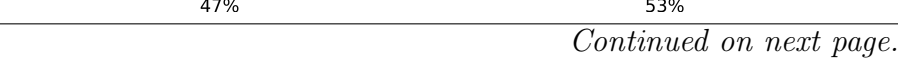
The reported resolution of this entry is 3.70 Å.

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	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	431	 60% 48% 52%
2	B	176	 6% 45% 54% .
3	C	156	 53% 47% 53%
4	E	113	 50% 45% 54% .
5	F	83	 54% 49% 51%
6	G	85	 91% 47% 53%


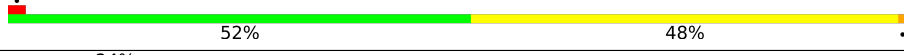
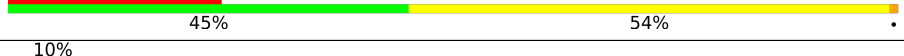


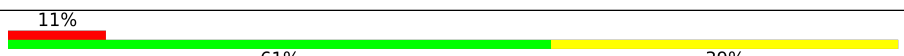







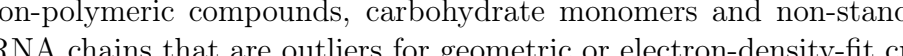
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Mol	Chain	Length	Quality of chain
6	X	85	55% 45%
7	H	112	51% 54% 44%
8	I	110	45% 47% 36% 14%
9	J	337	32% 47% 51%
10	K	33	64% 39% 61%
11	L	118	56% 47% 53%
12	M	687	52% 48% 52%
13	N	143	34% 60% 38%
14	O	212	61% 41% 58%
15	P	208	31% 47% 52%
16	Q	430	18% 43% 55%
17	S	70	63% 36%
18	T	95	47% 53% 47%
19	U	83	75% 25%
20	V	140	14% 65% 34%
21	W	138	65% 33%
22	Y	59	31% 64% 5%
23	Z	80	72% 28%
24	a	138	59% 40%
25	b	128	15% 43% 52%
26	c	153	52% 47%
27	d	171	65% 33%
28	e	97	10% 71% 29%
29	f	47	19% 62% 36%
30	g	119	50% 50%

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Mol	Chain	Length	Quality of chain
31	h	104	
32	i	347	
33	j	115	
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	137	
44	w	320	

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
45	SF4	A	501	-	-	X	-
45	SF4	B	302	-	-	X	-
45	SF4	M	801	-	-	X	-
46	FMN	A	502	-	-	X	-
47	PLX	b	201	-	-	X	-
49	NDP	J	401	-	-	X	-
50	FES	O	301	-	-	X	-
52	PEE	V	202	-	-	X	-
52	PEE	l	701	-	-	X	-

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 66789 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3322	2096	594	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1420	893	243	271	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1249	794	227	214	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	968	623	178	162	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	83	670	422	124	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	85	672	434	99	134	5	0	0
6	X	85	686	442	101	138	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	922	593	157	169	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	95	769	483	146	138	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	337	2712	1759	482	463	8	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	274	173	47	53	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	964	608	173	179	4	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	5274	3310	917	1009	38	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	1195	770	210	212	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	212	1643	1047	276	310	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1730	1117	297	313	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3460	2214	599	624	23	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	568	367	101	96	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	95	742	459	138	142	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	83	647	427	105	113	2	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	140	1038	668	178	187	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	138	1135	727	202	200	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	59	533	354	87	91	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	80	648	426	110	110	2	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	138	1174	771	199	202	2	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	124	1059	697	181	176	5	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	153	1236	795	208	222	11	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	171	1418	885	262	259	12	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	97	810	522	132	152	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	47	405	269	69	67	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	119	1004	658	173	169	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	104	863	546	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2735	1819	421	470	25	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	115	919	626	132	152	9	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	97	740	487	113	127	13	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4717	3119	742	823	33	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	174	1313	879	194	229	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	473	305	85	80	3	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	128	1066	685	192	187	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	172	1495	961	265	261	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3629	2411	569	619	30	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	318	2509	1678	380	435	16	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	169	1394	886	247	252	9	0	0

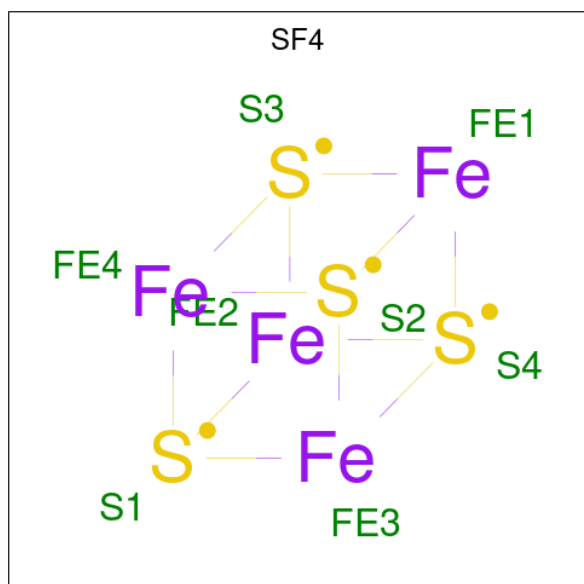
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	111	921	569	187	156	9	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

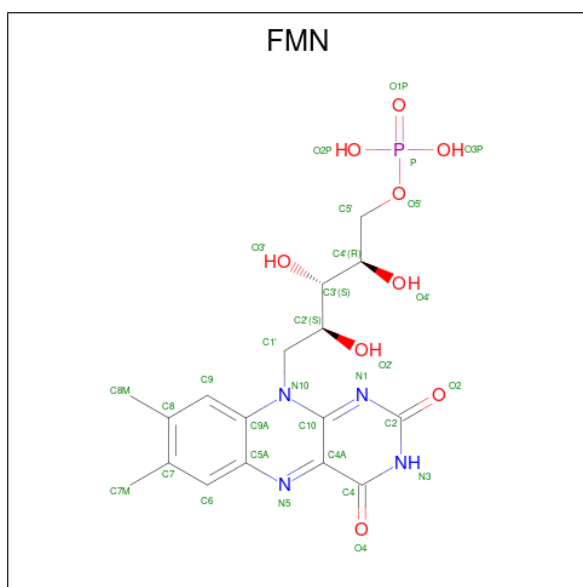
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2474	1573	429	464	8	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



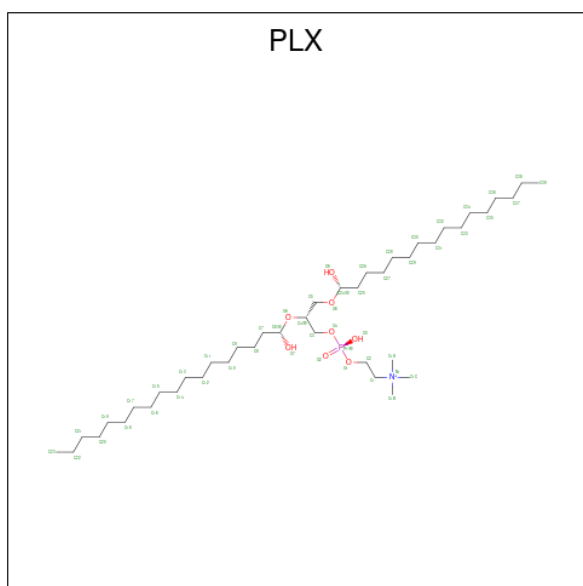
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 47 is (9R,11S)-9-({(1S)-1-HYDROXYHEXADECYL}OXY)METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



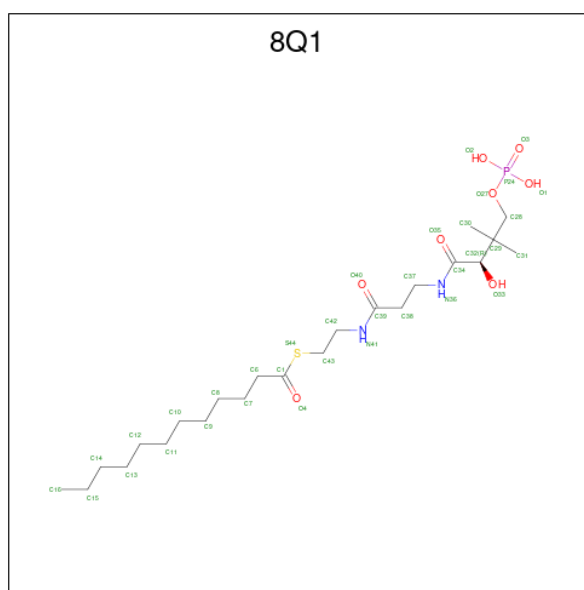
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	B	1	52	42	1	8	1	0
47	U	1	52	42	1	8	1	0

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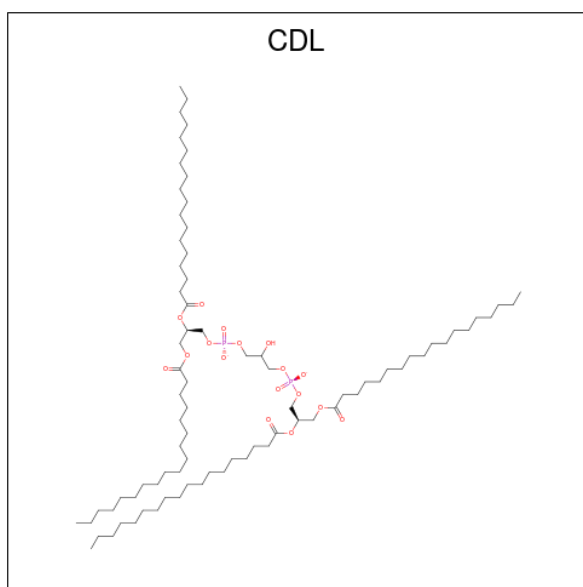
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



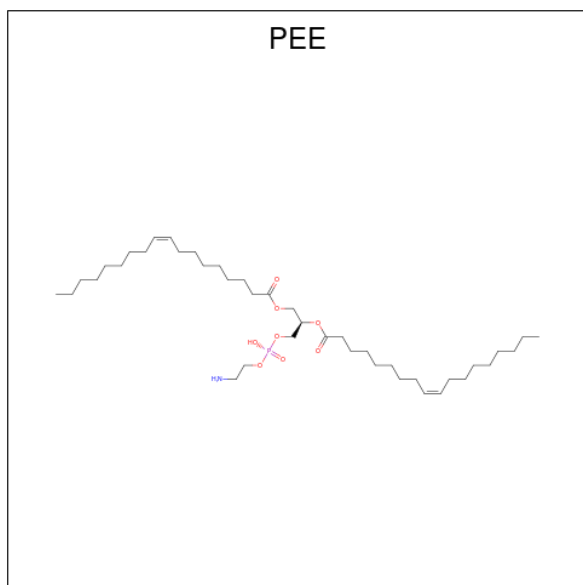
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

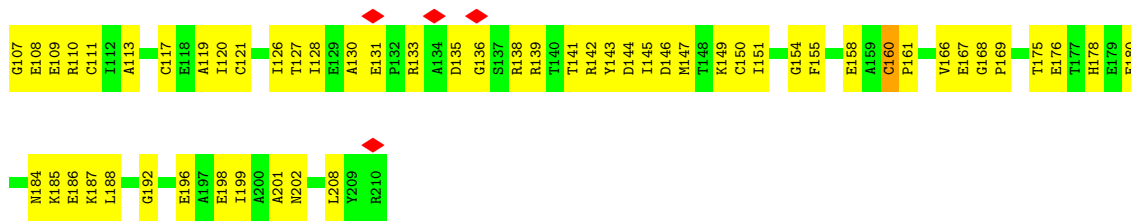


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	V	1	63	44	17	2	0
51	i	1	64	45	17	2	0
51	l	1	64	45	17	2	0
51	l	1	64	45	17	2	0
51	n	1	64	45	17	2	0

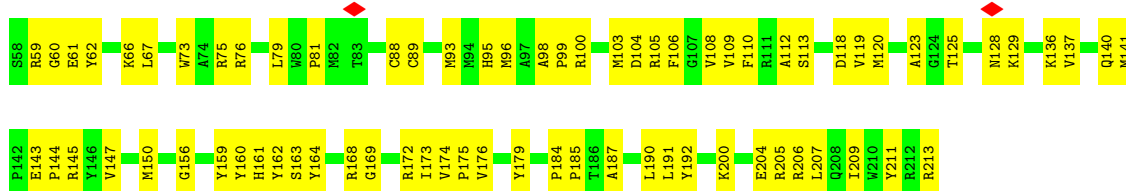
- Molecule 52 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



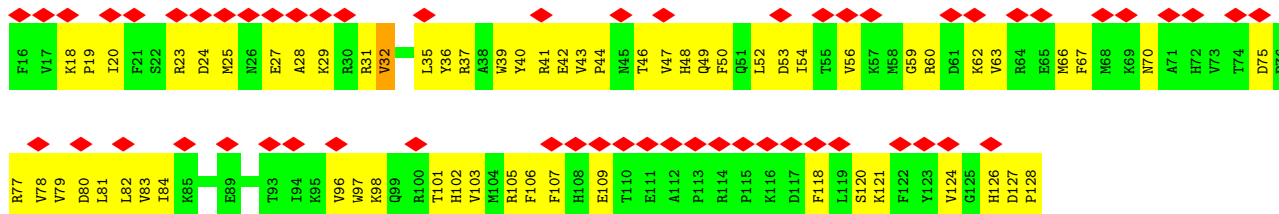
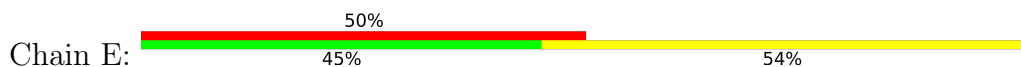
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	1	1	Total	C	N	O	P	0
			51	41	1	8	1	



- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



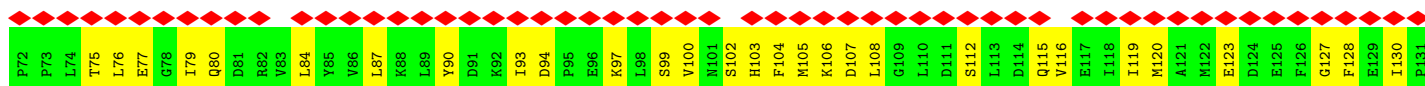
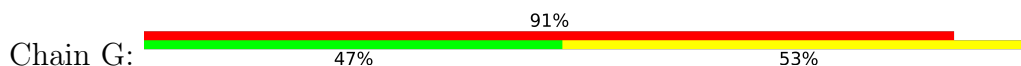
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial

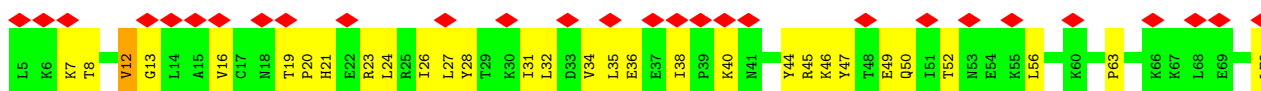




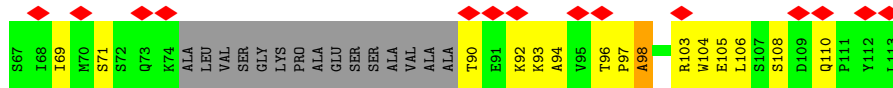
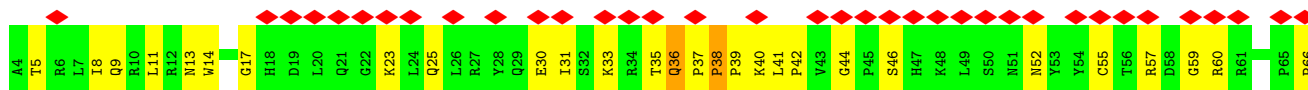
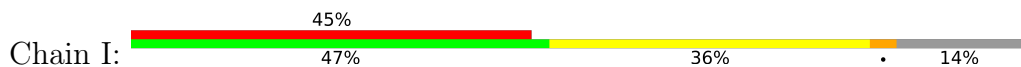
• Molecule 6: Acyl carrier protein, mitochondrial



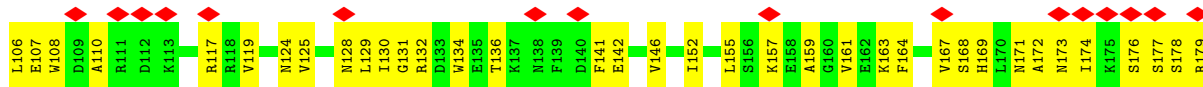
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

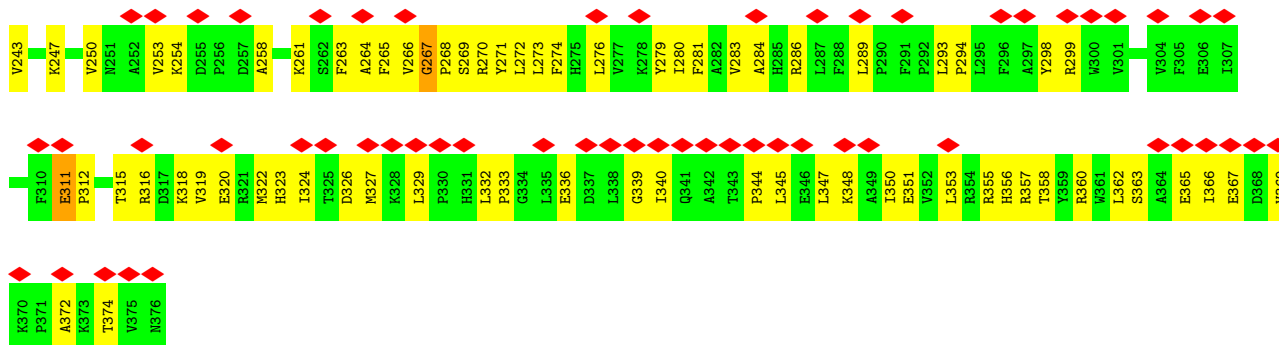


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

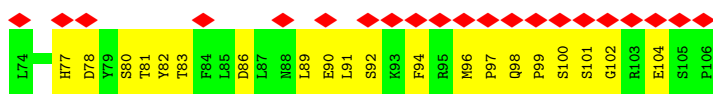


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

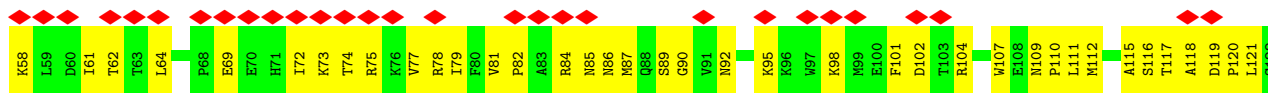




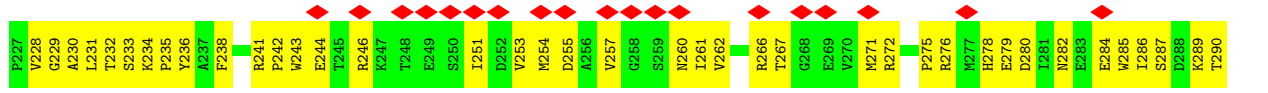
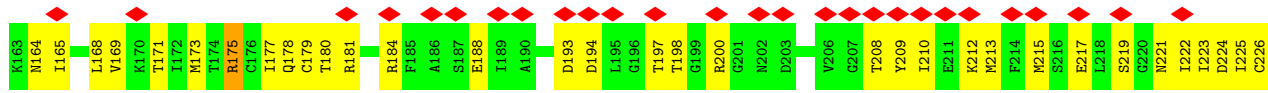
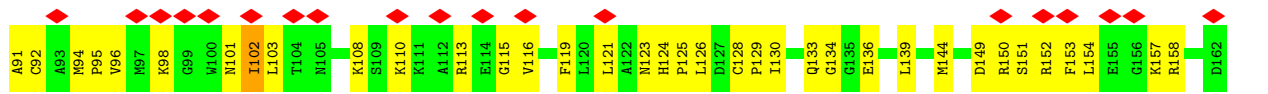
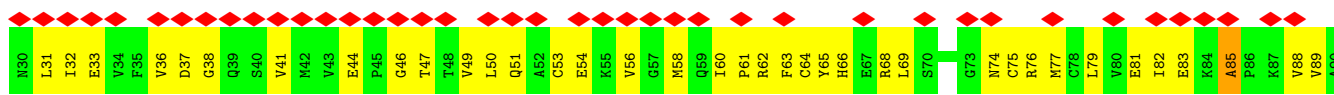
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

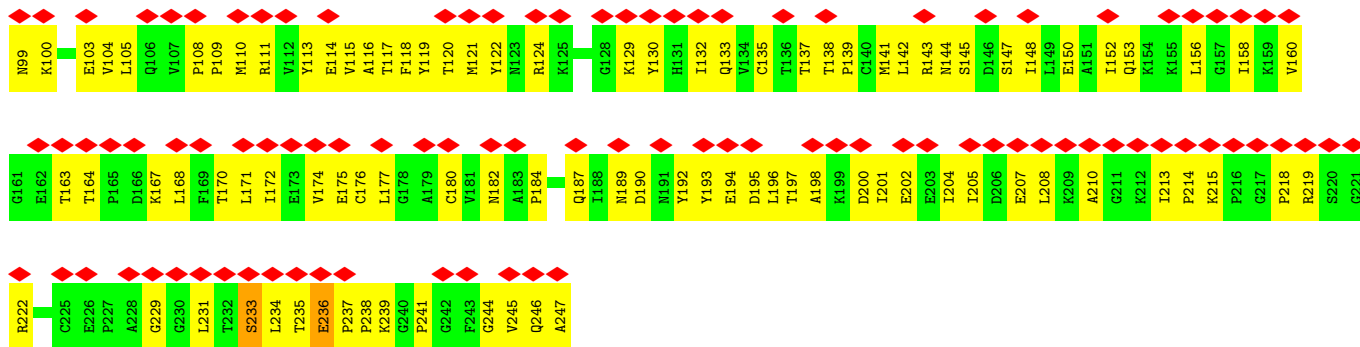


• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

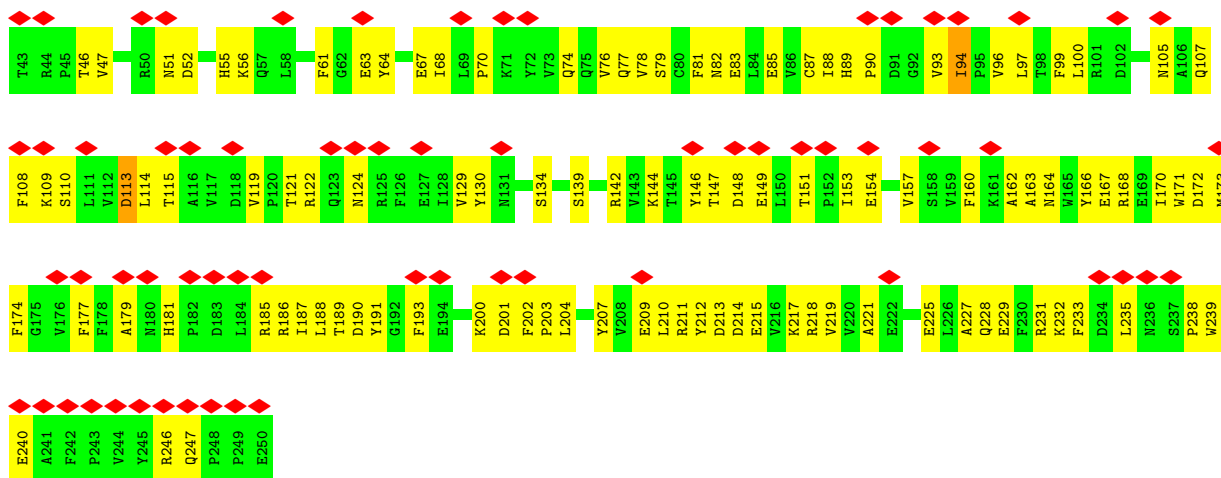


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

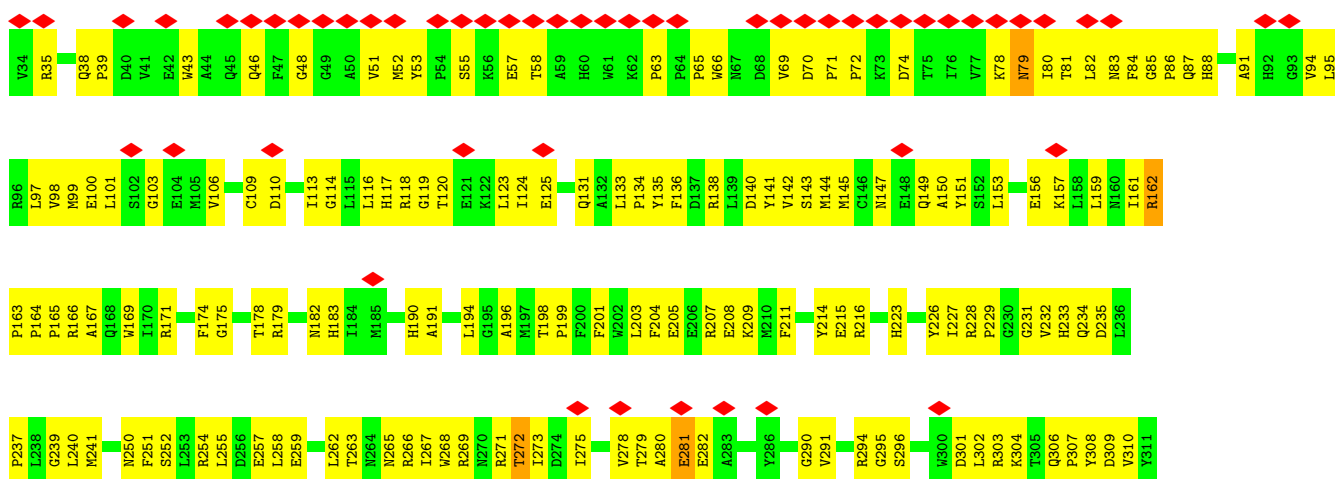


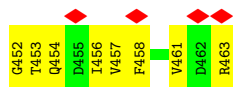
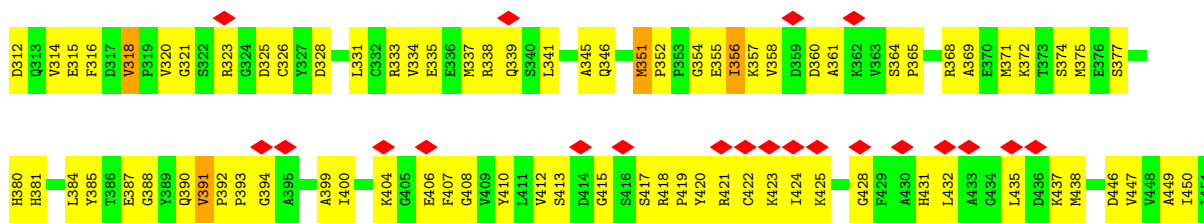


• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

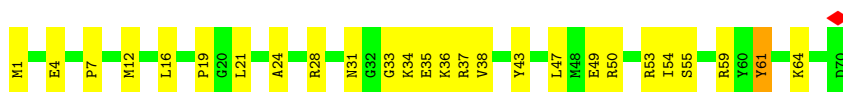


• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

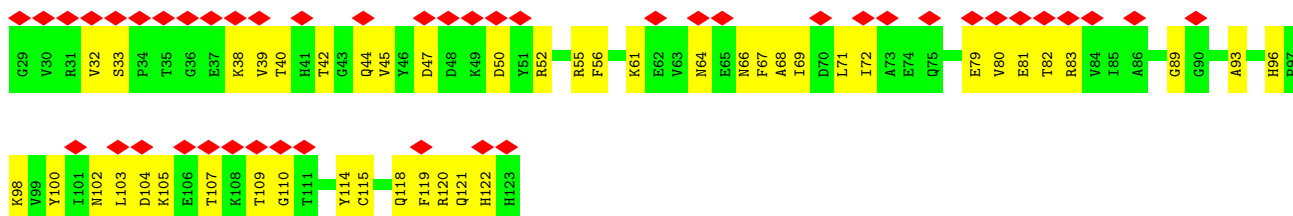




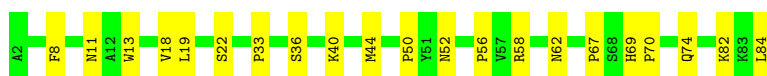
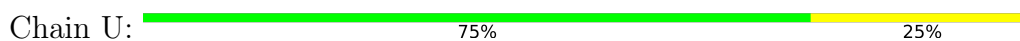
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



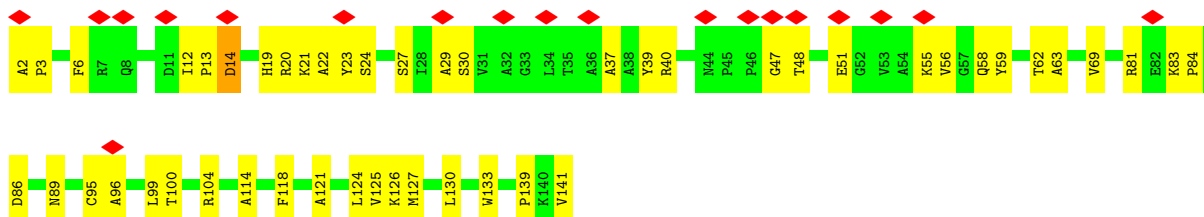
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

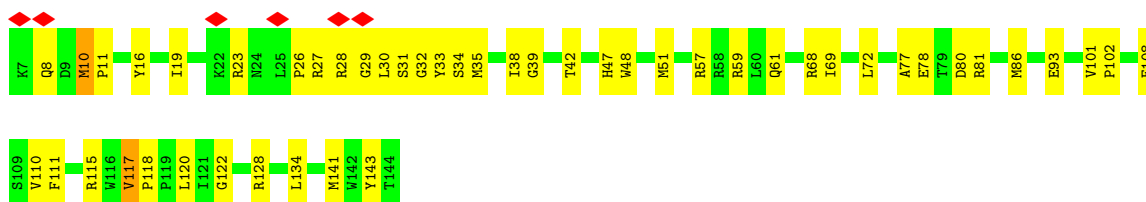


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W: 



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 



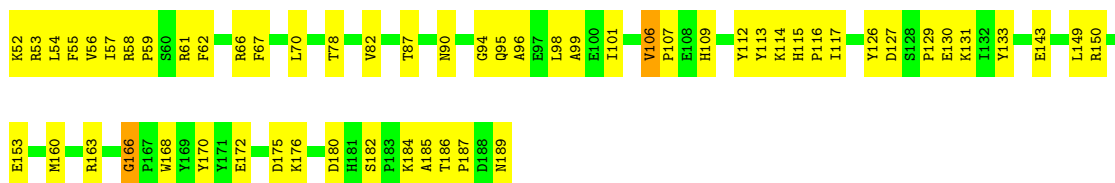
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 



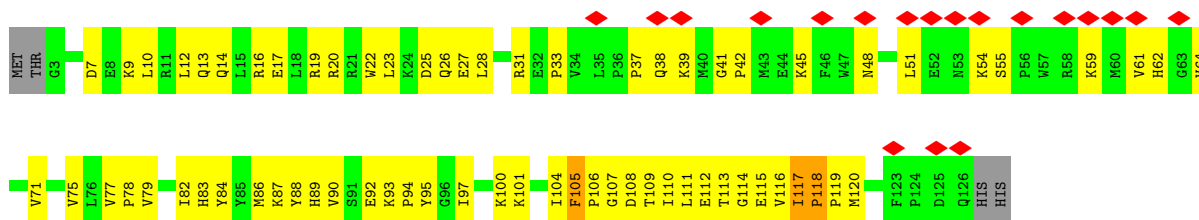
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



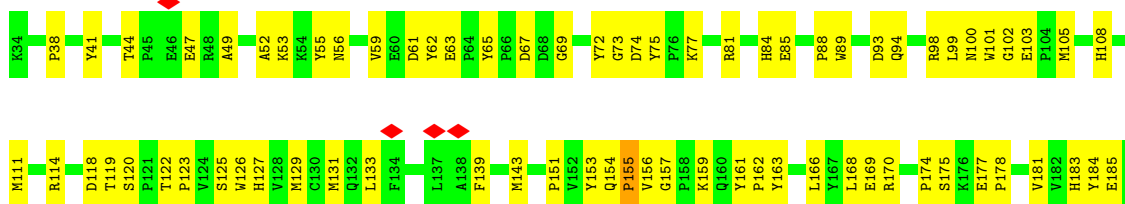
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 



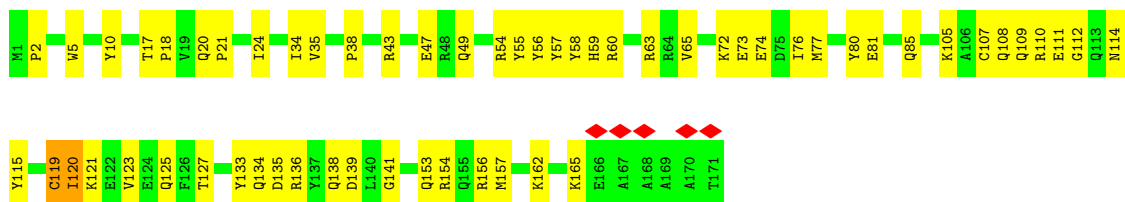
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



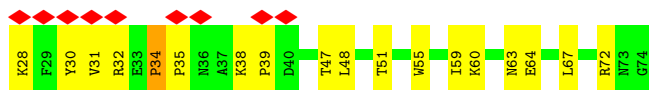
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



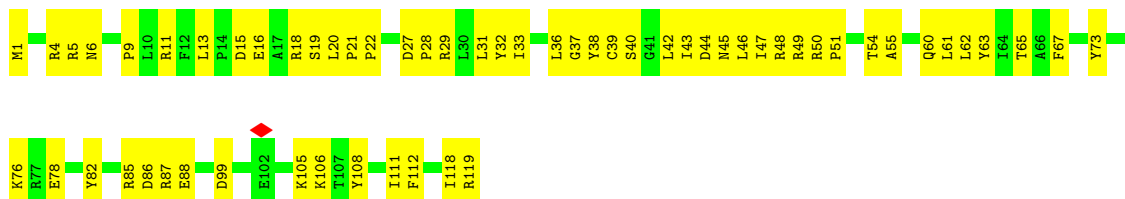
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



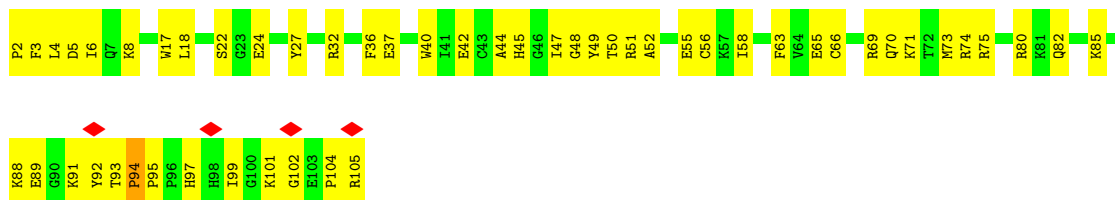
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 

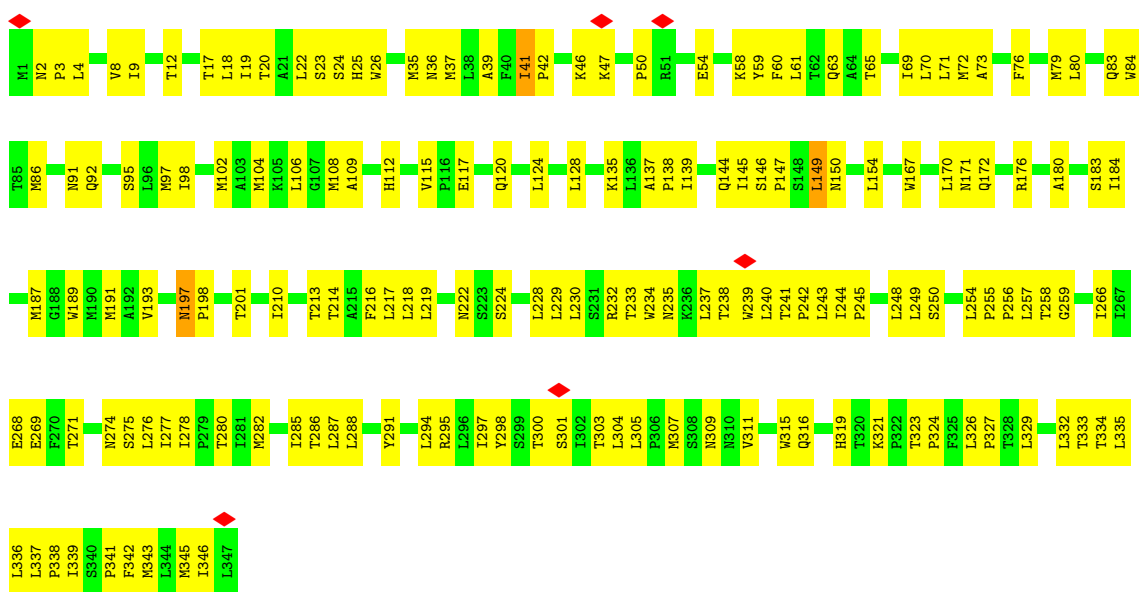


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

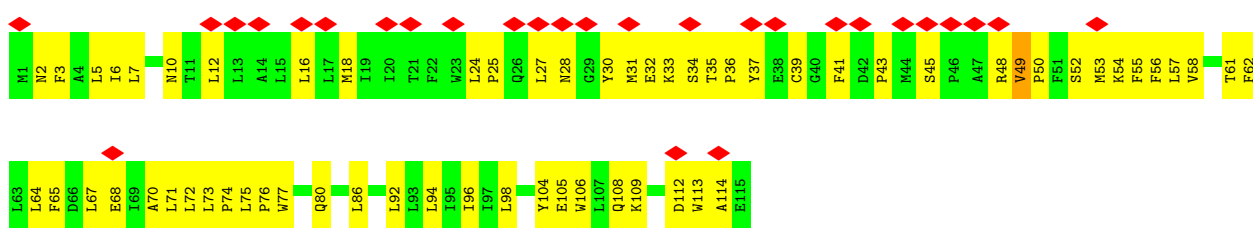
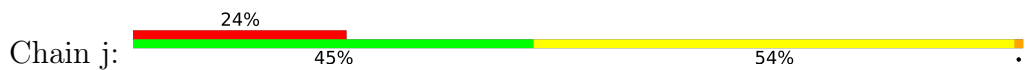
Chain h: 



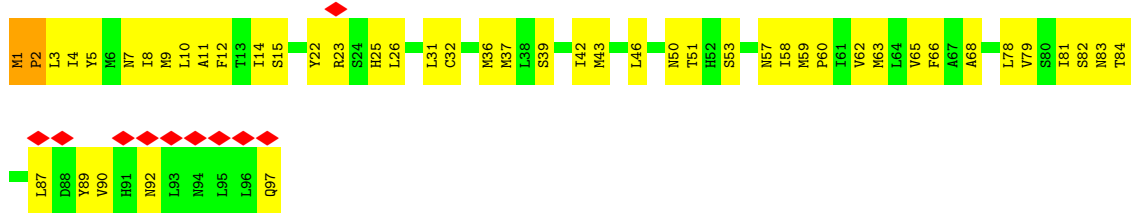
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2



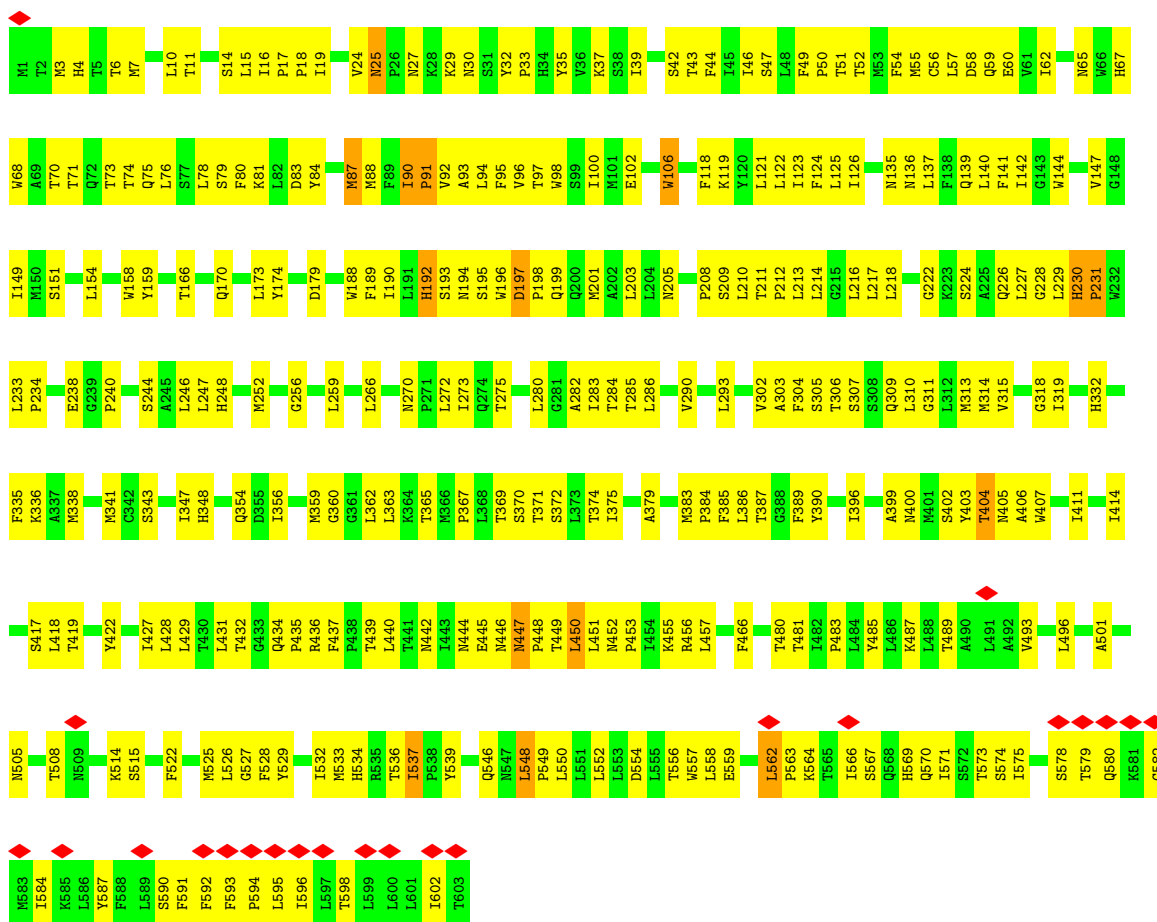
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



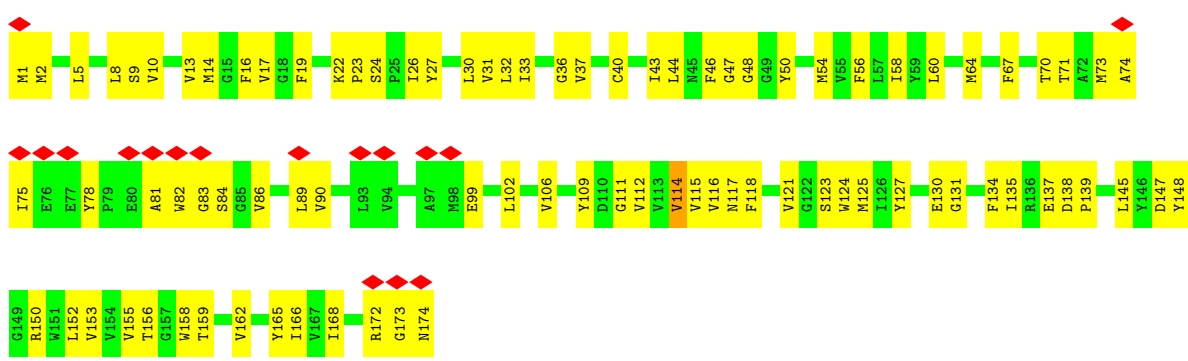
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

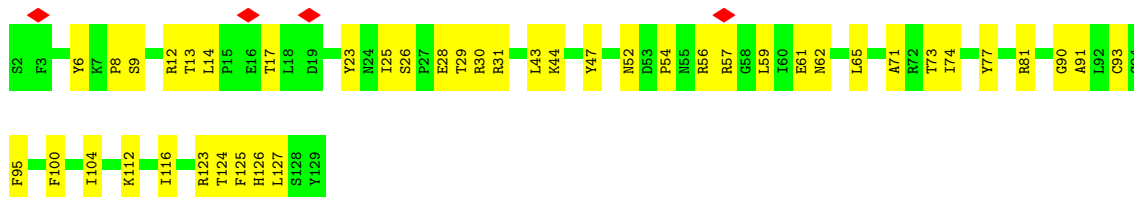


• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

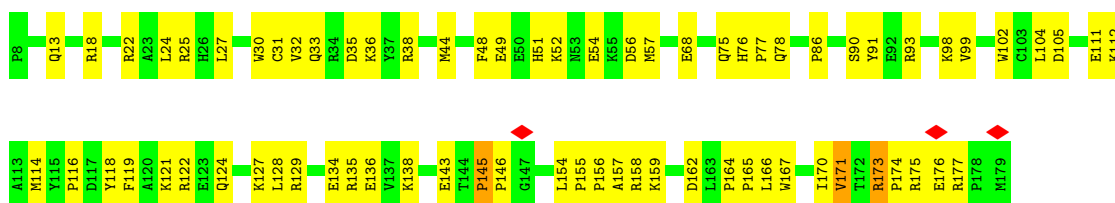




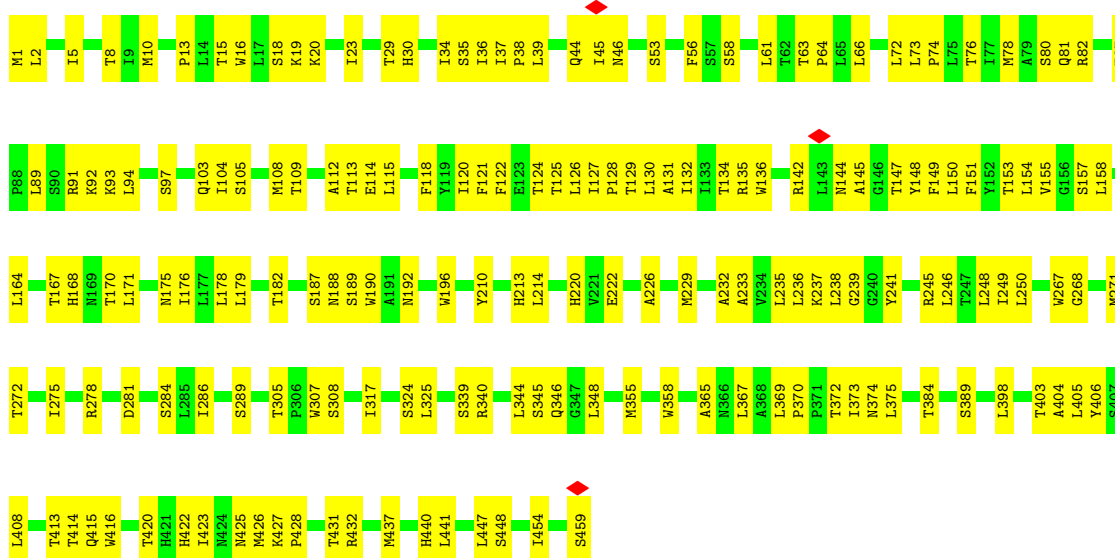
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

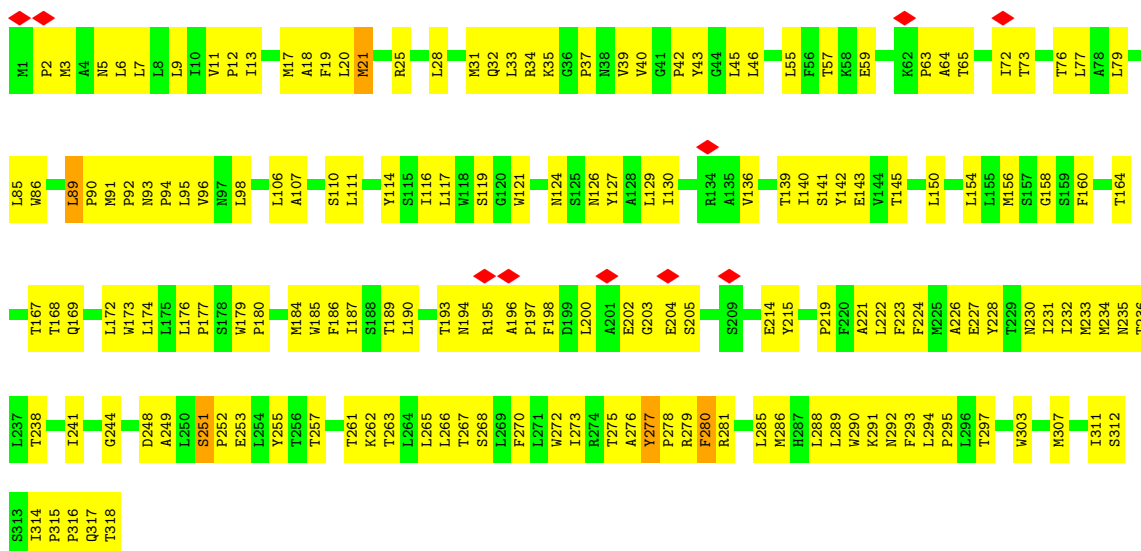


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

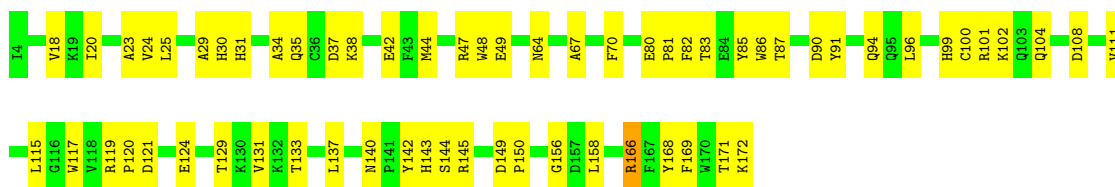


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

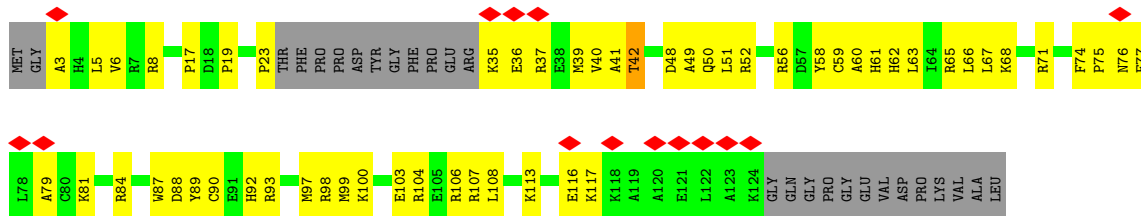




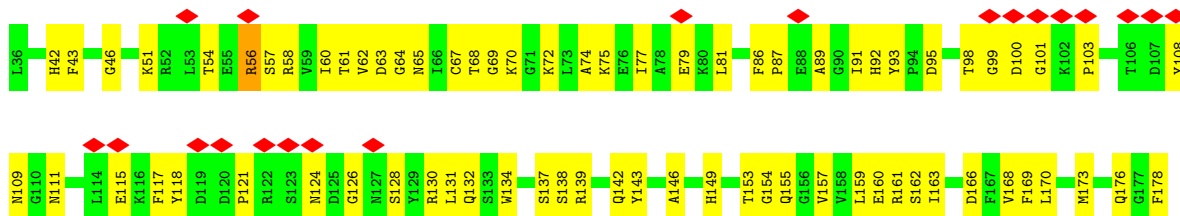
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

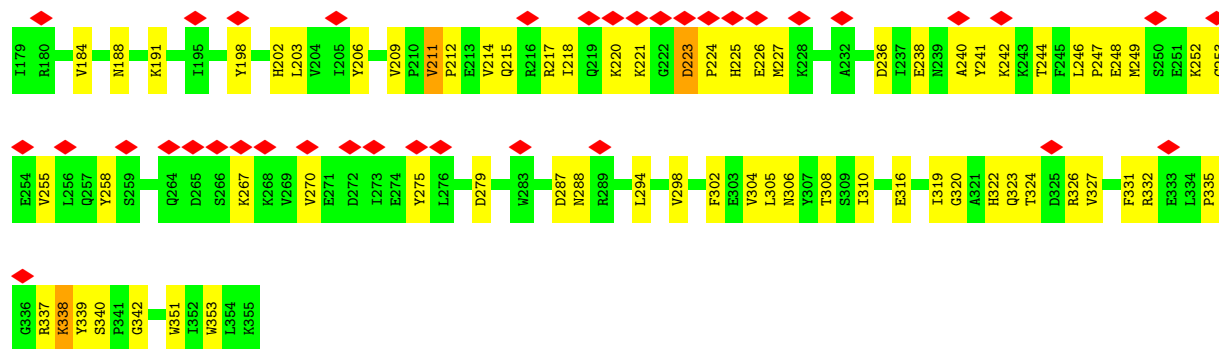


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0525	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PLX, NDP, 8Q1, FES, PEE, CDL, 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	0.39	0/3398	0.87	5/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.36	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	H	0.45	0/941	0.87	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	7/1681 (0.4%)
14	O	0.39	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.55	0/3552	1.01	15/4815 (0.3%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	T	0.38	0/755	0.79	0/1017
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	W	0.74	1/1166 (0.1%)	1.05	5/1579 (0.3%)
22	Y	0.61	0/559	1.16	7/763 (0.9%)
23	Z	0.56	0/669	0.82	0/899
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	d	0.78	0/1445	0.97	3/1945 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	l	0.84	4/4840 (0.1%)	1.03	29/6611 (0.4%)
36	m	0.82	0/1346	0.99	5/1832 (0.3%)
37	n	0.63	0/484	0.99	0/652
38	o	0.71	0/1093	0.89	0/1479
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	v	0.63	0/934	1.00	4/1241 (0.3%)
44	w	0.53	1/2533 (0.0%)	0.91	7/3440 (0.2%)
All	All	0.67	12/67276 (0.0%)	0.96	232/91300 (0.3%)

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
44	w	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.58	1.50	1.54
25	b	117	ILE	C-N	6.56	1.41	1.33
21	W	117	VAL	CA-CB	-6.07	1.49	1.54
40	r	37	ILE	CA-CB	-5.94	1.51	1.54
25	b	105	PHE	C-N	5.80	1.41	1.33

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	10	MET	CA-C-N	-10.85	109.21	120.38
21	W	10	MET	C-N-CA	-10.85	109.21	120.38
8	I	38	PRO	CA-C-N	10.35	130.66	119.28
8	I	38	PRO	C-N-CA	10.35	130.66	119.28
16	Q	162	ARG	CA-C-N	10.24	127.03	119.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

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	A	3322	0	3289	213	0
2	B	1420	0	1371	119	0
3	C	1249	0	1253	82	0
4	E	968	0	982	63	0
5	F	670	0	679	38	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	H	922	0	950	58	0
8	I	769	0	788	46	0
9	J	2712	0	2757	235	0
10	K	274	0	257	25	0
11	L	964	0	962	63	0
12	M	5274	0	5312	339	0
13	N	1195	0	1155	50	0
14	O	1643	0	1646	113	0
15	P	1730	0	1685	115	0
16	Q	3460	0	3419	310	0
17	S	568	0	567	39	0
18	T	742	0	723	40	0
19	U	647	0	653	17	0
20	V	1038	0	1027	36	0
21	W	1135	0	1129	56	0
22	Y	533	0	475	97	0
23	Z	648	0	627	19	0
24	a	1174	0	1177	105	0
25	b	1059	0	1079	126	0
26	c	1236	0	1092	81	0
27	d	1418	0	1375	120	0
28	e	810	0	772	35	0
29	f	405	0	407	19	0
30	g	1004	0	1008	64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	h	863	0	861	66	0
32	i	2735	0	2893	185	0
33	j	919	0	968	76	0
34	k	740	0	792	89	0
35	l	4717	0	4893	400	0
36	m	1313	0	1330	122	0
37	n	473	0	480	30	0
38	o	1066	0	1086	52	0
39	p	1495	0	1440	94	0
40	r	3629	0	3825	164	0
41	s	2509	0	2617	170	0
42	u	1394	0	1367	60	0
43	v	921	0	892	90	0
44	w	2474	0	2304	116	0
45	A	8	0	0	6	0
45	B	16	0	0	3	0
45	C	8	0	0	0	0
45	M	16	0	0	3	0
46	A	31	0	19	16	0
47	B	52	0	88	4	0
47	U	52	0	88	3	0
47	V	52	0	88	5	0
47	b	52	0	88	38	0
47	g	156	0	264	13	0
47	r	104	0	176	23	0
48	E	35	0	0	4	0
48	p	35	0	0	12	0
49	J	48	0	26	26	0
50	M	4	0	0	1	0
50	O	4	0	0	2	0
51	V	63	0	68	8	0
51	i	64	0	72	3	0
51	l	128	0	144	4	0
51	n	64	0	72	10	0
52	V	51	0	82	21	0
52	W	51	0	82	19	0
52	l	100	0	157	68	0
All	All	66789	0	67204	3729	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 28.

The worst 5 of 3729 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)
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.65
35:l:533:MET:CE	52:l:702:PEE:H36	1.25	1.58
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.57
24:a:55:PHE:HE2	39:p:118:TYR:CE2	1.17	1.56
24:a:55:PHE:CE2	39:p:118:TYR:CD2	1.91	1.55

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

30 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$
51	CDL	V	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
47	PLX	r	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
51	CDL	l	704	-	63,63,99	1.27	5 (7%)	69,75,111	1.02	4 (5%)
49	NDP	J	401	-	51,52,52	1.15	6 (11%)	71,80,80	1.56	10 (14%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
52	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
47	PLX	r	502	-	51,51,51	0.62	0	53,59,59	0.66	1 (1%)
52	PEE	W	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
47	PLX	g	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
51	CDL	i	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
47	PLX	B	303	-	51,51,51	0.79	1 (1%)	53,59,59	0.69	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
46	FMN	A	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	9 (18%)
48	8Q1	E	201	-	32,34,34	1.58	6 (18%)	39,43,43	1.42	7 (17%)
48	8Q1	p	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
50	FES	M	803	-	0,4,4	-	-	-	-	-
52	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
51	CDL	l	703	-	63,63,99	1.23	5 (7%)	69,75,111	1.08	4 (5%)
50	FES	O	301	14	0,4,4	-	-	-	-	-
47	PLX	g	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.60	1 (1%)
47	PLX	g	202	-	51,51,51	0.77	1 (1%)	53,59,59	0.62	1 (1%)
47	PLX	U	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
47	PLX	V	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.61	1 (1%)
52	PEE	l	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
47	PLX	b	201	-	51,51,51	0.55	0	53,59,59	0.64	0
51	CDL	n	101	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	4 (5%)

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
51	CDL	V	201	-	-	40/69/69/110	-
47	PLX	r	501	-	-	27/55/55/55	-
51	CDL	l	704	-	-	42/74/74/110	-
49	NDP	J	401	-	-	15/34/77/77	0/5/5/5
52	PEE	l	701	-	-	31/52/52/54	-
45	SF4	B	302	2	-	-	0/6/5/5
47	PLX	r	502	-	-	36/55/55/55	-
52	PEE	W	201	-	-	29/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
47	PLX	g	201	-	-	24/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
51	CDL	i	401	-	-	39/74/74/110	-
47	PLX	B	303	-	-	22/55/55/55	-
48	8Q1	p	201	-	-	19/41/41/41	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
48	8Q1	E	201	-	-	18/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
50	FES	M	803	-	-	-	0/1/1/1
52	PEE	V	202	-	-	26/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
51	CDL	l	703	-	-	36/74/74/110	-
50	FES	O	301	14	-	-	0/1/1/1
47	PLX	g	203	-	-	22/55/55/55	-
47	PLX	g	202	-	-	26/55/55/55	-
47	PLX	U	101	-	-	22/55/55/55	-
47	PLX	V	203	-	-	26/55/55/55	-
52	PEE	l	702	-	-	27/54/54/54	-
47	PLX	b	201	-	-	26/55/55/55	-
51	CDL	n	101	-	-	32/74/74/110	-

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	201	8Q1	C39-N41	5.03	1.45	1.33
48	p	201	8Q1	C34-N36	4.93	1.45	1.33
48	E	201	8Q1	C34-N36	4.88	1.45	1.33
48	E	201	8Q1	C39-N41	4.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	502	FMN	C9A-C5A	4.60	1.48	1.41

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	p	201	8Q1	C6-C1-S44	5.93	120.47	113.40
49	J	401	NDP	C5A-C4A-N3A	-5.84	118.68	126.72
49	J	401	NDP	N3A-C4A-N9A	4.76	135.26	127.17
48	E	201	8Q1	C6-C1-S44	4.50	118.77	113.40
52	l	702	PEE	O2-C10-C11	4.38	120.95	111.48

There are no chirality outliers.

5 of 592 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	B	303	PLX	C2-O1-P1-O4

There are no ring outliers.

28 monomers are involved in 285 short contacts:

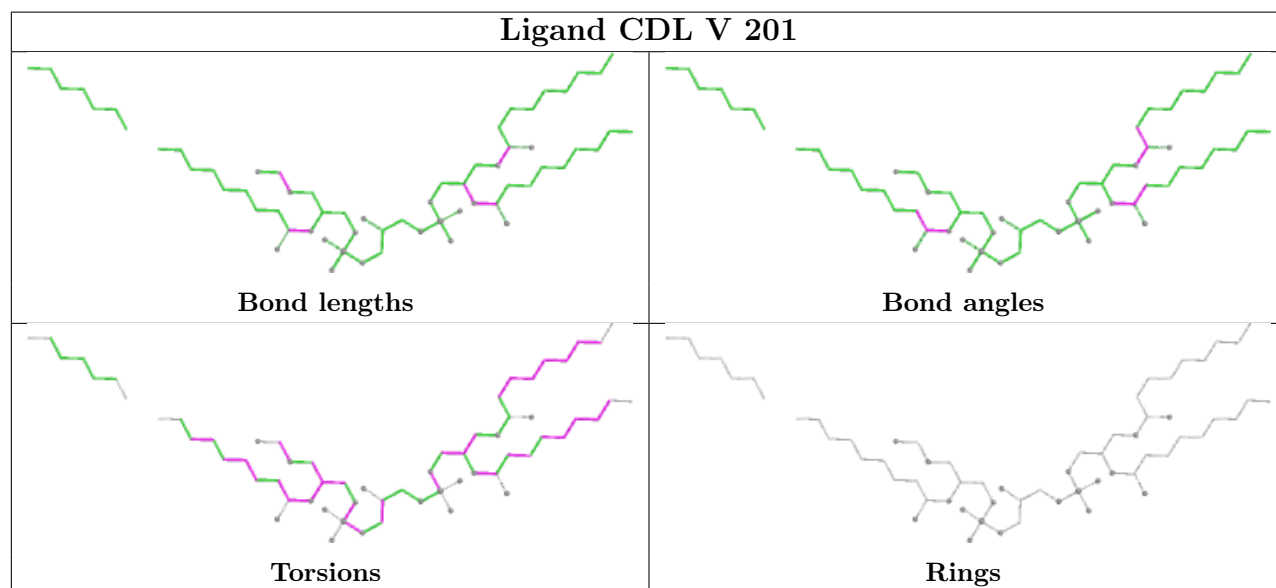
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	V	201	CDL	8	0
47	r	501	PLX	6	0
51	l	704	CDL	2	0
49	J	401	NDP	26	0
45	B	302	SF4	2	0
52	l	701	PEE	50	0
47	r	502	PLX	17	0
52	W	201	PEE	19	0
45	B	301	SF4	1	0
47	g	201	PLX	2	0
45	A	501	SF4	6	0
51	i	401	CDL	3	0
47	B	303	PLX	4	0
45	M	801	SF4	3	0
46	A	502	FMN	16	0
48	E	201	8Q1	4	0

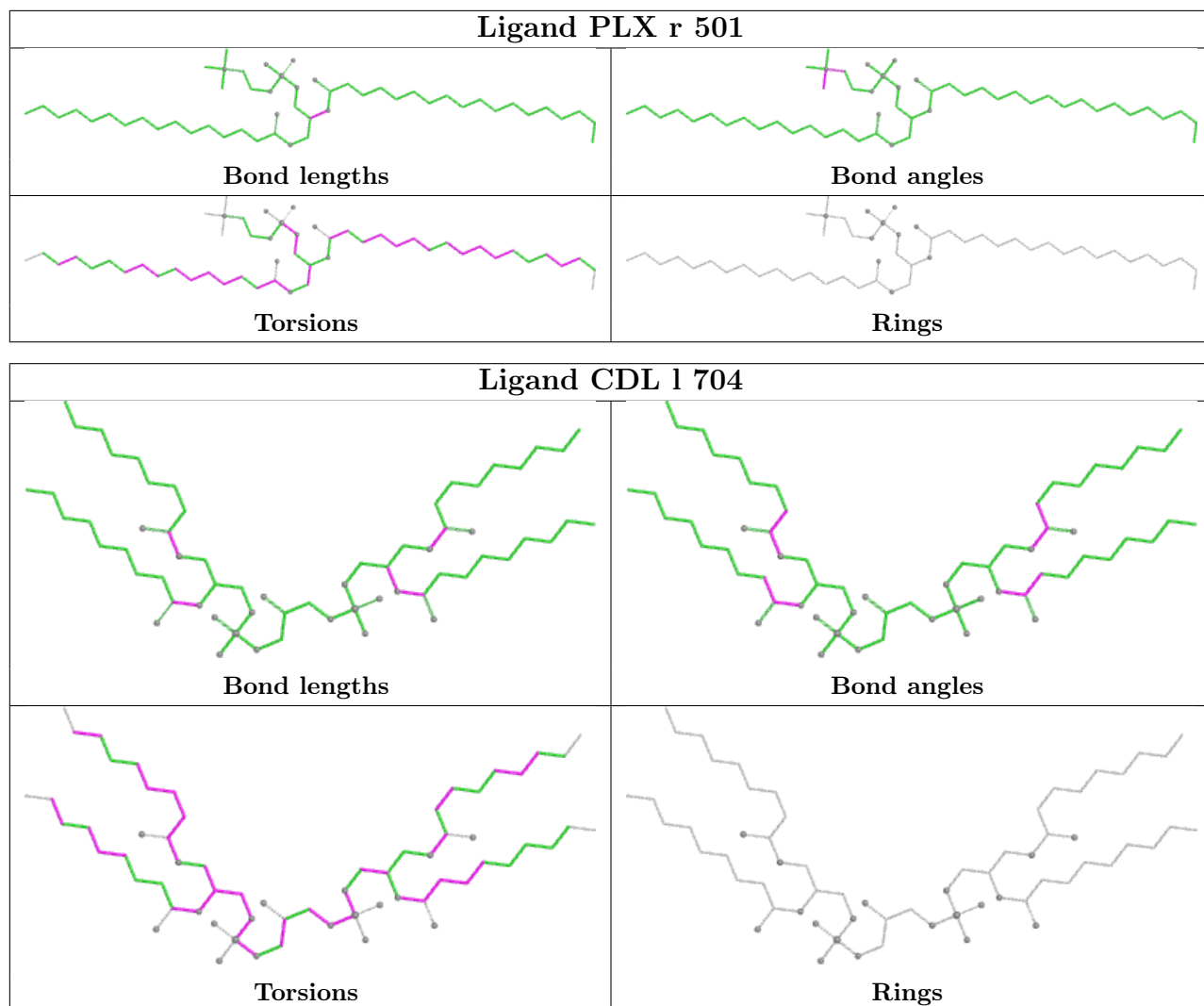
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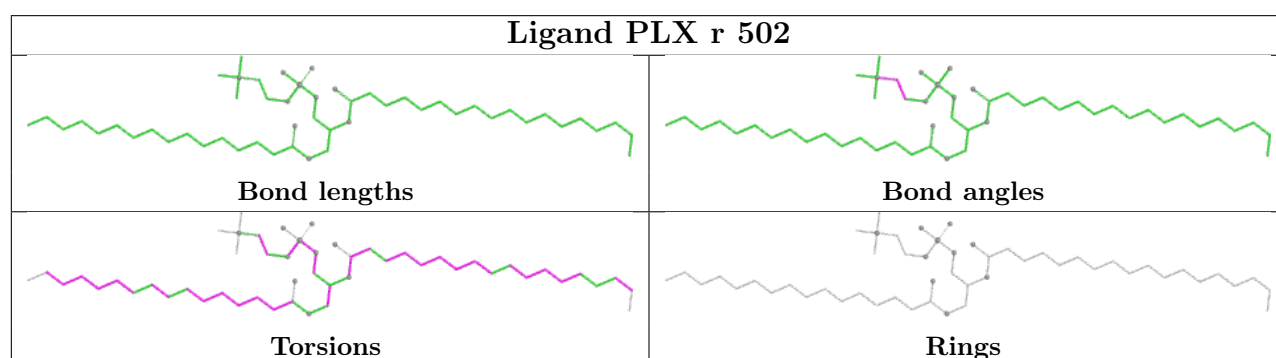
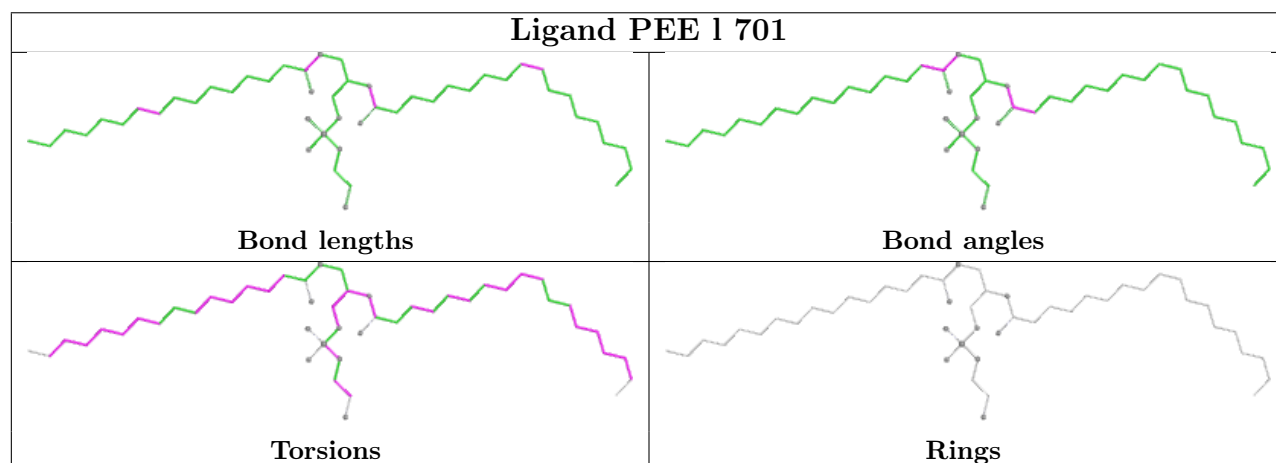
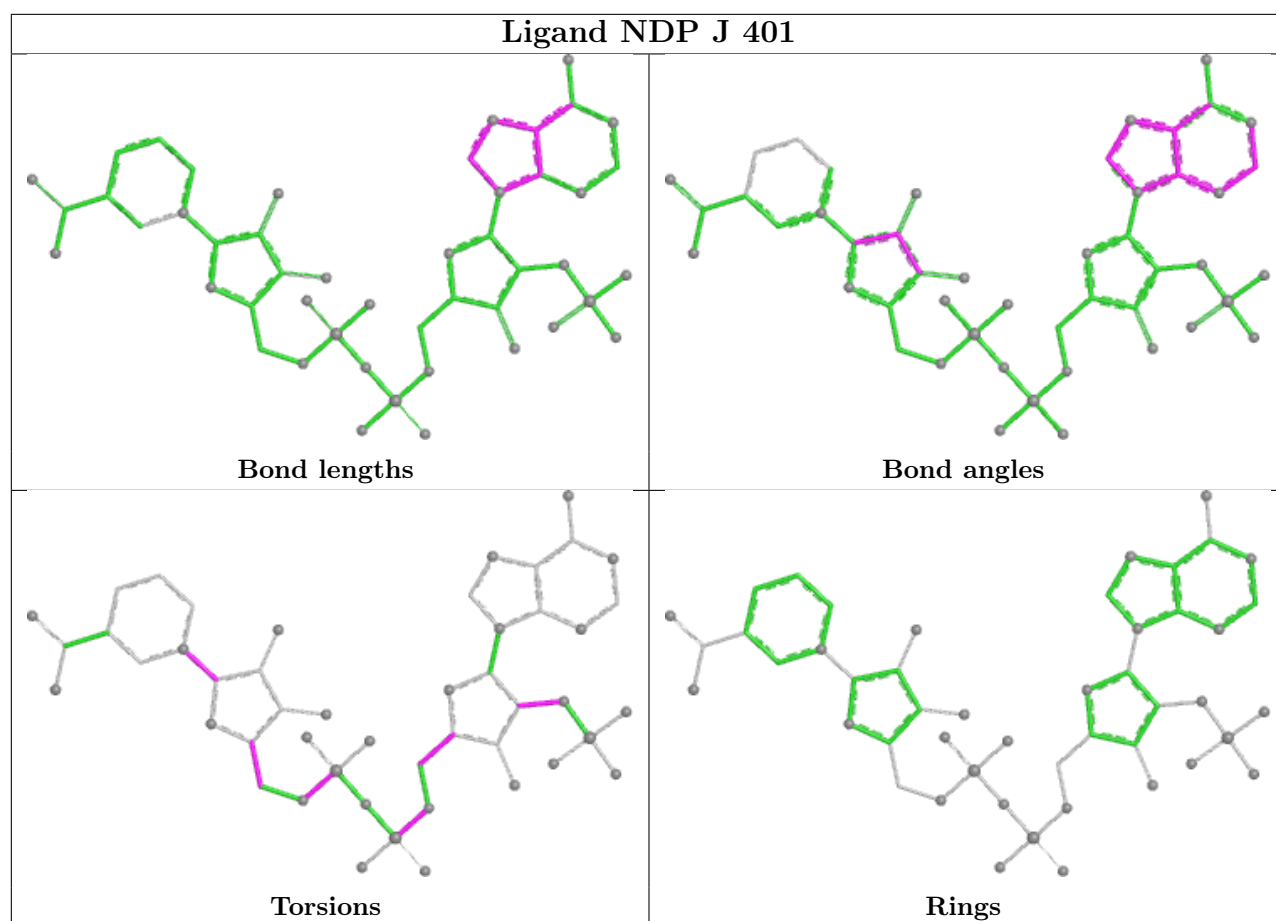
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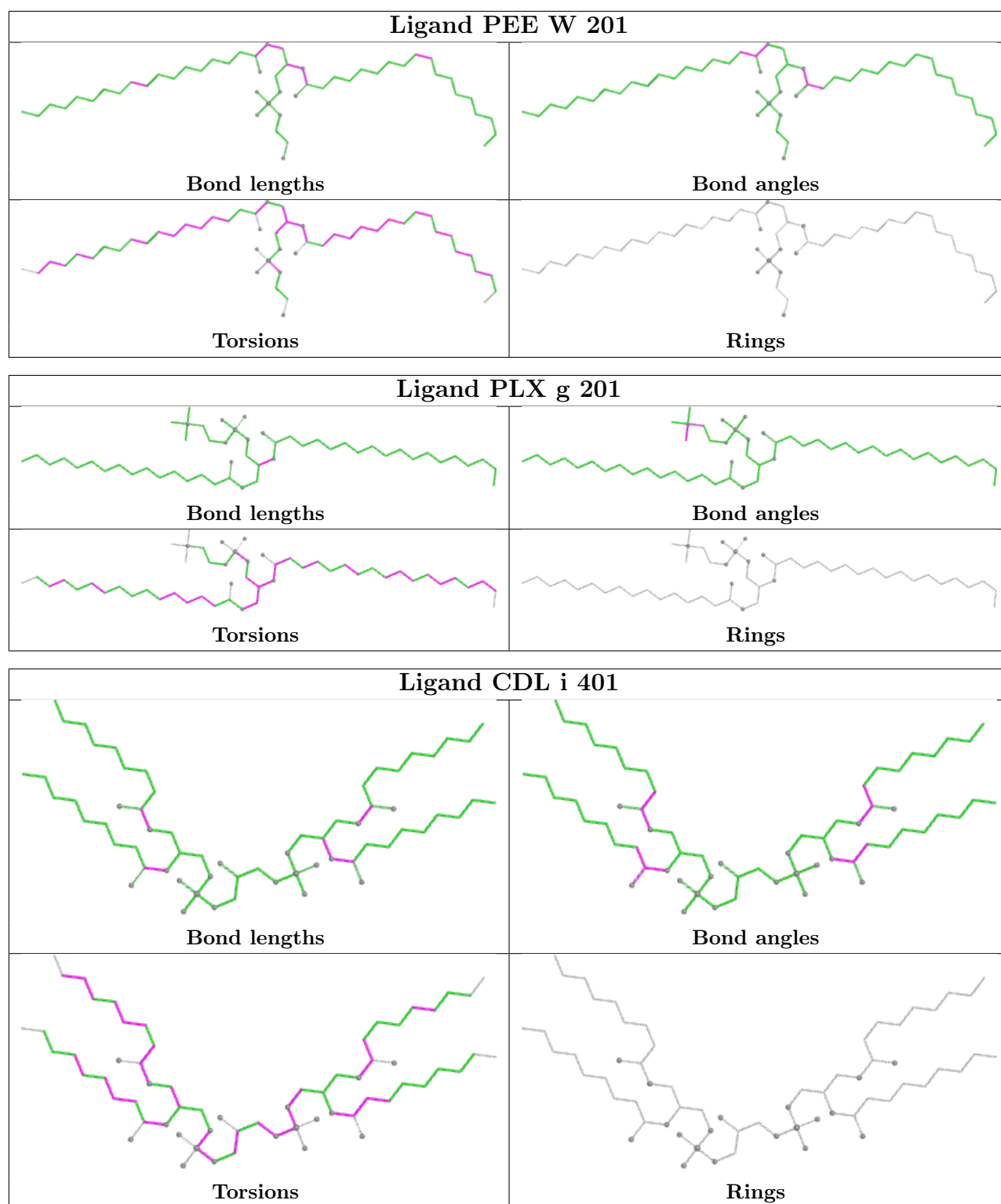
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	p	201	8Q1	12	0
50	M	803	FES	1	0
52	V	202	PEE	21	0
51	l	703	CDL	2	0
50	O	301	FES	2	0
47	g	203	PLX	8	0
47	g	202	PLX	3	0
47	U	101	PLX	3	0
47	V	203	PLX	5	0
52	l	702	PEE	18	0
47	b	201	PLX	38	0
51	n	101	CDL	10	0

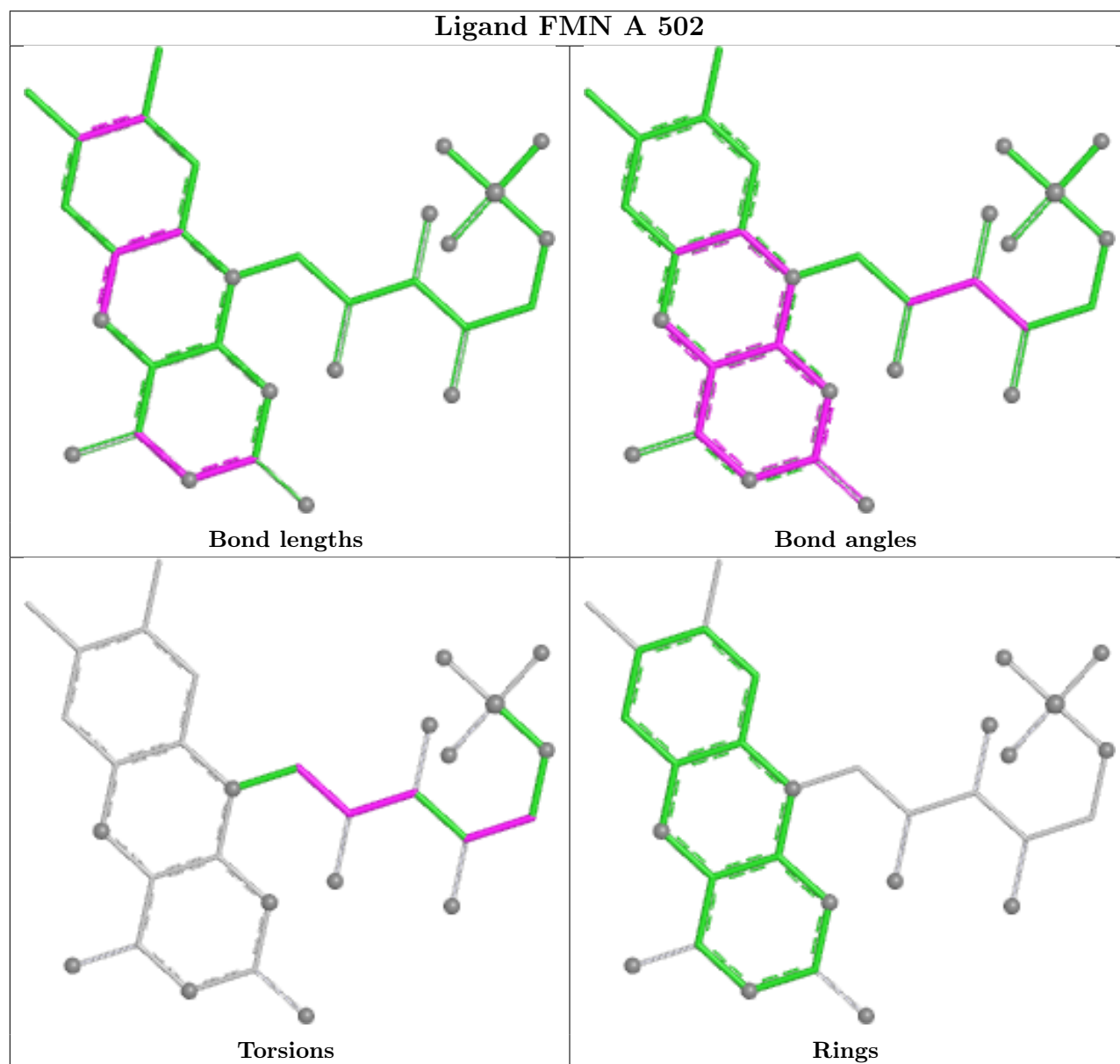
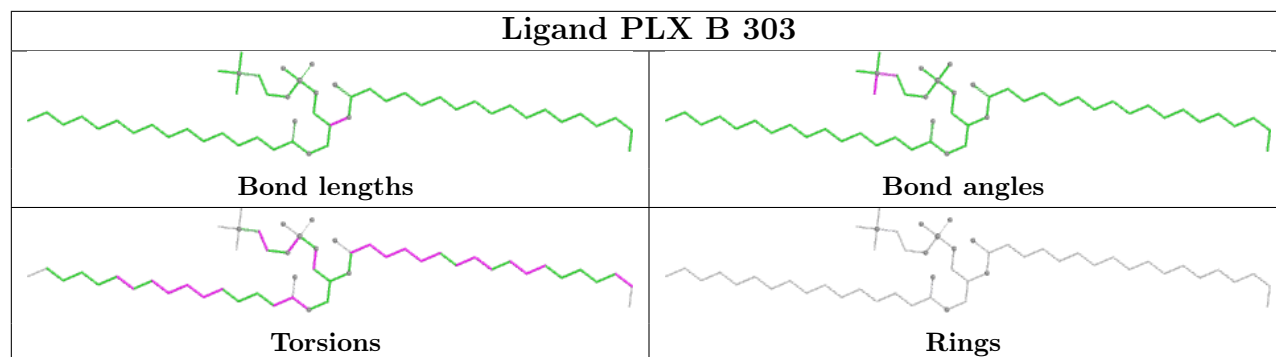
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

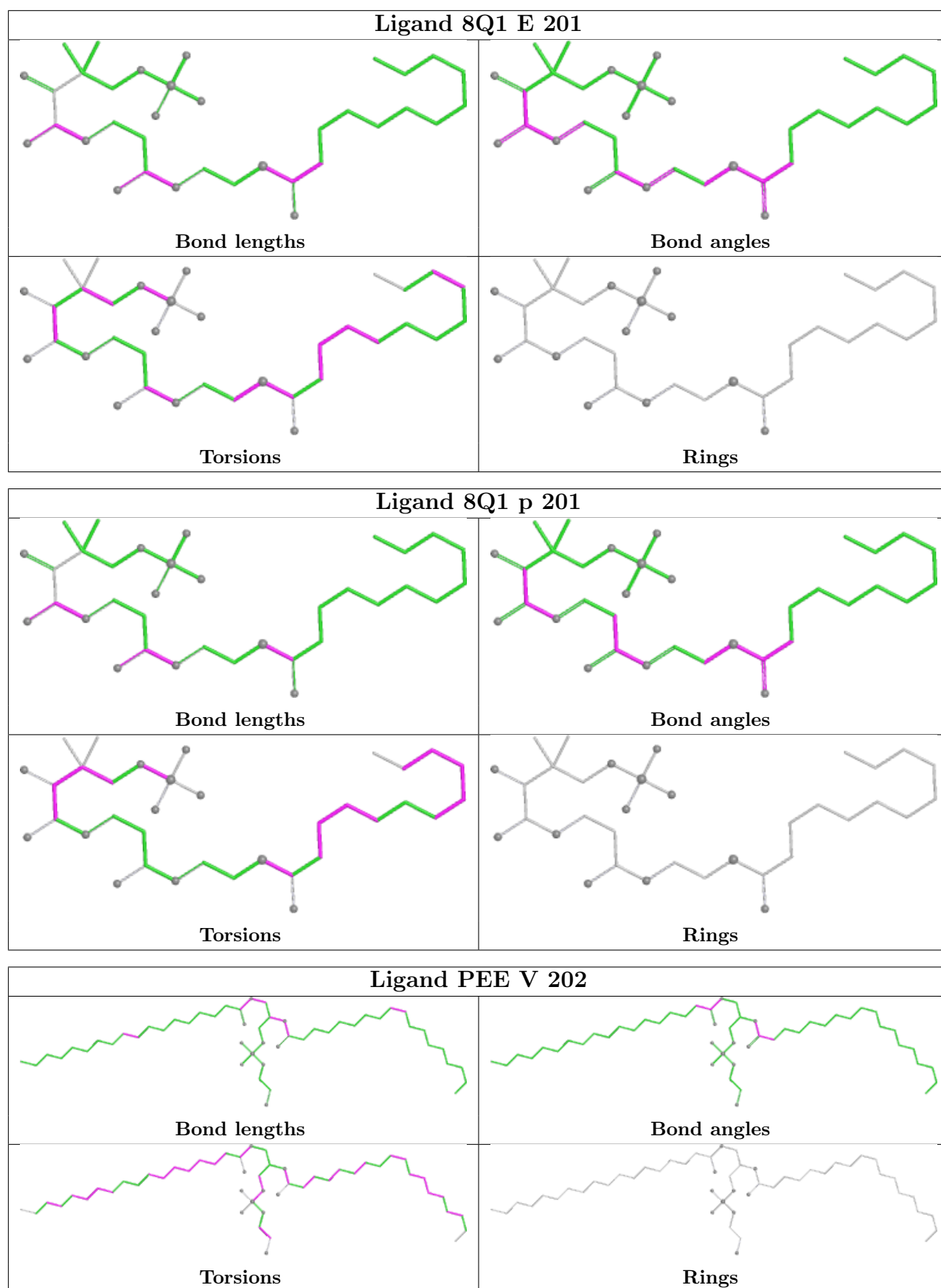


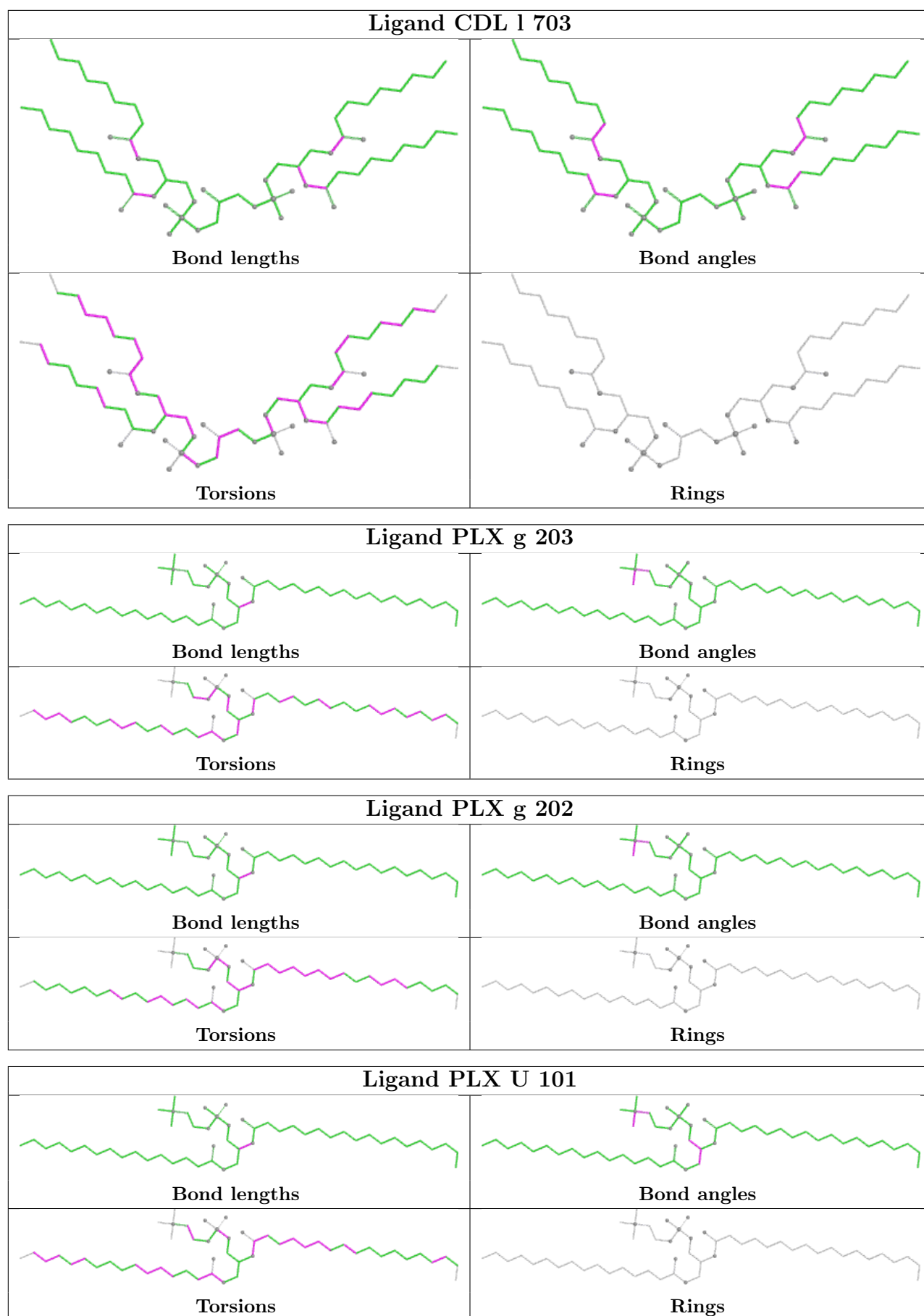


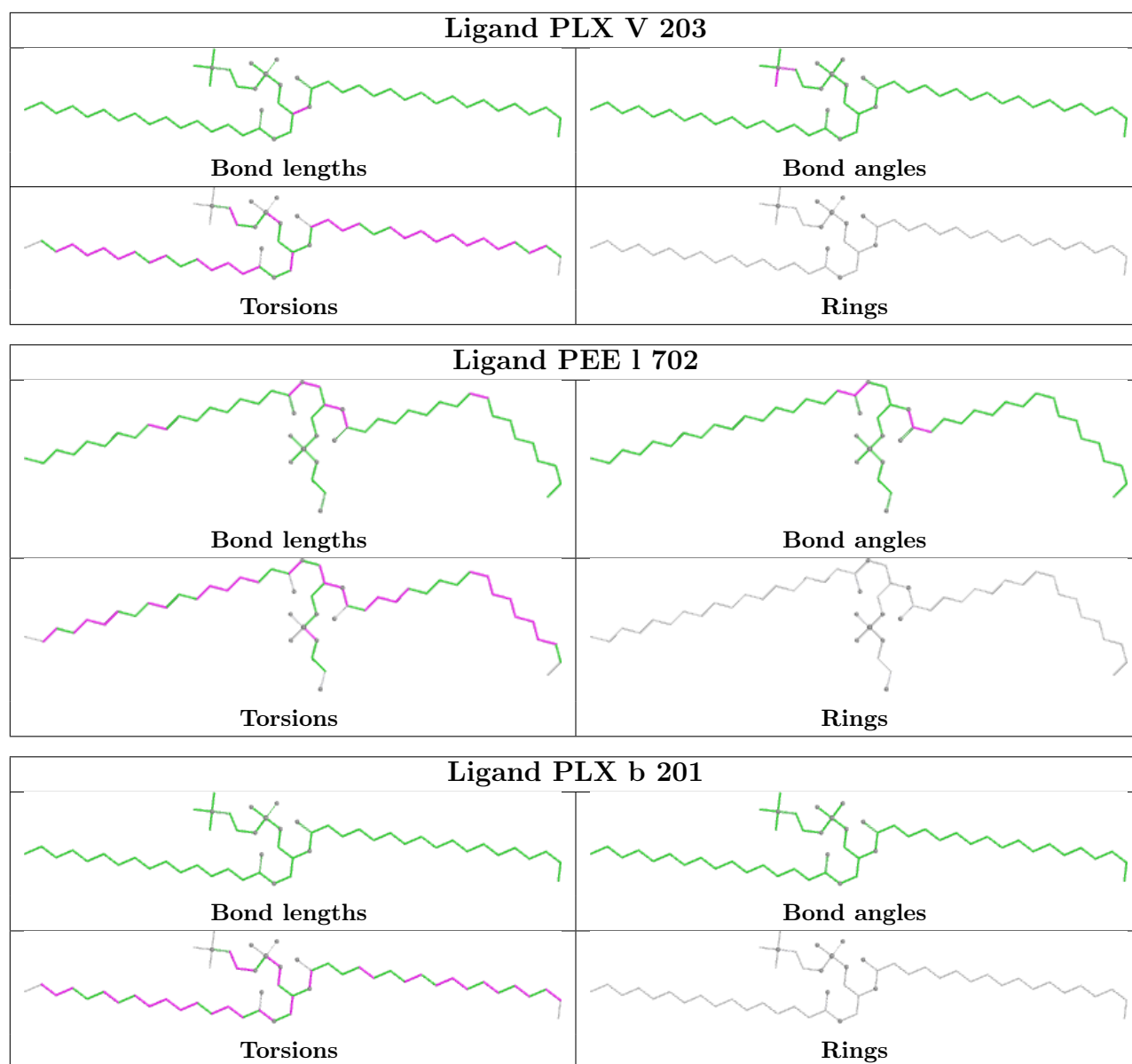


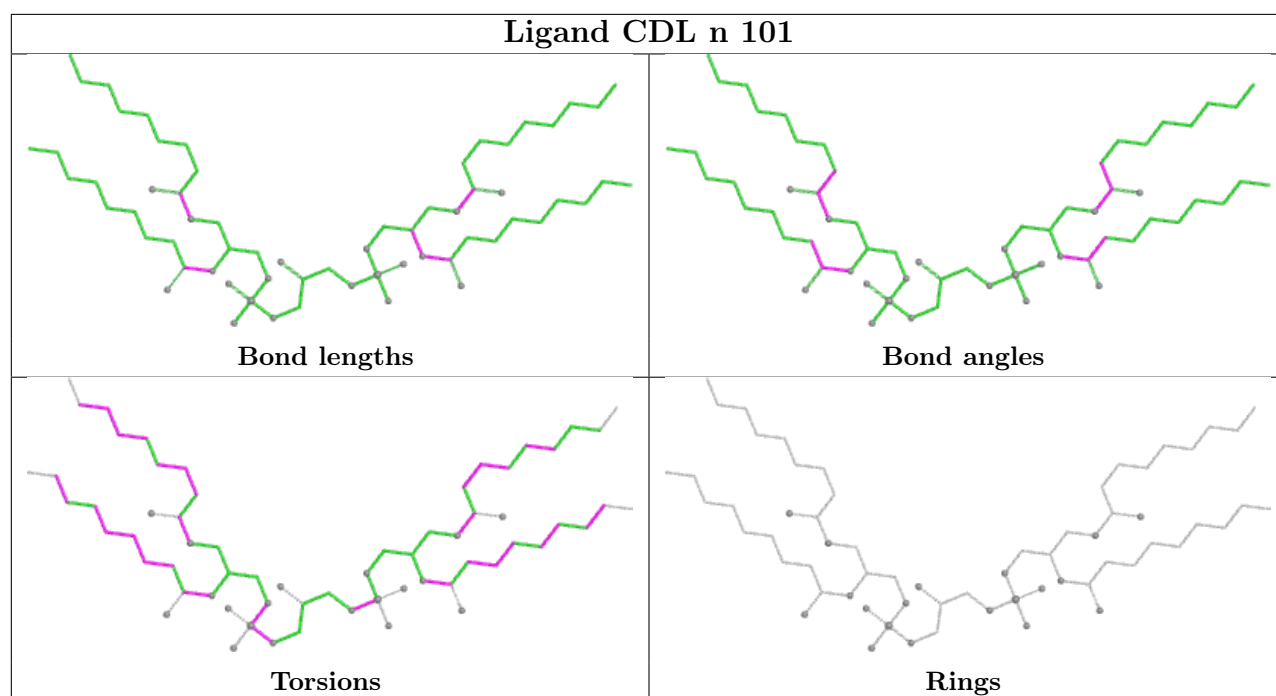












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

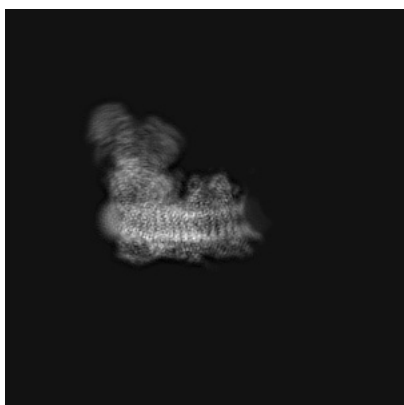
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6773. These allow visual inspection of the internal detail of the map and identification of artifacts.

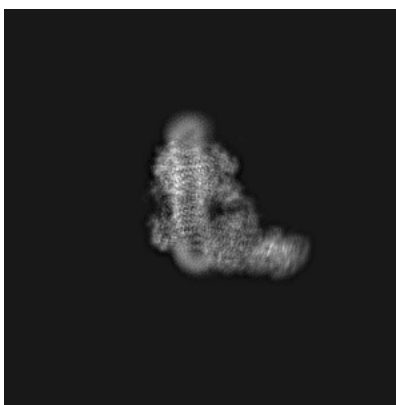
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

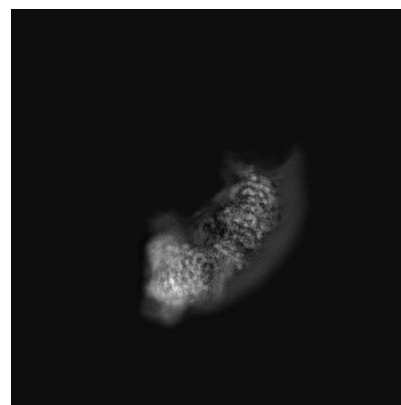
6.1.1 Primary map



X



Y



Z

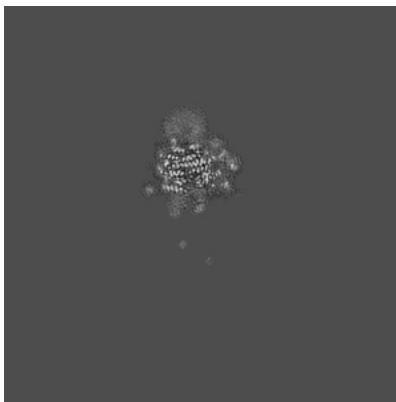
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

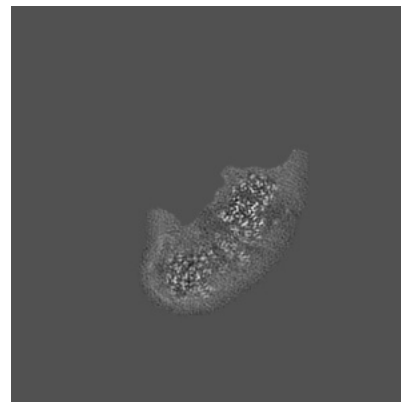
6.2.1 Primary map



X Index: 240



Y Index: 240

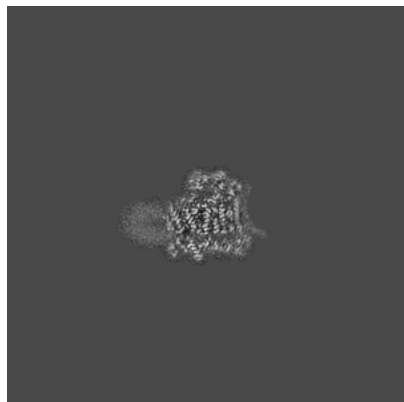


Z Index: 240

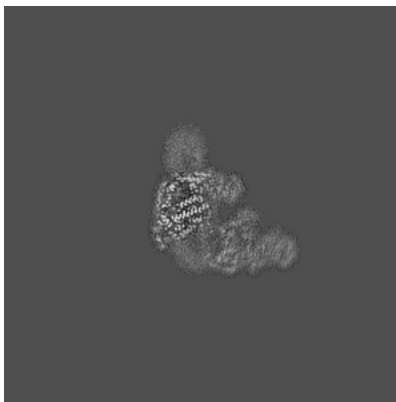
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

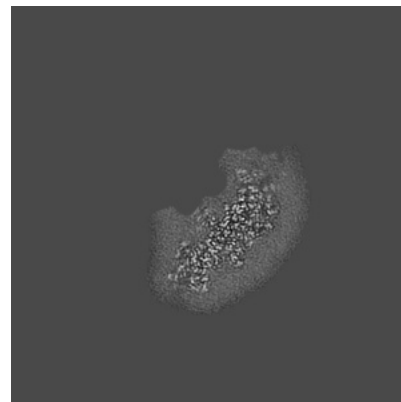
6.3.1 Primary map



X Index: 290



Y Index: 183

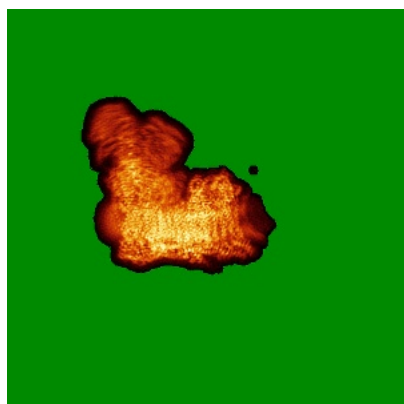


Z Index: 208

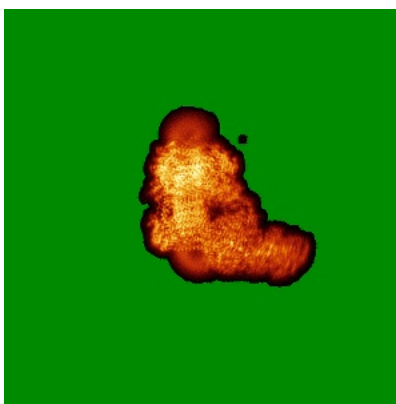
The images above show the largest variance slices of the map in three orthogonal directions.

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

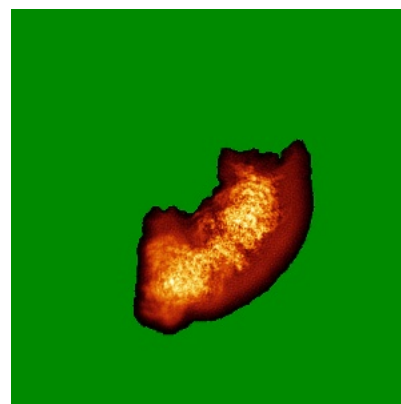
6.4.1 Primary map



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

This section was not generated.

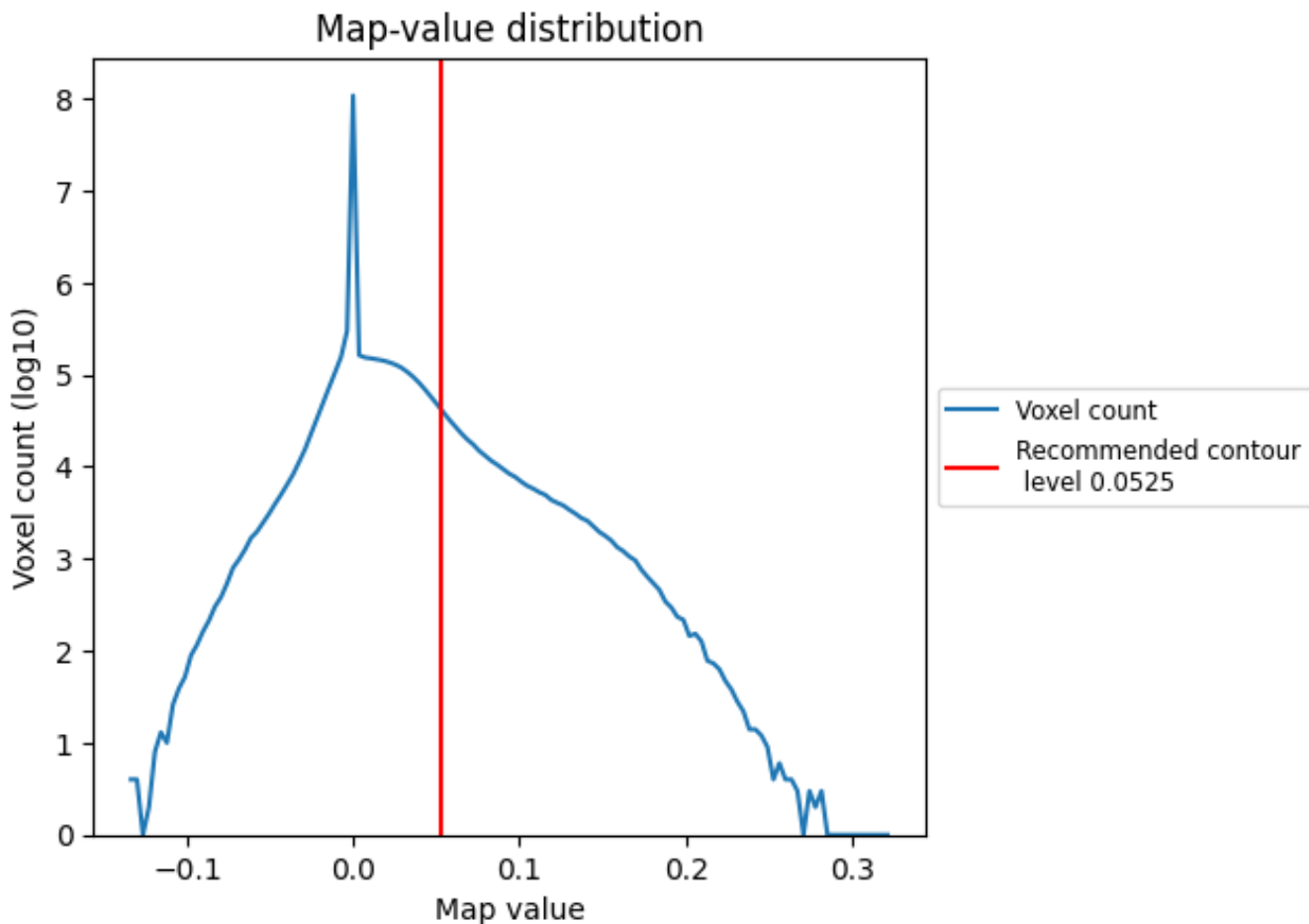
6.6 Mask visualisation

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

7 Map analysis [i](#)

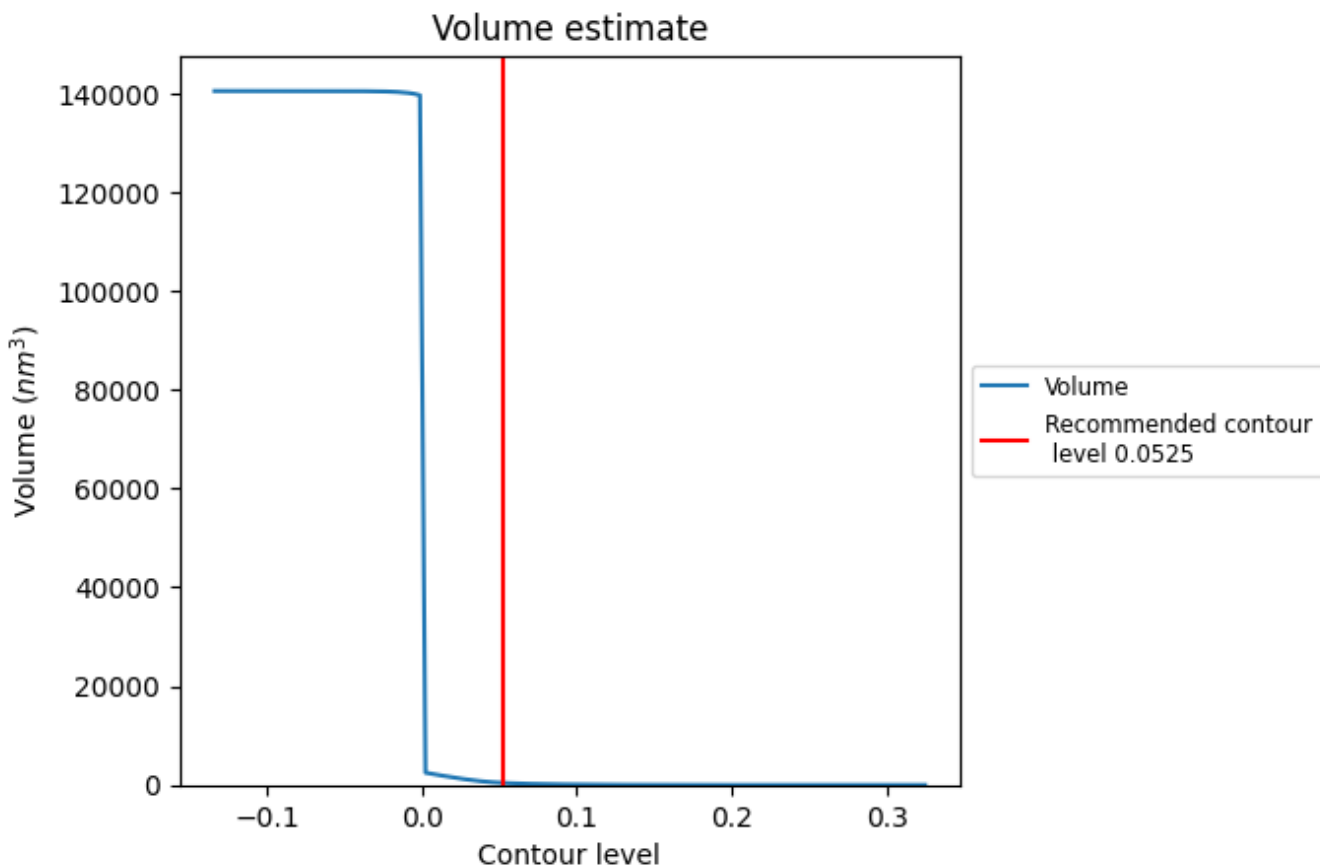
This section contains the results of statistical analysis of the map.

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.

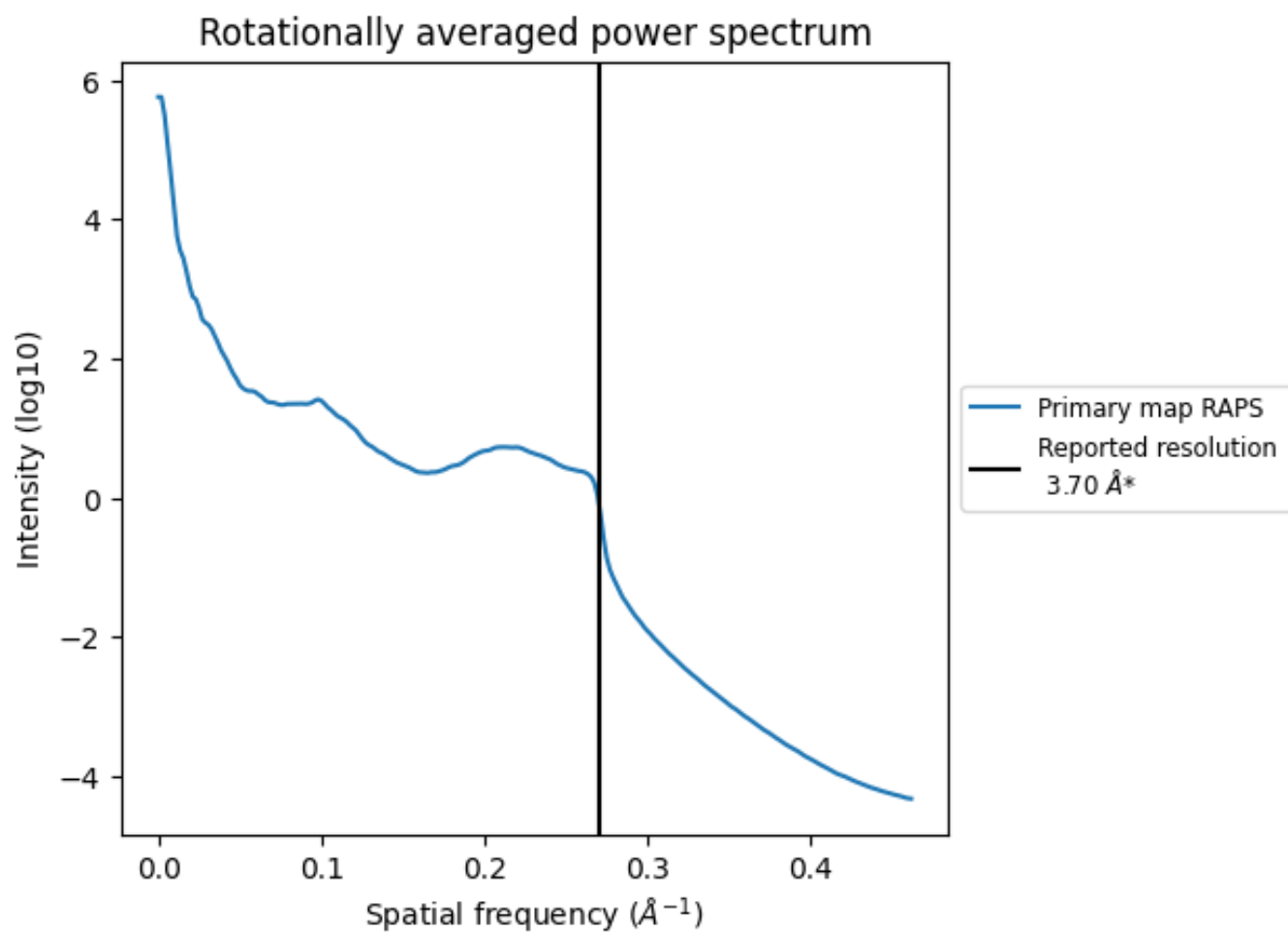
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 372 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.270\AA^{-1}

8 Fourier-Shell correlation

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

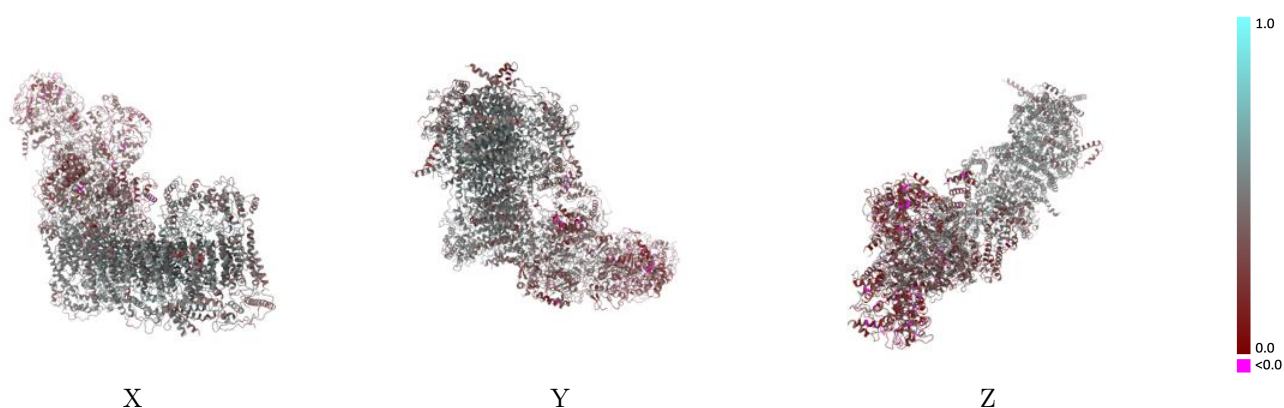
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6773 and PDB model 5XTD. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

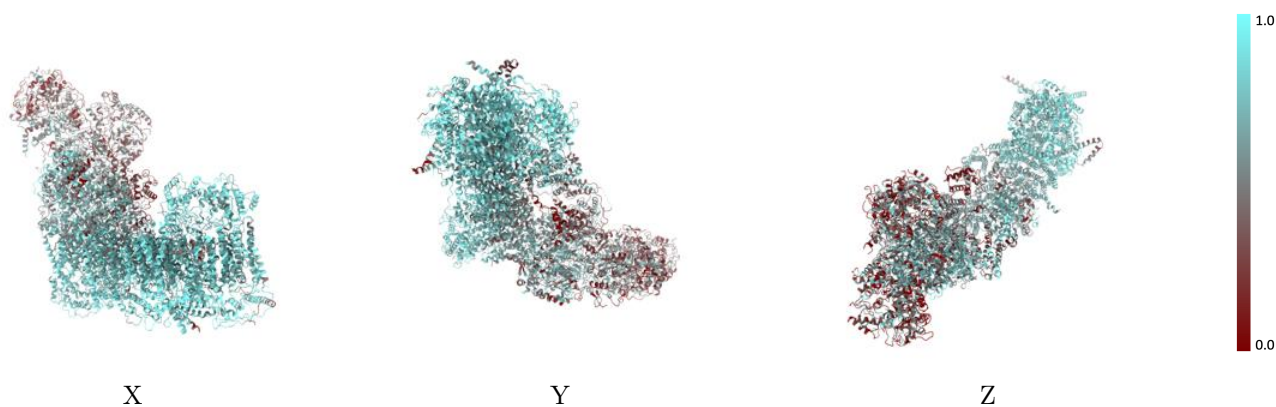
This section was not generated.

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



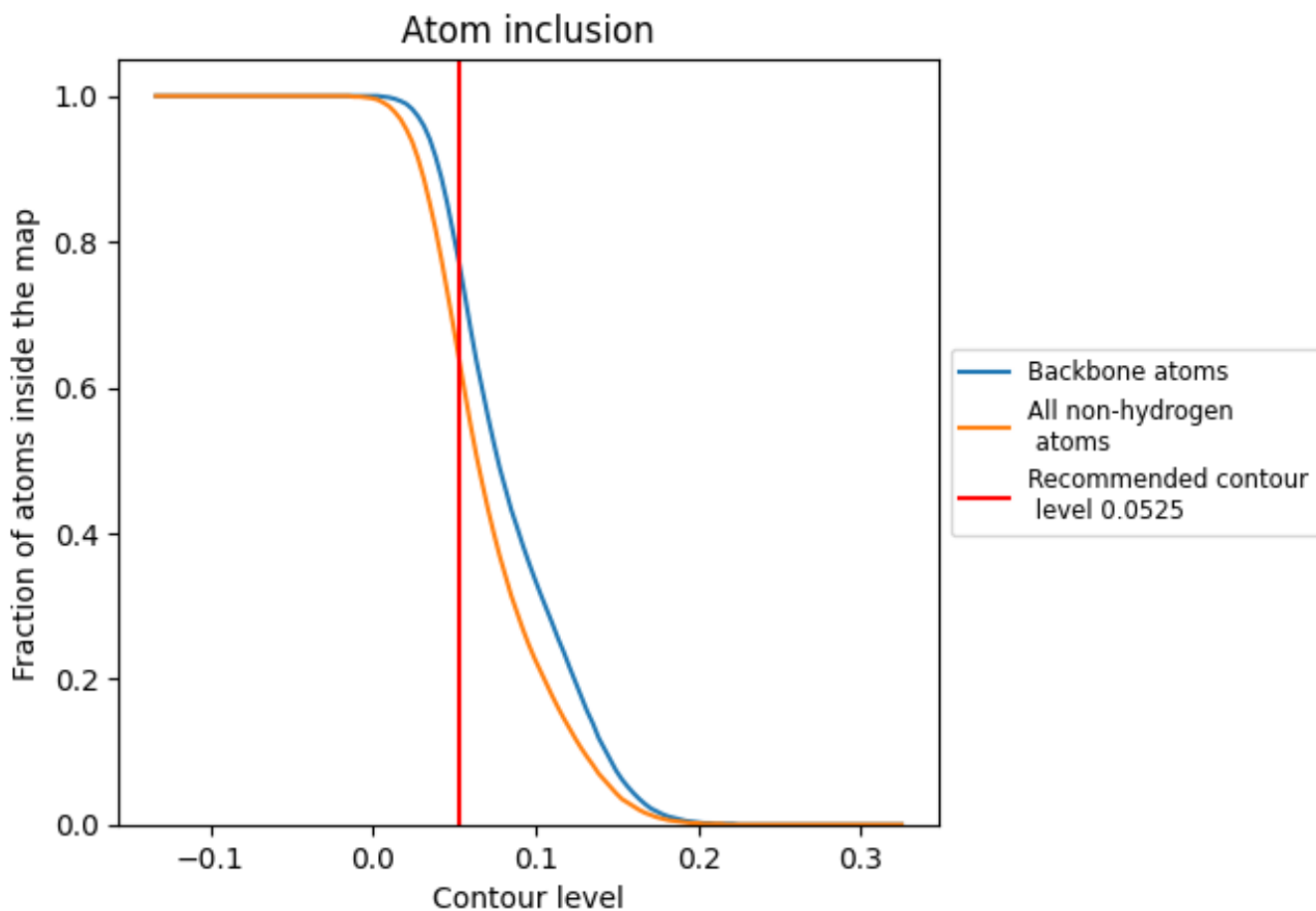
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0525).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0525) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.4010
A	 0.3440	 0.2340
B	 0.7530	 0.4320
C	 0.7910	 0.4590
E	 0.3910	 0.3140
F	 0.3690	 0.2200
G	 0.1290	 0.2310
H	 0.4360	 0.2870
I	 0.4070	 0.3250
J	 0.5260	 0.3290
K	 0.3020	 0.2340
L	 0.3510	 0.2970
M	 0.4030	 0.2840
N	 0.5340	 0.3760
O	 0.3390	 0.2460
P	 0.5330	 0.3350
Q	 0.6230	 0.3820
S	 0.8200	 0.4740
T	 0.4140	 0.3560
U	 0.7870	 0.4510
V	 0.6180	 0.4430
W	 0.8030	 0.4550
X	 0.7880	 0.4390
Y	 0.8360	 0.4350
Z	 0.7600	 0.4170
a	 0.8660	 0.5000
b	 0.7050	 0.3980
c	 0.8320	 0.4840
d	 0.8260	 0.4620
e	 0.7660	 0.4730
f	 0.6670	 0.3950
g	 0.7960	 0.4890
h	 0.8170	 0.4660
i	 0.7810	 0.5020
j	 0.6040	 0.4120



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Chain	Atom inclusion	Q-score
k	 0.7110	 0.4750
l	 0.7560	 0.4770
m	 0.7010	 0.4490
n	 0.7370	 0.4510
o	 0.7890	 0.4710
p	 0.8180	 0.4600
r	 0.8290	 0.5080
s	 0.7680	 0.4730
u	 0.8410	 0.4560
v	 0.7170	 0.3930
w	 0.6340	 0.3910