



## wwPDB EM Validation Summary Report ⓘ

Jul 6, 2024 – 04:01 PM EDT

PDB ID : 8UEZ  
EMDB ID : EMD-42176  
Title : In-situ complex I, Active-Q10 (State-delta)  
Authors : Zheng, W.; Zhu, J.; Zhang, K.  
Deposited on : 2023-10-02  
Resolution : 3.50 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:

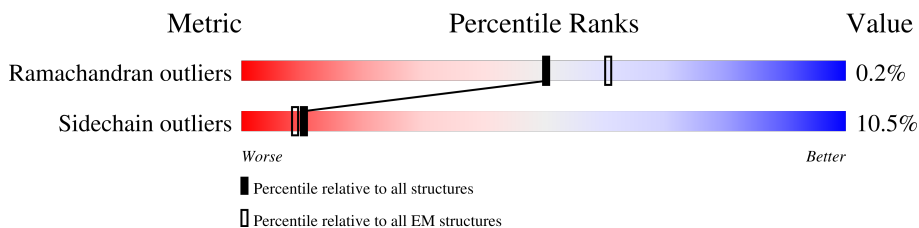
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 3.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1A	115	28% 90% 10%
2	1B	258	56% 40%
3	1C	264	74% 5% 21%
4	1D	476	10% 83% 7% 10%
5	1E	249	81% 5% 14%
6	1F	464	88% 5% 7%
7	1G	727	88% 8%
8	1H	318	9% 91% 9%
9	1I	239	68% 6% 26%

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Mol	Chain	Length	Quality of chain
10	1J	175	21% 83% 17%
11	1K	98	7% 87% 13%
12	1L	606	36% 87% 13%
13	1M	459	8% 91% 9%
14	1N	347	• 91% 9%
15	1O	357	32% 80% 10% 10%
16	1P	377	10% 84% 6% 9%
17	1Q	175	7% 66% 7% 26%
18	1R	123	9% 67% 11% 22%
19	1S	99	6% 78% 10% 12%
20	1T	156	26% 45% 10% 46%
20	1U	156	37% 51% • 45%
21	1V	116	9% 90% 9% •
22	1W	128	8% 80% 9% 10%
23	1X	172	6% 89% 10% •
24	1Y	141	11% 93% 6% •
25	1Z	144	5% 90% 8% •
26	1a	70	• 89% 11%
27	1b	84	12% 94% 5% •
28	1c	76	21% 57% 8% 36%
29	1d	123	6% 88% 11% •
30	1e	106	• 84% 9% 7%
31	1f	135	15% 37% • 58%
32	1g	154	18% 55% 10% 35%
33	1h	189	15% 66% 7% 27%

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Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

## 2 Entry composition i

There are 58 unique types of molecules in this entry. The entry contains 67334 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	115	916	616	134	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	155	1242	791	226	211	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1740	1125	297	316	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	429	3452	2207	593	628	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1E	214	1658	1058	278	312	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1F	432	3325	2100	592	613	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1G	699	5362	3360	933	1029	40	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1H	318	2504	1673	385	425	21	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	1I	176	1412	887	243	269	13	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	1J	175	1339	898	190	238	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1K	98	750	494	113	129	14	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1L	606	4818	3195	746	826	51	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1M	459	3632	2411	572	610	39	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	1N	347	2712	1783	420	463	46	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	1O	320	2590	1649	440	491	10	0	0

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	1P	342	2751	1783	481	478	9	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	1Q	129	1047	659	186	199	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1Y	139	1016	648	173	189	6	0	0

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1Z	141	1168	752	202	205	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1a	70	562	361	101	94	6	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	1b	83	643	417	110	115	1	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	1c	49	417	276	71	70	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	1d	121	996	648	172	170	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1d	-2	ACE	-	acetylation	UNP A0A480JRW3

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	1e	99	816	519	151	140	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	1f	57	487	316	89	80	2	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	1g	100	835	535	138	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	1h	138	1151	754	195	199	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	1i	127	1100	723	194	181	2	0	0

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	1j	71	601	394	99	107	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	1k	81	649	422	110	116	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	1l	156	1310	847	213	242	8	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		
38	1m	128	1062	691	182	189	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	1n	172	1495	956	273	258	8	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	1o	122	1045	650	198	187	10	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	1p	173	1449	908	263	270	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	1q	145	1212	775	219	213	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	1r	96	767	483	144	137	3	0	0

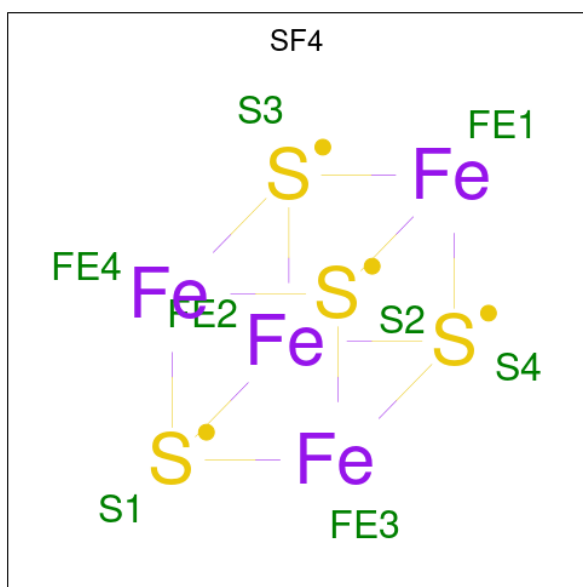
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1r	0	ACE	-	insertion	UNP A0A8W4F7N8

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1s	45	382	238	70	73	1	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1B	1	8	4	4	0
45	1F	1	8	4	4	0
45	1G	1	8	4	4	0
45	1G	1	8	4	4	0
45	1I	1	8	4	4	0
45	1I	1	8	4	4	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



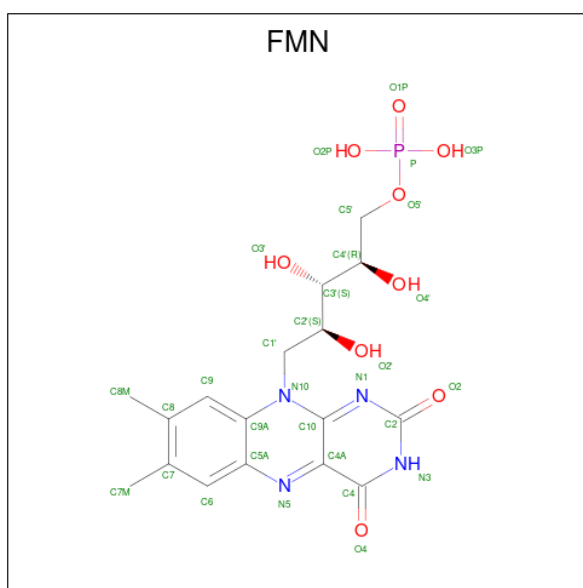
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	1B	1	34	24	1	8	1	0
46	1L	1	46	36	1	8	1	0
46	1M	1	35	25	1	8	1	0
46	1d	1	39	29	1	8	1	0
46	1f	1	25	15	1	8	1	0
46	1q	1	48	38	1	8	1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
47	1E	1	Total	Fe	S	0
			4	2	2	
47	1G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).

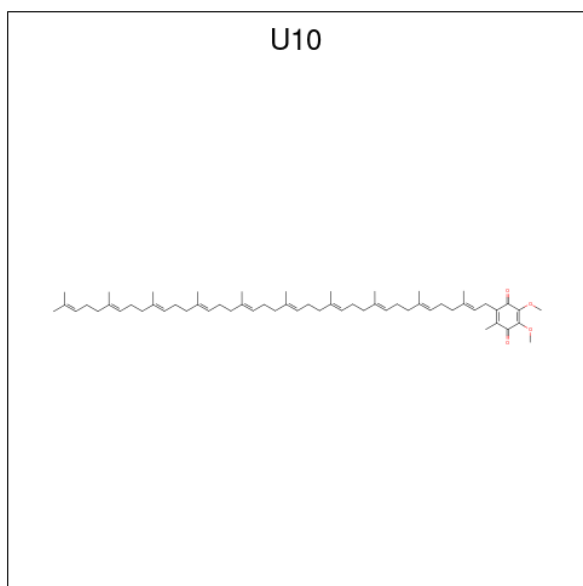


Mol	Chain	Residues	Atoms				AltConf	
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is POTASSIUM ION (three-letter code: K) (formula: K).

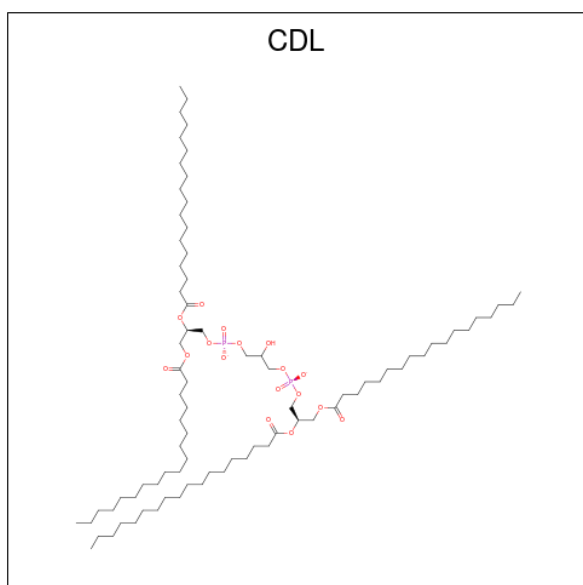
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

- Molecule 50 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

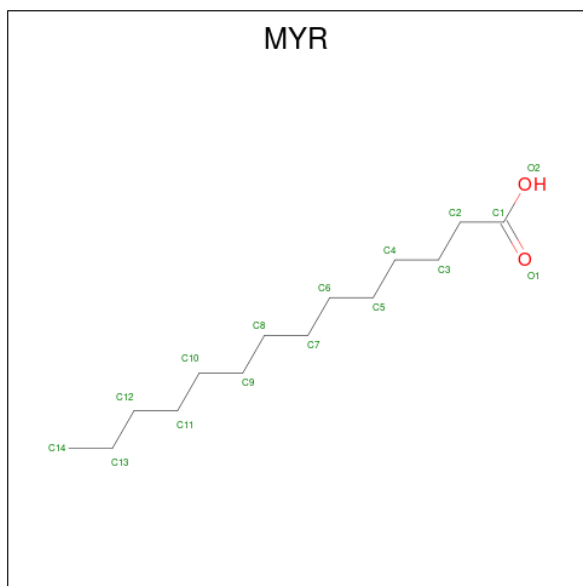
- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).





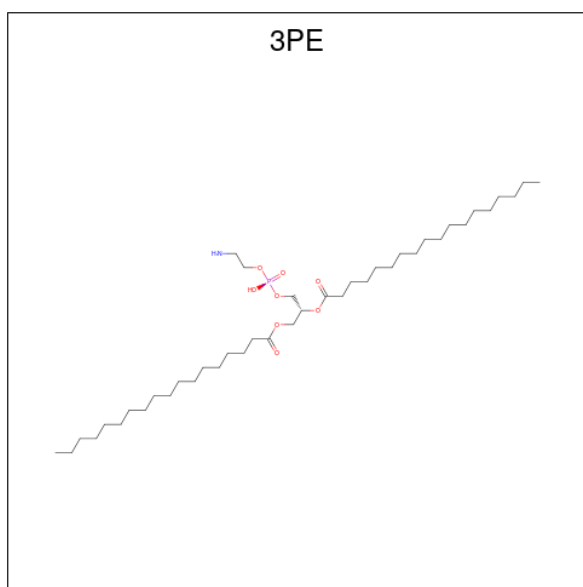
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1O	1	Total	C	O	P	0
			67	48	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



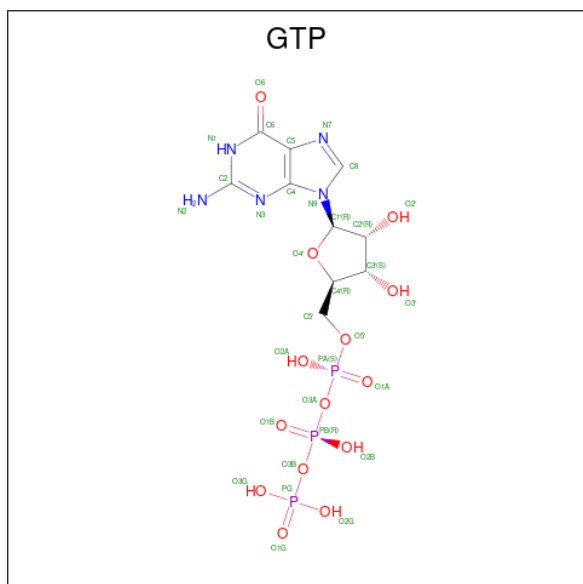
Mol	Chain	Residues	Atoms			AltConf
52	1L	1	Total	C	O	0
			15	14	1	

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	1M	1	38	28	1	8	1	0
53	1Y	1	35	25	1	8	1	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

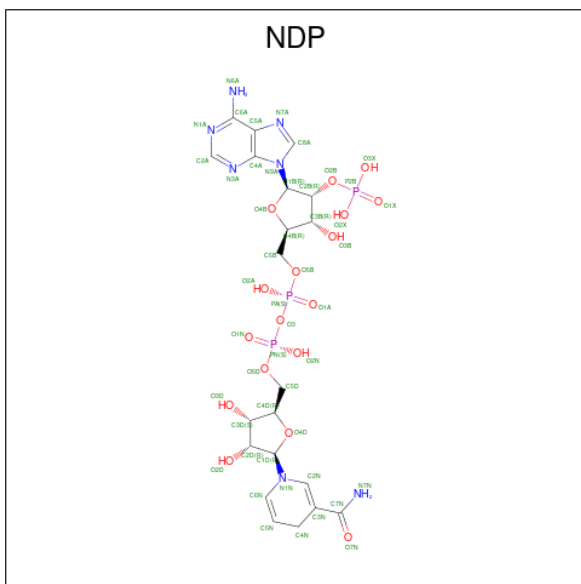


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	10	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	1O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

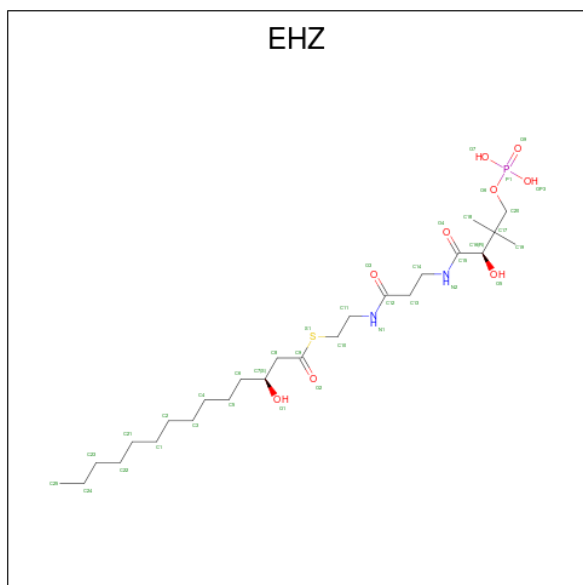


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	1R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

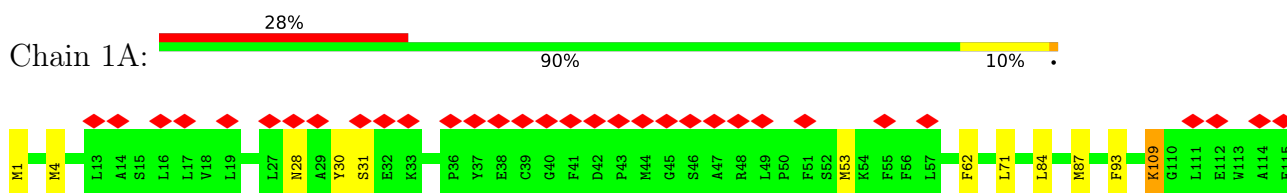


Mol	Chain	Residues	Atoms					AltConf		
			Total	C	N	O	P		S	
58	1W	1	Total	37	25	2	8	1	1	0
58	1n	1	Total	37	25	2	8	1	1	0

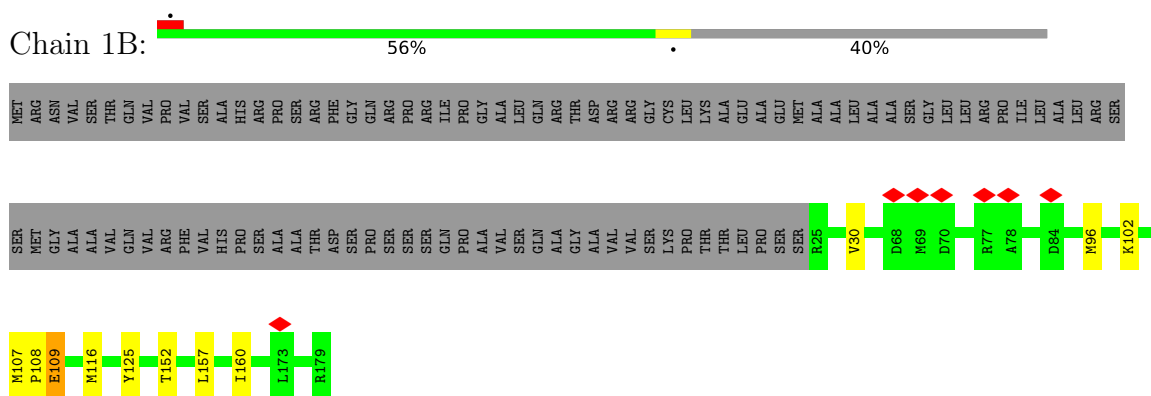
### 3 Residue-property plots

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.

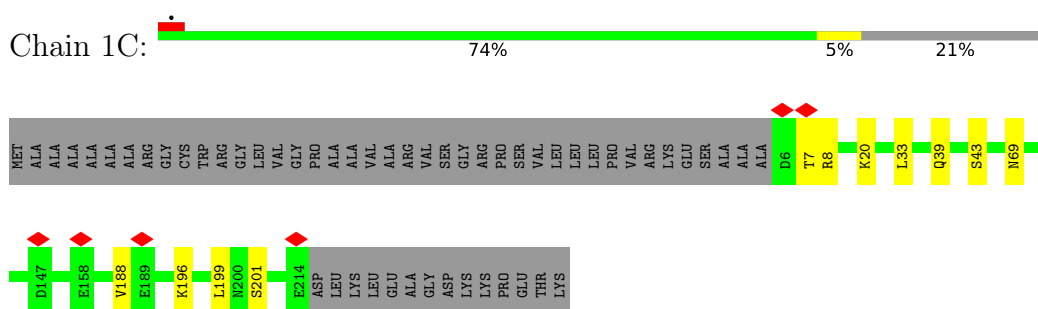
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



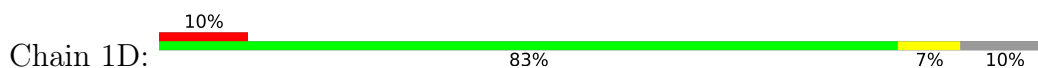
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

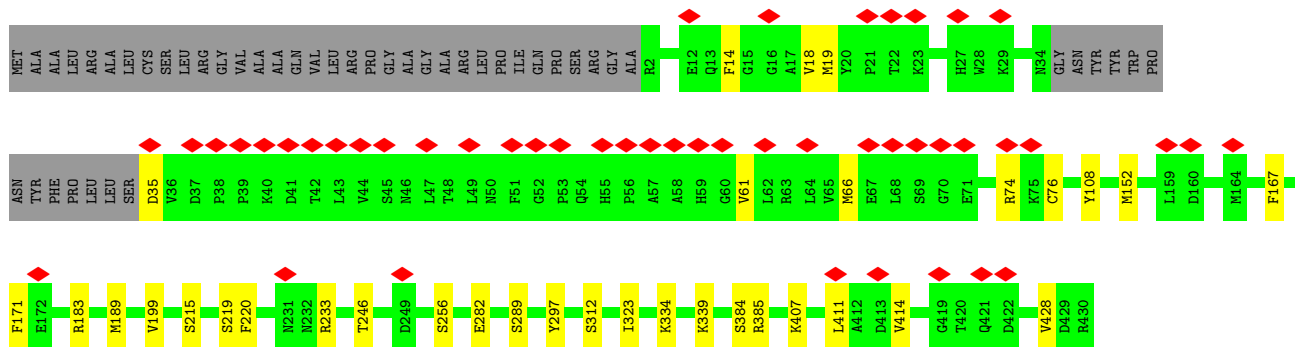


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

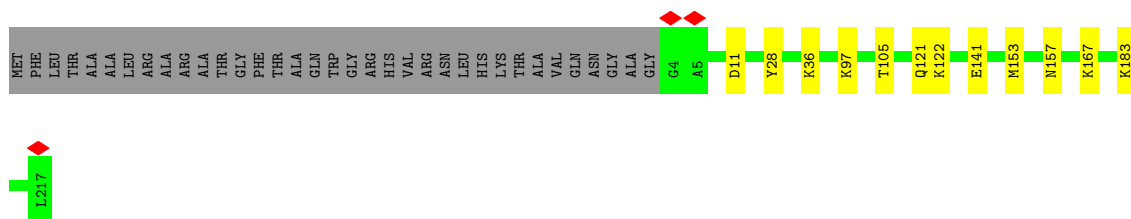
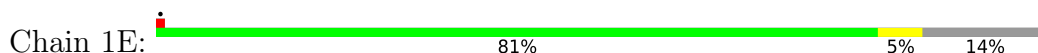


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

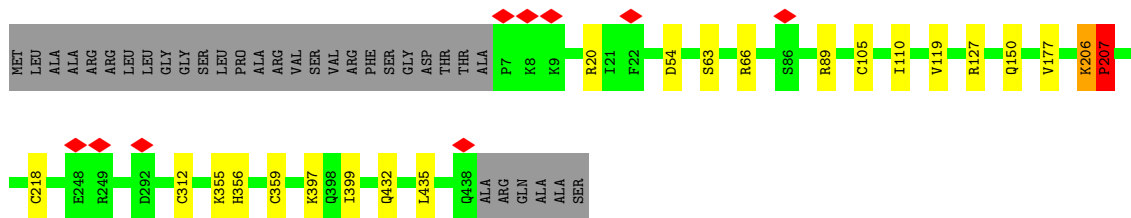
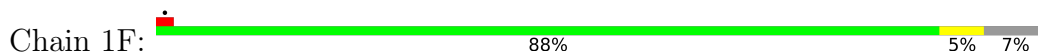




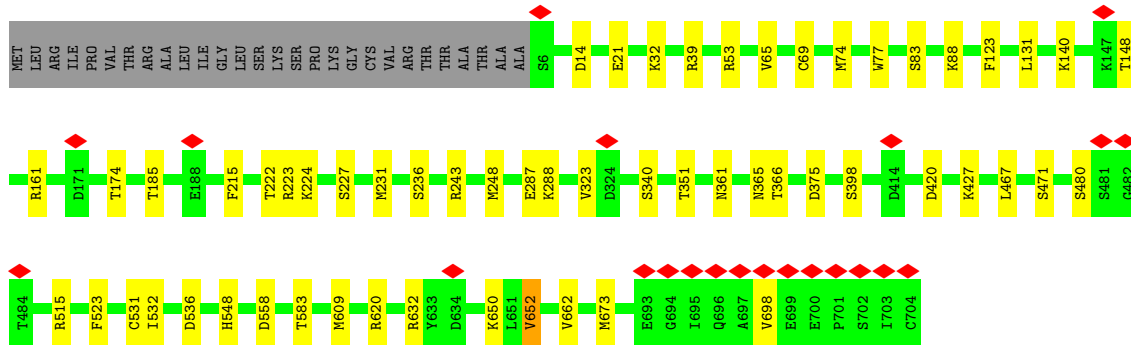
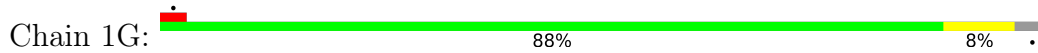
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



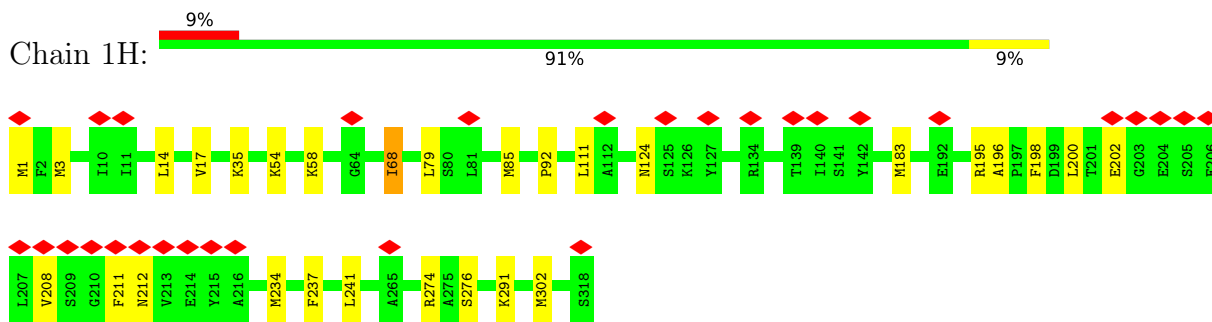
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



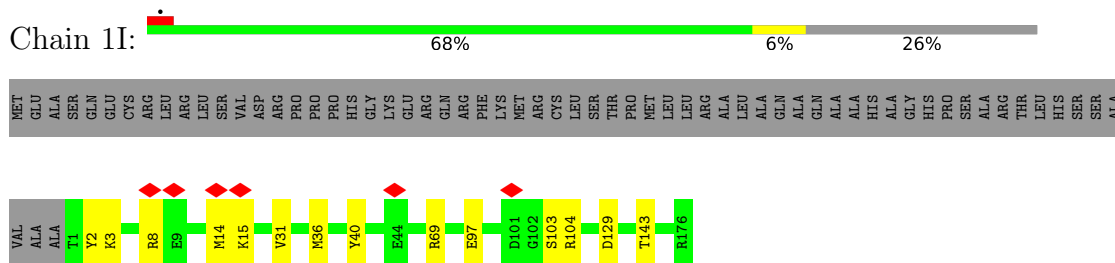
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



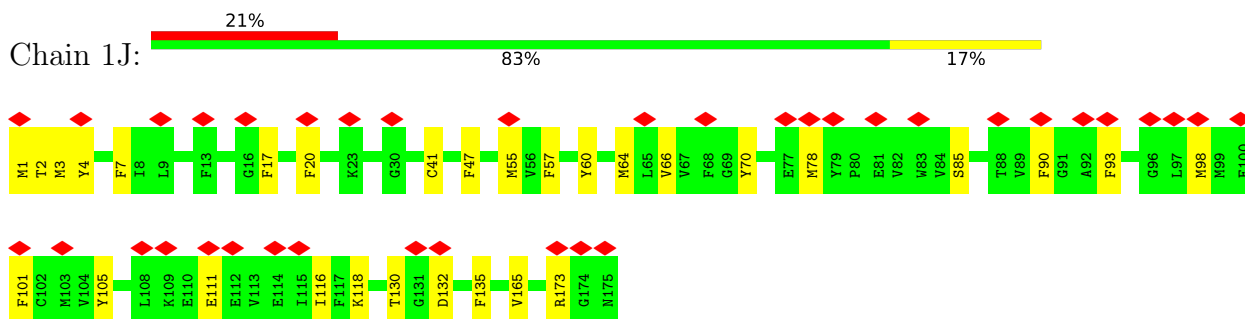
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



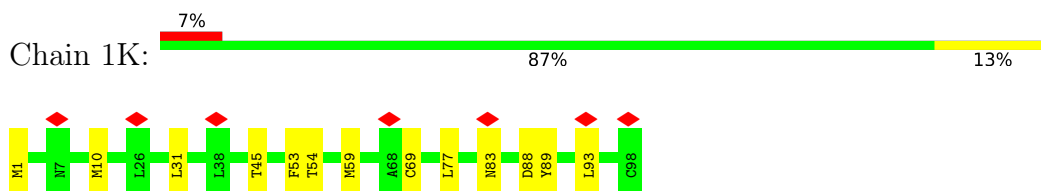
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



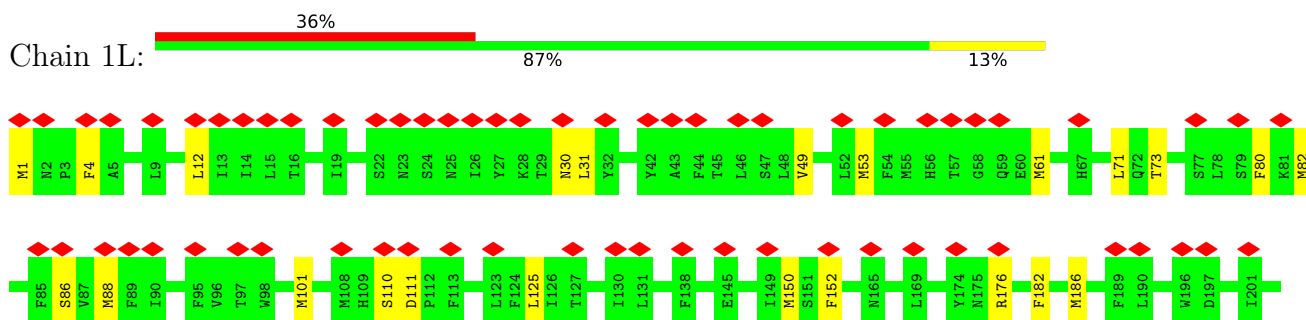
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

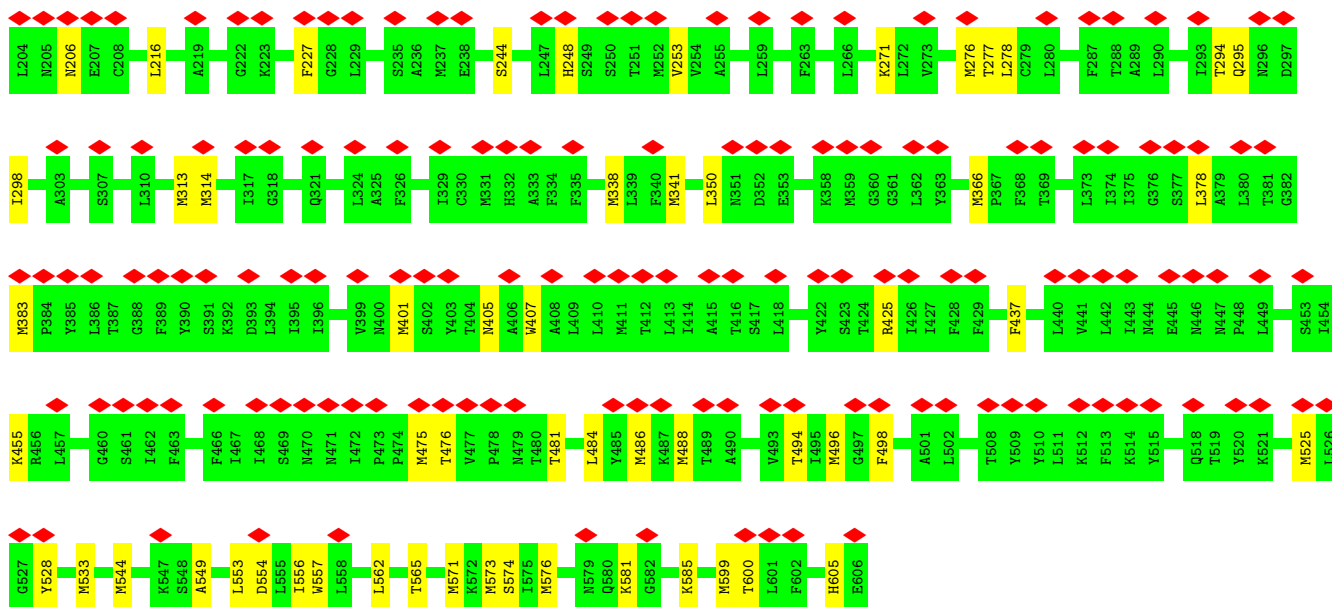


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

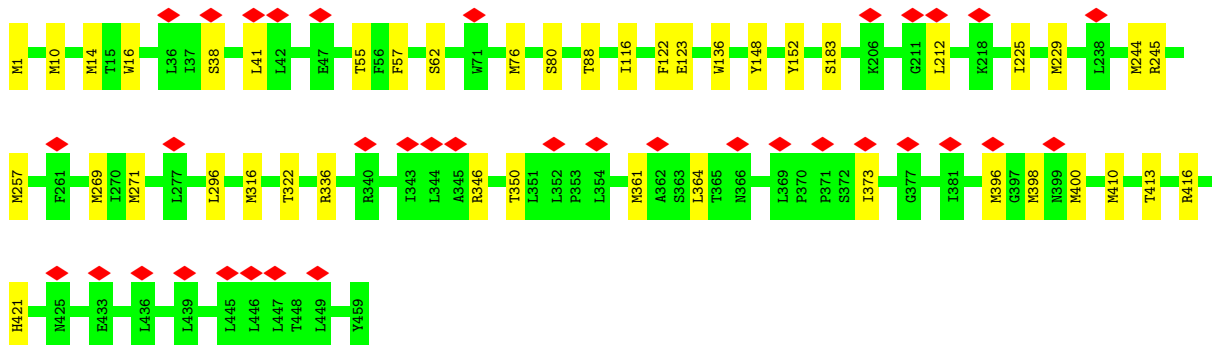
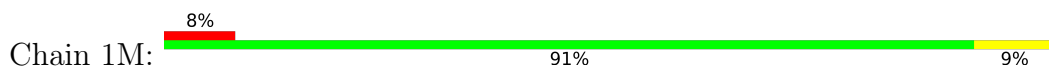


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

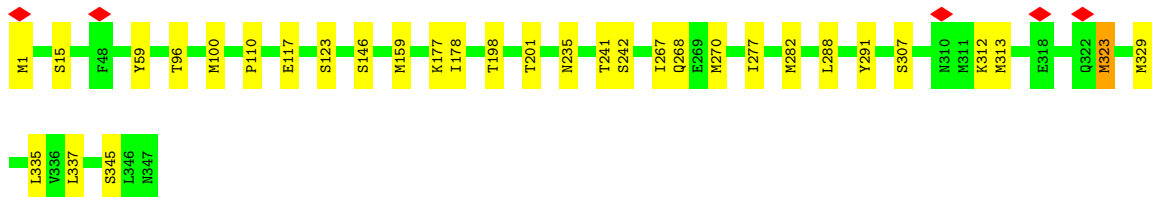




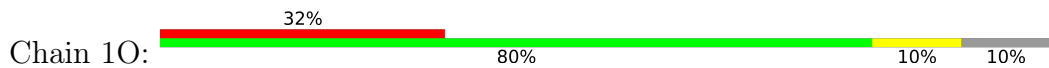
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



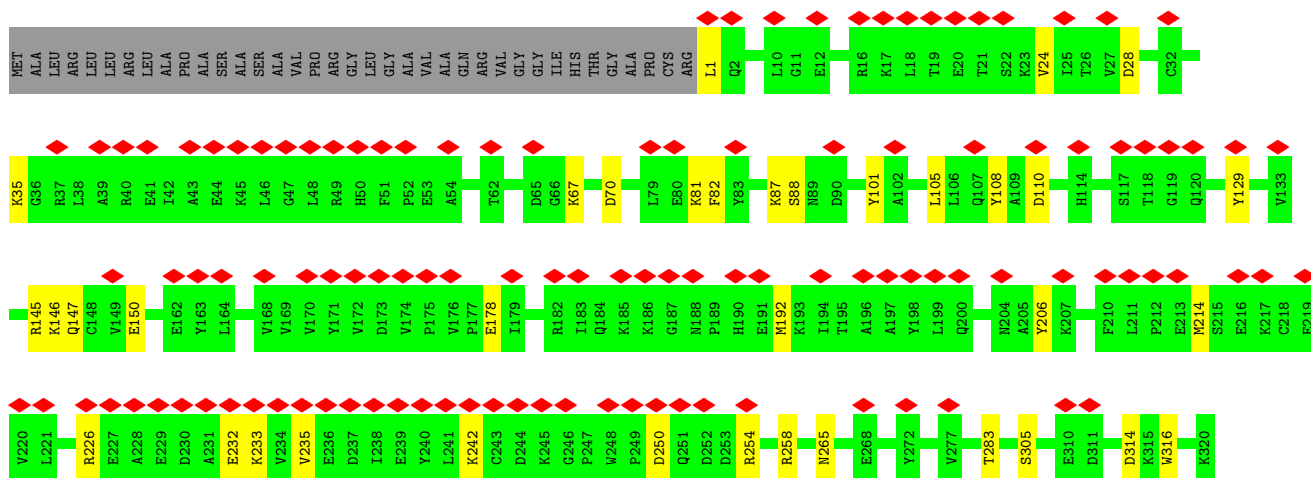
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



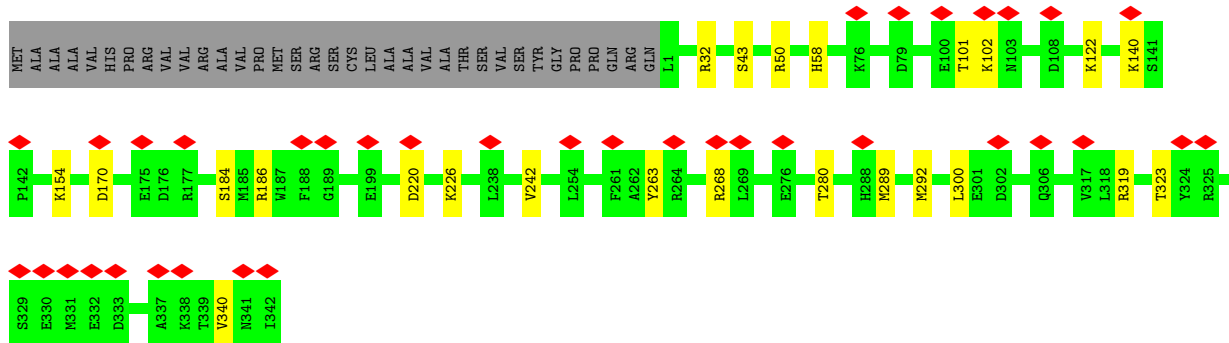
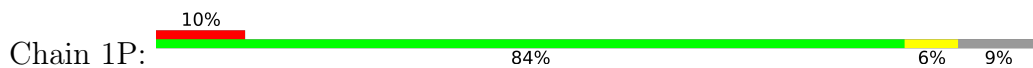
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



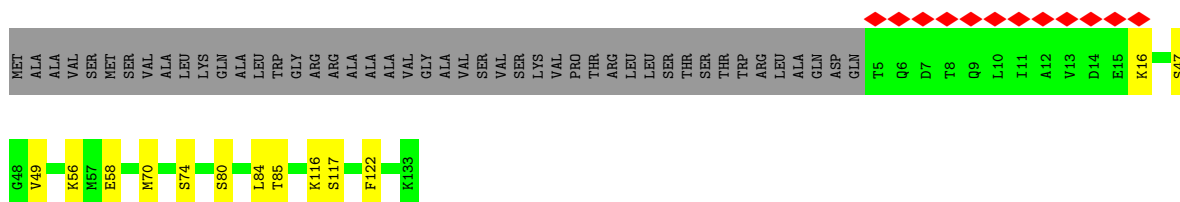




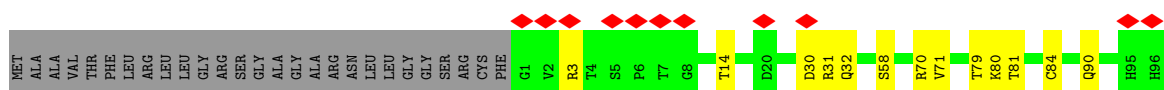
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



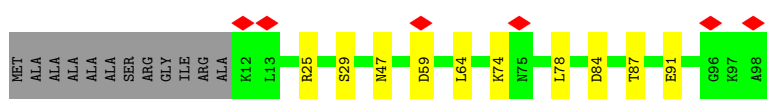
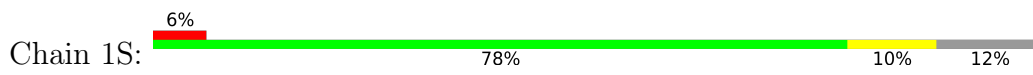
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



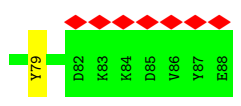
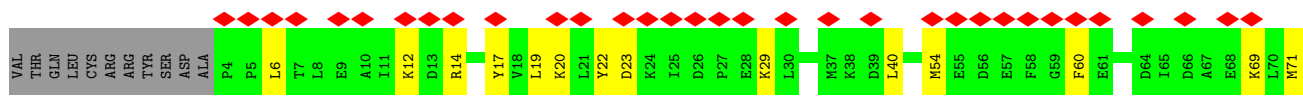
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



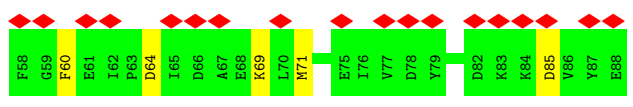
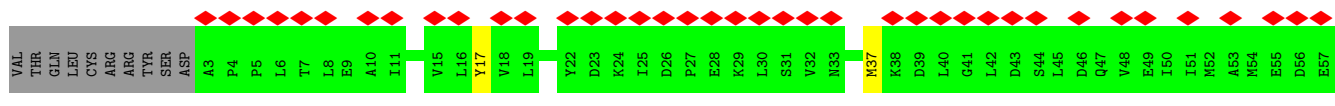
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



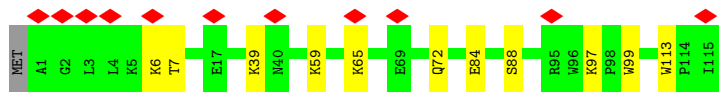
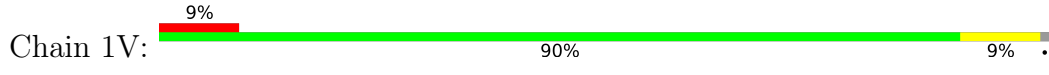
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



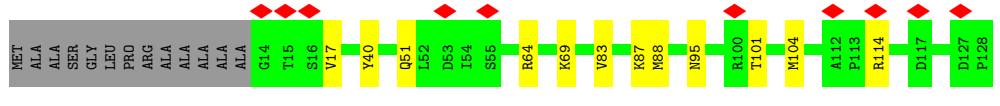
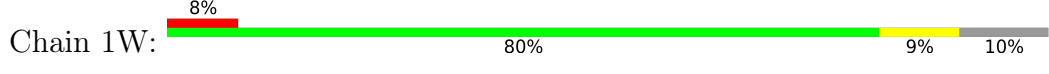
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



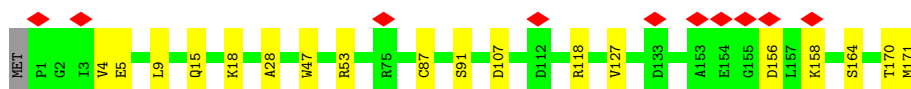
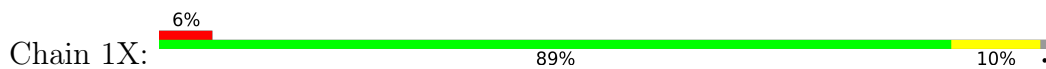
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



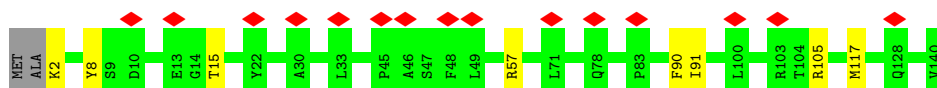
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



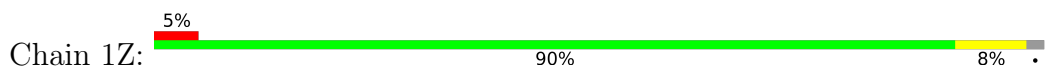
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



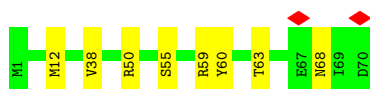
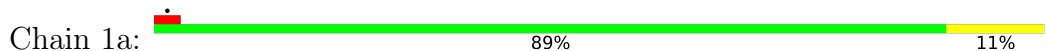
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



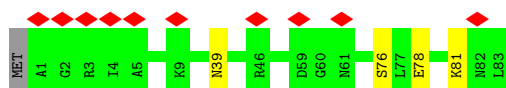
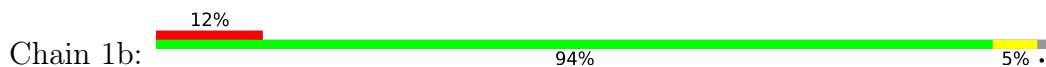
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



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



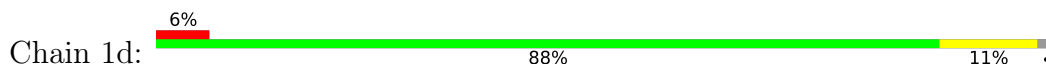
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

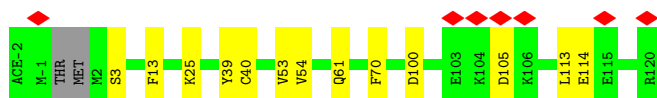


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

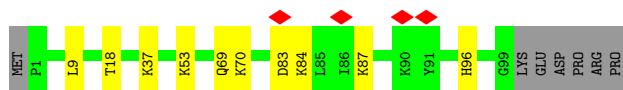
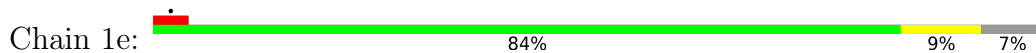


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

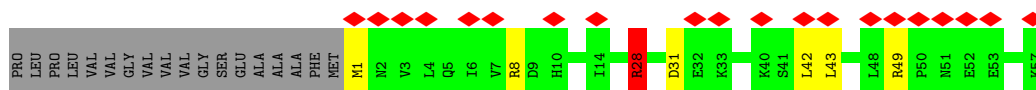




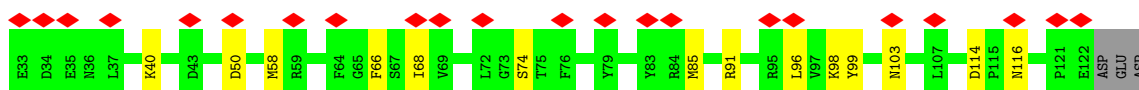
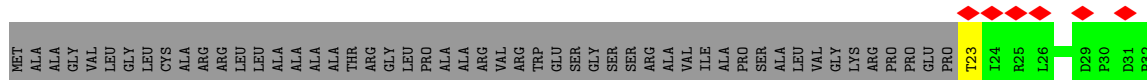
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



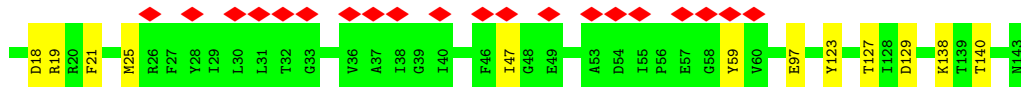
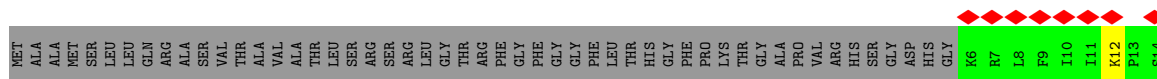
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



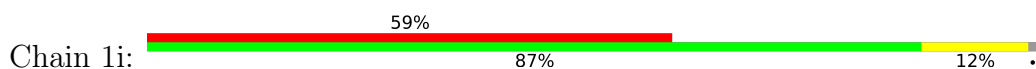
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

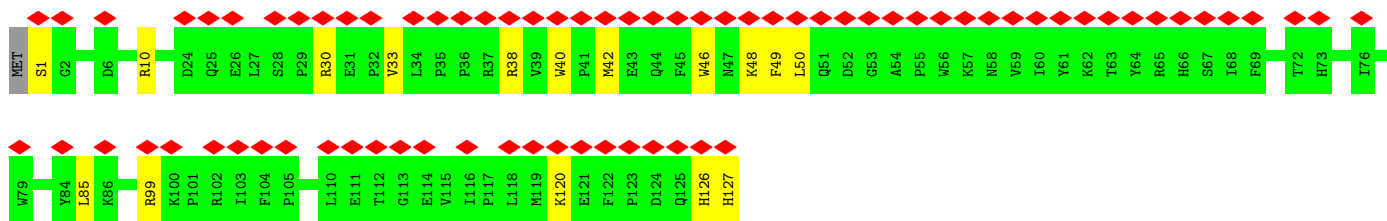


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

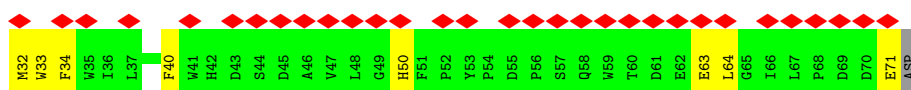
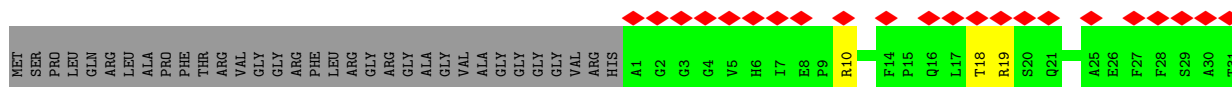


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

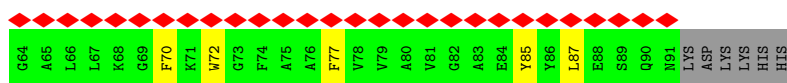
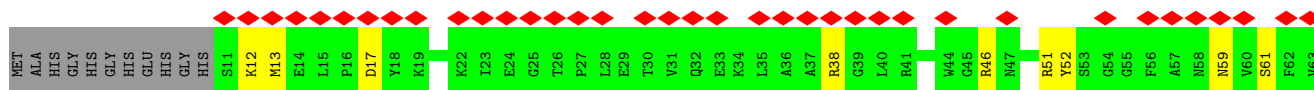




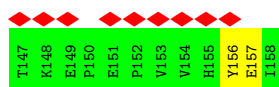
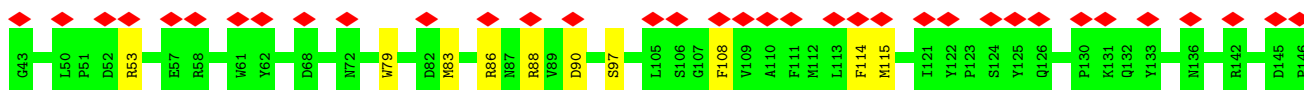
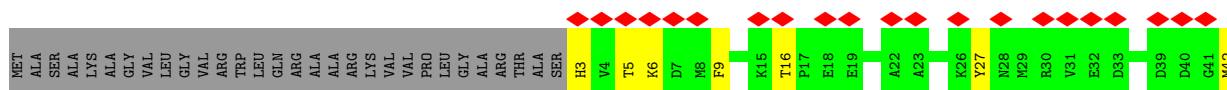
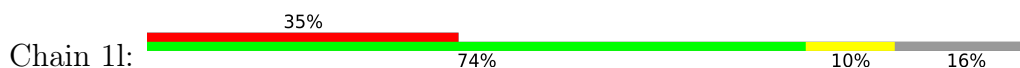
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

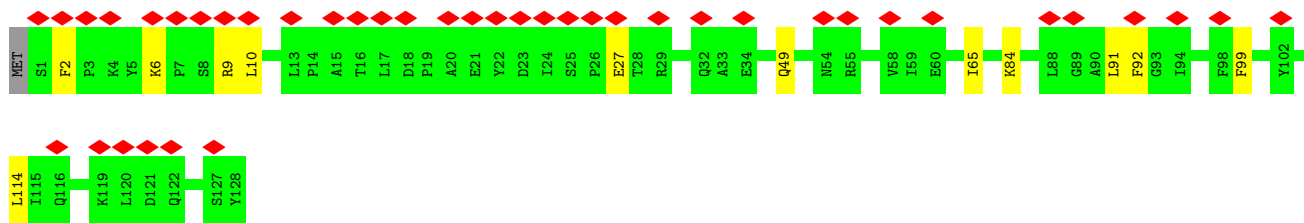


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

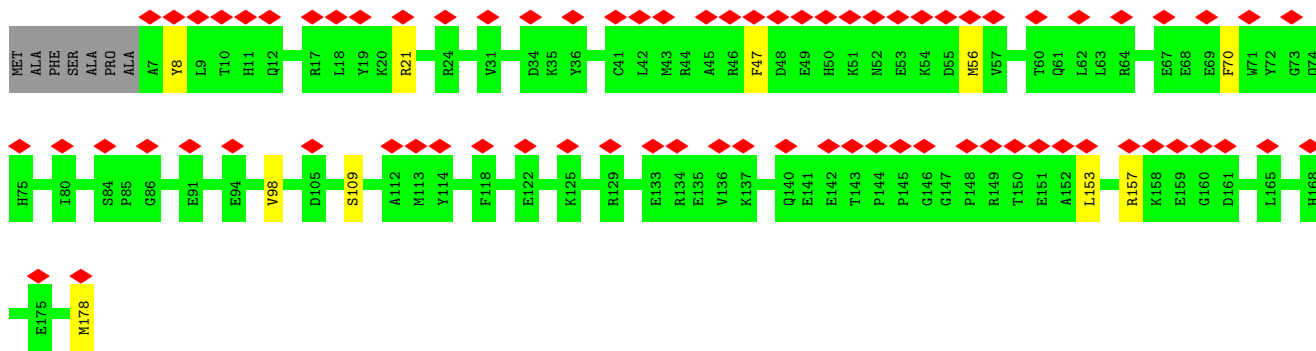
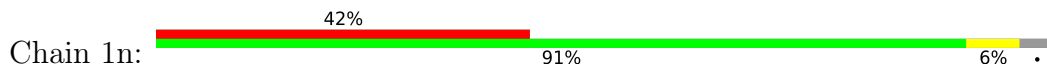


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

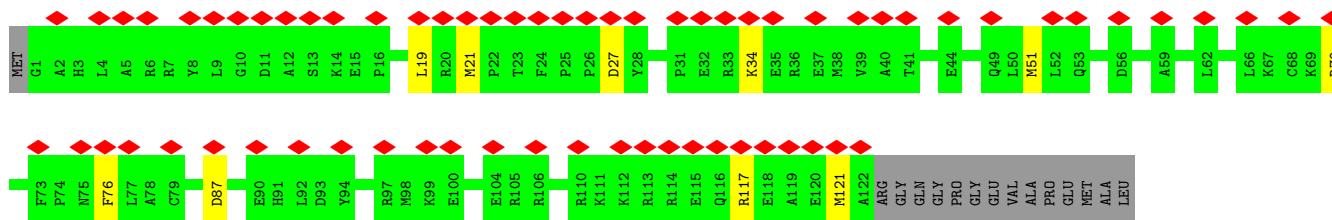
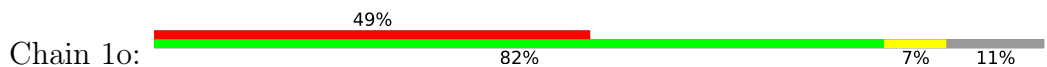




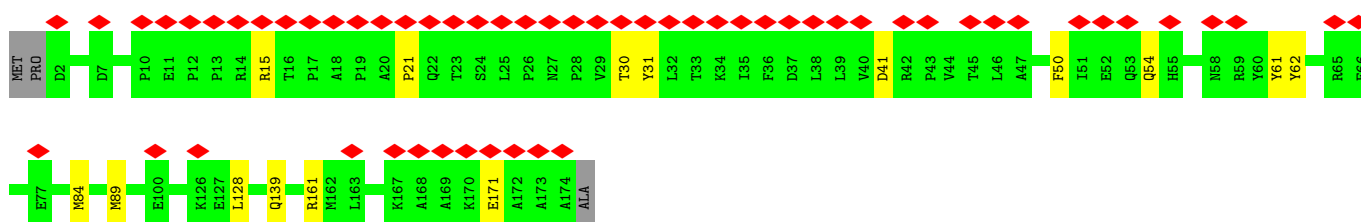
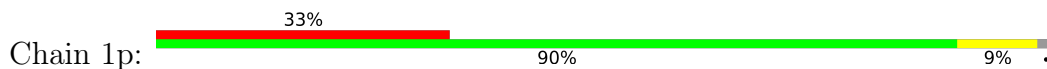
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



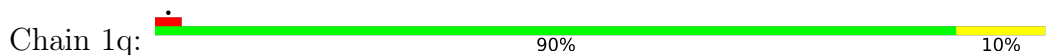
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

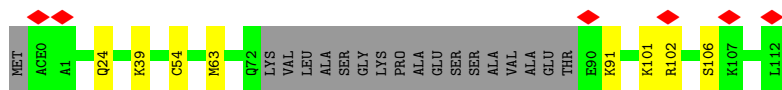
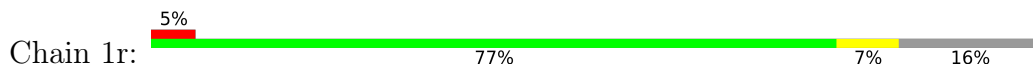


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

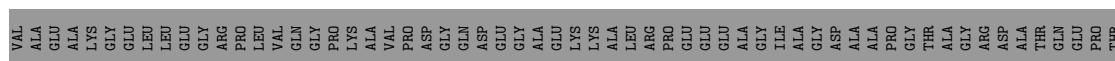
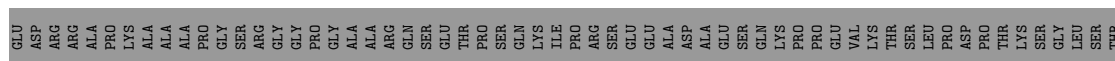
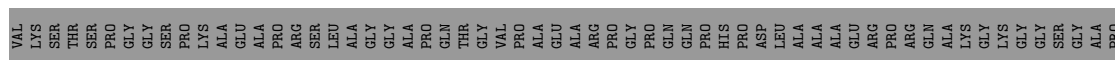
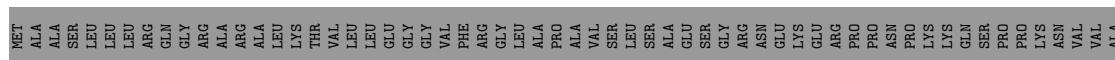




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	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)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.011	Depositor
Minimum map value	-0.198	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	556.0, 556.0, 556.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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: PC1, CDL, ZN, U10, FES, EHZ, FMN, K, MG, NDP, 3PE, GTP, SF4, SAC, MYR, FME, ACE

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	1A	0.35	0/930	0.57	0/1271
2	1B	0.32	0/1273	0.56	0/1722
3	1C	0.29	0/1791	0.50	0/2439
4	1D	0.31	0/3545	0.53	1/4806 (0.0%)
5	1E	0.28	0/1698	0.49	0/2311
6	1F	0.59	5/3401 (0.1%)	0.88	6/4595 (0.1%)
7	1G	0.31	1/5451 (0.0%)	0.50	0/7387
8	1H	0.35	0/2566	0.52	1/3509 (0.0%)
9	1I	0.34	0/1443	0.52	0/1952
10	1J	0.35	0/1364	0.57	0/1850
11	1K	0.35	0/751	0.58	0/1018
12	1L	0.28	0/4939	0.57	1/6718 (0.0%)
13	1M	0.29	0/3713	0.54	0/5063
14	1N	0.32	1/2765 (0.0%)	0.57	2/3758 (0.1%)
15	1O	0.29	0/2650	0.55	0/3588
16	1P	0.29	0/2828	0.51	0/3834
17	1Q	0.31	0/1070	0.55	0/1446
18	1R	0.29	0/755	0.54	0/1018
19	1S	0.25	0/711	0.52	0/956
20	1T	0.39	0/701	0.55	0/946
20	1U	0.29	0/706	0.51	0/954
21	1V	0.34	0/946	0.59	0/1281
22	1W	0.30	0/995	0.55	0/1340
23	1X	0.53	1/1436 (0.1%)	0.49	0/1938
24	1Y	0.35	0/1037	0.56	0/1404
25	1Z	0.30	0/1199	0.52	0/1617
26	1a	0.29	0/577	0.47	0/777
27	1b	0.36	1/664 (0.2%)	0.54	0/912
28	1c	0.33	0/430	0.67	0/581
29	1d	0.30	0/1024	0.60	1/1383 (0.1%)
30	1e	0.27	0/836	0.51	0/1118
31	1f	0.28	0/499	0.68	2/673 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	1g	0.27	0/858	0.57	0/1165
33	1h	0.27	0/1184	0.51	0/1603
34	1i	0.30	0/1131	0.57	0/1541
35	1j	0.64	2/627 (0.3%)	0.58	0/858
36	1k	0.33	0/668	0.58	0/903
37	1l	0.27	0/1365	0.52	0/1867
38	1m	0.31	0/1092	0.56	0/1481
39	1n	0.25	0/1549	0.52	0/2098
40	1o	0.26	0/1069	0.56	0/1430
41	1p	0.25	0/1481	0.50	0/1997
42	1q	0.34	0/1253	0.57	0/1704
43	1r	0.30	0/782	0.57	0/1057
44	1s	0.97	5/394 (1.3%)	1.35	5/533 (0.9%)
All	All	0.34	16/68147 (0.0%)	0.57	19/92402 (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
2	1B	0	2
6	1F	0	2
8	1H	0	1
21	1V	0	1
31	1f	0	1
All	All	0	7

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1F	207	PRO	CG-CD	-24.61	0.69	1.50
23	1X	87	CYS	CB-SG	-17.34	1.52	1.82
44	1s	32	PRO	CG-CD	-11.48	1.12	1.50
6	1F	207	PRO	CB-CG	10.31	2.01	1.50
35	1j	71	GLU	CD-OE1	-10.11	1.14	1.25

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1F	207	PRO	CA-N-CD	-28.82	71.15	111.50
6	1F	207	PRO	CB-CG-CD	-27.30	0.04	106.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1s	32	PRO	CA-N-CD	-19.47	84.24	111.50
6	1F	206	LYS	C-N-CD	16.44	162.92	128.40
6	1F	207	PRO	N-CA-CB	-14.12	86.35	103.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	108	PRO	Peptide
2	1B	109	GLU	Peptide
6	1F	206	LYS	Peptide
6	1F	207	PRO	Mainchain
8	1H	196	ALA	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	1A	113/115 (98%)	103 (91%)	9 (8%)	1 (1%)	17	56
2	1B	153/258 (59%)	138 (90%)	15 (10%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100
4	1D	427/476 (90%)	402 (94%)	25 (6%)	0	100	100
5	1E	212/249 (85%)	195 (92%)	16 (8%)	1 (0%)	29	68
6	1F	430/464 (93%)	414 (96%)	16 (4%)	0	100	100
7	1G	697/727 (96%)	655 (94%)	41 (6%)	1 (0%)	51	84
8	1H	316/318 (99%)	292 (92%)	21 (7%)	3 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
10	1J	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	9	42
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	552 (91%)	47 (8%)	5 (1%)	19	58
13	1M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	1N	345/347 (99%)	322 (93%)	22 (6%)	1 (0%)	41	75
15	1O	318/357 (89%)	298 (94%)	20 (6%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	64
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
29	1d	117/123 (95%)	104 (89%)	12 (10%)	1 (1%)	17	56
30	1e	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
31	1f	55/135 (41%)	49 (89%)	6 (11%)	0	100	100
32	1g	98/154 (64%)	83 (85%)	14 (14%)	1 (1%)	15	54
33	1h	136/189 (72%)	126 (93%)	10 (7%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
37	1l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	1m	126/129 (98%)	114 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	1o	120/137 (88%)	110 (92%)	10 (8%)	0	100	100
41	1p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
43	1r	90/114 (79%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	38 (88%)	4 (9%)	1 (2%)	6	36
All	All	8194/9744 (84%)	7656 (93%)	519 (6%)	19 (0%)	50	81

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
7	1G	652	VAL
8	1H	68	ILE
8	1H	92	PRO
10	1J	2	THR

### 5.3.2 Protein sidechains [i](#)

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	1A	99/99 (100%)	88 (89%)	11 (11%)	6	28
2	1B	131/212 (62%)	121 (92%)	10 (8%)	13	43
3	1C	190/227 (84%)	177 (93%)	13 (7%)	16	48
4	1D	371/405 (92%)	338 (91%)	33 (9%)	9	37
5	1E	183/207 (88%)	172 (94%)	11 (6%)	19	52
6	1F	346/368 (94%)	324 (94%)	22 (6%)	17	50
7	1G	588/610 (96%)	531 (90%)	57 (10%)	8	33
8	1H	274/274 (100%)	250 (91%)	24 (9%)	10	38
9	1I	151/201 (75%)	137 (91%)	14 (9%)	9	35
10	1J	140/140 (100%)	114 (81%)	26 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1K	84/84 (100%)	72 (86%)	12 (14%)	3	19
12	1L	539/539 (100%)	467 (87%)	72 (13%)	4	21
13	1M	408/408 (100%)	366 (90%)	42 (10%)	7	32
14	1N	310/310 (100%)	280 (90%)	30 (10%)	8	33
15	1O	283/307 (92%)	247 (87%)	36 (13%)	4	22
16	1P	296/323 (92%)	272 (92%)	24 (8%)	11	41
17	1Q	117/152 (77%)	104 (89%)	13 (11%)	6	28
18	1R	79/97 (81%)	66 (84%)	13 (16%)	2	13
19	1S	77/82 (94%)	67 (87%)	10 (13%)	4	21
20	1T	79/133 (59%)	64 (81%)	15 (19%)	1	8
20	1U	79/133 (59%)	72 (91%)	7 (9%)	9	37
21	1V	100/101 (99%)	90 (90%)	10 (10%)	7	32
22	1W	107/112 (96%)	95 (89%)	12 (11%)	6	27
23	1X	153/154 (99%)	137 (90%)	16 (10%)	7	31
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	12	41
25	1Z	123/124 (99%)	111 (90%)	12 (10%)	8	33
26	1a	58/58 (100%)	50 (86%)	8 (14%)	3	20
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	62
28	1c	45/66 (68%)	39 (87%)	6 (13%)	4	21
29	1d	107/109 (98%)	96 (90%)	11 (10%)	7	32
30	1e	87/94 (93%)	77 (88%)	10 (12%)	5	26
31	1f	54/113 (48%)	48 (89%)	6 (11%)	6	28
32	1g	92/129 (71%)	78 (85%)	14 (15%)	3	17
33	1h	121/158 (77%)	108 (89%)	13 (11%)	6	30
34	1i	119/120 (99%)	104 (87%)	15 (13%)	4	22
35	1j	62/84 (74%)	52 (84%)	10 (16%)	2	14
36	1k	63/76 (83%)	49 (78%)	14 (22%)	1	5
37	1l	141/161 (88%)	122 (86%)	19 (14%)	4	21
38	1m	113/114 (99%)	101 (89%)	12 (11%)	6	30
39	1n	156/160 (98%)	146 (94%)	10 (6%)	17	50
40	1o	110/120 (92%)	100 (91%)	10 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1p	154/156 (99%)	139 (90%)	15 (10%)	8	33
42	1q	131/131 (100%)	116 (88%)	15 (12%)	5	26
43	1r	85/98 (87%)	77 (91%)	8 (9%)	8	35
44	1s	44/351 (12%)	37 (84%)	7 (16%)	2	14
All	All	7219/8272 (87%)	6460 (90%)	759 (10%)	10	31

5 of 759 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	1S	25	ARG
29	1d	39	TYR
20	1T	17	TYR
18	1R	90	GLN
23	1X	15	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
37	1l	78	HIS
43	1r	46	HIS
38	1m	78	ASN
40	1o	75	ASN
15	1O	72	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	FME	1A	1	1	8,9,10	0.49	0	7,9,11	1.07	1 (14%)
12	FME	1L	1	12	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
34	SAC	1i	1	-	7,8,9	0.51	0	8,9,11	1.93	2 (25%)
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.02	1 (14%)
8	FME	1H	1	8	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
10	FME	1J	1	10	8,9,10	0.51	0	7,9,11	1.18	1 (14%)
11	FME	1K	1	11	8,9,10	0.52	0	7,9,11	1.02	1 (14%)
14	FME	1N	1	14	8,9,10	0.50	0	7,9,11	0.99	1 (14%)

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
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
34	SAC	1i	1	-	-	6/7/8/10	-
13	FME	1M	1	13	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
10	FME	1J	1	10	-	1/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	CA-N-C1A	3.70	129.98	123.15
34	1i	1	SAC	O-C-CA	-2.91	117.14	124.78
1	1A	1	FME	O-C-CA	-2.57	118.05	124.78
11	1K	1	FME	O-C-CA	-2.50	118.21	124.78
12	1L	1	FME	O-C-CA	-2.49	118.25	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
34	1i	1	SAC	C-CA-CB-OG
34	1i	1	SAC	C2A-C1A-N-CA
34	1i	1	SAC	OAC-C1A-N-CA
34	1i	1	SAC	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
53	3PE	1M	502	-	37,37,50	0.30	0	40,42,55	0.41	0
51	CDL	1O	403	-	66,66,99	0.98	3 (4%)	72,78,111	1.38	5 (6%)
45	SF4	1F	502	6	0,12,12	-	-	-	-	-
56	NDP	1P	501	-	45,52,52	0.63	0	53,80,80	0.75	2 (3%)
46	PC1	1L	702	-	45,45,53	0.29	0	51,53,61	0.33	0
58	EHZ	1n	201	-	29,36,37	0.21	0	35,44,47	0.94	1 (2%)
45	SF4	1B	201	2	0,12,12	-	-	-	-	-
51	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.43	0
47	FES	1E	301	5	0,4,4	-	-	-	-	-
46	PC1	1q	201	-	47,47,53	0.29	0	53,55,61	0.31	0
46	PC1	1f	101	-	24,24,53	0.36	0	30,32,61	0.65	0
53	3PE	1Y	201	-	34,34,50	0.46	0	37,39,55	0.88	2 (5%)
45	SF4	1G	801	7	0,12,12	-	-	-	-	-
45	SF4	1G	802	7	0,12,12	-	-	-	-	-
46	PC1	1M	501	-	34,34,53	0.32	0	40,42,61	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1I	202	9	0,12,12	-	-	-		
51	CDL	1H	702	-	50,50,99	0.36	0	56,62,111	0.59	1 (1%)
52	MYR	1L	701	-	14,14,15	0.32	0	13,13,15	0.40	0
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.90	1 (3%)
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.34	0
58	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.02	1 (2%)
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
47	FES	1G	804	7	0,4,4	-	-	-		
46	PC1	1d	201	-	38,38,53	0.32	0	44,46,61	0.48	0
50	U10	1H	701	-	63,63,63	0.59	1 (1%)	76,79,79	0.74	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
53	3PE	1M	502	-	-	5/41/41/54	-
51	CDL	1O	403	-	-	15/76/76/110	-
56	NDP	1P	501	-	-	5/30/77/77	0/5/5/5
45	SF4	1F	502	6	-	-	0/6/5/5
46	PC1	1L	702	-	-	9/49/49/57	-
58	EHZ	1n	201	-	-	10/42/44/45	-
45	SF4	1B	201	2	-	-	0/6/5/5
51	CDL	1a	101	-	-	6/71/71/110	-
47	FES	1E	301	5	-	-	0/1/1/1
46	PC1	1q	201	-	-	11/51/51/57	-
46	PC1	1f	101	-	-	5/27/27/57	-
53	3PE	1Y	201	-	-	12/38/38/54	-
45	SF4	1G	801	7	-	-	0/6/5/5
45	SF4	1G	802	7	-	-	0/6/5/5
46	PC1	1M	501	-	-	4/38/38/57	-
52	MYR	1L	701	-	-	2/11/12/13	-
45	SF4	1I	201	9	-	-	0/6/5/5
51	CDL	1H	702	-	-	10/61/61/110	-
54	GTP	1O	401	55	-	0/18/38/38	0/3/3/3
45	SF4	1I	202	9	-	-	0/6/5/5
46	PC1	1B	202	-	-	14/37/37/57	-

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	1W	201	-	-	5/42/44/45	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
47	FES	1G	804	7	-	-	0/1/1/1
46	PC1	1d	201	-	-	13/42/42/57	-
50	U10	1H	701	-	-	22/63/87/87	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	1O	403	CDL	C71-CB7	5.23	1.66	1.50
51	1O	403	CDL	OB9-CB7	4.75	1.36	1.22
54	1O	401	GTP	C5-C6	-2.60	1.42	1.47
50	1H	701	U10	C4-C5	-2.60	1.41	1.48
51	1O	403	CDL	OB8-CB7	2.06	1.39	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1O	403	CDL	OB8-CB7-C71	-7.06	89.76	111.91
58	1W	201	EHZ	C10-S1-C9	5.55	119.14	101.87
51	1O	403	CDL	OB8-CB7-OB9	5.54	137.58	123.59
51	1O	403	CDL	OB8-CB6-CB4	5.11	123.31	108.43
58	1n	201	EHZ	C10-S1-C9	5.09	117.73	101.87

There are no chirality outliers.

5 of 149 torsion outliers are listed below:

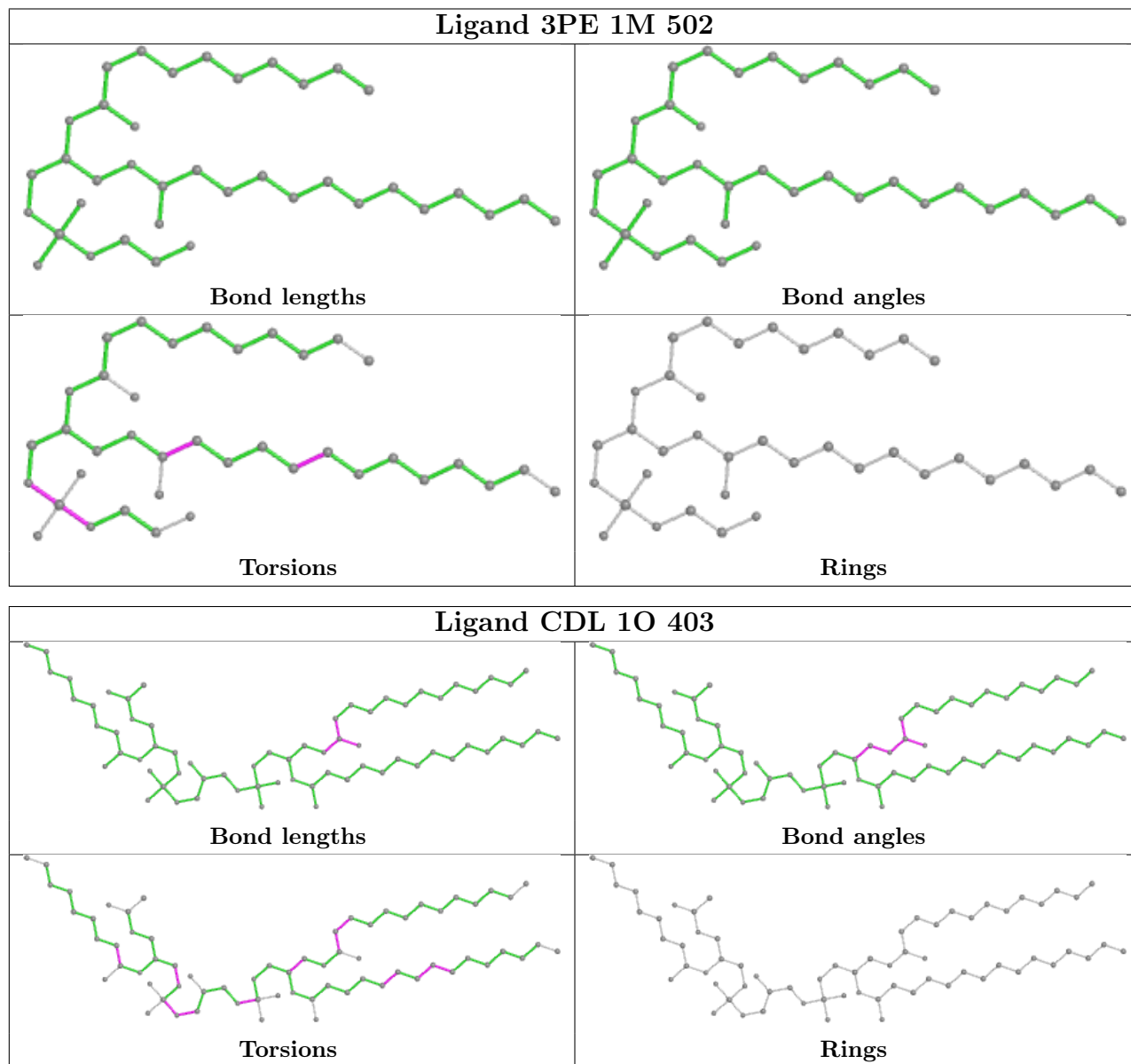
Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C11-O13-P-O14
46	1B	202	PC1	C2-C1-O11-P
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3
46	1L	702	PC1	C11-O13-P-O14

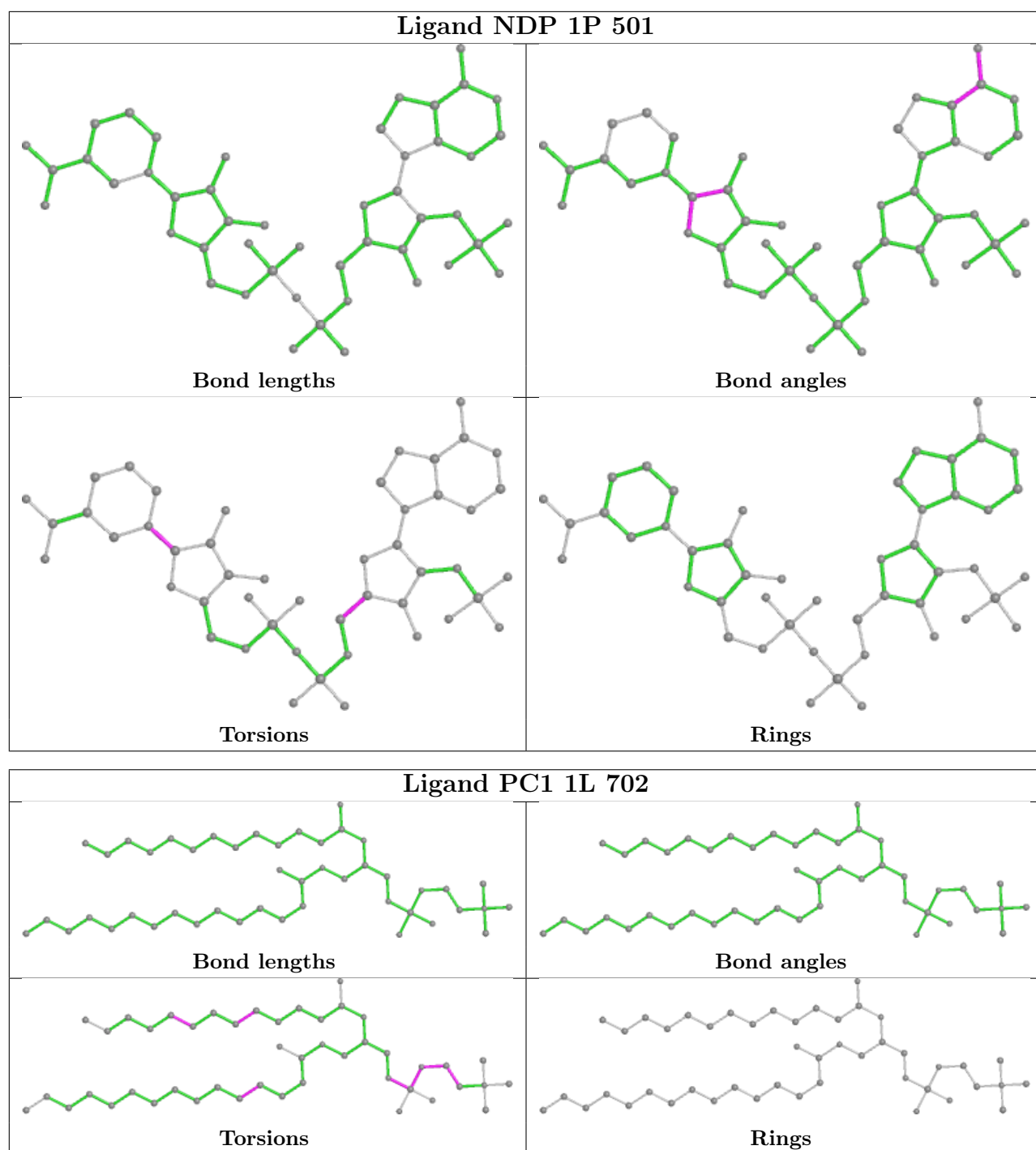
There are no ring outliers.

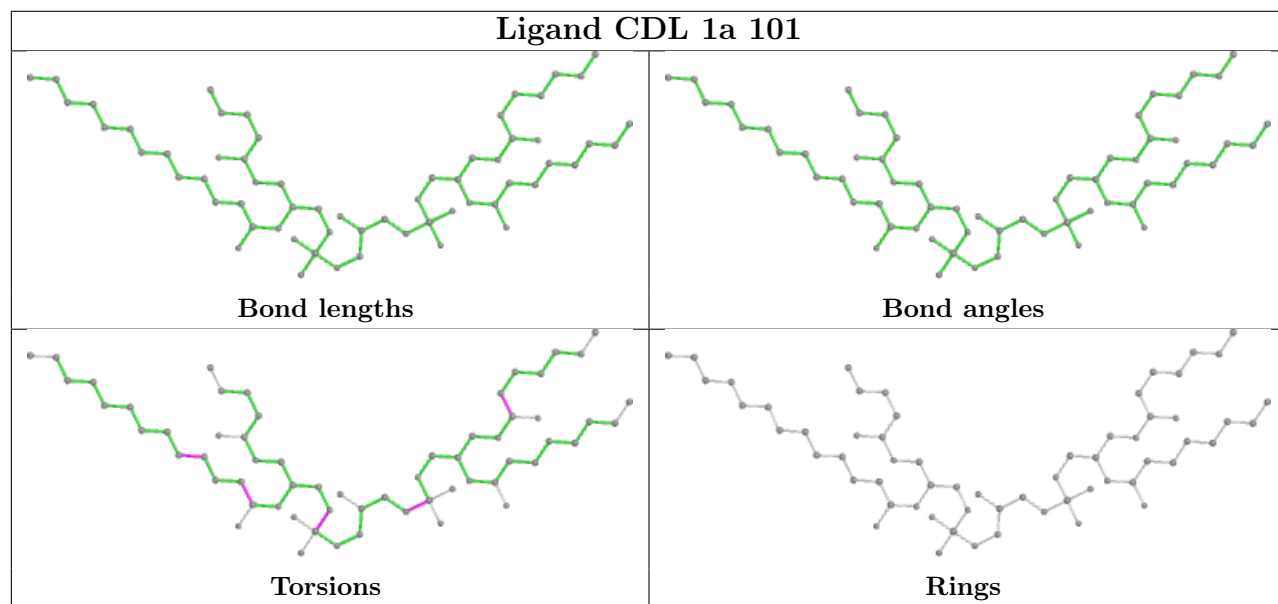
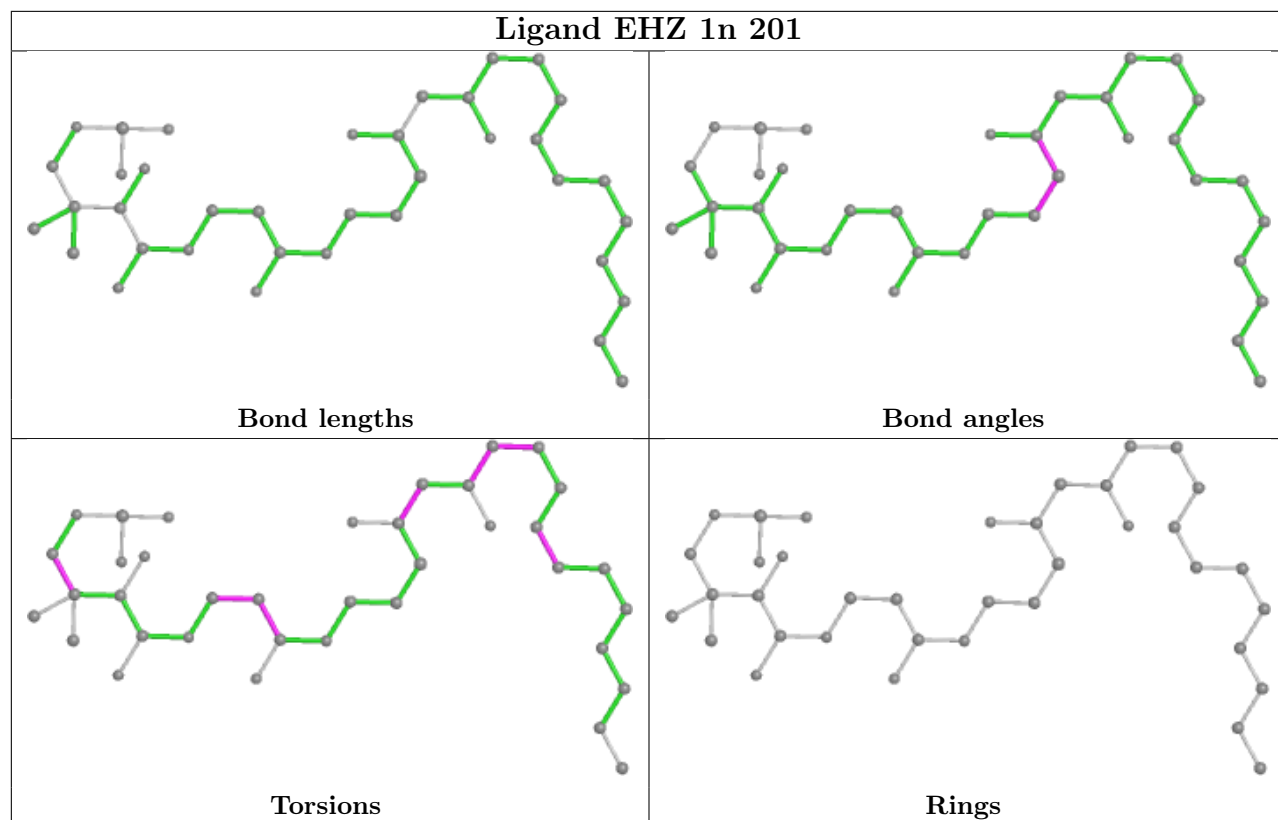
No monomer is involved in short contacts.

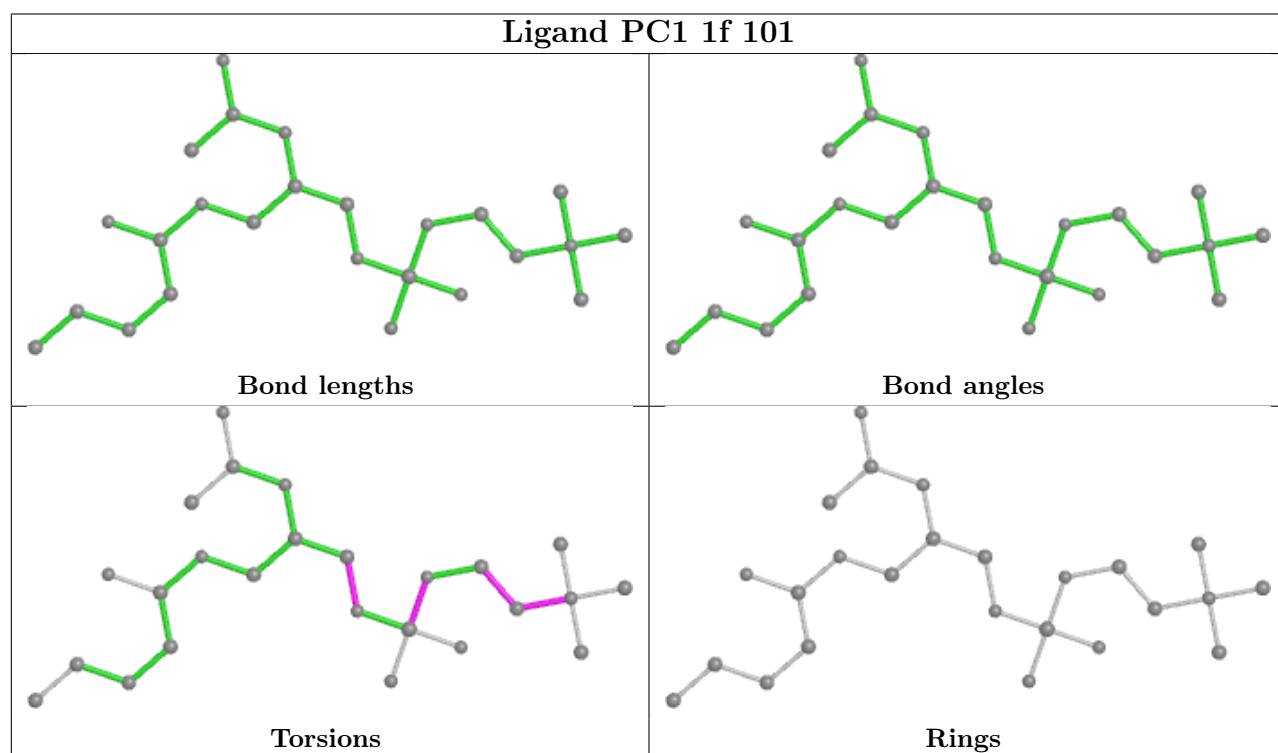
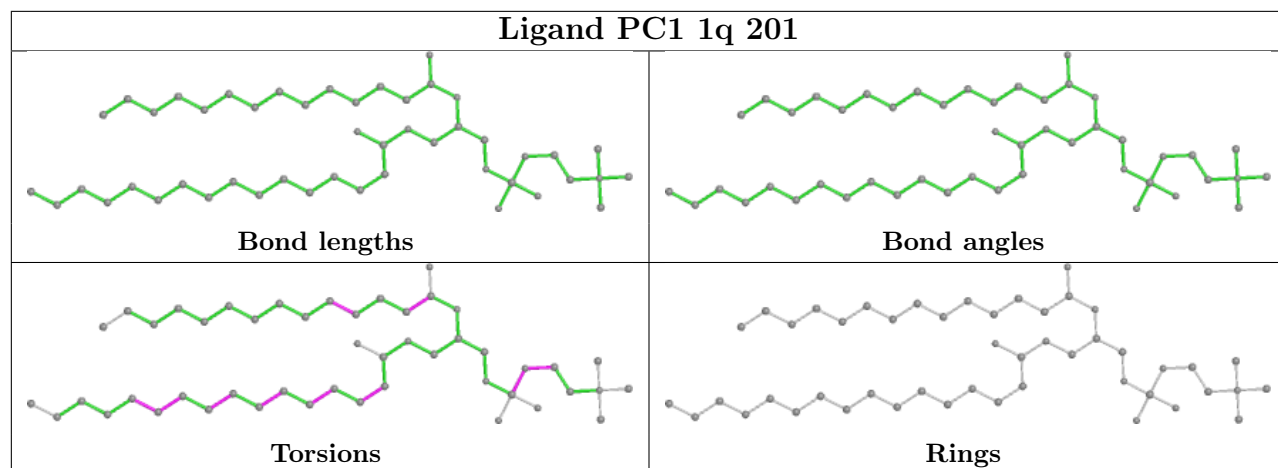
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

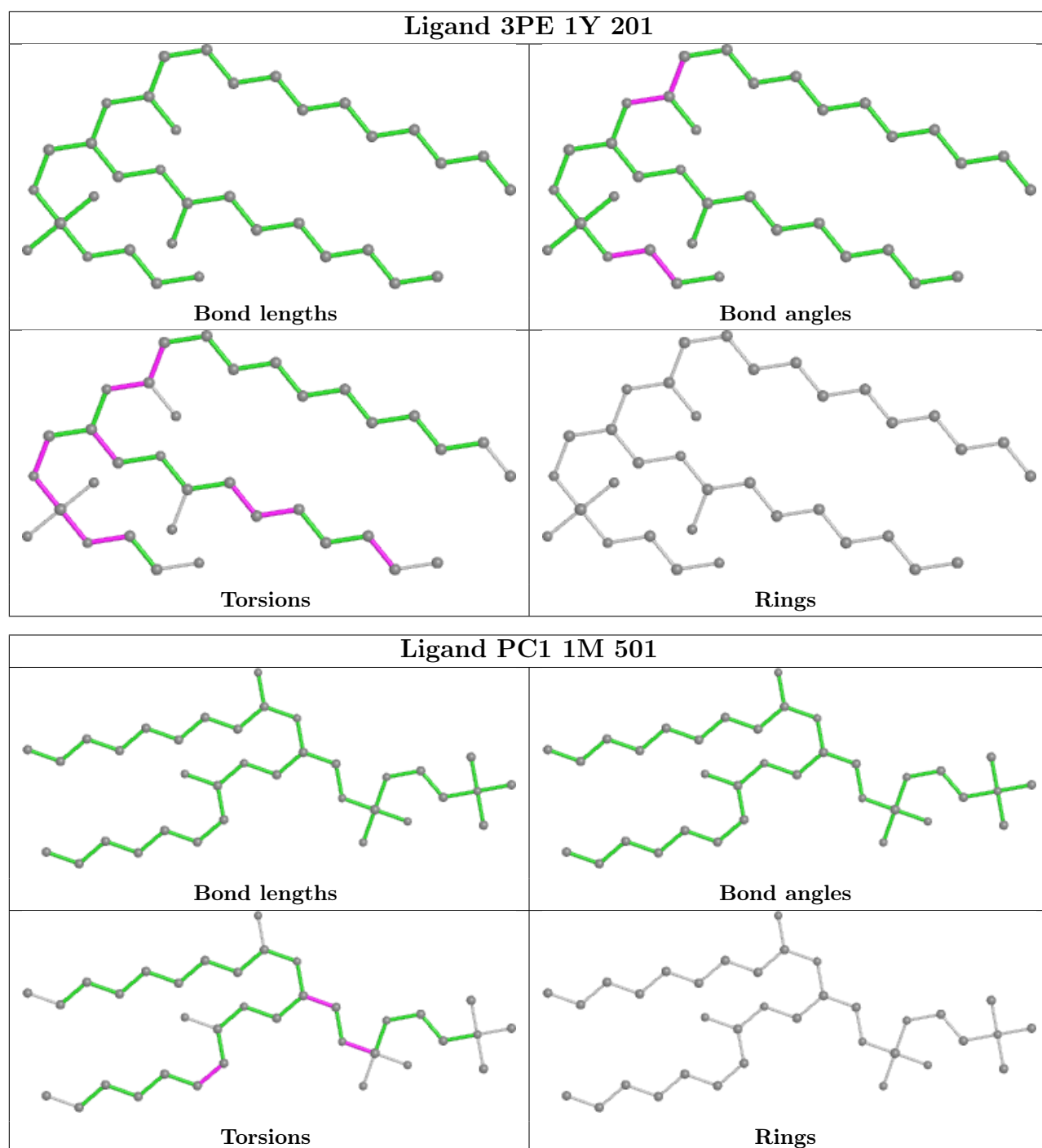
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



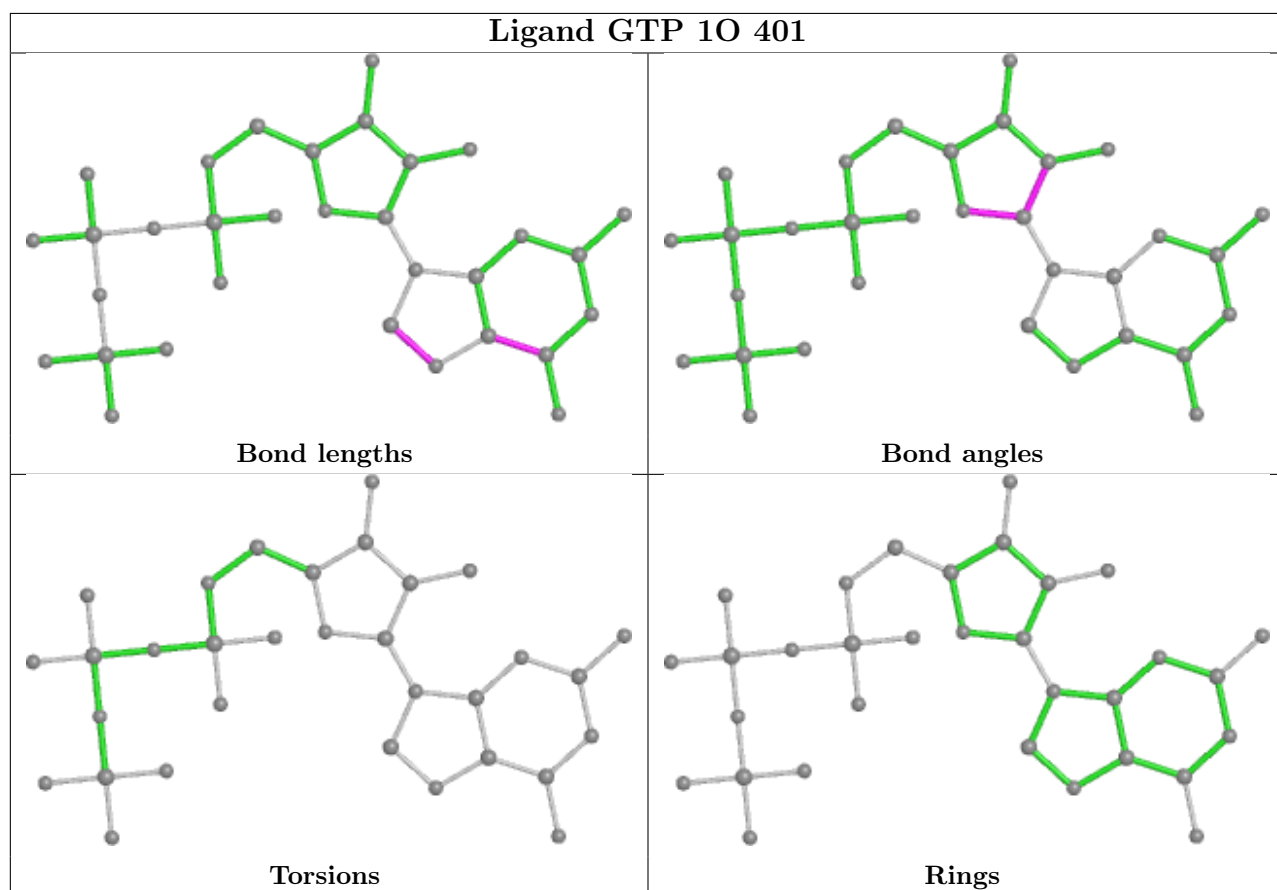
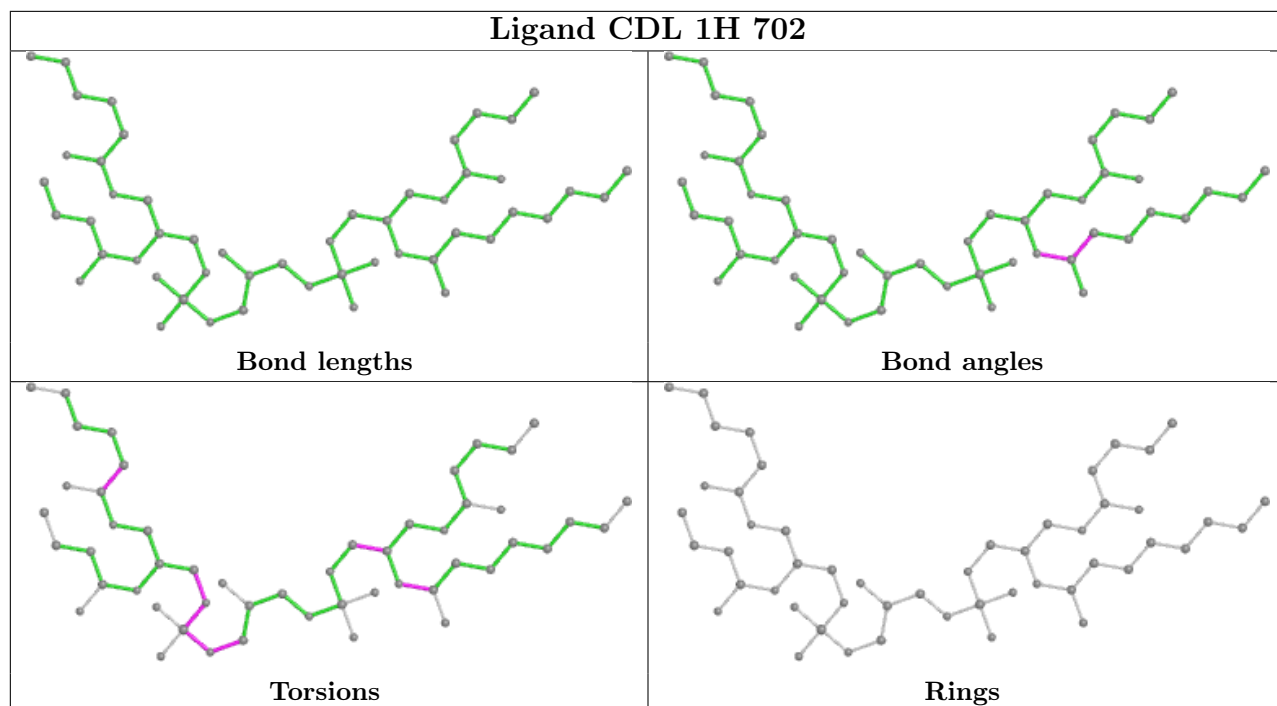


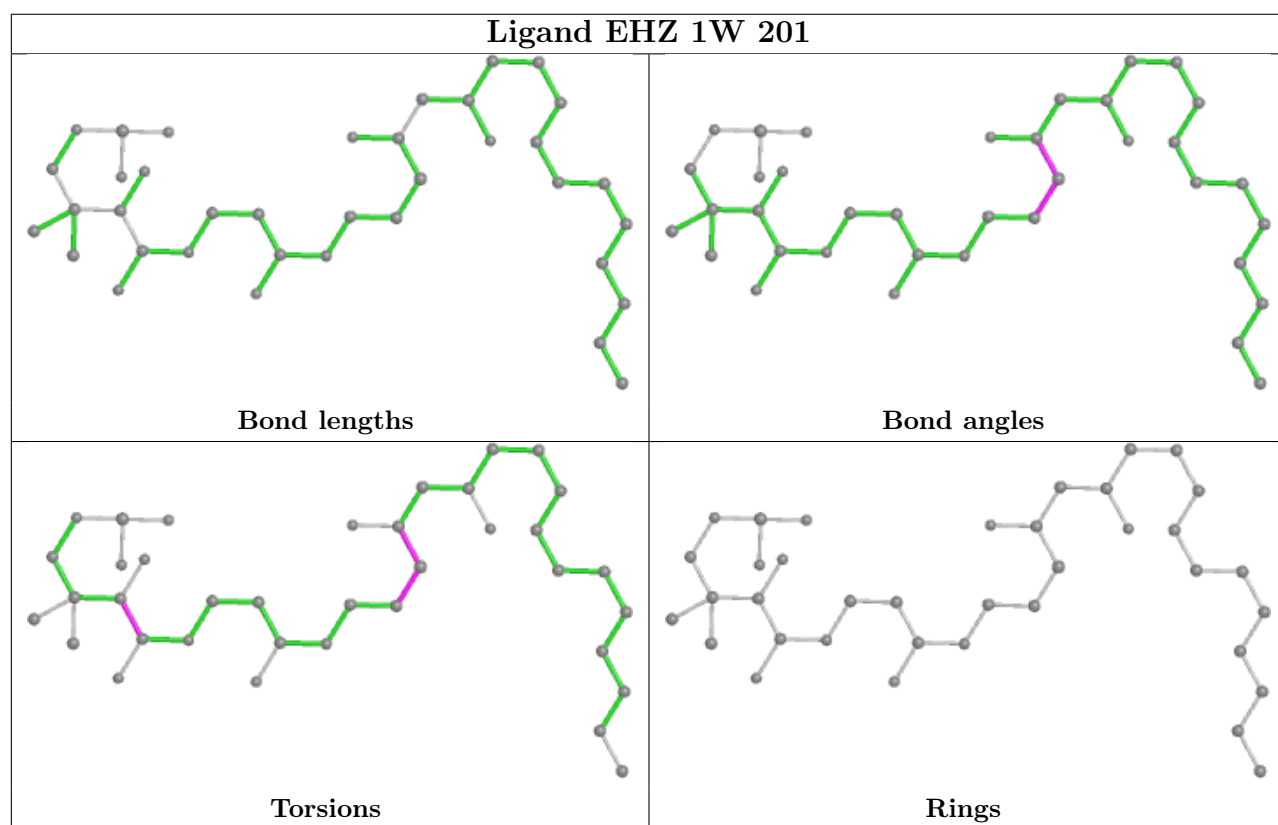
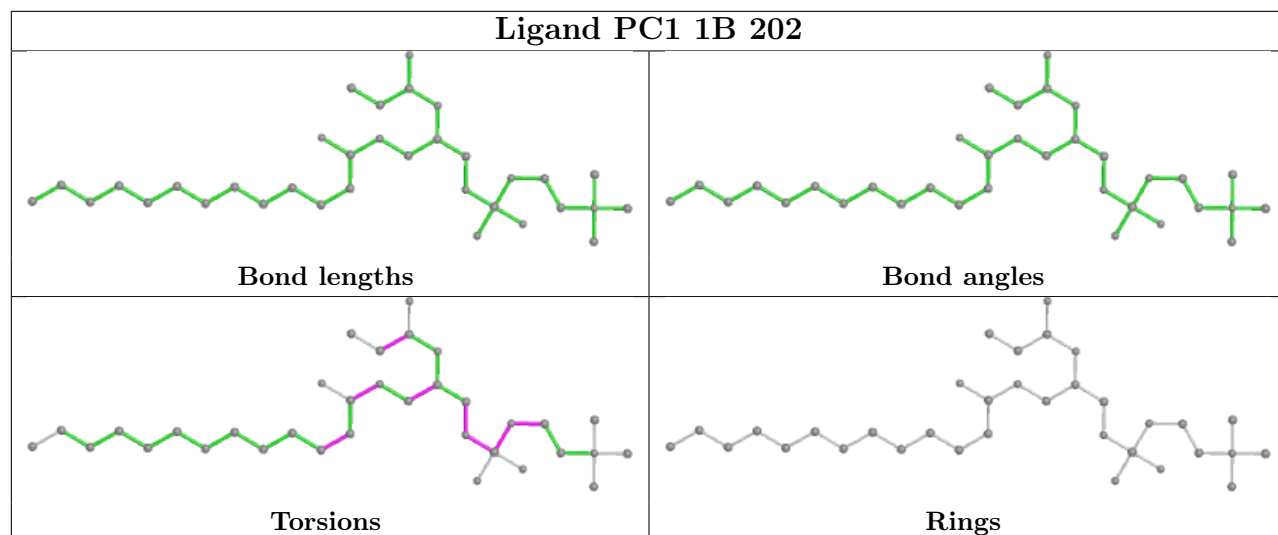


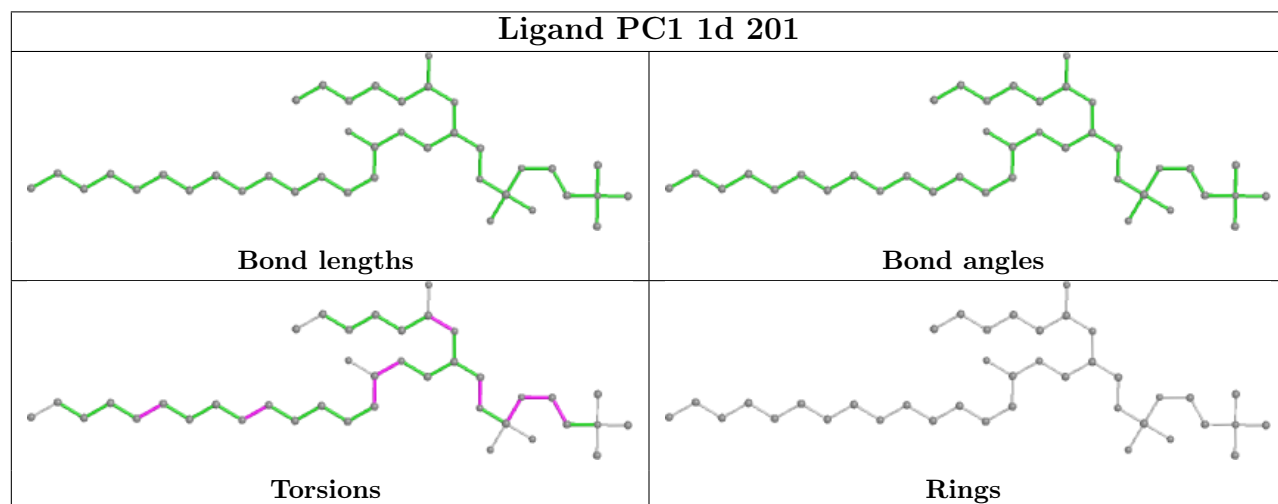
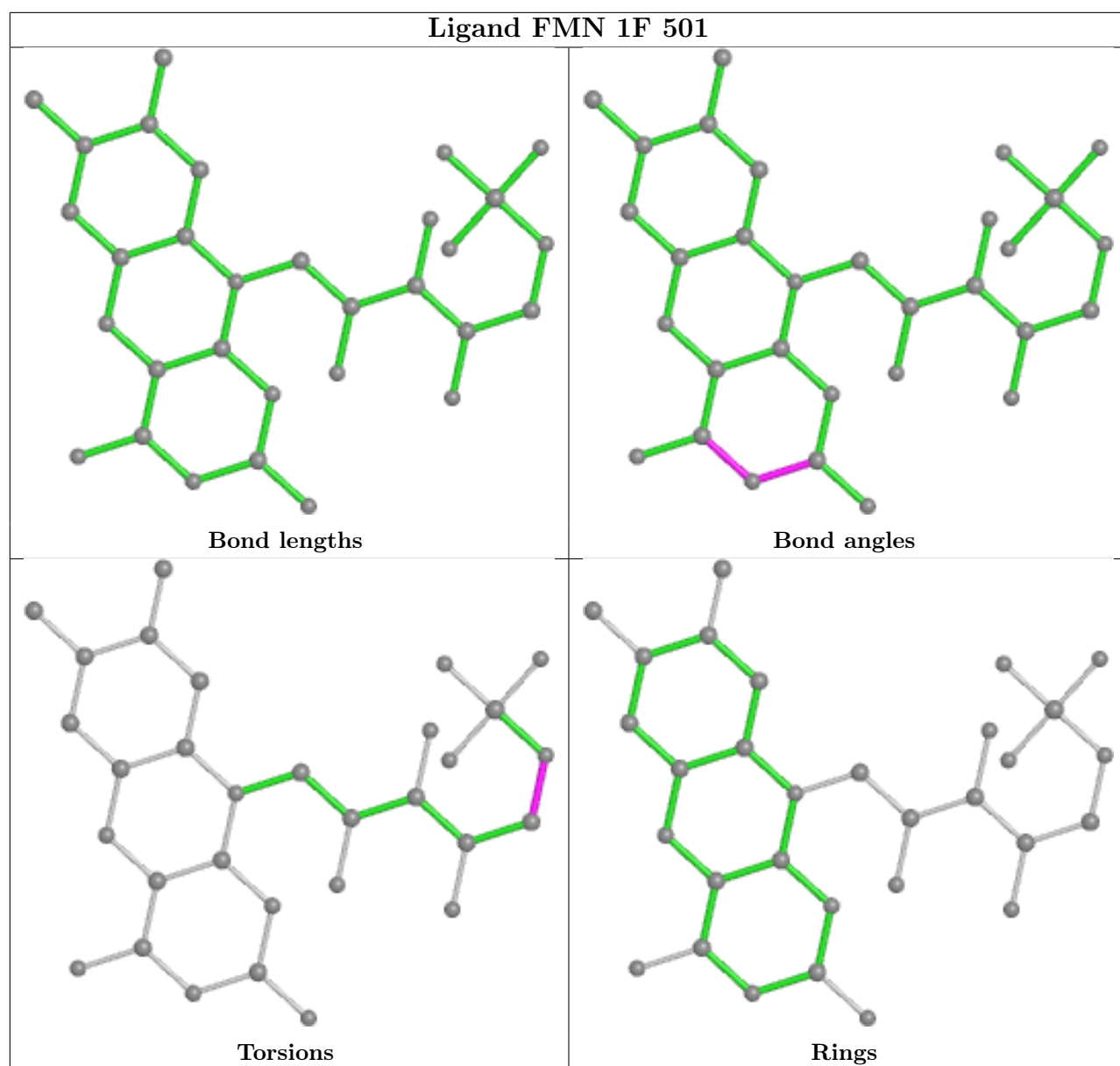


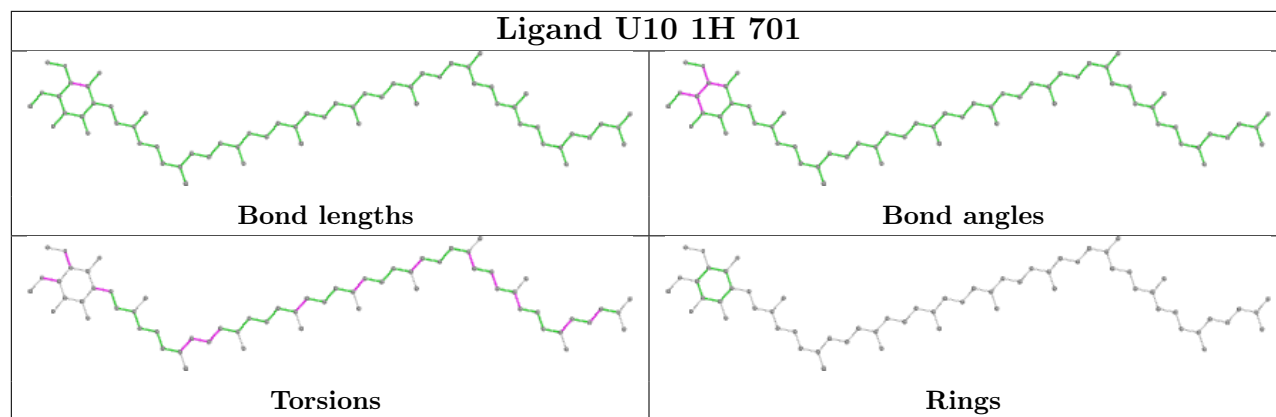












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	1r	1
34	1i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	6.44
1	1i	1:SAC	C	2:GLY	N	3.63

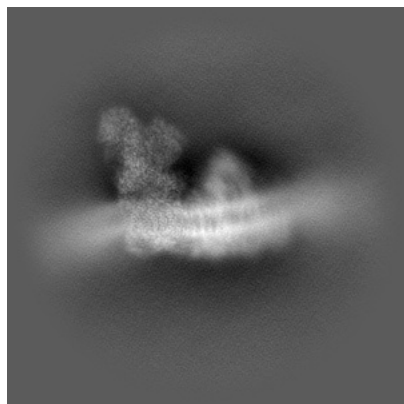
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42176. These allow visual inspection of the internal detail of the map and identification of artifacts.

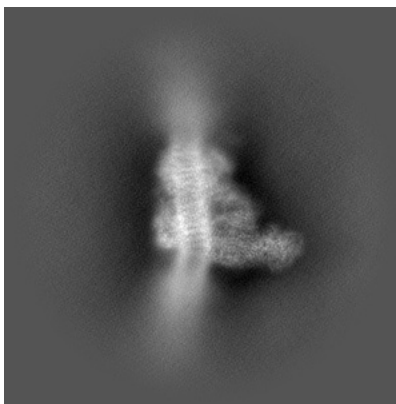
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

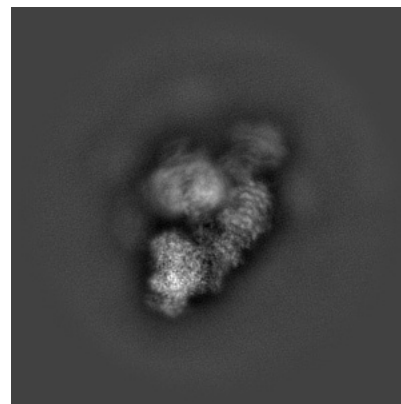
#### 6.1.1 Primary map



X

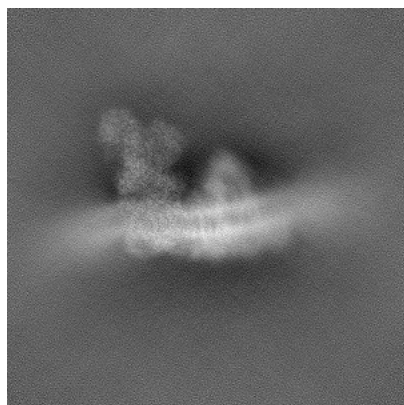


Y

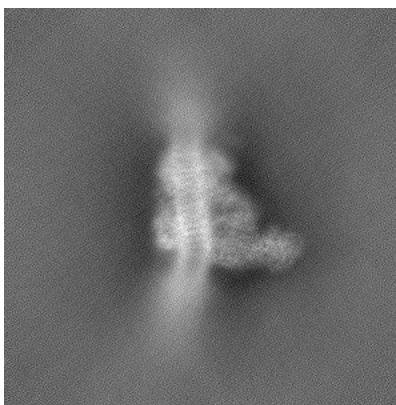


Z

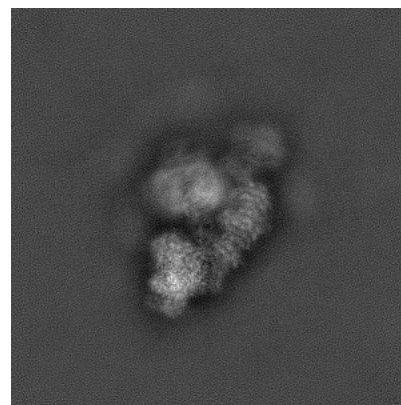
#### 6.1.2 Raw map



X



Y

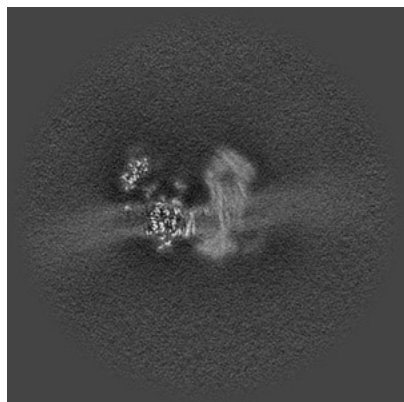


Z

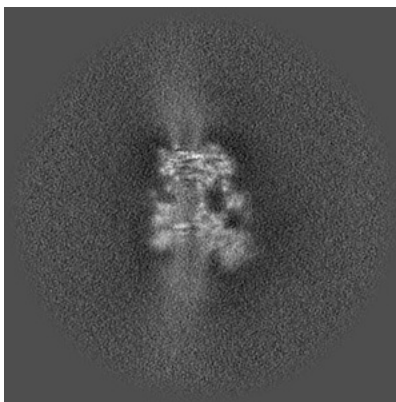
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

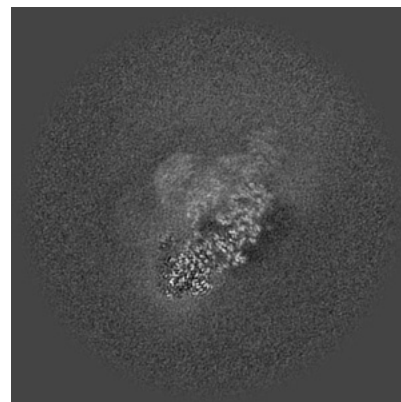
### 6.2.1 Primary map



X Index: 200

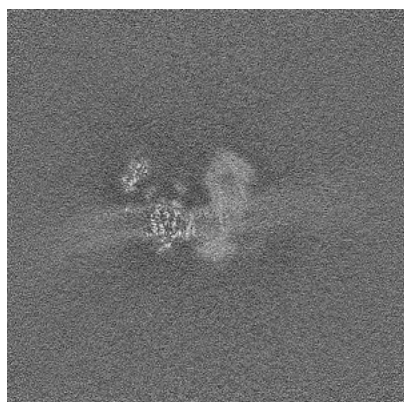


Y Index: 200

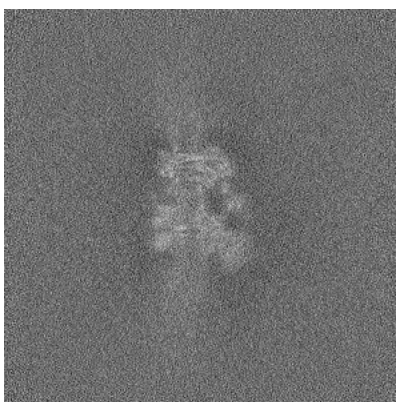


Z Index: 200

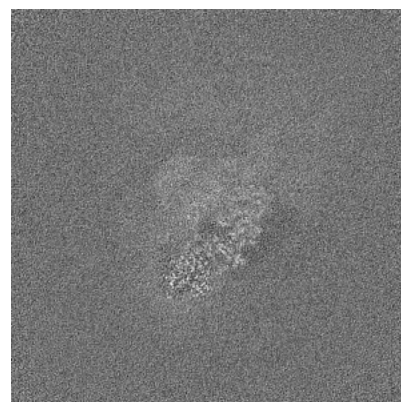
### 6.2.2 Raw map



X Index: 200



Y Index: 200

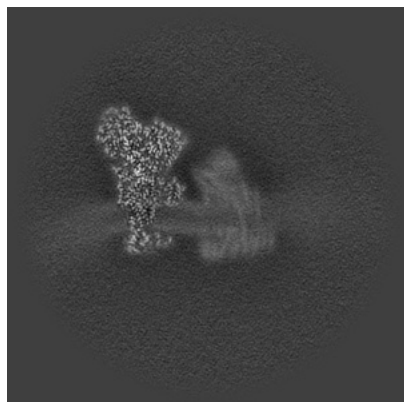


Z Index: 200

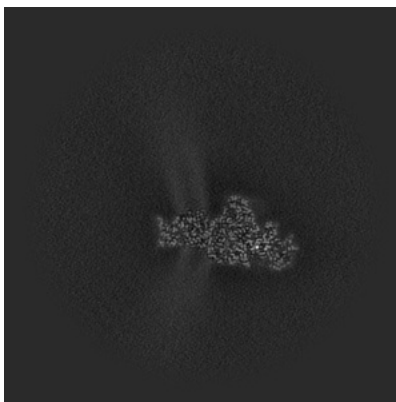
The images above show central slices of the map in three orthogonal directions.

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

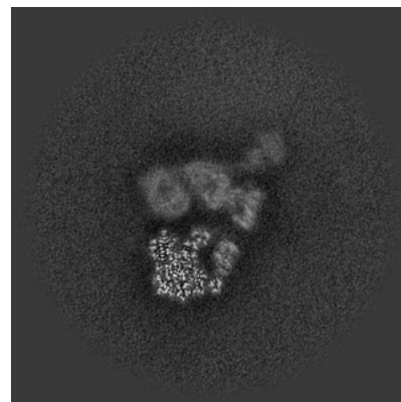
### 6.3.1 Primary map



X Index: 163

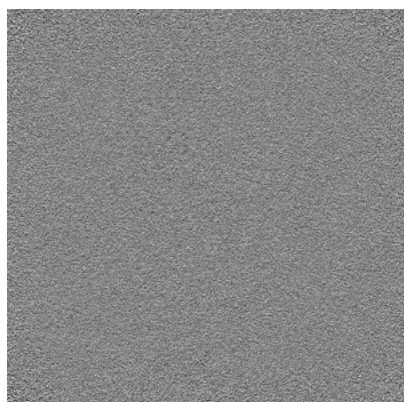


Y Index: 127

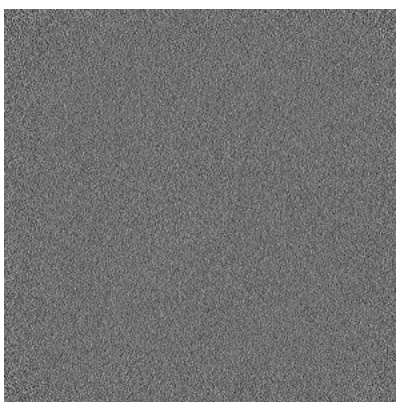


Z Index: 225

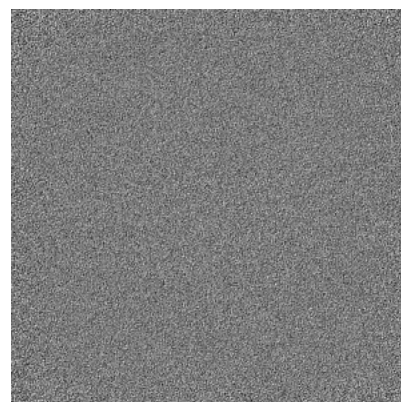
### 6.3.2 Raw map



X Index: 0



Y Index: 0

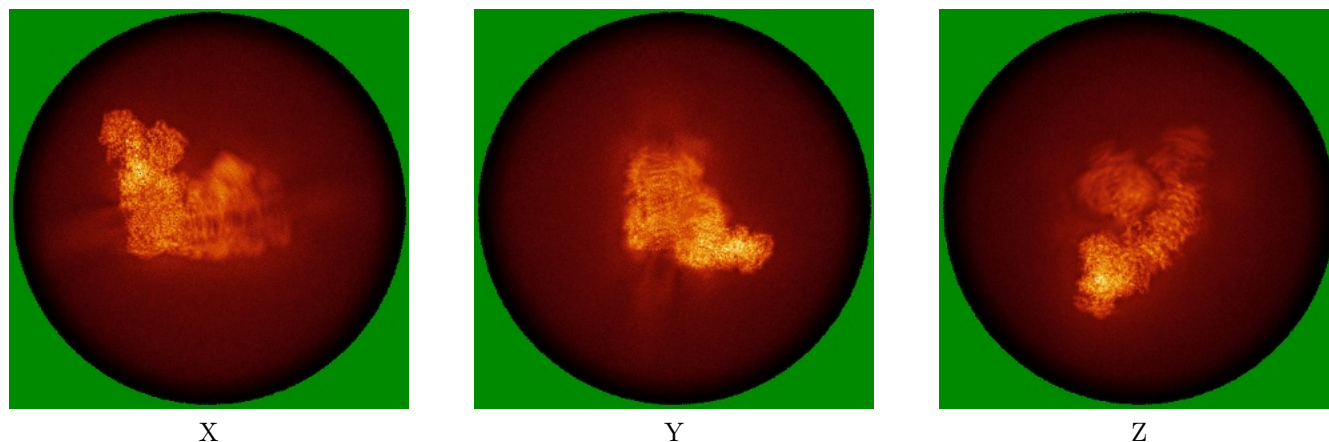


Z Index: 0

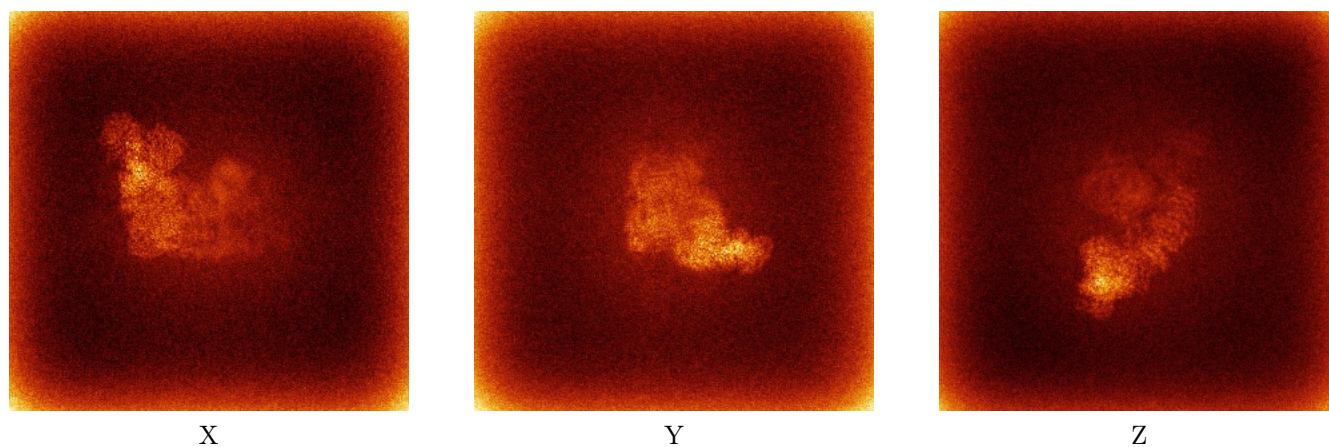
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



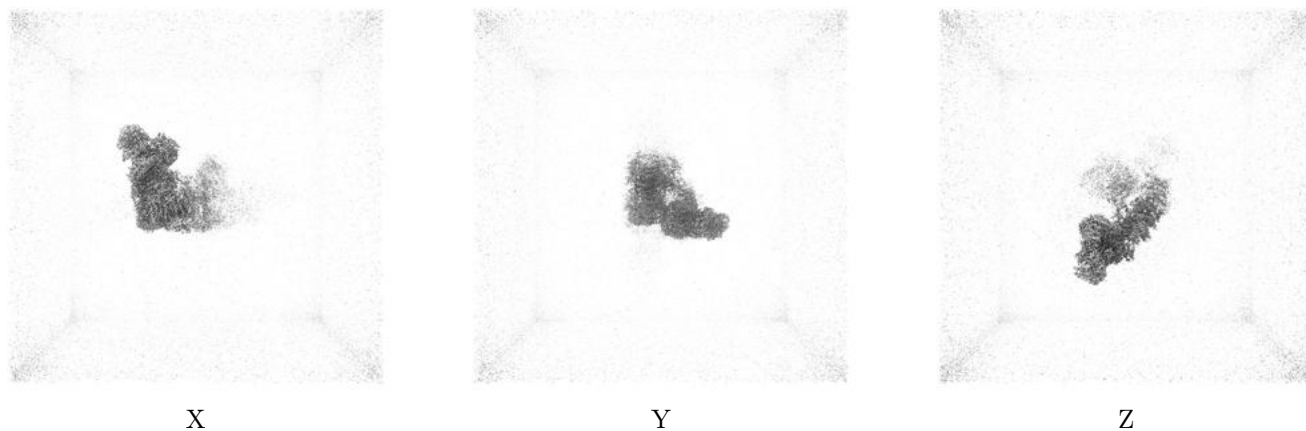
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

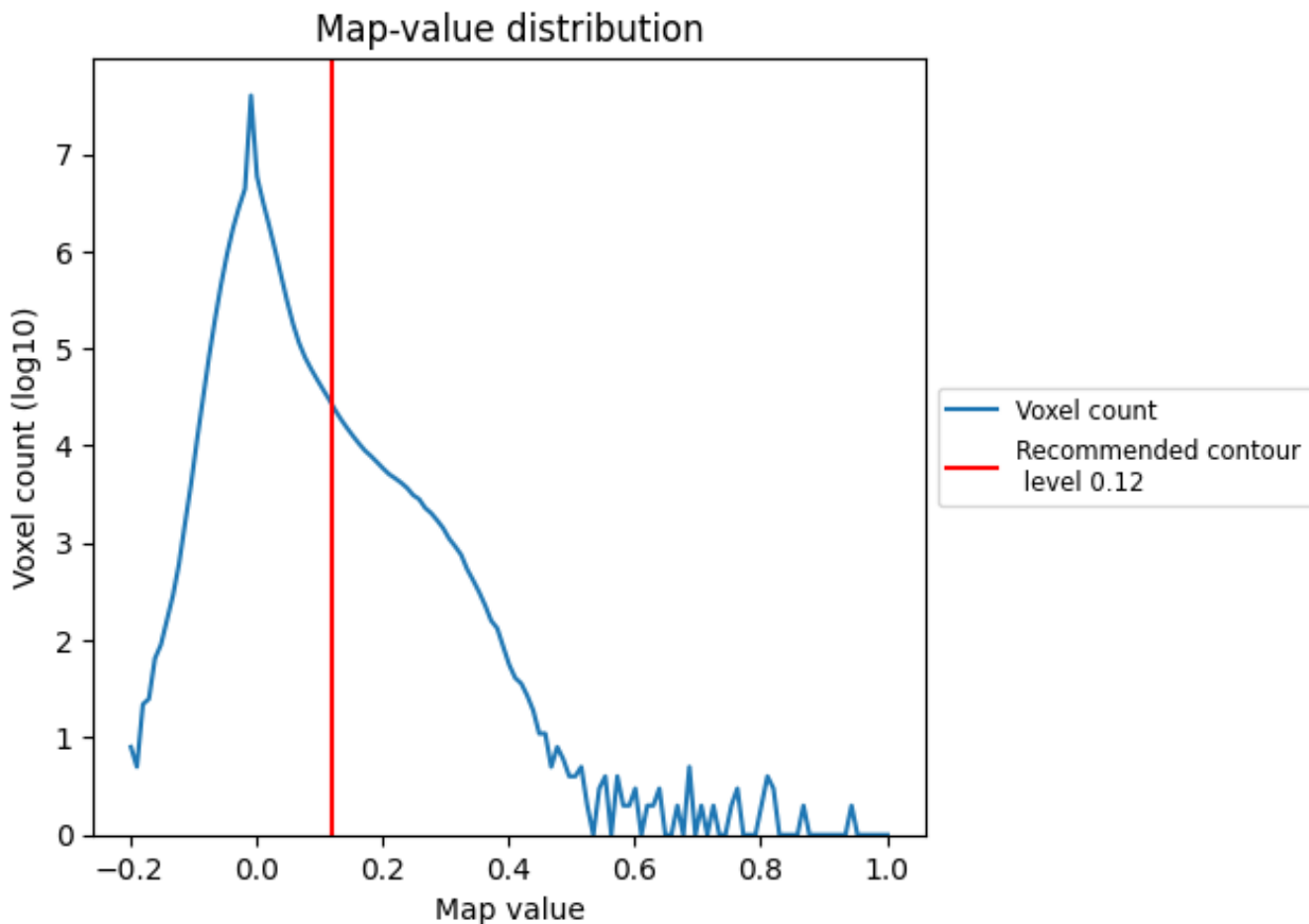
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

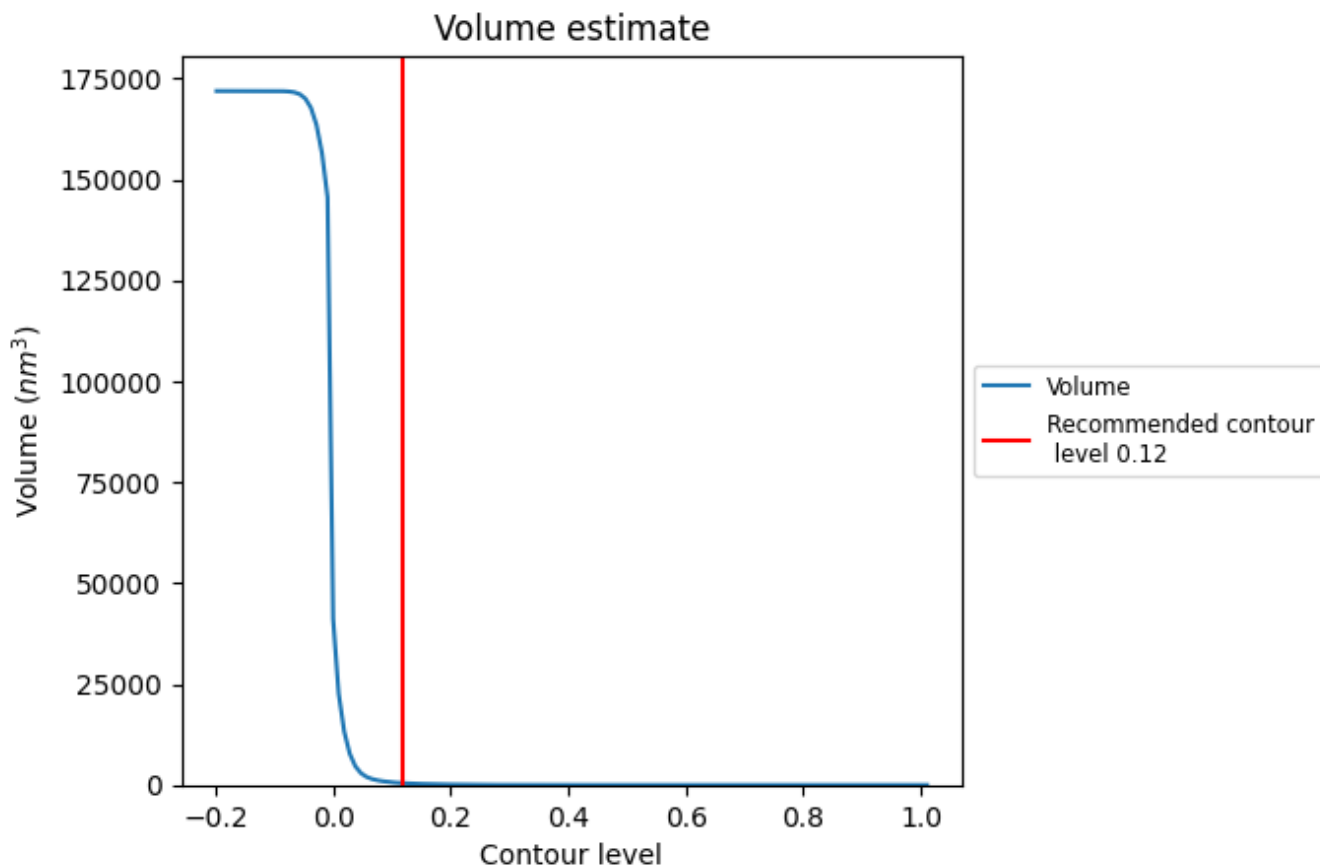
This section contains the results of statistical analysis of the map.

### 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.

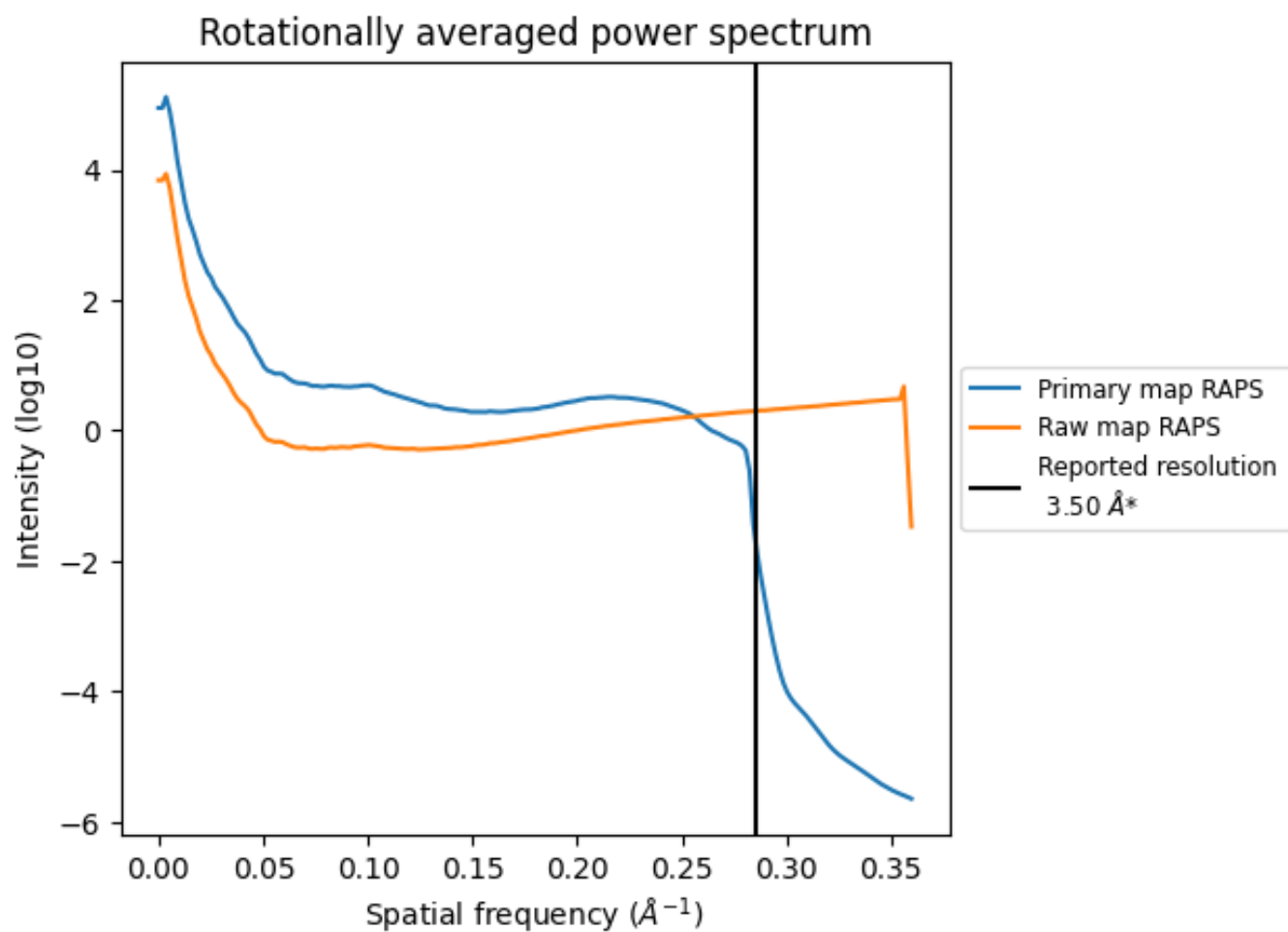
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 437 nm<sup>3</sup>; this corresponds to an approximate mass of 394 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

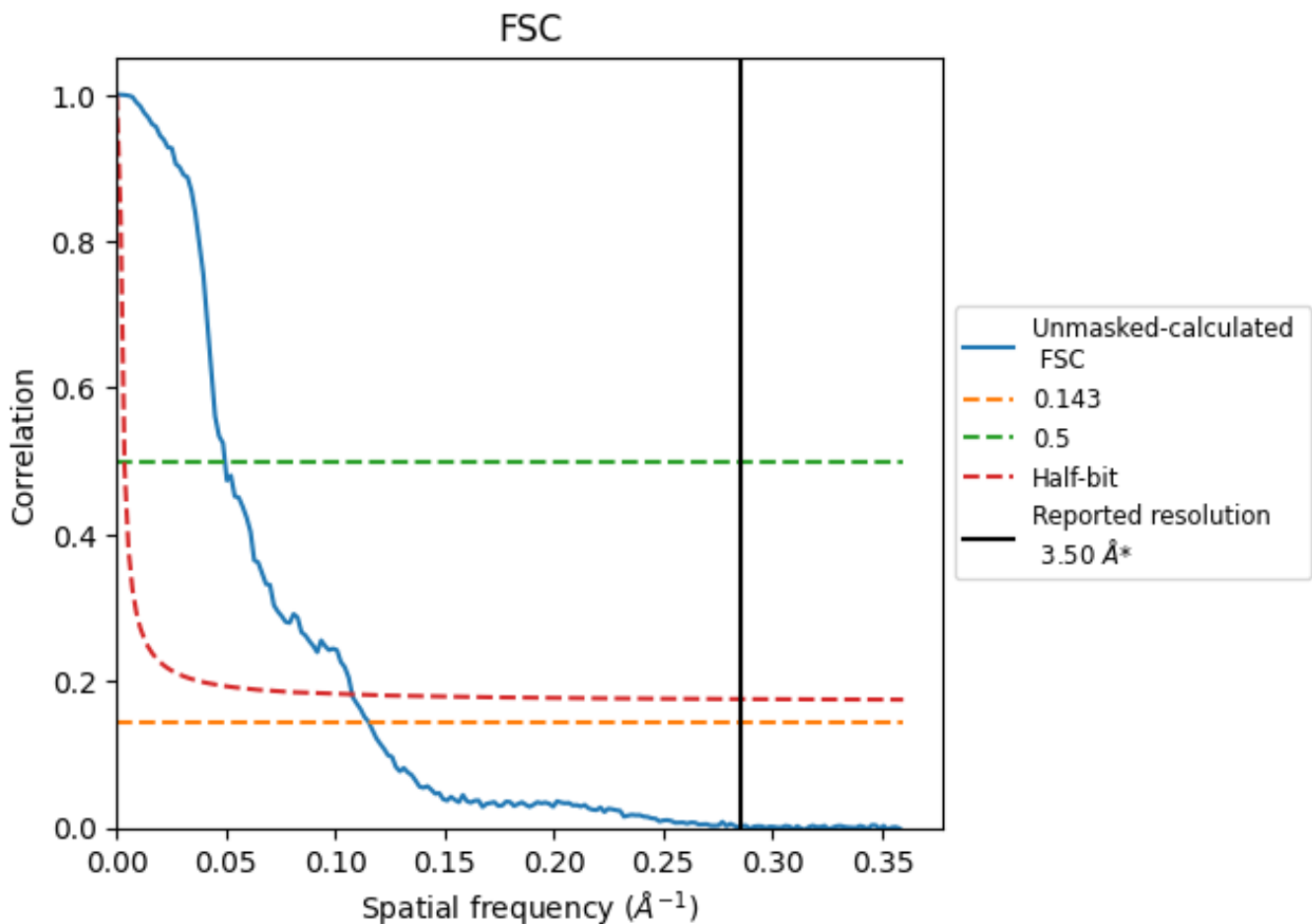


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

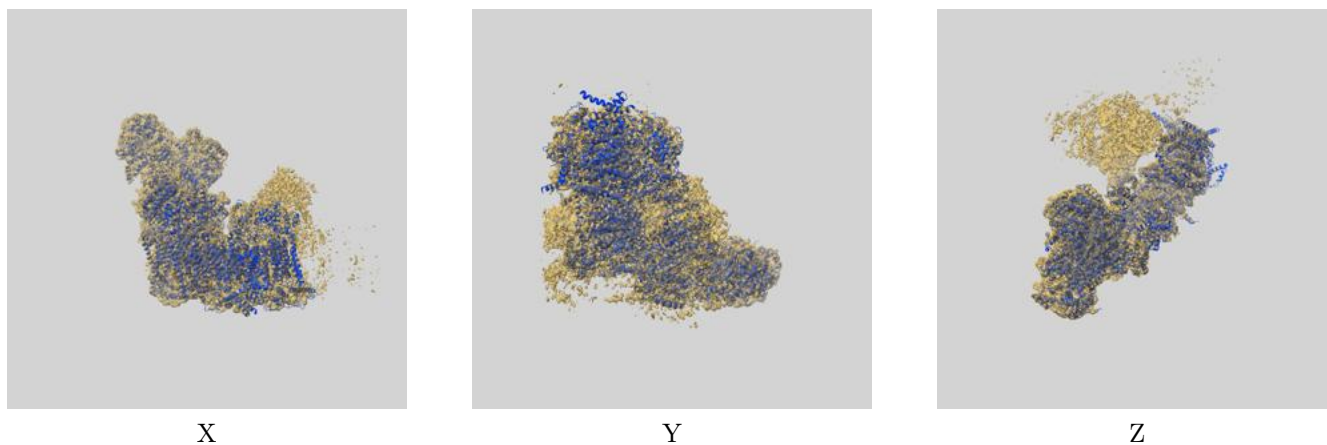
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.67	20.24	9.29

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.67 differs from the reported value 3.5 by more than 10 %

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

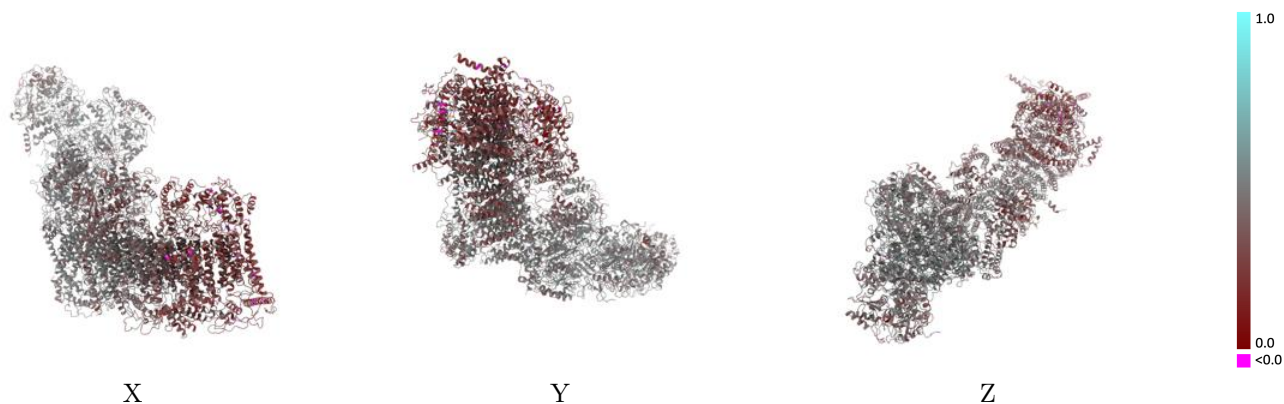
This section contains information regarding the fit between EMDB map EMD-42176 and PDB model 8UEZ. Per-residue inclusion information can be found in section 3 on page 21.

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



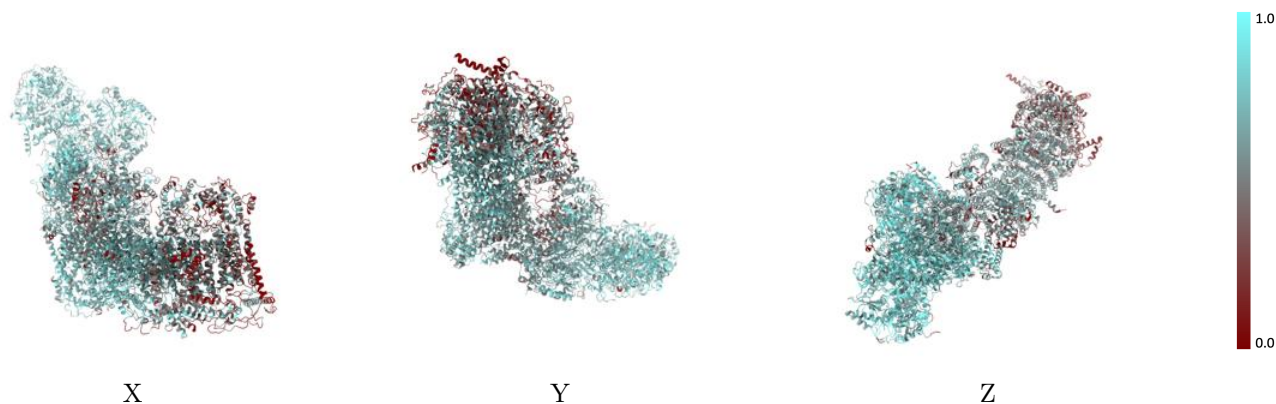
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

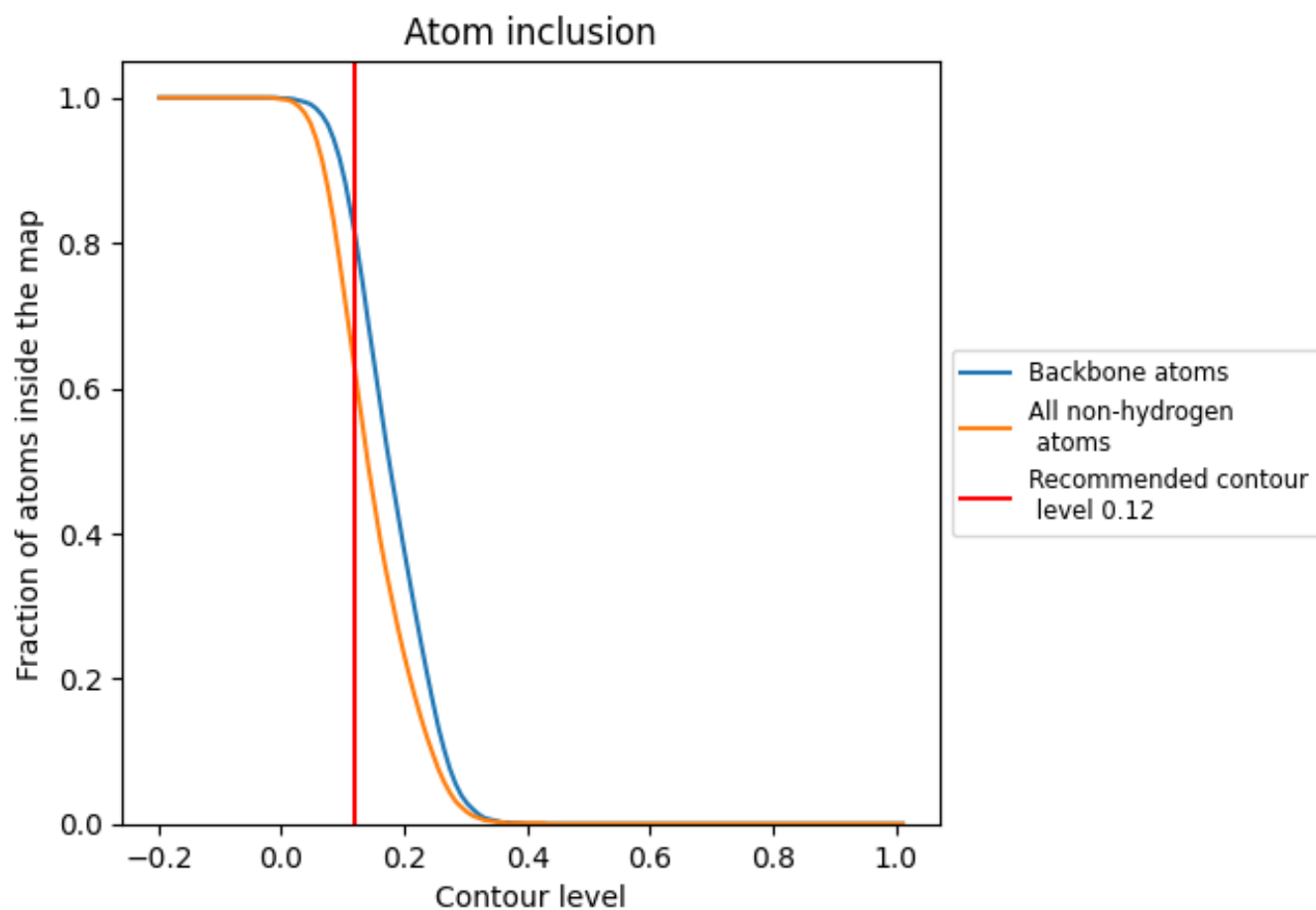
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.12).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 62% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6230	 0.4010
1A	 0.5080	 0.4400
1B	 0.6810	 0.4650
1C	 0.7470	 0.4810
1D	 0.6960	 0.4630
1E	 0.7530	 0.4310
1F	 0.7600	 0.4330
1G	 0.7680	 0.4620
1H	 0.6370	 0.4520
1I	 0.7930	 0.4780
1J	 0.5660	 0.4110
1K	 0.6560	 0.4220
1L	 0.4650	 0.2850
1M	 0.6410	 0.3930
1N	 0.7170	 0.4480
1O	 0.4580	 0.3360
1P	 0.6340	 0.4620
1Q	 0.6640	 0.4610
1R	 0.7260	 0.4720
1S	 0.7300	 0.4200
1T	 0.4410	 0.3560
1U	 0.3490	 0.2370
1V	 0.6490	 0.4250
1W	 0.6380	 0.4360
1X	 0.7470	 0.4320
1Y	 0.6080	 0.3420
1Z	 0.7450	 0.4470
1a	 0.7460	 0.4700
1b	 0.6920	 0.4520
1c	 0.4900	 0.3690
1d	 0.6970	 0.4220
1e	 0.7200	 0.4420
1f	 0.4750	 0.3600
1g	 0.5180	 0.3530
1h	 0.6120	 0.3860



*Continued on next page...*

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Chain	Atom inclusion	Q-score
1i	 0.2920	 0.2750
1j	 0.2660	 0.2590
1k	 0.2150	 0.2400
1l	 0.4720	 0.2970
1m	 0.4870	 0.2980
1n	 0.4540	 0.2740
1o	 0.4030	 0.2470
1p	 0.5130	 0.3290
1q	 0.7440	 0.4730
1r	 0.7510	 0.4730
1s	 0.7090	 0.4110