



Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 12:12 PM EDT

PDB ID : 8UER
EMDB ID : EMD-42168
Title : In-situ complex I with Q10 (State-gamma)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.50 Å (reported)

This is a Full wwPDB EM Validation 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:

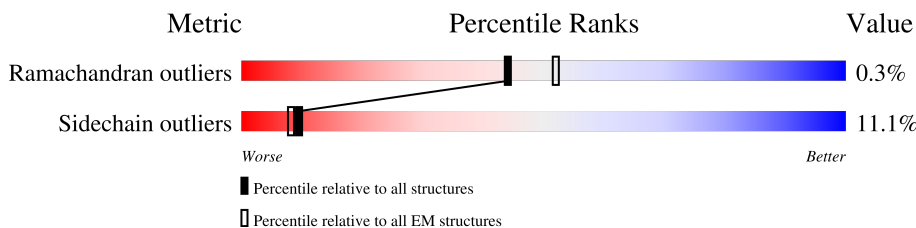
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 ≥ 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	
2	1B	255	
3	1C	264	
4	1D	476	
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	

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Mol	Chain	Length	Quality of chain
10	1J	175	50% 85% 15%
11	1K	98	39% 87% 13%
12	1L	606	92% 91% 9%
13	1M	459	56% 89% 11%
14	1N	347	19% 92% 8%
15	1O	357	68% 81% 9% 10%
16	1P	377	28% 83% 8% 9%
17	1Q	175	21% 66% 7% 26%
18	1R	123	15% 68% 10% 22%
19	1S	99	22% 75% 13% 12%
20	1T	156	45% 49% 6% 46%
20	1U	156	55% 46% 8% 45%
21	1V	116	38% 90% 9%
22	1W	128	41% 77% 13% 10%
23	1X	172	28% 92% 7%
24	1Y	141	66% 91% 8%
25	1Z	144	23% 86% 12%
26	1a	70	16% 93% 7%
27	1b	84	37% 89% 10%
28	1c	76	38% 53% 12% 36%
29	1d	123	30% 89% 10%
30	1e	106	23% 84% 9% 7%
31	1f	135	31% 34% 8% 58%
32	1g	154	60% 52% 11% 35%
33	1h	189	48% 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

There are 58 unique types of molecules in this entry. The entry contains 67436 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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	?	-	PRO	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8

- 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
			Total	C	N	O	S		
18	1R	96	741	452	140	146	3	0	0

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

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

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

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

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

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

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

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

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

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

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	S		
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

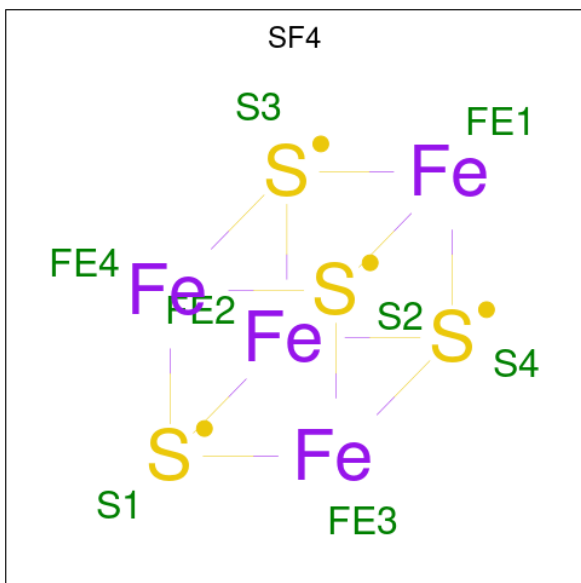
There is a discrepancy between the modelled and reference sequences:

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: Fe₄S₄).



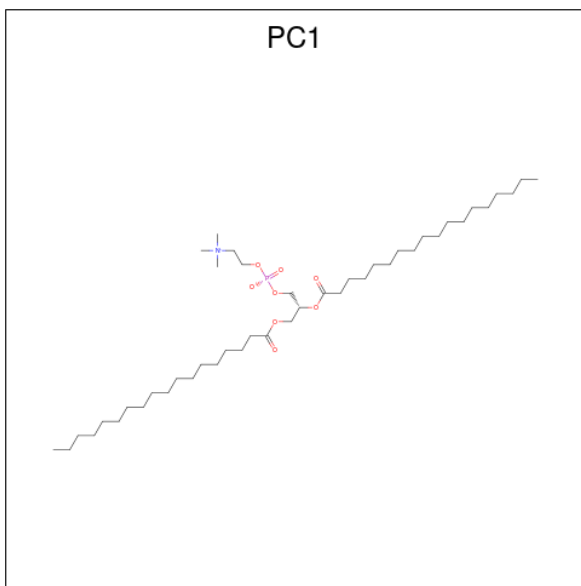
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1B	1	8	4	4	0
45	1F	1	8	4	4	0
45	1G	1	8	4	4	0
45	1G	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
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: $C_{44}H_{88}NO_8P$).



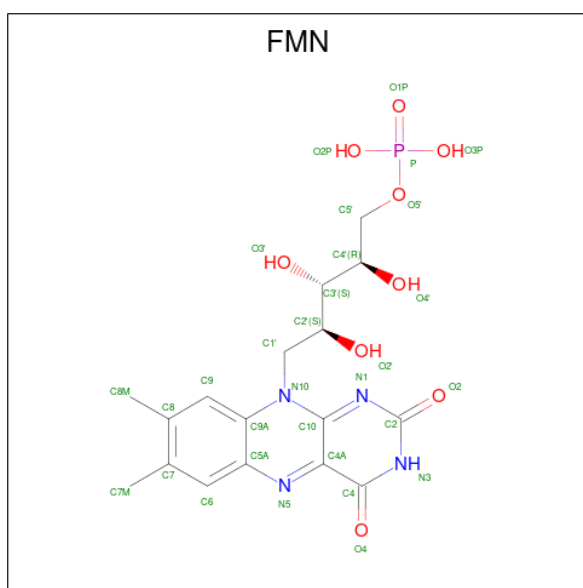
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	1B	1	34	24	1	8	1	0
46	1Y	1	35	25	1	8	1	0
46	1d	1	39	29	1	8	1	0
46	1h	1	34	24	1	8	1	0
46	1m	1	46	36	1	8	1	0
46	1q	1	48	38	1	8	1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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: C₁₇H₂₁N₄O₉P).

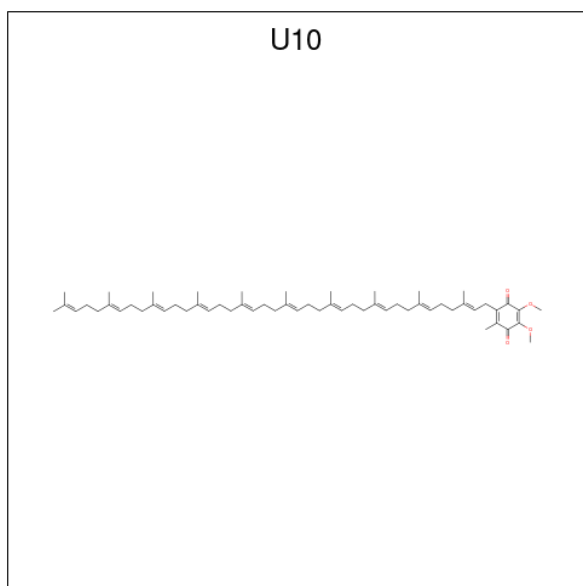


Mol	Chain	Residues	Atoms				AltConf	
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

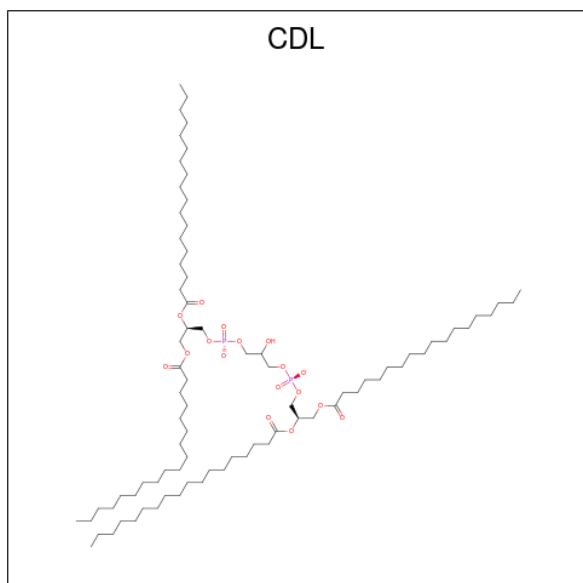
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

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



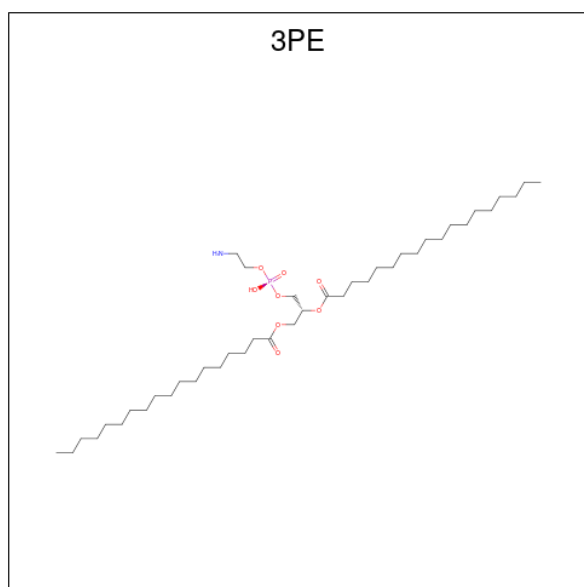
Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

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



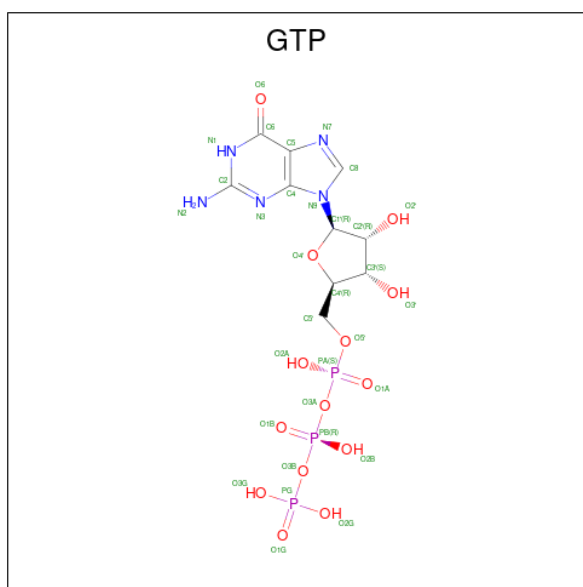
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	1H	1	51	32	17	2	0
51	1O	1	67	48	17	2	0
51	1a	1	61	42	17	2	0

- Molecule 52 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	
52	1N	1	38	28	1	8	1	0
52	1Y	1	35	25	1	8	1	0
52	1g	1	51	41	1	8	1	0
52	1n	1	42	32	1	8	1	0

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

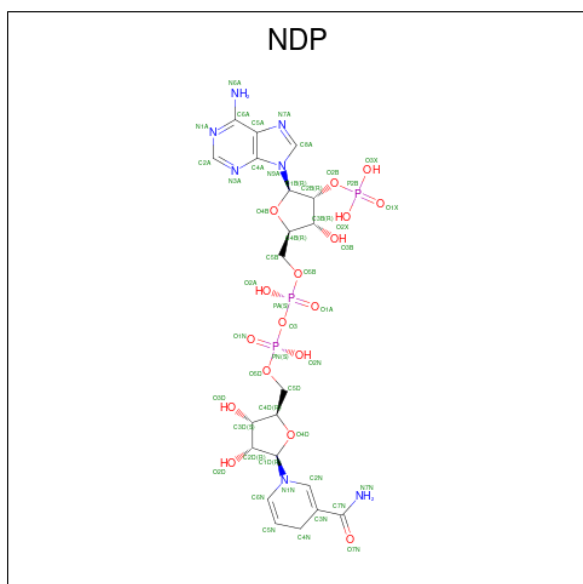


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
53	10	1	32	10	5	14	3	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	10	1	1	1	0

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

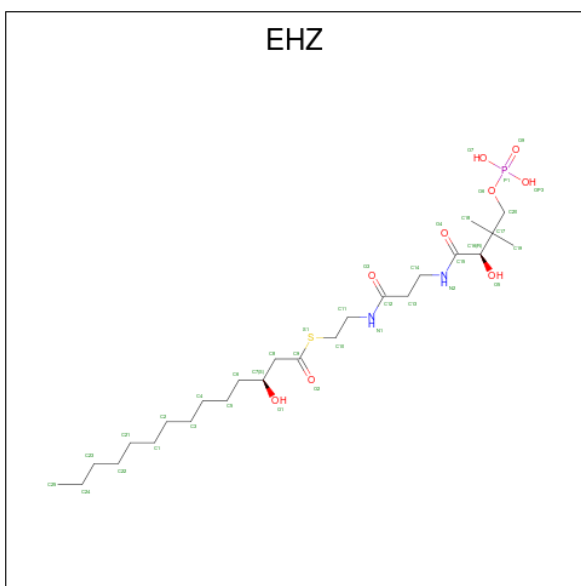


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

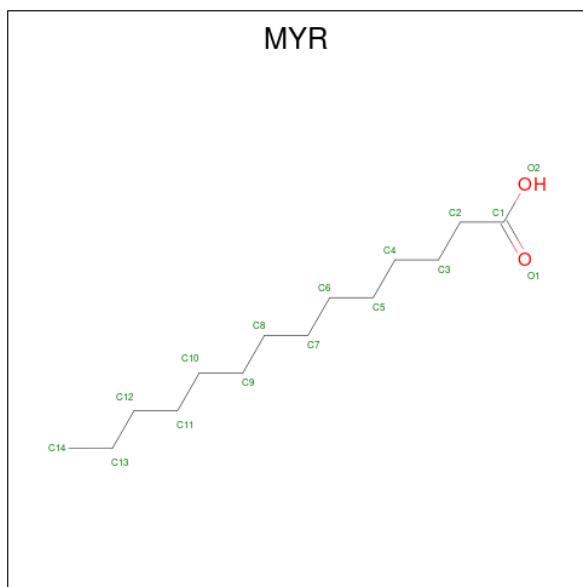
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- Molecule 57 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: C₂₅H₄₉N₂O₉PS).



Mol	Chain	Residues	Atoms						AltConf
57	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).

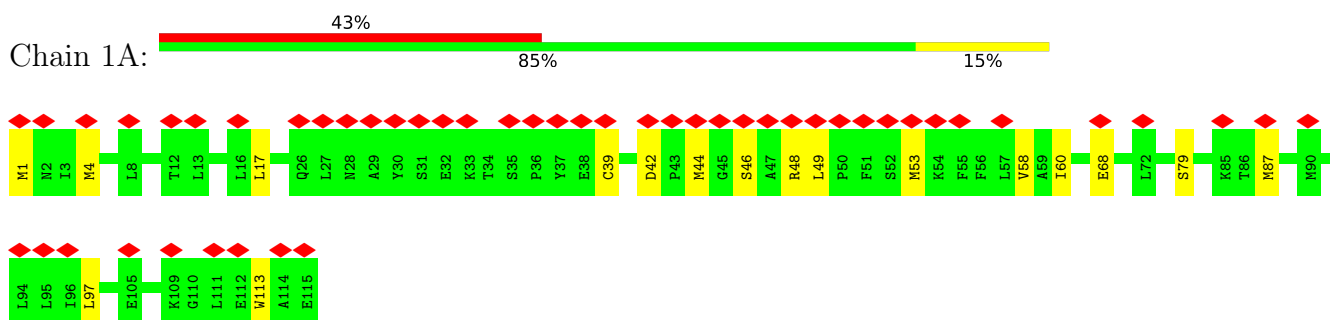


Mol	Chain	Residues	Atoms			AltConf
58	11	1	Total	C	O	0
			15	14	1	

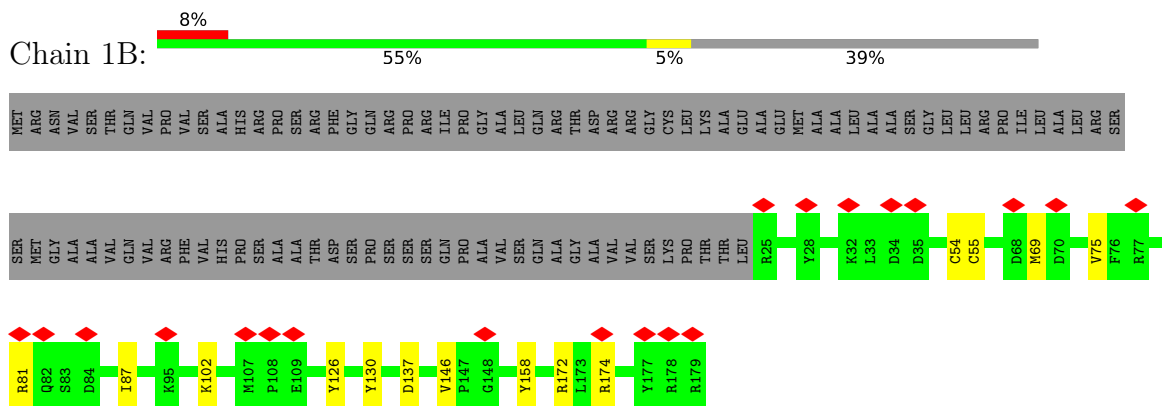
3 Residue-property plots i

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

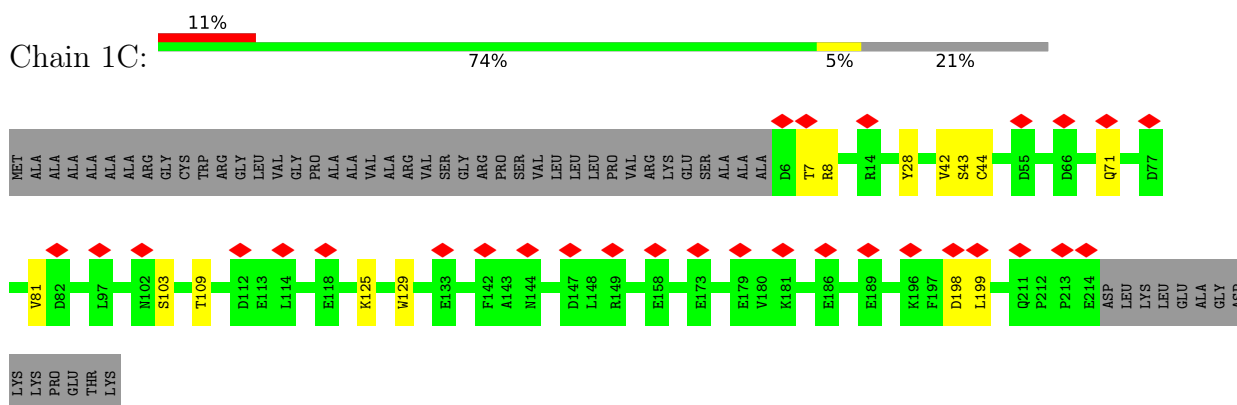
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



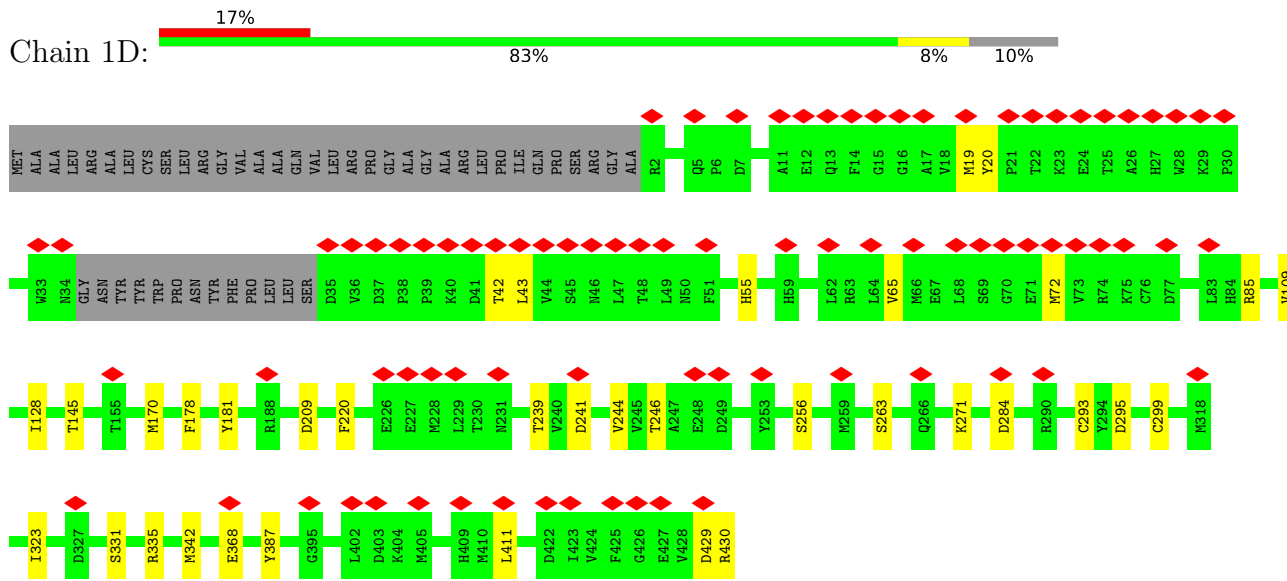
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



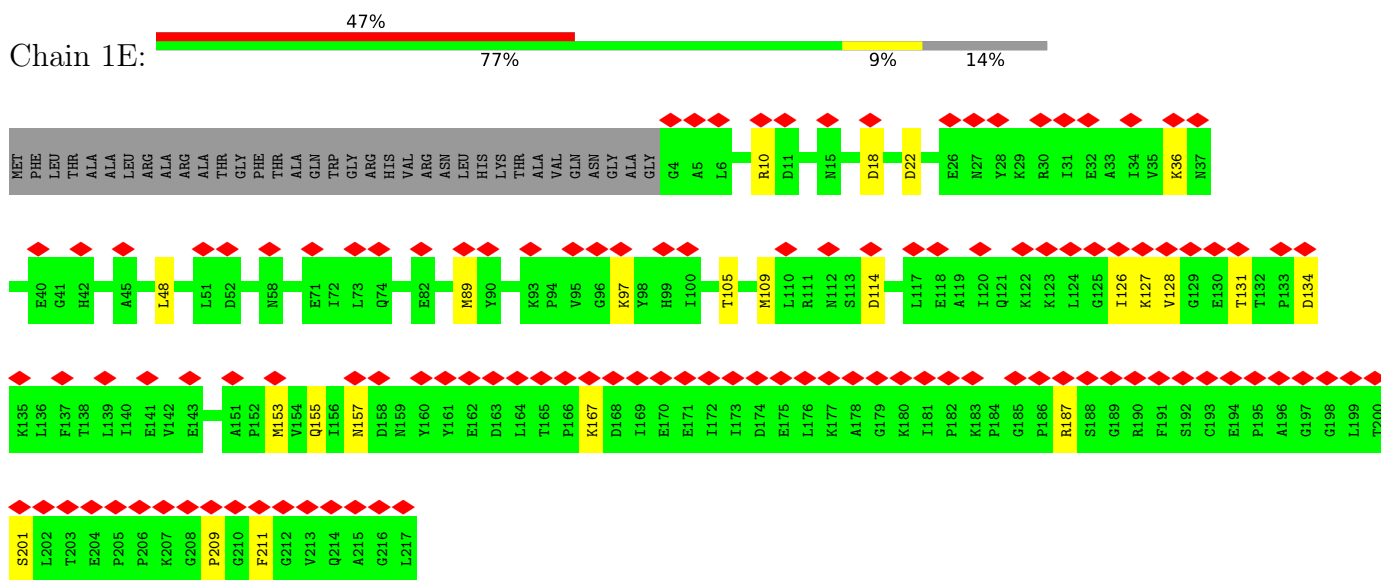
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



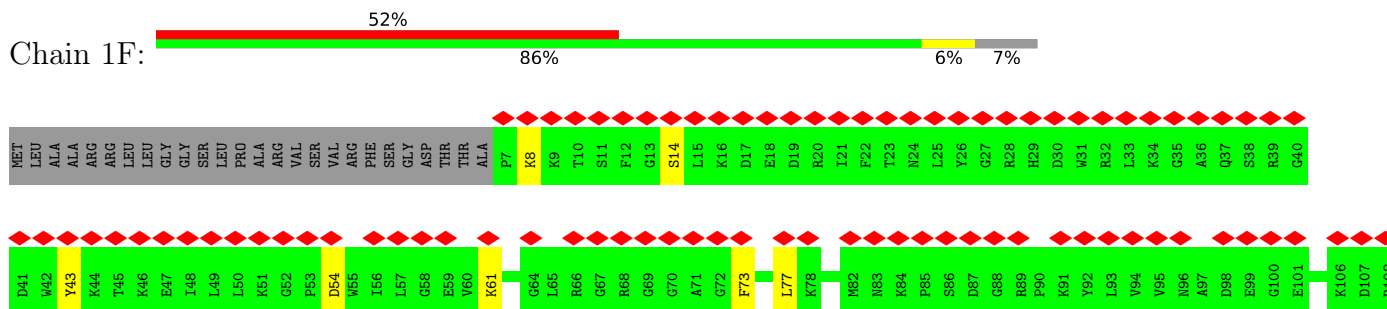
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

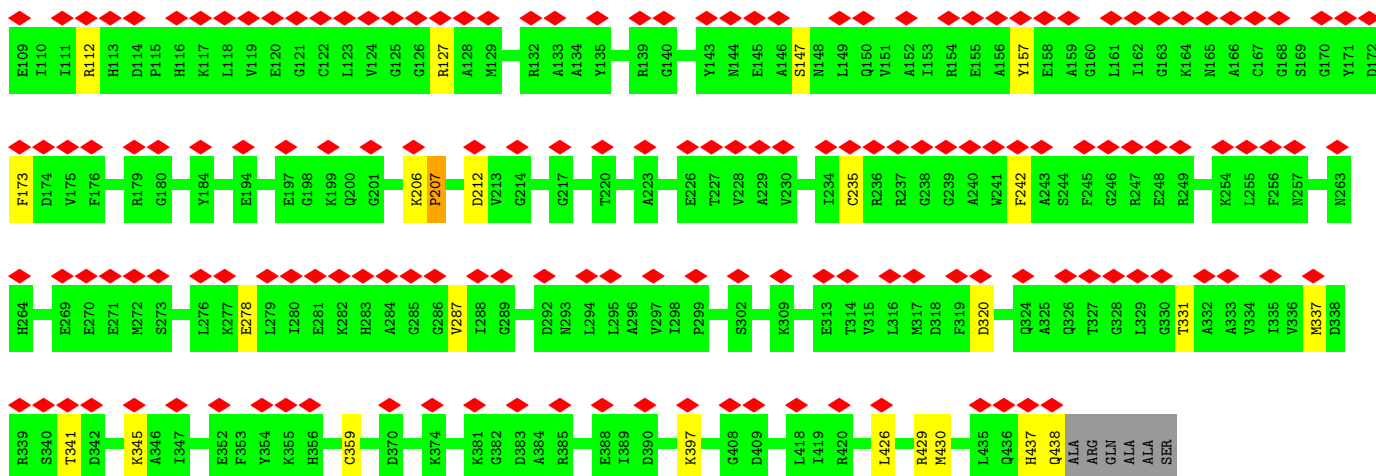


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

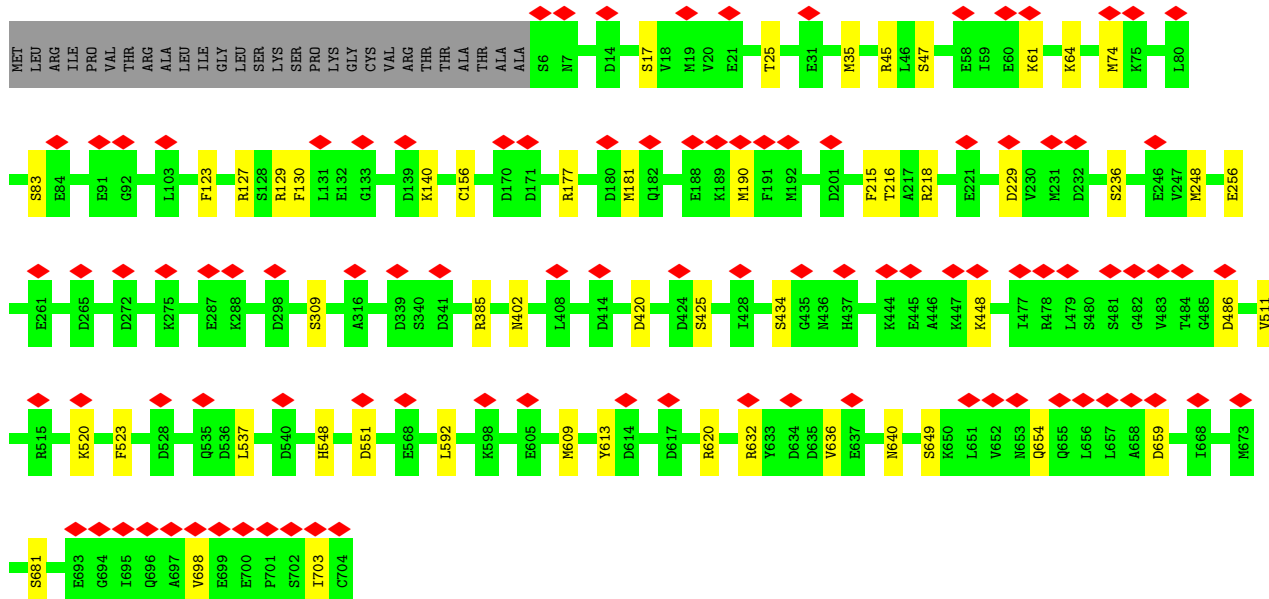
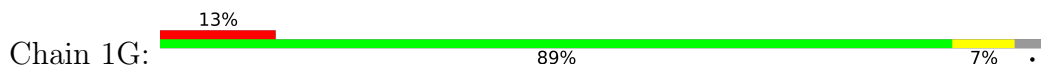


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

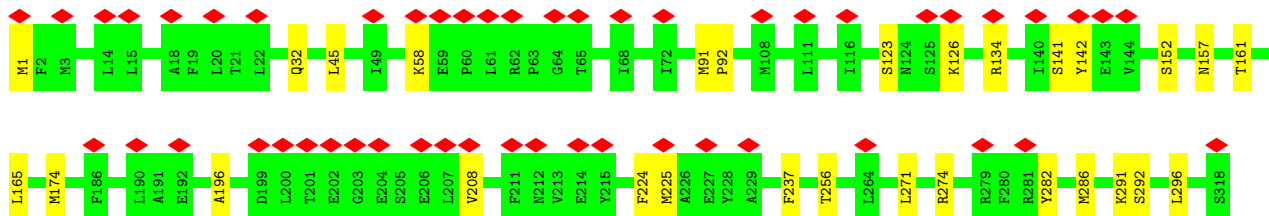
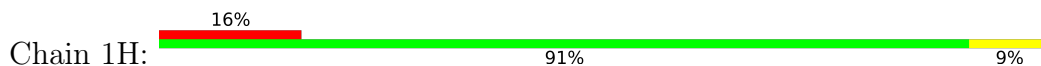




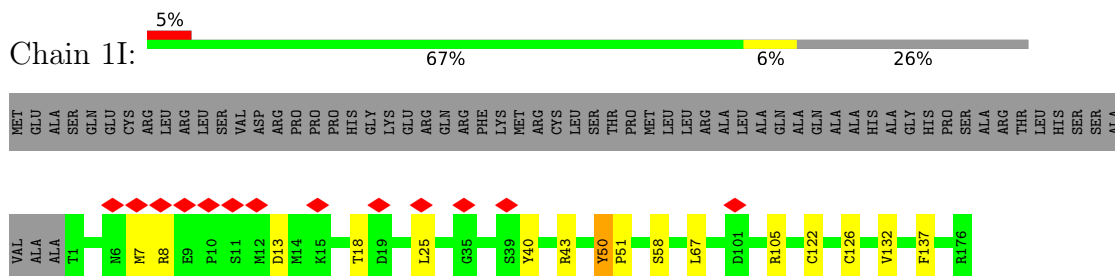
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



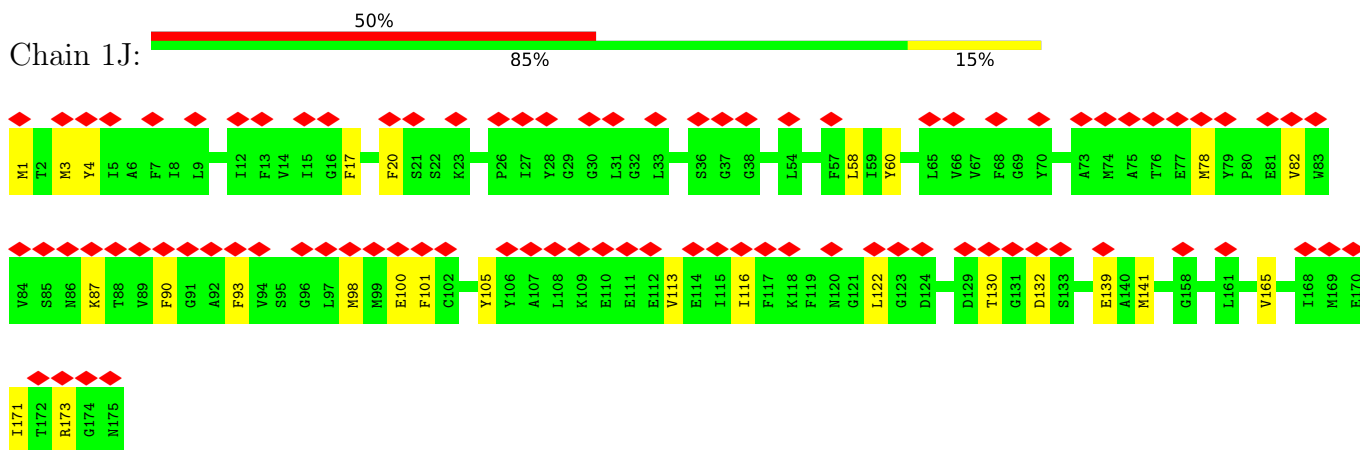
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



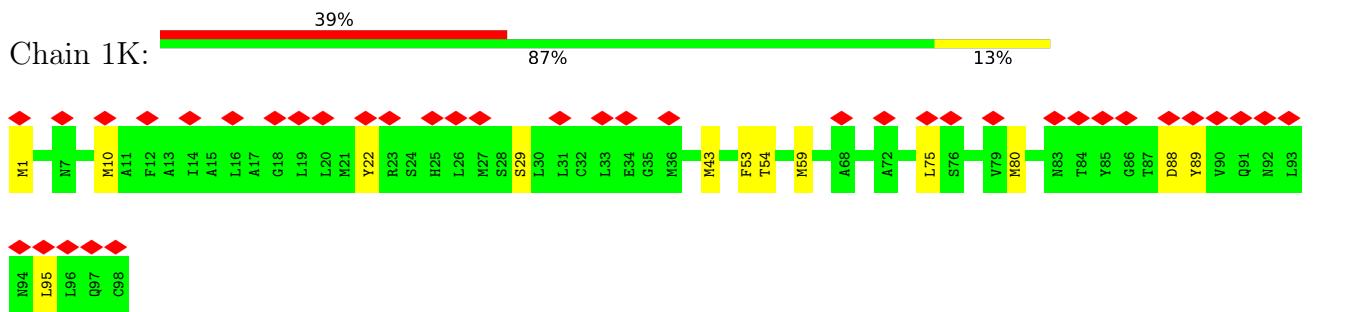
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



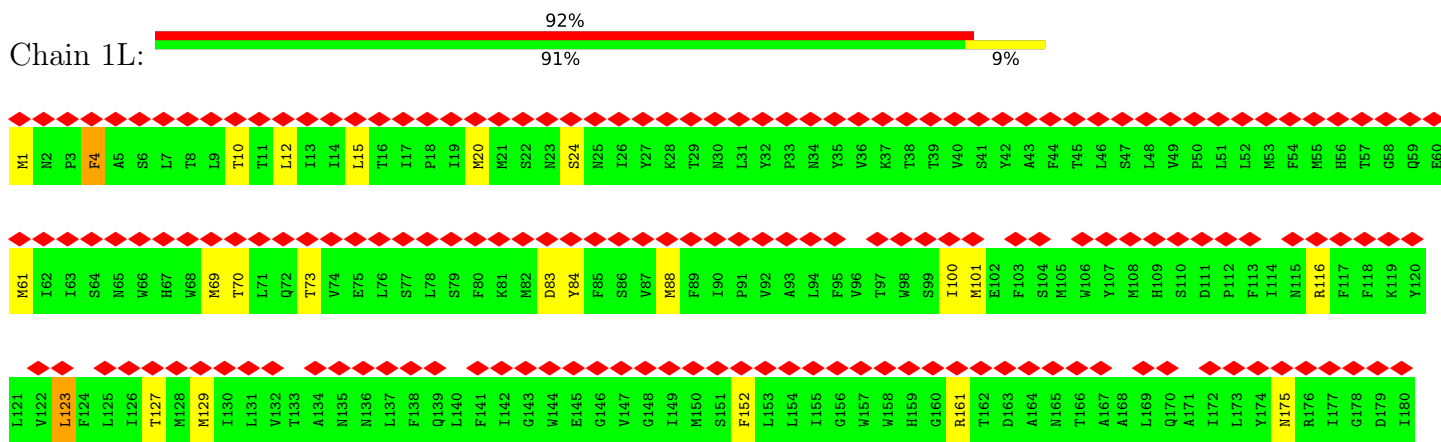
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

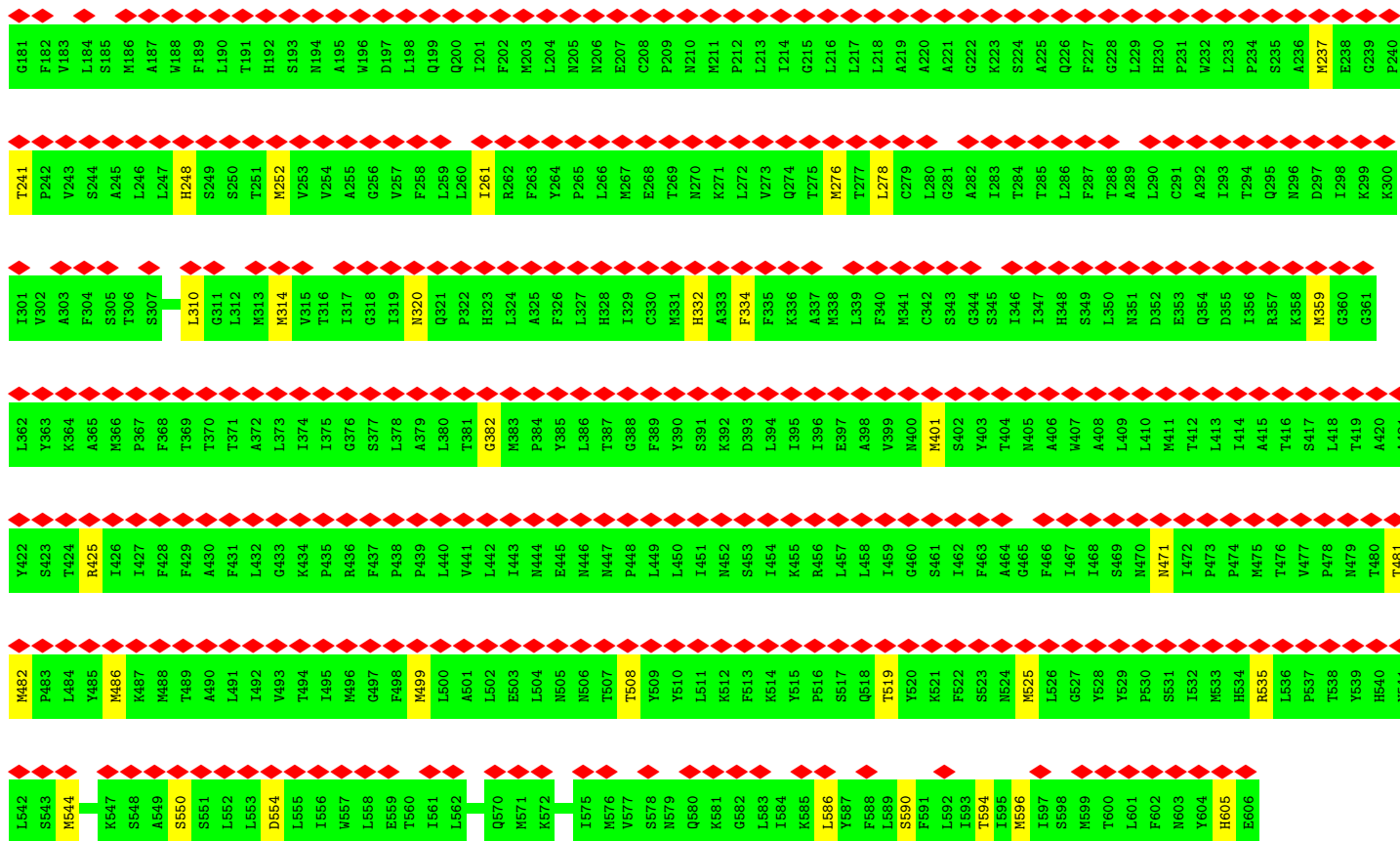


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

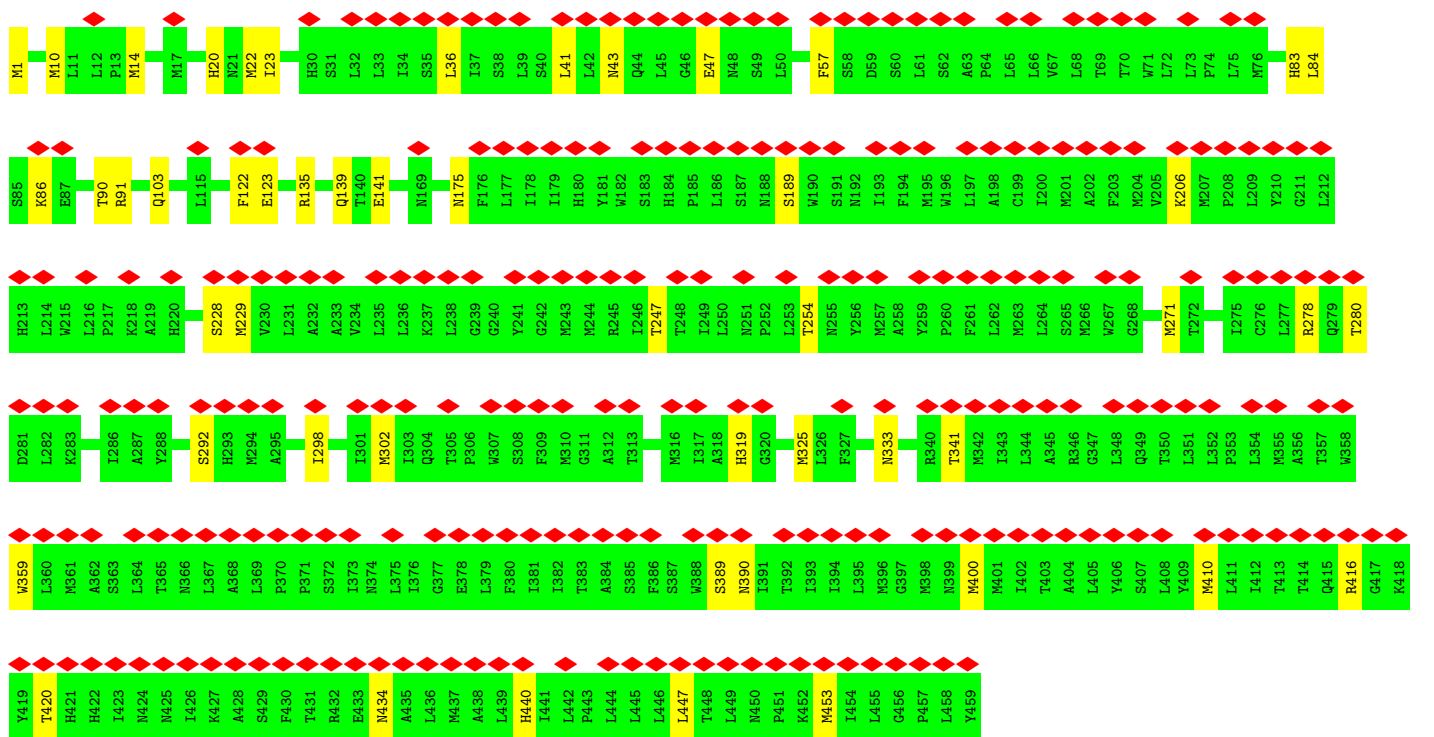
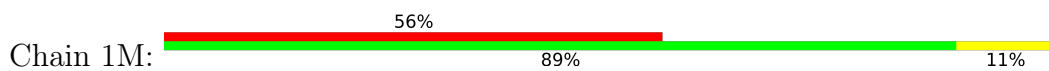


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

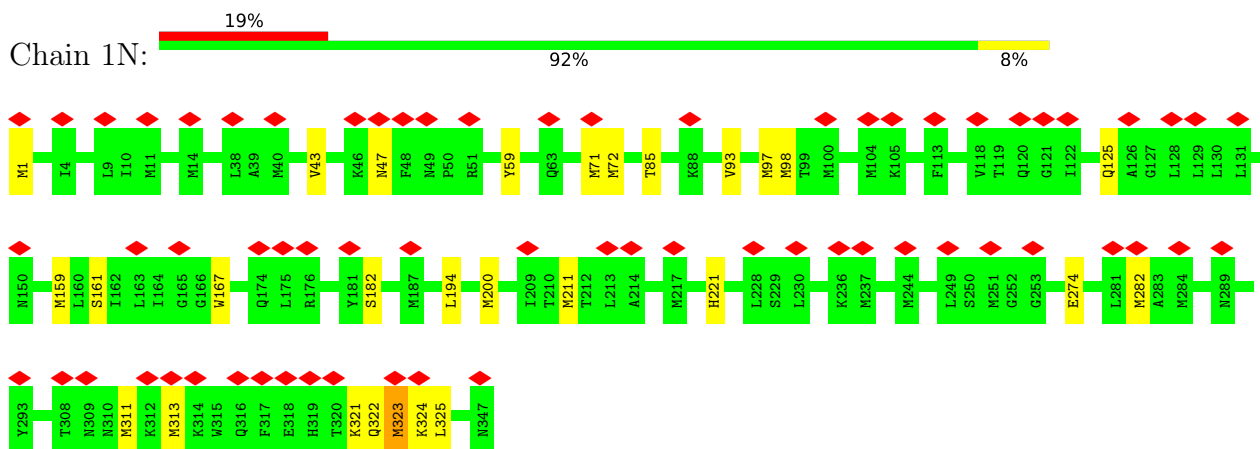




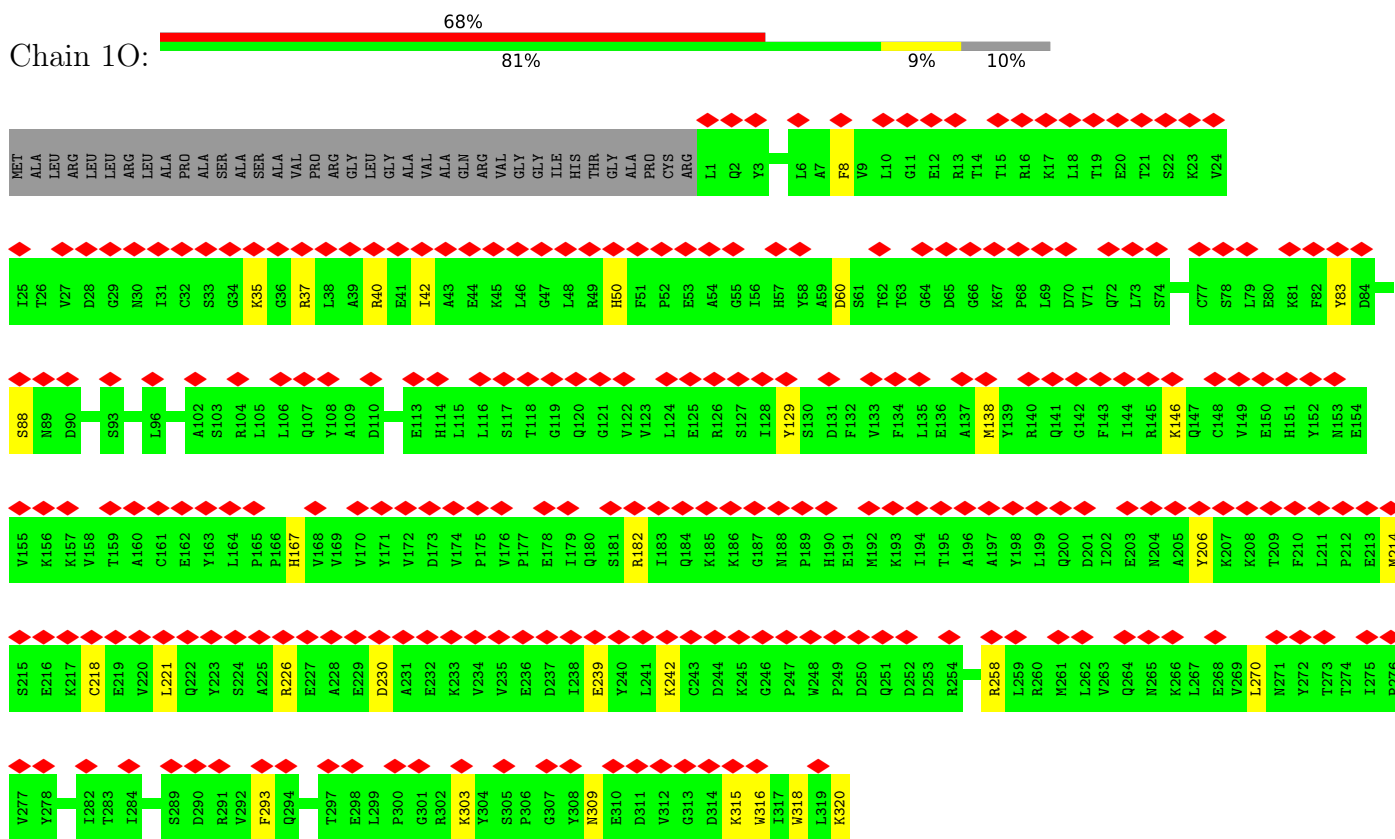
● Molecule 13: NADH-ubiquinone oxidoreductase chain 4



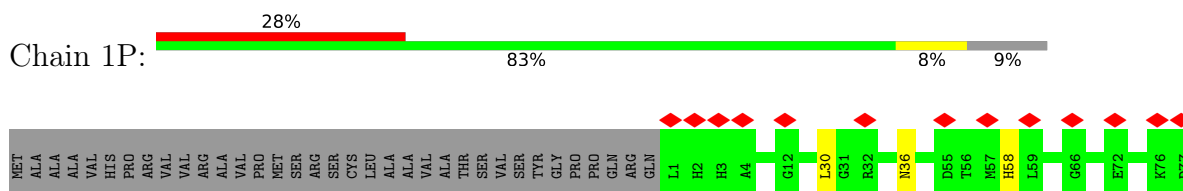
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

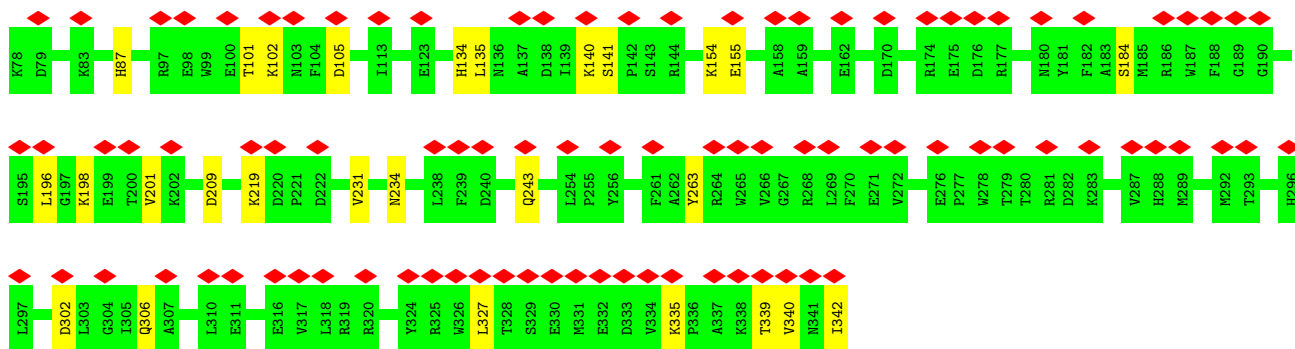


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

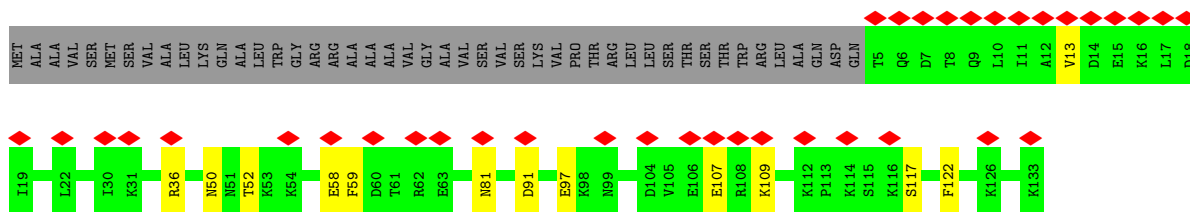


- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

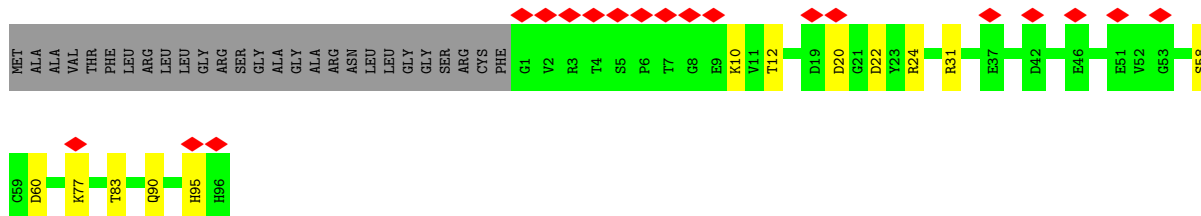




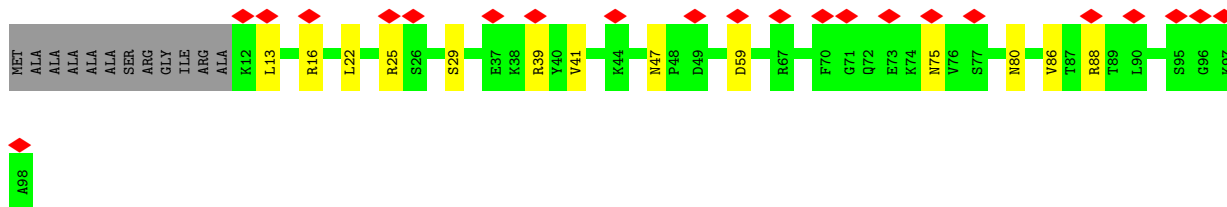
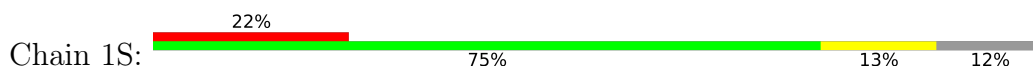
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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



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

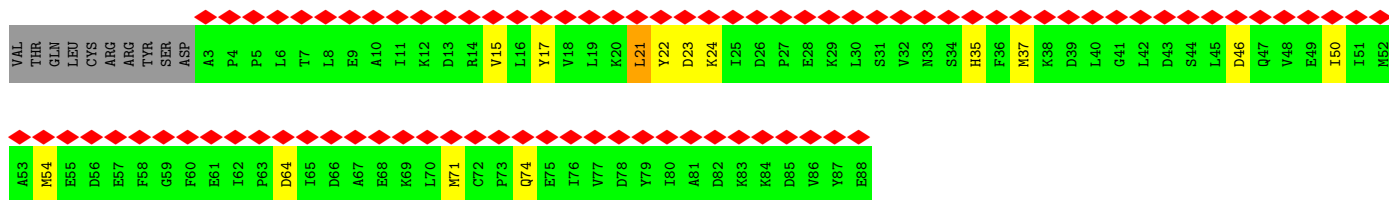


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

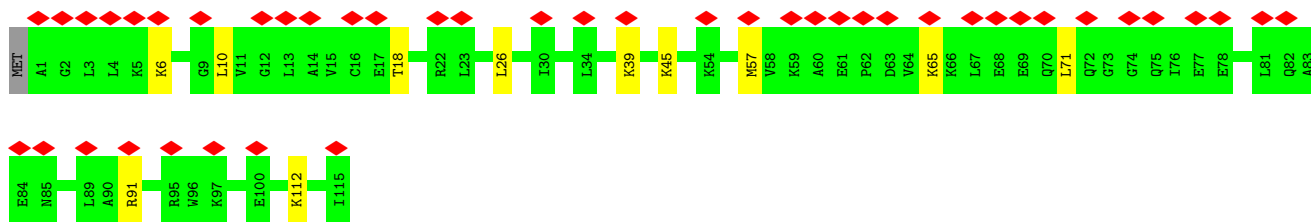
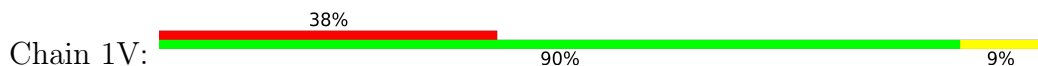




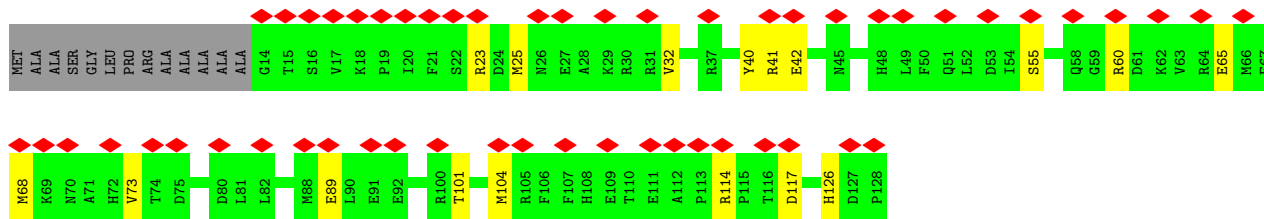
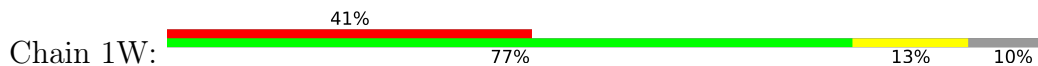
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



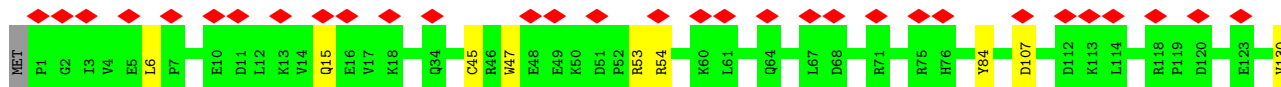
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

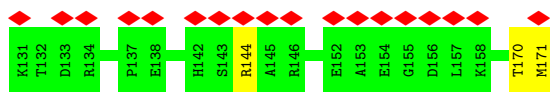


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

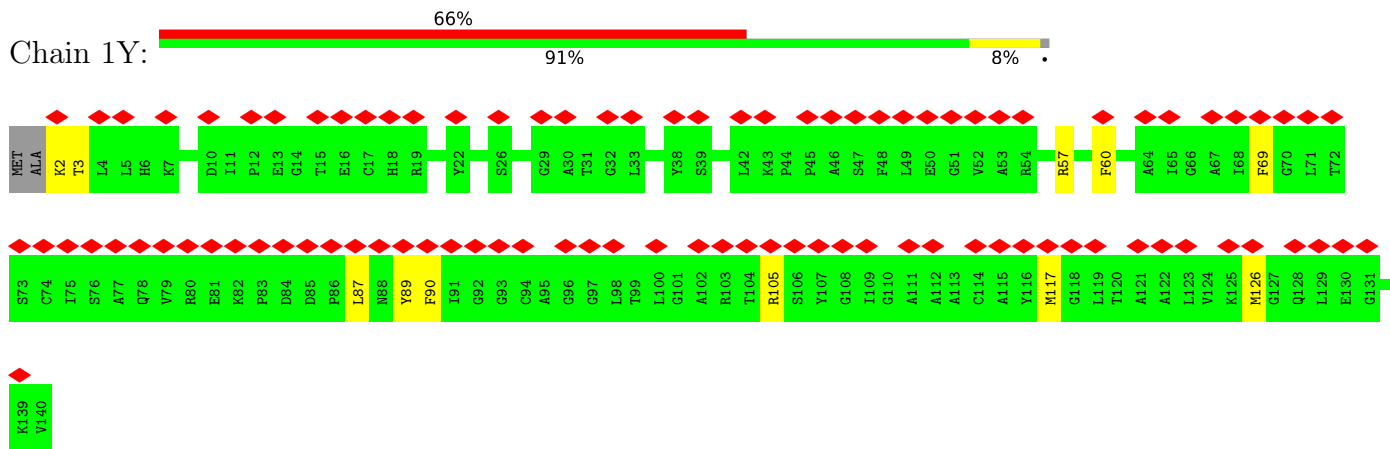


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

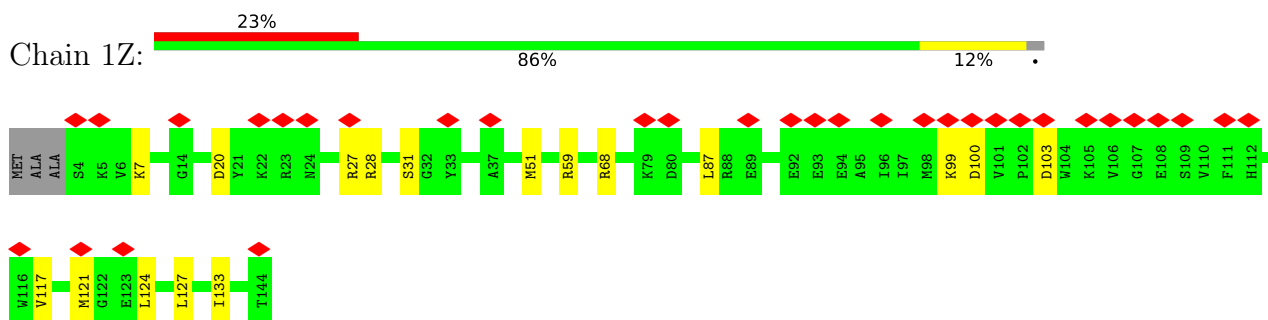




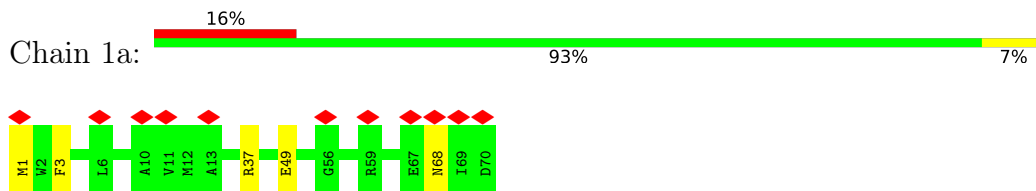
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



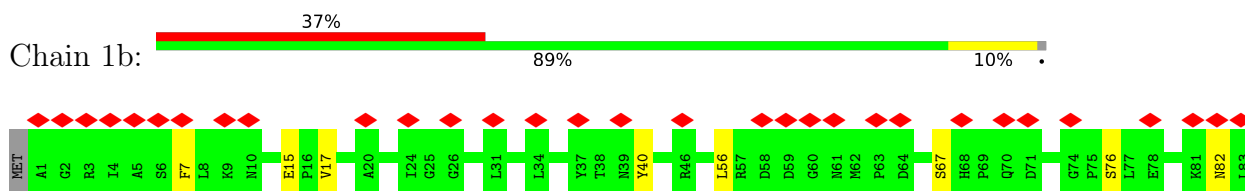
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



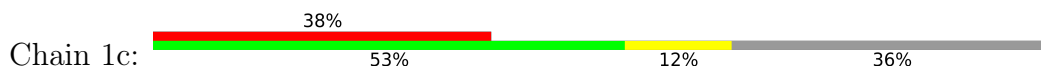
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

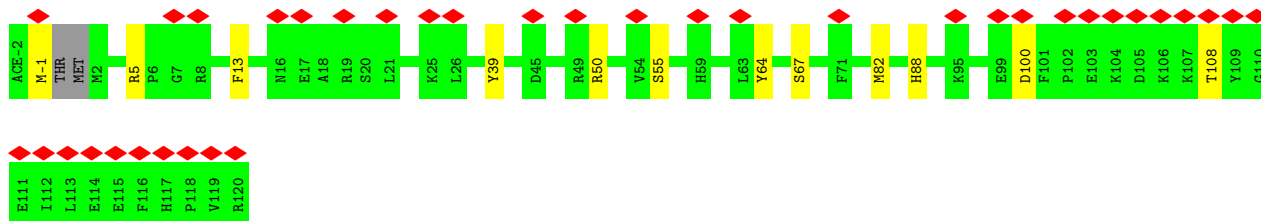
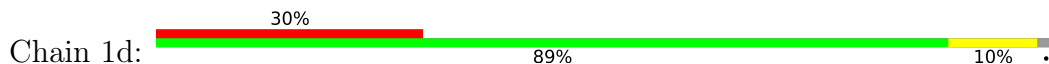


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

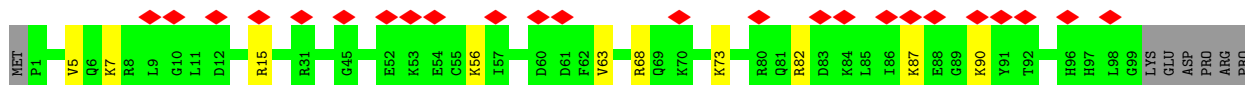
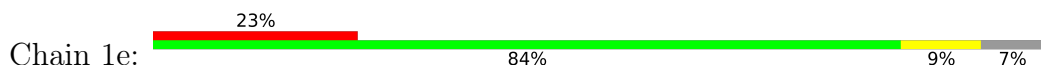




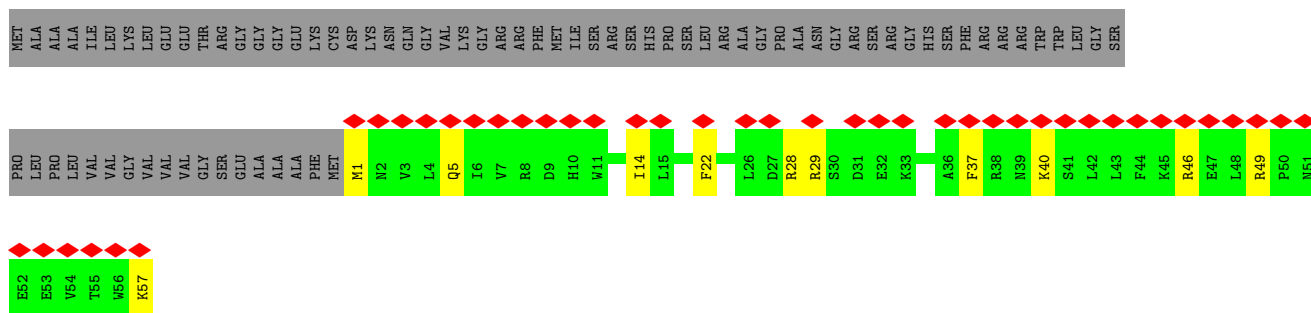
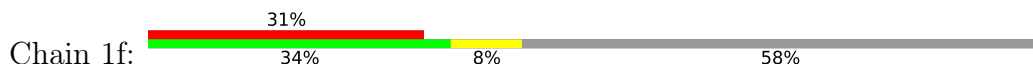
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



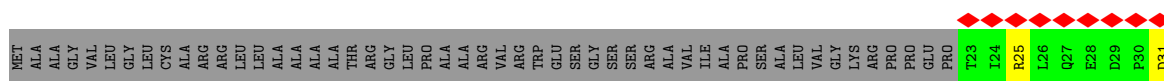
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

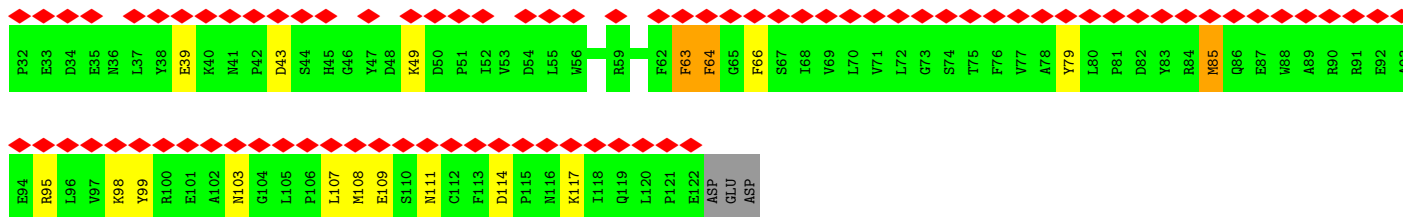


• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

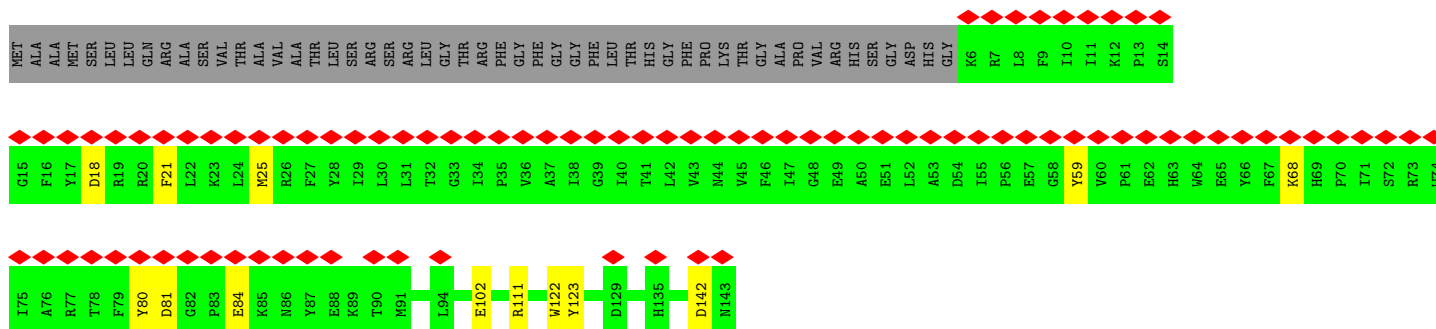


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

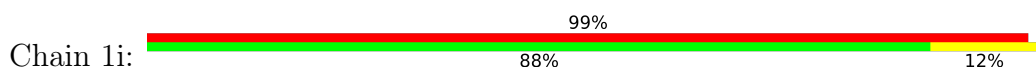




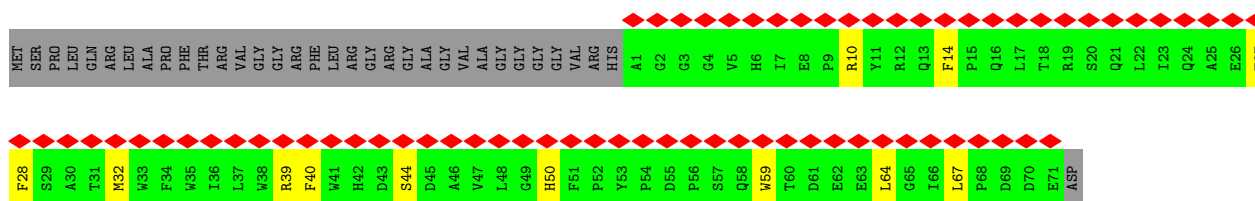
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



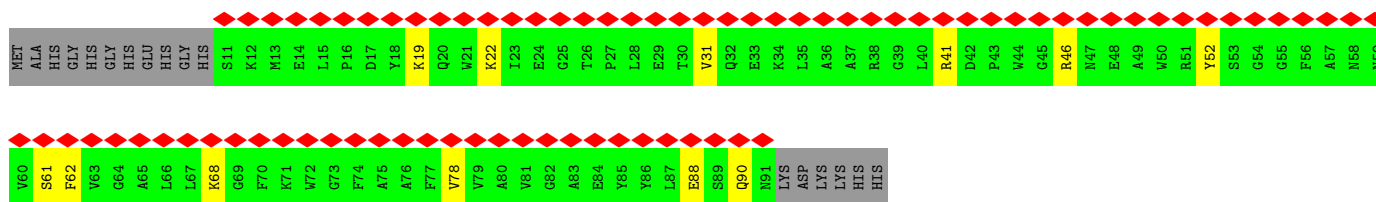
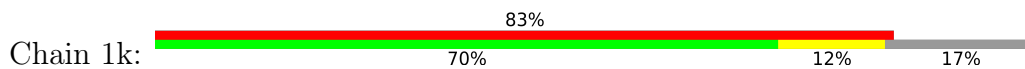
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



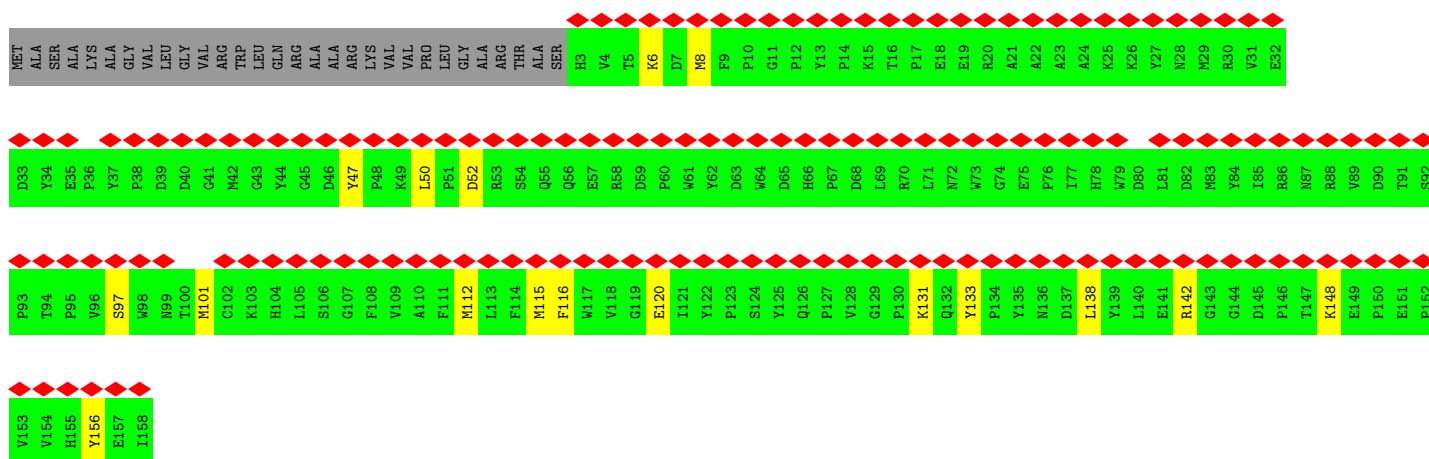
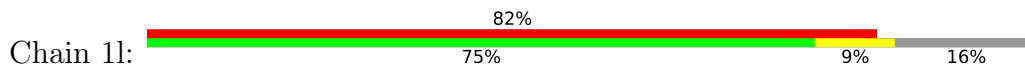
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



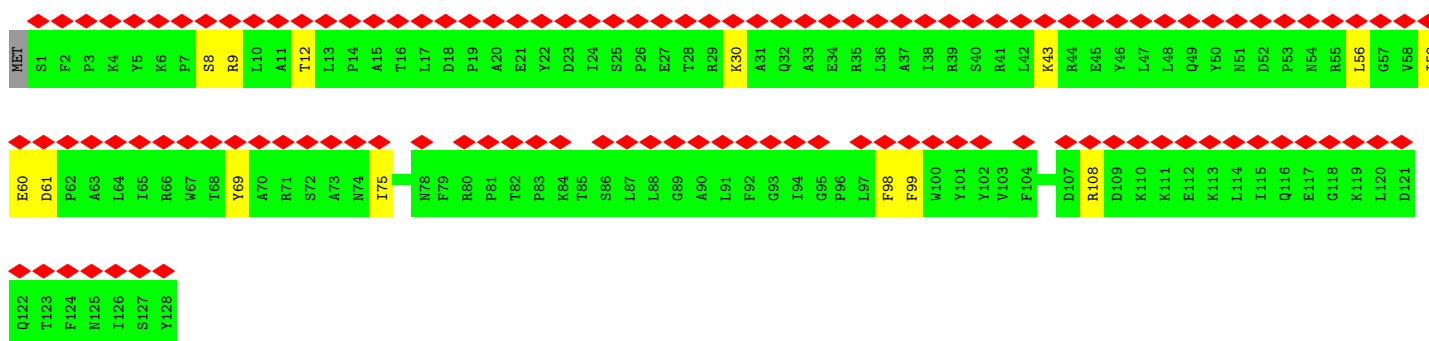
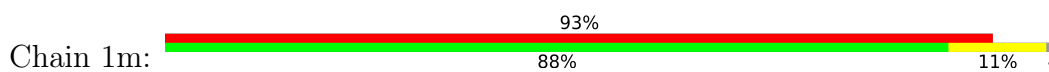
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



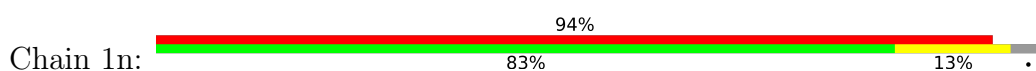
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

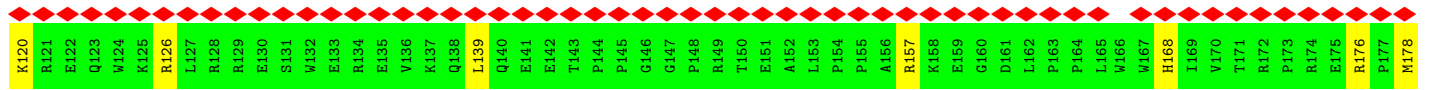
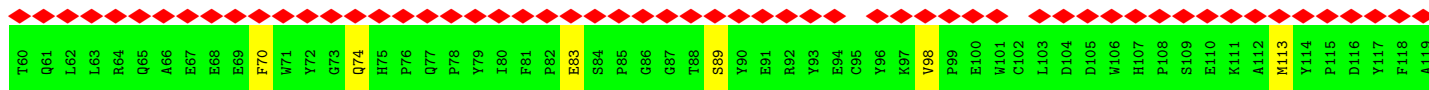


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

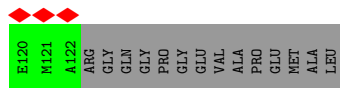
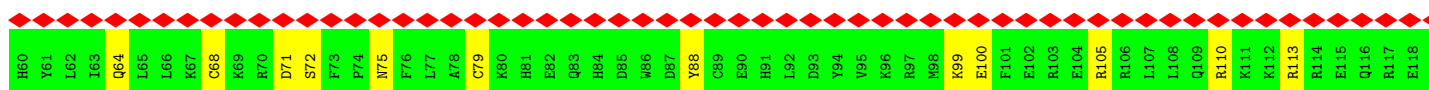
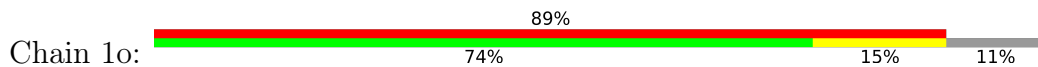


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

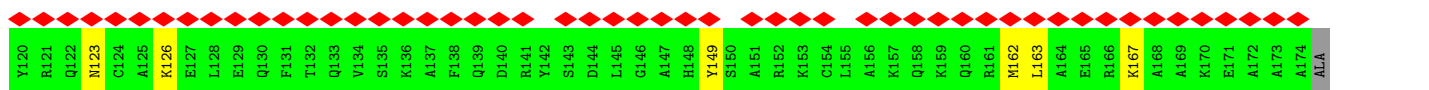
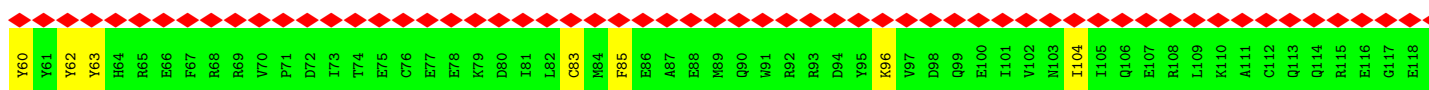
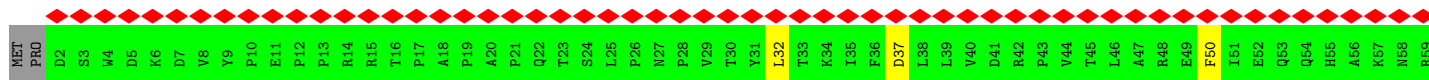
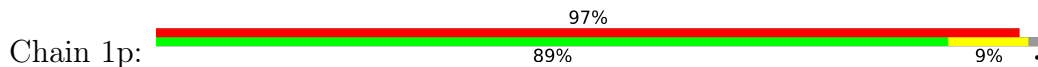




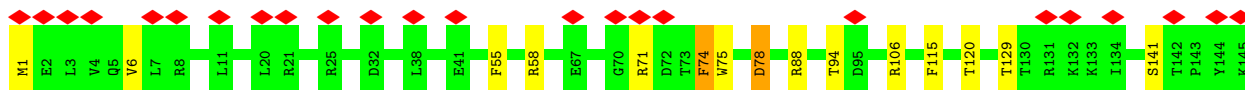
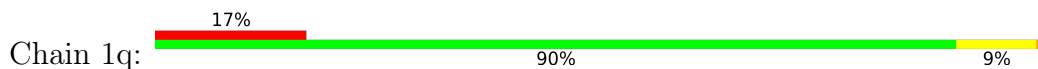
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



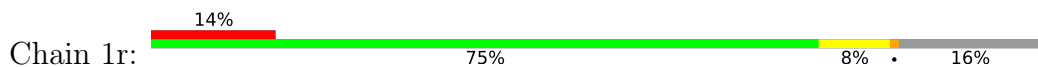
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	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	0.924	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, U10, MG, FES, 3PE, FMN, NDP, SF4, ACE, FME, SAC, GTP, K, PC1, CDL, ZN, EHZ

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	0.29	0/930	0.62	0/1271
2	1B	0.32	0/1273	0.62	0/1722
3	1C	0.29	0/1791	0.54	0/2439
4	1D	0.29	0/3545	0.53	0/4806
5	1E	0.28	0/1698	0.55	0/2311
6	1F	0.27	0/3401	0.53	0/4595
7	1G	0.27	0/5451	0.54	0/7387
8	1H	0.28	0/2566	0.54	0/3509
9	1I	0.30	0/1443	0.52	0/1952
10	1J	0.30	0/1364	0.59	0/1850
11	1K	0.28	0/751	0.68	0/1018
12	1L	0.26	0/4939	0.59	5/6718 (0.1%)
13	1M	0.26	0/3713	0.62	1/5063 (0.0%)
14	1N	0.30	0/2765	0.62	3/3758 (0.1%)
15	1O	0.29	0/2650	0.57	0/3588
16	1P	0.27	0/2828	0.52	0/3834
17	1Q	0.29	0/1070	0.56	1/1446 (0.1%)
18	1R	0.28	0/755	0.60	0/1018
19	1S	0.27	0/711	0.61	0/956
20	1T	0.30	0/701	0.72	0/946
20	1U	0.31	0/706	0.71	1/954 (0.1%)
21	1V	0.28	0/946	0.54	0/1281
22	1W	0.30	0/995	0.65	0/1340
23	1X	0.26	0/1436	0.50	0/1938
24	1Y	0.27	0/1037	0.60	0/1404
25	1Z	0.28	0/1199	0.59	0/1617
26	1a	0.26	0/577	0.49	0/777
27	1b	0.26	0/664	0.56	0/912
28	1c	0.28	0/430	0.67	0/581
29	1d	0.29	0/1024	0.55	0/1383
30	1e	0.28	0/836	0.57	0/1118
31	1f	0.29	0/499	0.70	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.34	0/858	0.71	1/1165 (0.1%)
33	1h	0.26	0/1184	0.56	0/1603
34	1i	0.29	0/1131	0.67	0/1541
35	1j	0.27	0/627	0.63	0/858
36	1k	0.26	0/668	0.54	0/903
37	1l	0.27	0/1365	0.58	1/1867 (0.1%)
38	1m	0.28	0/1092	0.55	0/1481
39	1n	0.28	0/1549	0.62	0/2098
40	1o	0.33	1/1069 (0.1%)	0.73	3/1430 (0.2%)
41	1p	0.27	0/1481	0.55	1/1997 (0.1%)
42	1q	0.29	0/1253	0.59	1/1704 (0.1%)
43	1r	0.31	0/782	0.70	1/1057 (0.1%)
44	1s	0.28	0/394	0.69	1/533 (0.2%)
All	All	0.28	1/68147 (0.0%)	0.58	20/92402 (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
6	1F	0	2
8	1H	0	1
9	1I	0	1
14	1N	0	1
42	1q	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1o	26	PRO	CG-CD	-6.41	1.29	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1o	26	PRO	N-CD-CG	-10.96	86.76	103.20
13	1M	84	LEU	CA-CB-CG	8.82	135.59	115.30
20	1U	21	LEU	CA-CB-CG	8.31	134.42	115.30
43	1r	110	PRO	CA-N-CD	-7.87	100.48	111.50
32	1g	85	MET	CB-CG-SD	7.38	134.54	112.40
14	1N	323	MET	CA-CB-CG	6.41	124.20	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1o	26	PRO	CA-CB-CG	-6.40	91.84	104.00
12	1L	310	LEU	CA-CB-CG	6.16	129.47	115.30
37	1l	138	LEU	CA-CB-CG	6.12	129.36	115.30
40	1o	26	PRO	CA-N-CD	-5.92	103.21	111.50
12	1L	123	LEU	CA-CB-CG	5.78	128.60	115.30
14	1N	323	MET	N-CA-CB	5.78	121.00	110.60
12	1L	12	LEU	CA-CB-CG	5.76	128.54	115.30
12	1L	382	GLY	C-N-CA	-5.69	107.47	121.70
17	1Q	91	ASP	CB-CG-OD2	5.44	123.19	118.30
12	1L	278	LEU	CA-CB-CG	5.30	127.49	115.30
42	1q	78	ASP	CB-CG-OD2	5.21	122.99	118.30
41	1p	163	LEU	CA-CB-CG	5.10	127.04	115.30
14	1N	159	MET	CA-CB-CG	5.04	121.87	113.30
44	1s	58	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
6	1F	207	PRO	Peptide
8	1H	141	SER	Peptide
9	1I	50	TYR	Peptide
14	1N	322	GLN	Peptide
42	1q	74	PHE	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%)	102 (90%)	10 (9%)	1 (1%)	17	56
2	1B	153/255 (60%)	138 (90%)	14 (9%)	1 (1%)	22	61
3	1C	207/264 (78%)	196 (95%)	11 (5%)	0	100	100
4	1D	427/476 (90%)	407 (95%)	20 (5%)	0	100	100
5	1E	212/249 (85%)	192 (91%)	19 (9%)	1 (0%)	29	68
6	1F	430/464 (93%)	401 (93%)	28 (6%)	1 (0%)	47	81
7	1G	697/727 (96%)	633 (91%)	62 (9%)	2 (0%)	41	75
8	1H	316/318 (99%)	299 (95%)	14 (4%)	3 (1%)	17	56
9	1I	174/239 (73%)	160 (92%)	12 (7%)	2 (1%)	14	52
10	1J	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	9	42
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	541 (90%)	62 (10%)	1 (0%)	47	81
13	1M	457/459 (100%)	431 (94%)	25 (6%)	1 (0%)	47	81
14	1N	345/347 (99%)	320 (93%)	23 (7%)	2 (1%)	25	64
15	1O	318/357 (89%)	287 (90%)	31 (10%)	0	100	100
16	1P	340/377 (90%)	316 (93%)	24 (7%)	0	100	100
17	1Q	127/175 (73%)	119 (94%)	8 (6%)	0	100	100
18	1R	94/123 (76%)	81 (86%)	13 (14%)	0	100	100
19	1S	85/99 (86%)	68 (80%)	17 (20%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	17	56
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
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%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	112 (96%)	5 (4%)	0	100	100
30	1e	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	1g	98/154 (64%)	84 (86%)	12 (12%)	2 (2%)	7	39
33	1h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	1i	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	58 (84%)	11 (16%)	0	100	100
36	1k	79/98 (81%)	71 (90%)	8 (10%)	0	100	100
37	1l	154/186 (83%)	130 (84%)	24 (16%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	157 (92%)	12 (7%)	1 (1%)	25	64
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	1q	143/145 (99%)	136 (95%)	6 (4%)	1 (1%)	22	61
43	1r	90/114 (79%)	85 (94%)	4 (4%)	1 (1%)	14	52
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
All	All	8194/9741 (84%)	7570 (92%)	600 (7%)	24 (0%)	44	75

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	46	SER
8	1H	92	PRO
8	1H	196	ALA
10	1J	113	VAL
10	1J	122	LEU
13	1M	23	ILE
14	1N	324	LYS
14	1N	323	MET
5	1E	157	ASN
7	1G	256	GLU
12	1L	4	PHE
7	1G	654	GLN
42	1q	75	TRP
2	1B	172	ARG
8	1H	208	VAL
9	1I	50	TYR
9	1I	51	PRO
32	1g	64	PHE
43	1r	110	PRO

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Mol	Chain	Res	Type
21	1V	112	LYS
32	1g	63	PHE
39	1n	31	VAL
6	1F	207	PRO
10	1J	116	ILE

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%)	84 (85%)	15 (15%)	3 17
2	1B	131/209 (63%)	118 (90%)	13 (10%)	8 33
3	1C	190/227 (84%)	176 (93%)	14 (7%)	13 44
4	1D	371/405 (92%)	335 (90%)	36 (10%)	8 33
5	1E	183/207 (88%)	161 (88%)	22 (12%)	5 24
6	1F	346/368 (94%)	317 (92%)	29 (8%)	11 40
7	1G	588/610 (96%)	538 (92%)	50 (8%)	10 39
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%)	118 (84%)	22 (16%)	2 15
11	1K	84/84 (100%)	72 (86%)	12 (14%)	3 19
12	1L	539/539 (100%)	488 (90%)	51 (10%)	8 34
13	1M	408/408 (100%)	361 (88%)	47 (12%)	5 26
14	1N	310/310 (100%)	287 (93%)	23 (7%)	13 44
15	1O	283/307 (92%)	252 (89%)	31 (11%)	6 29
16	1P	296/323 (92%)	266 (90%)	30 (10%)	7 32
17	1Q	117/152 (77%)	105 (90%)	12 (10%)	7 32
18	1R	79/97 (81%)	67 (85%)	12 (15%)	3 17
19	1S	77/82 (94%)	64 (83%)	13 (17%)	2 12
20	1T	79/133 (59%)	70 (89%)	9 (11%)	5 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1U	79/133 (59%)	65 (82%)	14 (18%)	2	10
21	1V	100/101 (99%)	90 (90%)	10 (10%)	7	32
22	1W	107/112 (96%)	90 (84%)	17 (16%)	2	14
23	1X	153/154 (99%)	141 (92%)	12 (8%)	12	42
24	1Y	101/102 (99%)	90 (89%)	11 (11%)	6	29
25	1Z	123/124 (99%)	106 (86%)	17 (14%)	3	20
26	1a	58/58 (100%)	53 (91%)	5 (9%)	10	38
27	1b	69/70 (99%)	61 (88%)	8 (12%)	5	26
28	1c	45/66 (68%)	36 (80%)	9 (20%)	1	7
29	1d	107/109 (98%)	95 (89%)	12 (11%)	6	27
30	1e	87/94 (93%)	77 (88%)	10 (12%)	5	26
31	1f	54/113 (48%)	43 (80%)	11 (20%)	1	6
32	1g	92/129 (71%)	72 (78%)	20 (22%)	1	5
33	1h	121/158 (77%)	108 (89%)	13 (11%)	6	30
34	1i	119/120 (99%)	105 (88%)	14 (12%)	5	25
35	1j	62/84 (74%)	50 (81%)	12 (19%)	1	7
36	1k	63/76 (83%)	51 (81%)	12 (19%)	1	8
37	1l	141/161 (88%)	125 (89%)	16 (11%)	6	27
38	1m	113/114 (99%)	99 (88%)	14 (12%)	4	23
39	1n	156/160 (98%)	134 (86%)	22 (14%)	3	19
40	1o	110/120 (92%)	90 (82%)	20 (18%)	1	9
41	1p	154/156 (99%)	139 (90%)	15 (10%)	8	33
42	1q	131/131 (100%)	117 (89%)	14 (11%)	6	30
43	1r	85/98 (87%)	76 (89%)	9 (11%)	6	30
44	1s	44/351 (12%)	36 (82%)	8 (18%)	1	9
All	All	7219/8269 (87%)	6415 (89%)	804 (11%)	9	28

All (804) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	4	MET
1	1A	17	LEU
1	1A	39	CYS

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Mol	Chain	Res	Type
1	1A	42	ASP
1	1A	44	MET
1	1A	48	ARG
1	1A	49	LEU
1	1A	53	MET
1	1A	58	VAL
1	1A	60	ILE
1	1A	68	GLU
1	1A	79	SER
1	1A	87	MET
1	1A	97	LEU
1	1A	113	TRP
2	1B	54	CYS
2	1B	55	CYS
2	1B	69	MET
2	1B	75	VAL
2	1B	81	ARG
2	1B	87	ILE
2	1B	102	LYS
2	1B	126	TYR
2	1B	130	TYR
2	1B	137	ASP
2	1B	146	VAL
2	1B	158	TYR
2	1B	174	ARG
3	1C	7	THR
3	1C	8	ARG
3	1C	28	TYR
3	1C	42	VAL
3	1C	43	SER
3	1C	44	CYS
3	1C	71	GLN
3	1C	81	VAL
3	1C	103	SER
3	1C	109	THR
3	1C	125	LYS
3	1C	129	TRP
3	1C	198	ASP
3	1C	199	LEU
4	1D	19	MET
4	1D	20	TYR
4	1D	42	THR

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Mol	Chain	Res	Type
4	1D	43	LEU
4	1D	55	HIS
4	1D	65	VAL
4	1D	72	MET
4	1D	85	ARG
4	1D	109	VAL
4	1D	128	ILE
4	1D	145	THR
4	1D	170	MET
4	1D	178	PHE
4	1D	181	TYR
4	1D	209	ASP
4	1D	220	PHE
4	1D	239	THR
4	1D	241	ASP
4	1D	244	VAL
4	1D	246	THR
4	1D	256	SER
4	1D	263	SER
4	1D	271	LYS
4	1D	284	ASP
4	1D	293	CYS
4	1D	295	ASP
4	1D	299	CYS
4	1D	323	ILE
4	1D	331	SER
4	1D	335	ARG
4	1D	342	MET
4	1D	368	GLU
4	1D	387	TYR
4	1D	411	LEU
4	1D	429	ASP
4	1D	430	ARG
5	1E	10	ARG
5	1E	18	ASP
5	1E	22	ASP
5	1E	36	LYS
5	1E	48	LEU
5	1E	89	MET
5	1E	97	LYS
5	1E	105	THR
5	1E	109	MET

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Mol	Chain	Res	Type
5	1E	114	ASP
5	1E	126	ILE
5	1E	127	LYS
5	1E	128	VAL
5	1E	131	THR
5	1E	134	ASP
5	1E	153	MET
5	1E	155	GLN
5	1E	167	LYS
5	1E	187	ARG
5	1E	201	SER
5	1E	209	PRO
5	1E	211	PHE
6	1F	8	LYS
6	1F	14	SER
6	1F	43	TYR
6	1F	54	ASP
6	1F	61	LYS
6	1F	73	PHE
6	1F	77	LEU
6	1F	112	ARG
6	1F	127	ARG
6	1F	147	SER
6	1F	157	TYR
6	1F	173	PHE
6	1F	212	ASP
6	1F	235	CYS
6	1F	242	PHE
6	1F	278	GLU
6	1F	287	VAL
6	1F	320	ASP
6	1F	331	THR
6	1F	337	MET
6	1F	341	THR
6	1F	345	LYS
6	1F	359	CYS
6	1F	397	LYS
6	1F	426	LEU
6	1F	429	ARG
6	1F	430	MET
6	1F	437	HIS
6	1F	438	GLN

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Mol	Chain	Res	Type
7	1G	17	SER
7	1G	25	THR
7	1G	35	MET
7	1G	45	ARG
7	1G	47	SER
7	1G	61	LYS
7	1G	64	LYS
7	1G	74	MET
7	1G	83	SER
7	1G	123	PHE
7	1G	127	ARG
7	1G	129	ARG
7	1G	130	PHE
7	1G	140	LYS
7	1G	156	CYS
7	1G	177	ARG
7	1G	181	MET
7	1G	190	MET
7	1G	215	PHE
7	1G	216	THR
7	1G	218	ARG
7	1G	229	ASP
7	1G	236	SER
7	1G	248	MET
7	1G	309	SER
7	1G	385	ARG
7	1G	402	ASN
7	1G	420	ASP
7	1G	425	SER
7	1G	434	SER
7	1G	448	LYS
7	1G	486	ASP
7	1G	511	VAL
7	1G	520	LYS
7	1G	523	PHE
7	1G	537	LEU
7	1G	548	HIS
7	1G	551	ASP
7	1G	592	LEU
7	1G	609	MET
7	1G	613	TYR
7	1G	620	ARG

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Mol	Chain	Res	Type
7	1G	632	ARG
7	1G	636	VAL
7	1G	640	ASN
7	1G	649	SER
7	1G	659	ASP
7	1G	681	SER
7	1G	698	VAL
7	1G	703	ILE
8	1H	32	GLN
8	1H	45	LEU
8	1H	58	LYS
8	1H	91	MET
8	1H	123	SER
8	1H	126	LYS
8	1H	134	ARG
8	1H	142	TYR
8	1H	152	SER
8	1H	157	ASN
8	1H	161	THR
8	1H	165	LEU
8	1H	174	MET
8	1H	224	PHE
8	1H	225	MET
8	1H	237	PHE
8	1H	256	THR
8	1H	271	LEU
8	1H	274	ARG
8	1H	282	TYR
8	1H	286	MET
8	1H	291	LYS
8	1H	292	SER
8	1H	296	LEU
9	1I	7	MET
9	1I	8	ARG
9	1I	13	ASP
9	1I	18	THR
9	1I	25	LEU
9	1I	40	TYR
9	1I	43	ARG
9	1I	58	SER
9	1I	67	LEU
9	1I	105	ARG

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Mol	Chain	Res	Type
9	1I	122	CYS
9	1I	126	CYS
9	1I	132	VAL
9	1I	137	PHE
10	1J	3	MET
10	1J	4	TYR
10	1J	17	PHE
10	1J	20	PHE
10	1J	58	LEU
10	1J	60	TYR
10	1J	78	MET
10	1J	82	VAL
10	1J	87	LYS
10	1J	90	PHE
10	1J	93	PHE
10	1J	98	MET
10	1J	100	GLU
10	1J	101	PHE
10	1J	105	TYR
10	1J	130	THR
10	1J	132	ASP
10	1J	139	GLU
10	1J	141	MET
10	1J	165	VAL
10	1J	171	ILE
10	1J	173	ARG
11	1K	10	MET
11	1K	22	TYR
11	1K	29	SER
11	1K	43	MET
11	1K	53	PHE
11	1K	54	THR
11	1K	59	MET
11	1K	75	LEU
11	1K	80	MET
11	1K	88	ASP
11	1K	89	TYR
11	1K	95	LEU
12	1L	4	PHE
12	1L	10	THR
12	1L	15	LEU
12	1L	20	MET

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Mol	Chain	Res	Type
12	1L	24	SER
12	1L	61	MET
12	1L	69	MET
12	1L	70	THR
12	1L	73	THR
12	1L	83	ASP
12	1L	84	TYR
12	1L	88	MET
12	1L	100	ILE
12	1L	101	MET
12	1L	116	ARG
12	1L	123	LEU
12	1L	127	THR
12	1L	129	MET
12	1L	152	PHE
12	1L	161	ARG
12	1L	175	ASN
12	1L	237	MET
12	1L	241	THR
12	1L	248	HIS
12	1L	252	MET
12	1L	261	ILE
12	1L	276	MET
12	1L	314	MET
12	1L	320	ASN
12	1L	332	HIS
12	1L	334	PHE
12	1L	359	MET
12	1L	401	MET
12	1L	425	ARG
12	1L	471	ASN
12	1L	481	THR
12	1L	482	MET
12	1L	486	MET
12	1L	499	MET
12	1L	508	THR
12	1L	519	THR
12	1L	525	MET
12	1L	535	ARG
12	1L	544	MET
12	1L	550	SER
12	1L	554	ASP

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Mol	Chain	Res	Type
12	1L	586	LEU
12	1L	590	SER
12	1L	594	THR
12	1L	596	MET
12	1L	605	HIS
13	1M	10	MET
13	1M	14	MET
13	1M	20	HIS
13	1M	22	MET
13	1M	36	LEU
13	1M	41	LEU
13	1M	43	ASN
13	1M	47	GLU
13	1M	57	PHE
13	1M	83	HIS
13	1M	86	LYS
13	1M	90	THR
13	1M	91	ARG
13	1M	103	GLN
13	1M	122	PHE
13	1M	123	GLU
13	1M	135	ARG
13	1M	139	GLN
13	1M	141	GLU
13	1M	175	ASN
13	1M	189	SER
13	1M	206	LYS
13	1M	228	SER
13	1M	229	MET
13	1M	247	THR
13	1M	254	THR
13	1M	271	MET
13	1M	278	ARG
13	1M	280	THR
13	1M	292	SER
13	1M	298	ILE
13	1M	302	MET
13	1M	319	HIS
13	1M	325	MET
13	1M	333	ASN
13	1M	341	THR
13	1M	359	TRP

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Mol	Chain	Res	Type
13	1M	389	SER
13	1M	390	ASN
13	1M	400	MET
13	1M	410	MET
13	1M	416	ARG
13	1M	420	THR
13	1M	434	ASN
13	1M	440	HIS
13	1M	447	LEU
13	1M	453	MET
14	1N	43	VAL
14	1N	47	ASN
14	1N	59	TYR
14	1N	71	MET
14	1N	72	MET
14	1N	85	THR
14	1N	93	VAL
14	1N	97	MET
14	1N	98	MET
14	1N	125	GLN
14	1N	161	SER
14	1N	167	TRP
14	1N	182	SER
14	1N	194	LEU
14	1N	200	MET
14	1N	211	MET
14	1N	221	HIS
14	1N	274	GLU
14	1N	282	MET
14	1N	311	MET
14	1N	313	MET
14	1N	321	LYS
14	1N	325	LEU
15	1O	8	PHE
15	1O	35	LYS
15	1O	37	ARG
15	1O	40	ARG
15	1O	42	ILE
15	1O	50	HIS
15	1O	60	ASP
15	1O	83	TYR
15	1O	88	SER

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Mol	Chain	Res	Type
15	1O	129	TYR
15	1O	138	MET
15	1O	146	LYS
15	1O	167	HIS
15	1O	182	ARG
15	1O	206	TYR
15	1O	214	MET
15	1O	218	CYS
15	1O	221	LEU
15	1O	226	ARG
15	1O	230	ASP
15	1O	239	GLU
15	1O	242	LYS
15	1O	258	ARG
15	1O	270	LEU
15	1O	293	PHE
15	1O	303	LYS
15	1O	309	ASN
15	1O	315	LYS
15	1O	316	TRP
15	1O	318	TRP
15	1O	320	LYS
16	1P	30	LEU
16	1P	36	ASN
16	1P	58	HIS
16	1P	87	HIS
16	1P	101	THR
16	1P	102	LYS
16	1P	105	ASP
16	1P	134	HIS
16	1P	135	LEU
16	1P	140	LYS
16	1P	141	SER
16	1P	154	LYS
16	1P	155	GLU
16	1P	184	SER
16	1P	196	LEU
16	1P	198	LYS
16	1P	201	VAL
16	1P	209	ASP
16	1P	219	LYS
16	1P	231	VAL

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Mol	Chain	Res	Type
16	1P	234	ASN
16	1P	243	GLN
16	1P	263	TYR
16	1P	302	ASP
16	1P	306	GLN
16	1P	327	LEU
16	1P	335	LYS
16	1P	339	THR
16	1P	340	VAL
16	1P	342	ILE
17	1Q	13	VAL
17	1Q	36	ARG
17	1Q	50	ASN
17	1Q	52	THR
17	1Q	58	GLU
17	1Q	59	PHE
17	1Q	81	ASN
17	1Q	97	GLU
17	1Q	107	GLU
17	1Q	109	LYS
17	1Q	117	SER
17	1Q	122	PHE
18	1R	10	LYS
18	1R	12	THR
18	1R	20	ASP
18	1R	22	ASP
18	1R	24	ARG
18	1R	31	ARG
18	1R	58	SER
18	1R	60	ASP
18	1R	77	LYS
18	1R	83	THR
18	1R	90	GLN
18	1R	95	HIS
19	1S	13	LEU
19	1S	16	ARG
19	1S	22	LEU
19	1S	25	ARG
19	1S	29	SER
19	1S	39	ARG
19	1S	41	VAL
19	1S	47	ASN

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Mol	Chain	Res	Type
19	1S	59	ASP
19	1S	75	ASN
19	1S	80	ASN
19	1S	86	VAL
19	1S	88	ARG
20	1T	7	THR
20	1T	17	TYR
20	1T	22	TYR
20	1T	24	LYS
20	1T	31	SER
20	1T	47	GLN
20	1T	64	ASP
20	1T	69	LYS
20	1T	79	TYR
20	1U	15	VAL
20	1U	17	TYR
20	1U	21	LEU
20	1U	22	TYR
20	1U	23	ASP
20	1U	24	LYS
20	1U	35	HIS
20	1U	37	MET
20	1U	46	ASP
20	1U	50	ILE
20	1U	54	MET
20	1U	64	ASP
20	1U	71	MET
20	1U	74	GLN
21	1V	6	LYS
21	1V	10	LEU
21	1V	18	THR
21	1V	26	LEU
21	1V	39	LYS
21	1V	45	LYS
21	1V	57	MET
21	1V	65	LYS
21	1V	71	LEU
21	1V	91	ARG
22	1W	23	ARG
22	1W	25	MET
22	1W	32	VAL
22	1W	40	TYR

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Mol	Chain	Res	Type
22	1W	41	ARG
22	1W	42	GLU
22	1W	55	SER
22	1W	60	ARG
22	1W	65	GLU
22	1W	68	MET
22	1W	73	VAL
22	1W	89	GLU
22	1W	101	THR
22	1W	104	MET
22	1W	114	ARG
22	1W	117	ASP
22	1W	126	HIS
23	1X	6	LEU
23	1X	15	GLN
23	1X	45	CYS
23	1X	47	TRP
23	1X	53	ARG
23	1X	54	ARG
23	1X	84	TYR
23	1X	107	ASP
23	1X	130	VAL
23	1X	144	ARG
23	1X	170	THR
23	1X	171	MET
24	1Y	2	LYS
24	1Y	3	THR
24	1Y	57	ARG
24	1Y	60	PHE
24	1Y	69	PHE
24	1Y	87	LEU
24	1Y	89	TYR
24	1Y	90	PHE
24	1Y	105	ARG
24	1Y	117	MET
24	1Y	126	MET
25	1Z	7	LYS
25	1Z	20	ASP
25	1Z	27	ARG
25	1Z	28	ARG
25	1Z	31	SER
25	1Z	51	MET

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Mol	Chain	Res	Type
25	1Z	59	ARG
25	1Z	68	ARG
25	1Z	87	LEU
25	1Z	99	LYS
25	1Z	100	ASP
25	1Z	103	ASP
25	1Z	117	VAL
25	1Z	121	MET
25	1Z	124	LEU
25	1Z	127	LEU
25	1Z	133	ILE
26	1a	1	MET
26	1a	3	PHE
26	1a	37	ARG
26	1a	49	GLU
26	1a	68	ASN
27	1b	7	PHE
27	1b	15	GLU
27	1b	17	VAL
27	1b	40	TYR
27	1b	56	LEU
27	1b	67	SER
27	1b	76	SER
27	1b	82	ASN
28	1c	1	LYS
28	1c	2	PHE
28	1c	5	ARG
28	1c	15	LEU
28	1c	26	PHE
28	1c	30	TYR
28	1c	40	LEU
28	1c	42	TYR
28	1c	44	ARG
29	1d	-1	MET
29	1d	5	ARG
29	1d	13	PHE
29	1d	39	TYR
29	1d	50	ARG
29	1d	55	SER
29	1d	64	TYR
29	1d	67	SER
29	1d	82	MET

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Mol	Chain	Res	Type
29	1d	88	HIS
29	1d	100	ASP
29	1d	108	THR
30	1e	5	VAL
30	1e	7	LYS
30	1e	15	ARG
30	1e	56	LYS
30	1e	63	VAL
30	1e	68	ARG
30	1e	73	LYS
30	1e	82	ARG
30	1e	87	LYS
30	1e	90	LYS
31	1f	1	MET
31	1f	5	GLN
31	1f	14	ILE
31	1f	22	PHE
31	1f	28	ARG
31	1f	29	ARG
31	1f	37	PHE
31	1f	40	LYS
31	1f	46	ARG
31	1f	49	ARG
31	1f	57	LYS
32	1g	25	ARG
32	1g	31	ASP
32	1g	39	GLU
32	1g	43	ASP
32	1g	49	LYS
32	1g	63	PHE
32	1g	64	PHE
32	1g	66	PHE
32	1g	79	TYR
32	1g	85	MET
32	1g	95	ARG
32	1g	98	LYS
32	1g	99	TYR
32	1g	103	ASN
32	1g	107	LEU
32	1g	108	MET
32	1g	109	GLU
32	1g	111	ASN

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Mol	Chain	Res	Type
32	1g	114	ASP
32	1g	117	LYS
33	1h	18	ASP
33	1h	21	PHE
33	1h	25	MET
33	1h	59	TYR
33	1h	68	LYS
33	1h	80	TYR
33	1h	81	ASP
33	1h	84	GLU
33	1h	102	GLU
33	1h	111	ARG
33	1h	122	TRP
33	1h	123	TYR
33	1h	142	ASP
34	1i	3	TYR
34	1i	13	GLN
34	1i	23	LYS
34	1i	24	ASP
34	1i	30	ARG
34	1i	42	MET
34	1i	48	LYS
34	1i	69	PHE
34	1i	86	LYS
34	1i	100	LYS
34	1i	104	PHE
34	1i	112	THR
34	1i	116	ILE
34	1i	126	HIS
35	1j	10	ARG
35	1j	14	PHE
35	1j	27	PHE
35	1j	28	PHE
35	1j	32	MET
35	1j	39	ARG
35	1j	40	PHE
35	1j	44	SER
35	1j	50	HIS
35	1j	59	TRP
35	1j	64	LEU
35	1j	67	LEU
36	1k	19	LYS

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Mol	Chain	Res	Type
36	1k	22	LYS
36	1k	31	VAL
36	1k	41	ARG
36	1k	46	ARG
36	1k	52	TYR
36	1k	61	SER
36	1k	62	PHE
36	1k	68	LYS
36	1k	78	VAL
36	1k	88	GLU
36	1k	90	GLN
37	1l	6	LYS
37	1l	8	MET
37	1l	47	TYR
37	1l	50	LEU
37	1l	52	ASP
37	1l	97	SER
37	1l	101	MET
37	1l	112	MET
37	1l	115	MET
37	1l	116	PHE
37	1l	120	GLU
37	1l	131	LYS
37	1l	133	TYR
37	1l	142	ARG
37	1l	148	LYS
37	1l	156	TYR
38	1m	8	SER
38	1m	9	ARG
38	1m	12	THR
38	1m	30	LYS
38	1m	43	LYS
38	1m	56	LEU
38	1m	59	ILE
38	1m	60	GLU
38	1m	61	ASP
38	1m	69	TYR
38	1m	75	ILE
38	1m	98	PHE
38	1m	99	PHE
38	1m	108	ARG
39	1n	8	TYR

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Mol	Chain	Res	Type
39	1n	12	GLN
39	1n	21	ARG
39	1n	37	ARG
39	1n	47	PHE
39	1n	48	ASP
39	1n	49	GLU
39	1n	54	LYS
39	1n	56	MET
39	1n	70	PHE
39	1n	74	GLN
39	1n	83	GLU
39	1n	89	SER
39	1n	98	VAL
39	1n	113	MET
39	1n	120	LYS
39	1n	126	ARG
39	1n	139	LEU
39	1n	157	ARG
39	1n	168	HIS
39	1n	176	ARG
39	1n	178	MET
40	1o	19	LEU
40	1o	28	TYR
40	1o	30	PHE
40	1o	38	MET
40	1o	41	THR
40	1o	45	MET
40	1o	51	MET
40	1o	58	CYS
40	1o	64	GLN
40	1o	68	CYS
40	1o	71	ASP
40	1o	72	SER
40	1o	75	ASN
40	1o	79	CYS
40	1o	88	TYR
40	1o	99	LYS
40	1o	100	GLU
40	1o	105	ARG
40	1o	110	ARG
40	1o	113	ARG
41	1p	32	LEU

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Mol	Chain	Res	Type
41	1p	37	ASP
41	1p	50	PHE
41	1p	60	TYR
41	1p	62	TYR
41	1p	63	TYR
41	1p	83	CYS
41	1p	85	PHE
41	1p	96	LYS
41	1p	104	ILE
41	1p	123	ASN
41	1p	126	LYS
41	1p	149	TYR
41	1p	162	MET
41	1p	167	LYS
42	1q	1	MET
42	1q	6	VAL
42	1q	55	PHE
42	1q	58	ARG
42	1q	71	ARG
42	1q	74	PHE
42	1q	78	ASP
42	1q	88	ARG
42	1q	94	THR
42	1q	106	ARG
42	1q	115	PHE
42	1q	120	THR
42	1q	129	THR
42	1q	141	SER
43	1r	10	LEU
43	1r	23	LEU
43	1r	32	LYS
43	1r	49	SER
43	1r	53	TYR
43	1r	54	CYS
43	1r	63	MET
43	1r	102	ARG
43	1r	108	ASP
44	1s	39	ARG
44	1s	40	ASN
44	1s	41	LEU
44	1s	43	HIS
44	1s	51	PHE

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Mol	Chain	Res	Type
44	1s	58	LEU
44	1s	71	GLN
44	1s	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	61	HIS
5	1E	91	ASN
5	1E	101	GLN
5	1E	214	GLN
6	1F	150	GLN
6	1F	200	GLN
6	1F	436	GLN
7	1G	36	GLN
7	1G	100	ASN
7	1G	101	HIS
7	1G	436	ASN
7	1G	459	GLN
7	1G	517	ASN
7	1G	618	GLN
10	1J	120	ASN
11	1K	50	ASN
12	1L	34	ASN
12	1L	248	HIS
13	1M	293	HIS
13	1M	415	GLN
14	1N	204	ASN
14	1N	310	ASN
15	1O	309	ASN
16	1P	180	ASN
16	1P	321	HIS
20	1T	35	HIS
21	1V	110	GLN
22	1W	99	GLN
25	1Z	8	GLN
26	1a	68	ASN
30	1e	44	HIS
32	1g	45	HIS
33	1h	124	GLN
37	1l	104	HIS
39	1n	32	HIS

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Mol	Chain	Res	Type
39	1n	107	HIS
39	1n	140	GLN
39	1n	168	HIS
40	1o	109	GLN
41	1p	54	GLN
42	1q	87	HIS
43	1r	12	ASN
43	1r	24	GLN
43	1r	109	GLN
44	1s	40	ASN

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
14	FME	1N	1	14	8,9,10	0.56	0	7,9,11	1.02	1 (14%)
34	SAC	1i	1	-	7,8,9	0.55	0	8,9,11	1.06	1 (12%)
1	FME	1A	1	1	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
10	FME	1J	1	10	8,9,10	0.52	0	7,9,11	0.93	1 (14%)
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	0.91	1 (14%)
12	FME	1L	1	12	8,9,10	0.53	0	7,9,11	0.99	1 (14%)
11	FME	1K	1	11	8,9,10	0.47	0	7,9,11	1.04	1 (14%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.15	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
14	FME	1N	1	14	-	3/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
1	FME	1A	1	1	-	1/7/9/11	-
10	FME	1J	1	10	-	1/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.91	117.15	124.78
8	1H	1	FME	O-C-CA	-2.76	117.56	124.78
11	1K	1	FME	O-C-CA	-2.59	117.99	124.78
12	1L	1	FME	O-C-CA	-2.54	118.12	124.78
1	1A	1	FME	O-C-CA	-2.51	118.19	124.78
14	1N	1	FME	O-C-CA	-2.44	118.37	124.78
10	1J	1	FME	O-C-CA	-2.42	118.43	124.78
13	1M	1	FME	O-C-CA	-2.29	118.77	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	1K	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
14	1N	1	FME	N-CA-CB-CG
14	1N	1	FME	C-CA-CB-CG
10	1J	1	FME	N-CA-CB-CG
13	1M	1	FME	N-CA-CB-CG
12	1L	1	FME	CA-CB-CG-SD
1	1A	1	FME	CB-CG-SD-CE

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 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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
57	EHZ	1n	201	-	29,36,37	0.16	0	35,44,47	1.17	1 (2%)
58	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.38	0
45	SF4	1I	201	9	0,12,12	-	-	-		
51	CDL	1O	403	-	66,66,99	0.36	0	72,78,111	0.53	0
45	SF4	1F	502	6	0,12,12	-	-	-		
47	FES	1G	803	7	0,4,4	-	-	-		
46	PC1	1h	201	-	33,33,53	0.31	0	39,41,61	0.44	0
46	PC1	1m	201	-	45,45,53	0.28	0	51,53,61	0.36	0
57	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.23	1 (2%)
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.33	0
45	SF4	1G	802	7	0,12,12	-	-	-		
46	PC1	1q	201	-	47,47,53	0.37	0	53,55,61	0.54	1 (1%)
52	3PE	1g	201	-	50,50,50	0.27	0	53,55,55	0.98	3 (5%)
52	3PE	1n	202	-	41,41,50	0.29	0	44,46,55	0.43	0
51	CDL	1H	402	-	50,50,99	0.36	0	56,62,111	0.54	1 (1%)
48	FMN	1F	501	-	33,33,33	0.58	0	48,50,50	0.66	1 (2%)
50	U10	1H	401	-	63,63,63	0.56	1 (1%)	76,79,79	0.82	4 (5%)
45	SF4	1B	201	2	0,12,12	-	-	-		
55	NDP	1P	501	-	45,52,52	0.60	0	53,80,80	0.70	1 (1%)
45	SF4	1G	801	7	0,12,12	-	-	-		
47	FES	1E	301	5	0,4,4	-	-	-		
52	3PE	1Y	202	-	34,34,50	0.30	0	37,39,55	0.56	1 (2%)
51	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.53	0
46	PC1	1d	201	-	38,38,53	0.31	0	44,46,61	0.50	0
52	3PE	1N	401	-	37,37,50	0.32	0	40,42,55	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	1I	202	9	0,12,12	-	-	-		
53	GTP	1O	401	54	26,34,34	0.95	2 (7%)	32,54,54	0.84	0
46	PC1	1Y	201	-	34,34,53	0.33	0	40,42,61	0.37	0

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
57	EHZ	1n	201	-	-	2/42/44/45	-
58	MYR	1l	201	-	-	1/11/12/13	-
45	SF4	1I	201	9	-	-	0/6/5/5
51	CDL	1O	403	-	-	15/76/76/110	-
45	SF4	1F	502	6	-	-	0/6/5/5
47	FES	1G	803	7	-	-	0/1/1/1
46	PC1	1h	201	-	-	4/36/36/57	-
57	EHZ	1W	201	-	-	17/42/44/45	-
46	PC1	1m	201	-	-	9/49/49/57	-
46	PC1	1B	202	-	-	13/37/37/57	-
45	SF4	1G	802	7	-	-	0/6/5/5
46	PC1	1q	201	-	-	18/51/51/57	-
52	3PE	1g	201	-	-	12/54/54/54	-
52	3PE	1n	202	-	-	7/45/45/54	-
51	CDL	1H	402	-	-	8/61/61/110	-
48	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
50	U10	1H	401	-	-	6/63/87/87	0/1/1/1
55	NDP	1P	501	-	-	5/30/77/77	0/5/5/5
45	SF4	1B	201	2	-	-	0/6/5/5
45	SF4	1G	801	7	-	-	0/6/5/5
47	FES	1E	301	5	-	-	0/1/1/1
52	3PE	1Y	202	-	-	14/38/38/54	-
51	CDL	1a	101	-	-	18/71/71/110	-
46	PC1	1d	201	-	-	13/42/42/57	-
52	3PE	1N	401	-	-	4/41/41/54	-
45	SF4	1I	202	9	-	-	0/6/5/5
53	GTP	1O	401	54	-	3/18/38/38	0/3/3/3
46	PC1	1Y	201	-	-	11/38/38/57	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1O	401	GTP	C5-C6	-2.58	1.42	1.47
50	1H	401	U10	C4-C5	-2.50	1.41	1.48
53	1O	401	GTP	C8-N7	-2.12	1.31	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1W	201	EHZ	C10-S1-C9	6.71	122.76	101.87
57	1n	201	EHZ	C10-S1-C9	6.49	122.07	101.87
52	1g	201	3PE	O21-C21-C22	4.52	121.23	111.50
52	1g	201	3PE	O21-C2-C3	3.44	120.86	108.40
52	1g	201	3PE	O21-C21-O22	-2.77	117.01	123.70
50	1H	401	U10	O3-C3-C2	2.65	125.54	116.56
50	1H	401	U10	O4-C4-C5	-2.62	107.69	116.56
55	1P	501	NDP	C5A-C6A-N6A	2.19	123.69	120.35
50	1H	401	U10	C4-C3-C2	-2.18	116.39	120.68
51	1H	402	CDL	OB6-CB5-C51	2.15	116.13	111.50
50	1H	401	U10	O4-C4-C3	2.14	131.70	123.64
46	1q	201	PC1	O21-C21-C22	-2.05	107.09	111.50
48	1F	501	FMN	C4-N3-C2	-2.03	121.90	125.64
52	1Y	202	3PE	O21-C2-C3	2.02	115.72	108.40

There are no chirality outliers.

All (182) 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	1Y	201	PC1	C1-O11-P-O14
46	1Y	201	PC1	O32-C31-O31-C3
46	1Y	201	PC1	C32-C31-O31-C3
46	1d	201	PC1	O13-C11-C12-N
46	1d	201	PC1	O22-C21-O21-C2
46	1d	201	PC1	C22-C21-O21-C2
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1h	201	PC1	C1-O11-P-O12
46	1h	201	PC1	C1-O11-P-O14
46	1h	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	1m	201	PC1	C11-O13-P-O14
46	1m	201	PC1	C1-O11-P-O14
46	1q	201	PC1	C11-O13-P-O14
48	1F	501	FMN	N10-C1'-C2'-O2'
48	1F	501	FMN	N10-C1'-C2'-C3'
51	1H	402	CDL	C1-CA2-OA2-PA1
51	1H	402	CDL	CA3-OA5-PA1-OA3
51	1H	402	CDL	OB7-CB5-OB6-CB4
51	1H	402	CDL	C51-CB5-OB6-CB4
51	1O	403	CDL	CA2-OA2-PA1-OA3
51	1O	403	CDL	CA2-OA2-PA1-OA5
51	1O	403	CDL	CB2-OB2-PB2-OB5
51	1a	101	CDL	CB2-OB2-PB2-OB3
51	1a	101	CDL	CB2-OB2-PB2-OB5
52	1g	201	3PE	O22-C21-O21-C2
52	1g	201	3PE	C22-C21-O21-C2
57	1W	201	EHZ	N2-C15-C16-C17
57	1W	201	EHZ	N2-C15-C16-O5
57	1W	201	EHZ	O4-C15-C16-C17
57	1W	201	EHZ	O4-C15-C16-O5
57	1W	201	EHZ	C15-C16-C17-C19
57	1W	201	EHZ	C15-C16-C17-C20
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
52	1g	201	3PE	O21-C2-C3-O31
51	1a	101	CDL	CB7-C71-C72-C73
51	1O	403	CDL	CB7-C71-C72-C73
50	1H	401	U10	C4-C3-O3-C3M
46	1B	202	PC1	C1-O11-P-O13
52	1Y	202	3PE	C1-O11-P-O13
46	1d	201	PC1	C22-C23-C24-C25
53	1O	401	GTP	C4'-C5'-O5'-PA
46	1q	201	PC1	C33-C34-C35-C36
46	1m	201	PC1	C25-C26-C27-C28
52	1Y	202	3PE	C34-C35-C36-C37
46	1q	201	PC1	C32-C33-C34-C35
46	1q	201	PC1	C3A-C3B-C3C-C3D
52	1g	201	3PE	C21-C22-C23-C24
51	1O	403	CDL	C55-C56-C57-C58
46	1q	201	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
51	1a	101	CDL	OB5-CB3-CB4-OB6
46	1B	202	PC1	C31-C32-C33-C34
46	1Y	201	PC1	C1-O11-P-O13
46	1Y	201	PC1	C2-C1-O11-P
50	1H	401	U10	C2-C3-O3-C3M
57	1W	201	EHZ	O3-C12-C13-C14
52	1Y	202	3PE	C1-C2-C3-O31
52	1g	201	3PE	C1-C2-C3-O31
46	1d	201	PC1	C3A-C3B-C3C-C3D
51	1a	101	CDL	CB5-C51-C52-C53
51	1O	403	CDL	C52-C53-C54-C55
51	1O	403	CDL	C71-C72-C73-C74
52	1g	201	3PE	C2-C1-O11-P
51	1H	402	CDL	OB5-CB3-CB4-OB6
46	1d	201	PC1	C33-C34-C35-C36
46	1q	201	PC1	O11-C1-C2-C3
50	1H	401	U10	C20-C19-C21-C22
57	1W	201	EHZ	C13-C14-N2-C15
46	1q	201	PC1	C1-O11-P-O13
51	1O	403	CDL	CB3-OB5-PB2-OB2
51	1O	403	CDL	C78-C79-C80-C81
51	1O	403	CDL	OB6-CB4-CB6-OB8
52	1n	202	3PE	O21-C2-C3-O31
46	1q	201	PC1	C39-C3A-C3B-C3C
52	1n	202	3PE	C21-C22-C23-C24
51	1H	402	CDL	OB5-CB3-CB4-CB6
51	1a	101	CDL	OB5-CB3-CB4-CB6
50	1H	401	U10	C18-C19-C21-C22
52	1Y	202	3PE	C32-C33-C34-C35
52	1Y	202	3PE	O31-C31-C32-C33
46	1Y	201	PC1	C1-C2-C3-O31
46	1h	201	PC1	C2-C1-O11-P
51	1a	101	CDL	CB3-CB4-CB6-OB8
52	1N	401	3PE	C2-C1-O11-P
46	1q	201	PC1	O11-C1-C2-O21
52	1g	201	3PE	O11-C1-C2-O21
52	1n	202	3PE	C26-C27-C28-C29
55	1P	501	NDP	C2D-C1D-N1N-C6N
51	1H	402	CDL	CA3-OA5-PA1-OA2
46	1d	201	PC1	C2-C1-O11-P
51	1a	101	CDL	CB4-CB3-OB5-PB2
46	1Y	201	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
51	1O	403	CDL	CB2-OB2-PB2-OB4
52	1Y	202	3PE	C1-O11-P-O14
46	1B	202	PC1	C12-C11-O13-P
52	1N	401	3PE	C12-C11-O13-P
52	1Y	202	3PE	C12-C11-O13-P
52	1g	201	3PE	C12-C11-O13-P
52	1n	202	3PE	C12-C11-O13-P
46	1B	202	PC1	O21-C21-C22-C23
46	1q	201	PC1	C21-C22-C23-C24
46	1Y	201	PC1	O13-C11-C12-N
46	1m	201	PC1	O13-C11-C12-N
51	1O	403	CDL	CB3-CB4-CB6-OB8
46	1Y	201	PC1	O21-C2-C3-O31
46	1m	201	PC1	O21-C2-C3-O31
52	1Y	202	3PE	O21-C2-C3-O31
51	1H	402	CDL	CA4-CA3-OA5-PA1
51	1a	101	CDL	CA4-CA3-OA5-PA1
57	1W	201	EHZ	N1-C12-C13-C14
46	1B	202	PC1	C11-O13-P-O11
46	1m	201	PC1	C11-O13-P-O11
46	1m	201	PC1	C1-O11-P-O13
46	1q	201	PC1	C11-O13-P-O11
51	1a	101	CDL	CA3-OA5-PA1-OA2
52	1Y	202	3PE	C11-O13-P-O11
52	1n	202	3PE	C1-O11-P-O13
51	1a	101	CDL	CA7-C31-C32-C33
55	1P	501	NDP	O4D-C1D-N1N-C6N
51	1O	403	CDL	C71-CB7-OB8-CB6
52	1Y	202	3PE	C2-C3-O31-C31
46	1B	202	PC1	O22-C21-C22-C23
52	1Y	202	3PE	C27-C28-C29-C2A
46	1q	201	PC1	C37-C38-C39-C3A
46	1B	202	PC1	C1-C2-C3-O31
52	1n	202	3PE	C22-C23-C24-C25
55	1P	501	NDP	C2D-C1D-N1N-C2N
57	1W	201	EHZ	C2-C1-C21-C22
52	1Y	202	3PE	C23-C24-C25-C26
50	1H	401	U10	C5-C4-O4-C4M
57	1W	201	EHZ	C11-C10-S1-C9
51	1O	403	CDL	C53-C54-C55-C56
46	1d	201	PC1	C23-C24-C25-C26
53	1O	401	GTP	O4'-C4'-C5'-O5'

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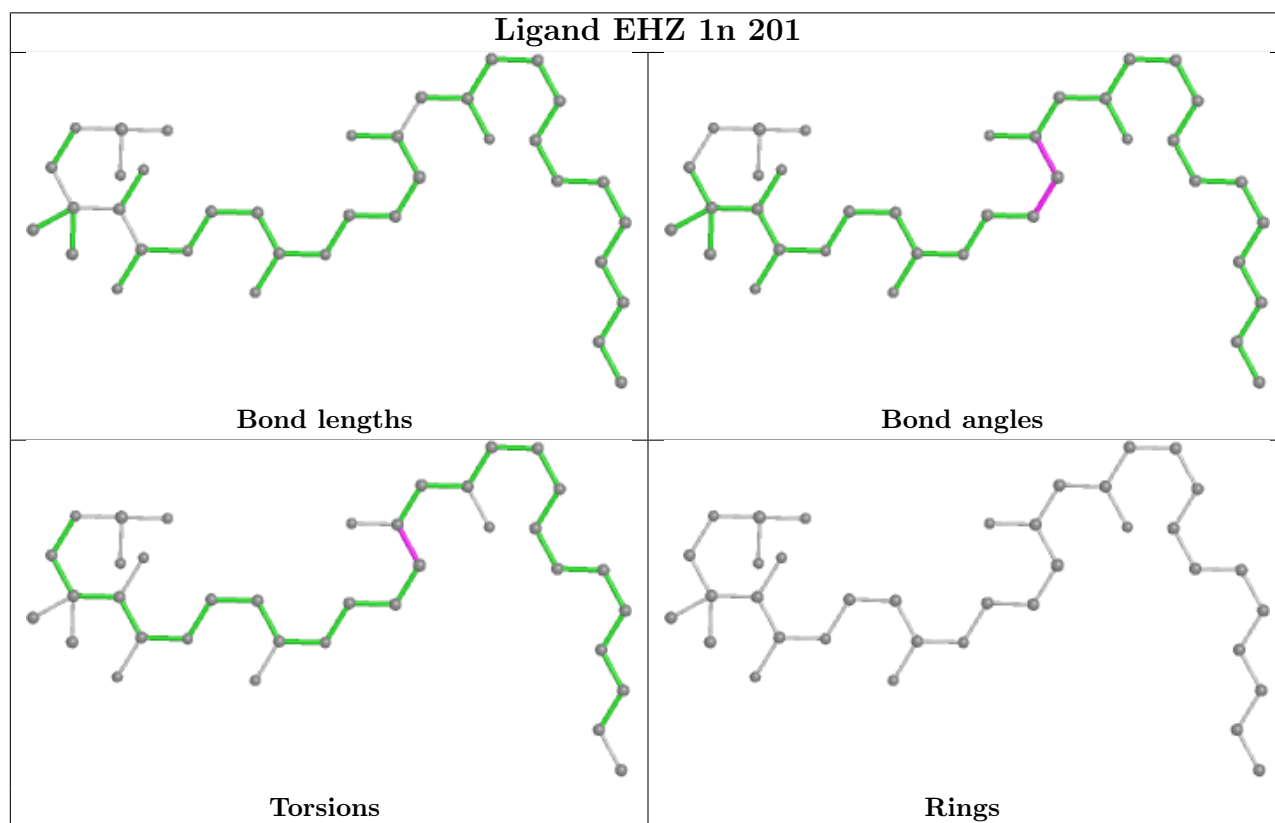
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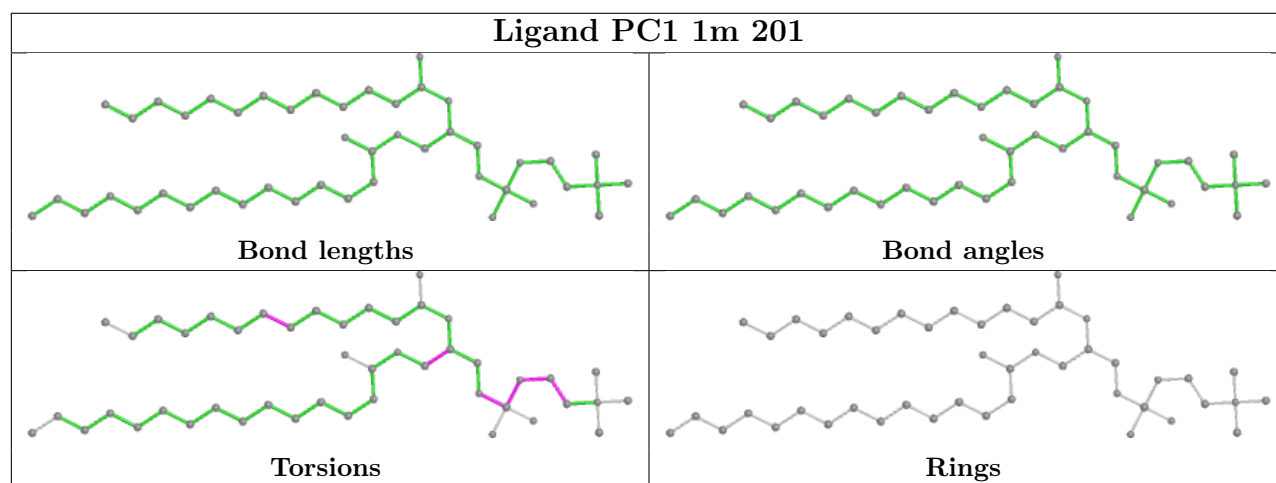
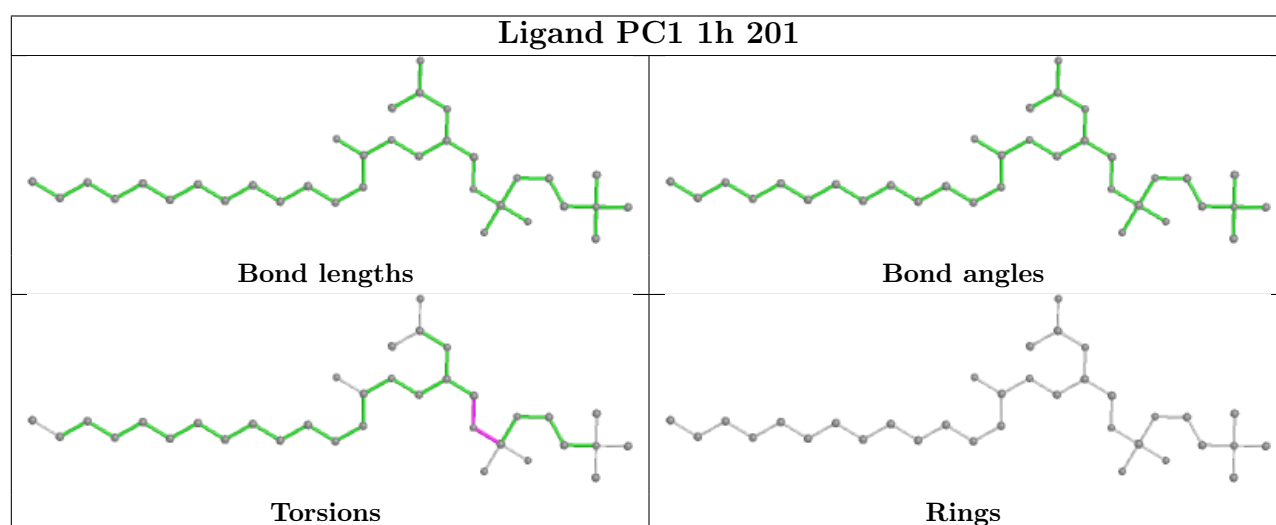
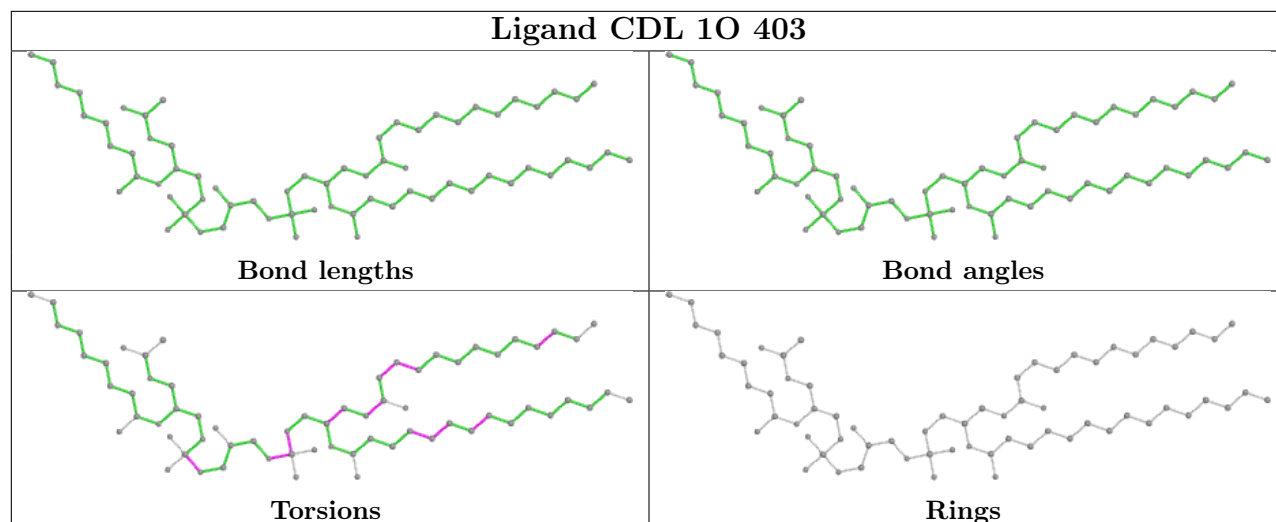
Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C36-C37-C38-C39
53	1O	401	GTP	C3'-C4'-C5'-O5'
52	1g	201	3PE	C1-C2-O21-C21
57	1W	201	EHZ	C10-C11-N1-C12
52	1N	401	3PE	O11-C1-C2-O21
57	1W	201	EHZ	C15-C16-C17-C18
57	1W	201	EHZ	O5-C16-C17-C18
51	1a	101	CDL	CA5-C11-C12-C13
58	1l	201	MYR	C6-C7-C8-C9
50	1H	401	U10	C26-C27-C28-C29
46	1m	201	PC1	C1-C2-C3-O31
51	1a	101	CDL	C12-C13-C14-C15
46	1B	202	PC1	C1-O11-P-O14
46	1q	201	PC1	C1-O11-P-O14
51	1O	403	CDL	CB3-OB5-PB2-OB3
51	1a	101	CDL	CA3-OA5-PA1-OA3
51	1a	101	CDL	CB3-OB5-PB2-OB3
52	1n	202	3PE	C1-O11-P-O14
55	1P	501	NDP	O4B-C4B-C5B-O5B
52	1g	201	3PE	C25-C26-C27-C28
51	1a	101	CDL	C12-C11-CA5-OA6
51	1a	101	CDL	C19-C20-C21-C22
46	1q	201	PC1	O22-C21-C22-C23
46	1Y	201	PC1	C33-C34-C35-C36
52	1N	401	3PE	C33-C34-C35-C36
46	1m	201	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
52	1Y	202	3PE	C3-C2-O21-C21
46	1d	201	PC1	C35-C36-C37-C38
52	1Y	202	3PE	O32-C31-C32-C33
46	1q	201	PC1	C22-C23-C24-C25
46	1q	201	PC1	O31-C31-C32-C33
57	1W	201	EHZ	S1-C10-C11-N1
46	1d	201	PC1	O32-C31-C32-C33
46	1d	201	PC1	O31-C31-C32-C33
46	1q	201	PC1	O32-C31-C32-C33
55	1P	501	NDP	O4D-C1D-N1N-C2N
51	1a	101	CDL	C17-C18-C19-C20
52	1g	201	3PE	C38-C39-C3A-C3B
46	1Y	201	PC1	C34-C35-C36-C37
52	1g	201	3PE	O31-C31-C32-C33

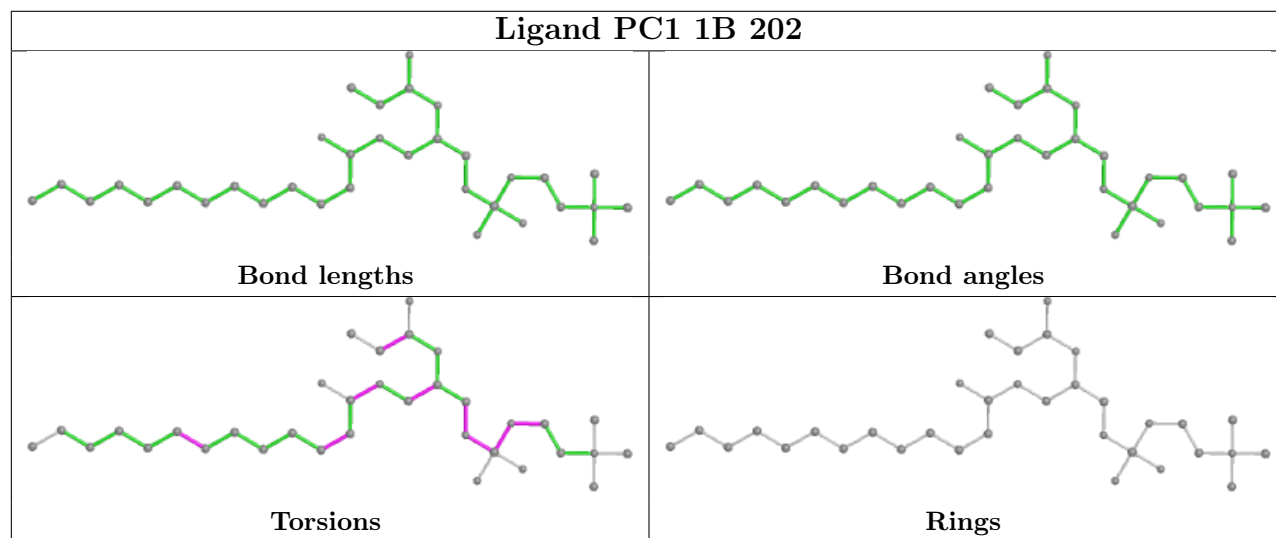
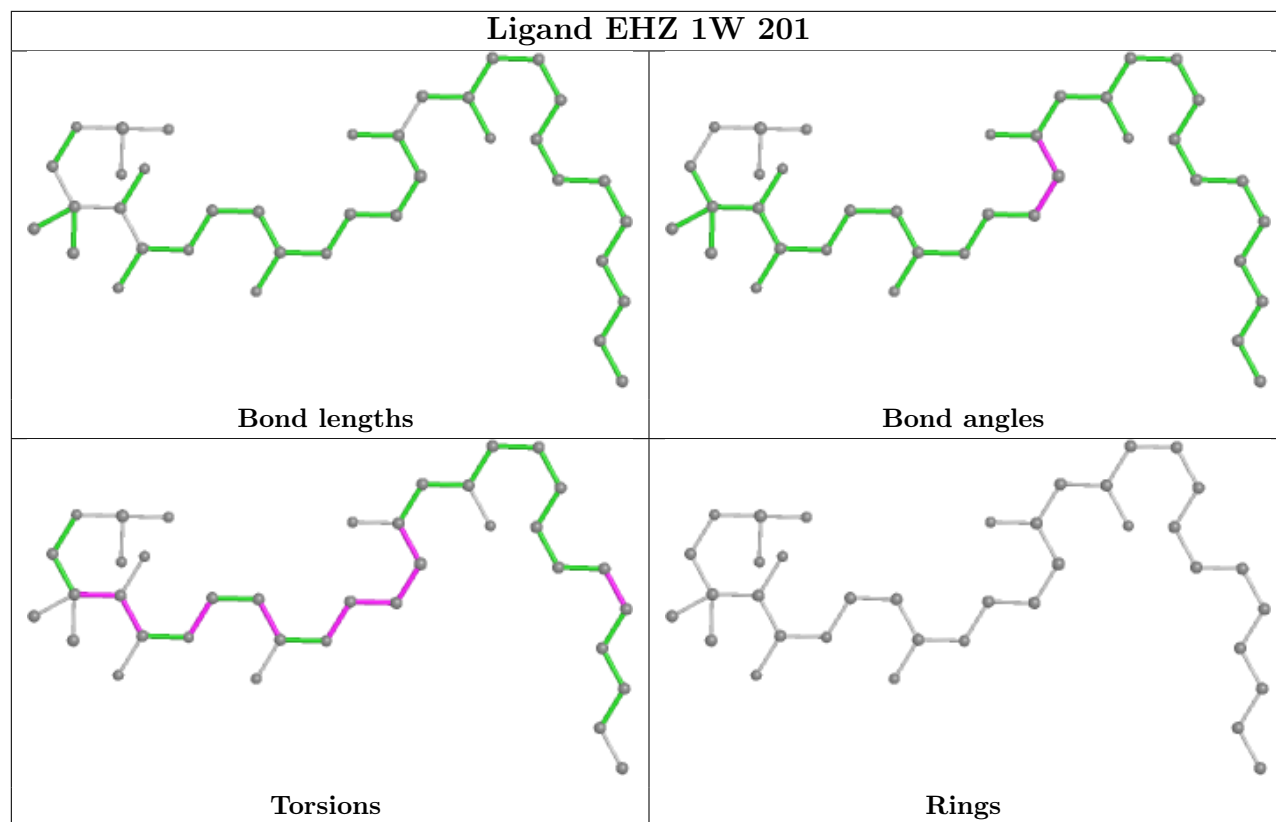
There are no ring outliers.

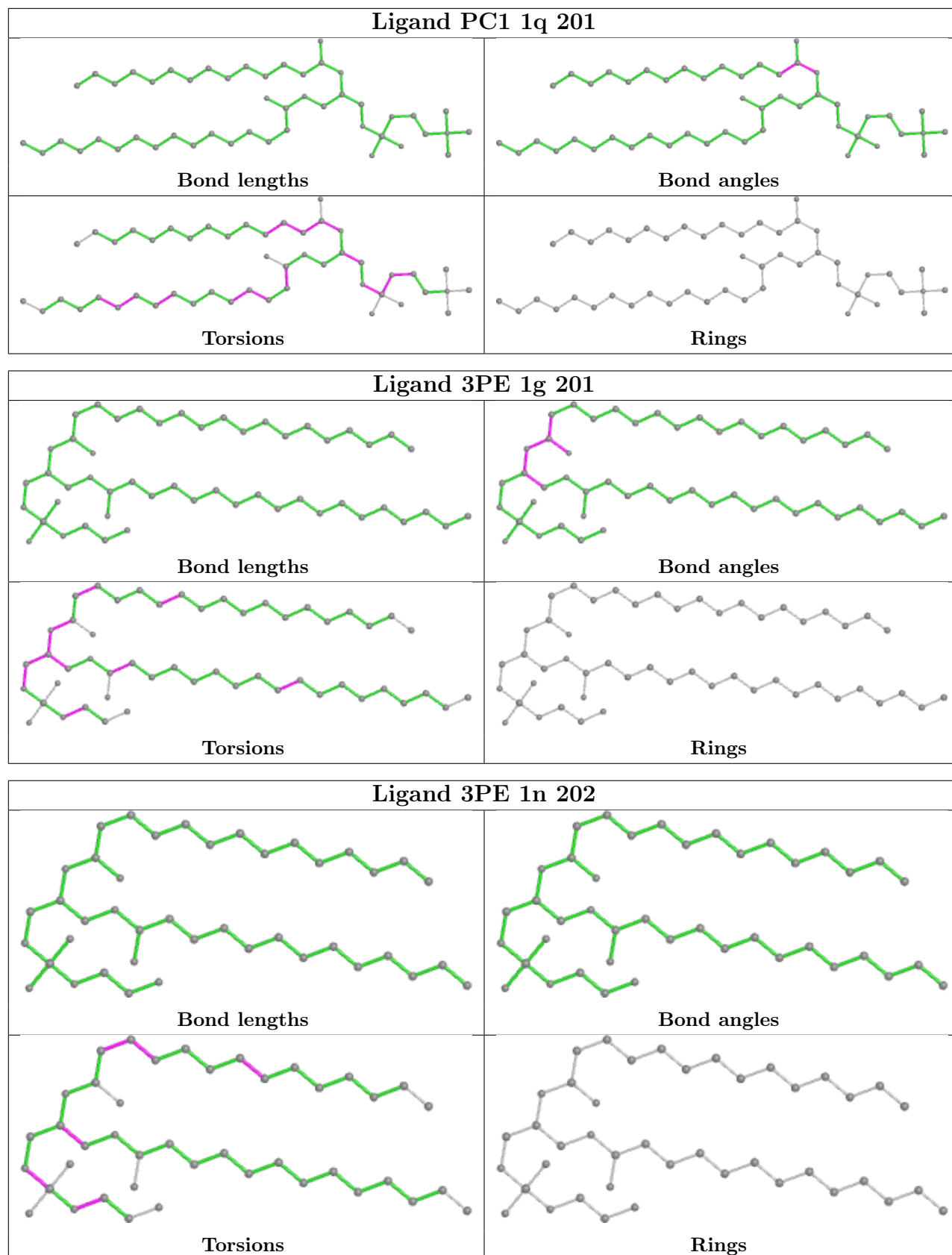
No monomer is involved in short contacts.

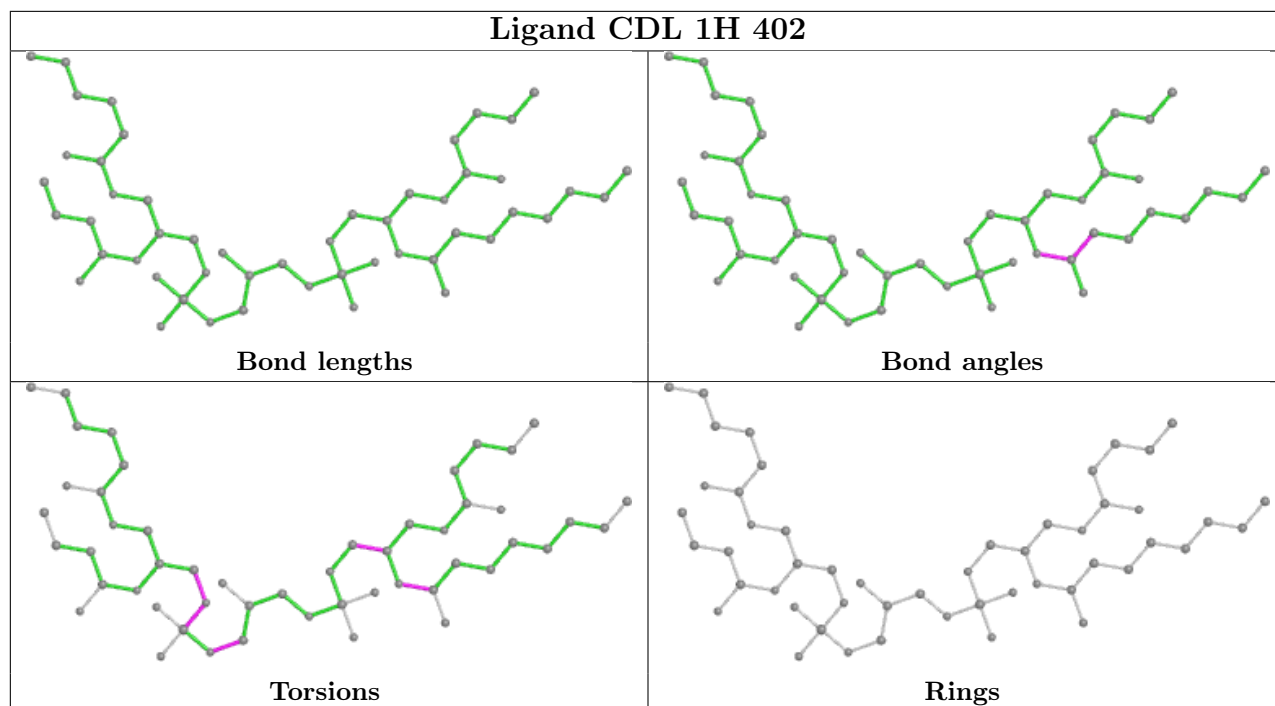
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

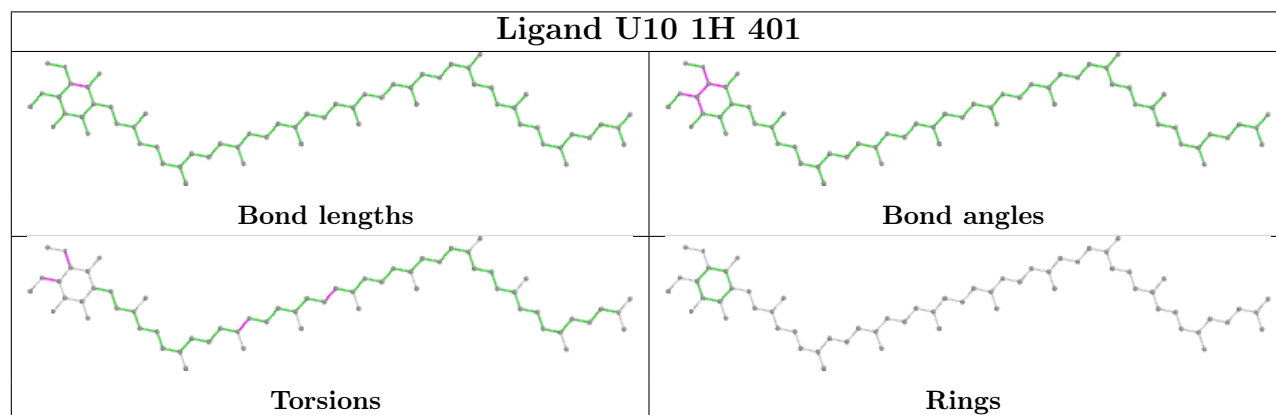
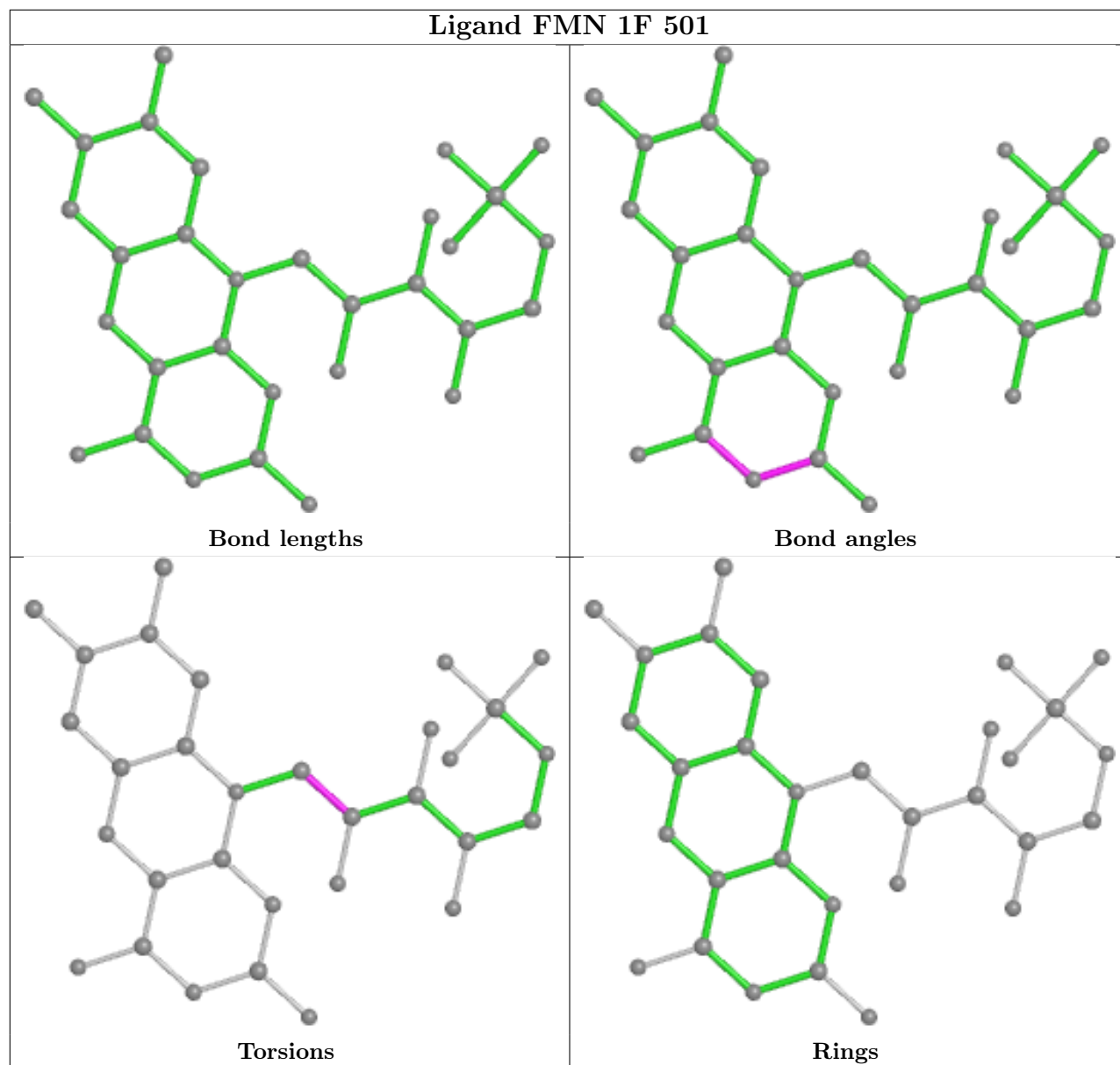


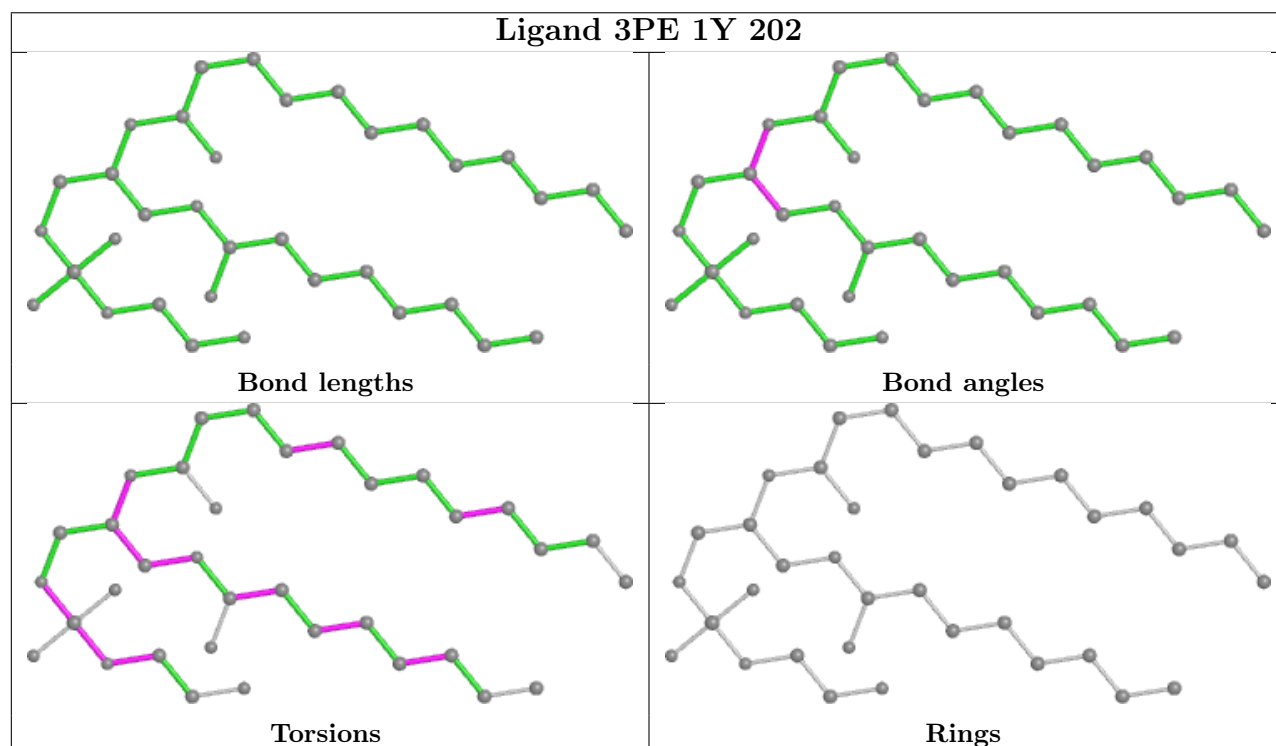
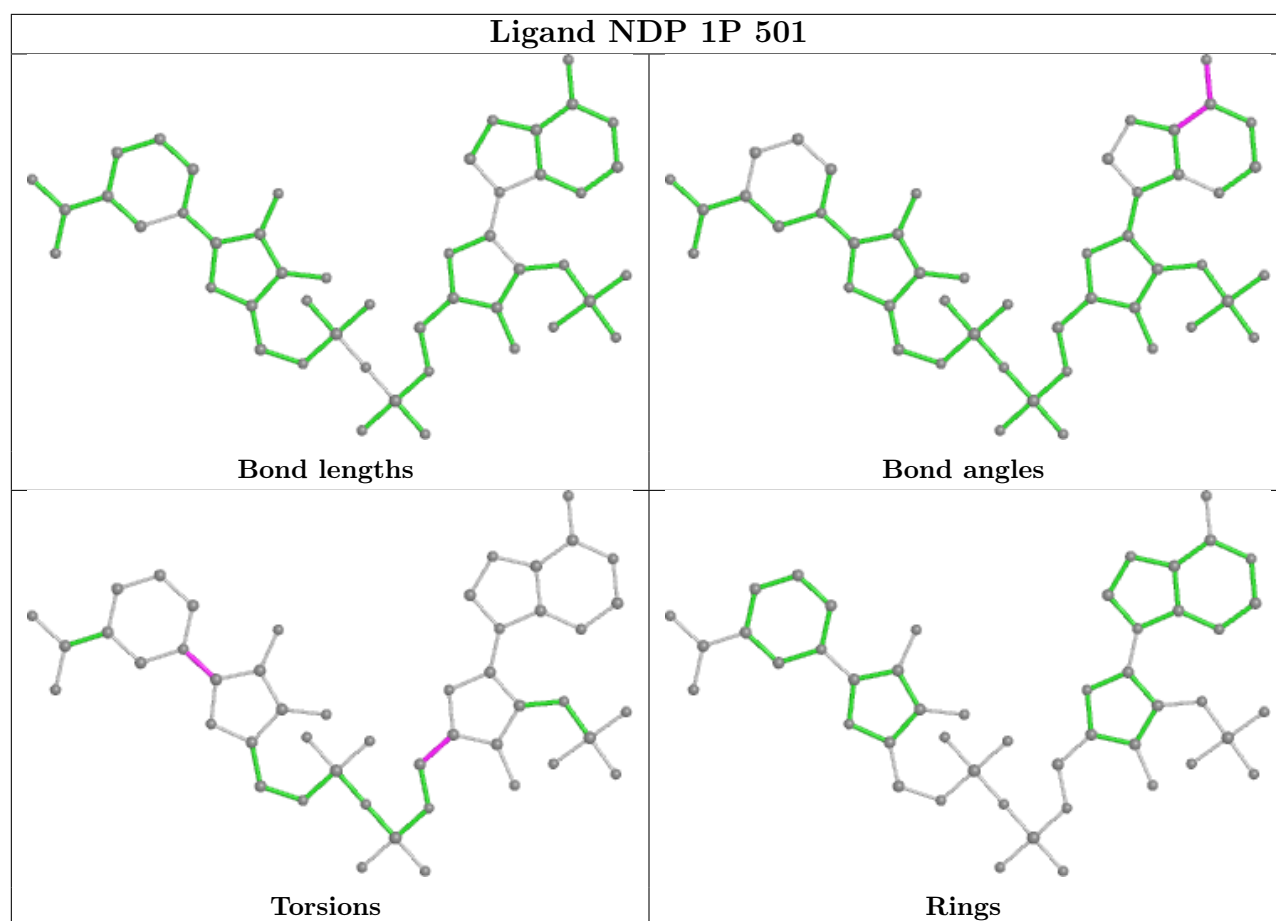


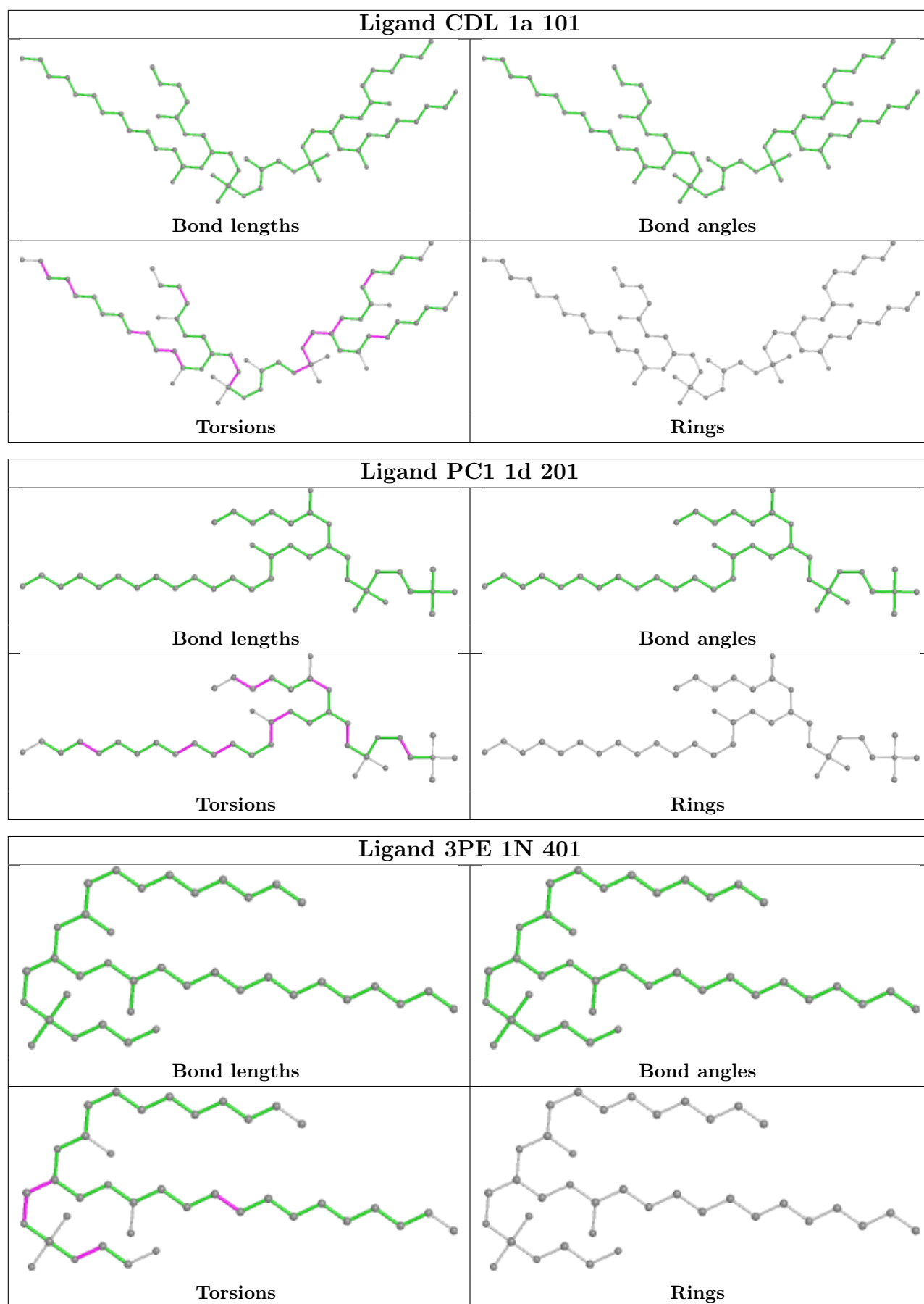


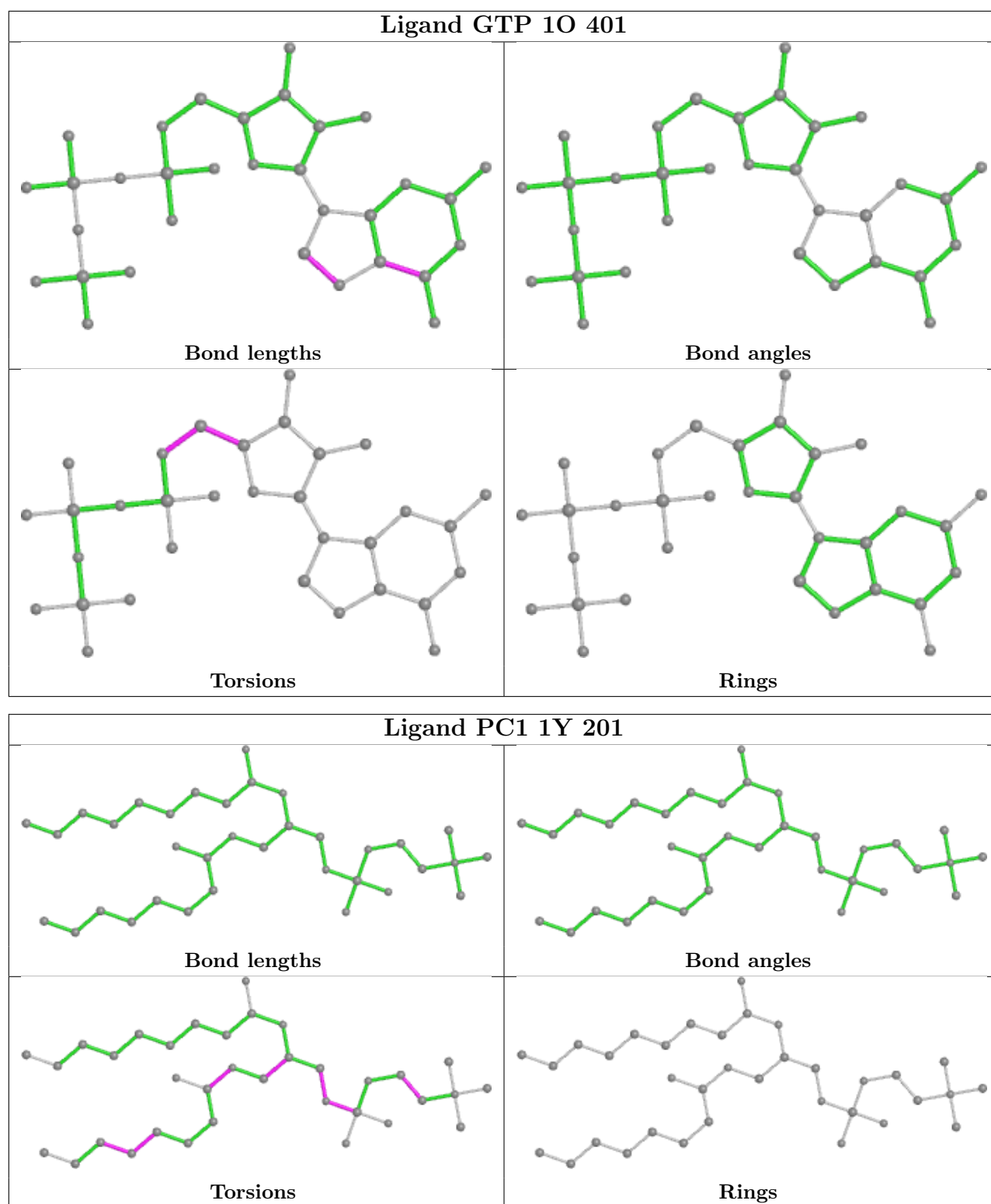












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	7.02
1	1i	1:SAC	C	2:GLY	N	4.04

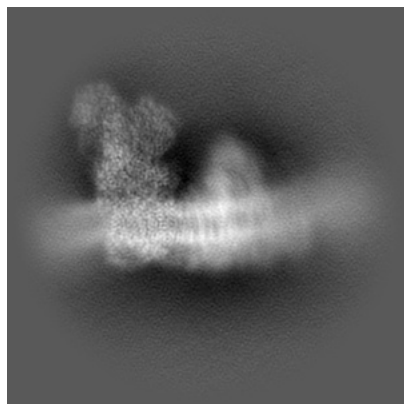
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42168. These allow visual inspection of the internal detail of the map and identification of artifacts.

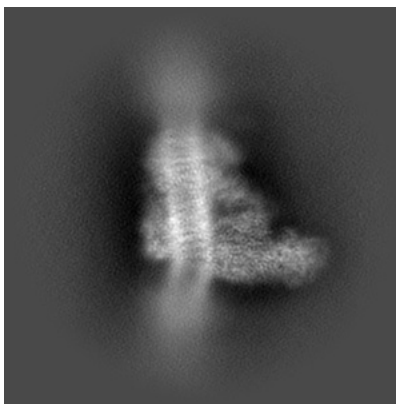
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

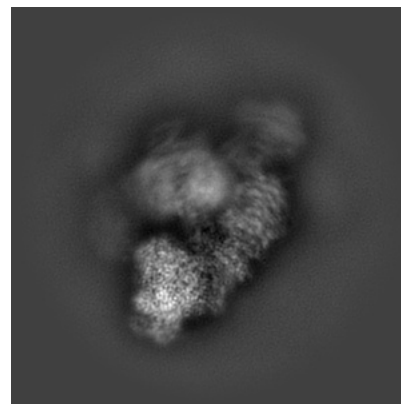
6.1.1 Primary map



X

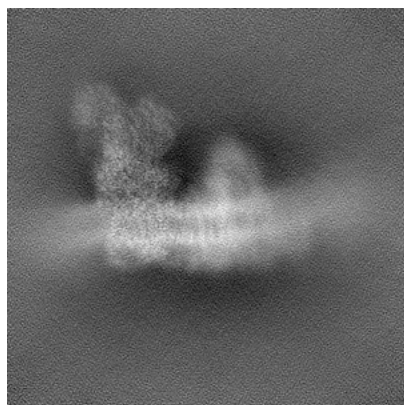


Y

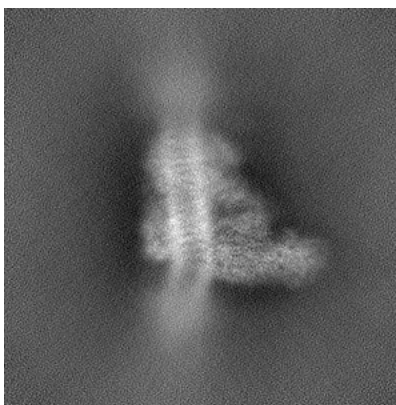


Z

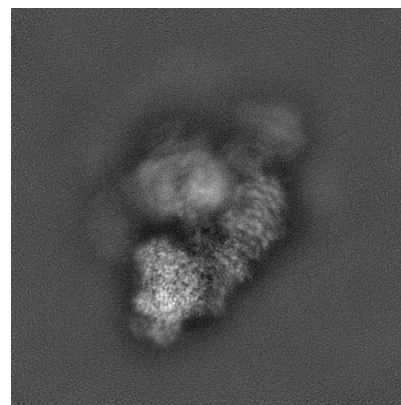
6.1.2 Raw map



X



Y

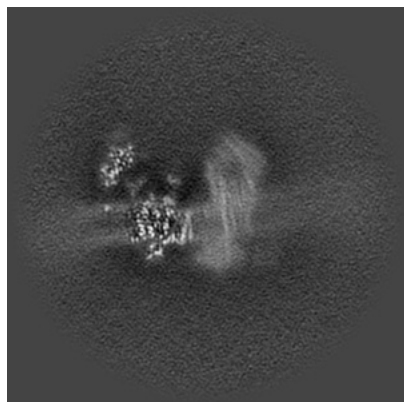


Z

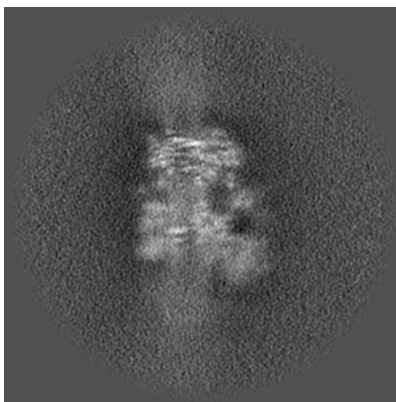
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

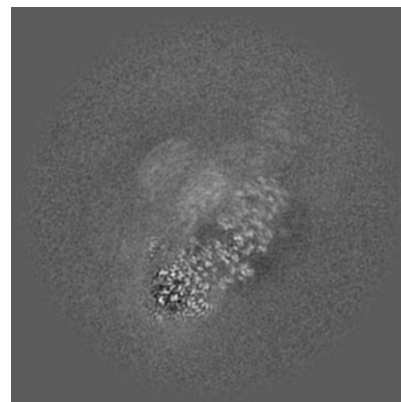
6.2.1 Primary map



X Index: 160

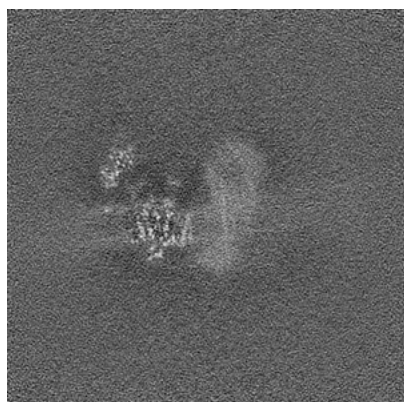


Y Index: 160

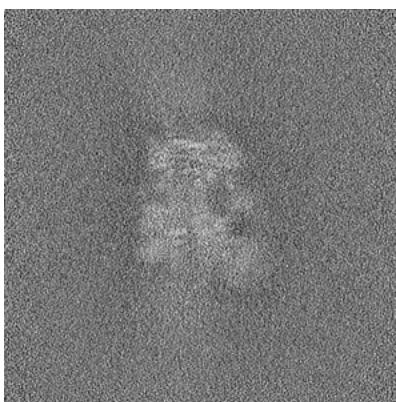


Z Index: 160

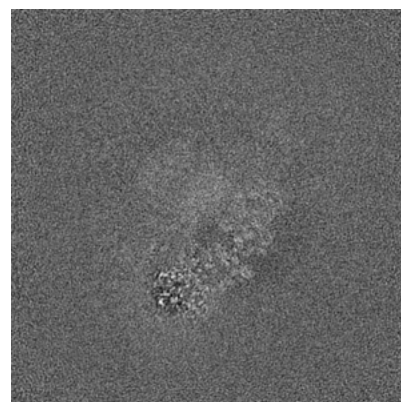
6.2.2 Raw map



X Index: 160



Y Index: 160

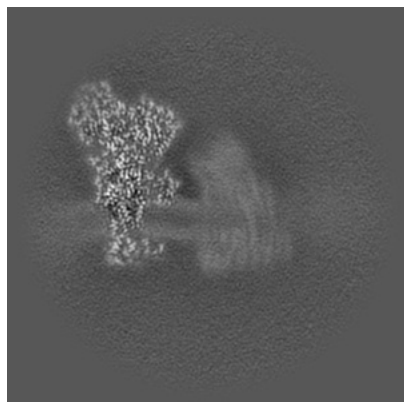


Z Index: 160

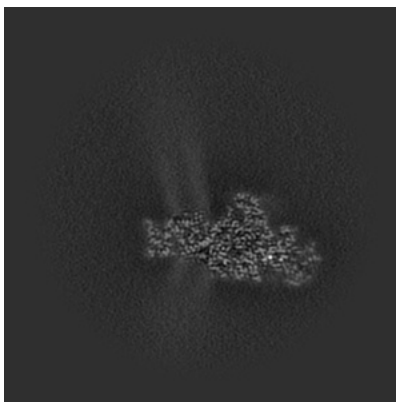
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

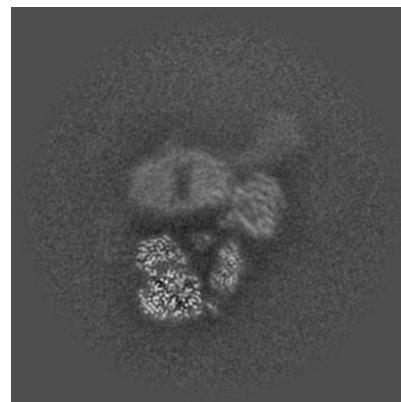
6.3.1 Primary map



X Index: 123

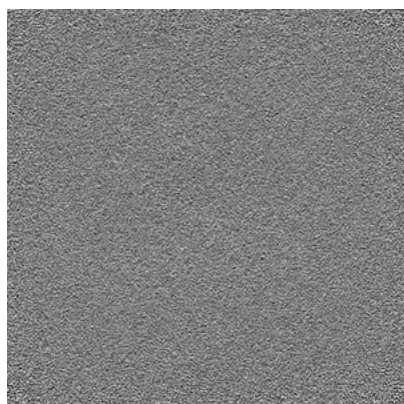


Y Index: 87

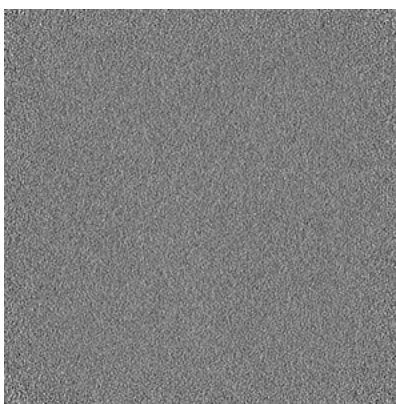


Z Index: 177

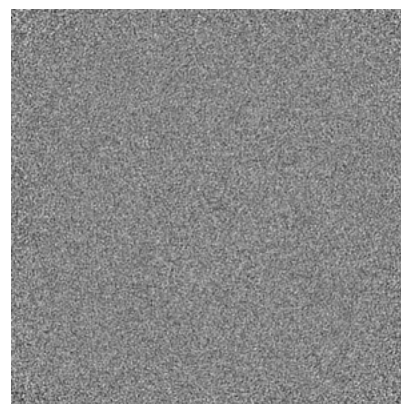
6.3.2 Raw map



X Index: 0



Y Index: 0

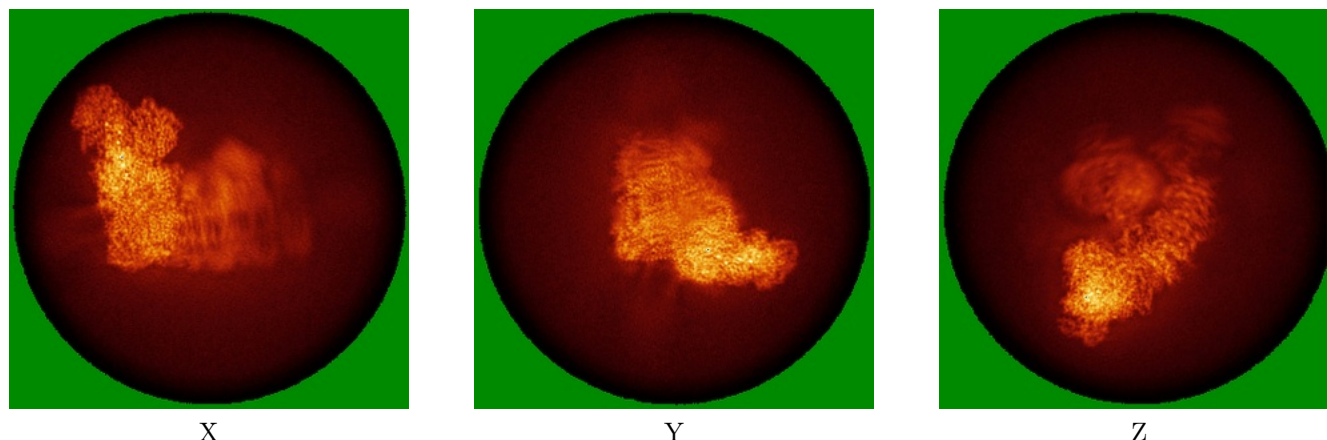


Z Index: 0

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

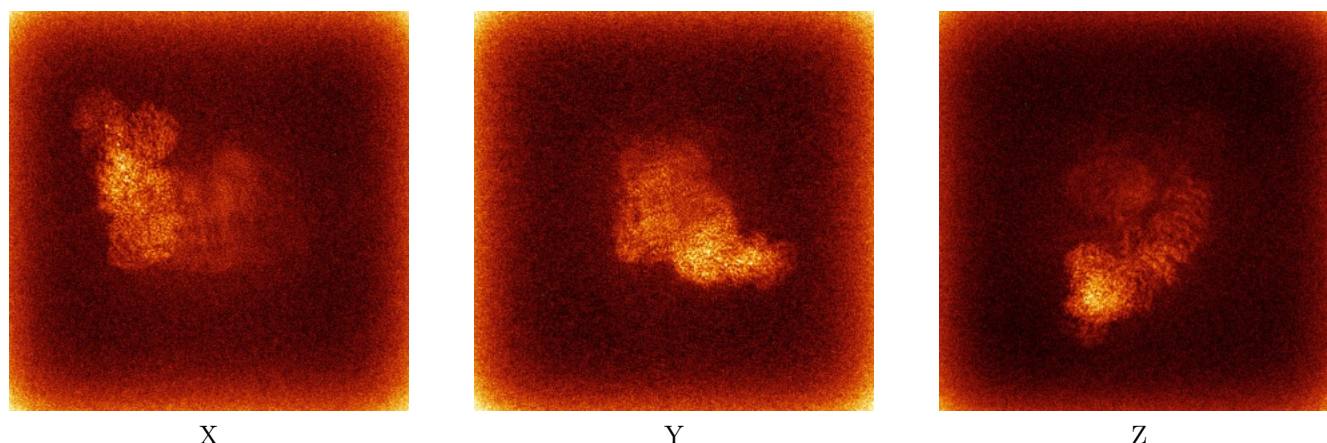


X

Y

Z

6.4.2 Raw map



X

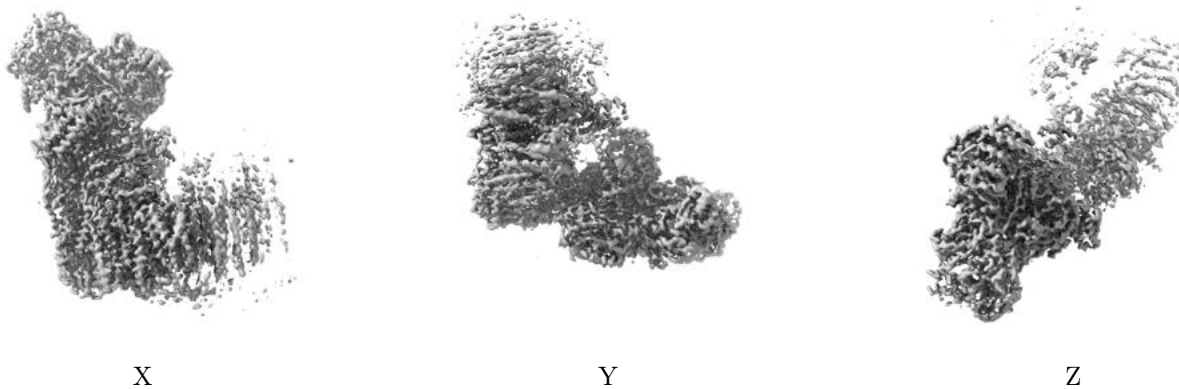
Y

Z

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

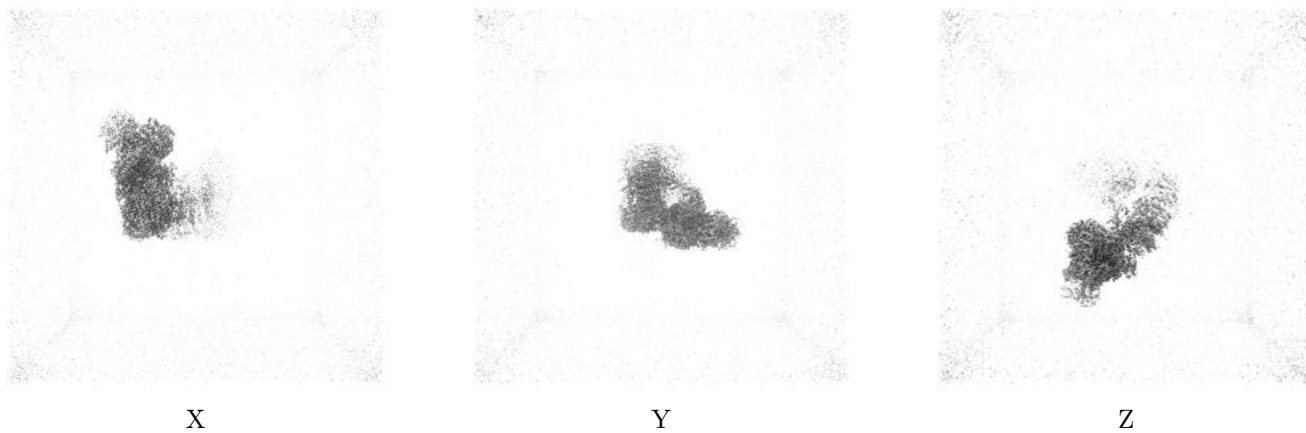
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 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.

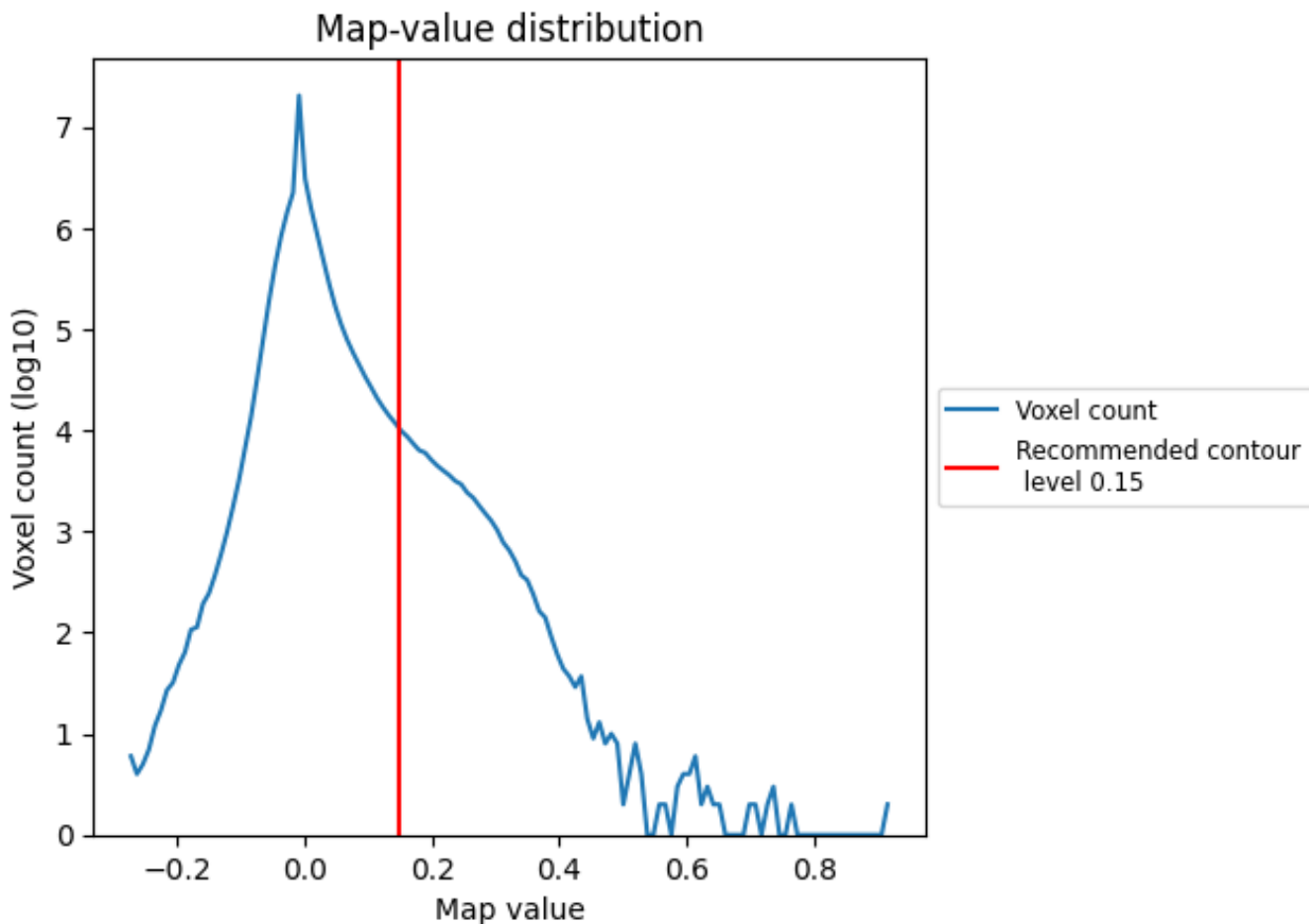
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

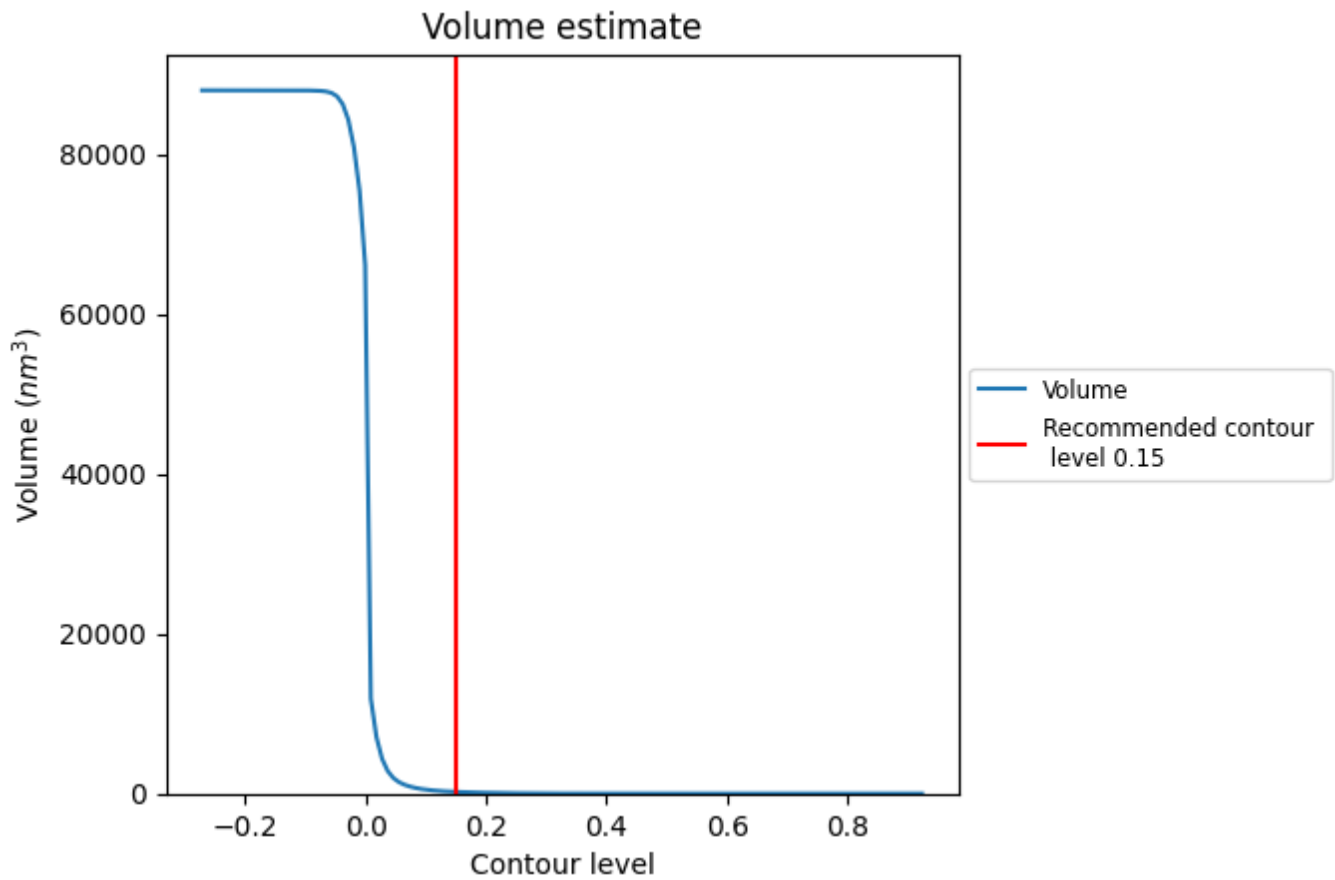
This section contains the results of statistical analysis of the map.

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.

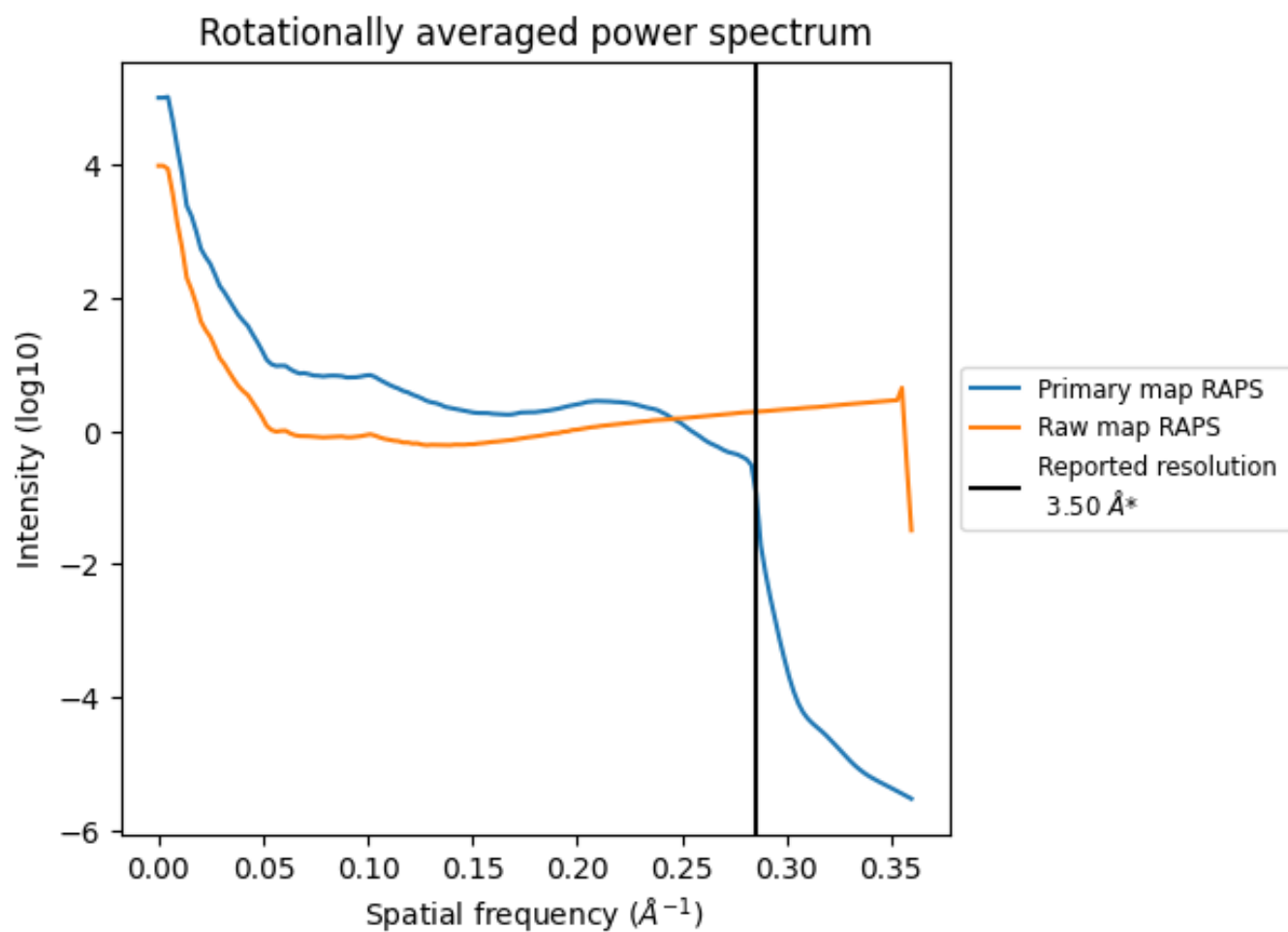
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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

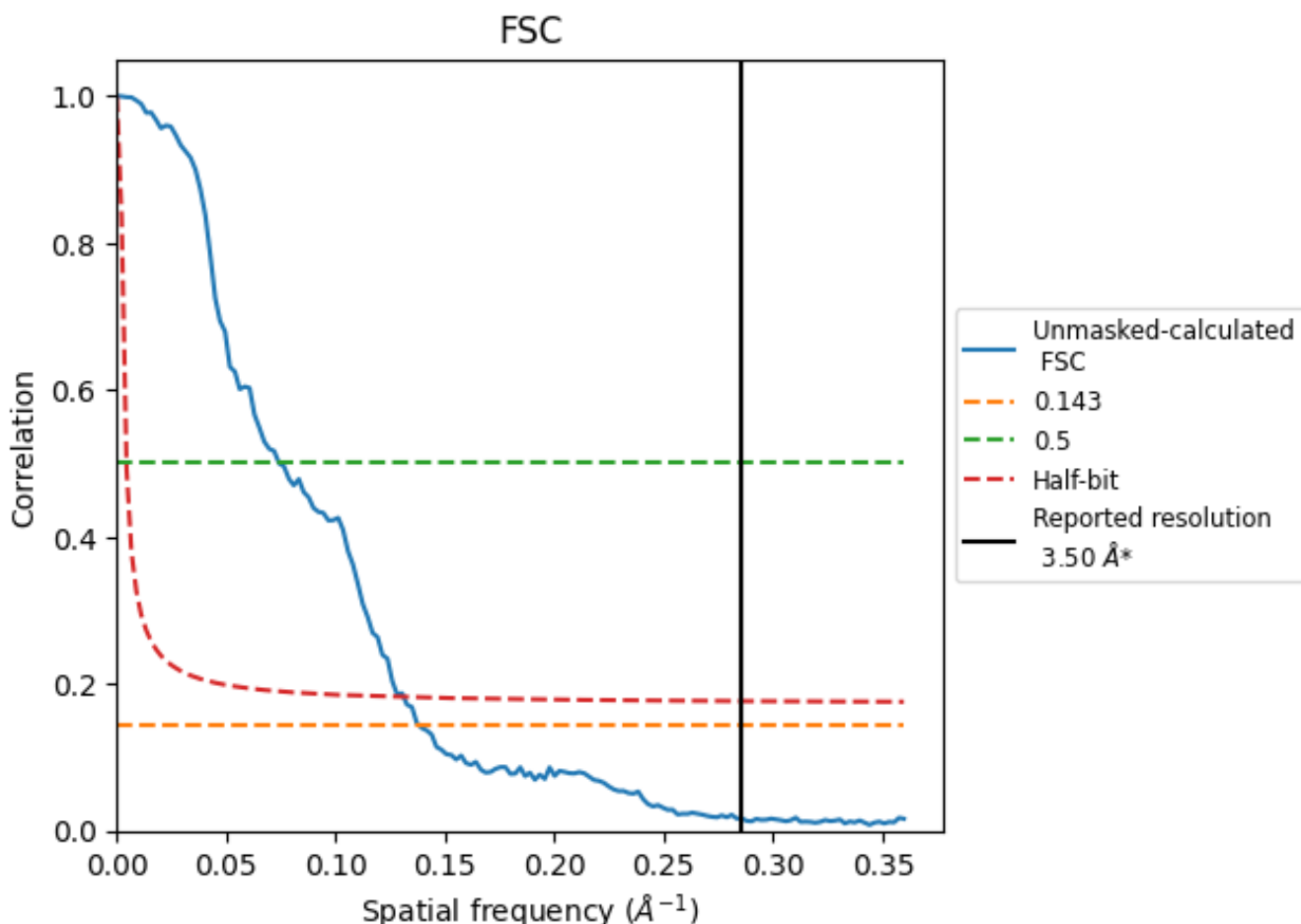


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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⁻¹

8.2 Resolution estimates [i](#)

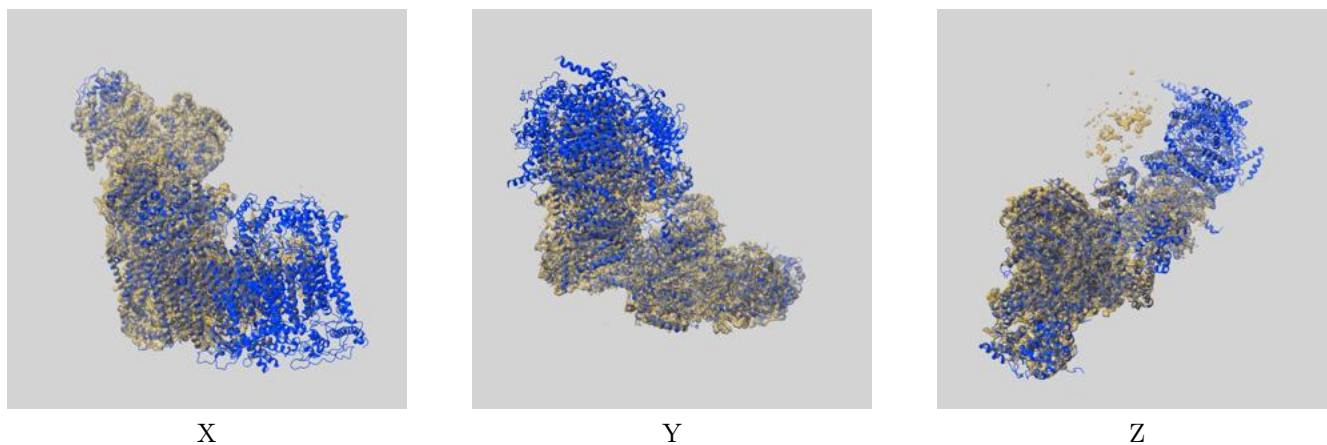
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.24	13.48	7.63

*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 7.24 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

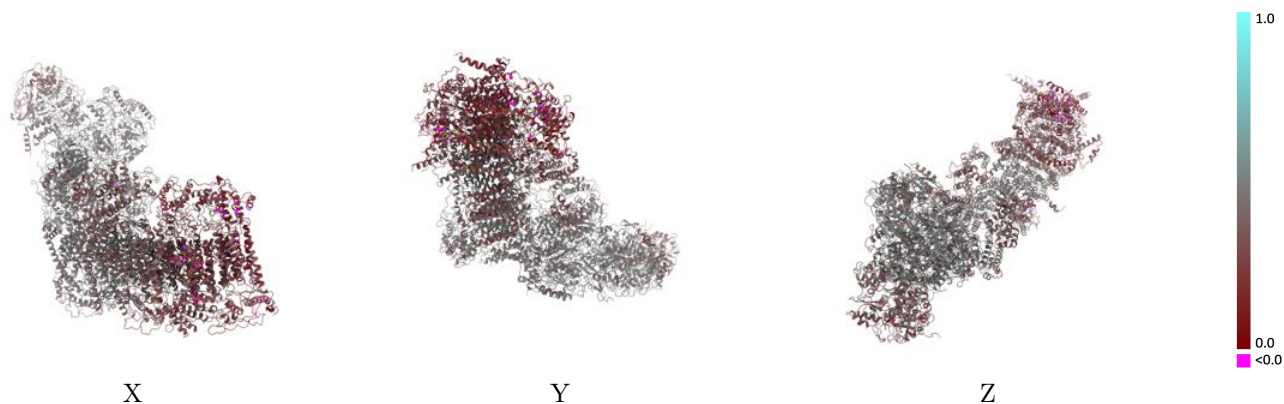
This section contains information regarding the fit between EMDB map EMD-42168 and PDB model 8UER. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



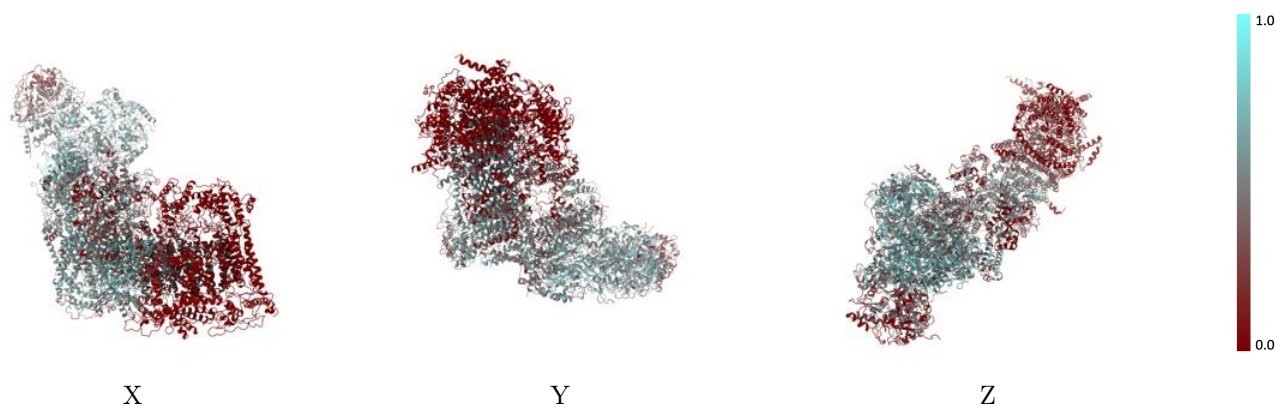
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



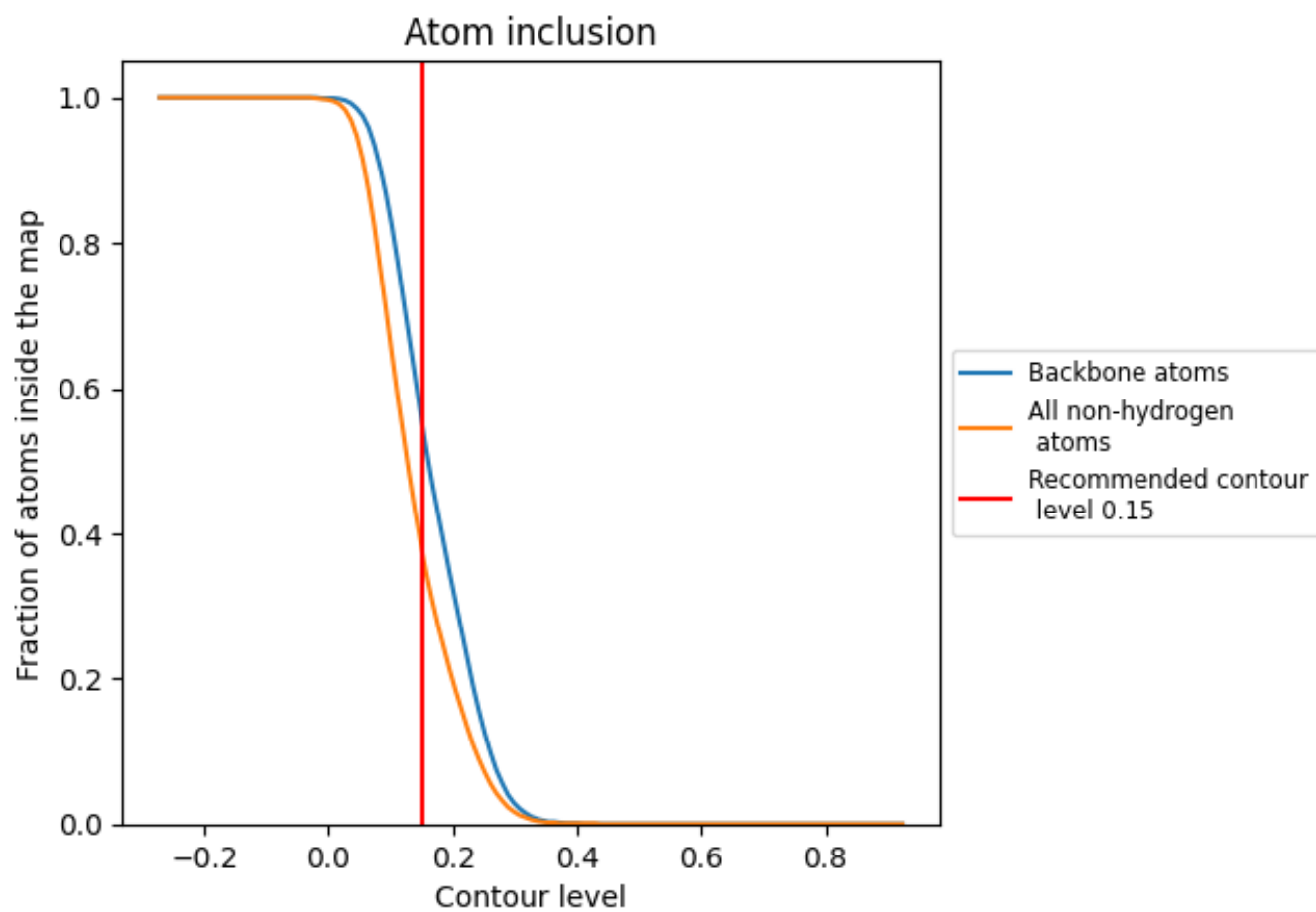
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3800	 0.3880
1A	 0.4340	 0.4320
1B	 0.6100	 0.4560
1C	 0.5770	 0.4740
1D	 0.5810	 0.4590
1E	 0.3490	 0.3930
1F	 0.3610	 0.3930
1G	 0.5870	 0.4470
1H	 0.5560	 0.4510
1I	 0.6800	 0.4600
1J	 0.4030	 0.4130
1K	 0.4480	 0.4110
1L	 0.1050	 0.2710
1M	 0.3520	 0.3820
1N	 0.5370	 0.4410
1O	 0.2470	 0.3480
1P	 0.5000	 0.4580
1Q	 0.4720	 0.4510
1R	 0.5400	 0.4590
1S	 0.5320	 0.4170
1T	 0.2300	 0.3430
1U	 0.0020	 0.2200
1V	 0.4610	 0.4300
1W	 0.4200	 0.4200
1X	 0.5060	 0.4250
1Y	 0.2750	 0.3430
1Z	 0.5740	 0.4340
1a	 0.5880	 0.4480
1b	 0.4780	 0.4270
1c	 0.3100	 0.3700
1d	 0.4660	 0.4150
1e	 0.5380	 0.4350
1f	 0.2250	 0.3370
1g	 0.1330	 0.3280
1h	 0.2770	 0.3750



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Chain	Atom inclusion	Q-score
1i	 0.0090	 0.2600
1j	 0.0000	 0.2620
1k	 0.0000	 0.2080
1l	 0.0550	 0.2770
1m	 0.1150	 0.2940
1n	 0.0290	 0.2450
1o	 0.0020	 0.2220
1p	 0.0430	 0.3140
1q	 0.6100	 0.4560
1r	 0.5980	 0.4600
1s	 0.2210	 0.3810