



# wwPDB EM Validation Summary Report ⓘ

Jun 13, 2024 – 10:58 AM EDT

PDB ID : 8UEV  
EMDB ID : EMD-42172  
Title : In-situ complex I, Deactive class04  
Authors : Zheng, W.; Zhu, J.; Zhang, K.  
Deposited on : 2023-10-02  
Resolution : 3.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

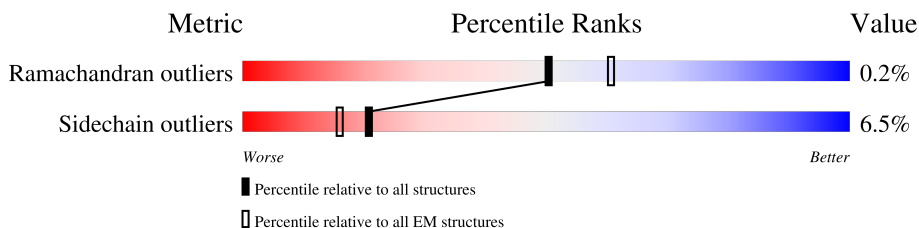
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	16% (red), 70% (green), 6% (yellow), 23% (grey)
2	1B	258	15% (red), 54% (green), 6% (yellow), 40% (grey)
3	1C	264	42% (red), 75% (green), 5% (yellow), 21% (grey)
4	1D	476	28% (red), 86% (green), 10% (grey)
5	1E	249	85% (red), 78% (green), 7% (yellow), 14% (grey)
6	1F	464	92% (red), 86% (green), 7% (yellow), 7% (grey)
7	1G	727	69% (red), 89% (green), 7% (yellow), 1% (grey)
8	1H	318	14% (red), 89% (green), 5% (yellow), 7% (grey)
9	1I	239	13% (red), 68% (green), 5% (yellow), 26% (grey)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	1J	175	30% 94% 6%
11	1K	98	11% 93% 7%
12	1L	606	95% 5%
13	1M	459	97% .
14	1N	347	96% .
15	1O	357	48% 84% 5% 10%
16	1P	377	62% 83% 7% 9%
17	1Q	175	52% 70% 26%
18	1R	123	54% 74% 22%
19	1S	99	84% 84% 12%
20	1T	156	46% 50% 46%
20	1U	156	6% 49% 6% 45%
21	1V	116	83% 91% 9% .
22	1W	128	62% 79% 10% 10%
23	1X	172	24% 94% 6% .
24	1Y	141	96% ..
25	1Z	144	24% 92% 6% .
26	1a	70	13% 91% 9%
27	1b	84	30% 95% ..
28	1c	76	26% 61% 36%
29	1d	123	7% 94% ..
30	1e	106	14% 84% 9% 7%
31	1f	135	16% 39% 58%
32	1g	154	14% 58% 6% 35%
33	1h	189	11% 66% 6% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	1i	128	<p>51% 94% 5% ..</p>
35	1j	105	<p>21% 65% 32%</p>
36	1k	98	<p>28% 74% 8% 17%</p>
37	1l	186	<p>13% 78% 5% 16%</p>
38	1m	129	<p>5% 94% 5% .</p>
39	1n	179	<p>11% 90% 6% .</p>
40	1o	137	<p>29% 83% 6% 11%</p>
41	1p	176	<p>18% 95% . .</p>
42	1q	145	<p>48% 90% 9% .</p>
43	1r	114	<p>47% 73% 11% 16%</p>
44	1s	471	<p>10% 9% 90%</p>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67103 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	88	707	484	101	117	5	0	0

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1H	297	2344	1571	363	389	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
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	1l	156	1310	847	213	242	8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	1m	128	1062	691	182	189	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	1n	172	1495	956	273	258	8	0	0

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

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

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

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

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

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

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

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

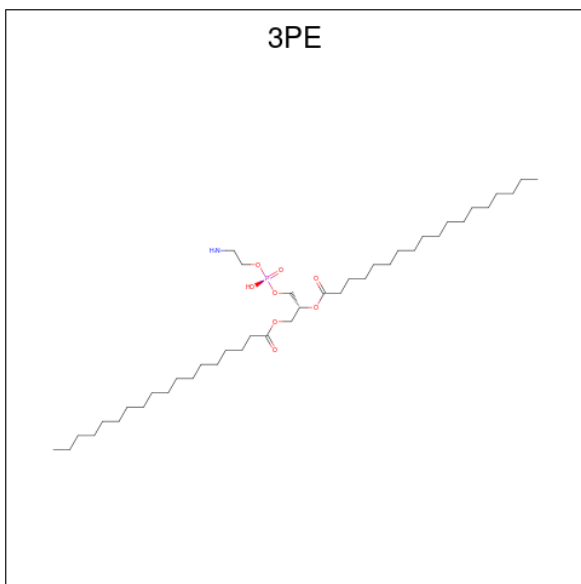
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 45 is 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	
45	1A	1	47	37	1	8	1	0
45	1L	1	46	36	1	8	1	0
45	1L	1	42	32	1	8	1	0
45	1N	1	51	41	1	8	1	0
45	1Y	1	31	21	1	8	1	0
45	1Y	1	51	41	1	8	1	0

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



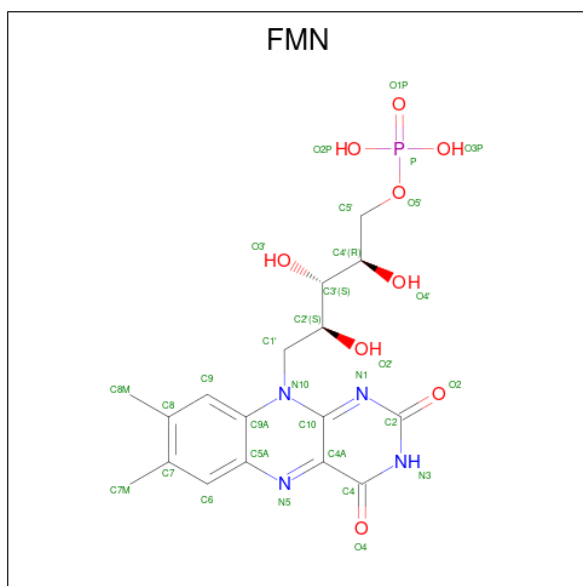
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
46	1B	1	8	4	4	0
46	1F	1	8	4	4	0
46	1G	1	8	4	4	0
46	1G	1	8	4	4	0
46	1I	1	8	4	4	0
46	1I	1	8	4	4	0

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



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

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

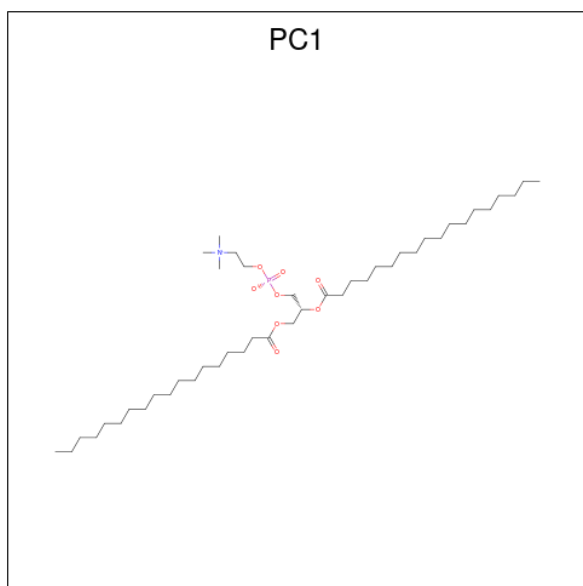


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

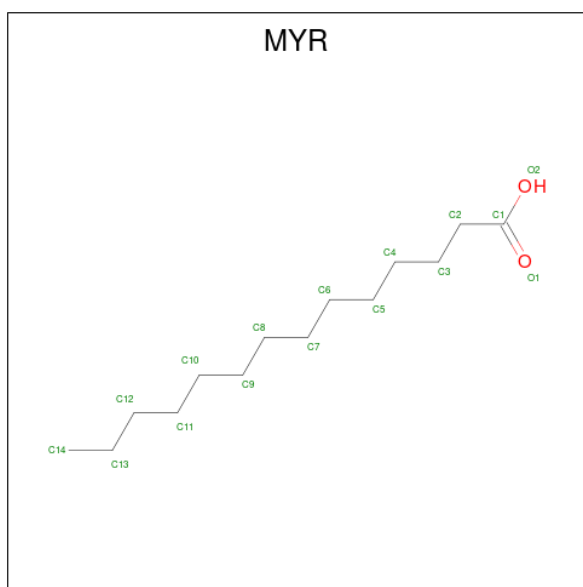
- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

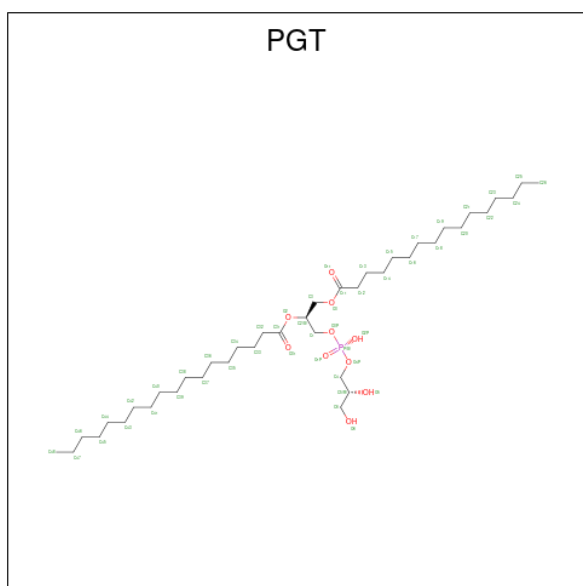
- Molecule 51 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).





Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	1L	1	15	14	1	0

- Molecule 52 is (1S)-2-[[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula:  $C_{40}H_{79}O_{10}P$ ).



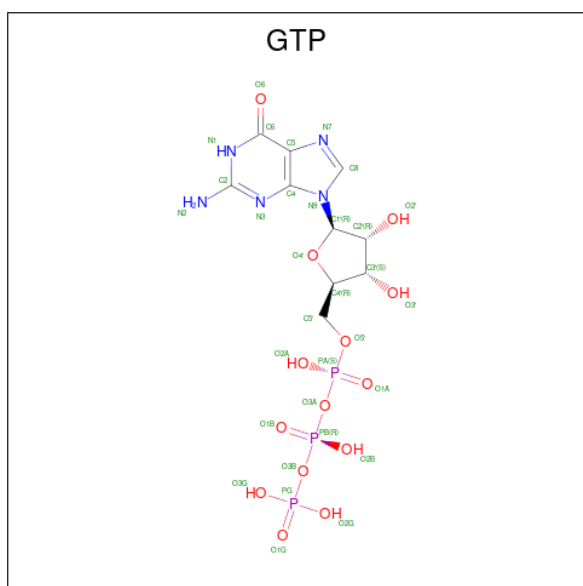
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	1M	1	51	40	10	1	0

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	1N	1	77	58	17	2	0
53	1r	1	61	42	17	2	0

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

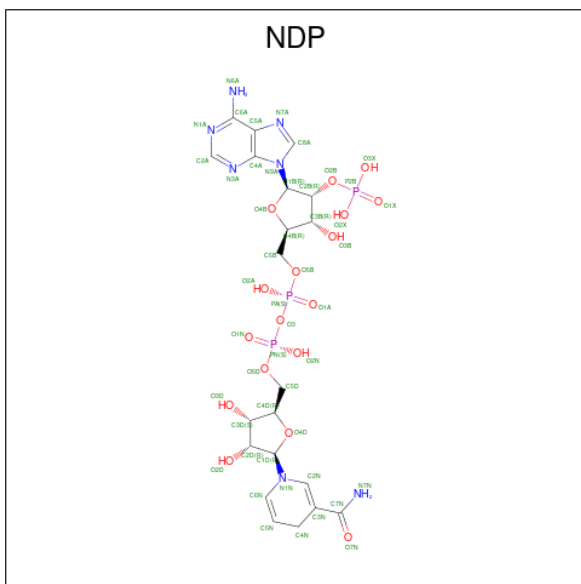


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	10	1	32	10	5	14	3	0

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

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

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

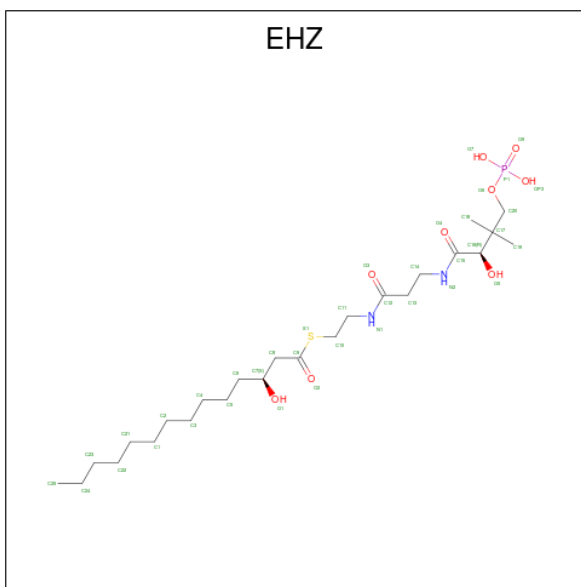


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

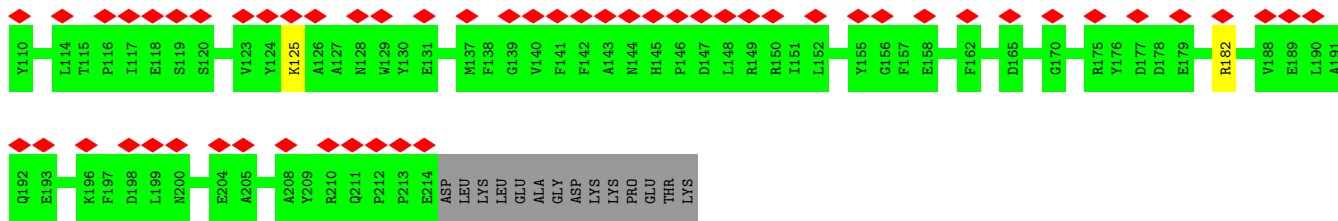
Mol	Chain	Residues	Atoms		AltConf
57	1R	1	Total	Zn	0
			1	1	

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

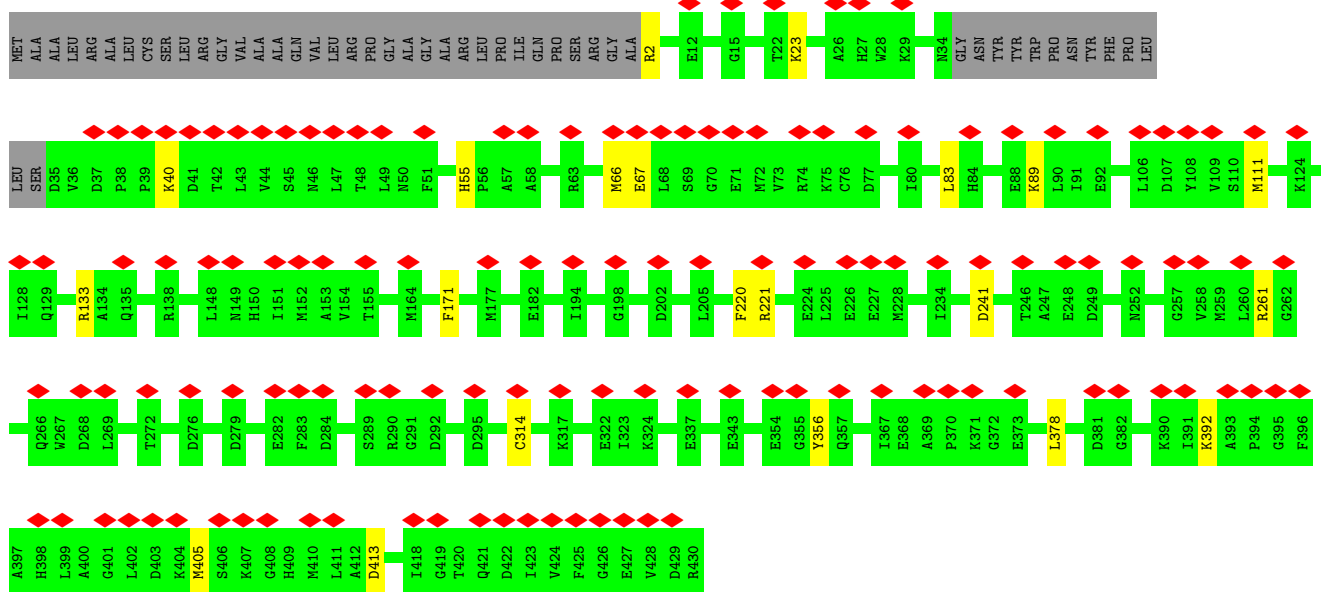
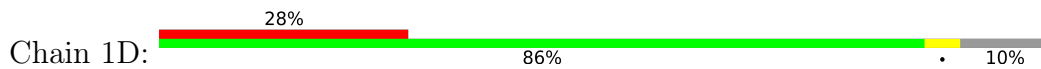


Mol	Chain	Residues	Atoms					AltConf		
			Total	C	N	O	P		S	
58	1W	1	Total	37	25	2	8	1	1	0
58	1n	1	Total	37	25	2	8	1	1	0

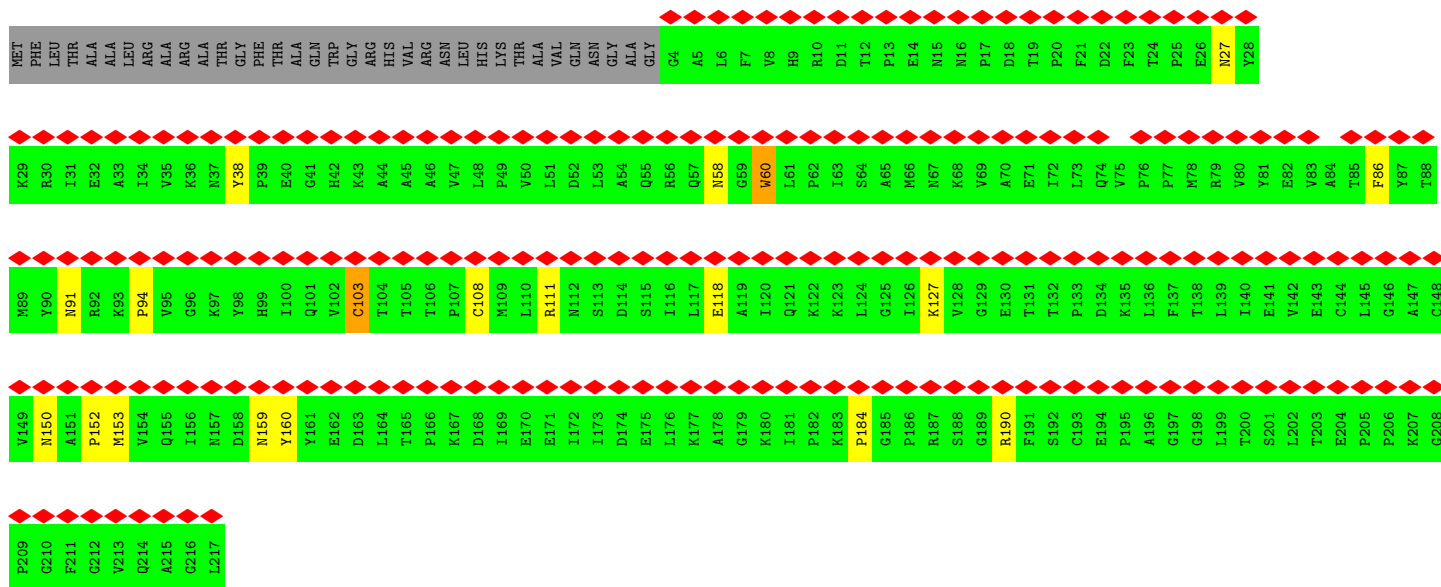
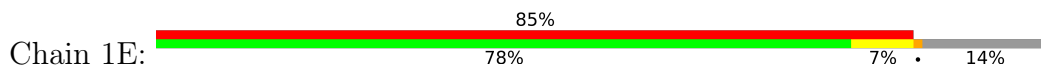




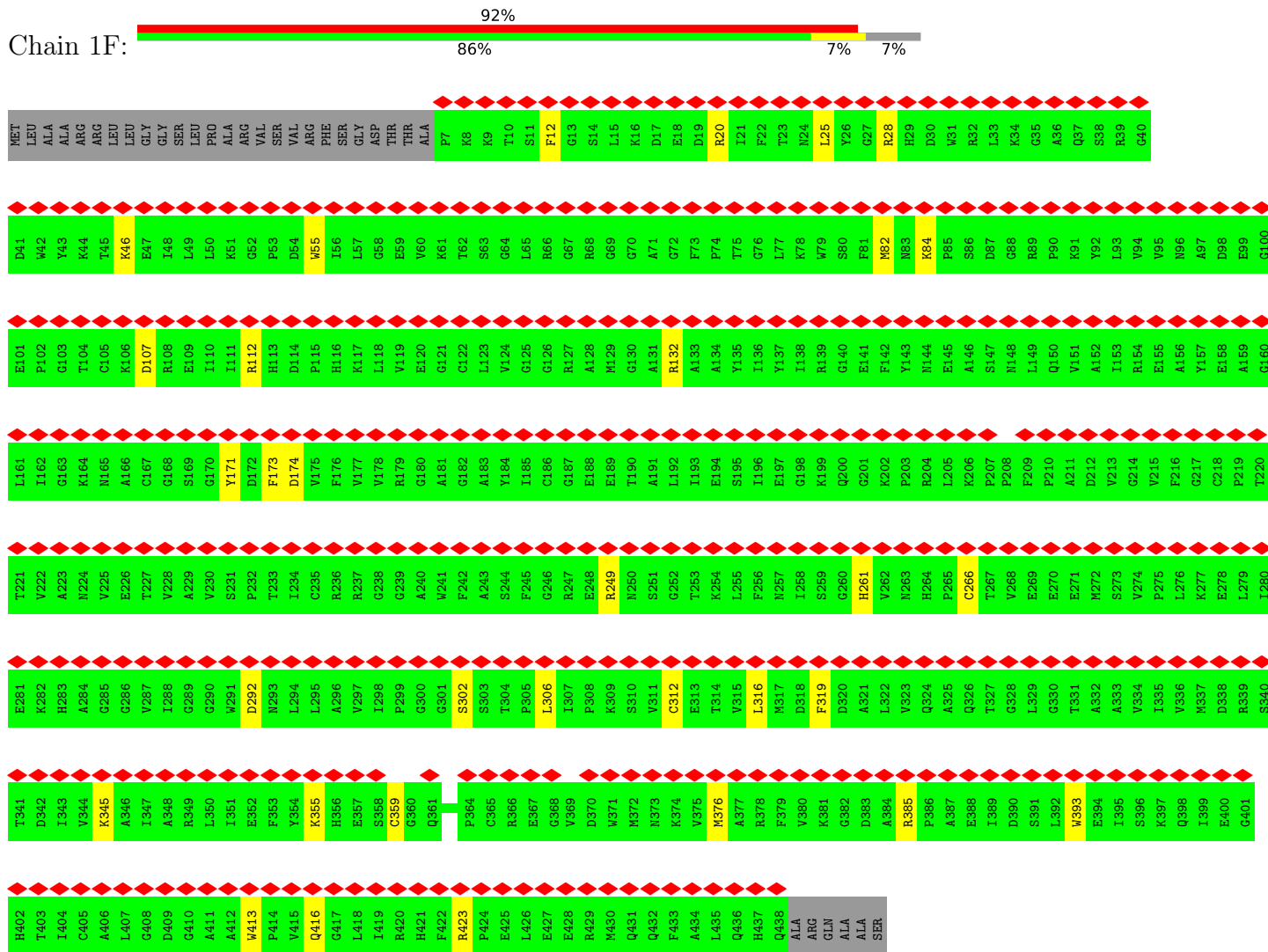
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



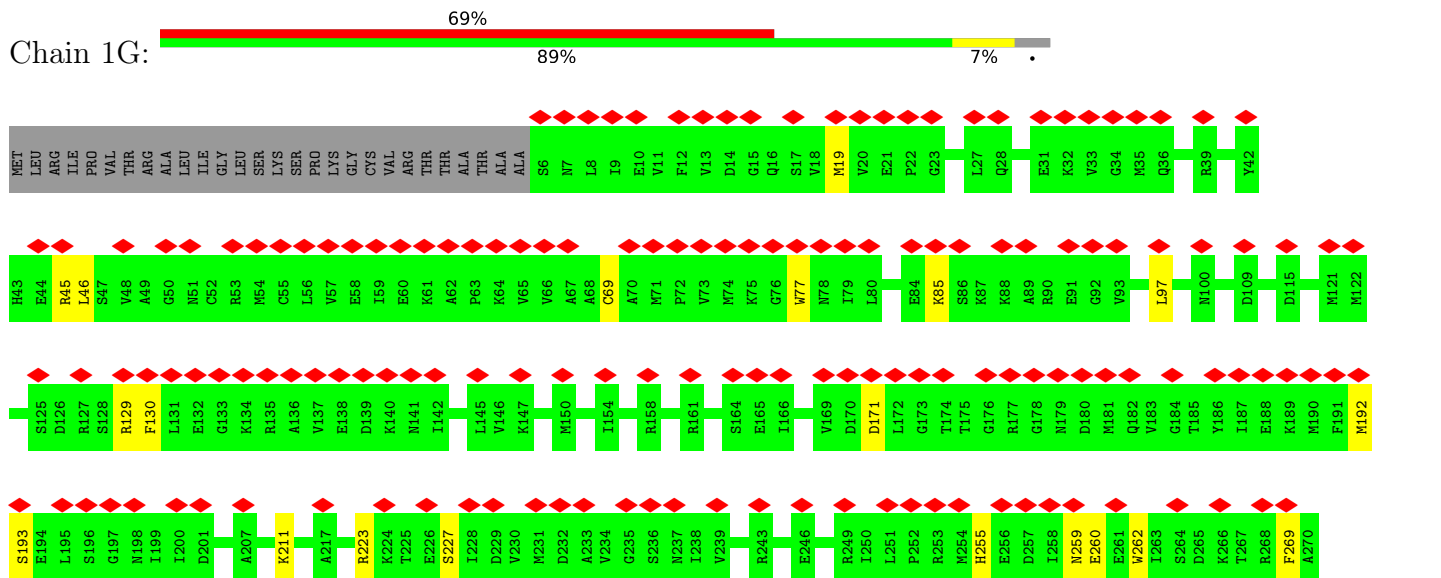
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

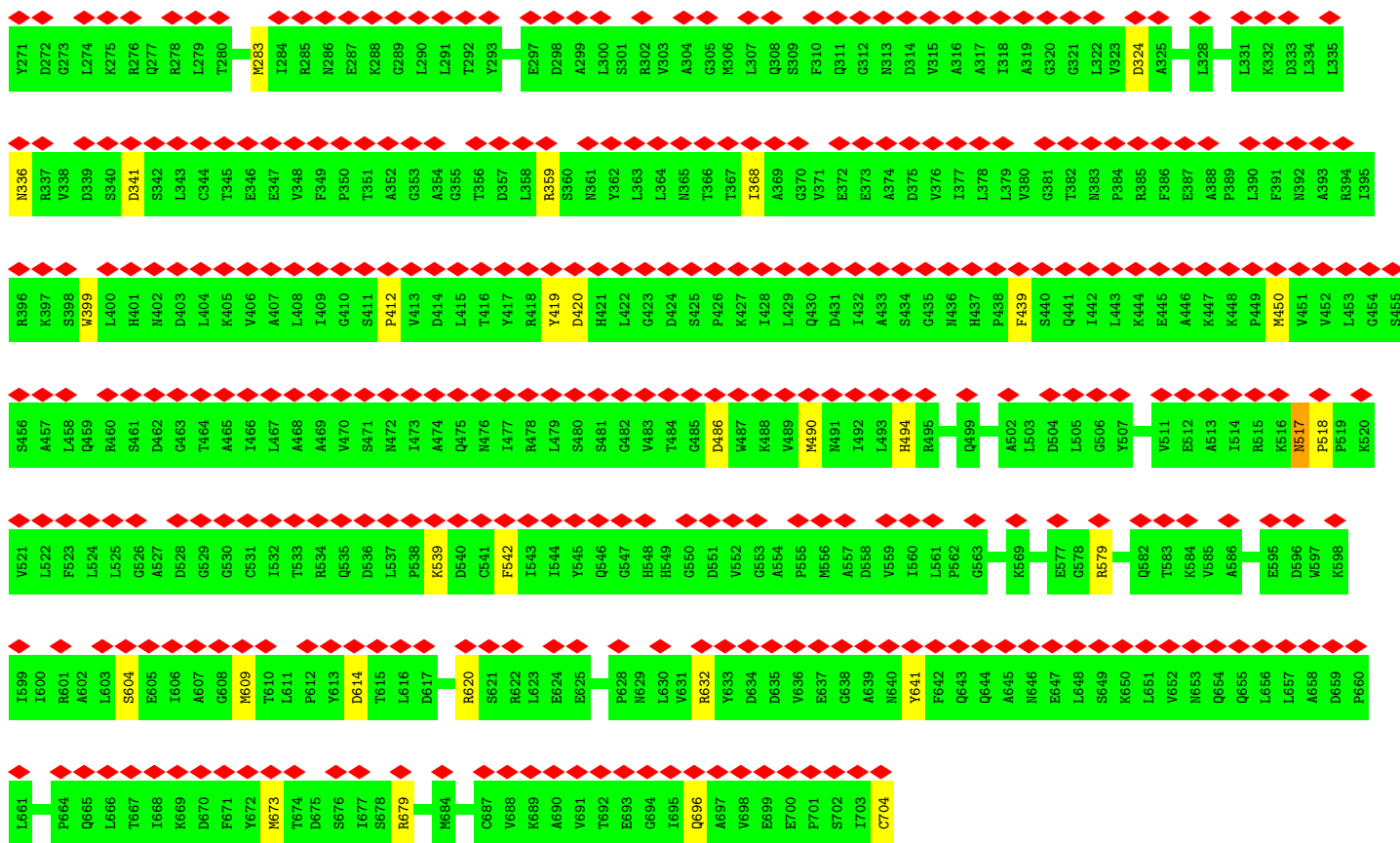


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

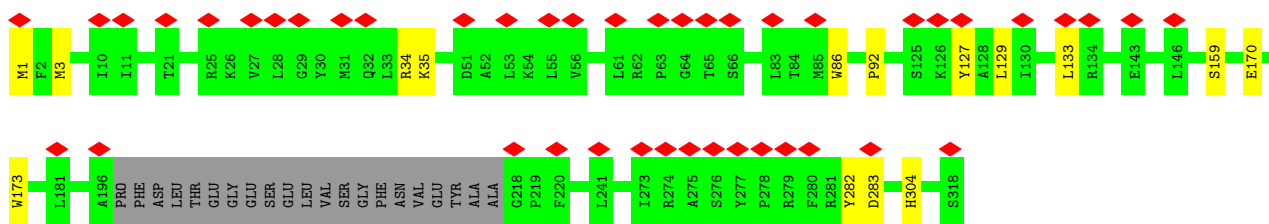
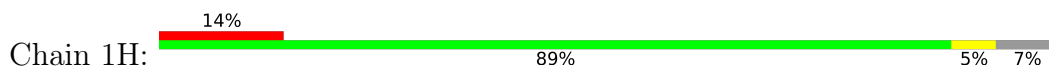


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

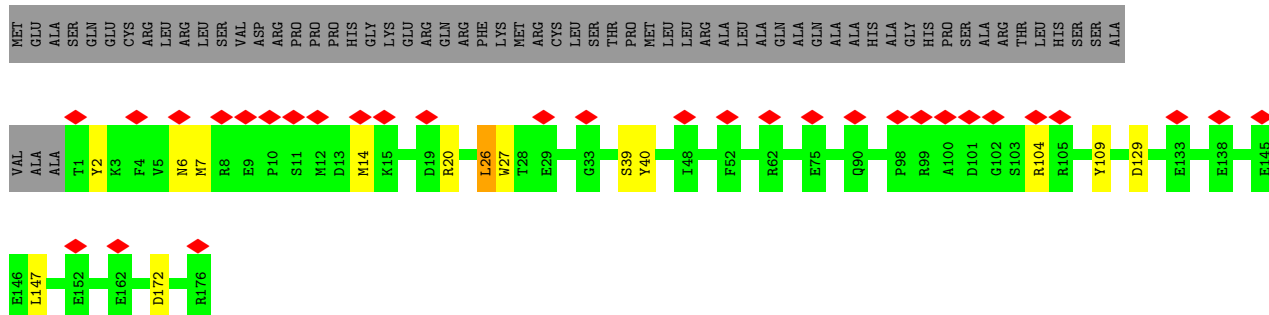




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

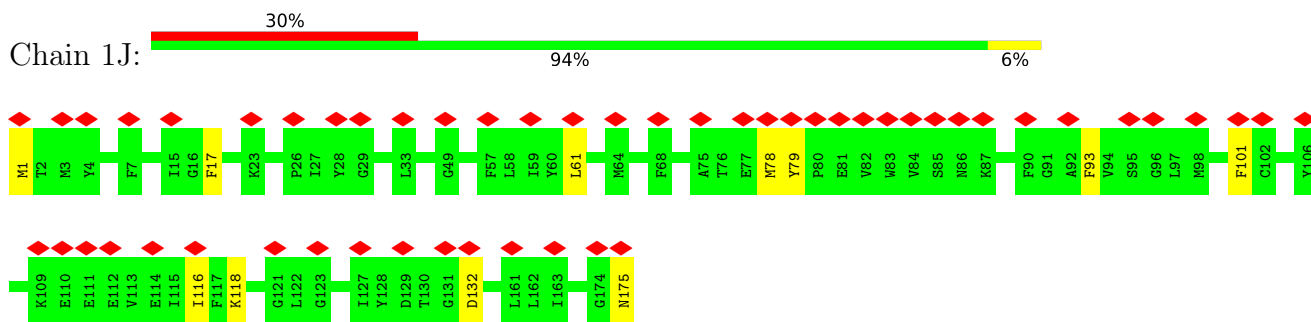


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

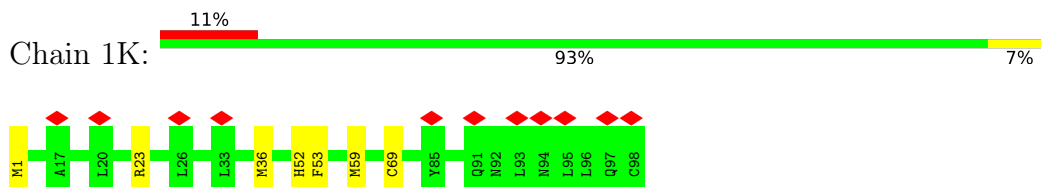




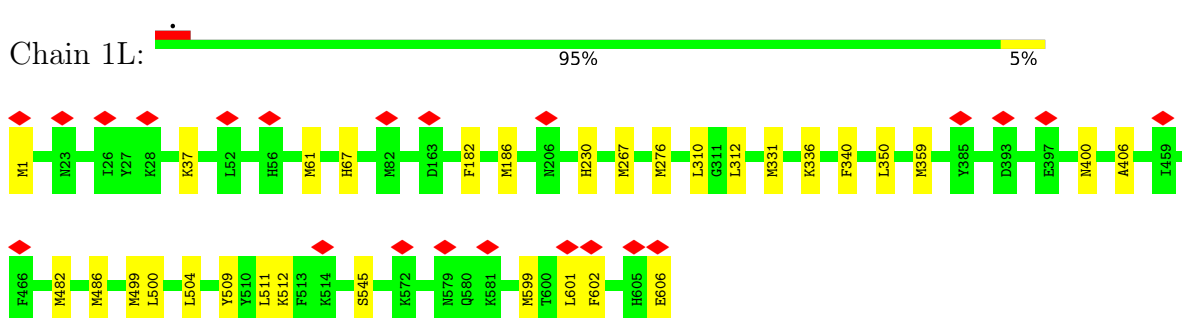
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



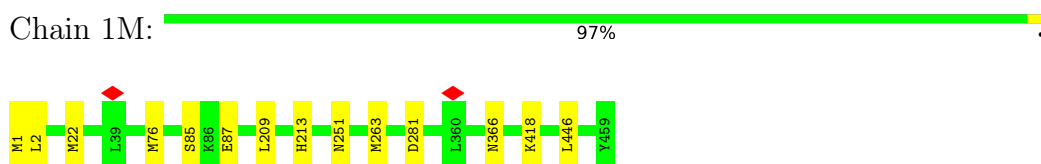
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



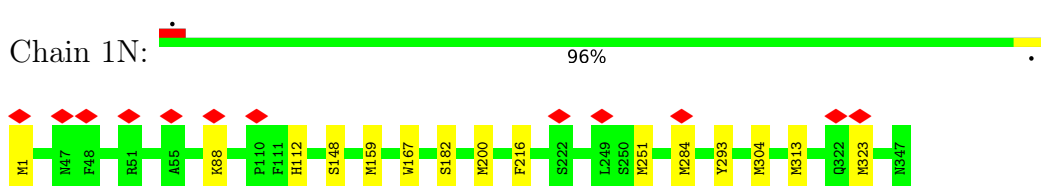
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



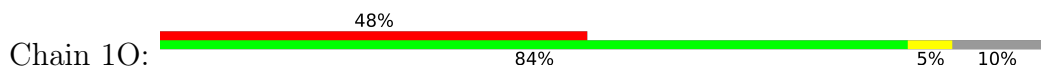
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

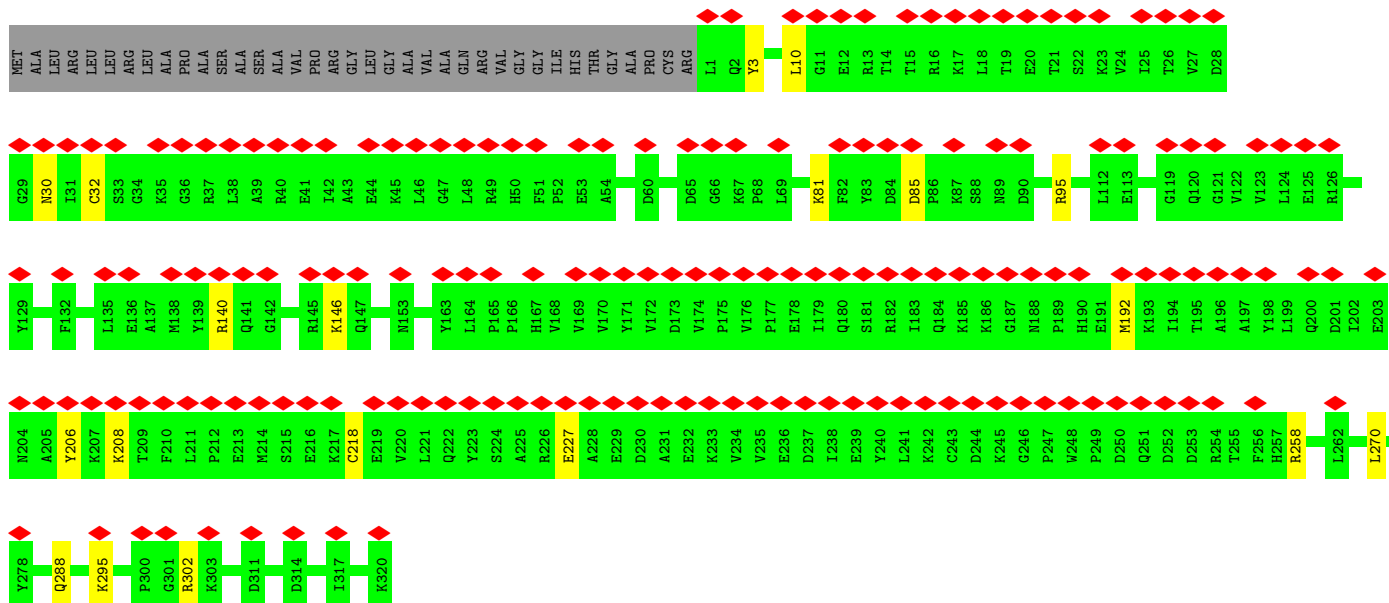


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

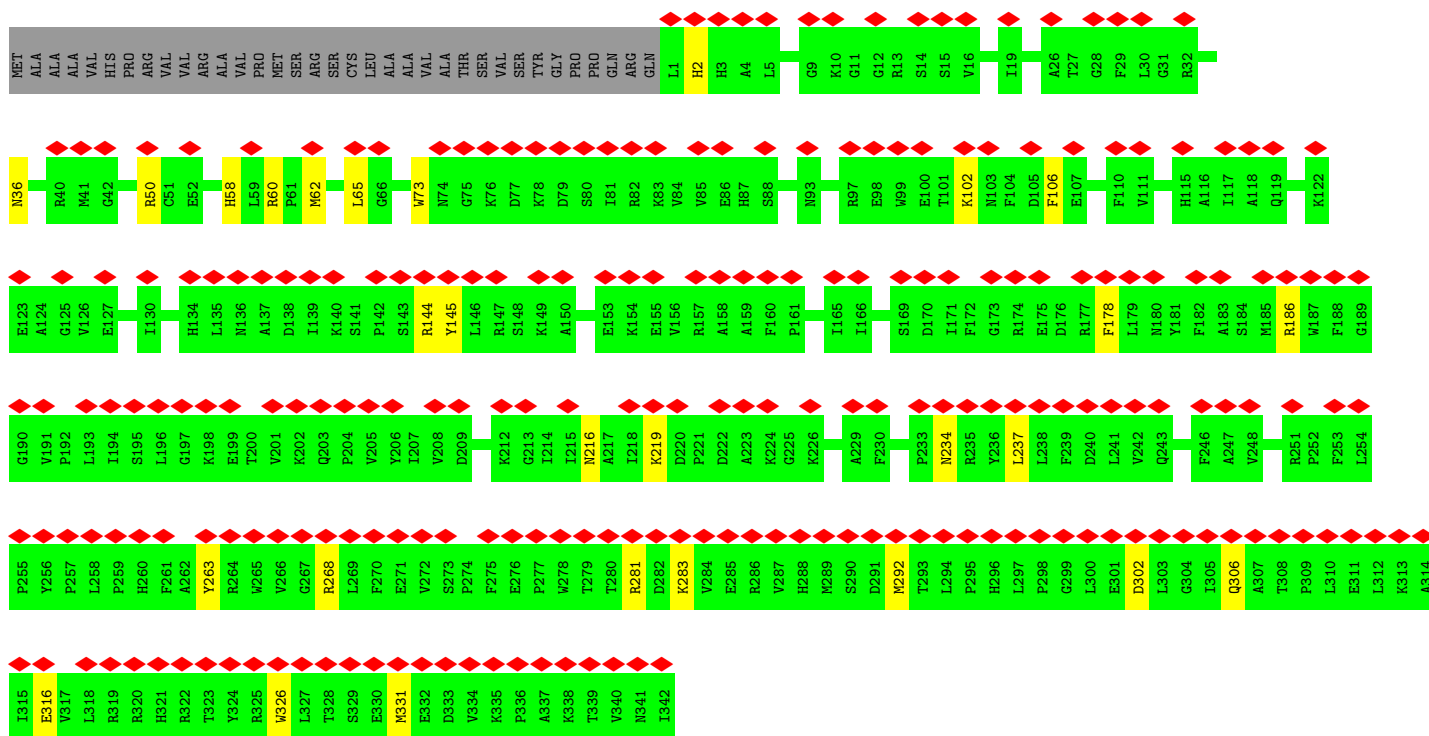
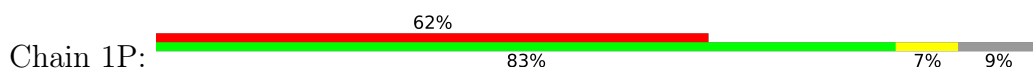


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

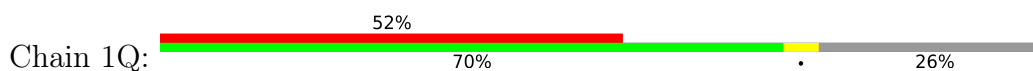


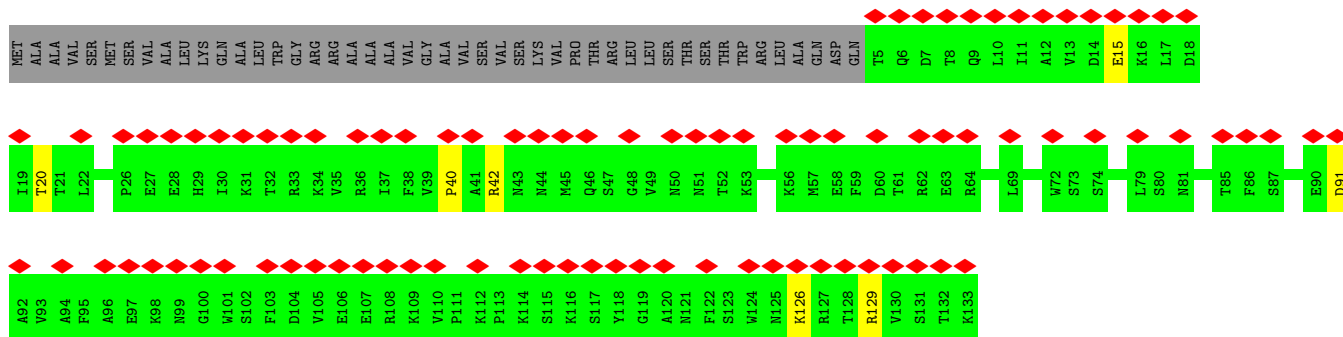


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

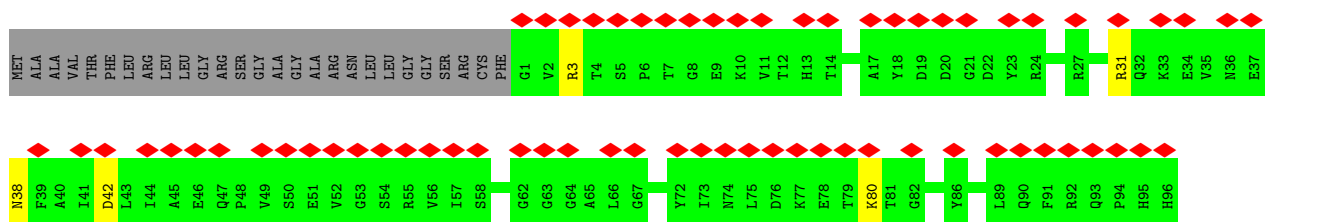
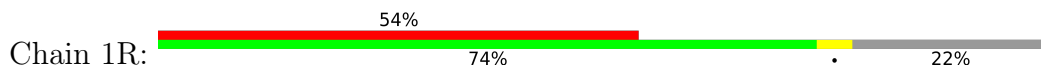


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

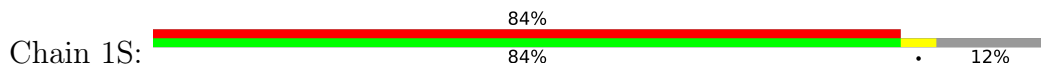




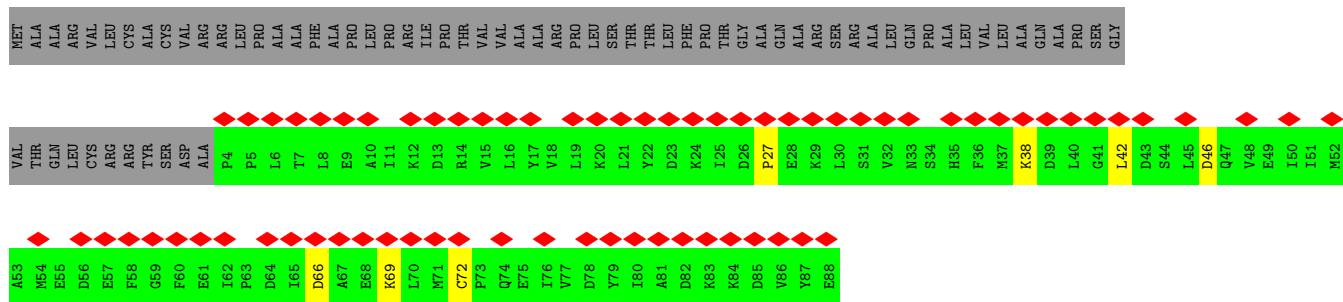
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

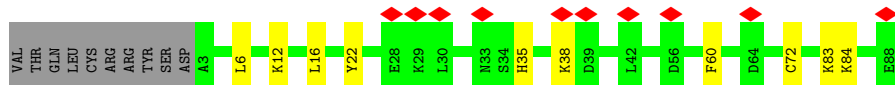
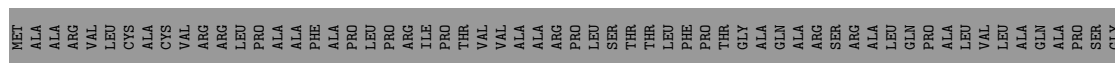


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

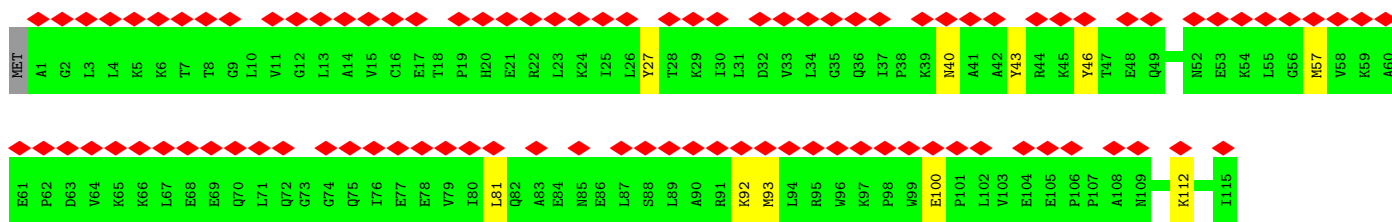
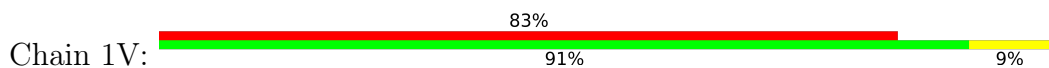


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

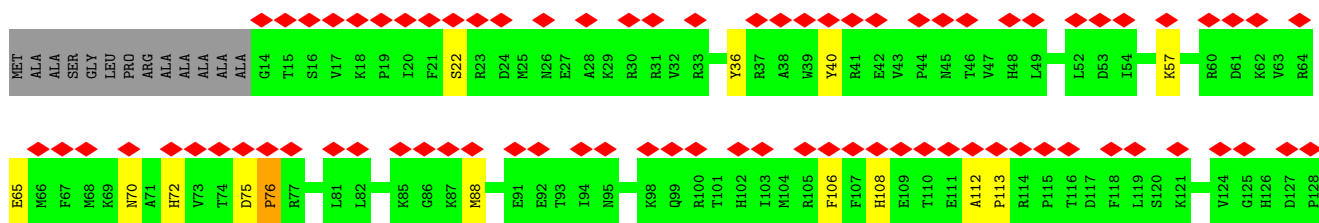
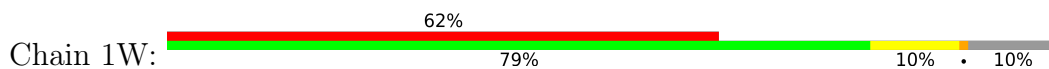




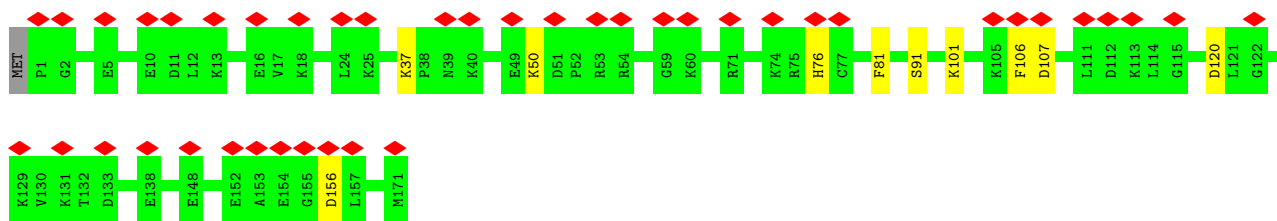
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



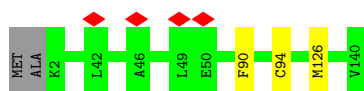
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



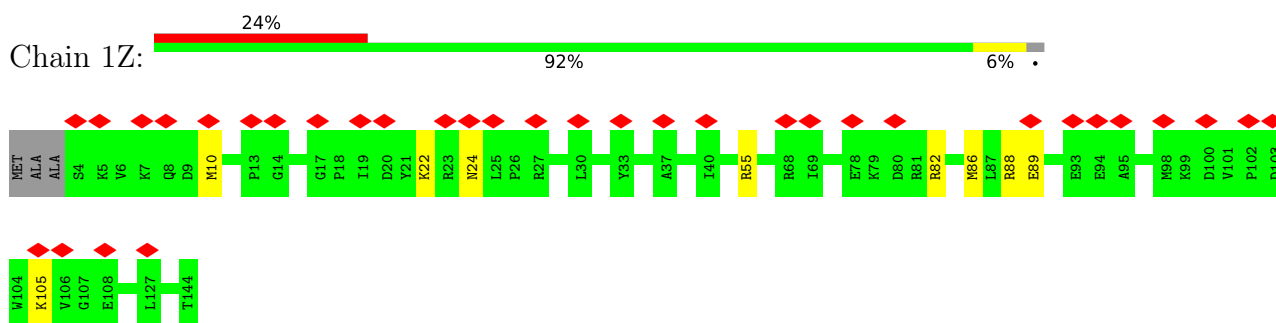
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



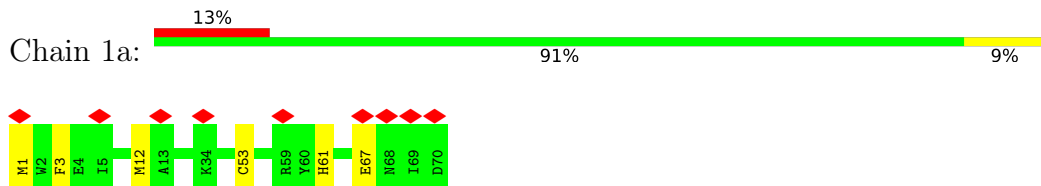
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



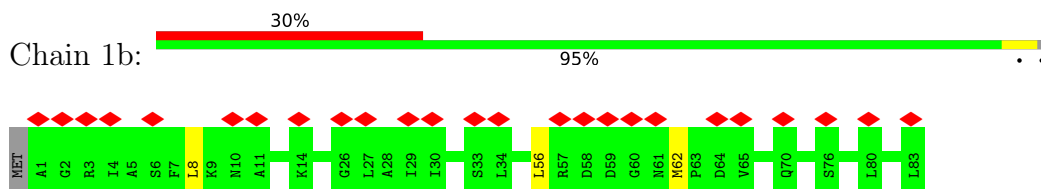
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



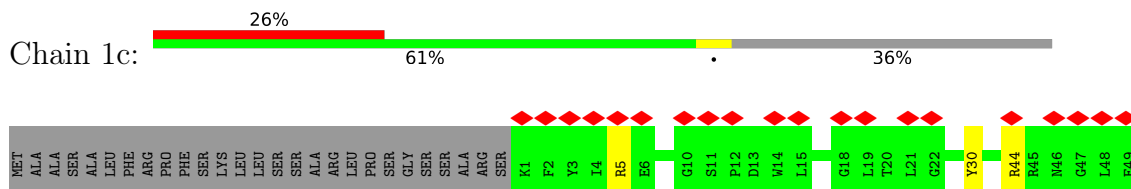
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



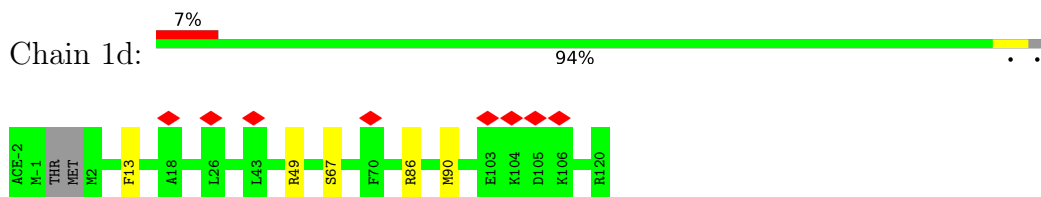
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



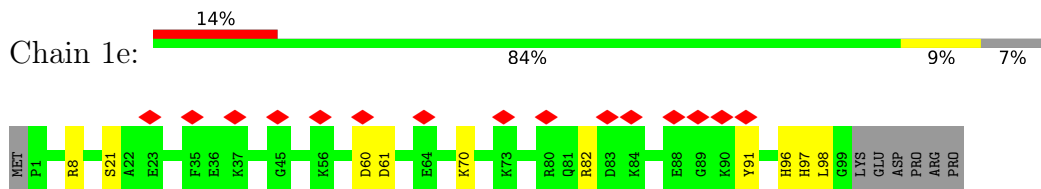
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

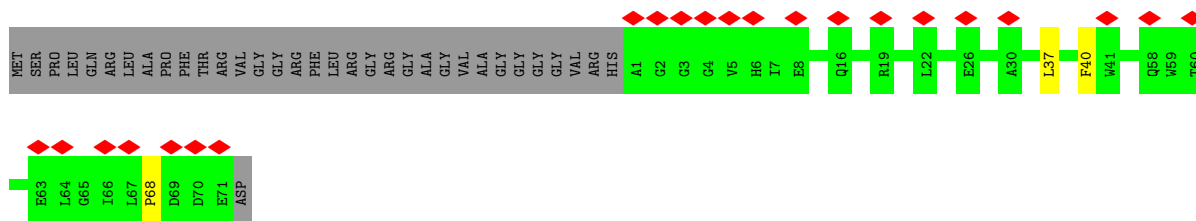


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

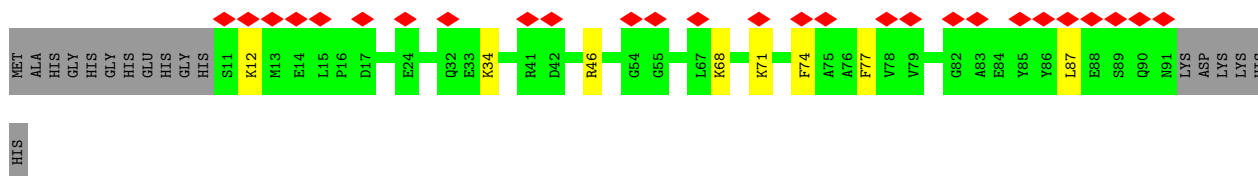
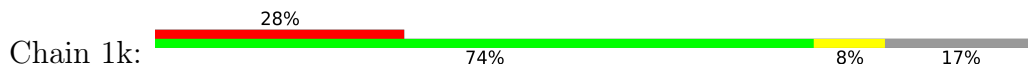


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

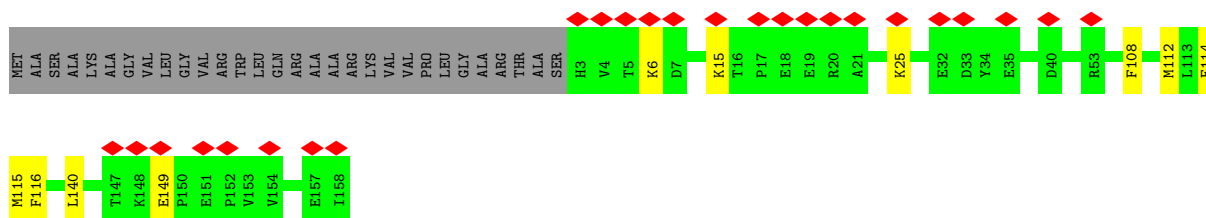
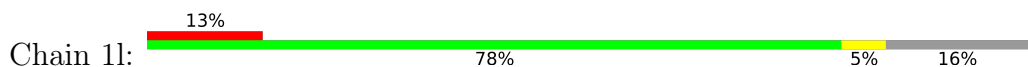




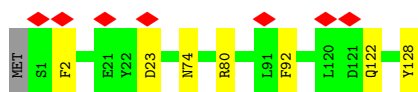
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



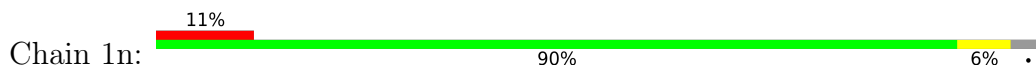
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



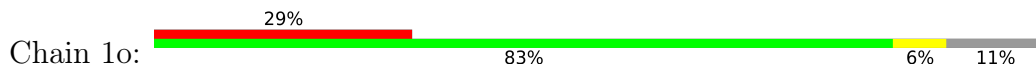
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



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







VAL	GLU	VAL	VAL	PRO
LYS	ASP	ALA	ALA	ALA
SER	ARG	PRO	ALA	ALA
THR	ARG	ARG	GLU	GLU
SER	ARG	GLY	ALA	ALA
ALA	ALA	LYS	LYS	LYS
PRO	PRO	PRO	GLU	GLU
GLY	LYS	ALA	LEU	LEU
GLY	ALA	SER	LEU	LEU
ALA	ALA	ALA	LEU	LEU
SER	ALA	PRO	GLY	GLY
GLU	ALA	THR	VAL	VAL
ALA	ARG	PRO	GLN	GLN
PRO	GLY	GLY	GLY	GLY
LYS	PRO	ALA	PRO	PRO
ALA	GLY	ALA	PRO	PRO
ALA	GLY	ARG	LYS	LYS
ALA	ALA	LEU	ALA	ALA
GLY	ALA	LEU	VAL	VAL
GLY	ALA	PRO	ALA	ALA
ARG	ARG	PRO	PRO	PRO
GLN	THR	THR	ASP	ASP
GLN	THR	PRO	GLY	GLY
THR	THR	GLN	GLN	GLN
GLY	PRO	GLU	ASP	ASP
VAL	SER	THR	GLU	GLU
GLN	GLN	GLY	GLY	GLY
ALA	LYS	ALA	ALA	ALA
ALA	ILE	GLU	GLU	GLU
ALA	PRO	ARG	LYS	LYS
ALA	ARG	PRO	LYS	LYS
ARG	ARG	LEU	ALA	ALA
PRO	SER	GLY	ALA	ALA
PRO	GLY	ALA	LEU	LEU
GLU	GLU	GLU	LEU	LEU
ALA	ALA	VAL	PRO	PRO
GLN	GLN	PRO	GLY	GLY
ASP	ASP	GLY	ILE	ILE
ALA	ALA	ALA	GLY	GLY
ALA	ALA	ASP	GLY	GLY
ALA	ALA	THR	ALA	ALA
VAL	VAL	ALA	ASP	ASP
LEU	LEU	ALA	ALA	ALA
LEU	LEU	ALA	ALA	ALA
LEU	LEU	THR	THR	THR
GLY	GLY	ALA	ALA	ALA
GLY	GLY	ARG	ARG	ARG
GLY	GLY	ALA	ALA	ALA
GLY	GLY	ALA	ALA	ALA
GLY	GLY	ASP	ASP	ASP
GLY	GLY	THR	THR	THR
GLY	GLY	ALA	ALA	ALA
GLY	GLY	THR	THR	THR
SER	SER	GLN	GLN	GLN
GLY	GLY	GLN	GLN	GLN
SER	SER	ALA	ALA	ALA
GLY	GLY	ALA	ALA	ALA
LEU	LEU	GLU	GLU	GLU
SER	SER	PRO	PRO	PRO
THR	THR	THR	THR	THR



PRO	PRO	PRO	PRO	PRO
ALA	ALA	ALA	ALA	ALA
ALA	ALA	ALA	ALA	ALA
ALA	ALA	ALA	ALA	ALA
ALA	ALA	ALA	ALA	ALA
E31	P32	F33	D34	N35
S36	T37	Y38	R39	M40
L41	Q42	H43	H44	E45
Y46	S47	T48	Y49	T50
F51	L52	D53	L54	N55
V56	E57	L58	S59	K60
F61	R62	M63	P64	Q65
P66	S67	S68	G69	R70
Q71	S72	P73	R74	H75

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37000	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	0.909	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.30	0/713	0.53	0/975
2	1B	0.45	2/1273 (0.2%)	0.66	1/1722 (0.1%)
3	1C	0.29	0/1791	0.57	0/2439
4	1D	0.30	0/3545	0.54	1/4806 (0.0%)
5	1E	0.44	3/1698 (0.2%)	0.72	5/2311 (0.2%)
6	1F	0.32	0/3401	0.58	1/4595 (0.0%)
7	1G	0.42	4/5451 (0.1%)	0.66	10/7387 (0.1%)
8	1H	0.28	0/2401	0.50	0/3282
9	1I	0.31	0/1443	0.63	1/1952 (0.1%)
10	1J	0.31	0/1364	0.52	0/1850
11	1K	0.31	0/751	0.59	0/1018
12	1L	0.27	0/4939	0.52	2/6718 (0.0%)
13	1M	0.26	0/3713	0.47	0/5063
14	1N	0.30	0/2765	0.53	0/3758
15	1O	0.35	1/2650 (0.0%)	0.52	0/3588
16	1P	0.30	0/2828	0.54	1/3834 (0.0%)
17	1Q	0.32	0/1070	0.62	1/1446 (0.1%)
18	1R	0.28	0/755	0.57	0/1018
19	1S	0.30	0/711	0.65	1/956 (0.1%)
20	1T	0.50	1/701 (0.1%)	0.78	2/946 (0.2%)
20	1U	0.29	0/706	0.53	1/954 (0.1%)
21	1V	0.27	0/946	0.49	0/1281
22	1W	1.28	5/995 (0.5%)	1.39	7/1340 (0.5%)
23	1X	0.27	0/1436	0.52	0/1938
24	1Y	0.24	0/1037	0.46	0/1404
25	1Z	0.27	0/1199	0.55	0/1617
26	1a	0.39	0/577	1.04	2/777 (0.3%)
27	1b	0.27	0/664	0.53	0/912
28	1c	0.32	0/430	0.61	0/581
29	1d	0.32	0/1024	0.52	0/1383
30	1e	0.25	0/836	0.53	0/1118
31	1f	0.27	0/499	0.58	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	1g	0.35	0/858	0.65	0/1165
33	1h	0.33	1/1184 (0.1%)	0.52	0/1603
34	1i	1.14	6/1131 (0.5%)	1.31	7/1541 (0.5%)
35	1j	0.28	0/627	0.58	2/858 (0.2%)
36	1k	0.28	0/668	0.55	0/903
37	1l	0.27	0/1365	0.47	0/1867
38	1m	0.27	0/1092	0.50	0/1481
39	1n	0.37	2/1549 (0.1%)	0.69	2/2098 (0.1%)
40	1o	0.26	0/1069	0.55	0/1430
41	1p	0.27	0/1481	0.54	0/1997
42	1q	0.32	0/1253	0.65	2/1704 (0.1%)
43	1r	0.34	0/782	0.62	0/1057
44	1s	0.27	0/394	0.54	0/533
All	All	0.38	25/67765 (0.0%)	0.61	49/91879 (0.1%)

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
5	1E	0	1
13	1M	0	1
34	1i	0	1
42	1q	0	1
All	All	0	4

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1W	76	PRO	CG-CD	-24.74	0.69	1.50
34	1i	54	ALA	C-N	23.84	1.79	1.34
22	1W	75	ASP	C-N	19.93	1.72	1.34
34	1i	55	PRO	CG-CD	-19.67	0.85	1.50
22	1W	76	PRO	N-CD	13.94	1.67	1.47

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	55	PRO	CA-N-CD	-27.55	72.92	111.50
34	1i	55	PRO	CB-CG-CD	-27.29	0.05	106.50
22	1W	76	PRO	CB-CG-CD	-25.73	6.17	106.50

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1a	1	MET	CG-SD-CE	-23.03	63.36	100.20
22	1W	76	PRO	CA-N-CD	-21.45	81.47	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1E	152	PRO	Peptide
13	1M	251	ASN	Peptide
34	1i	55	PRO	Mainchain
42	1q	143	PRO	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	84/115 (73%)	80 (95%)	4 (5%)	0	100	100
2	1B	153/258 (59%)	137 (90%)	16 (10%)	0	100	100
3	1C	207/264 (78%)	194 (94%)	13 (6%)	0	100	100
4	1D	427/476 (90%)	394 (92%)	33 (8%)	0	100	100
5	1E	212/249 (85%)	191 (90%)	21 (10%)	0	100	100
6	1F	430/464 (93%)	398 (93%)	31 (7%)	1 (0%)	47	78
7	1G	697/727 (96%)	643 (92%)	50 (7%)	4 (1%)	25	62
8	1H	293/318 (92%)	279 (95%)	12 (4%)	2 (1%)	22	59
9	1I	174/239 (73%)	163 (94%)	11 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	25	62
11	1K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	1L	604/606 (100%)	556 (92%)	45 (8%)	3 (0%)	29	66
13	1M	457/459 (100%)	440 (96%)	16 (4%)	1 (0%)	47	78
14	1N	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
15	1O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	305 (90%)	35 (10%)	0	100	100
17	1Q	127/175 (73%)	111 (87%)	15 (12%)	1 (1%)	19	56
18	1R	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	1U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	17	54
22	1W	113/128 (88%)	103 (91%)	9 (8%)	1 (1%)	17	54
23	1X	169/172 (98%)	159 (94%)	10 (6%)	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%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	7 (7%)	1 (1%)	15	51
33	1h	136/189 (72%)	128 (94%)	8 (6%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	72 (91%)	7 (9%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	25	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
42	1q	143/145 (99%)	129 (90%)	11 (8%)	3 (2%)	7	38
43	1r	90/114 (79%)	83 (92%)	7 (8%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8142/9744 (84%)	7572 (93%)	550 (7%)	20 (0%)	50	78

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	259	ASN
8	1H	92	PRO
12	1L	406	ALA
13	1M	2	LEU
17	1Q	20	THR

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	76/99 (77%)	70 (92%)	6 (8%)	12	42
2	1B	131/212 (62%)	117 (89%)	14 (11%)	6	30
3	1C	190/227 (84%)	178 (94%)	12 (6%)	18	49
4	1D	371/405 (92%)	351 (95%)	20 (5%)	22	54
5	1E	183/207 (88%)	170 (93%)	13 (7%)	14	45
6	1F	346/368 (94%)	316 (91%)	30 (9%)	10	38
7	1G	588/610 (96%)	547 (93%)	41 (7%)	15	45
8	1H	257/274 (94%)	245 (95%)	12 (5%)	26	56
9	1I	151/201 (75%)	137 (91%)	14 (9%)	9	35
10	1J	140/140 (100%)	131 (94%)	9 (6%)	17	48
11	1K	84/84 (100%)	78 (93%)	6 (7%)	14	45

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1L	539/539 (100%)	514 (95%)	25 (5%)	27	57
13	1M	408/408 (100%)	397 (97%)	11 (3%)	44	68
14	1N	310/310 (100%)	296 (96%)	14 (4%)	27	57
15	1O	283/307 (92%)	265 (94%)	18 (6%)	17	48
16	1P	296/323 (92%)	269 (91%)	27 (9%)	9	36
17	1Q	117/152 (77%)	112 (96%)	5 (4%)	29	58
18	1R	79/97 (81%)	74 (94%)	5 (6%)	18	49
19	1S	77/82 (94%)	74 (96%)	3 (4%)	32	60
20	1T	79/133 (59%)	73 (92%)	6 (8%)	13	43
20	1U	79/133 (59%)	70 (89%)	9 (11%)	5	27
21	1V	100/101 (99%)	91 (91%)	9 (9%)	9	37
22	1W	107/112 (96%)	97 (91%)	10 (9%)	9	35
23	1X	153/154 (99%)	143 (94%)	10 (6%)	17	48
24	1Y	101/102 (99%)	98 (97%)	3 (3%)	41	66
25	1Z	123/124 (99%)	114 (93%)	9 (7%)	14	44
26	1a	58/58 (100%)	53 (91%)	5 (9%)	10	39
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	58
28	1c	45/66 (68%)	42 (93%)	3 (7%)	16	47
29	1d	107/109 (98%)	102 (95%)	5 (5%)	26	56
30	1e	87/94 (93%)	77 (88%)	10 (12%)	5	27
31	1f	54/113 (48%)	50 (93%)	4 (7%)	13	44
32	1g	92/129 (71%)	83 (90%)	9 (10%)	8	33
33	1h	121/158 (77%)	108 (89%)	13 (11%)	6	30
34	1i	119/120 (99%)	115 (97%)	4 (3%)	37	64
35	1j	62/84 (74%)	61 (98%)	1 (2%)	62	80
36	1k	63/76 (83%)	55 (87%)	8 (13%)	4	23
37	1l	141/161 (88%)	131 (93%)	10 (7%)	14	45
38	1m	113/114 (99%)	106 (94%)	7 (6%)	18	49
39	1n	156/160 (98%)	148 (95%)	8 (5%)	24	55
40	1o	110/120 (92%)	102 (93%)	8 (7%)	14	44
41	1p	154/156 (99%)	148 (96%)	6 (4%)	32	60

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1q	131/131 (100%)	122 (93%)	9 (7%)	15	46
43	1r	85/98 (87%)	72 (85%)	13 (15%)	2	17
44	1s	44/351 (12%)	42 (96%)	2 (4%)	27	57
All	All	7179/8272 (87%)	6710 (94%)	469 (6%)	21	48

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	1O	81	LYS
41	1p	133	GLN
20	1T	42	LEU
40	1o	111	LYS
36	1k	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
19	1S	75	ASN
44	1s	43	HIS
29	1d	88	HIS
44	1s	40	ASN
42	1q	69	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
8	FME	1H	1	8	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
34	SAC	1i	1	-	7,8,9	0.54	0	8,9,11	1.04	1 (12%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	0.94	1 (14%)
14	FME	1N	1	14	8,9,10	0.53	0	7,9,11	1.03	1 (14%)
13	FME	1M	1	13	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
10	FME	1J	1	10	8,9,10	0.53	0	7,9,11	0.97	1 (14%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	1.06	1 (14%)
1	FME	1A	1	1	8,9,10	0.50	0	7,9,11	1.02	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
8	FME	1H	1	8	-	0/7/9/11	-
34	SAC	1i	1	-	-	2/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
10	FME	1J	1	10	-	3/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.87	117.26	124.78
12	1L	1	FME	O-C-CA	-2.61	117.93	124.78
13	1M	1	FME	O-C-CA	-2.53	118.15	124.78
10	1J	1	FME	O-C-CA	-2.51	118.20	124.78
1	1A	1	FME	O-C-CA	-2.50	118.23	124.78

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	CB-CG-SD-CE
11	1K	1	FME	CB-CG-SD-CE
34	1i	1	SAC	C-CA-N-C1A
34	1i	1	SAC	CB-CA-N-C1A

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	$\# Z  > 2$
56	NDP	1P	501	-	45,52,52	0.62	0	53,80,80	0.87	2 (3%)
48	FMN	1F	501	-	33,33,33	0.58	0	48,50,50	0.64	0
58	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.27	1 (2%)
47	FES	1G	803	7	0,4,4	-	-	-	-	-
46	SF4	1I	201	9	0,12,12	-	-	-	-	-
45	3PE	1Y	202	-	50,50,50	0.26	0	53,55,55	0.31	0
46	SF4	1I	202	9	0,12,12	-	-	-	-	-
50	PC1	1I	203	-	53,53,53	0.26	0	59,61,61	0.32	0
45	3PE	1L	702	-	45,45,50	0.28	0	48,50,55	0.31	0
47	FES	1E	301	5	0,4,4	-	-	-	-	-
46	SF4	1B	201	2	0,12,12	-	-	-	-	-
58	EHZ	1n	201	-	29,36,37	0.18	0	35,44,47	1.20	1 (2%)
50	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.39	0
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0
46	SF4	1G	802	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.44	0
45	3PE	1Y	201	-	30,30,50	0.35	0	33,35,55	0.65	1 (3%)
46	SF4	1F	502	6	0,12,12	-	-	-	-	-
45	3PE	1L	704	-	41,41,50	0.30	0	44,46,55	1.28	5 (11%)
45	3PE	1N	401	-	50,50,50	0.26	0	53,55,55	0.37	0
53	CDL	1r	201	-	60,60,99	0.84	3 (5%)	66,72,111	1.10	4 (6%)
53	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.37	0
51	MYR	1L	701	-	14,14,15	0.34	0	13,13,15	0.41	0
50	PC1	1f	101	-	45,45,53	0.26	0	51,53,61	0.35	0
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.86	1 (3%)
52	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.49	0
50	PC1	1L	703	-	43,43,53	0.29	0	49,51,61	0.38	0
46	SF4	1G	801	7	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	NDP	1P	501	-	-	11/30/77/77	0/5/5/5
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
58	EHZ	1W	201	-	-	8/42/44/45	-
47	FES	1G	803	7	-	-	0/1/1/1
46	SF4	1I	201	9	-	-	0/6/5/5
45	3PE	1Y	202	-	-	8/54/54/54	-
46	SF4	1I	202	9	-	-	0/6/5/5
50	PC1	1I	203	-	-	16/57/57/57	-
45	3PE	1L	702	-	-	4/49/49/54	-
47	FES	1E	301	5	-	-	0/1/1/1
46	SF4	1B	201	2	-	-	0/6/5/5
58	EHZ	1n	201	-	-	8/42/44/45	-
50	PC1	1I	204	-	-	4/47/47/57	-
45	3PE	1A	201	-	-	3/50/50/54	-
50	PC1	1J	201	-	-	3/38/38/57	-
46	SF4	1G	802	7	-	-	0/6/5/5
45	3PE	1Y	201	-	-	9/34/34/54	-
46	SF4	1F	502	6	-	-	0/6/5/5
45	3PE	1L	704	-	-	7/45/45/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1N	401	-	-	10/54/54/54	-
53	CDL	1r	201	-	-	16/71/71/110	-
53	CDL	1N	402	-	-	8/87/87/110	-
51	MYR	1L	701	-	-	1/11/12/13	-
50	PC1	1f	101	-	-	13/49/49/57	-
54	GTP	1O	401	55	-	0/18/38/38	0/3/3/3
52	PGT	1M	501	-	-	23/55/55/55	-
50	PC1	1L	703	-	-	8/47/47/57	-
46	SF4	1G	801	7	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1r	201	CDL	OB5-CB3	4.73	1.63	1.44
54	1O	401	GTP	C5-C6	-2.59	1.42	1.47
53	1r	201	CDL	OB2-CB2	2.19	1.53	1.44
53	1r	201	CDL	PB2-OB4	-2.18	1.45	1.55
54	1O	401	GTP	C8-N7	-2.07	1.31	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1n	201	EHZ	C10-S1-C9	6.79	123.01	101.87
58	1W	201	EHZ	C10-S1-C9	6.74	122.86	101.87
45	1L	704	3PE	O21-C21-C22	6.30	125.08	111.50
53	1r	201	CDL	OB4-PB2-OB2	4.45	128.41	107.75
53	1r	201	CDL	OB5-PB2-OB3	-4.25	92.48	109.07

There are no chirality outliers.

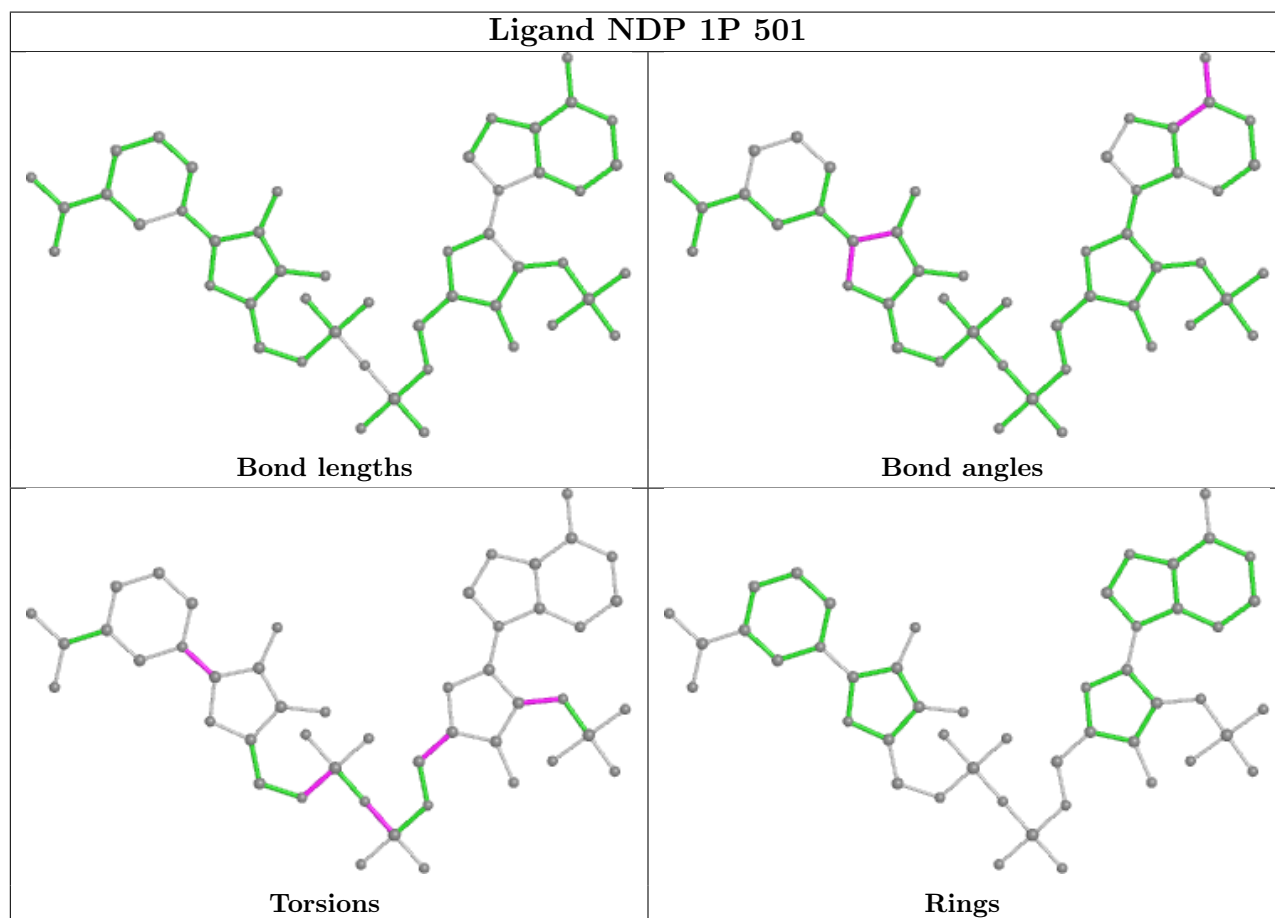
5 of 161 torsion outliers are listed below:

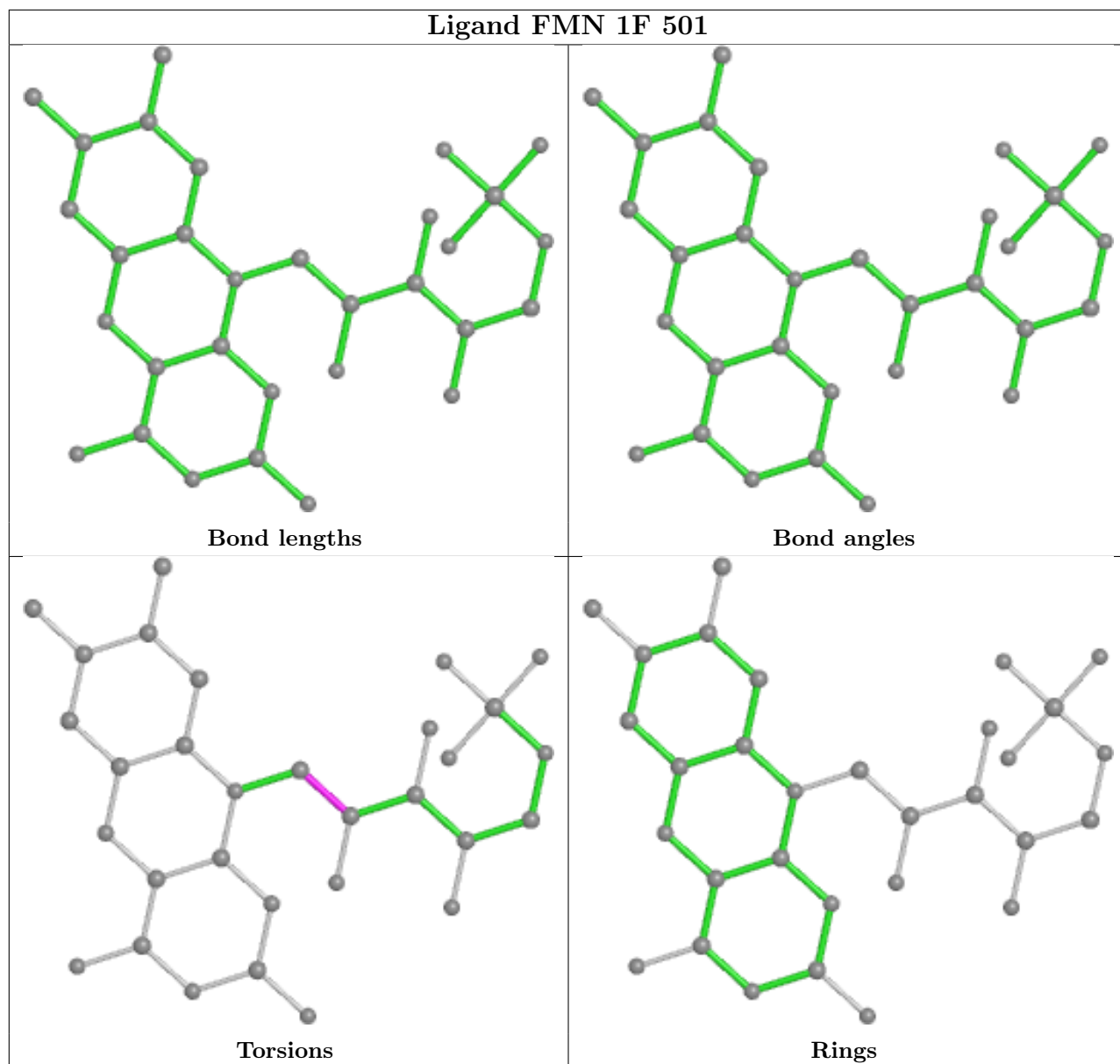
Mol	Chain	Res	Type	Atoms
45	1L	704	3PE	O22-C21-O21-C2
45	1L	704	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	201	3PE	C1-O11-P-O14
45	1Y	201	3PE	O32-C31-O31-C3

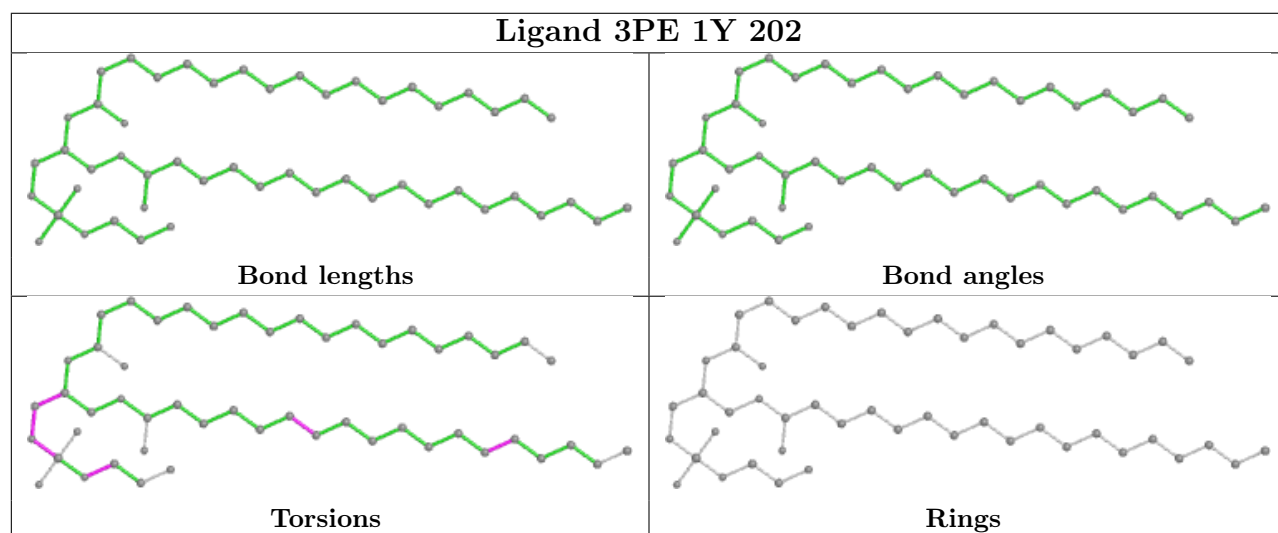
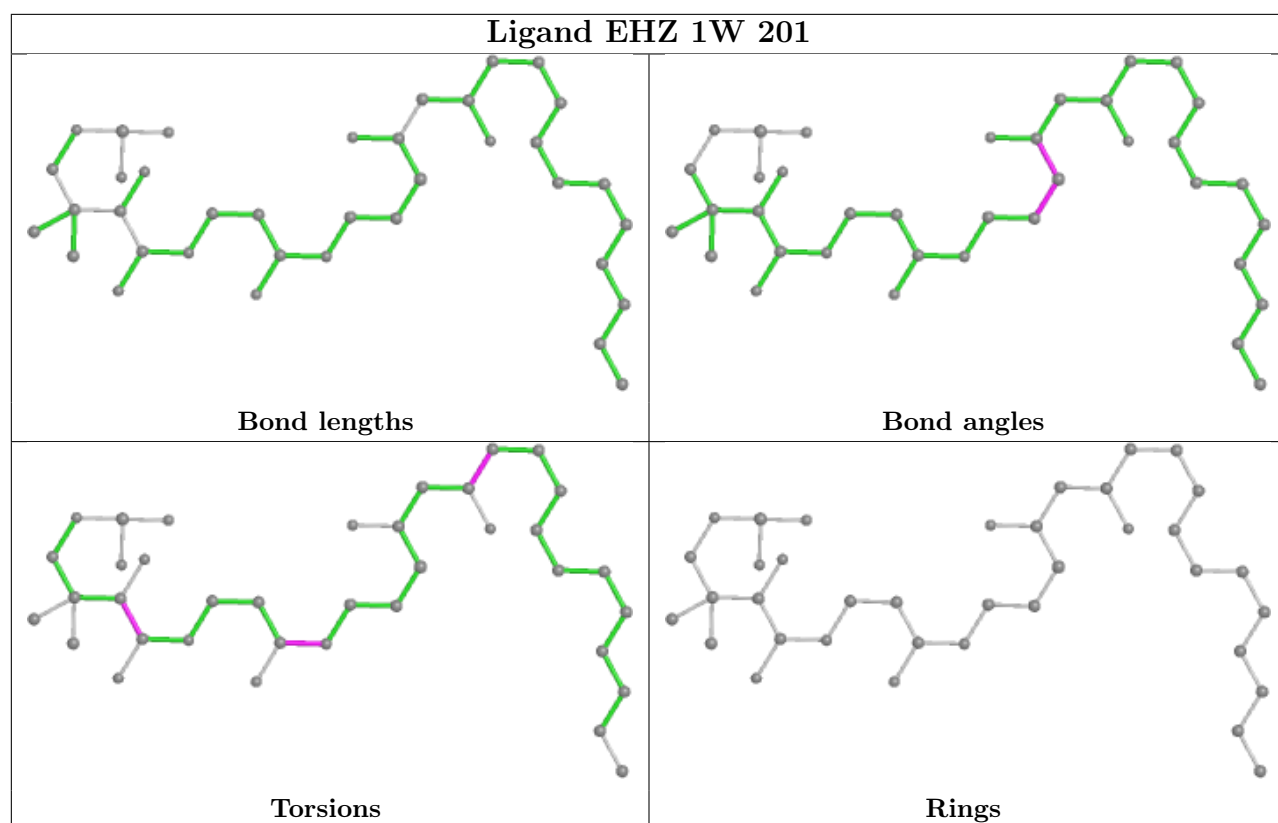
There are no ring outliers.

No monomer is involved in short contacts.

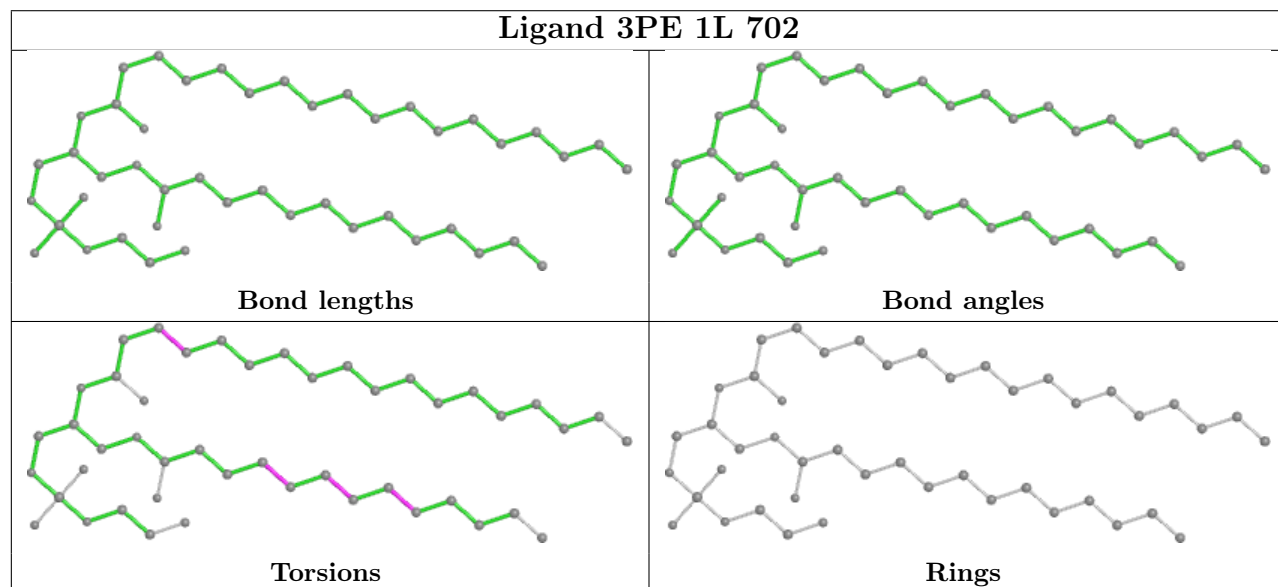
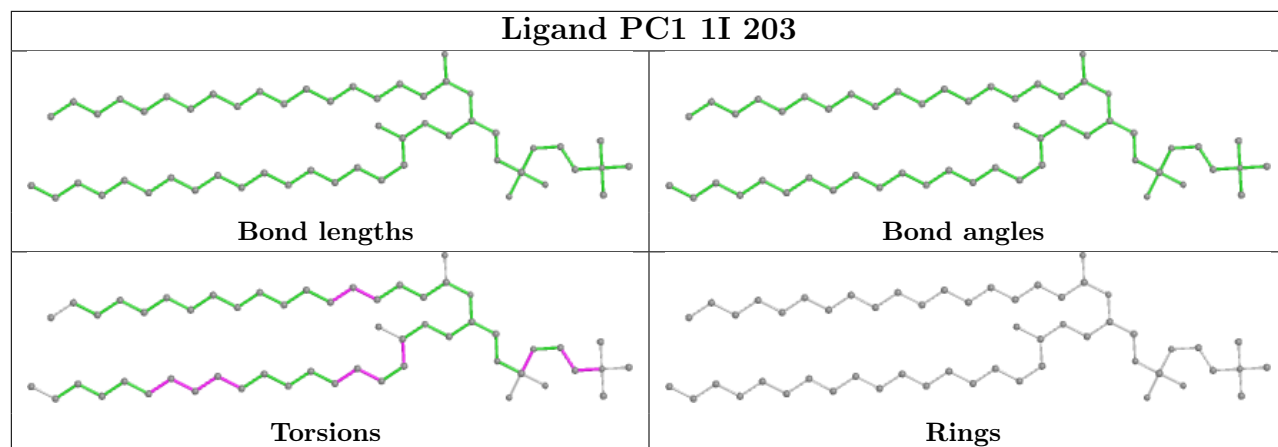
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

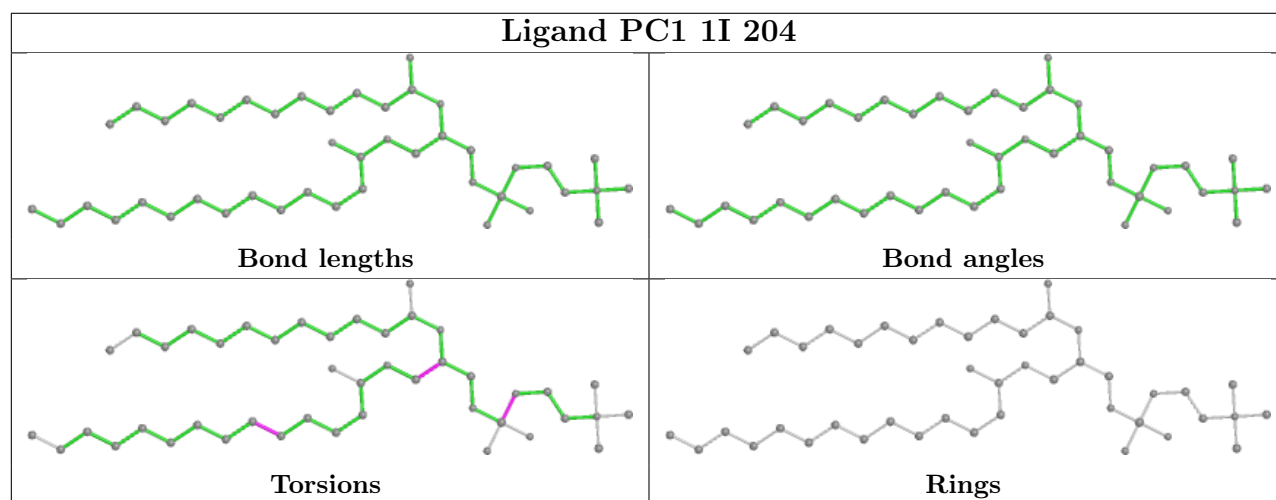
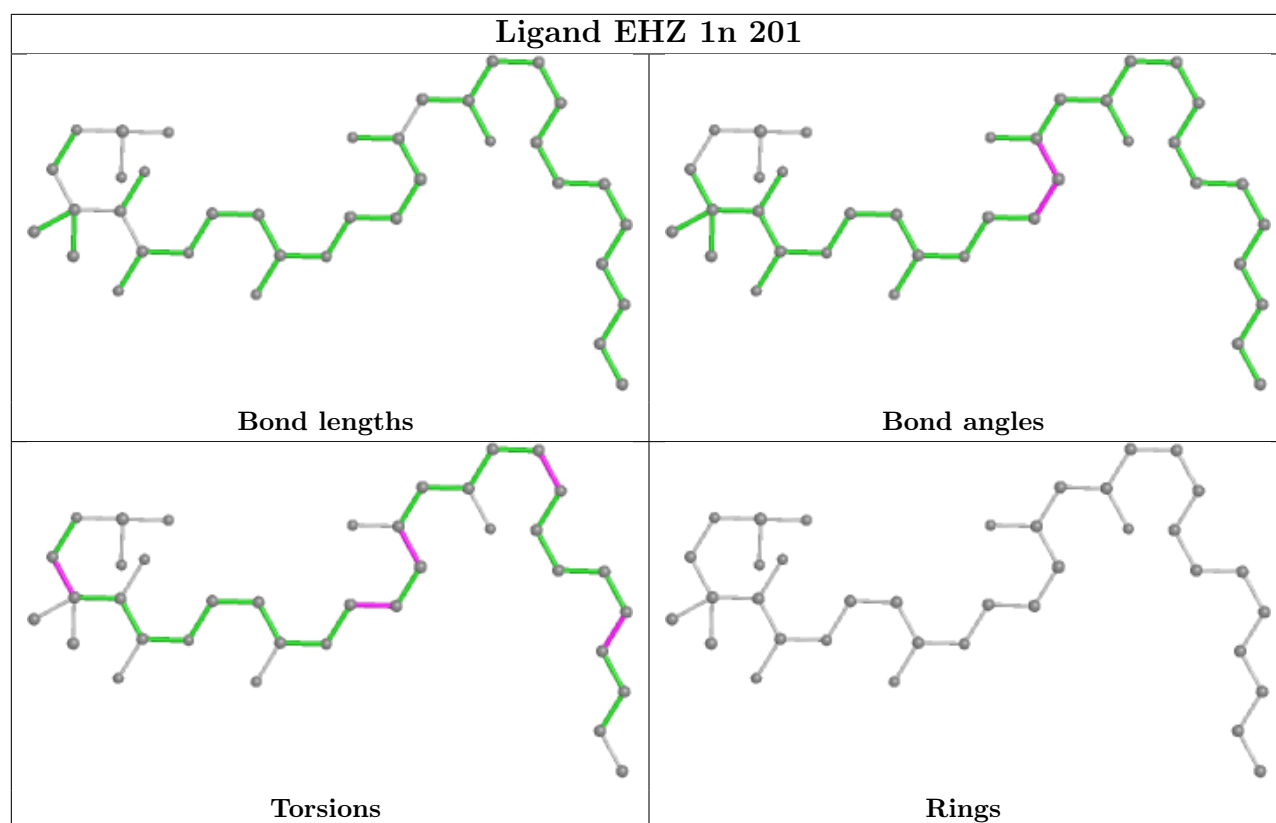


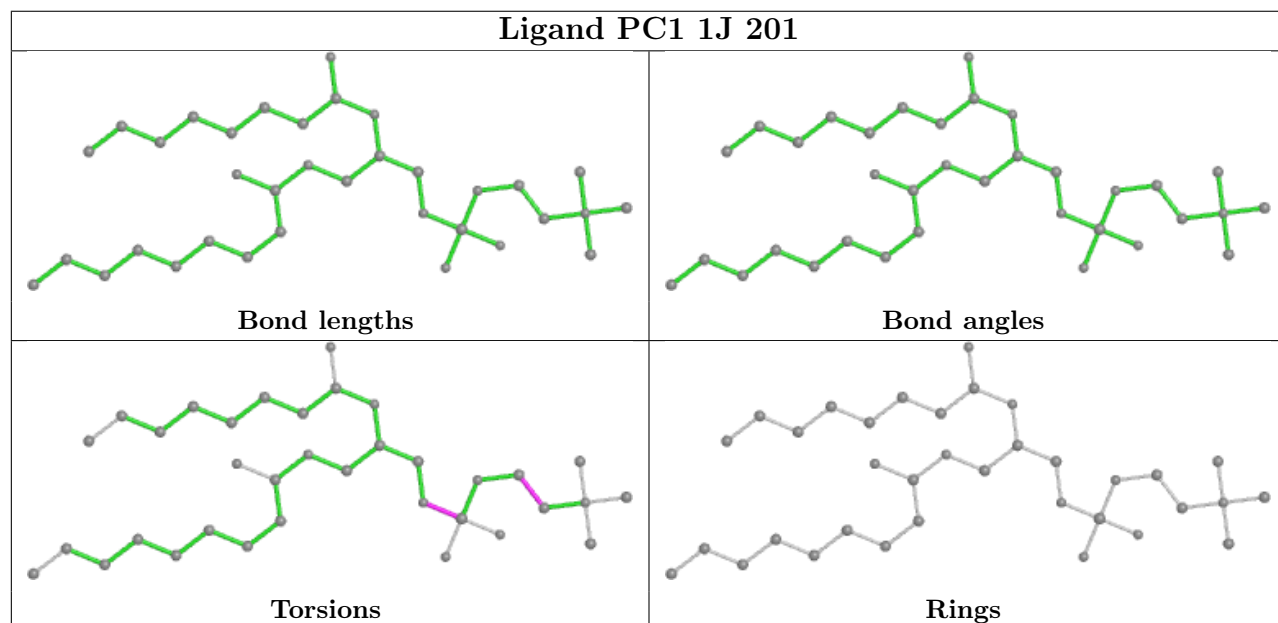
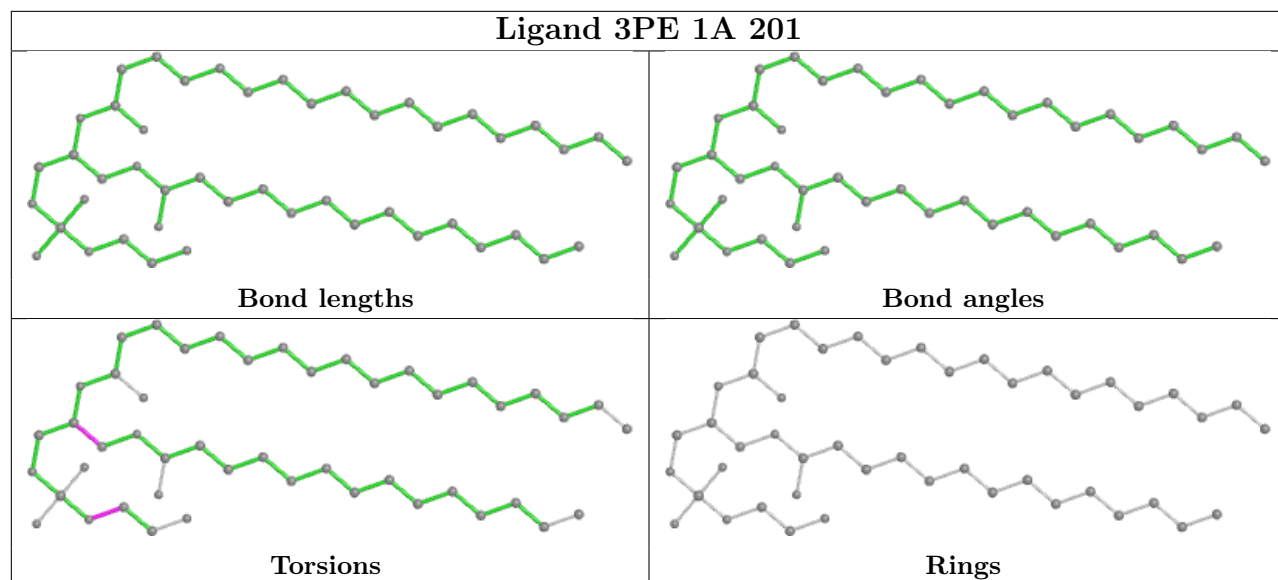


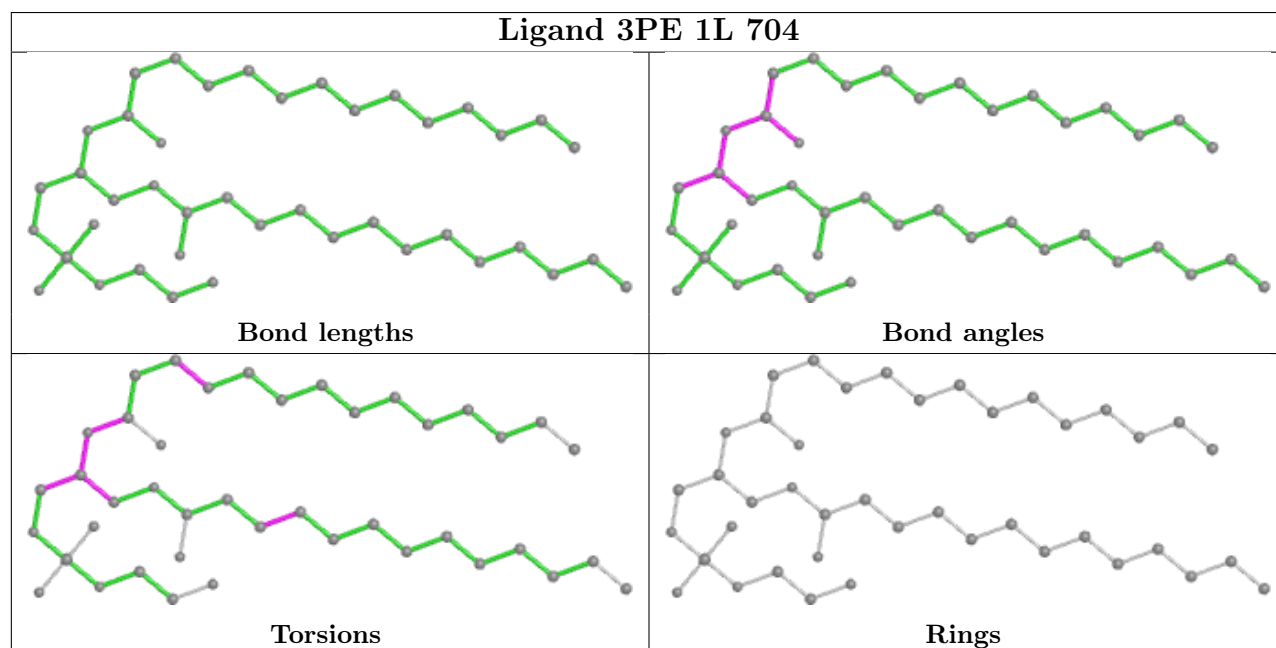
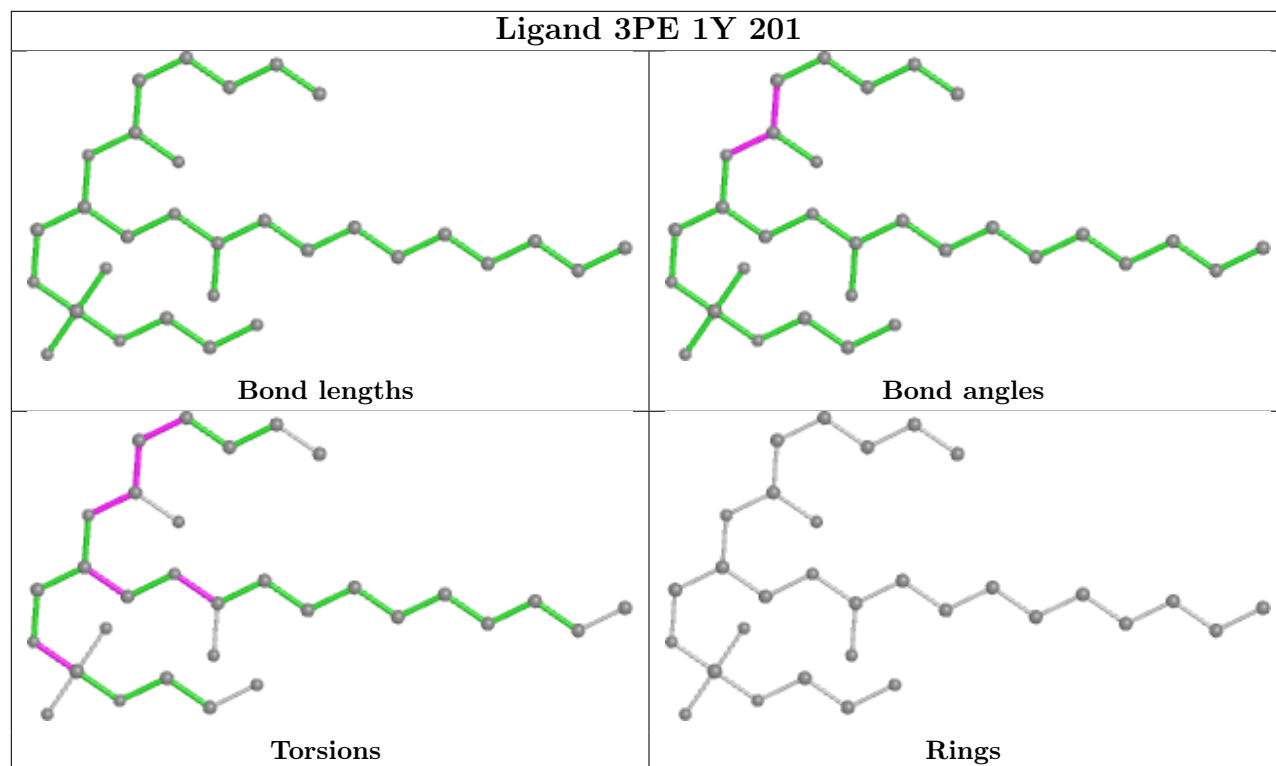


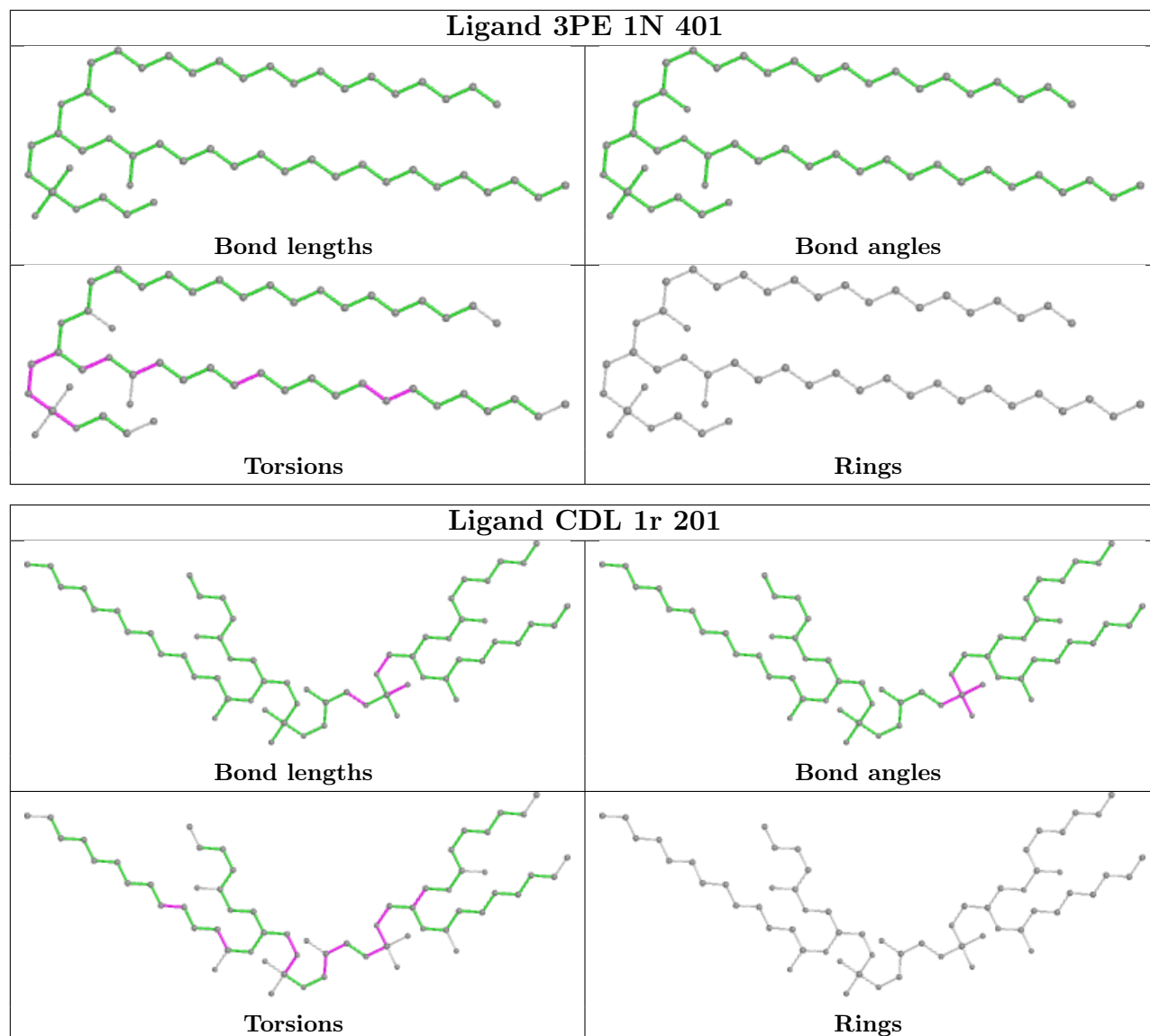


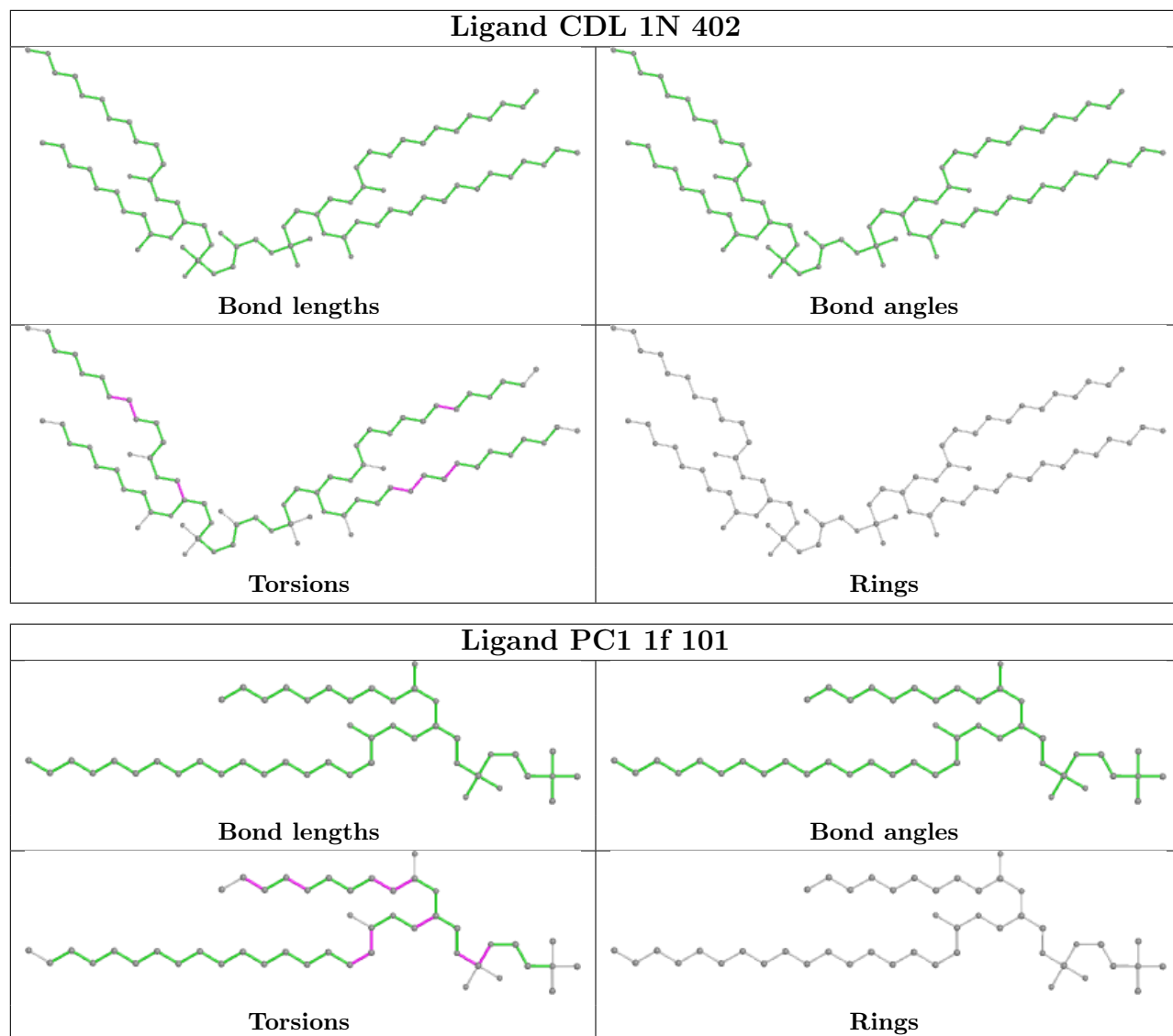


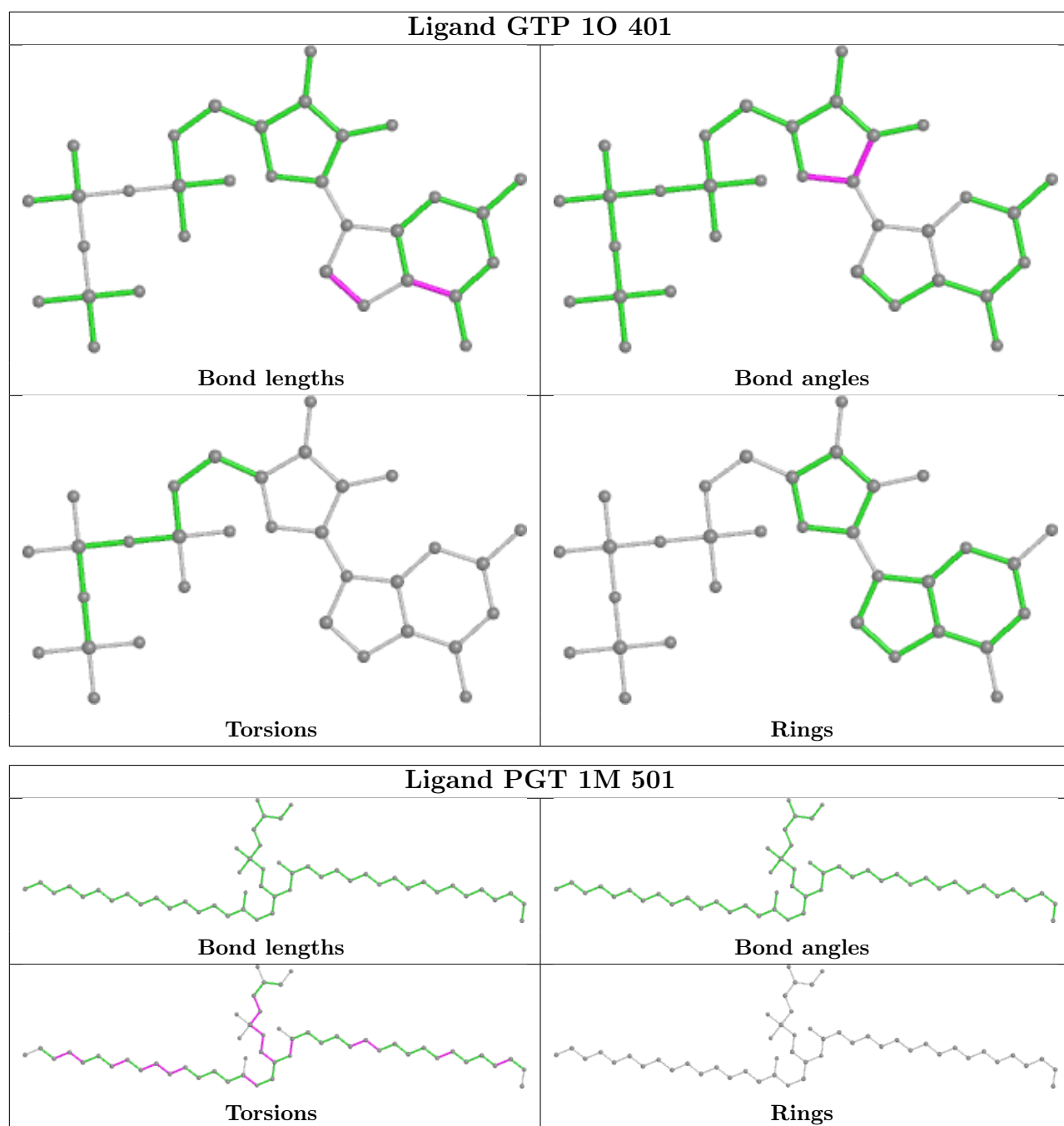


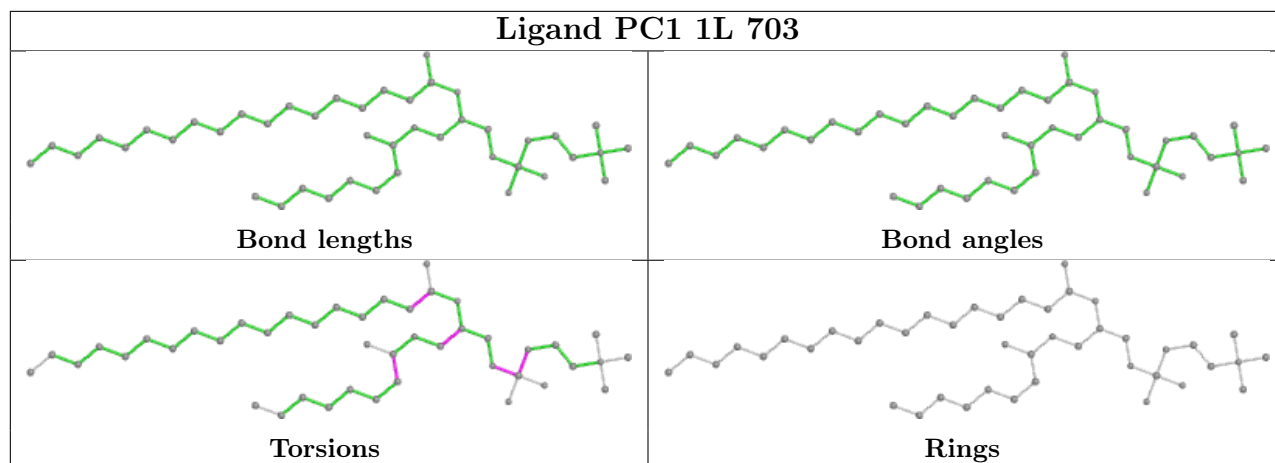












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	2
43	1r	1
22	1W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	4.03
1	1r	1:ALA	C	2:SER	N	3.12
1	1i	54:ALA	C	55:PRO	N	1.79
1	1W	75:ASP	C	76:PRO	N	1.72



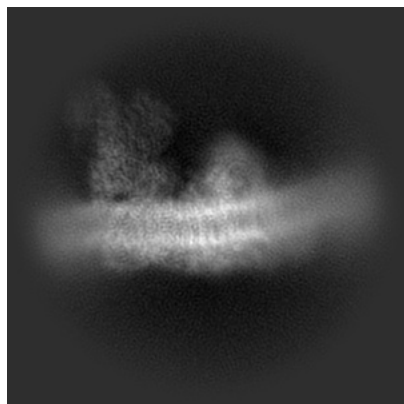
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42172. These allow visual inspection of the internal detail of the map and identification of artifacts.

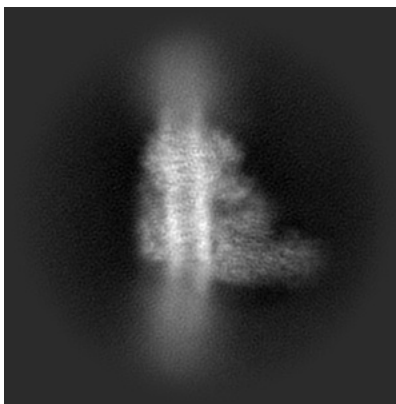
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

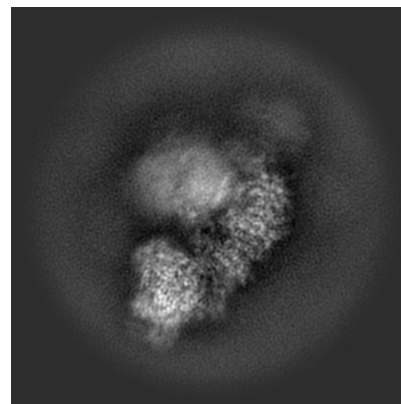
#### 6.1.1 Primary map



X

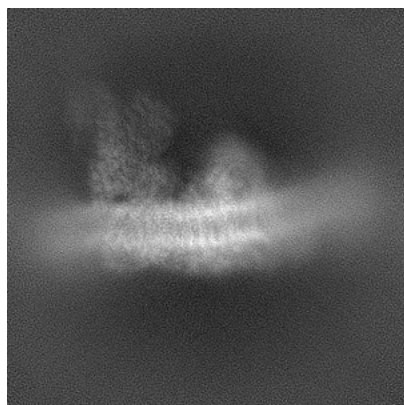


Y

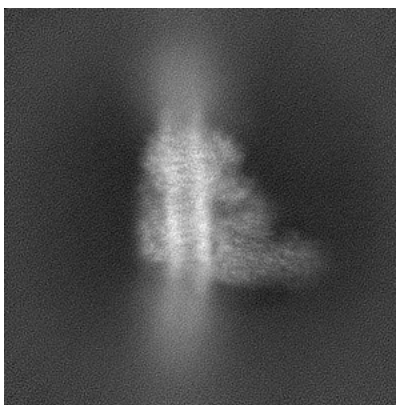


Z

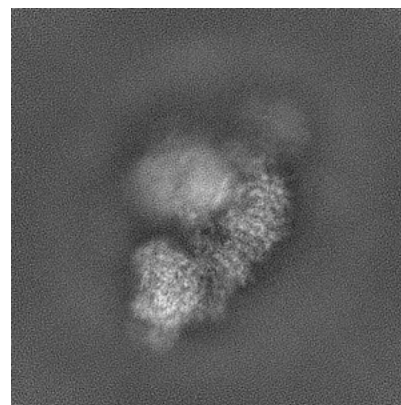
#### 6.1.2 Raw map



X



Y

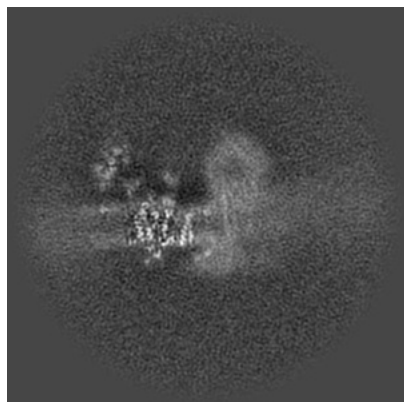


Z

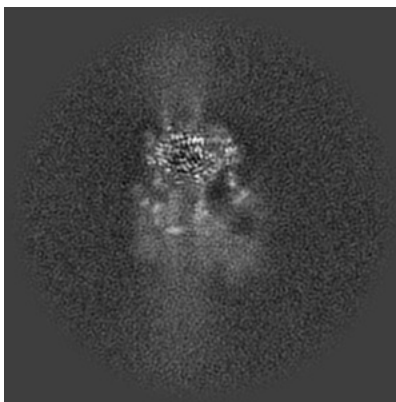
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

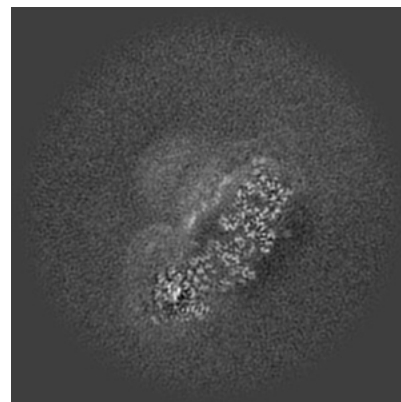
### 6.2.1 Primary map



X Index: 160

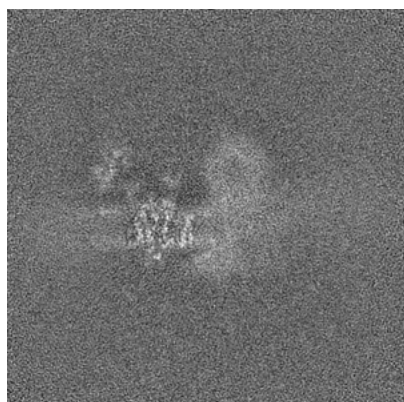


Y Index: 160

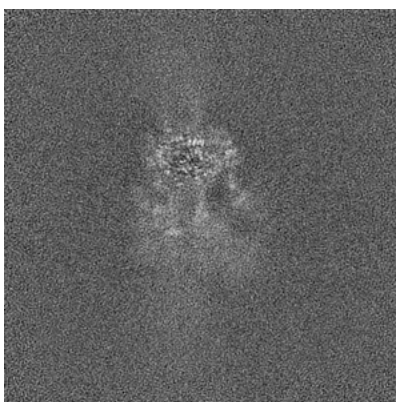


Z Index: 160

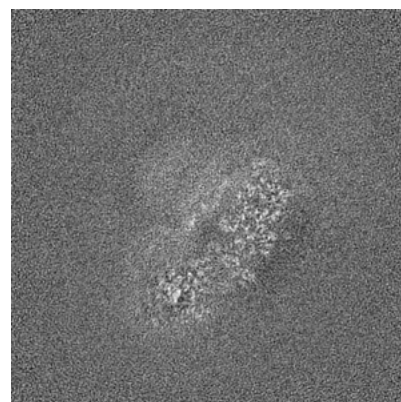
### 6.2.2 Raw map



X Index: 160



Y Index: 160

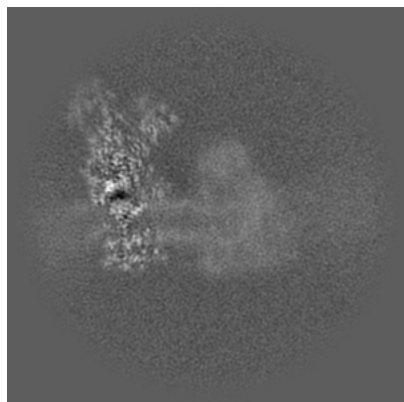


Z Index: 160

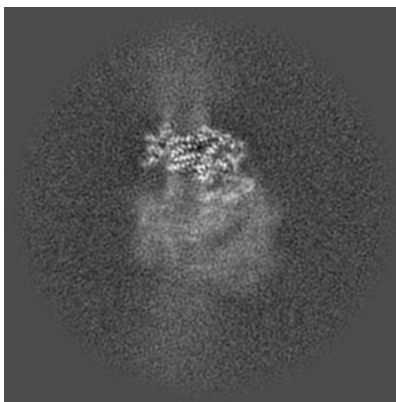
The images above show central slices of the map in three orthogonal directions.

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

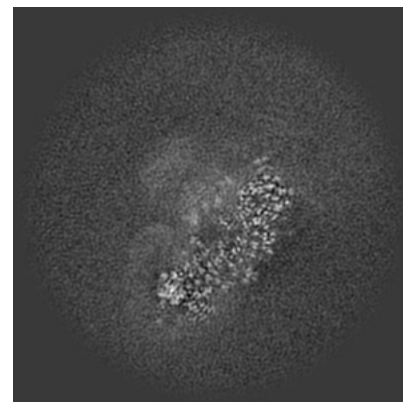
### 6.3.1 Primary map



X Index: 129

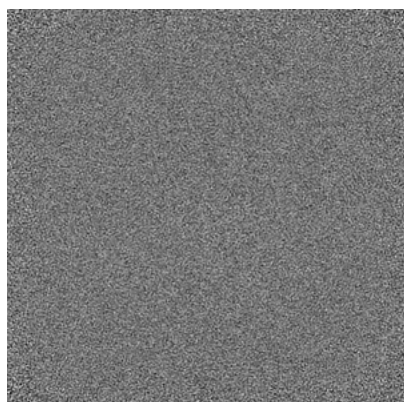


Y Index: 171

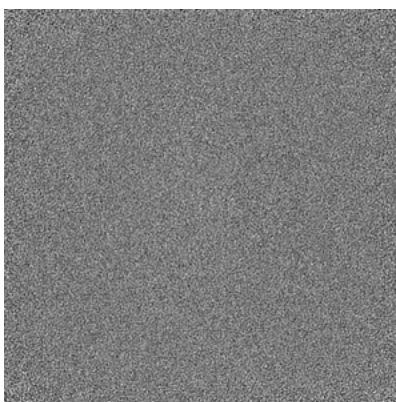


Z Index: 158

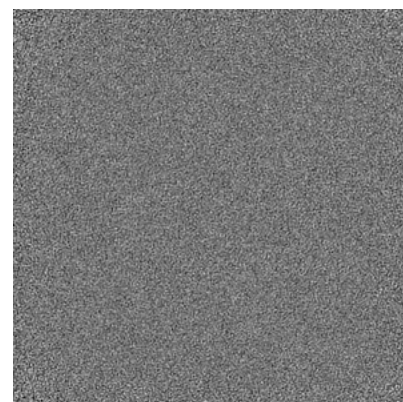
### 6.3.2 Raw map



X Index: 0



Y Index: 0



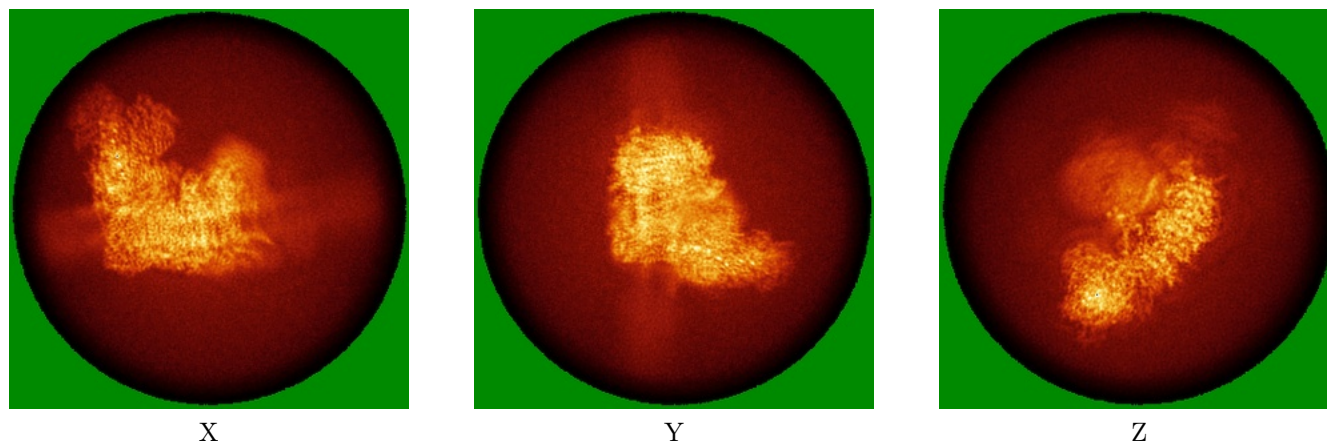
Z Index: 0

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

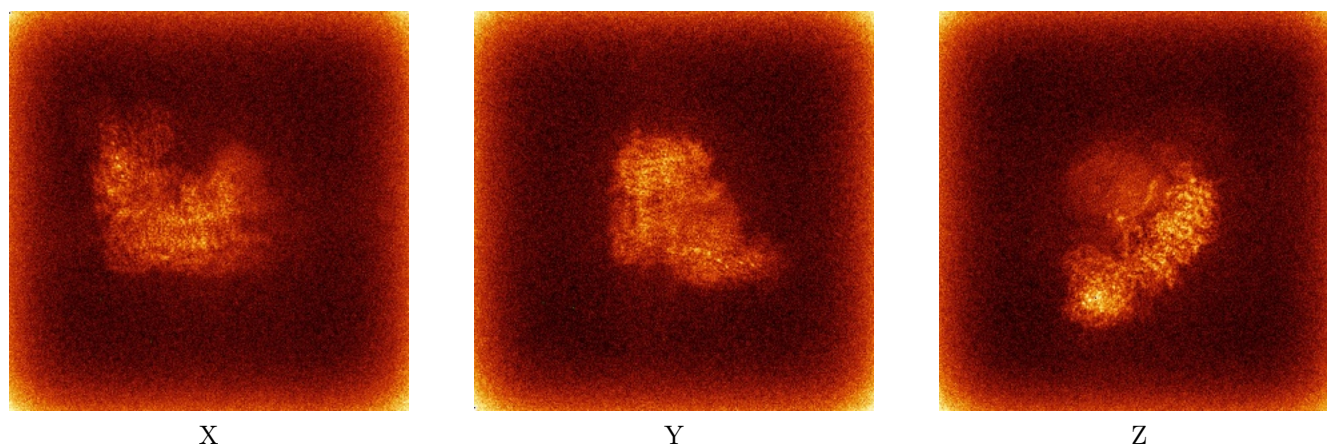


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



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

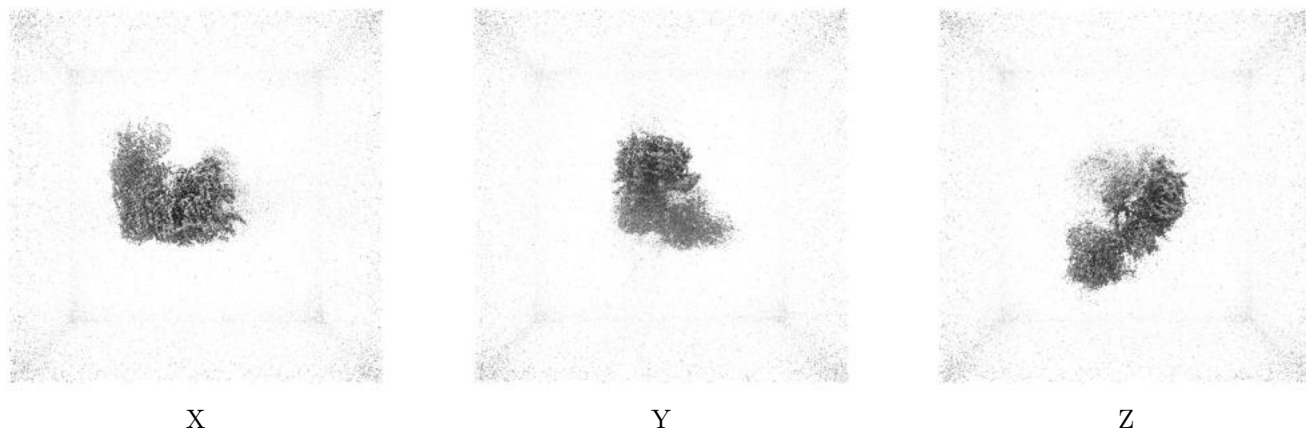
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

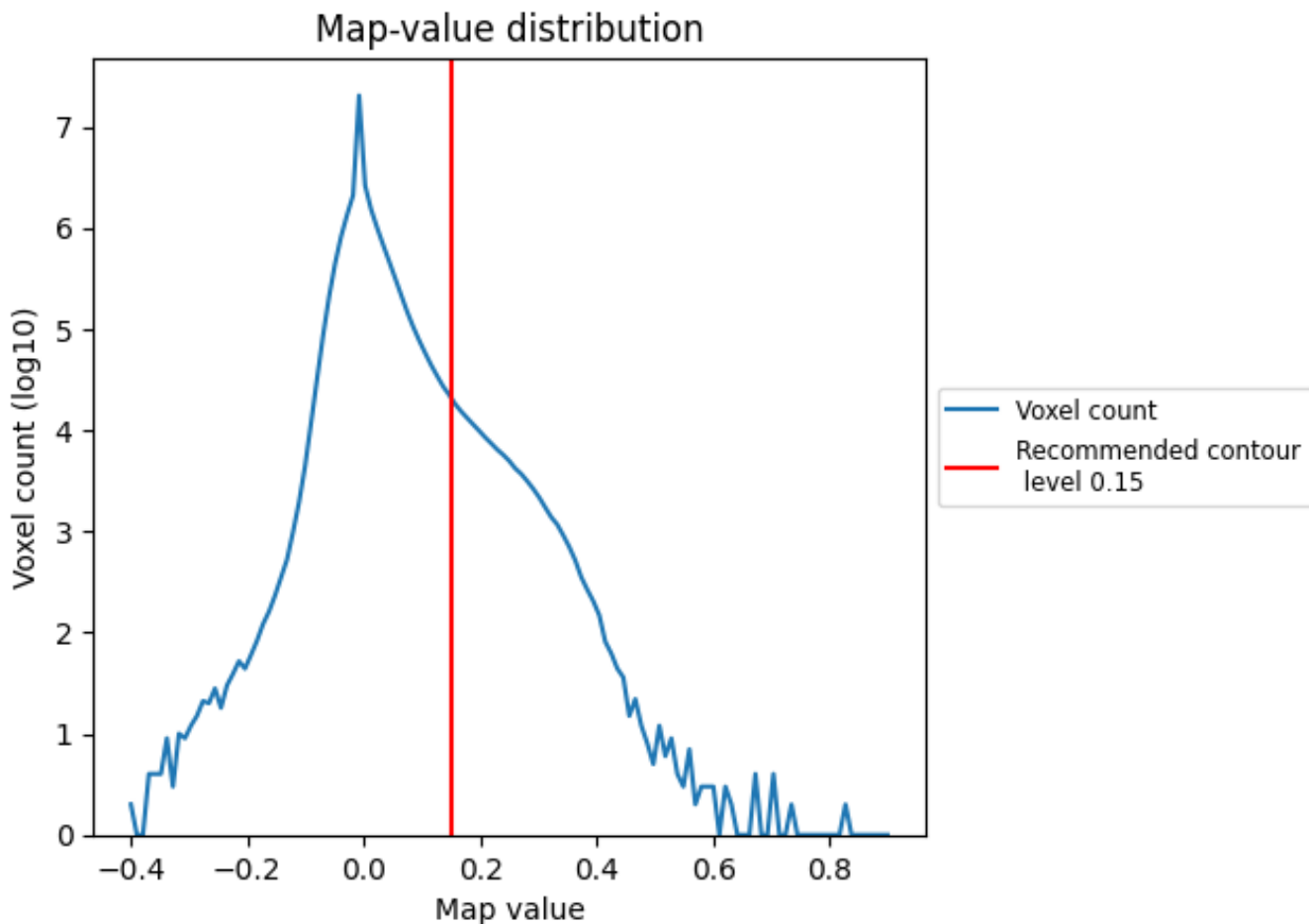
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

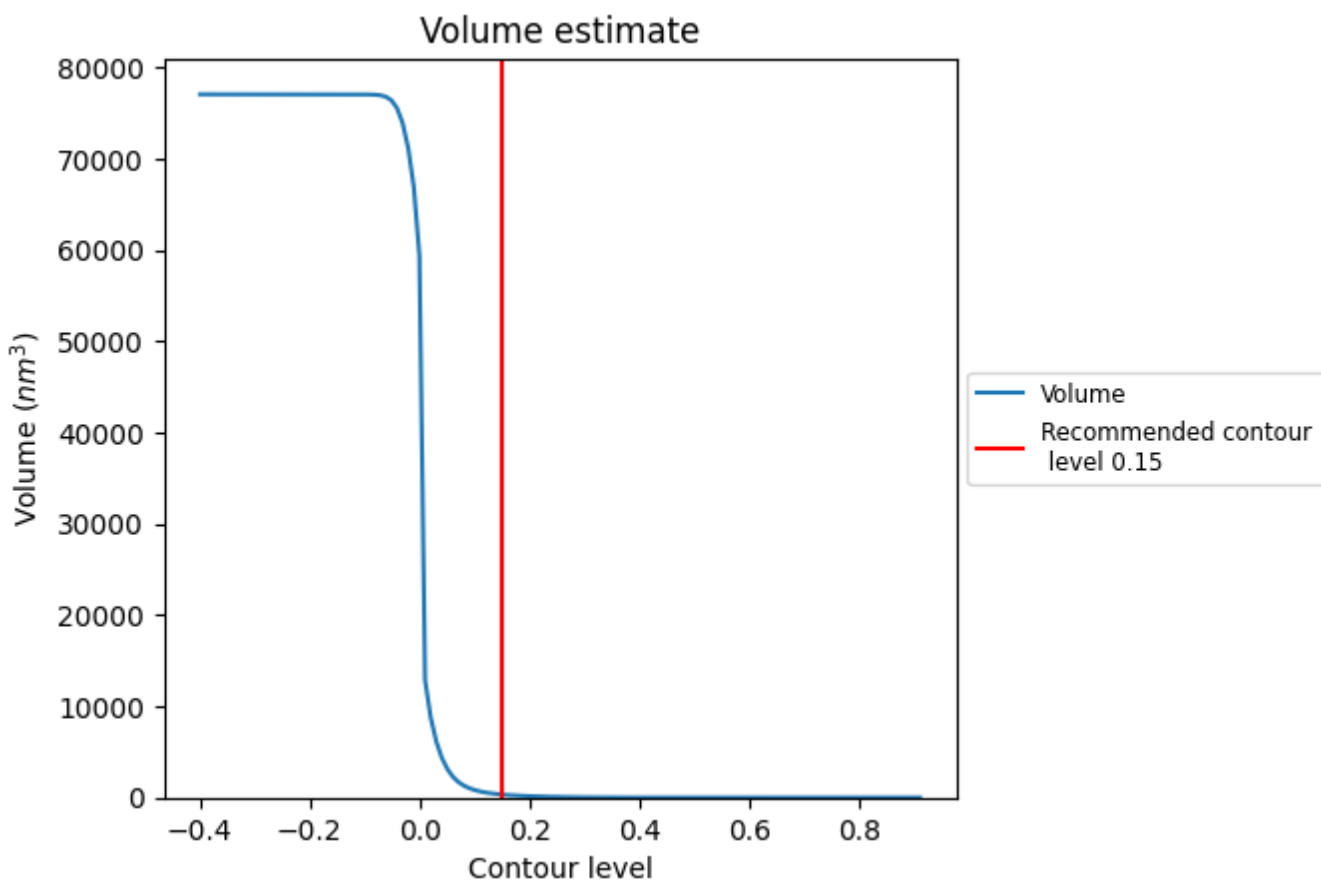
This section contains the results of statistical analysis of the map.

### 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.

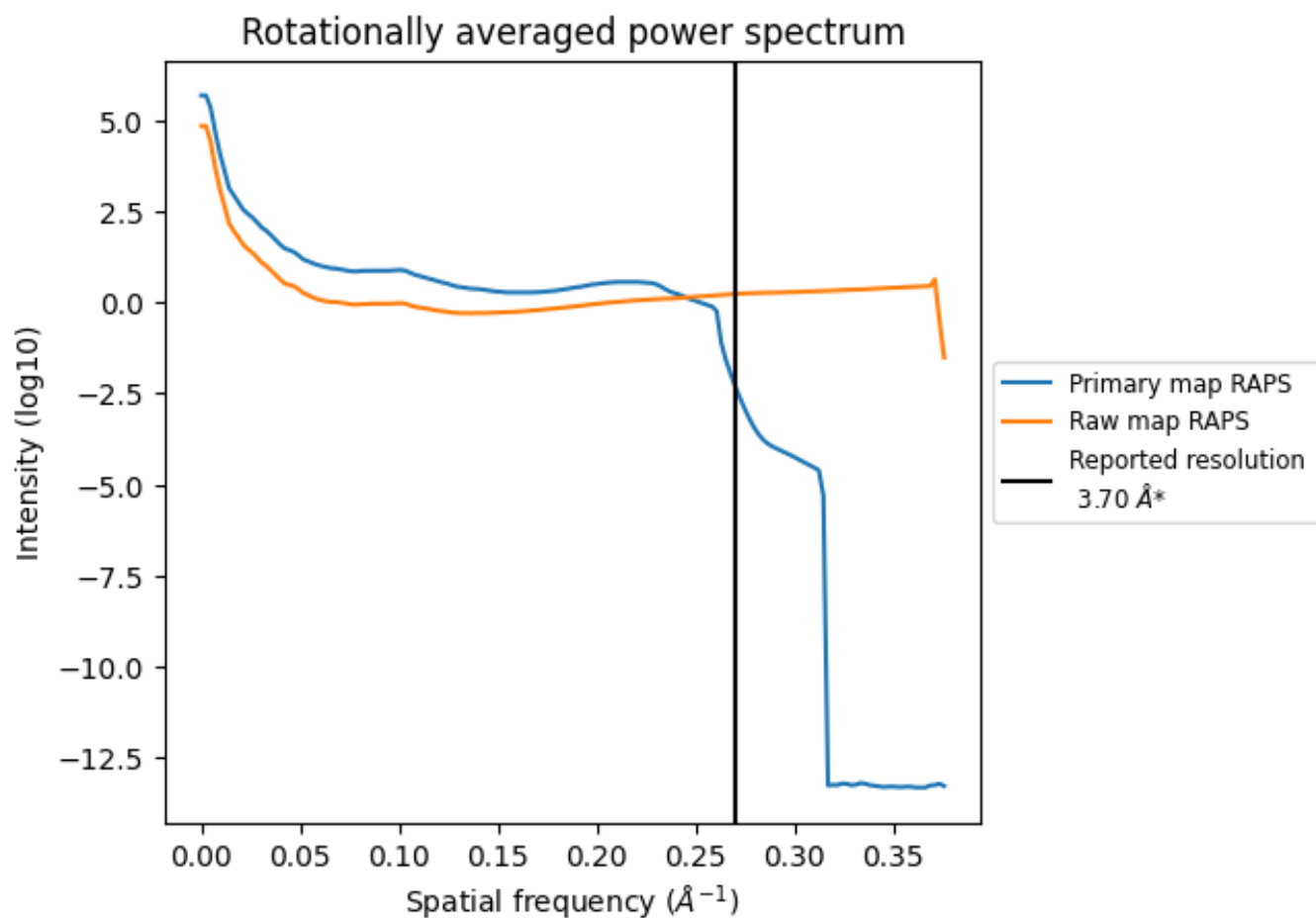
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 329 nm<sup>3</sup>; this corresponds to an approximate mass of 297 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i



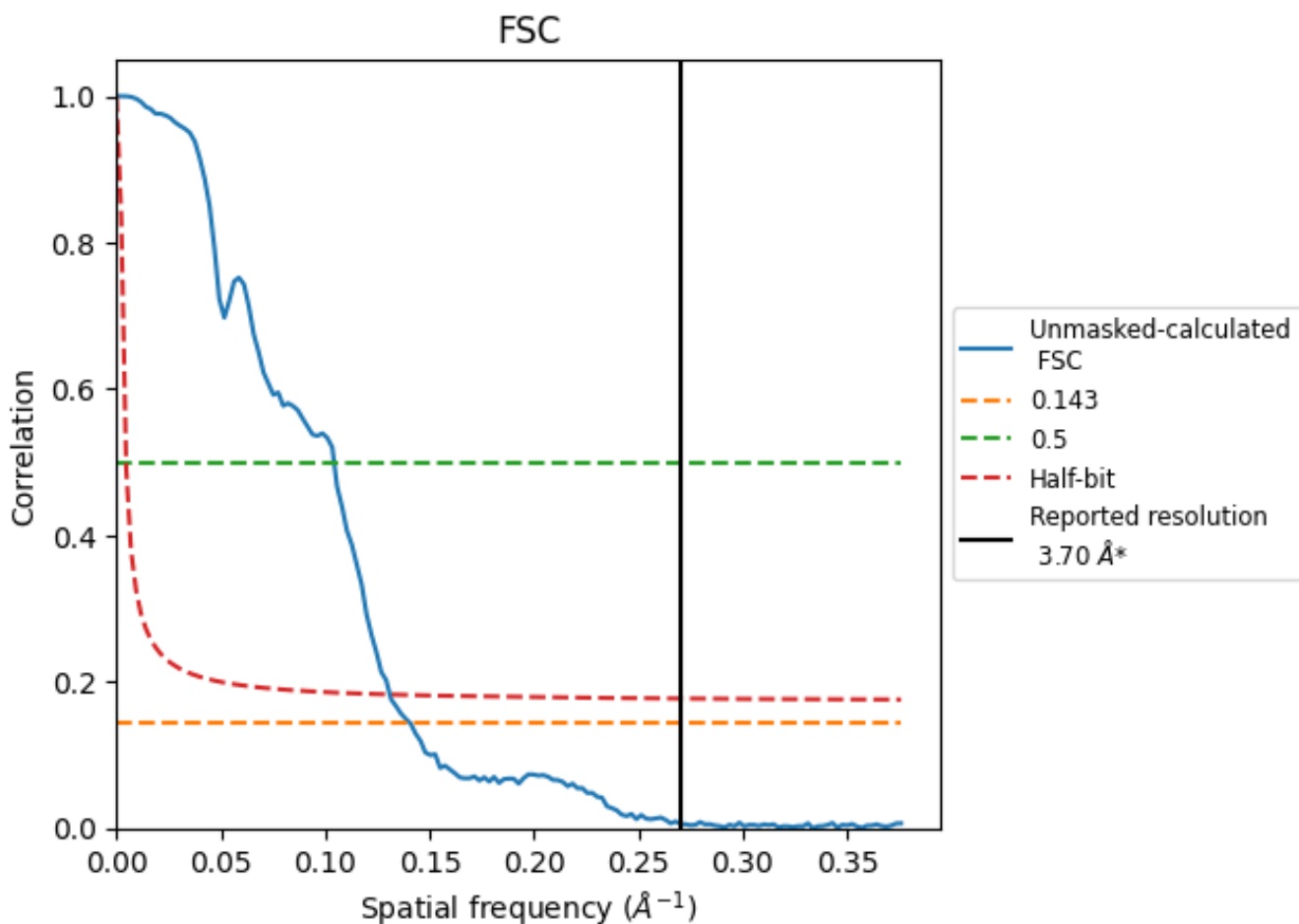
\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

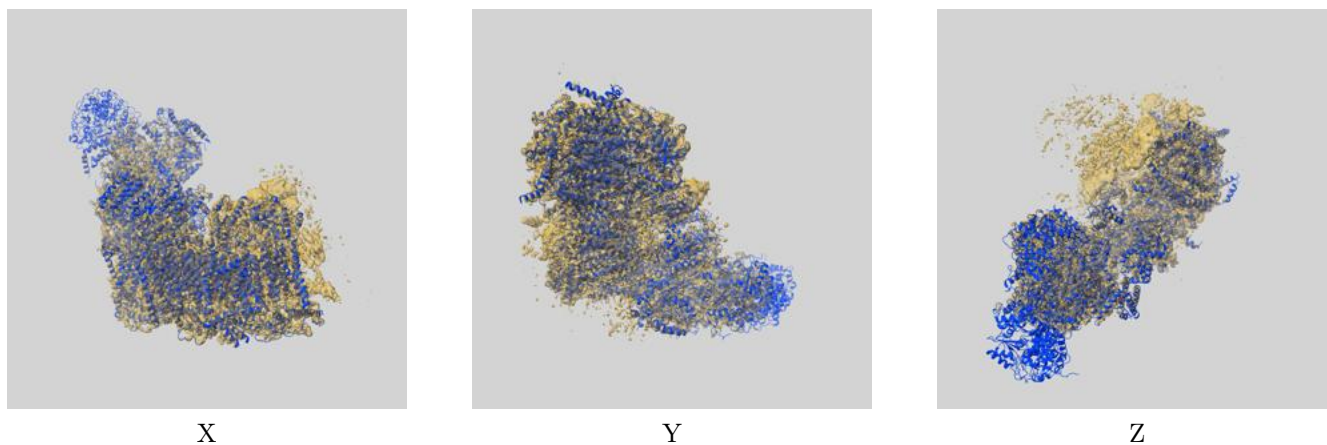
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.11	9.59	7.63

\*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 7.11 differs from the reported value 3.7 by more than 10 %

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

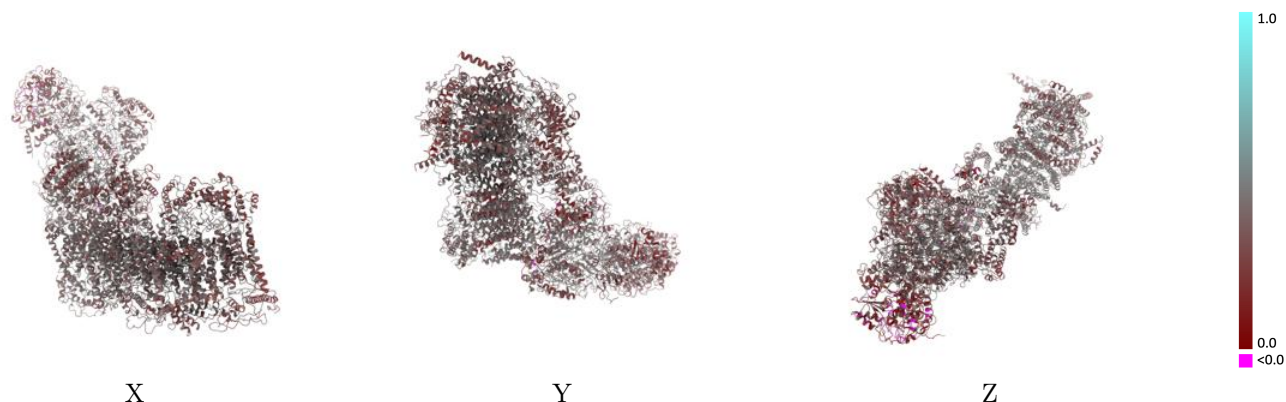
This section contains information regarding the fit between EMDB map EMD-42172 and PDB model 8UEV. Per-residue inclusion information can be found in section 3 on page 21.

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



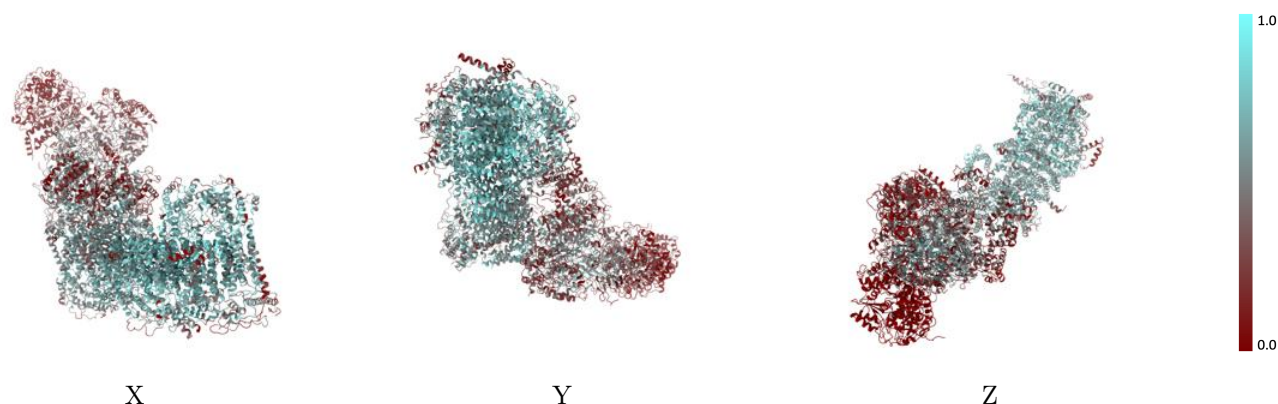
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



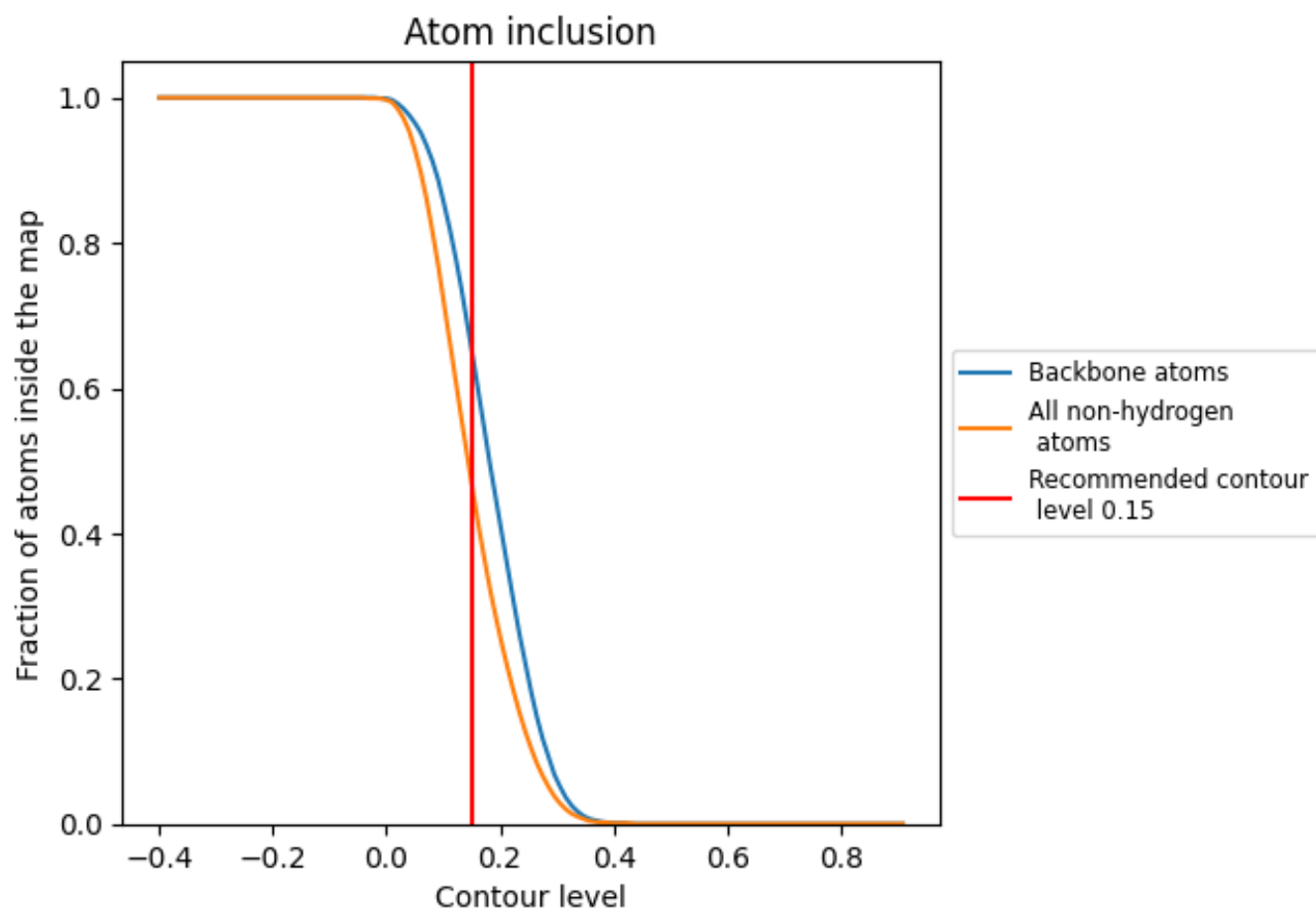
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 65% of all backbone atoms, 47% 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	 0.4700	 0.3720
1A	 0.5330	 0.3980
1B	 0.5360	 0.4120
1C	 0.3790	 0.4050
1D	 0.5130	 0.3900
1E	 0.0170	 0.2640
1F	 0.0260	 0.2420
1G	 0.2700	 0.3560
1H	 0.6000	 0.4040
1I	 0.5430	 0.4040
1J	 0.4900	 0.3710
1K	 0.5900	 0.4010
1L	 0.7030	 0.4000
1M	 0.7470	 0.4290
1N	 0.6660	 0.4180
1O	 0.3710	 0.3540
1P	 0.2900	 0.3420
1Q	 0.2780	 0.3820
1R	 0.2670	 0.4000
1S	 0.1250	 0.2970
1T	 0.2030	 0.2660
1U	 0.6350	 0.3460
1V	 0.2070	 0.3340
1W	 0.2910	 0.3410
1X	 0.5300	 0.4010
1Y	 0.6650	 0.3700
1Z	 0.5480	 0.4060
1a	 0.6560	 0.4080
1b	 0.5310	 0.4090
1c	 0.4360	 0.3760
1d	 0.6810	 0.4150
1e	 0.5760	 0.4250
1f	 0.4550	 0.3590
1g	 0.6000	 0.3840
1h	 0.6400	 0.3980



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
1i	 0.3950	 0.3490
1j	 0.5200	 0.3690
1k	 0.5260	 0.3480
1l	 0.6480	 0.3910
1m	 0.6980	 0.3850
1n	 0.6530	 0.3660
1o	 0.4940	 0.3250
1p	 0.6120	 0.3770
1q	 0.4190	 0.4040
1r	 0.3430	 0.3900
1s	 0.0000	 0.2230