wwPDB EM Validation Summary Report

Jun 13, 2024 – 11:03 AM EDT

PDB ID	:	8UET
EMDB ID	:	EMD-42170
Title	:	In-situ complex I, Deactive class02
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*
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:

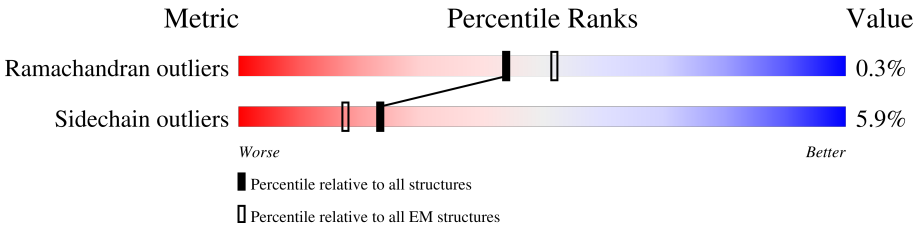
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	23% 70% 5% 24%
2	1B	258	16% 56% • 40%
3	1C	264	39% 75% • 21%
4	1D	476	28% 85% • 12%
5	1E	249	85% 82% • 14%
6	1F	464	91% 88% 5% 7%
7	1G	727	66% 88% 8% •
8	1H	318	13% 95% 5%
9	1I	239	10% 69% 5% 26%

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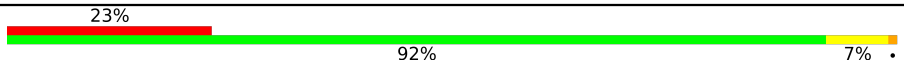
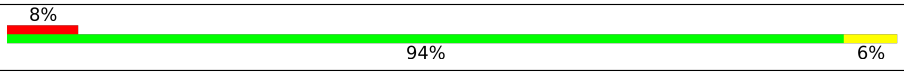
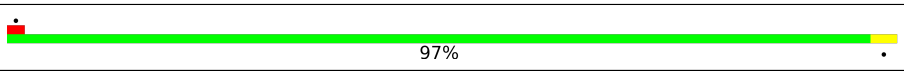
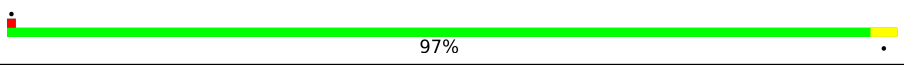
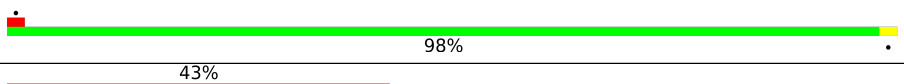
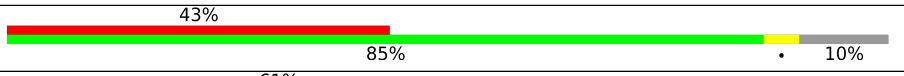
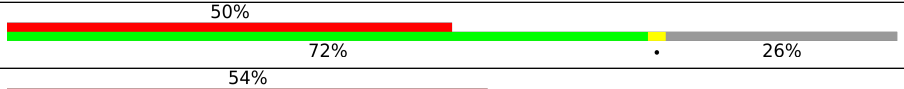
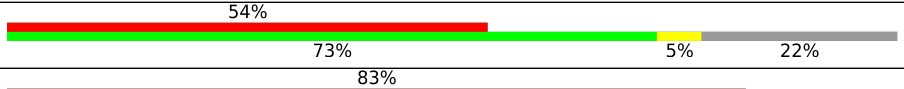
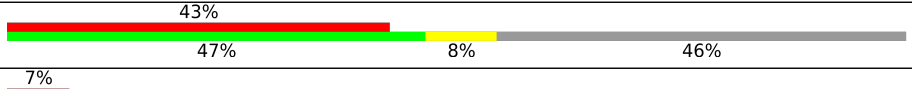
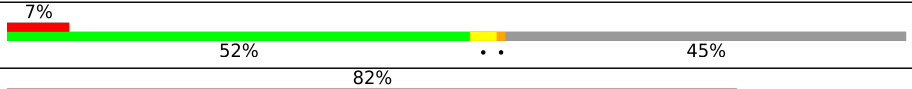
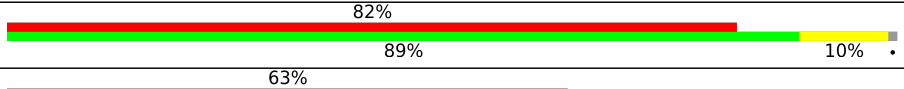
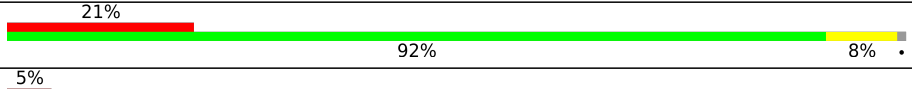
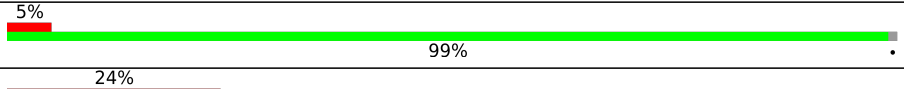
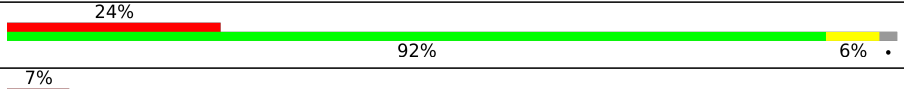
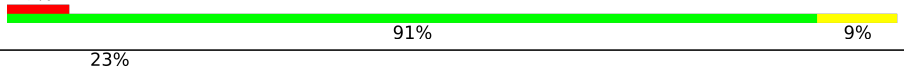
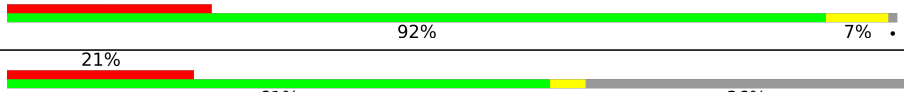
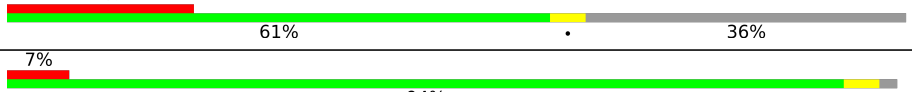
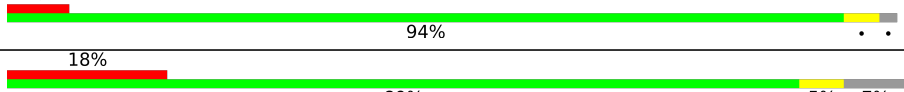
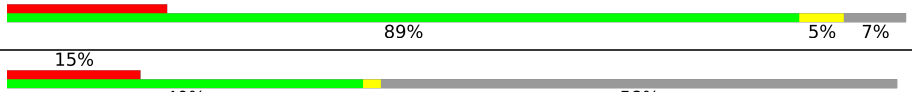
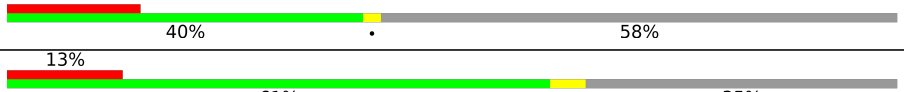
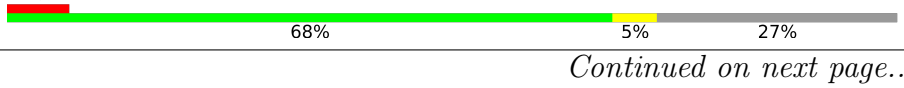
Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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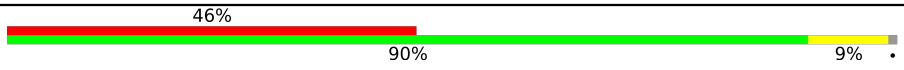
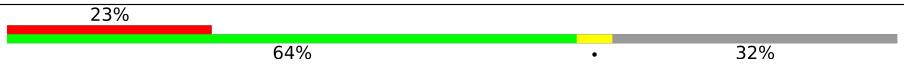
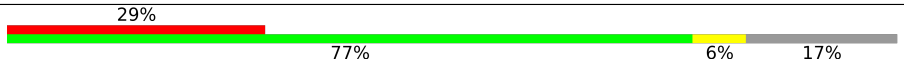
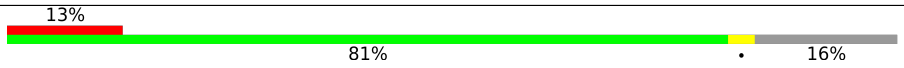
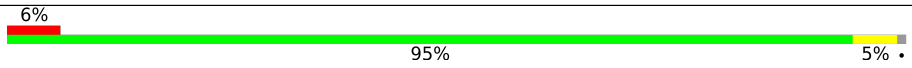
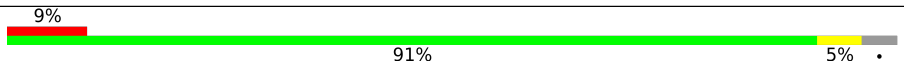
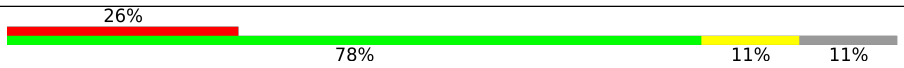
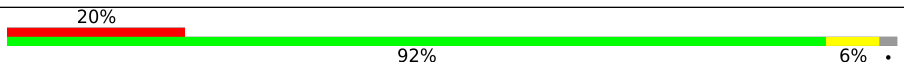
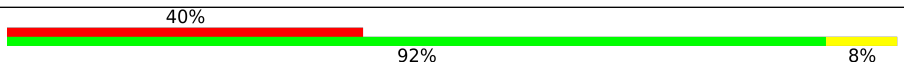
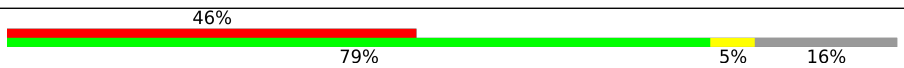
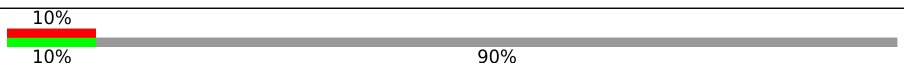
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67180 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	87	700	479	100	116	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	418	3376	2159	577	616	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
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

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

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

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

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

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

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

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

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

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

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

- 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
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

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

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

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

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

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

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

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

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

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

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

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
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

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

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

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
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

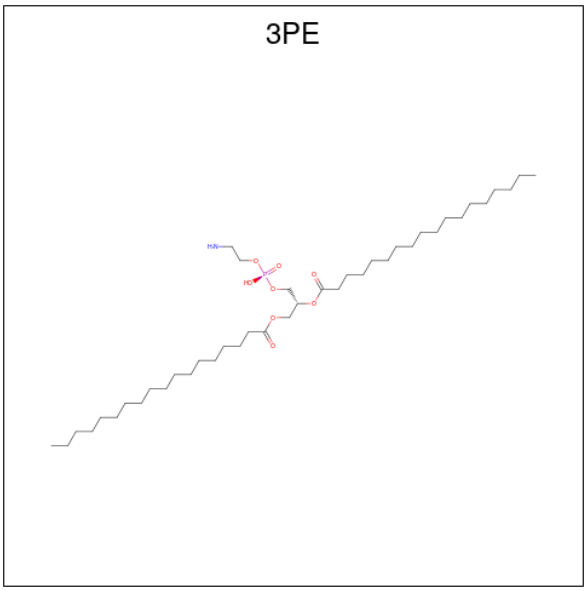
There is a discrepancy between the modelled and reference sequences:

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

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

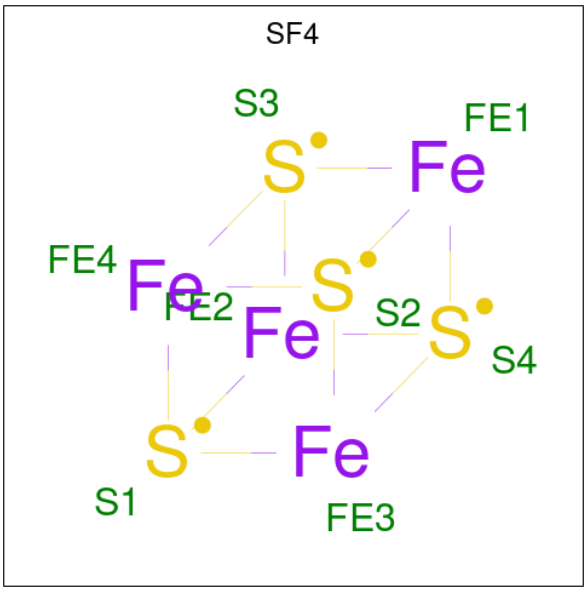
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



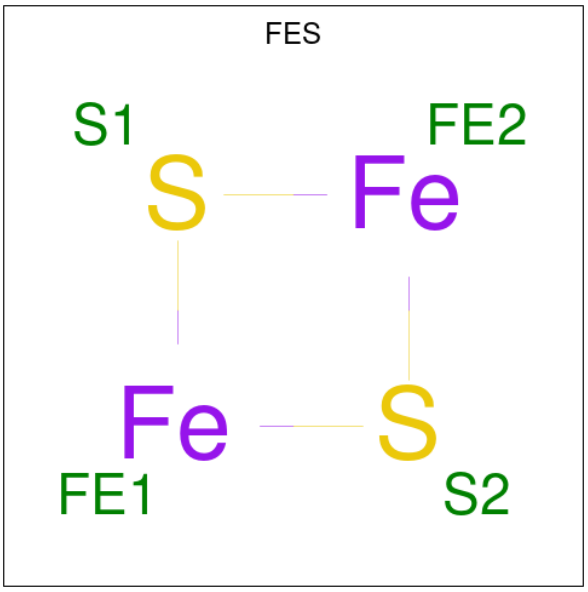
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



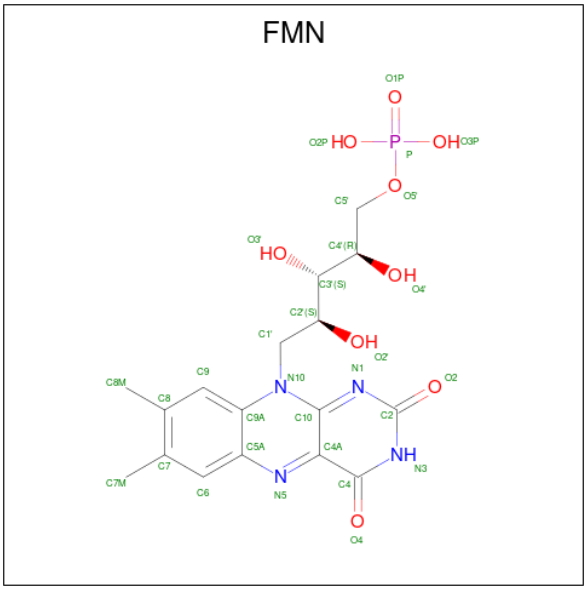
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total Fe S 8 4 4	0
46	1F	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0

- 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: $C_{17}H_{21}N_4O_9P$).

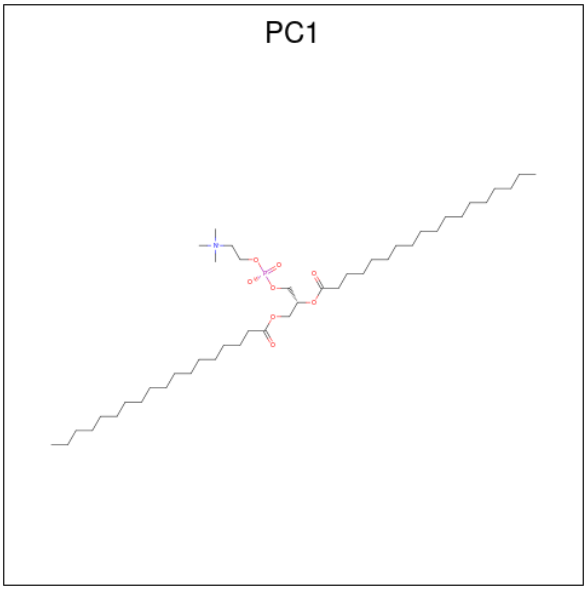


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

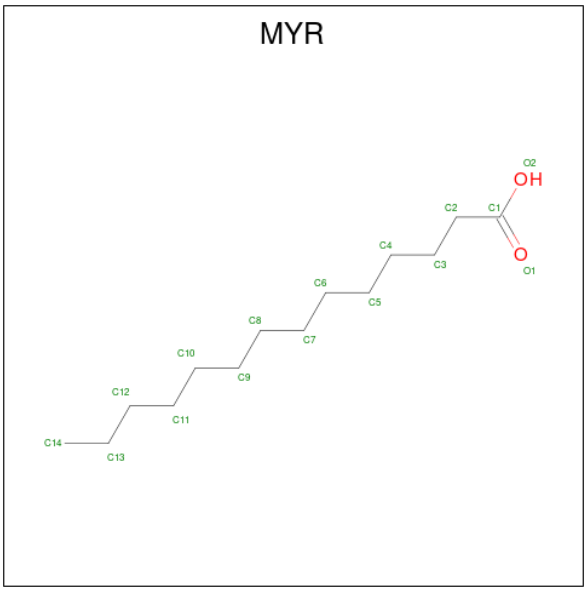
Mol	Chain	Residues	Atoms	AltConf
49	1G	1	Total K 1 1	0

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



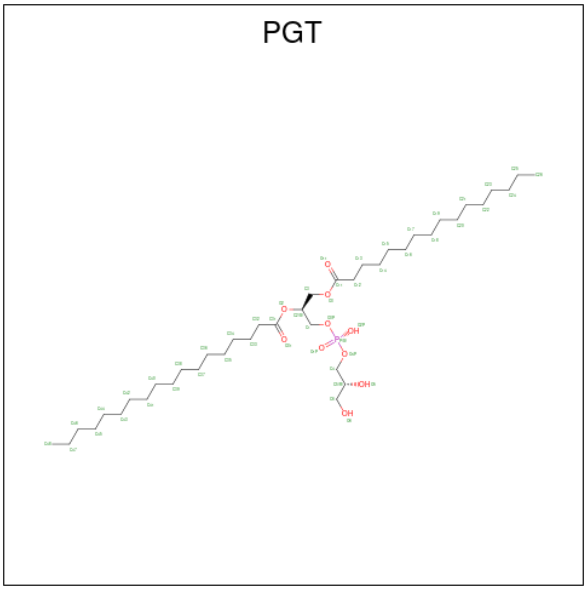
Mol	Chain	Residues	Atoms	AltConf
50	1H	1	Total C N O P 54 44 1 8 1	0
50	1I	1	Total C N O P 44 34 1 8 1	0
50	1J	1	Total C N O P 35 25 1 8 1	0
50	1M	1	Total C N O P 44 34 1 8 1	0
50	1f	1	Total C N O P 46 36 1 8 1	0

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



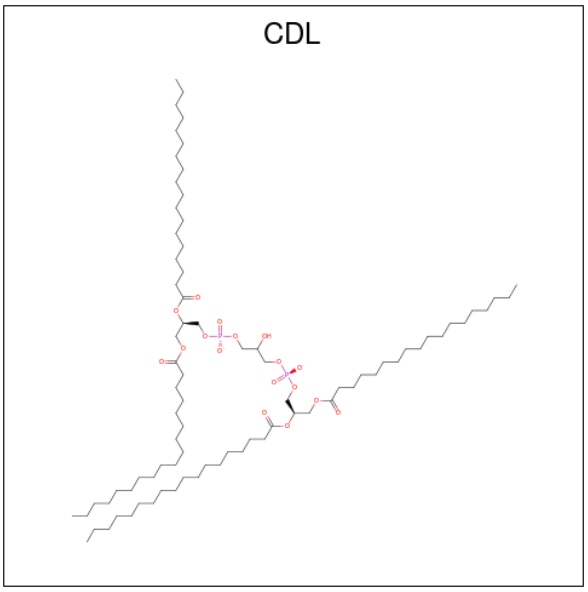
Mol	Chain	Residues	Atoms			AltConf
51	1L	1	Total	C	O	0
			15	14	1	

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



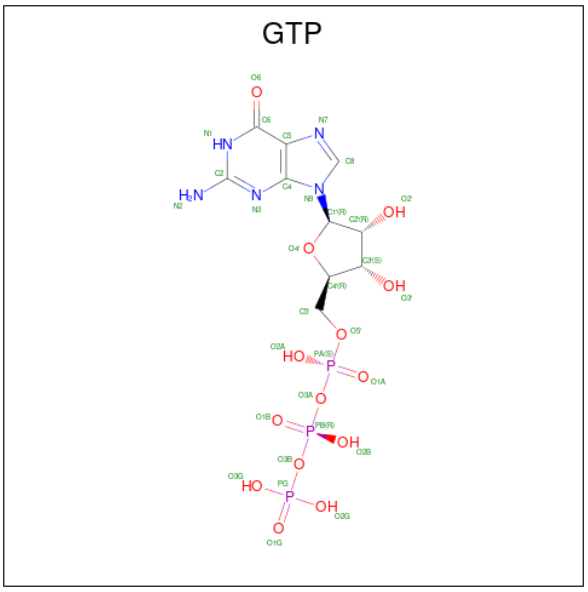
Mol	Chain	Residues	Atoms				AltConf
52	1M	1	Total	C	O	P	0
			51	40	10	1	

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



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

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

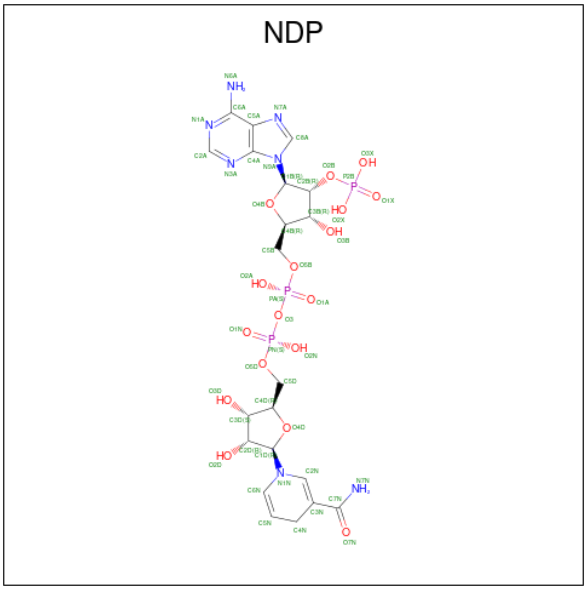


Mol	Chain	Residues	Atoms					AltConf
54	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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: $C_{21}H_{30}N_7O_{17}P_3$).

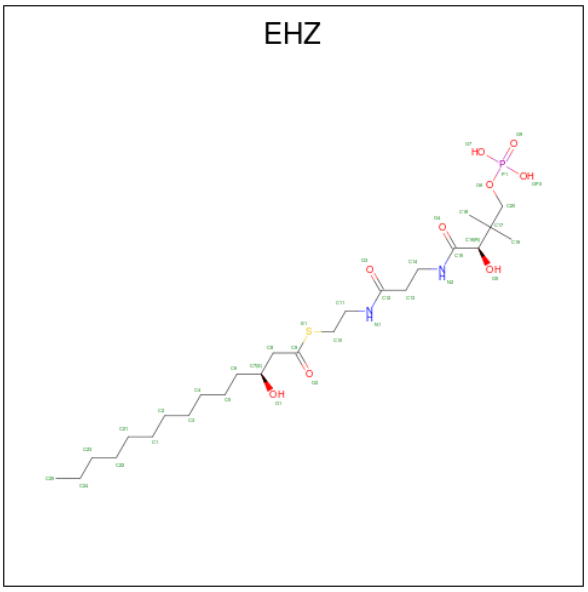


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- 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-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



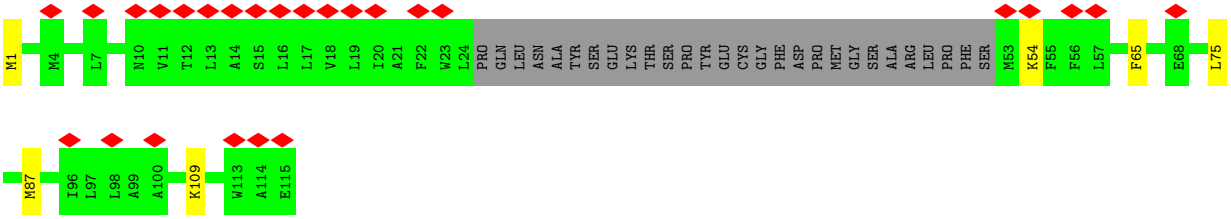
Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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.

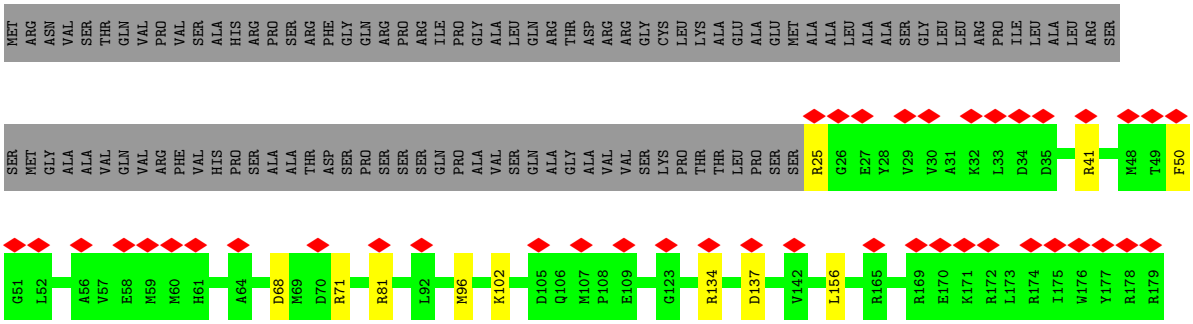
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain 1A:



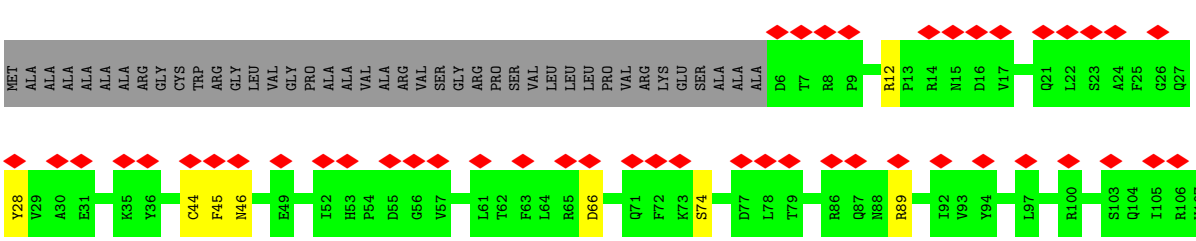
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

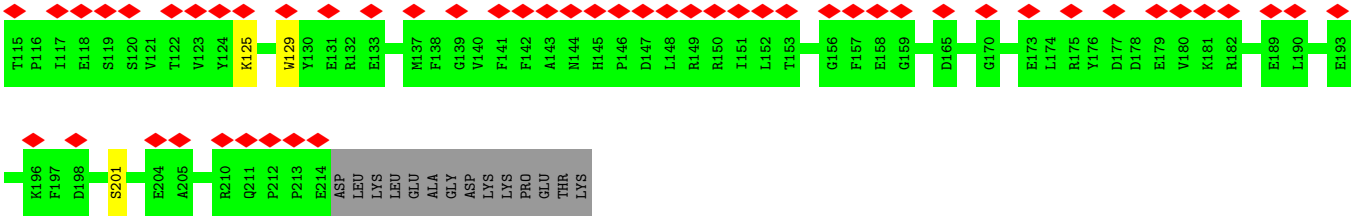
Chain 1B:



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

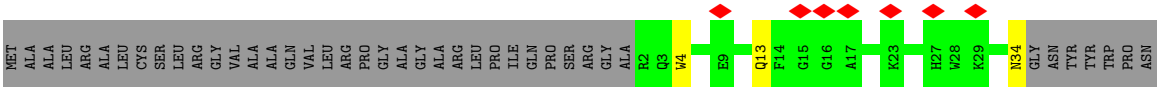
Chain 1C:

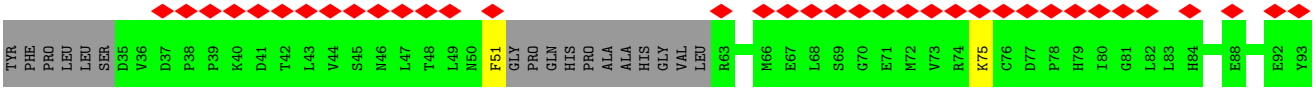


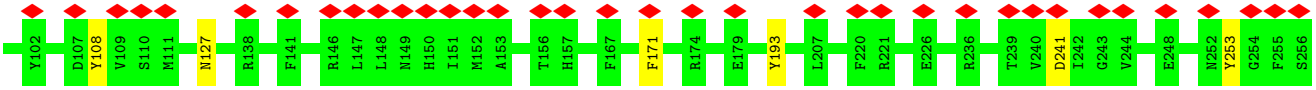


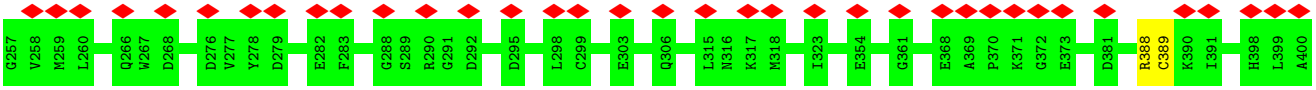
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

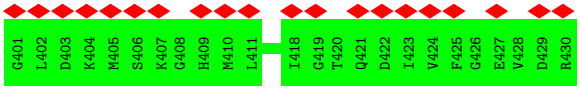
Chain 1D:





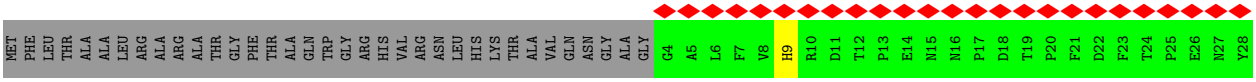


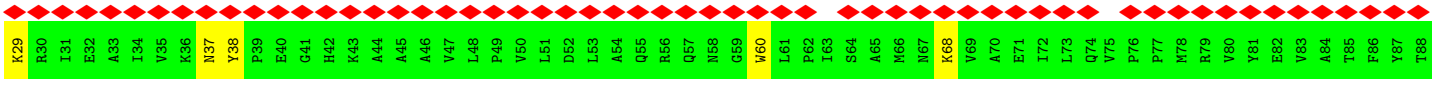


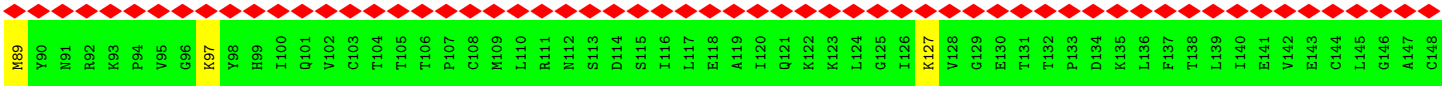


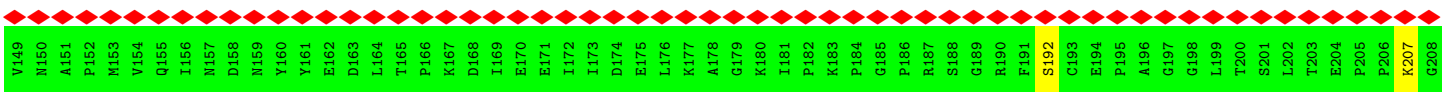
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

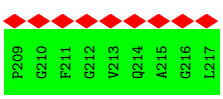
Chain 1E:





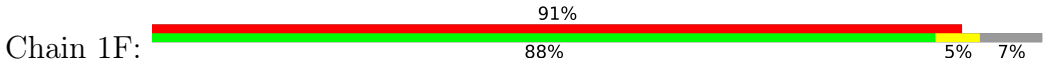


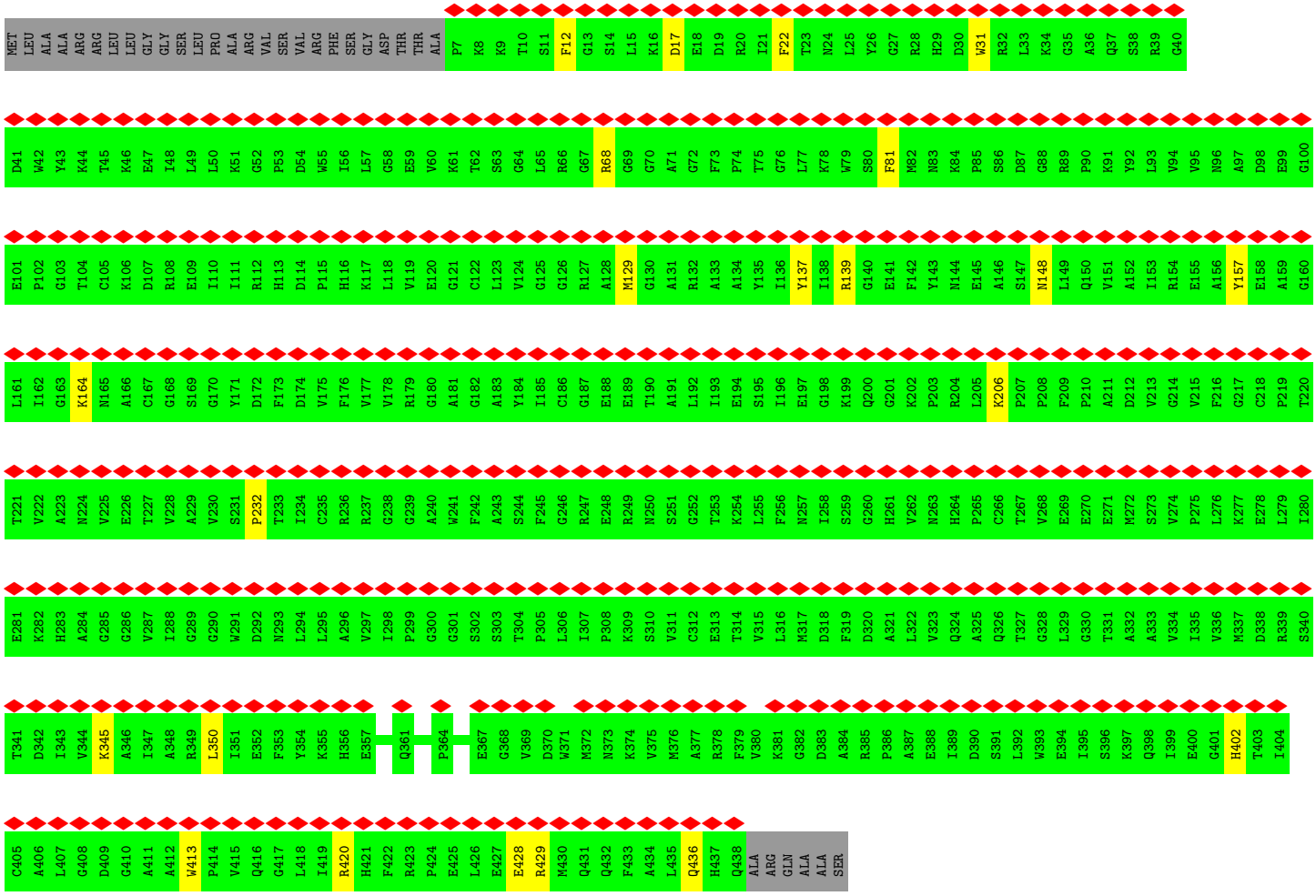




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

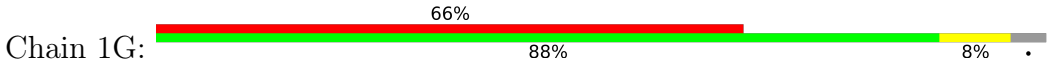
Chain 1F:

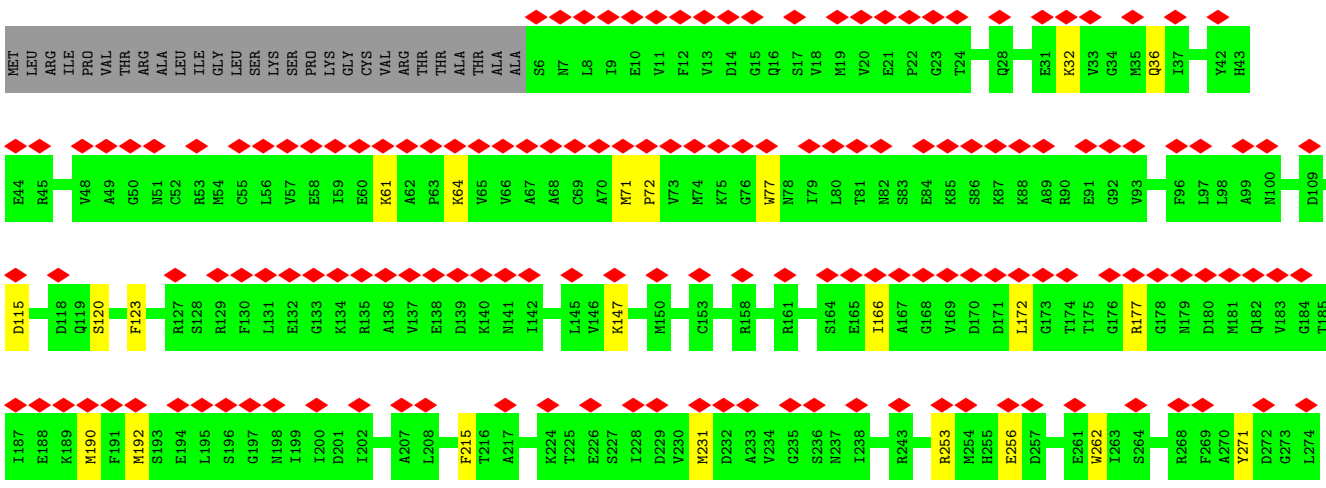


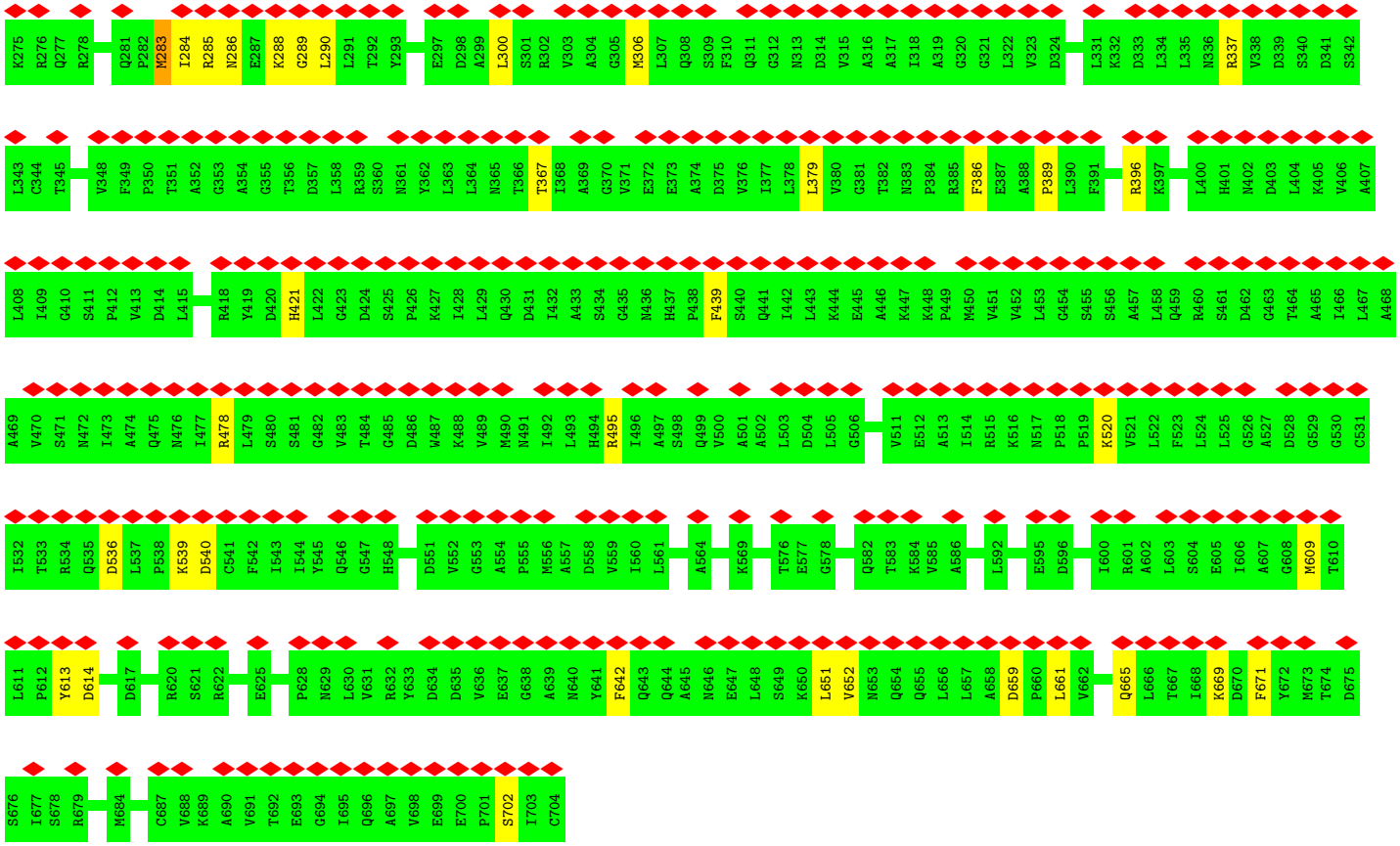


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G:

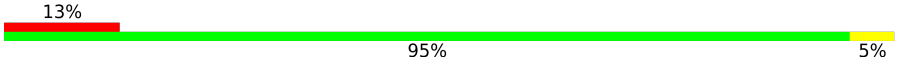


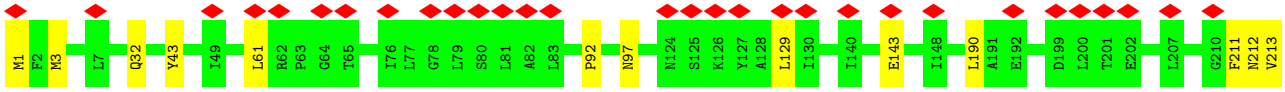


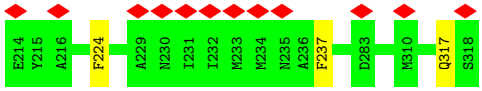


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:

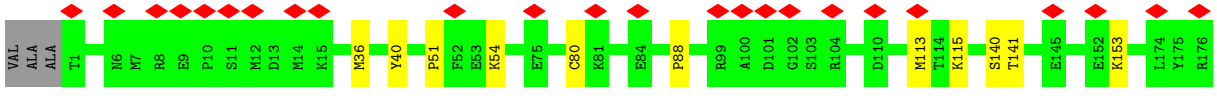






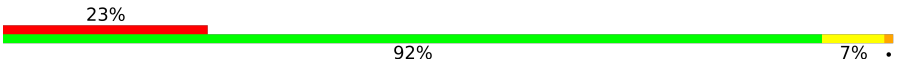
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

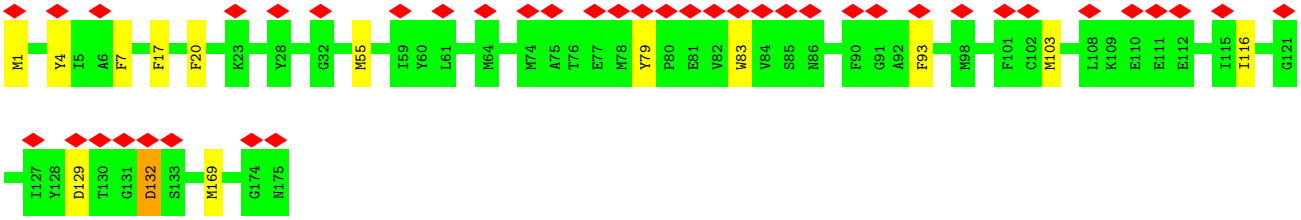
Chain 1I:



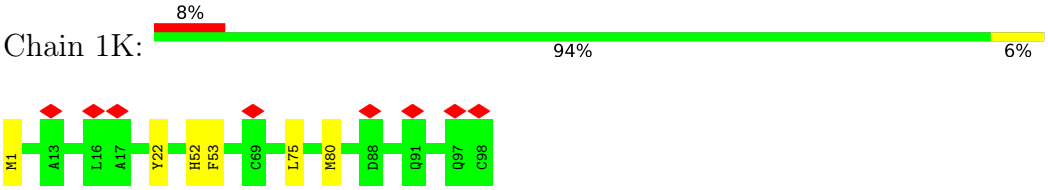
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:

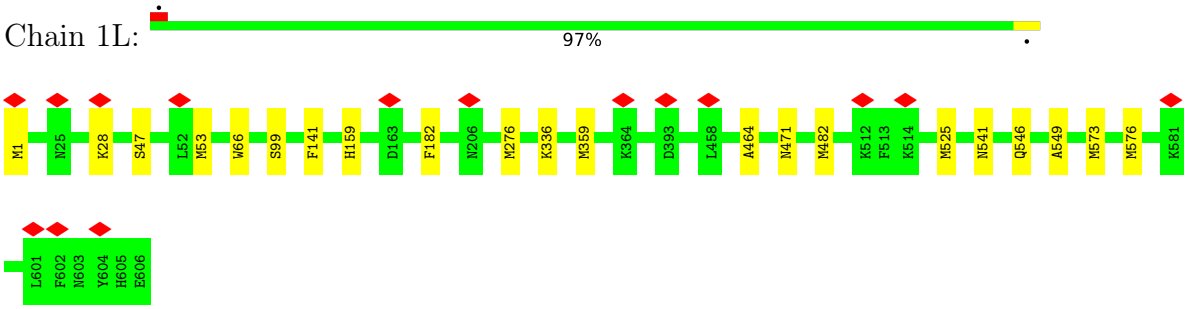




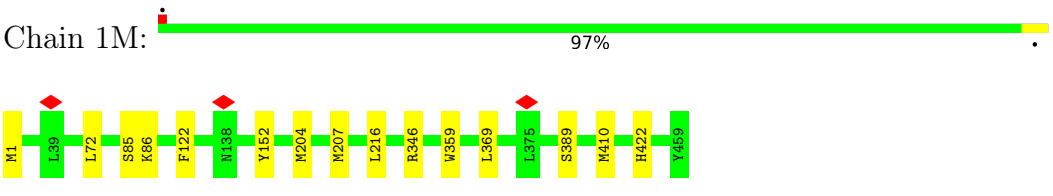
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



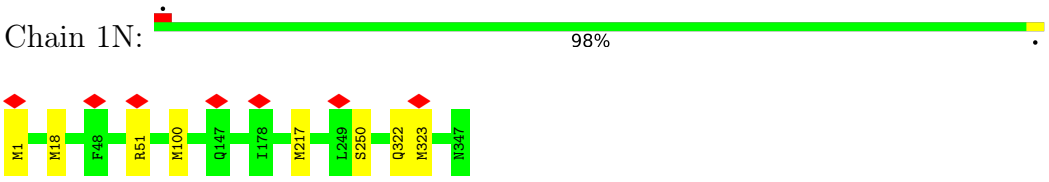
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



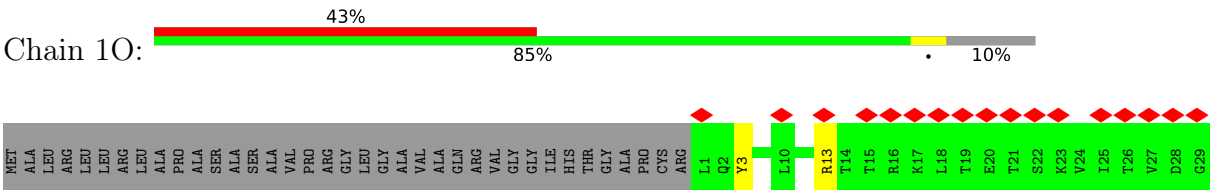
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

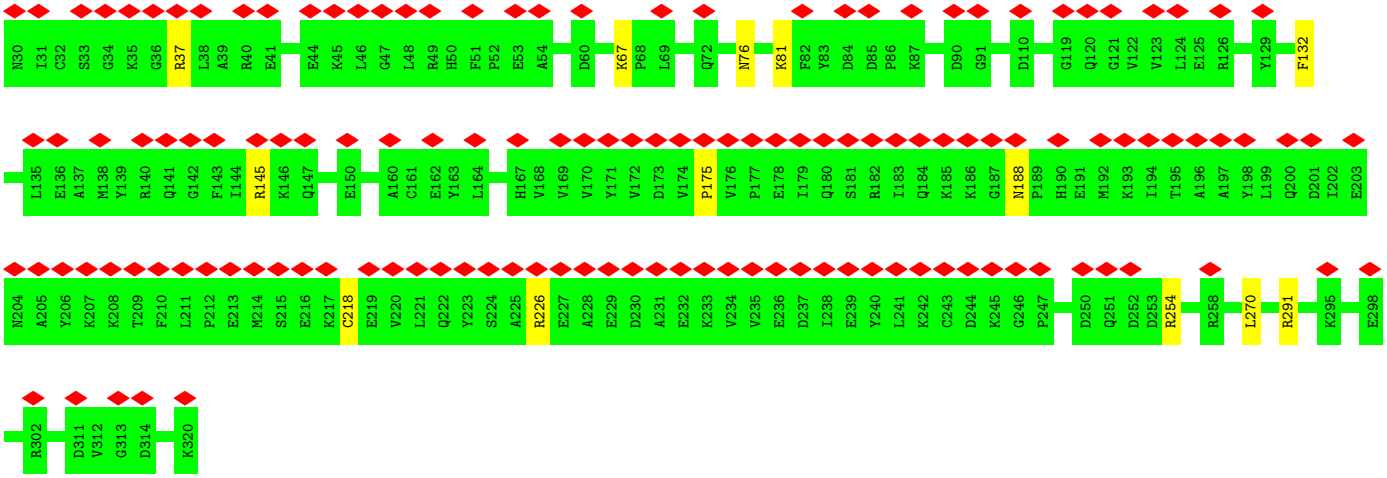


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



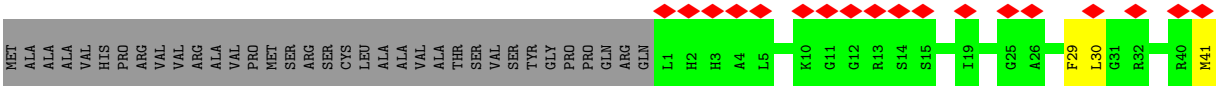
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





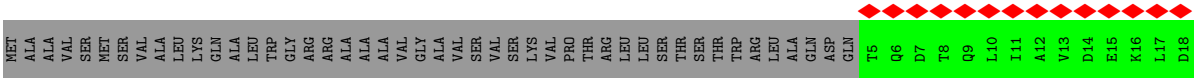
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

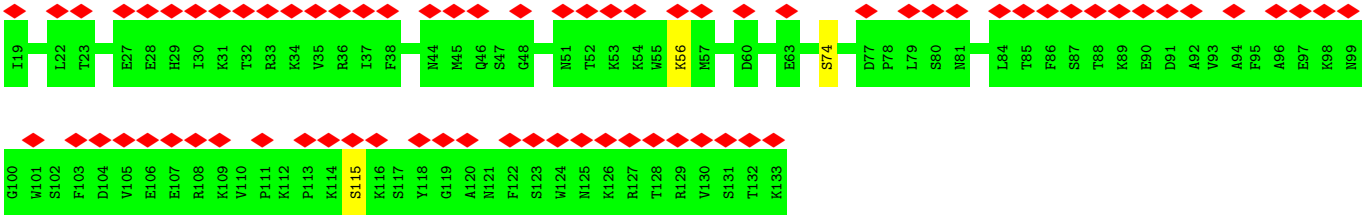
Chain 1P:



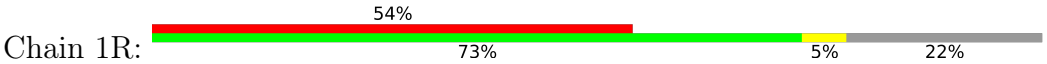
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

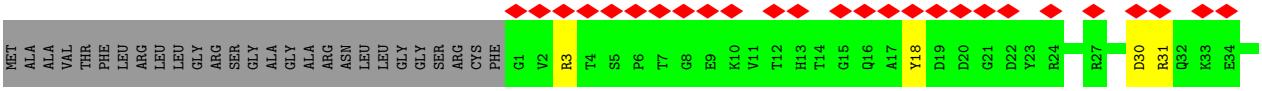
Chain 1Q:



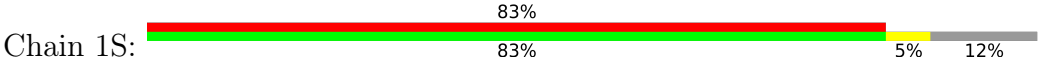


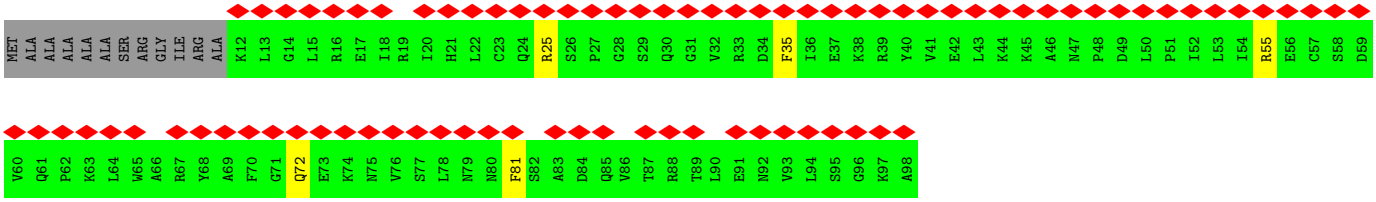
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



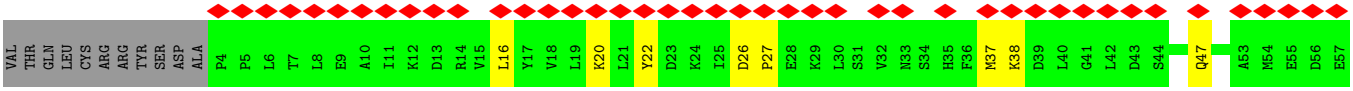


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

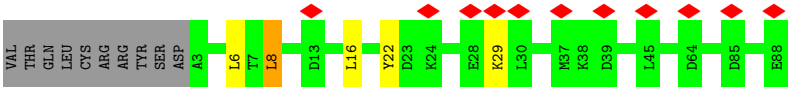




• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

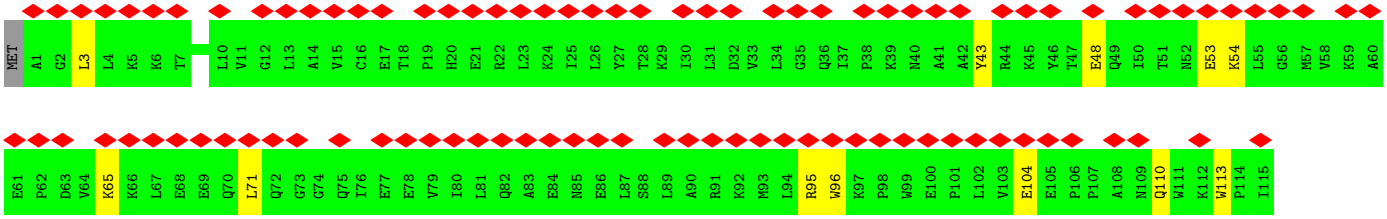


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



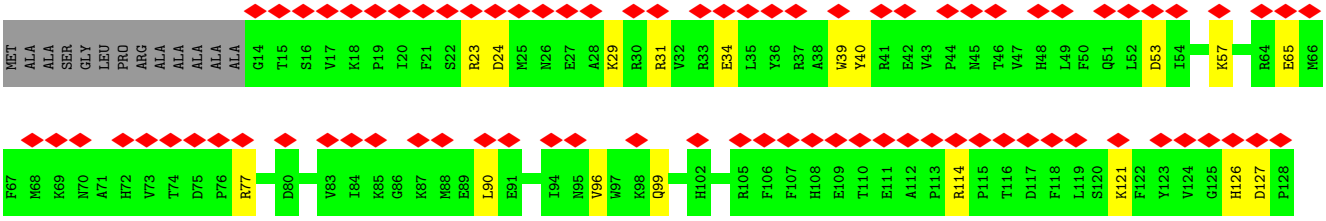
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:



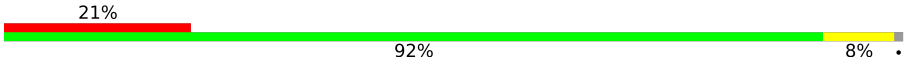
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

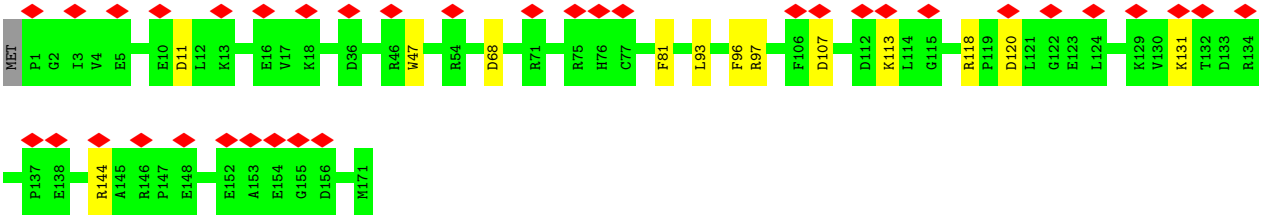
Chain 1W:



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

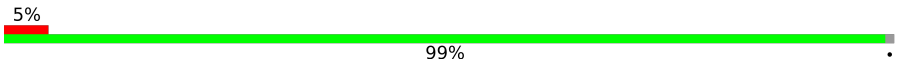
Chain 1X:

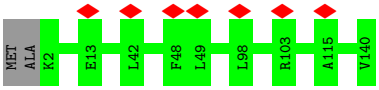




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

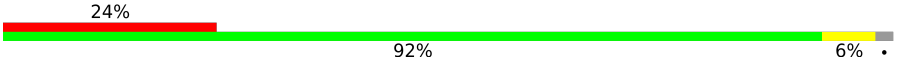
Chain 1Y:

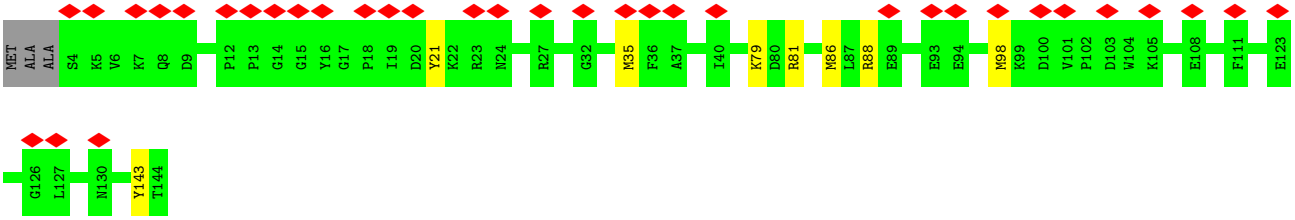




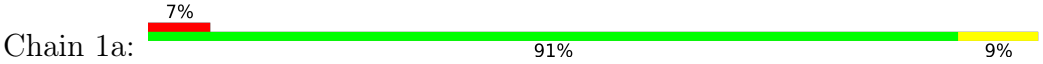
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

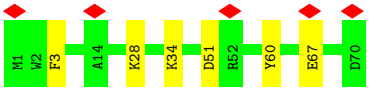
Chain 1Z:



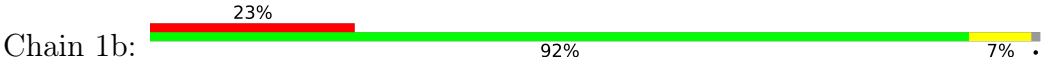


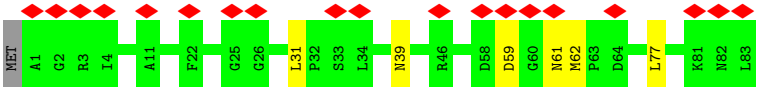
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



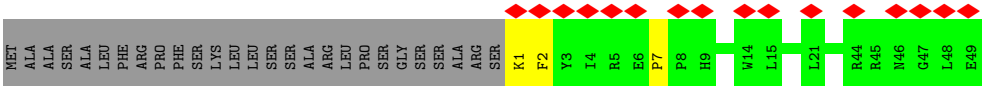


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

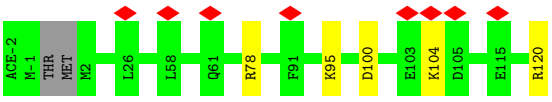




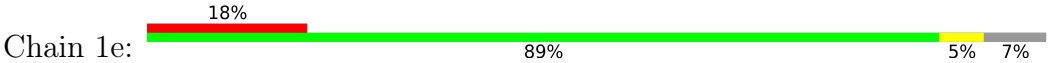
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

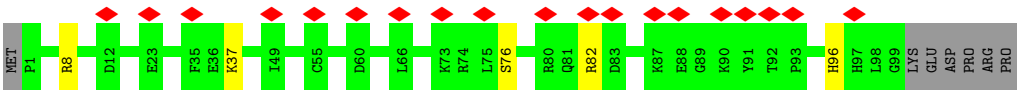


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

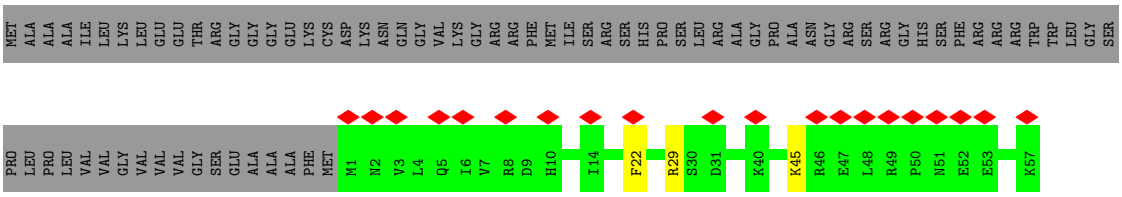


• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



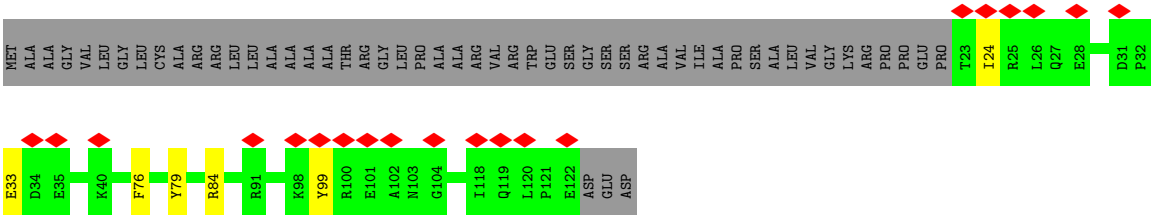


• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



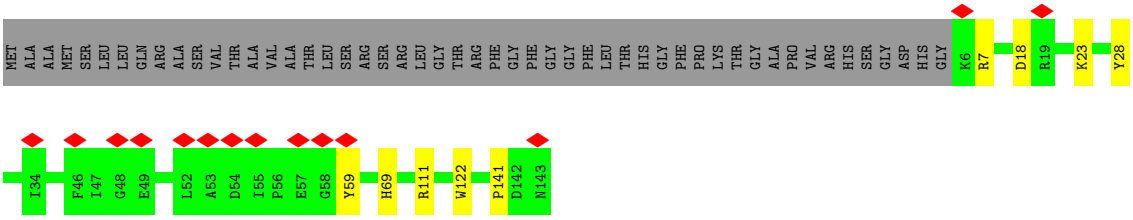
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



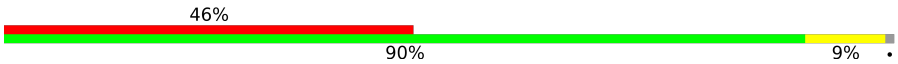
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

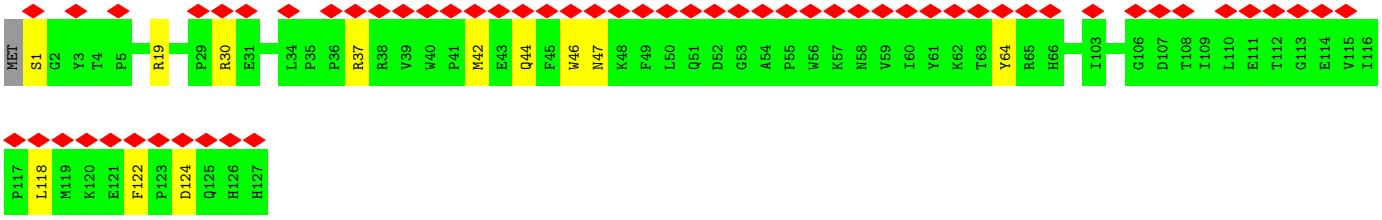
Chain 1h:



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

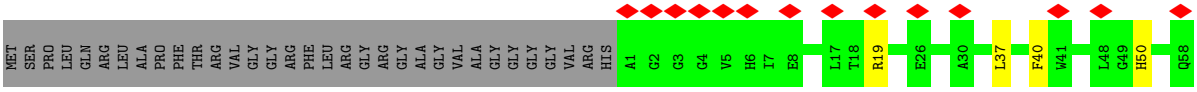
Chain 1i:

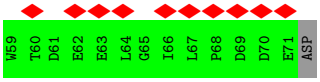




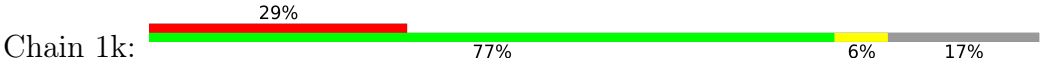
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

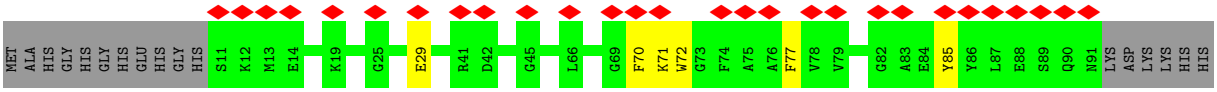
Chain 1j:



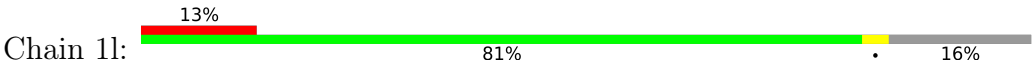


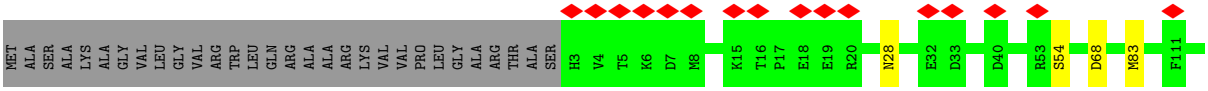
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

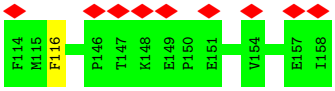




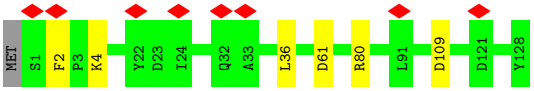
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



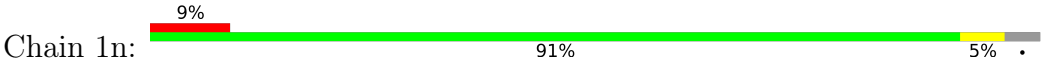




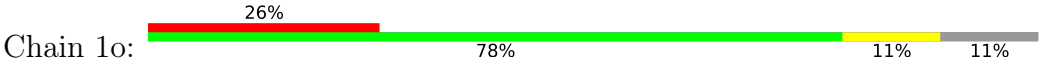
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

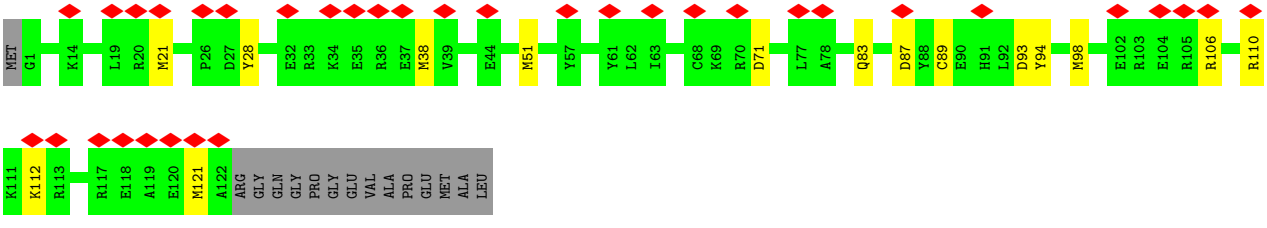


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



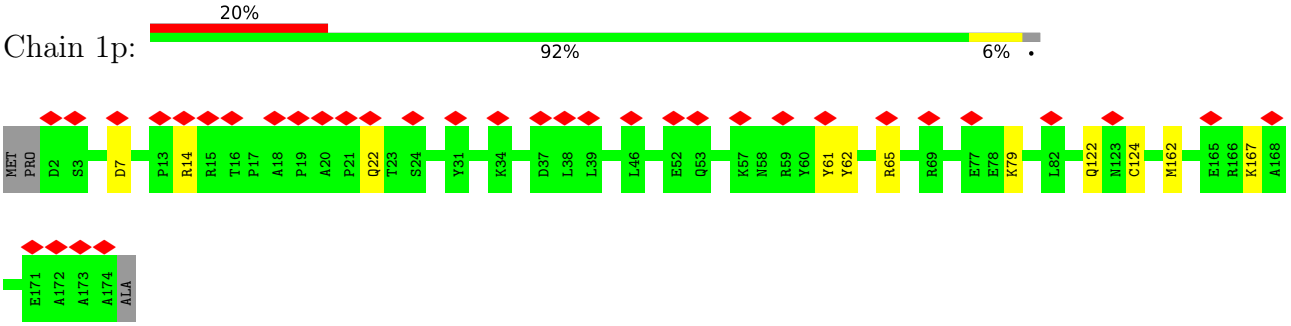
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





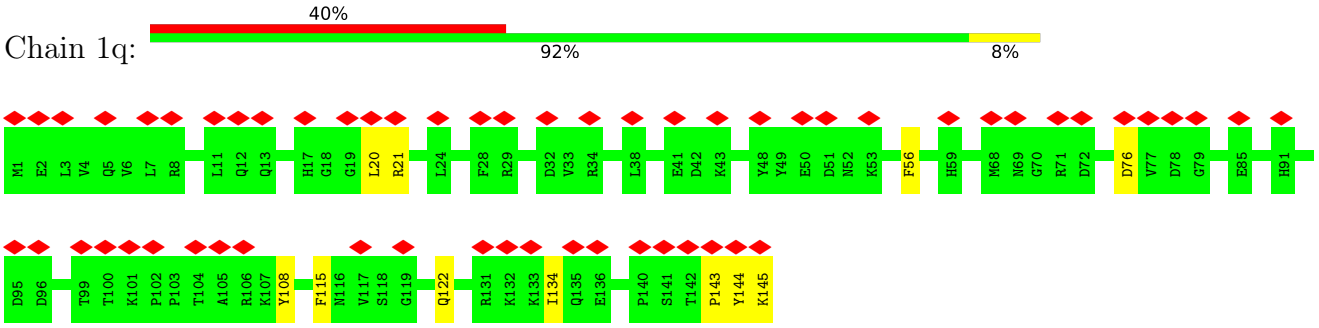
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p:



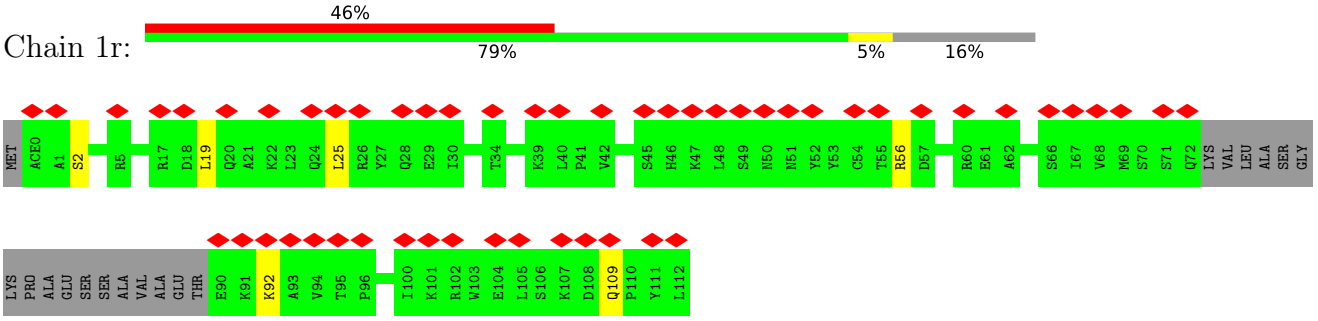
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:



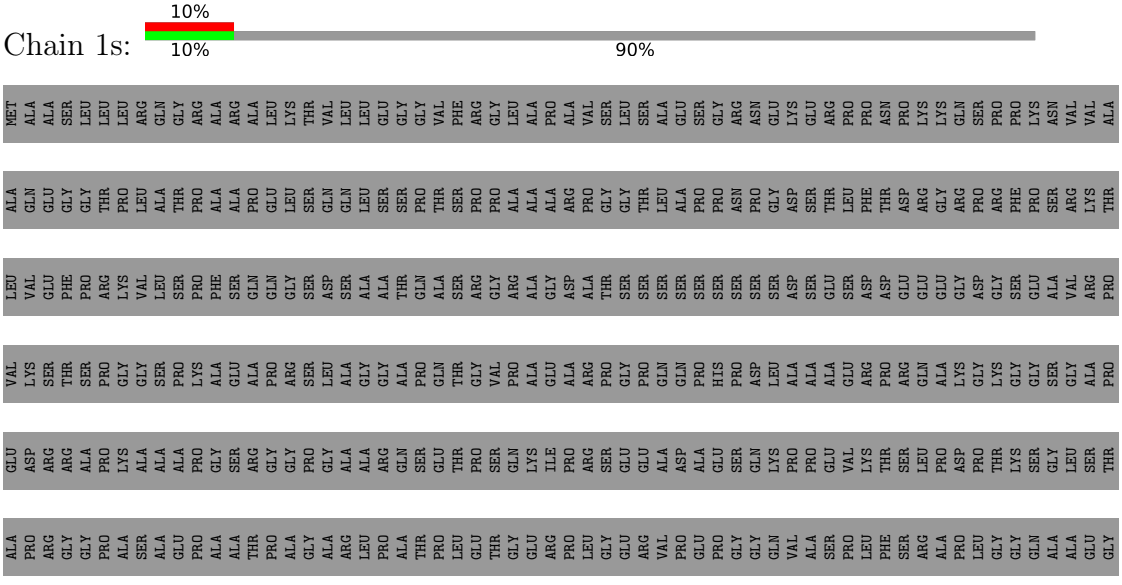
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

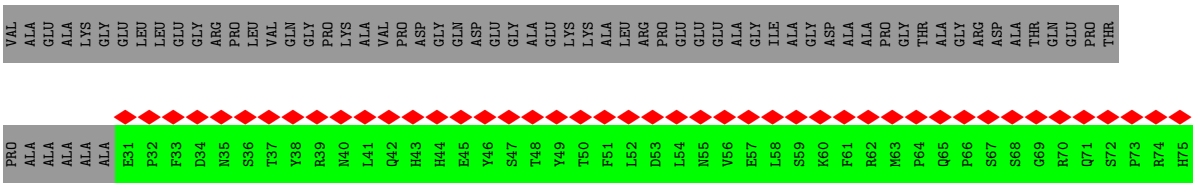
Chain 1r:



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

Chain 1s:




VAL ALA GLU ALA LYS GLY GLU LEU LEU GLU GLY ARG PRO LEU VAL GLN GLY PRO LYS ALA VAL PRO ASP GLY GLN ASP GLU GLY ALA GLU LYS LYS ALA LEU ARG PRO GLU GLU GLU ALA GLY ILE ALA GLY ASP ALA ALA PRO GLY THR ALA GLY ARG ASP ALA THR GLN GLU PRO THR
PRO ALA ALA ALA ALA ALA E31 P32 F33 D34 N35 S36 T37 Y38 R39 N40 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 (i)

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 ($e^-/Å^2$)	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	0.935	Depositor
Minimum map value	-0.432	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	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

5.1 Standard geometry

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

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	0.25	0/705	0.51	0/963
2	1B	0.32	0/1273	0.60	0/1722
3	1C	0.30	0/1791	0.56	0/2439
4	1D	0.30	0/3464	0.54	0/4692
5	1E	0.27	0/1698	0.52	0/2311
6	1F	0.26	0/3401	0.53	1/4595 (0.0%)
7	1G	0.29	1/5451 (0.0%)	0.60	5/7387 (0.1%)
8	1H	0.29	0/2566	0.54	0/3509
9	1I	0.38	0/1443	0.69	3/1952 (0.2%)
10	1J	0.29	0/1364	0.55	1/1850 (0.1%)
11	1K	0.29	0/751	0.58	0/1018
12	1L	0.28	0/4939	0.49	0/6718
13	1M	0.27	0/3713	0.48	0/5063
14	1N	0.27	0/2765	0.51	0/3758
15	1O	0.27	0/2650	0.53	1/3588 (0.0%)
16	1P	0.28	0/2828	0.56	1/3834 (0.0%)
17	1Q	0.29	0/1070	0.60	0/1446
18	1R	0.28	0/755	0.56	0/1018
19	1S	0.28	0/711	0.71	1/956 (0.1%)
20	1T	0.33	0/701	0.72	2/946 (0.2%)
20	1U	0.27	0/706	0.55	1/954 (0.1%)
21	1V	0.26	0/946	0.59	0/1281
22	1W	0.30	0/995	0.63	0/1340
23	1X	0.26	0/1436	0.52	0/1938
24	1Y	0.29	0/1037	0.48	0/1404
25	1Z	0.28	0/1199	0.54	0/1617
26	1a	0.28	0/577	0.52	0/777
27	1b	0.29	0/664	0.55	0/912
28	1c	0.28	0/430	0.57	1/581 (0.2%)
29	1d	0.29	0/1024	0.52	0/1383
30	1e	0.27	0/836	0.53	0/1118
31	1f	0.24	0/499	0.62	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.28	0/858	0.56	0/1165
33	1h	0.34	0/1184	0.63	2/1603 (0.1%)
34	1i	0.28	0/1131	0.58	0/1541
35	1j	0.25	0/627	0.51	0/858
36	1k	0.27	0/668	0.52	0/903
37	1l	0.27	0/1365	0.50	0/1867
38	1m	0.28	0/1092	0.53	1/1481 (0.1%)
39	1n	0.27	0/1549	0.52	0/2098
40	1o	0.28	0/1069	0.55	0/1430
41	1p	0.27	0/1481	0.52	0/1997
42	1q	0.32	0/1253	0.64	2/1704 (0.1%)
43	1r	0.29	0/782	0.65	0/1057
44	1s	0.25	0/394	0.52	0/533
All	All	0.28	1/67841 (0.0%)	0.55	22/91980 (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	1
7	1G	0	2
13	1M	0	1
21	1V	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1G	389	PRO	CG-CD	-5.26	1.33	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1h	141	PRO	CA-N-CD	-10.69	96.53	111.50
9	1I	51	PRO	CA-N-CD	-10.46	96.86	111.50
9	1I	51	PRO	N-CD-CG	-9.48	88.98	103.20
20	1T	27	PRO	CA-N-CD	-9.46	98.26	111.50
7	1G	389	PRO	CA-N-CD	-8.39	99.75	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
7	1G	284	ILE	Peptide
7	1G	286	ASN	Peptide
13	1M	207	MET	Peptide
21	1V	113	TRP	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	83/115 (72%)	78 (94%)	3 (4%)	2 (2%)	6 35
2	1B	153/258 (59%)	140 (92%)	13 (8%)	0	100 100
3	1C	207/264 (78%)	192 (93%)	15 (7%)	0	100 100
4	1D	414/476 (87%)	380 (92%)	34 (8%)	0	100 100
5	1E	212/249 (85%)	193 (91%)	19 (9%)	0	100 100
6	1F	430/464 (93%)	397 (92%)	33 (8%)	0	100 100
7	1G	697/727 (96%)	620 (89%)	71 (10%)	6 (1%)	17 54
8	1H	316/318 (99%)	290 (92%)	24 (8%)	2 (1%)	25 62
9	1I	174/239 (73%)	164 (94%)	10 (6%)	0	100 100
10	1J	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	25 62
11	1K	96/98 (98%)	90 (94%)	6 (6%)	0	100 100
12	1L	604/606 (100%)	557 (92%)	44 (7%)	3 (0%)	29 66
13	1M	457/459 (100%)	436 (95%)	20 (4%)	1 (0%)	47 78
14	1N	345/347 (99%)	326 (94%)	19 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	1O	318/357 (89%)	288 (91%)	30 (9%)	0	100	100
16	1P	340/377 (90%)	304 (89%)	35 (10%)	1 (0%)	41	74
17	1Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
18	1R	94/123 (76%)	83 (88%)	10 (11%)	1 (1%)	14	50
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	99 (88%)	14 (12%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	6 (5%)	1 (1%)	17	54
23	1X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	1Y	137/141 (97%)	129 (94%)	8 (6%)	0	100	100
25	1Z	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
26	1a	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	94 (97%)	3 (3%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	89 (91%)	8 (8%)	1 (1%)	15	51
33	1h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	1i	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
35	1j	69/105 (66%)	63 (91%)	5 (7%)	1 (1%)	11	45
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	141 (92%)	13 (8%)	0	100	100
38	1m	126/129 (98%)	116 (92%)	10 (8%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	7 (4%)	0	100	100
40	1o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	1p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	11 (8%)	1 (1%)	22	59
43	1r	90/114 (79%)	82 (91%)	8 (9%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8151/9744 (84%)	7525 (92%)	605 (7%)	21 (0%)	44 74

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
7	1G	652	VAL
7	1G	671	PHE
8	1H	92	PRO
12	1L	464	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	75/99 (76%)	72 (96%)	3 (4%)	31 60
2	1B	131/212 (62%)	120 (92%)	11 (8%)	11 40
3	1C	190/227 (84%)	179 (94%)	11 (6%)	20 52
4	1D	364/405 (90%)	351 (96%)	13 (4%)	35 63
5	1E	183/207 (88%)	172 (94%)	11 (6%)	19 50
6	1F	346/368 (94%)	326 (94%)	20 (6%)	20 52
7	1G	588/610 (96%)	542 (92%)	46 (8%)	12 42
8	1H	274/274 (100%)	261 (95%)	13 (5%)	26 56
9	1I	151/201 (75%)	141 (93%)	10 (7%)	16 48
10	1J	140/140 (100%)	128 (91%)	12 (9%)	10 39
11	1K	84/84 (100%)	79 (94%)	5 (6%)	19 50
12	1L	539/539 (100%)	522 (97%)	17 (3%)	39 65
13	1M	408/408 (100%)	396 (97%)	12 (3%)	42 66
14	1N	310/310 (100%)	303 (98%)	7 (2%)	50 71
15	1O	283/307 (92%)	269 (95%)	14 (5%)	25 56
16	1P	296/323 (92%)	273 (92%)	23 (8%)	12 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	1Q	117/152 (77%)	114 (97%)	3 (3%)	46	69
18	1R	79/97 (81%)	74 (94%)	5 (6%)	18	49
19	1S	77/82 (94%)	73 (95%)	4 (5%)	23	55
20	1T	79/133 (59%)	68 (86%)	11 (14%)	3	20
20	1U	79/133 (59%)	74 (94%)	5 (6%)	18	49
21	1V	100/101 (99%)	89 (89%)	11 (11%)	6	29
22	1W	107/112 (96%)	90 (84%)	17 (16%)	2	16
23	1X	153/154 (99%)	140 (92%)	13 (8%)	10	40
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	115 (94%)	8 (6%)	17	48
26	1a	58/58 (100%)	52 (90%)	6 (10%)	7	31
27	1b	69/70 (99%)	63 (91%)	6 (9%)	10	38
28	1c	45/66 (68%)	43 (96%)	2 (4%)	28	58
29	1d	107/109 (98%)	102 (95%)	5 (5%)	26	56
30	1e	87/94 (93%)	82 (94%)	5 (6%)	20	52
31	1f	54/113 (48%)	51 (94%)	3 (6%)	21	53
32	1g	92/129 (71%)	87 (95%)	5 (5%)	22	54
33	1h	121/158 (77%)	113 (93%)	8 (7%)	16	48
34	1i	119/120 (99%)	108 (91%)	11 (9%)	9	36
35	1j	62/84 (74%)	59 (95%)	3 (5%)	25	56
36	1k	63/76 (83%)	57 (90%)	6 (10%)	8	34
37	1l	141/161 (88%)	136 (96%)	5 (4%)	36	63
38	1m	113/114 (99%)	108 (96%)	5 (4%)	28	58
39	1n	156/160 (98%)	147 (94%)	9 (6%)	20	52
40	1o	110/120 (92%)	95 (86%)	15 (14%)	3	21
41	1p	154/156 (99%)	143 (93%)	11 (7%)	14	45
42	1q	131/131 (100%)	123 (94%)	8 (6%)	18	50
43	1r	85/98 (87%)	79 (93%)	6 (7%)	14	45
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7188/8272 (87%)	6764 (94%)	424 (6%)	23	51

5 of 424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	1R	3	ARG
23	1X	68	ASP
41	1p	7	ASP
19	1S	72	GLN
21	1V	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
21	1V	70	GLN
33	1h	124	GLN
21	1V	85	ASN
27	1b	45	ASN
38	1m	78	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	$\#\|Z\| > 2$
34	SAC	1i	1	-	7,8,9	0.53	0	8,9,11	1.08	1 (12%)
8	FME	1H	1	8	8,9,10	0.61	0	7,9,11	1.06	1 (14%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	1.05	1 (14%)
11	FME	1K	1	11	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
14	FME	1N	1	14	8,9,10	0.50	0	7,9,11	0.94	1 (14%)
1	FME	1A	1	1	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.02	1 (14%)
10	FME	1J	1	10	8,9,10	0.52	0	7,9,11	0.96	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
34	SAC	1i	1	-	-	2/7/8/10	-
8	FME	1H	1	8	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1i	1	SAC	O-C-CA	-2.98	116.97	124.78
11	1K	1	FME	O-C-CA	-2.62	117.92	124.78
8	1H	1	FME	O-C-CA	-2.61	117.95	124.78
12	1L	1	FME	O-C-CA	-2.58	118.02	124.78
10	1J	1	FME	O-C-CA	-2.54	118.13	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
10	1J	1	FME	N-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
34	1i	1	SAC	CB-CA-N-C1A
10	1J	1	FME	C-CA-CB-CG

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	$\#\|Z\| > 2$
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.88	1 (3%)
56	NDP	1P	501	-	45,52,52	0.61	0	53,80,80	0.72	1 (1%)
58	EHZ	1n	201	-	29,36,37	0.16	0	35,44,47	1.29	2 (5%)
47	FES	1E	301	5	0,4,4	-	-	-		
46	SF4	1G	801	7	0,12,12	-	-	-		
50	PC1	1f	101	-	45,45,53	0.27	0	51,53,61	0.34	0
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.39	0
50	PC1	1H	401	-	53,53,53	0.27	0	59,61,61	0.32	0
47	FES	1G	803	7	0,4,4	-	-	-		
53	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.36	0
50	PC1	1M	502	-	43,43,53	0.29	0	49,51,61	0.44	0
50	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.39	0
53	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.41	0
48	FMN	1F	501	-	33,33,33	0.57	0	48,50,50	0.65	0
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.32	0
58	EHZ	1W	201	-	29,36,37	0.18	0	35,44,47	1.12	1 (2%)
46	SF4	1F	502	6	0,12,12	-	-	-		
45	3PE	1L	703	-	30,30,50	0.36	0	33,35,55	0.59	0
45	3PE	1L	702	-	45,45,50	0.29	0	48,50,55	0.32	0
46	SF4	1I	202	9	0,12,12	-	-	-		
51	MYR	1L	701	-	14,14,15	0.33	0	13,13,15	0.38	0
45	3PE	1L	704	-	41,41,50	0.30	0	44,46,55	1.29	5 (11%)
52	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.48	0
46	SF4	1B	201	2	0,12,12	-	-	-		
46	SF4	1G	802	7	0,12,12	-	-	-		
45	3PE	1Y	201	-	50,50,50	0.27	0	53,55,55	0.42	0
46	SF4	1I	201	9	0,12,12	-	-	-		
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.40	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
54	GTP	1O	401	55	-	3/18/38/38	0/3/3/3
56	NDP	1P	501	-	-	9/30/77/77	0/5/5/5
58	EHZ	1n	201	-	-	13/42/44/45	-
47	FES	1E	301	5	-	-	0/1/1/1
46	SF4	1G	801	7	-	-	0/6/5/5
50	PC1	1f	101	-	-	7/49/49/57	-
45	3PE	1A	201	-	-	3/50/50/54	-
50	PC1	1H	401	-	-	5/57/57/57	-
47	FES	1G	803	7	-	-	0/1/1/1
53	CDL	1N	402	-	-	9/87/87/110	-
50	PC1	1M	502	-	-	8/47/47/57	-
50	PC1	1I	203	-	-	6/47/47/57	-
53	CDL	1a	101	-	-	13/71/71/110	-
46	SF4	1I	201	9	-	-	0/6/5/5
48	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
50	PC1	1J	201	-	-	5/38/38/57	-
46	SF4	1F	502	6	-	-	0/6/5/5
45	3PE	1L	703	-	-	8/34/34/54	-
45	3PE	1L	702	-	-	2/49/49/54	-
51	MYR	1L	701	-	-	1/11/12/13	-
46	SF4	1I	202	9	-	-	0/6/5/5
45	3PE	1L	704	-	-	7/45/45/54	-
52	PGT	1M	501	-	-	23/55/55/55	-
46	SF4	1B	201	2	-	-	0/6/5/5
46	SF4	1G	802	7	-	-	0/6/5/5
45	3PE	1Y	201	-	-	9/54/54/54	-
58	EHZ	1W	201	-	-	6/42/44/45	-
45	3PE	1N	401	-	-	9/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1O	401	GTP	C5-C6	-2.60	1.42	1.47
54	1O	401	GTP	C8-N7	-2.08	1.31	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	1L	704	3PE	O21-C21-C22	6.45	125.41	111.50
58	1W	201	EHZ	C10-S1-C9	6.15	121.03	101.87
58	1n	201	EHZ	C10-S1-C9	6.11	120.90	101.87
58	1n	201	EHZ	C14-C13-C12	3.06	117.46	112.36
54	1O	401	GTP	O4'-C1'-C2'	-2.73	102.93	106.93

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

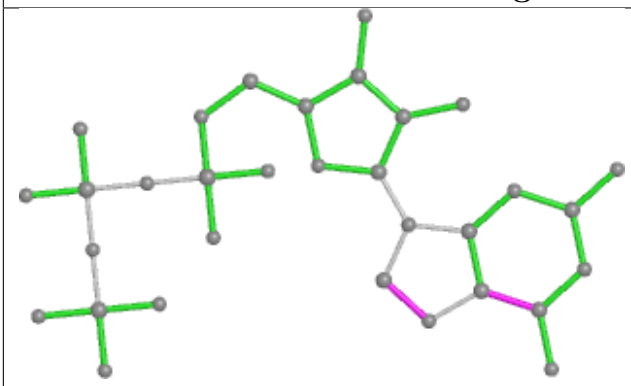
Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	C1-O11-P-O14
45	1L	703	3PE	O32-C31-O31-C3
45	1L	703	3PE	C32-C31-O31-C3
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2

There are no ring outliers.

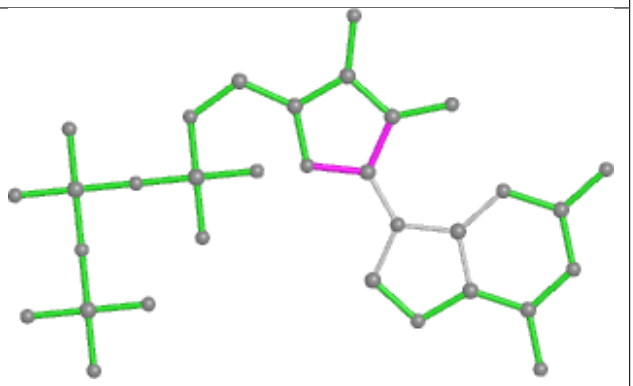
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

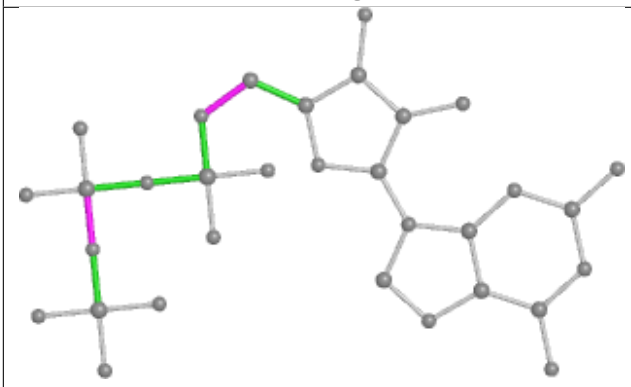
Ligand GTP 1O 401



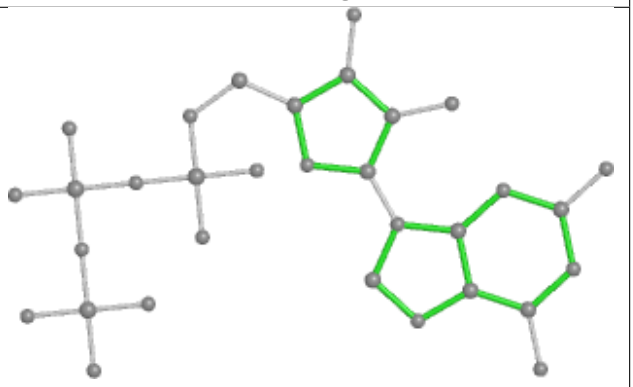
Bond lengths



Bond angles

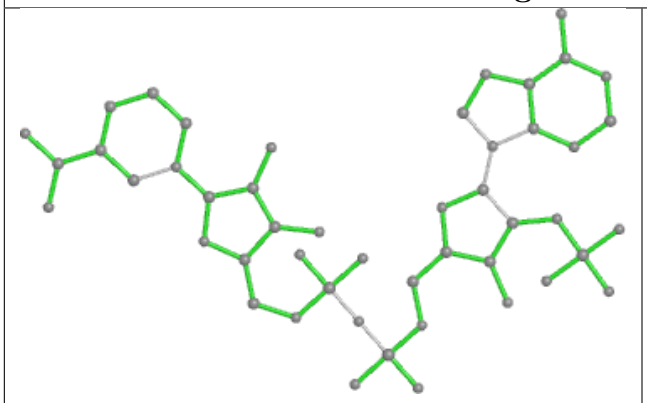


Torsions

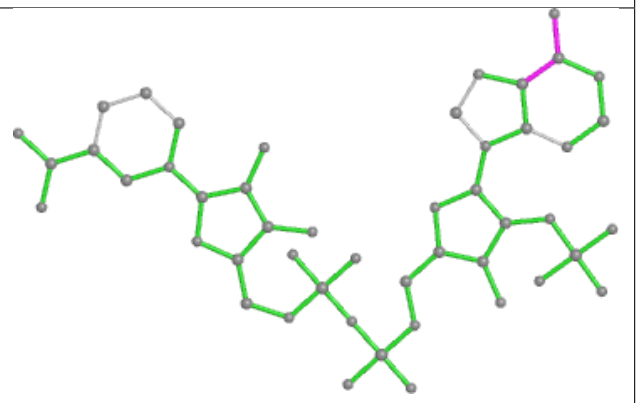


Rings

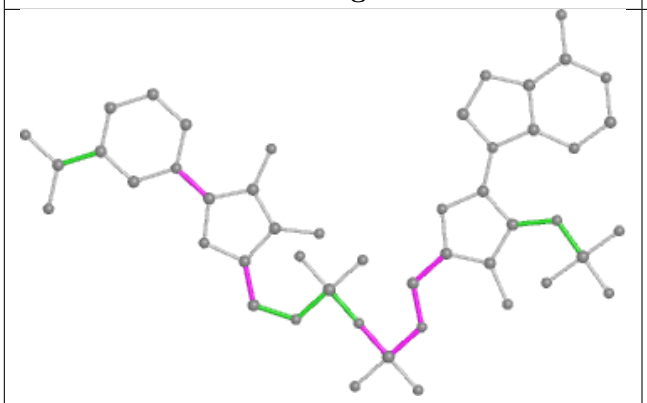
Ligand NDP 1P 501



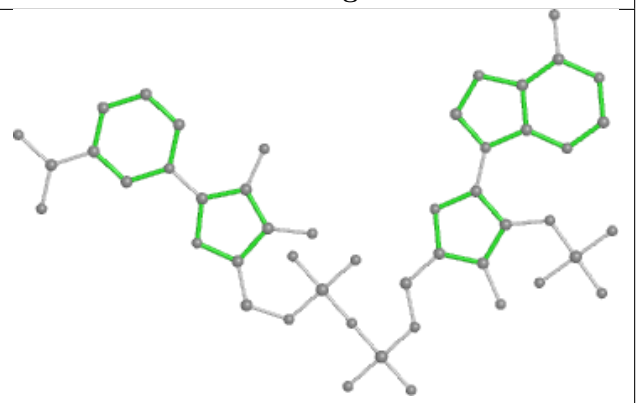
Bond lengths



Bond angles

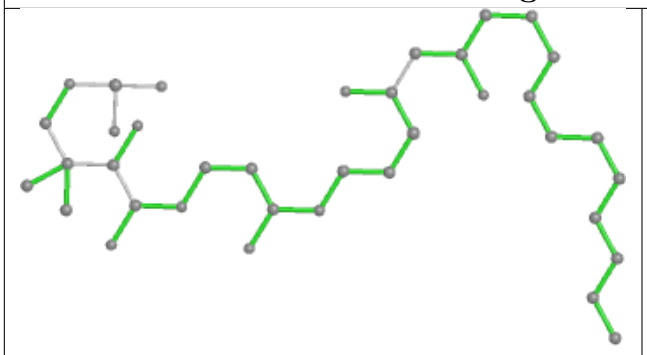


Torsions

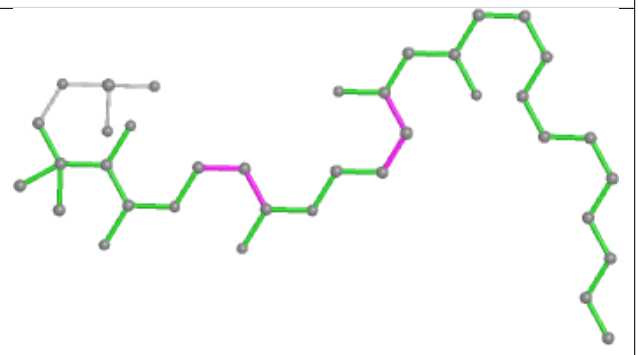


Rings

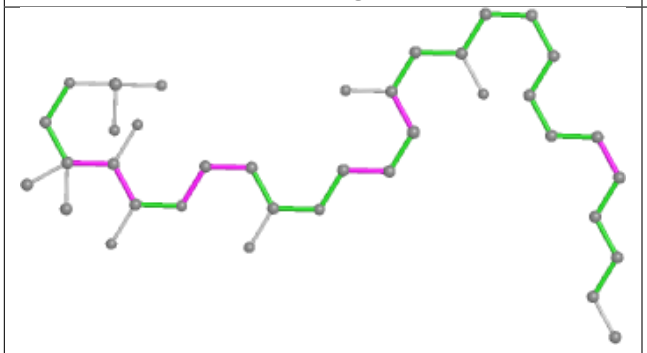
Ligand EHZ 1n 201



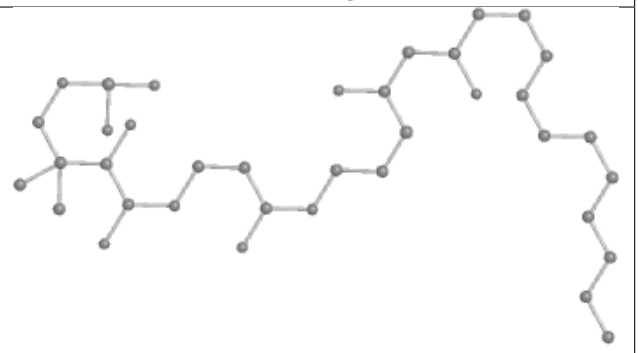
Bond lengths



Bond angles

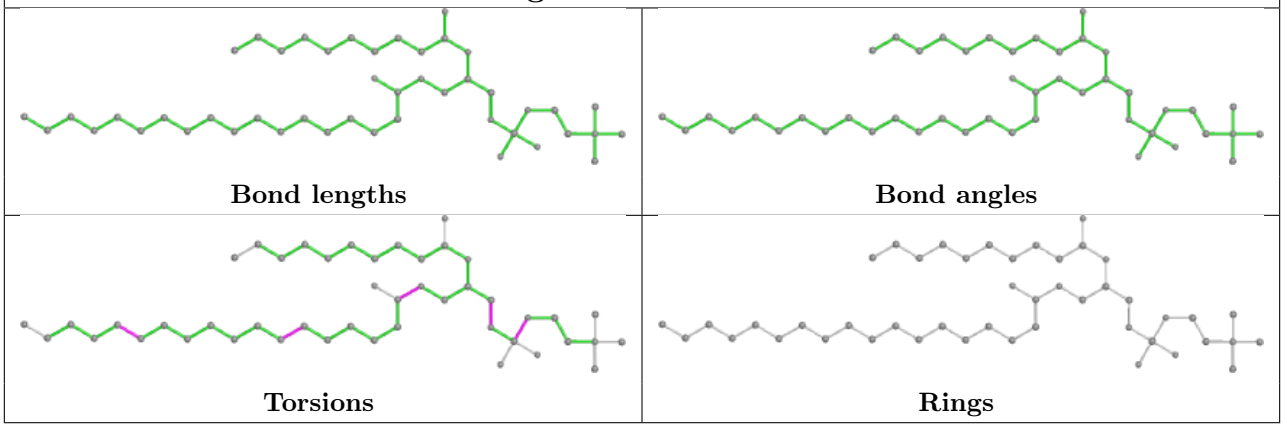


Torsions

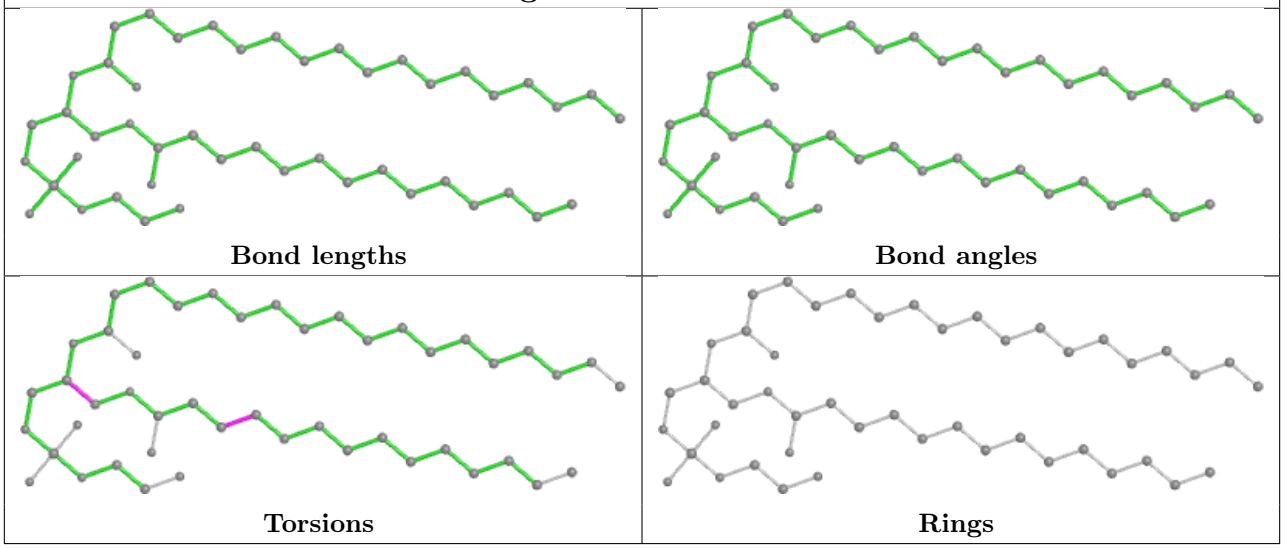


Rings

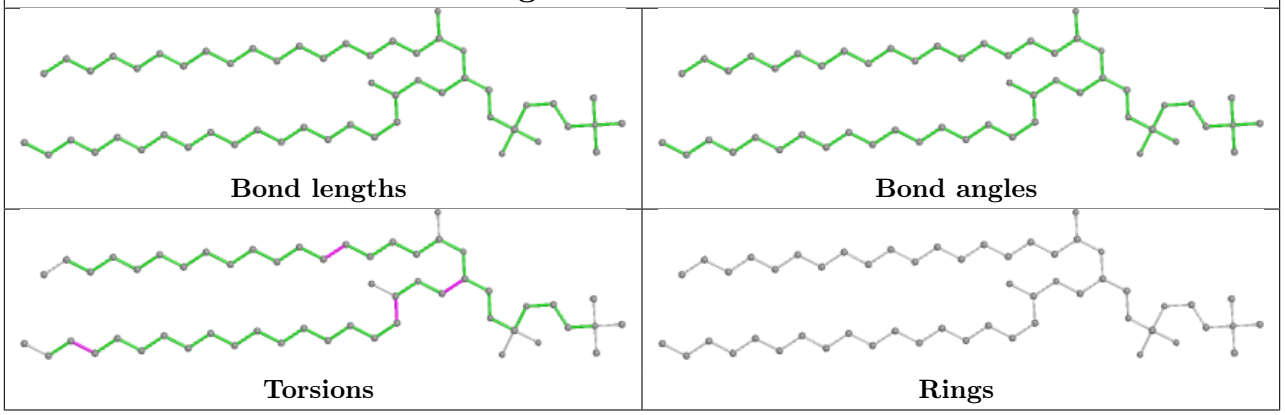
Ligand PC1 1f 101



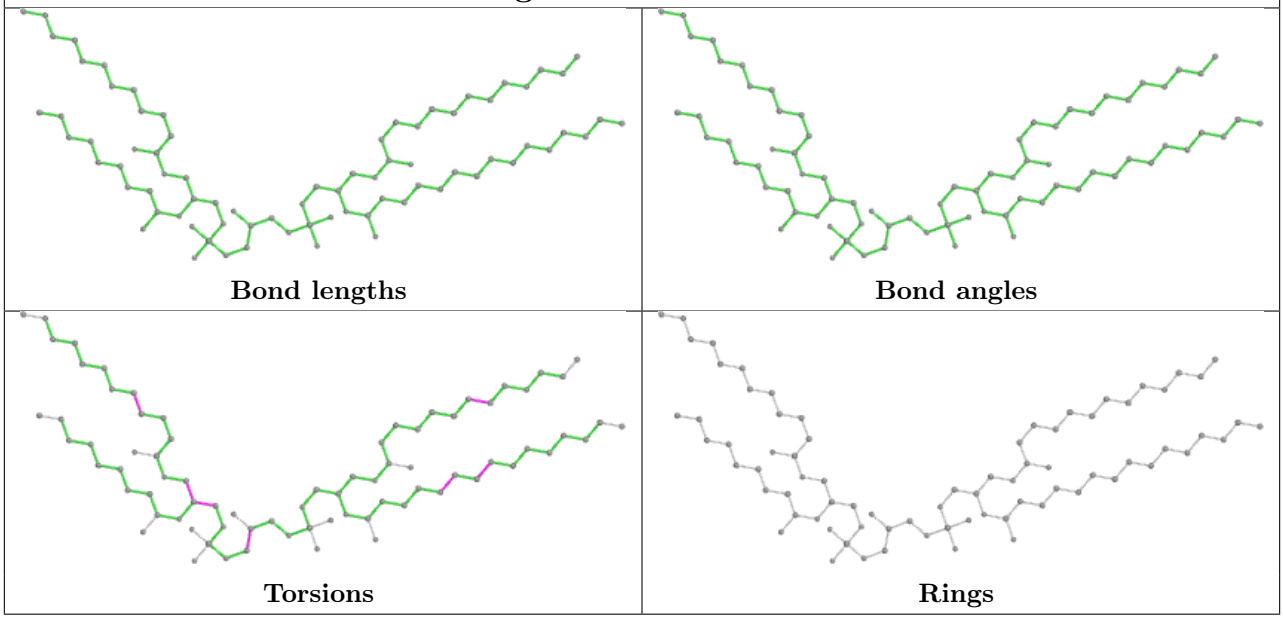
Ligand 3PE 1A 201



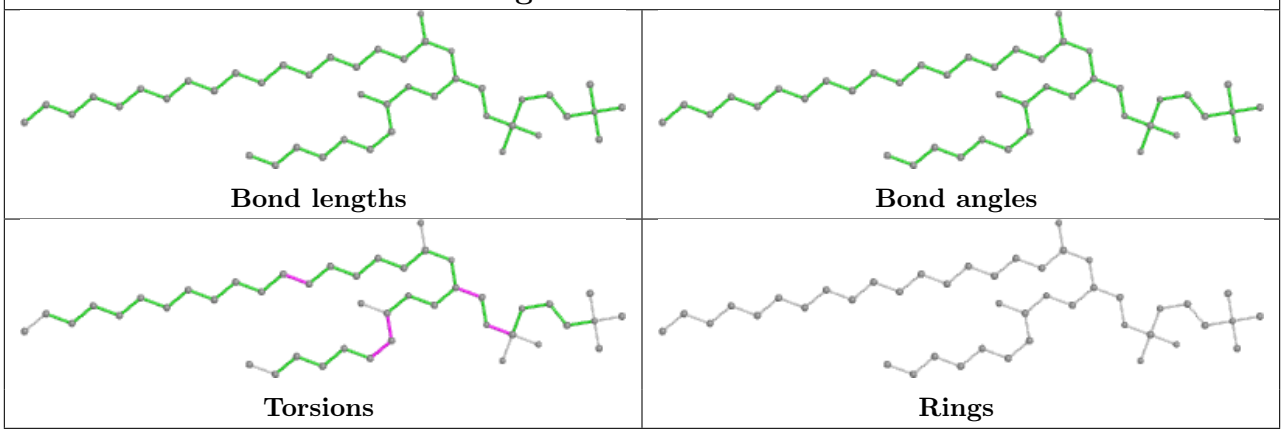
Ligand PC1 1H 401



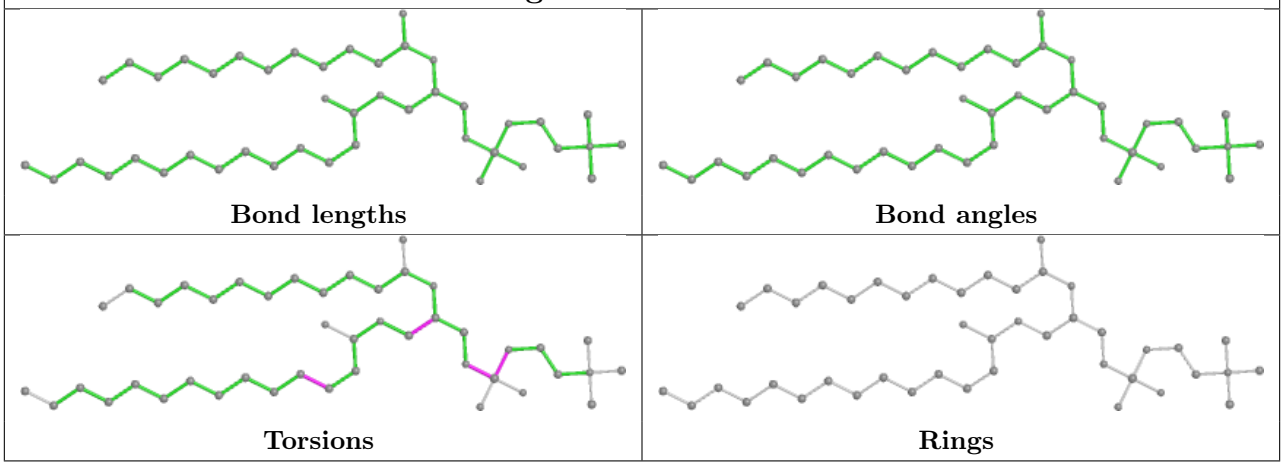
Ligand CDL 1N 402



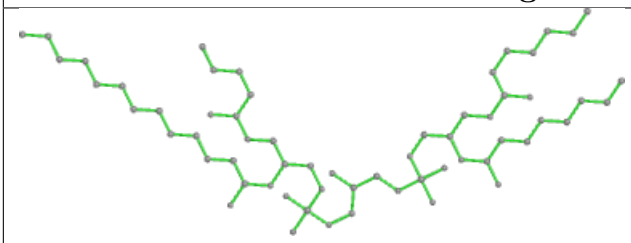
Ligand PC1 1M 502



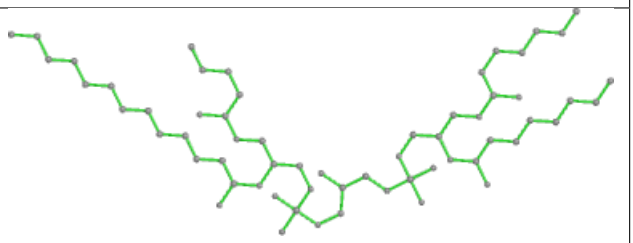
Ligand PC1 1I 203



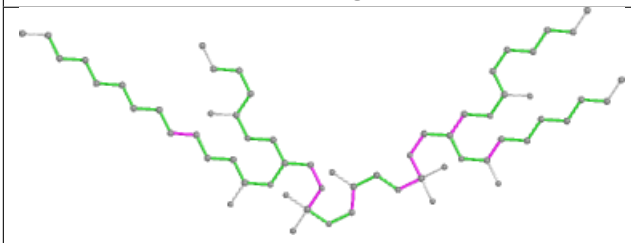
Ligand CDL 1a 101



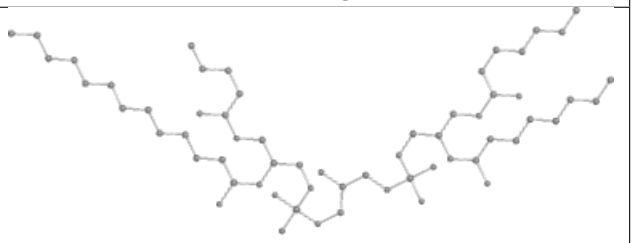
Bond lengths



Bond angles

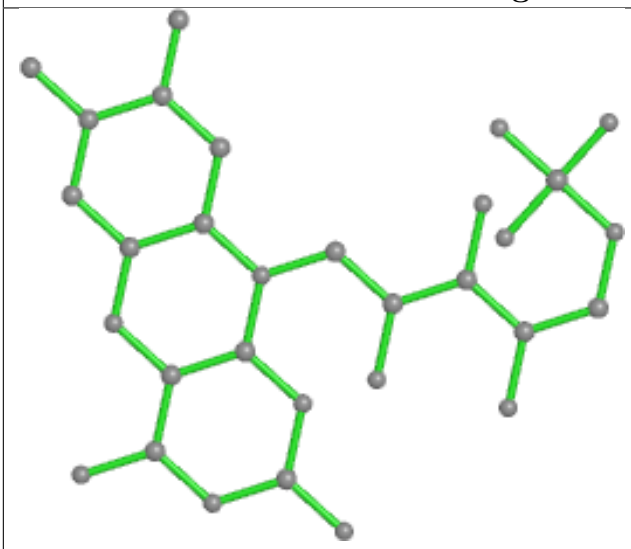


Torsions

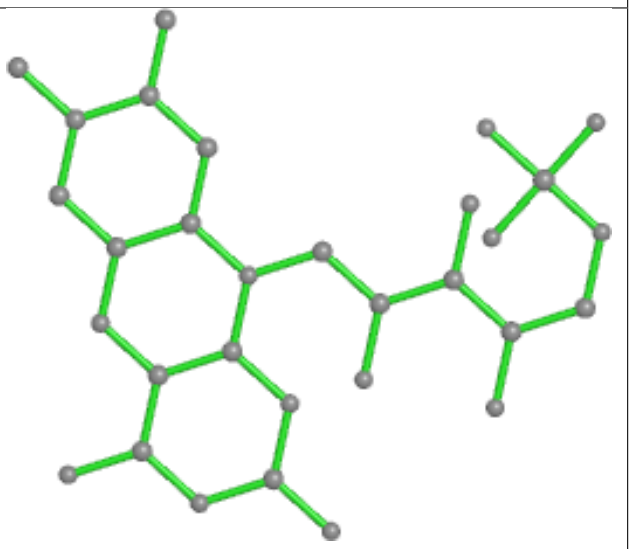


Rings

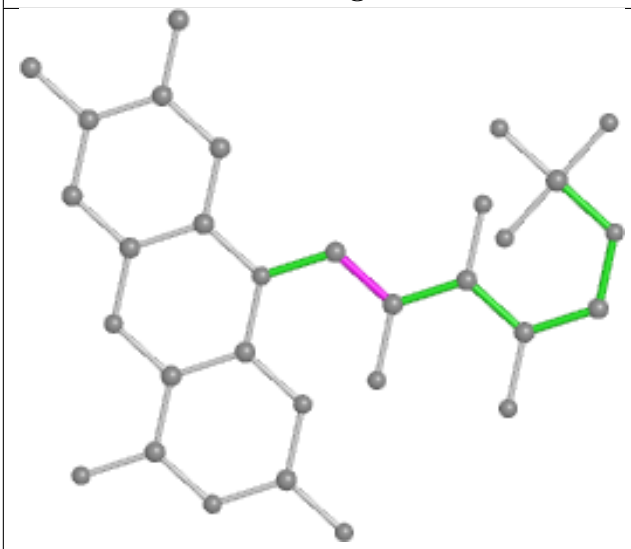
Ligand FMN 1F 501



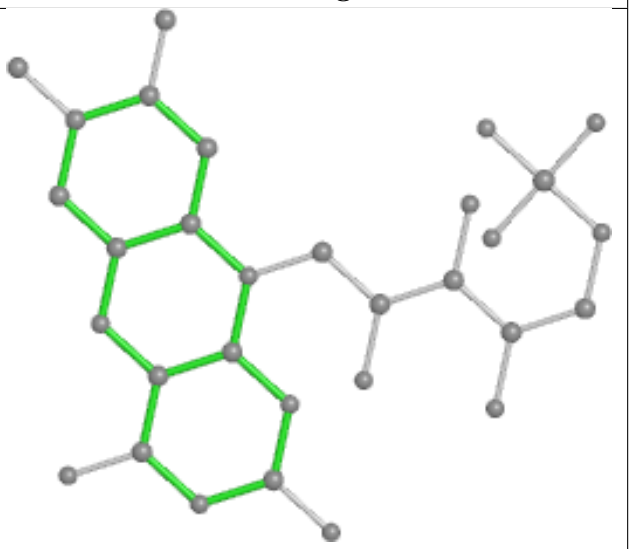
Bond lengths



Bond angles

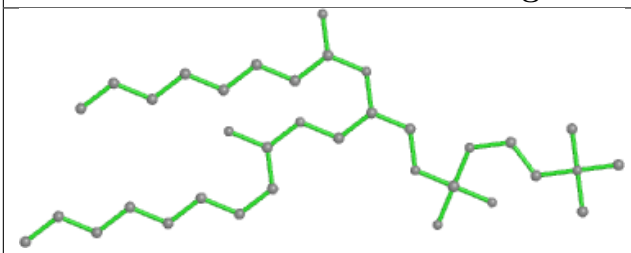


Torsions

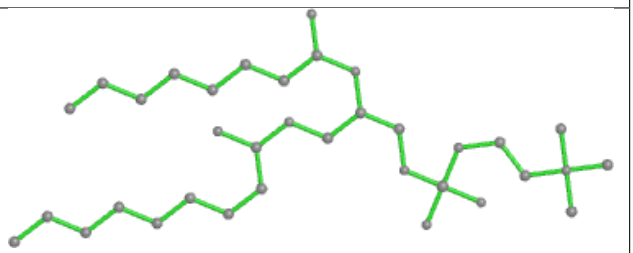


Rings

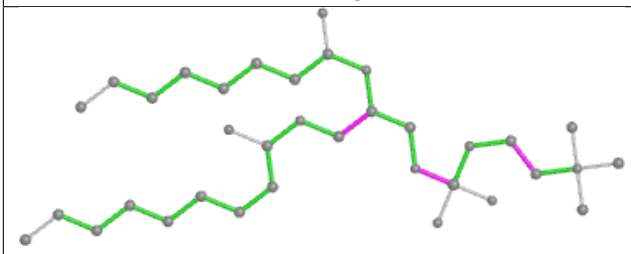
Ligand PC1 1J 201



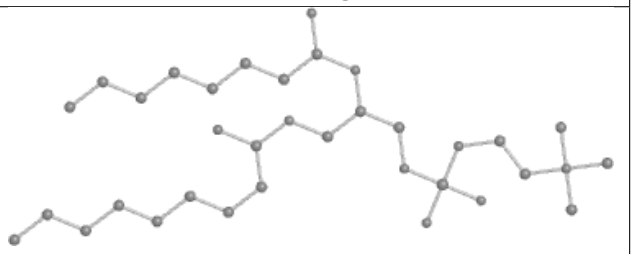
Bond lengths



Bond angles

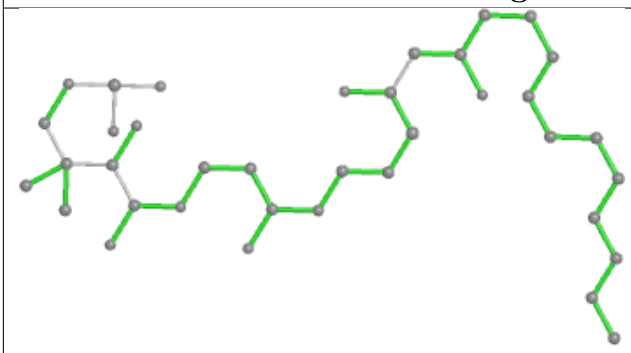


Torsions

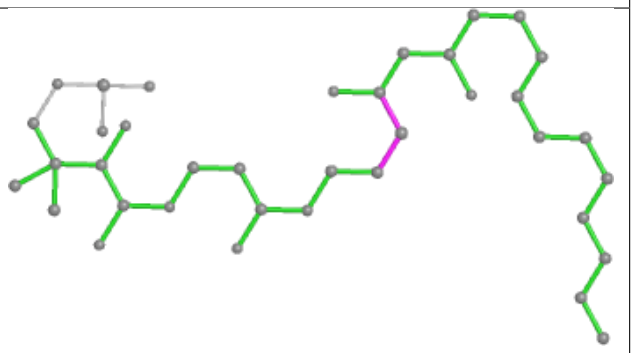


Rings

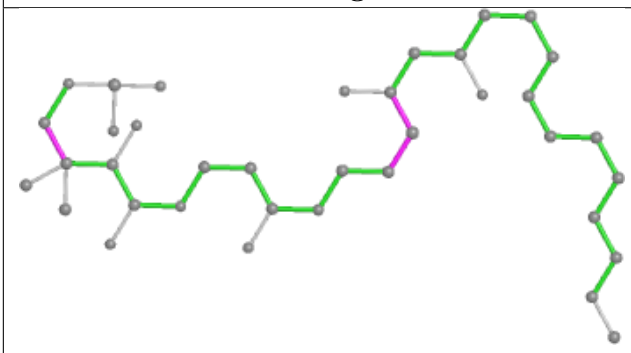
Ligand EHZ 1W 201



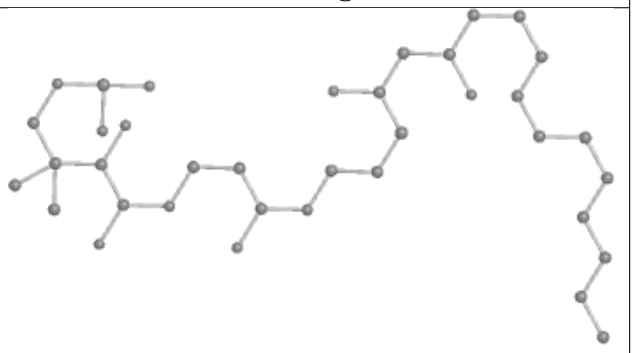
Bond lengths



Bond angles

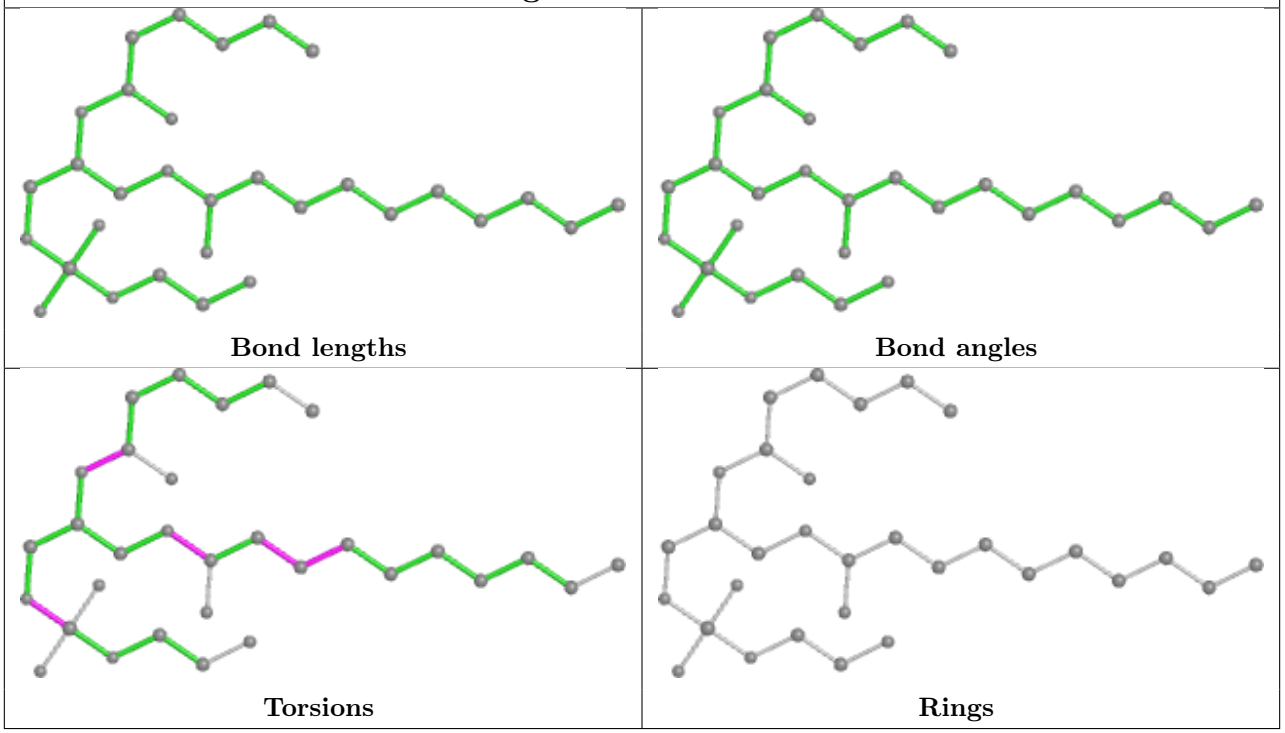


Torsions

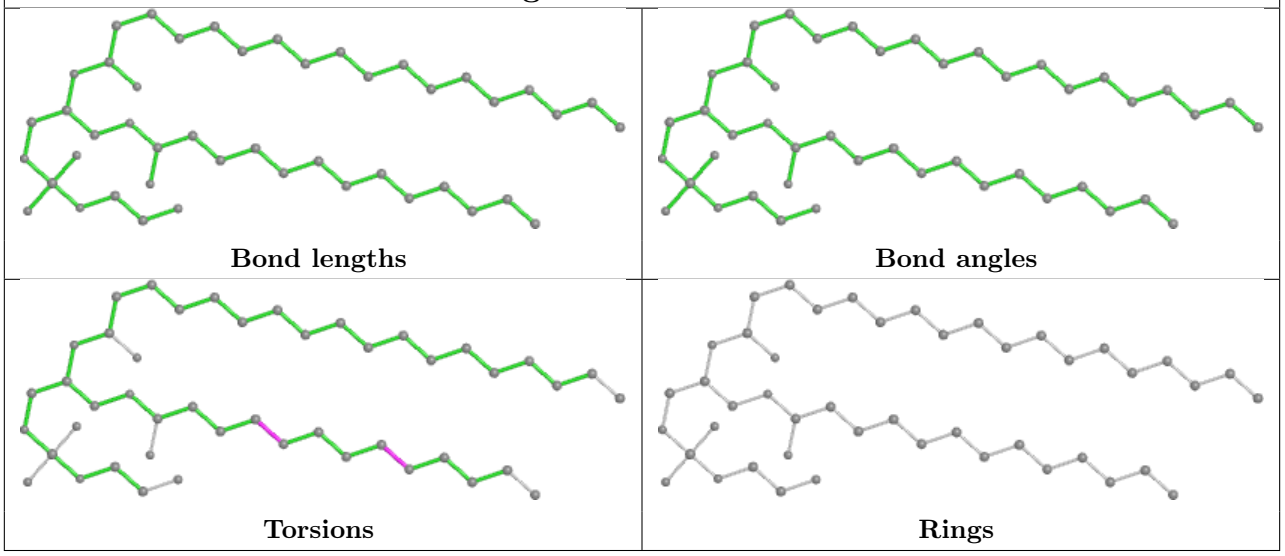


Rings

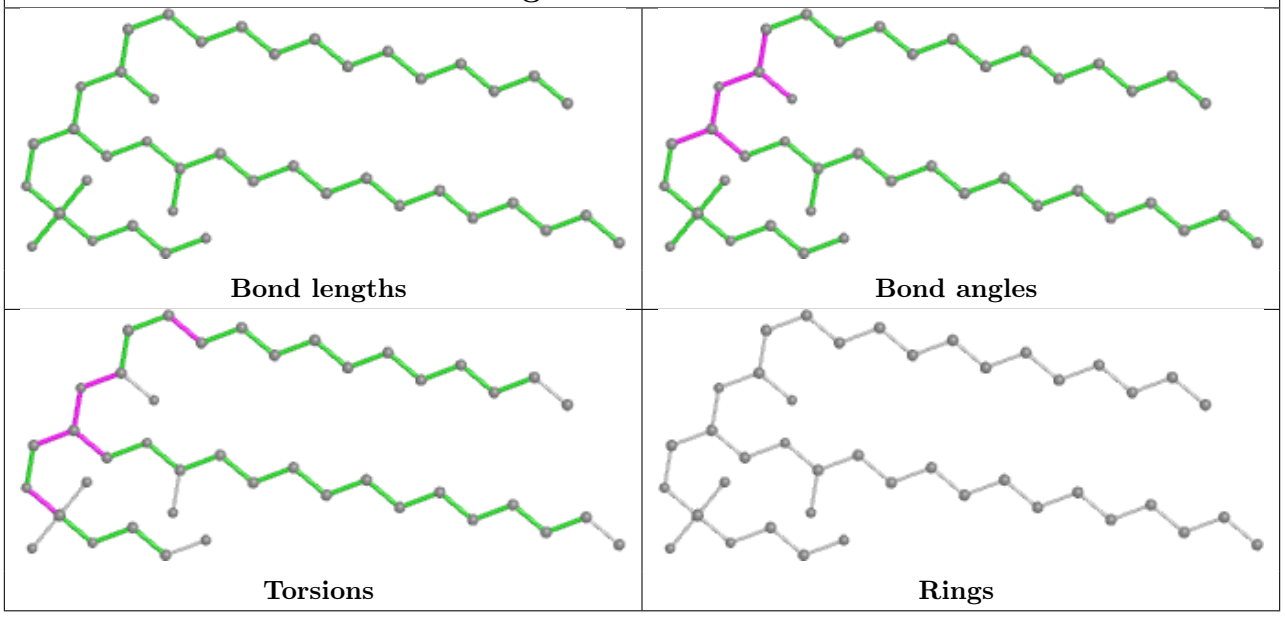
Ligand 3PE 1L 703



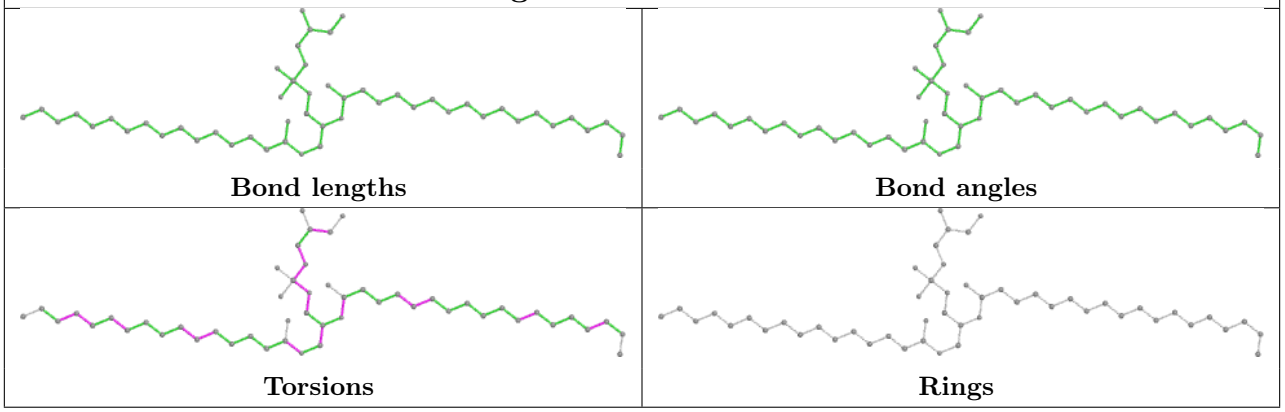
Ligand 3PE 1L 702



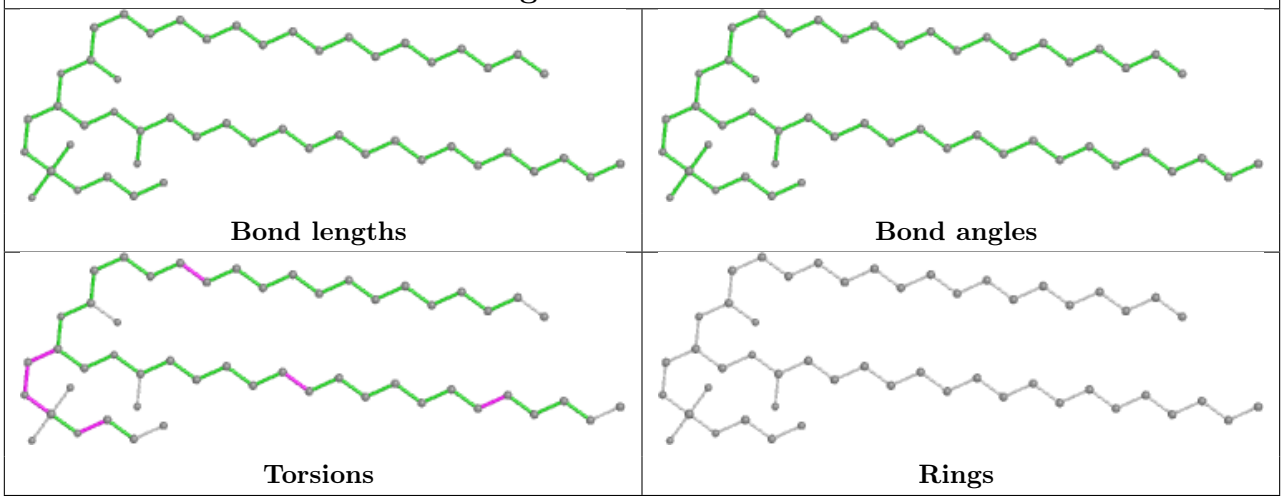
Ligand 3PE 1L 704



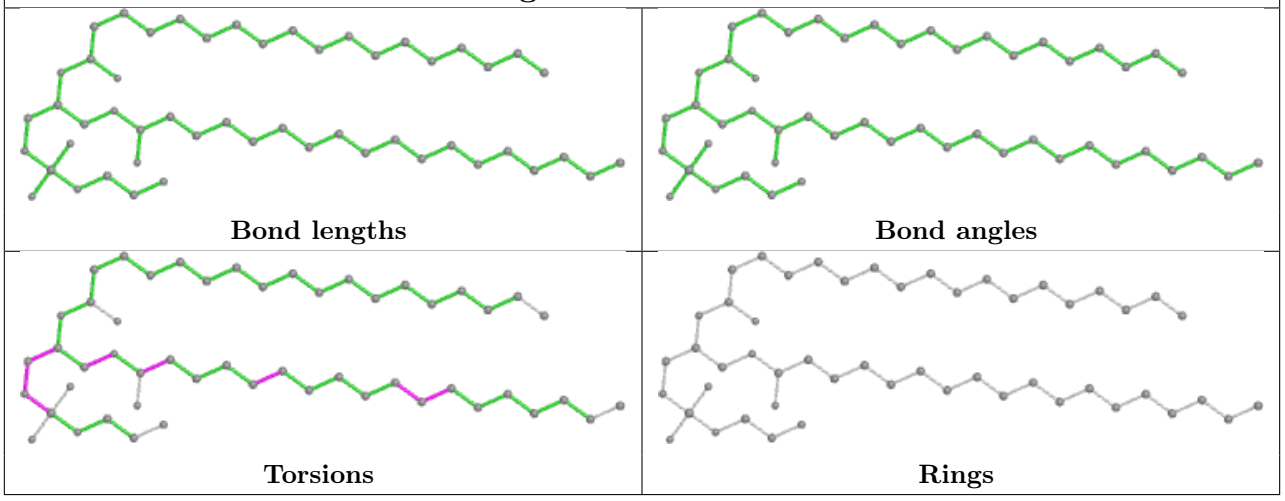
Ligand PGT 1M 501



Ligand 3PE 1Y 201



Ligand 3PE 1N 401



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	1
43	1r	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	3.33
1	1r	1:ALA	C	2:SER	N	2.79

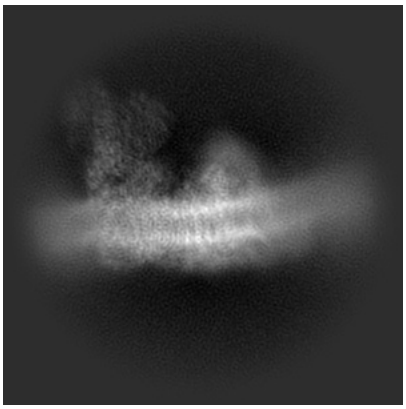
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42170. These allow visual inspection of the internal detail of the map and identification of artifacts.

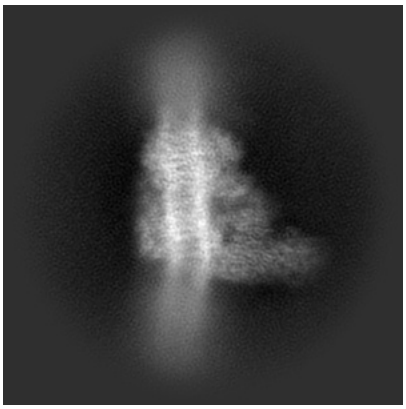
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

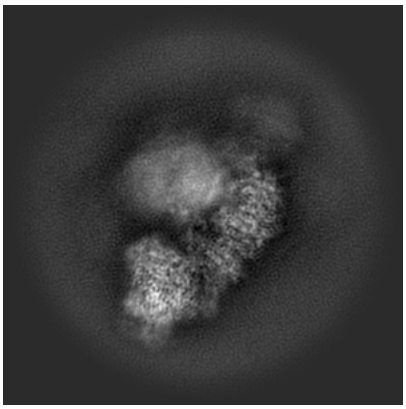
6.1.1 Primary map



X

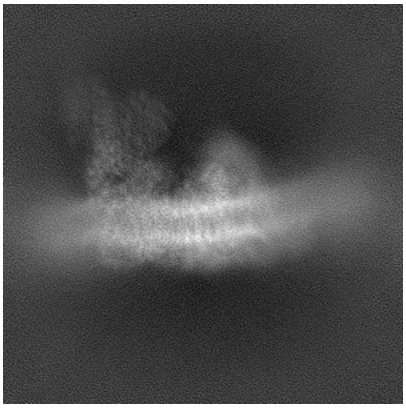


Y

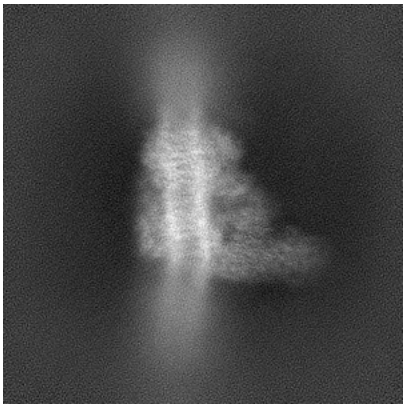


Z

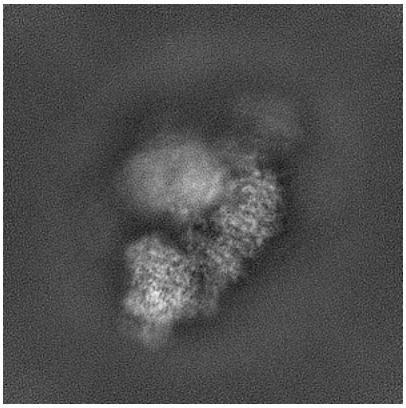
6.1.2 Raw map



X



Y

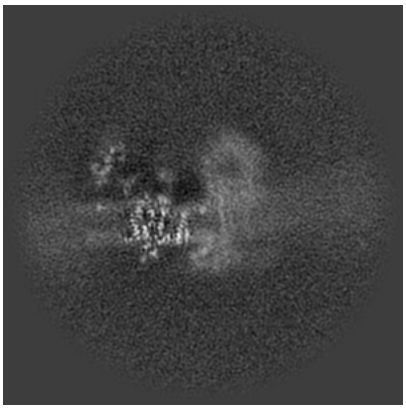


Z

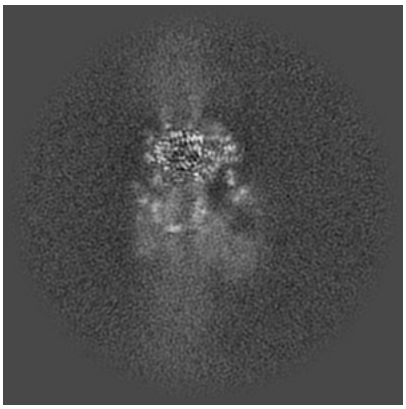
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

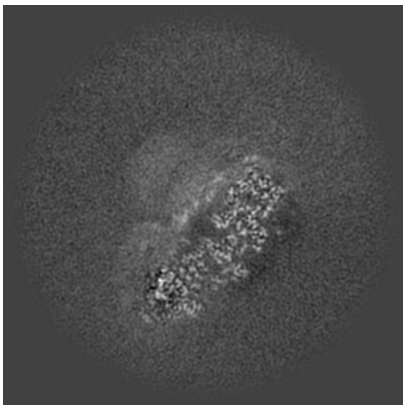
6.2.1 Primary map



X Index: 160



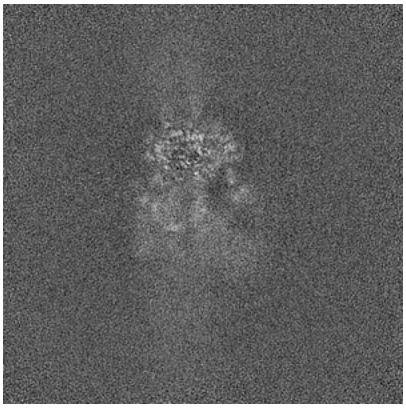
Y Index: 160



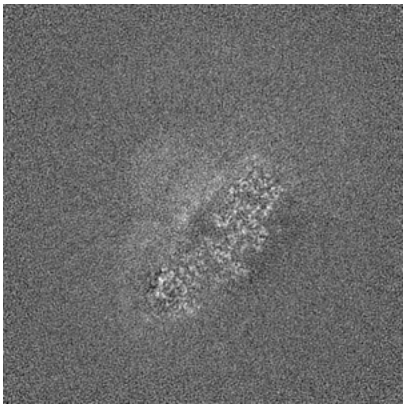
Z Index: 160

6.2.2 Raw map

X Index: 160



Y Index: 160

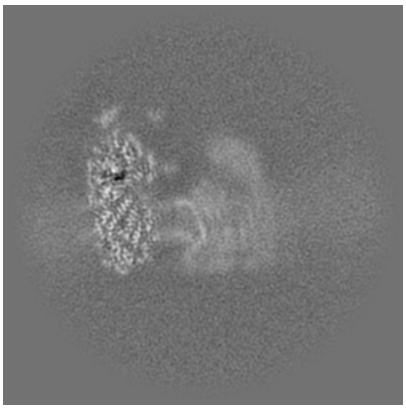


Z Index: 160

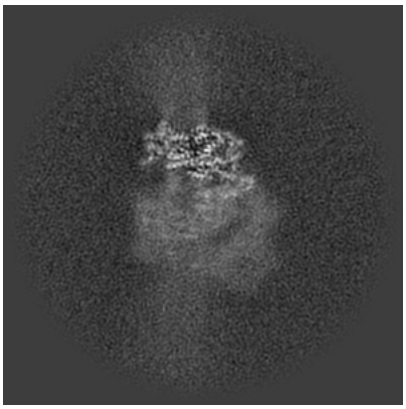
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

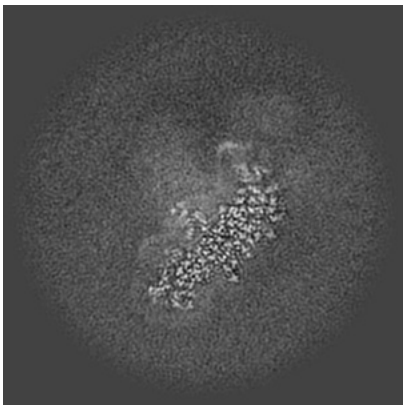
6.3.1 Primary map



X Index: 140

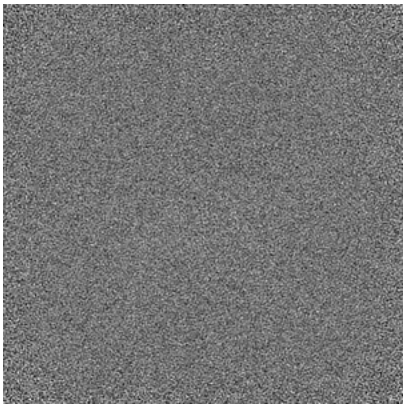


Y Index: 172

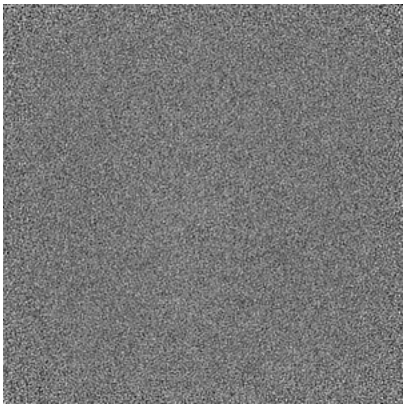


Z Index: 134

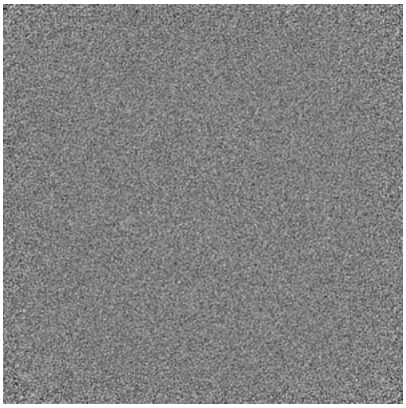
6.3.2 Raw map



X Index: 0



Y Index: 0

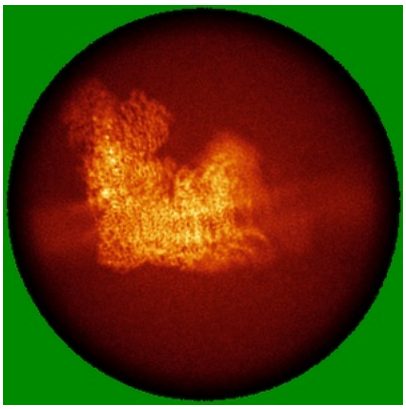


Z Index: 0

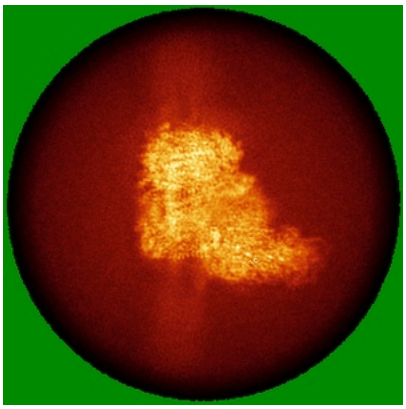
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

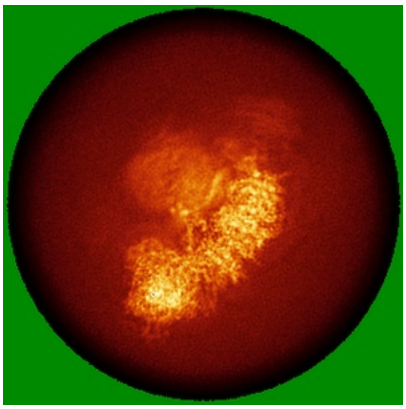
6.4.1 Primary map



X

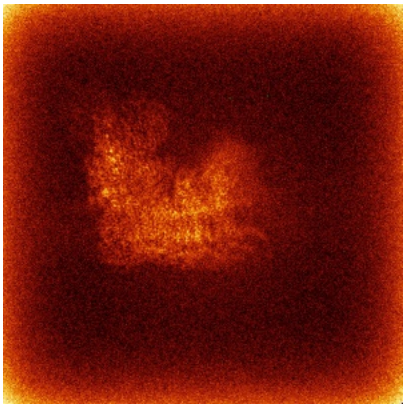


Y

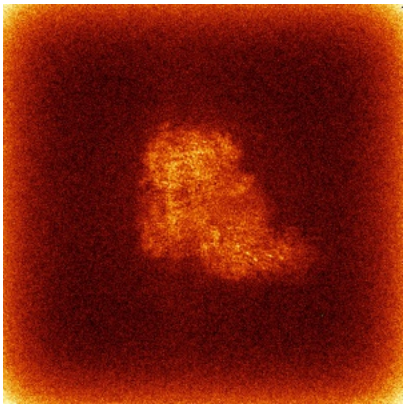


Z

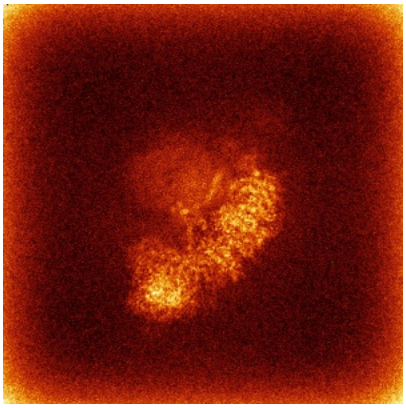
6.4.2 Raw map



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

X Y Z

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

6.5.2 Raw map

X Y Z

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.

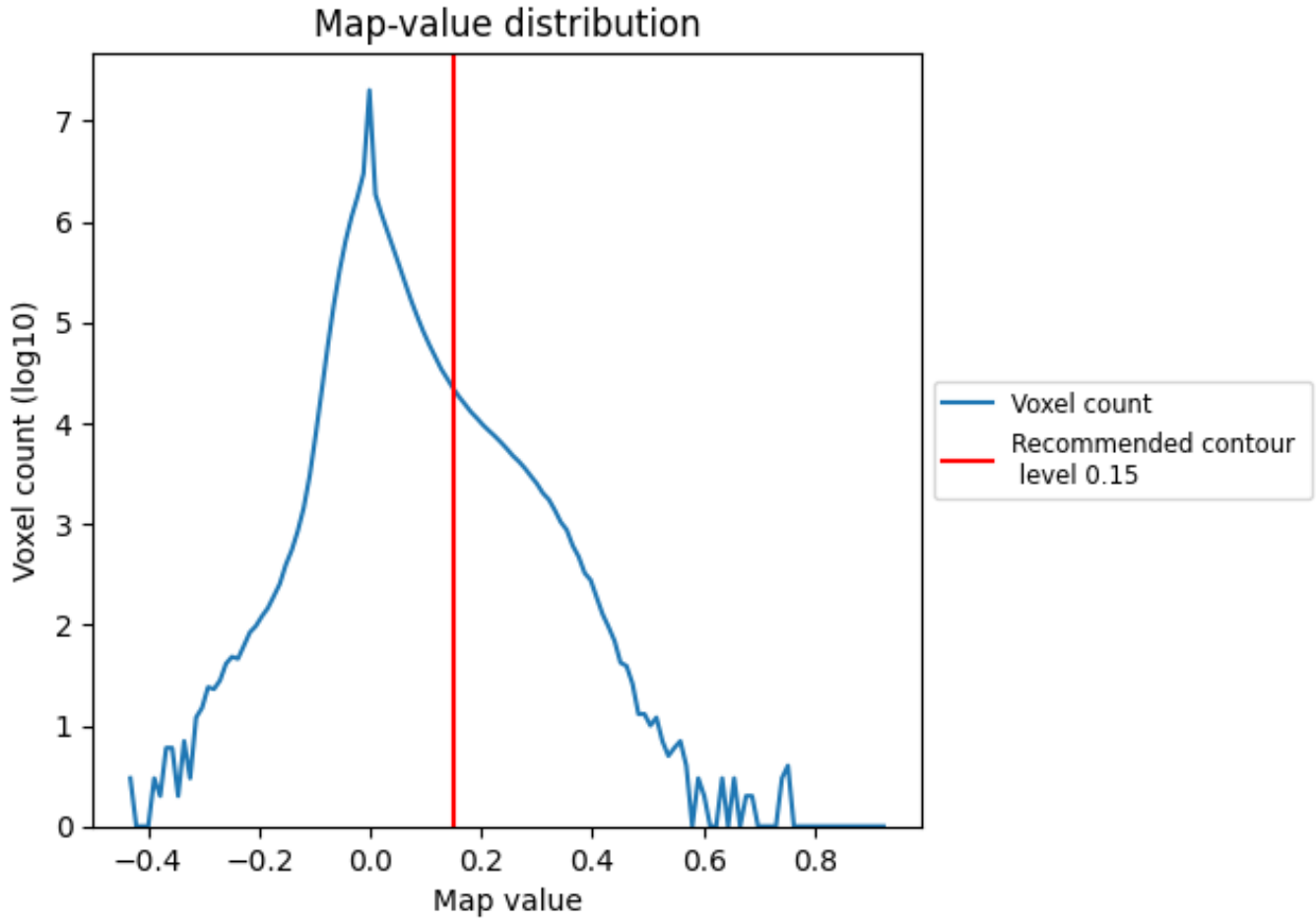
6.6 Mask visualisation (i)

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

7 Map analysis

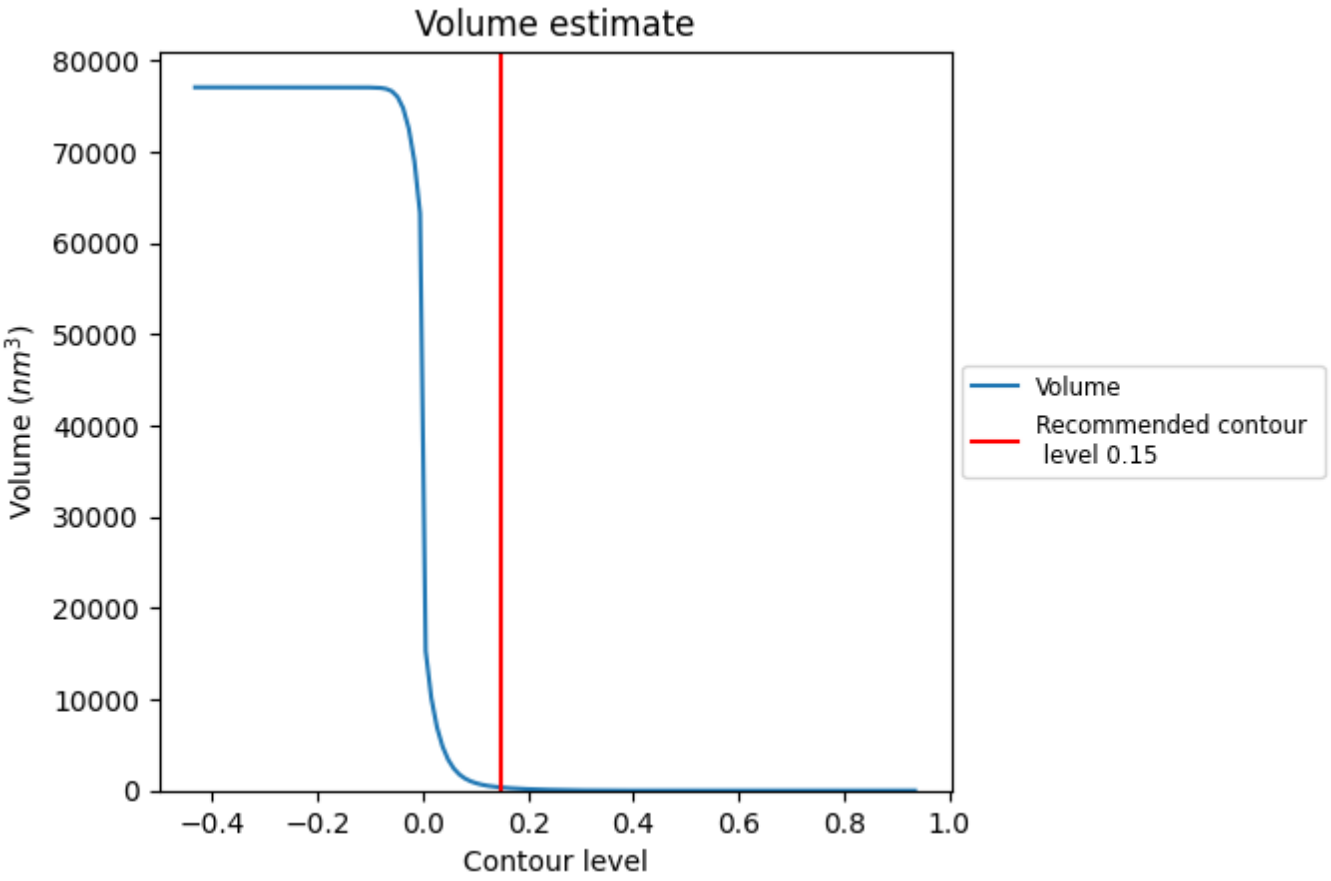
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

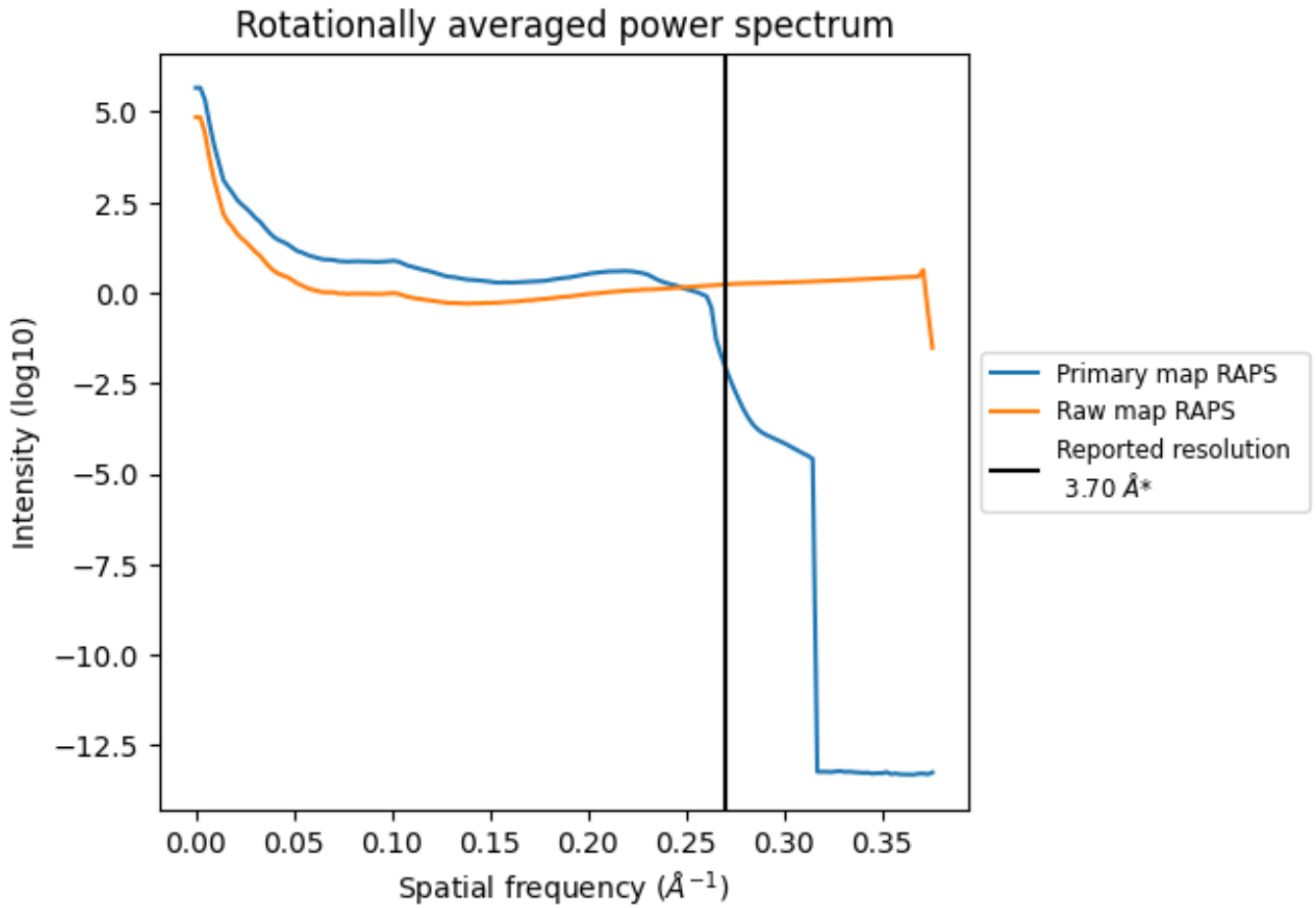
7.2 Volume estimate (i)



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 304 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)

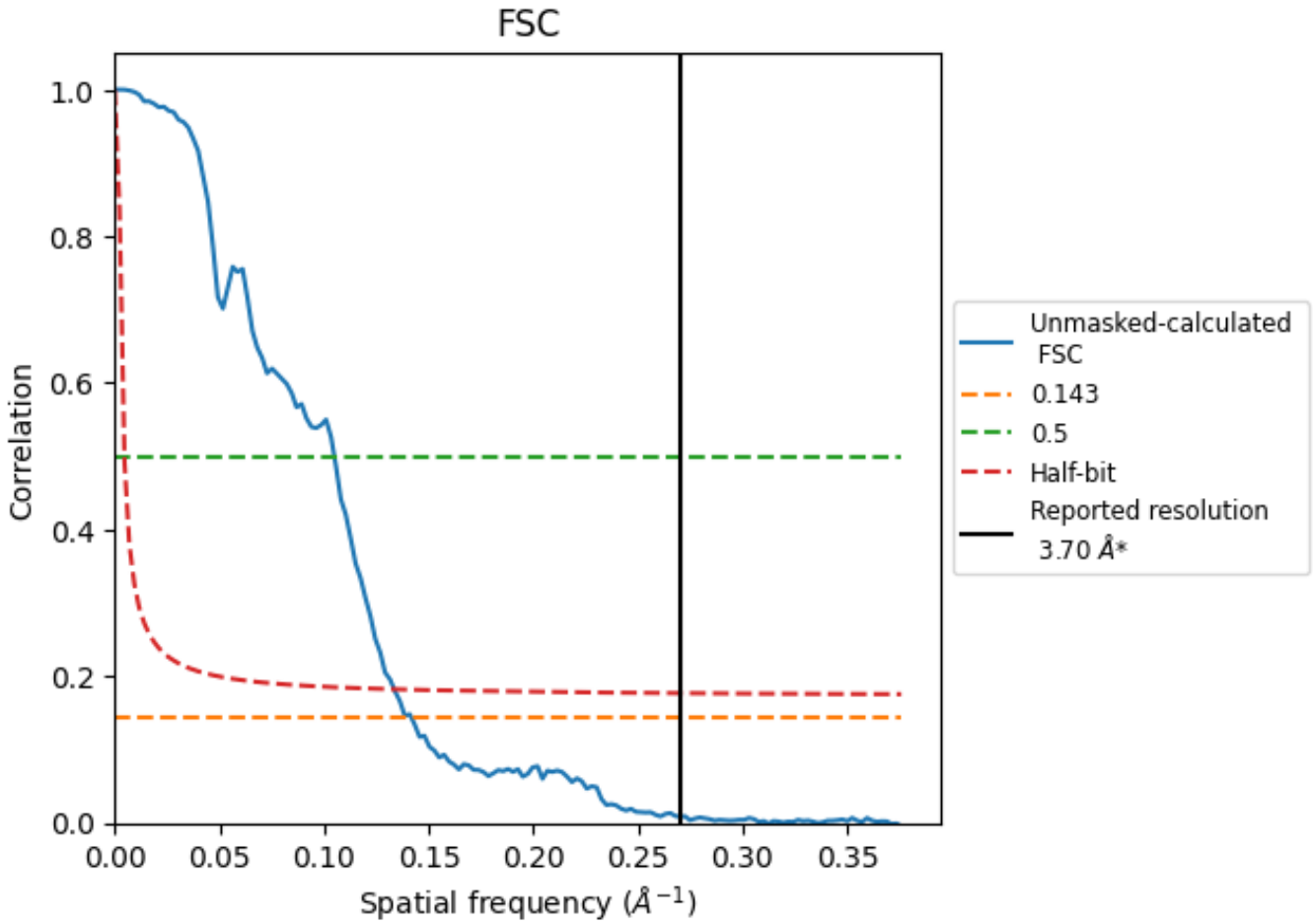


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

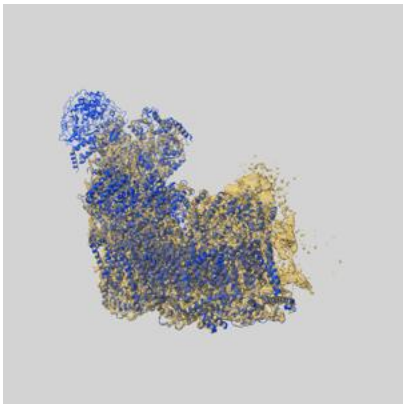
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.05	9.53	7.49

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

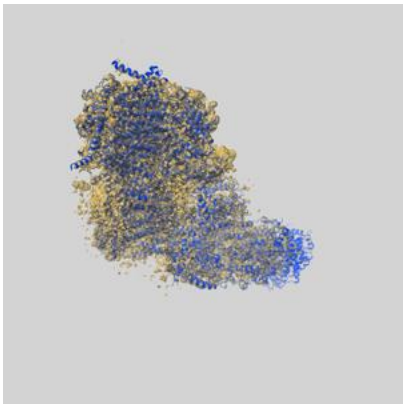
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42170 and PDB model 8UET. Per-residue inclusion information can be found in section 3 on page 21.

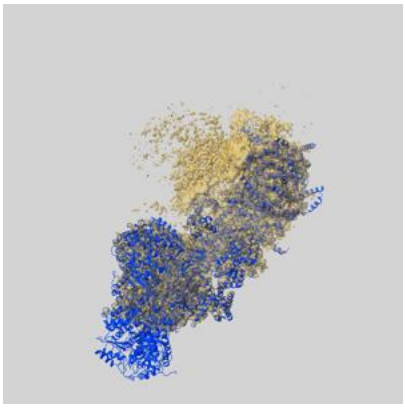
9.1 Map-model overlay



X



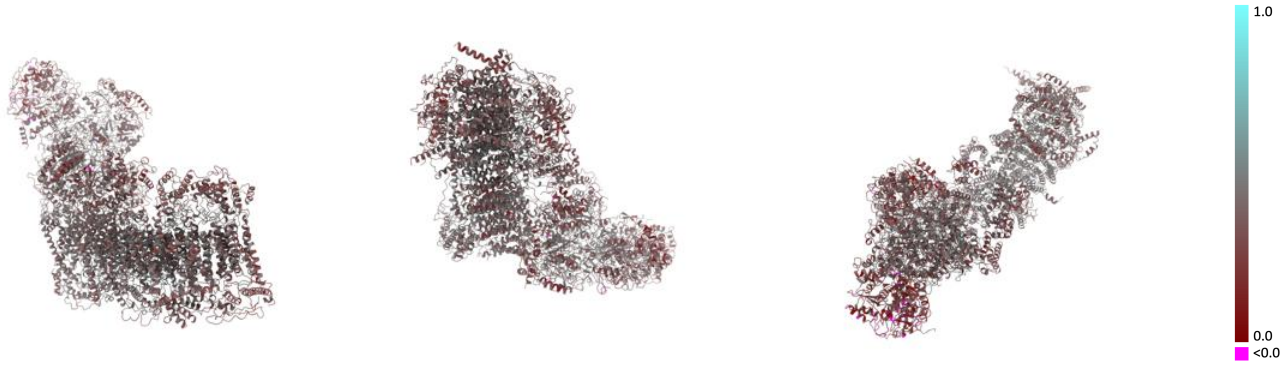
Y



Z

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.

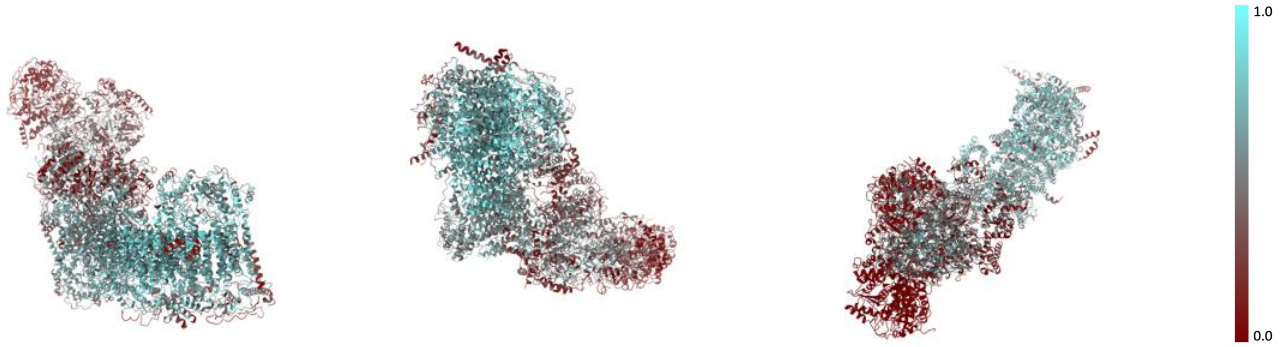
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

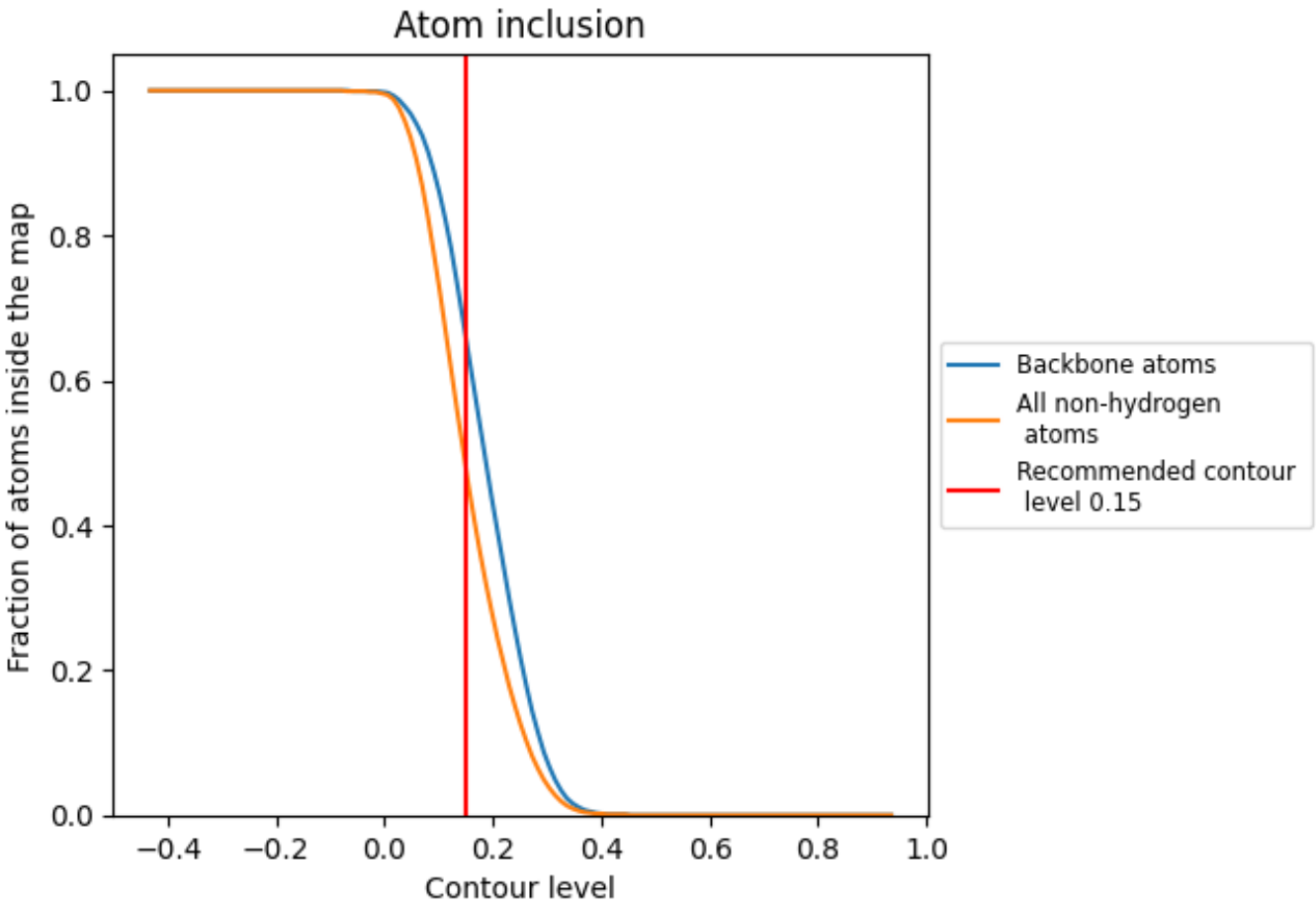
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 66% of all backbone atoms, 48% 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	0.4800	0.3770
1A	0.4830	0.4010
1B	0.5470	0.4180
1C	0.3960	0.4030
1D	0.4800	0.3900
1E	0.0280	0.2870
1F	0.0360	0.2590
1G	0.2840	0.3580
1H	0.6170	0.4070
1I	0.5820	0.4160
1J	0.5090	0.3870
1K	0.6140	0.4060
1L	0.7190	0.4070
1M	0.7590	0.4370
1N	0.6800	0.4280
1O	0.3880	0.3560
1P	0.2990	0.3370
1Q	0.3150	0.3830
1R	0.2950	0.4120
1S	0.1410	0.2900
1T	0.2340	0.2780
1U	0.6150	0.3370
1V	0.2060	0.3380
1W	0.3060	0.3340
1X	0.5480	0.4050
1Y	0.6740	0.3790
1Z	0.5480	0.4150
1a	0.6110	0.4090
1b	0.5370	0.4110
1c	0.4680	0.3690
1d	0.6670	0.4240
1e	0.5960	0.4280
1f	0.4620	0.3840
1g	0.6020	0.3950
1h	0.6730	0.4090

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Chain	Atom inclusion	Q-score
1i	0.3890	0.3470
1j	0.5240	0.3740
1k	0.5120	0.3590
1l	0.6540	0.3980
1m	0.7090	0.3890
1n	0.6720	0.3670
1o	0.5030	0.3170
1p	0.6070	0.3830
1q	0.4470	0.4090
1r	0.3790	0.4020
1s	0.0000	0.2520