wwPDB EM Validation Summary Report (i)

Aug 4, 2026 – 08:28 PM EDT

PDB ID	:	8UER / pdb_00008uer
EMDB ID	:	EMD-42168
Title	:	In-situ complex I with Q10 (State-gamma)
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-10-02
Resolution	:	3.50 Å(reported)

This is a 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 (i) 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 (1)) were used in the production of this report:

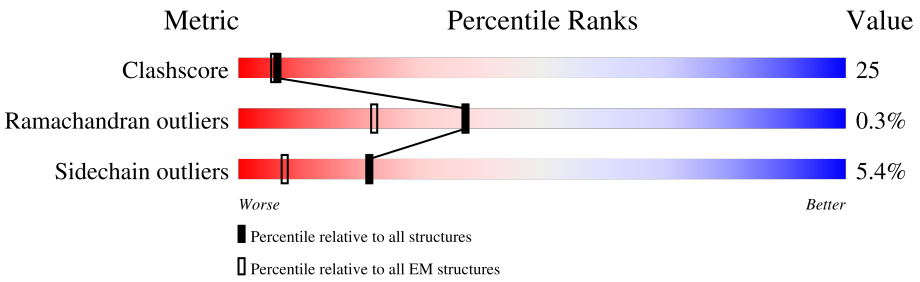
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

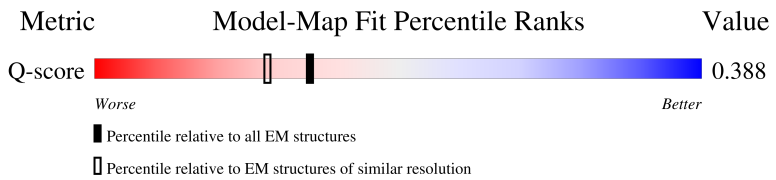
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	43%, 45%, 50%, •
2	1B	255	8%, 33%, 25%, •, 39%
3	1C	264	11%, 52%, 25%, •, 21%
4	1D	476	17%, 51%, 36%, •, 10%

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Mol	Chain	Length	Quality of chain
5	1E	249	47% 45% 40% 14%
6	1F	464	52% 52% 39% 7%
7	1G	727	13% 55% 39%
8	1H	318	16% 50% 46%
9	1I	239	5% 35% 36% 26%
10	1J	175	50% 52% 45%
11	1K	98	39% 40% 54% 6%
12	1L	606	92% 36% 61%
13	1M	459	56% 36% 59%
14	1N	347	19% 42% 55%
15	1O	357	68% 40% 48% 10%
16	1P	377	28% 56% 32% 9%
17	1Q	175	21% 48% 25% 26%
18	1R	123	15% 50% 28% 22%
19	1S	99	22% 39% 45% 12%
20	1T	156	45% 22% 31% 46%
20	1U	156	55% 18% 32% 45%
21	1V	116	38% 52% 45%
22	1W	128	41% 51% 36% 10%
23	1X	172	28% 61% 37%
24	1Y	141	66% 48% 49%
25	1Z	144	23% 54% 42%
26	1a	70	16% 67% 30%
27	1b	84	37% 68% 27%
28	1c	76	38% 32% 30% 36%

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Mol	Chain	Length	Quality of chain
29	1d	123	30% 61% 34%
30	1e	106	23% 53% 38% 7%
31	1f	135	31% 17% 23% 58%
32	1g	154	60% 22% 40% 35%
33	1h	189	48% 40% 31% 27%
34	1i	128	99% 36% 62%
35	1j	105	68% 36% 29% 32%
36	1k	98	83% 34% 48% 17%
37	1l	186	82% 40% 41% 16%
38	1m	129	93% 45% 50% 5%
39	1n	179	94% 39% 54%
40	1o	137	89% 35% 50% 11%
41	1p	176	97% 51% 47%
42	1q	145	17% 67% 30%
43	1r	114	14% 57% 25% 16%
44	1s	471	7% 5% 5% 90%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1F	502	-	-	X	-
45	SF4	1G	801	-	-	X	-
45	SF4	1G	802	-	-	X	-
45	SF4	1I	201	-	-	X	-
45	SF4	1I	202	-	-	X	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

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

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

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

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

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

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

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

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

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

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

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

8, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

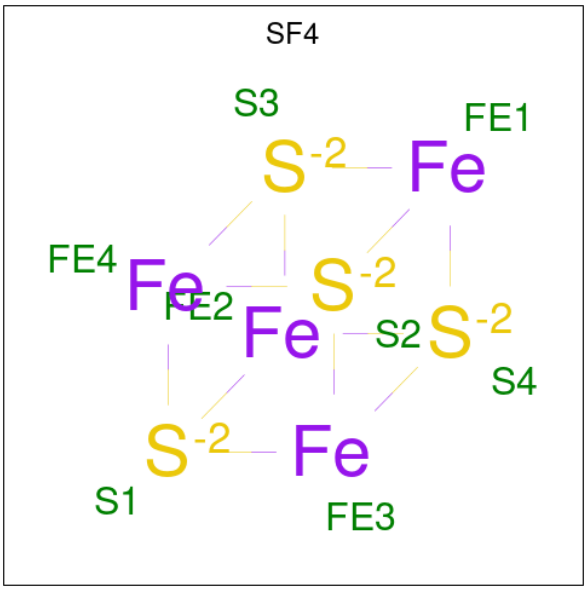
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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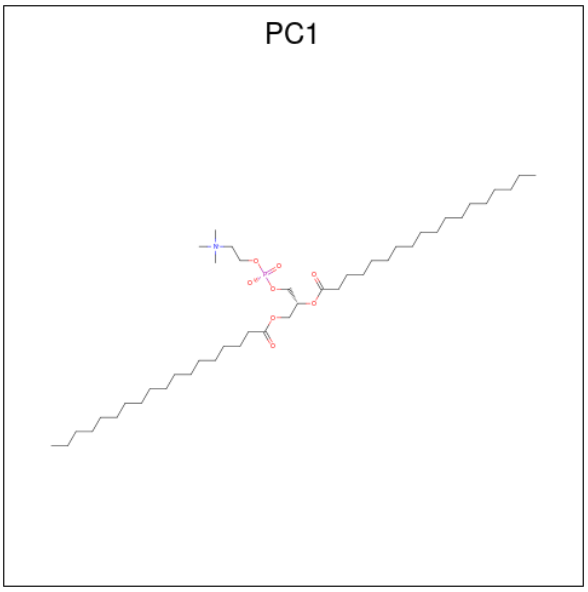
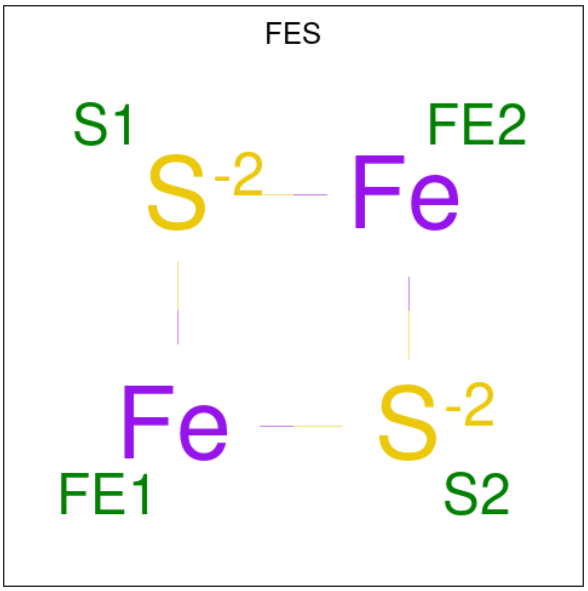
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1I	1	8	4	4	0
			Total	Fe	S	
45	1I	1	8	4	4	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



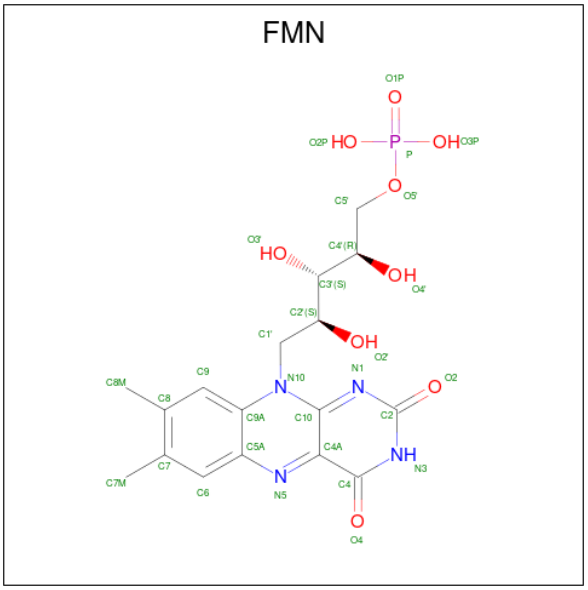
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	1B	1	34	24	1	8	1	0
			Total	C	N	O	P	
46	1Y	1	35	25	1	8	1	0
			Total	C	N	O	P	
46	1d	1	39	29	1	8	1	0
			Total	C	N	O	P	
46	1h	1	34	24	1	8	1	0
			Total	C	N	O	P	
46	1m	1	46	36	1	8	1	0
			Total	C	N	O	P	
46	1q	1	48	38	1	8	1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

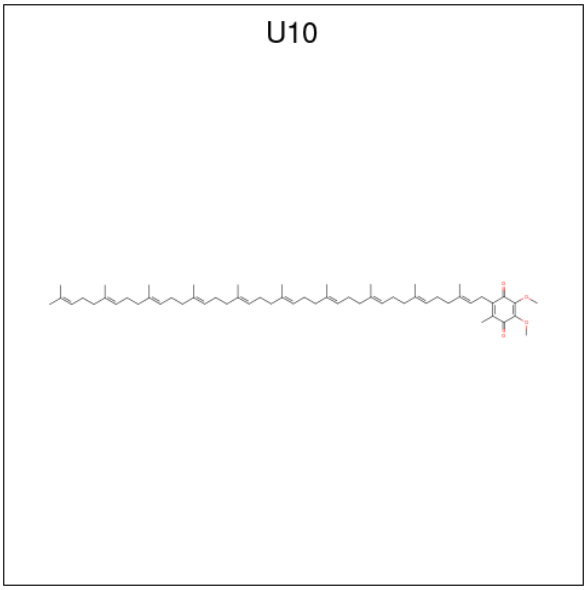


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	1F	1	31	17	4	9	1	0

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

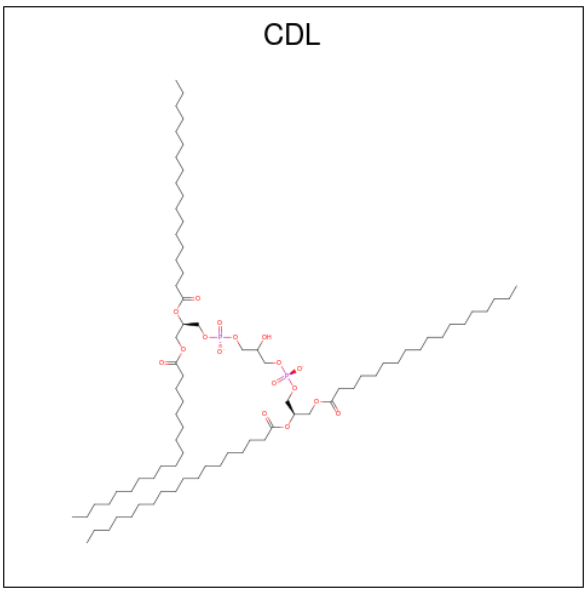
Mol	Chain	Residues	Atoms			AltConf
			Total	K		
49	1G	1	1	1		0

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



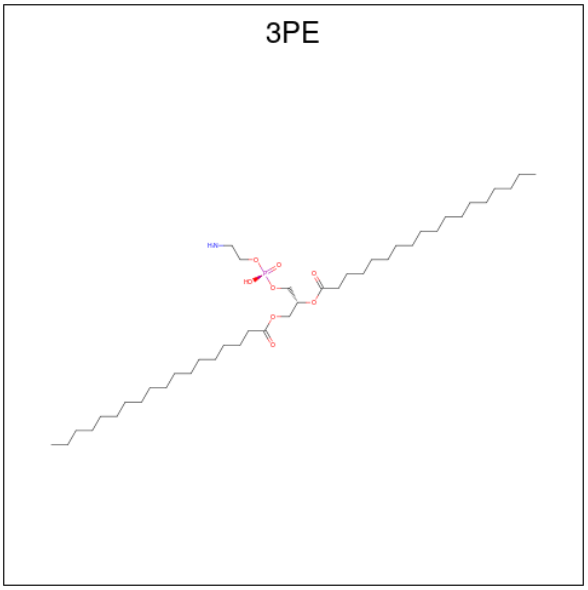
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	1H	1	63	59	4	0

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



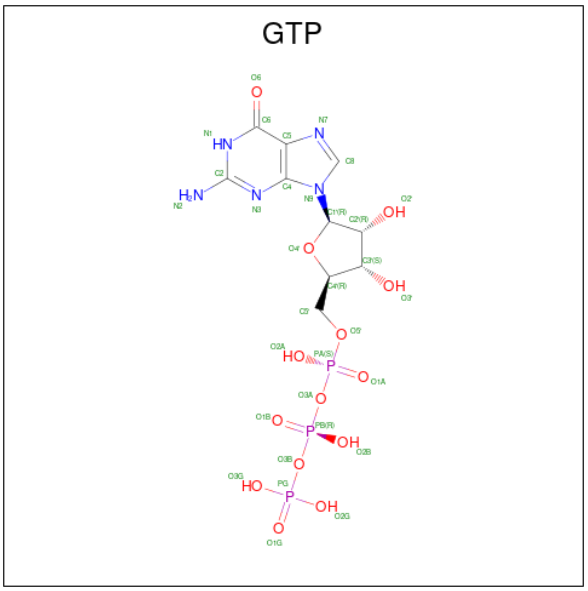
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total 51	C 32	O 17	P 2	0
51	1O	1	Total 67	C 48	O 17	P 2	0
51	1a	1	Total 61	C 42	O 17	P 2	0

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
52	1N	1	Total 38	C 28	N 1	O 8	P 1	0
52	1Y	1	Total 35	C 25	N 1	O 8	P 1	0
52	1g	1	Total 51	C 41	N 1	O 8	P 1	0
52	1n	1	Total 42	C 32	N 1	O 8	P 1	0

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

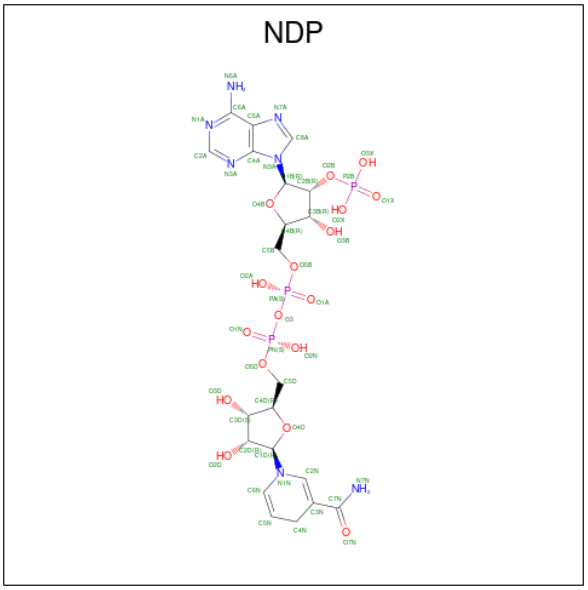


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	1O	1	32	10	5	14	3	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

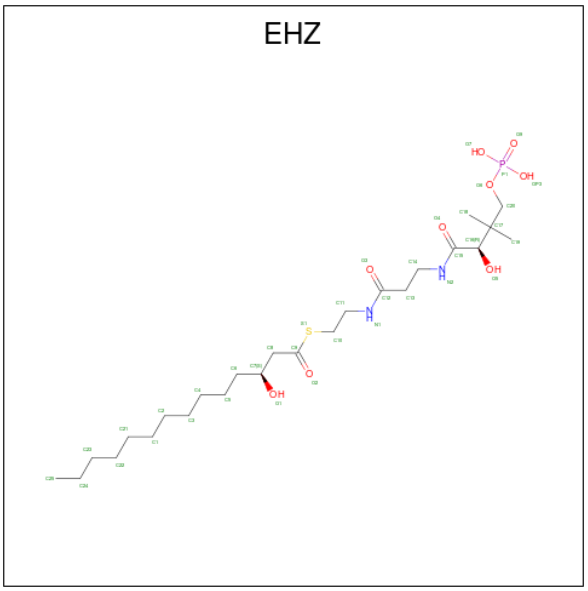


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	1P	1	48	21	7	17	3	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

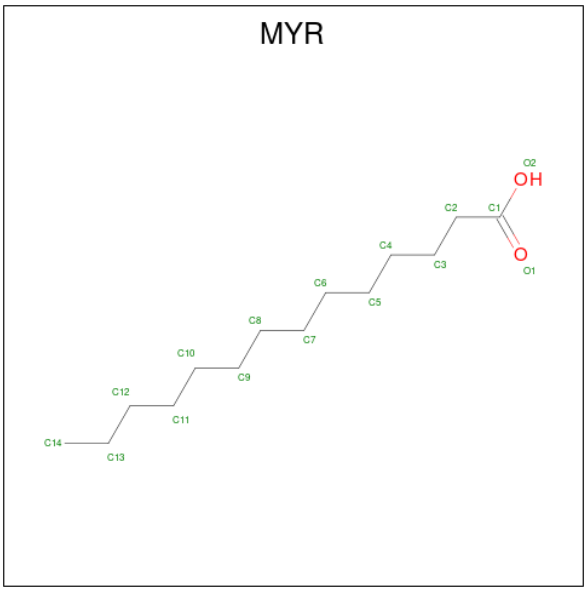
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
56	1R	1	1	1	0

- Molecule 57 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



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

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



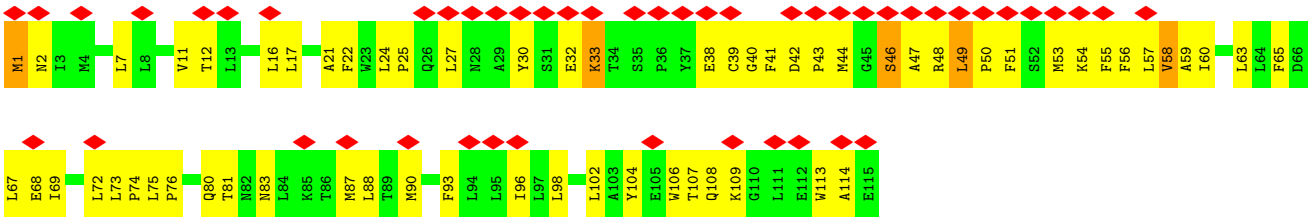
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	1l	1	15	14	1	0

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.

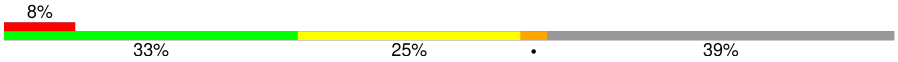
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

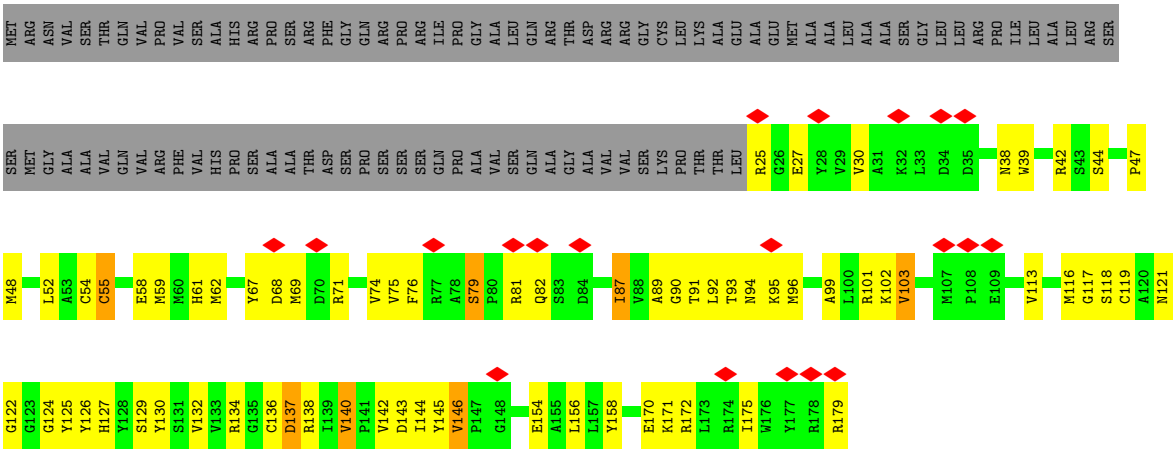
Chain 1A:



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

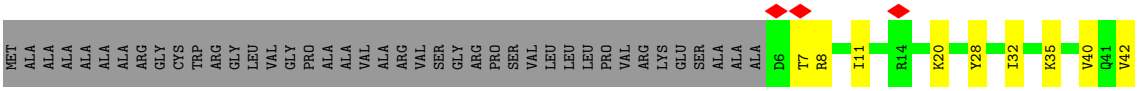
Chain 1B:

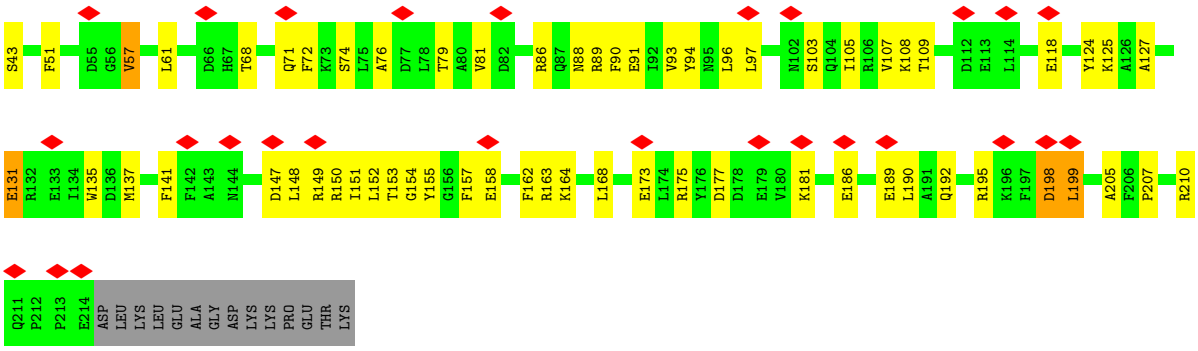




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

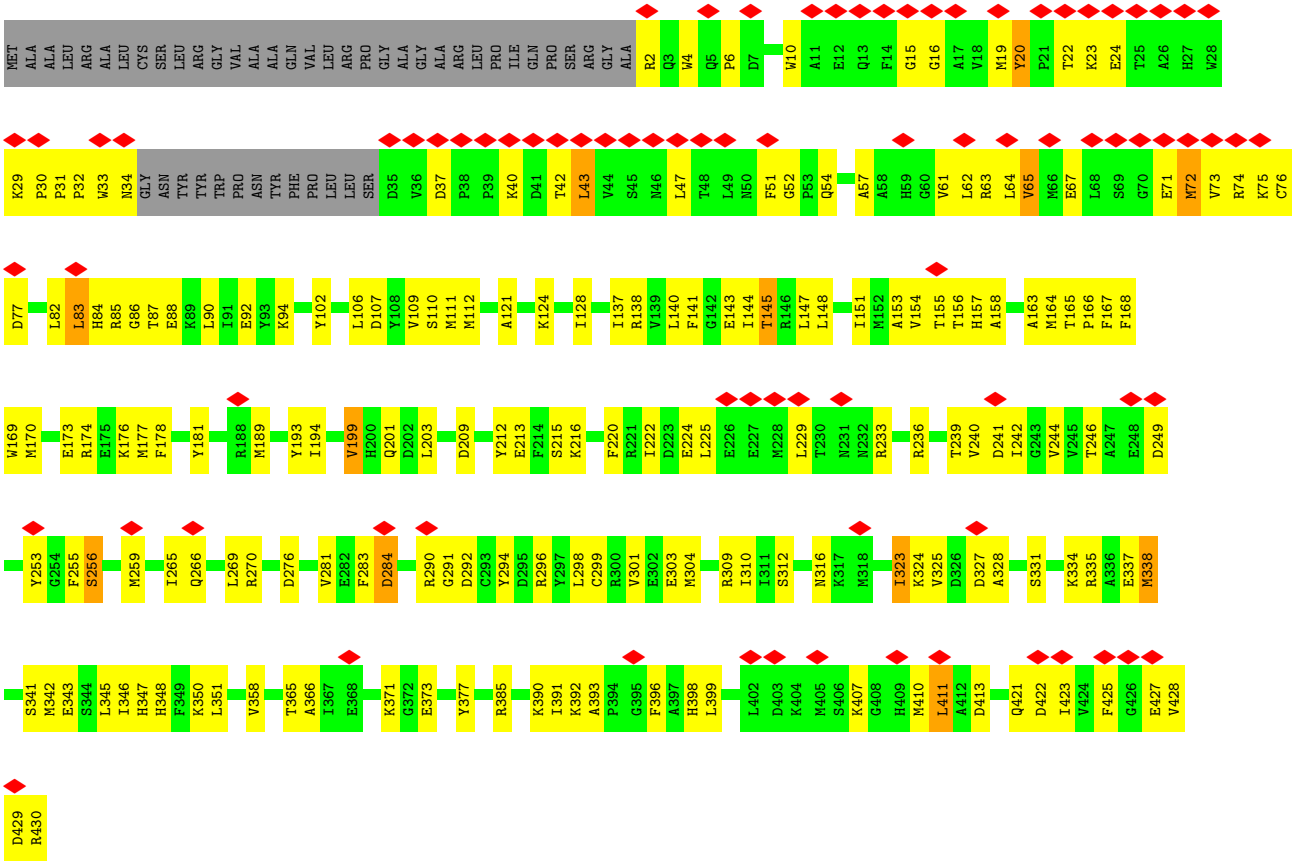
Chain 1C:





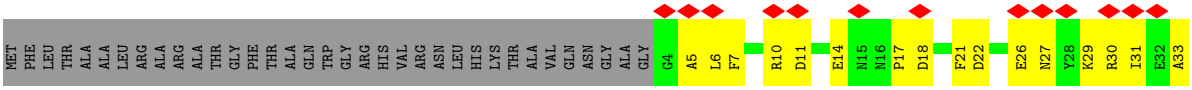
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

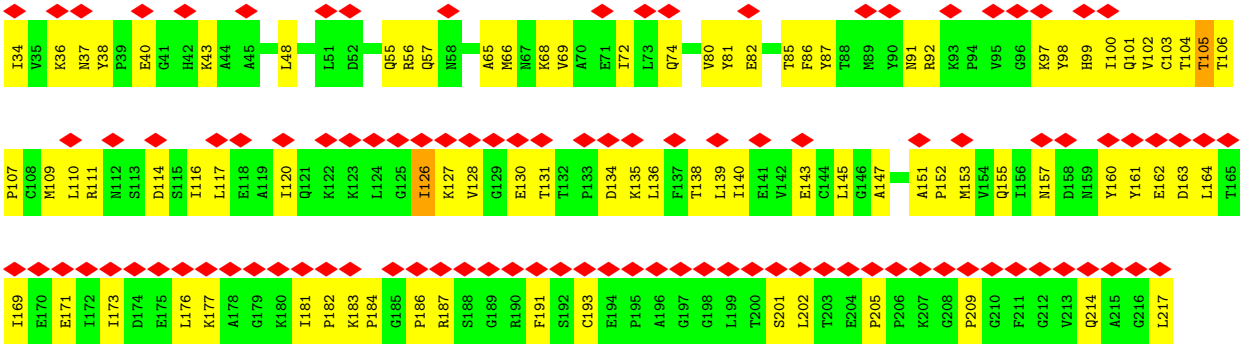
Chain 1D:



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

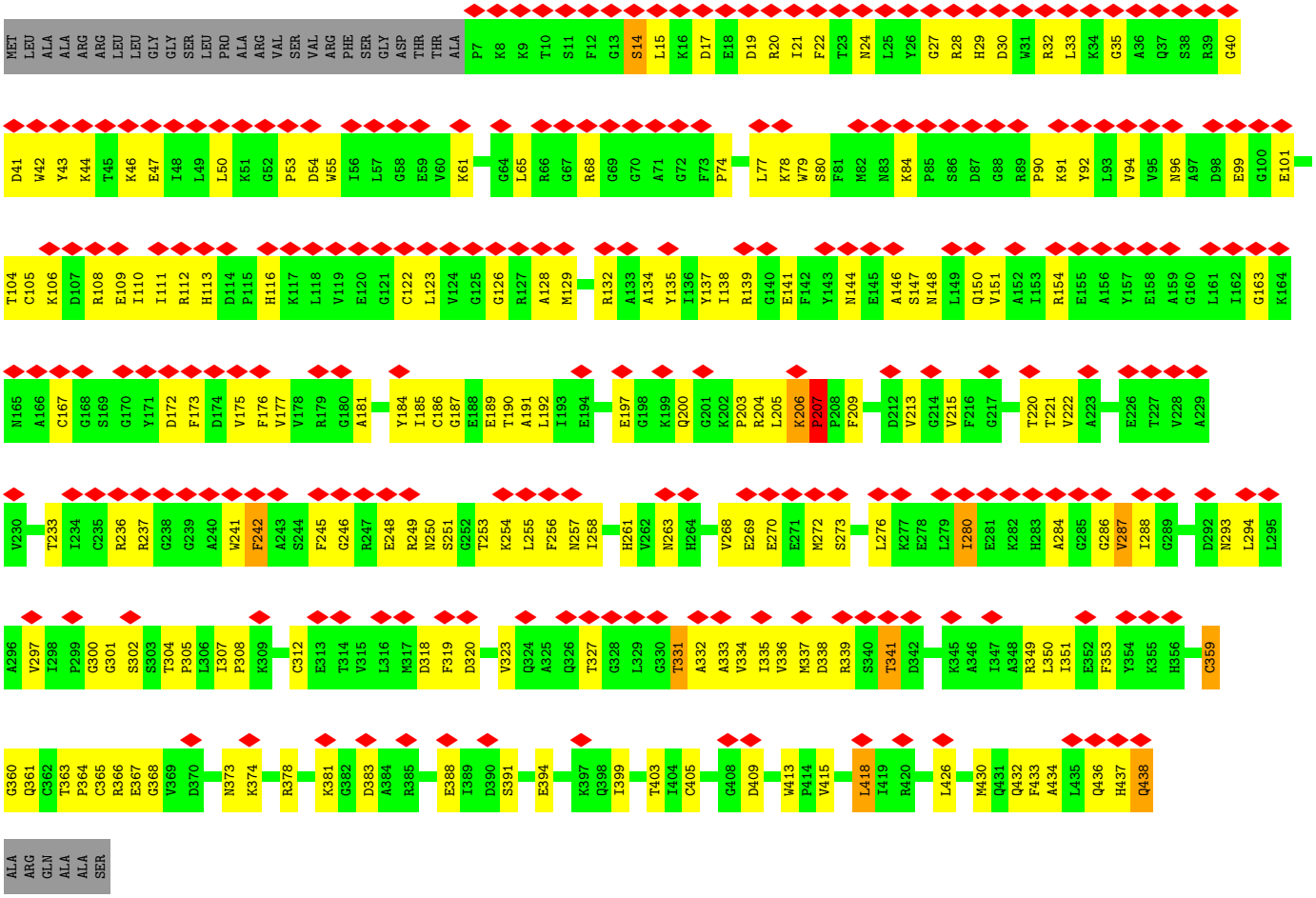
Chain 1E:





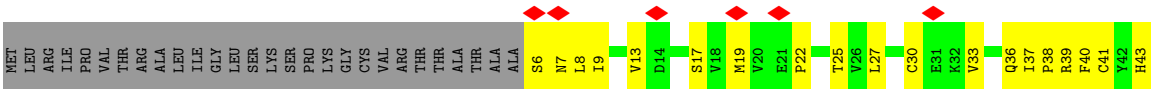
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

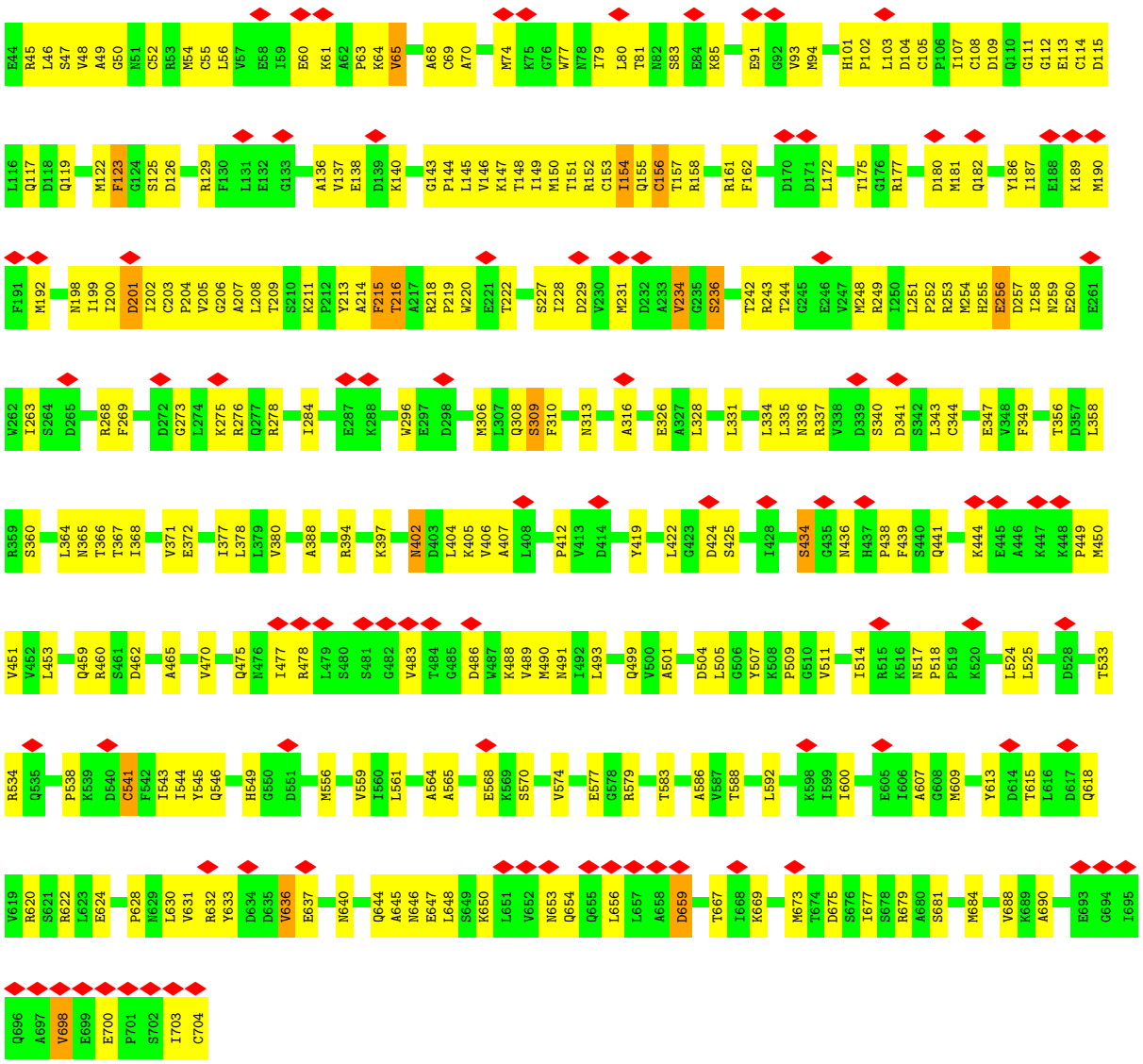
Chain 1F:



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

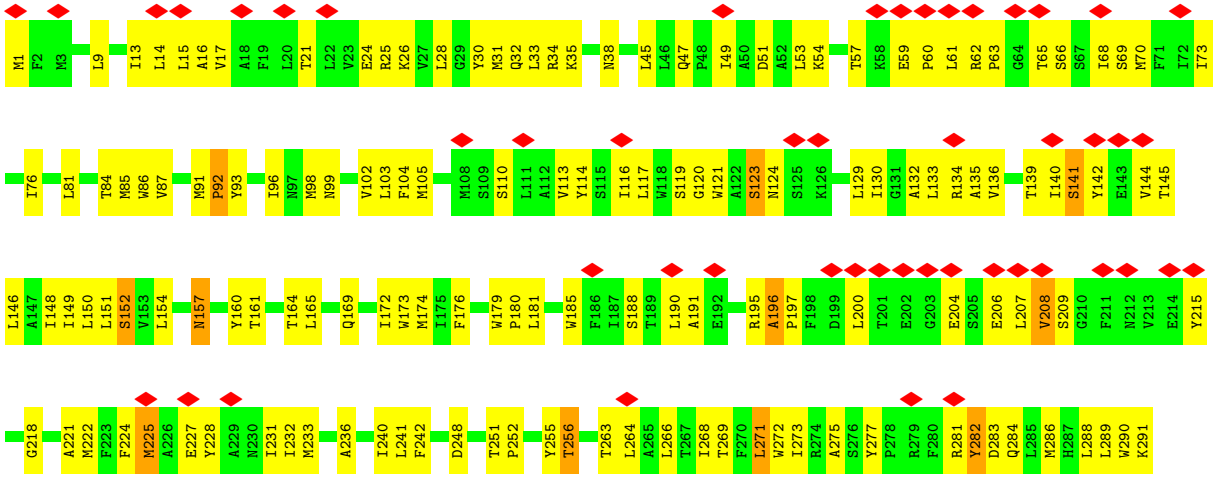
Chain 1G:

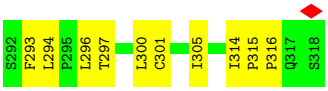




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

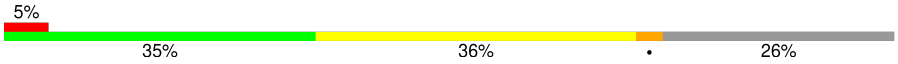
Chain 1H:

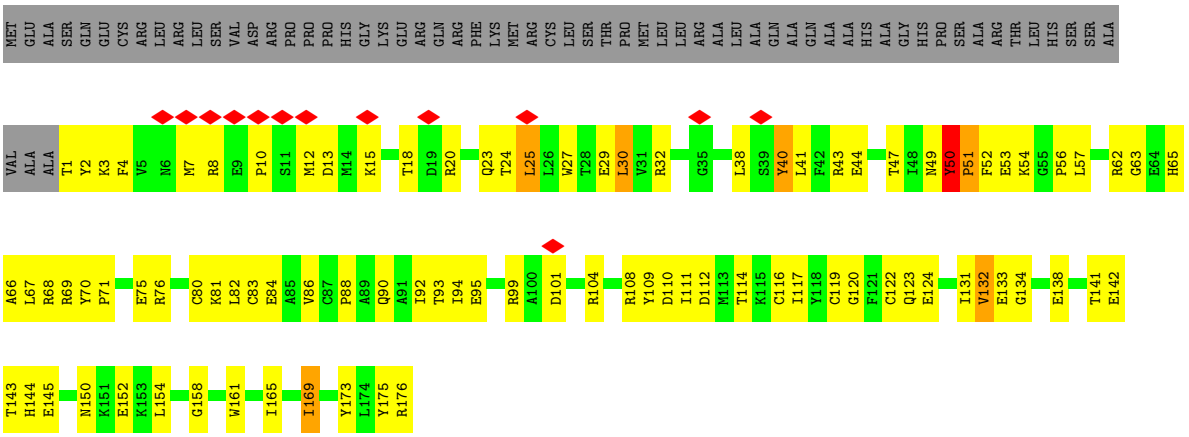




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

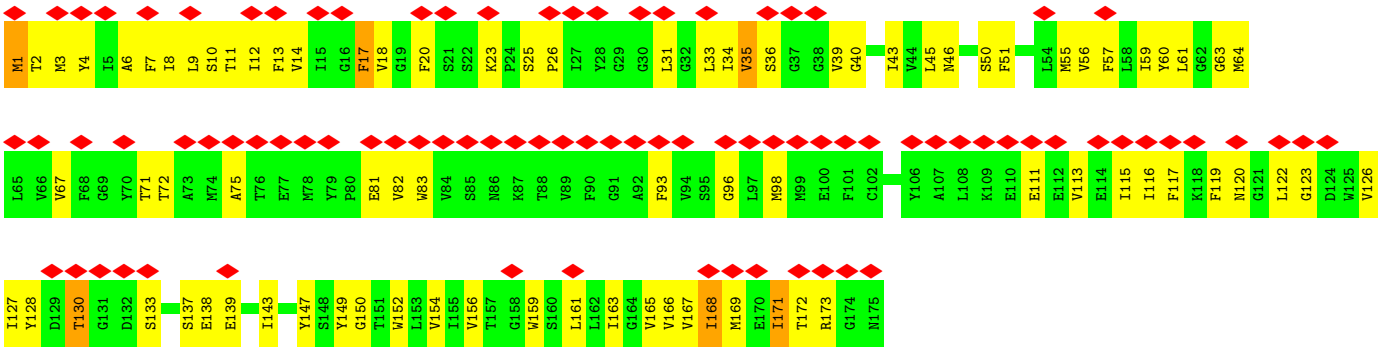
Chain 1I:





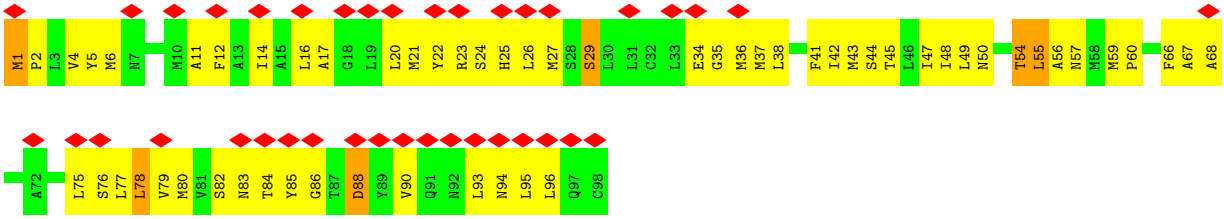
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:



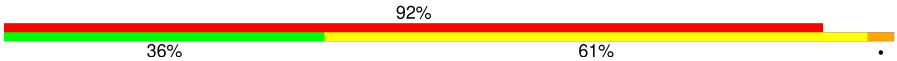
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:



M1 N2 P3 F4 A5 S6 L7 T8 L9 T10 T11 L12 I13 I14 L15 T16 I17 P18 I19 M20 M21 S22 N23 S24 N25 I26 Y27 K28 T29 N30 L31 Y32 P33 N34 Y35 V36 K37 T38 T39 V40 S41 Y42 A43 F44 T45 L46 S47 L48 V49 P50 L51 L52 M53 F54 M55 H56 T57 G58 Q59 E60

M61 I62 I63 S64 N65 W66 H67 W68 M69 T70 L71 Q72 T73 V74 E75 L76 S77 L78 S79 F80 K81 M82 D83 Y84 F85 S86 V87 M88 F89 I90 P91 V92 A93 L94 F95 V96 T97 W98 S99 I100 M101 E102 F103 S104 M105 W106 Y107 M108 H109 S110 D111 P112 F113 I114 N115 R116 F117 F118 K119 Y120

L121 V122 L123 F124 L125 I126 T127 M128 M129 I130 L131 V132 T133 A134 N135 N136 L137 F138 Q139 L140 F141 I142 G143 W144 E145 G146 V147 G148 I149 M150 S151 F152 L153 L154 I155 G156 W157 W158 H159 G160 R161 T162 D163 A164 N165 T166 A167 A168 L169 Q170 A171 I172 L173 Y174 N175 R176 I177 G178 D179 I180

G181 F182 V183 L184 S185 M186 A187 W188 F189 L190 T191 H192 S193 N194 A195 W196 D197 L198 Q199 Q200 I201 F202 M203 L204 N205 N206 E207 C208 P209 N210 M211 P212 L213 I214 G215 L216 L217 L218 A219 A220 A221 G222 K223 S224 A225 Q226 F227 G228 L229 H230 P231 W232 L233 P234 S235 A236 M237 E238 G239 P240

T241 P242 V243 S244 A245 L246 L247 H248 S249 S250 T251 M252 V253 V254 A255 G256 V257 F258 L259 L260 I261 R262 F263 Y264 P265 L266 M267 E268 T269 N270 K271 L272 V273 Q274 T275 M276 T277 L278 C279 L280 G281 A282 I283 T284 T285 L286 F287 T288 A289 L290 C291 A292 I293 T294 Q295 N296 D297 T298 K299 K300

I301 V302 A303 F304 S305 T306 S307 S308 Q309 L310 G311 L312 M313 M314 V315 T316 I317 G318 I319 N320 Q321 P322 H323 L324 A325 F326 L327 H328 I329 C330 M331 H332 A333 F334 F335 K336 A337 M338 L339 F340 M341 C342 S343 G344 S345 I346 I347 H348 S349 L350 N351 D352 E353 Q354 D355 I356 R357 K358 M359 G360

G361 L362 Y363 K364 A365 M366 P367 F368 T369 T370 T371 A372 L373 I374 I375 G376 S377 L378 A379 L380 T381 G382 M383 P384 Y385 L386 T387 G388 F389 Y390 S391 K392 D393 L394 I395 I396 E397 A398 V399 N400 M401 S402 Y403 T404 N405 A406 W407 A408 L409 L410 M411 T412 L413 I414 A415 T416 S417 L418 T419 A420

A421 Y422 S423 T424 R425 I426 I427 F428 F429 A430 F431 L432 G433 K434 P435 R436 F437 P438 P439 L440 V441 L442 I443 N444 E445 N446 N447 P448 L449 L450 I451 N452 S453 I454 K455 R456 L457 L458 I459 G460 S461 I462 F463 A464 G465 F466 I467 I468 S469 N470 N471 I472 P473 P474 M475 T476 V477 P478 N479 T480

T481 M482 P483 L484 Y485 M486 K487 M488 T489 A490 L491 I492 V493 T494 I495 M496 G497 F498 M499 L500 A501 L502 E503 L504 N505 N506 T507 T508 Y509 Y510 L511 K512 F513 K514 Y515 P516 S517 Q518 T519 Y520 K521 F522 S523 N524 M525 L526 G527 Y528 Y529 P530 S531 I532 M533 H534 R535 L536 P537 T538 Y539 H540

N541 L542 S543 M544 K547 S548 A549 S550 S551 L552 L553 D554 L555 I556 W557 L558 E559 T560 I561 L562 P563 T566 S567 F568 I569 Q570 M571 K572 M573 S574 I575 M576 V577 S578 N579 Q580 K581 G582 L583 T584 K585 L586 Y587 F588 L589 S590 F591 L592 I593 T594 I595 M596 I597 S598 M599 T600 L601 F602

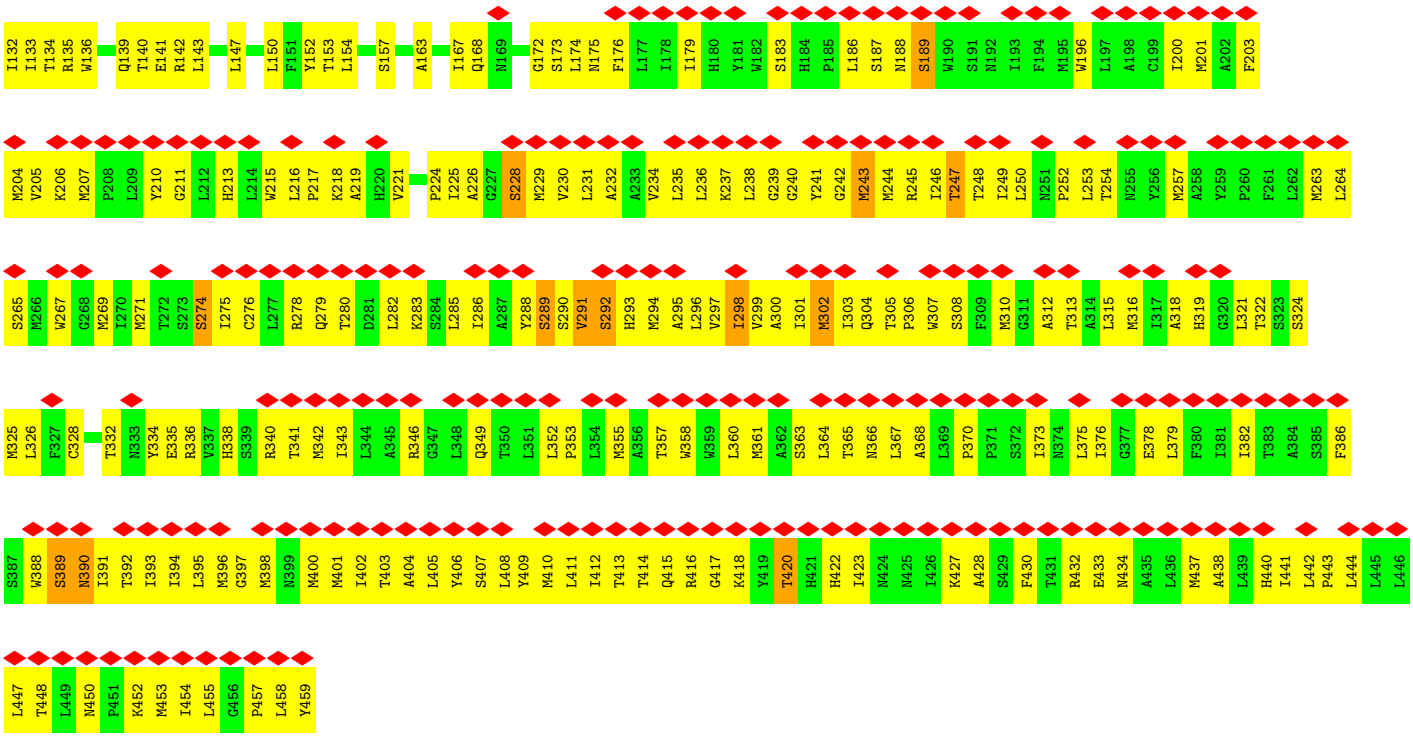
N603 Y604 H605 E606

- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:

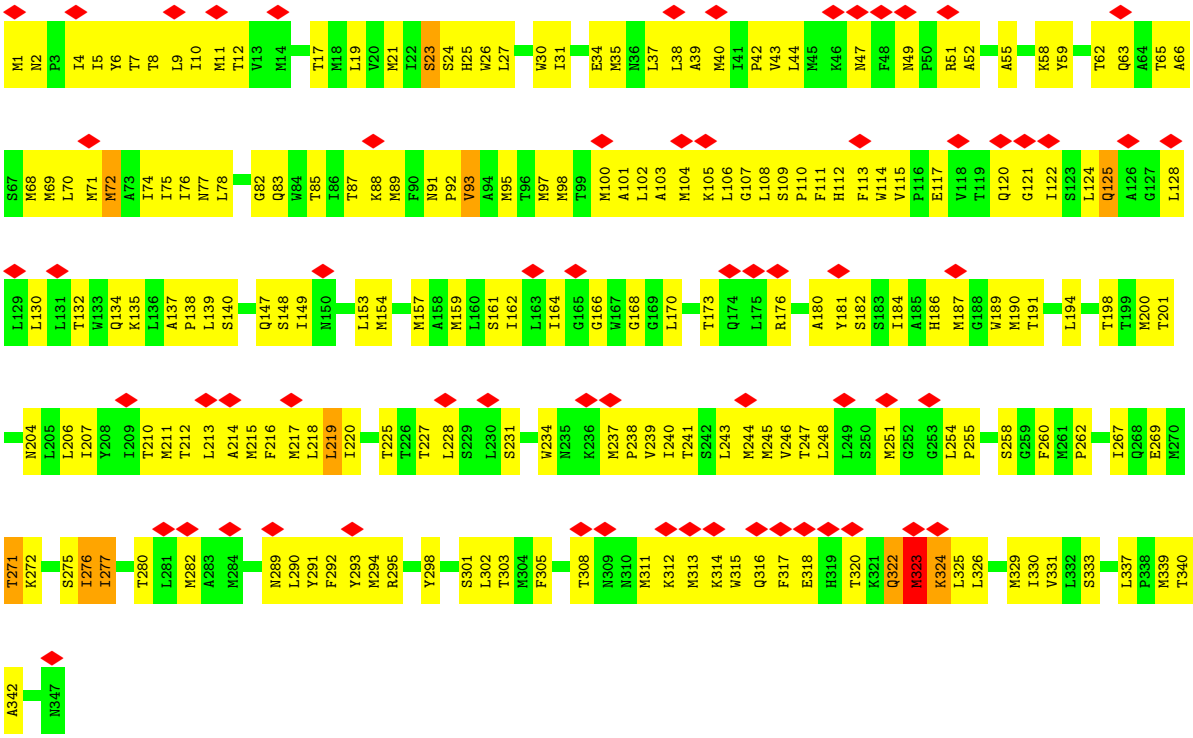
M1 L2 K3 I4 I5 I6 P7 T8 T9 M10 L11 L12 P13 M14 T15 W16 M17 S18 M22 I23 W24 I25 N26 H30 S31 L32 L33 I34 S35 L36 I37 S38 L39 S40 L41 L42 N43 Q44 L45 G46 E47 N48 S49 L50 N51 F52 S53 L54 F57 S58 D59 S60 L61 S62 A63 P64 L65

L66 V67 L68 T69 T70 W71 L72 L73 P74 L75 M76 L77 M78 A79 S80 H83 L84 S85 K86 E87 T88 T89 T90 R91 K92 K93 L94 Y95 L99 I100 L101 L102 Q103 L104 F105 L106 I107 M108 T109 F110 T111 E114 L115 I116 L117 F118 Y119 F122 E123 L126 V127 P128 T129 L130 I131



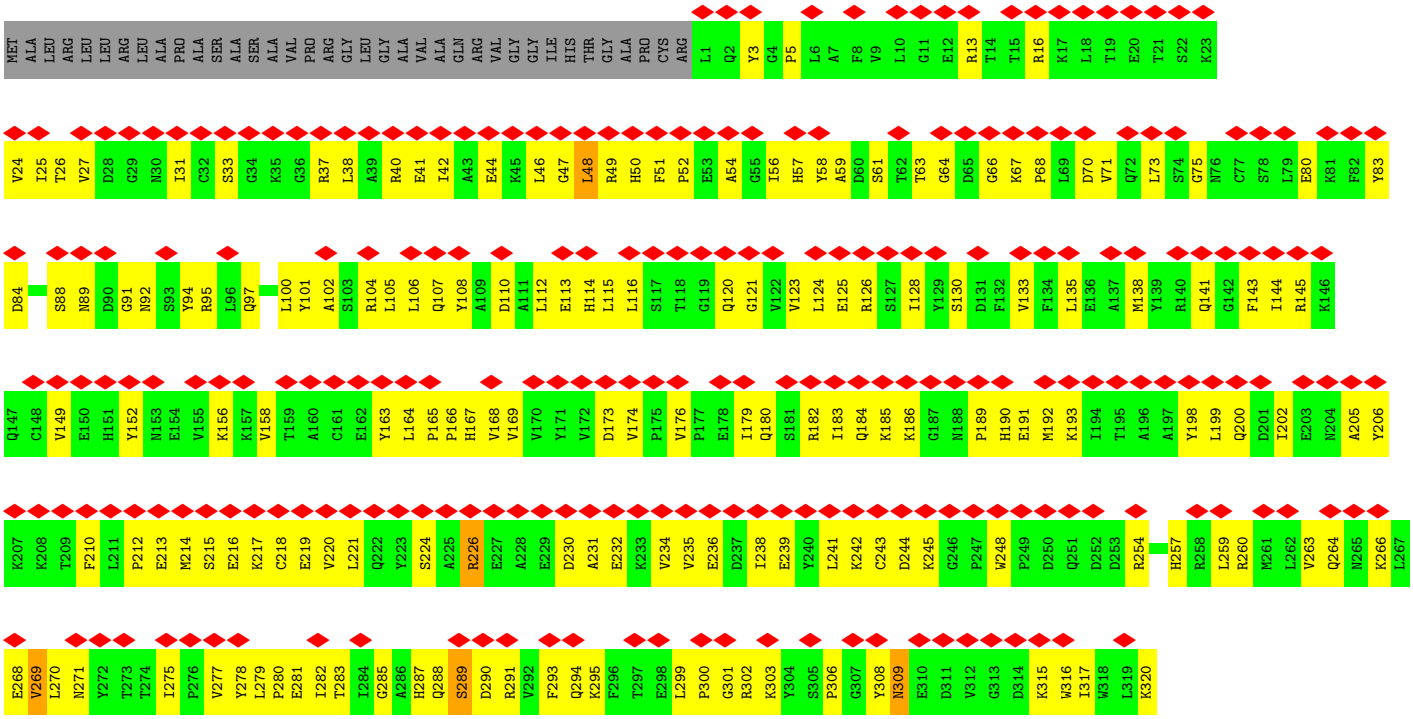
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:



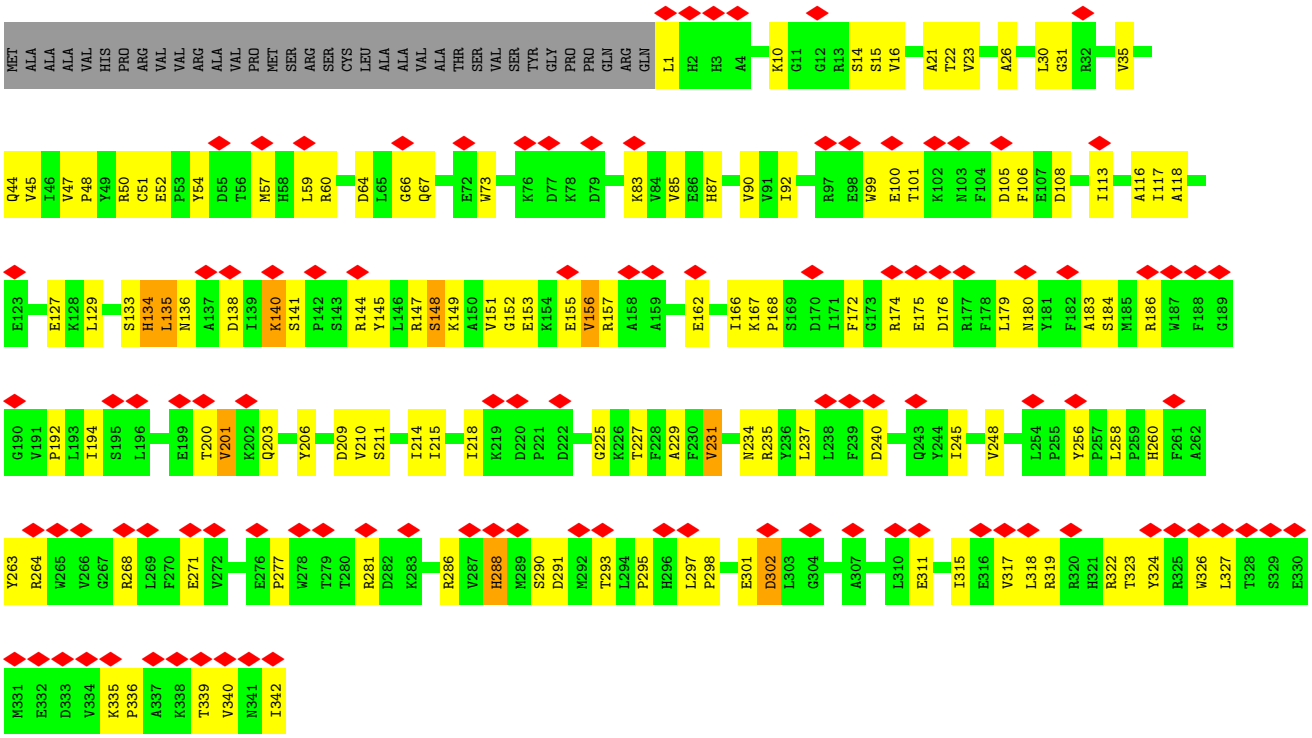
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:



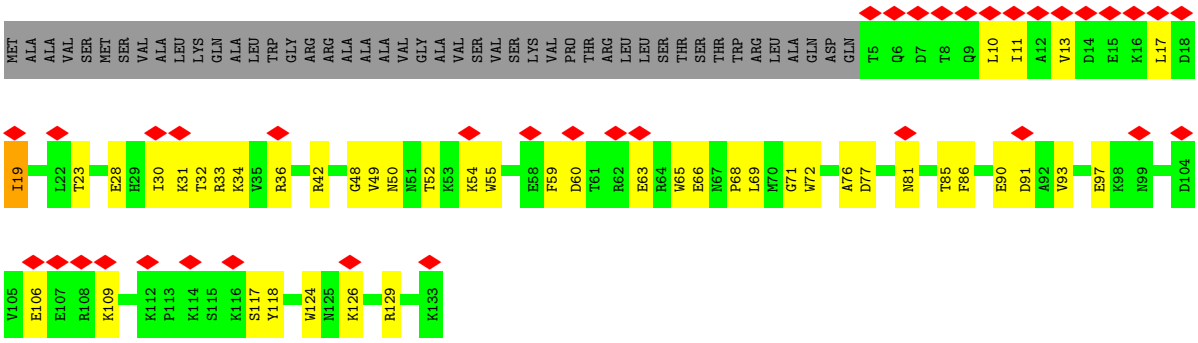
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



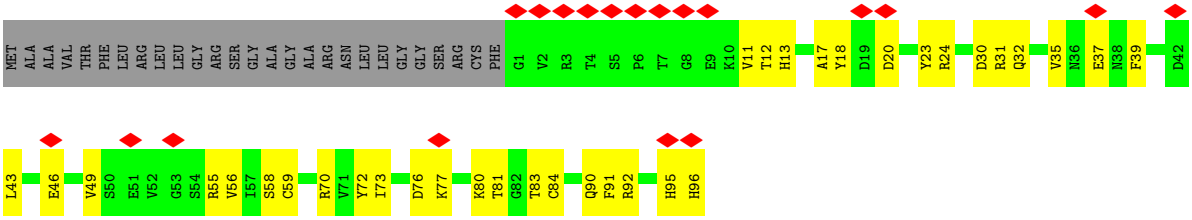
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



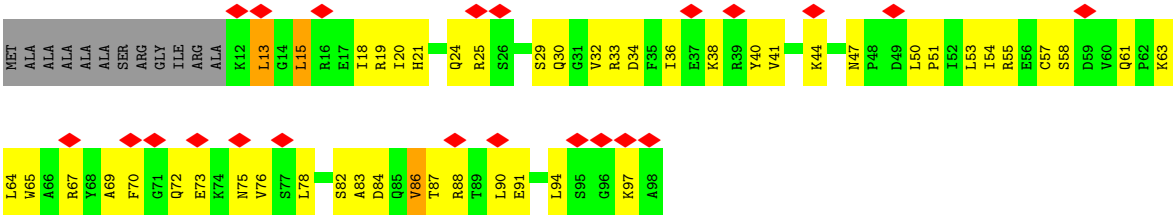
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



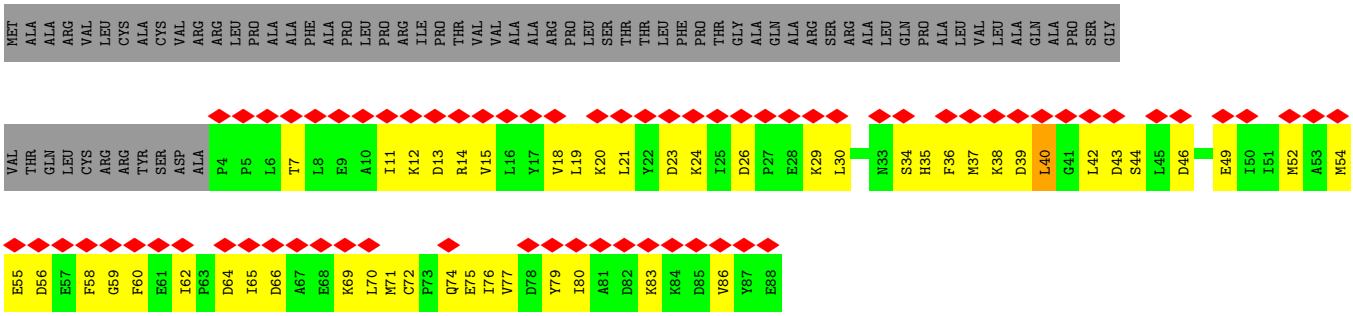
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



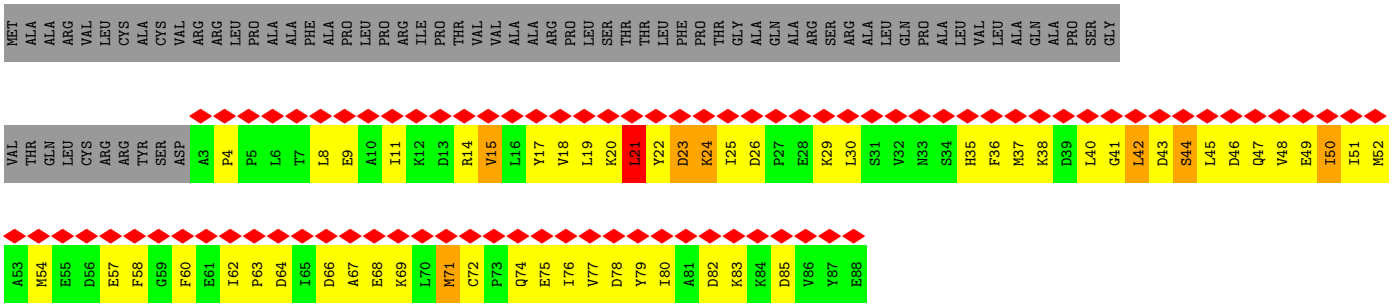
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T:



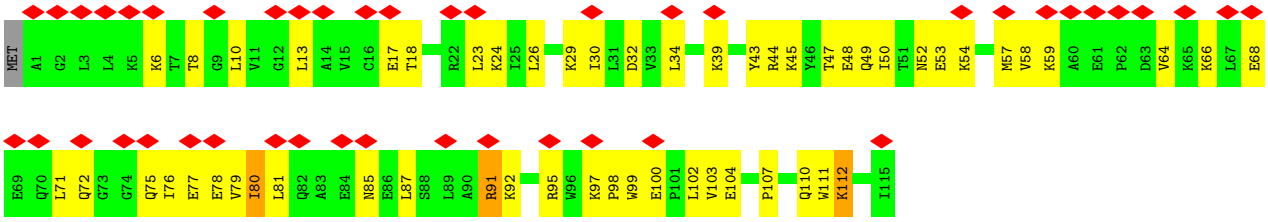
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U:



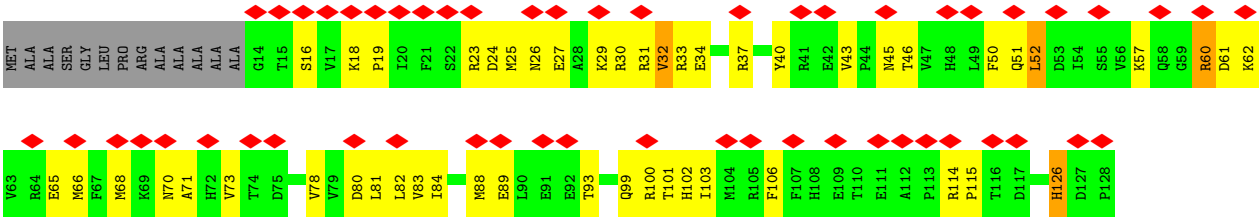
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:



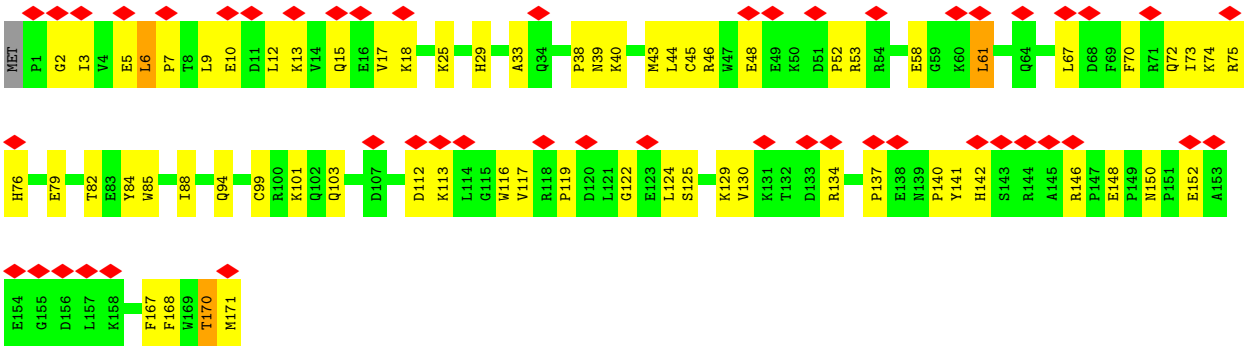
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain 1W:



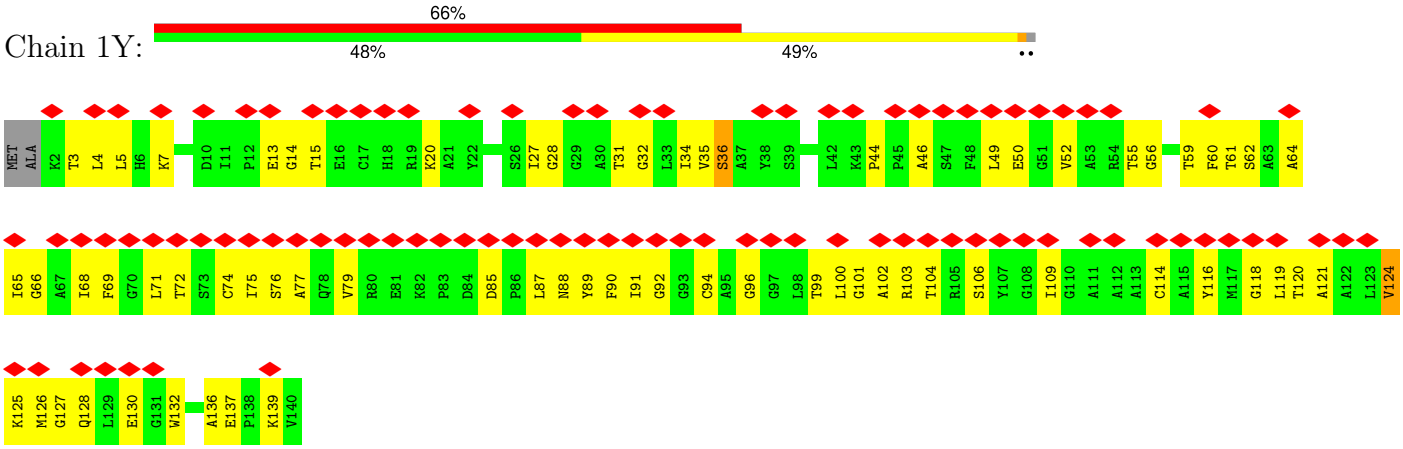
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X:



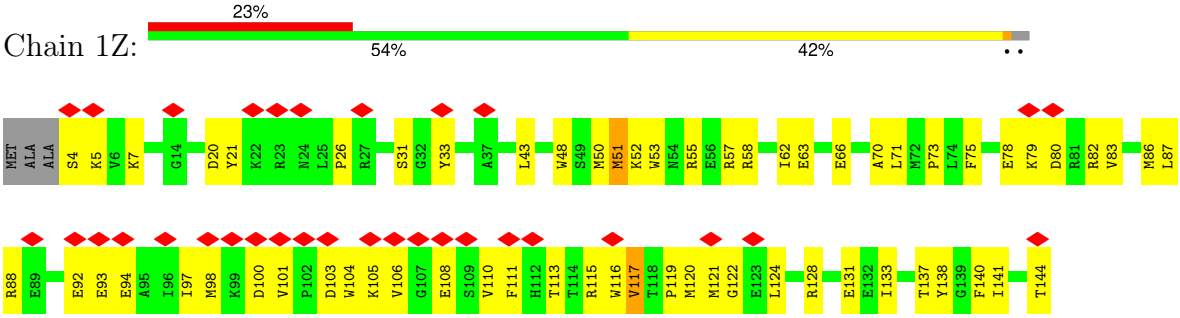
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:



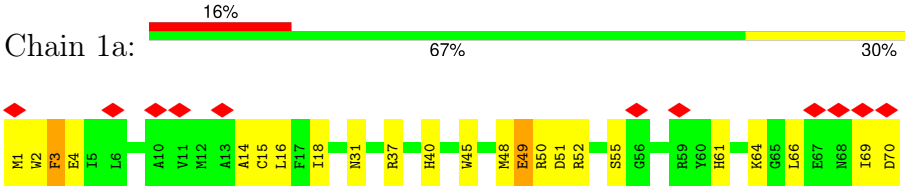
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:



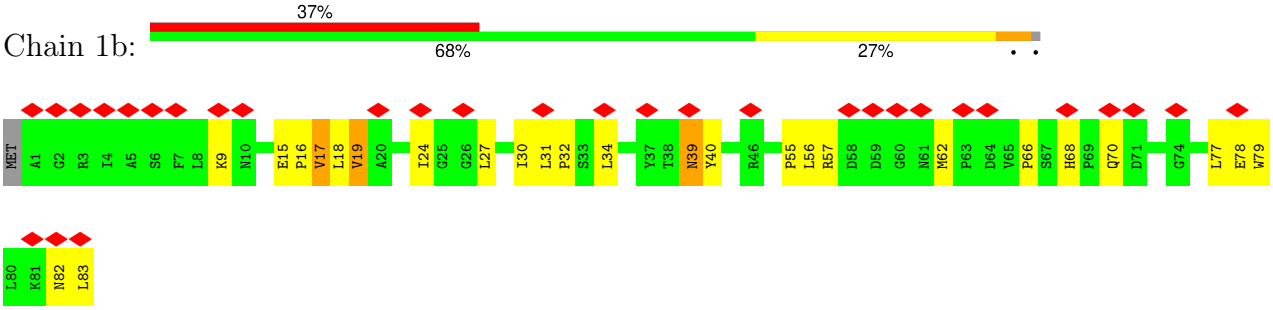
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a:



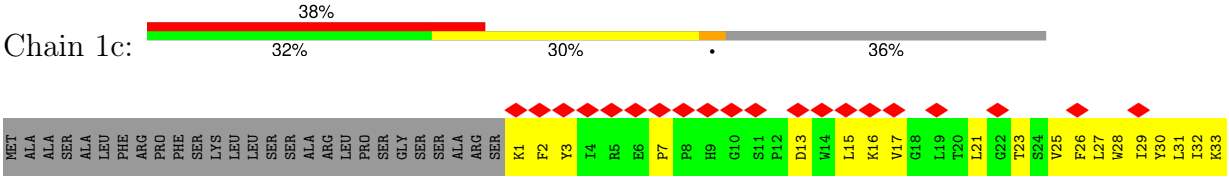
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

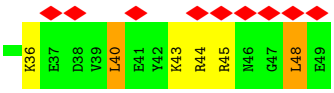
Chain 1b:



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

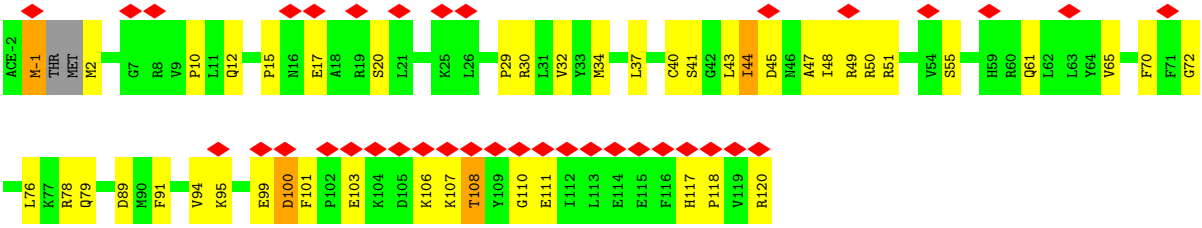
Chain 1c:





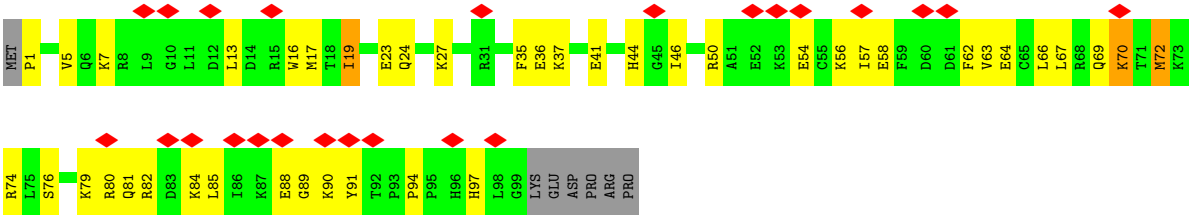
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d:



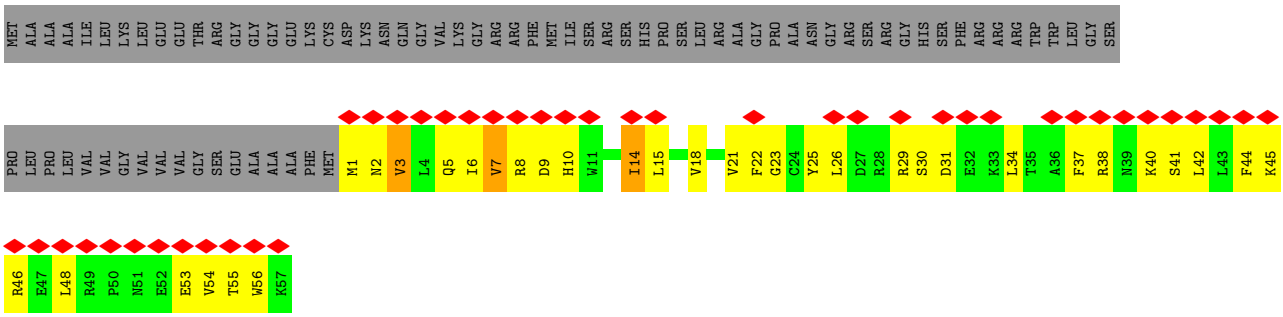
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:



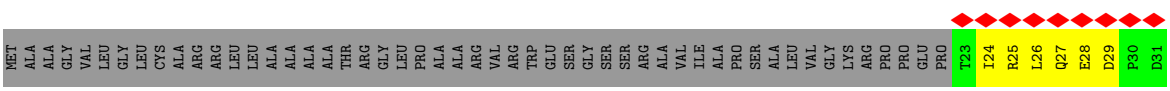
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

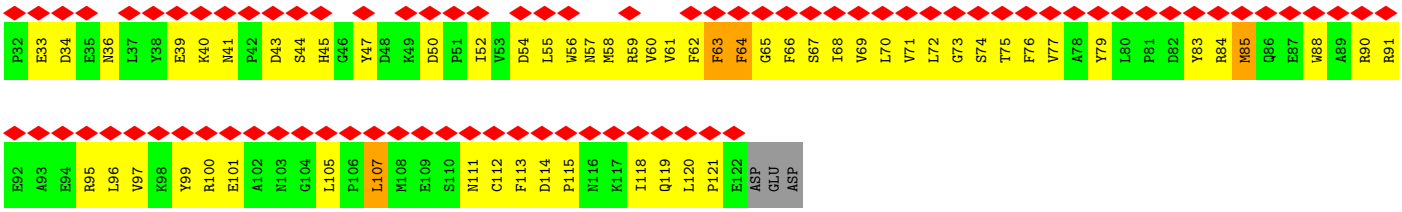
Chain 1f:



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

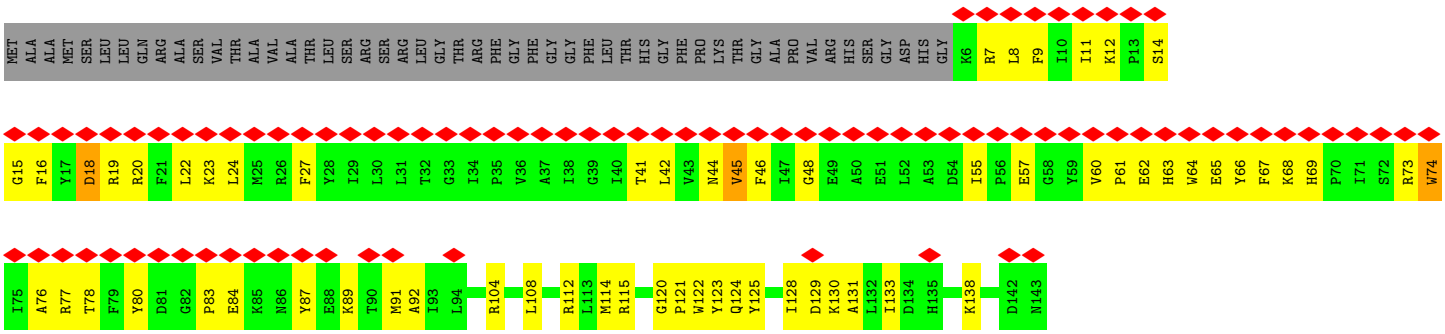
Chain 1g:





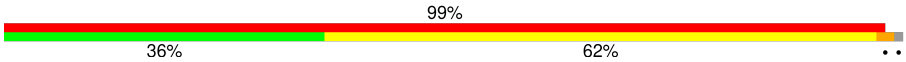
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

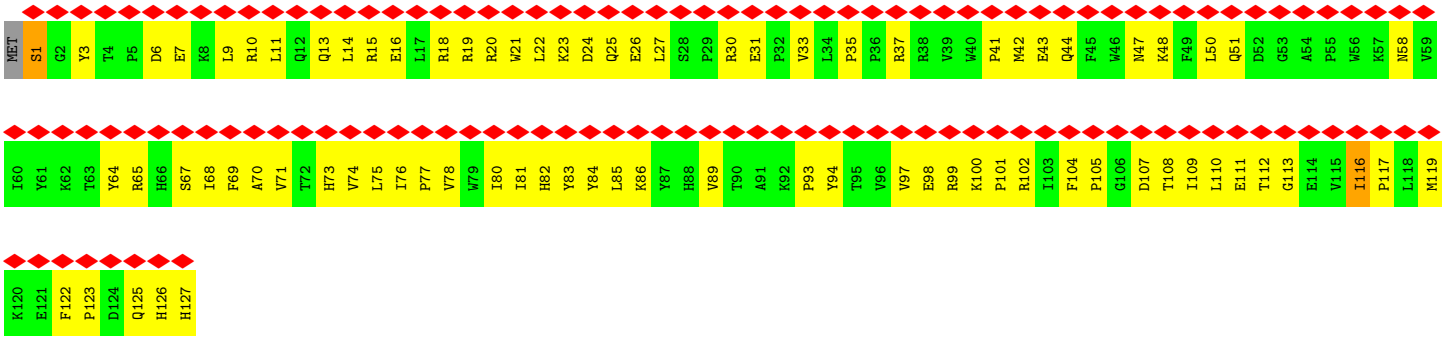
Chain 1h:



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

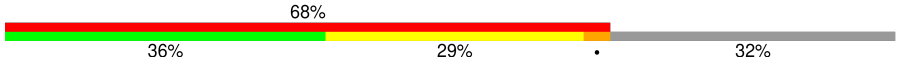
Chain 1i:

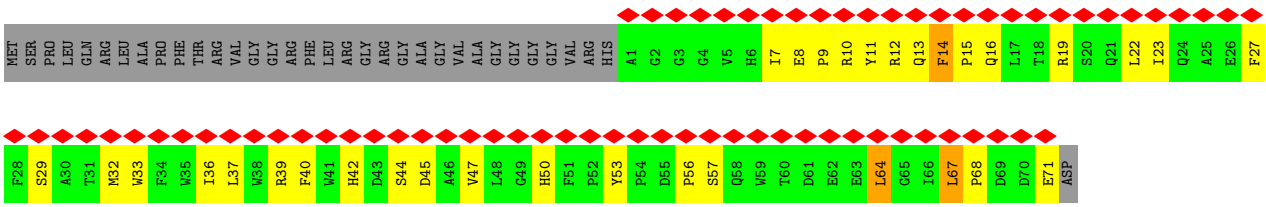




• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

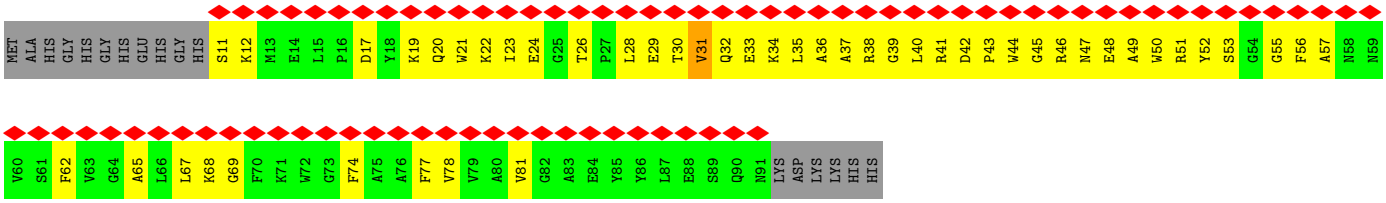
Chain 1j:





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

Chain 1k:

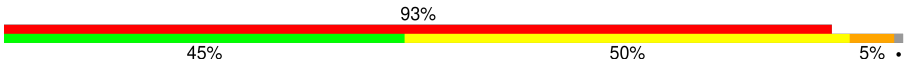


• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l:

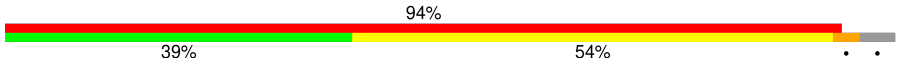
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

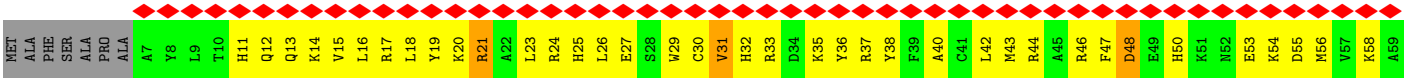
Chain 1m:

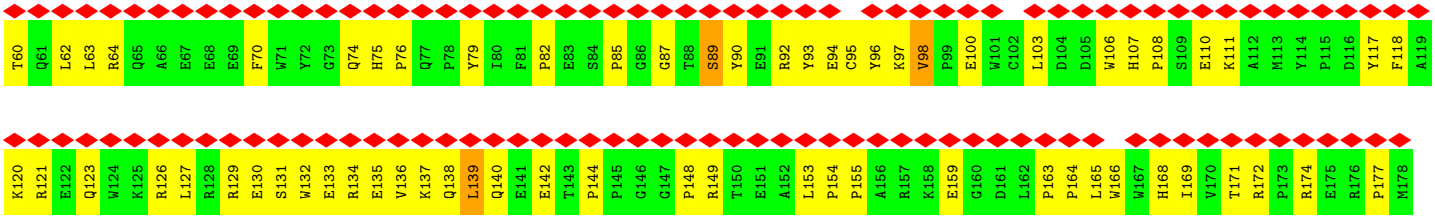


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n:





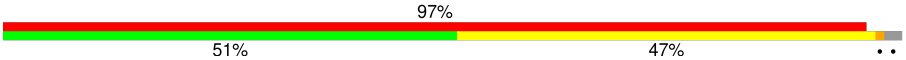


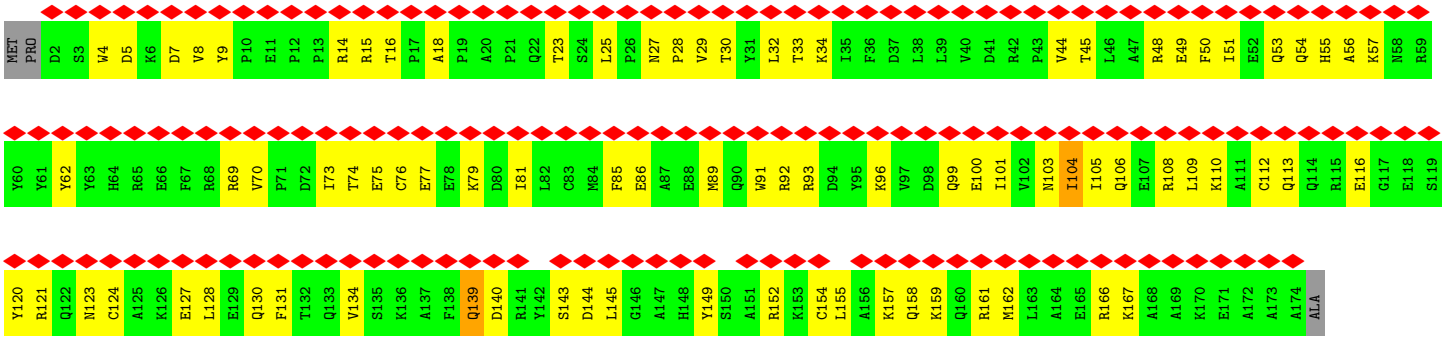
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:

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

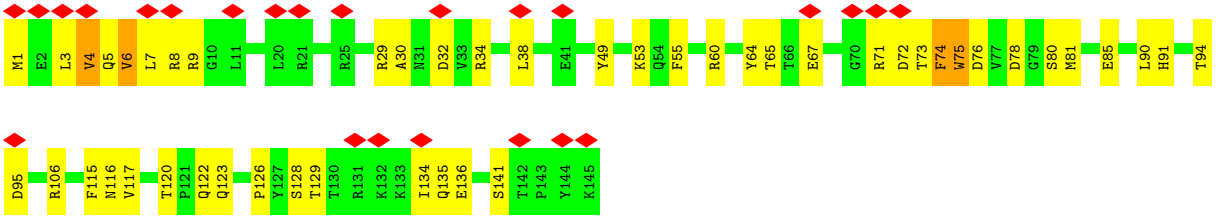
Chain 1p:





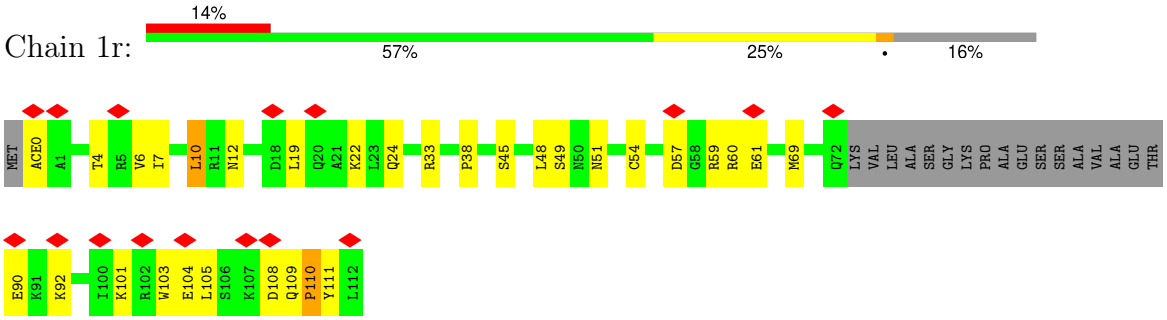
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:



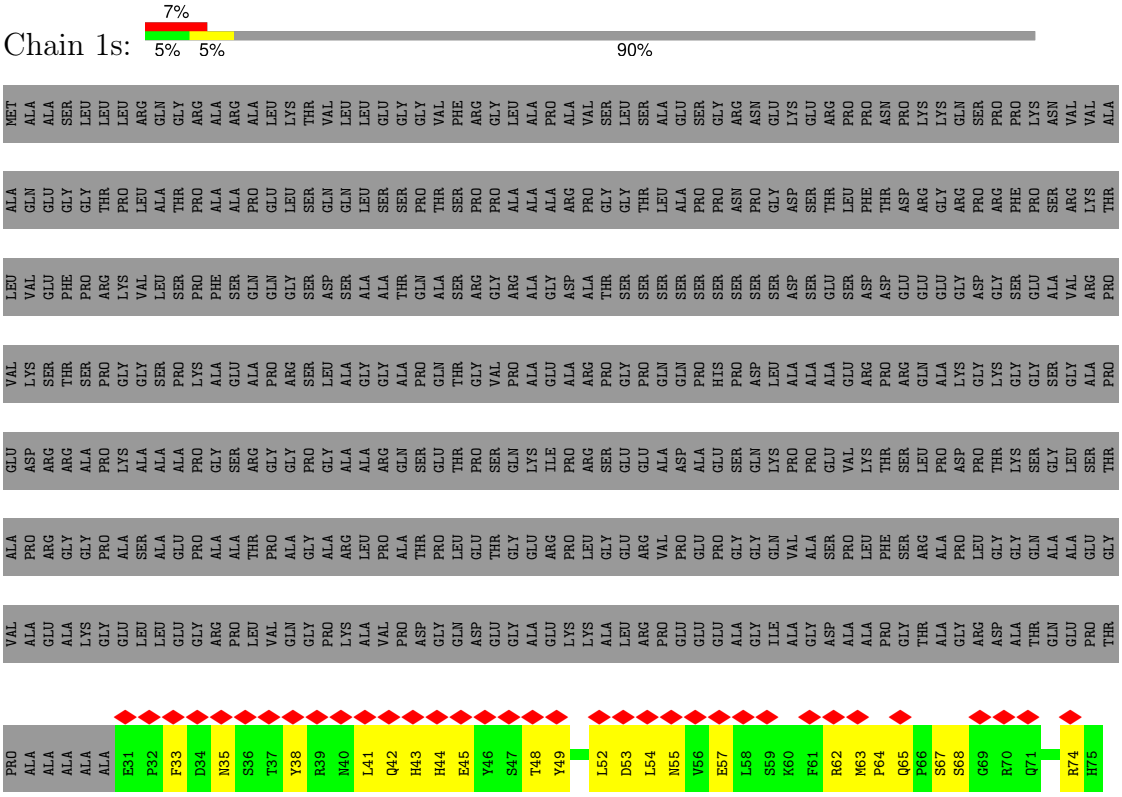
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 1r:



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

Chain 1s:



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	0.924	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.20	0/930	0.55	1/1271 (0.1%)
2	1B	0.21	0/1273	0.44	0/1722
3	1C	0.17	0/1791	0.38	0/2439
4	1D	0.17	0/3545	0.36	1/4806 (0.0%)
5	1E	0.16	0/1698	0.40	0/2311
6	1F	0.15	0/3401	0.38	0/4595
7	1G	0.16	0/5451	0.39	0/7387
8	1H	0.19	0/2566	0.43	0/3509
9	1I	0.19	0/1443	0.39	0/1952
10	1J	0.18	0/1364	0.49	0/1850
11	1K	0.21	0/751	0.57	0/1018
12	1L	0.18	0/4939	0.52	2/6718 (0.0%)
13	1M	0.18	0/3713	0.51	1/5063 (0.0%)
14	1N	0.22	0/2765	0.53	2/3758 (0.1%)
15	1O	0.17	0/2650	0.47	1/3588 (0.0%)
16	1P	0.14	0/2828	0.33	0/3834
17	1Q	0.17	0/1070	0.43	0/1446
18	1R	0.15	0/755	0.43	0/1018
19	1S	0.17	0/711	0.45	0/956
20	1T	0.22	0/701	0.67	0/946
20	1U	0.24	0/706	0.68	2/954 (0.2%)
21	1V	0.17	0/946	0.43	0/1281
22	1W	0.19	0/995	0.52	0/1340
23	1X	0.13	0/1436	0.34	0/1938
24	1Y	0.16	0/1037	0.47	0/1404
25	1Z	0.17	0/1199	0.41	0/1617
26	1a	0.17	0/577	0.32	0/777
27	1b	0.14	0/664	0.42	0/912
28	1c	0.19	0/430	0.56	0/581
29	1d	0.17	0/1024	0.39	0/1383
30	1e	0.19	0/836	0.47	0/1118
31	1f	0.21	0/499	0.60	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.23	0/858	0.66	1/1165 (0.1%)
33	1h	0.15	0/1184	0.40	0/1603
34	1i	0.19	0/1131	0.55	0/1541
35	1j	0.20	0/627	0.54	0/858
36	1k	0.14	0/668	0.40	0/903
37	1l	0.17	0/1365	0.50	0/1867
38	1m	0.16	0/1092	0.41	0/1481
39	1n	0.17	0/1549	0.50	0/2098
40	1o	0.25	1/1069 (0.1%)	0.61	3/1430 (0.2%)
41	1p	0.14	0/1481	0.37	0/1997
42	1q	0.16	0/1253	0.40	0/1704
43	1r	0.21	0/782	0.54	1/1057 (0.1%)
44	1s	0.17	0/394	0.55	0/533
All	All	0.18	1/68147 (0.0%)	0.46	15/92402 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1F	0	2
8	1H	0	1
9	1I	0	1
14	1N	0	1
42	1q	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1o	26	PRO	CG-CD	-6.25	1.29	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	1o	26	PRO	N-CD-CG	-10.96	86.76	103.20
43	1r	110	PRO	CA-N-CD	-8.22	100.48	112.00
32	1g	85	MET	CB-CG-SD	7.28	134.54	112.70
40	1o	26	PRO	CA-CB-CG	-6.67	91.84	104.50
40	1o	26	PRO	CA-N-CD	-6.28	103.21	112.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
6	1F	207	PRO	Peptide
8	1H	141	SER	Peptide
9	1I	50	TYR	Peptide
14	1N	322	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	62	0
2	1B	1242	0	1249	70	0
3	1C	1740	0	1691	56	0
4	1D	3452	0	3389	169	0
5	1E	1658	0	1662	94	0
6	1F	3325	0	3288	162	0
7	1G	5362	0	5388	243	0
8	1H	2504	0	2602	144	0
9	1I	1412	0	1366	94	0
10	1J	1339	0	1337	93	0
11	1K	750	0	798	65	0
12	1L	4818	0	4953	386	0
13	1M	3632	0	3836	300	0
14	1N	2712	0	2868	199	0
15	1O	2590	0	2556	160	0
16	1P	2751	0	2776	86	0
17	1Q	1047	0	1042	35	0
18	1R	741	0	704	22	0
19	1S	700	0	719	40	0
20	1T	689	0	687	58	0
20	1U	694	0	691	78	0
21	1V	927	0	972	47	0
22	1W	971	0	975	56	0
23	1X	1398	0	1378	58	0
24	1Y	1016	0	1020	55	0
25	1Z	1168	0	1161	77	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	1a	562	0	557	24	0
27	1b	643	0	645	25	0
28	1c	417	0	425	28	0
29	1d	996	0	989	46	0
30	1e	816	0	823	52	0
31	1f	487	0	498	35	0
32	1g	835	0	795	69	0
33	1h	1151	0	1164	72	0
34	1i	1100	0	1106	95	0
35	1j	601	0	546	41	0
36	1k	649	0	626	62	0
37	1l	1310	0	1204	100	0
38	1m	1062	0	1075	85	0
39	1n	1495	0	1434	128	0
40	1o	1045	0	1018	89	0
41	1p	1449	0	1416	97	0
42	1q	1212	0	1174	40	0
43	1r	767	0	791	26	0
44	1s	382	0	351	24	0
45	1B	8	0	0	1	0
45	1F	8	0	0	3	0
45	1G	16	0	0	8	0
45	1I	16	0	0	4	0
46	1B	34	0	42	1	0
46	1Y	35	0	44	2	0
46	1d	39	0	50	9	0
46	1h	34	0	42	2	0
46	1m	46	0	64	6	0
46	1q	48	0	68	2	0
47	1E	4	0	0	1	0
47	1G	4	0	0	1	0
48	1F	31	0	19	2	0
49	1G	1	0	0	0	0
50	1H	63	0	90	11	0
51	1H	51	0	46	2	0
51	1O	67	0	78	8	0
51	1a	61	0	64	4	0
52	1N	38	0	50	6	0
52	1Y	35	0	43	2	0
52	1g	51	0	81	5	0
52	1n	42	0	52	4	0
53	1O	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1O	1	0	0	0	0
55	1P	48	0	26	1	0
56	1R	1	0	0	0	0
57	1W	37	0	0	1	0
57	1n	37	0	0	0	0
58	1l	15	0	27	1	0
All	All	67436	0	67593	3425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 3425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:217:MET:HE3	51:1O:403:CDL:H711	1.36	1.04
10:1J:172:THR:HA	11:1K:80:MET:HE1	1.45	0.94
13:1M:450:ASN:HB3	13:1M:453:MET:HE1	1.50	0.93
7:1G:156:CYS:HB2	45:1G:802:SF4:S4	2.09	0.91
23:1X:6:LEU:HB2	25:1Z:88:ARG:HH21	1.34	0.90

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1A	113/115 (98%)	102 (90%)	10 (9%)	1 (1%)	14 47
2	1B	153/255 (60%)	138 (90%)	14 (9%)	1 (1%)	18 51
3	1C	207/264 (78%)	196 (95%)	11 (5%)	0	100 100
4	1D	427/476 (90%)	407 (95%)	20 (5%)	0	100 100
5	1E	212/249 (85%)	192 (91%)	19 (9%)	1 (0%)	24 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	1F	430/464 (93%)	401 (93%)	28 (6%)	1 (0%)	43	74
7	1G	697/727 (96%)	633 (91%)	62 (9%)	2 (0%)	36	67
8	1H	316/318 (99%)	299 (95%)	14 (4%)	3 (1%)	14	47
9	1I	174/239 (73%)	160 (92%)	12 (7%)	2 (1%)	11	43
10	1J	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	7	35
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	541 (90%)	62 (10%)	1 (0%)	43	74
13	1M	457/459 (100%)	431 (94%)	25 (6%)	1 (0%)	43	74
14	1N	345/347 (99%)	320 (93%)	23 (7%)	2 (1%)	21	54
15	1O	318/357 (89%)	287 (90%)	31 (10%)	0	100	100
16	1P	340/377 (90%)	316 (93%)	24 (7%)	0	100	100
17	1Q	127/175 (73%)	119 (94%)	8 (6%)	0	100	100
18	1R	94/123 (76%)	81 (86%)	13 (14%)	0	100	100
19	1S	85/99 (86%)	68 (80%)	17 (20%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	14	47
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	112 (96%)	5 (4%)	0	100	100
30	1e	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100
32	1g	98/154 (64%)	84 (86%)	12 (12%)	2 (2%)	6	32
33	1h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	1i	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	58 (84%)	11 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1k	79/98 (81%)	71 (90%)	8 (10%)	0	100	100
37	1l	154/186 (83%)	130 (84%)	24 (16%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	157 (92%)	12 (7%)	1 (1%)	21	54
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	1q	143/145 (99%)	136 (95%)	6 (4%)	1 (1%)	18	51
43	1r	90/114 (79%)	85 (94%)	4 (4%)	1 (1%)	11	43
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
All	All	8194/9741 (84%)	7570 (92%)	600 (7%)	24 (0%)	37	67

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	46	SER
8	1H	92	PRO
8	1H	196	ALA
10	1J	113	VAL
10	1J	122	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	90 (91%)	9 (9%)	9	32
2	1B	131/209 (63%)	120 (92%)	11 (8%)	10	34
3	1C	190/227 (84%)	178 (94%)	12 (6%)	16	42
4	1D	371/405 (92%)	341 (92%)	30 (8%)	11	35
5	1E	183/207 (88%)	175 (96%)	8 (4%)	25	51
6	1F	346/368 (94%)	334 (96%)	12 (4%)	32	57
7	1G	588/610 (96%)	559 (95%)	29 (5%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1H	274/274 (100%)	262 (96%)	12 (4%)	25	51
9	1I	151/201 (75%)	141 (93%)	10 (7%)	15	41
10	1J	140/140 (100%)	130 (93%)	10 (7%)	13	38
11	1K	84/84 (100%)	77 (92%)	7 (8%)	10	34
12	1L	539/539 (100%)	512 (95%)	27 (5%)	22	48
13	1M	408/408 (100%)	380 (93%)	28 (7%)	14	39
14	1N	310/310 (100%)	294 (95%)	16 (5%)	21	47
15	1O	283/307 (92%)	272 (96%)	11 (4%)	28	54
16	1P	296/323 (92%)	273 (92%)	23 (8%)	11	36
17	1Q	117/152 (77%)	112 (96%)	5 (4%)	26	51
18	1R	79/97 (81%)	76 (96%)	3 (4%)	29	55
19	1S	77/82 (94%)	70 (91%)	7 (9%)	9	32
20	1T	79/133 (59%)	74 (94%)	5 (6%)	16	42
20	1U	79/133 (59%)	71 (90%)	8 (10%)	7	28
21	1V	100/101 (99%)	93 (93%)	7 (7%)	14	39
22	1W	107/112 (96%)	101 (94%)	6 (6%)	19	46
23	1X	153/154 (99%)	147 (96%)	6 (4%)	28	54
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	28	54
25	1Z	123/124 (99%)	116 (94%)	7 (6%)	18	45
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	57
27	1b	69/70 (99%)	66 (96%)	3 (4%)	26	51
28	1c	45/66 (68%)	43 (96%)	2 (4%)	25	51
29	1d	107/109 (98%)	99 (92%)	8 (8%)	12	37
30	1e	87/94 (93%)	82 (94%)	5 (6%)	18	45
31	1f	54/113 (48%)	51 (94%)	3 (6%)	19	46
32	1g	92/129 (71%)	88 (96%)	4 (4%)	26	51
33	1h	121/158 (77%)	118 (98%)	3 (2%)	42	63
34	1i	119/120 (99%)	114 (96%)	5 (4%)	26	52
35	1j	62/84 (74%)	58 (94%)	4 (6%)	15	42
36	1k	63/76 (83%)	61 (97%)	2 (3%)	34	59
37	1l	141/161 (88%)	135 (96%)	6 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	1m	113/114 (99%)	106 (94%)	7 (6%)	16	43
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	59
40	1o	110/120 (92%)	103 (94%)	7 (6%)	16	42
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	62
42	1q	131/131 (100%)	124 (95%)	7 (5%)	20	47
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32	57
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7219/8269 (87%)	6826 (95%)	393 (5%)	21	46

5 of 393 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	1O	309	ASN
21	1V	50	ILE
16	1P	140	LYS
18	1R	12	THR
23	1X	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
37	1l	104	HIS
43	1r	109	GLN
39	1n	107	HIS
41	1p	130	GLN
12	1L	248	HIS

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	$\#\|Z\| > 2$
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.89	1 (12%)
14	FME	1N	1	14,10	8,9,10	0.59	0	8,9,11	0.95	1 (12%)
34	SAC	1i	1	-	7,8,9	0.58	0	7,9,11	1.15	1 (14%)
11	FME	1K	1	11	8,9,10	0.51	0	8,9,11	1.00	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.00	1 (12%)
12	FME	1L	1	12	8,9,10	0.57	0	8,9,11	0.94	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.89	1 (12%)
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	1.11	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FME	1J	1	10	-	1/7/9/11	-
14	FME	1N	1	14,10	-	3/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1i	1	SAC	O-C-CA	-2.96	117.15	124.77
8	1H	1	FME	O-C-CA	-2.81	117.56	124.77
11	1K	1	FME	O-C-CA	-2.64	117.99	124.77
12	1L	1	FME	O-C-CA	-2.58	118.12	124.77
1	1A	1	FME	O-C-CA	-2.56	118.19	124.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	1K	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
14	1N	1	FME	N-CA-CB-CG
14	1N	1	FME	C-CA-CB-CG
10	1J	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	1J	1	FME	1	0
34	1i	1	SAC	1	0
11	1K	1	FME	1	0
1	1A	1	FME	1	0
13	1M	1	FME	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
46	PC1	1q	201	42	47,47,53	0.37	0	53,55,61	0.55	1 (1%)
47	FES	1E	301	5	0,4,4	-	-	-		
57	EHZ	1W	201	-	31,36,37	0.19	0	36,44,47	1.27	1 (2%)
52	3PE	1N	401	-	37,37,50	0.32	0	40,42,55	0.39	0
46	PC1	1m	201	38,12	45,45,53	0.28	0	51,53,61	0.36	0
57	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.21	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	GTP	1O	401	54	33,34,34	0.60	0	50,54,54	0.64	0
45	SF4	1I	202	9	0,12,12	-	-	-		
50	U10	1H	401	-	63,63,63	0.58	2 (3%)	78,79,79	0.85	5 (6%)
45	SF4	1B	201	2	0,12,12	-	-	-		
47	FES	1G	803	7	0,4,4	-	-	-		
46	PC1	1Y	201	24	34,34,53	0.32	0	40,42,61	0.37	0
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.66	1 (2%)
52	3PE	1n	202	39,12	41,41,50	0.29	0	44,46,55	0.43	0
52	3PE	1g	201	32	50,50,50	0.28	0	53,55,55	0.99	3 (5%)
46	PC1	1h	201	-	33,33,53	0.31	0	39,41,61	0.45	0
51	CDL	1O	403	14,15	66,66,99	0.37	0	72,78,111	0.54	1 (1%)
45	SF4	1G	801	7	0,12,12	-	-	-		
46	PC1	1d	201	14,30,29	38,38,53	0.31	0	44,46,61	0.51	0
51	CDL	1a	101	26	60,60,99	0.33	0	66,72,111	0.54	0
52	3PE	1Y	202	24	34,34,50	0.31	0	37,39,55	0.56	1 (2%)
55	NDP	1P	501	-	51,52,52	0.51	0	71,80,80	0.79	2 (2%)
58	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.30	0
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.33	0
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
45	SF4	1F	502	6	0,12,12	-	-	-		
51	CDL	1H	402	-	50,50,99	0.36	0	56,62,111	0.55	1 (1%)

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
46	PC1	1q	201	42	-	15/51/51/57	-
47	FES	1E	301	5	-	-	0/1/1/1
57	EHZ	1W	201	-	-	16/42/44/45	-
46	PC1	1m	201	38,12	-	6/49/49/57	-
57	EHZ	1n	201	-	-	2/42/44/45	-
53	GTP	1O	401	54	-	3/22/38/38	0/3/3/3
51	CDL	1H	402	-	-	7/61/61/110	-
50	U10	1H	401	-	-	6/63/87/87	0/1/1/1
45	SF4	1I	202	9	-	-	0/6/5/5
45	SF4	1B	201	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	FES	1G	803	7	-	-	0/1/1/1
46	PC1	1Y	201	24	-	11/38/38/57	-
48	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
52	3PE	1n	202	39,12	-	6/45/45/54	-
52	3PE	1g	201	32	-	11/54/54/54	-
46	PC1	1h	201	-	-	4/36/36/57	-
51	CDL	1O	403	14,15	-	15/76/76/110	-
45	SF4	1G	801	7	-	-	0/6/5/5
46	PC1	1d	201	14,30,29	-	13/42/42/57	-
51	CDL	1a	101	26	-	17/71/71/110	-
55	NDP	1P	501	-	-	3/34/77/77	0/5/5/5
52	3PE	1Y	202	24	-	13/38/38/54	-
58	MYR	1l	201	-	-	2/12/12/13	-
46	PC1	1B	202	-	-	11/37/37/57	-
45	SF4	1G	802	7	-	-	0/6/5/5
45	SF4	1I	201	9	-	-	0/6/5/5
45	SF4	1F	502	6	-	-	0/6/5/5
52	3PE	1N	401	-	-	4/41/41/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1H	401	U10	C4-C5	-2.48	1.41	1.48
50	1H	401	U10	C4-C3	2.10	1.44	1.36

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1W	201	EHZ	C10-S1-C9	7.08	122.76	101.84
57	1n	201	EHZ	C10-S1-C9	6.84	122.07	101.84
55	1P	501	NDP	P2B-O2B-C2B	-4.77	110.69	123.43
52	1g	201	3PE	O21-C21-C22	4.51	121.23	111.48
52	1g	201	3PE	O21-C2-C3	3.49	120.86	108.34

There are no chirality outliers.

5 of 167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C11-O13-P-O14

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

There are no ring outliers.

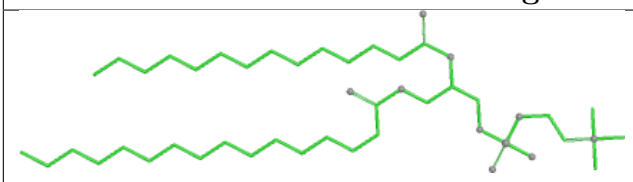
27 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1q	201	PC1	2	0
47	1E	301	FES	1	0
57	1W	201	EHZ	1	0
52	1N	401	3PE	6	0
46	1m	201	PC1	6	0
53	1O	401	GTP	3	0
45	1I	202	SF4	2	0
50	1H	401	U10	11	0
45	1B	201	SF4	1	0
47	1G	803	FES	1	0
46	1Y	201	PC1	2	0
48	1F	501	FMN	2	0
52	1n	202	3PE	4	0
52	1g	201	3PE	5	0
46	1h	201	PC1	2	0
51	1O	403	CDL	8	0
45	1G	801	SF4	3	0
46	1d	201	PC1	9	0
51	1a	101	CDL	4	0
52	1Y	202	3PE	2	0
55	1P	501	NDP	1	0
58	1l	201	MYR	1	0
46	1B	202	PC1	1	0
45	1I	201	SF4	2	0
45	1G	802	SF4	5	0
45	1F	502	SF4	3	0
51	1H	402	CDL	2	0

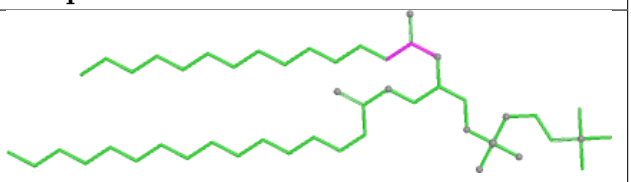
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

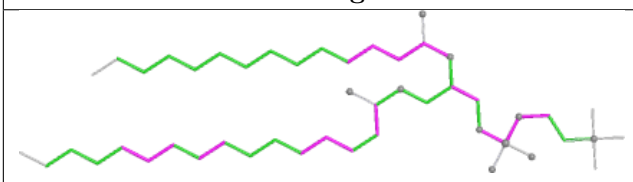
Ligand PC1 1q 201



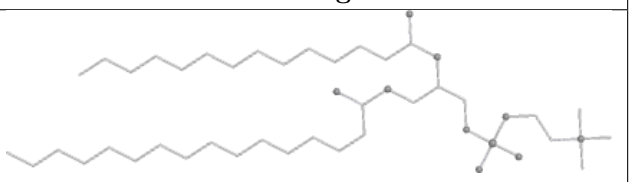
Bond lengths



Bond angles

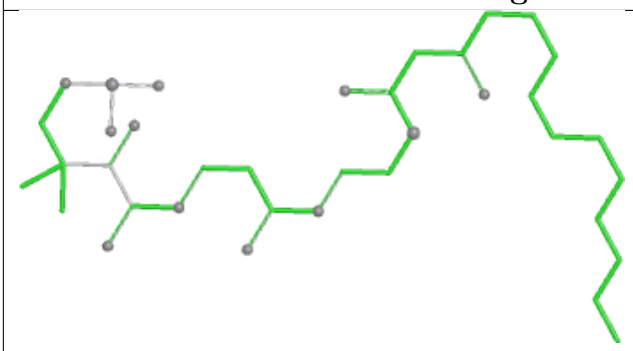


Torsions

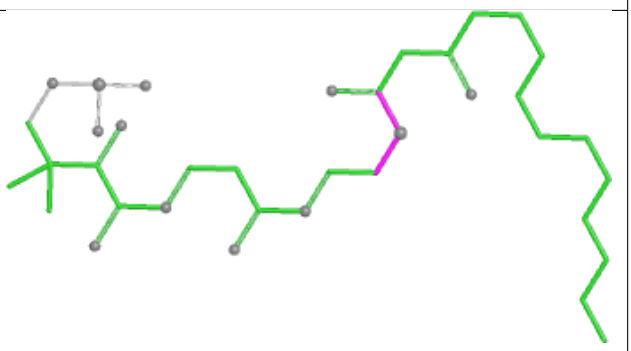


Rings

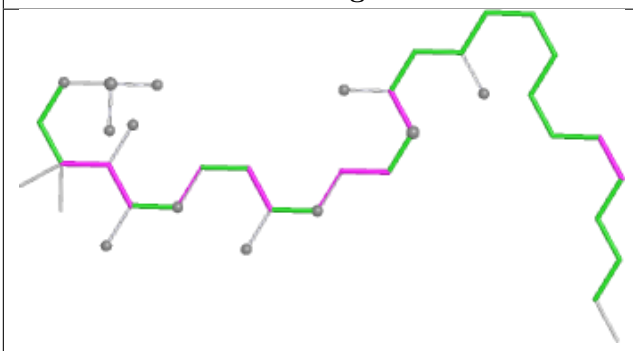
Ligand EHZ 1W 201



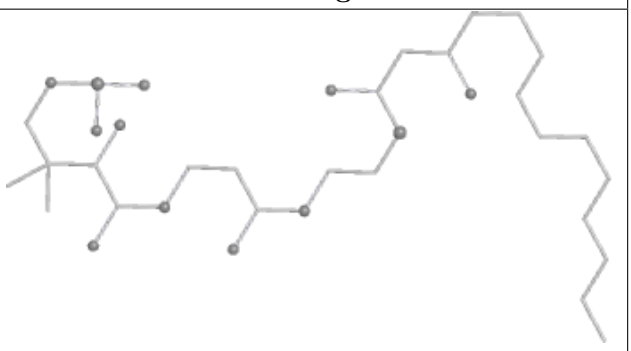
Bond lengths



Bond angles

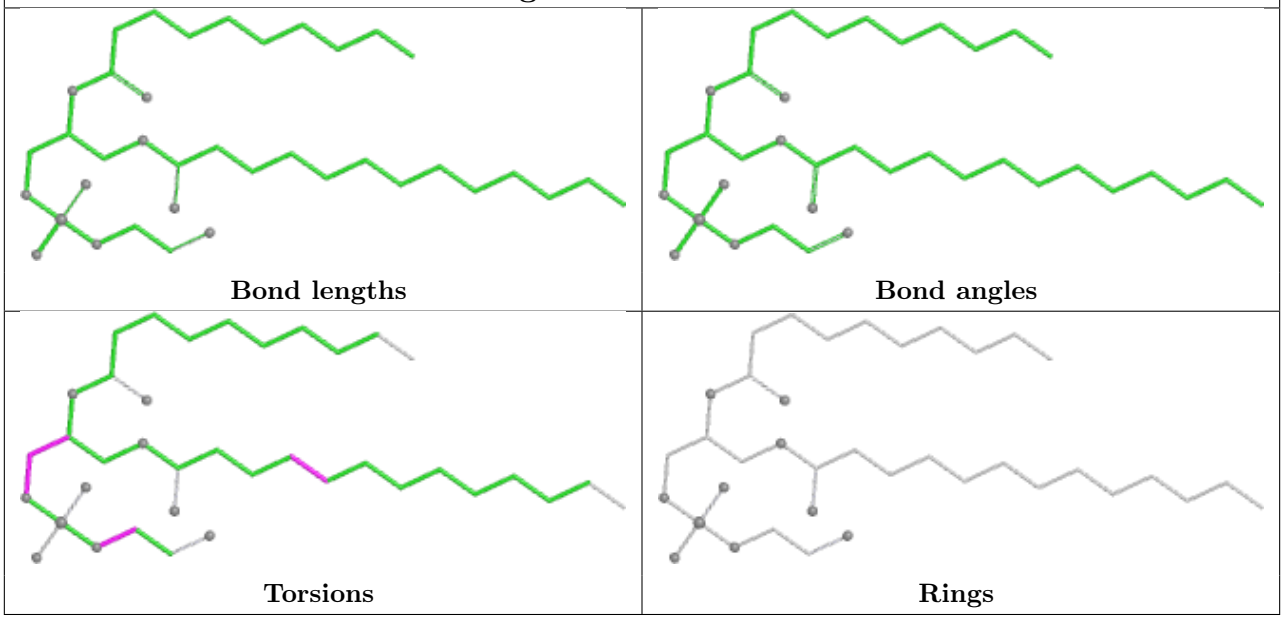


Torsions

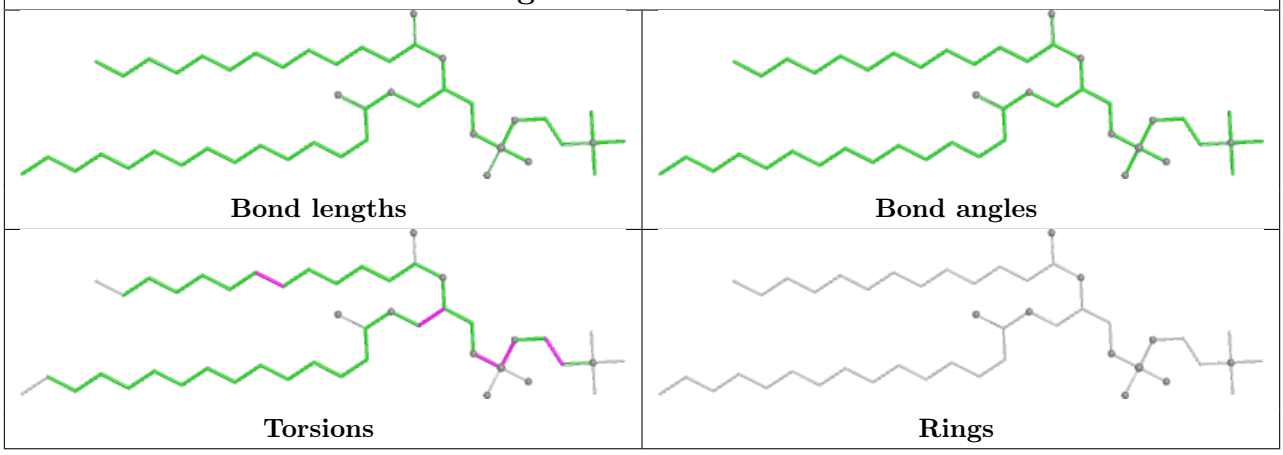


Rings

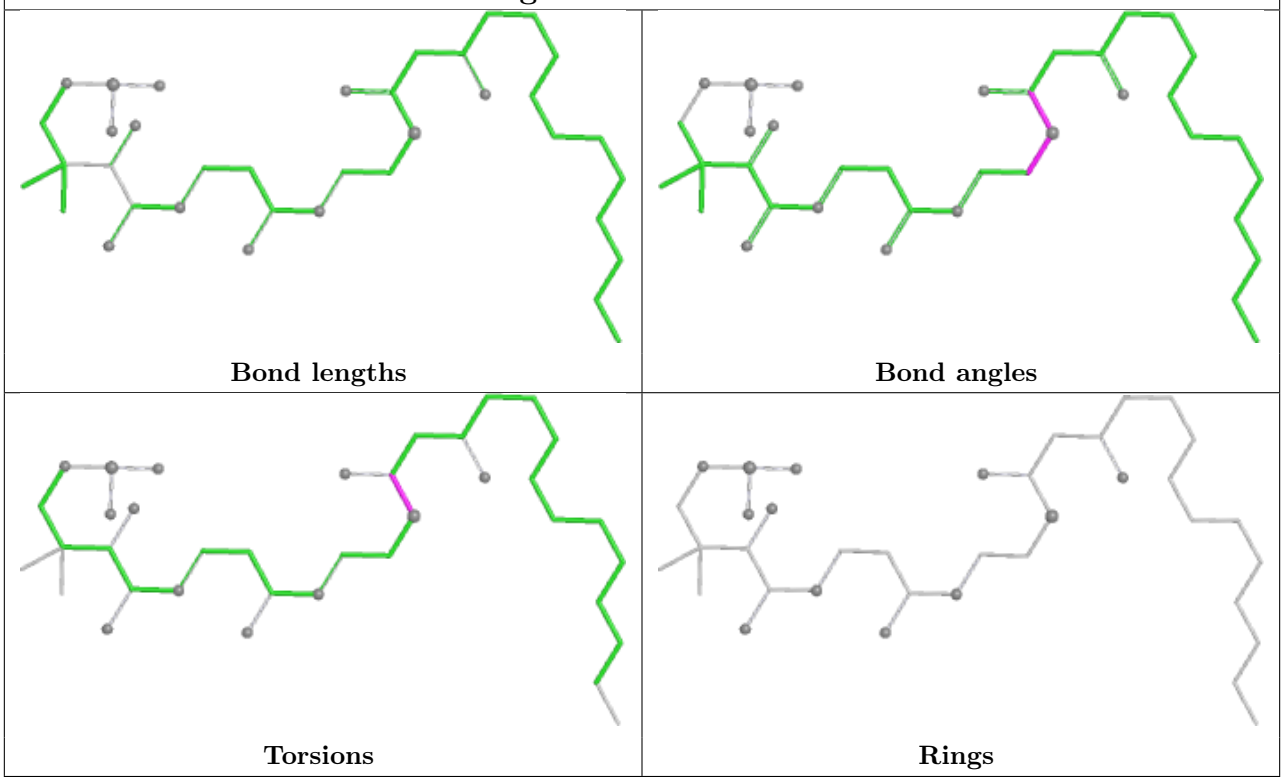
Ligand 3PE 1N 401



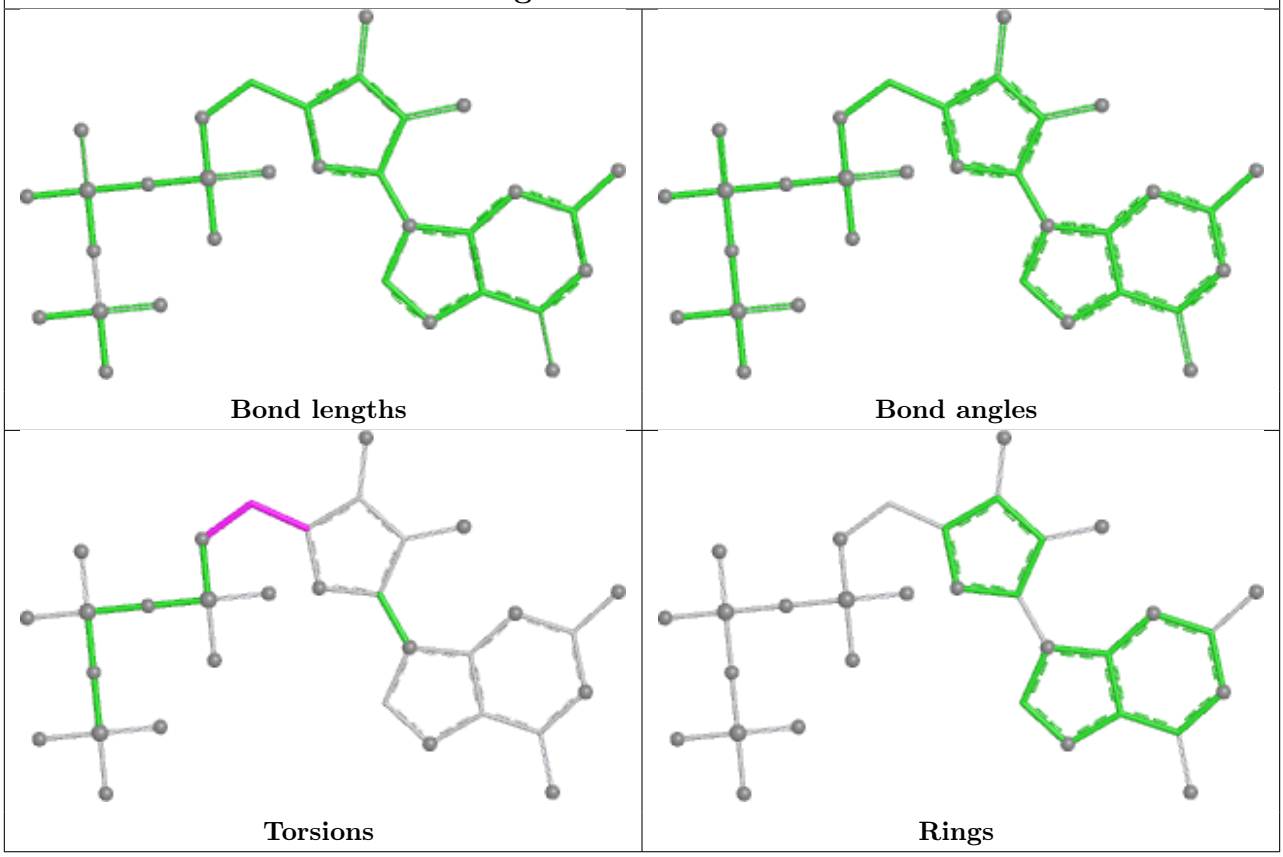
Ligand PC1 1m 201

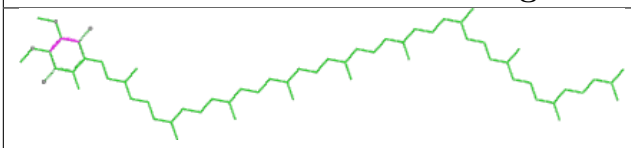
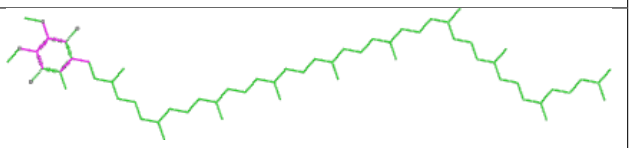
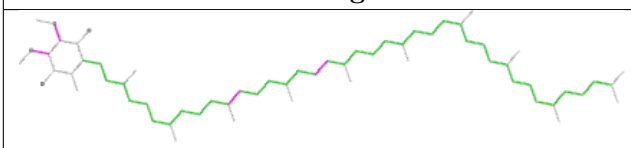
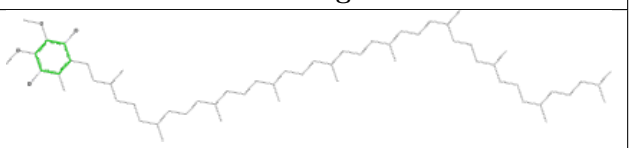


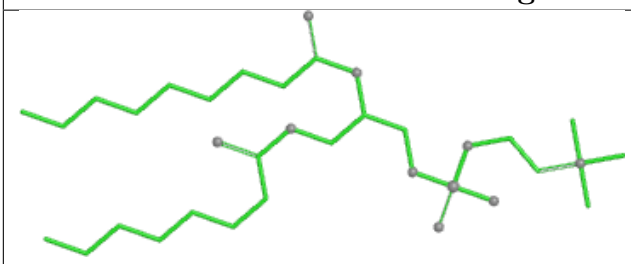
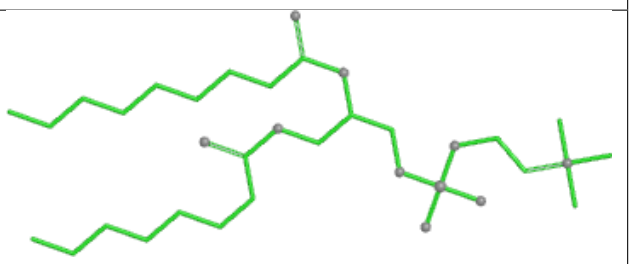
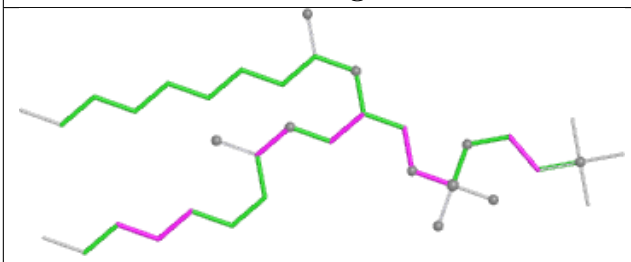
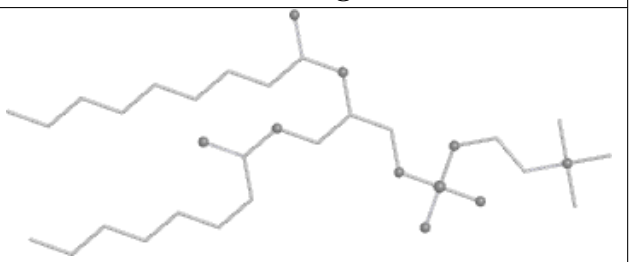
Ligand EHZ 1n 201

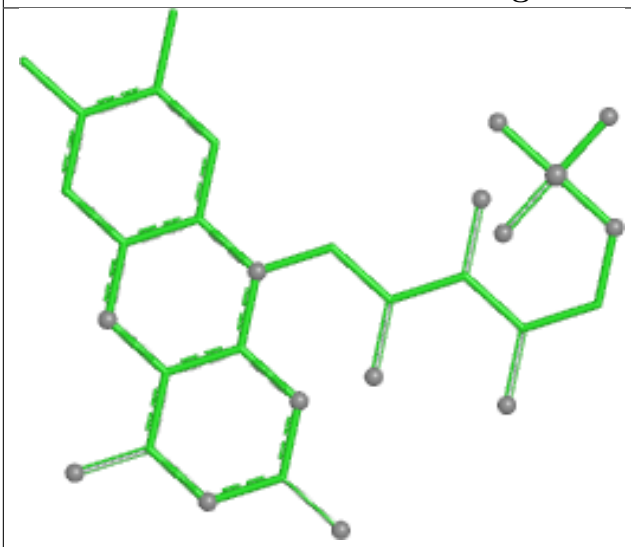
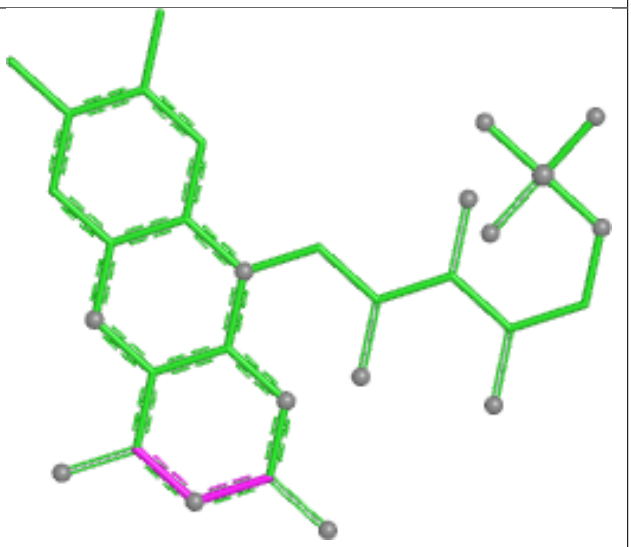
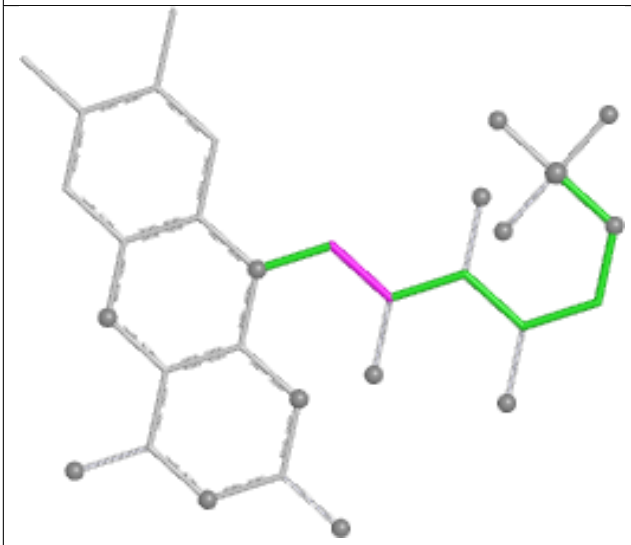
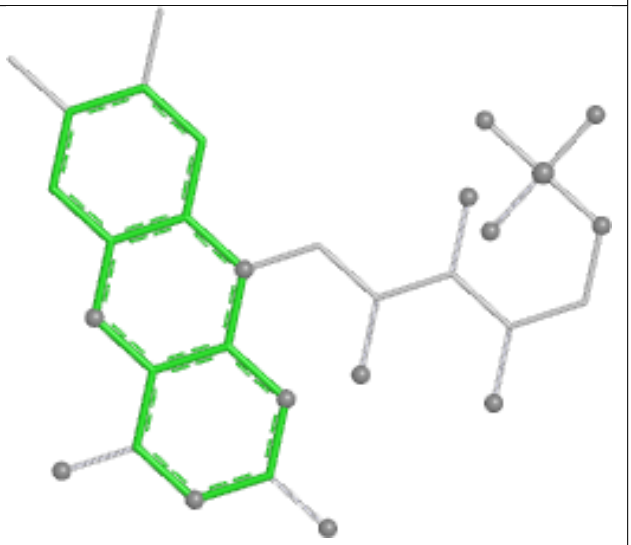


Ligand GTP 1O 401

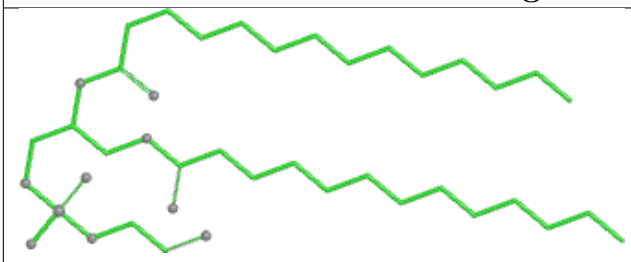


Ligand U10 1H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

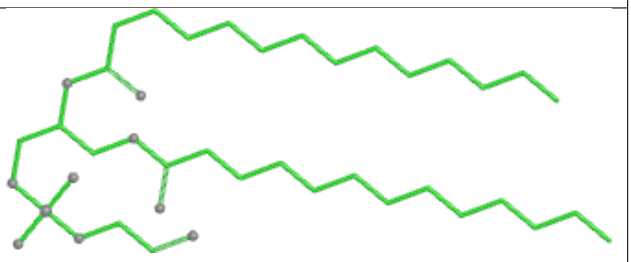
Ligand PC1 1Y 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN 1F 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

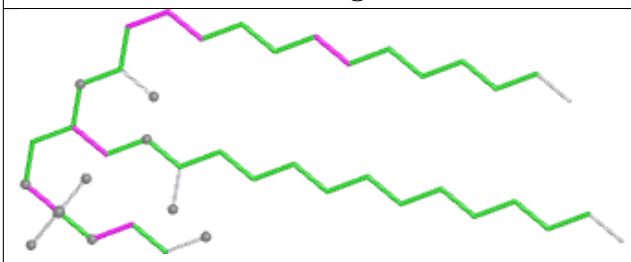
Ligand 3PE 1n 202



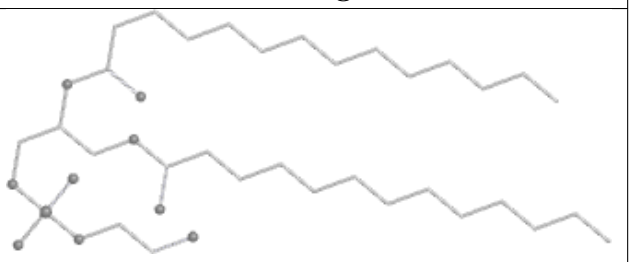
Bond lengths



Bond angles

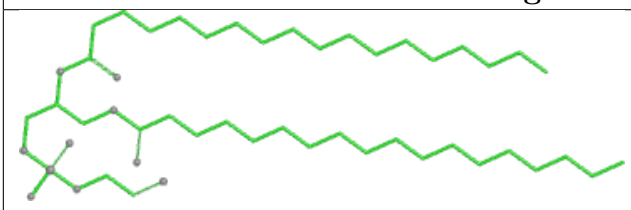


Torsions

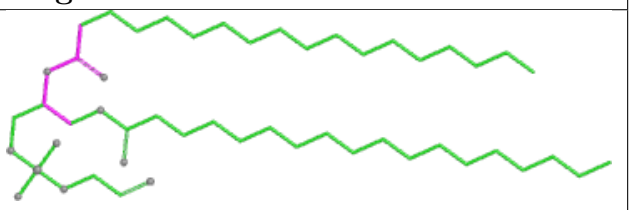


Rings

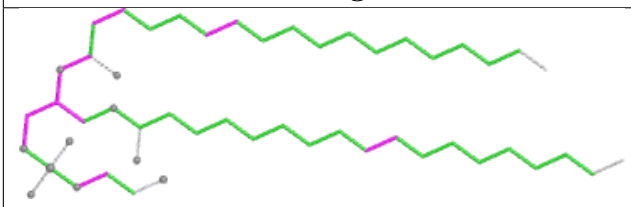
Ligand 3PE 1g 201



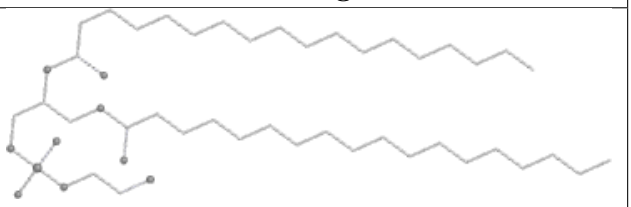
Bond lengths



Bond angles

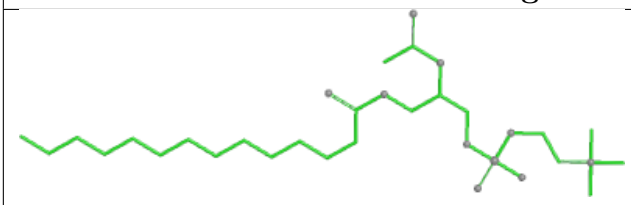


Torsions

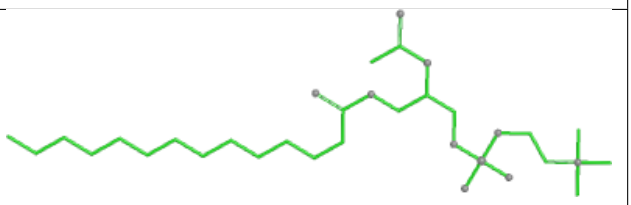


Rings

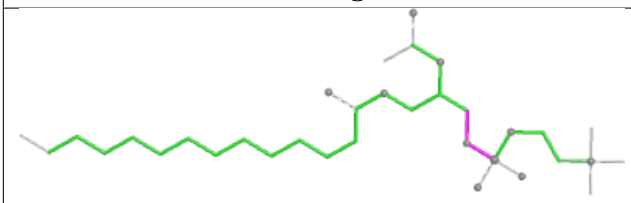
Ligand PC1 1h 201



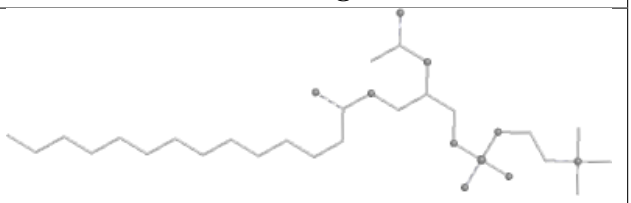
Bond lengths



Bond angles

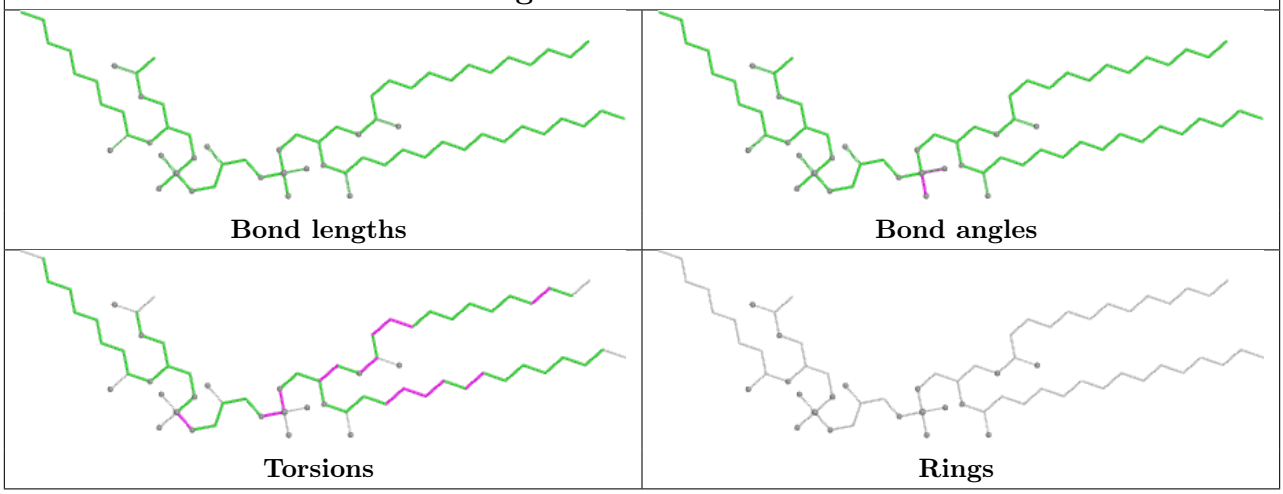


Torsions

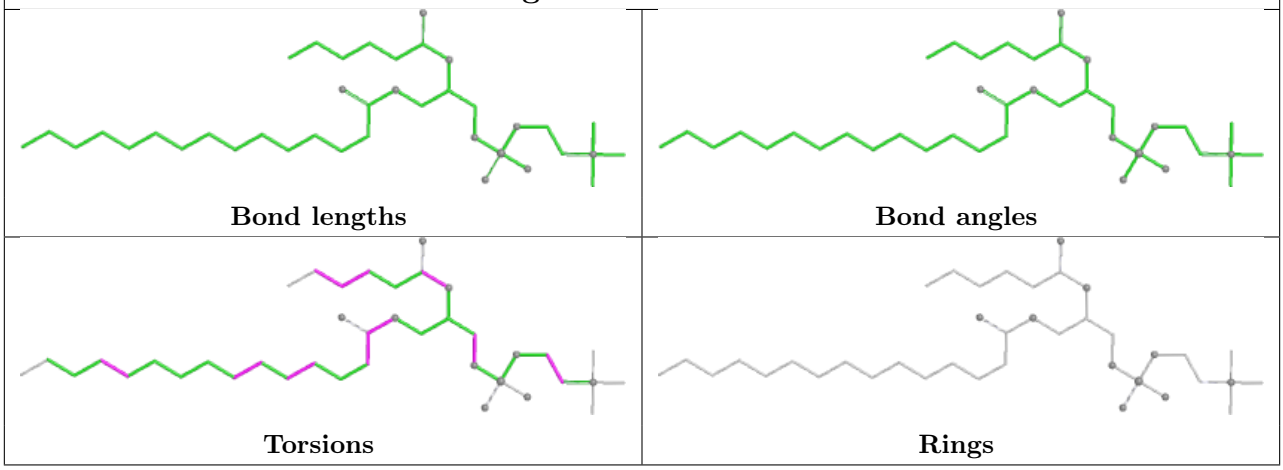


Rings

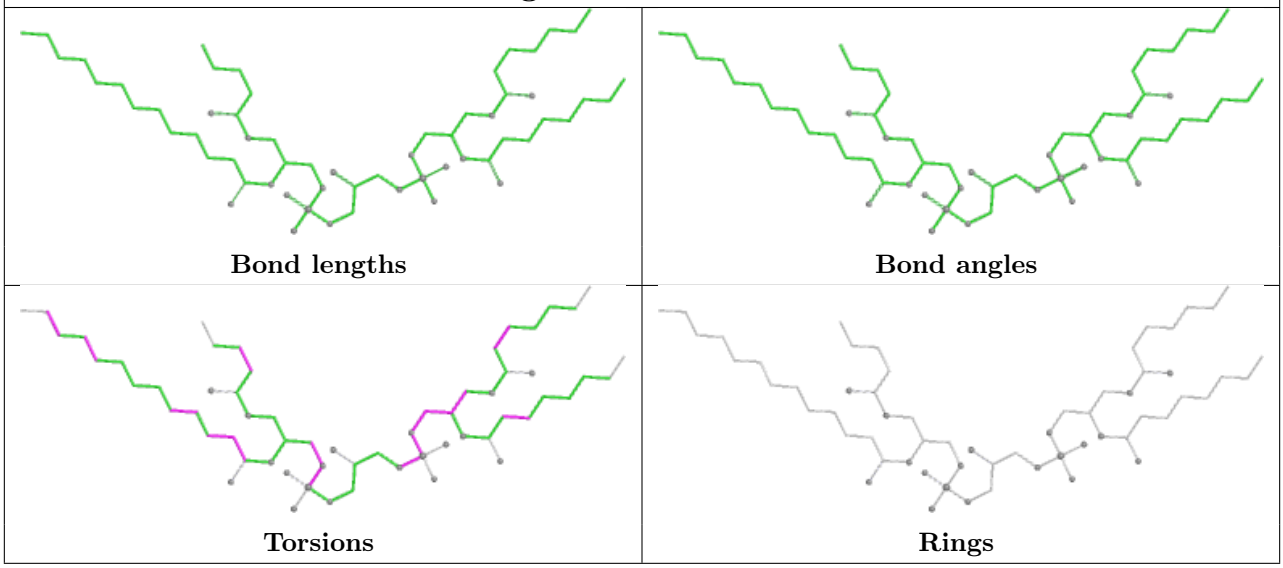
Ligand CDL 1O 403



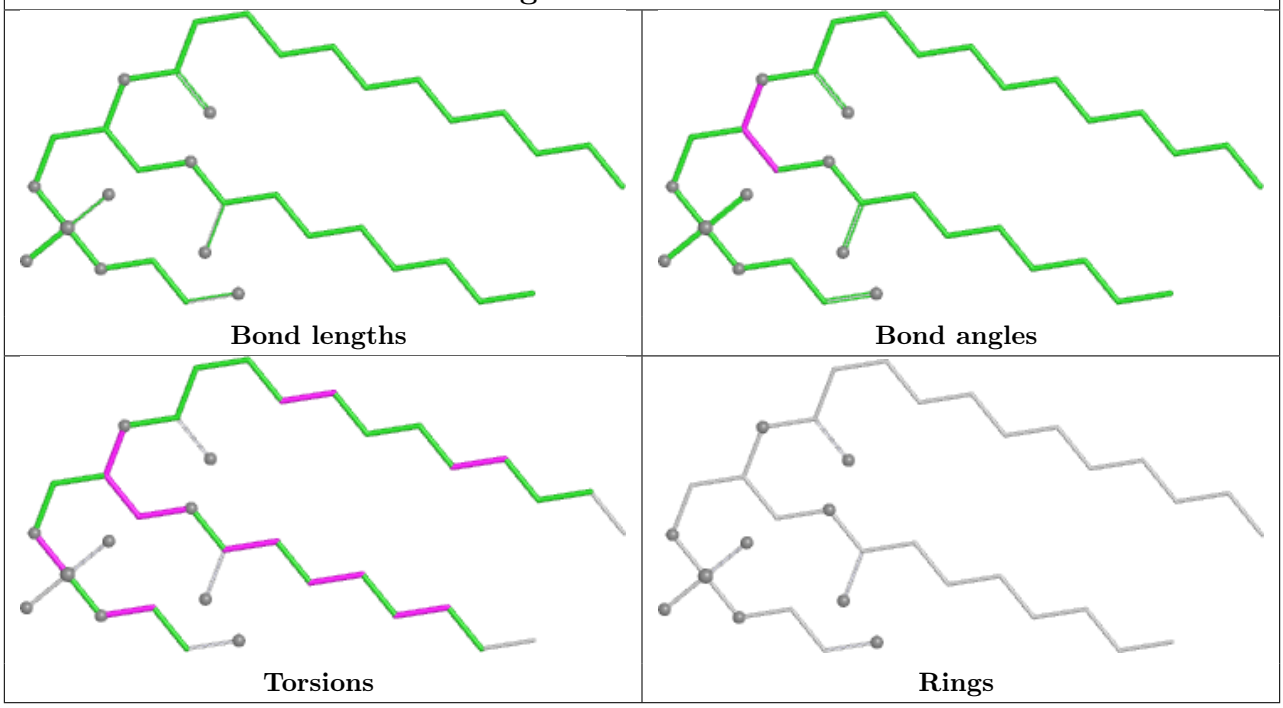
Ligand PC1 1d 201



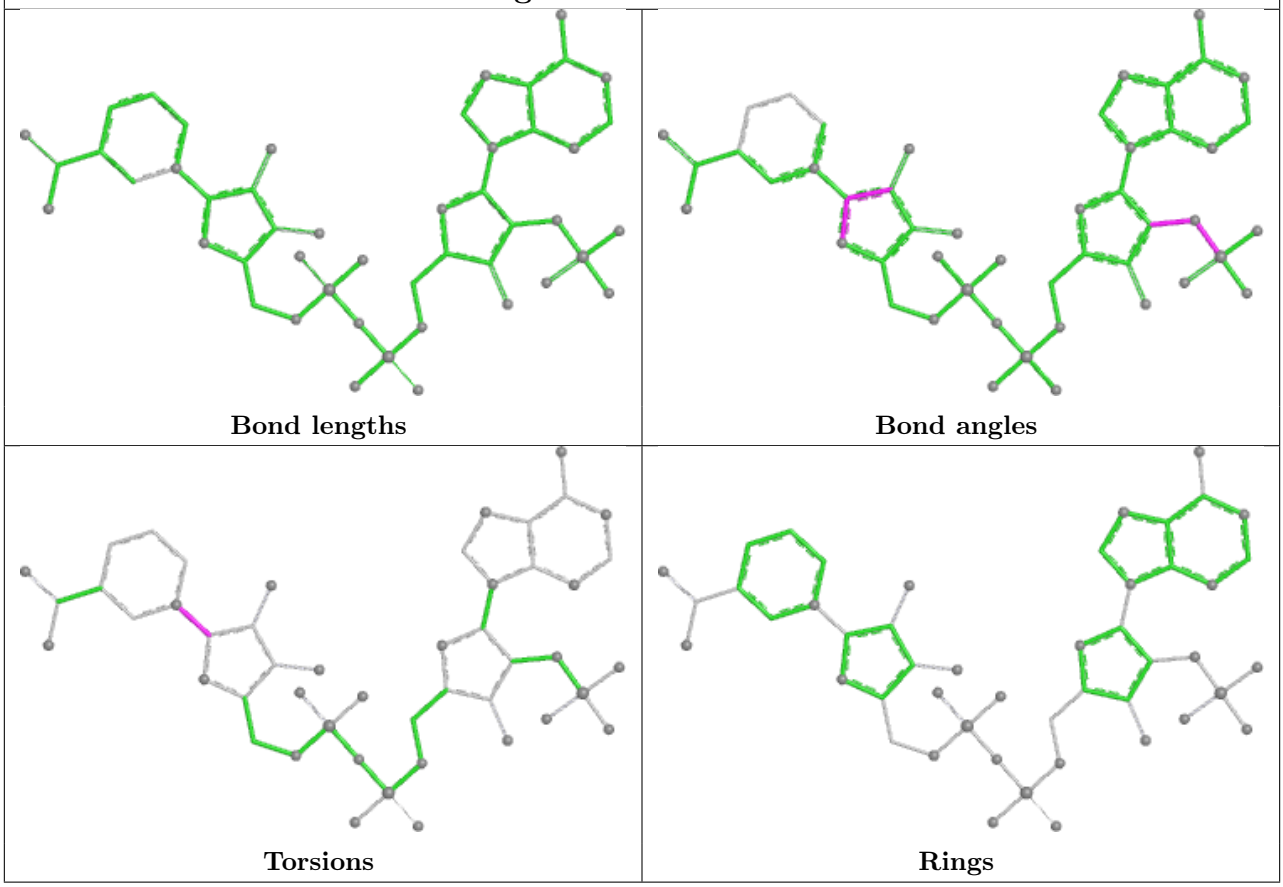
Ligand CDL 1a 101

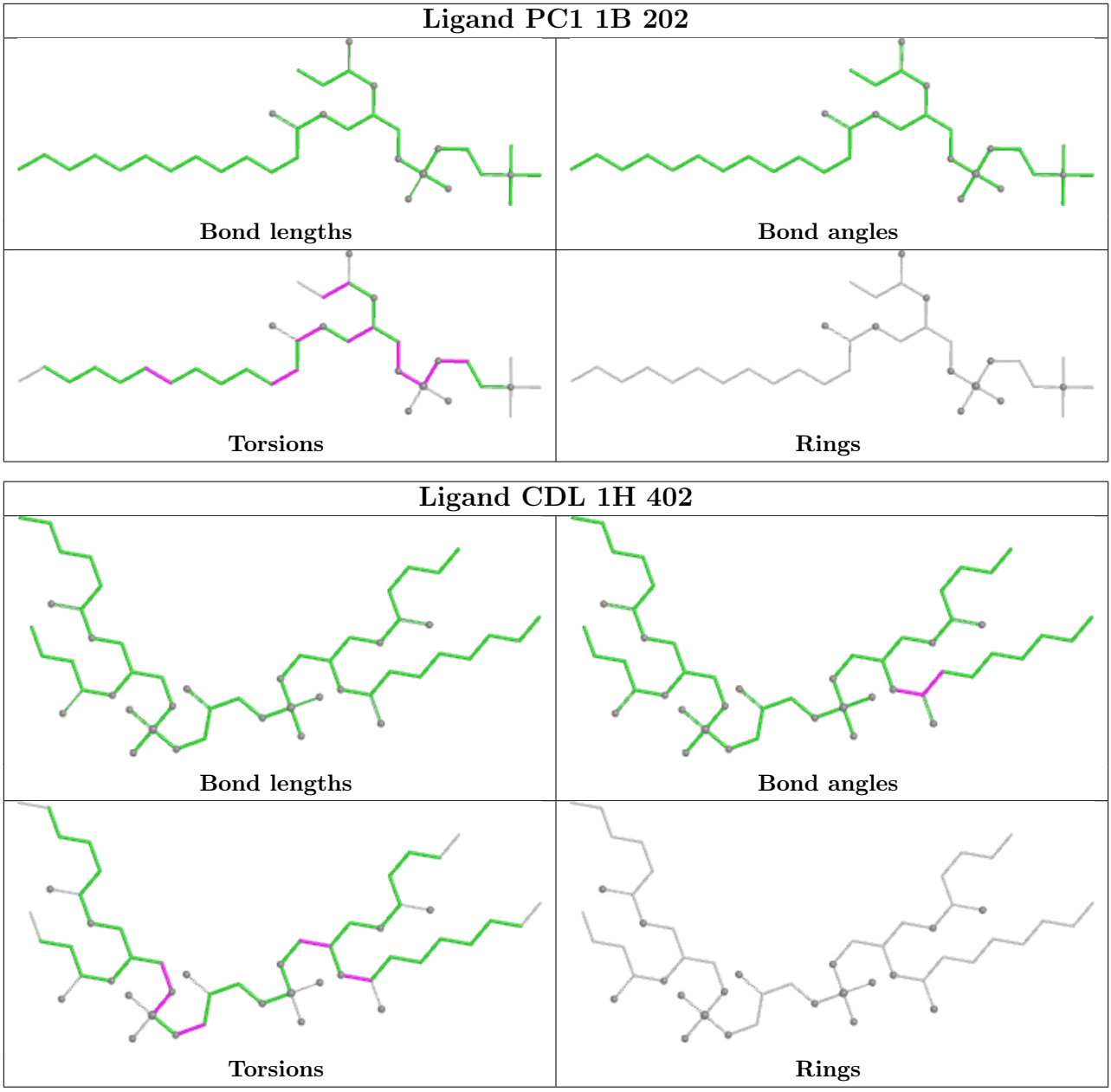


Ligand 3PE 1Y 202



Ligand NDP 1P 501





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	7.02
1	1i	1:SAC	C	2:GLY	N	4.04

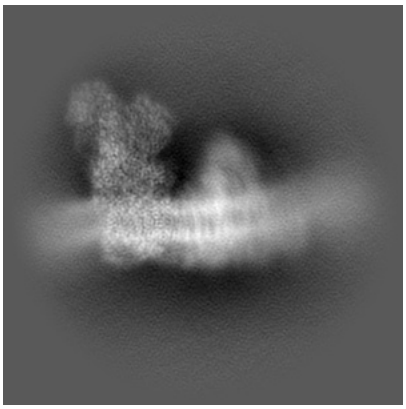
6 Map visualisation (i)

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

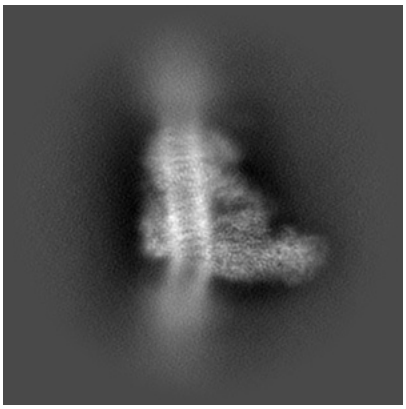
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

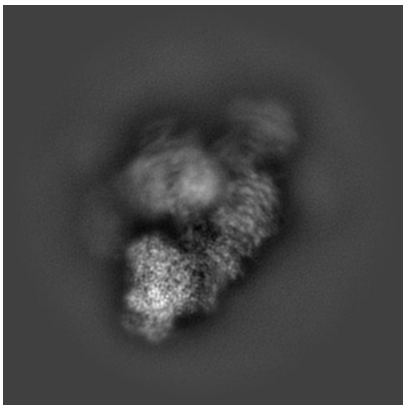
6.1.1 Primary map



X

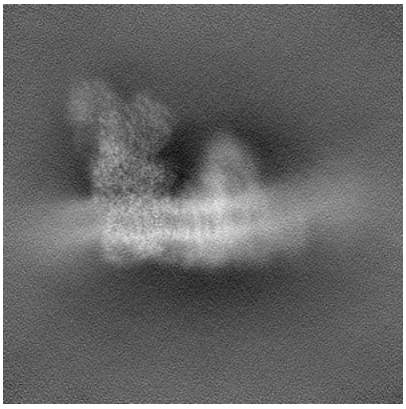


Y



Z

6.1.2 Raw map



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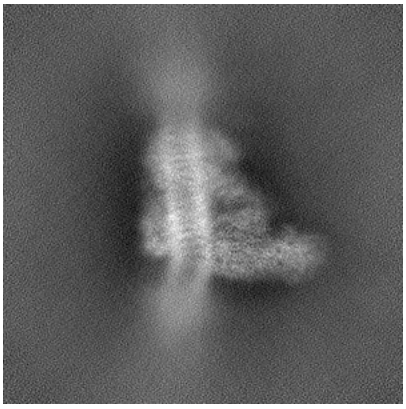
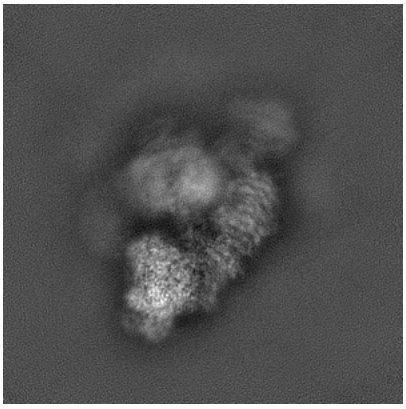


Y

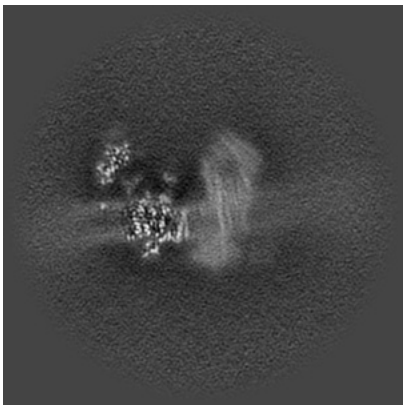


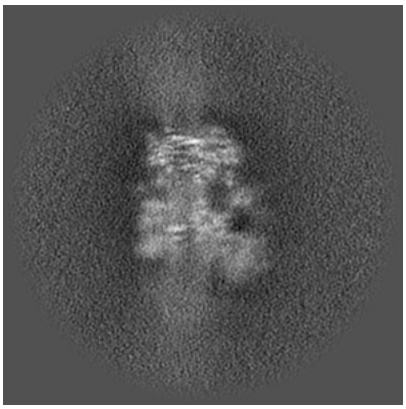
Z

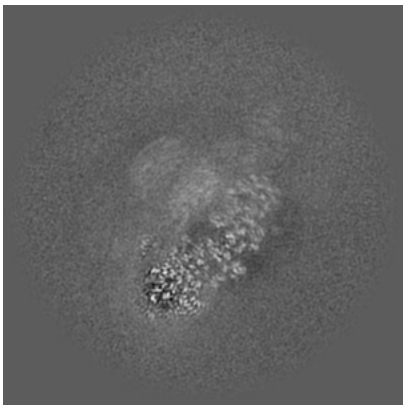
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

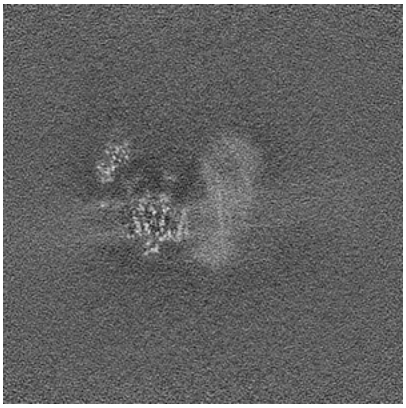
6.2.1 Primary map

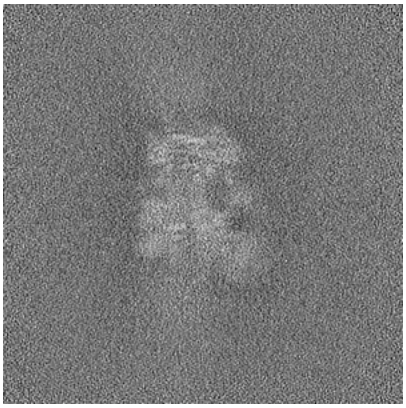

X Index: 160

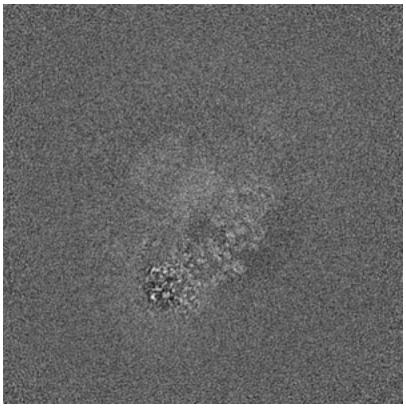

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

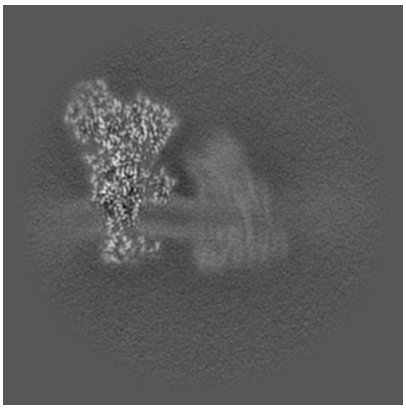

Y Index: 160


Z Index: 160

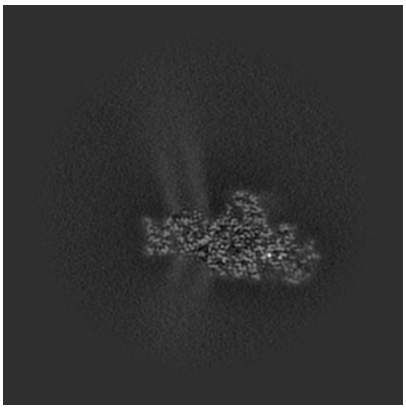
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

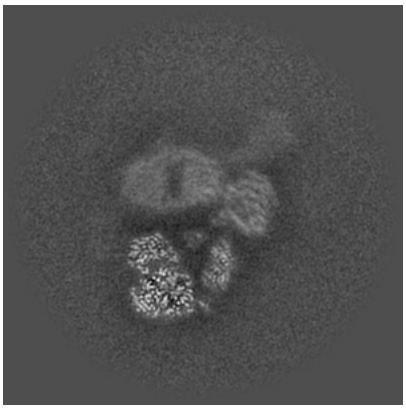
6.3.1 Primary map



X Index: 123

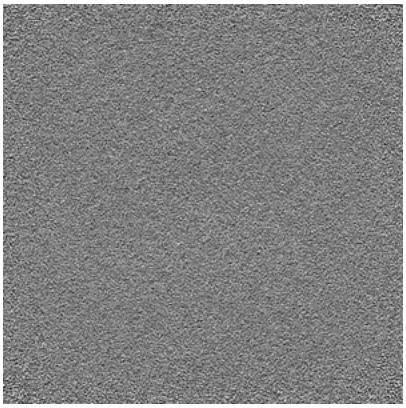


Y Index: 87

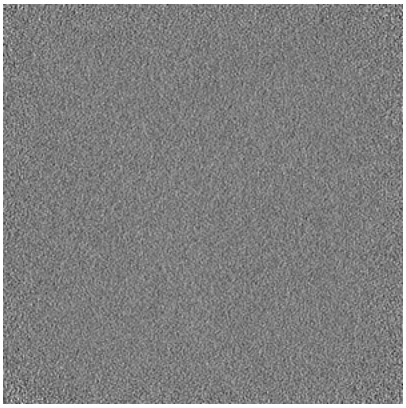


Z Index: 177

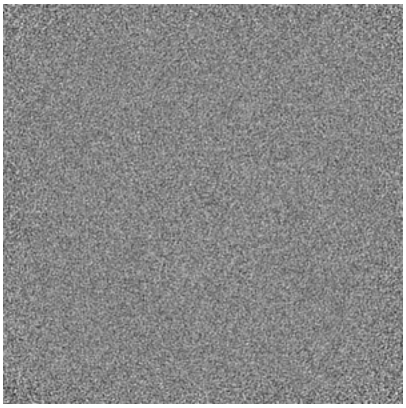
6.3.2 Raw map



X Index: 0



Y Index: 0

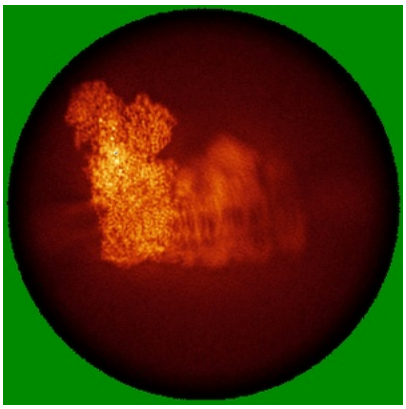


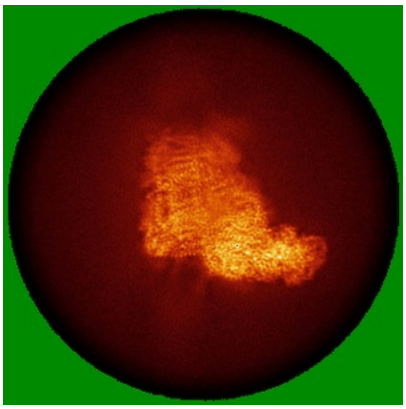
Z Index: 0

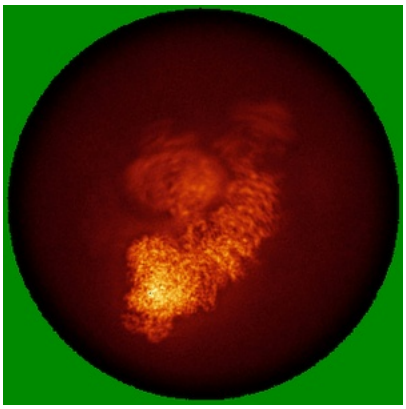
The images above show the largest variance slices of the map in three orthogonal directions.

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

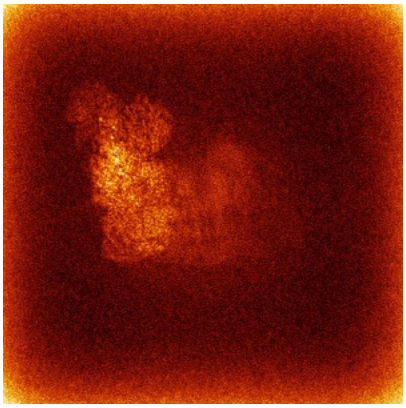
6.4.1 Primary map

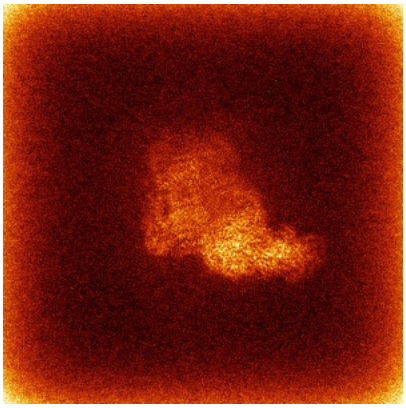

X

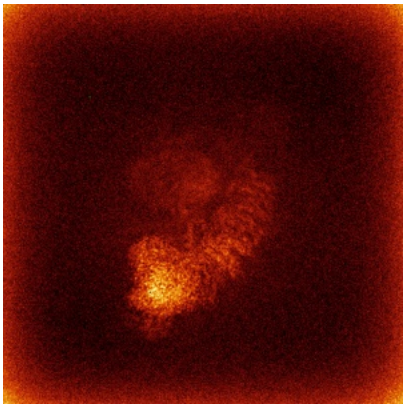

Y


Z

6.4.2 Raw map


X


Y


Z

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

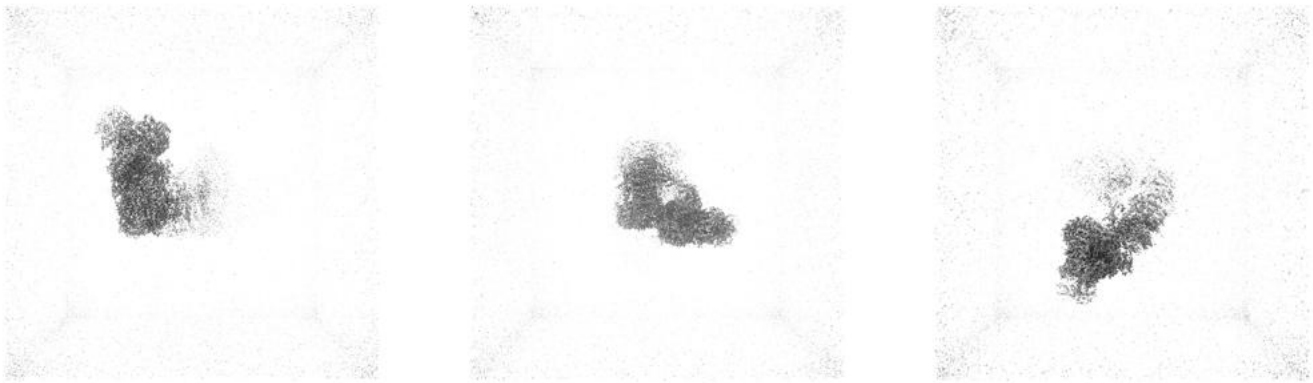
6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

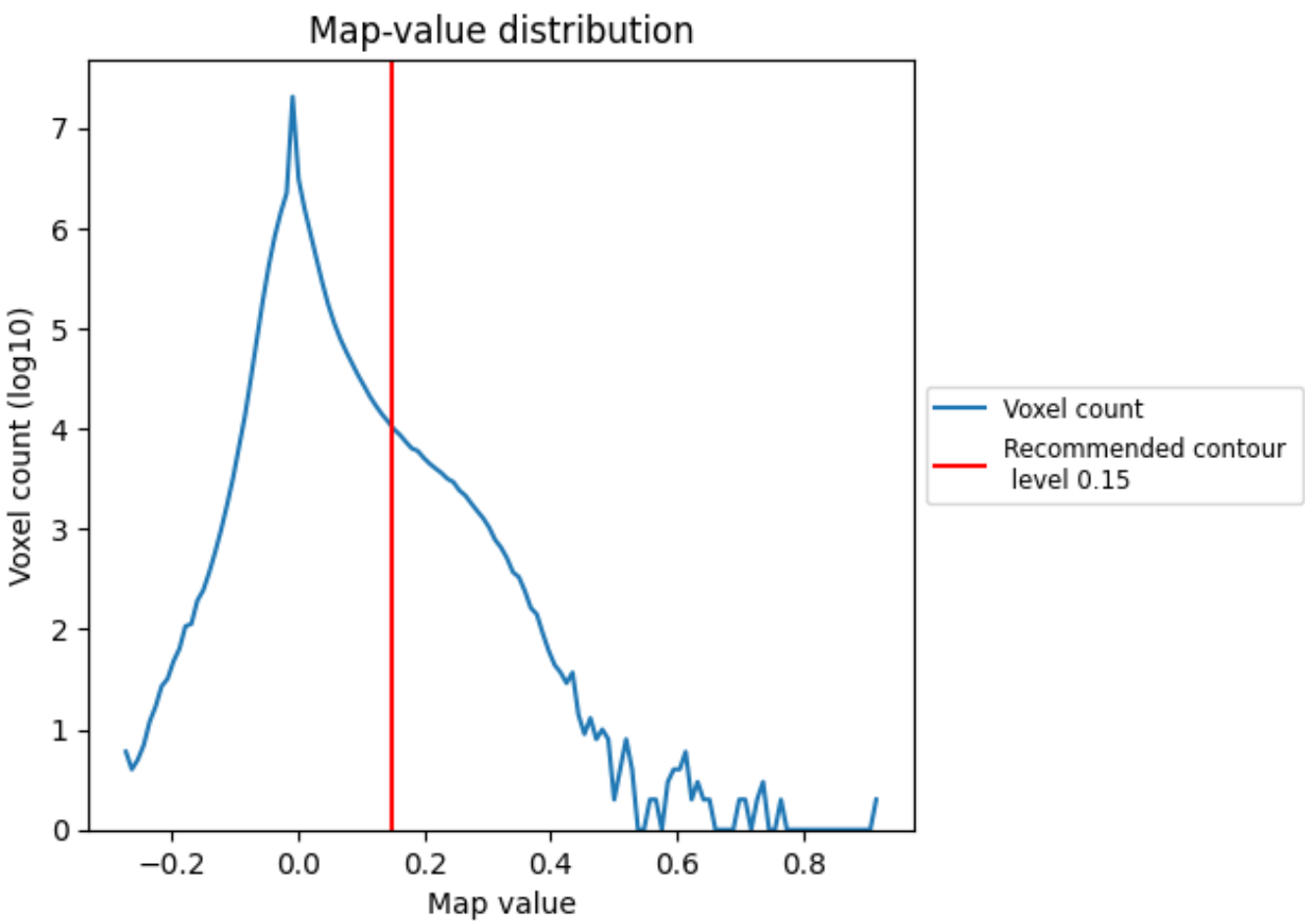
6.6 Mask visualisation (i)

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

7 Map analysis (i)

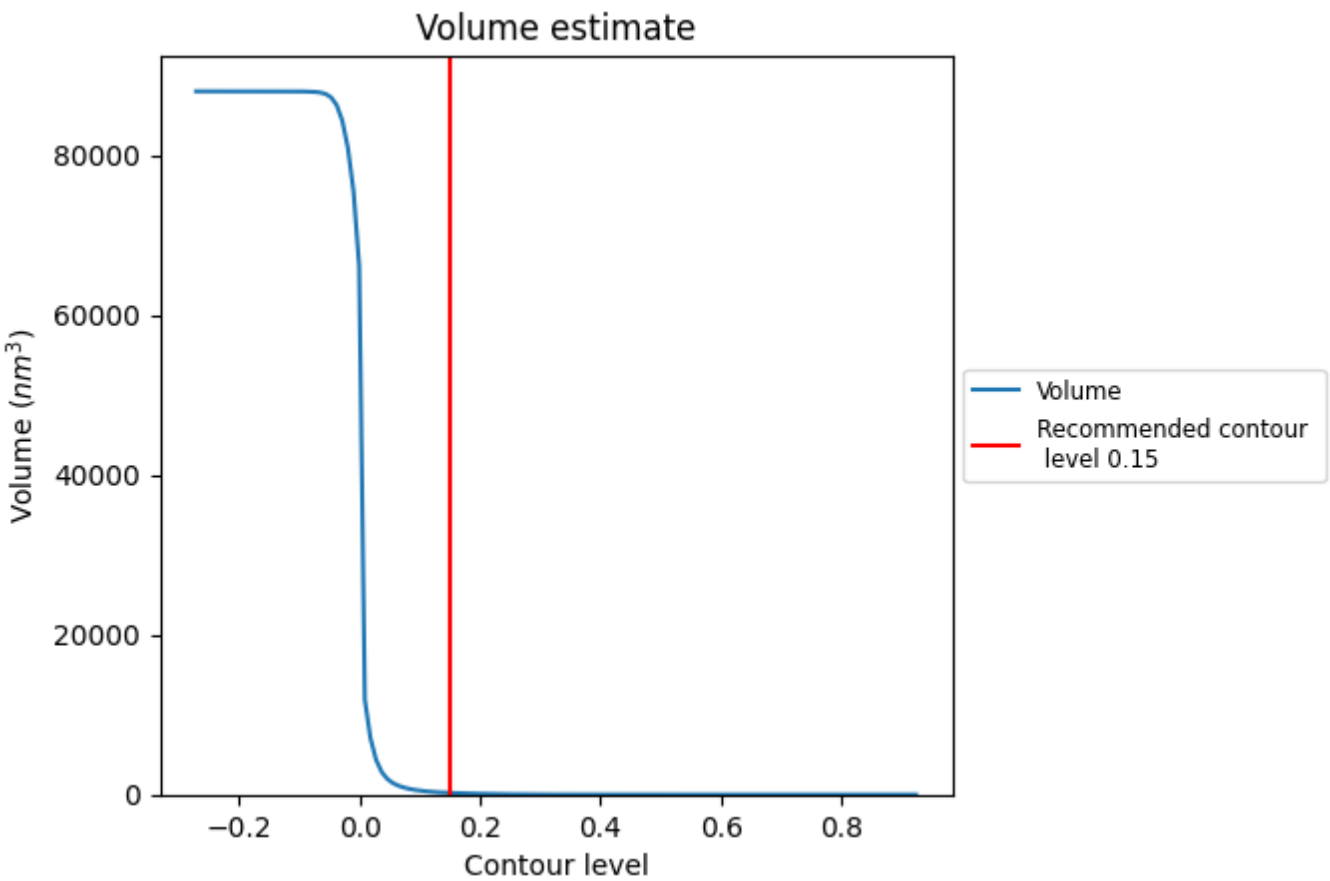
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

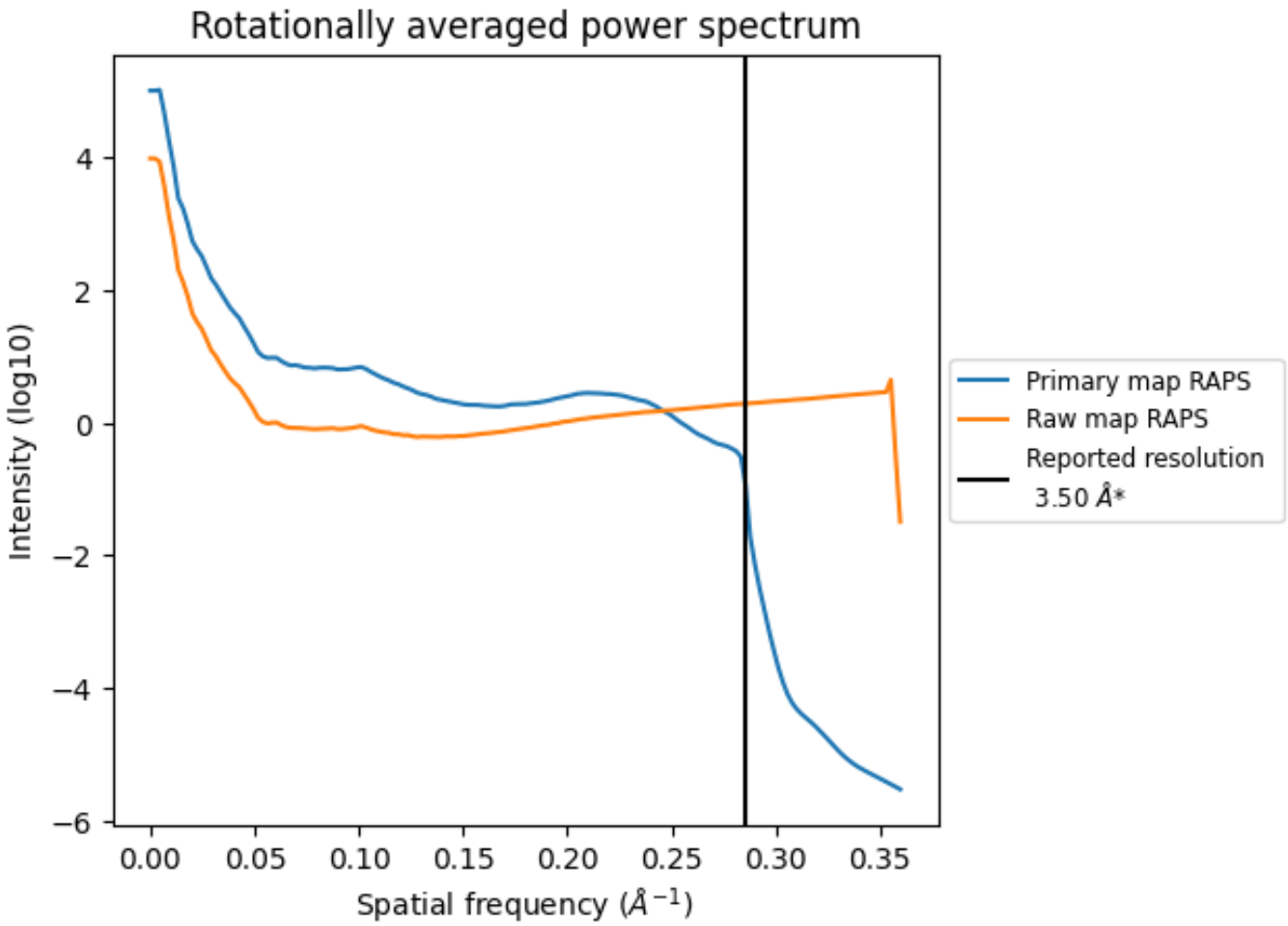
7.2 Volume estimate (i)



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 kDa.

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

7.3 Rotationally averaged power spectrum (i)

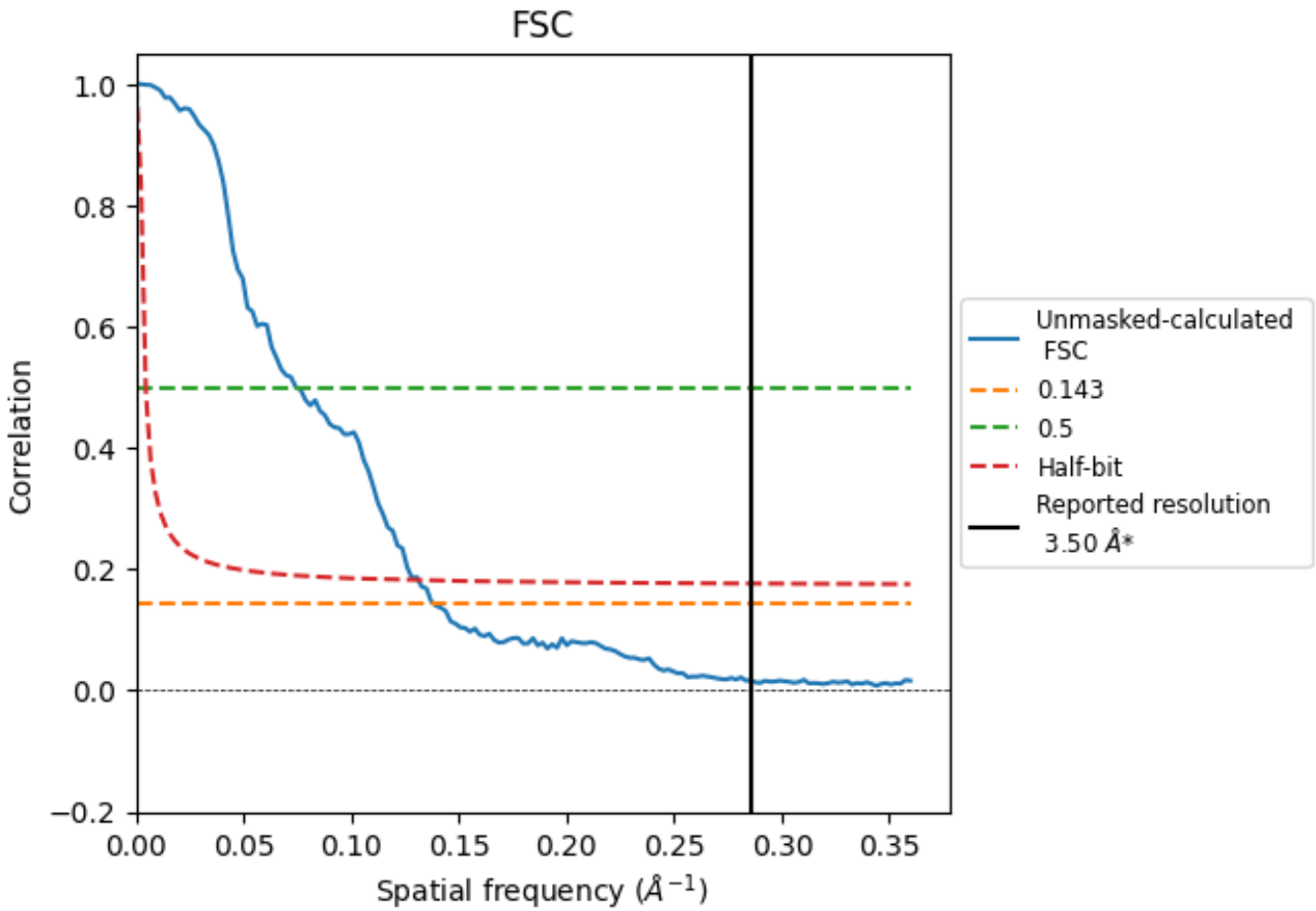


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

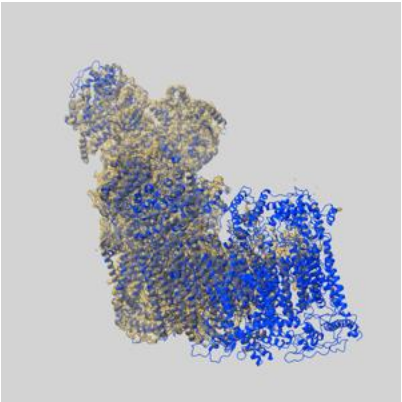
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.24	13.48	7.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.24 differs from the reported value 3.5 by more than 10 %

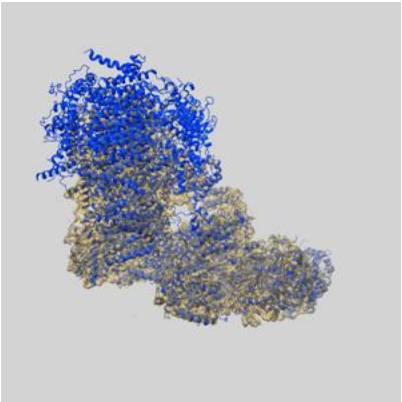
9 Map-model fit (i)

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

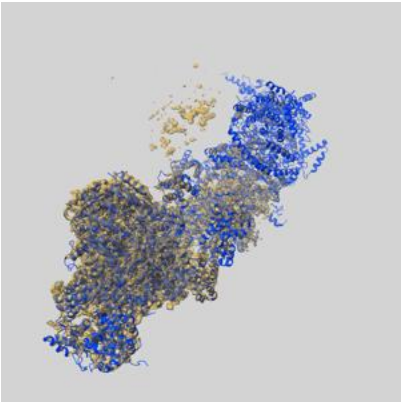
9.1 Map-model overlay (i)



X



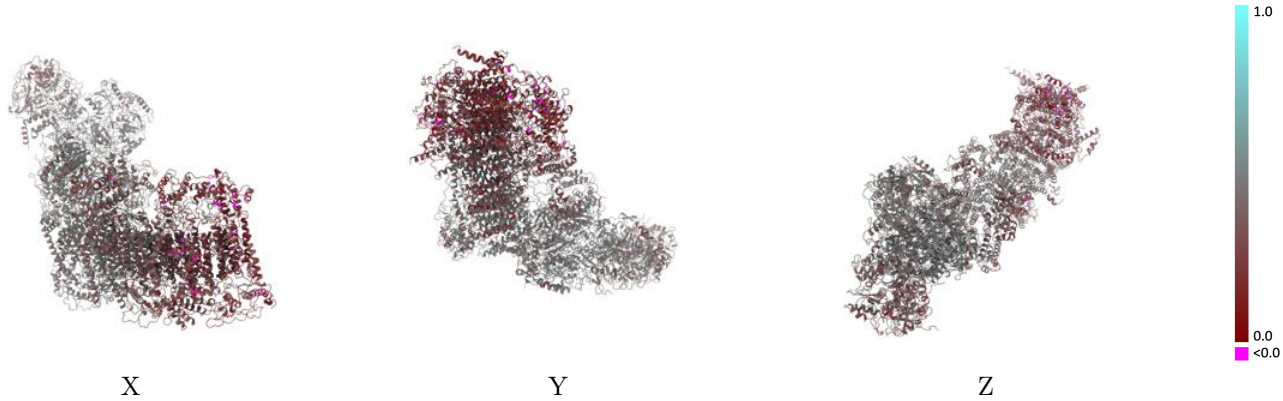
Y



Z

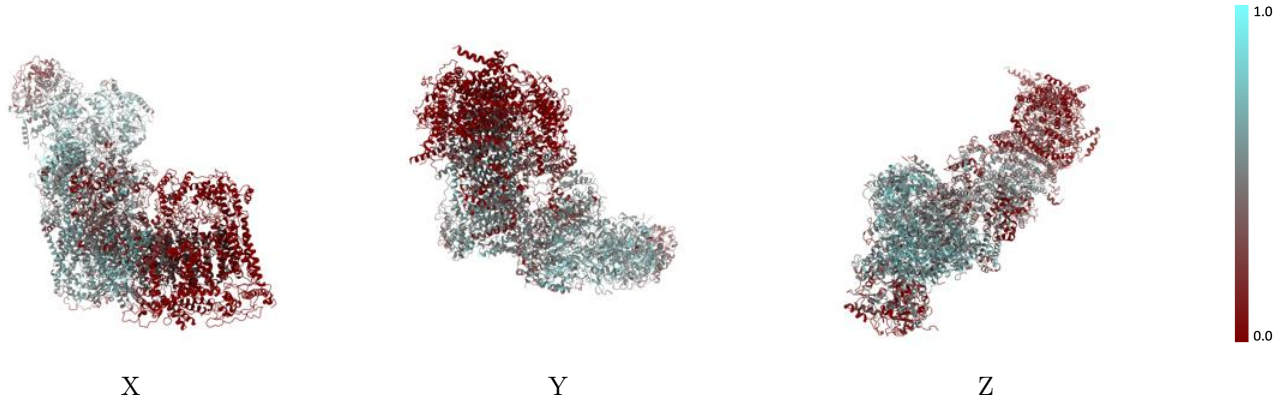
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



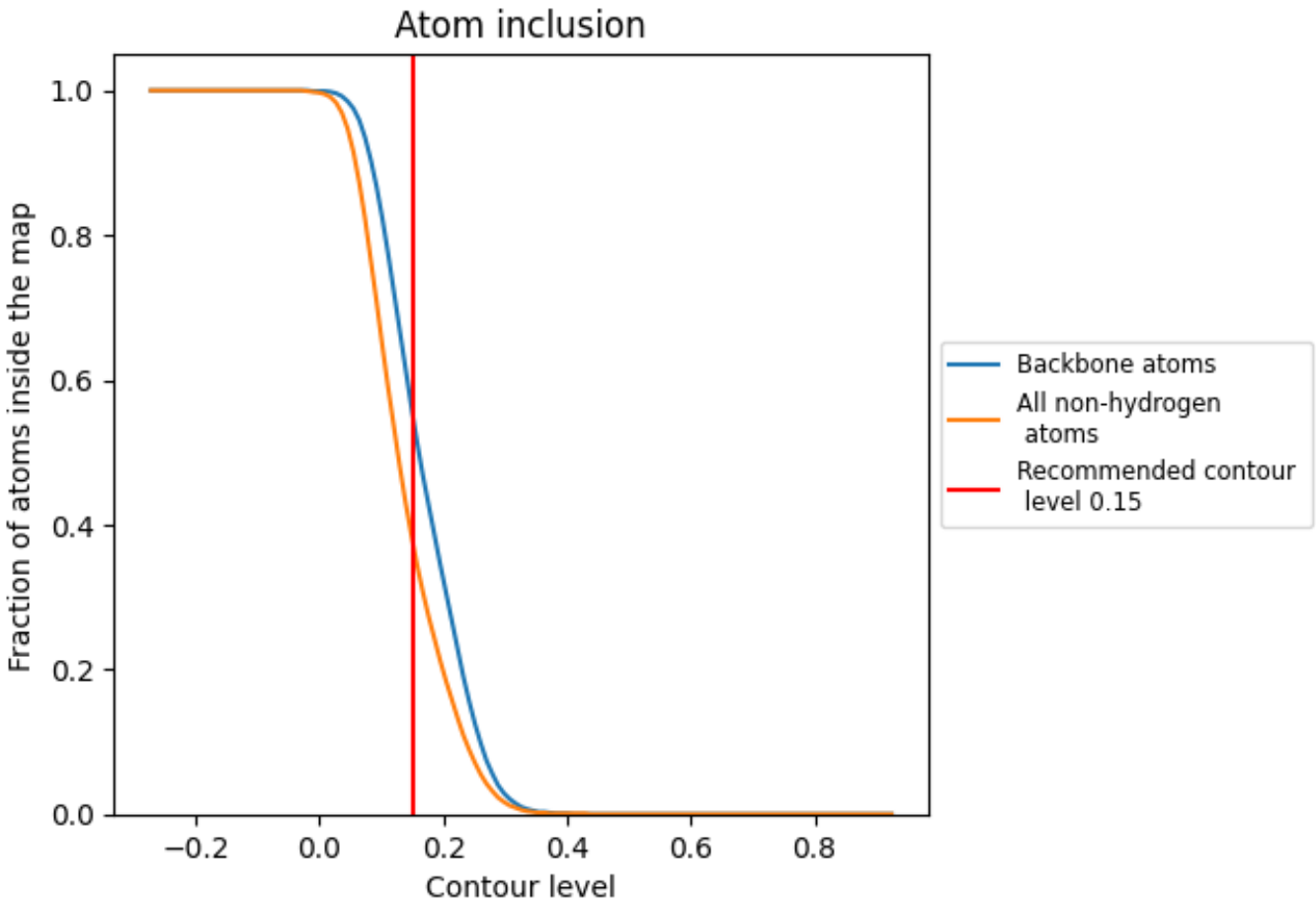
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

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

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

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