wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 08:50 am GMT

PDB ID	:	7AK6
EMDB ID	:	EMD-11811
Title	:	Cryo-EM structure of ND6-P25L mutant respiratory complex I from Mus musculus at 3.8 A
Authors	:	Yin, Z.; Bridges, H.R.; Grba, D.; Hirst, J.
Deposited on	:	2020-09-29
Resolution	:	3.82 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:

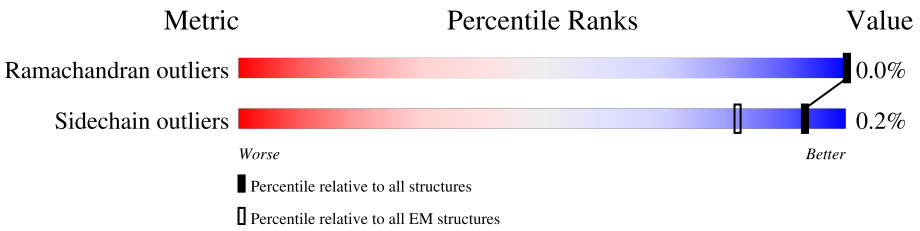
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.82 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	52% 79% • 19%
2	B	224	16% 69% 31%
3	C	263	19% 78% 21%
4	D	463	25% 90% 10%
5	E	248	55% 85% 15%
6	F	464	56% 92% 8%
7	G	727	41% 94% 6%
8	H	318	45% 96% •
9	I	212	16% 84% 16%

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Mol	Chain	Length	Quality of chain
10	J	172	68% 99%
11	K	98	50% 99%
12	L	607	61% 100%
13	M	459	36% 100%
14	N	345	32% 99%
15	O	355	50% 90% 10%
16	P	377	47% 76% 24%
17	Q	175	26% 71% 29%
18	R	116	34% 80% 19%
19	S	99	73% 83% 17%
20	T	156	44% 46% 54%
20	U	156	48% 56% 44%
21	V	116	62% 97%
22	W	131	53% 86% 13%
23	X	172	59% 99%
24	Y	143	85% 98%
25	Z	144	43% 97%
26	a	68	46% 100%
27	b	84	60% 98%
28	c	76	43% 61% 39%
29	d	120	49% 99%
30	e	106	42% 97%
31	f	57	63% 89% 11%
32	g	151	40% 68% 32%
33	h	189	30% 72% 28%

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Mol	Chain	Length	Quality of chain
34	i	128	55% 73% 26%
35	j	105	55% 59% 41%
36	k	104	67% 73% 26%
37	l	186	54% 84% 16%
38	m	129	69% 97%
39	n	179	68% 98%
40	o	137	72% 83% 17%
41	p	176	56% 95% 5%
42	q	145	48% 98%
43	r	112	48% 85% 14%
44	s	104	32% 38% 62%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 65323 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	A	93	761	527	105	124	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	793	222	212	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

- 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	D	417	3369	2155	576	614	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1639	1043	275	310	11	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	F	428	3301	2080	590	609	22	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	G	686	5281	3313	917	1010	41	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	H	305	2441	1642	367	411	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	I	178	1408	885	243	268	12	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	J	171	1278	858	185	220	15	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	K	98	737	477	112	137	11	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	L	606	4800	3182	746	827	45	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	M	459	3632	2408	567	617	40	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	N	344	2696	1791	416	452	37	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	O	319	2599	1668	430	491	10	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	288	2281	1453	412	409	7	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	Q	125	1015	642	179	190	4	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	R	94	738	458	135	142	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	S	82	659	413	125	118	3	0	0

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	72	584	376	86	117	5	0	0
20	U	88	706	453	104	144	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	112	915	596	152	164	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	W	114	970	619	180	165	6	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	X	171	1396	889	250	247	10	0	0

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1037	662	175	192	8	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	139	1152	741	204	199	8	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	a	68	556	360	99	93	4	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	b	82	643	422	104	113	4	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	S		
28	c	46	381	249	66	65	1	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	d	119	985	645	167	164	9	0	0

- 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	e	104	870	550	161	151	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	51	433	278	78	75	2	0	0

- 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	g	102	858	555	137	162	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	h	137	1153	756	192	202	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	i	95	802	524	138	137	3	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	62	537	355	88	93	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	k	77	626	414	106	104	2	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	l	156	1312	846	219	236	11	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	m	125	1044	673	188	183	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	n	176	1527	976	274	266	11	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	o	114	984	620	185	171	8	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	p	168	1424	896	256	264	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	q	143	1192	766	212	210	4	0	0

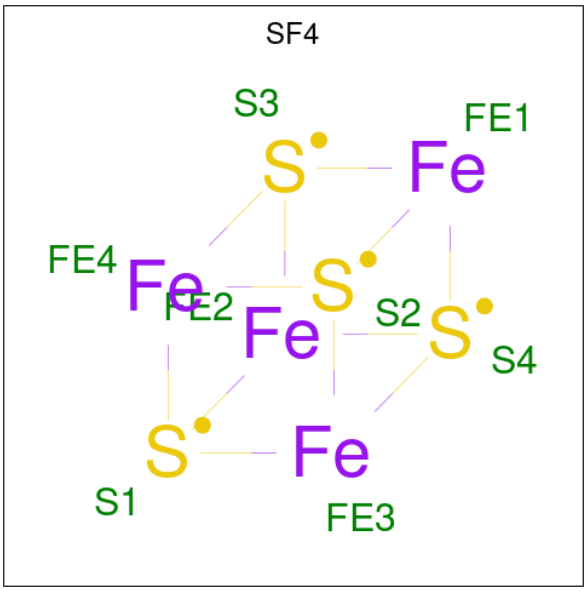
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	96	776	490	145	138	3	0	0

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

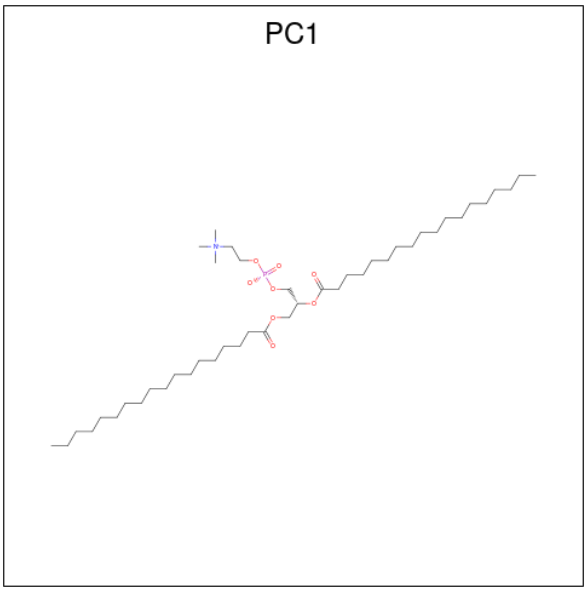
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	s	39	329	207	59	63	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



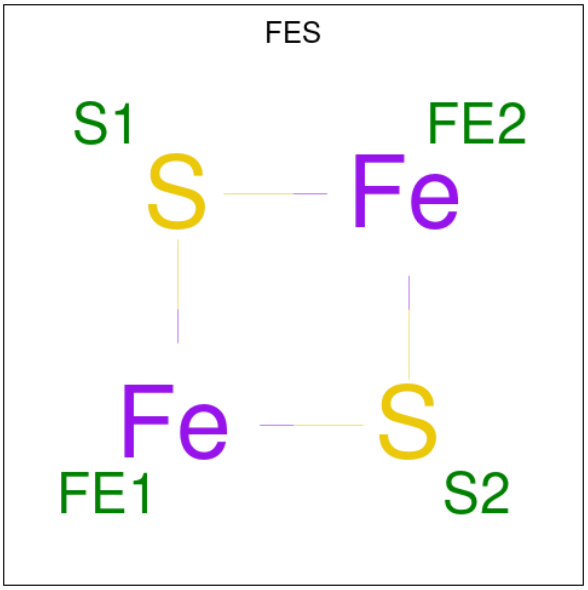
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	B	1	8	4	4	0
45	F	1	8	4	4	0
45	G	1	16	8	8	0
45	G	1	16	8	8	0
45	I	1	16	8	8	0
45	I	1	16	8	8	0

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



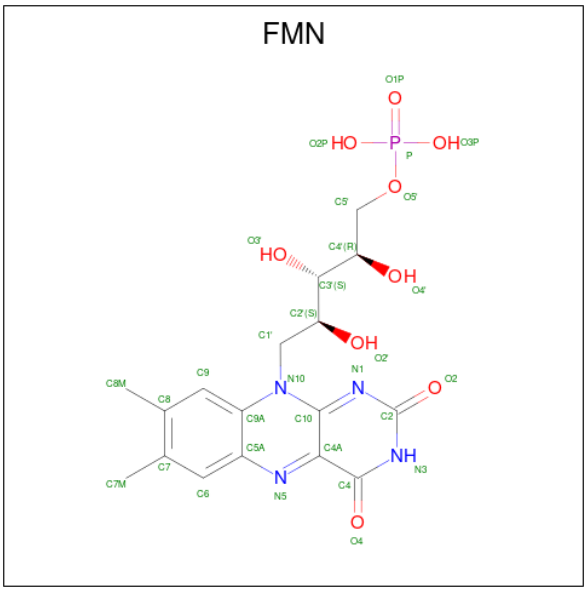
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	B	1	26	16	1	8	1	0

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



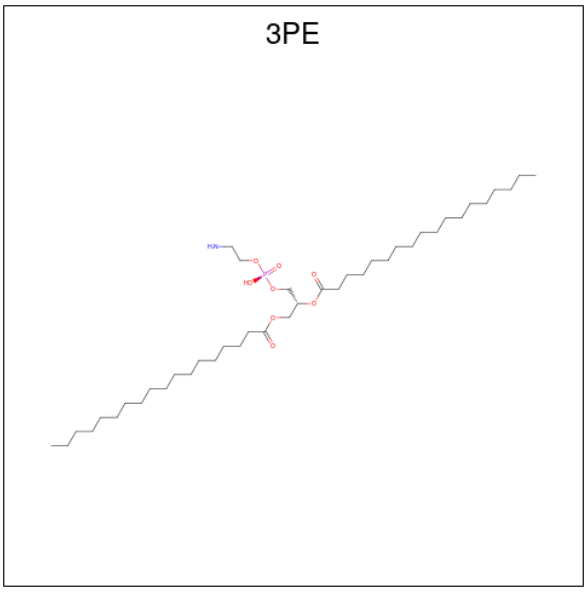
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	E	1	4	2	2	0
			Total	Fe	S	
47	G	1	4	2	2	0

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



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

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	H	1	42	32	1	8	1	0
			Total	C	N	O	P	
49	J	1	38	28	1	8	1	0

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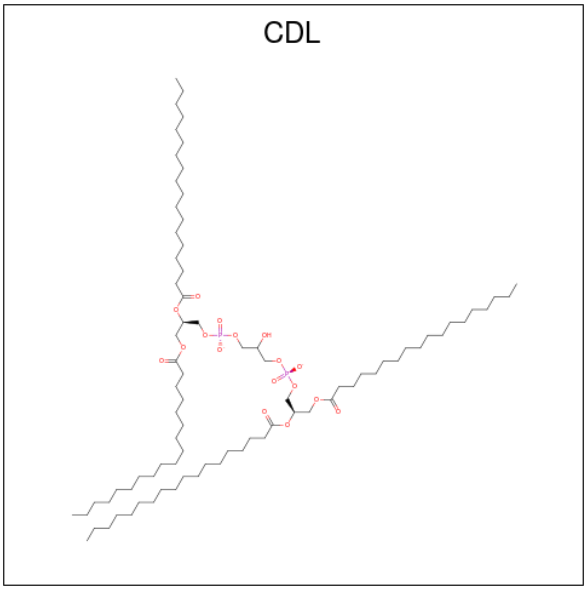
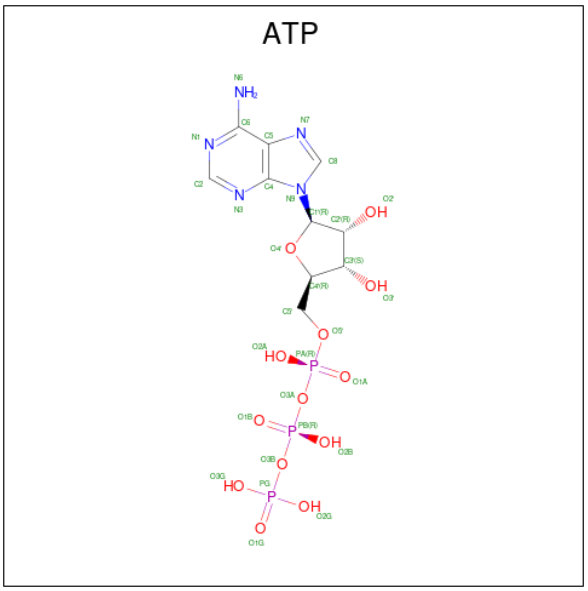
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	L	1	45	35	1	8	1	0
49	M	1	38	28	1	8	1	0

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



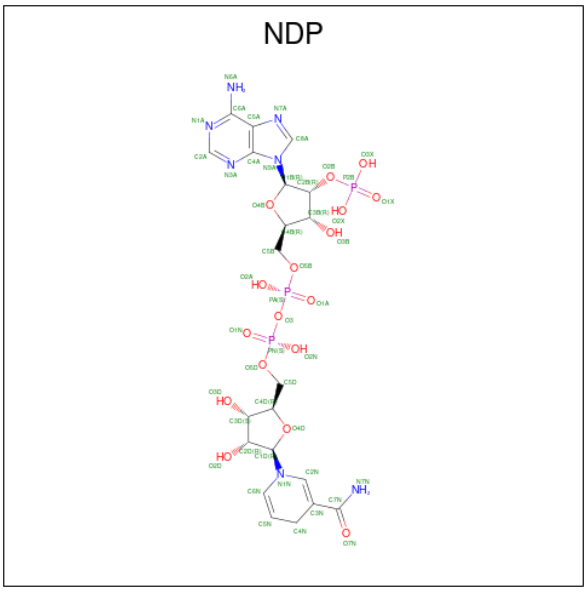
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
50	L	1	54	35	17	2	0
50	d	1	50	31	17	2	0

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	O	1	31	10	5	13	3	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

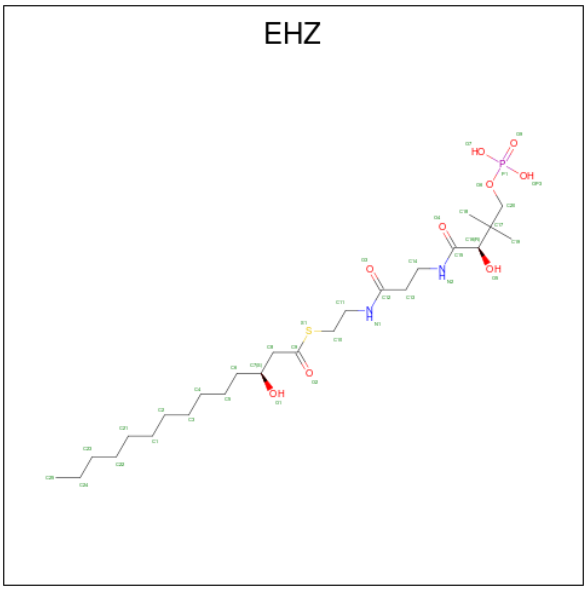


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	P	1	48	21	7	17	3	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



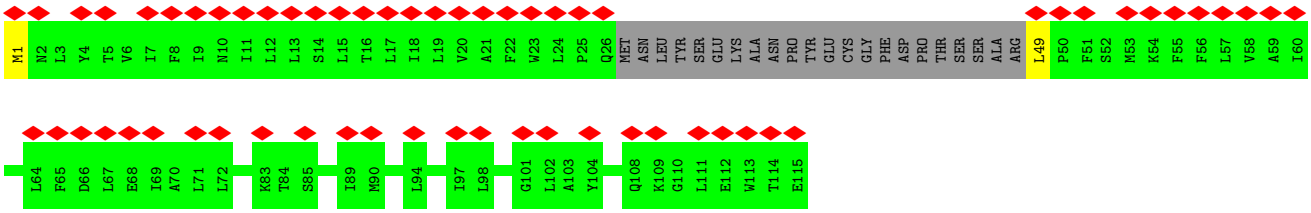
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
54	T	1	37	25	2	8	1	1	0
			Total	C	N	O	P	S	
54	U	1	37	25	2	8	1	1	0

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.

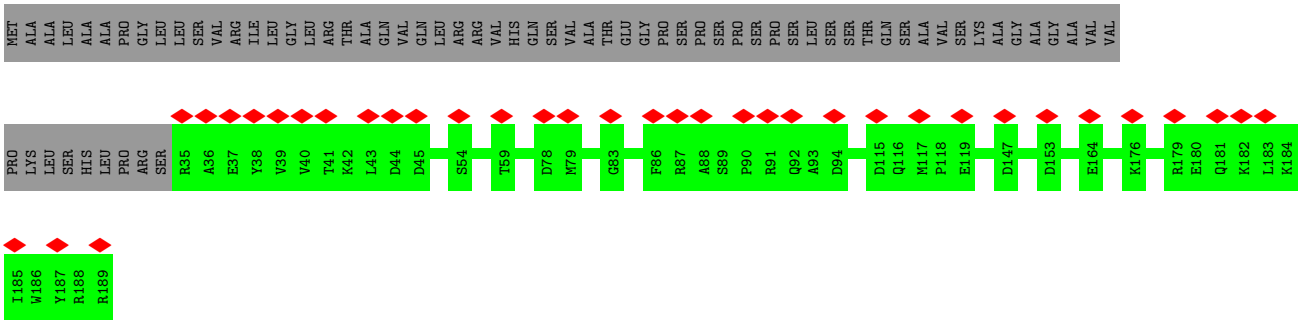
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 52% 79% • 19%



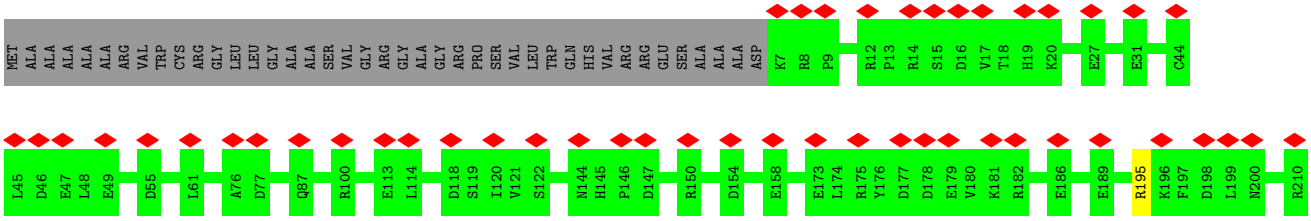
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

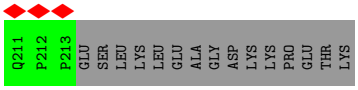
Chain B: 16% 69% 31%



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

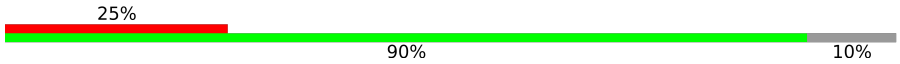
Chain C: 19% 78% 21%

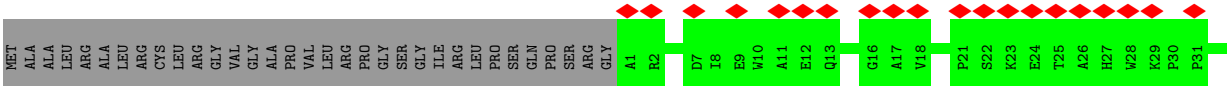


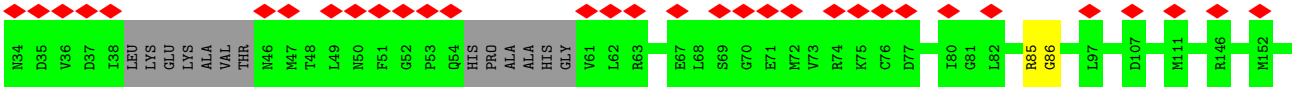


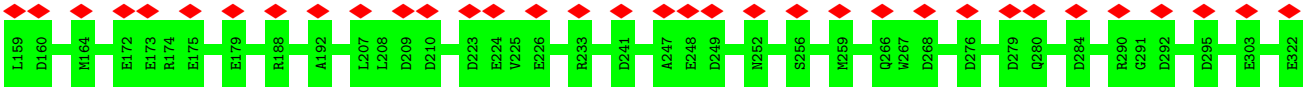
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

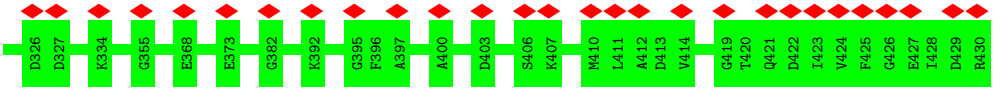
Chain D:





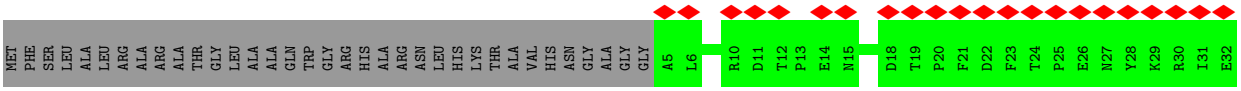


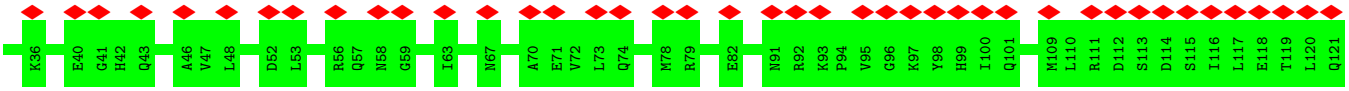


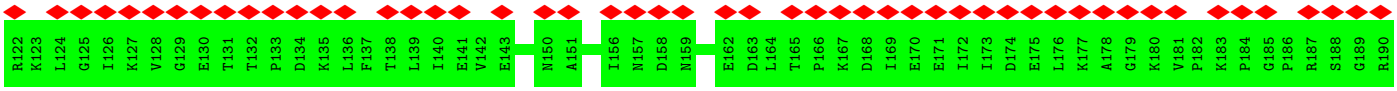


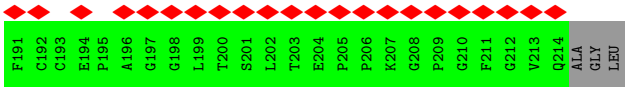
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



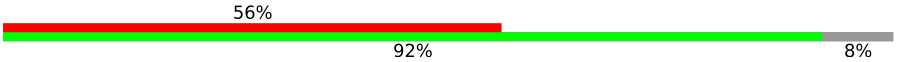


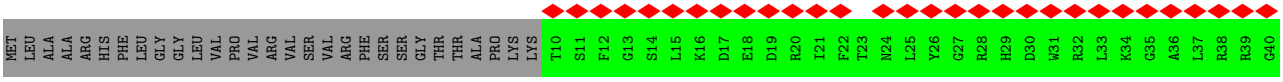




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:





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H113 D114 P115 H116 K117 L118 V119 E120 G121 C122 G126 R127 A128 M129 G130 A131 G140 E141 E145 A146 S147 N148 I153 R154 E155 A156 Y157 E158 A159 G160 L161 I162 G163 K164 N165 A166 C167 G168 S169 D170 Y171 D172 F173 D174 R179 G180 A181 G182 E189 E194 S195 I196 E197

G201 R204 L205 K206 F209 D212 G217 N224 V225 E226 A229 V230 S231 C235 R236 R237 G238 G239 T240 V241 F242 A243 G244 F245 G246 R247 E248 R249 N250 S251 G252 T253 K254 N257 I258 S259 G260 H261 V262 N263 H264 P265 E269 E270 E271 M272 S273 V274 P275 L276

K277 E278 L279 I280 E281 K282 H283 A284 G285 G286 V287 T288 G289 G290 W291 D292 N293 L294 L295 A296 G300 G301 S302 S303 L306 K309 S310 V311 C312 E313 T314 V315 L316 M317 D318 F319 D320 A321 L322 V323 Q324 A325 Q326 T327 G328 L329 G330 T331 A332 A333 M337 D338 R339 S340 T341 D342

I343 V344 K345 A346 H356 D370 N373 V380 K381 G382 D383 A384 R385 P386 A387 D390 K397 D409 G410 I419 R420 H421 F422 R423 P424 E425 L426 E427 D428 R429 M430 Q431 R432 F433 A434 Q435 Q436 H437 ARG ALA TRP GLN ALA ALA SER

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

Chain G: 41% 94% 6%

MET LEU ARG ILE PRO ILE LYS ARG ALA LEU ILE GLY LEU SER ASN SER PRO LYS GLY TYR VAL ARG THR THR GLY THR ALA ALA SER N7 L8 I9 E10 V11 F12 V13 D14 G15 Q16 M19 V20 E21 P22 G23 E44 E58 I59 E60 K61 A62 P63 K64 M74 K75 G76 W77

N78 N82 S128 R129 F130 L131 E132 E138 D139 K140 N141 K147 G168 V169 D170 D171 N179 D180 M181 Q182 E188 K189 M190 F191 M192 S193 E194 L195 S196 D201 R223 D229 Y230 M231 D232 A233 R243 T244 M254 H255 E256 D265 L274 E281

R285 N286 E287 K288 G289 L290 Y293 E297 D298 A304 G305 M306 L307 Q308 N309 F310 E311 G312 N313 A314 V315 A316 A319 G320 G321 L322 V323 D324 D333 L334 L335 N336 K337 V338 D339 S340 D341 N342 L343 E346 E347 I348 F349 P350 T351 E352 G353 A354 G355 T356 D357 L358 R359 S360

N365 T366 T367 I368 A369 G370 V371 E372 E373 A374 D375 G381 T382 N383 E387 A388 P389 L390 R394 N402 D403 S411 P412 V413 D414 L415 T416 Y417 R418 Y419 D420 H421 L422 G423 D424 S425 P426 K427 I428 L429 Q430 D431 I432 A433 S434 G435 R436 H437 S438 F439 C440 E441 V442 L443

K444 D445 A446 K447 K448 G454 S455 L458 Q459 R460 D461 D462 G463 A464 A465 I466 L467 V468 A469 V470 S471 N472 M473 V474 Q475 K476 I477 R478 V479 T480 T481 G482 V483 A484 A485 E486 M490 N491 I492 L493 H494 R495 I496 A497 S498 D504 L505 K508 P509 G510 V511 E512 A513 I514 R515

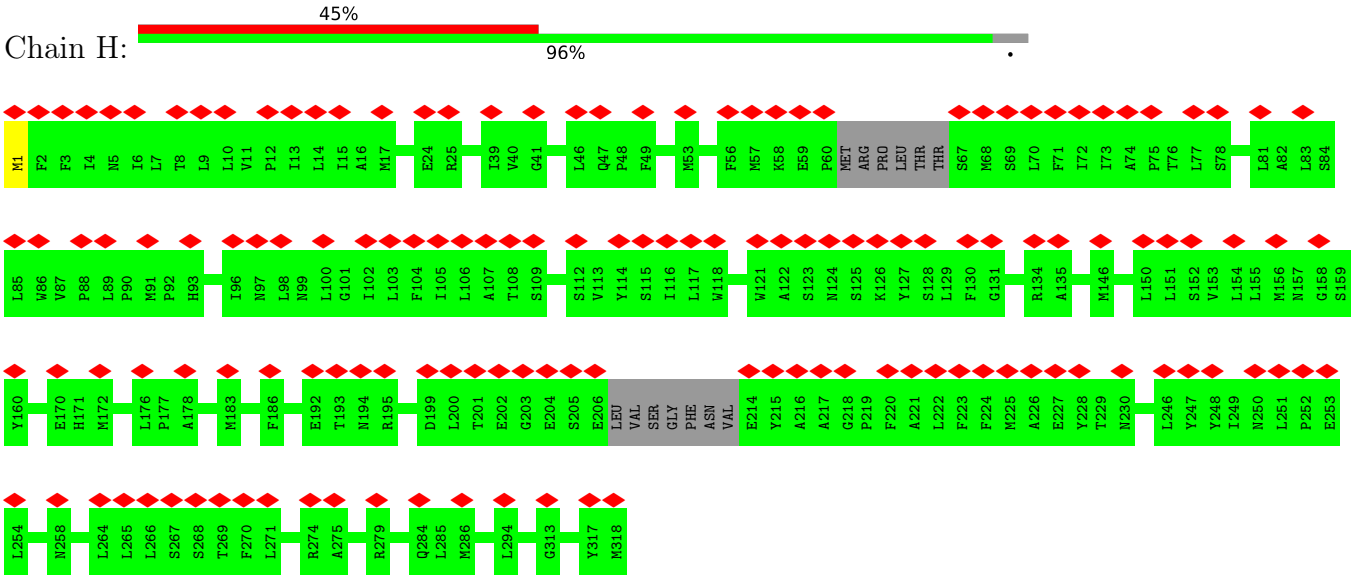
K516 N517 P518 P519 K520 M521 L522 L525 G526 A527 D528 G529 G530 C531 I532 T533 R534 Q535 D536 L537 P538 K539 D540 C541 F542 D551 V552 G553 A554 P555 M556 A557 D558 G563 A564 N575 T576 E577 G591 L592 E595 D596 W597 K598 E605 I606 A607 G608 I609 T610 L611 P612 Y613

D614 T615 L616 D617 R620 N621 R622 L623 E624 E625 M629 R632 Y633 D634 D635 I636 E637 E638 T639 N640 Y641 F642 Q643 Q644 A645 S646 E647 K650 L651 V652 M653 Q654 E655 V656 L657 A658 D659 P660 L661 V662 P663 P664 Q665 L666 T667 I668 K669 D670 M673 T674 D675 S676 I677 S678 R679

Q682 T683 M684 A685 K686 A690 V691 T692 GLU GLY ALA GLN ALA VAL GLU GLU PRO SER ILE CYS

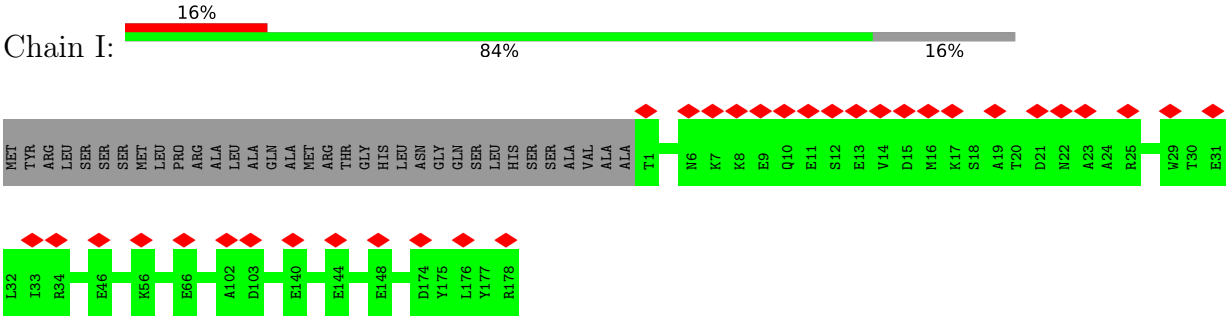
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



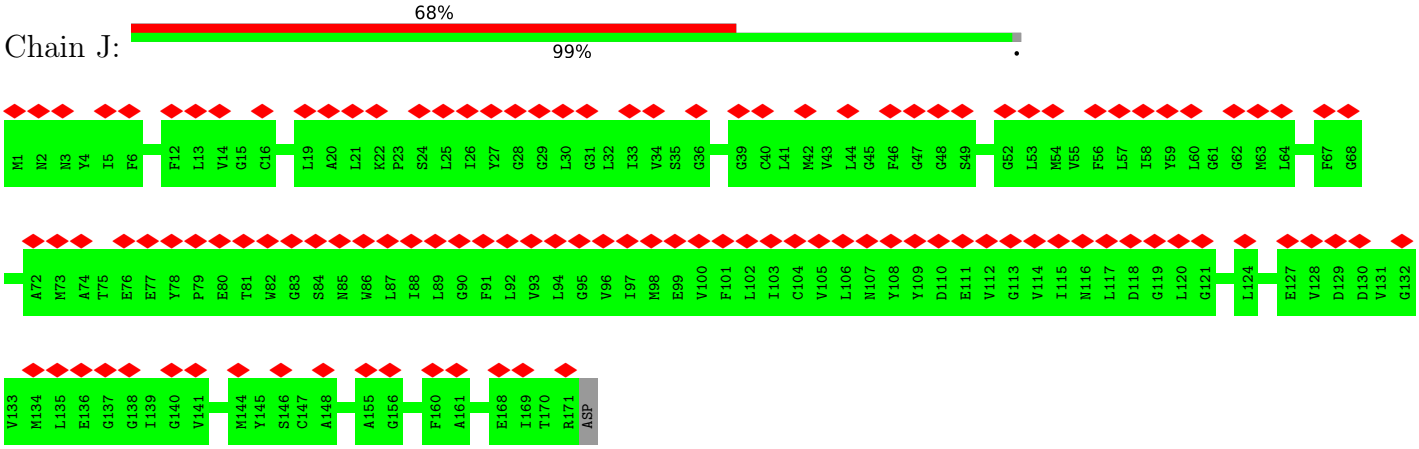
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



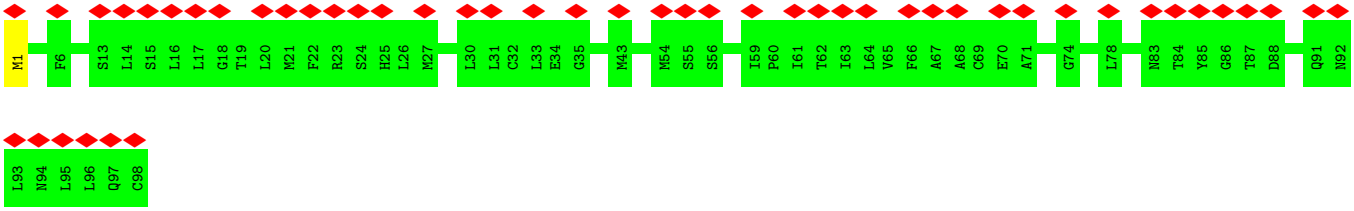
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



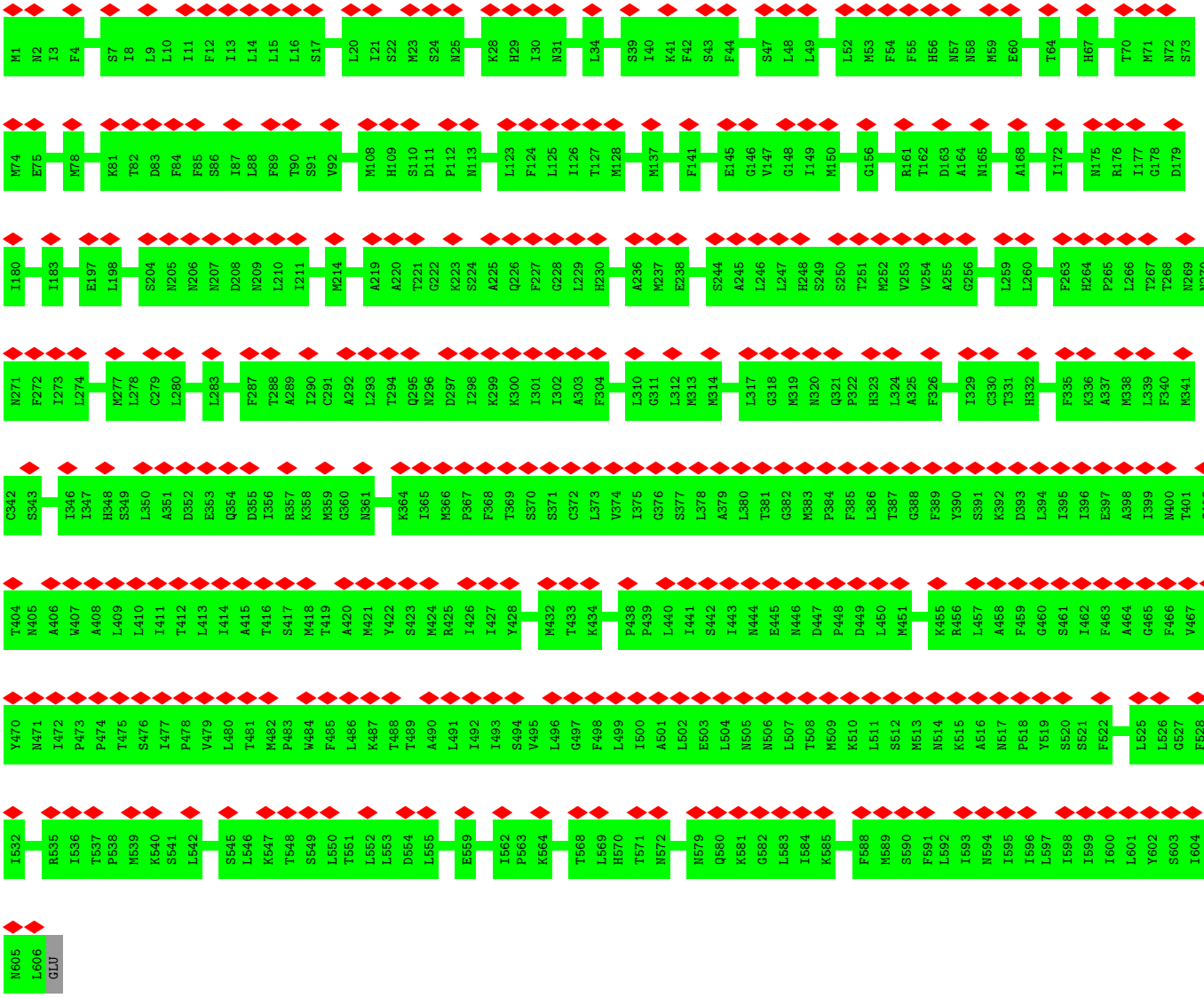
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



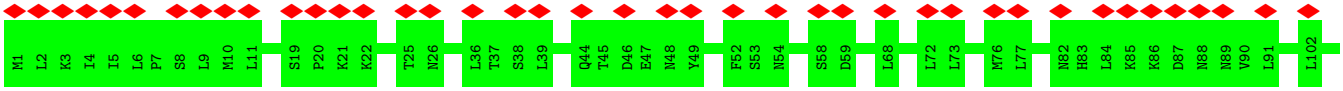
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

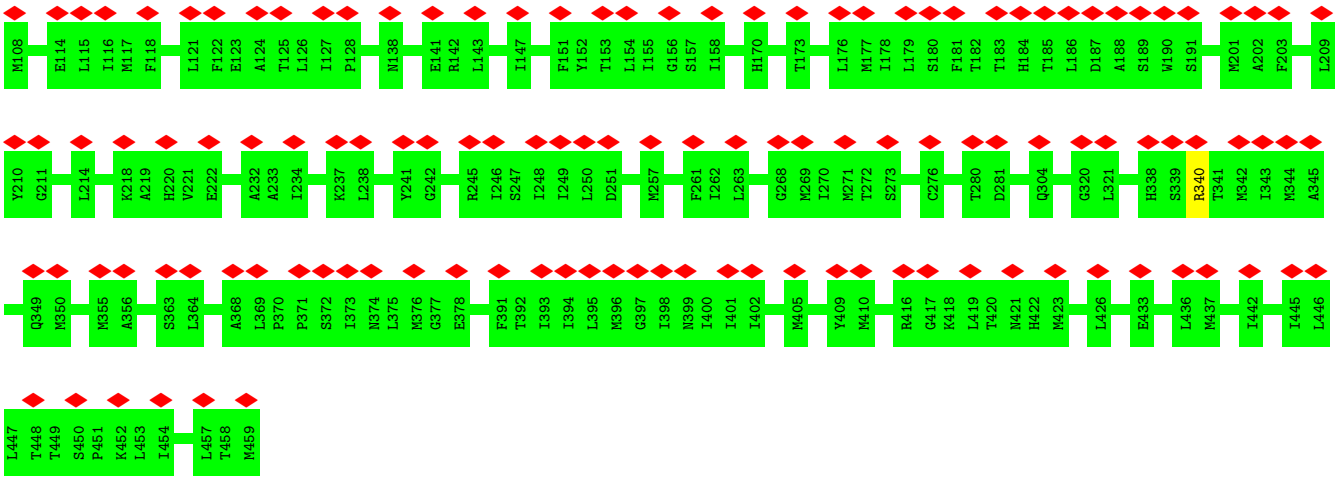
Chain L: 61% 100%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

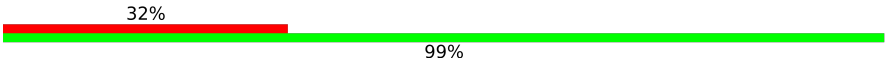
Chain M: 36% 100%

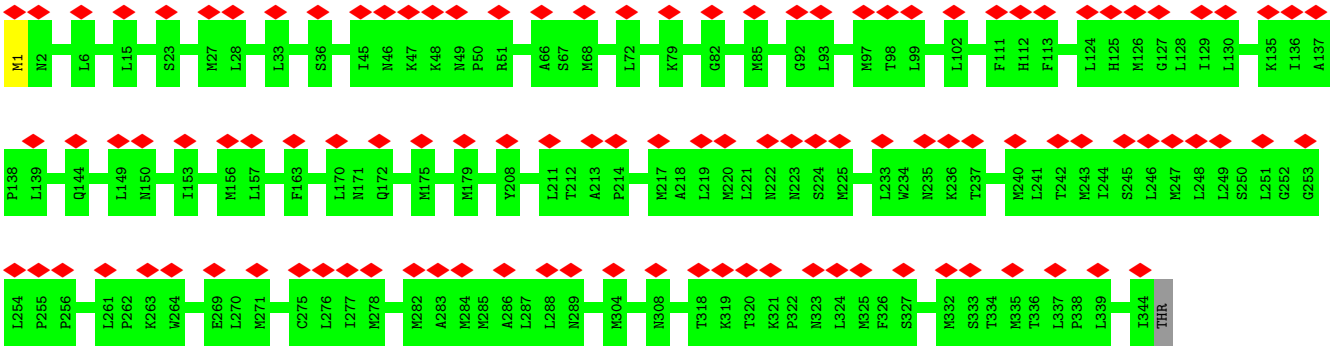




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

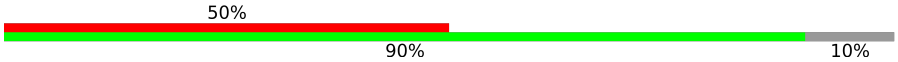
Chain N:

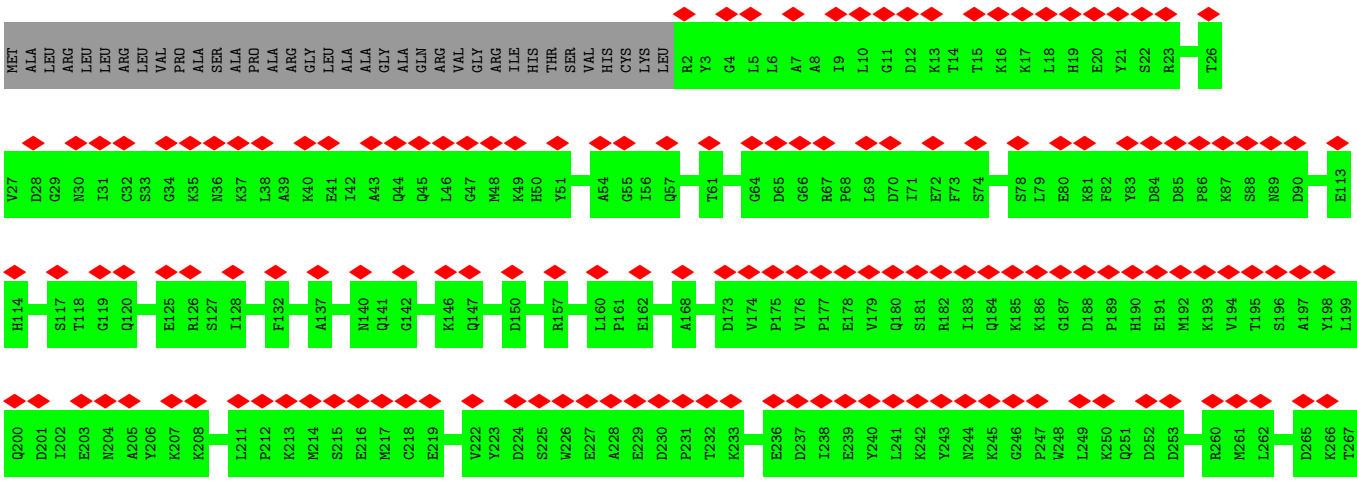




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

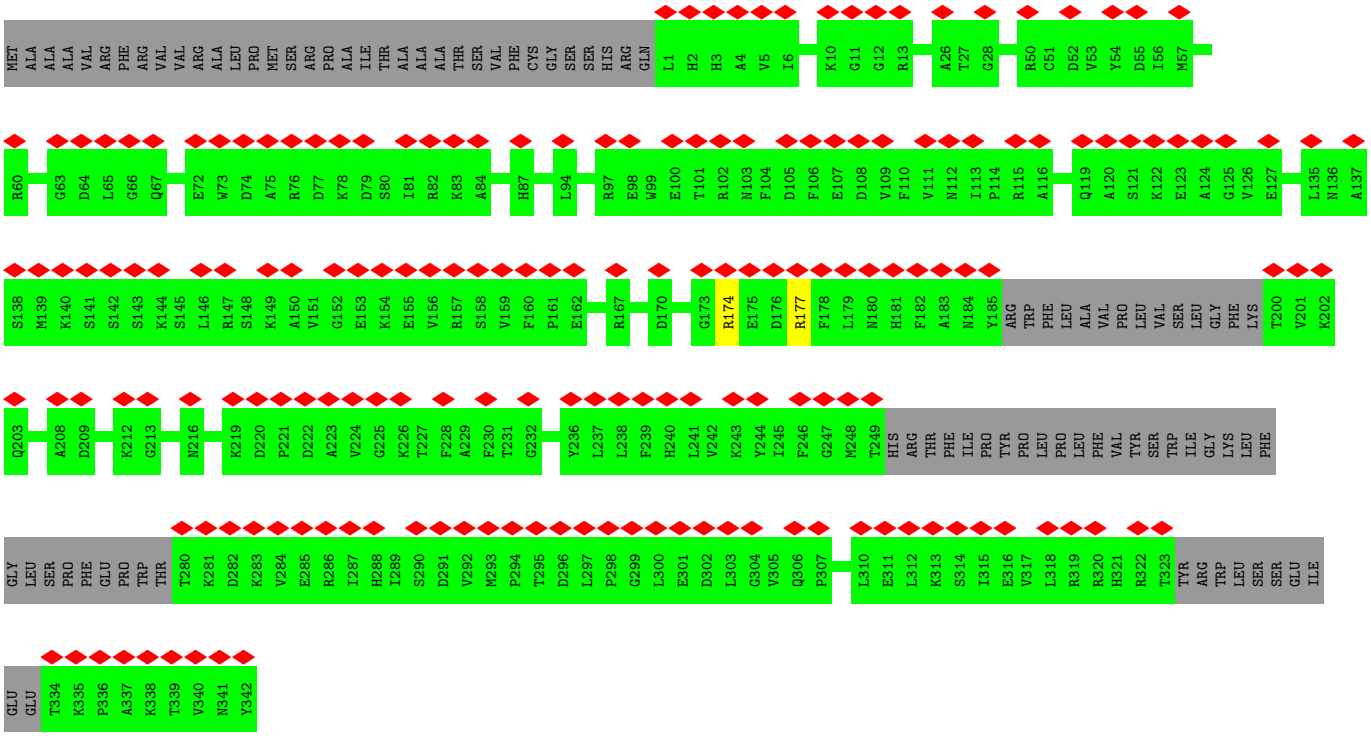
Chain O:





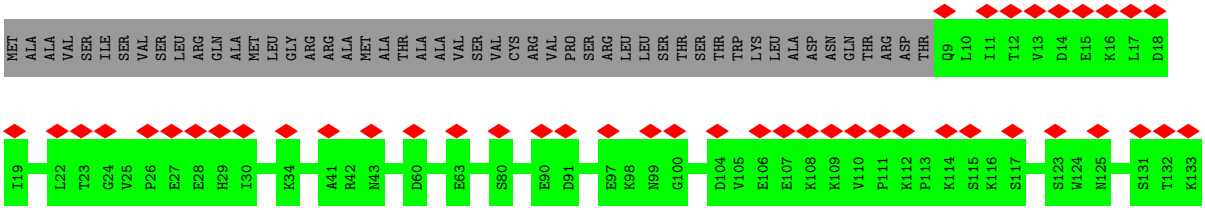
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



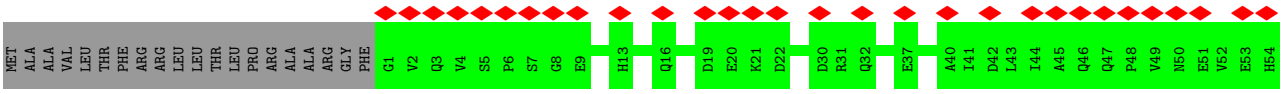
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

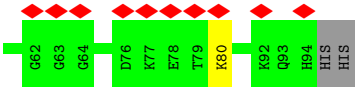
Chain Q:



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

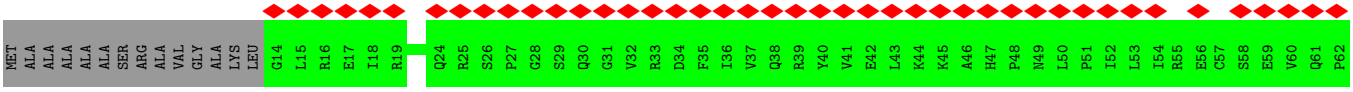
Chain R:

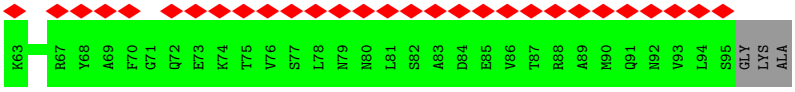




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

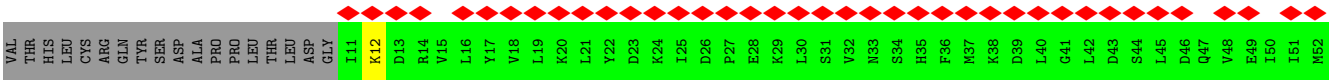
Chain S:

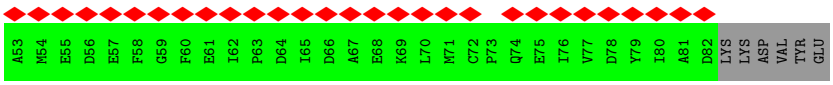




• Molecule 20: Acyl carrier protein, mitochondrial

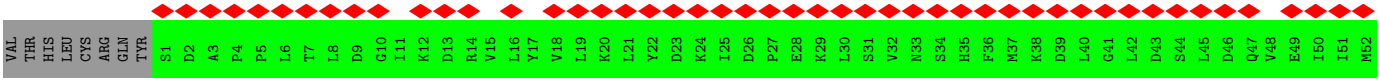
Chain T:

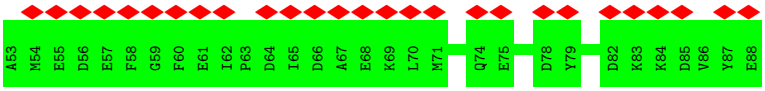




• Molecule 20: Acyl carrier protein, mitochondrial

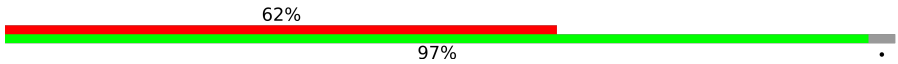
Chain U:

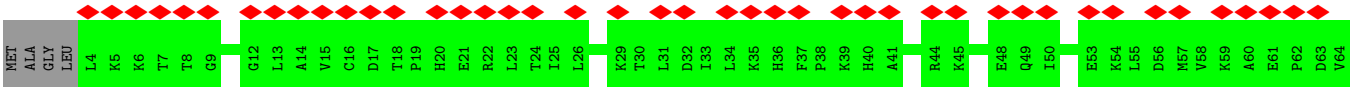


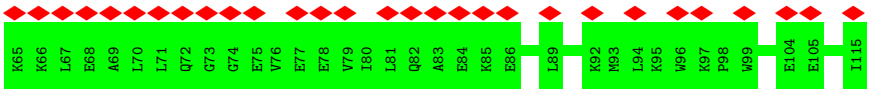


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:

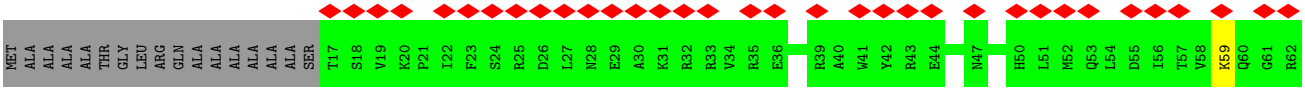


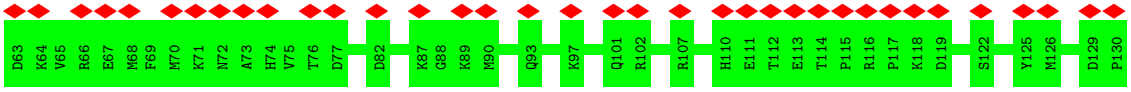




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

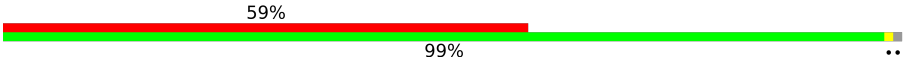
Chain W:

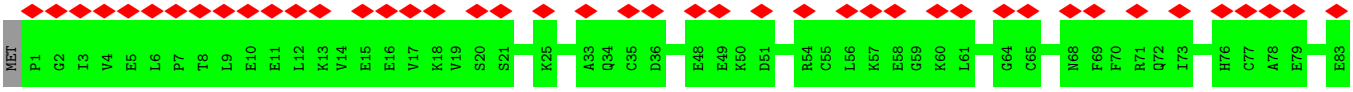


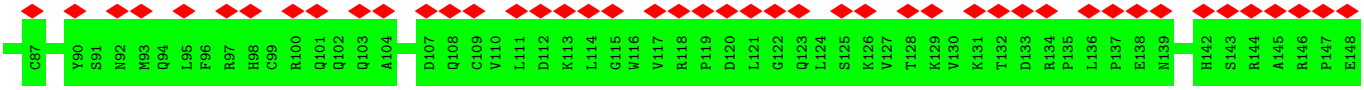


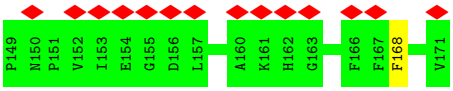
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



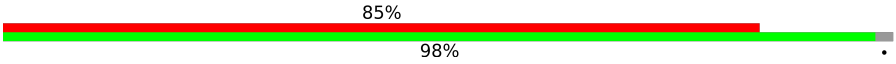


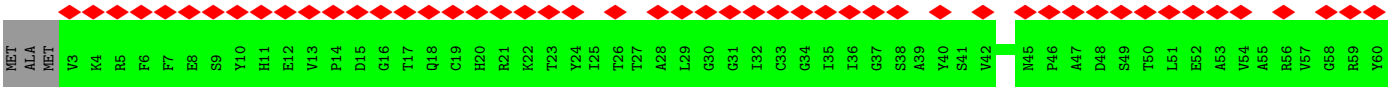


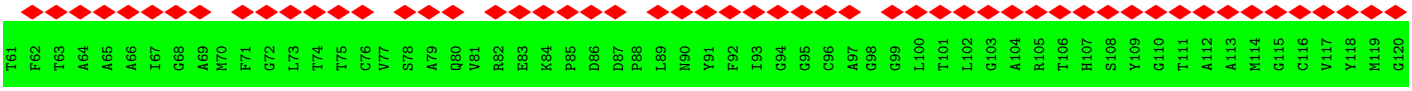


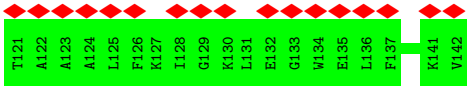
• Molecule 24: MCG5603

Chain Y:



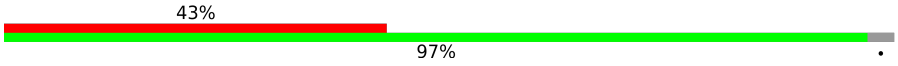


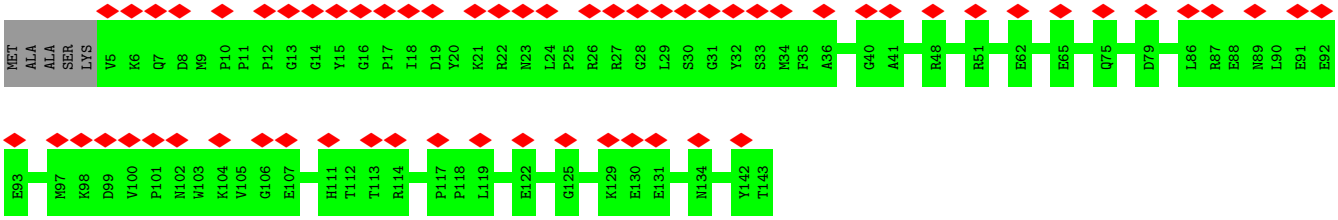




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

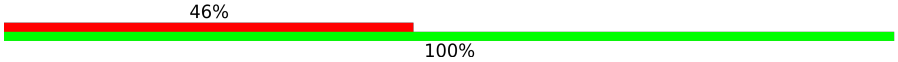
Chain Z:

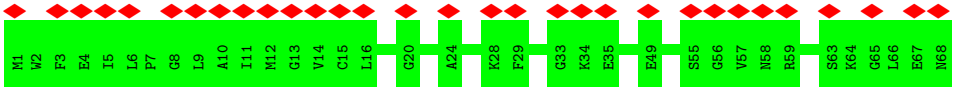




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

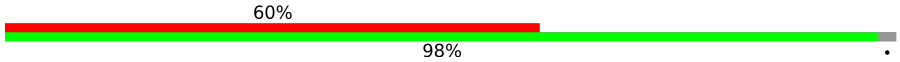
Chain a:

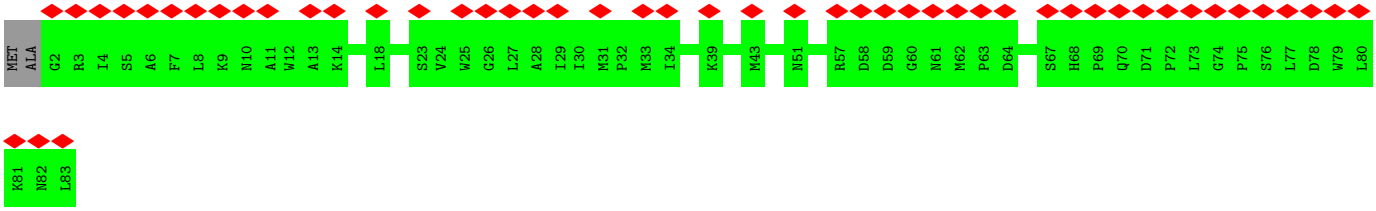




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

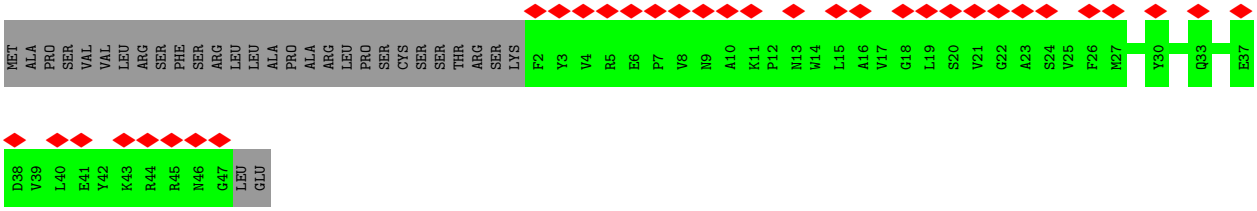
Chain b:





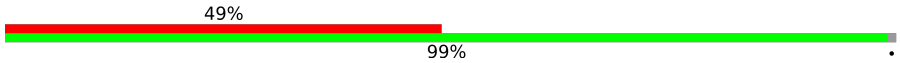
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

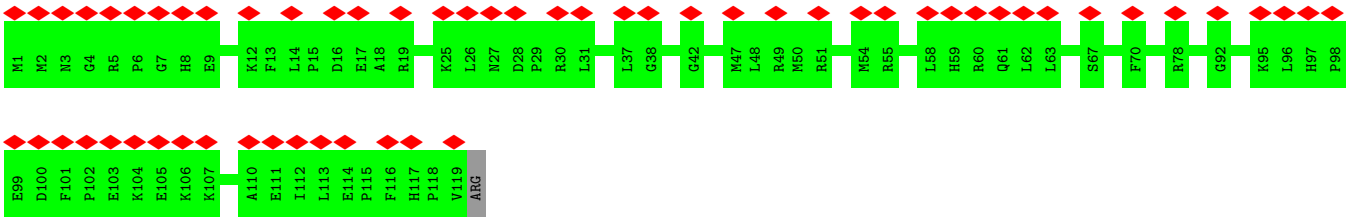
Chain c:



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

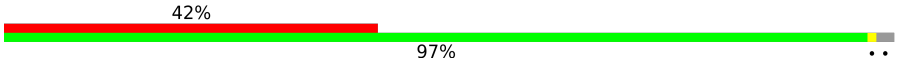
Chain d:

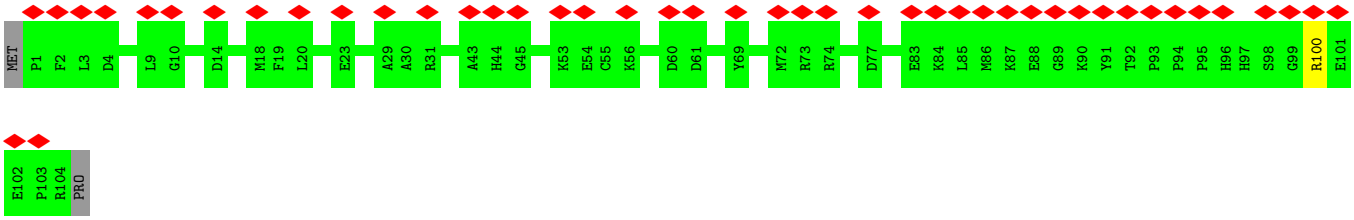




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

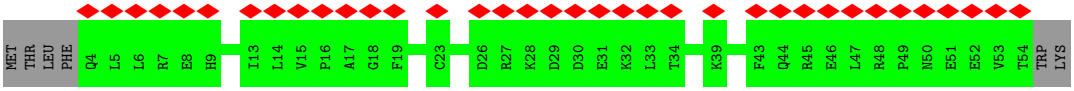
Chain e:





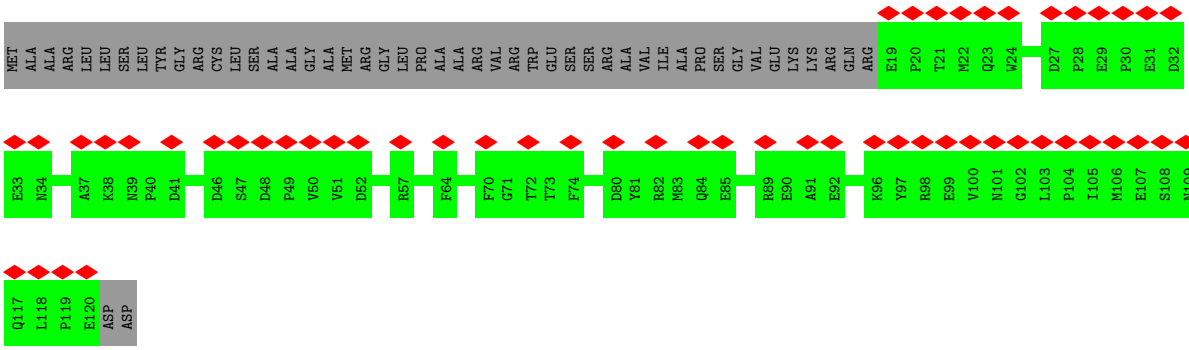
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



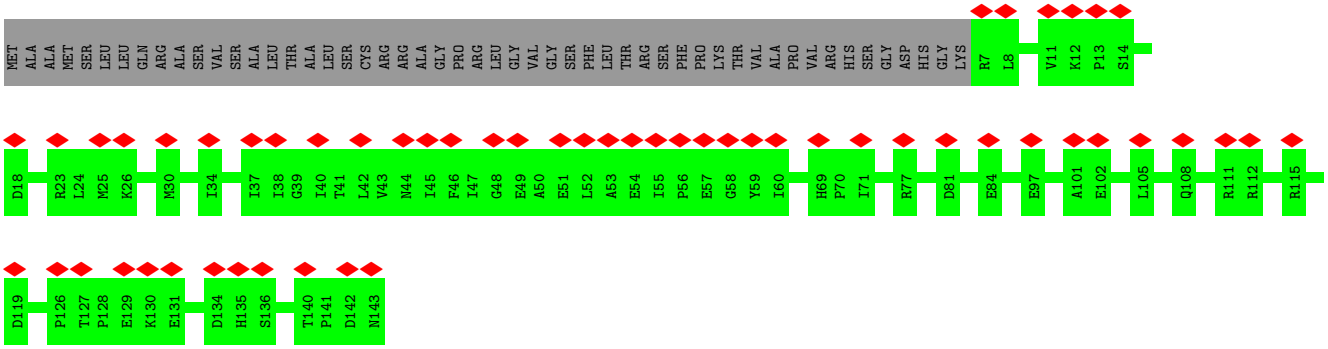
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



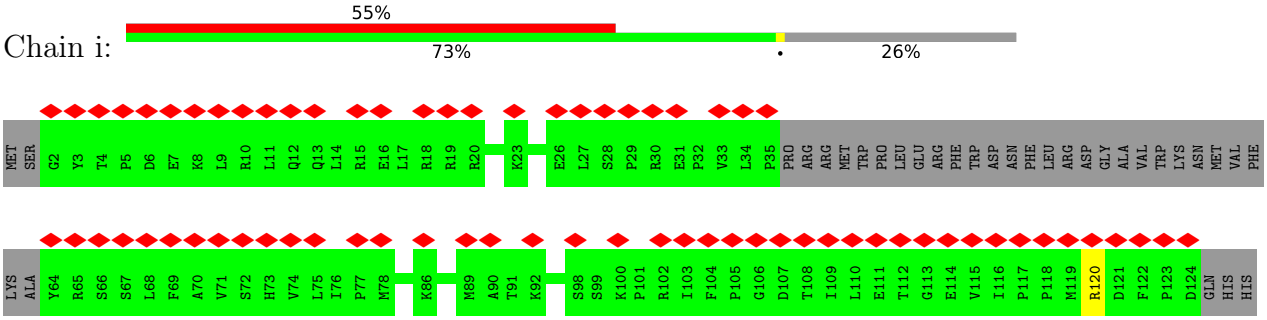
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



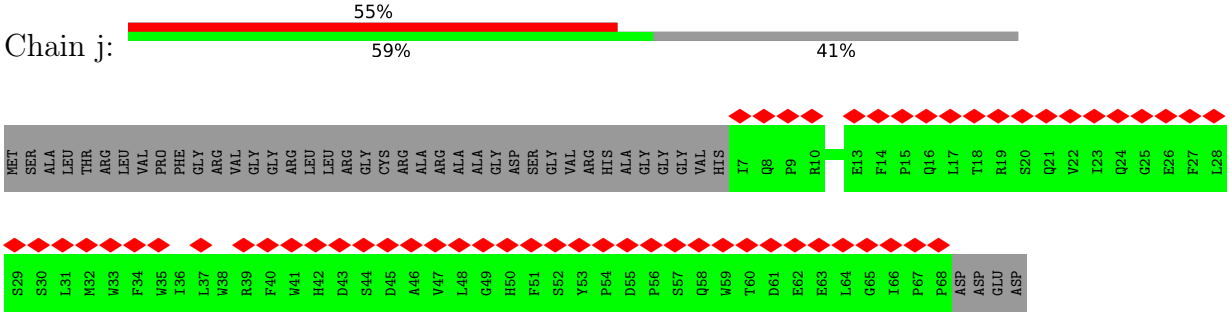
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



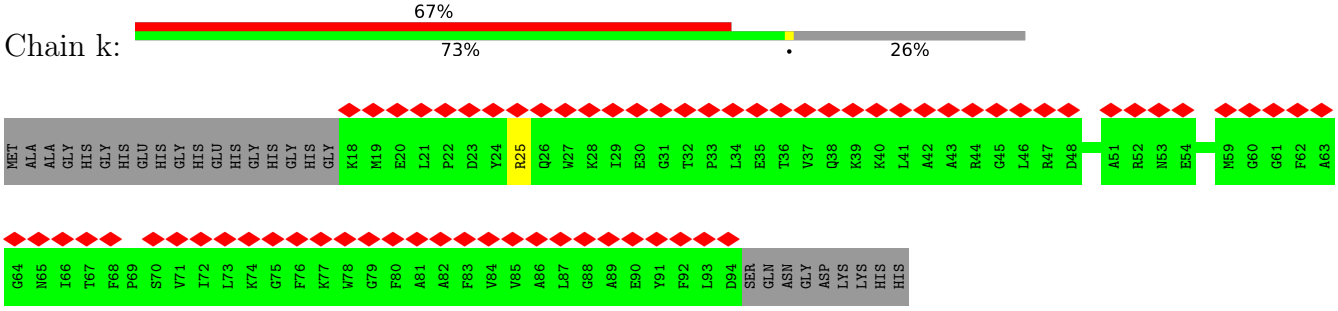
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



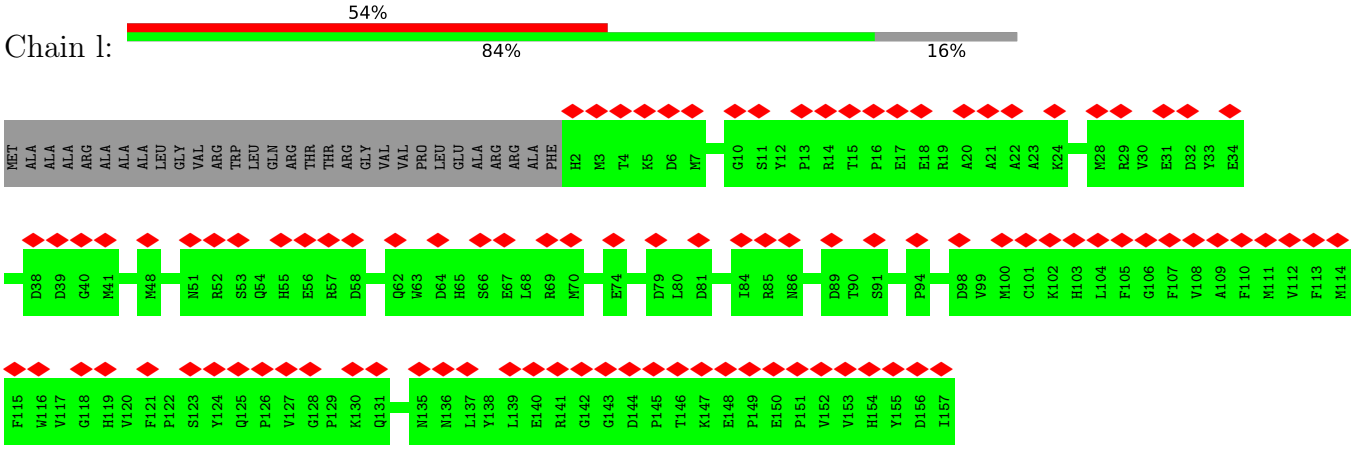
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



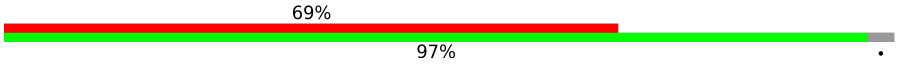
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

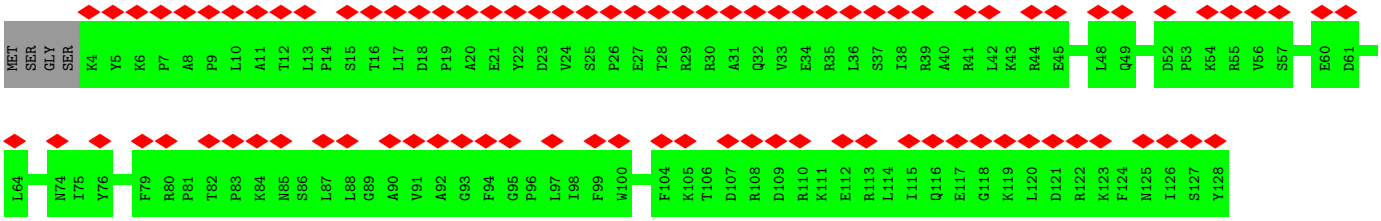
Chain l:



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

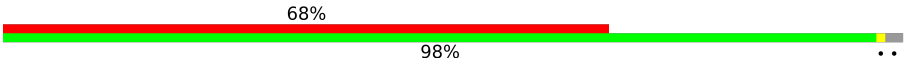
Chain m:

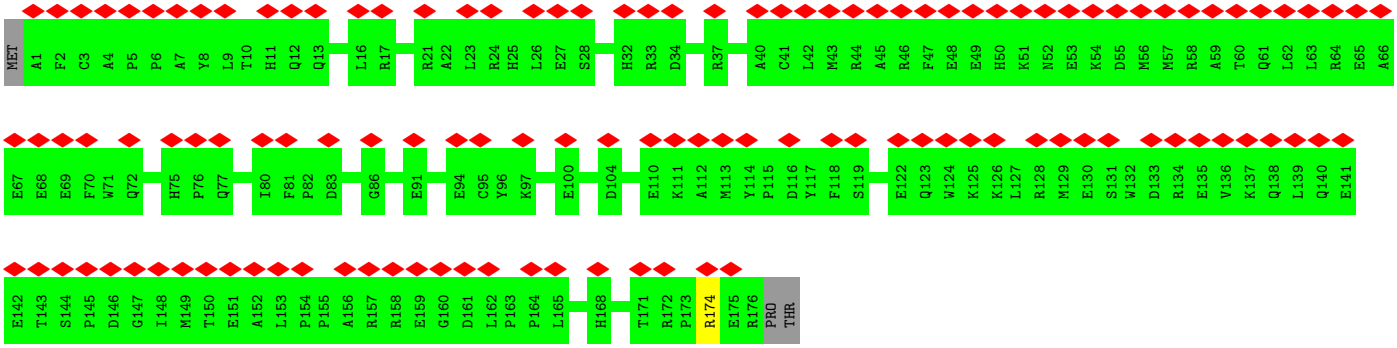




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

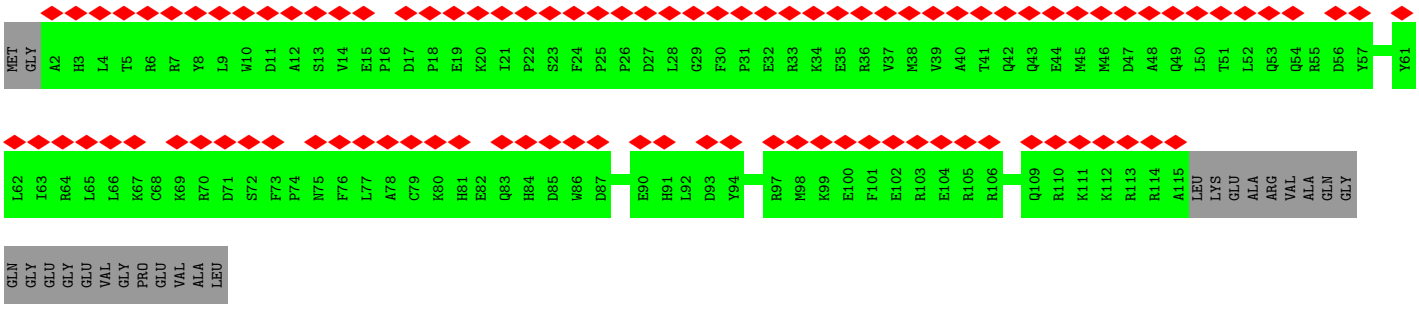
Chain n:





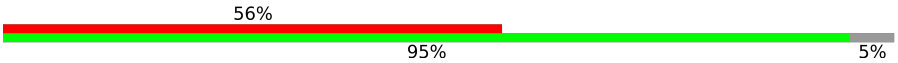
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

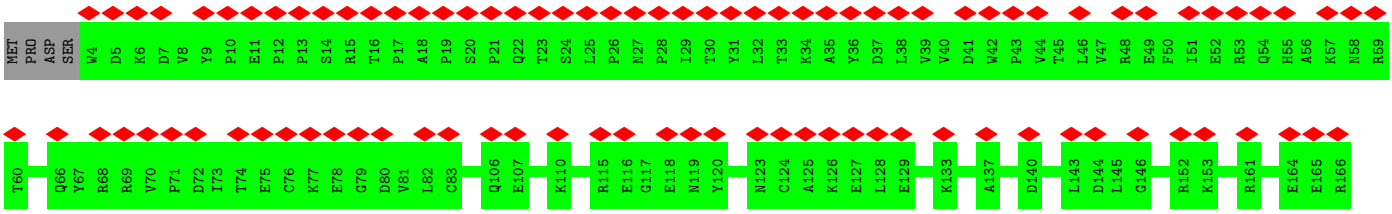
Chain o:

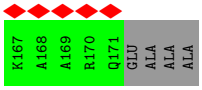


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:

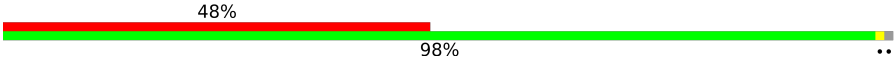


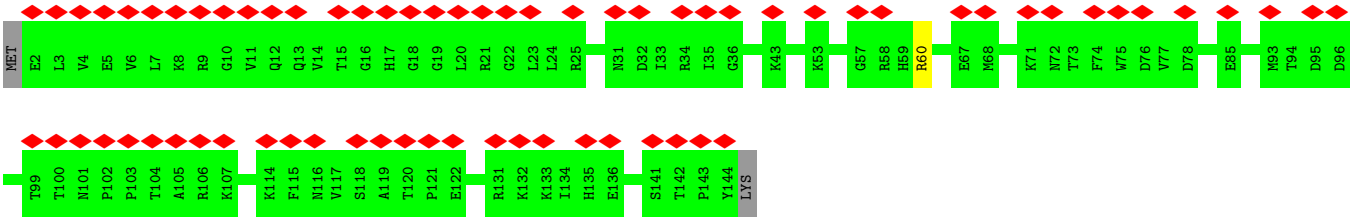




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

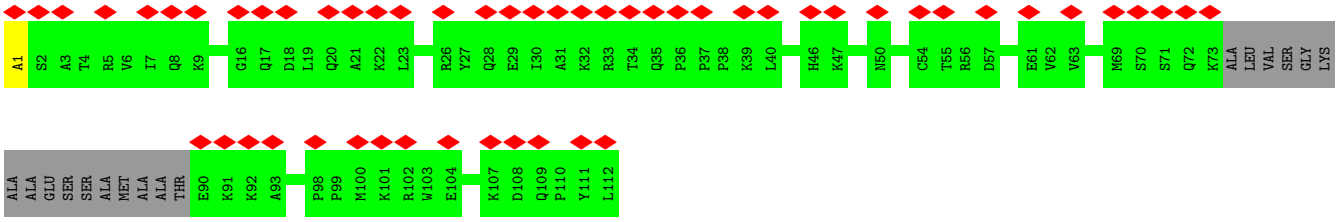
Chain q:





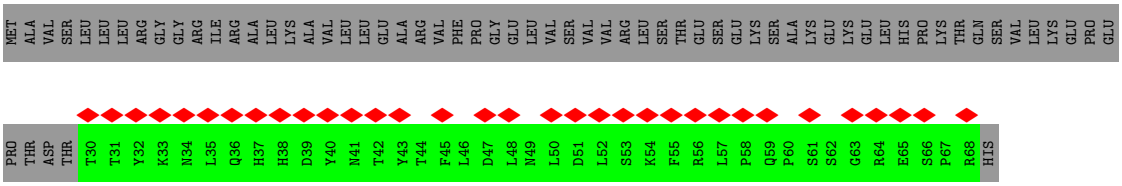
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25629	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 ($e^-/Å^2$)	50.015	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0268	Depositor
Map size (Å)	474.30002, 474.30002, 474.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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: ZN, EHZ, NDP, 2MR, ATP, FMN, SF4, FES, CDL, AYA, PC1, FME, 3PE

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	A	0.31	0/771	0.52	2/1054 (0.2%)
2	B	0.43	0/1272	0.48	0/1722
3	C	0.38	0/1771	0.47	0/2412
4	D	0.37	0/3440	0.45	0/4656
5	E	0.31	0/1679	0.45	0/2288
6	F	0.31	0/3376	0.46	0/4561
7	G	0.34	0/5368	0.47	0/7273
8	H	0.33	0/2504	0.43	0/3420
9	I	0.41	0/1438	0.48	0/1946
10	J	0.32	0/1297	0.44	0/1764
11	K	0.31	0/738	0.43	0/1002
12	L	0.31	0/4913	0.45	0/6686
13	M	0.31	0/3709	0.46	0/5052
14	N	0.33	0/2748	0.44	0/3741
15	O	0.32	0/2666	0.44	0/3615
16	P	0.32	0/2329	0.47	0/3145
17	Q	0.32	0/1038	0.47	0/1401
18	R	0.34	0/751	0.46	0/1011
19	S	0.27	0/670	0.47	0/904
20	T	0.28	0/593	0.44	0/799
20	U	0.29	0/718	0.41	0/970
21	V	0.31	0/937	0.42	0/1270
22	W	0.31	0/993	0.45	0/1335
23	X	0.30	0/1434	0.44	0/1937
24	Y	0.29	0/1061	0.45	0/1439
25	Z	0.32	0/1183	0.44	0/1597
26	a	0.34	0/569	0.43	0/766
27	b	0.29	0/666	0.41	0/914
28	c	0.30	0/392	0.40	0/533
29	d	0.34	0/1017	0.44	0/1373
30	e	0.30	0/892	0.45	0/1187
31	f	0.28	0/443	0.44	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.33	0/887	0.42	0/1209
33	h	0.33	0/1188	0.42	0/1610
34	i	0.30	0/828	0.45	0/1125
35	j	0.27	0/561	0.41	0/768
36	k	0.28	0/646	0.43	0/873
37	l	0.31	0/1367	0.41	0/1866
38	m	0.31	0/1073	0.45	0/1455
39	n	0.30	0/1581	0.41	0/2140
40	o	0.27	0/1009	0.42	0/1355
41	p	0.33	0/1457	0.42	0/1969
42	q	0.35	0/1234	0.45	0/1681
43	r	0.31	0/786	0.43	0/1062
44	s	0.27	0/338	0.45	0/458
All	All	0.33	0/66331	0.45	2/89940 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	49	LEU	CB-CG-CD1	5.60	120.51	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/115 (77%)	83 (93%)	6 (7%)	0	100	100
2	B	153/224 (68%)	136 (89%)	17 (11%)	0	100	100
3	C	205/263 (78%)	181 (88%)	24 (12%)	0	100	100
4	D	410/463 (89%)	379 (92%)	30 (7%)	1 (0%)	47	78
5	E	208/248 (84%)	180 (86%)	28 (14%)	0	100	100
6	F	426/464 (92%)	385 (90%)	41 (10%)	0	100	100
7	G	684/727 (94%)	617 (90%)	67 (10%)	0	100	100
8	H	299/318 (94%)	267 (89%)	32 (11%)	0	100	100
9	I	176/212 (83%)	157 (89%)	19 (11%)	0	100	100
10	J	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
11	K	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
12	L	604/607 (100%)	544 (90%)	60 (10%)	0	100	100
13	M	457/459 (100%)	411 (90%)	46 (10%)	0	100	100
14	N	342/345 (99%)	316 (92%)	26 (8%)	0	100	100
15	O	317/355 (89%)	283 (89%)	34 (11%)	0	100	100
16	P	280/377 (74%)	244 (87%)	36 (13%)	0	100	100
17	Q	123/175 (70%)	111 (90%)	12 (10%)	0	100	100
18	R	92/116 (79%)	84 (91%)	8 (9%)	0	100	100
19	S	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
20	T	70/156 (45%)	62 (89%)	8 (11%)	0	100	100
20	U	86/156 (55%)	75 (87%)	11 (13%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	169/172 (98%)	153 (90%)	15 (9%)	1 (1%)	25	62
24	Y	138/143 (96%)	129 (94%)	9 (6%)	0	100	100
25	Z	137/144 (95%)	126 (92%)	11 (8%)	0	100	100
26	a	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
27	b	80/84 (95%)	69 (86%)	11 (14%)	0	100	100
28	c	44/76 (58%)	41 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
30	e	102/106 (96%)	87 (85%)	15 (15%)	0	100	100
31	f	49/57 (86%)	41 (84%)	8 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	100/151 (66%)	88 (88%)	12 (12%)	0	100	100
33	h	135/189 (71%)	121 (90%)	14 (10%)	0	100	100
34	i	91/128 (71%)	71 (78%)	20 (22%)	0	100	100
35	j	60/105 (57%)	55 (92%)	5 (8%)	0	100	100
36	k	75/104 (72%)	69 (92%)	6 (8%)	0	100	100
37	l	154/186 (83%)	132 (86%)	22 (14%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	174/179 (97%)	162 (93%)	12 (7%)	0	100	100
40	o	112/137 (82%)	95 (85%)	17 (15%)	0	100	100
41	p	166/176 (94%)	151 (91%)	15 (9%)	0	100	100
42	q	141/145 (97%)	122 (86%)	19 (14%)	0	100	100
43	r	92/112 (82%)	80 (87%)	12 (13%)	0	100	100
44	s	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
All	All	7950/9211 (86%)	7148 (90%)	800 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	168	PHE
4	D	86	GLY

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	A	84/103 (82%)	84 (100%)	0	100	100
2	B	131/185 (71%)	131 (100%)	0	100	100
3	C	189/227 (83%)	188 (100%)	1 (0%)	88	94
4	D	361/394 (92%)	361 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	578/610 (95%)	575 (100%)	3 (0%)	88	94
8	H	267/279 (96%)	267 (100%)	0	100	100
9	I	145/178 (82%)	145 (100%)	0	100	100
10	J	131/137 (96%)	131 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100
13	M	414/414 (100%)	413 (100%)	1 (0%)	93	97
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	249/325 (77%)	247 (99%)	2 (1%)	81	89
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	78 (99%)	1 (1%)	69	82
19	S	73/80 (91%)	73 (100%)	0	100	100
20	T	67/135 (50%)	66 (98%)	1 (2%)	65	80
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	107 (99%)	1 (1%)	78	88
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	58/58 (100%)	58 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	40/67 (60%)	40 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	92/94 (98%)	91 (99%)	1 (1%)	73	85
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	90/120 (75%)	89 (99%)	1 (1%)	73	85
35	j	58/87 (67%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	60/78 (77%)	59 (98%)	1 (2%)	60	78
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	161/164 (98%)	160 (99%)	1 (1%)	86	92
40	o	106/121 (88%)	106 (100%)	0	100	100
41	p	153/158 (97%)	153 (100%)	0	100	100
42	q	129/131 (98%)	128 (99%)	1 (1%)	81	89
43	r	86/95 (90%)	86 (100%)	0	100	100
44	s	38/95 (40%)	38 (100%)	0	100	100
All	All	7060/7946 (89%)	7045 (100%)	15 (0%)	93	97

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	R	80	LYS
39	n	174	ARG
20	T	12	LYS
42	q	60	ARG
34	i	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
23	X	34	GLN
33	h	44	ASN
23	X	102	GLN
25	Z	89	ASN
37	l	71	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

9 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	$\#\|Z\| > 2$
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	1.35	1 (14%)
43	AYA	r	1	43	6,7,8	1.29	1 (16%)	5,8,10	1.26	1 (20%)
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.72	2 (40%)
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	0.67	0
14	FME	N	1	14	8,9,10	0.89	0	7,9,11	1.22	1 (14%)
1	FME	A	1	1	8,9,10	0.89	0	7,9,11	1.46	1 (14%)
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.93	0
8	FME	H	1	8	8,9,10	0.93	0	7,9,11	1.13	1 (14%)
10	FME	J	1	10	8,9,10	0.92	0	7,9,11	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	3/7/9/11	-
43	AYA	r	1	43	-	1/4/6/8	-
4	2MR	D	85	4	-	3/10/13/15	-
13	FME	M	1	13	-	1/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.31	1.45	1.34
4	D	85	2MR	CZ-NH2	4.94	1.44	1.33
43	r	1	AYA	CA-N	-2.54	1.43	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	C-CA-N	3.12	115.36	109.73
11	K	1	FME	C-CA-N	2.90	114.97	109.73
4	D	85	2MR	CD-NE-CZ	2.87	128.79	123.41
43	r	1	AYA	CB-CA-N	2.50	112.39	109.61
4	D	85	2MR	NE-CZ-NH2	-2.46	117.23	119.48

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#\|Z\| > 2$
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	9 (18%)
49	3PE	L	701	-	44,44,50	0.90	4 (9%)	47,49,55	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	EHZ	T	201	20	29,36,37	1.69	5 (17%)	35,44,47	1.53	4 (11%)
45	SF4	B	201	2	0,12,12	-	-	-		
49	3PE	J	401	-	37,37,50	0.99	4 (10%)	40,42,55	1.11	2 (5%)
47	FES	E	301	5	0,4,4	-	-	-		
50	CDL	d	201	-	49,49,99	1.22	7 (14%)	55,61,111	1.35	5 (9%)
49	3PE	M	501	-	37,37,50	0.99	4 (10%)	40,42,55	1.10	2 (5%)
45	SF4	I	202	9	0,12,12	-	-	-		
47	FES	G	803	7	0,4,4	-	-	-		
45	SF4	I	201	9	0,12,12	-	-	-		
54	EHZ	U	201	20	29,36,37	1.72	5 (17%)	35,44,47	1.55	6 (17%)
45	SF4	G	801	7	0,12,12	-	-	-		
49	3PE	H	401	-	41,41,50	0.95	4 (9%)	44,46,55	1.26	4 (9%)
50	CDL	L	702	-	53,53,99	1.18	8 (15%)	59,65,111	1.13	4 (6%)
46	PC1	B	202	-	25,25,53	1.36	4 (16%)	31,33,61	1.10	2 (6%)
45	SF4	G	802	7	0,12,12	-	-	-		
51	ATP	O	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.73	5 (16%)
52	NDP	P	501	-	45,52,52	2.23	5 (11%)	53,80,80	1.76	8 (15%)
45	SF4	F	502	6	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FMN	F	501	-	-	10/18/18/18	0/3/3/3
49	3PE	L	701	-	-	25/48/48/54	-
54	EHZ	T	201	20	-	15/42/44/45	-
45	SF4	B	201	2	-	-	0/6/5/5
49	3PE	J	401	-	-	18/41/41/54	-
47	FES	E	301	5	-	-	0/1/1/1
50	CDL	d	201	-	-	22/59/59/110	-
49	3PE	M	501	-	-	23/41/41/54	-
45	SF4	I	202	9	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	I	201	9	-	-	0/6/5/5
54	EHZ	U	201	20	-	24/42/44/45	-
45	SF4	G	801	7	-	-	0/6/5/5
49	3PE	H	401	-	-	13/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CDL	L	702	-	-	25/64/64/110	-
46	PC1	B	202	-	-	15/29/29/57	-
45	SF4	G	802	7	-	-	0/6/5/5
51	ATP	O	401	-	-	5/18/38/38	0/3/3/3
52	NDP	P	501	-	-	9/30/77/77	0/5/5/5
45	SF4	F	502	6	-	-	0/6/5/5

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.32	1.82	1.59
54	U	201	EHZ	C15-N2	5.60	1.45	1.33
54	T	201	EHZ	C15-N2	5.51	1.45	1.33
54	U	201	EHZ	C12-N1	5.38	1.45	1.33
54	T	201	EHZ	C12-N1	5.28	1.45	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	PN-O3-PA	-7.51	107.07	132.83
54	T	201	EHZ	C8-C9-S1	5.46	120.39	113.63
54	U	201	EHZ	C8-C9-S1	5.36	120.26	113.63
50	d	201	CDL	OA6-CA5-C11	4.75	119.83	111.09
49	L	701	3PE	O21-C21-C22	4.64	121.51	111.50

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	O13-C11-C12-N
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'

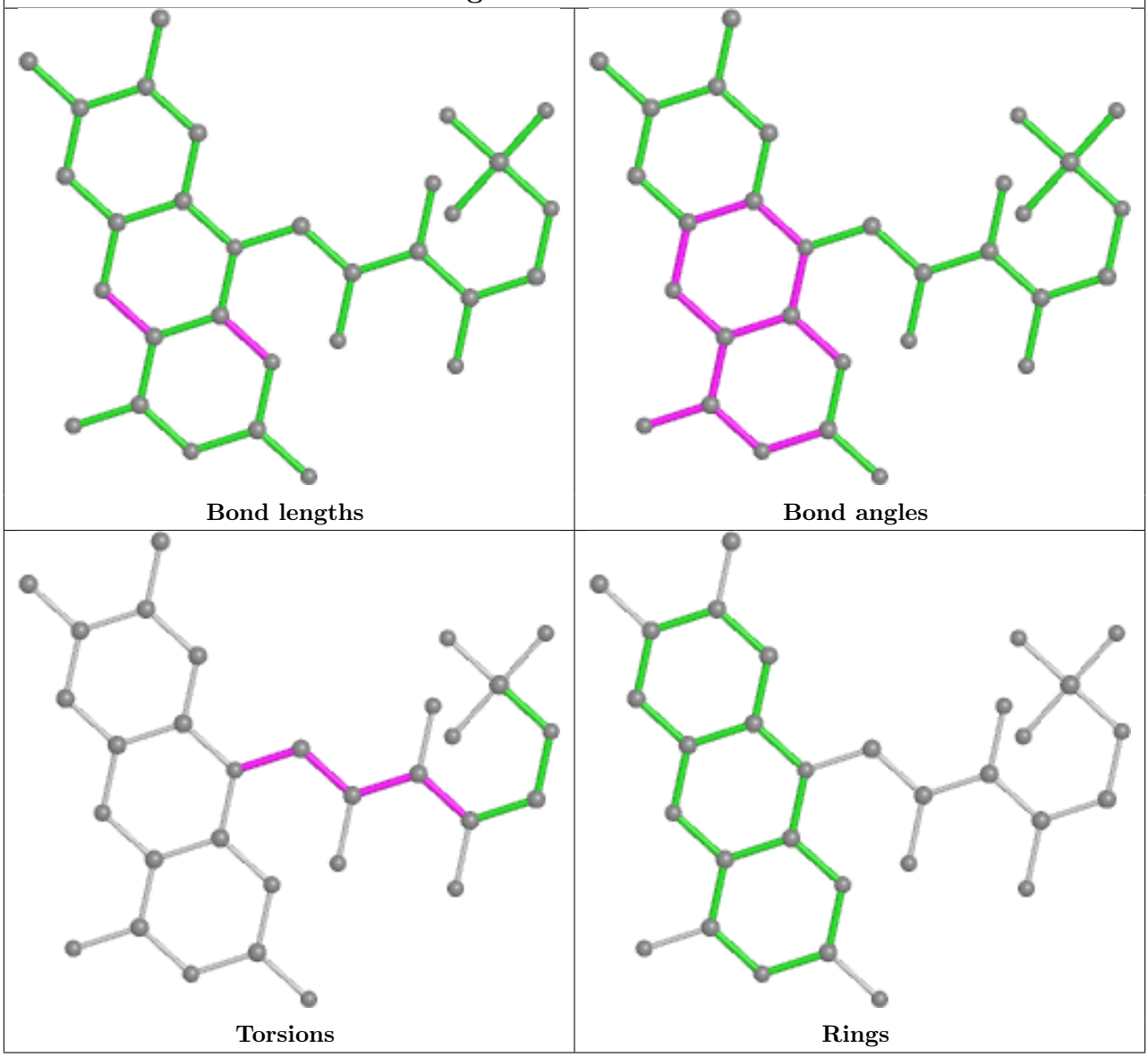
There are no ring outliers.

No monomer is involved in short contacts.

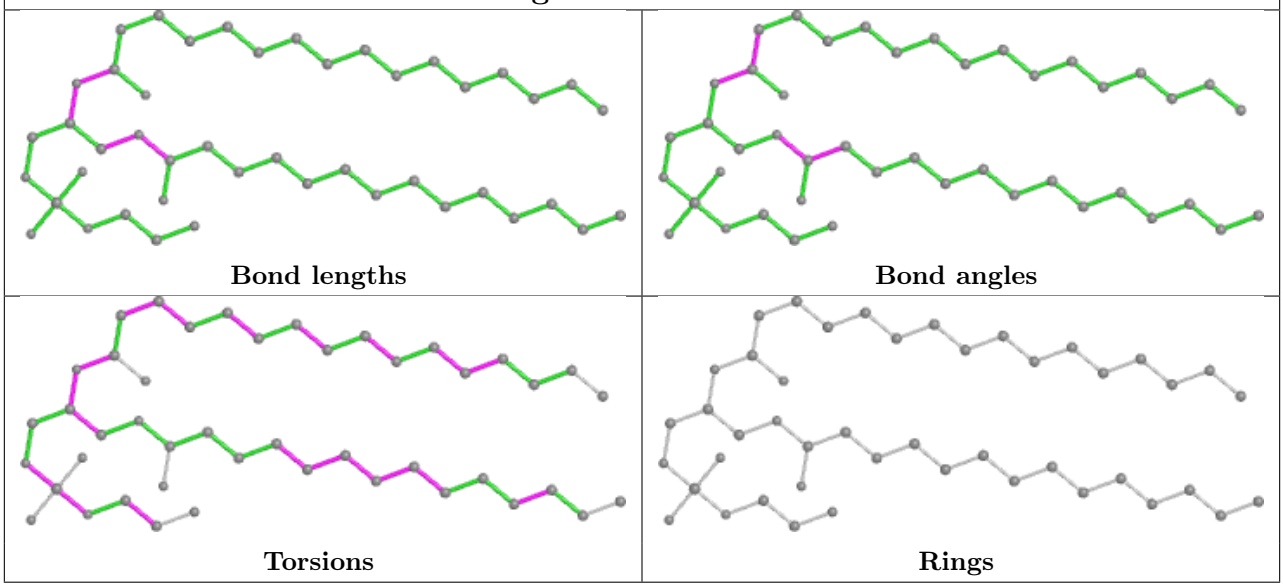
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

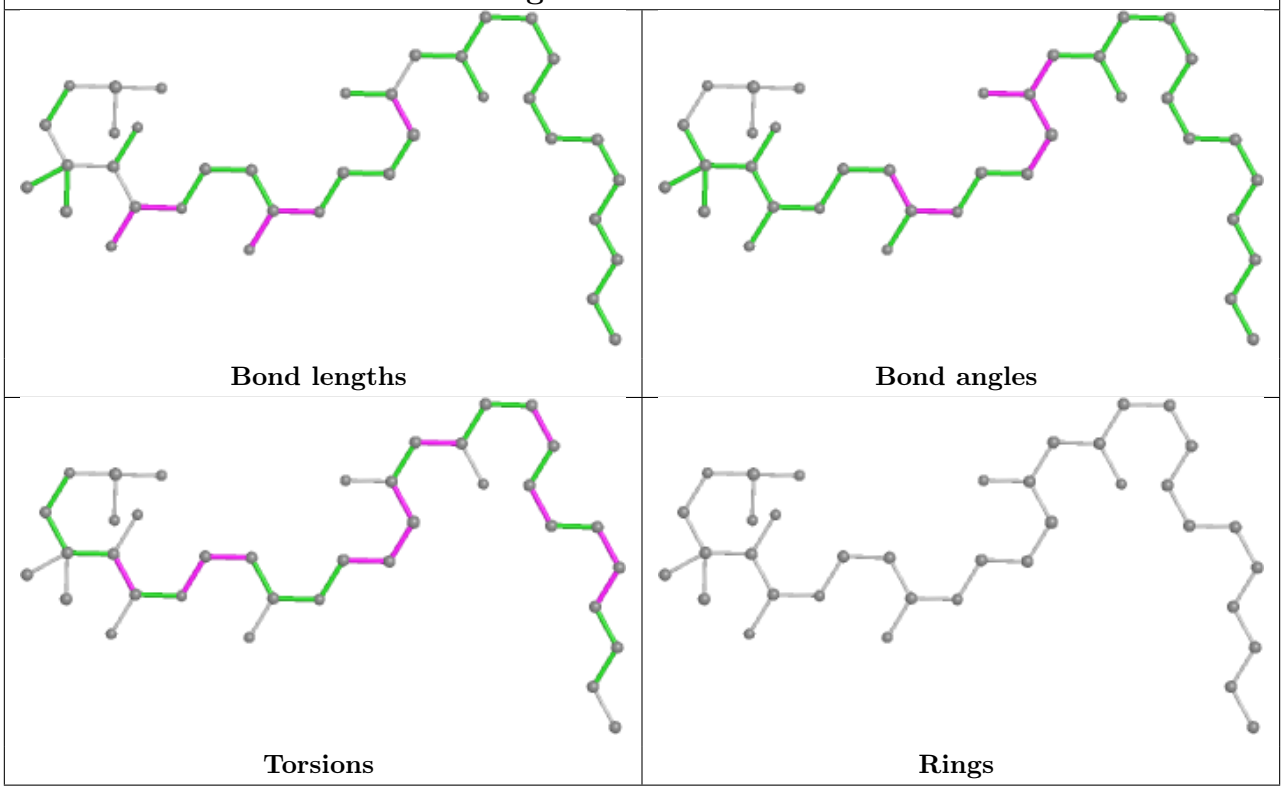
Ligand FMN F 501



Ligand 3PE L 701



Ligand EHZ T 201



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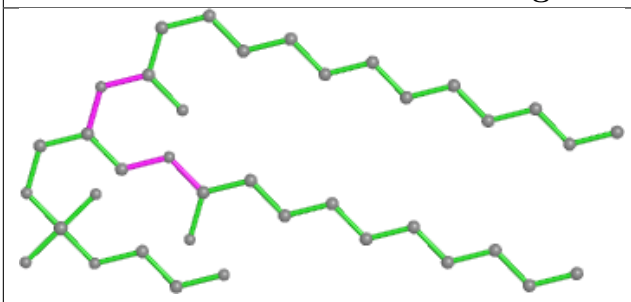
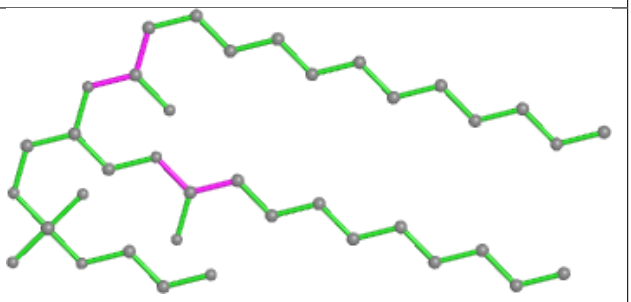
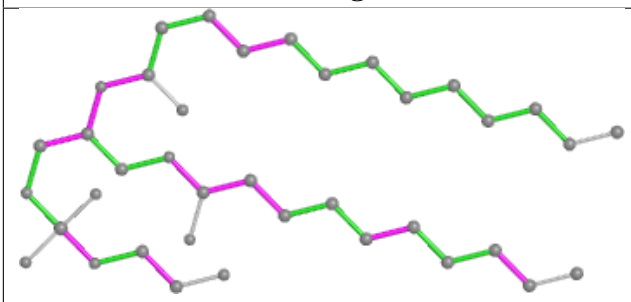
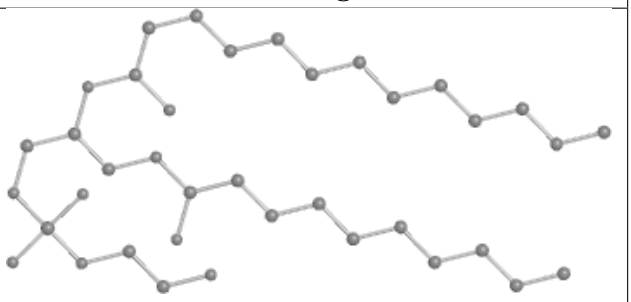
 Bond lengths	 Bond angles
 Torsions	 Rings

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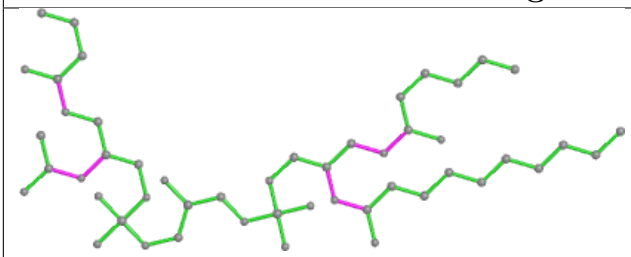
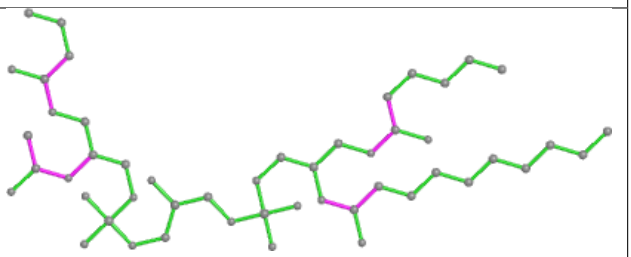
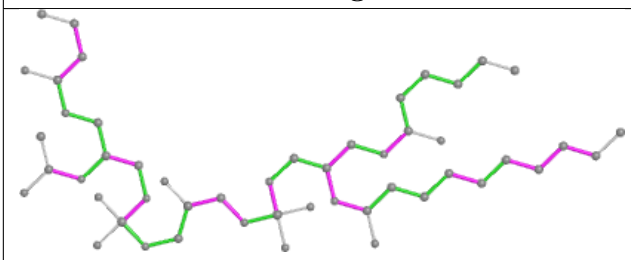
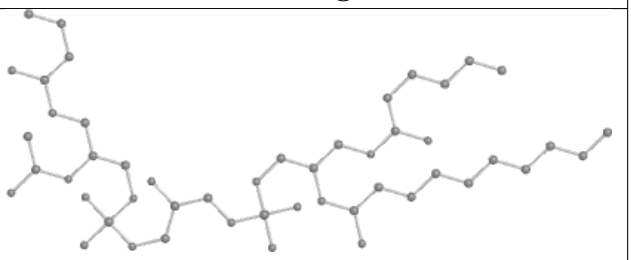
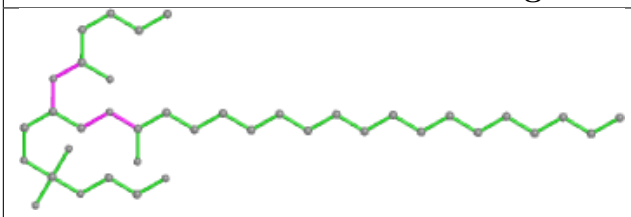
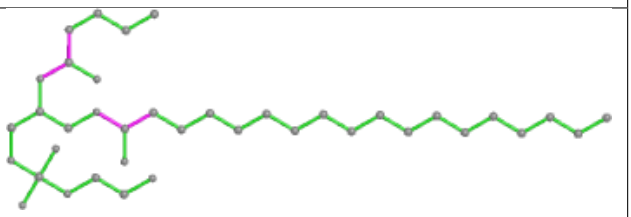
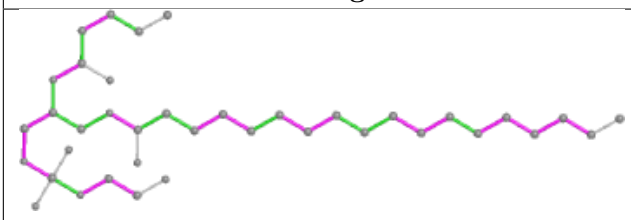
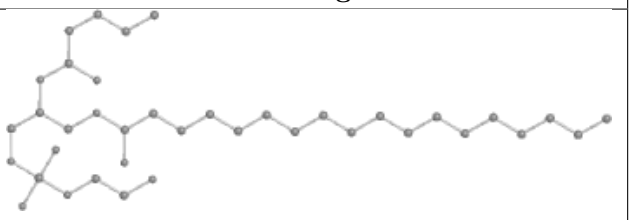
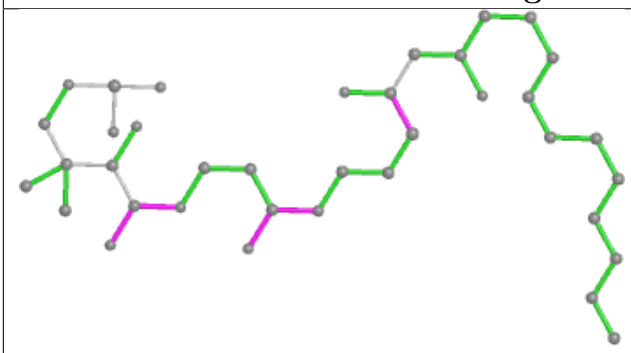
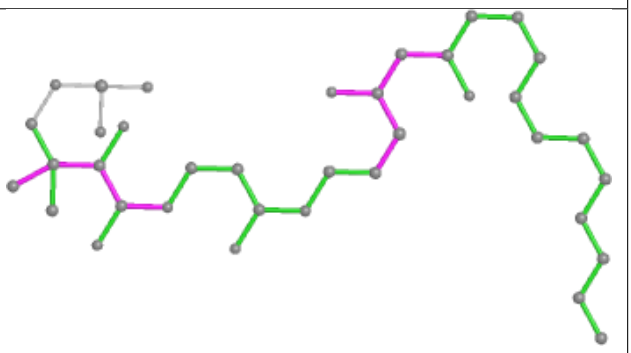
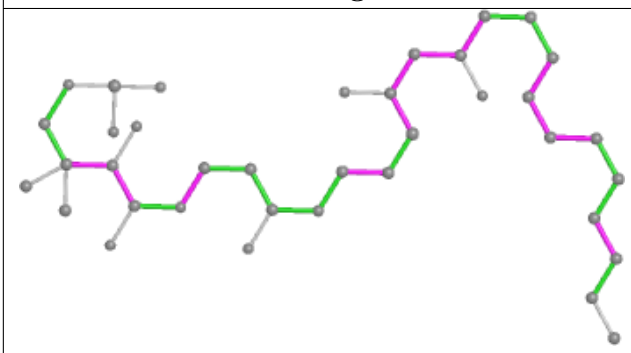
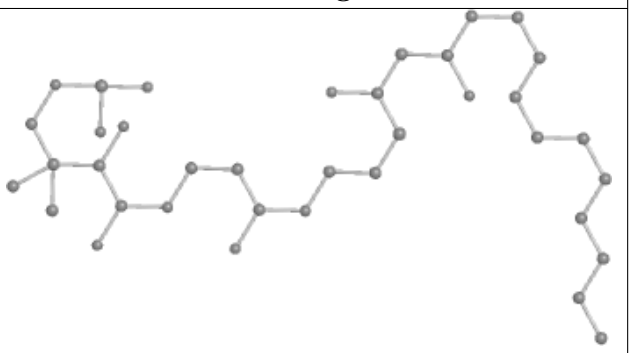
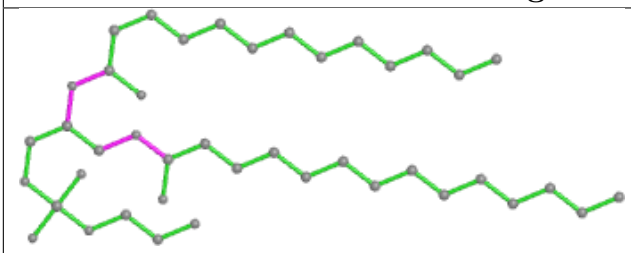
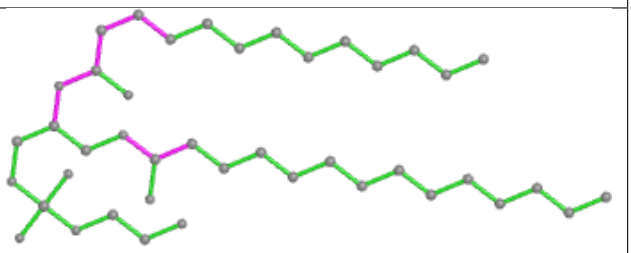
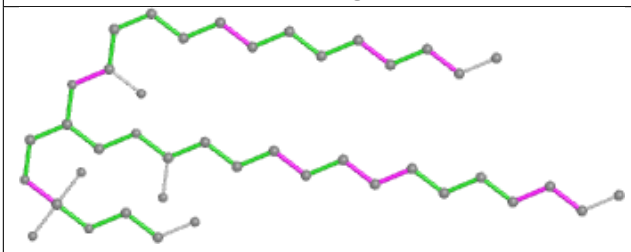
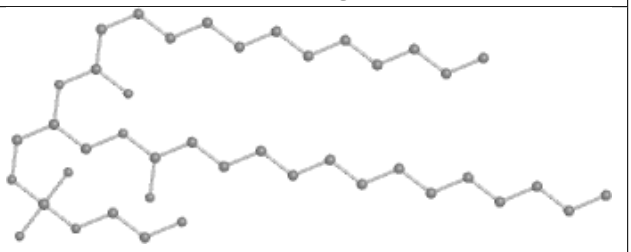
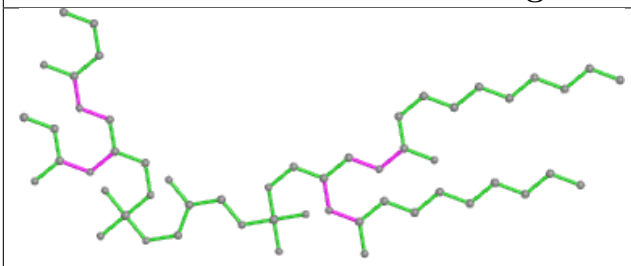
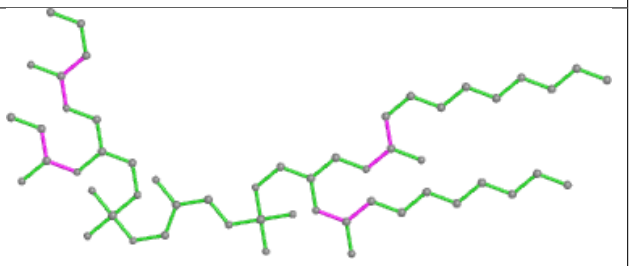
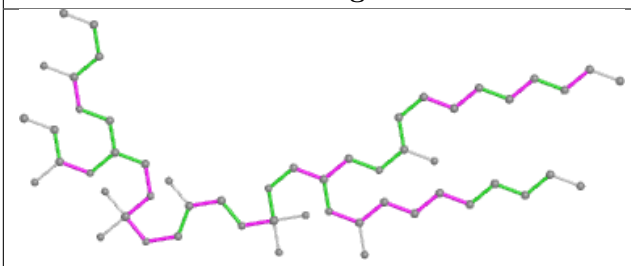
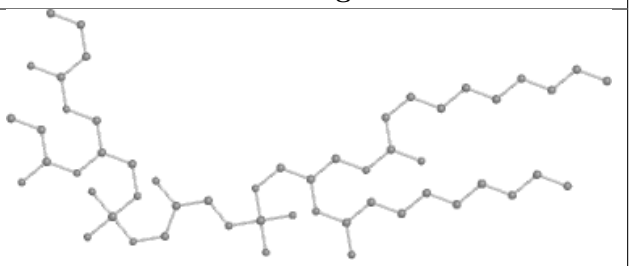
 Bond lengths	 Bond angles
 Torsions	 Rings

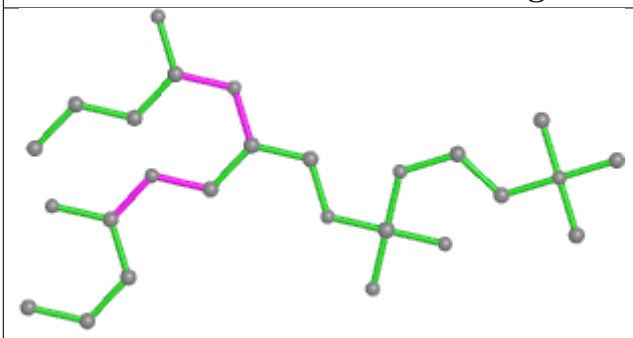
Ligand 3PE M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EHZ U 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

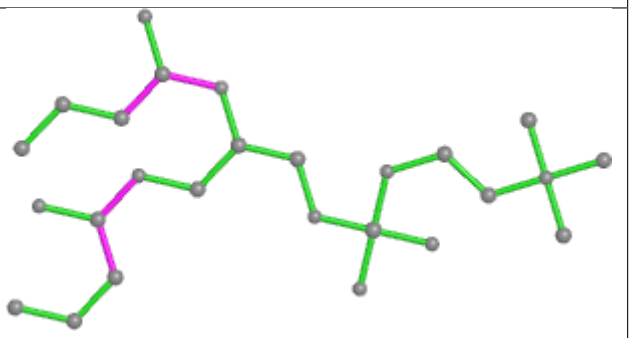
Ligand 3PE H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL L 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

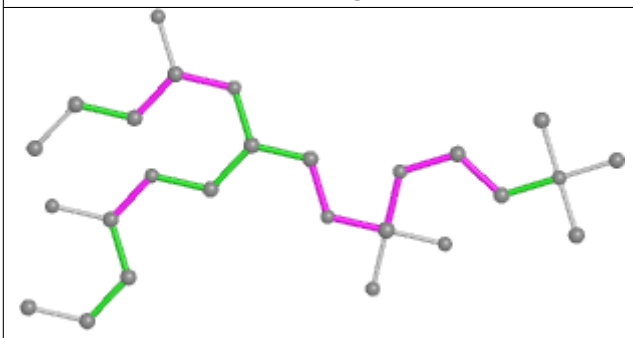
Ligand PC1 B 202



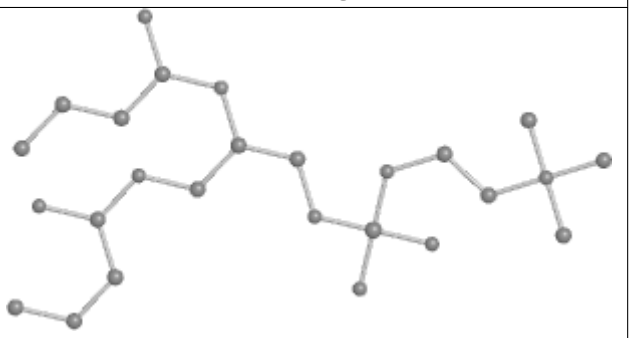
Bond lengths



Bond angles

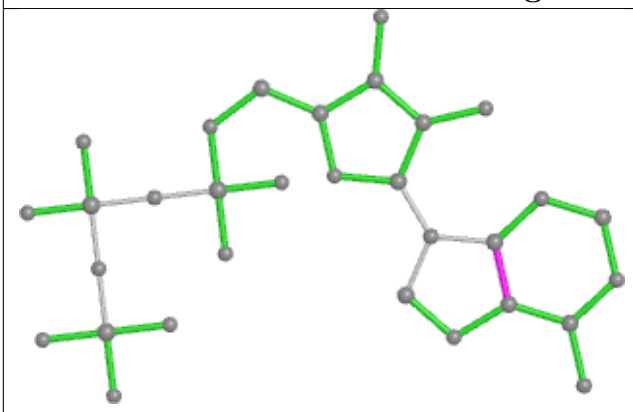


Torsions

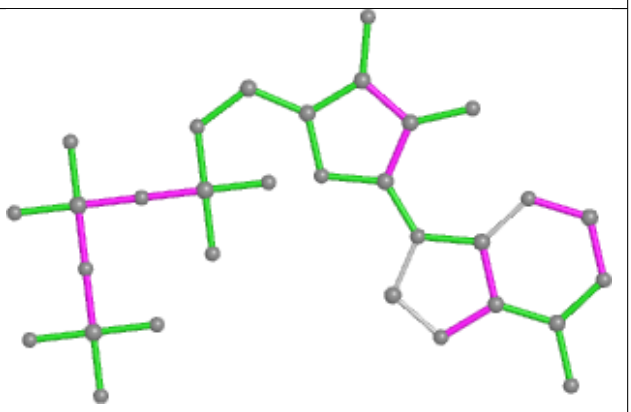


Rings

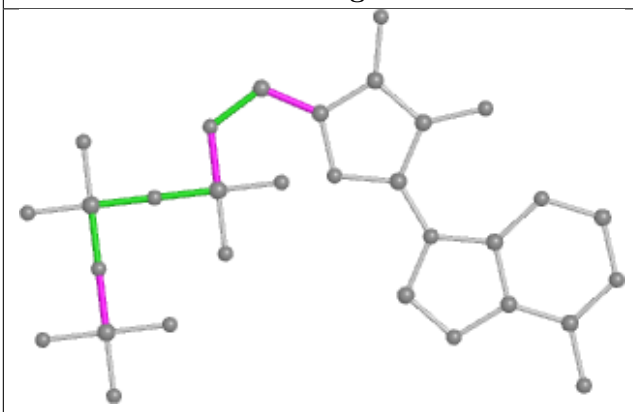
Ligand ATP O 401



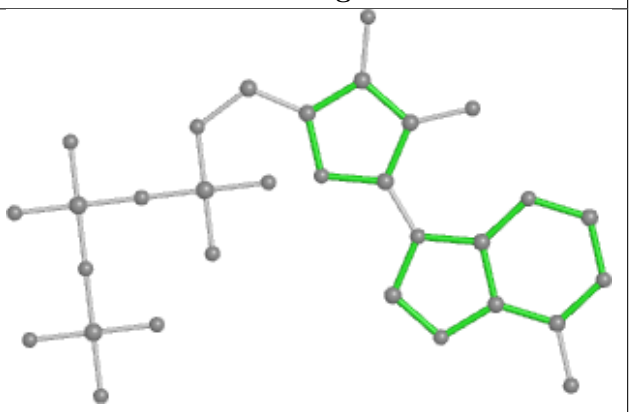
Bond lengths



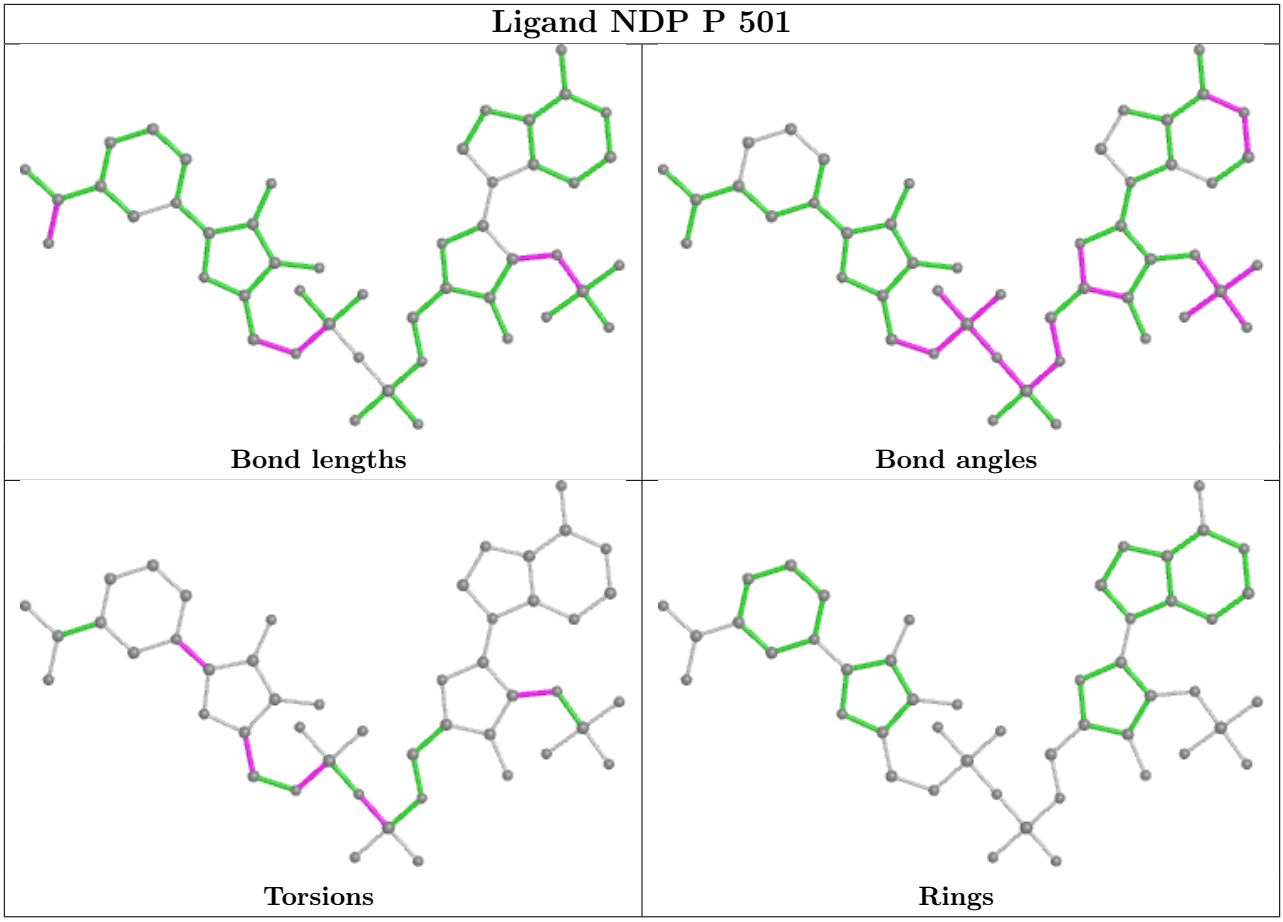
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

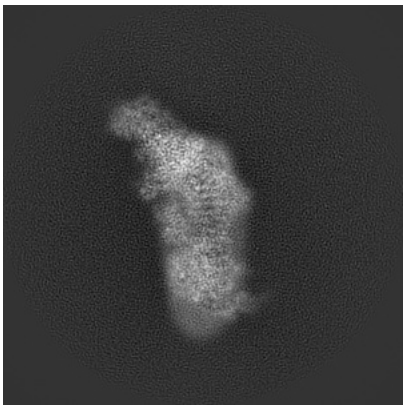
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11811. These allow visual inspection of the internal detail of the map and identification of artifacts.

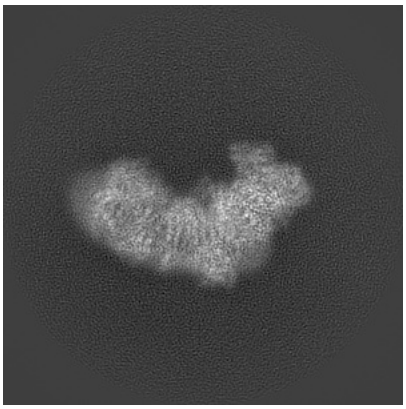
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

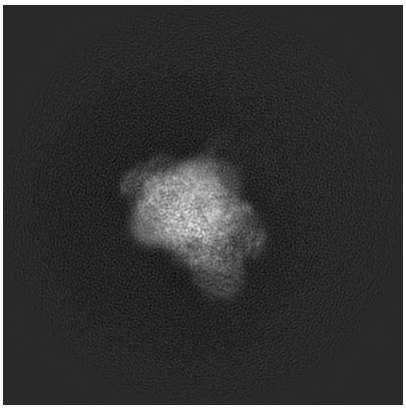
6.1.1 Primary map



X

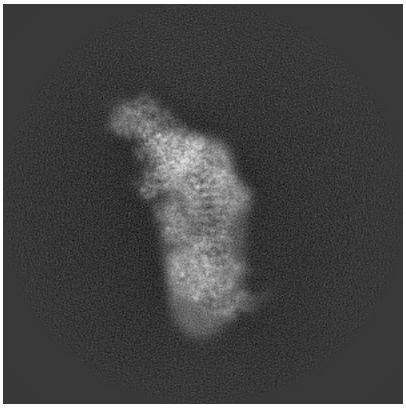


Y

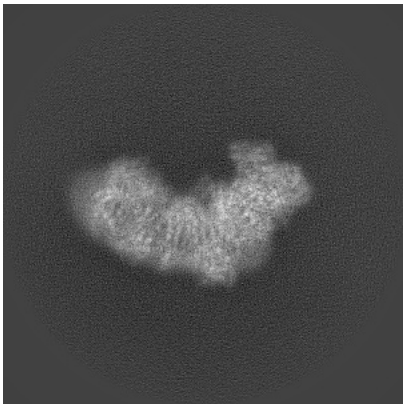


Z

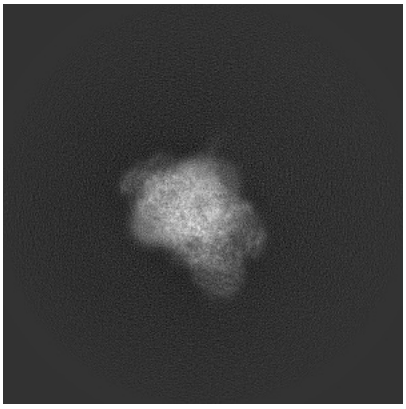
6.1.2 Raw map



X



Y

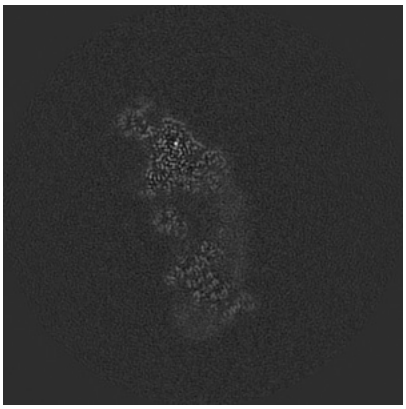


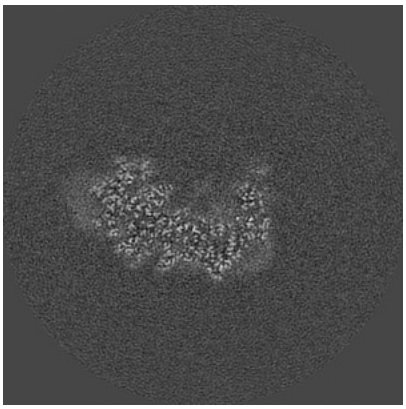
Z

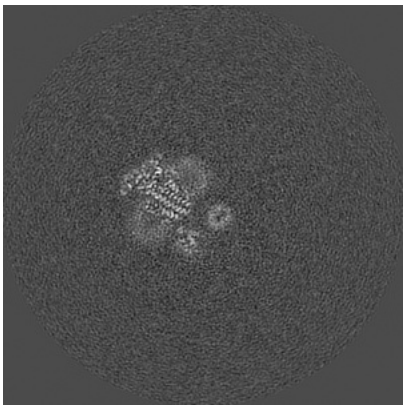
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

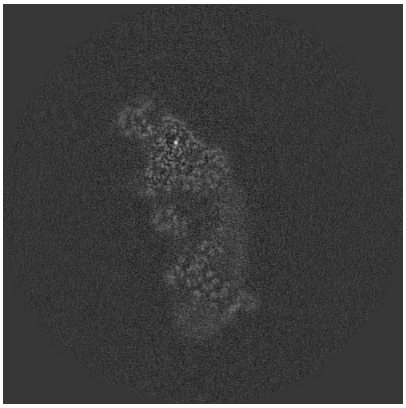
6.2.1 Primary map

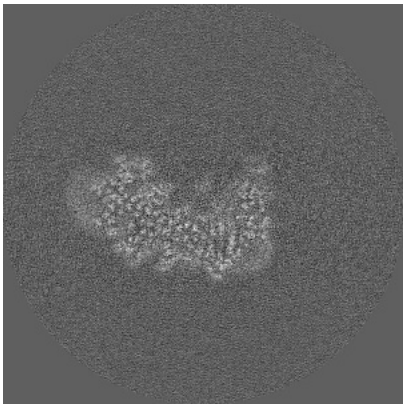

X Index: 225

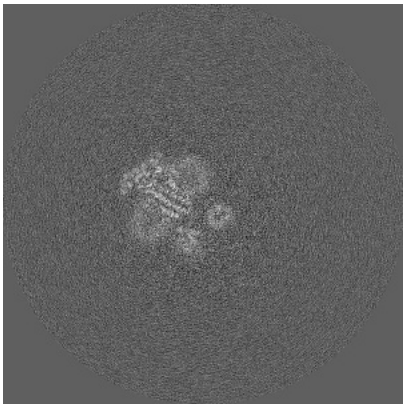

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

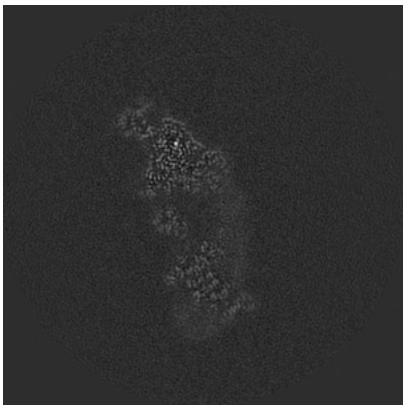

Y Index: 225

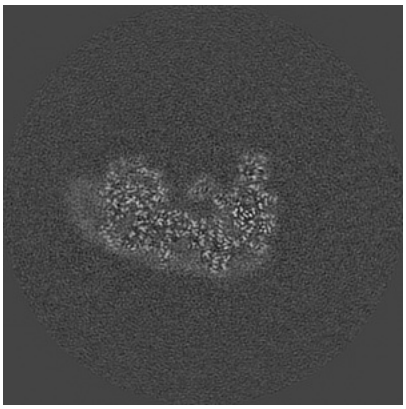

Z Index: 225

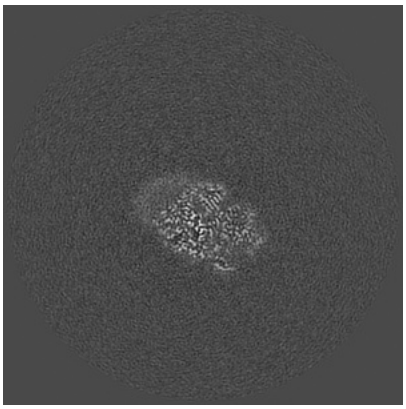
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

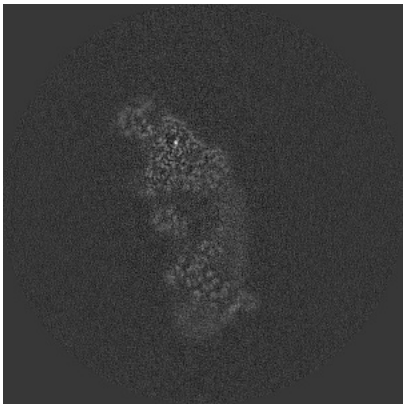
6.3.1 Primary map

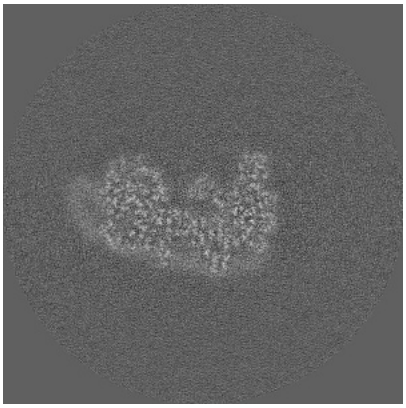

X Index: 225

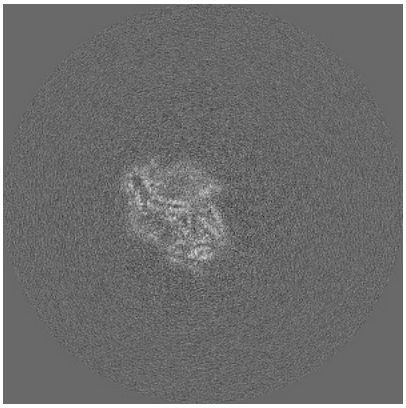

Y Index: 216


Z Index: 279

6.3.2 Raw map


X Index: 225

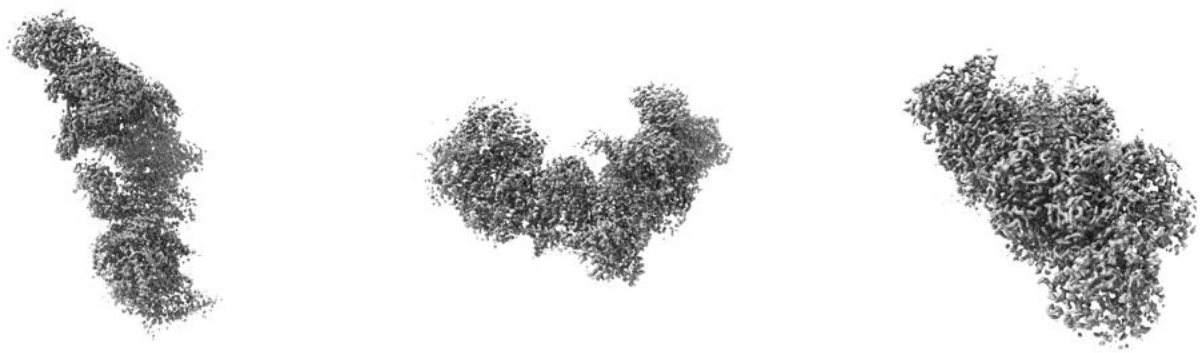

Y Index: 216


Z Index: 245

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

6.4 Orthogonal surface views (i)

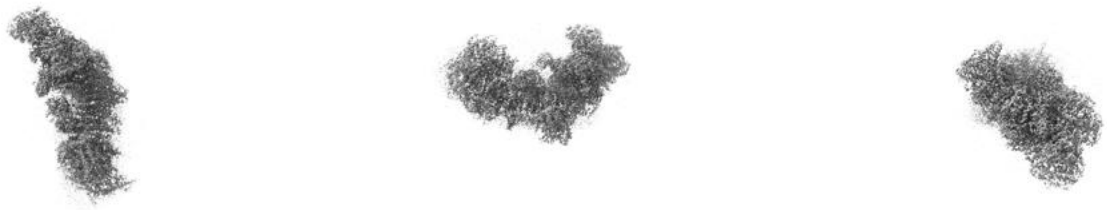
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0268. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

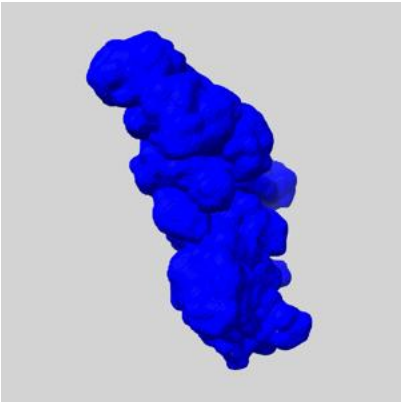
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

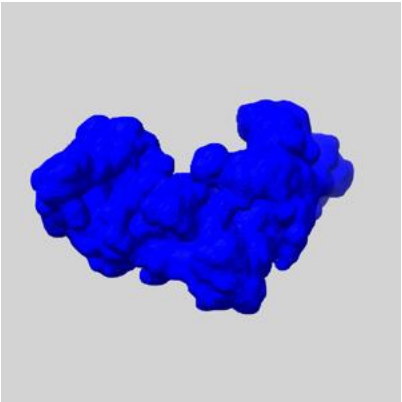
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

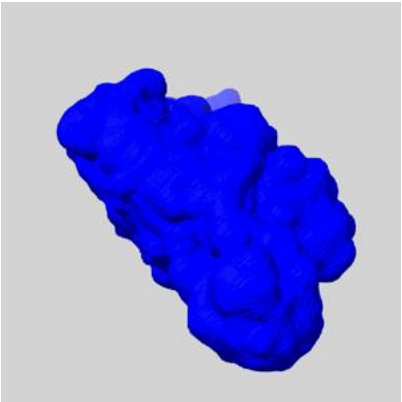
6.5.1 emd_11811_msk_1.map (i)



X



Y

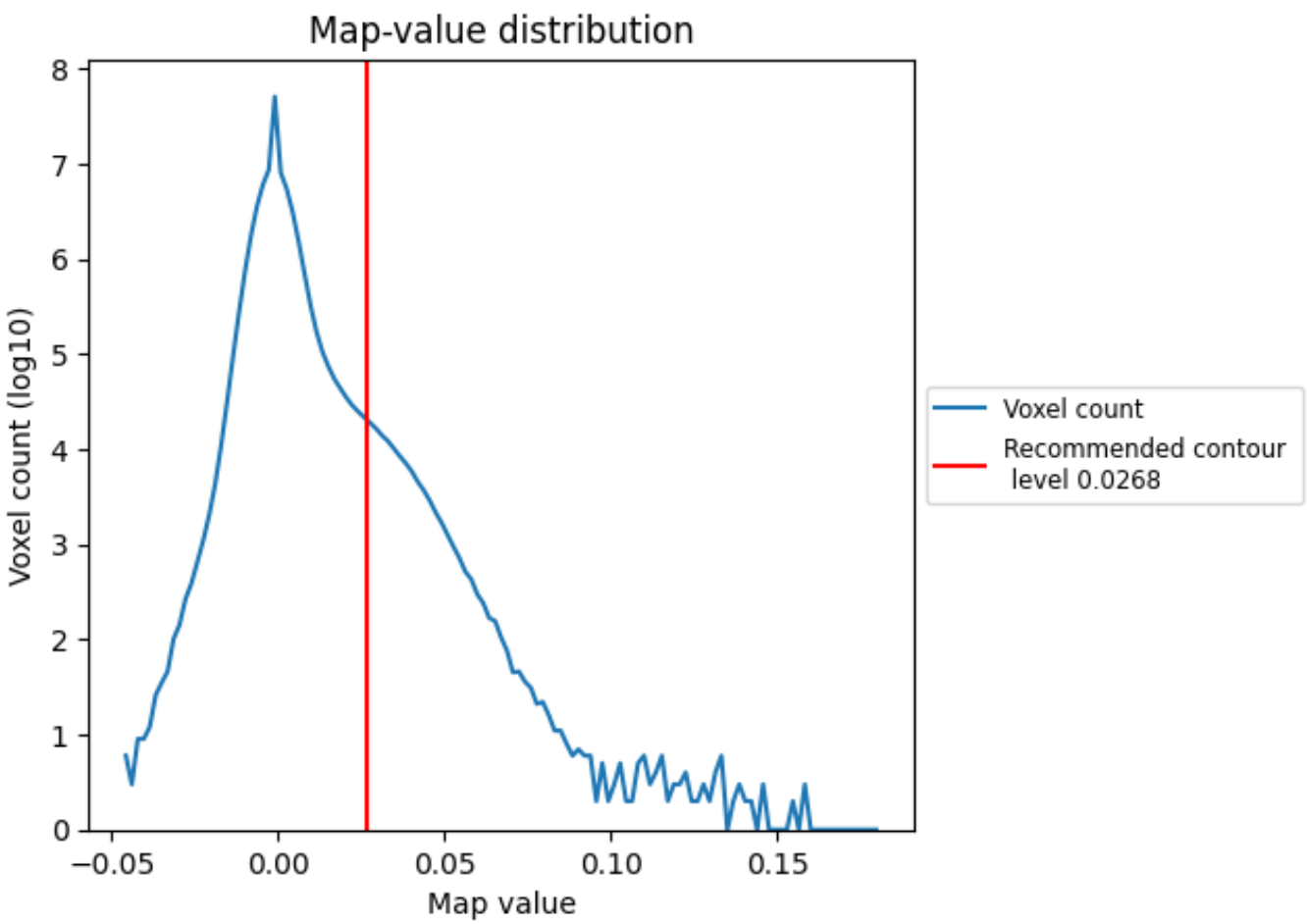


Z

7 Map analysis (i)

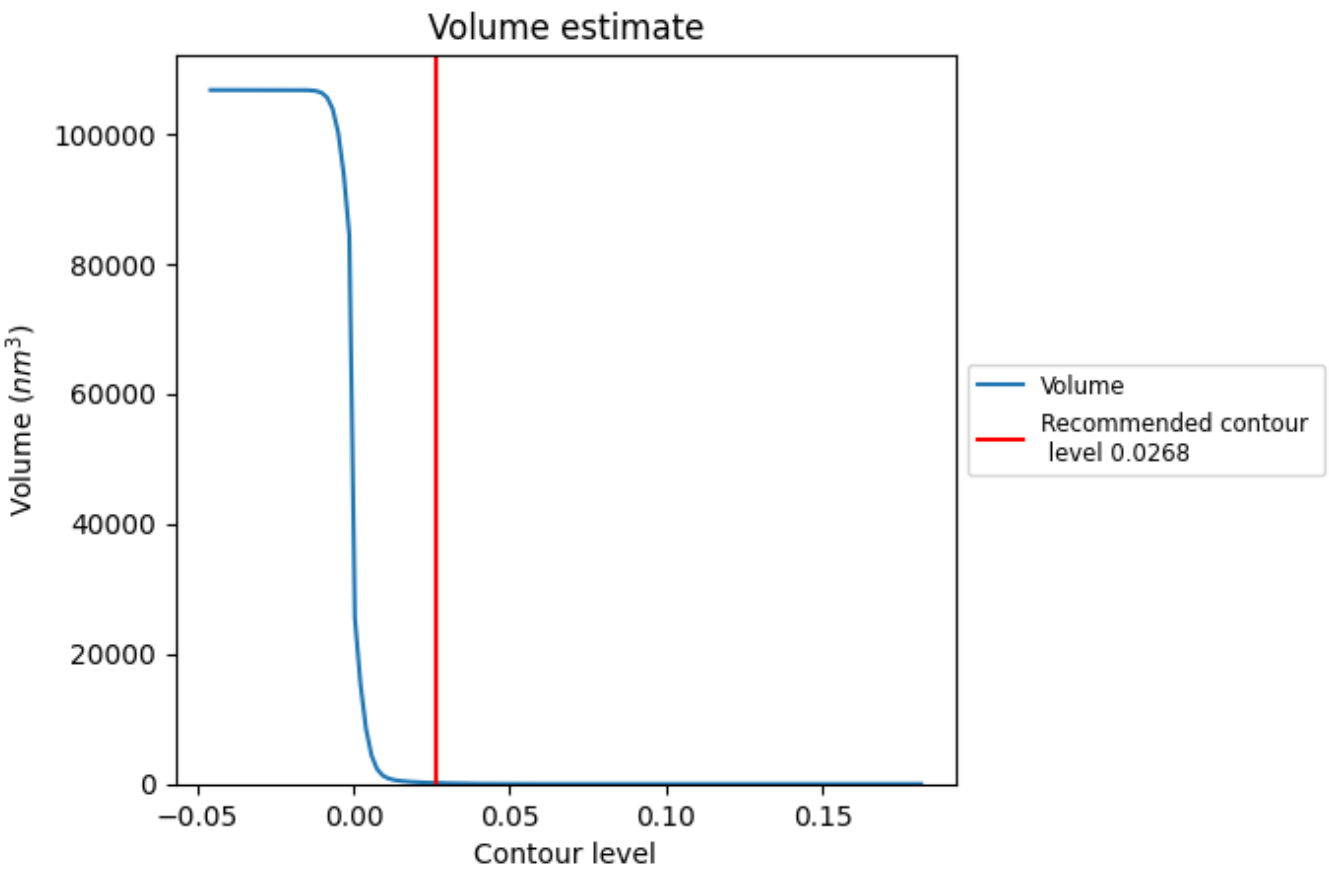
This section contains the results of statistical analysis of the map.

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.

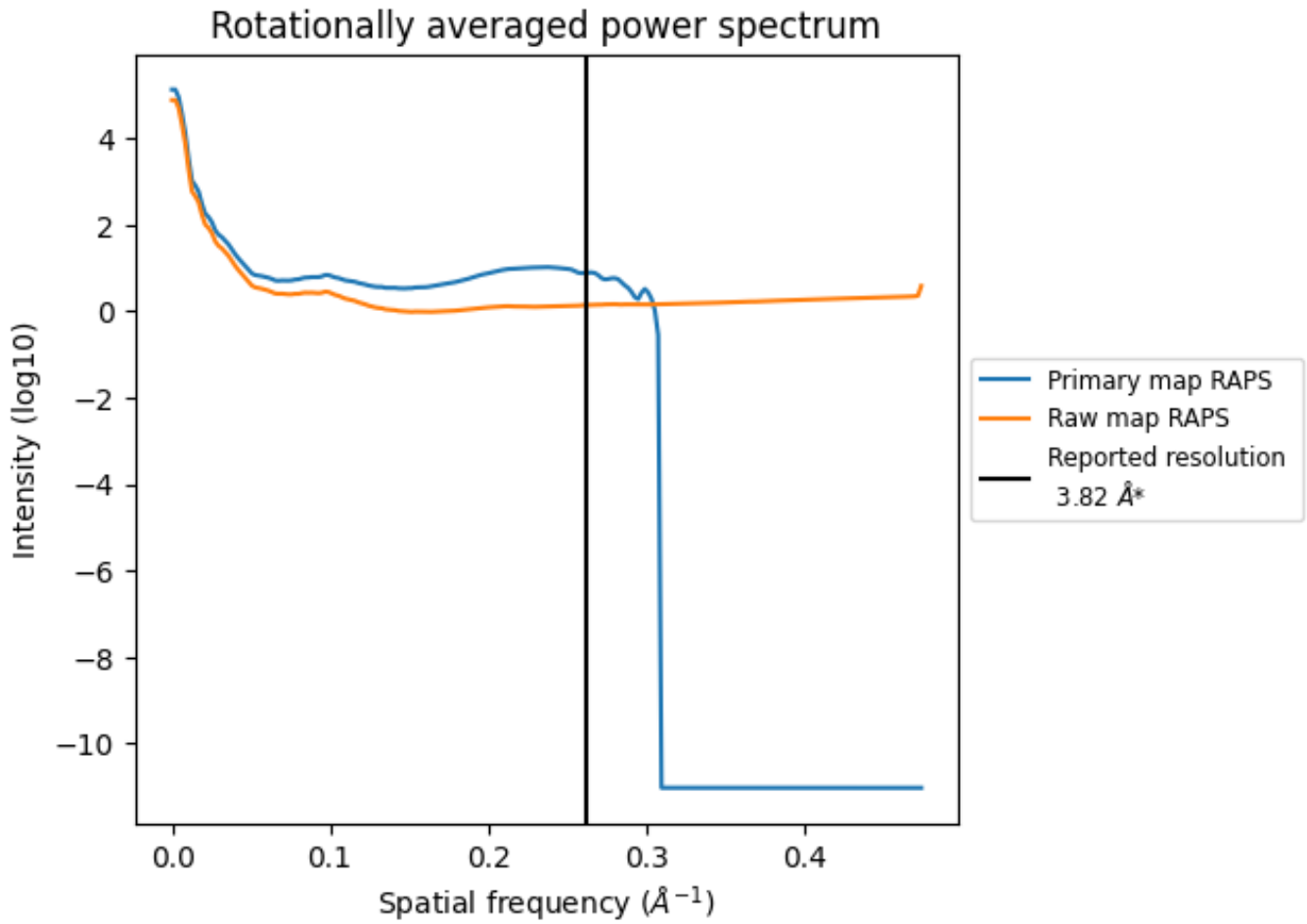
7.2 Volume estimate (i)



The volume at the recommended contour level is 146 nm^3; this corresponds to an approximate mass of 132 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)

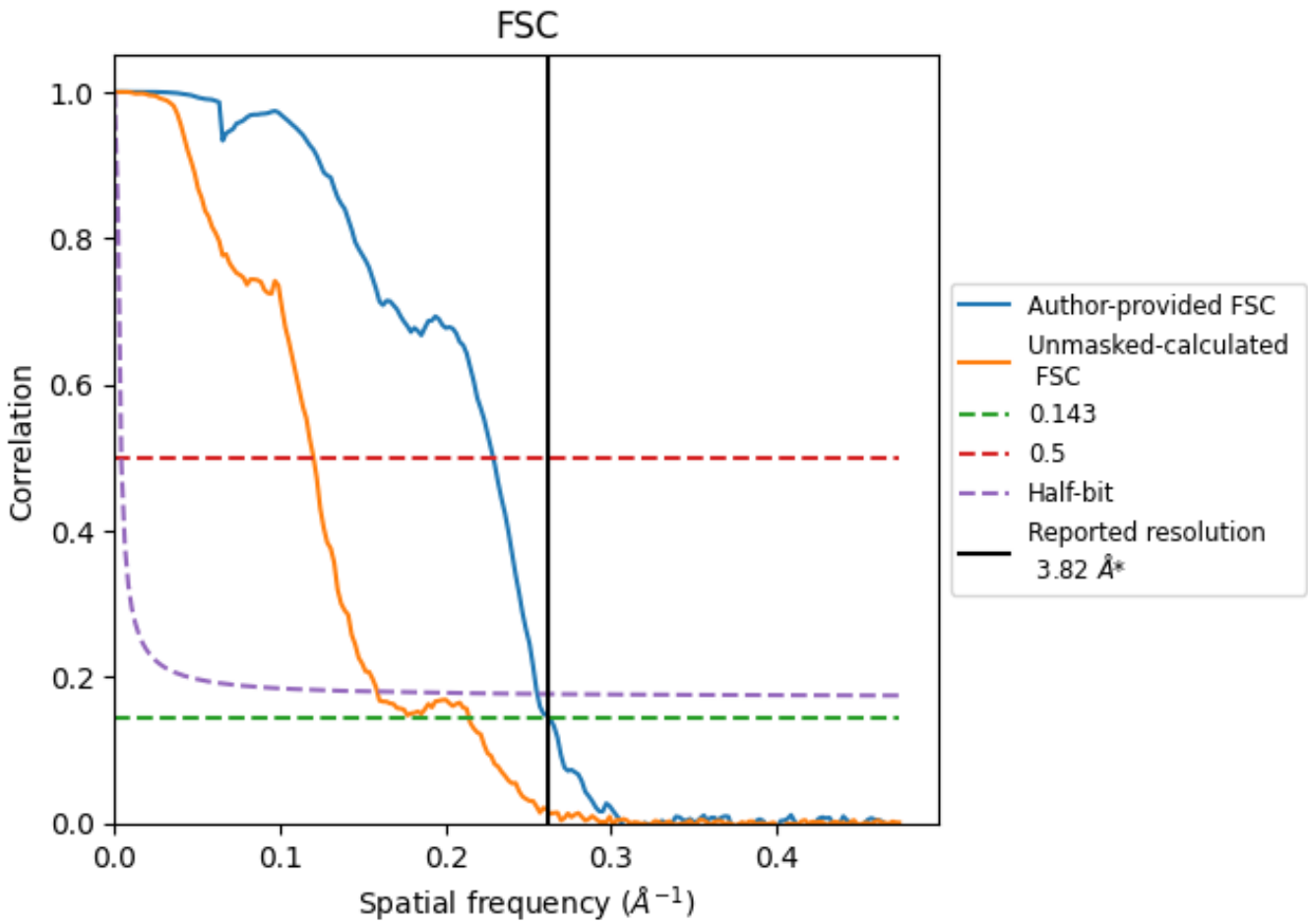


*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

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 0.262 Å^{-1}

8.2 Resolution estimates (i)

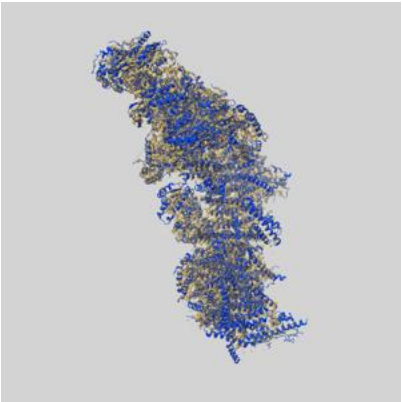
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.80	4.37	3.91
Unmasked-calculated*	4.66	8.31	6.30

*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 4.66 differs from the reported value 3.82 by more than 10 %

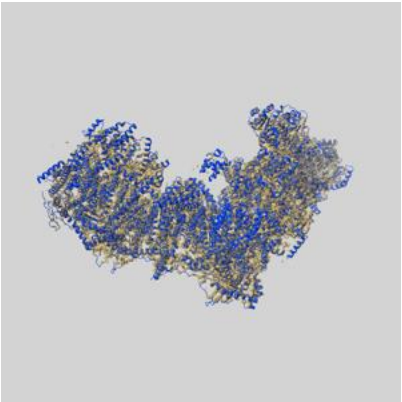
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11811 and PDB model 7AK6. Per-residue inclusion information can be found in section 3 on page 18.

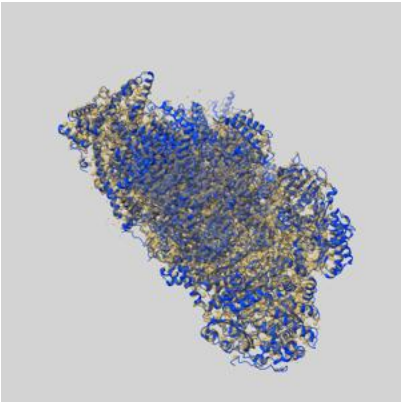
9.1 Map-model overlay (i)



X



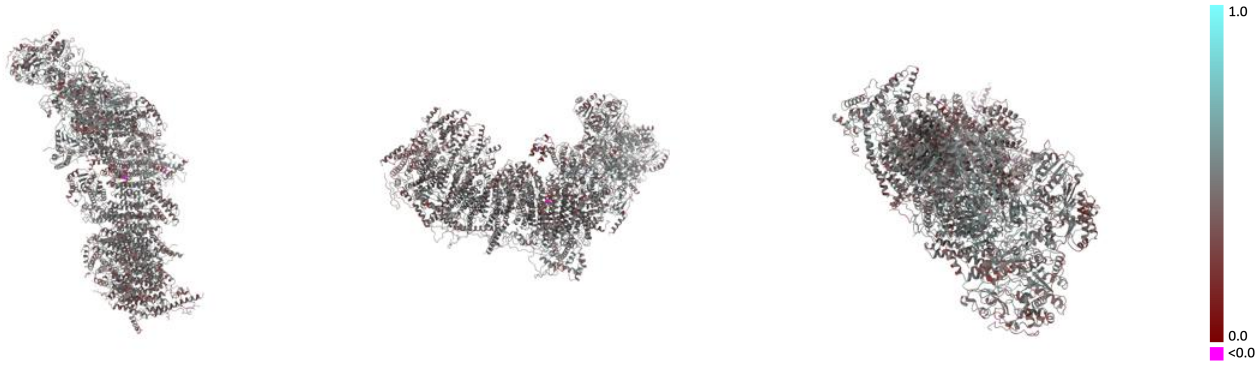
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

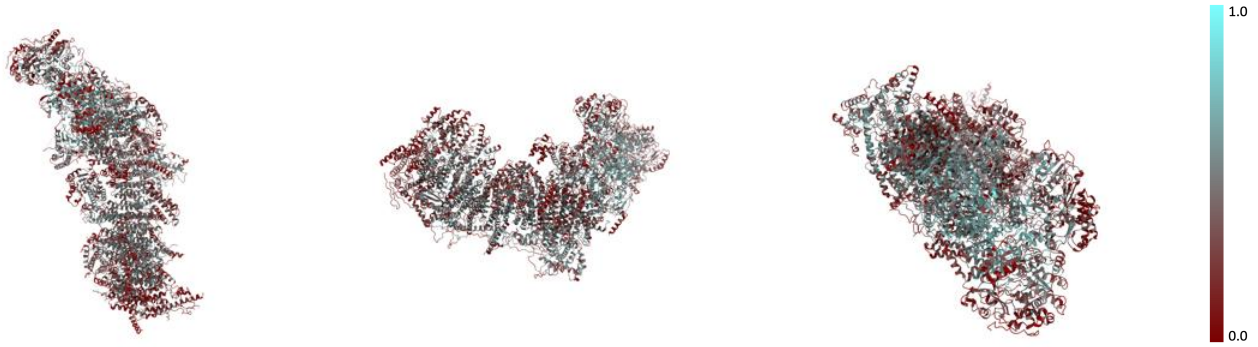
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

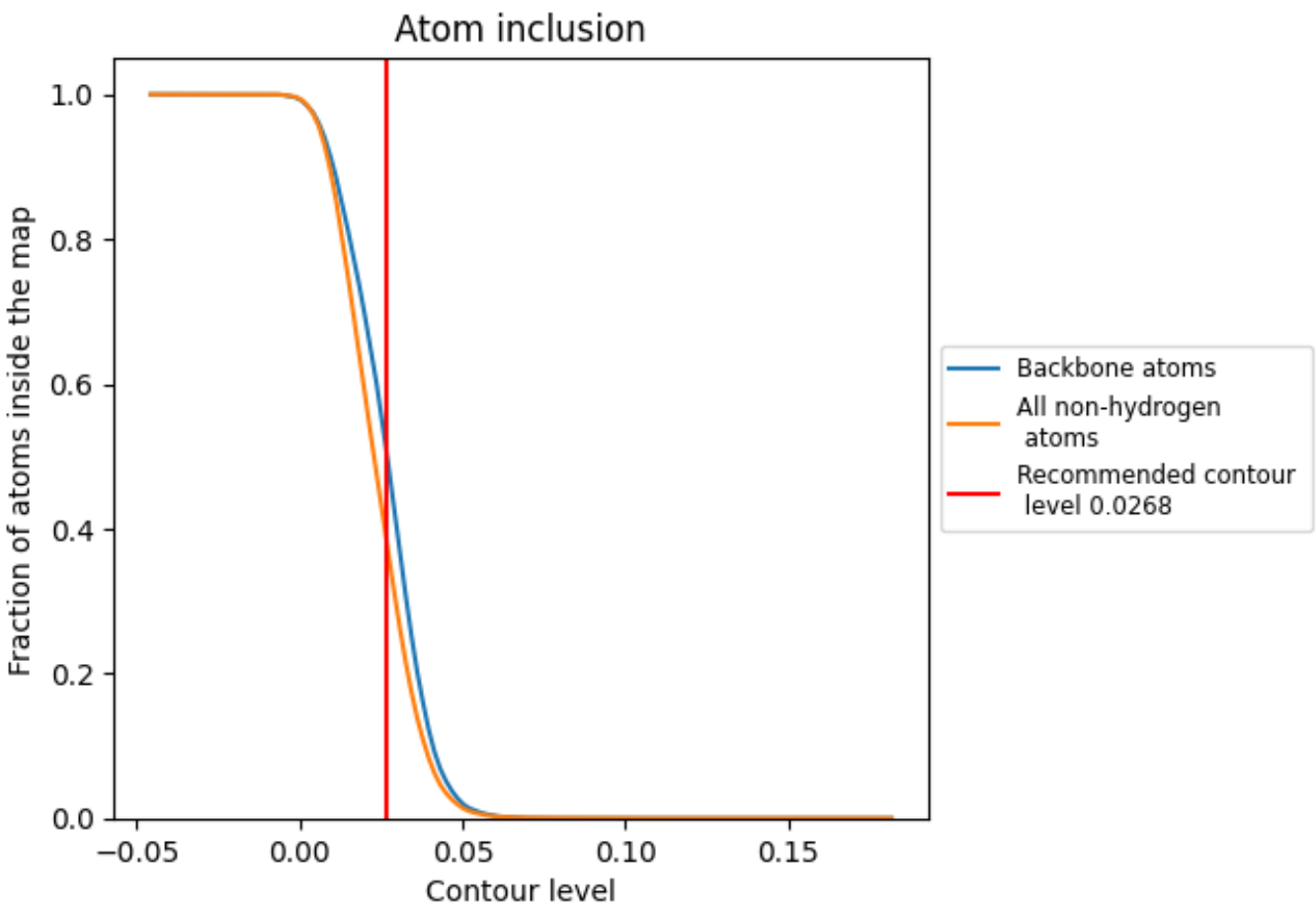
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0268).

9.4 Atom inclusion (i)



At the recommended contour level, 50% 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 (0.0268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3806	0.4470
A	0.3086	0.4300
B	0.5678	0.4850
C	0.5343	0.4930
D	0.5195	0.4770
E	0.3038	0.4230
F	0.3491	0.4430
G	0.4310	0.4570
H	0.4023	0.4510
I	0.5887	0.4930
J	0.2757	0.4190
K	0.3847	0.4600
L	0.3495	0.4400
M	0.4608	0.4670
N	0.4800	0.4640
O	0.3607	0.4480
P	0.3408	0.4350
Q	0.4416	0.4760
R	0.4400	0.4750
S	0.1922	0.3990
T	0.0763	0.3060
U	0.1927	0.3950
V	0.3271	0.4380
W	0.3422	0.4330
X	0.3477	0.4540
Y	0.2183	0.4140
Z	0.4403	0.4540
a	0.4264	0.4560
b	0.3339	0.4240
c	0.2811	0.4230
d	0.3778	0.4630
e	0.3950	0.4520
f	0.2803	0.4130
g	0.3513	0.4440
h	0.4255	0.4620

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Chain	Atom inclusion	Q-score
i	0.2655	0.4070
j	0.1648	0.3950
k	0.1675	0.4170
l	0.3216	0.4450
m	0.2955	0.4260
n	0.3130	0.4290
o	0.2065	0.3850
p	0.3539	0.4300
q	0.4262	0.4660
r	0.3952	0.4560
s	0.2250	0.4390