Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 12:06 PM EDT

PDB ID	:	8UEQ
EMDB ID	:	EMD-42167
Title	:	In-situ complex I with Q10 (State-beta)
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-10-02
Resolution	:	3.40 Å(reported)

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

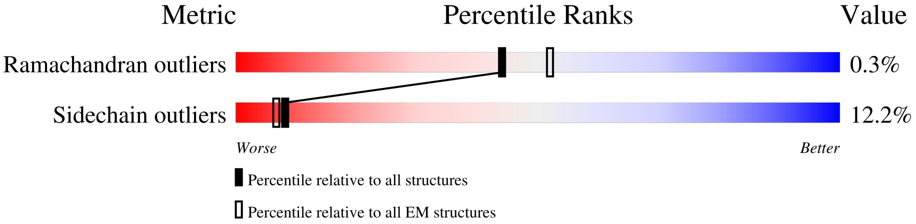
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

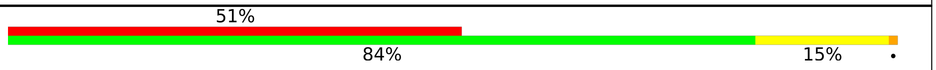
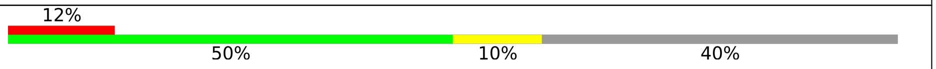
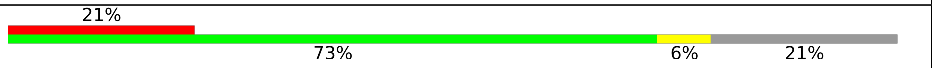
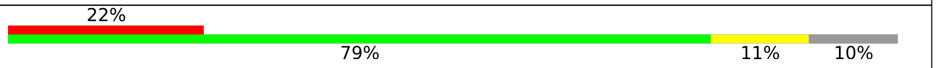
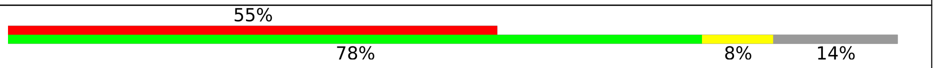
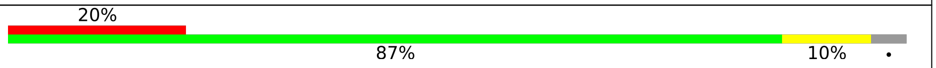
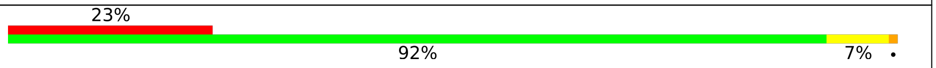
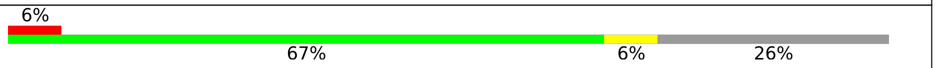
The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	115	
2	1B	258	
3	1C	264	
4	1D	476	
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	

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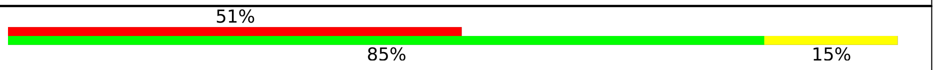
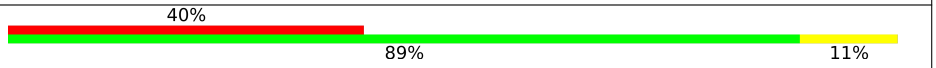
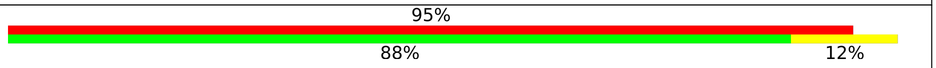
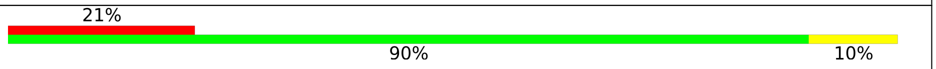
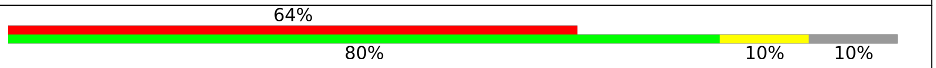
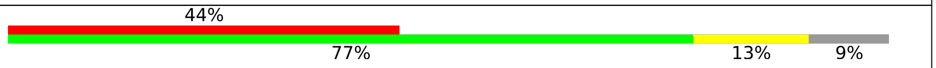
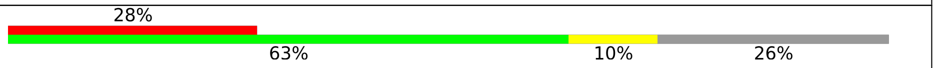
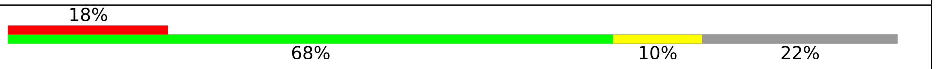
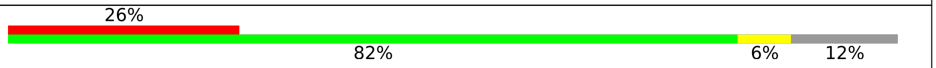
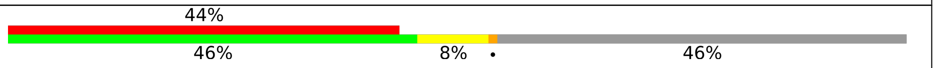
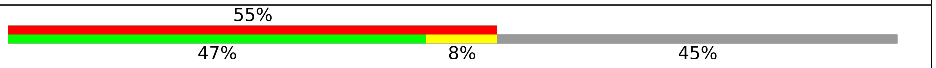
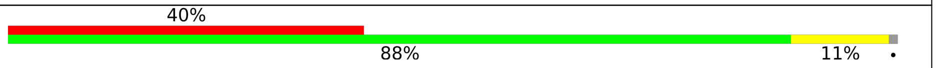
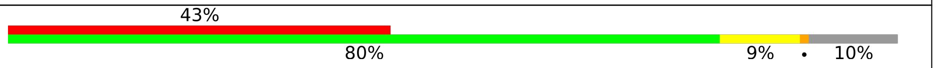
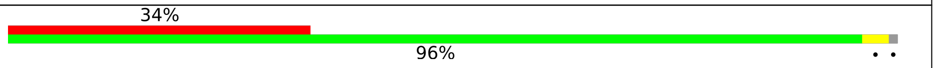
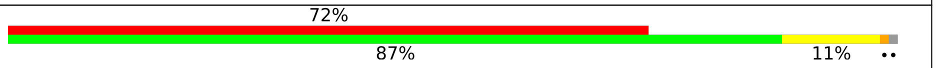
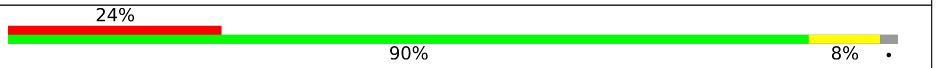
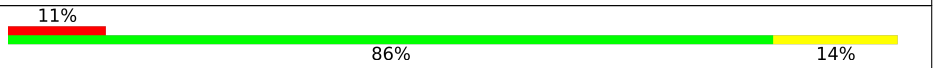
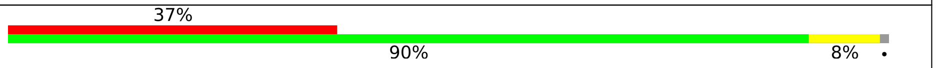
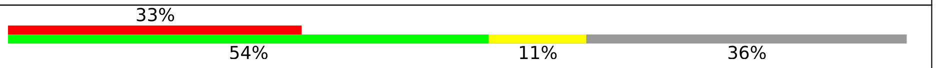
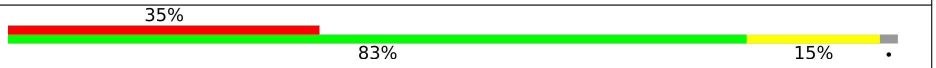
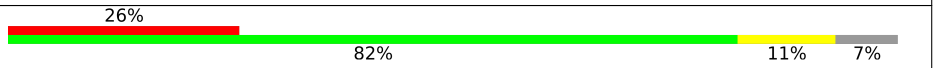
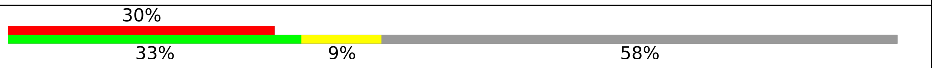
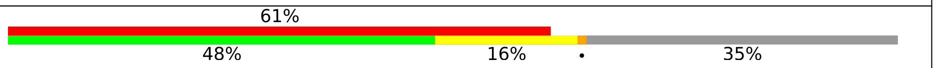
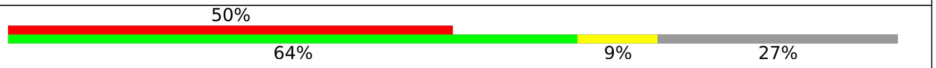
Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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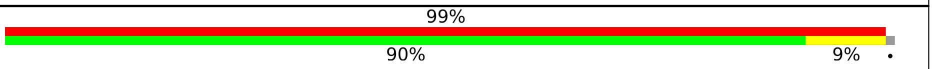
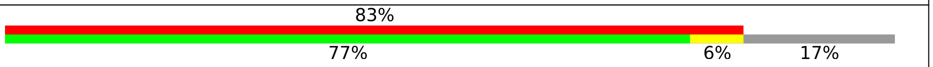
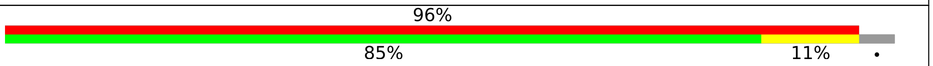
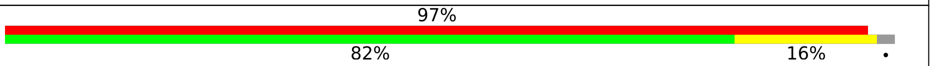
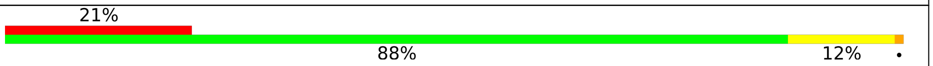
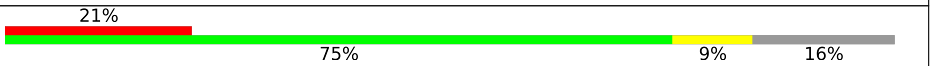
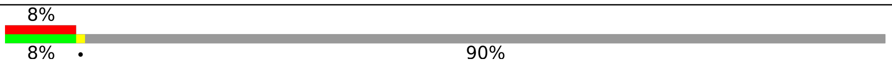
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67142 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

- 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
5	1E	214	Total 1658	C 1058	N 278	O 312	S 10	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

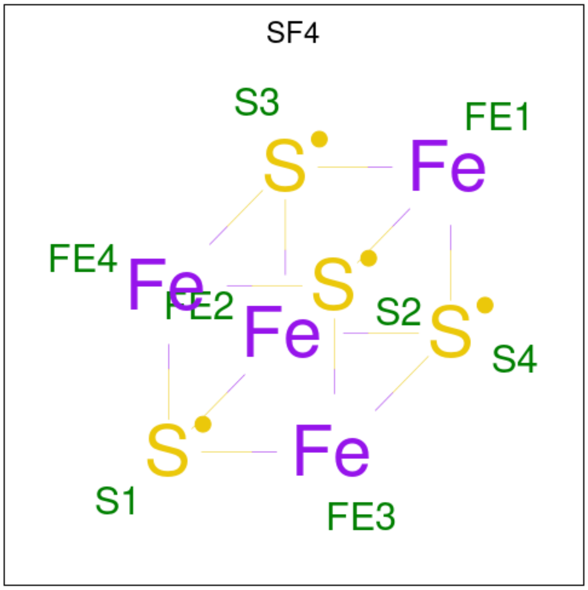
There is a discrepancy between the modelled and reference sequences:

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

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

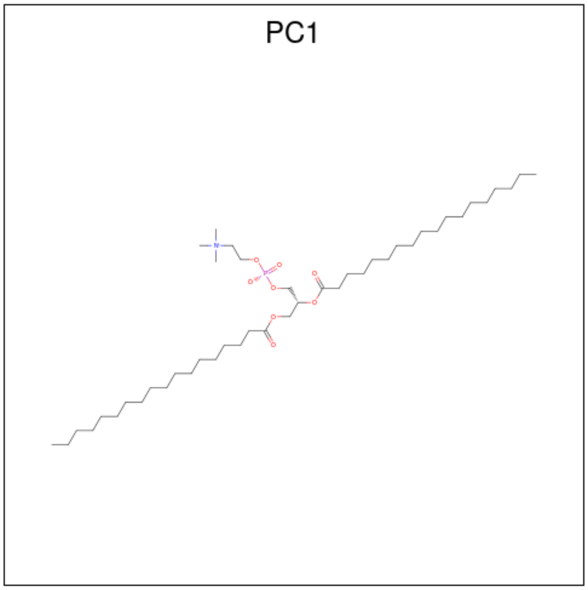
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1s	45	382	238	70	73	1	0	0

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



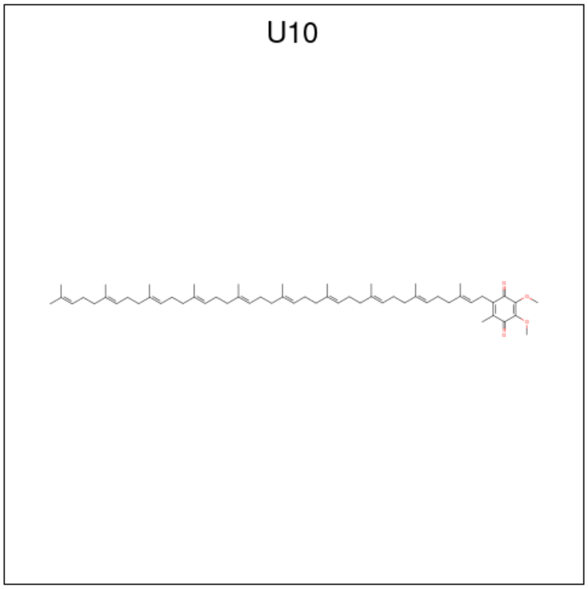
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1B	1	8	4	4	0
45	1F	1	8	4	4	0
45	1G	1	8	4	4	0
45	1G	1	8	4	4	0
45	1I	1	8	4	4	0
45	1I	1	8	4	4	0

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



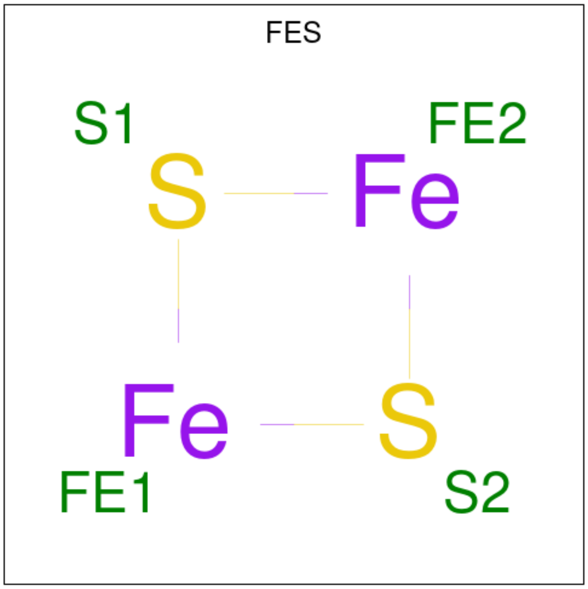
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total C N O P 34 24 1 8 1	0
46	1d	1	Total C N O P 39 29 1 8 1	0
46	1q	1	Total C N O P 48 38 1 8 1	0

- Molecule 47 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



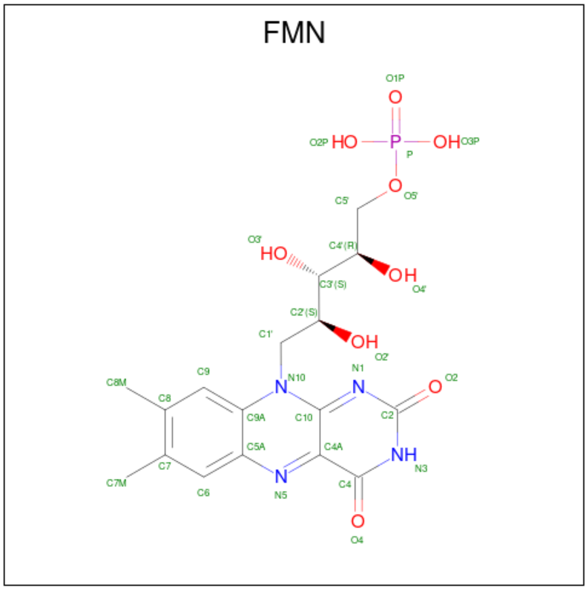
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	1D	1	63	59	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	1E	1	4	2	2	0
48	1G	1	4	2	2	0

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

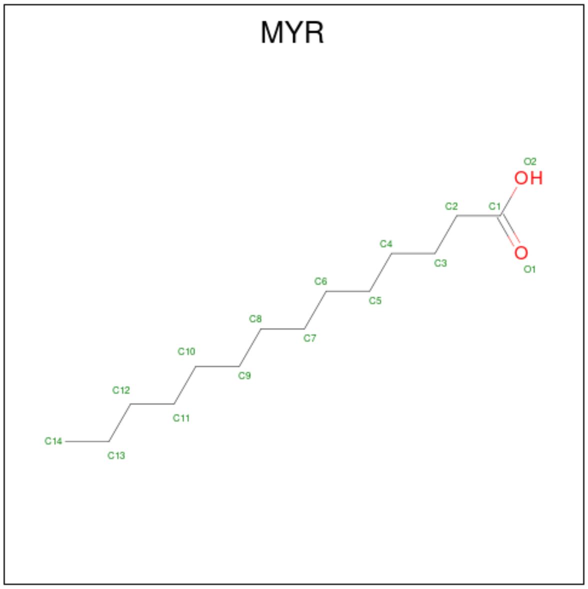


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	1F	1	31	17	4	9	1	0

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

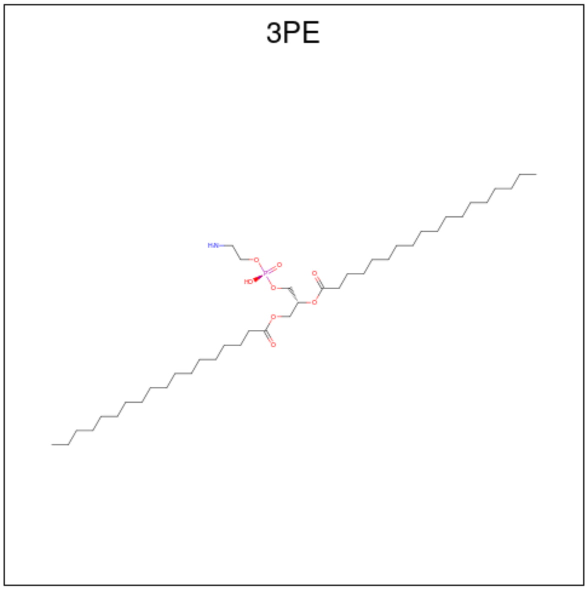
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
50	1G	1	1	1	0

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



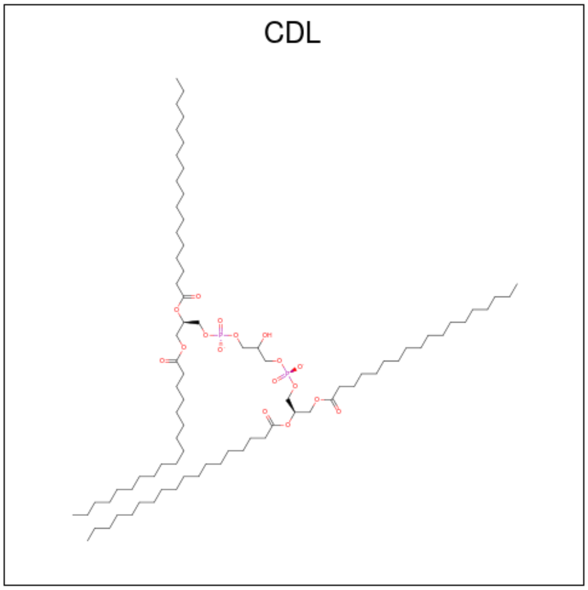
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	1L	1	15	14	1	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	1M	1	38	28	1	8	1	0

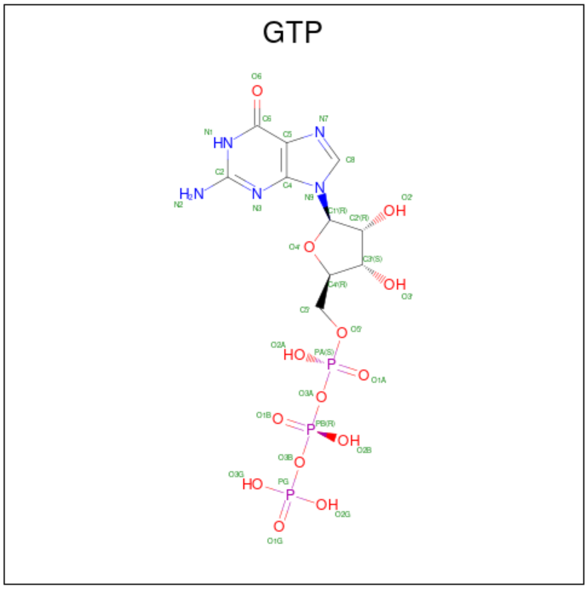
- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	1N	1	67	48	17	2	0
53	1a	1	61	42	17	2	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$C_{10}H_{16}N_5O_{14}P_3$).

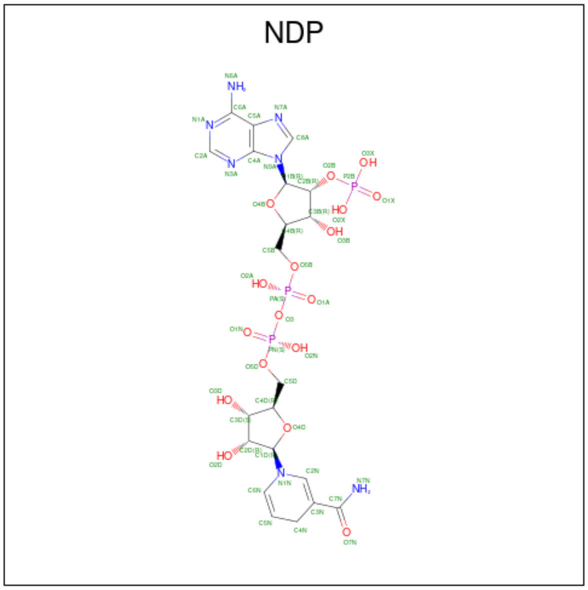


Mol	Chain	Residues	Atoms	AltConf
54	1O	1	Total C N O P 32 10 5 14 3	0

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

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

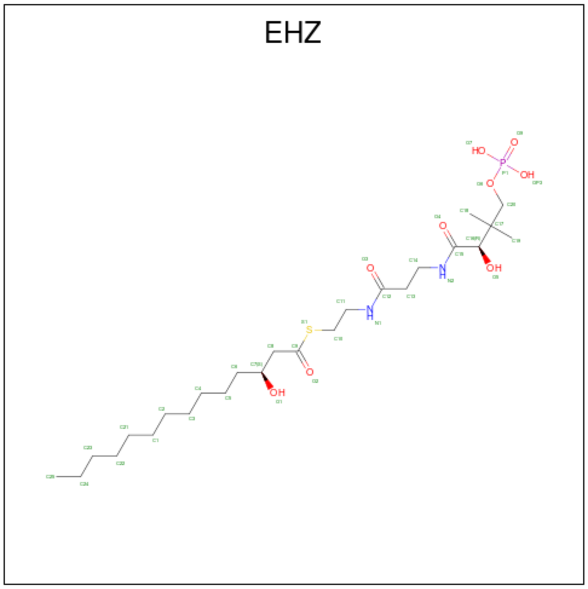


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	1P	1	48	21	7	17	3	0

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

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

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

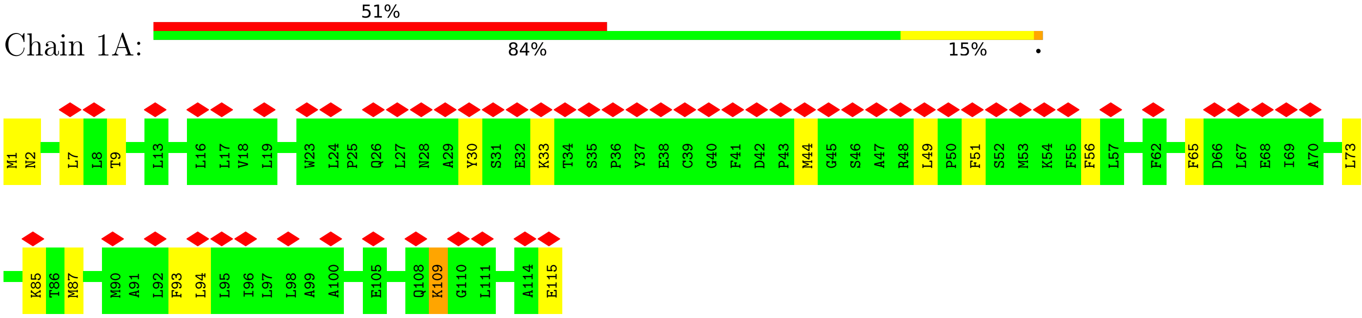


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	1W	1	37	25	2	8	1	1	0
			Total	C	N	O	P	S	
58	1n	1	37	25	2	8	1	1	0

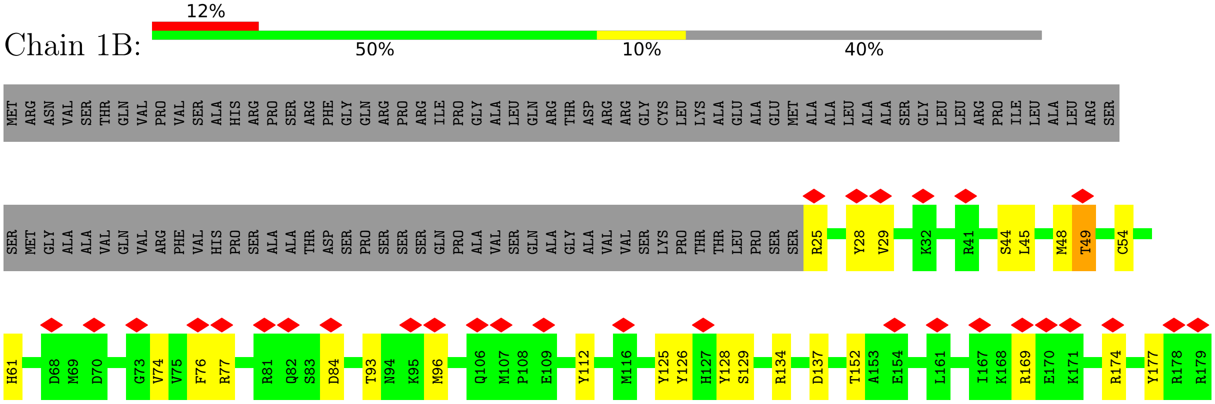
3 Residue-property plots ⓘ

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

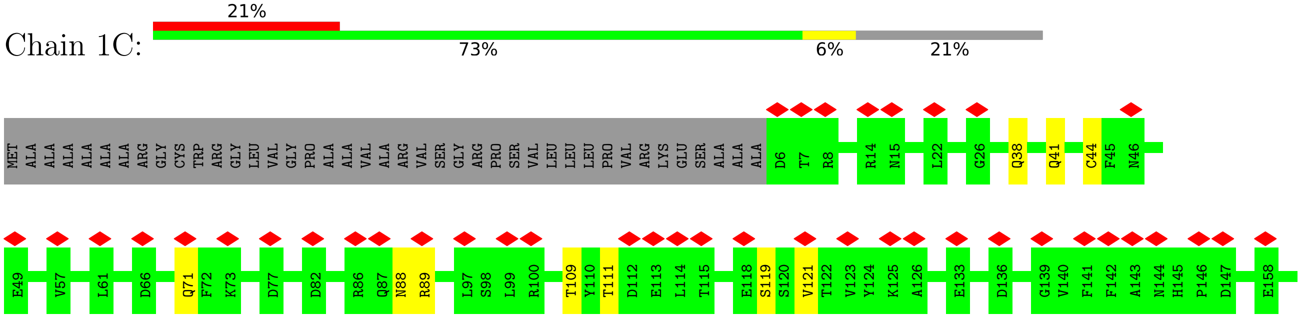
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

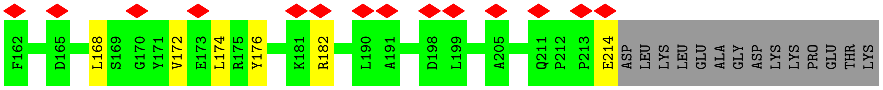


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



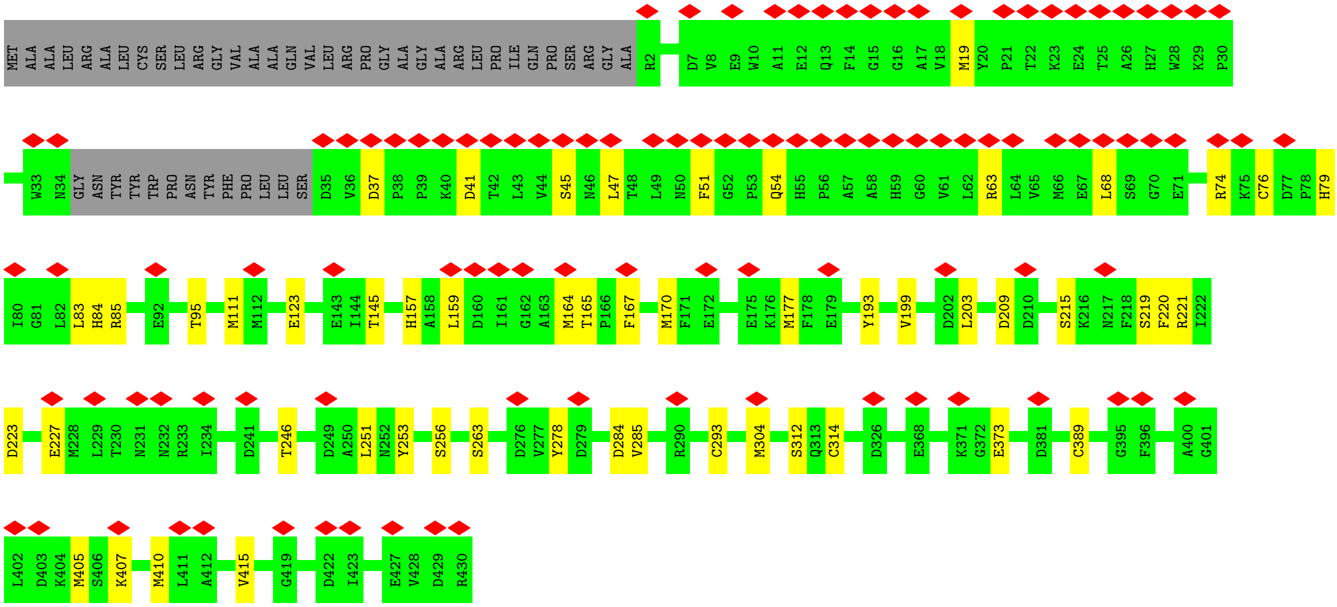
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





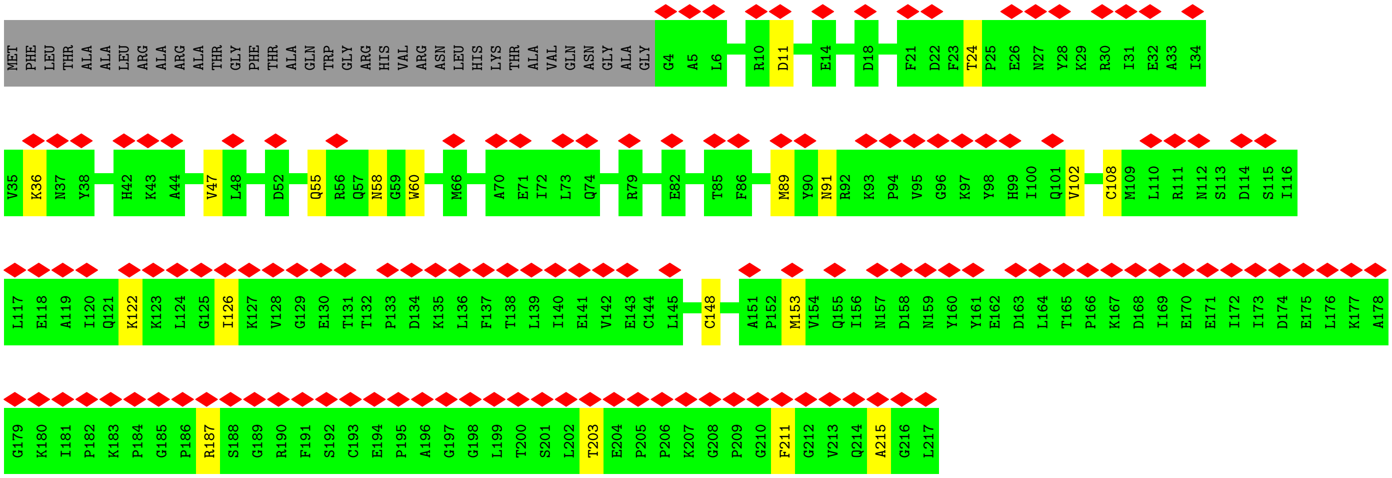
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:



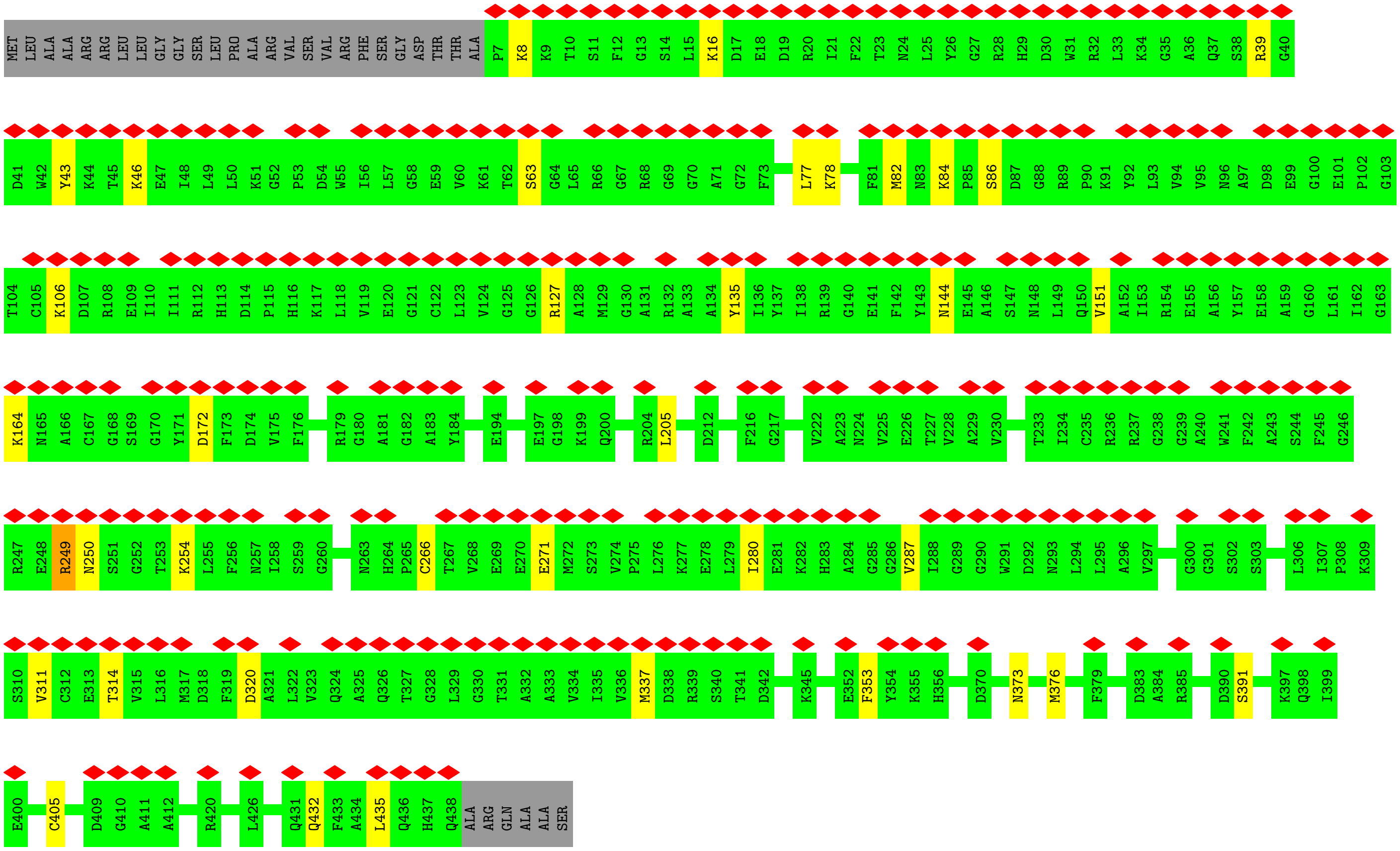
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E:



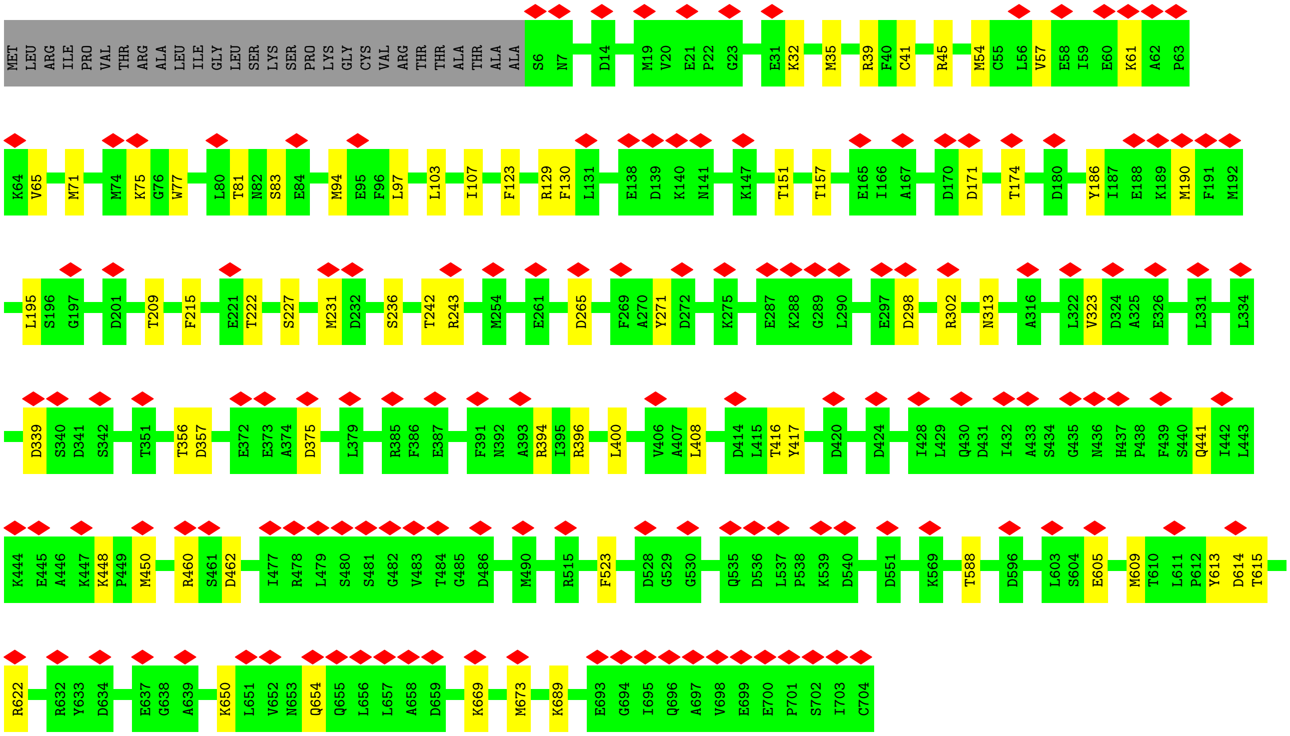
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F:

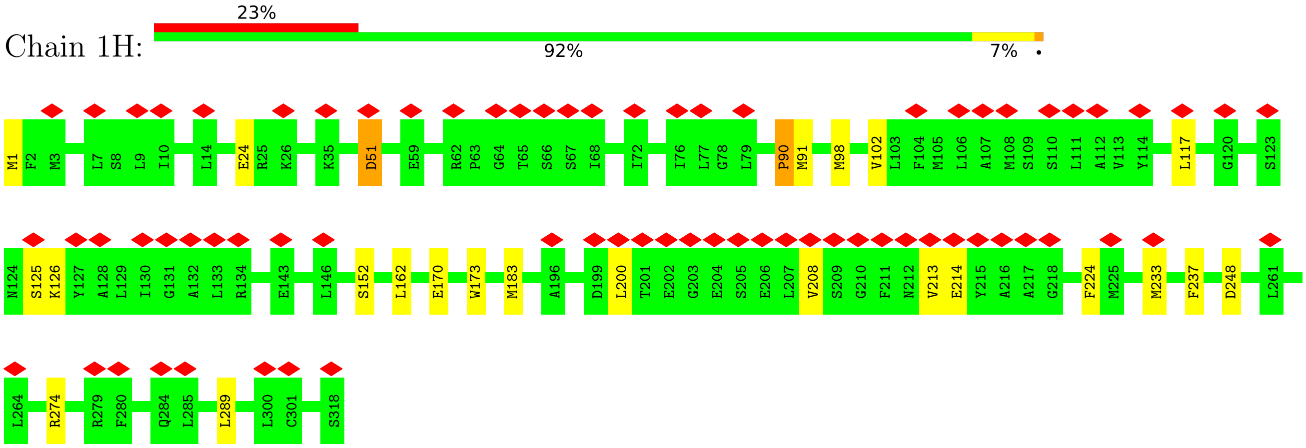


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

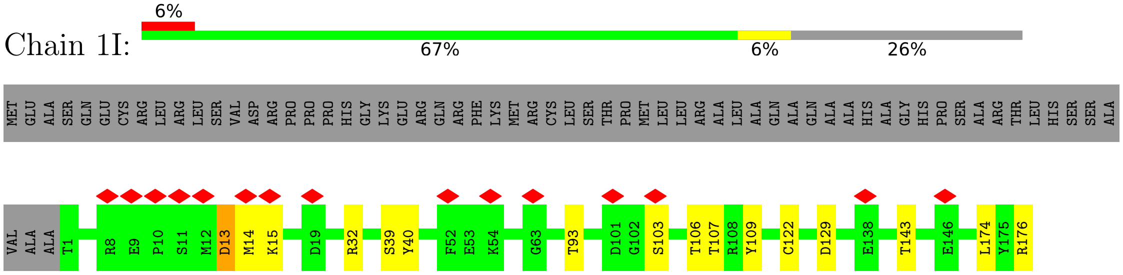
Chain 1G:



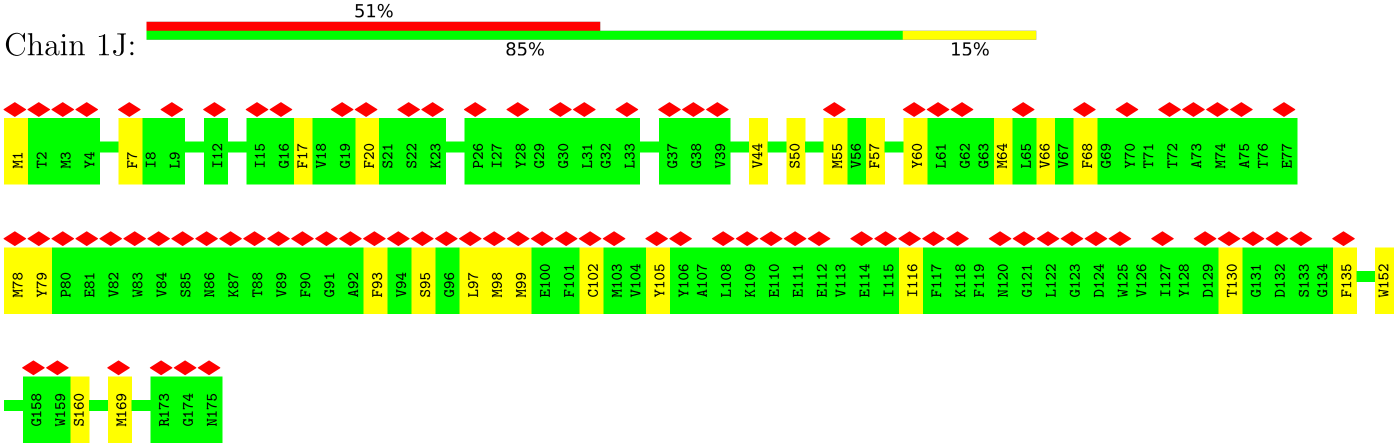
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



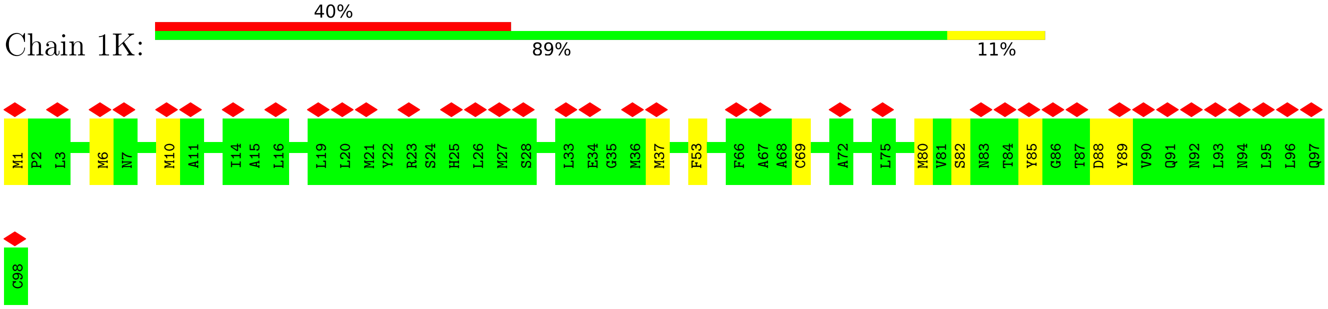
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

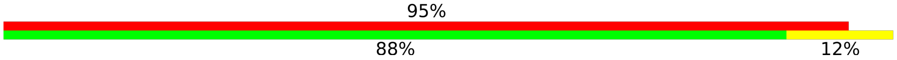


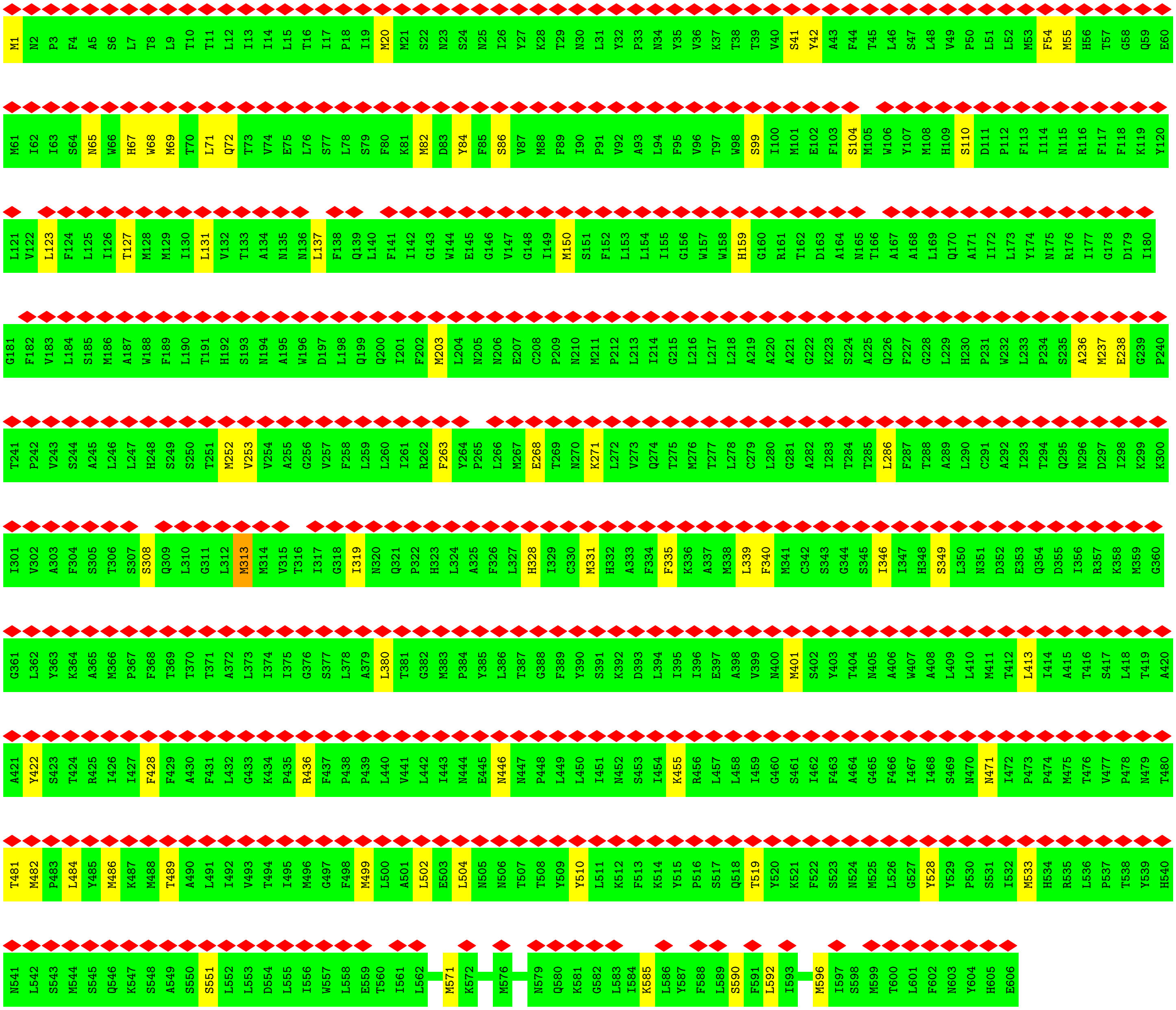
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

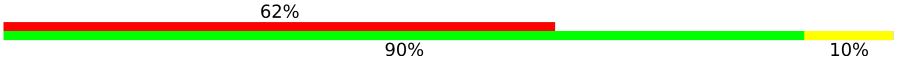
Chain 1L:

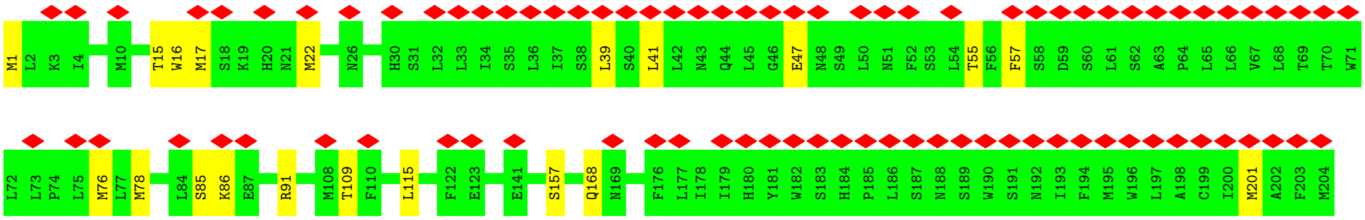


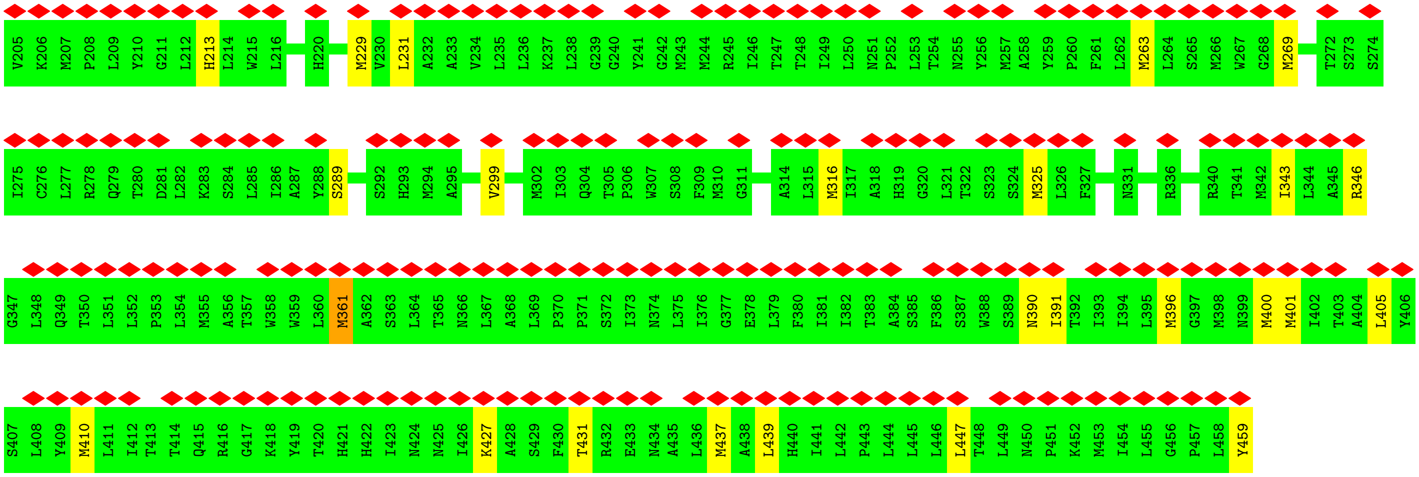


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:

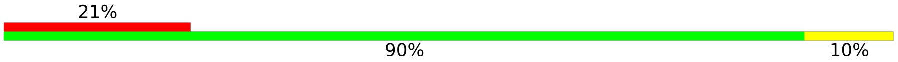


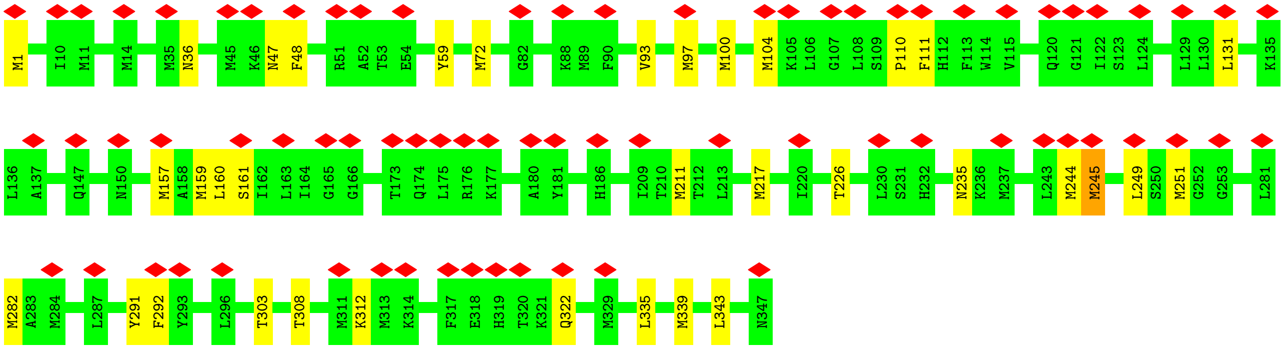




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

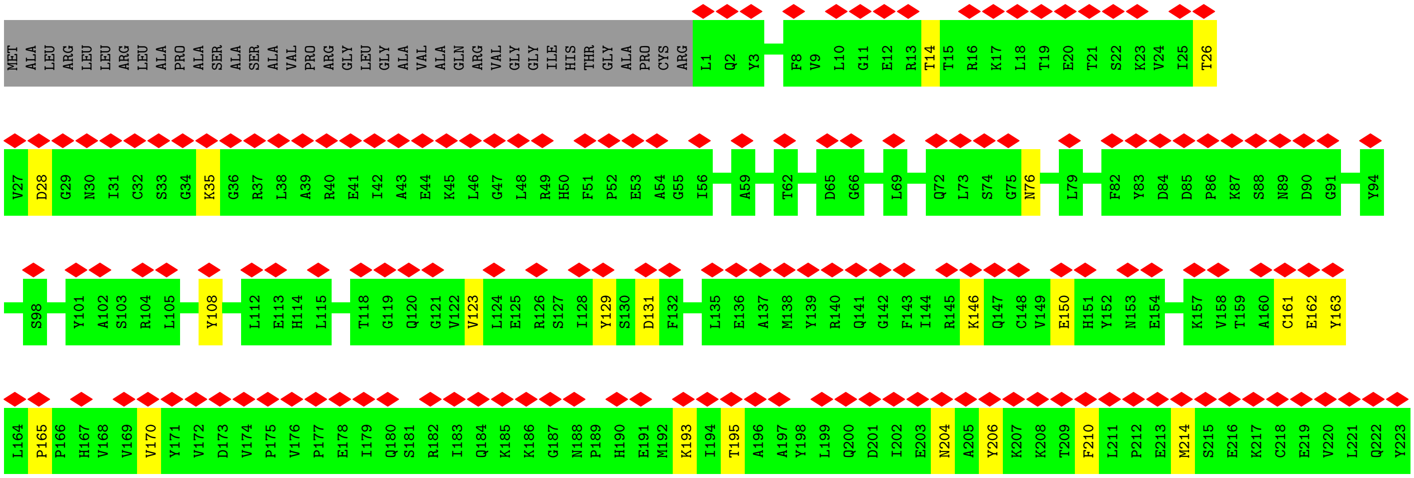
Chain 1N:

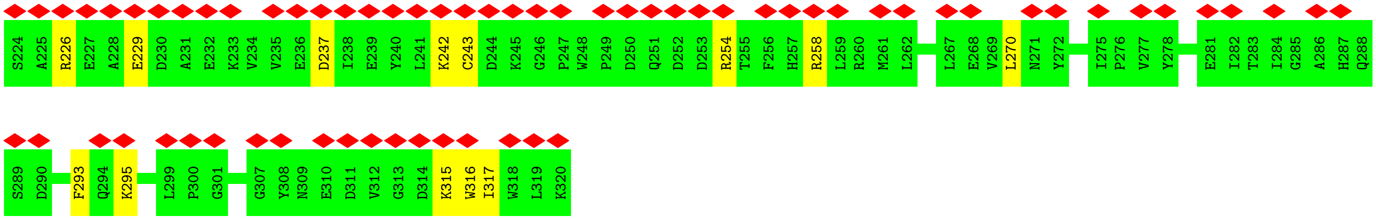




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

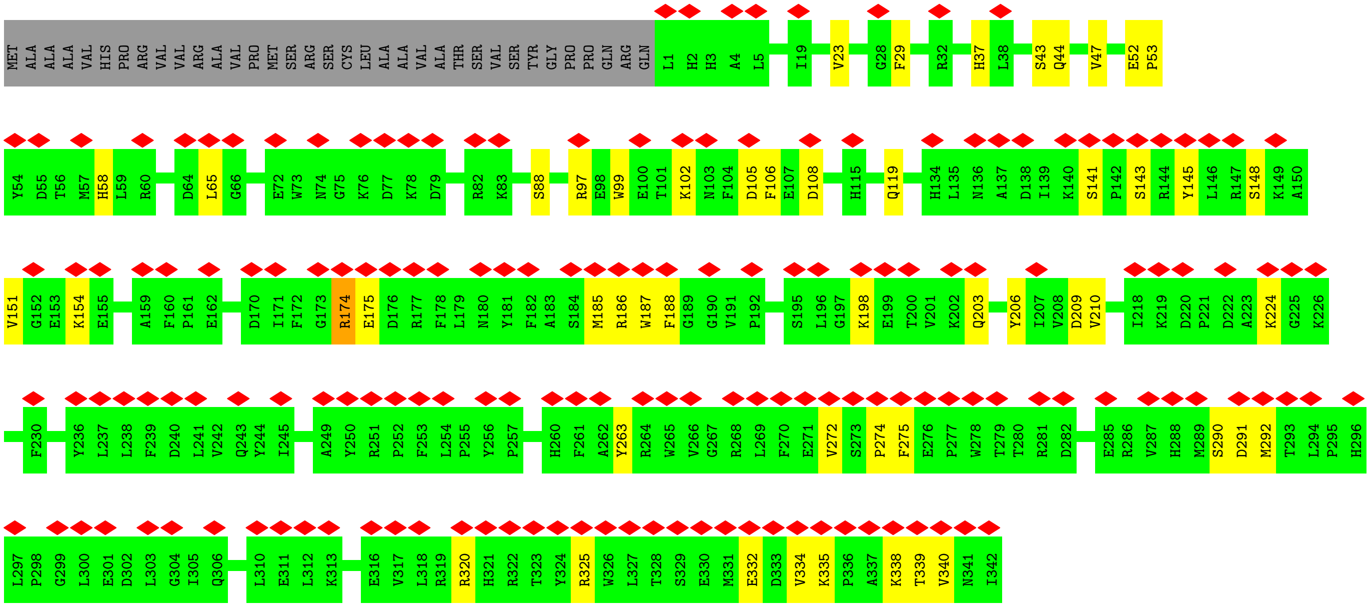
Chain 1O:





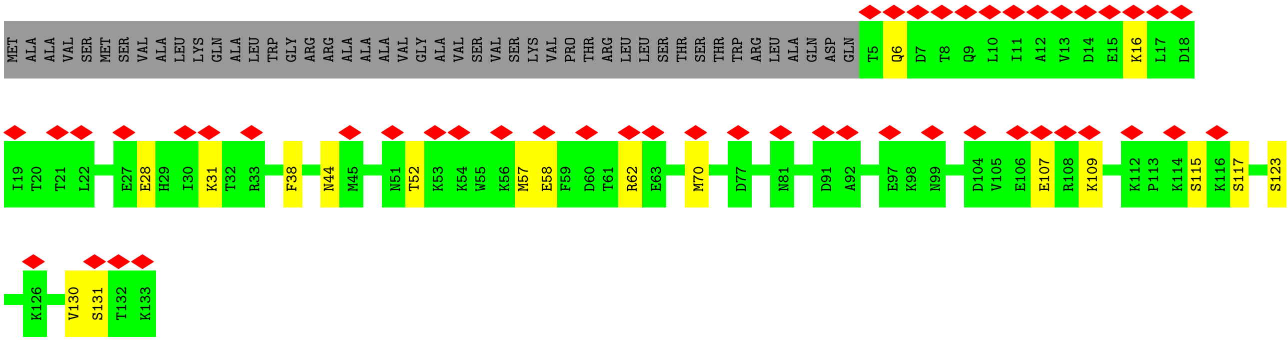
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



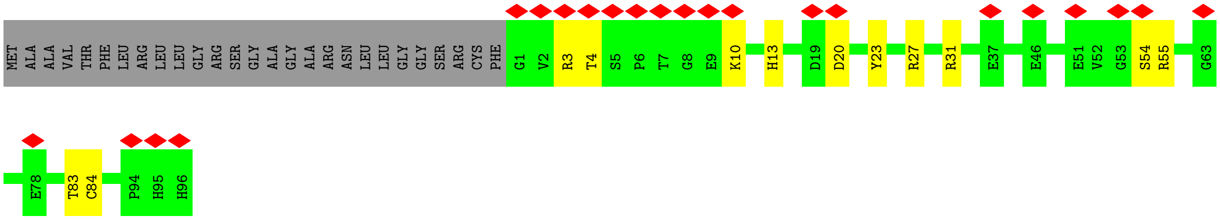
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



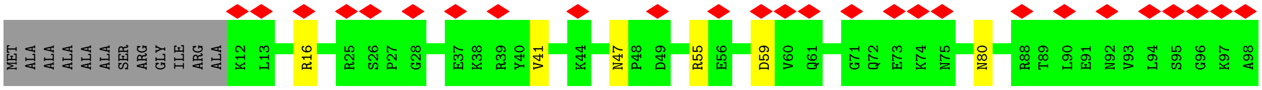
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



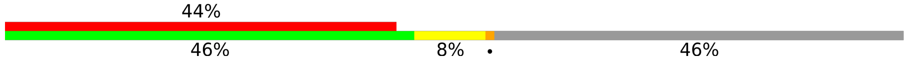
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

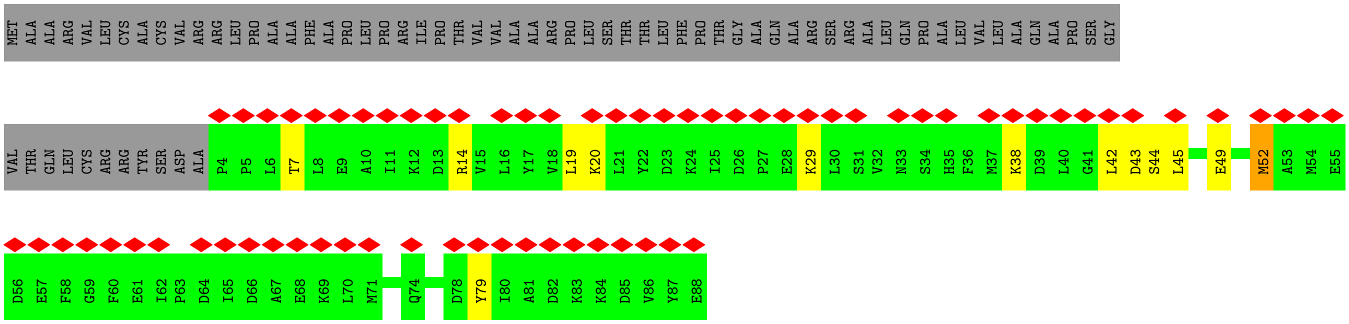
Chain 1S:



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

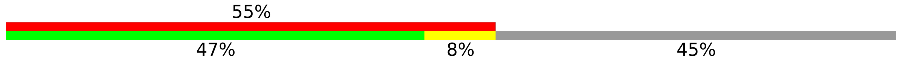
Chain 1T:

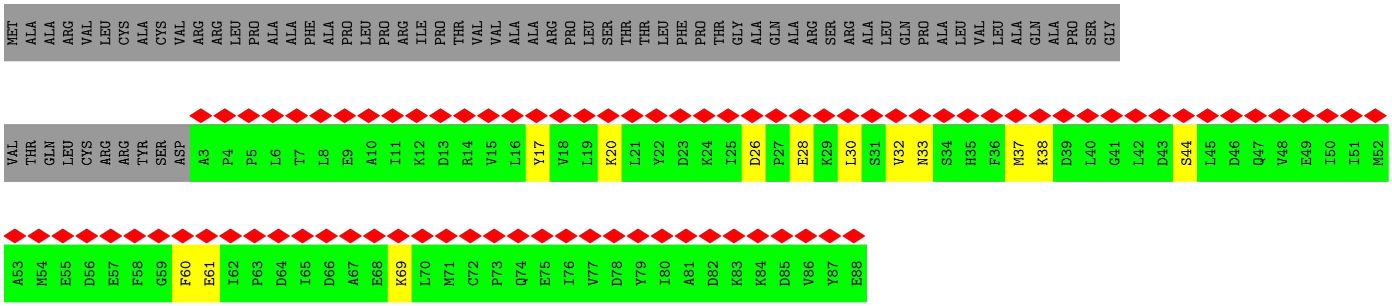




- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

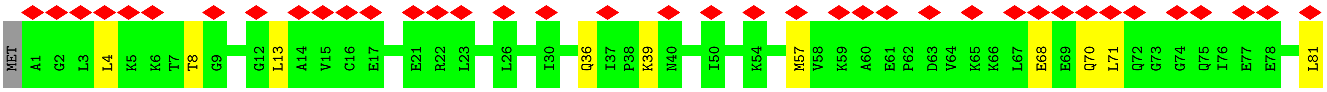
Chain 1U:

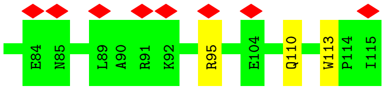




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

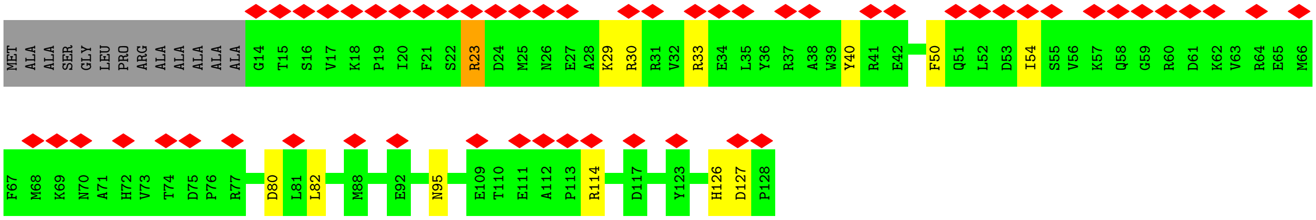
Chain 1V:





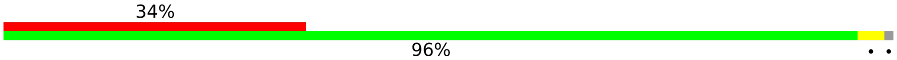
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

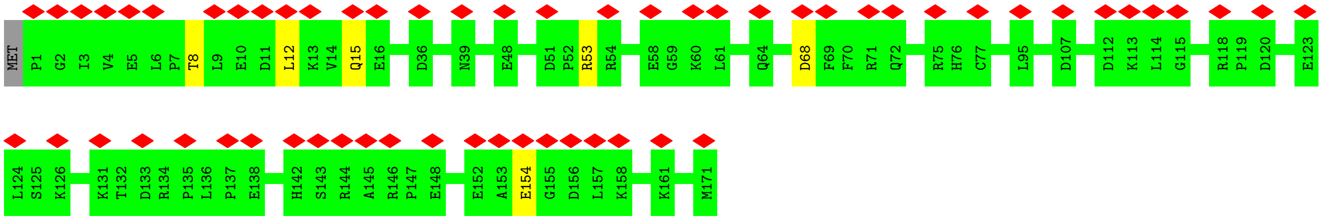
Chain 1W:



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

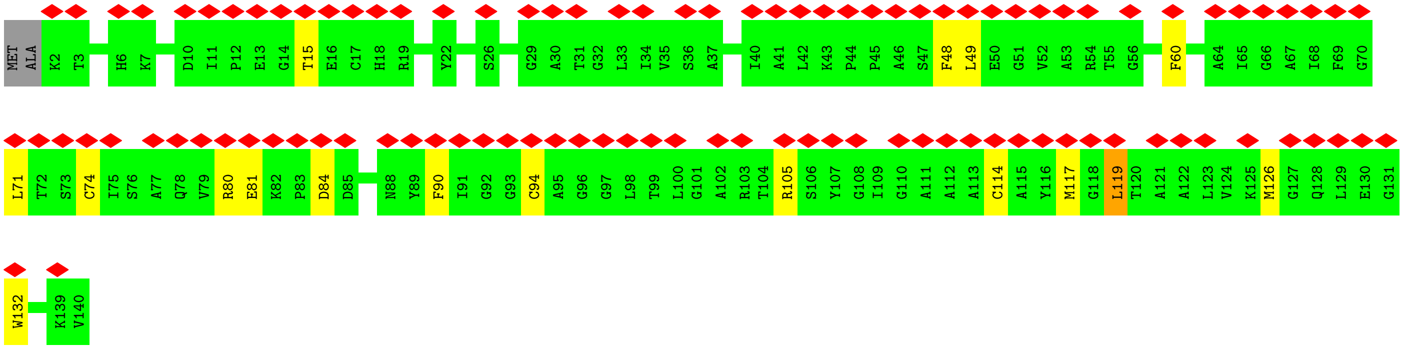
Chain 1X:





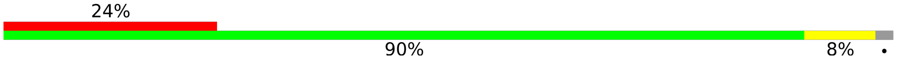
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

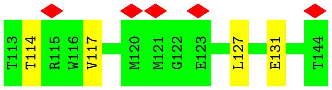
Chain 1Y:



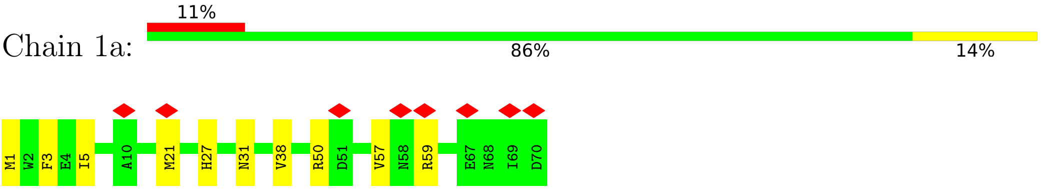
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:

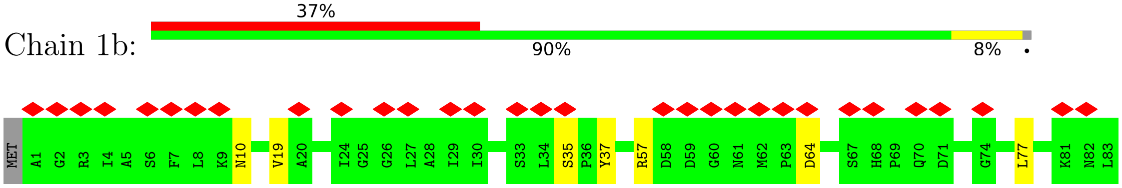




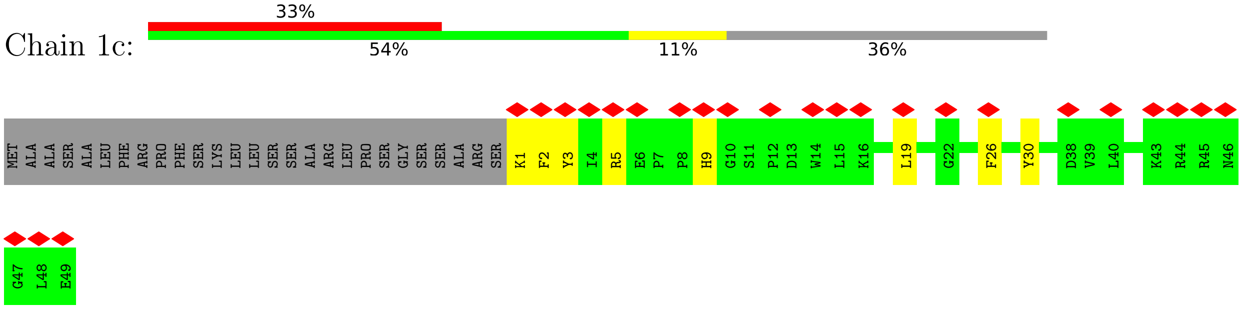
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



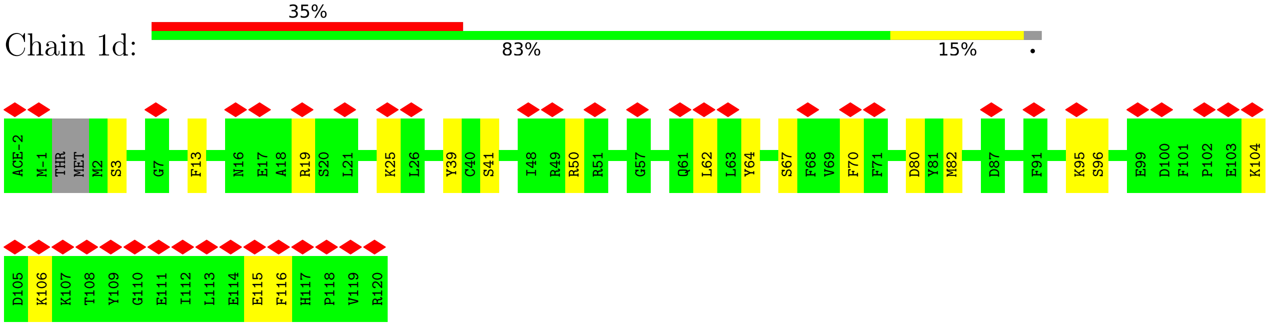
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



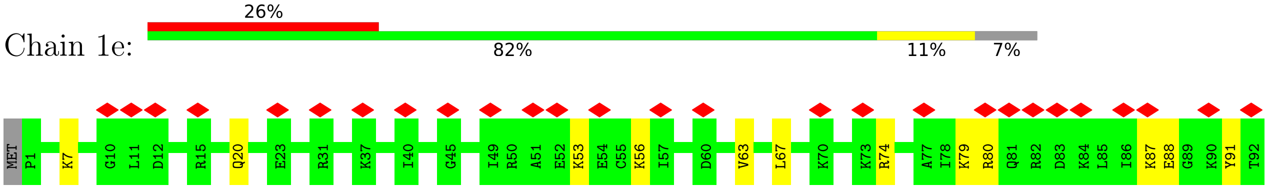
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

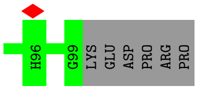


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

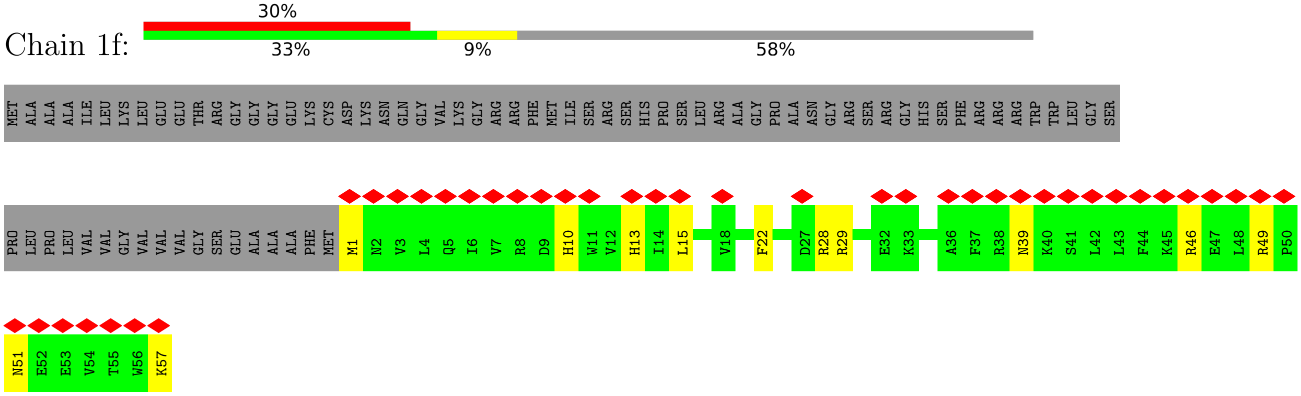


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

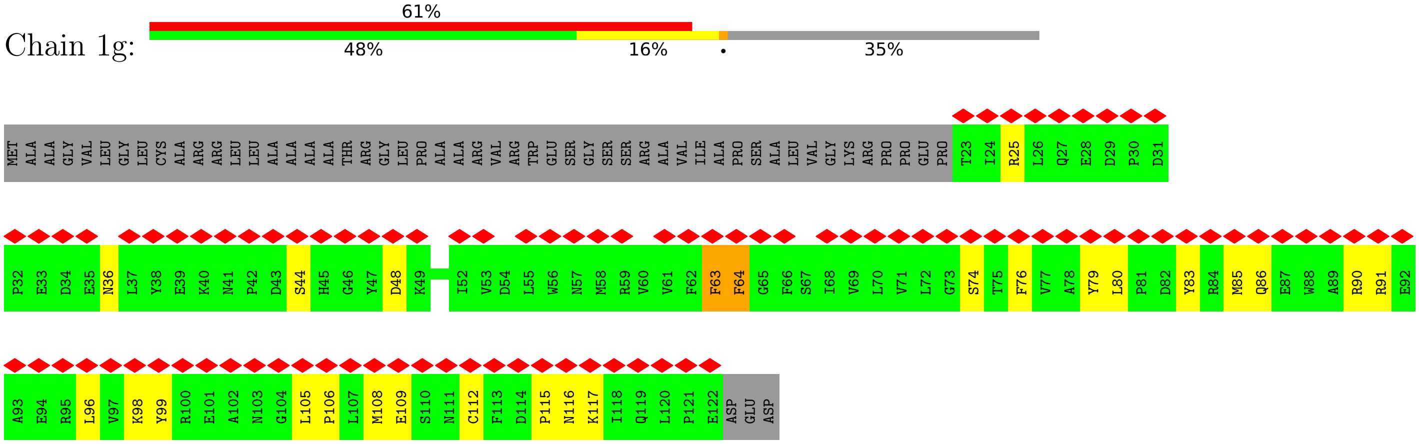




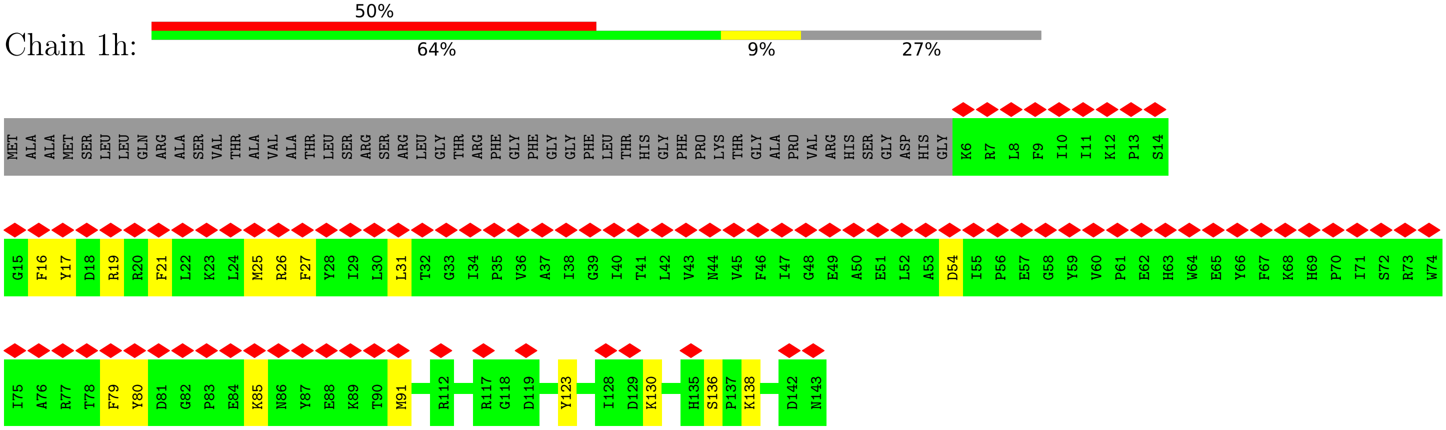
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



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

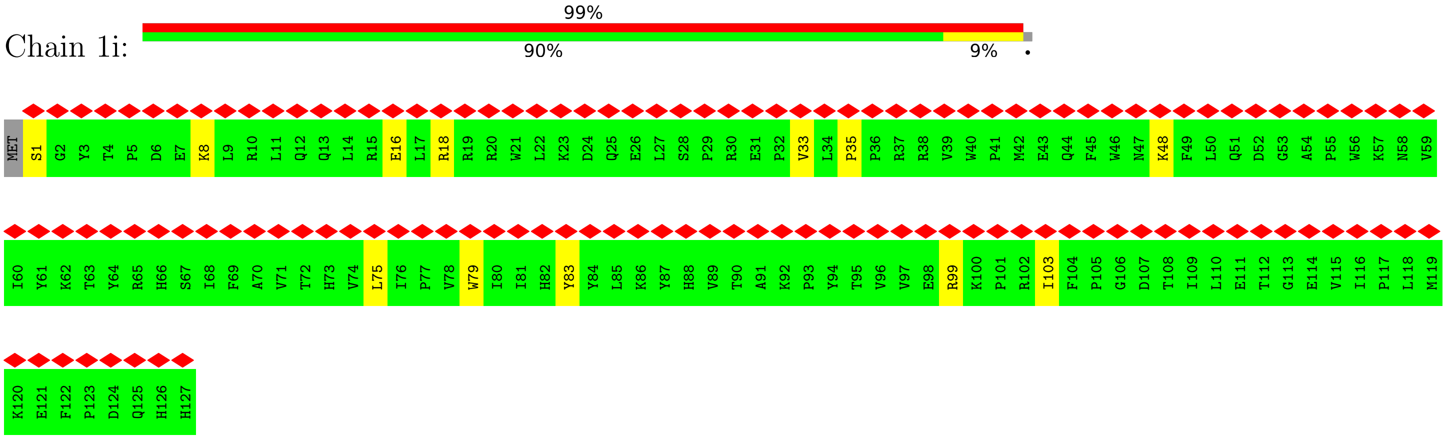


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



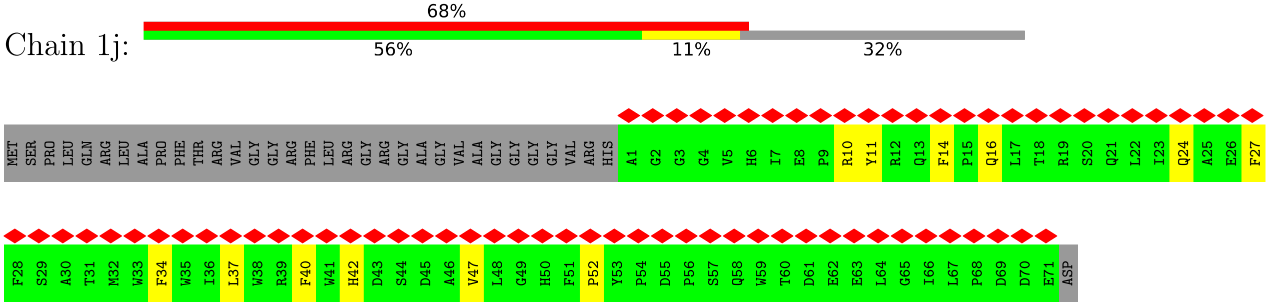
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



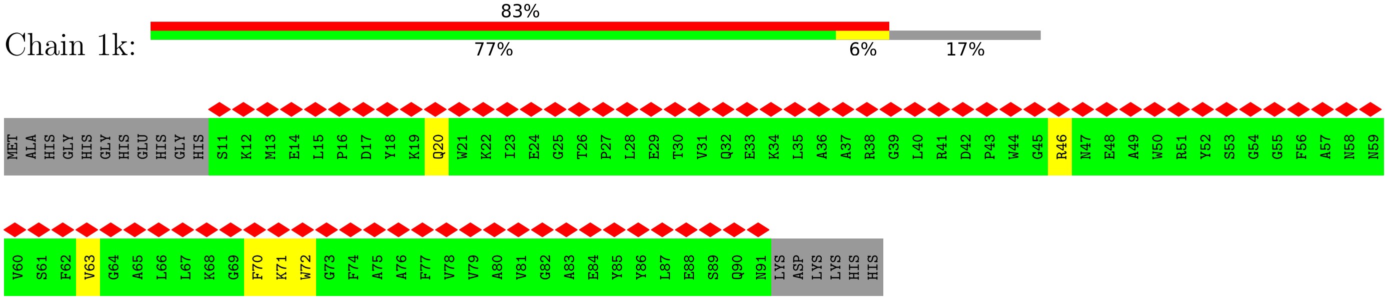
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



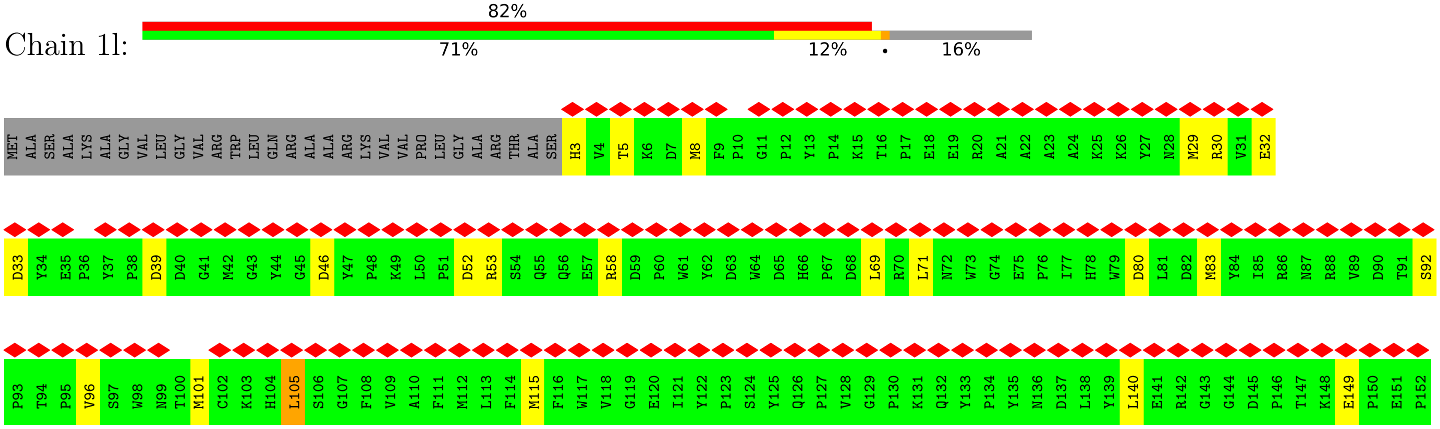
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



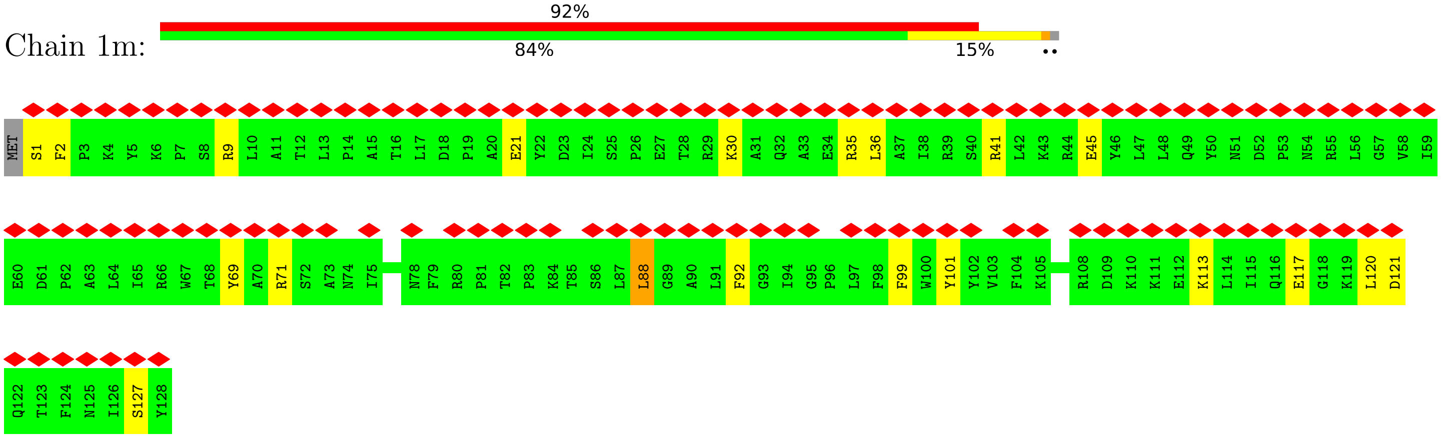
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l:



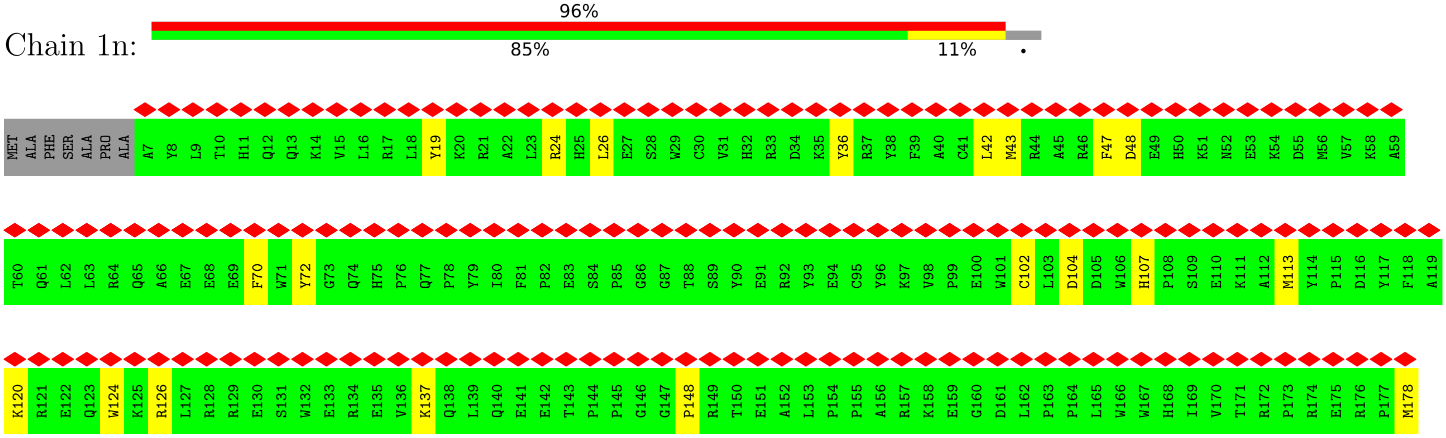
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m:



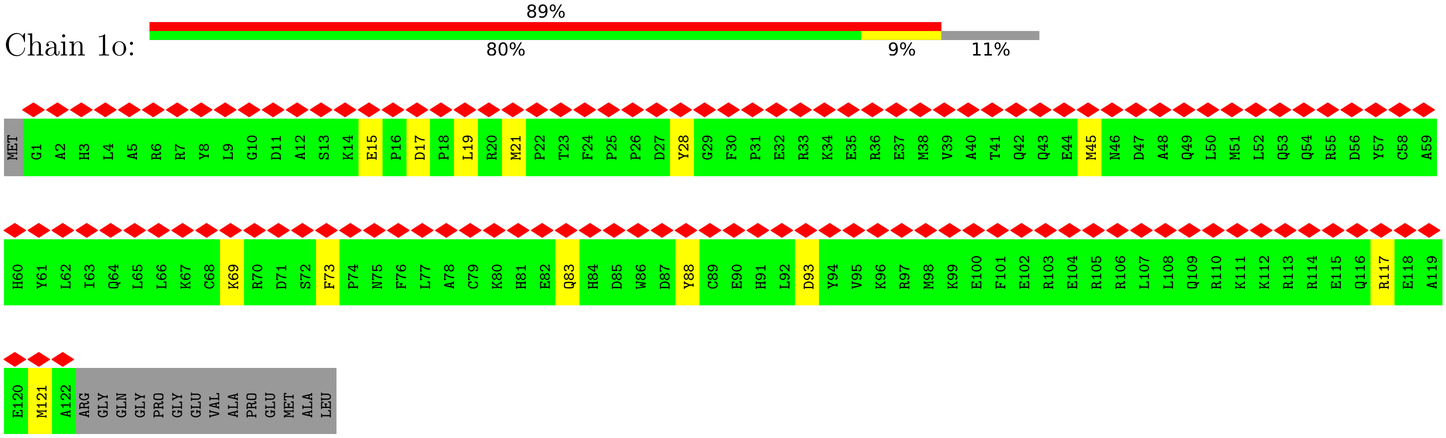
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n:



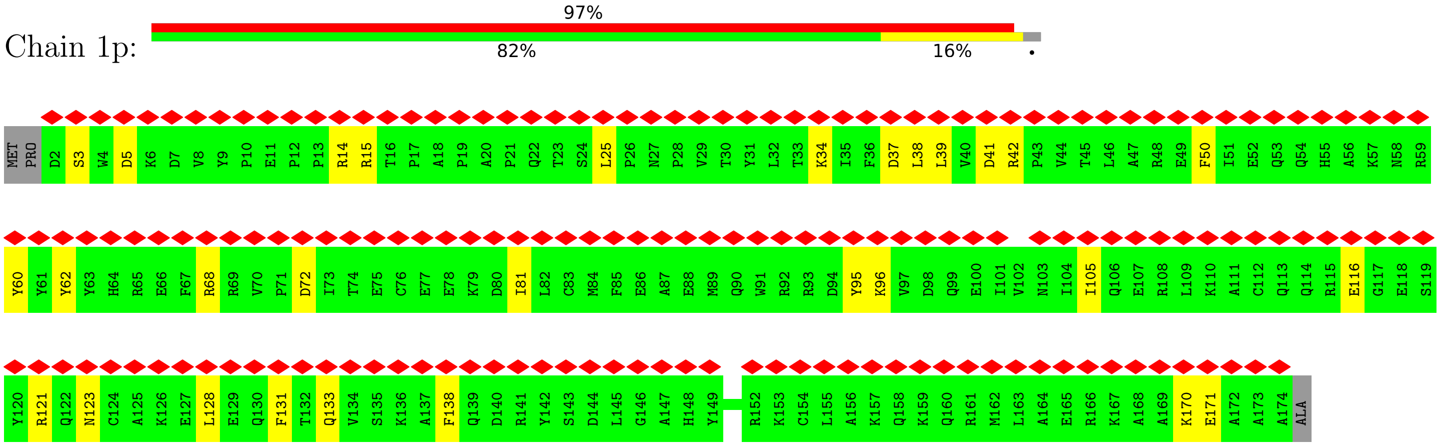
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:



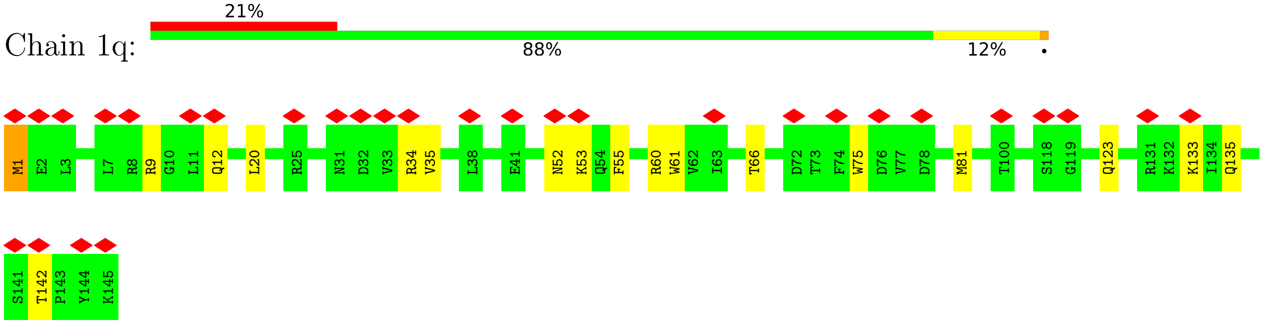
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p:



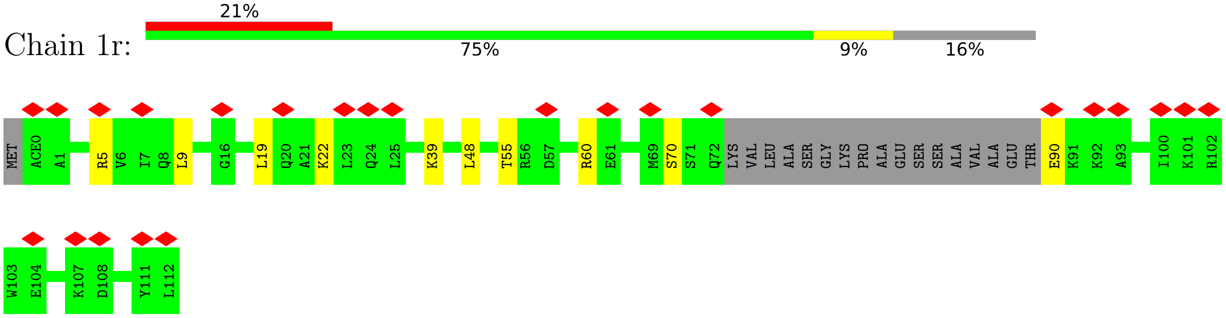
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:



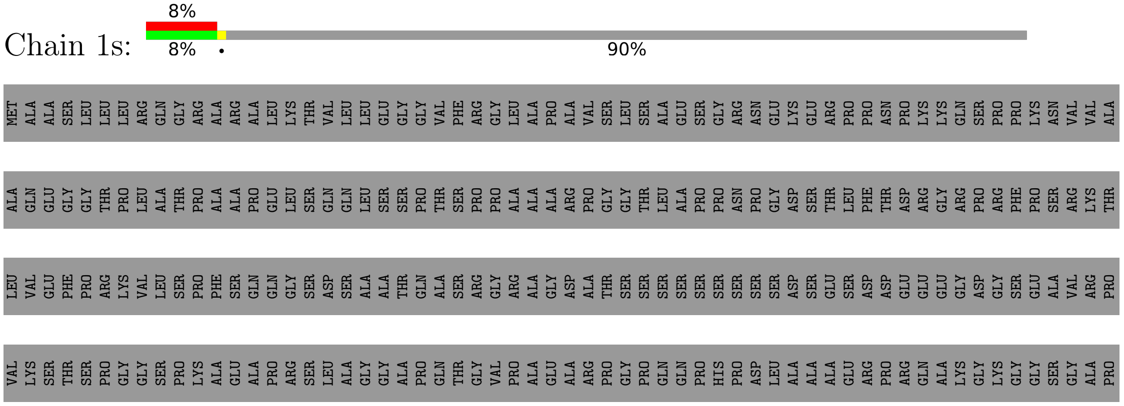
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

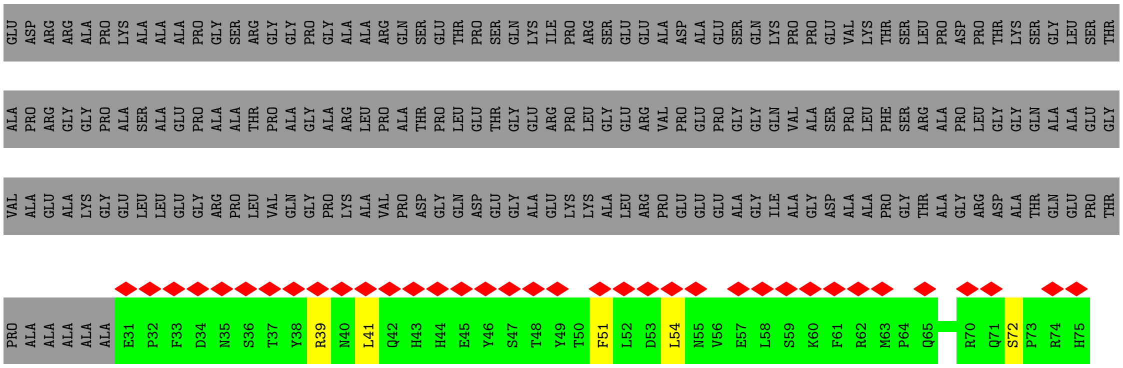
Chain 1r:



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

Chain 1s:





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

ALA PRO ARG GLY GLY PRO ALA SER ALA GLU PRO ALA ALA THR PRO ALA GLY ALA ARG LEU PRO ALA THR PRO LEU GLU THR GLY GLU ARG PRO LEU GLY GLU ARG VAL PRO GLU PRO GLY GLY GLN VAL ALA SER PRO LEU PHE SER ARG ALA PRO LEU GLY GLY GLN ALA ALA GLU GLY

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

PRO ALA ALA ALA ALA ALA E31 P32 F33 D34 N35 S36 T37 Y38 R39 N40 L41 Q42 H43 H44 E45 Y46 S47 T48 Y49 T50 F51 L52 D53 L54 N55 V56 E57 L58 S59 K60 F61 R62 M63 P64 Q65 R70 Q71 S72 P73 R74 H75

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	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	0.898	Depositor
Minimum map value	-0.238	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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1A	0.30	0/930	0.69	1/1271 (0.1%)
2	1B	0.32	0/1273	0.64	1/1722 (0.1%)
3	1C	0.29	0/1791	0.54	0/2439
4	1D	0.32	0/3545	0.65	3/4806 (0.1%)
5	1E	0.27	0/1698	0.55	0/2311
6	1F	0.28	0/3401	0.55	0/4595
7	1G	0.26	0/5451	0.57	3/7387 (0.0%)
8	1H	0.66	4/2566 (0.2%)	0.84	6/3509 (0.2%)
9	1I	0.29	0/1443	0.57	1/1952 (0.1%)
10	1J	0.33	0/1364	0.63	1/1850 (0.1%)
11	1K	0.36	0/751	0.81	2/1018 (0.2%)
12	1L	0.29	0/4939	0.68	9/6718 (0.1%)
13	1M	0.28	0/3713	0.70	7/5063 (0.1%)
14	1N	0.32	0/2765	0.73	5/3758 (0.1%)
15	1O	0.31	0/2650	0.59	1/3588 (0.0%)
16	1P	0.37	2/2828 (0.1%)	0.65	5/3834 (0.1%)
17	1Q	0.29	0/1070	0.59	0/1446
18	1R	0.26	0/755	0.56	0/1018
19	1S	0.28	0/711	0.59	0/956
20	1T	0.40	0/701	0.83	1/946 (0.1%)
20	1U	0.32	0/706	0.65	0/954
21	1V	0.30	0/946	0.62	1/1281 (0.1%)
22	1W	0.35	0/995	0.79	2/1340 (0.1%)
23	1X	0.27	0/1436	0.57	0/1938
24	1Y	0.32	0/1037	0.70	3/1404 (0.2%)
25	1Z	0.28	0/1199	0.61	0/1617
26	1a	0.26	0/577	0.49	0/777
27	1b	0.31	0/664	0.64	0/912
28	1c	0.28	0/430	0.84	1/581 (0.2%)
29	1d	0.30	0/1024	0.57	0/1383
30	1e	0.29	0/836	0.66	0/1118
31	1f	0.29	0/499	0.67	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
32	1g	0.54	1/858 (0.1%)	0.98	6/1165 (0.5%)
33	1h	0.30	0/1184	0.61	0/1603
34	1i	0.34	0/1131	0.73	1/1541 (0.1%)
35	1j	0.38	0/627	0.81	2/858 (0.2%)
36	1k	0.31	0/668	0.62	0/903
37	1l	0.28	0/1365	0.62	1/1867 (0.1%)
38	1m	0.31	0/1092	0.67	1/1481 (0.1%)
39	1n	0.28	0/1549	0.68	2/2098 (0.1%)
40	1o	0.27	0/1069	0.62	0/1430
41	1p	0.28	0/1481	0.62	2/1997 (0.1%)
42	1q	0.29	0/1253	0.57	1/1704 (0.1%)
43	1r	0.28	0/782	0.59	0/1057
44	1s	0.26	0/394	0.58	0/533
All	All	0.32	7/68147 (0.0%)	0.65	69/92402 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1D	0	1
8	1H	0	1
21	1V	0	1
22	1W	0	1
34	1i	0	1
39	1n	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1H	90	PRO	CB-CG	21.64	2.58	1.50
8	1H	90	PRO	CG-CD	-16.49	0.96	1.50
32	1g	106	PRO	CG-CD	-10.16	1.17	1.50
16	1P	53	PRO	CG-CD	-8.72	1.21	1.50
8	1H	90	PRO	N-CD	7.93	1.58	1.47
16	1P	274	PRO	CG-CD	-5.50	1.32	1.50
8	1H	90	PRO	N-CA	-5.22	1.38	1.47

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1H	90	PRO	CB-CG-CD	-27.27	0.16	106.50
8	1H	90	PRO	CA-N-CD	-17.82	86.54	111.50
32	1g	106	PRO	CA-N-CD	-12.62	93.83	111.50
16	1P	274	PRO	CA-N-CD	-12.07	94.60	111.50
8	1H	90	PRO	CA-CB-CG	-11.58	81.99	104.00
35	1j	52	PRO	CA-N-CD	-11.32	95.65	111.50
16	1P	53	PRO	CA-N-CD	-11.15	95.89	111.50
34	1i	35	PRO	CA-N-CD	-10.75	96.45	111.50
39	1n	24	ARG	C-N-CA	10.32	147.50	121.70
22	1W	54	ILE	CG1-CB-CG2	-9.73	90.00	111.40
32	1g	106	PRO	N-CD-CG	-9.71	88.63	103.20
16	1P	53	PRO	N-CD-CG	-8.97	89.75	103.20
15	1O	165	PRO	CA-N-CD	-8.21	100.00	111.50
8	1H	90	PRO	N-CA-CB	-7.95	93.75	103.30
28	1c	19	LEU	CA-CB-CG	7.86	133.38	115.30
14	1N	251	MET	CA-CB-CG	7.82	126.59	113.30
12	1L	123	LEU	CA-CB-CG	7.66	132.92	115.30
35	1j	37	LEU	CB-CG-CD2	-7.59	98.10	111.00
11	1K	10	MET	CA-CB-CG	7.24	125.61	113.30
24	1Y	119	LEU	CA-CB-CG	7.14	131.73	115.30
12	1L	413	LEU	CB-CG-CD2	-7.13	98.88	111.00
4	1D	83	LEU	CA-CB-CG	7.04	131.50	115.30
39	1n	113	MET	CA-CB-CG	6.89	125.02	113.30
16	1P	274	PRO	N-CD-CG	-6.84	92.94	103.20
4	1D	47	LEU	CA-CB-CG	6.83	131.01	115.30
13	1M	325	MET	CA-CB-CG	6.49	124.34	113.30
12	1L	339	LEU	CA-CB-CG	6.46	130.16	115.30
32	1g	105	LEU	CA-CB-CG	6.45	130.14	115.30
14	1N	72	MET	CG-SD-CE	6.41	110.45	100.20
12	1L	236	ALA	C-N-CA	-6.31	105.91	121.70
32	1g	115	PRO	CA-N-CD	-6.28	102.72	111.50
10	1J	97	LEU	CA-CB-CG	6.24	129.65	115.30
13	1M	39	LEU	CA-CB-CG	6.20	129.57	115.30
14	1N	244	MET	CA-CB-CG	6.16	123.77	113.30
16	1P	53	PRO	CA-CB-CG	-6.15	92.32	104.00
13	1M	231	LEU	CA-CB-CG	6.11	129.35	115.30
32	1g	106	PRO	CA-CB-CG	-6.09	92.42	104.00
37	1l	105	LEU	CA-CB-CG	6.07	129.27	115.30
38	1m	88	LEU	CA-CB-CG	6.04	129.20	115.30
4	1D	405	MET	CA-CB-CG	5.93	123.38	113.30
8	1H	51	ASP	CB-CG-OD2	5.62	123.36	118.30
7	1G	171	ASP	CB-CG-OD2	5.57	123.31	118.30
11	1K	6	MET	CG-SD-CE	5.57	109.11	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1M	41	LEU	CA-CB-CG	5.56	128.09	115.30
7	1G	97	LEU	CB-CG-CD2	-5.51	101.63	111.00
2	1B	48	MET	CB-CG-SD	5.49	128.86	112.40
12	1L	592	LEU	CA-CB-CG	5.48	127.91	115.30
20	1T	52	MET	CA-CB-CG	5.43	122.54	113.30
1	1A	7	LEU	CA-CB-CG	5.42	127.77	115.30
13	1M	439	LEU	CA-CB-CG	5.32	127.54	115.30
13	1M	361	MET	CA-CB-CG	5.31	122.33	113.30
22	1W	82	LEU	CA-CB-CG	5.27	127.42	115.30
12	1L	319	ILE	CG1-CB-CG2	-5.26	99.82	111.40
12	1L	380	LEU	CA-CB-CG	5.26	127.39	115.30
42	1q	1	MET	CB-CG-SD	5.25	128.16	112.40
32	1g	96	LEU	CA-CB-CG	5.24	127.35	115.30
12	1L	313	MET	CA-CB-CG	5.22	122.17	113.30
9	1I	13	ASP	CB-CG-OD1	5.21	122.99	118.30
14	1N	160	LEU	CA-CB-CG	5.20	127.25	115.30
14	1N	245	MET	CB-CG-SD	5.19	127.98	112.40
24	1Y	119	LEU	CB-CG-CD2	5.18	119.81	111.00
8	1H	162	LEU	CA-CB-CG	5.17	127.19	115.30
21	1V	81	LEU	CA-CB-CG	5.15	127.14	115.30
41	1p	38	LEU	CA-CB-CG	5.10	127.04	115.30
12	1L	504	LEU	CA-CB-CG	5.02	126.85	115.30
24	1Y	71	LEU	CA-CB-CG	5.01	126.83	115.30
7	1G	103	LEU	CA-CB-CG	5.01	126.82	115.30
13	1M	405	LEU	CA-CB-CG	5.00	126.81	115.30
41	1p	37	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1D	74	ARG	Sidechain
8	1H	90	PRO	Peptide
21	1V	113	TRP	Peptide
22	1W	23	ARG	Sidechain
34	1i	99	ARG	Sidechain
39	1n	42	LEU	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	95 (84%)	16 (14%)	2 (2%)	8	32
2	1B	153/258 (59%)	137 (90%)	15 (10%)	1 (1%)	22	55
3	1C	207/264 (78%)	186 (90%)	20 (10%)	1 (0%)	29	61
4	1D	427/476 (90%)	390 (91%)	37 (9%)	0	100	100
5	1E	212/249 (85%)	193 (91%)	18 (8%)	1 (0%)	29	61
6	1F	430/464 (93%)	408 (95%)	21 (5%)	1 (0%)	47	78
7	1G	697/727 (96%)	645 (92%)	48 (7%)	4 (1%)	25	57
8	1H	316/318 (99%)	291 (92%)	23 (7%)	2 (1%)	25	57
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100
10	1J	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	25	57
11	1K	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
12	1L	604/606 (100%)	543 (90%)	59 (10%)	2 (0%)	41	72
13	1M	457/459 (100%)	436 (95%)	20 (4%)	1 (0%)	47	78
14	1N	345/347 (99%)	320 (93%)	24 (7%)	1 (0%)	41	72
15	1O	318/357 (89%)	300 (94%)	18 (6%)	0	100	100
16	1P	340/377 (90%)	315 (93%)	23 (7%)	2 (1%)	25	57
17	1Q	127/175 (73%)	113 (89%)	14 (11%)	0	100	100
18	1R	94/123 (76%)	85 (90%)	9 (10%)	0	100	100
19	1S	85/99 (86%)	73 (86%)	12 (14%)	0	100	100
20	1T	83/156 (53%)	74 (89%)	9 (11%)	0	100	100
20	1U	84/156 (54%)	76 (90%)	8 (10%)	0	100	100
21	1V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	1X	169/172 (98%)	153 (90%)	16 (10%)	0	100	100
24	1Y	137/141 (97%)	128 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	1Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	1a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	49 (89%)	6 (11%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	8 (8%)	2 (2%)	7	30
33	1h	136/189 (72%)	120 (88%)	16 (12%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	60 (87%)	9 (13%)	0	100	100
36	1k	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
37	1l	154/186 (83%)	139 (90%)	15 (10%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	154 (91%)	15 (9%)	1 (1%)	25	57
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
41	1p	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
42	1q	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
43	1r	90/114 (79%)	85 (94%)	5 (6%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
All	All	8194/9744 (84%)	7564 (92%)	608 (7%)	22 (0%)	44	72

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1C	121	VAL
7	1G	416	THR
7	1G	460	ARG
7	1G	650	LYS
8	1H	170	GLU
13	1M	390	ASN
39	1n	148	PRO
1	1A	109	LYS
2	1B	49	THR
7	1G	186	TYR

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Mol	Chain	Res	Type
10	1J	116	ILE
16	1P	174	ARG
32	1g	64	PHE
6	1F	249	ARG
12	1L	551	SER
12	1L	72	GLN
1	1A	44	MET
5	1E	215	ALA
32	1g	63	PHE
14	1N	110	PRO
8	1H	208	VAL
16	1P	23	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	99/99 (100%)	84 (85%)	15 (15%)	3 11
2	1B	131/212 (62%)	106 (81%)	25 (19%)	1 4
3	1C	190/227 (84%)	175 (92%)	15 (8%)	12 39
4	1D	371/405 (92%)	321 (86%)	50 (14%)	4 14
5	1E	183/207 (88%)	165 (90%)	18 (10%)	8 28
6	1F	346/368 (94%)	309 (89%)	37 (11%)	6 24
7	1G	588/610 (96%)	525 (89%)	63 (11%)	6 24
8	1H	274/274 (100%)	254 (93%)	20 (7%)	14 43
9	1I	151/201 (75%)	135 (89%)	16 (11%)	6 24
10	1J	140/140 (100%)	116 (83%)	24 (17%)	2 8
11	1K	84/84 (100%)	76 (90%)	8 (10%)	8 29
12	1L	539/539 (100%)	479 (89%)	60 (11%)	6 22
13	1M	408/408 (100%)	371 (91%)	37 (9%)	9 32
14	1N	310/310 (100%)	281 (91%)	29 (9%)	8 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	1O	283/307 (92%)	249 (88%)	34 (12%)	5	19
16	1P	296/323 (92%)	248 (84%)	48 (16%)	2	9
17	1Q	117/152 (77%)	99 (85%)	18 (15%)	2	11
18	1R	79/97 (81%)	67 (85%)	12 (15%)	3	11
19	1S	77/82 (94%)	71 (92%)	6 (8%)	12	39
20	1T	79/133 (59%)	66 (84%)	13 (16%)	2	9
20	1U	79/133 (59%)	66 (84%)	13 (16%)	2	9
21	1V	100/101 (99%)	89 (89%)	11 (11%)	6	23
22	1W	107/112 (96%)	96 (90%)	11 (10%)	7	26
23	1X	153/154 (99%)	147 (96%)	6 (4%)	32	61
24	1Y	101/102 (99%)	85 (84%)	16 (16%)	2	10
25	1Z	123/124 (99%)	111 (90%)	12 (10%)	8	28
26	1a	58/58 (100%)	48 (83%)	10 (17%)	2	8
27	1b	69/70 (99%)	62 (90%)	7 (10%)	7	27
28	1c	45/66 (68%)	38 (84%)	7 (16%)	2	11
29	1d	107/109 (98%)	88 (82%)	19 (18%)	2	6
30	1e	87/94 (93%)	75 (86%)	12 (14%)	3	14
31	1f	54/113 (48%)	42 (78%)	12 (22%)	1	2
32	1g	92/129 (71%)	70 (76%)	22 (24%)	0	2
33	1h	121/158 (77%)	104 (86%)	17 (14%)	3	13
34	1i	119/120 (99%)	110 (92%)	9 (8%)	13	41
35	1j	62/84 (74%)	52 (84%)	10 (16%)	2	10
36	1k	63/76 (83%)	57 (90%)	6 (10%)	8	29
37	1l	141/161 (88%)	117 (83%)	24 (17%)	2	8
38	1m	113/114 (99%)	93 (82%)	20 (18%)	2	6
39	1n	156/160 (98%)	140 (90%)	16 (10%)	7	26
40	1o	110/120 (92%)	97 (88%)	13 (12%)	5	19
41	1p	154/156 (99%)	127 (82%)	27 (18%)	2	7
42	1q	131/131 (100%)	113 (86%)	18 (14%)	3	14
43	1r	85/98 (87%)	75 (88%)	10 (12%)	5	19
44	1s	44/351 (12%)	39 (89%)	5 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7219/8272 (87%)	6338 (88%)	881 (12%)	8 18

All (881) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	2	ASN
1	1A	9	THR
1	1A	30	TYR
1	1A	33	LYS
1	1A	49	LEU
1	1A	51	PHE
1	1A	56	PHE
1	1A	65	PHE
1	1A	73	LEU
1	1A	85	LYS
1	1A	87	MET
1	1A	93	PHE
1	1A	94	LEU
1	1A	109	LYS
1	1A	115	GLU
2	1B	25	ARG
2	1B	28	TYR
2	1B	29	VAL
2	1B	44	SER
2	1B	45	LEU
2	1B	49	THR
2	1B	54	CYS
2	1B	61	HIS
2	1B	74	VAL
2	1B	76	PHE
2	1B	77	ARG
2	1B	84	ASP
2	1B	93	THR
2	1B	96	MET
2	1B	112	TYR
2	1B	125	TYR
2	1B	126	TYR
2	1B	128	TYR
2	1B	129	SER
2	1B	134	ARG
2	1B	137	ASP
2	1B	152	THR

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Mol	Chain	Res	Type
2	1B	169	ARG
2	1B	174	ARG
2	1B	177	TYR
3	1C	38	GLN
3	1C	41	GLN
3	1C	44	CYS
3	1C	71	GLN
3	1C	88	ASN
3	1C	89	ARG
3	1C	109	THR
3	1C	111	THR
3	1C	119	SER
3	1C	168	LEU
3	1C	172	VAL
3	1C	174	LEU
3	1C	176	TYR
3	1C	182	ARG
3	1C	214	GLU
4	1D	19	MET
4	1D	37	ASP
4	1D	41	ASP
4	1D	45	SER
4	1D	51	PHE
4	1D	54	GLN
4	1D	63	ARG
4	1D	68	LEU
4	1D	76	CYS
4	1D	79	HIS
4	1D	84	HIS
4	1D	85	ARG
4	1D	95	THR
4	1D	111	MET
4	1D	123	GLU
4	1D	145	THR
4	1D	157	HIS
4	1D	159	LEU
4	1D	164	MET
4	1D	165	THR
4	1D	167	PHE
4	1D	170	MET
4	1D	177	MET
4	1D	193	TYR

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Mol	Chain	Res	Type
4	1D	199	VAL
4	1D	203	LEU
4	1D	209	ASP
4	1D	215	SER
4	1D	219	SER
4	1D	220	PHE
4	1D	221	ARG
4	1D	223	ASP
4	1D	227	GLU
4	1D	246	THR
4	1D	251	LEU
4	1D	253	TYR
4	1D	256	SER
4	1D	263	SER
4	1D	278	TYR
4	1D	284	ASP
4	1D	285	VAL
4	1D	293	CYS
4	1D	304	MET
4	1D	312	SER
4	1D	314	CYS
4	1D	373	GLU
4	1D	389	CYS
4	1D	407	LYS
4	1D	410	MET
4	1D	415	VAL
5	1E	11	ASP
5	1E	24	THR
5	1E	36	LYS
5	1E	47	VAL
5	1E	55	GLN
5	1E	58	ASN
5	1E	60	TRP
5	1E	89	MET
5	1E	91	ASN
5	1E	102	VAL
5	1E	108	CYS
5	1E	122	LYS
5	1E	126	ILE
5	1E	148	CYS
5	1E	153	MET
5	1E	187	ARG

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Mol	Chain	Res	Type
5	1E	203	THR
5	1E	211	PHE
6	1F	8	LYS
6	1F	16	LYS
6	1F	39	ARG
6	1F	43	TYR
6	1F	46	LYS
6	1F	63	SER
6	1F	77	LEU
6	1F	78	LYS
6	1F	82	MET
6	1F	84	LYS
6	1F	86	SER
6	1F	106	LYS
6	1F	127	ARG
6	1F	135	TYR
6	1F	144	ASN
6	1F	151	VAL
6	1F	164	LYS
6	1F	172	ASP
6	1F	205	LEU
6	1F	249	ARG
6	1F	250	ASN
6	1F	254	LYS
6	1F	266	CYS
6	1F	271	GLU
6	1F	280	ILE
6	1F	287	VAL
6	1F	311	VAL
6	1F	314	THR
6	1F	320	ASP
6	1F	337	MET
6	1F	353	PHE
6	1F	373	ASN
6	1F	376	MET
6	1F	391	SER
6	1F	405	CYS
6	1F	432	GLN
6	1F	435	LEU
7	1G	32	LYS
7	1G	35	MET
7	1G	39	ARG

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Mol	Chain	Res	Type
7	1G	41	CYS
7	1G	45	ARG
7	1G	54	MET
7	1G	57	VAL
7	1G	61	LYS
7	1G	65	VAL
7	1G	71	MET
7	1G	75	LYS
7	1G	77	TRP
7	1G	81	THR
7	1G	83	SER
7	1G	94	MET
7	1G	107	ILE
7	1G	123	PHE
7	1G	129	ARG
7	1G	130	PHE
7	1G	151	THR
7	1G	157	THR
7	1G	174	THR
7	1G	190	MET
7	1G	195	LEU
7	1G	209	THR
7	1G	215	PHE
7	1G	222	THR
7	1G	227	SER
7	1G	231	MET
7	1G	236	SER
7	1G	242	THR
7	1G	243	ARG
7	1G	265	ASP
7	1G	271	TYR
7	1G	298	ASP
7	1G	302	ARG
7	1G	313	ASN
7	1G	323	VAL
7	1G	339	ASP
7	1G	356	THR
7	1G	357	ASP
7	1G	375	ASP
7	1G	394	ARG
7	1G	396	ARG
7	1G	400	LEU

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Mol	Chain	Res	Type
7	1G	408	LEU
7	1G	417	TYR
7	1G	441	GLN
7	1G	448	LYS
7	1G	450	MET
7	1G	462	ASP
7	1G	523	PHE
7	1G	588	THR
7	1G	605	GLU
7	1G	609	MET
7	1G	613	TYR
7	1G	614	ASP
7	1G	615	THR
7	1G	622	ARG
7	1G	654	GLN
7	1G	669	LYS
7	1G	673	MET
7	1G	689	LYS
8	1H	24	GLU
8	1H	51	ASP
8	1H	91	MET
8	1H	98	MET
8	1H	102	VAL
8	1H	117	LEU
8	1H	125	SER
8	1H	126	LYS
8	1H	152	SER
8	1H	173	TRP
8	1H	183	MET
8	1H	200	LEU
8	1H	213	VAL
8	1H	214	GLU
8	1H	224	PHE
8	1H	233	MET
8	1H	237	PHE
8	1H	248	ASP
8	1H	274	ARG
8	1H	289	LEU
9	1I	13	ASP
9	1I	14	MET
9	1I	15	LYS
9	1I	32	ARG

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Mol	Chain	Res	Type
9	1I	39	SER
9	1I	40	TYR
9	1I	93	THR
9	1I	103	SER
9	1I	106	THR
9	1I	107	THR
9	1I	109	TYR
9	1I	122	CYS
9	1I	129	ASP
9	1I	143	THR
9	1I	174	LEU
9	1I	176	ARG
10	1J	7	PHE
10	1J	17	PHE
10	1J	20	PHE
10	1J	44	VAL
10	1J	50	SER
10	1J	55	MET
10	1J	57	PHE
10	1J	60	TYR
10	1J	64	MET
10	1J	66	VAL
10	1J	68	PHE
10	1J	78	MET
10	1J	79	TYR
10	1J	93	PHE
10	1J	95	SER
10	1J	98	MET
10	1J	99	MET
10	1J	102	CYS
10	1J	105	TYR
10	1J	130	THR
10	1J	135	PHE
10	1J	152	TRP
10	1J	160	SER
10	1J	169	MET
11	1K	37	MET
11	1K	53	PHE
11	1K	69	CYS
11	1K	80	MET
11	1K	82	SER
11	1K	85	TYR

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Mol	Chain	Res	Type
11	1K	88	ASP
11	1K	89	TYR
12	1L	20	MET
12	1L	41	SER
12	1L	42	TYR
12	1L	54	PHE
12	1L	55	MET
12	1L	65	ASN
12	1L	67	HIS
12	1L	68	TRP
12	1L	69	MET
12	1L	71	LEU
12	1L	82	MET
12	1L	84	TYR
12	1L	86	SER
12	1L	99	SER
12	1L	104	SER
12	1L	110	SER
12	1L	127	THR
12	1L	131	LEU
12	1L	137	LEU
12	1L	150	MET
12	1L	159	HIS
12	1L	203	MET
12	1L	237	MET
12	1L	238	GLU
12	1L	252	MET
12	1L	253	VAL
12	1L	263	PHE
12	1L	268	GLU
12	1L	271	LYS
12	1L	286	LEU
12	1L	308	SER
12	1L	313	MET
12	1L	328	HIS
12	1L	331	MET
12	1L	335	PHE
12	1L	340	PHE
12	1L	346	ILE
12	1L	349	SER
12	1L	401	MET
12	1L	422	TYR

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Mol	Chain	Res	Type
12	1L	428	PHE
12	1L	436	ARG
12	1L	446	ASN
12	1L	455	LYS
12	1L	471	ASN
12	1L	481	THR
12	1L	482	MET
12	1L	484	LEU
12	1L	486	MET
12	1L	489	THR
12	1L	499	MET
12	1L	502	LEU
12	1L	510	TYR
12	1L	519	THR
12	1L	528	TYR
12	1L	533	MET
12	1L	571	MET
12	1L	585	LYS
12	1L	590	SER
12	1L	596	MET
13	1M	15	THR
13	1M	16	TRP
13	1M	17	MET
13	1M	22	MET
13	1M	47	GLU
13	1M	55	THR
13	1M	57	PHE
13	1M	76	MET
13	1M	78	MET
13	1M	85	SER
13	1M	86	LYS
13	1M	91	ARG
13	1M	109	THR
13	1M	115	LEU
13	1M	157	SER
13	1M	168	GLN
13	1M	201	MET
13	1M	213	HIS
13	1M	229	MET
13	1M	263	MET
13	1M	269	MET
13	1M	289	SER

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Mol	Chain	Res	Type
13	1M	299	VAL
13	1M	316	MET
13	1M	343	ILE
13	1M	346	ARG
13	1M	361	MET
13	1M	391	ILE
13	1M	396	MET
13	1M	400	MET
13	1M	401	MET
13	1M	410	MET
13	1M	427	LYS
13	1M	431	THR
13	1M	437	MET
13	1M	447	LEU
13	1M	459	TYR
14	1N	36	ASN
14	1N	47	ASN
14	1N	48	PHE
14	1N	59	TYR
14	1N	93	VAL
14	1N	97	MET
14	1N	100	MET
14	1N	104	MET
14	1N	111	PHE
14	1N	131	LEU
14	1N	157	MET
14	1N	159	MET
14	1N	161	SER
14	1N	211	MET
14	1N	217	MET
14	1N	226	THR
14	1N	235	ASN
14	1N	245	MET
14	1N	249	LEU
14	1N	282	MET
14	1N	291	TYR
14	1N	292	PHE
14	1N	303	THR
14	1N	308	THR
14	1N	312	LYS
14	1N	322	GLN
14	1N	335	LEU

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Mol	Chain	Res	Type
14	1N	339	MET
14	1N	343	LEU
15	1O	14	THR
15	1O	26	THR
15	1O	28	ASP
15	1O	35	LYS
15	1O	76	ASN
15	1O	108	TYR
15	1O	123	VAL
15	1O	129	TYR
15	1O	131	ASP
15	1O	146	LYS
15	1O	150	GLU
15	1O	161	CYS
15	1O	162	GLU
15	1O	163	TYR
15	1O	170	VAL
15	1O	193	LYS
15	1O	195	THR
15	1O	204	ASN
15	1O	206	TYR
15	1O	210	PHE
15	1O	214	MET
15	1O	226	ARG
15	1O	229	GLU
15	1O	237	ASP
15	1O	242	LYS
15	1O	243	CYS
15	1O	254	ARG
15	1O	258	ARG
15	1O	270	LEU
15	1O	293	PHE
15	1O	295	LYS
15	1O	315	LYS
15	1O	316	TRP
15	1O	317	ILE
16	1P	29	PHE
16	1P	37	HIS
16	1P	43	SER
16	1P	44	GLN
16	1P	47	VAL
16	1P	52	GLU

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Mol	Chain	Res	Type
16	1P	58	HIS
16	1P	65	LEU
16	1P	88	SER
16	1P	97	ARG
16	1P	99	TRP
16	1P	102	LYS
16	1P	105	ASP
16	1P	106	PHE
16	1P	108	ASP
16	1P	119	GLN
16	1P	141	SER
16	1P	143	SER
16	1P	145	TYR
16	1P	148	SER
16	1P	151	VAL
16	1P	154	LYS
16	1P	174	ARG
16	1P	175	GLU
16	1P	185	MET
16	1P	186	ARG
16	1P	187	TRP
16	1P	188	PHE
16	1P	198	LYS
16	1P	203	GLN
16	1P	206	TYR
16	1P	209	ASP
16	1P	210	VAL
16	1P	224	LYS
16	1P	263	TYR
16	1P	272	VAL
16	1P	275	PHE
16	1P	290	SER
16	1P	291	ASP
16	1P	292	MET
16	1P	320	ARG
16	1P	325	ARG
16	1P	332	GLU
16	1P	334	VAL
16	1P	335	LYS
16	1P	338	LYS
16	1P	339	THR
16	1P	340	VAL

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Mol	Chain	Res	Type
17	1Q	6	GLN
17	1Q	16	LYS
17	1Q	28	GLU
17	1Q	31	LYS
17	1Q	38	PHE
17	1Q	44	ASN
17	1Q	52	THR
17	1Q	57	MET
17	1Q	58	GLU
17	1Q	62	ARG
17	1Q	70	MET
17	1Q	107	GLU
17	1Q	109	LYS
17	1Q	115	SER
17	1Q	117	SER
17	1Q	123	SER
17	1Q	130	VAL
17	1Q	131	SER
18	1R	3	ARG
18	1R	4	THR
18	1R	10	LYS
18	1R	13	HIS
18	1R	20	ASP
18	1R	23	TYR
18	1R	27	ARG
18	1R	31	ARG
18	1R	54	SER
18	1R	55	ARG
18	1R	83	THR
18	1R	84	CYS
19	1S	16	ARG
19	1S	41	VAL
19	1S	47	ASN
19	1S	55	ARG
19	1S	59	ASP
19	1S	80	ASN
20	1T	7	THR
20	1T	14	ARG
20	1T	19	LEU
20	1T	20	LYS
20	1T	29	LYS
20	1T	38	LYS

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Mol	Chain	Res	Type
20	1T	42	LEU
20	1T	43	ASP
20	1T	44	SER
20	1T	45	LEU
20	1T	49	GLU
20	1T	52	MET
20	1T	79	TYR
20	1U	17	TYR
20	1U	20	LYS
20	1U	26	ASP
20	1U	28	GLU
20	1U	30	LEU
20	1U	32	VAL
20	1U	33	ASN
20	1U	37	MET
20	1U	38	LYS
20	1U	44	SER
20	1U	60	PHE
20	1U	61	GLU
20	1U	69	LYS
21	1V	4	LEU
21	1V	8	THR
21	1V	13	LEU
21	1V	36	GLN
21	1V	39	LYS
21	1V	57	MET
21	1V	68	GLU
21	1V	70	GLN
21	1V	71	LEU
21	1V	95	ARG
21	1V	110	GLN
22	1W	23	ARG
22	1W	29	LYS
22	1W	30	ARG
22	1W	33	ARG
22	1W	40	TYR
22	1W	50	PHE
22	1W	80	ASP
22	1W	95	ASN
22	1W	114	ARG
22	1W	126	HIS
22	1W	127	ASP

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Mol	Chain	Res	Type
23	1X	8	THR
23	1X	12	LEU
23	1X	15	GLN
23	1X	53	ARG
23	1X	68	ASP
23	1X	154	GLU
24	1Y	15	THR
24	1Y	48	PHE
24	1Y	49	LEU
24	1Y	60	PHE
24	1Y	74	CYS
24	1Y	80	ARG
24	1Y	81	GLU
24	1Y	84	ASP
24	1Y	90	PHE
24	1Y	94	CYS
24	1Y	105	ARG
24	1Y	114	CYS
24	1Y	117	MET
24	1Y	119	LEU
24	1Y	126	MET
24	1Y	132	TRP
25	1Z	20	ASP
25	1Z	28	ARG
25	1Z	30	LEU
25	1Z	50	MET
25	1Z	72	MET
25	1Z	85	GLN
25	1Z	109	SER
25	1Z	110	VAL
25	1Z	114	THR
25	1Z	117	VAL
25	1Z	127	LEU
25	1Z	131	GLU
26	1a	1	MET
26	1a	3	PHE
26	1a	5	ILE
26	1a	21	MET
26	1a	27	HIS
26	1a	31	ASN
26	1a	38	VAL
26	1a	50	ARG

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Mol	Chain	Res	Type
26	1a	57	VAL
26	1a	59	ARG
27	1b	10	ASN
27	1b	19	VAL
27	1b	35	SER
27	1b	37	TYR
27	1b	57	ARG
27	1b	64	ASP
27	1b	77	LEU
28	1c	1	LYS
28	1c	2	PHE
28	1c	3	TYR
28	1c	5	ARG
28	1c	9	HIS
28	1c	26	PHE
28	1c	30	TYR
29	1d	3	SER
29	1d	13	PHE
29	1d	19	ARG
29	1d	25	LYS
29	1d	39	TYR
29	1d	41	SER
29	1d	50	ARG
29	1d	62	LEU
29	1d	64	TYR
29	1d	67	SER
29	1d	70	PHE
29	1d	80	ASP
29	1d	82	MET
29	1d	95	LYS
29	1d	96	SER
29	1d	104	LYS
29	1d	106	LYS
29	1d	115	GLU
29	1d	116	PHE
30	1e	7	LYS
30	1e	20	GLN
30	1e	53	LYS
30	1e	56	LYS
30	1e	63	VAL
30	1e	67	LEU
30	1e	74	ARG

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Mol	Chain	Res	Type
30	1e	79	LYS
30	1e	80	ARG
30	1e	87	LYS
30	1e	88	GLU
30	1e	91	TYR
31	1f	1	MET
31	1f	10	HIS
31	1f	13	HIS
31	1f	15	LEU
31	1f	22	PHE
31	1f	28	ARG
31	1f	29	ARG
31	1f	39	ASN
31	1f	46	ARG
31	1f	49	ARG
31	1f	51	ASN
31	1f	57	LYS
32	1g	25	ARG
32	1g	36	ASN
32	1g	44	SER
32	1g	48	ASP
32	1g	63	PHE
32	1g	64	PHE
32	1g	74	SER
32	1g	76	PHE
32	1g	79	TYR
32	1g	80	LEU
32	1g	83	TYR
32	1g	85	MET
32	1g	86	GLN
32	1g	90	ARG
32	1g	91	ARG
32	1g	98	LYS
32	1g	99	TYR
32	1g	108	MET
32	1g	109	GLU
32	1g	112	CYS
32	1g	116	ASN
32	1g	117	LYS
33	1h	16	PHE
33	1h	17	TYR
33	1h	19	ARG

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Mol	Chain	Res	Type
33	1h	21	PHE
33	1h	25	MET
33	1h	26	ARG
33	1h	27	PHE
33	1h	31	LEU
33	1h	54	ASP
33	1h	79	PHE
33	1h	80	TYR
33	1h	85	LYS
33	1h	91	MET
33	1h	123	TYR
33	1h	130	LYS
33	1h	136	SER
33	1h	138	LYS
34	1i	8	LYS
34	1i	16	GLU
34	1i	18	ARG
34	1i	33	VAL
34	1i	48	LYS
34	1i	75	LEU
34	1i	79	TRP
34	1i	83	TYR
34	1i	103	ILE
35	1j	10	ARG
35	1j	11	TYR
35	1j	14	PHE
35	1j	16	GLN
35	1j	24	GLN
35	1j	27	PHE
35	1j	34	PHE
35	1j	40	PHE
35	1j	42	HIS
35	1j	47	VAL
36	1k	20	GLN
36	1k	46	ARG
36	1k	63	VAL
36	1k	70	PHE
36	1k	71	LYS
36	1k	72	TRP
37	1l	3	HIS
37	1l	5	THR
37	1l	8	MET

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Mol	Chain	Res	Type
37	1l	29	MET
37	1l	30	ARG
37	1l	32	GLU
37	1l	33	ASP
37	1l	39	ASP
37	1l	46	ASP
37	1l	52	ASP
37	1l	53	ARG
37	1l	58	ARG
37	1l	69	LEU
37	1l	71	LEU
37	1l	80	ASP
37	1l	83	MET
37	1l	92	SER
37	1l	96	VAL
37	1l	101	MET
37	1l	105	LEU
37	1l	115	MET
37	1l	140	LEU
37	1l	149	GLU
37	1l	156	TYR
38	1m	1	SER
38	1m	2	PHE
38	1m	9	ARG
38	1m	21	GLU
38	1m	30	LYS
38	1m	35	ARG
38	1m	36	LEU
38	1m	41	ARG
38	1m	45	GLU
38	1m	69	TYR
38	1m	71	ARG
38	1m	88	LEU
38	1m	92	PHE
38	1m	99	PHE
38	1m	101	TYR
38	1m	113	LYS
38	1m	117	GLU
38	1m	120	LEU
38	1m	121	ASP
38	1m	127	SER
39	1n	19	TYR

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Mol	Chain	Res	Type
39	1n	26	LEU
39	1n	36	TYR
39	1n	43	MET
39	1n	47	PHE
39	1n	48	ASP
39	1n	70	PHE
39	1n	72	TYR
39	1n	102	CYS
39	1n	104	ASP
39	1n	107	HIS
39	1n	120	LYS
39	1n	124	TRP
39	1n	126	ARG
39	1n	137	LYS
39	1n	178	MET
40	1o	15	GLU
40	1o	17	ASP
40	1o	19	LEU
40	1o	21	MET
40	1o	28	TYR
40	1o	45	MET
40	1o	69	LYS
40	1o	73	PHE
40	1o	83	GLN
40	1o	88	TYR
40	1o	93	ASP
40	1o	117	ARG
40	1o	121	MET
41	1p	3	SER
41	1p	5	ASP
41	1p	14	ARG
41	1p	15	ARG
41	1p	25	LEU
41	1p	34	LYS
41	1p	39	LEU
41	1p	41	ASP
41	1p	42	ARG
41	1p	50	PHE
41	1p	60	TYR
41	1p	62	TYR
41	1p	68	ARG
41	1p	72	ASP

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Mol	Chain	Res	Type
41	1p	81	ILE
41	1p	95	TYR
41	1p	96	LYS
41	1p	105	ILE
41	1p	116	GLU
41	1p	121	ARG
41	1p	123	ASN
41	1p	128	LEU
41	1p	131	PHE
41	1p	133	GLN
41	1p	138	PHE
41	1p	170	LYS
41	1p	171	GLU
42	1q	1	MET
42	1q	9	ARG
42	1q	12	GLN
42	1q	20	LEU
42	1q	34	ARG
42	1q	35	VAL
42	1q	52	ASN
42	1q	53	LYS
42	1q	55	PHE
42	1q	60	ARG
42	1q	61	TRP
42	1q	66	THR
42	1q	75	TRP
42	1q	81	MET
42	1q	123	GLN
42	1q	133	LYS
42	1q	135	GLN
42	1q	142	THR
43	1r	5	ARG
43	1r	9	LEU
43	1r	19	LEU
43	1r	22	LYS
43	1r	39	LYS
43	1r	48	LEU
43	1r	55	THR
43	1r	60	ARG
43	1r	70	SER
43	1r	90	GLU
44	1s	39	ARG

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Mol	Chain	Res	Type
44	1s	41	LEU
44	1s	51	PHE
44	1s	54	LEU
44	1s	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	1C	38	GLN
3	1C	200	ASN
4	1D	114	ASN
4	1D	149	ASN
4	1D	348	HIS
5	1E	112	ASN
6	1F	257	ASN
7	1G	277	GLN
7	1G	392	ASN
7	1G	436	ASN
12	1L	165	ASN
12	1L	506	ASN
13	1M	44	GLN
13	1M	48	ASN
13	1M	293	HIS
13	1M	415	GLN
14	1N	63	GLN
14	1N	268	GLN
15	1O	200	GLN
15	1O	271	ASN
16	1P	180	ASN
17	1Q	6	GLN
20	1T	74	GLN
21	1V	85	ASN
22	1W	48	HIS
22	1W	58	GLN
23	1X	103	GLN
31	1f	39	ASN
32	1g	116	ASN
34	1i	12	GLN
35	1j	16	GLN
37	1l	136	ASN
39	1n	74	GLN
40	1o	84	HIS

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Mol	Chain	Res	Type
41	1p	27	ASN
41	1p	54	GLN
41	1p	55	HIS
41	1p	133	GLN
42	1q	135	GLN
43	1r	35	GLN
43	1r	46	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	FME	1A	1	1	8,9,10	0.53	0	7,9,11	1.01	1 (14%)
10	FME	1J	1	10	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
14	FME	1N	1	14	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
8	FME	1H	1	8	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
13	FME	1M	1	13	8,9,10	0.50	0	7,9,11	0.91	1 (14%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
12	FME	1L	1	12	8,9,10	0.52	0	7,9,11	1.02	1 (14%)
34	SAC	1i	1	-	7,8,9	0.53	0	8,9,11	1.07	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
1	FME	1A	1	1	-	1/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
13	FME	1M	1	13	-	2/7/9/11	-
11	FME	1K	1	11	-	2/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
34	SAC	1i	1	-	-	3/7/8/10	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1i	1	SAC	O-C-CA	-2.92	117.12	124.78
8	1H	1	FME	O-C-CA	-2.69	117.74	124.78
1	1A	1	FME	O-C-CA	-2.54	118.11	124.78
12	1L	1	FME	O-C-CA	-2.52	118.18	124.78
11	1K	1	FME	O-C-CA	-2.48	118.27	124.78
14	1N	1	FME	O-C-CA	-2.44	118.38	124.78
10	1J	1	FME	O-C-CA	-2.41	118.45	124.78
13	1M	1	FME	O-C-CA	-2.25	118.88	124.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O-C-CA-CB
8	1H	1	FME	O-C-CA-CB
10	1J	1	FME	N-CA-CB-CG
10	1J	1	FME	C-CA-CB-CG
11	1K	1	FME	O-C-CA-CB
12	1L	1	FME	O-C-CA-CB
13	1M	1	FME	N-CA-CB-CG
34	1i	1	SAC	O-C-CA-CB
11	1K	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-N-C1A
34	1i	1	SAC	CB-CA-N-C1A

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
45	SF4	1F	502	6	0,12,12	-	-	-		
45	SF4	1G	801	7	0,12,12	-	-	-		
49	FMN	1F	501	-	33,33,33	0.58	0	48,50,50	0.66	1 (2%)
48	FES	1E	301	5	0,4,4	-	-	-		
48	FES	1G	803	7	0,4,4	-	-	-		
53	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.42	0
47	U10	1D	501	-	63,63,63	0.58	2 (3%)	76,79,79	0.74	4 (5%)
45	SF4	1I	201	9	0,12,12	-	-	-		
51	MYR	1L	701	-	14,14,15	0.35	0	13,13,15	0.39	0
56	NDP	1P	501	-	45,52,52	0.60	0	53,80,80	0.76	2 (3%)
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.88	1 (3%)
58	EHZ	1W	201	-	29,36,37	0.18	0	35,44,47	1.30	1 (2%)
58	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.09	2 (5%)
52	3PE	1M	501	-	37,37,50	0.30	0	40,42,55	0.38	0
46	PC1	1d	201	-	38,38,53	0.30	0	44,46,61	0.38	0
45	SF4	1B	201	2	0,12,12	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
53	CDL	1N	401	-	66,66,99	0.31	0	72,78,111	0.42	0
46	PC1	1q	201	-	47,47,53	0.30	0	53,55,61	0.41	0
45	SF4	1I	202	9	0,12,12	-	-	-		
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.33	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
45	SF4	1F	502	6	-	-	0/6/5/5
45	SF4	1G	801	7	-	-	0/6/5/5
49	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
48	FES	1E	301	5	-	-	0/1/1/1
48	FES	1G	803	7	-	-	0/1/1/1
53	CDL	1a	101	-	-	11/71/71/110	-
47	U10	1D	501	-	-	15/63/87/87	0/1/1/1
45	SF4	1I	201	9	-	-	0/6/5/5
51	MYR	1L	701	-	-	0/11/12/13	-
56	NDP	1P	501	-	-	3/30/77/77	0/5/5/5
54	GTP	1O	401	55	-	1/18/38/38	0/3/3/3
58	EHZ	1W	201	-	-	12/42/44/45	-
58	EHZ	1n	201	-	-	9/42/44/45	-
52	3PE	1M	501	-	-	6/41/41/54	-
46	PC1	1d	201	-	-	14/42/42/57	-
45	SF4	1B	201	2	-	-	0/6/5/5
45	SF4	1G	802	7	-	-	0/6/5/5
53	CDL	1N	401	-	-	25/76/76/110	-
46	PC1	1q	201	-	-	16/51/51/57	-
45	SF4	1I	202	9	-	-	0/6/5/5
46	PC1	1B	202	-	-	12/37/37/57	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1O	401	GTP	C5-C6	-2.54	1.42	1.47
47	1D	501	U10	C4-C5	-2.53	1.41	1.48
54	1O	401	GTP	C8-N7	-2.08	1.31	1.35
47	1D	501	U10	C6-C5	-2.02	1.41	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1W	201	EHZ	C10-S1-C9	7.23	124.38	101.87
58	1n	201	EHZ	C10-S1-C9	5.64	119.42	101.87
56	1P	501	NDP	O4D-C1D-C2D	-2.77	100.60	106.64
54	1O	401	GTP	O4'-C1'-C2'	-2.73	102.94	106.93
47	1D	501	U10	O3-C3-C2	2.70	125.69	116.56
47	1D	501	U10	O4-C4-C5	-2.41	108.42	116.56
47	1D	501	U10	C4-C3-C2	-2.20	116.35	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1P	501	NDP	C5A-C6A-N6A	2.18	123.66	120.35
58	1n	201	EHZ	C14-C13-C12	2.12	115.89	112.36
47	1D	501	U10	O4-C4-C3	2.06	131.40	123.64
49	1F	501	FMN	C4-N3-C2	-2.02	121.92	125.64

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C2-C1-O11-P
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3
46	1d	201	PC1	C11-O13-P-O14
46	1d	201	PC1	O22-C21-O21-C2
46	1d	201	PC1	C22-C21-O21-C2
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1q	201	PC1	C11-O13-P-O14
46	1q	201	PC1	O32-C31-O31-C3
46	1q	201	PC1	C32-C31-O31-C3
47	1D	501	U10	C12-C11-C9-C8
47	1D	501	U10	C12-C11-C9-C10
47	1D	501	U10	C34-C36-C37-C38
49	1F	501	FMN	N10-C1'-C2'-O2'
49	1F	501	FMN	N10-C1'-C2'-C3'
52	1M	501	3PE	C12-C11-O13-P
53	1N	401	CDL	CA2-OA2-PA1-OA4
58	1W	201	EHZ	O1-C7-C8-C9
58	1W	201	EHZ	N2-C15-C16-C17
58	1W	201	EHZ	N2-C15-C16-O5
58	1W	201	EHZ	O4-C15-C16-C17
58	1W	201	EHZ	O2-C9-S1-C10
58	1W	201	EHZ	C8-C9-S1-C10
58	1n	201	EHZ	O1-C7-C8-C9
58	1n	201	EHZ	C13-C12-N1-C11
53	1N	401	CDL	O1-C1-CA2-OA2
47	1D	501	U10	C40-C39-C41-C42
47	1D	501	U10	C45-C44-C46-C47
47	1D	501	U10	C38-C39-C41-C42
47	1D	501	U10	C43-C44-C46-C47
47	1D	501	U10	C24-C26-C27-C28
58	1n	201	EHZ	O3-C12-N1-C11

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Mol	Chain	Res	Type	Atoms
53	1N	401	CDL	CB2-C1-CA2-OA2
53	1N	401	CDL	CB5-C51-C52-C53
53	1N	401	CDL	C1-CA2-OA2-PA1
47	1D	501	U10	C4-C3-O3-C3M
46	1q	201	PC1	C1-O11-P-O13
53	1N	401	CDL	CA2-OA2-PA1-OA5
46	1B	202	PC1	C31-C32-C33-C34
53	1N	401	CDL	C74-C75-C76-C77
53	1N	401	CDL	C1-CB2-OB2-PB2
53	1N	401	CDL	C14-C15-C16-C17
52	1M	501	3PE	C24-C25-C26-C27
53	1N	401	CDL	C31-CA7-OA8-CA6
52	1M	501	3PE	C31-C32-C33-C34
53	1N	401	CDL	C57-C58-C59-C60
53	1N	401	CDL	OA9-CA7-OA8-CA6
46	1B	202	PC1	C1-O11-P-O13
52	1M	501	3PE	C11-O13-P-O11
56	1P	501	NDP	O4D-C1D-N1N-C6N
46	1q	201	PC1	O11-C1-C2-C3
47	1D	501	U10	C2-C3-O3-C3M
58	1W	201	EHZ	O4-C15-C16-O5
53	1a	101	CDL	CA7-C31-C32-C33
46	1d	201	PC1	C2-C1-O11-P
46	1q	201	PC1	C3B-C3C-C3D-C3E
46	1d	201	PC1	C22-C23-C24-C25
53	1N	401	CDL	OB5-CB3-CB4-OB6
47	1D	501	U10	C9-C11-C12-C13
53	1N	401	CDL	CB4-CB3-OB5-PB2
53	1N	401	CDL	C52-C51-CB5-OB6
53	1a	101	CDL	C12-C13-C14-C15
46	1B	202	PC1	C1-C2-C3-O31
46	1q	201	PC1	O11-C1-C2-O21
53	1N	401	CDL	C72-C71-CB7-OB8
58	1W	201	EHZ	O3-C12-C13-C14
58	1W	201	EHZ	C15-C16-C17-C19
58	1W	201	EHZ	N1-C12-C13-C14
46	1d	201	PC1	C11-O13-P-O11
46	1q	201	PC1	C11-O13-P-O11
46	1q	201	PC1	C1-O11-P-O14
52	1M	501	3PE	C11-O13-P-O12
53	1N	401	CDL	CA2-OA2-PA1-OA3
58	1W	201	EHZ	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
58	1n	201	EHZ	C6-C7-C8-C9
46	1B	202	PC1	C12-C11-O13-P
46	1d	201	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
58	1W	201	EHZ	C15-C16-C17-C20
46	1d	201	PC1	O13-C11-C12-N
46	1q	201	PC1	O13-C11-C12-N
46	1q	201	PC1	C24-C25-C26-C27
46	1d	201	PC1	C35-C36-C37-C38
46	1B	202	PC1	O21-C2-C3-O31
53	1a	101	CDL	OA6-CA4-CA6-OA8
58	1n	201	EHZ	C2-C3-C4-C5
46	1B	202	PC1	C11-O13-P-O11
53	1a	101	CDL	CA3-OA5-PA1-OA2
53	1a	101	CDL	CB2-OB2-PB2-OB5
52	1M	501	3PE	C2-C1-O11-P
53	1N	401	CDL	C12-C13-C14-C15
53	1a	101	CDL	CA4-CA3-OA5-PA1
58	1n	201	EHZ	C10-C11-N1-C12
53	1N	401	CDL	CA2-C1-CB2-OB2
58	1n	201	EHZ	C19-C17-C20-O6
46	1B	202	PC1	O21-C21-C22-C23
58	1n	201	EHZ	C11-C10-S1-C9
53	1N	401	CDL	OB5-CB3-CB4-CB6
46	1q	201	PC1	C23-C24-C25-C26
56	1P	501	NDP	O4D-C4D-C5D-O5D
58	1n	201	EHZ	C1-C21-C22-C23
46	1q	201	PC1	O21-C21-C22-C23
47	1D	501	U10	C5-C4-O4-C4M
53	1N	401	CDL	C72-C71-CB7-OB9
53	1N	401	CDL	C12-C11-CA5-OA6
46	1B	202	PC1	O22-C21-C22-C23
53	1N	401	CDL	C56-C57-C58-C59
54	1O	401	GTP	PB-O3A-PA-O2A
47	1D	501	U10	C46-C47-C48-C49
46	1d	201	PC1	C39-C3A-C3B-C3C
46	1q	201	PC1	O22-C21-C22-C23
46	1B	202	PC1	C1-O11-P-O14
46	1d	201	PC1	C11-O13-P-O12
53	1a	101	CDL	CA3-OA5-PA1-OA3
56	1P	501	NDP	O4B-C4B-C5B-O5B
47	1D	501	U10	C36-C37-C38-C39

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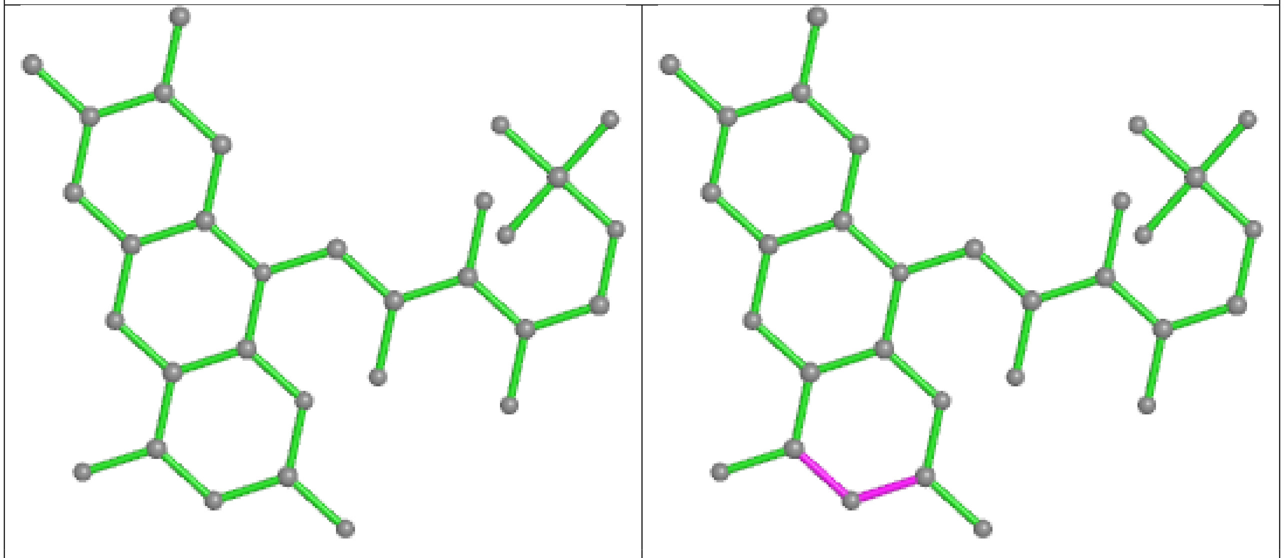
Mol	Chain	Res	Type	Atoms
46	1q	201	PC1	C3-C2-O21-C21
53	1a	101	CDL	C13-C14-C15-C16
53	1N	401	CDL	C12-C11-CA5-OA7
53	1N	401	CDL	C52-C51-CB5-OB7
53	1a	101	CDL	C12-C11-CA5-OA6
53	1a	101	CDL	C72-C71-CB7-OB8
47	1D	501	U10	C31-C32-C33-C34
46	1d	201	PC1	O31-C31-C32-C33
53	1a	101	CDL	C72-C71-CB7-OB9

There are no ring outliers.

No monomer is involved in short contacts.

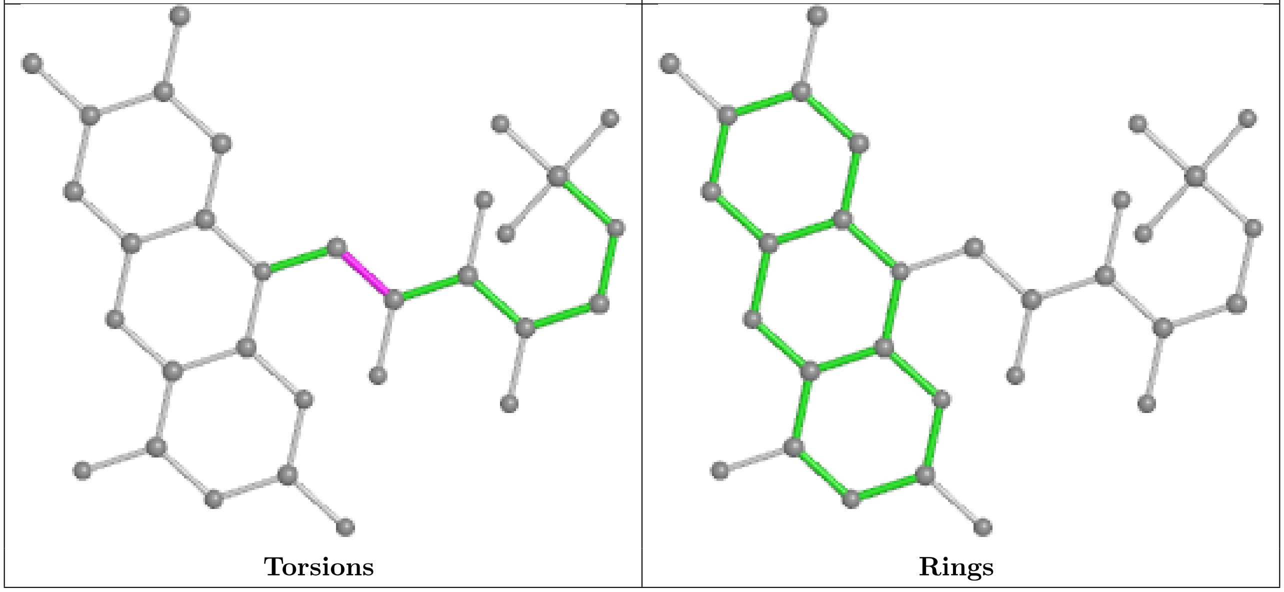
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1F 501



Bond lengths

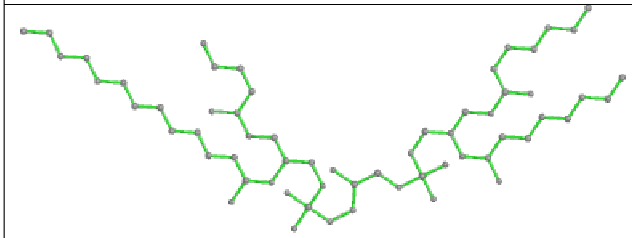
Bond angles



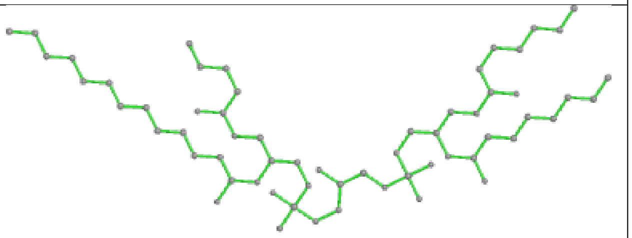
Torsions

Rings

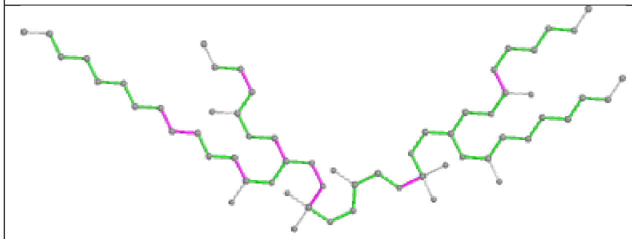
Ligand CDL 1a 101



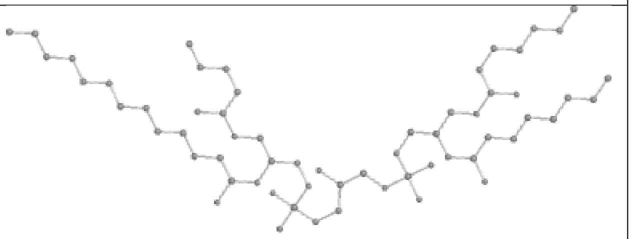
Bond lengths



Bond angles

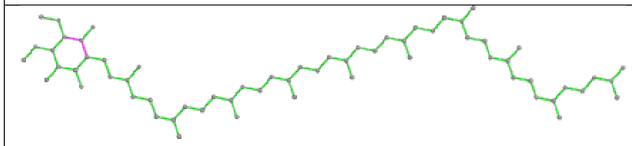


Torsions

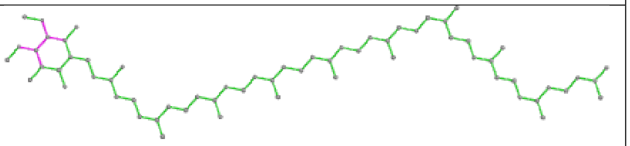


Rings

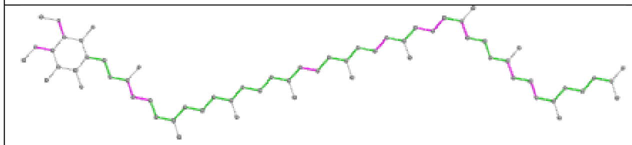
Ligand U10 1D 501



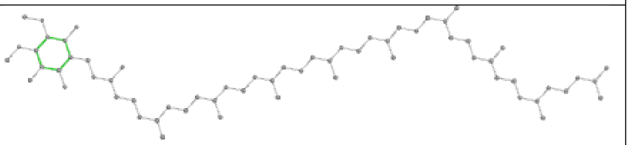
Bond lengths



Bond angles

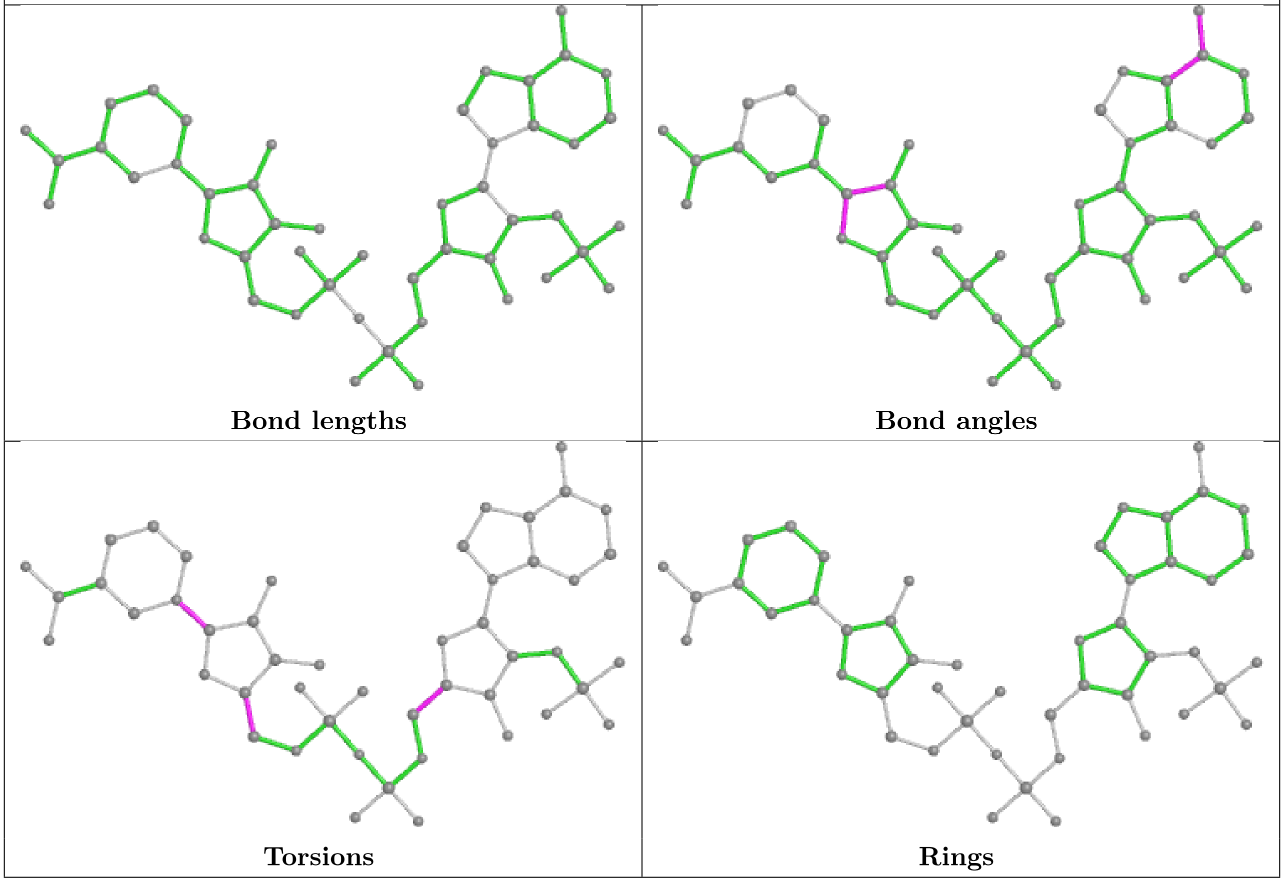


Torsions



Rings

Ligand NDP 1P 501



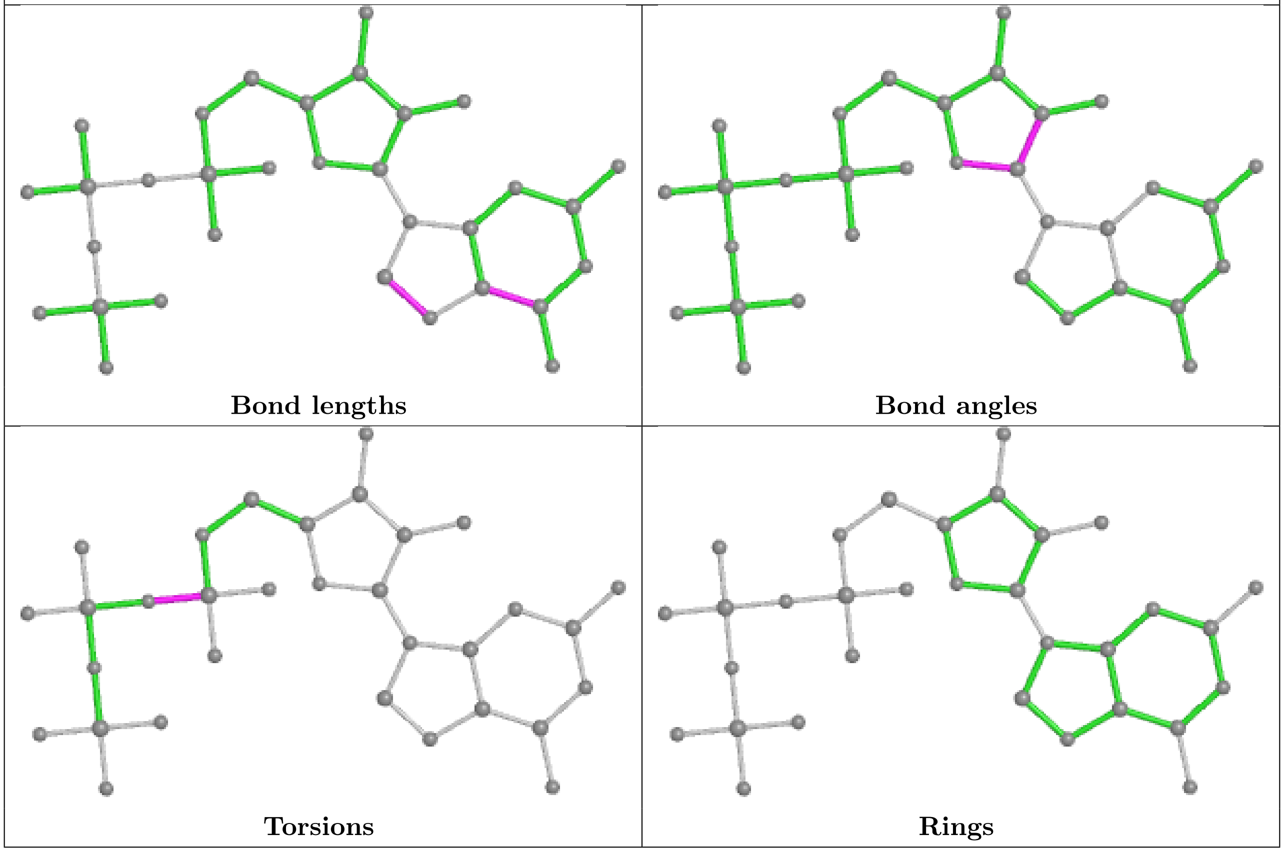
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP 1O 401



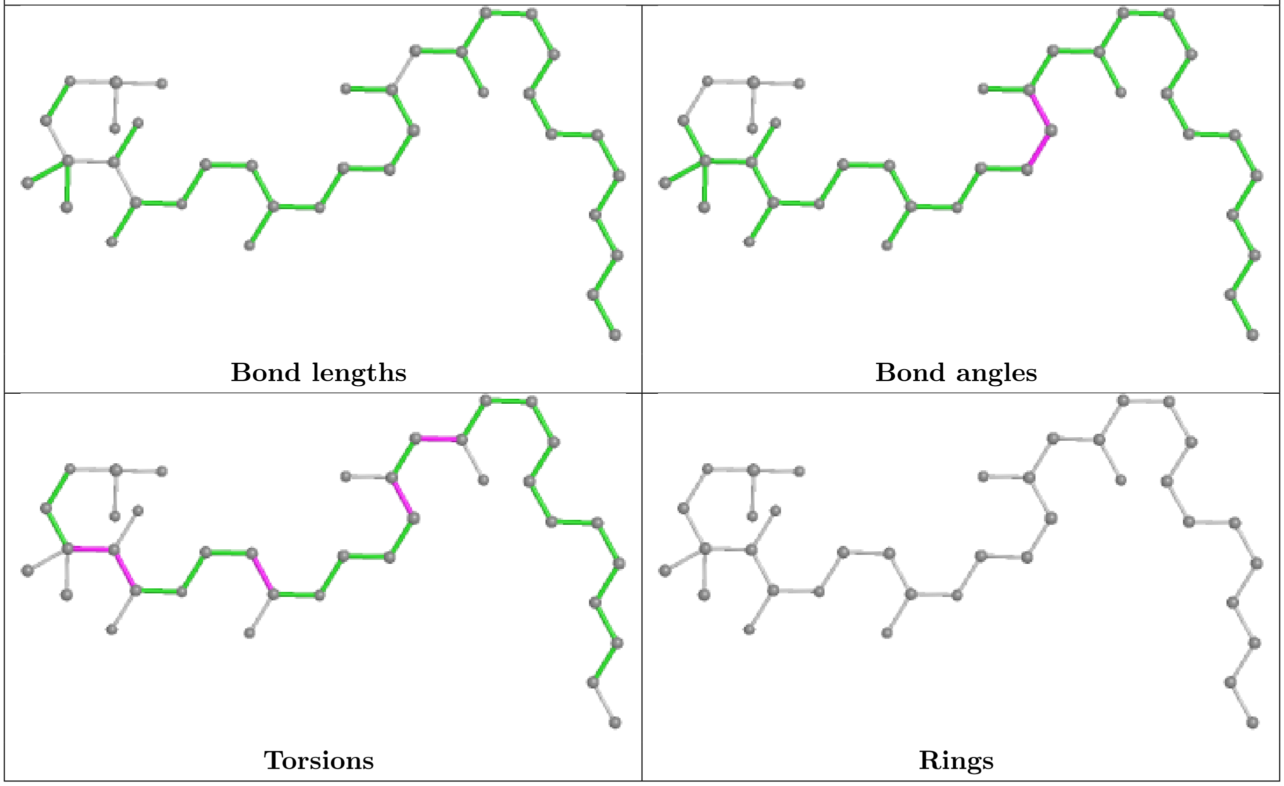
Bond lengths

Bond angles

Torsions

Rings

Ligand EHZ 1W 201



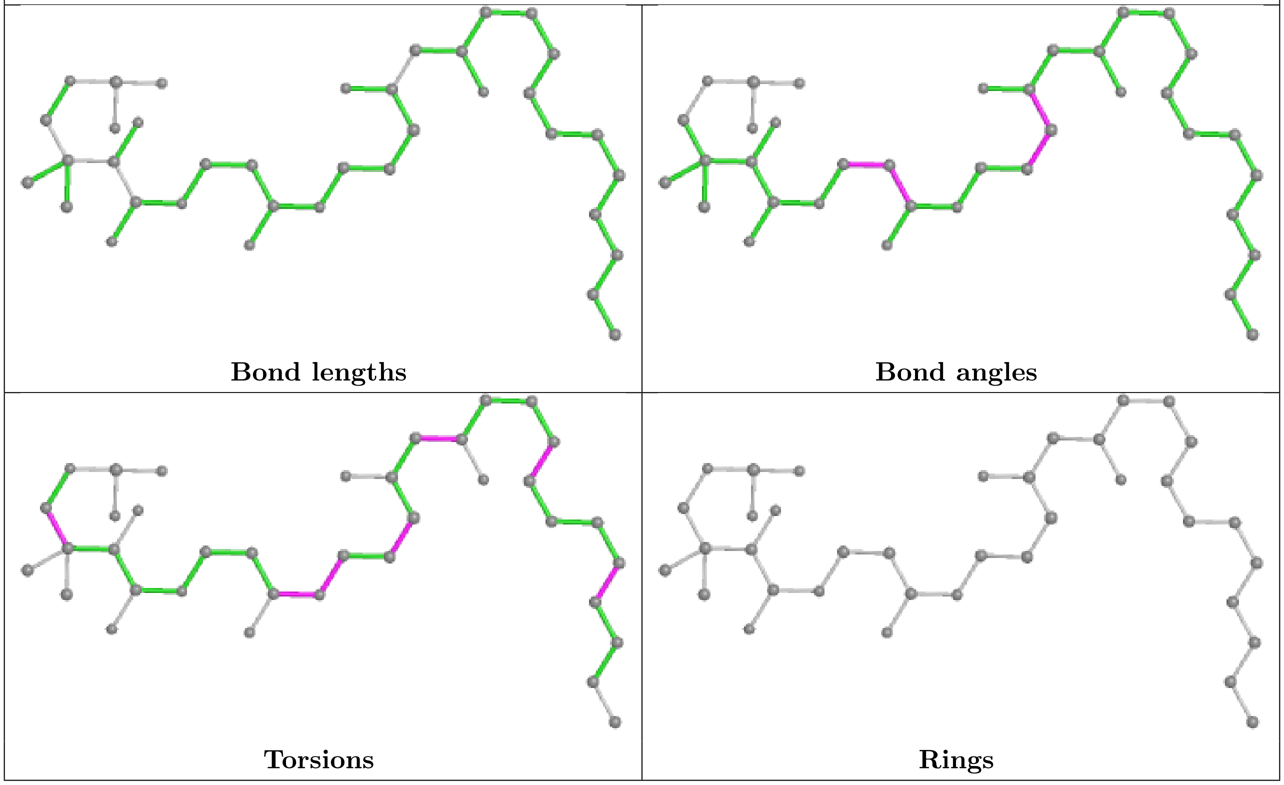
Bond lengths

Bond angles

Torsions

Rings

Ligand EHZ 1n 201



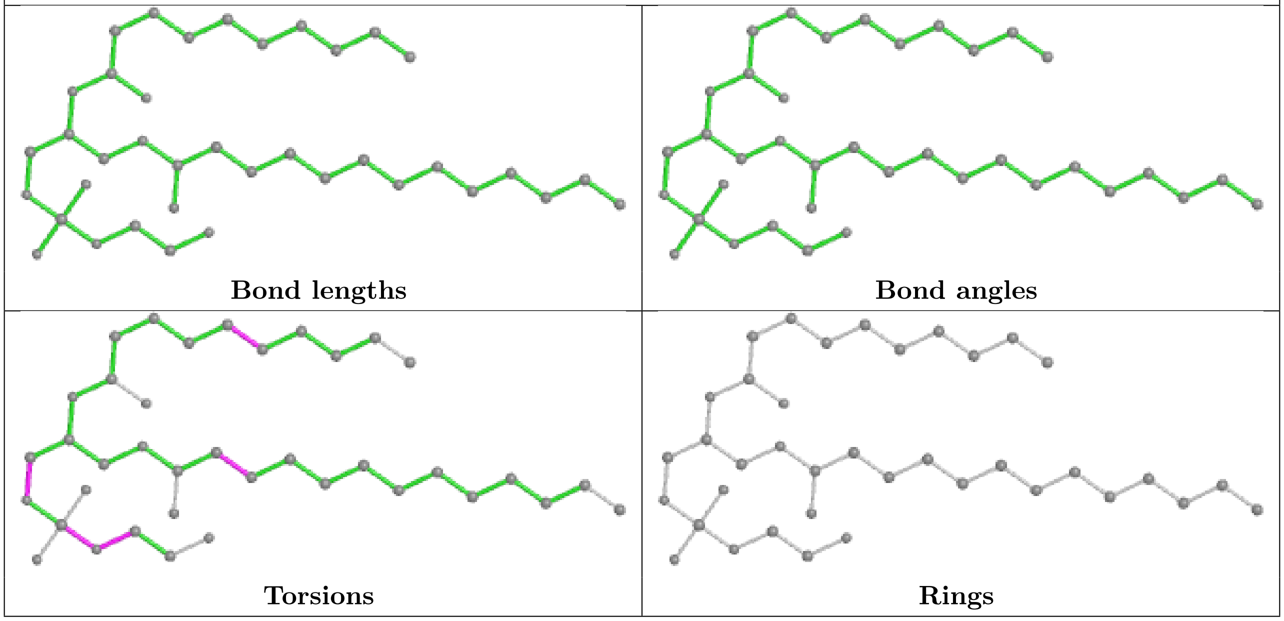
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 1M 501



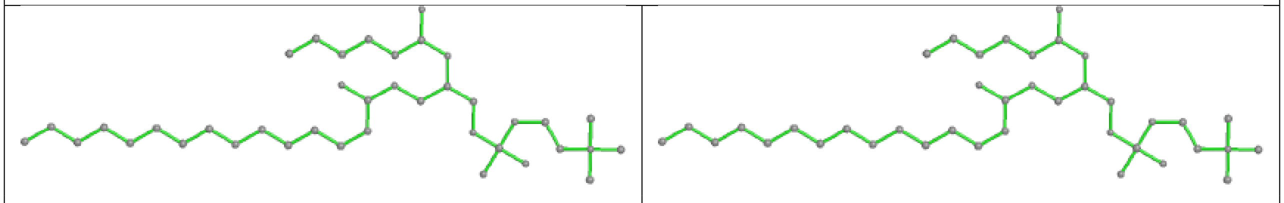
Bond lengths

Bond angles

Torsions

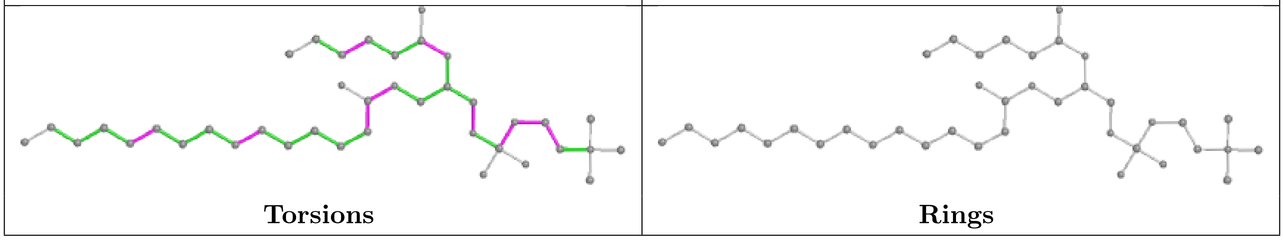
Rings

Ligand PC1 1d 201



Bond lengths

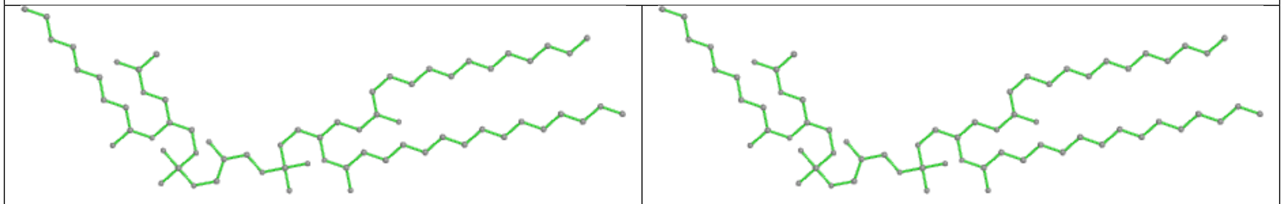
Bond angles



Torsions

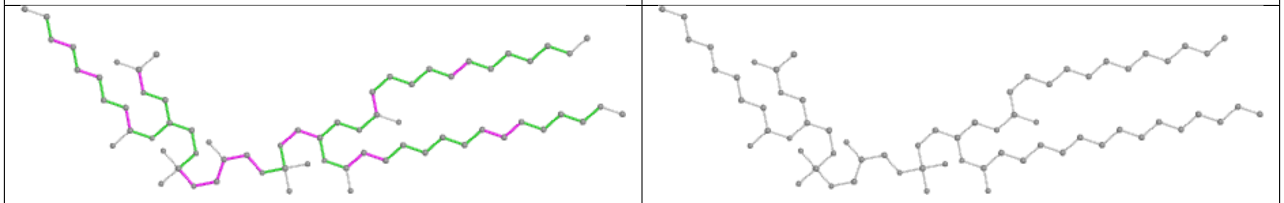
Rings

Ligand CDL 1N 401



Bond lengths

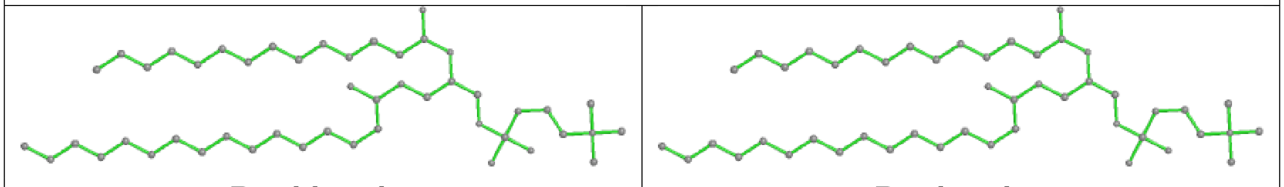
Bond angles



Torsions

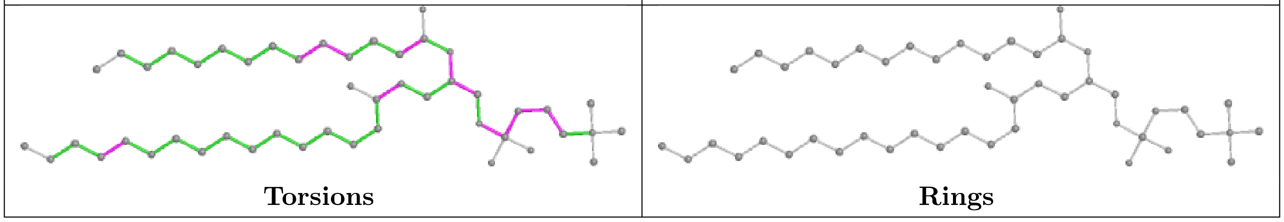
Rings

Ligand PC1 1q 201



Bond lengths

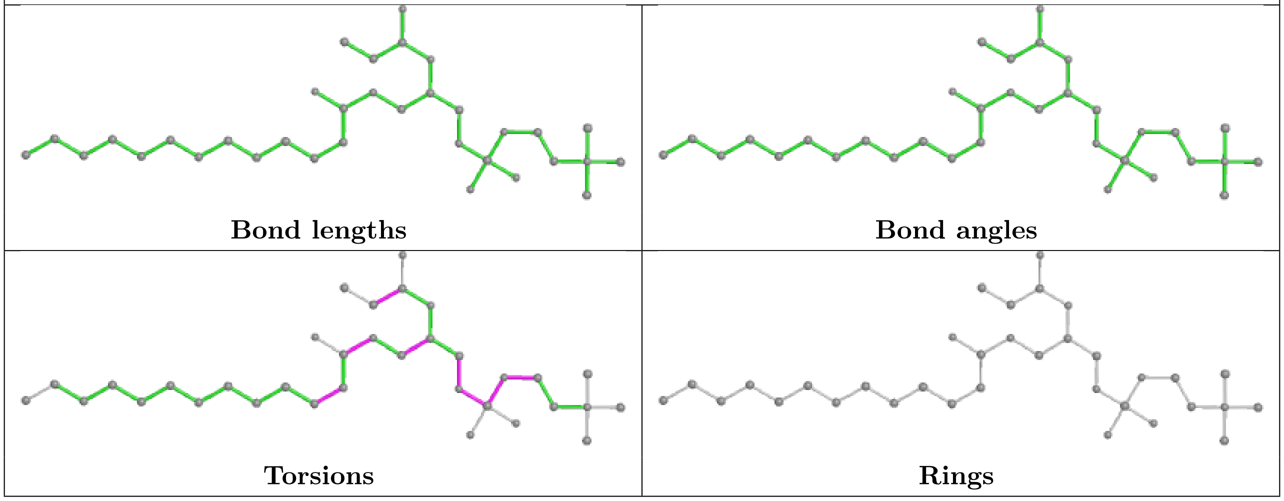
Bond angles



Torsions

Rings

Ligand PC1 1B 202



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	9.77
1	1i	1:SAC	C	2:GLY	N	3.19

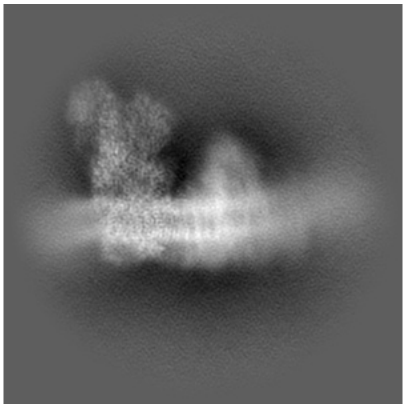
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-42167. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map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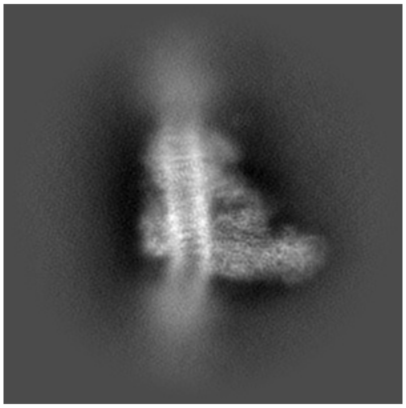
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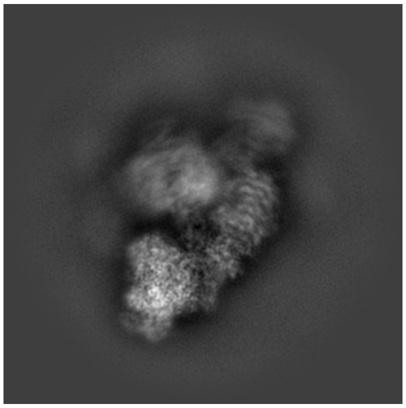
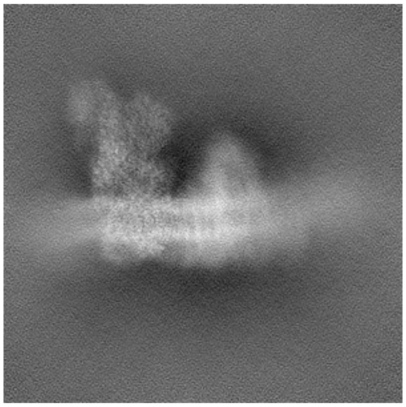
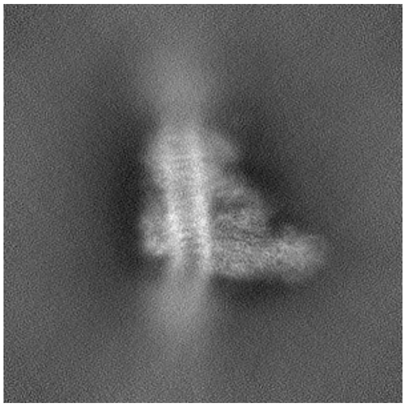
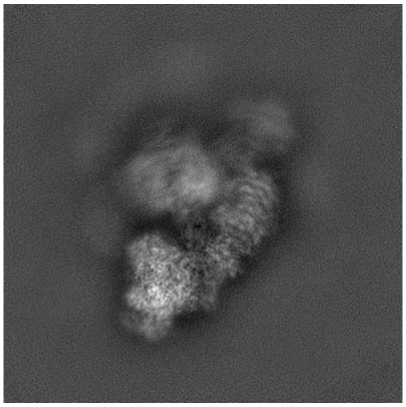

Z

6.1.2 Raw map


X

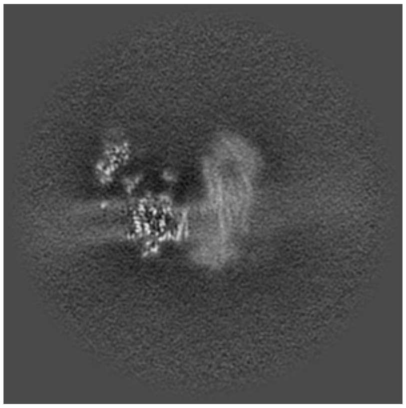

Y


Z

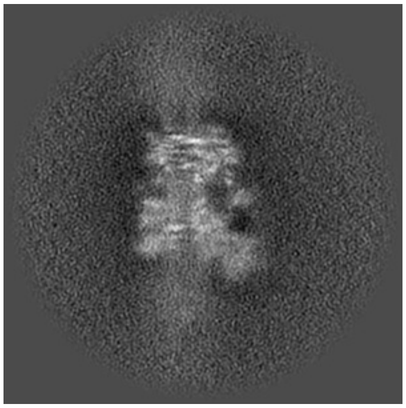
The images above show the map projected in three orthogonal directions.

6.2 Central slices

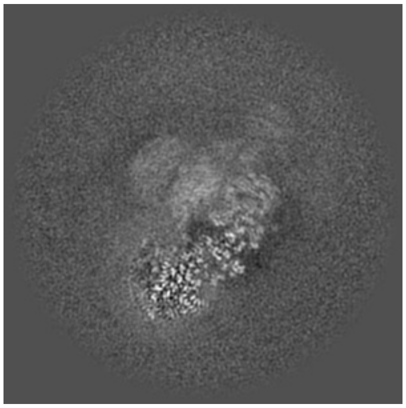
6.2.1 Primary map



X Index: 160

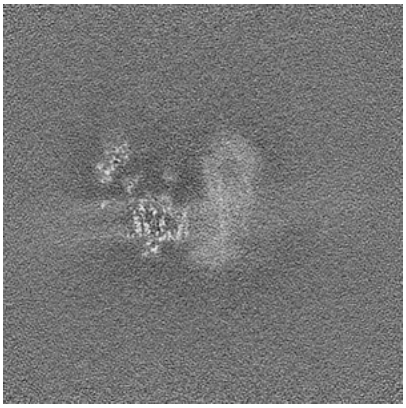


Y Index: 160

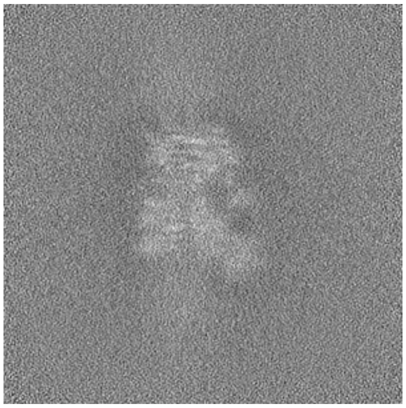


Z Index: 160

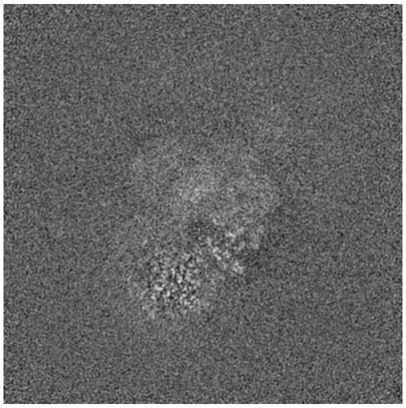
6.2.2 Raw map



X Index: 160



Y Index: 160

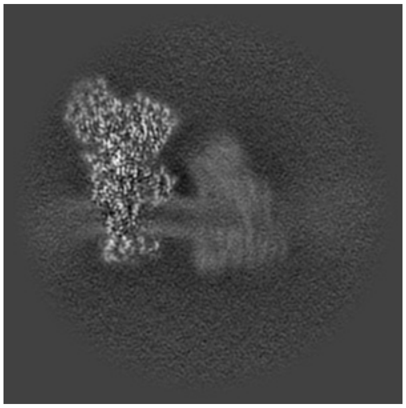


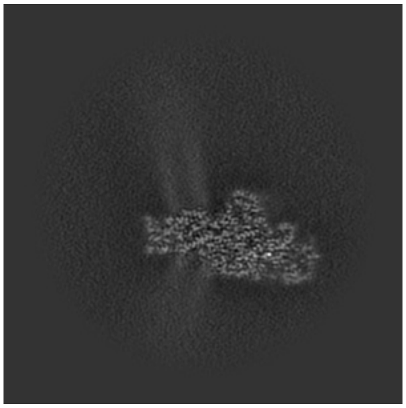
Z Index: 160

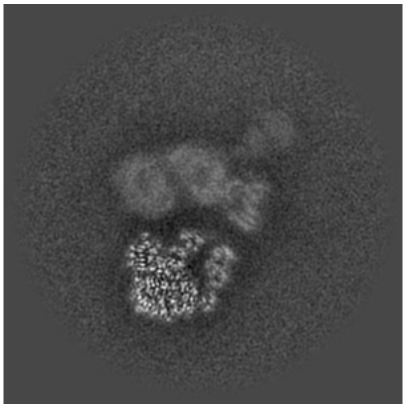
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

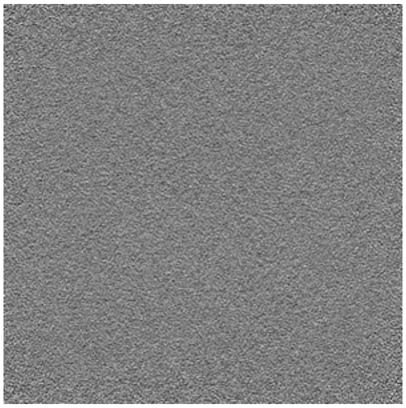
6.3.1 Primary map

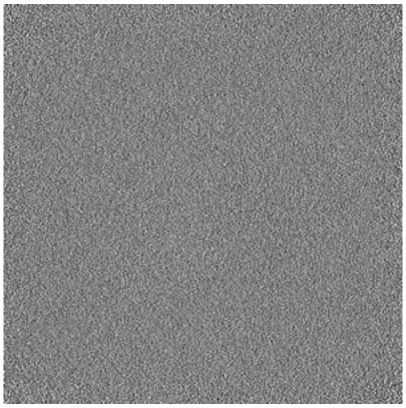

X Index: 123

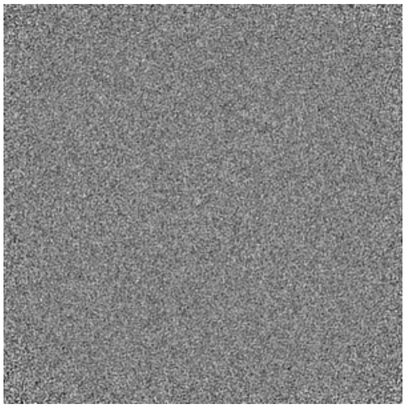

Y Index: 86


Z Index: 184

6.3.2 Raw map


X Index: 0

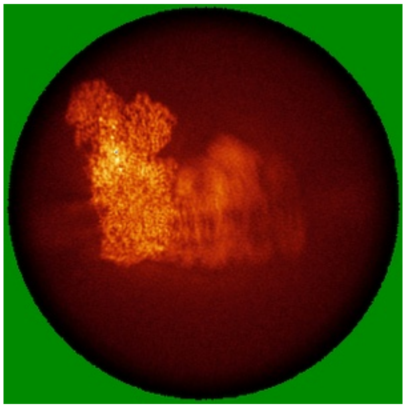

Y Index: 0

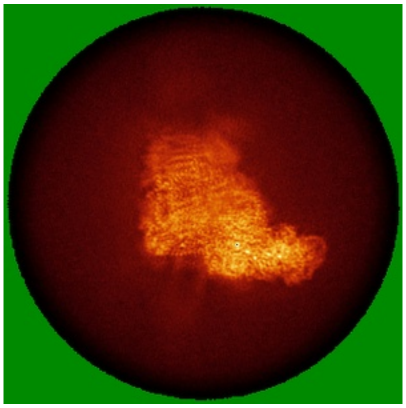

Z Index: 0

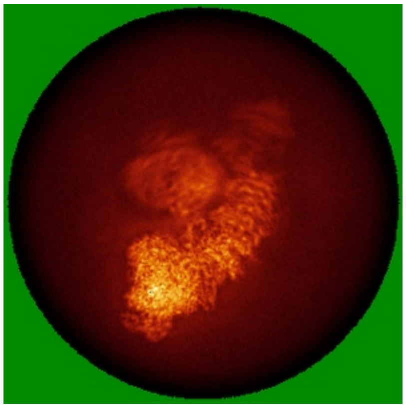
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

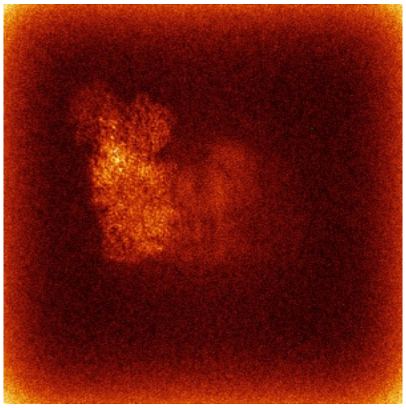
6.4.1 Primary map

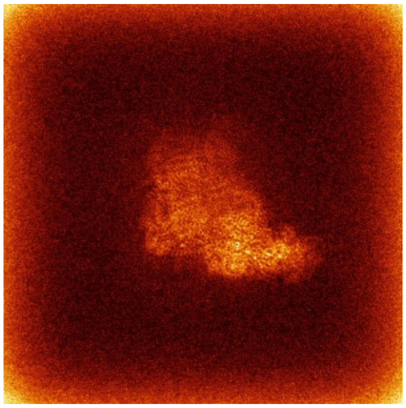

X

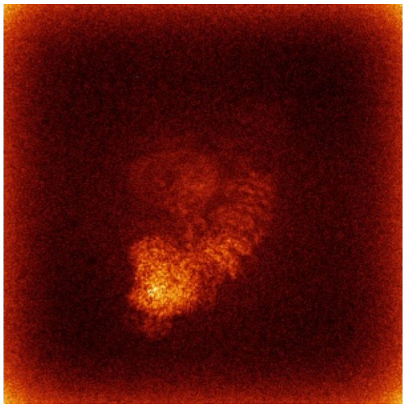

Y


Z

6.4.2 Raw map


X

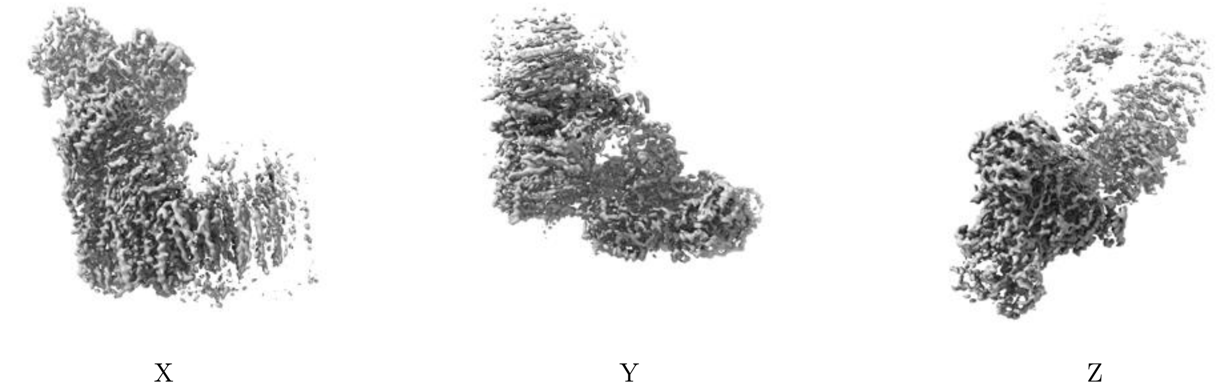

Y


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.

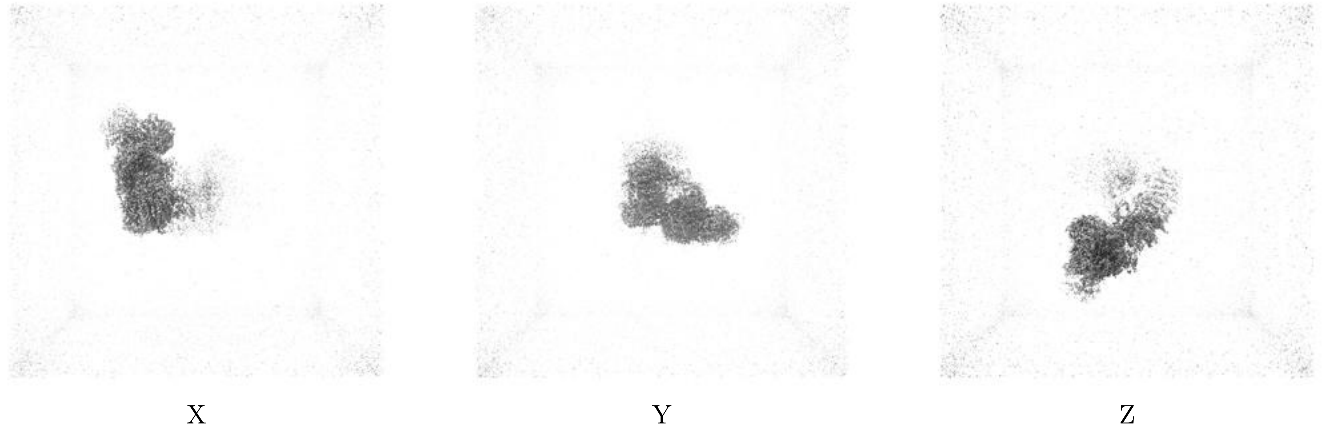
6.5 Orthogonal surface views ⓘ

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.

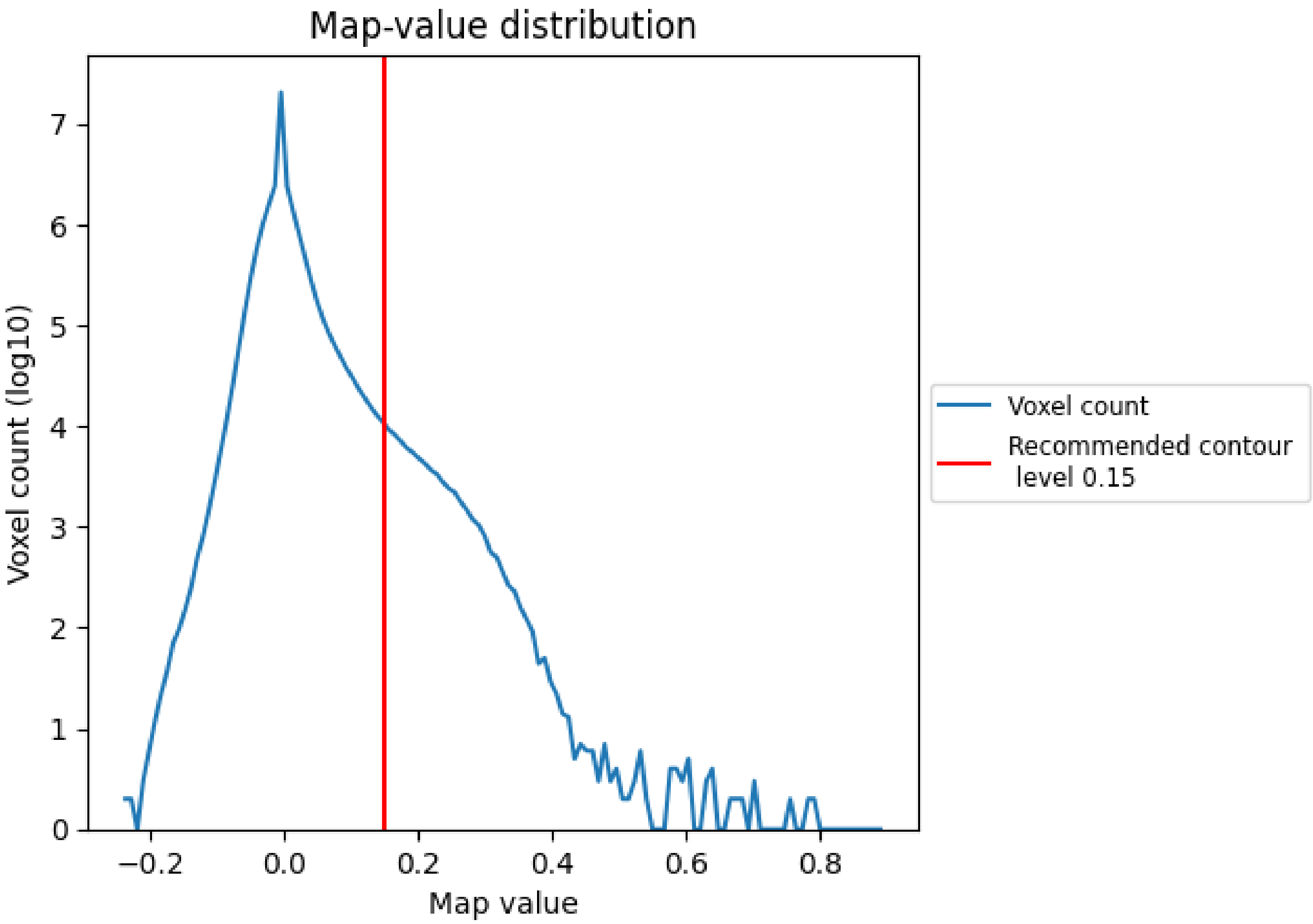
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

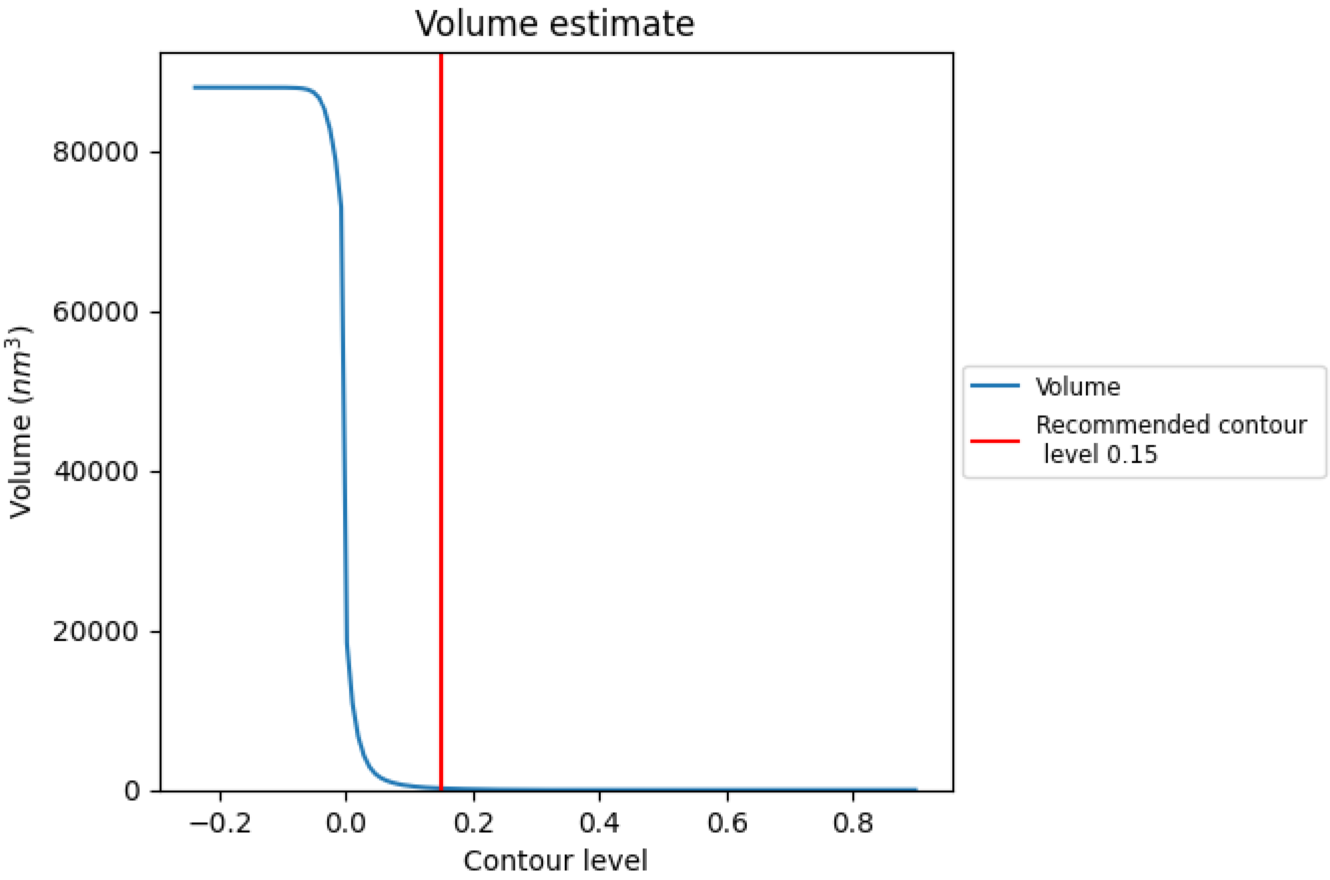
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

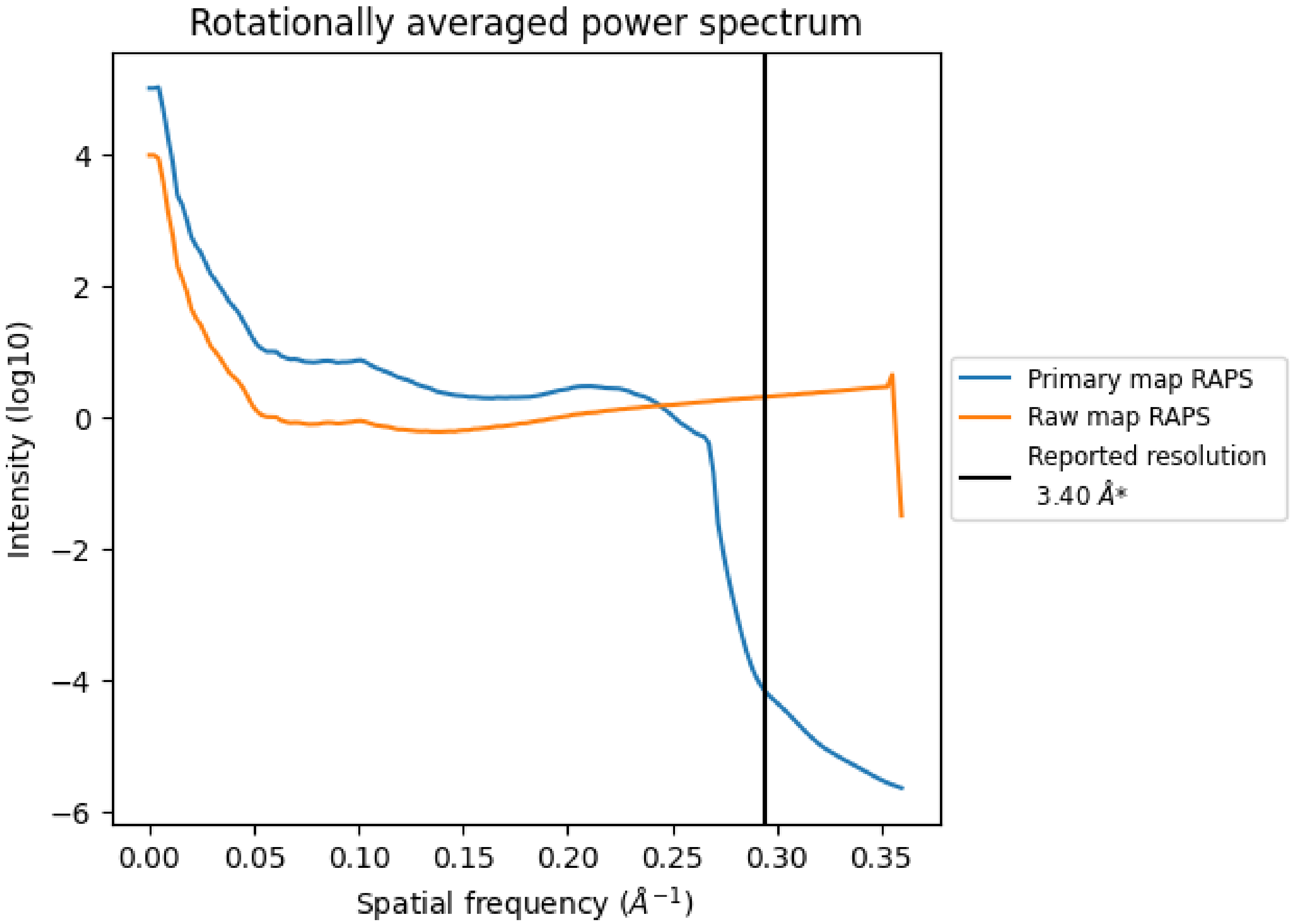
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 183 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 ⓘ

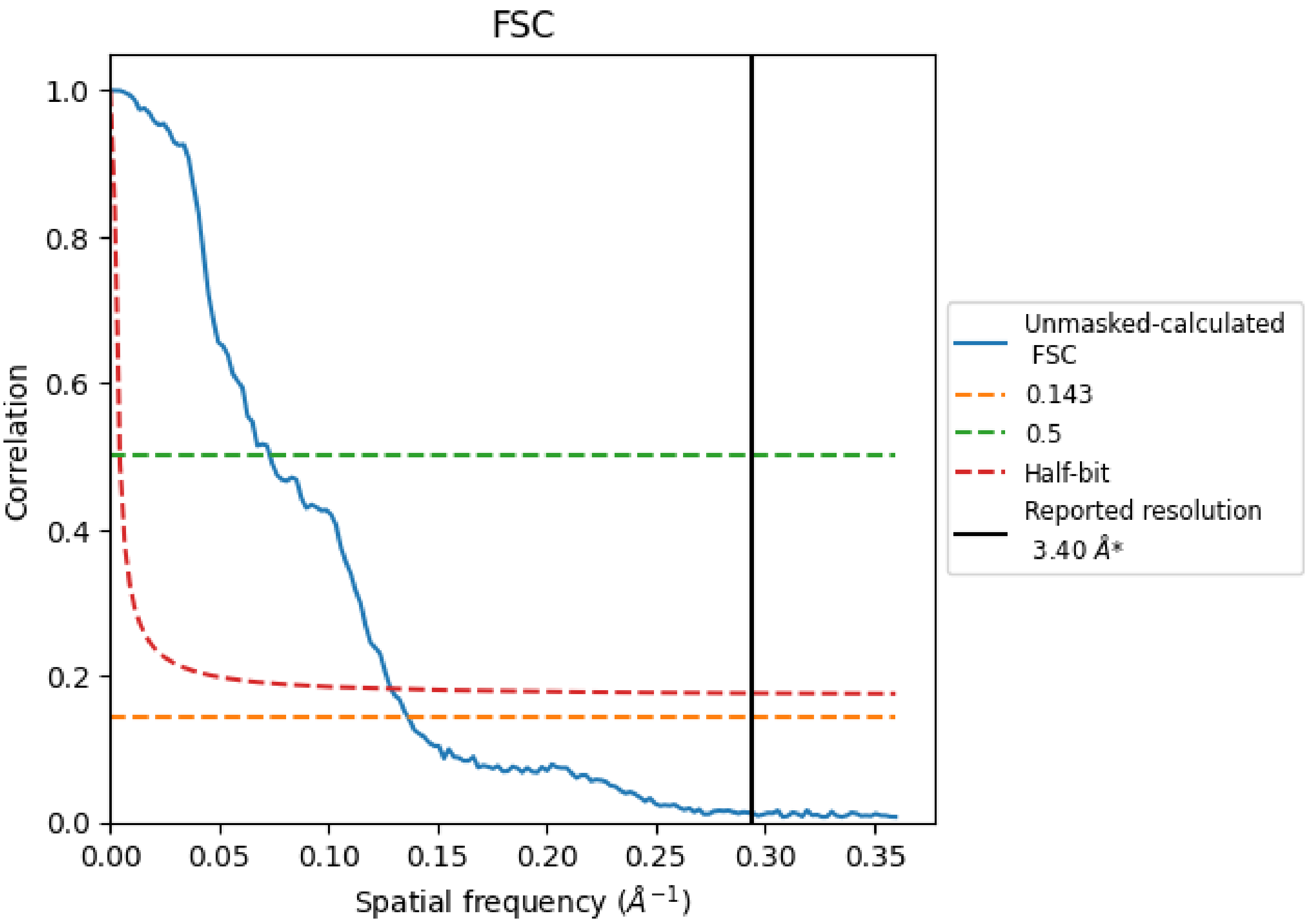


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates ⓘ

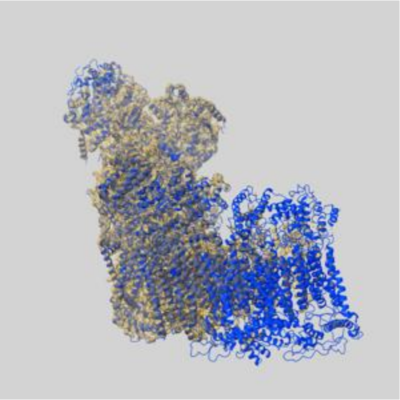
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.33	13.64	7.76

*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 7.33 differs from the reported value 3.4 by more than 10 %

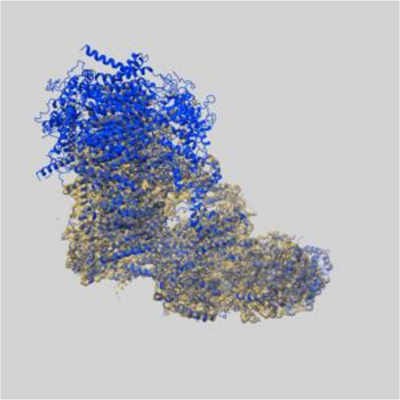
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-42167 and PDB model 8UEQ. Per-residue inclusion information can be found in section 3 on page 21.

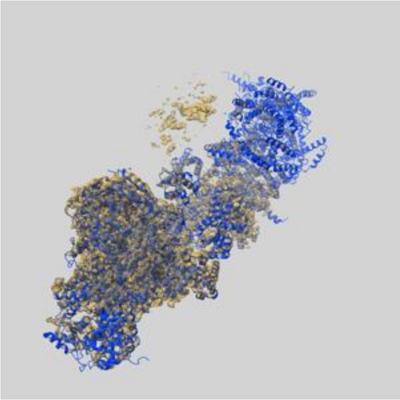
9.1 Map-model overlay ⓘ



X



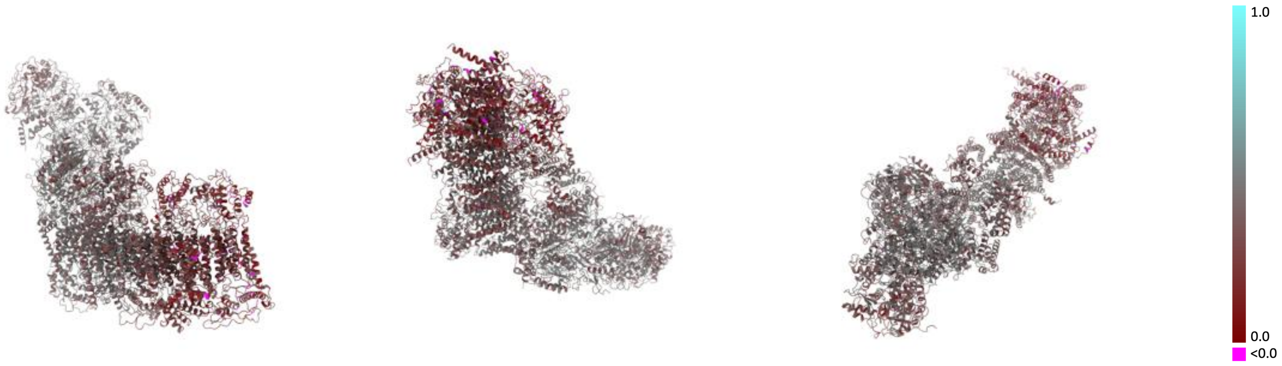
Y



Z

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

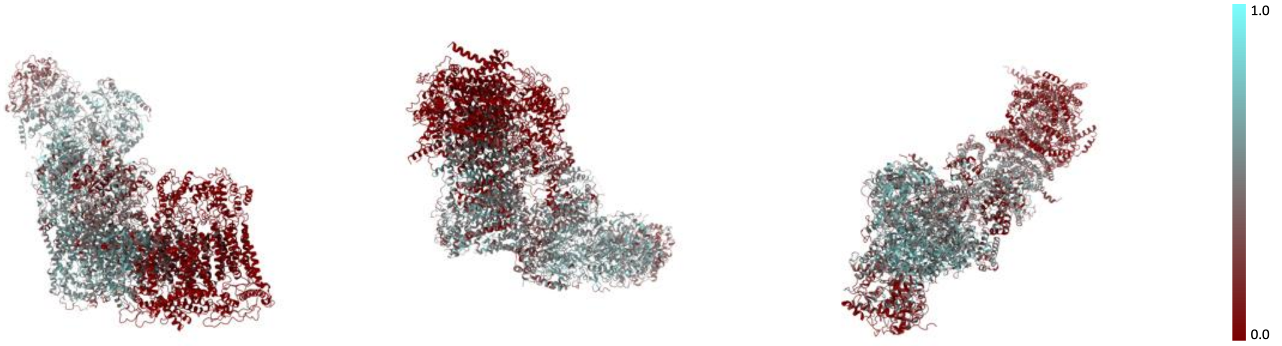
9.2 Q-score mapped to coordinate model ⓘ



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.

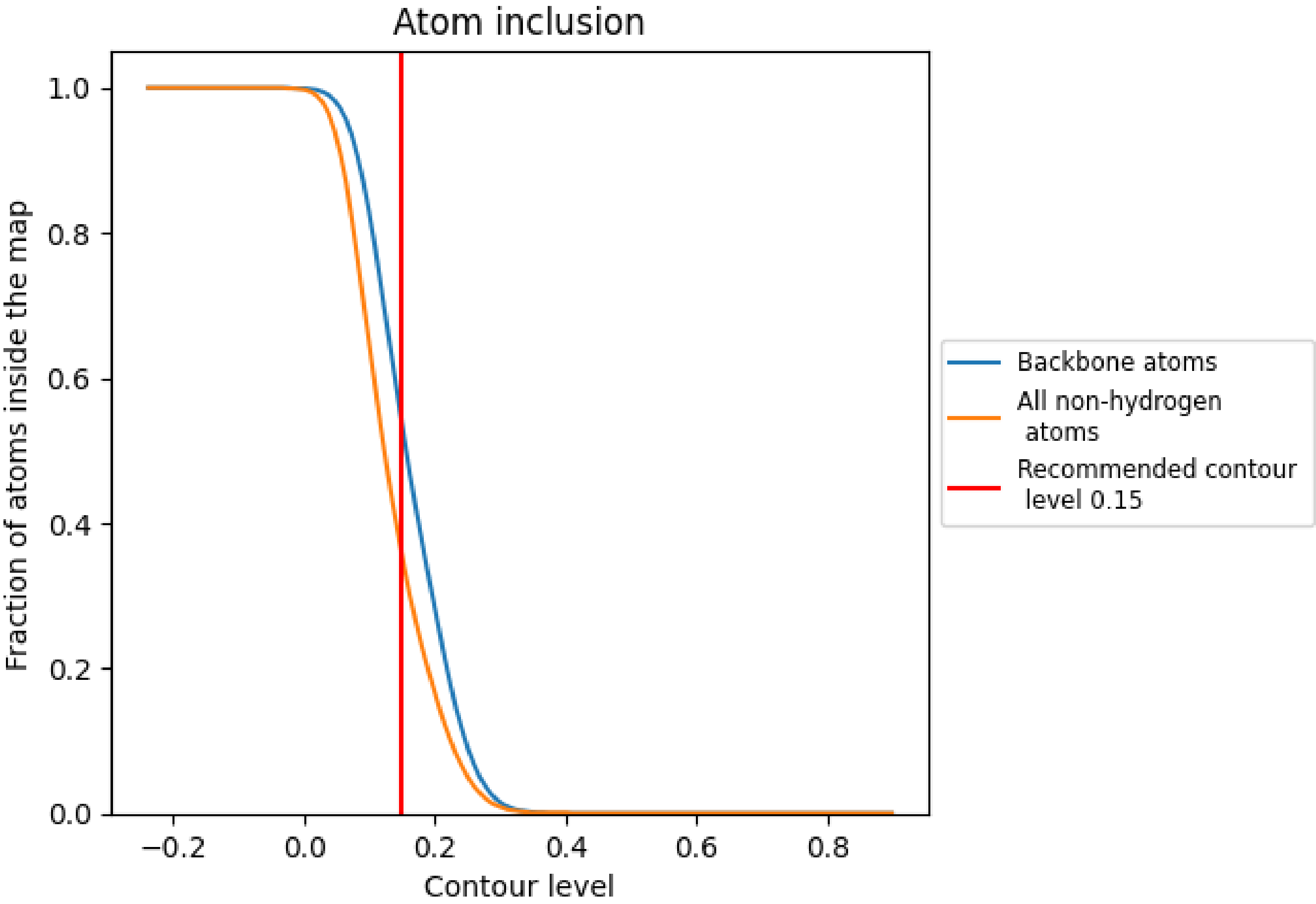
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



At the recommended contour level, 53% of all backbone atoms, 35% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.3540	0.3660
1A	0.3730	0.3490
1B	0.5570	0.4360
1C	0.5160	0.4470
1D	0.5310	0.4200
1E	0.2900	0.3700
1F	0.3130	0.3700
1G	0.5490	0.4250
1H	0.5340	0.4130
1I	0.6600	0.4360
1J	0.3670	0.3700
1K	0.4530	0.3930
1L	0.0860	0.2640
1M	0.3200	0.3550
1N	0.5210	0.4200
1O	0.2810	0.3560
1P	0.4190	0.4130
1Q	0.4350	0.4370
1R	0.4940	0.4280
1S	0.5020	0.3930
1T	0.2020	0.3220
1U	0.0020	0.2440
1V	0.4310	0.3990
1W	0.4090	0.3910
1X	0.4860	0.3970
1Y	0.2720	0.3290
1Z	0.5460	0.4150
1a	0.5650	0.4070
1b	0.4610	0.4110
1c	0.3420	0.3590
1d	0.4500	0.4020
1e	0.5160	0.4190
1f	0.2370	0.3460
1g	0.1060	0.3090
1h	0.2390	0.3490

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Chain	Atom inclusion	Q-score
1i	0.0060	0.2390
1j	0.0020	0.2440
1k	0.0020	0.1830
1l	0.0560	0.2550
1m	0.1060	0.2740
1n	0.0210	0.2250
1o	0.0040	0.2250
1p	0.0360	0.2900
1q	0.5810	0.4250
1r	0.5630	0.4430
1s	0.1560	0.3570