Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 10:59 AM EDT

PDB ID	:	8UES
EMDB ID	:	EMD-42169
Title	:	In-situ complex I, Deactive class01
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-10-02
Resolution	:	3.60 Å(reported)

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

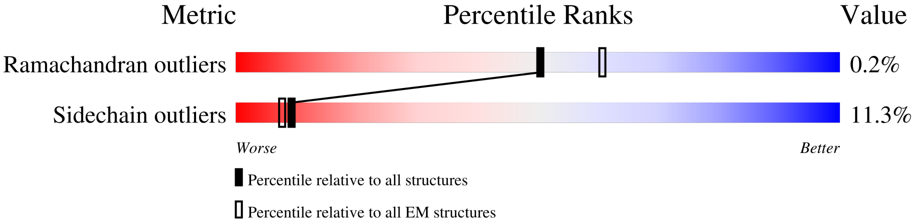
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

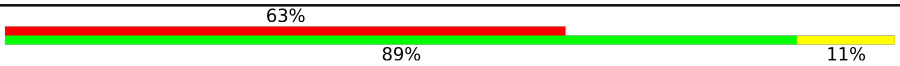
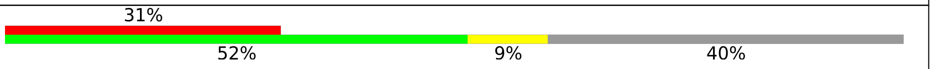
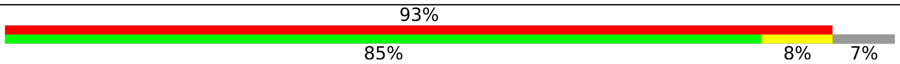
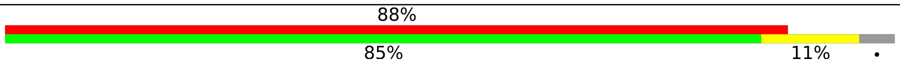
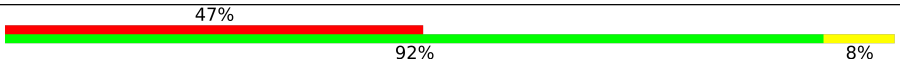
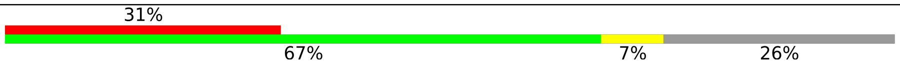
The reported resolution of this entry is 3.60 Å.

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	 63% 89% 11%
2	1B	258	 31% 52% 9% 40%
3	1C	264	 70% 73% 6% 21%
4	1D	476	 57% 82% 8% 10%
5	1E	249	 86% 75% 11% 14%
6	1F	464	 93% 85% 8% 7%
7	1G	727	 88% 85% 11% •
8	1H	318	 47% 92% 8%
9	1I	239	 31% 67% 7% 26%

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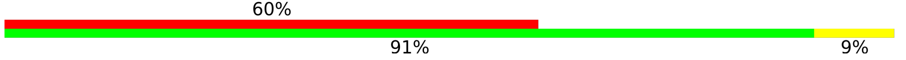
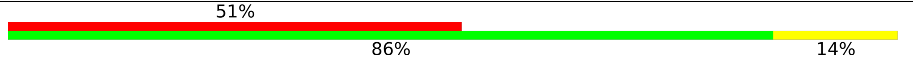
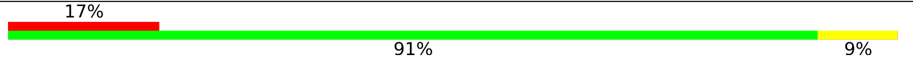
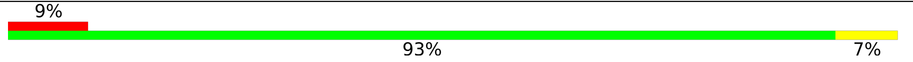
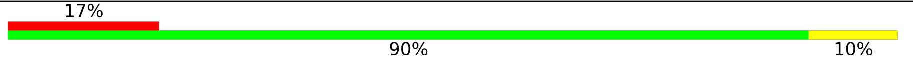
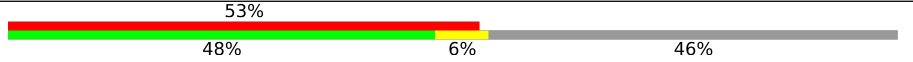
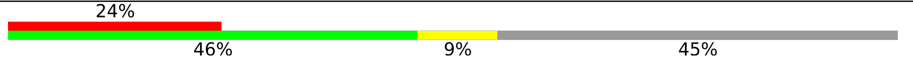
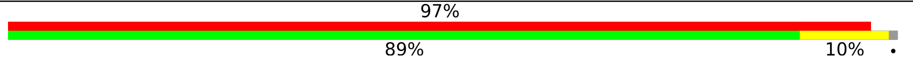
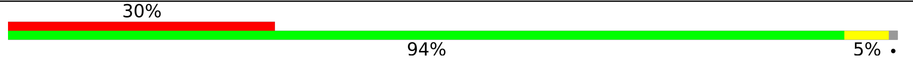
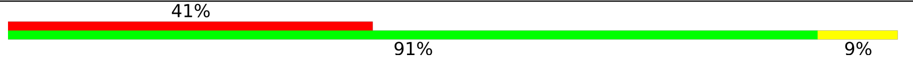
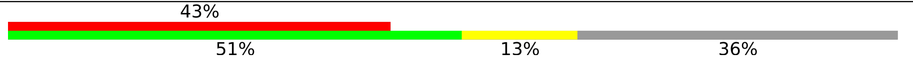
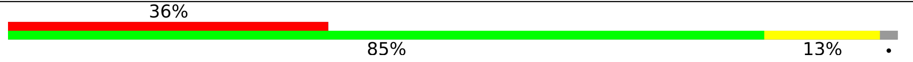
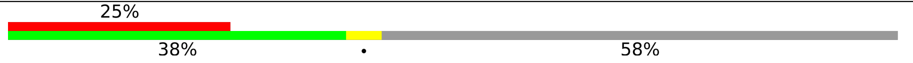
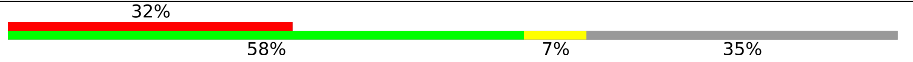
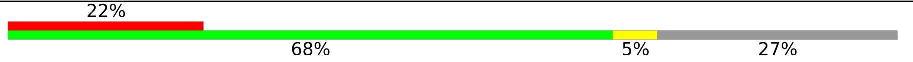
Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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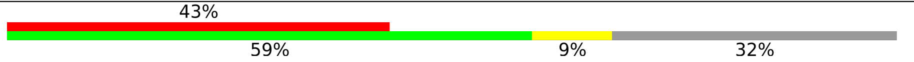
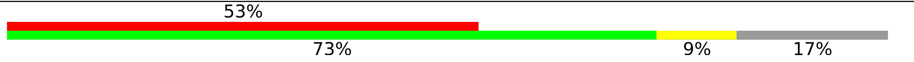
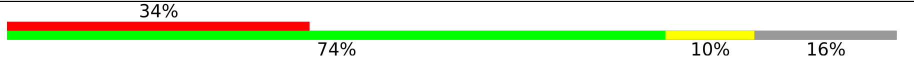
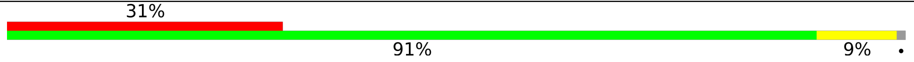
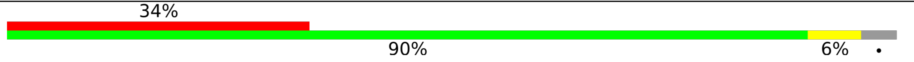
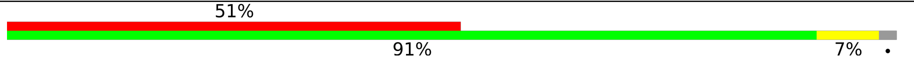
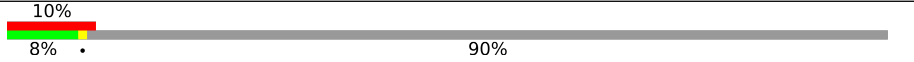
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67472 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
			Total	C	N	O	S		
5	1E	214	1658	1058	278	312	10	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

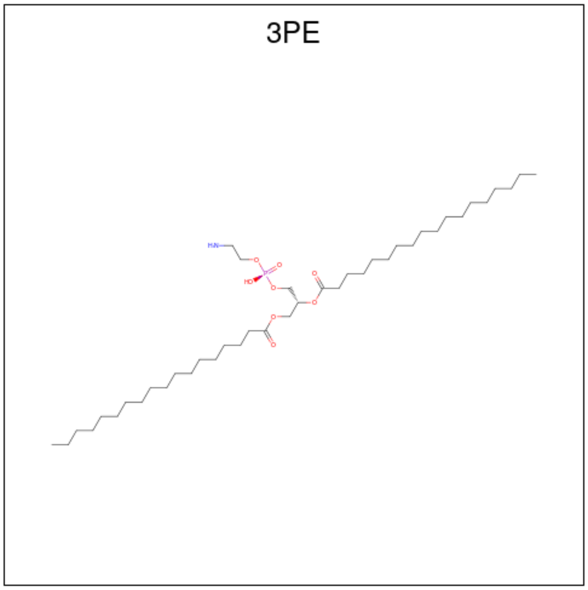
There is a discrepancy between the modelled and reference sequences:

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

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

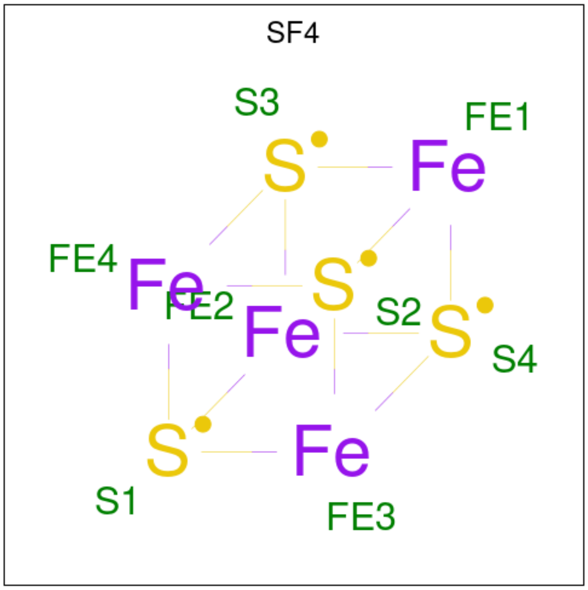
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total 382	C 238	N 70	O 73	S 1	0	0

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



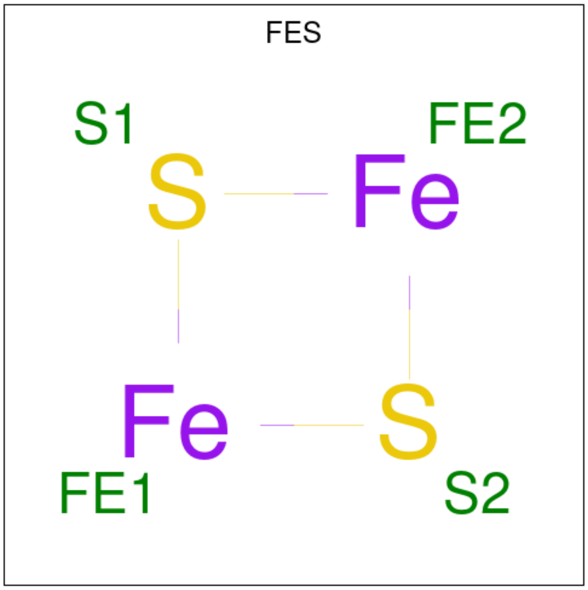
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total 47	C 37	N 1	O 8	P 1	0
45	1L	1	Total 46	C 36	N 1	O 8	P 1	0
45	1L	1	Total 42	C 32	N 1	O 8	P 1	0
45	1N	1	Total 51	C 41	N 1	O 8	P 1	0
45	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
45	1Y	1	Total 51	C 41	N 1	O 8	P 1	0

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



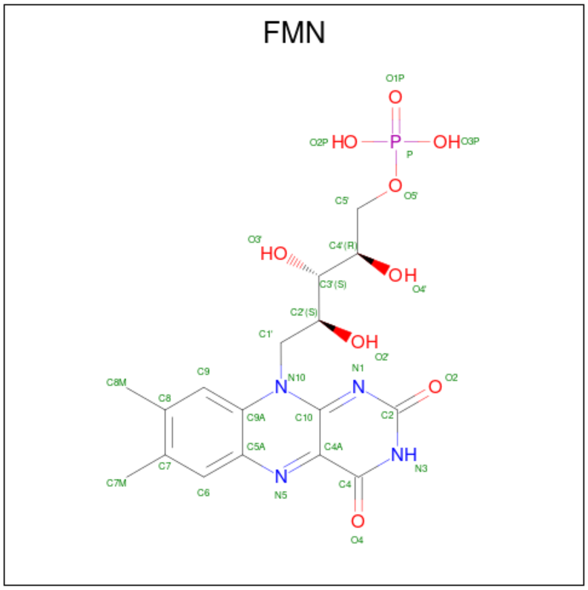
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total Fe S 8 4 4	0
46	1F	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0

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



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

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

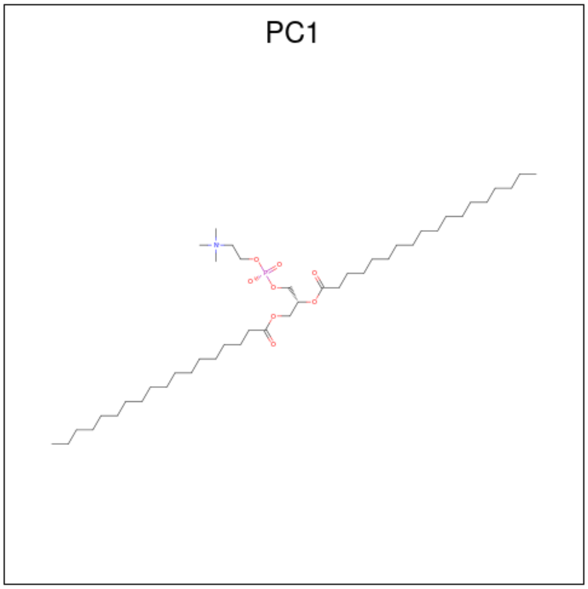


Mol	Chain	Residues	Atoms	AltConf
48	1F	1	Total C N O P 31 17 4 9 1	0

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

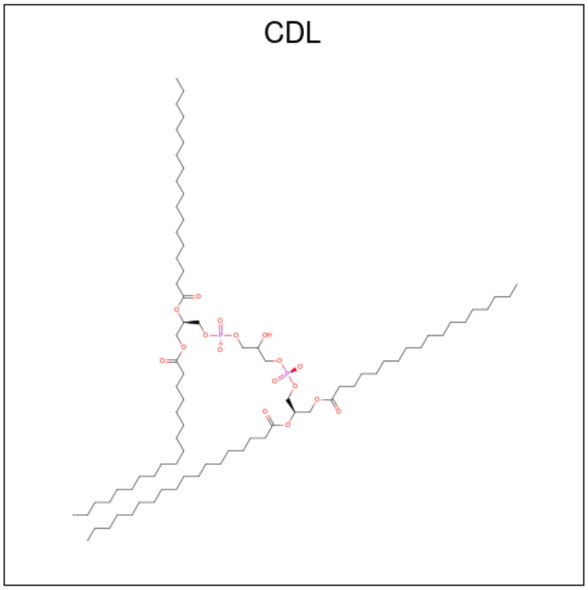
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total 1	K 1	0

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



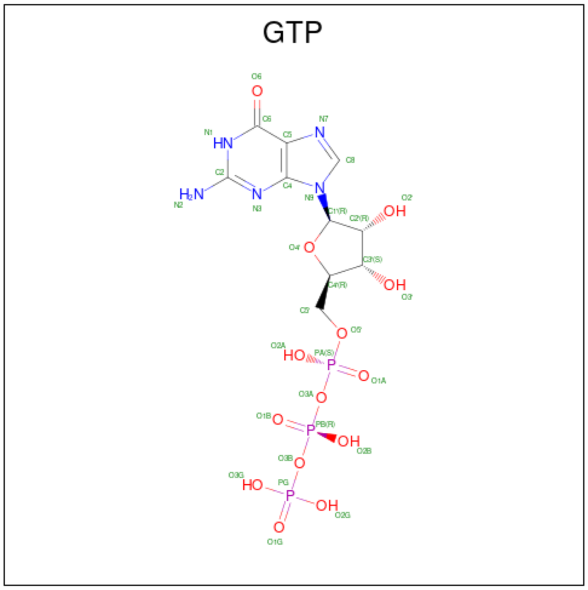
Mol	Chain	Residues	Atoms					AltConf
50	1I	1	Total 54	C 44	N 1	O 8	P 1	0
50	1I	1	Total 44	C 34	N 1	O 8	P 1	0
50	1J	1	Total 35	C 25	N 1	O 8	P 1	0
50	1L	1	Total 44	C 34	N 1	O 8	P 1	0
50	1f	1	Total 46	C 36	N 1	O 8	P 1	0

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



Mol	Chain	Residues	Atoms	AltConf
51	1N	1	Total C O P 77 58 17 2	0
51	1q	1	Total C O P 61 42 17 2	0

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

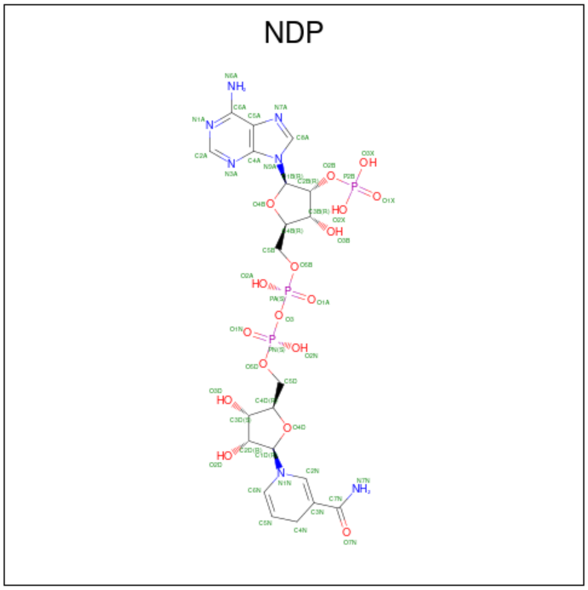


Mol	Chain	Residues	Atoms	AltConf
52	1O	1	Total C N O P 32 10 5 14 3	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	1O	1	1	1	0

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

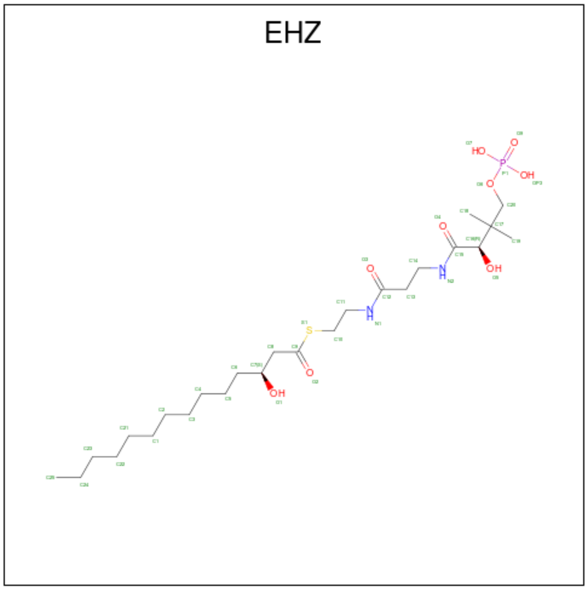


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	1P	1	48	21	7	17	3	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

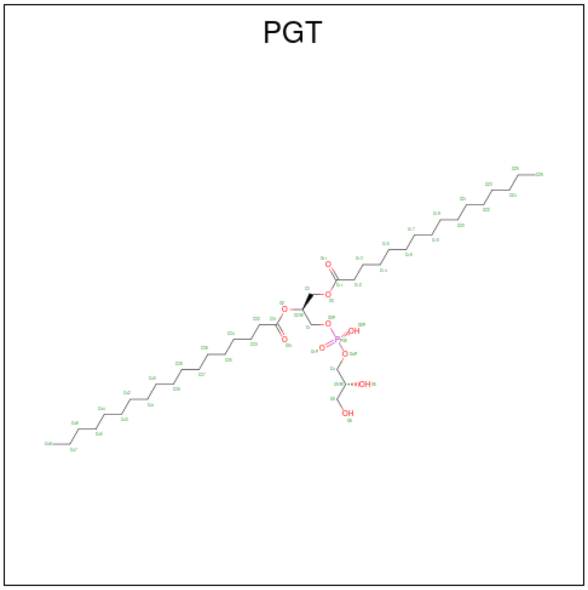
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	1R	1	1	1	0

- Molecule 56 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: $C_{25}H_{49}N_2O_9PS$).



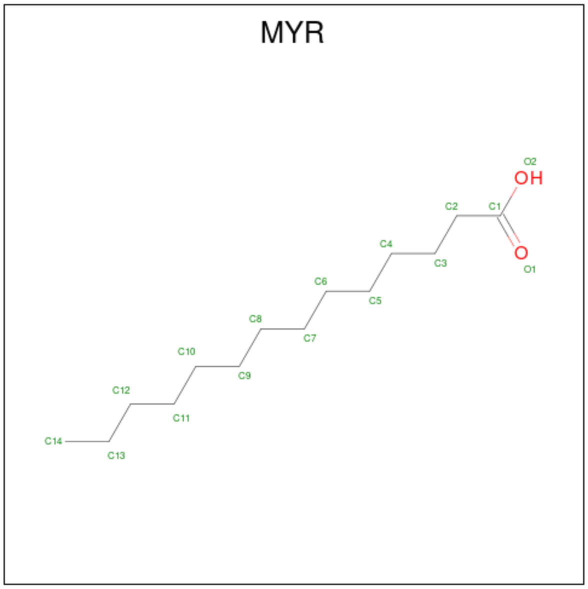
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
56	1W	1	37	25	2	8	1	1	0
56	1n	1	37	25	2	8	1	1	0

- Molecule 57 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
57	1Y	1	51	40	10	1	0

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

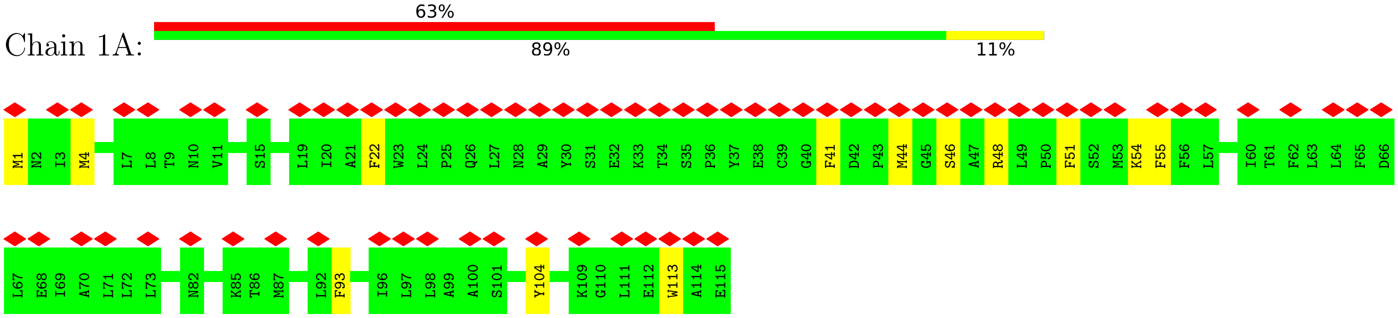


Mol	Chain	Residues	Atoms	AltConf
58	1l	1	Total C O 15 14 1	0

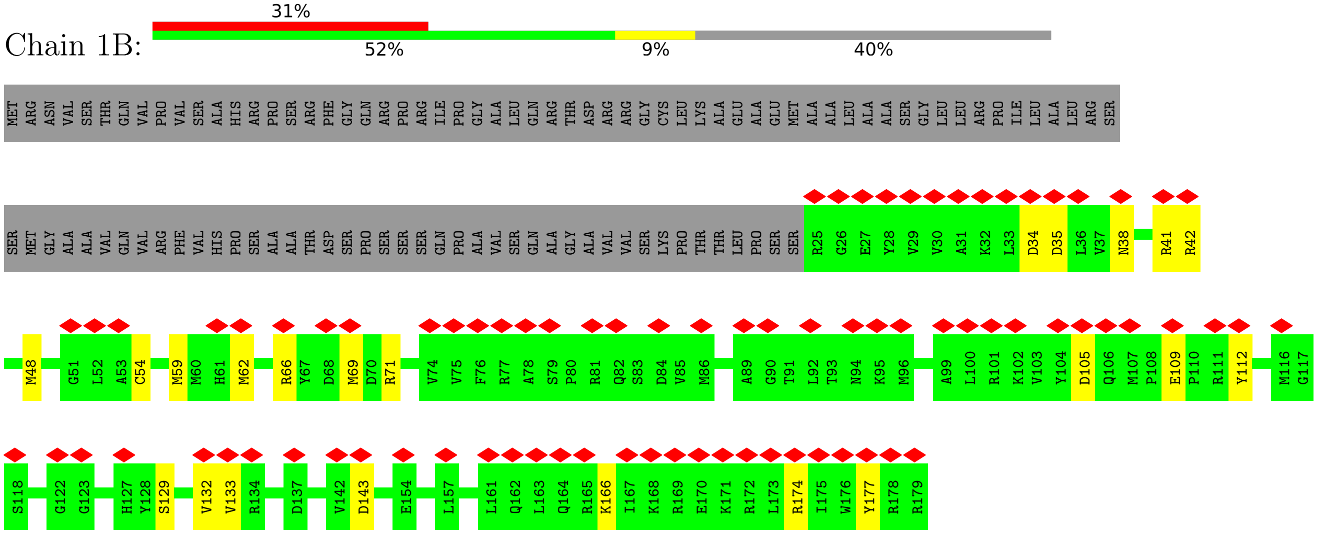
3 Residue-property plots ⓘ

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.

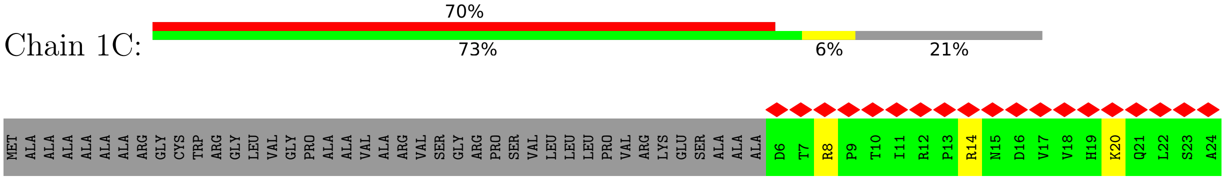
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

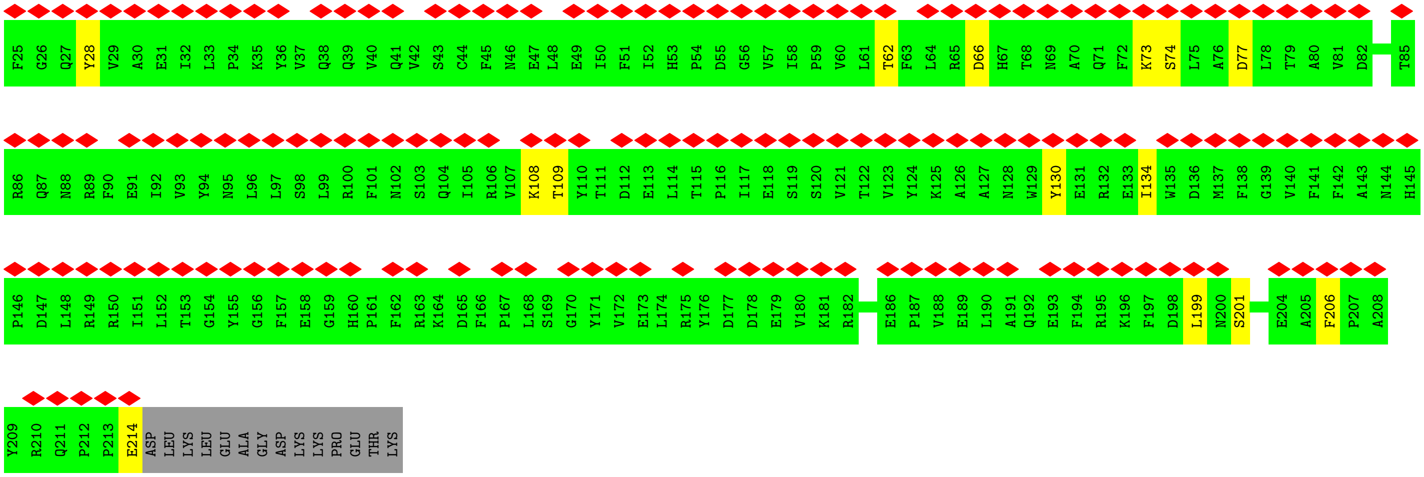


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



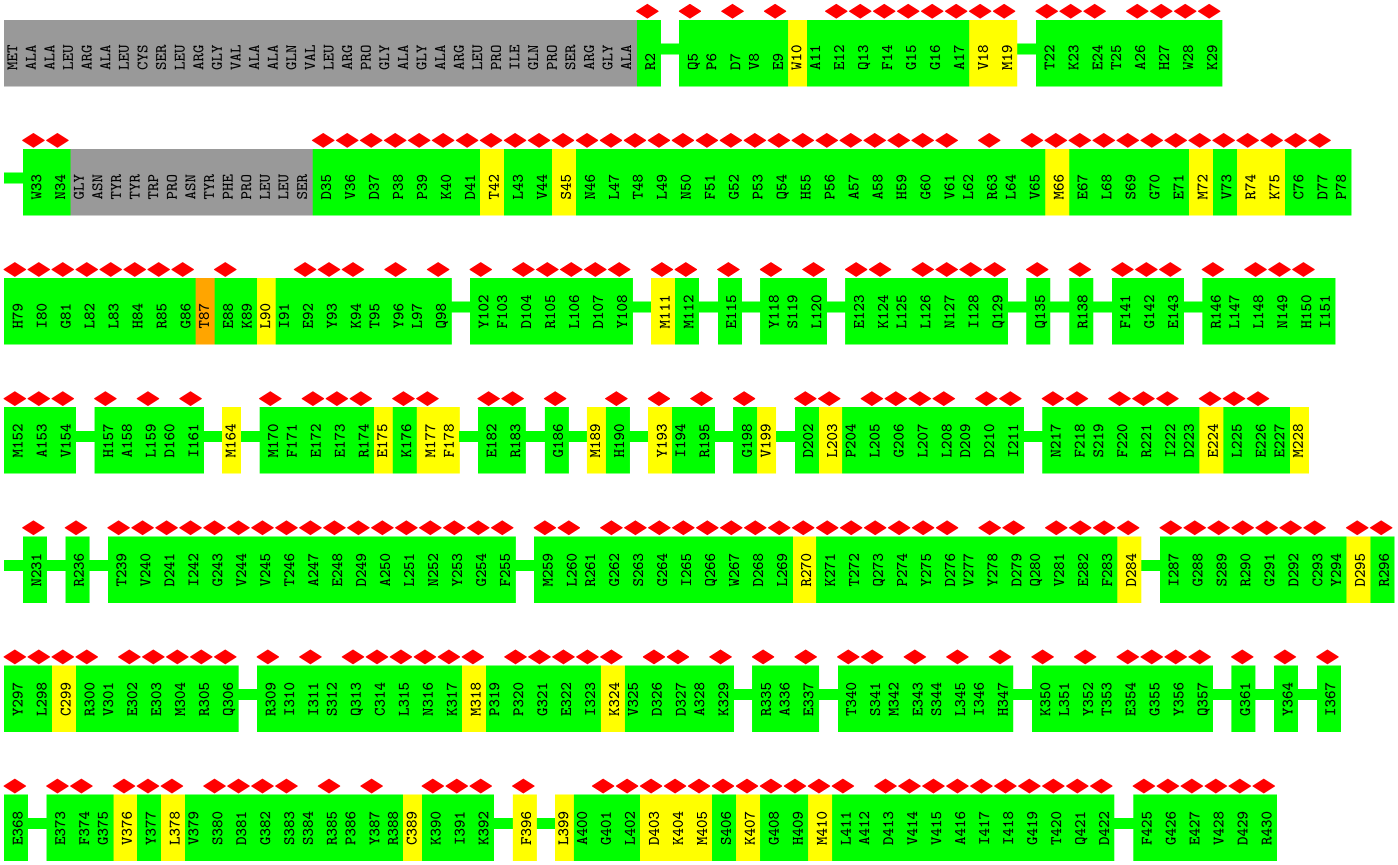
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





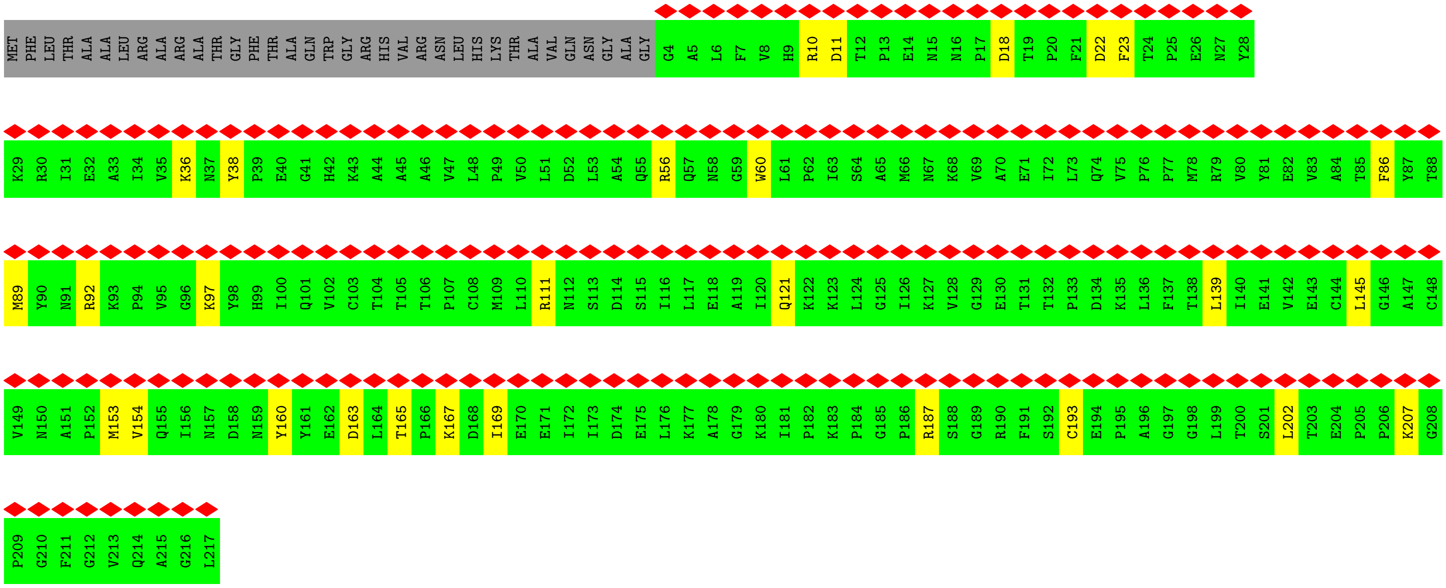
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:



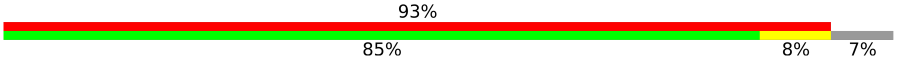
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

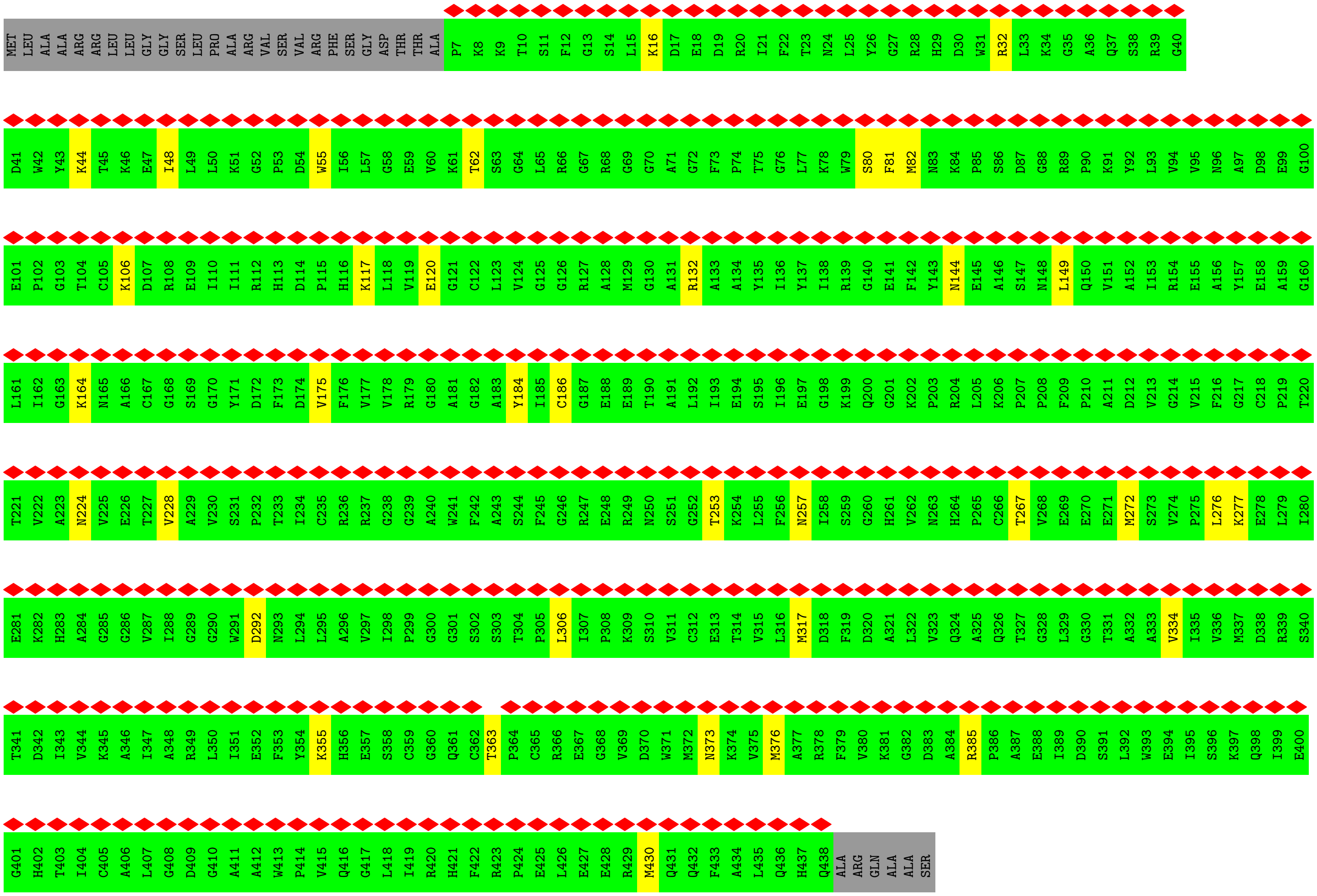
Chain 1E:



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

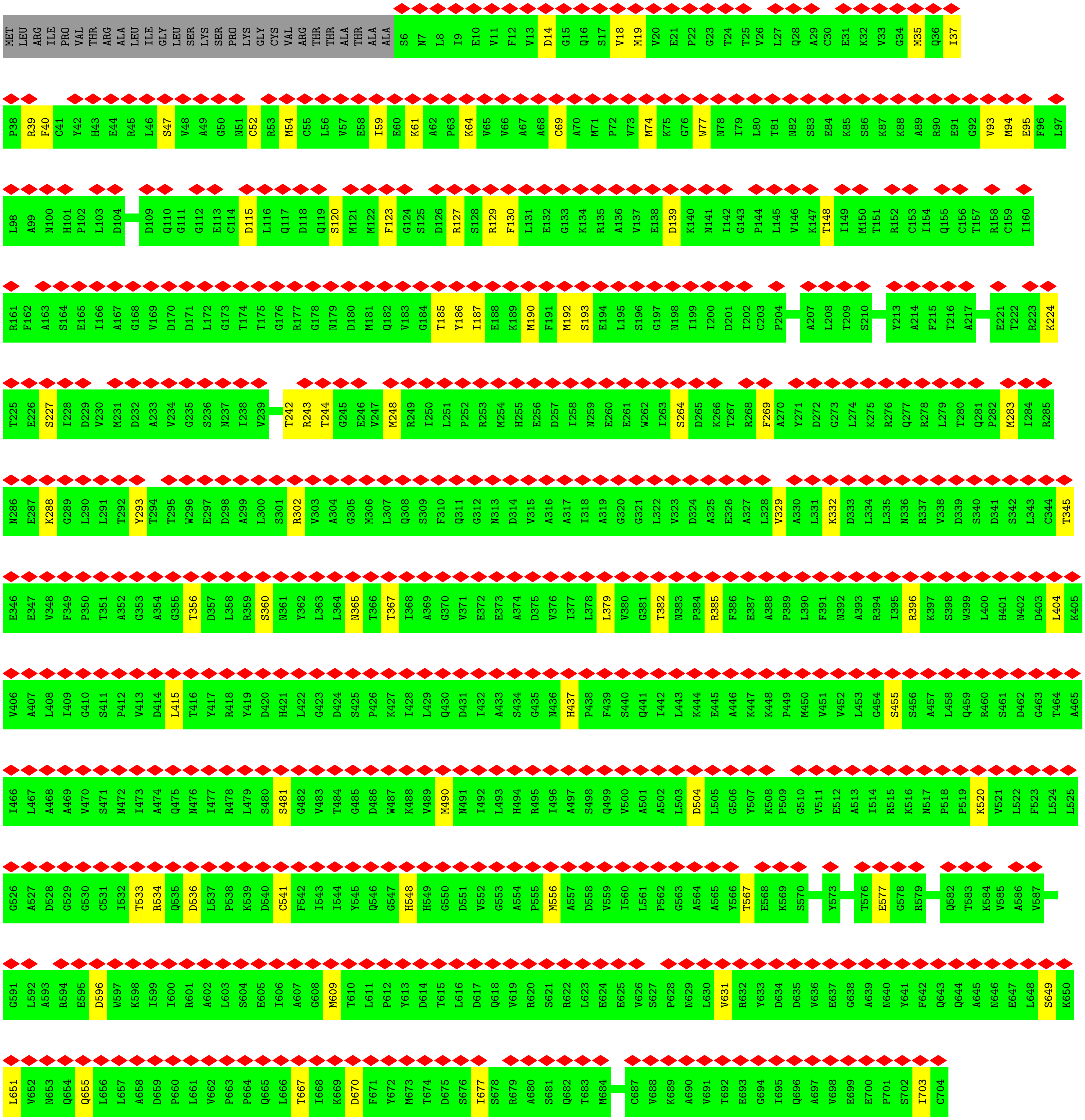
Chain 1F:





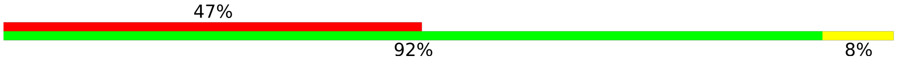
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

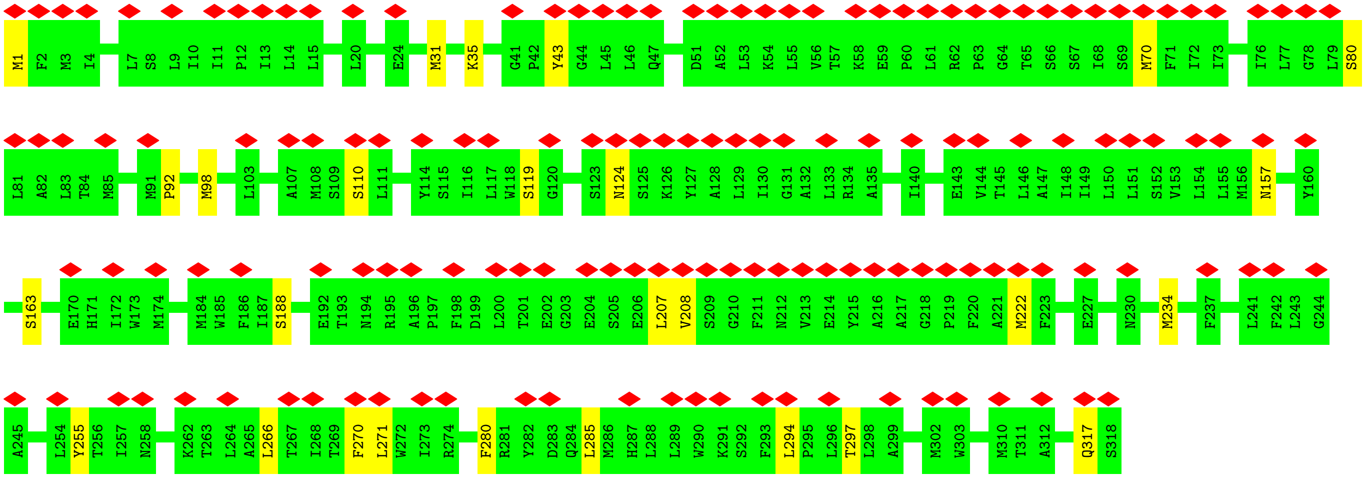
Chain 1G:



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

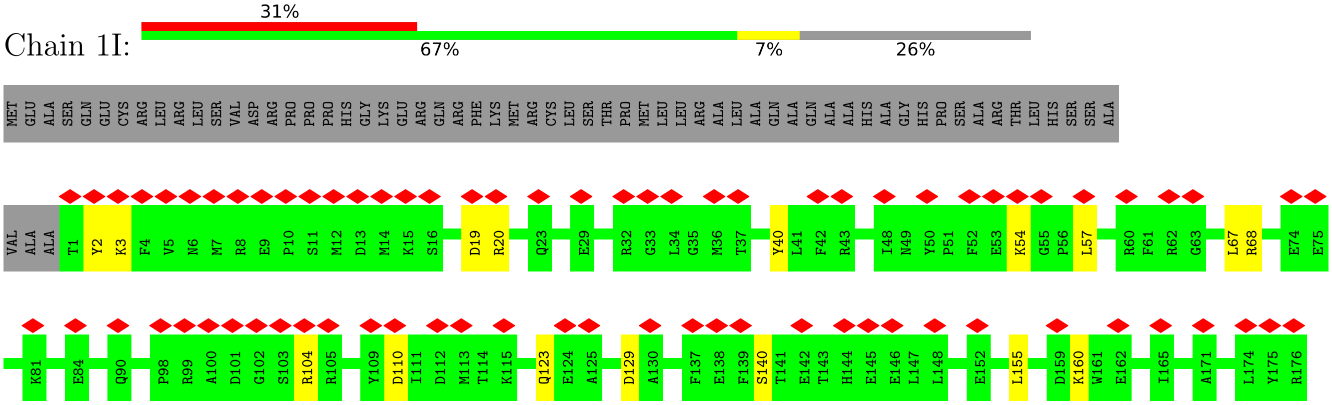
Chain 1H:





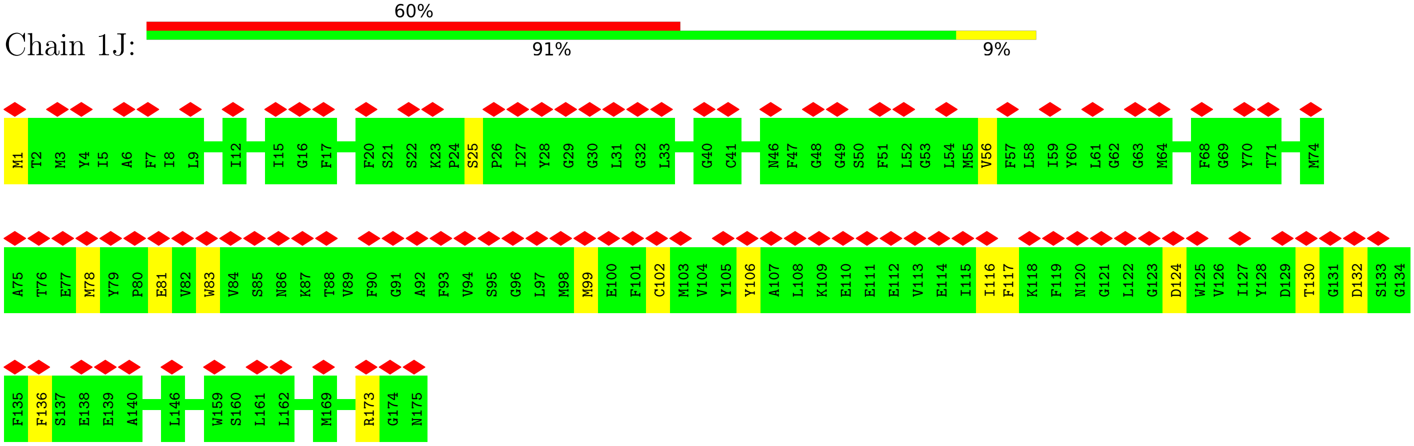
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:



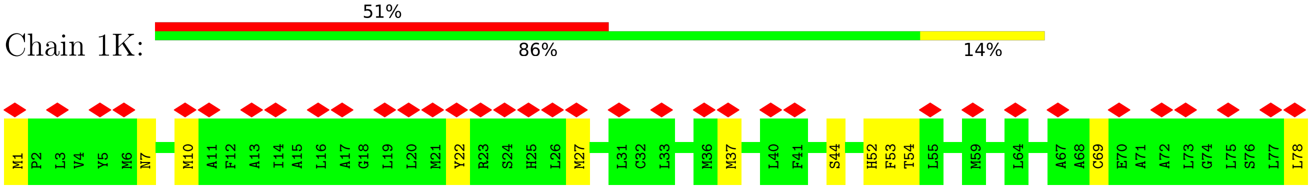
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

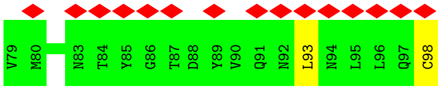
Chain 1J:



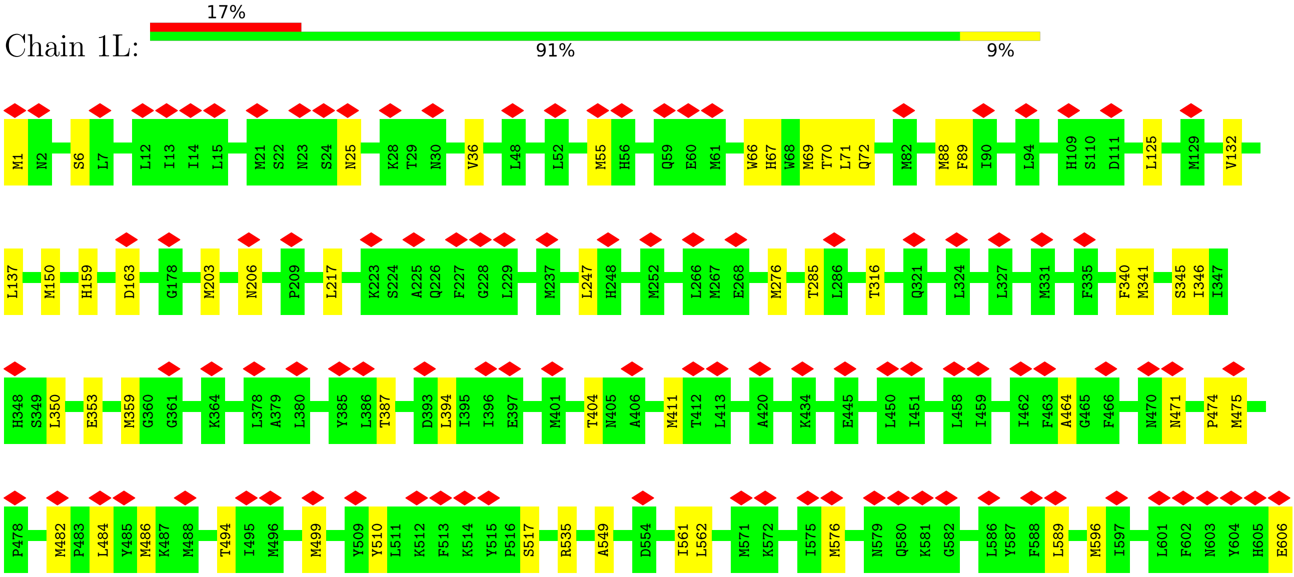
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:

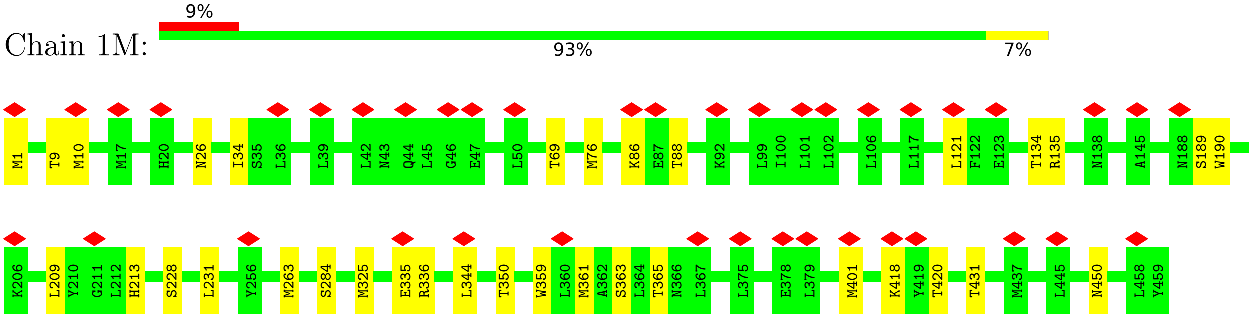




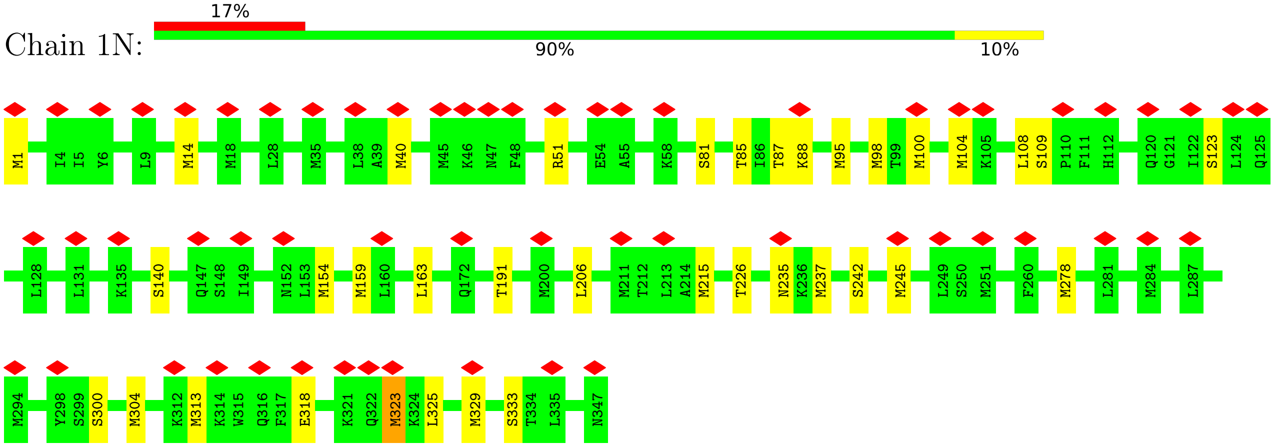
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

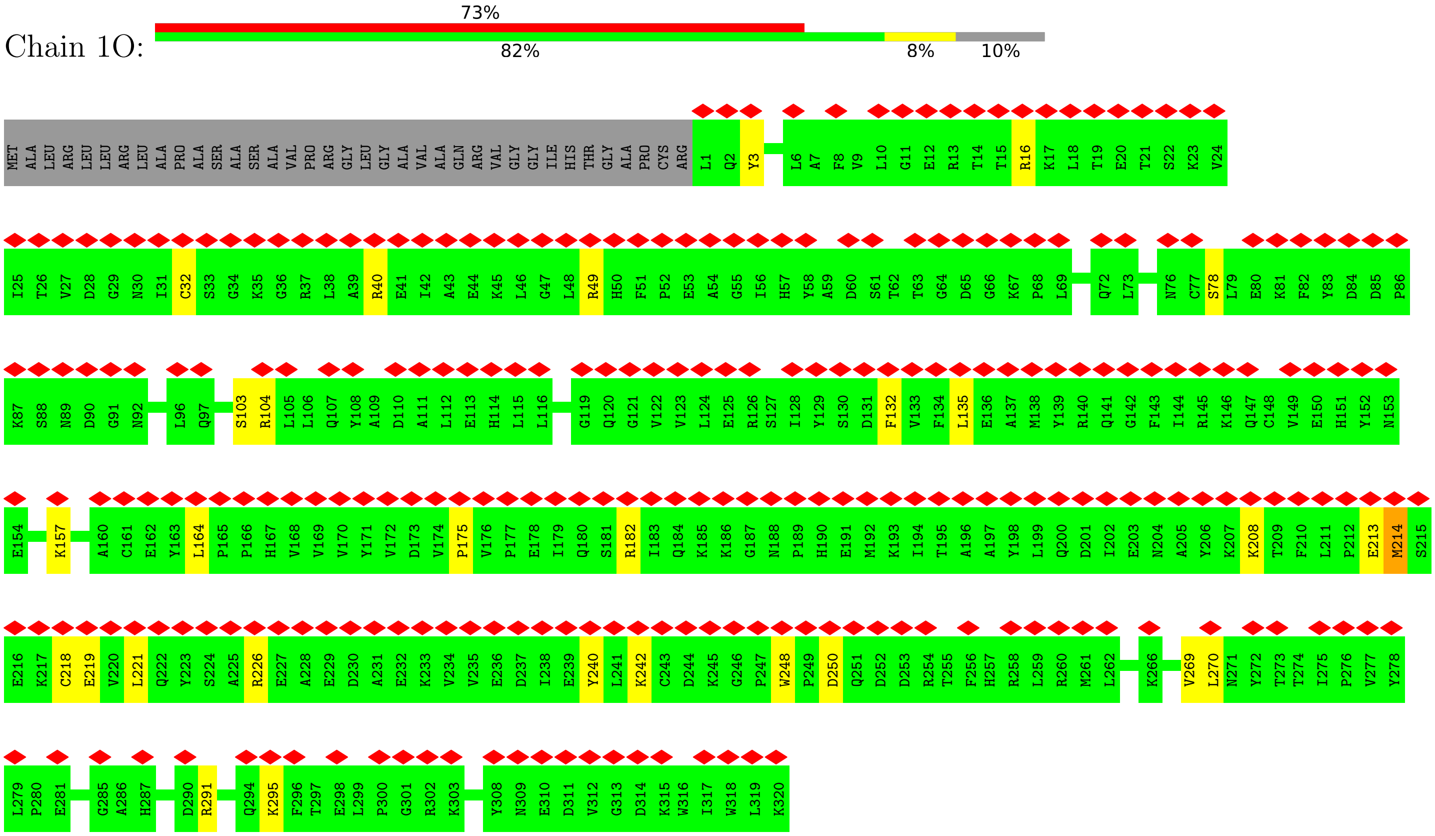


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



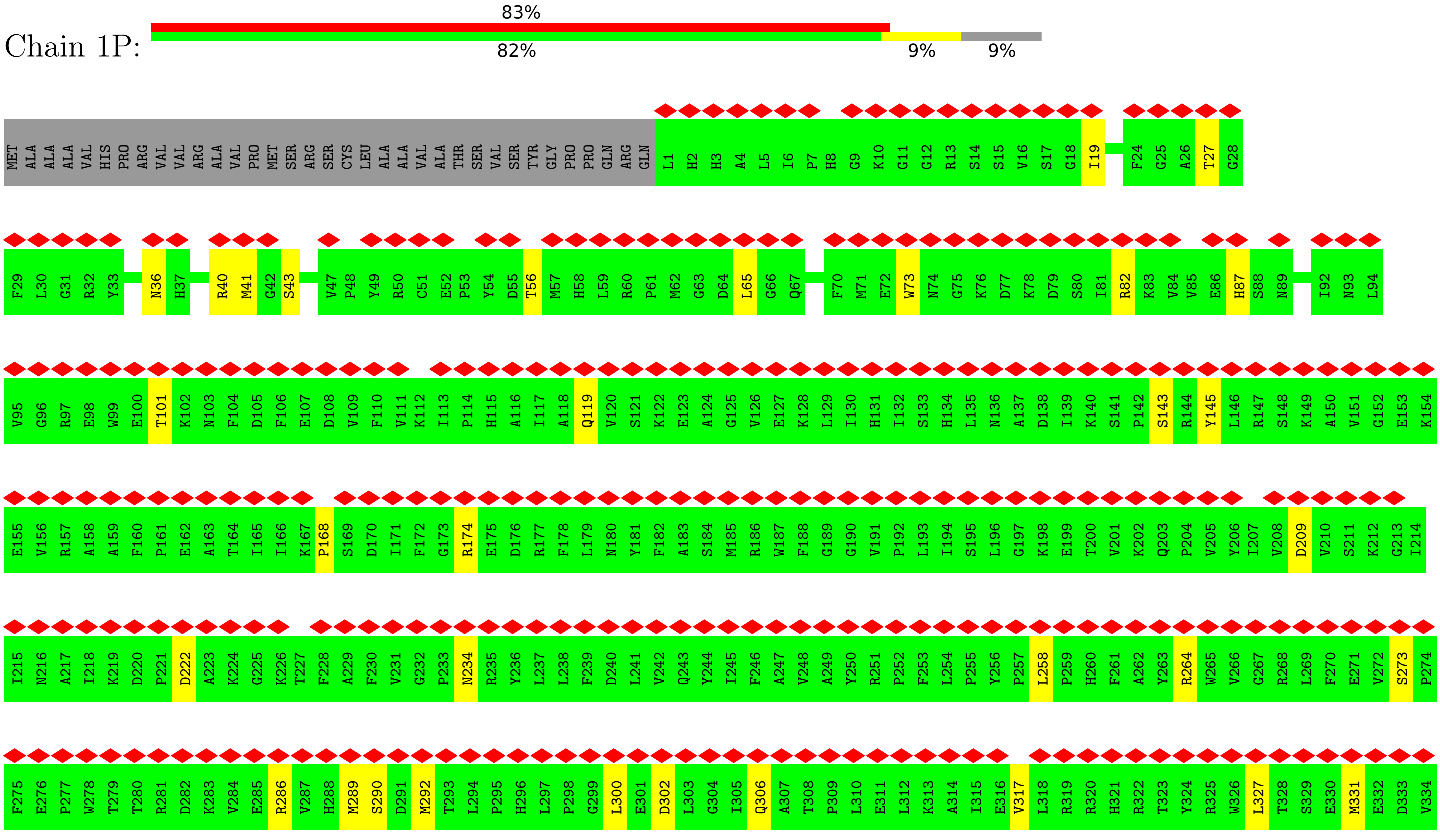
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

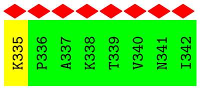
Chain 1O:



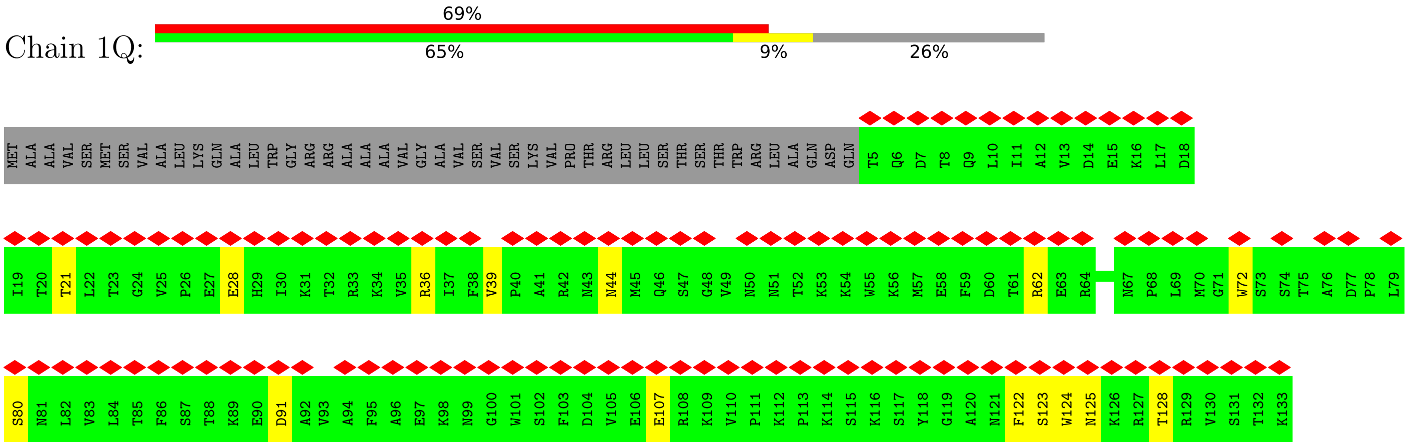
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:

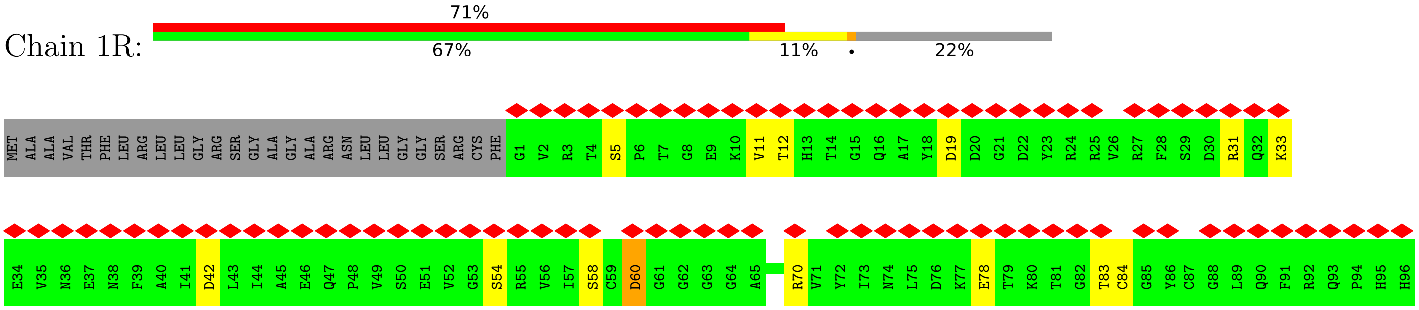




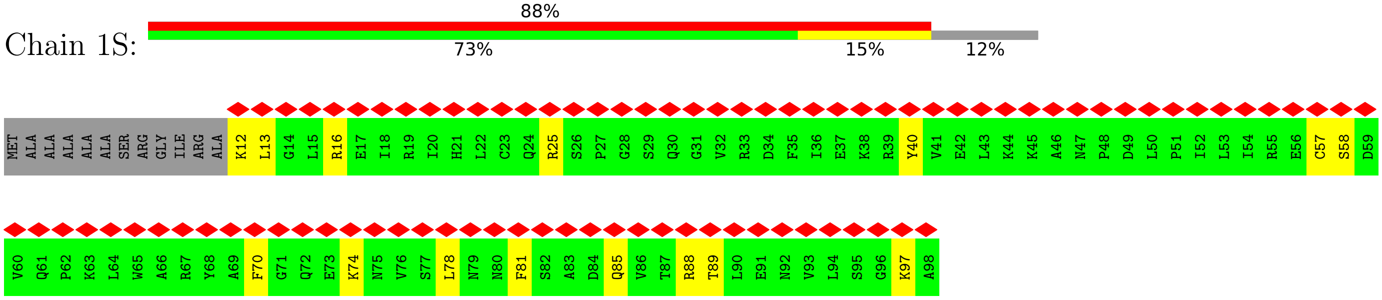
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



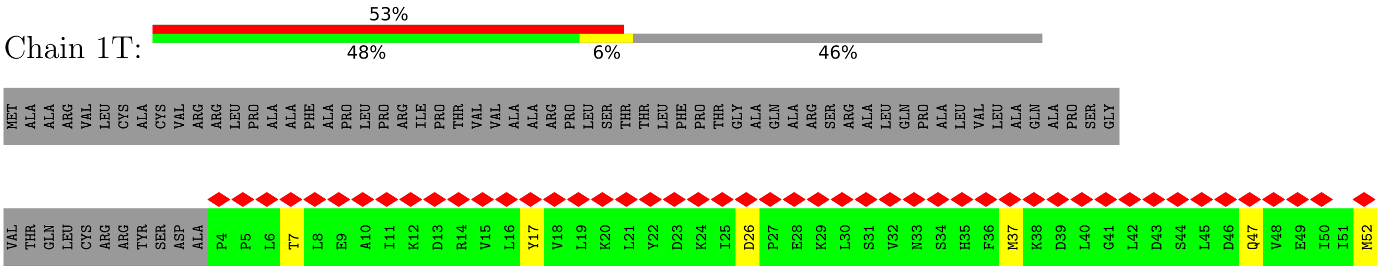
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

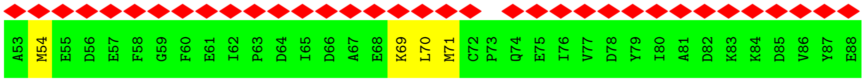


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

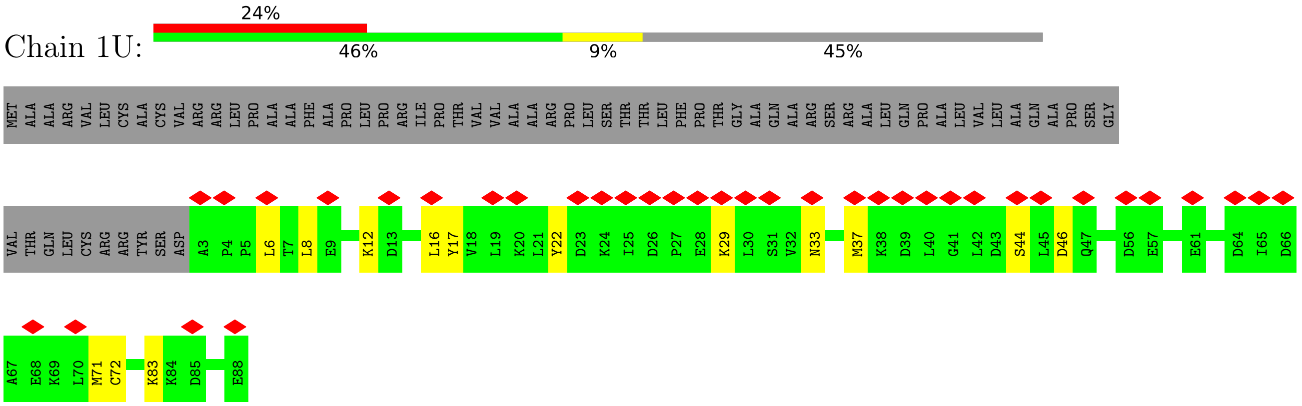


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

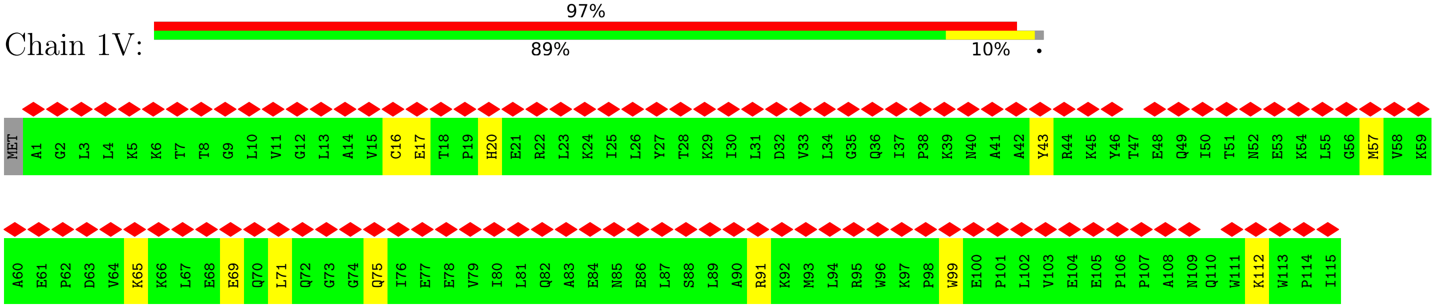




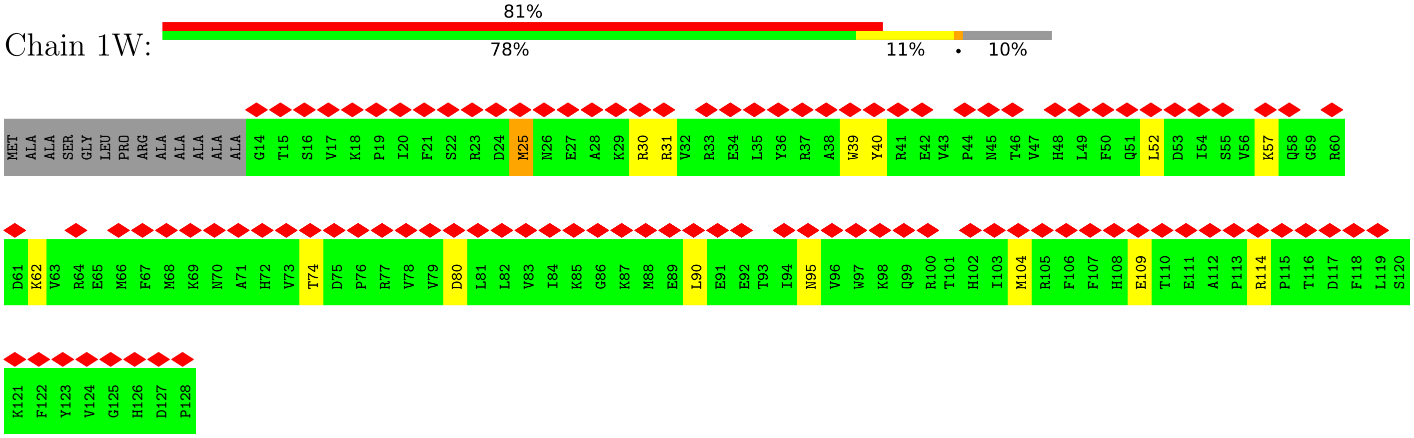
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



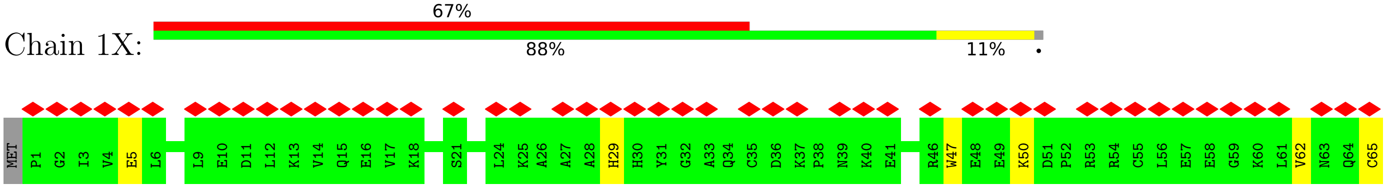
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

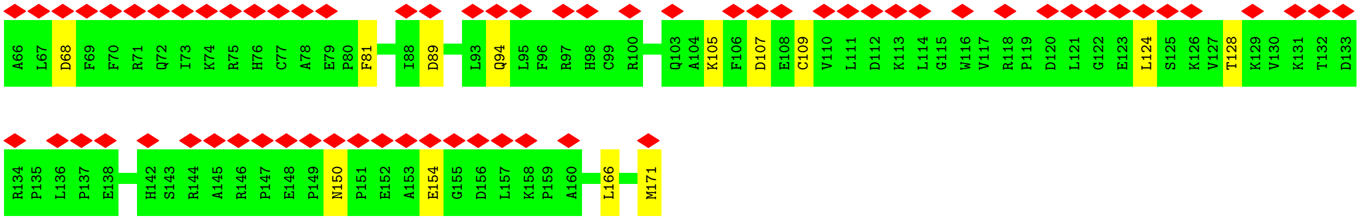


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



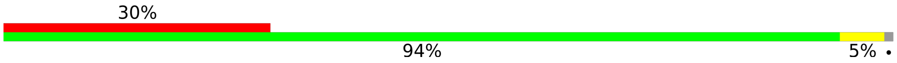
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

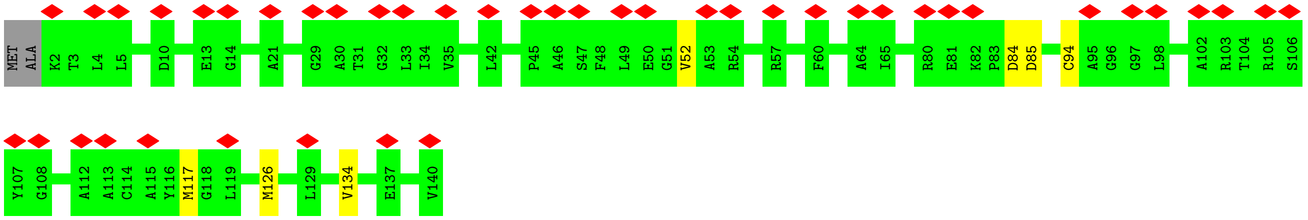




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

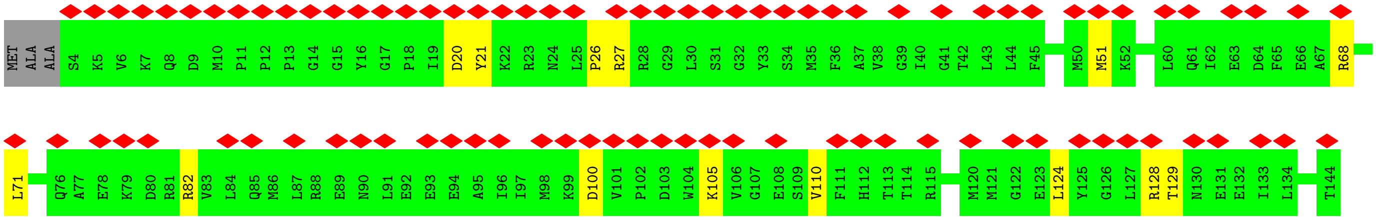
Chain 1Y:





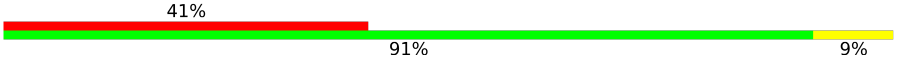
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

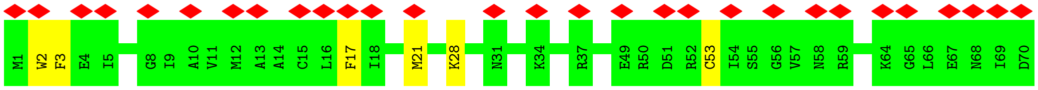
Chain 1Z:



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

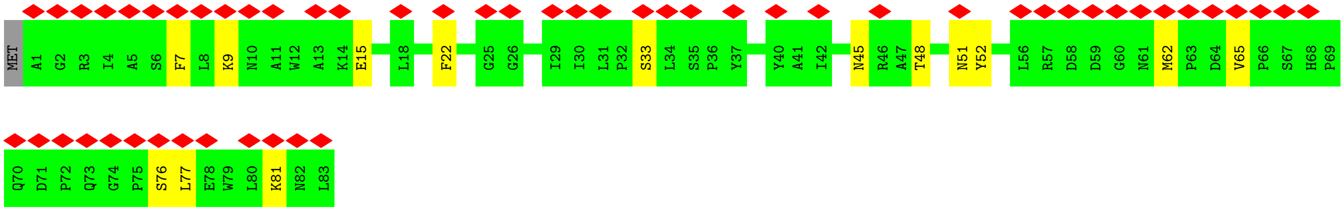
Chain 1a:





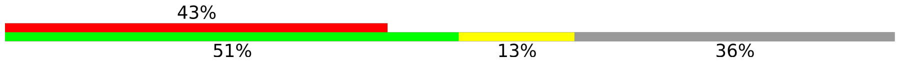
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

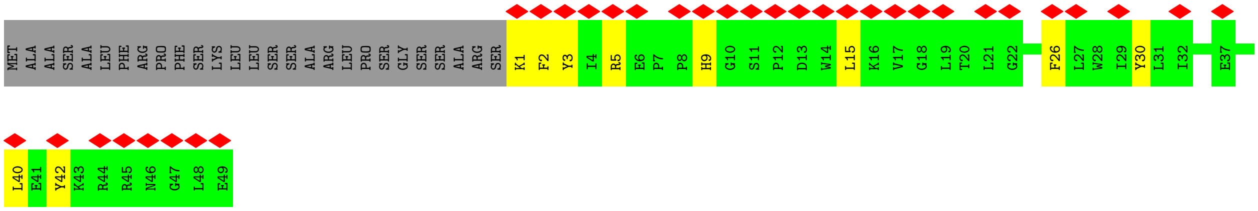
Chain 1b:



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

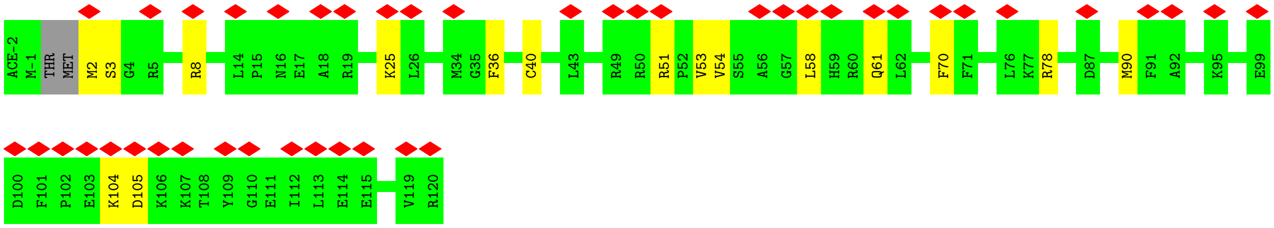
Chain 1c:





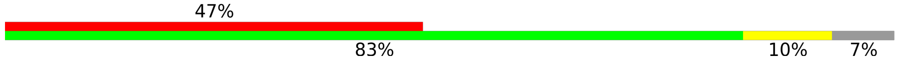
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

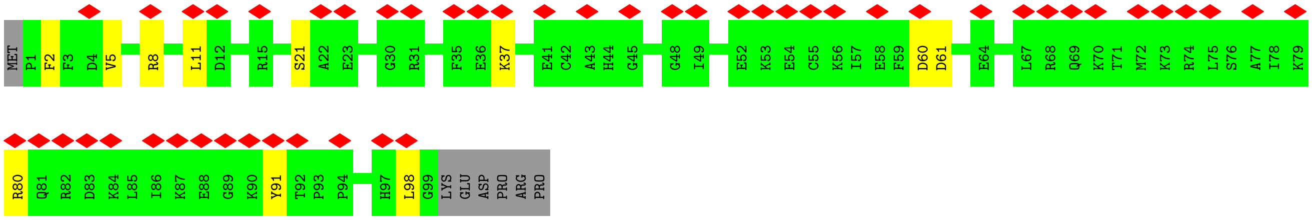
Chain 1d:



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

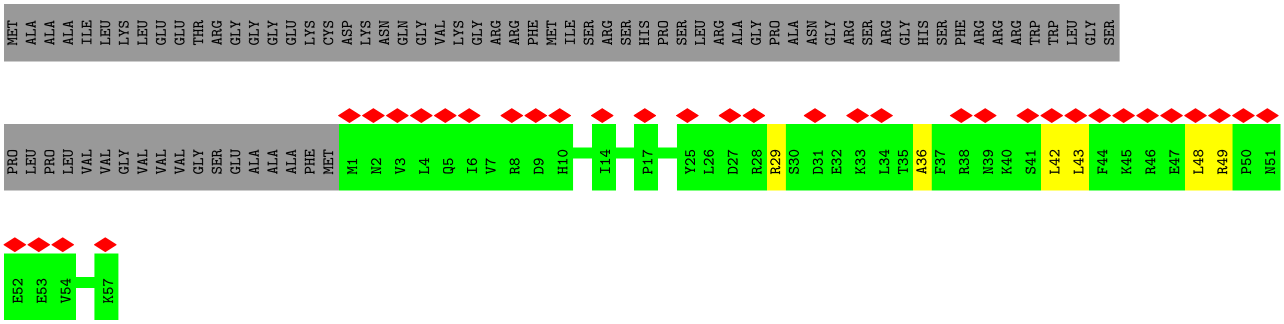
Chain 1e:





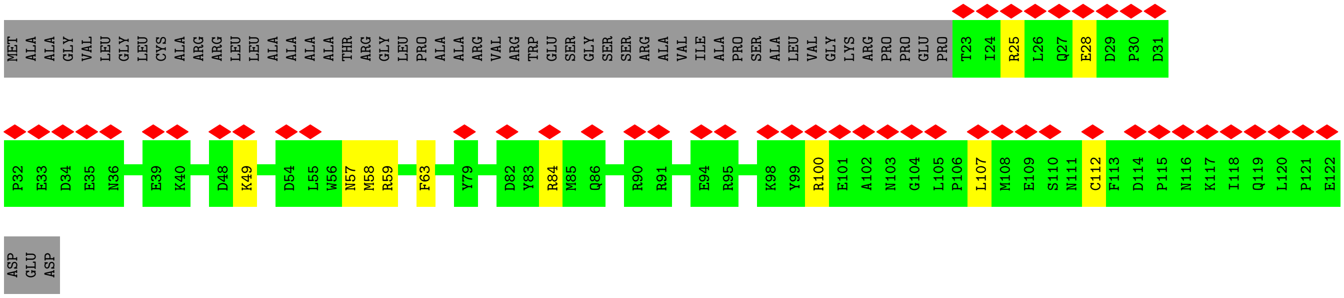
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f:



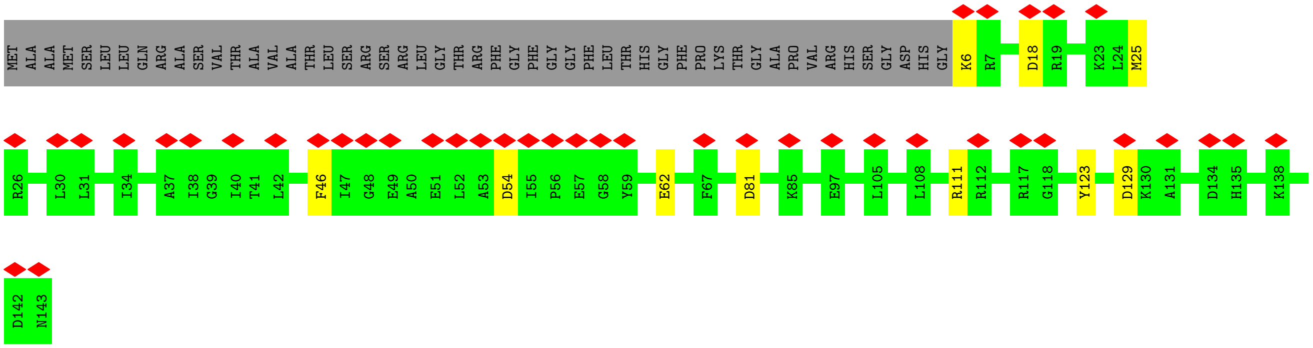
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



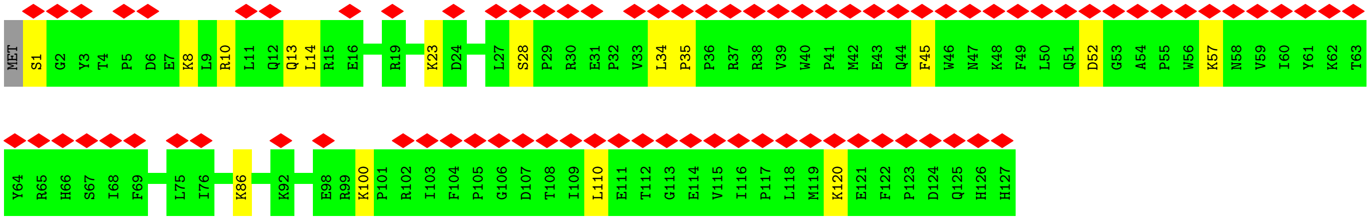
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



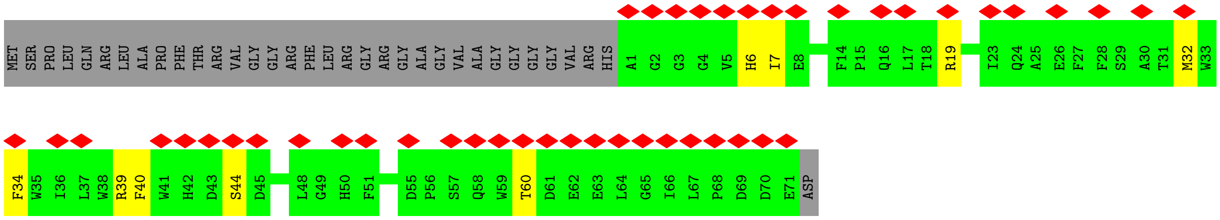
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



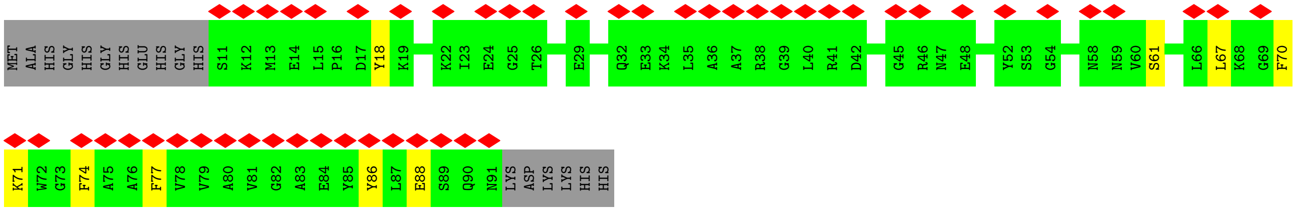
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



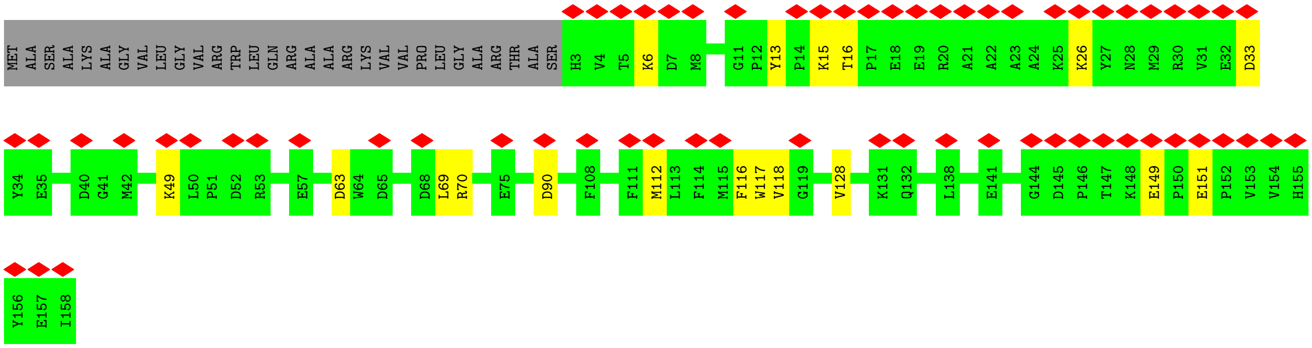
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



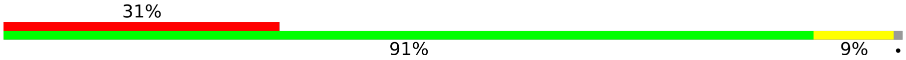
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

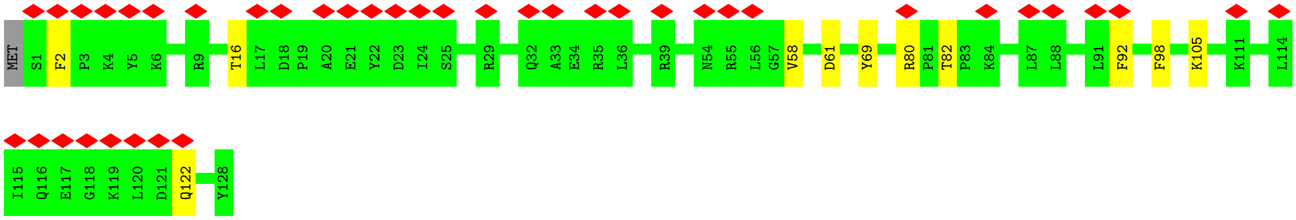
Chain 1l:



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

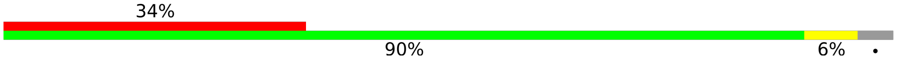
Chain 1m:

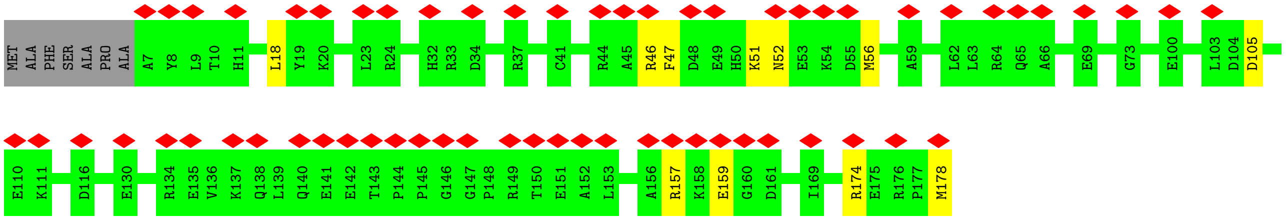




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

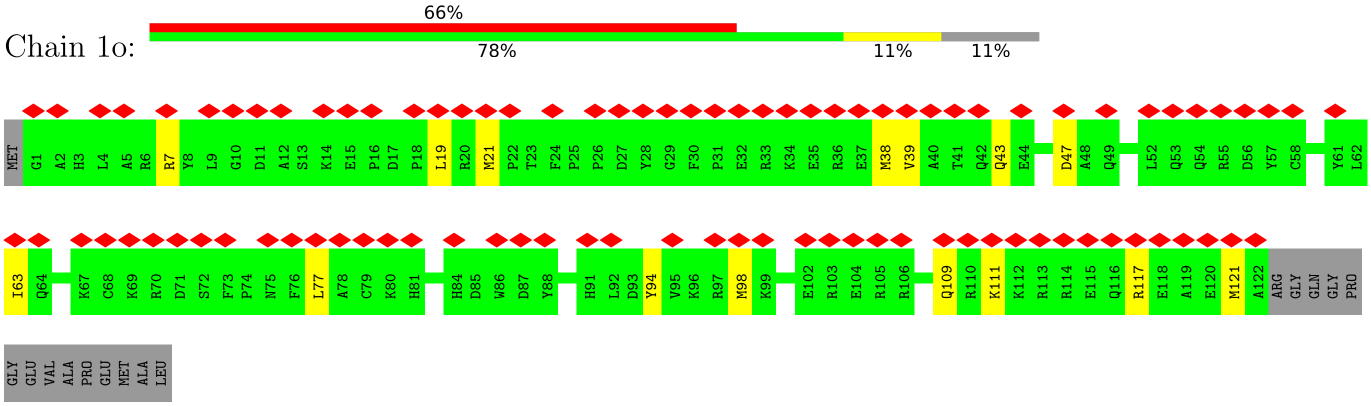
Chain 1n:





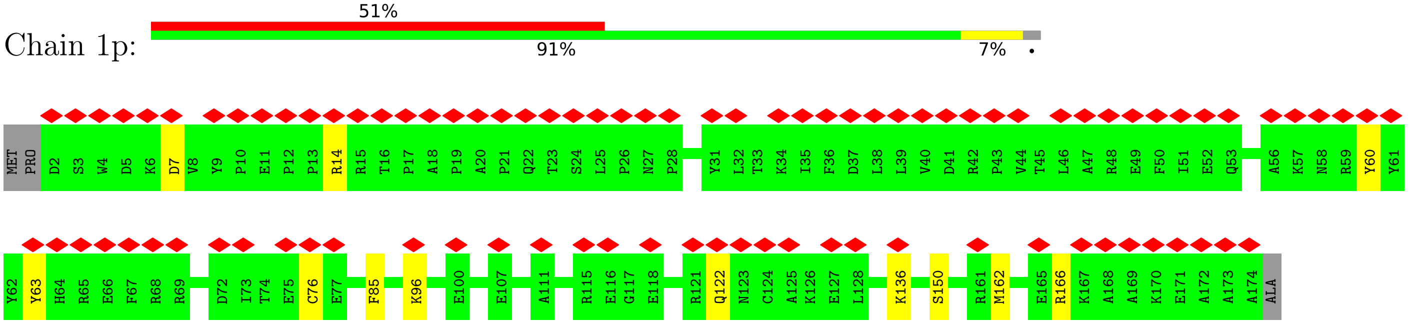
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:



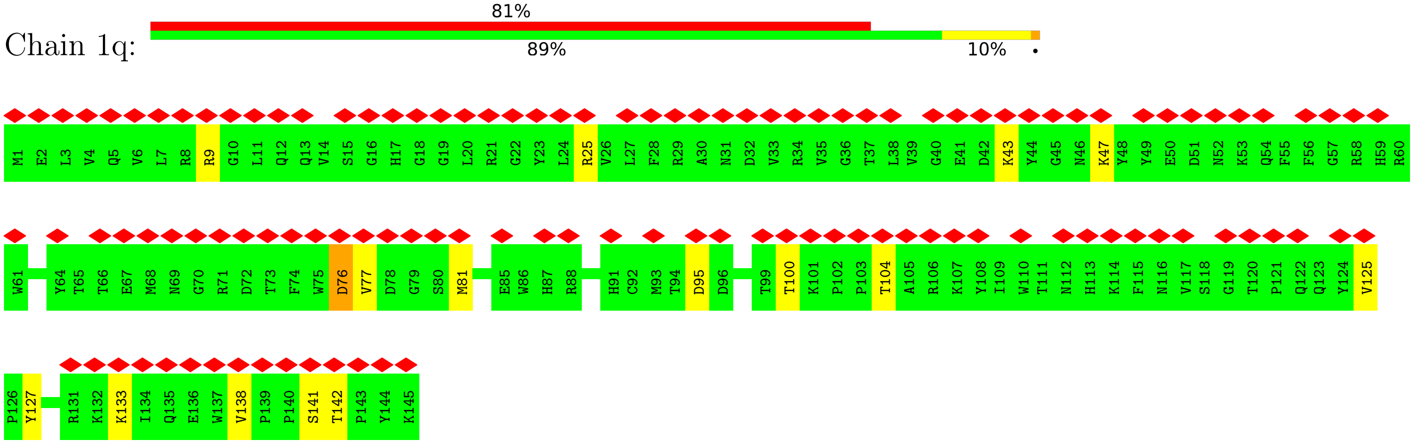
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p:



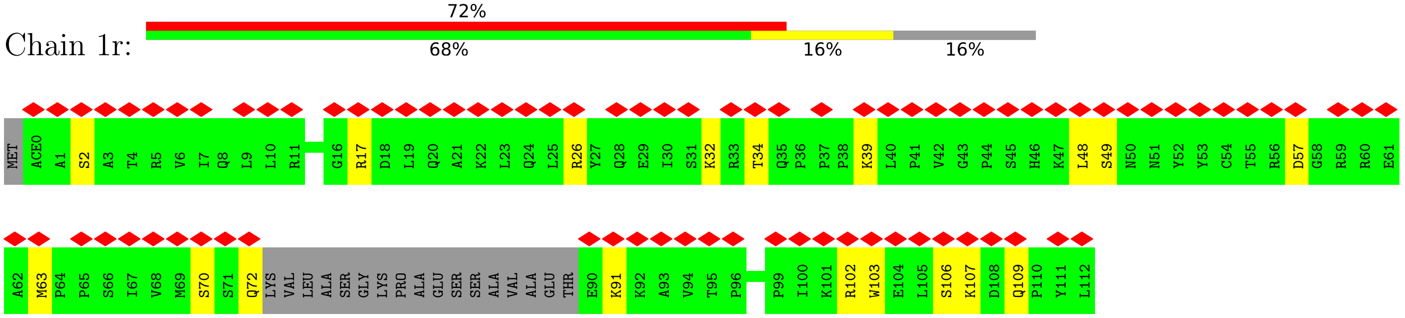
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:

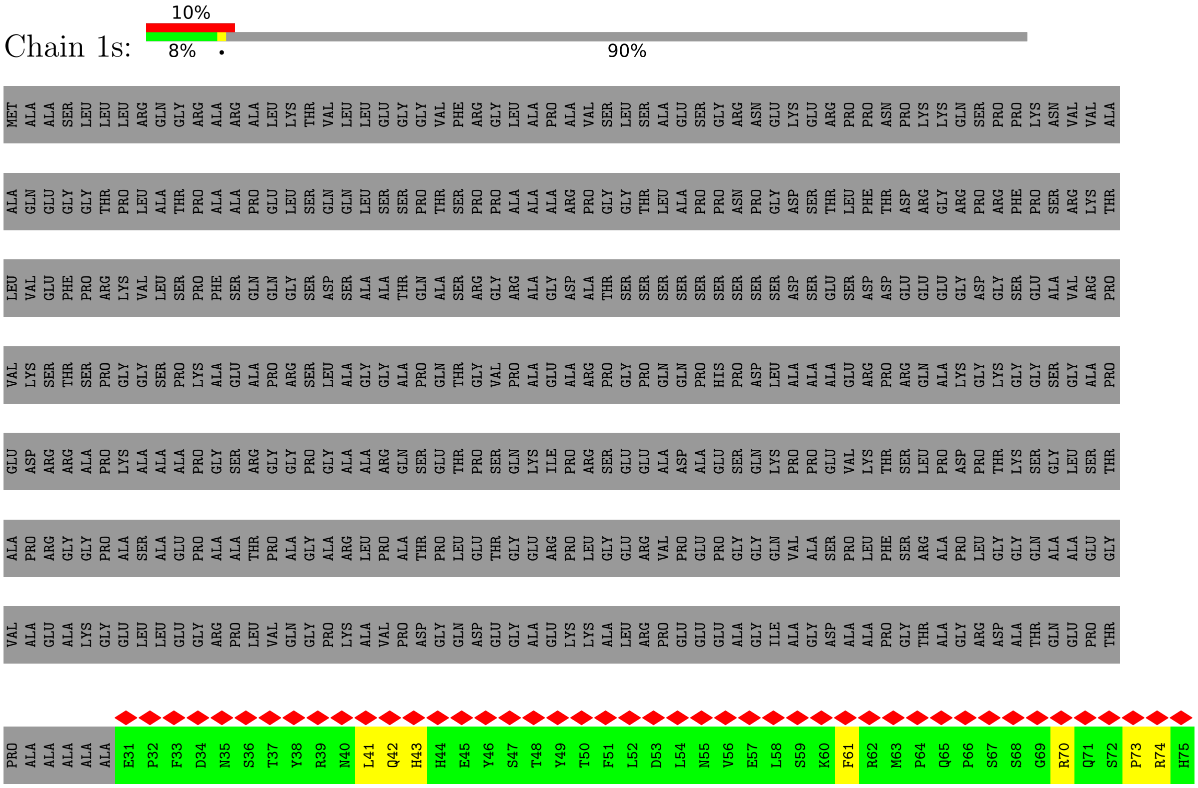


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 1r:



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


Chain 1s:
10%
8%
•
90%
MET ALA ALA SER LEU LEU LEU ARG GLN GLY ARG ALA ARG ALA LEU LYS THR VAL LEU LEU GLU GLY GLY VAL PHE ARG GLY LEU ALA PRO ALA VAL SER LEU SER ALA GLU SER GLY ARG ASN GLU LYS GLU ARG PRO PRO ASN PRO LYS LYS GLN SER PRO PRO LYS ASN VAL VAL ALA
ALA GLN GLU GLY GLY THR PRO LEU ALA THR PRO ALA ALA PRO GLU LEU SER GLN GLN LEU SER SER PRO THR SER PRO PRO ALA ALA ARG PRO GLY GLY THR LEU ALA PRO PRO ASN PRO GLY ASP SER THR LEU PHE THR ASP ARG GLY ARG PRO ARG PHE PRO SER ARG LYS THR
LEU VAL GLU PHE PRO ARG LYS VAL LEU SER PRO PHE SER GLN GLN GLY SER ASP SER ALA ALA THR GLN ALA SER ARG GLY ARG ALA GLY ASP ALA THR SER SER SER SER SER SER SER SER ASP SER GLU SER ASP ASP GLU GLU GLU GLY ASP GLY SER GLU ALA VAL ARG PRO
VAL LYS SER THR SER PRO GLY GLY SER PRO LYS ALA GLU ALA PRO ARG SER LEU ALA GLY GLY ALA PRO GLN THR GLY VAL PRO ALA GLU ALA ARG PRO GLY PRO GLN GLN PRO HIS PRO ASP LEU ALA ALA ALA GLU ARG PRO ARG GLN ALA LYS GLY LYS GLY GLY SER SER GLY ALA PRO
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 GLU ALA GLY ILE ALA GLY ASP ALA ALA PRO GLY THR ALA GLY ARG ASP ALA THR GLN GLU PRO THR
PRO ALA ALA ALA ALA ALA E31 P32 F33 D34 N35 S36 T37 Y38 R39 N40 L41 Q42 H43 H44 E45 Y46 S47 T48 Y49 T50 F51 L52 D53 L54 N55 V56 E57 L58 S59 K60 F61 R62 M63 P64 Q65 P66 S67 S68 G69 R70 Q71 S72 P73 R74 H75

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35000	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	0.594	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.29	0/930	0.62	0/1271
2	1B	0.32	0/1273	0.65	0/1722
3	1C	0.30	0/1791	0.58	0/2439
4	1D	0.29	0/3545	0.58	0/4806
5	1E	0.28	0/1698	0.58	1/2311 (0.0%)
6	1F	0.26	0/3401	0.56	2/4595 (0.0%)
7	1G	0.26	0/5451	0.60	0/7387
8	1H	0.28	0/2566	0.55	0/3509
9	1I	0.31	0/1443	0.58	0/1952
10	1J	0.30	0/1364	0.52	0/1850
11	1K	0.29	0/751	0.61	1/1018 (0.1%)
12	1L	0.28	0/4939	0.58	2/6718 (0.0%)
13	1M	0.27	0/3713	0.52	1/5063 (0.0%)
14	1N	0.27	0/2765	0.58	1/3758 (0.0%)
15	1O	0.27	0/2650	0.55	1/3588 (0.0%)
16	1P	0.27	0/2828	0.58	0/3834
17	1Q	0.31	0/1070	0.64	0/1446
18	1R	0.28	0/755	0.63	1/1018 (0.1%)
19	1S	0.30	0/711	0.80	1/956 (0.1%)
20	1T	0.26	0/701	0.60	0/946
20	1U	0.27	0/706	0.64	1/954 (0.1%)
21	1V	0.28	0/946	0.61	1/1281 (0.1%)
22	1W	0.32	0/995	0.76	1/1340 (0.1%)
23	1X	0.28	0/1436	0.53	1/1938 (0.1%)
24	1Y	0.25	0/1037	0.50	1/1404 (0.1%)
25	1Z	0.36	1/1199 (0.1%)	0.75	3/1617 (0.2%)
26	1a	0.32	0/577	0.63	1/777 (0.1%)
27	1b	0.28	0/664	0.58	0/912
28	1c	0.27	0/430	0.64	0/581
29	1d	0.29	0/1024	0.58	0/1383
30	1e	0.26	0/836	0.56	0/1118
31	1f	0.28	0/499	0.66	1/673 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.31	0/858	0.63	0/1165
33	1h	0.27	0/1184	0.53	1/1603 (0.1%)
34	1i	0.29	0/1131	0.59	1/1541 (0.1%)
35	1j	0.27	0/627	0.56	0/858
36	1k	0.30	0/668	0.59	0/903
37	1l	0.29	0/1365	0.56	0/1867
38	1m	0.28	0/1092	0.55	0/1481
39	1n	0.26	0/1549	0.56	1/2098 (0.0%)
40	1o	0.27	0/1069	0.59	0/1430
41	1p	0.27	0/1481	0.54	0/1997
42	1q	0.30	0/1253	0.63	1/1704 (0.1%)
43	1r	0.31	0/782	0.71	1/1057 (0.1%)
44	1s	0.32	0/394	0.71	1/533 (0.2%)
All	All	0.28	1/68147 (0.0%)	0.59	27/92402 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1Z	26	PRO	CG-CD	-5.63	1.32	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1Z	26	PRO	CA-N-CD	-12.73	93.67	111.50
12	1L	474	PRO	CA-N-CD	-9.39	98.35	111.50
25	1Z	26	PRO	N-CD-CG	-8.53	90.41	103.20
12	1L	350	LEU	CA-CB-CG	8.34	134.48	115.30
44	1s	73	PRO	CA-N-CD	-6.61	102.25	111.50
19	1S	78	LEU	CA-CB-CG	6.12	129.38	115.30
21	1V	112	LYS	CA-CB-CG	5.99	126.57	113.40
25	1Z	26	PRO	CA-CB-CG	-5.98	92.64	104.00
5	1E	202	LEU	CA-CB-CG	5.94	128.96	115.30
14	1N	323	MET	CA-CB-CG	5.86	123.26	113.30
42	1q	76	ASP	CB-CG-OD2	5.86	123.57	118.30
31	1f	48	LEU	CA-CB-CG	5.83	128.72	115.30
6	1F	149	LEU	CA-CB-CG	5.79	128.61	115.30
20	1U	6	LEU	CA-CB-CG	5.74	128.51	115.30
11	1K	93	LEU	CA-CB-CG	5.64	128.27	115.30
6	1F	292	ASP	CB-CG-OD1	5.60	123.34	118.30
34	1i	35	PRO	CA-N-CD	-5.54	103.74	111.50
39	1n	105	ASP	CB-CG-OD2	5.39	123.15	118.30
43	1r	63	MET	CB-CG-SD	5.39	128.58	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1O	214	MET	CA-CB-CG	5.37	122.42	113.30
24	1Y	84	ASP	CB-CG-OD1	5.29	123.06	118.30
33	1h	54	ASP	CB-CG-OD2	5.29	123.06	118.30
22	1W	25	MET	CA-CB-CG	5.21	122.16	113.30
13	1M	231	LEU	CA-CB-CG	5.18	127.22	115.30
26	1a	2	TRP	CD1-CG-CD2	-5.18	102.16	106.30
23	1X	109	CYS	CA-CB-SG	5.09	123.17	114.00
18	1R	60	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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%)	104 (92%)	9 (8%)	0	100	100
2	1B	153/258 (59%)	142 (93%)	11 (7%)	0	100	100
3	1C	207/264 (78%)	196 (95%)	11 (5%)	0	100	100
4	1D	427/476 (90%)	395 (92%)	31 (7%)	1 (0%)	47	79
5	1E	212/249 (85%)	192 (91%)	19 (9%)	1 (0%)	29	68
6	1F	430/464 (93%)	395 (92%)	35 (8%)	0	100	100
7	1G	697/727 (96%)	650 (93%)	44 (6%)	3 (0%)	34	71
8	1H	316/318 (99%)	291 (92%)	23 (7%)	2 (1%)	25	64
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	25	64
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	554 (92%)	47 (8%)	3 (0%)	29	68
13	1M	457/459 (100%)	437 (96%)	20 (4%)	0	100	100
14	1N	345/347 (99%)	323 (94%)	22 (6%)	0	100	100
15	1O	318/357 (89%)	293 (92%)	25 (8%)	0	100	100
16	1P	340/377 (90%)	320 (94%)	20 (6%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	80 (85%)	14 (15%)	0	100	100
19	1S	85/99 (86%)	78 (92%)	7 (8%)	0	100	100
20	1T	83/156 (53%)	75 (90%)	8 (10%)	0	100	100
20	1U	84/156 (54%)	76 (90%)	8 (10%)	0	100	100
21	1V	113/116 (97%)	101 (89%)	12 (11%)	0	100	100
22	1W	113/128 (88%)	103 (91%)	10 (9%)	0	100	100
23	1X	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
28	1c	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
29	1d	117/123 (95%)	111 (95%)	5 (4%)	1 (1%)	17	57
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	4 (7%)	1 (2%)	8	43
32	1g	98/154 (64%)	89 (91%)	8 (8%)	1 (1%)	15	55
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	1i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
38	1m	126/129 (98%)	117 (93%)	9 (7%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	1p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	134 (94%)	8 (6%)	1 (1%)	22	61
43	1r	90/114 (79%)	79 (88%)	11 (12%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
All	All	8194/9744 (84%)	7630 (93%)	549 (7%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1E	97	LYS
8	1H	92	PRO
29	1d	53	VAL
42	1q	142	THR
7	1G	47	SER
8	1H	208	VAL
32	1g	25	ARG
7	1G	186	TYR
31	1f	36	ALA
12	1L	464	ALA
4	1D	87	THR
7	1G	367	THR
12	1L	387	THR
12	1L	549	ALA
10	1J	116	ILE

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%)	87 (88%)	12 (12%)	5	26
2	1B	131/212 (62%)	109 (83%)	22 (17%)	2	14
3	1C	190/227 (84%)	173 (91%)	17 (9%)	9	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1D	371/405 (92%)	333 (90%)	38 (10%)	7	34
5	1E	183/207 (88%)	157 (86%)	26 (14%)	3	21
6	1F	346/368 (94%)	311 (90%)	35 (10%)	7	34
7	1G	588/610 (96%)	509 (87%)	79 (13%)	4	23
8	1H	274/274 (100%)	250 (91%)	24 (9%)	10	40
9	1I	151/201 (75%)	135 (89%)	16 (11%)	6	32
10	1J	140/140 (100%)	126 (90%)	14 (10%)	7	35
11	1K	84/84 (100%)	72 (86%)	12 (14%)	3	21
12	1L	539/539 (100%)	489 (91%)	50 (9%)	9	38
13	1M	408/408 (100%)	376 (92%)	32 (8%)	12	44
14	1N	310/310 (100%)	275 (89%)	35 (11%)	6	30
15	1O	283/307 (92%)	254 (90%)	29 (10%)	7	34
16	1P	296/323 (92%)	262 (88%)	34 (12%)	5	29
17	1Q	117/152 (77%)	102 (87%)	15 (13%)	4	24
18	1R	79/97 (81%)	65 (82%)	14 (18%)	2	11
19	1S	77/82 (94%)	63 (82%)	14 (18%)	1	10
20	1T	79/133 (59%)	69 (87%)	10 (13%)	4	24
20	1U	79/133 (59%)	66 (84%)	13 (16%)	2	15
21	1V	100/101 (99%)	89 (89%)	11 (11%)	6	31
22	1W	107/112 (96%)	92 (86%)	15 (14%)	3	21
23	1X	153/154 (99%)	135 (88%)	18 (12%)	5	28
24	1Y	101/102 (99%)	95 (94%)	6 (6%)	19	55
25	1Z	123/124 (99%)	110 (89%)	13 (11%)	6	32
26	1a	58/58 (100%)	53 (91%)	5 (9%)	10	41
27	1b	69/70 (99%)	55 (80%)	14 (20%)	1	8
28	1c	45/66 (68%)	35 (78%)	10 (22%)	1	6
29	1d	107/109 (98%)	92 (86%)	15 (14%)	3	21
30	1e	87/94 (93%)	76 (87%)	11 (13%)	4	24
31	1f	54/113 (48%)	50 (93%)	4 (7%)	13	46
32	1g	92/129 (71%)	82 (89%)	10 (11%)	6	32
33	1h	121/158 (77%)	112 (93%)	9 (7%)	13	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1i	119/120 (99%)	105 (88%)	14 (12%)	5	28
35	1j	62/84 (74%)	53 (86%)	9 (14%)	3	20
36	1k	63/76 (83%)	54 (86%)	9 (14%)	3	21
37	1l	141/161 (88%)	123 (87%)	18 (13%)	4	24
38	1m	113/114 (99%)	102 (90%)	11 (10%)	8	36
39	1n	156/160 (98%)	146 (94%)	10 (6%)	17	52
40	1o	110/120 (92%)	95 (86%)	15 (14%)	3	22
41	1p	154/156 (99%)	142 (92%)	12 (8%)	12	44
42	1q	131/131 (100%)	116 (88%)	15 (12%)	5	29
43	1r	85/98 (87%)	68 (80%)	17 (20%)	1	8
44	1s	44/351 (12%)	38 (86%)	6 (14%)	3	22
All	All	7219/8272 (87%)	6401 (89%)	818 (11%)	9	30

All (818) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	4	MET
1	1A	22	PHE
1	1A	41	PHE
1	1A	44	MET
1	1A	46	SER
1	1A	48	ARG
1	1A	51	PHE
1	1A	54	LYS
1	1A	55	PHE
1	1A	93	PHE
1	1A	104	TYR
1	1A	113	TRP
2	1B	34	ASP
2	1B	35	ASP
2	1B	38	ASN
2	1B	41	ARG
2	1B	42	ARG
2	1B	48	MET
2	1B	54	CYS
2	1B	59	MET
2	1B	62	MET
2	1B	66	ARG

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Mol	Chain	Res	Type
2	1B	69	MET
2	1B	71	ARG
2	1B	105	ASP
2	1B	109	GLU
2	1B	112	TYR
2	1B	129	SER
2	1B	132	VAL
2	1B	133	VAL
2	1B	143	ASP
2	1B	166	LYS
2	1B	174	ARG
2	1B	177	TYR
3	1C	8	ARG
3	1C	14	ARG
3	1C	20	LYS
3	1C	28	TYR
3	1C	62	THR
3	1C	66	ASP
3	1C	73	LYS
3	1C	74	SER
3	1C	77	ASP
3	1C	108	LYS
3	1C	109	THR
3	1C	130	TYR
3	1C	134	ILE
3	1C	199	LEU
3	1C	201	SER
3	1C	206	PHE
3	1C	214	GLU
4	1D	10	TRP
4	1D	18	VAL
4	1D	19	MET
4	1D	42	THR
4	1D	45	SER
4	1D	66	MET
4	1D	72	MET
4	1D	74	ARG
4	1D	75	LYS
4	1D	87	THR
4	1D	90	LEU
4	1D	111	MET
4	1D	164	MET

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Mol	Chain	Res	Type
4	1D	175	GLU
4	1D	177	MET
4	1D	178	PHE
4	1D	189	MET
4	1D	193	TYR
4	1D	199	VAL
4	1D	203	LEU
4	1D	224	GLU
4	1D	228	MET
4	1D	270	ARG
4	1D	284	ASP
4	1D	295	ASP
4	1D	299	CYS
4	1D	318	MET
4	1D	324	LYS
4	1D	376	VAL
4	1D	378	LEU
4	1D	389	CYS
4	1D	396	PHE
4	1D	399	LEU
4	1D	403	ASP
4	1D	404	LYS
4	1D	405	MET
4	1D	407	LYS
4	1D	410	MET
5	1E	10	ARG
5	1E	11	ASP
5	1E	18	ASP
5	1E	22	ASP
5	1E	23	PHE
5	1E	36	LYS
5	1E	38	TYR
5	1E	56	ARG
5	1E	60	TRP
5	1E	86	PHE
5	1E	89	MET
5	1E	92	ARG
5	1E	111	ARG
5	1E	121	GLN
5	1E	139	LEU
5	1E	145	LEU
5	1E	153	MET

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Mol	Chain	Res	Type
5	1E	154	VAL
5	1E	160	TYR
5	1E	163	ASP
5	1E	165	THR
5	1E	167	LYS
5	1E	169	ILE
5	1E	187	ARG
5	1E	193	CYS
5	1E	207	LYS
6	1F	16	LYS
6	1F	32	ARG
6	1F	44	LYS
6	1F	48	ILE
6	1F	55	TRP
6	1F	62	THR
6	1F	80	SER
6	1F	81	PHE
6	1F	82	MET
6	1F	106	LYS
6	1F	117	LYS
6	1F	120	GLU
6	1F	132	ARG
6	1F	144	ASN
6	1F	164	LYS
6	1F	175	VAL
6	1F	184	TYR
6	1F	186	CYS
6	1F	224	ASN
6	1F	228	VAL
6	1F	253	THR
6	1F	257	ASN
6	1F	267	THR
6	1F	272	MET
6	1F	276	LEU
6	1F	277	LYS
6	1F	306	LEU
6	1F	317	MET
6	1F	334	VAL
6	1F	355	LYS
6	1F	363	THR
6	1F	373	ASN
6	1F	376	MET

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Mol	Chain	Res	Type
6	1F	385	ARG
6	1F	430	MET
7	1G	14	ASP
7	1G	18	VAL
7	1G	19	MET
7	1G	35	MET
7	1G	37	ILE
7	1G	39	ARG
7	1G	40	PHE
7	1G	52	CYS
7	1G	54	MET
7	1G	59	ILE
7	1G	61	LYS
7	1G	64	LYS
7	1G	69	CYS
7	1G	74	MET
7	1G	77	TRP
7	1G	93	VAL
7	1G	94	MET
7	1G	95	GLU
7	1G	115	ASP
7	1G	120	SER
7	1G	123	PHE
7	1G	127	ARG
7	1G	129	ARG
7	1G	130	PHE
7	1G	139	ASP
7	1G	148	THR
7	1G	185	THR
7	1G	187	ILE
7	1G	190	MET
7	1G	192	MET
7	1G	193	SER
7	1G	224	LYS
7	1G	227	SER
7	1G	242	THR
7	1G	243	ARG
7	1G	244	THR
7	1G	248	MET
7	1G	264	SER
7	1G	269	PHE
7	1G	283	MET

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Mol	Chain	Res	Type
7	1G	288	LYS
7	1G	293	TYR
7	1G	302	ARG
7	1G	329	VAL
7	1G	332	LYS
7	1G	345	THR
7	1G	356	THR
7	1G	360	SER
7	1G	365	ASN
7	1G	379	LEU
7	1G	382	THR
7	1G	385	ARG
7	1G	396	ARG
7	1G	404	LEU
7	1G	415	LEU
7	1G	437	HIS
7	1G	455	SER
7	1G	481	SER
7	1G	490	MET
7	1G	504	ASP
7	1G	520	LYS
7	1G	533	THR
7	1G	534	ARG
7	1G	536	ASP
7	1G	541	CYS
7	1G	548	HIS
7	1G	556	MET
7	1G	567	THR
7	1G	577	GLU
7	1G	596	ASP
7	1G	609	MET
7	1G	631	VAL
7	1G	649	SER
7	1G	651	LEU
7	1G	655	GLN
7	1G	667	THR
7	1G	670	ASP
7	1G	677	ILE
7	1G	703	ILE
8	1H	31	MET
8	1H	35	LYS
8	1H	43	TYR

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Mol	Chain	Res	Type
8	1H	70	MET
8	1H	80	SER
8	1H	98	MET
8	1H	110	SER
8	1H	119	SER
8	1H	124	ASN
8	1H	157	ASN
8	1H	163	SER
8	1H	188	SER
8	1H	207	LEU
8	1H	222	MET
8	1H	234	MET
8	1H	255	TYR
8	1H	266	LEU
8	1H	270	PHE
8	1H	271	LEU
8	1H	280	PHE
8	1H	285	LEU
8	1H	294	LEU
8	1H	297	THR
8	1H	317	GLN
9	1I	2	TYR
9	1I	3	LYS
9	1I	19	ASP
9	1I	20	ARG
9	1I	40	TYR
9	1I	54	LYS
9	1I	57	LEU
9	1I	67	LEU
9	1I	68	ARG
9	1I	104	ARG
9	1I	110	ASP
9	1I	123	GLN
9	1I	129	ASP
9	1I	140	SER
9	1I	155	LEU
9	1I	160	LYS
10	1J	25	SER
10	1J	56	VAL
10	1J	78	MET
10	1J	81	GLU
10	1J	83	TRP

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Mol	Chain	Res	Type
10	1J	99	MET
10	1J	102	CYS
10	1J	106	TYR
10	1J	117	PHE
10	1J	124	ASP
10	1J	130	THR
10	1J	132	ASP
10	1J	136	PHE
10	1J	173	ARG
11	1K	7	ASN
11	1K	10	MET
11	1K	22	TYR
11	1K	27	MET
11	1K	37	MET
11	1K	44	SER
11	1K	52	HIS
11	1K	53	PHE
11	1K	54	THR
11	1K	69	CYS
11	1K	78	LEU
11	1K	98	CYS
12	1L	6	SER
12	1L	25	ASN
12	1L	36	VAL
12	1L	55	MET
12	1L	66	TRP
12	1L	67	HIS
12	1L	69	MET
12	1L	70	THR
12	1L	71	LEU
12	1L	72	GLN
12	1L	88	MET
12	1L	89	PHE
12	1L	125	LEU
12	1L	132	VAL
12	1L	137	LEU
12	1L	150	MET
12	1L	159	HIS
12	1L	163	ASP
12	1L	203	MET
12	1L	206	ASN
12	1L	217	LEU

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Mol	Chain	Res	Type
12	1L	247	LEU
12	1L	276	MET
12	1L	285	THR
12	1L	316	THR
12	1L	340	PHE
12	1L	341	MET
12	1L	345	SER
12	1L	346	ILE
12	1L	353	GLU
12	1L	359	MET
12	1L	394	LEU
12	1L	404	THR
12	1L	411	MET
12	1L	471	ASN
12	1L	475	MET
12	1L	482	MET
12	1L	484	LEU
12	1L	486	MET
12	1L	494	THR
12	1L	499	MET
12	1L	510	TYR
12	1L	517	SER
12	1L	535	ARG
12	1L	561	ILE
12	1L	562	LEU
12	1L	576	MET
12	1L	589	LEU
12	1L	596	MET
12	1L	606	GLU
13	1M	9	THR
13	1M	10	MET
13	1M	26	ASN
13	1M	34	ILE
13	1M	69	THR
13	1M	76	MET
13	1M	86	LYS
13	1M	88	THR
13	1M	121	LEU
13	1M	134	THR
13	1M	135	ARG
13	1M	189	SER
13	1M	190	TRP

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Mol	Chain	Res	Type
13	1M	209	LEU
13	1M	213	HIS
13	1M	228	SER
13	1M	263	MET
13	1M	284	SER
13	1M	325	MET
13	1M	335	GLU
13	1M	336	ARG
13	1M	344	LEU
13	1M	350	THR
13	1M	359	TRP
13	1M	361	MET
13	1M	363	SER
13	1M	365	THR
13	1M	401	MET
13	1M	418	LYS
13	1M	420	THR
13	1M	431	THR
13	1M	450	ASN
14	1N	14	MET
14	1N	40	MET
14	1N	51	ARG
14	1N	81	SER
14	1N	85	THR
14	1N	87	THR
14	1N	88	LYS
14	1N	95	MET
14	1N	98	MET
14	1N	100	MET
14	1N	104	MET
14	1N	108	LEU
14	1N	109	SER
14	1N	123	SER
14	1N	140	SER
14	1N	154	MET
14	1N	159	MET
14	1N	163	LEU
14	1N	191	THR
14	1N	206	LEU
14	1N	215	MET
14	1N	226	THR
14	1N	235	ASN

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Mol	Chain	Res	Type
14	1N	237	MET
14	1N	242	SER
14	1N	245	MET
14	1N	278	MET
14	1N	300	SER
14	1N	304	MET
14	1N	313	MET
14	1N	318	GLU
14	1N	323	MET
14	1N	325	LEU
14	1N	329	MET
14	1N	333	SER
15	1O	3	TYR
15	1O	16	ARG
15	1O	32	CYS
15	1O	40	ARG
15	1O	49	ARG
15	1O	78	SER
15	1O	103	SER
15	1O	104	ARG
15	1O	132	PHE
15	1O	135	LEU
15	1O	157	LYS
15	1O	164	LEU
15	1O	175	PRO
15	1O	182	ARG
15	1O	208	LYS
15	1O	213	GLU
15	1O	214	MET
15	1O	218	CYS
15	1O	219	GLU
15	1O	221	LEU
15	1O	226	ARG
15	1O	240	TYR
15	1O	242	LYS
15	1O	248	TRP
15	1O	250	ASP
15	1O	269	VAL
15	1O	270	LEU
15	1O	291	ARG
15	1O	295	LYS
16	1P	19	ILE

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Mol	Chain	Res	Type
16	1P	27	THR
16	1P	36	ASN
16	1P	40	ARG
16	1P	41	MET
16	1P	43	SER
16	1P	56	THR
16	1P	65	LEU
16	1P	73	TRP
16	1P	82	ARG
16	1P	87	HIS
16	1P	101	THR
16	1P	119	GLN
16	1P	143	SER
16	1P	145	TYR
16	1P	168	PRO
16	1P	174	ARG
16	1P	209	ASP
16	1P	222	ASP
16	1P	234	ASN
16	1P	258	LEU
16	1P	264	ARG
16	1P	273	SER
16	1P	286	ARG
16	1P	289	MET
16	1P	290	SER
16	1P	292	MET
16	1P	300	LEU
16	1P	302	ASP
16	1P	306	GLN
16	1P	317	VAL
16	1P	327	LEU
16	1P	331	MET
16	1P	335	LYS
17	1Q	21	THR
17	1Q	28	GLU
17	1Q	36	ARG
17	1Q	39	VAL
17	1Q	44	ASN
17	1Q	62	ARG
17	1Q	72	TRP
17	1Q	80	SER
17	1Q	91	ASP

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Mol	Chain	Res	Type
17	1Q	107	GLU
17	1Q	122	PHE
17	1Q	123	SER
17	1Q	124	TRP
17	1Q	125	ASN
17	1Q	128	THR
18	1R	5	SER
18	1R	11	VAL
18	1R	12	THR
18	1R	19	ASP
18	1R	31	ARG
18	1R	33	LYS
18	1R	42	ASP
18	1R	54	SER
18	1R	58	SER
18	1R	60	ASP
18	1R	70	ARG
18	1R	78	GLU
18	1R	83	THR
18	1R	84	CYS
19	1S	12	LYS
19	1S	13	LEU
19	1S	16	ARG
19	1S	25	ARG
19	1S	40	TYR
19	1S	57	CYS
19	1S	58	SER
19	1S	70	PHE
19	1S	74	LYS
19	1S	81	PHE
19	1S	85	GLN
19	1S	88	ARG
19	1S	89	THR
19	1S	97	LYS
20	1T	7	THR
20	1T	17	TYR
20	1T	26	ASP
20	1T	37	MET
20	1T	47	GLN
20	1T	52	MET
20	1T	54	MET
20	1T	69	LYS

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Mol	Chain	Res	Type
20	1T	70	LEU
20	1T	71	MET
20	1U	8	LEU
20	1U	12	LYS
20	1U	16	LEU
20	1U	17	TYR
20	1U	22	TYR
20	1U	29	LYS
20	1U	33	ASN
20	1U	37	MET
20	1U	44	SER
20	1U	46	ASP
20	1U	71	MET
20	1U	72	CYS
20	1U	83	LYS
21	1V	16	CYS
21	1V	17	GLU
21	1V	20	HIS
21	1V	43	TYR
21	1V	57	MET
21	1V	65	LYS
21	1V	69	GLU
21	1V	71	LEU
21	1V	75	GLN
21	1V	91	ARG
21	1V	99	TRP
22	1W	25	MET
22	1W	30	ARG
22	1W	31	ARG
22	1W	39	TRP
22	1W	40	TYR
22	1W	52	LEU
22	1W	57	LYS
22	1W	62	LYS
22	1W	74	THR
22	1W	80	ASP
22	1W	90	LEU
22	1W	95	ASN
22	1W	104	MET
22	1W	109	GLU
22	1W	114	ARG
23	1X	5	GLU

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Mol	Chain	Res	Type
23	1X	29	HIS
23	1X	47	TRP
23	1X	50	LYS
23	1X	62	VAL
23	1X	65	CYS
23	1X	68	ASP
23	1X	81	PHE
23	1X	89	ASP
23	1X	94	GLN
23	1X	105	LYS
23	1X	107	ASP
23	1X	124	LEU
23	1X	128	THR
23	1X	150	ASN
23	1X	154	GLU
23	1X	166	LEU
23	1X	171	MET
24	1Y	52	VAL
24	1Y	85	ASP
24	1Y	94	CYS
24	1Y	117	MET
24	1Y	126	MET
24	1Y	134	VAL
25	1Z	20	ASP
25	1Z	21	TYR
25	1Z	27	ARG
25	1Z	51	MET
25	1Z	68	ARG
25	1Z	71	LEU
25	1Z	82	ARG
25	1Z	100	ASP
25	1Z	105	LYS
25	1Z	110	VAL
25	1Z	124	LEU
25	1Z	128	ARG
25	1Z	129	THR
26	1a	3	PHE
26	1a	17	PHE
26	1a	21	MET
26	1a	28	LYS
26	1a	53	CYS
27	1b	7	PHE

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Mol	Chain	Res	Type
27	1b	9	LYS
27	1b	15	GLU
27	1b	22	PHE
27	1b	33	SER
27	1b	45	ASN
27	1b	48	THR
27	1b	51	ASN
27	1b	52	TYR
27	1b	62	MET
27	1b	65	VAL
27	1b	76	SER
27	1b	77	LEU
27	1b	81	LYS
28	1c	1	LYS
28	1c	2	PHE
28	1c	3	TYR
28	1c	5	ARG
28	1c	9	HIS
28	1c	15	LEU
28	1c	26	PHE
28	1c	30	TYR
28	1c	40	LEU
28	1c	42	TYR
29	1d	2	MET
29	1d	3	SER
29	1d	8	ARG
29	1d	25	LYS
29	1d	36	PHE
29	1d	40	CYS
29	1d	51	ARG
29	1d	54	VAL
29	1d	58	LEU
29	1d	61	GLN
29	1d	70	PHE
29	1d	78	ARG
29	1d	90	MET
29	1d	104	LYS
29	1d	105	ASP
30	1e	2	PHE
30	1e	5	VAL
30	1e	8	ARG
30	1e	11	LEU

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Mol	Chain	Res	Type
30	1e	21	SER
30	1e	37	LYS
30	1e	60	ASP
30	1e	61	ASP
30	1e	80	ARG
30	1e	91	TYR
30	1e	98	LEU
31	1f	29	ARG
31	1f	42	LEU
31	1f	43	LEU
31	1f	49	ARG
32	1g	28	GLU
32	1g	49	LYS
32	1g	57	ASN
32	1g	58	MET
32	1g	59	ARG
32	1g	63	PHE
32	1g	84	ARG
32	1g	100	ARG
32	1g	107	LEU
32	1g	112	CYS
33	1h	6	LYS
33	1h	18	ASP
33	1h	25	MET
33	1h	46	PHE
33	1h	62	GLU
33	1h	81	ASP
33	1h	111	ARG
33	1h	123	TYR
33	1h	129	ASP
34	1i	8	LYS
34	1i	10	ARG
34	1i	13	GLN
34	1i	14	LEU
34	1i	23	LYS
34	1i	28	SER
34	1i	34	LEU
34	1i	45	PHE
34	1i	52	ASP
34	1i	57	LYS
34	1i	86	LYS
34	1i	100	LYS

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Mol	Chain	Res	Type
34	1i	110	LEU
34	1i	120	LYS
35	1j	6	HIS
35	1j	7	ILE
35	1j	19	ARG
35	1j	32	MET
35	1j	34	PHE
35	1j	39	ARG
35	1j	40	PHE
35	1j	44	SER
35	1j	60	THR
36	1k	18	TYR
36	1k	61	SER
36	1k	67	LEU
36	1k	70	PHE
36	1k	71	LYS
36	1k	74	PHE
36	1k	77	PHE
36	1k	86	TYR
36	1k	88	GLU
37	1l	6	LYS
37	1l	13	TYR
37	1l	15	LYS
37	1l	16	THR
37	1l	26	LYS
37	1l	33	ASP
37	1l	49	LYS
37	1l	63	ASP
37	1l	69	LEU
37	1l	70	ARG
37	1l	90	ASP
37	1l	112	MET
37	1l	116	PHE
37	1l	117	TRP
37	1l	118	VAL
37	1l	128	VAL
37	1l	149	GLU
37	1l	151	GLU
38	1m	2	PHE
38	1m	16	THR
38	1m	58	VAL
38	1m	61	ASP

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Mol	Chain	Res	Type
38	1m	69	TYR
38	1m	80	ARG
38	1m	82	THR
38	1m	92	PHE
38	1m	98	PHE
38	1m	105	LYS
38	1m	122	GLN
39	1n	18	LEU
39	1n	46	ARG
39	1n	47	PHE
39	1n	51	LYS
39	1n	52	ASN
39	1n	56	MET
39	1n	157	ARG
39	1n	159	GLU
39	1n	174	ARG
39	1n	178	MET
40	1o	7	ARG
40	1o	19	LEU
40	1o	21	MET
40	1o	38	MET
40	1o	39	VAL
40	1o	43	GLN
40	1o	47	ASP
40	1o	63	ILE
40	1o	77	LEU
40	1o	94	TYR
40	1o	98	MET
40	1o	109	GLN
40	1o	111	LYS
40	1o	117	ARG
40	1o	121	MET
41	1p	7	ASP
41	1p	14	ARG
41	1p	60	TYR
41	1p	63	TYR
41	1p	76	CYS
41	1p	85	PHE
41	1p	96	LYS
41	1p	122	GLN
41	1p	136	LYS
41	1p	150	SER

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Mol	Chain	Res	Type
41	1p	162	MET
41	1p	166	ARG
42	1q	9	ARG
42	1q	25	ARG
42	1q	43	LYS
42	1q	47	LYS
42	1q	76	ASP
42	1q	77	VAL
42	1q	81	MET
42	1q	95	ASP
42	1q	100	THR
42	1q	104	THR
42	1q	125	VAL
42	1q	127	TYR
42	1q	133	LYS
42	1q	138	VAL
42	1q	141	SER
43	1r	2	SER
43	1r	17	ARG
43	1r	26	ARG
43	1r	32	LYS
43	1r	34	THR
43	1r	39	LYS
43	1r	48	LEU
43	1r	49	SER
43	1r	57	ASP
43	1r	70	SER
43	1r	72	GLN
43	1r	91	LYS
43	1r	102	ARG
43	1r	103	TRP
43	1r	106	SER
43	1r	107	LYS
43	1r	109	GLN
44	1s	41	LEU
44	1s	42	GLN
44	1s	43	HIS
44	1s	61	PHE
44	1s	70	ARG
44	1s	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	61	HIS
2	1B	106	GLN
3	1C	88	ASN
4	1D	114	ASN
4	1D	149	ASN
5	1E	121	GLN
6	1F	150	GLN
6	1F	224	ASN
12	1L	135	ASN
13	1M	168	GLN
13	1M	424	ASN
14	1N	36	ASN
14	1N	63	GLN
14	1N	77	ASN
14	1N	120	GLN
14	1N	134	GLN
14	1N	309	ASN
15	1O	76	ASN
15	1O	92	ASN
15	1O	147	GLN
16	1P	131	HIS
16	1P	180	ASN
16	1P	288	HIS
17	1Q	50	ASN
19	1S	61	GLN
21	1V	110	GLN
26	1a	46	ASN
29	1d	61	GLN
30	1e	97	HIS
37	1l	126	GLN
40	1o	3	HIS
41	1p	55	HIS
41	1p	158	GLN
42	1q	13	GLN
44	1s	55	ASN
44	1s	71	GLN

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	$\#\|Z\| > 2$
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.13	1 (14%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
34	SAC	1i	1	-	7,8,9	0.54	0	8,9,11	1.07	1 (12%)
14	FME	1N	1	14	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
11	FME	1K	1	11	8,9,10	0.53	0	7,9,11	1.04	1 (14%)
13	FME	1M	1	13	8,9,10	0.50	0	7,9,11	1.00	1 (14%)
10	FME	1J	1	10	8,9,10	0.52	0	7,9,11	0.95	1 (14%)
1	FME	1A	1	1	8,9,10	0.48	0	7,9,11	1.15	1 (14%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.92	117.13	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1H	1	FME	O-C-CA	-2.71	117.68	124.78
11	1K	1	FME	O-C-CA	-2.67	117.77	124.78
1	1A	1	FME	O-C-CA	-2.63	117.89	124.78
14	1N	1	FME	O-C-CA	-2.54	118.13	124.78
13	1M	1	FME	O-C-CA	-2.48	118.28	124.78
12	1L	1	FME	O-C-CA	-2.45	118.36	124.78
10	1J	1	FME	O-C-CA	-2.25	118.89	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	1M	1	FME	O-C-CA-CB
13	1M	1	FME	N-CA-CB-CG
11	1K	1	FME	CA-CB-CG-SD
1	1A	1	FME	CB-CG-SD-CE
13	1M	1	FME	CB-CA-N-CN

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 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	SF4	1B	201	2	0,12,12	-	-	-		
45	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
50	PC1	1L	702	-	43,43,53	0.30	0	49,51,61	0.35	0
46	SF4	1I	202	9	0,12,12	-	-	-		
45	3PE	1Y	202	-	30,30,50	0.35	0	33,35,55	0.64	1 (3%)
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.33	0
50	PC1	1f	101	-	45,45,53	0.28	0	51,53,61	0.36	0
45	3PE	1A	201	-	46,46,50	0.29	0	49,51,55	0.39	0
50	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.36	0
56	EHZ	1n	201	-	29,36,37	0.17	0	35,44,47	1.07	1 (2%)
51	CDL	1N	402	-	76,76,99	0.29	0	82,88,111	0.38	0
56	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.36	1 (2%)
46	SF4	1I	201	9	0,12,12	-	-	-		
48	FMN	1F	501	-	33,33,33	0.58	0	48,50,50	0.65	1 (2%)
47	FES	1E	301	5	0,4,4	-	-	-		
46	SF4	1G	802	7	0,12,12	-	-	-		
52	GTP	1O	401	53	26,34,34	0.96	2 (7%)	32,54,54	0.82	1 (3%)
45	3PE	1N	401	-	50,50,50	0.26	0	53,55,55	0.38	0
57	PGT	1Y	201	-	50,50,50	0.49	0	53,56,56	0.48	0
54	NDP	1P	501	-	45,52,52	0.62	0	53,80,80	0.77	2 (3%)
46	SF4	1F	502	6	0,12,12	-	-	-		
46	SF4	1G	801	7	0,12,12	-	-	-		
45	3PE	1L	703	-	41,41,50	0.31	0	44,46,55	1.25	5 (11%)
51	CDL	1q	201	-	60,60,99	0.32	0	66,72,111	0.84	4 (6%)
45	3PE	1Y	203	-	50,50,50	0.26	0	53,55,55	0.43	0
58	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.39	0
47	FES	1G	803	7	0,4,4	-	-	-		
50	PC1	1I	203	-	53,53,53	0.27	0	59,61,61	0.34	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
46	SF4	1B	201	2	-	-	0/6/5/5
45	3PE	1L	701	-	-	4/49/49/54	-
50	PC1	1L	702	-	-	6/47/47/57	-
50	PC1	1f	101	-	-	6/49/49/57	-
45	3PE	1Y	202	-	-	9/34/34/54	-
50	PC1	1J	201	-	-	3/38/38/57	-
46	SF4	1I	202	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1A	201	-	-	4/50/50/54	-
50	PC1	1I	204	-	-	3/47/47/57	-
56	EHZ	1n	201	-	-	10/42/44/45	-
51	CDL	1N	402	-	-	5/87/87/110	-
56	EHZ	1W	201	-	-	4/42/44/45	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
46	SF4	1I	201	9	-	-	0/6/5/5
47	FES	1E	301	5	-	-	0/1/1/1
46	SF4	1G	802	7	-	-	0/6/5/5
52	GTP	1O	401	53	-	3/18/38/38	0/3/3/3
45	3PE	1N	401	-	-	11/54/54/54	-
57	PGT	1Y	201	-	-	23/55/55/55	-
54	NDP	1P	501	-	-	8/30/77/77	0/5/5/5
46	SF4	1F	502	6	-	-	0/6/5/5
46	SF4	1G	801	7	-	-	0/6/5/5
45	3PE	1L	703	-	-	5/45/45/54	-
51	CDL	1q	201	-	-	16/71/71/110	-
45	3PE	1Y	203	-	-	9/54/54/54	-
58	MYR	1l	201	-	-	1/11/12/13	-
47	FES	1G	803	7	-	-	0/1/1/1
50	PC1	1I	203	-	-	5/57/57/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1O	401	GTP	C5-C6	-2.60	1.42	1.47
52	1O	401	GTP	C8-N7	-2.12	1.31	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1W	201	EHZ	C10-S1-C9	7.34	124.73	101.87
45	1L	703	3PE	O21-C21-C22	6.08	124.61	111.50
56	1n	201	EHZ	C10-S1-C9	5.78	119.86	101.87
51	1q	201	CDL	OB4-PB2-OB2	3.24	122.78	107.75
45	1L	703	3PE	O21-C21-O22	-2.64	117.32	123.70
54	1P	501	NDP	O4D-C1D-C2D	-2.59	100.98	106.64
45	1L	703	3PE	C2-O21-C21	2.54	124.04	117.79
51	1q	201	CDL	OB5-PB2-OB3	-2.35	99.89	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	1L	703	3PE	O21-C2-C1	2.34	116.86	108.40
54	1P	501	NDP	C5A-C6A-N6A	2.23	123.75	120.35
52	1O	401	GTP	O4'-C1'-C2'	-2.21	103.70	106.93
45	1Y	202	3PE	O21-C21-C22	2.18	116.20	111.50
51	1q	201	CDL	OA6-CA4-CA3	2.07	115.89	108.40
48	1F	501	FMN	C4-N3-C2	-2.04	121.87	125.64
51	1q	201	CDL	OB2-PB2-OB3	-2.02	101.18	109.07
45	1L	703	3PE	O21-C2-C3	2.01	115.68	108.40

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	202	3PE	C1-O11-P-O14
45	1Y	202	3PE	O32-C31-O31-C3
45	1Y	202	3PE	C32-C31-O31-C3
45	1Y	202	3PE	O22-C21-O21-C2
45	1Y	202	3PE	C22-C21-O21-C2
45	1Y	203	3PE	C1-O11-P-O14
50	1I	204	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O13
50	1L	702	PC1	C1-O11-P-O14
50	1f	101	PC1	O32-C31-O31-C3
50	1f	101	PC1	C32-C31-O31-C3
51	1N	402	CDL	OA6-CA4-CA6-OA8
51	1q	201	CDL	CA2-OA2-PA1-OA4
51	1q	201	CDL	CA2-OA2-PA1-OA5
51	1q	201	CDL	CA3-OA5-PA1-OA2
56	1W	201	EHZ	O2-C9-S1-C10
56	1W	201	EHZ	C8-C9-S1-C10
56	1n	201	EHZ	O2-C9-S1-C10
56	1n	201	EHZ	C8-C9-S1-C10
57	1Y	201	PGT	C32-C31-O2-C2
57	1Y	201	PGT	C5-C4-O4P-P
57	1Y	201	PGT	C4-C5-C6-O6
57	1Y	201	PGT	O5-C5-C6-O6
57	1Y	201	PGT	O11-C11-O3-C3
57	1Y	201	PGT	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
57	1Y	201	PGT	O31-C31-O2-C2
51	1q	201	CDL	O1-C1-CA2-OA2
52	1O	401	GTP	O4'-C4'-C5'-O5'
52	1O	401	GTP	C3'-C4'-C5'-O5'
45	1Y	203	3PE	C2-C1-O11-P
51	1q	201	CDL	CB2-C1-CA2-OA2
51	1q	201	CDL	CA2-C1-CB2-OB2
57	1Y	201	PGT	C1-O3P-P-O4P
57	1Y	201	PGT	C4-O4P-P-O3P
54	1P	501	NDP	C2D-C1D-N1N-C2N
54	1P	501	NDP	C2D-C1D-N1N-C6N
57	1Y	201	PGT	C40-C41-C42-C43
51	1q	201	CDL	O1-C1-CB2-OB2
57	1Y	201	PGT	C34-C35-C36-C37
57	1Y	201	PGT	C14-C15-C16-C17
57	1Y	201	PGT	C15-C16-C17-C18
50	1I	203	PC1	C24-C25-C26-C27
57	1Y	201	PGT	C21-C22-C23-C24
51	1q	201	CDL	C51-C52-C53-C54
56	1W	201	EHZ	C5-C6-C7-C8
45	1Y	203	3PE	C35-C36-C37-C38
56	1n	201	EHZ	C12-C13-C14-N2
57	1Y	201	PGT	C32-C33-C34-C35
45	1Y	203	3PE	C3C-C3D-C3E-C3F
57	1Y	201	PGT	C44-C45-C46-C47
45	1N	401	3PE	O31-C31-C32-C33
56	1n	201	EHZ	C18-C17-C20-O6
56	1n	201	EHZ	C19-C17-C20-O6
45	1L	703	3PE	O11-C1-C2-O21
50	1I	203	PC1	O31-C31-C32-C33
56	1n	201	EHZ	O3-C12-C13-C14
51	1q	201	CDL	C53-C54-C55-C56
51	1N	402	CDL	CA3-CA4-CA6-OA8
51	1q	201	CDL	OB5-CB3-CB4-OB6
52	1O	401	GTP	C4'-C5'-O5'-PA
54	1P	501	NDP	C3B-C2B-O2B-P2B
51	1q	201	CDL	OB5-CB3-CB4-CB6
45	1N	401	3PE	C2-C1-O11-P
51	1q	201	CDL	CA3-CA4-CA6-OA8
45	1Y	203	3PE	O11-C1-C2-O21
58	1l	201	MYR	C3-C4-C5-C6
45	1Y	203	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
50	1I	204	PC1	C1-O11-P-O13
50	1L	702	PC1	C1-O11-P-O13
54	1P	501	NDP	O4D-C1D-N1N-C6N
50	1L	702	PC1	C1-O11-P-O12
51	1q	201	CDL	CA2-OA2-PA1-OA3
51	1q	201	CDL	CA3-OA5-PA1-OA3
57	1Y	201	PGT	C1-O3P-P-O1P
57	1Y	201	PGT	C4-O4P-P-O1P
45	1A	201	3PE	C12-C11-O13-P
45	1Y	203	3PE	C12-C11-O13-P
54	1P	501	NDP	C1B-C2B-O2B-P2B
45	1N	401	3PE	C3A-C3B-C3C-C3D
54	1P	501	NDP	O4D-C1D-N1N-C2N
56	1n	201	EHZ	N1-C12-C13-C14
50	1J	201	PC1	O13-C11-C12-N
56	1n	201	EHZ	C16-C17-C20-O6
51	1N	402	CDL	C55-C56-C57-C58
45	1N	401	3PE	C34-C35-C36-C37
45	1Y	203	3PE	C24-C25-C26-C27
45	1A	201	3PE	C24-C25-C26-C27
45	1N	401	3PE	O11-C1-C2-O21
45	1N	401	3PE	C1-O11-P-O13
45	1Y	202	3PE	C1-O11-P-O13
50	1f	101	PC1	C11-O13-P-O11
45	1L	701	3PE	C22-C23-C24-C25
45	1N	401	3PE	C2-C3-O31-C31
56	1n	201	EHZ	C13-C14-N2-C15
45	1A	201	3PE	O21-C2-C3-O31
57	1Y	201	PGT	C2-C1-O3P-P
45	1L	703	3PE	C1-C2-C3-O31
50	1L	702	PC1	C1-C2-C3-O31
45	1L	703	3PE	C1-C2-O21-C21
57	1Y	201	PGT	C31-C32-C33-C34
51	1N	402	CDL	C76-C77-C78-C79
56	1n	201	EHZ	C11-C10-S1-C9
51	1q	201	CDL	OB6-CB4-CB6-OB8
45	1L	701	3PE	C33-C34-C35-C36
45	1Y	203	3PE	O11-C1-C2-C3
45	1N	401	3PE	O21-C2-C3-O31
45	1L	701	3PE	C35-C36-C37-C38
54	1P	501	NDP	O4D-C4D-C5D-O5D
51	1N	402	CDL	C53-C54-C55-C56

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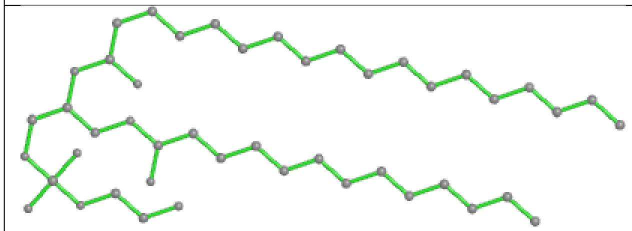
Mol	Chain	Res	Type	Atoms
51	1q	201	CDL	CB3-CB4-CB6-OB8
50	1I	203	PC1	O32-C31-C32-C33
45	1Y	202	3PE	O21-C2-C3-O31
45	1N	401	3PE	O32-C31-C32-C33
50	1I	204	PC1	C11-C12-N-C13
57	1Y	201	PGT	C41-C42-C43-C44
57	1Y	201	PGT	C39-C40-C41-C42
50	1f	101	PC1	C21-C22-C23-C24
50	1I	203	PC1	C3E-C3F-C3G-C3H
45	1N	401	3PE	C39-C3A-C3B-C3C
50	1f	101	PC1	C36-C37-C38-C39
50	1I	203	PC1	C1-O11-P-O14
50	1f	101	PC1	C11-O13-P-O14
56	1W	201	EHZ	C6-C7-C8-C9
54	1P	501	NDP	O4B-C4B-C5B-O5B
50	1L	702	PC1	O31-C31-C32-C33
45	1L	701	3PE	C37-C38-C39-C3A
57	1Y	201	PGT	C20-C21-C22-C23
45	1A	201	3PE	O21-C21-C22-C23
48	1F	501	FMN	N10-C1'-C2'-O2'
45	1Y	202	3PE	O22-C21-C22-C23
50	1L	702	PC1	O32-C31-C32-C33
45	1Y	202	3PE	O21-C21-C22-C23

There are no ring outliers.

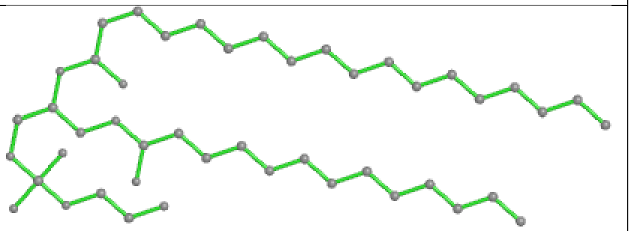
No monomer is involved in short contacts.

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.

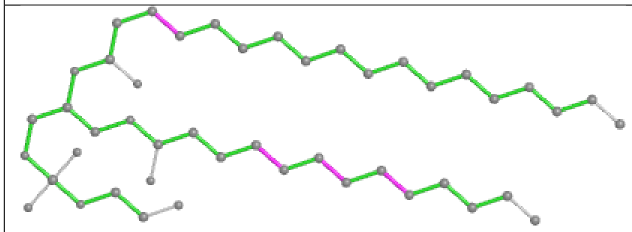
Ligand 3PE 1L 701



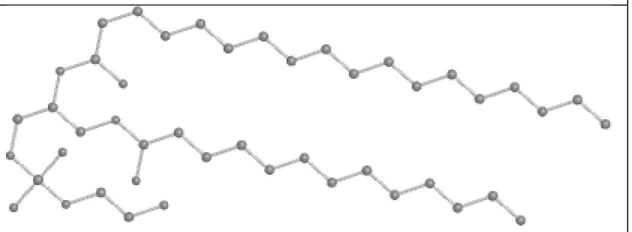
Bond lengths



Bond angles

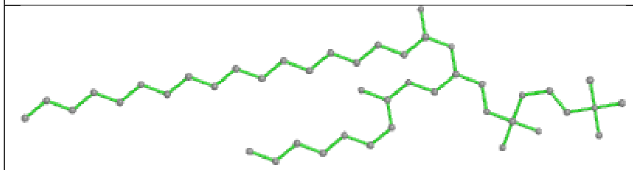


Torsions

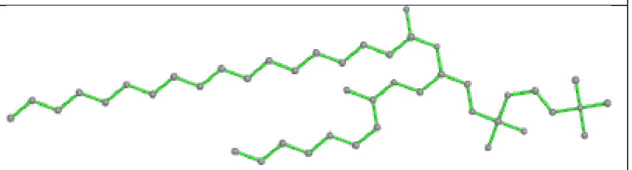


Rings

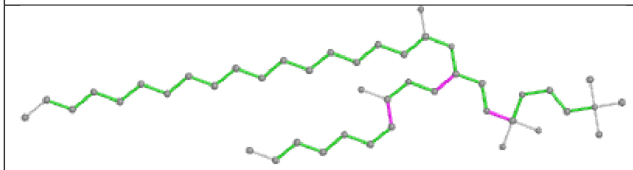
Ligand PC1 1L 702



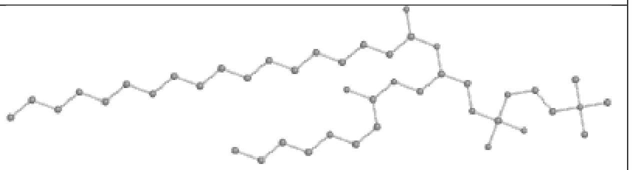
Bond lengths



Bond angles

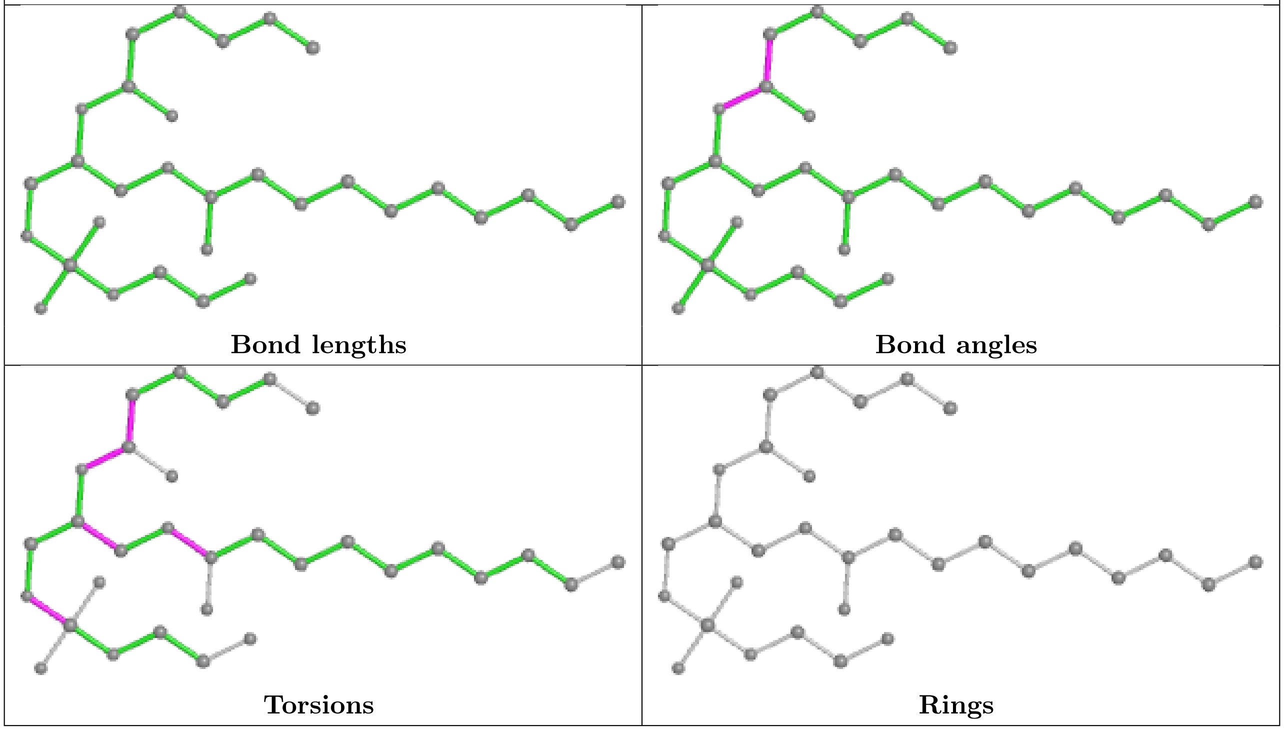


Torsions



Rings

Ligand 3PE 1Y 202



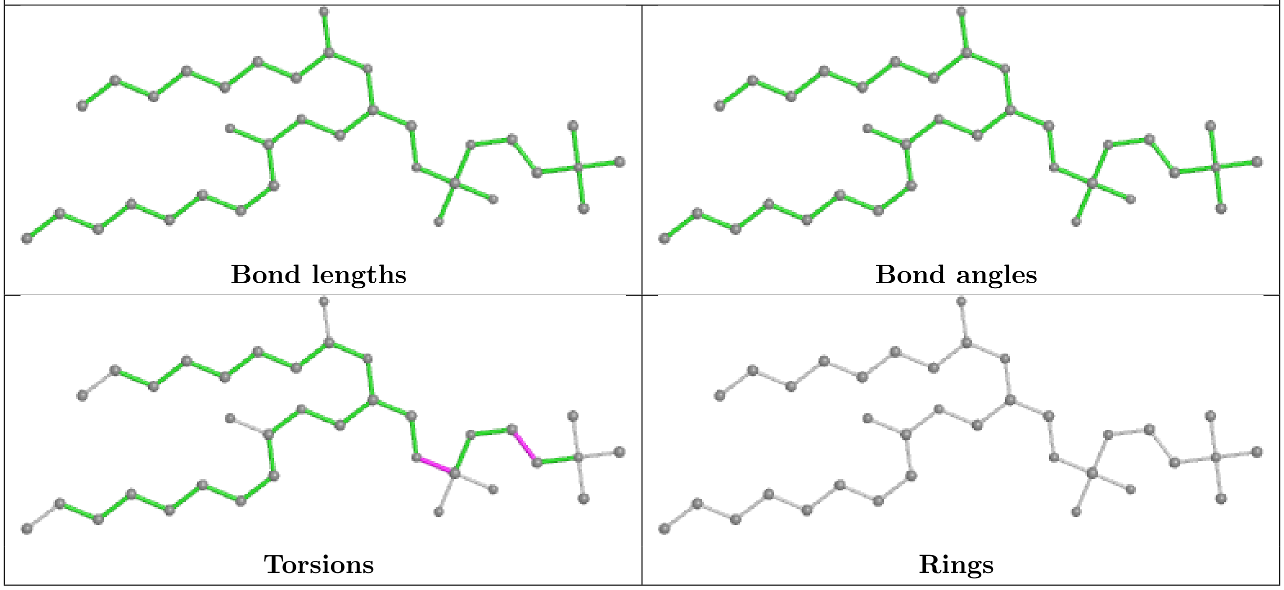
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 1J 201



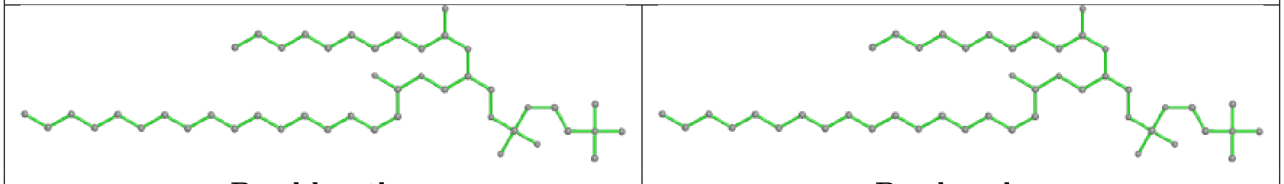
Bond lengths

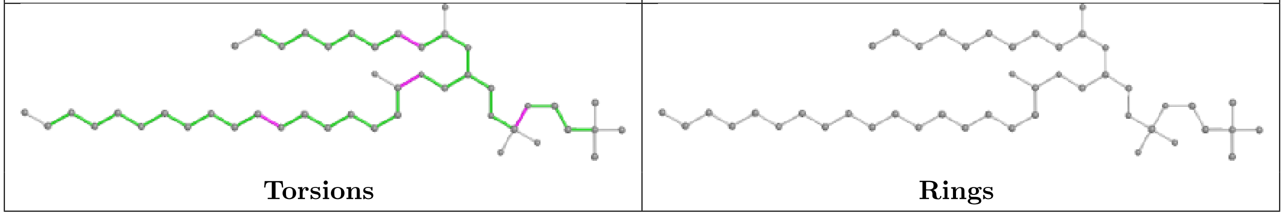
Bond angles

Torsions

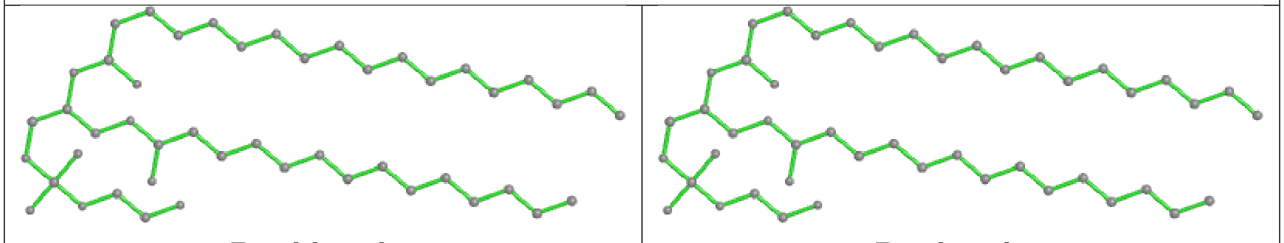
Rings

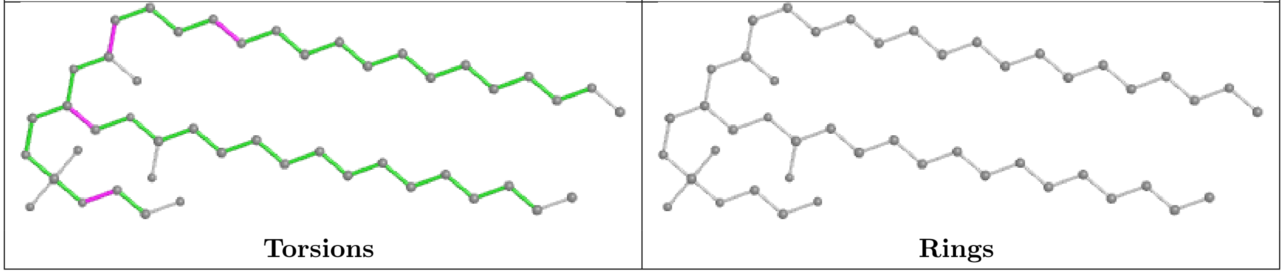
Ligand PC1 1f 101


Bond lengths Bond angles

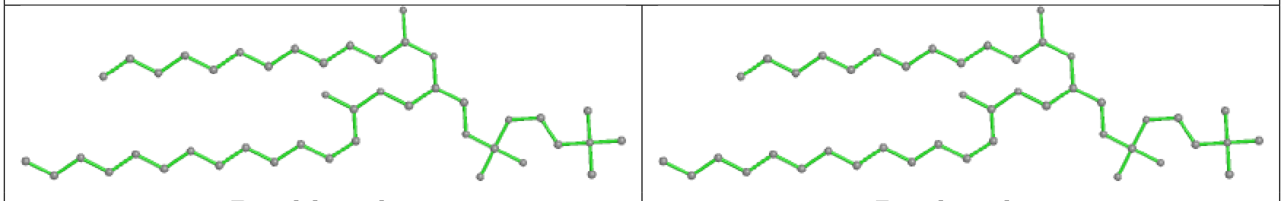

Torsions Rings

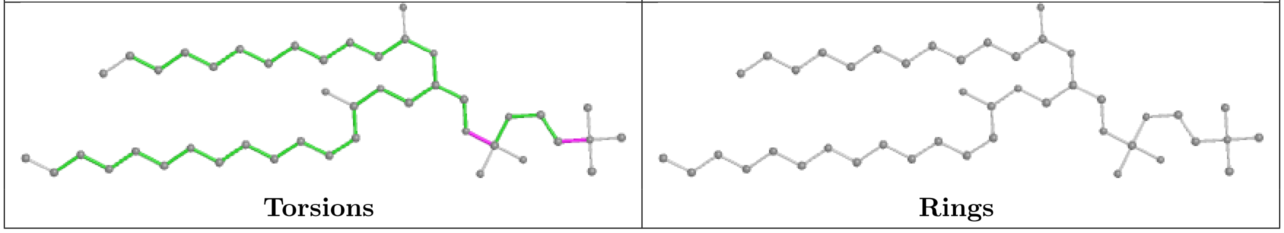
Ligand 3PE 1A 201


Bond lengths Bond angles

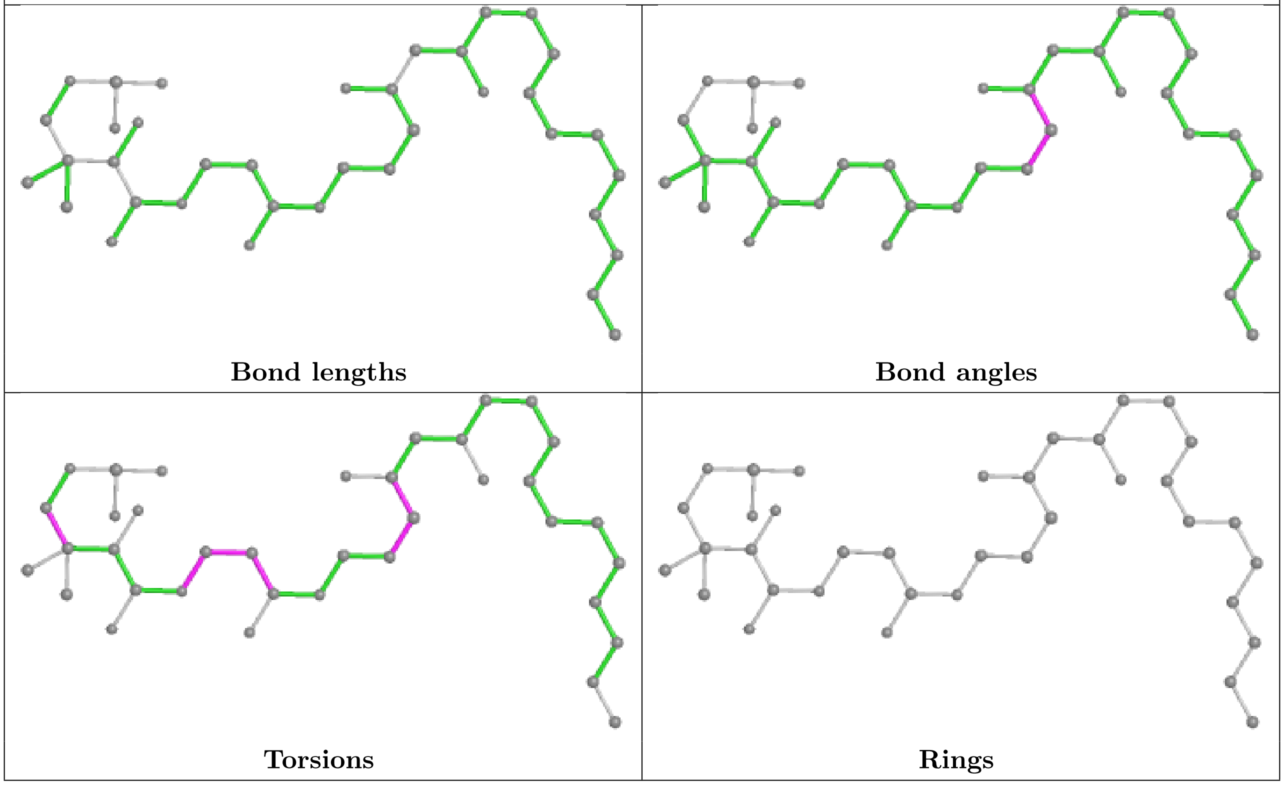

Torsions Rings

Ligand PC1 1I 204


Bond lengths Bond angles


Torsions Rings

Ligand EHZ 1n 201



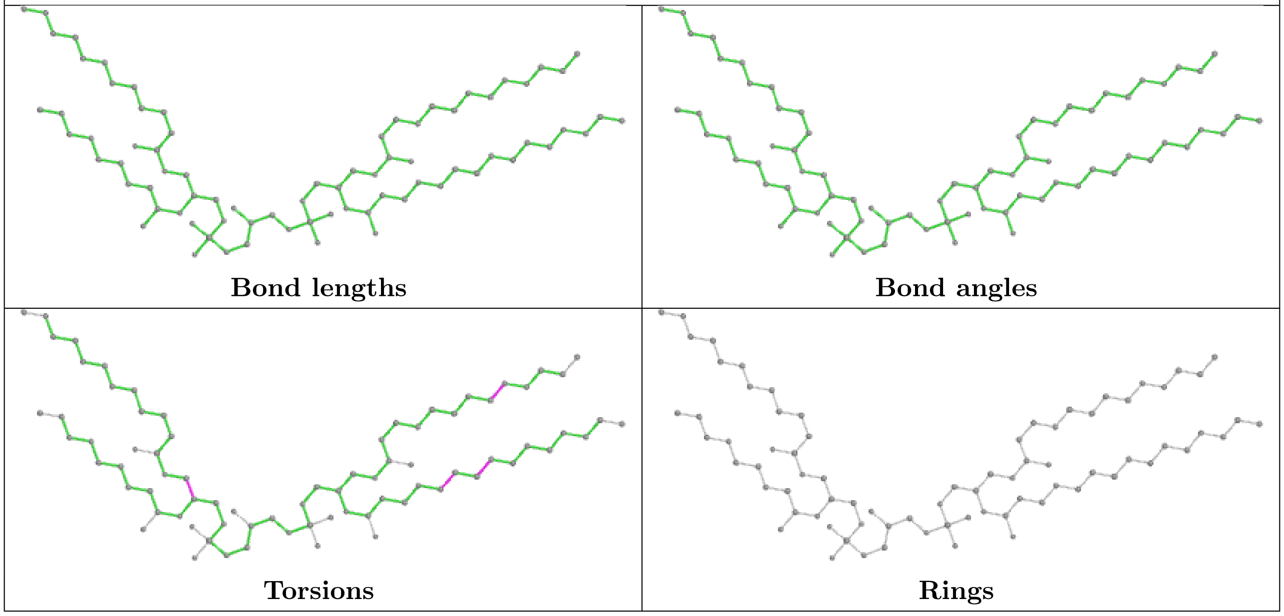
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL 1N 402



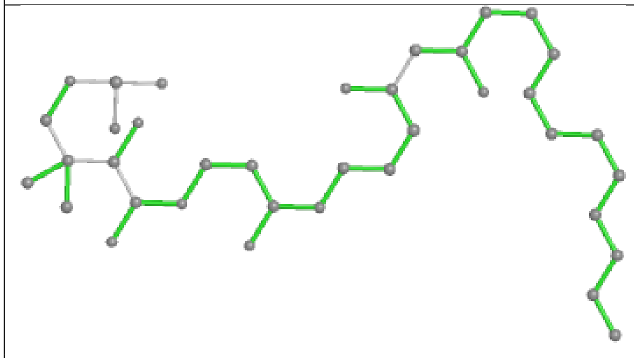
Bond lengths

Bond angles

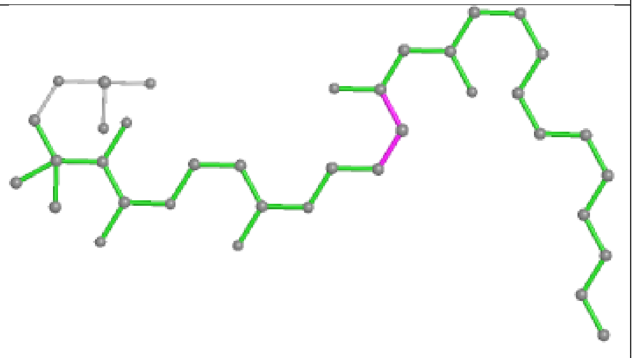
Torsions

Rings

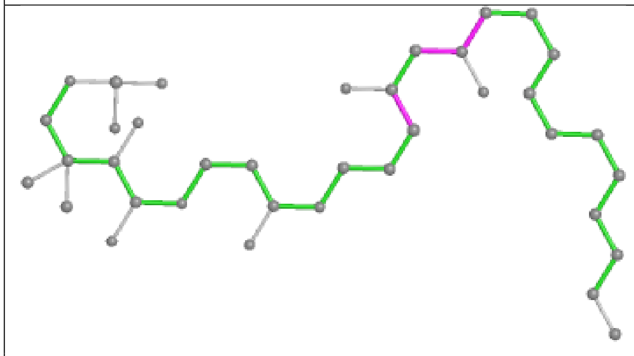
Ligand EHZ 1W 201



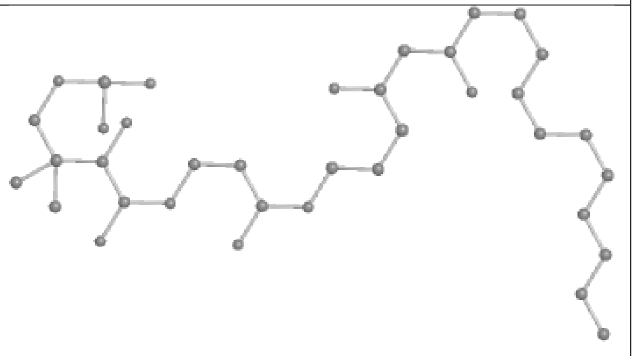
Bond lengths



Bond angles

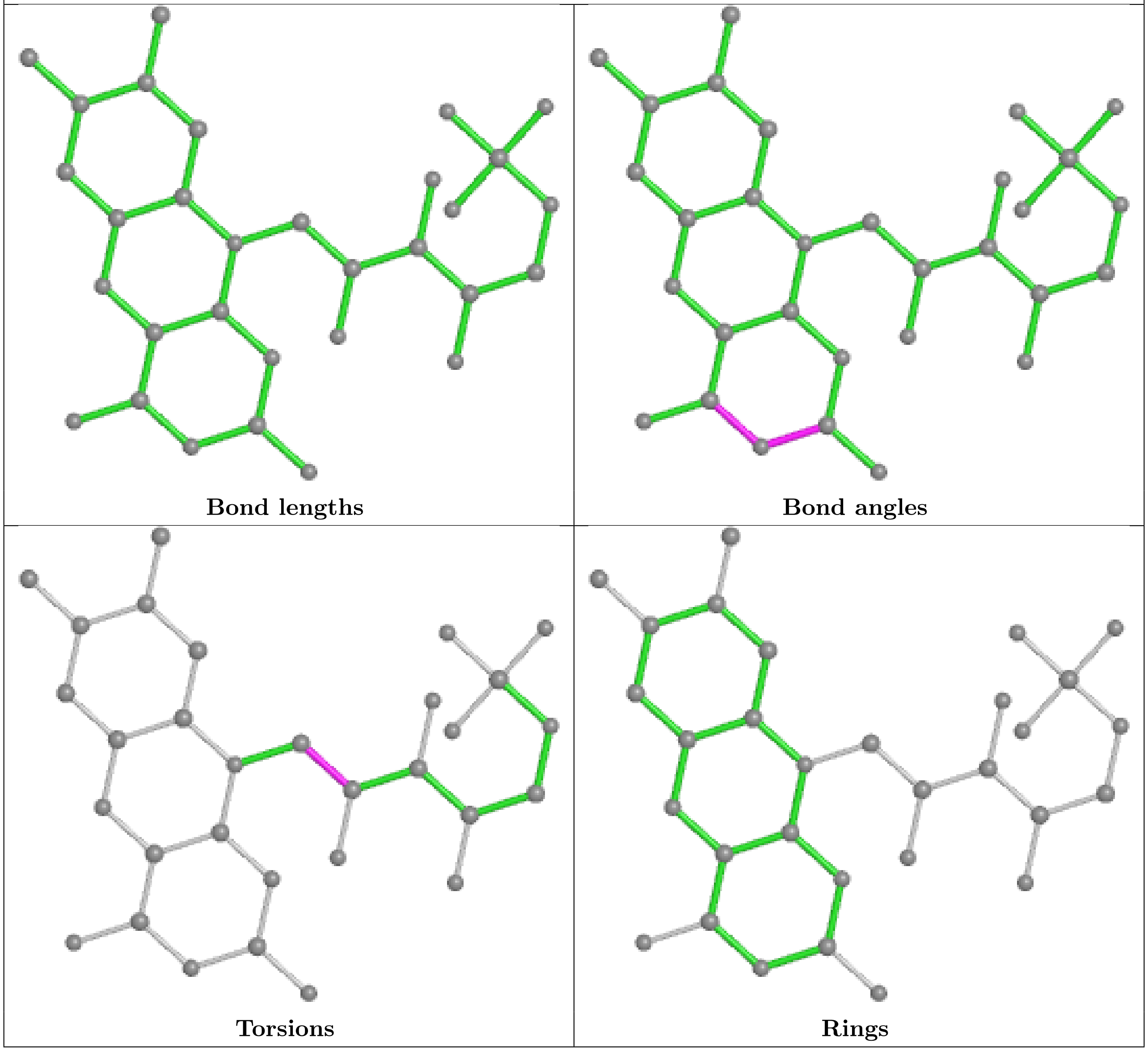


Torsions



Rings

Ligand FMN 1F 501



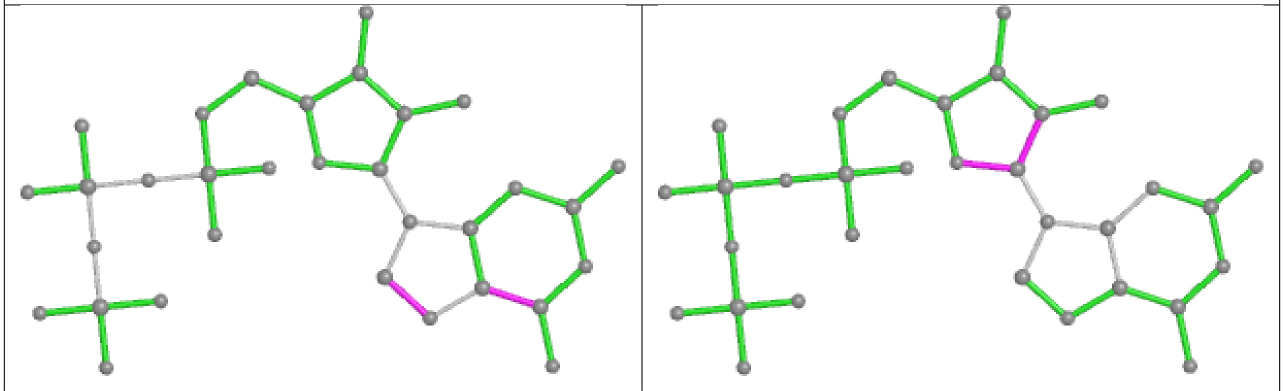
Bond lengths

Bond angles

Torsions

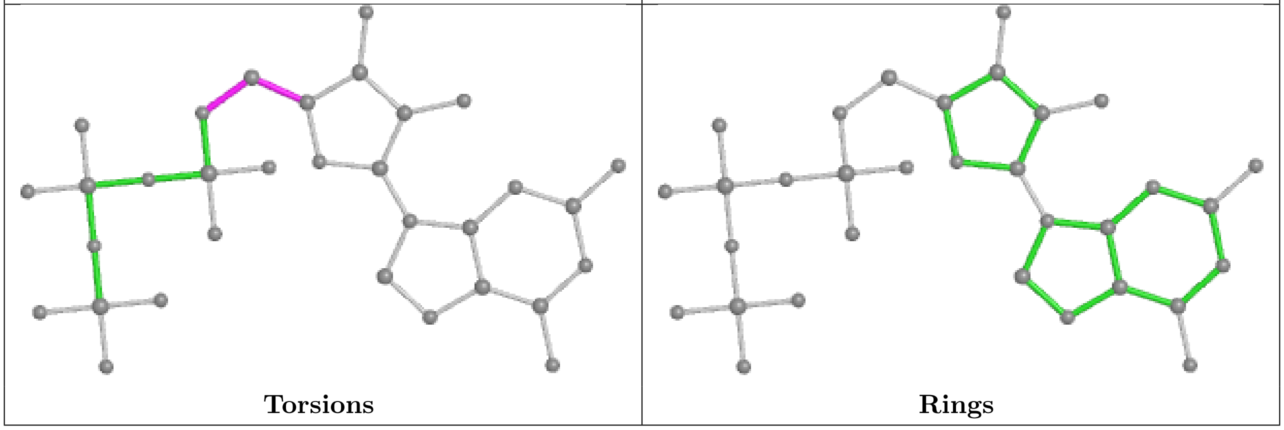
Rings

Ligand GTP 1O 401



Bond lengths

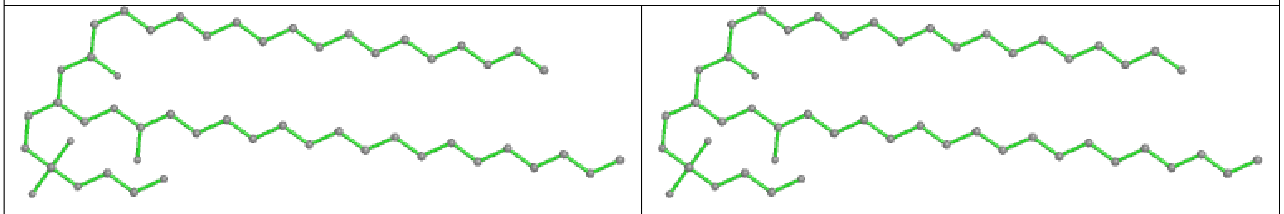
Bond angles



Torsions

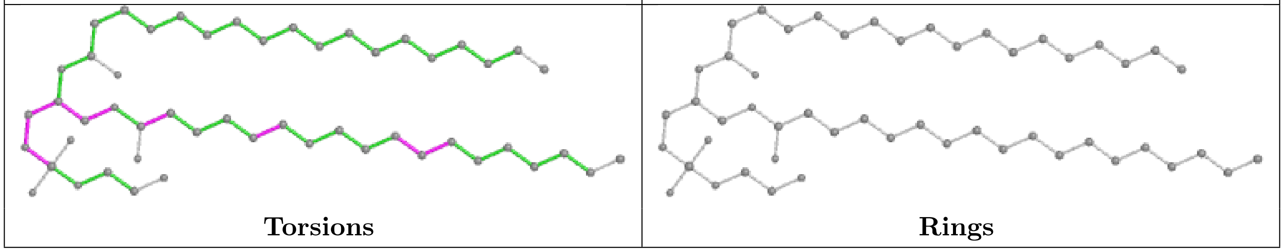
Rings

Ligand 3PE 1N 401



Bond lengths

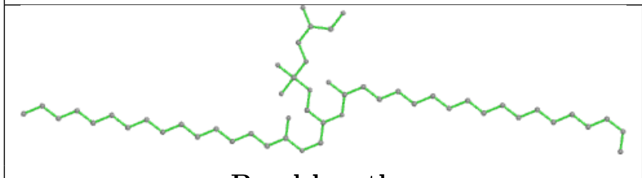
Bond angles



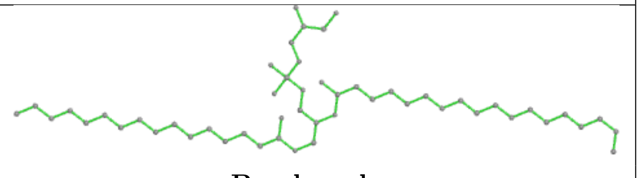
Torsions

Rings

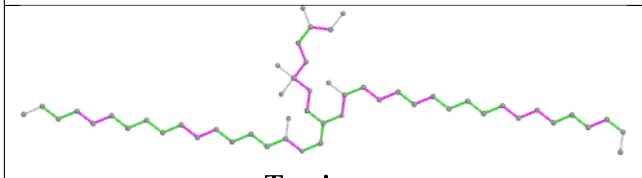
Ligand PGT 1Y 201



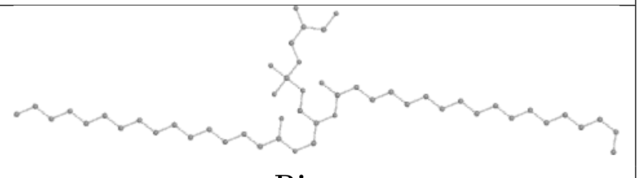
Bond lengths



Bond angles

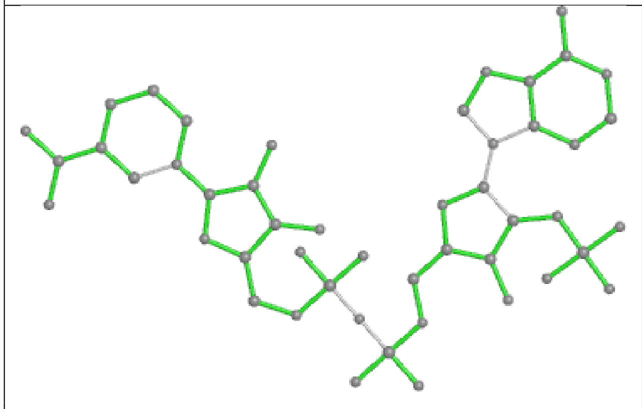


Torsions

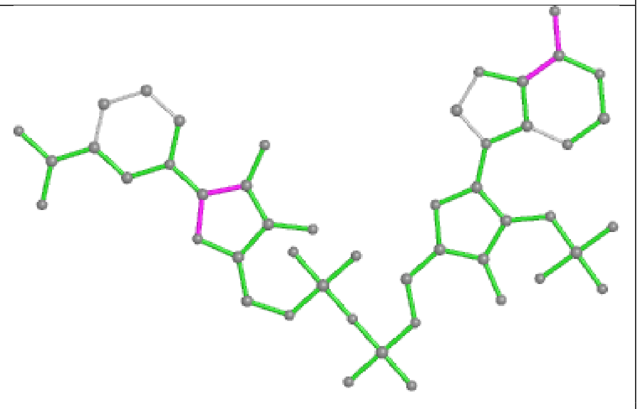


Rings

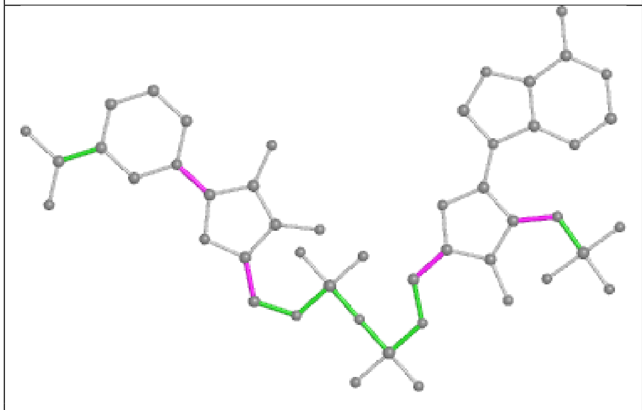
Ligand NDP 1P 501



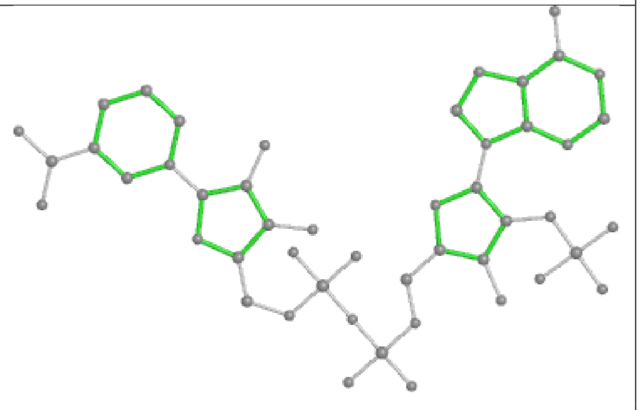
Bond lengths



Bond angles

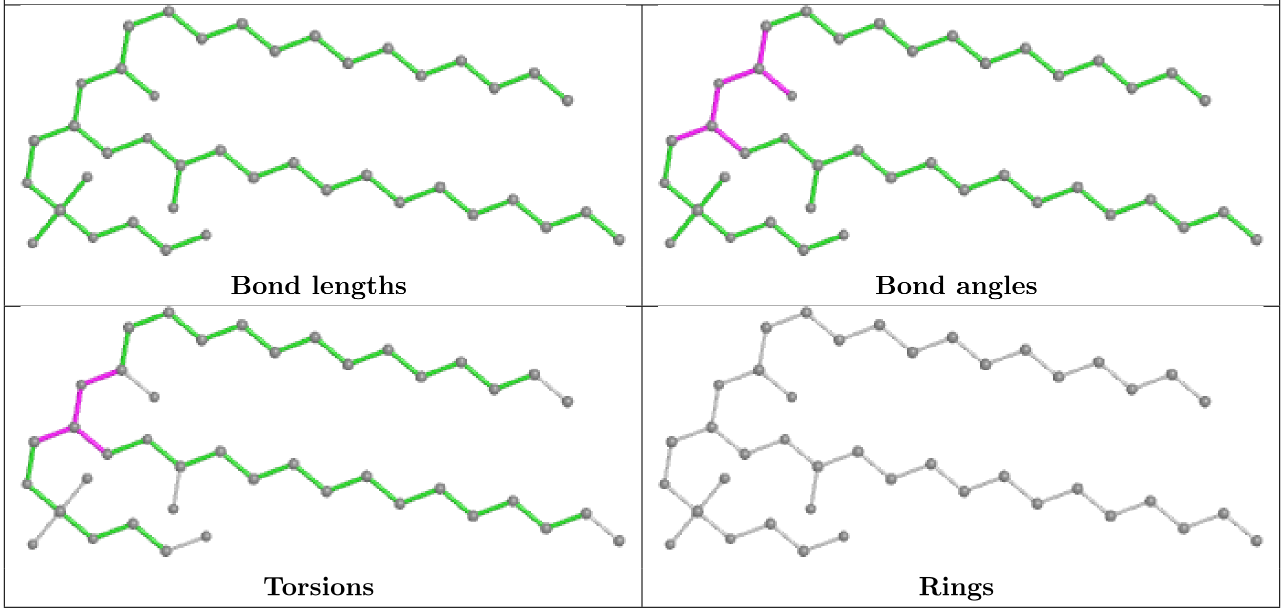


Torsions



Rings

Ligand 3PE 1L 703



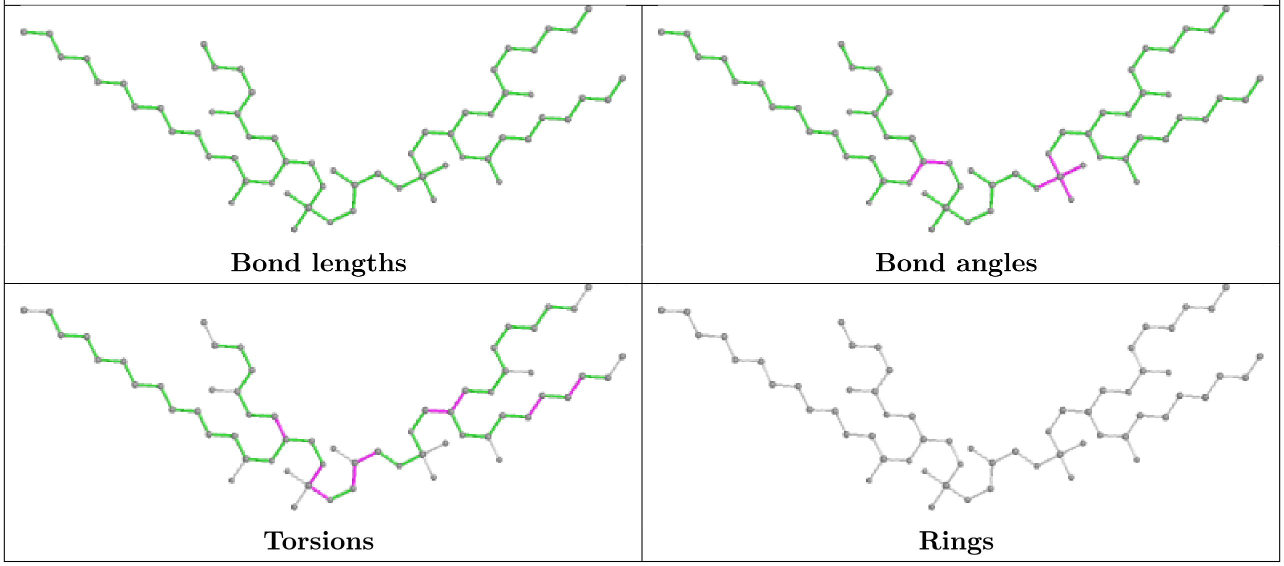
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL 1q 201



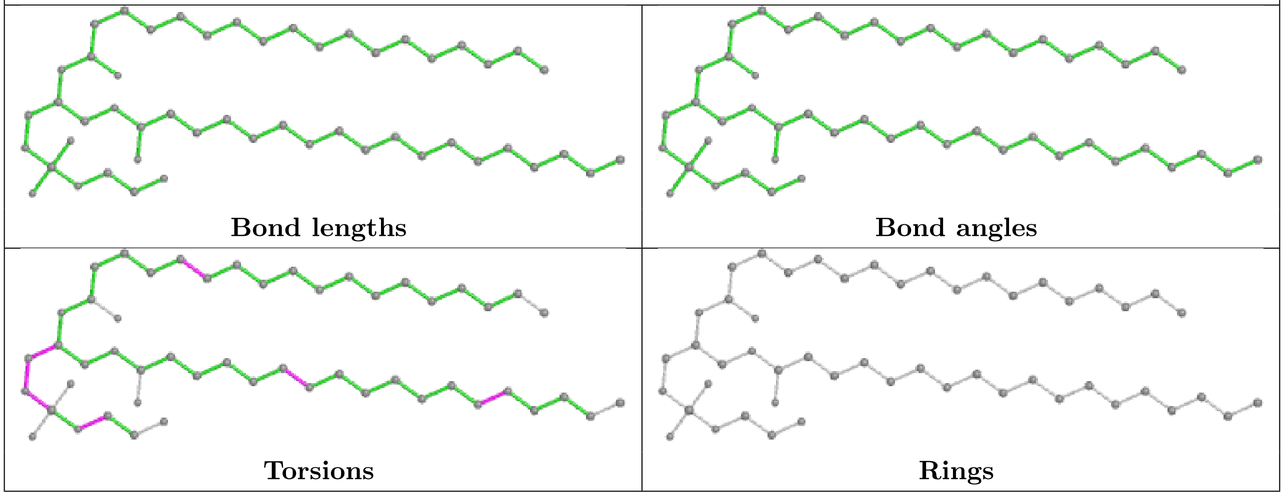
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 1Y 203



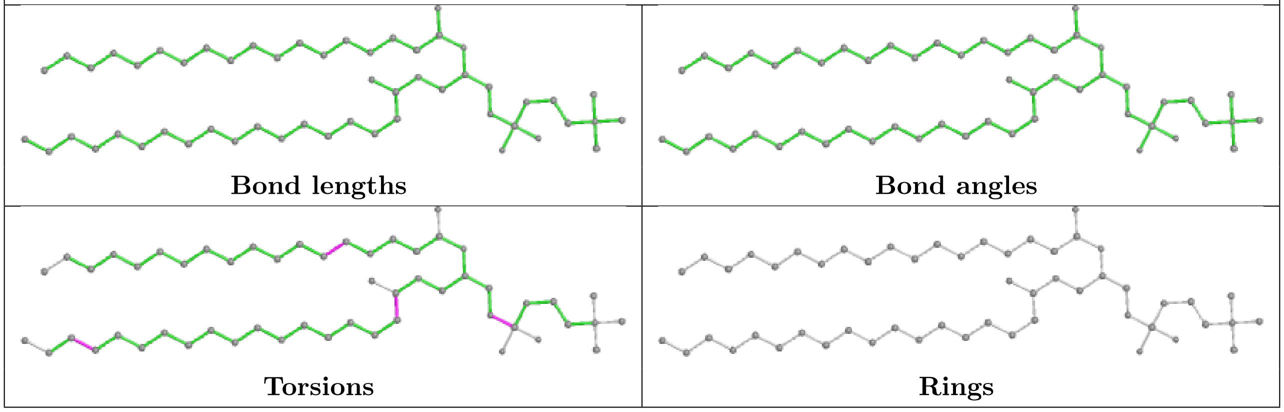
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 1I 203



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
34	1i	1
43	1r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	5.00
1	1r	1:ALA	C	2:SER	N	3.05

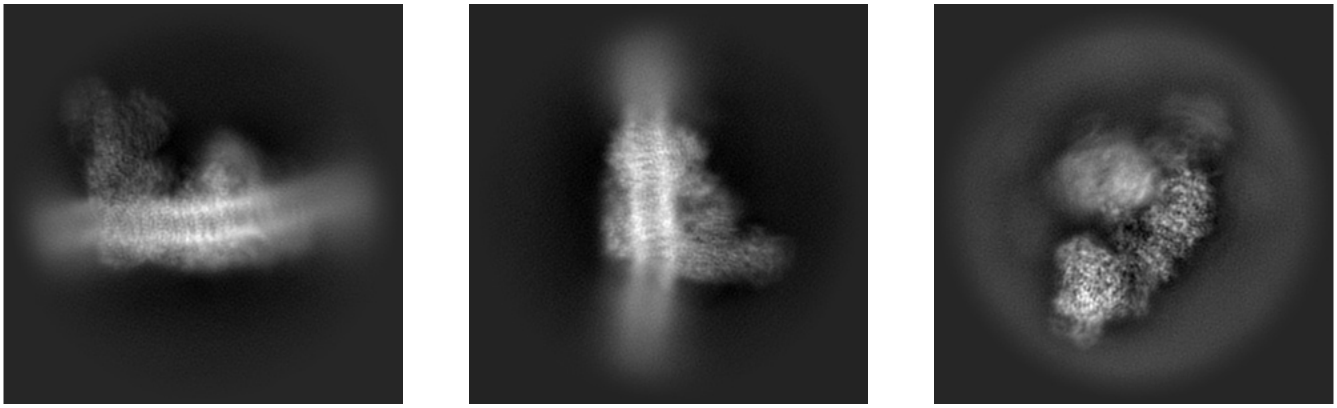
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-42169. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

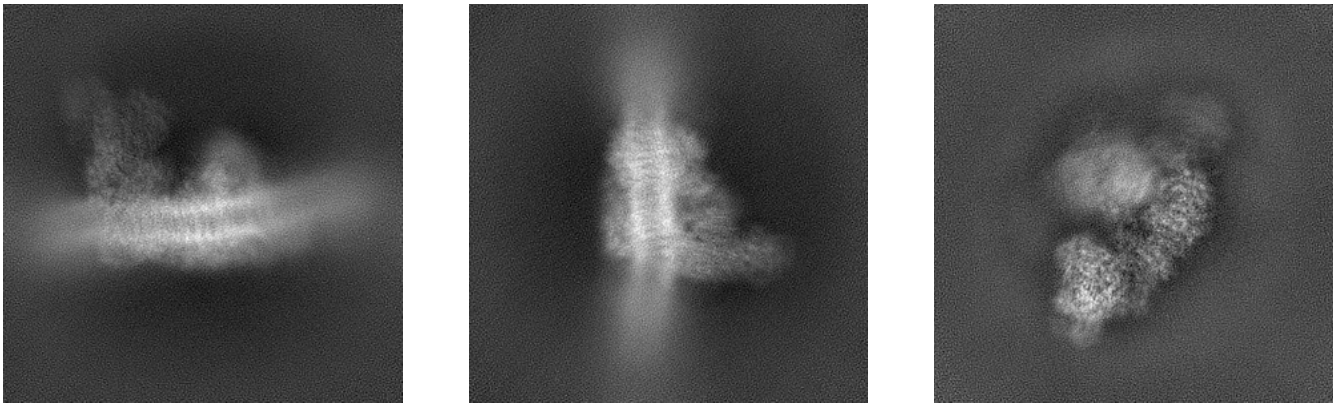
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

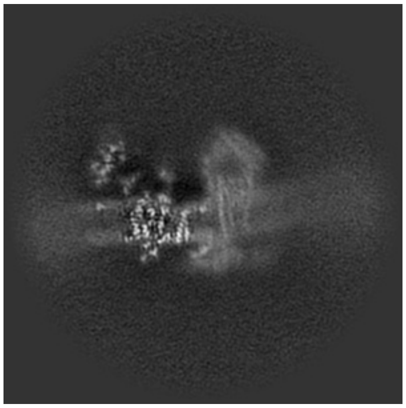


X Y Z

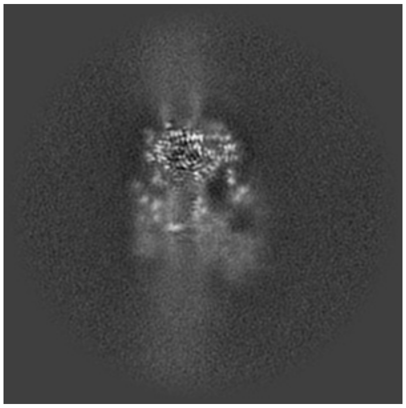
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

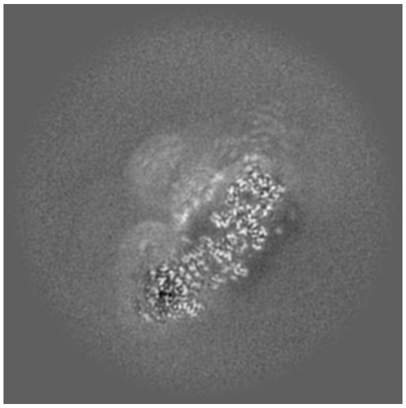
6.2.1 Primary map



X Index: 160

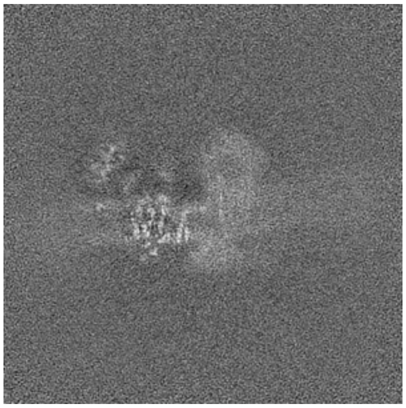


Y Index: 160

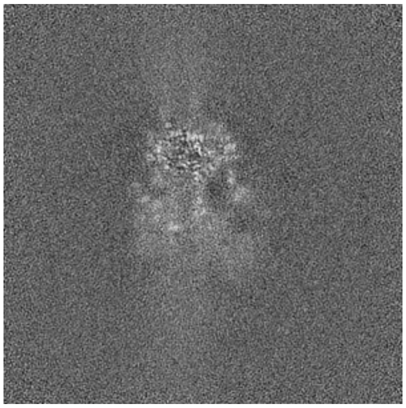


Z Index: 160

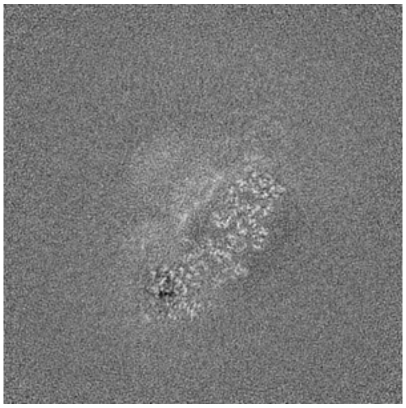
6.2.2 Raw map



X Index: 160



Y Index: 160

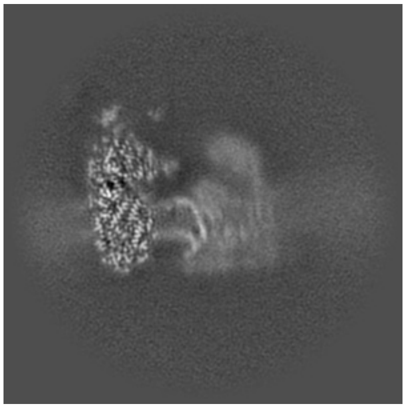


Z Index: 160

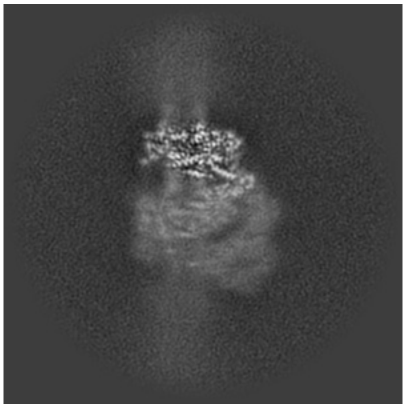
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

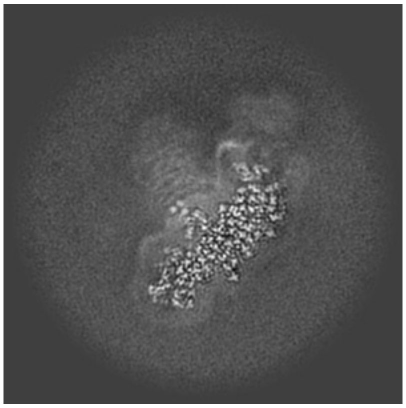
6.3.1 Primary map



X Index: 141

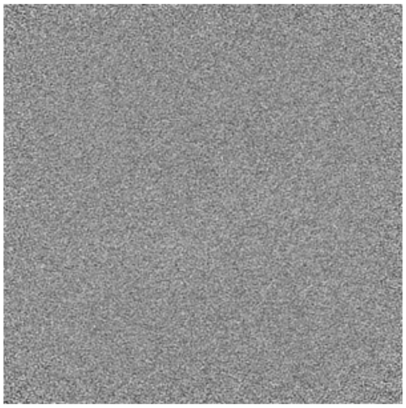


Y Index: 173

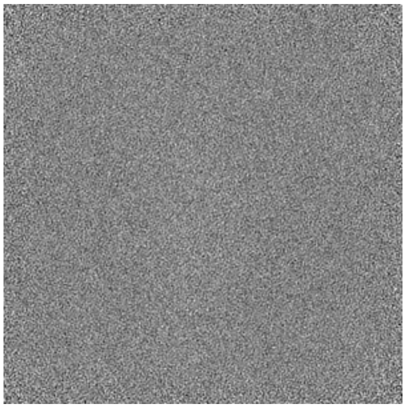


Z Index: 134

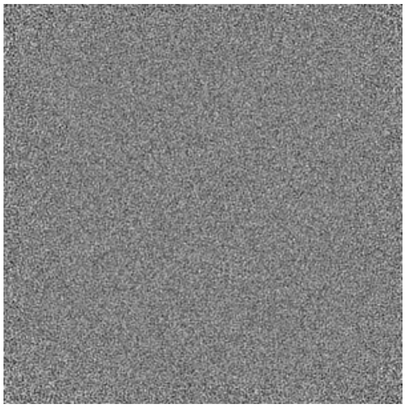
6.3.2 Raw map



X Index: 0



Y Index: 0

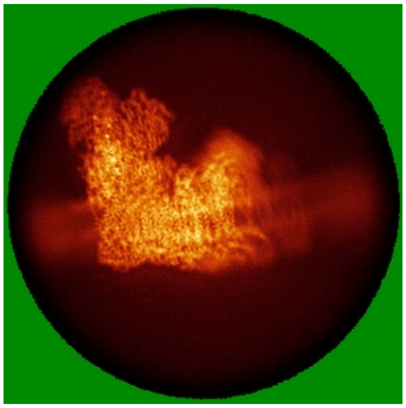


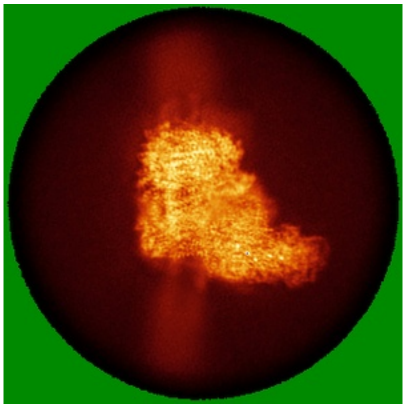
Z Index: 0

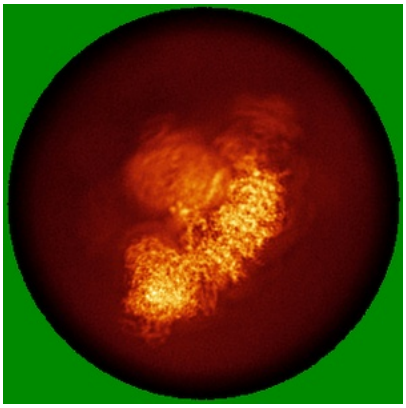
The images above show the largest variance slices of the map in three orthogonal directions.

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

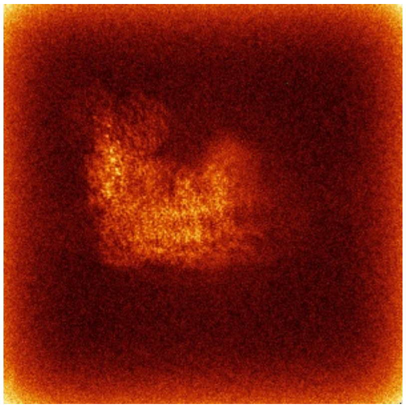
6.4.1 Primary map

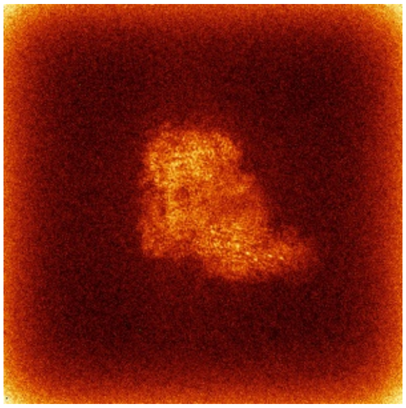

X

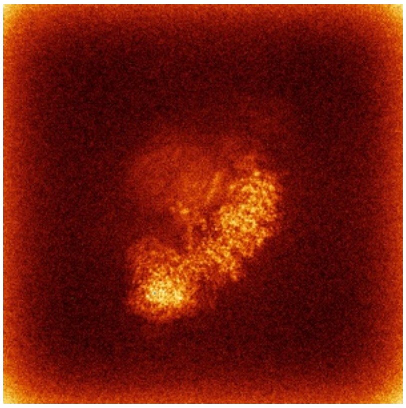

Y


Z

6.4.2 Raw map


X

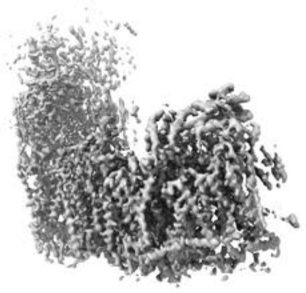

Y


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

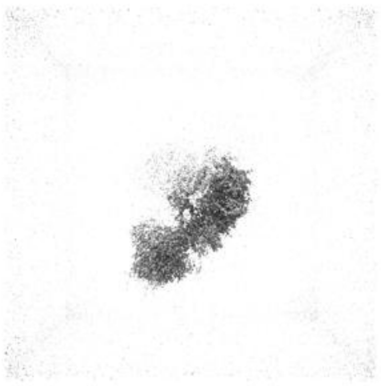
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

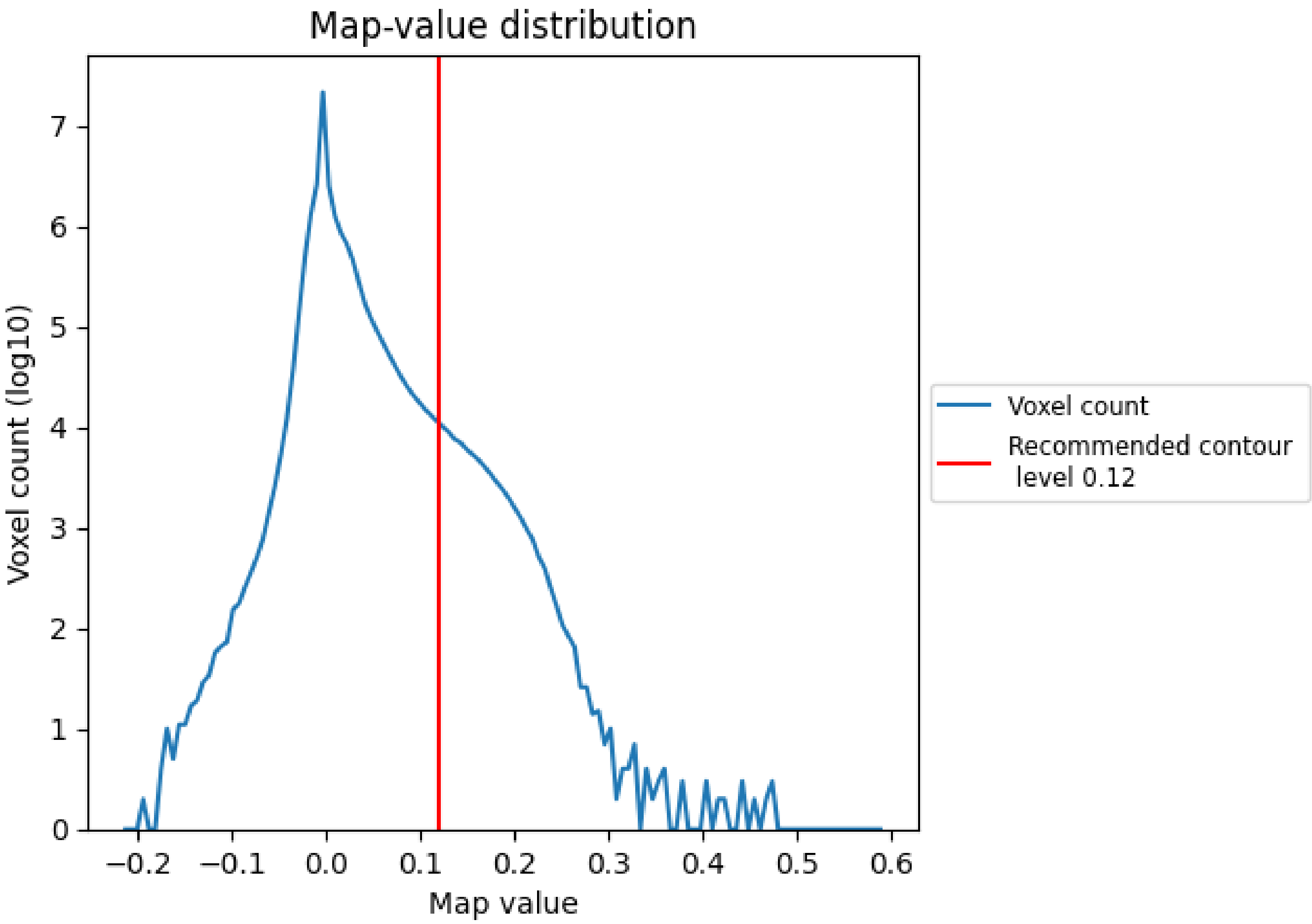
6.6 Mask visualisation

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

7 Map analysis ⓘ

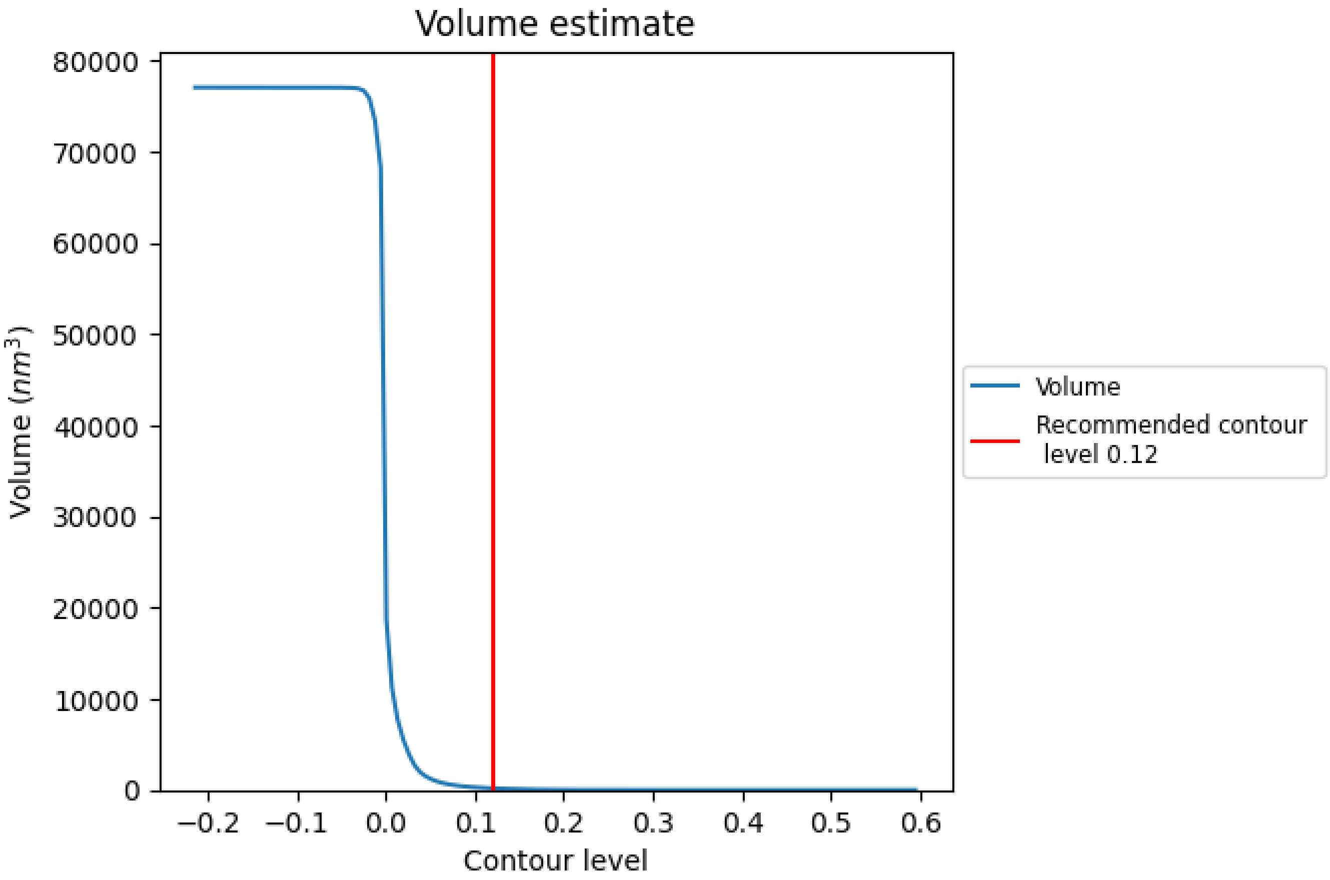
This section contains the results of statistical analysis of the map.

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.

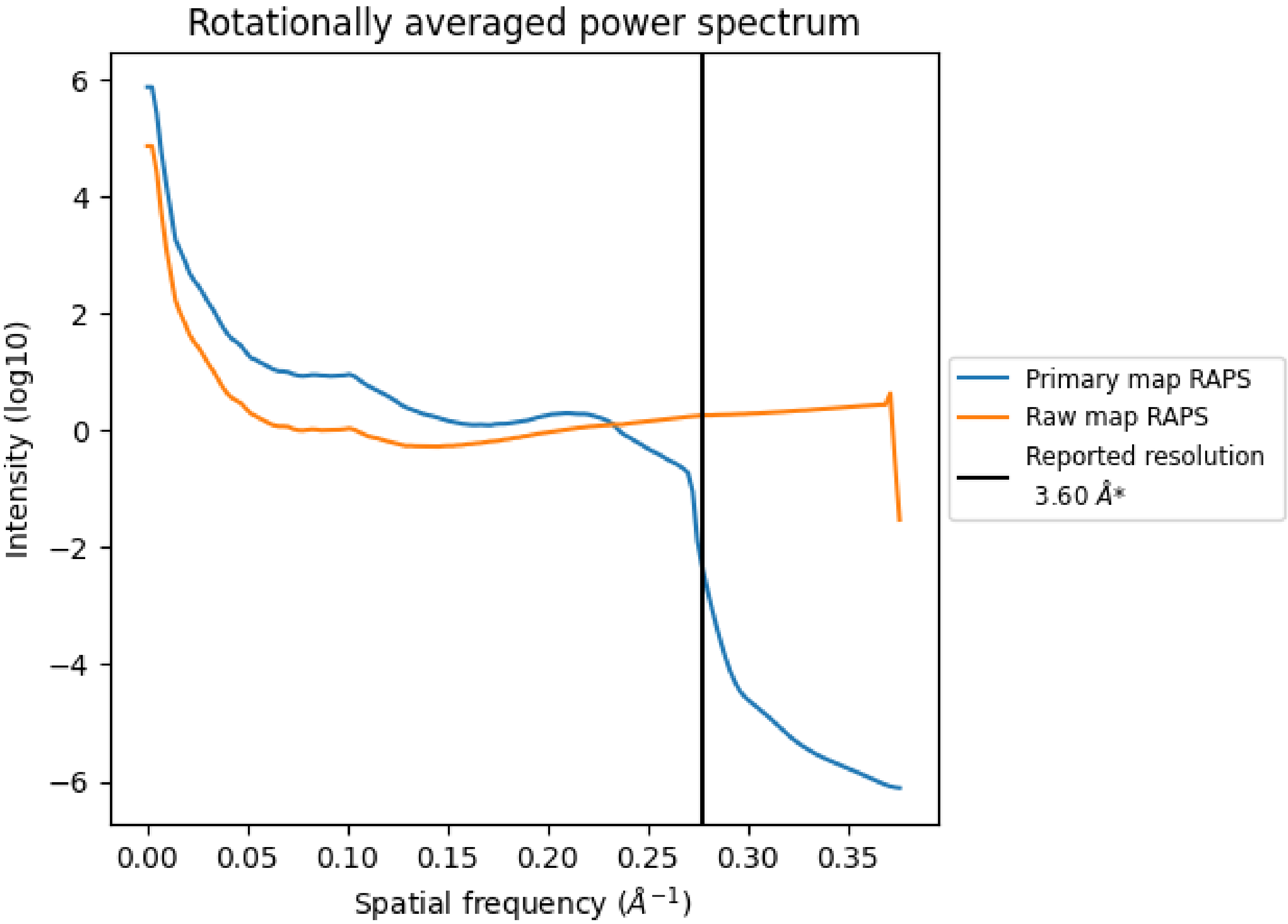
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 181 nm^3; this corresponds to an approximate mass of 163 kDa.

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

7.3 Rotationally averaged power spectrum (i)

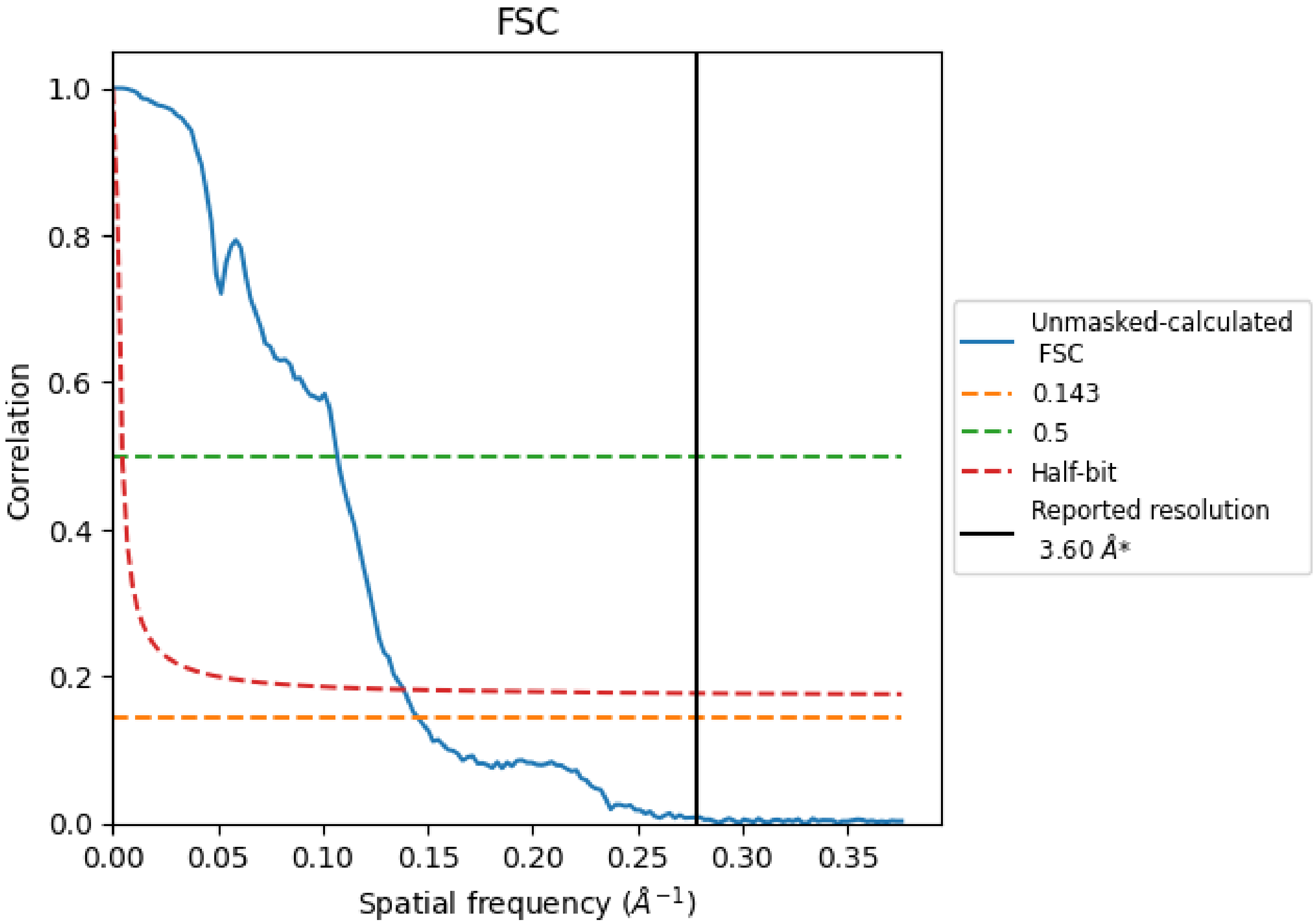


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates ⓘ

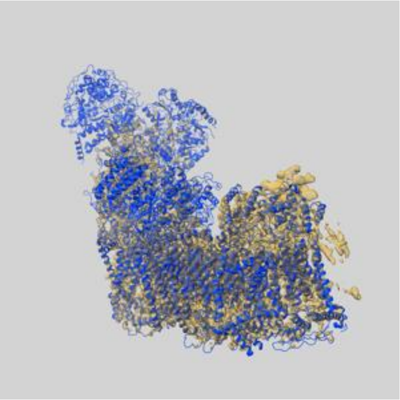
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.87	9.34	7.20

*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 6.87 differs from the reported value 3.6 by more than 10 %

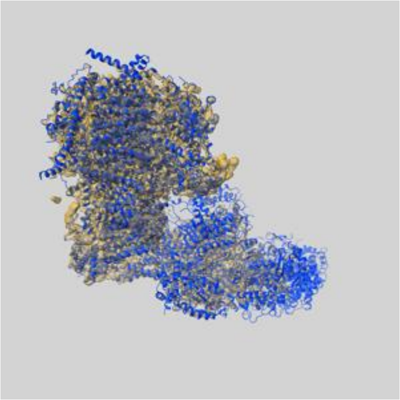
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-42169 and PDB model 8UES. Per-residue inclusion information can be found in section 3 on page 21.

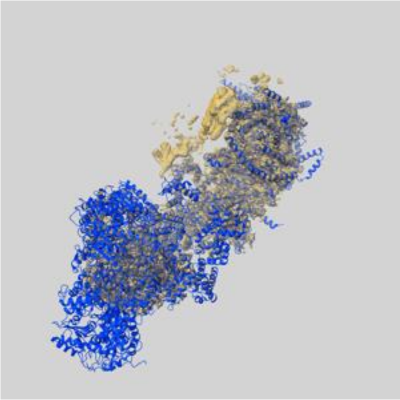
9.1 Map-model overlay ⓘ



X



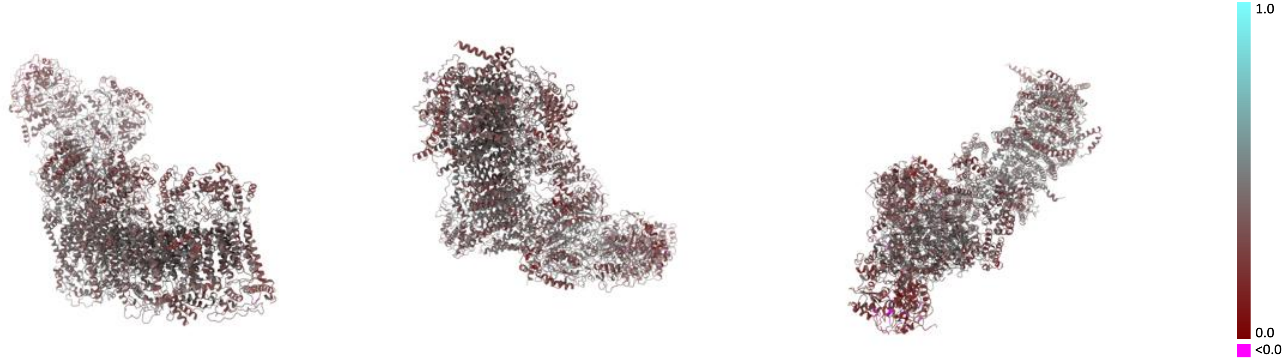
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

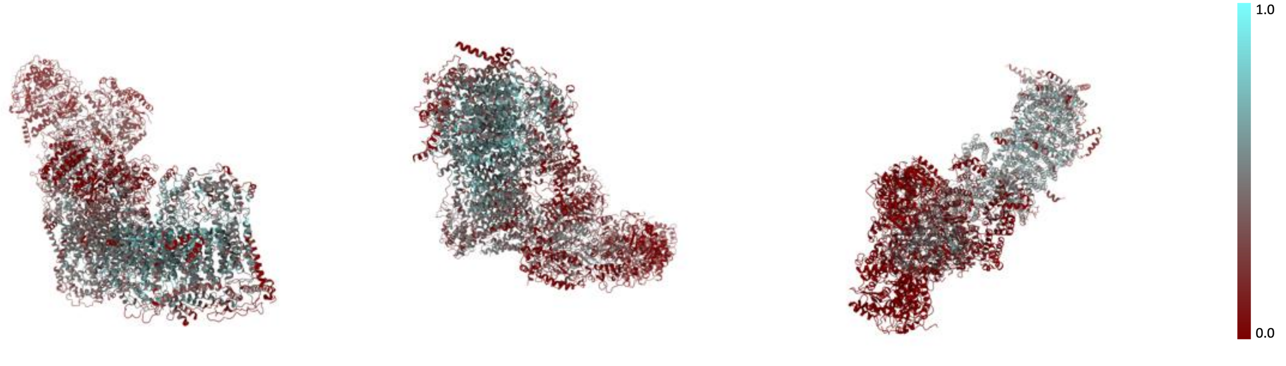
9.2 Q-score mapped to coordinate model ⓘ



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.

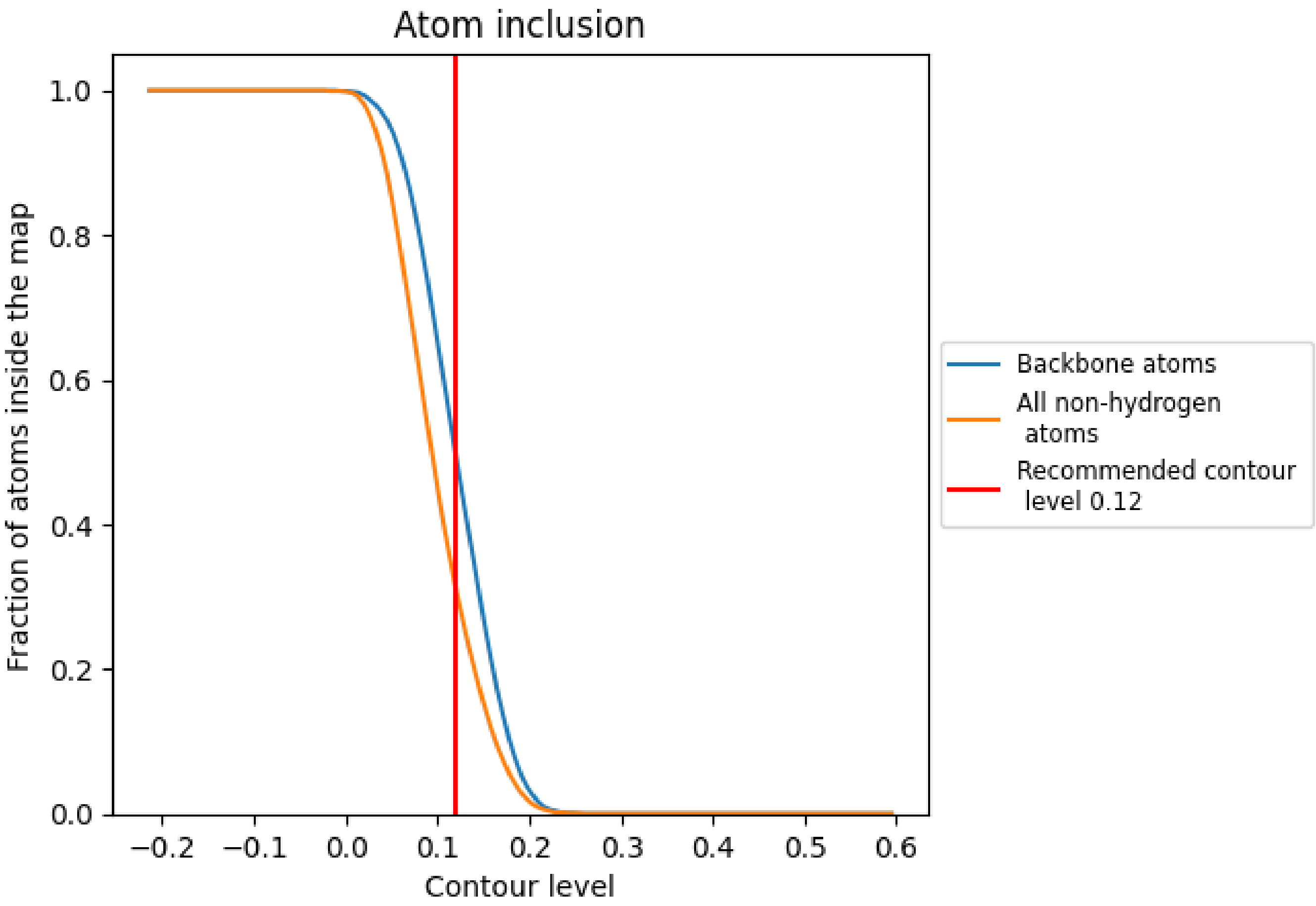
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 49% of all backbone atoms, 31% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3100	0.3800
1A	0.2840	0.3840
1B	0.3950	0.4320
1C	0.1910	0.4110
1D	0.3410	0.4120
1E	0.0040	0.2970
1F	0.0090	0.2810
1G	0.1260	0.3660
1H	0.4090	0.4160
1I	0.4090	0.4200
1J	0.3100	0.3730
1K	0.4190	0.4080
1L	0.5480	0.4000
1M	0.6040	0.4360
1N	0.5030	0.4250
1O	0.1880	0.3600
1P	0.1110	0.3450
1Q	0.1270	0.3760
1R	0.1550	0.4050
1S	0.0130	0.2940
1T	0.0410	0.2690
1U	0.4260	0.3490
1V	0.0510	0.3420
1W	0.1360	0.3460
1X	0.3390	0.4070
1Y	0.4450	0.3790
1Z	0.3580	0.4130
1a	0.4380	0.4050
1b	0.3230	0.4120
1c	0.2860	0.3610
1d	0.4730	0.4160
1e	0.4220	0.4270
1f	0.2900	0.3850
1g	0.4080	0.3800
1h	0.4720	0.4170

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Chain	Atom inclusion	Q-score
1i	0.2480	0.3510
1j	0.3160	0.3660
1k	0.3130	0.3460
1l	0.4300	0.3910
1m	0.5090	0.3760
1n	0.4620	0.3560
1o	0.2920	0.3240
1p	0.4050	0.3870
1q	0.2220	0.4100
1r	0.1870	0.4020
1s	0.0000	0.2530