Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 10:58 AM EDT

PDB ID	:	8UEV
EMDB ID	:	EMD-42172
Title	:	In-situ complex I, Deactive class04
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-10-02
Resolution	:	3.70 Å(reported)

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

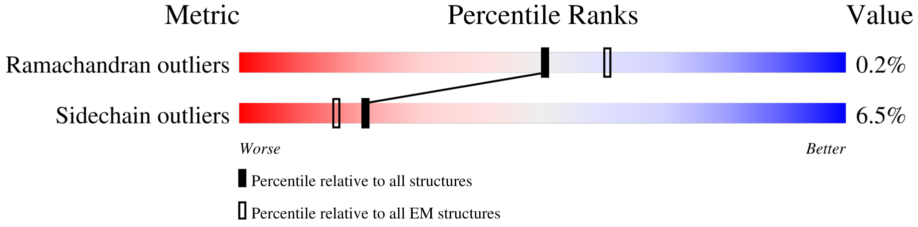
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

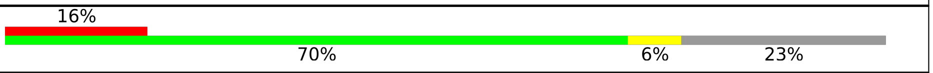
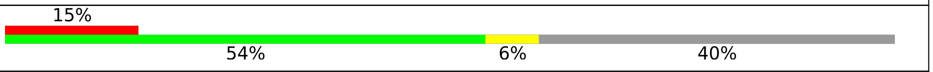
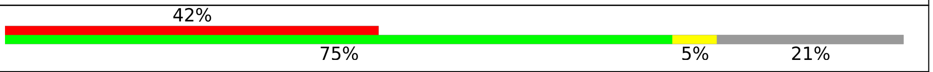
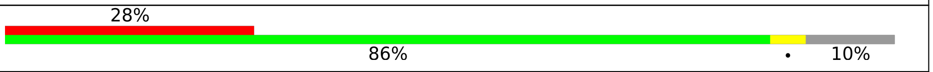
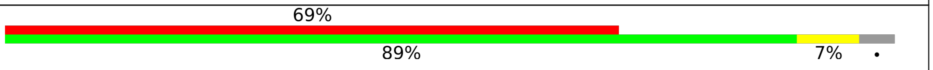
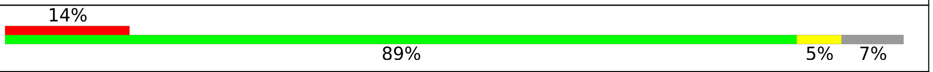
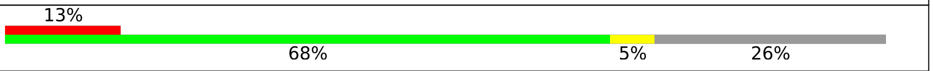
The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	115	 16% 70% 6% 23%
2	1B	258	 15% 54% 6% 40%
3	1C	264	 42% 75% 5% 21%
4	1D	476	 28% 86% • 10%
5	1E	249	 85% 78% 7% • 14%
6	1F	464	 92% 86% 7% 7%
7	1G	727	 69% 89% 7% •
8	1H	318	 14% 89% 5% 7%
9	1I	239	 13% 68% 5% 26%

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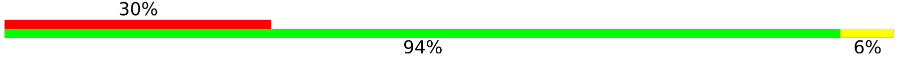
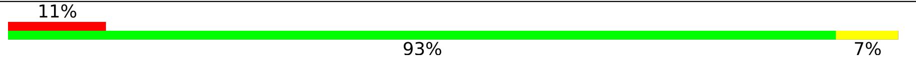
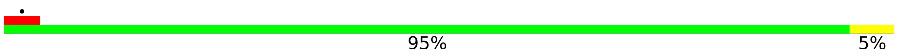
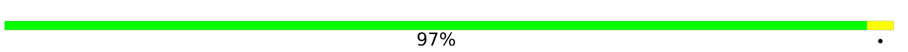
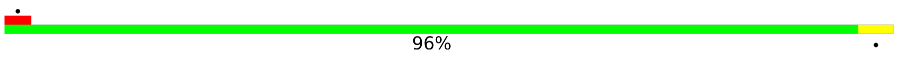
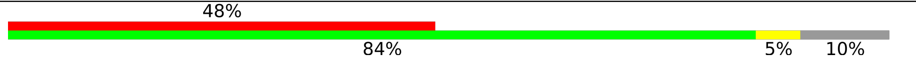
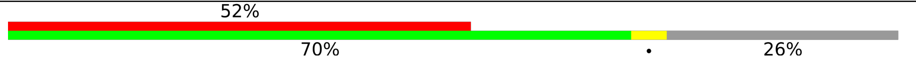
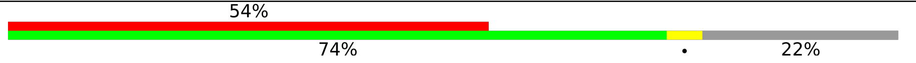
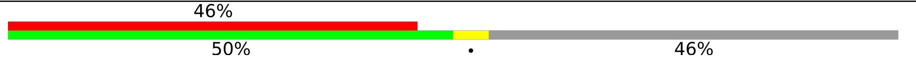
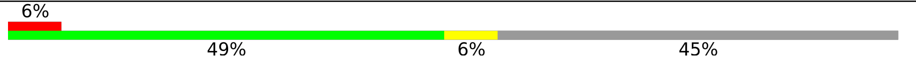
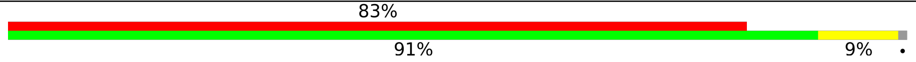
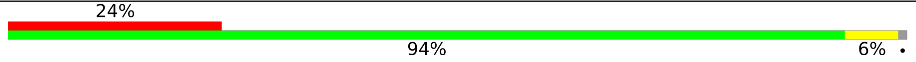
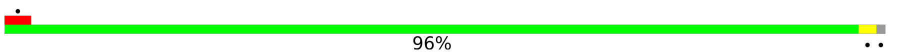
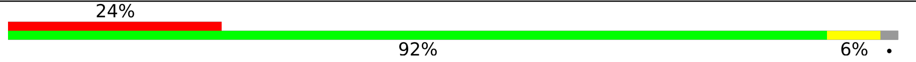
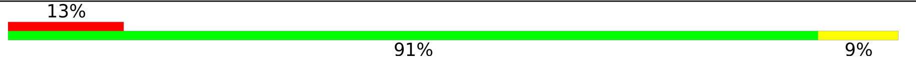
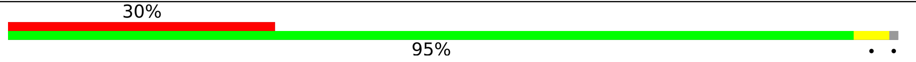
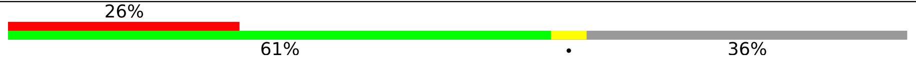
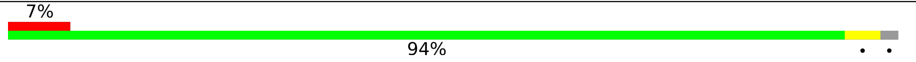
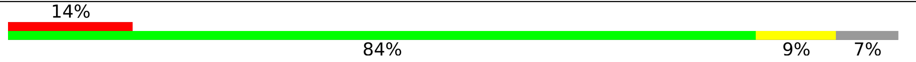
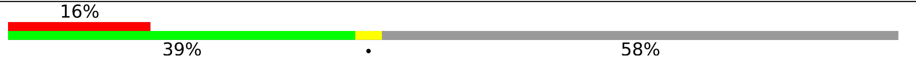
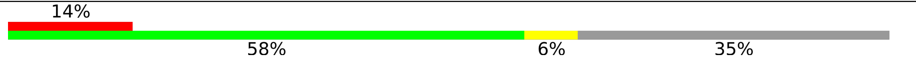
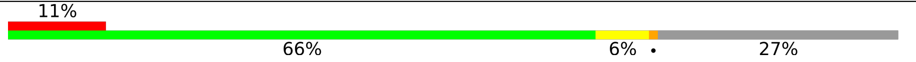
Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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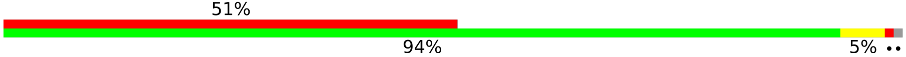
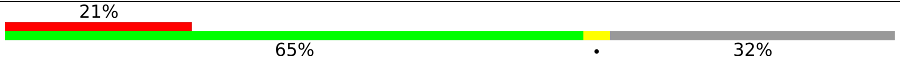
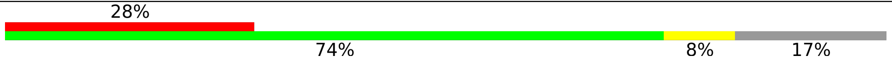
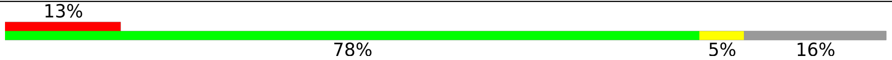
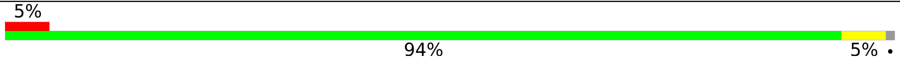
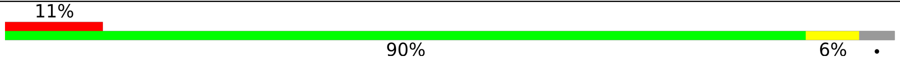
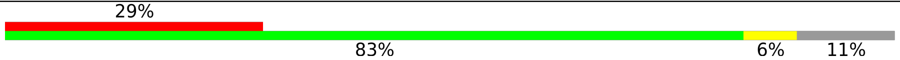
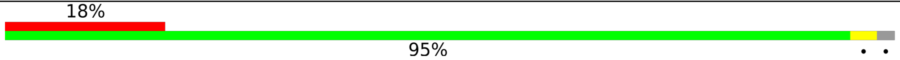
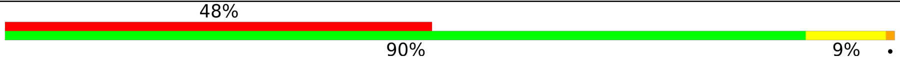
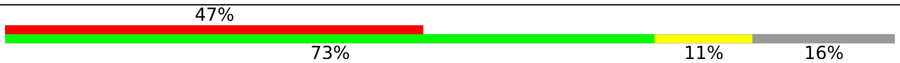
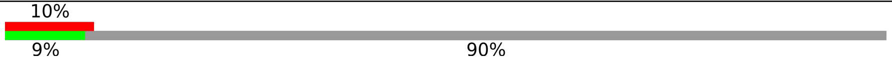
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

2 Entry composition ⓘ

There are 58 unique types of molecules in this entry. The entry contains 67103 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	88	707	484	101	117	5	0	0

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	297	Total 2344	C 1571	N 363	O 389	S 21	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

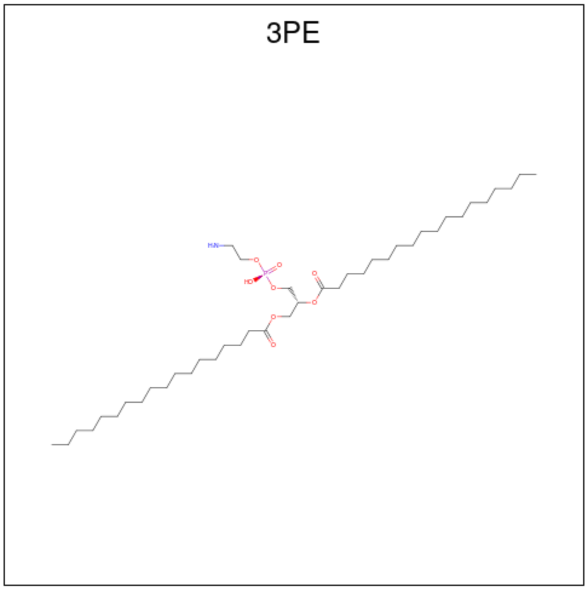
There is a discrepancy between the modelled and reference sequences:

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

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

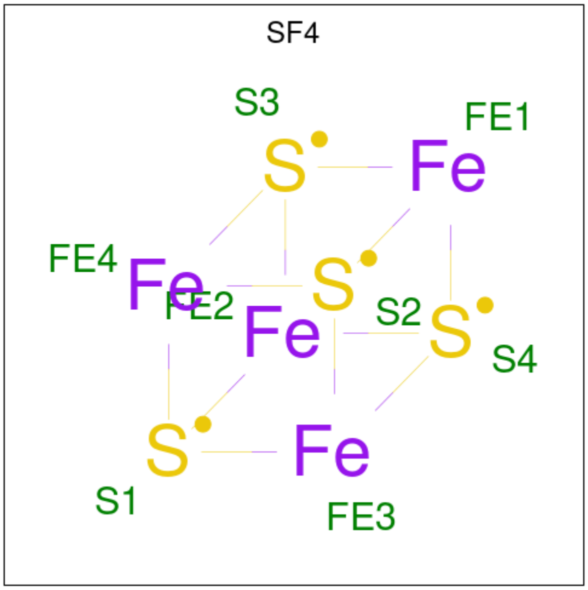
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1s	45	382	238	70	73	1	0	0

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



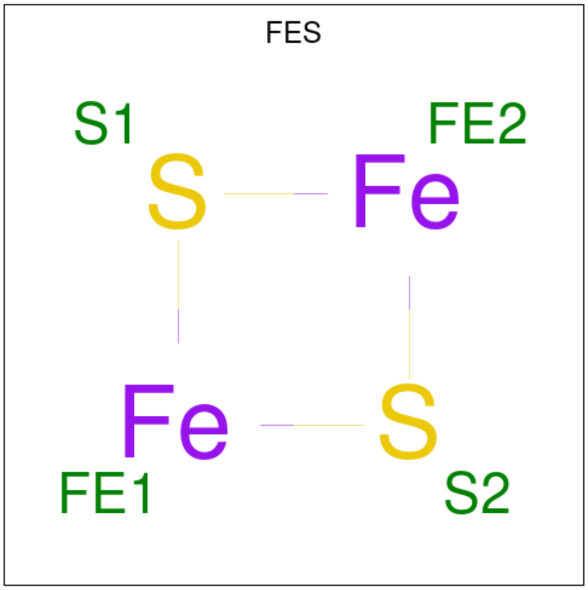
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	1A	1	47	37	1	8	1	0
45	1L	1	46	36	1	8	1	0
45	1L	1	42	32	1	8	1	0
45	1N	1	51	41	1	8	1	0
45	1Y	1	31	21	1	8	1	0
45	1Y	1	51	41	1	8	1	0

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



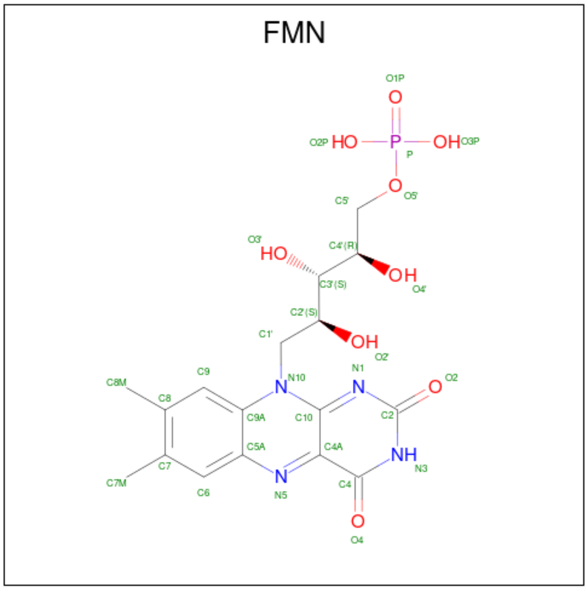
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total Fe S 8 4 4	0
46	1F	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0

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

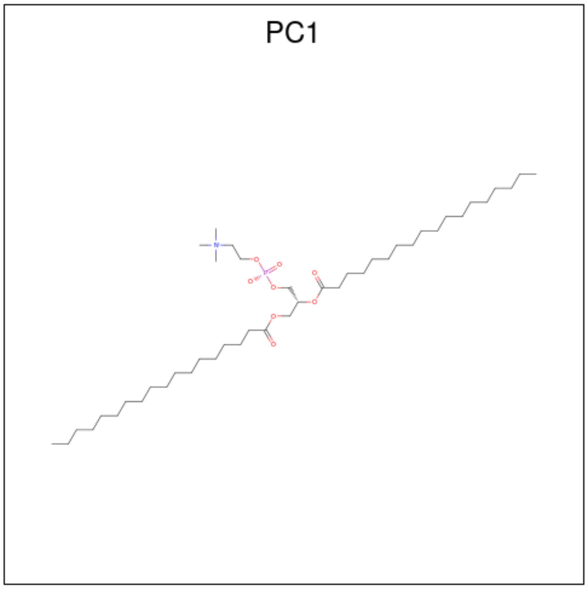


Mol	Chain	Residues	Atoms	AltConf
48	1F	1	Total C N O P 31 17 4 9 1	0

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

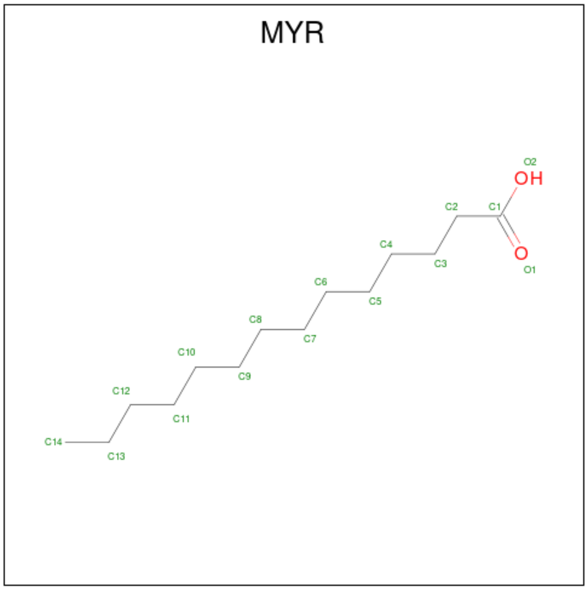
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total 1	K 1	0

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



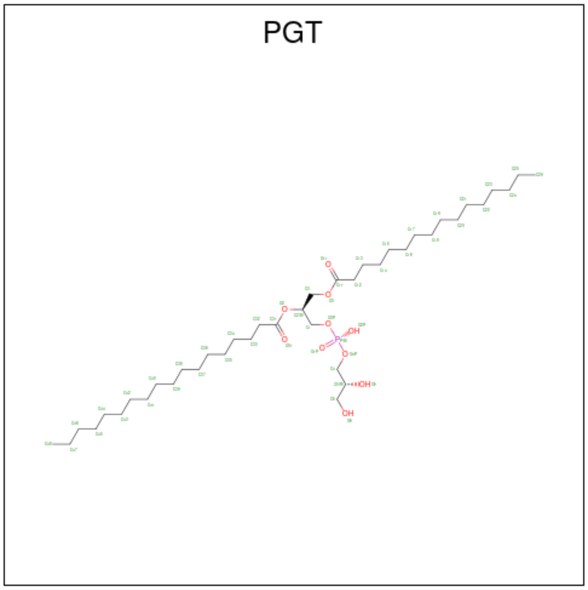
Mol	Chain	Residues	Atoms					AltConf
50	1I	1	Total 54	C 44	N 1	O 8	P 1	0
50	1I	1	Total 44	C 34	N 1	O 8	P 1	0
50	1J	1	Total 35	C 25	N 1	O 8	P 1	0
50	1L	1	Total 44	C 34	N 1	O 8	P 1	0
50	1f	1	Total 46	C 36	N 1	O 8	P 1	0

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



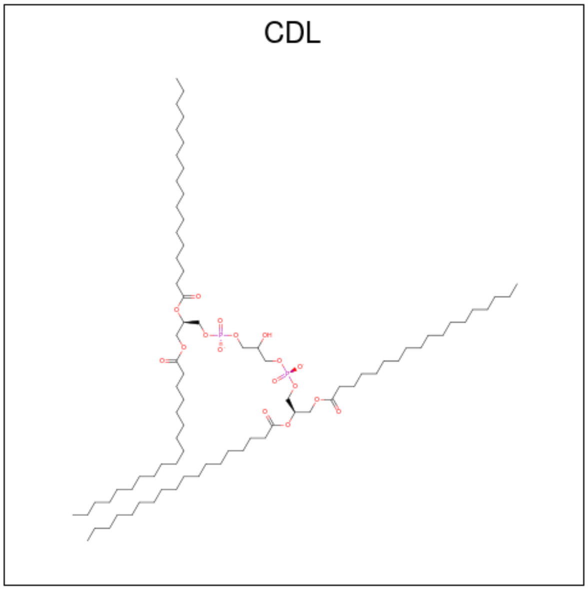
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	1L	1	15	14	1	0

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



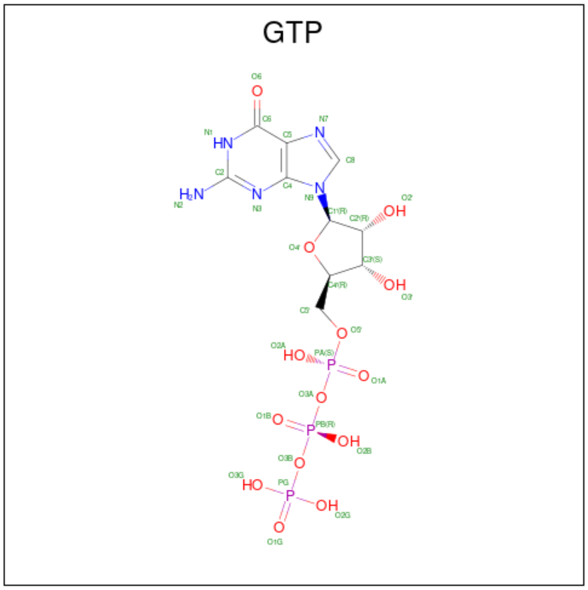
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	1M	1	51	40	10	1	0

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



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

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

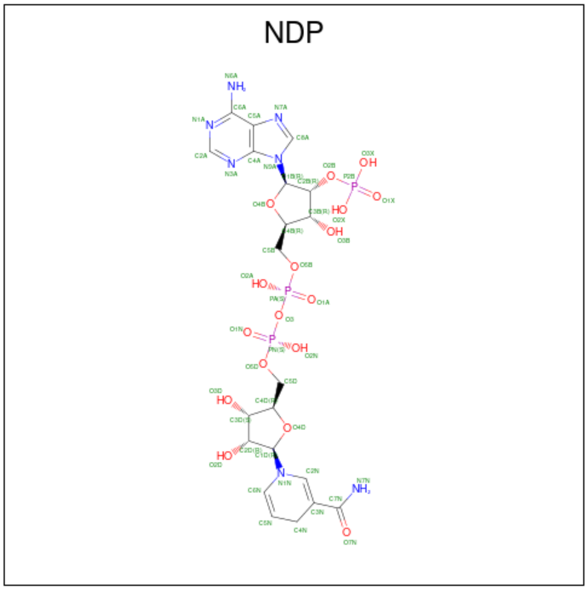


Mol	Chain	Residues	Atoms	AltConf
54	1O	1	Total C N O P 32 10 5 14 3	0

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

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

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

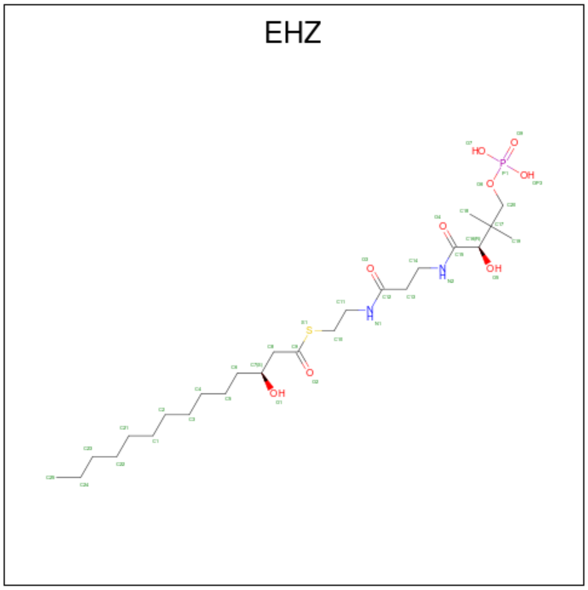


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	1P	1	48	21	7	17	3	0

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

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

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

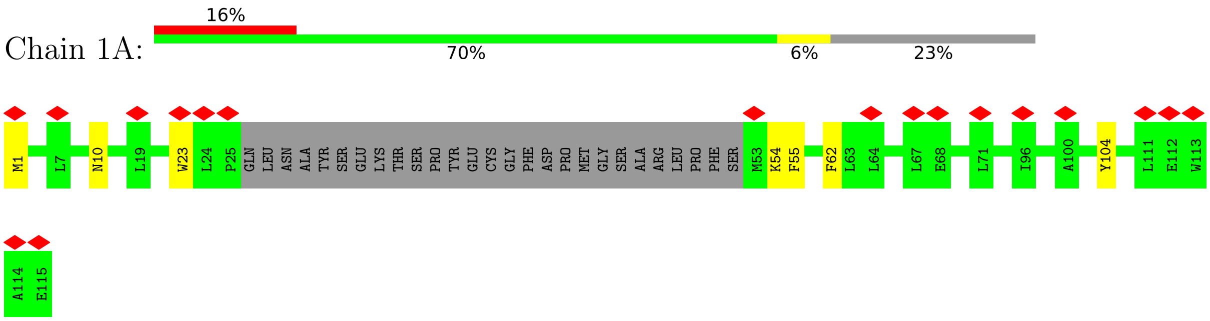


Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
58	1n	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

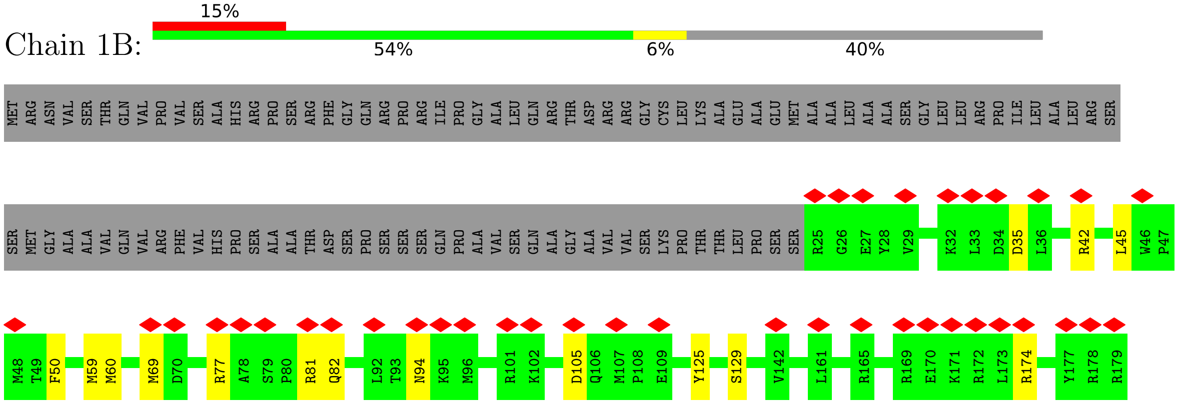
3 Residue-property plots ⓘ

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.

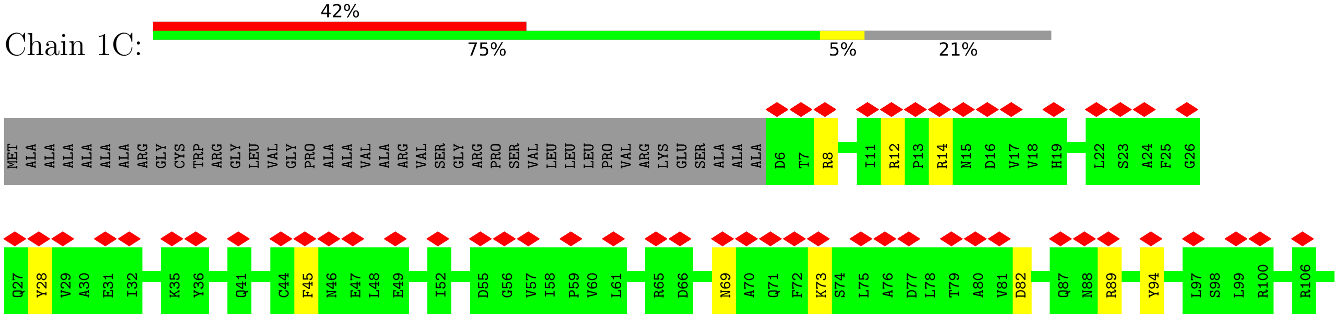
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

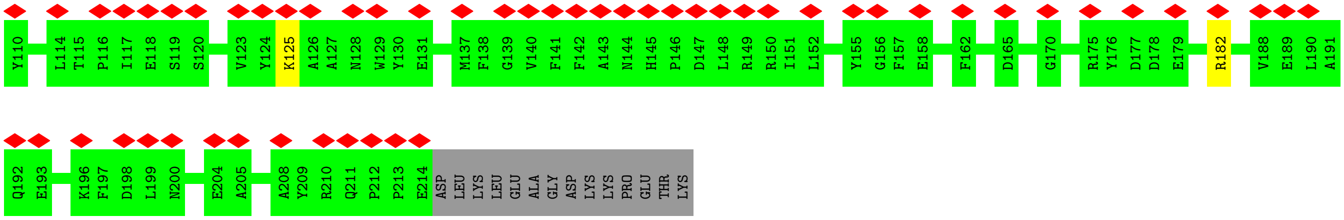


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



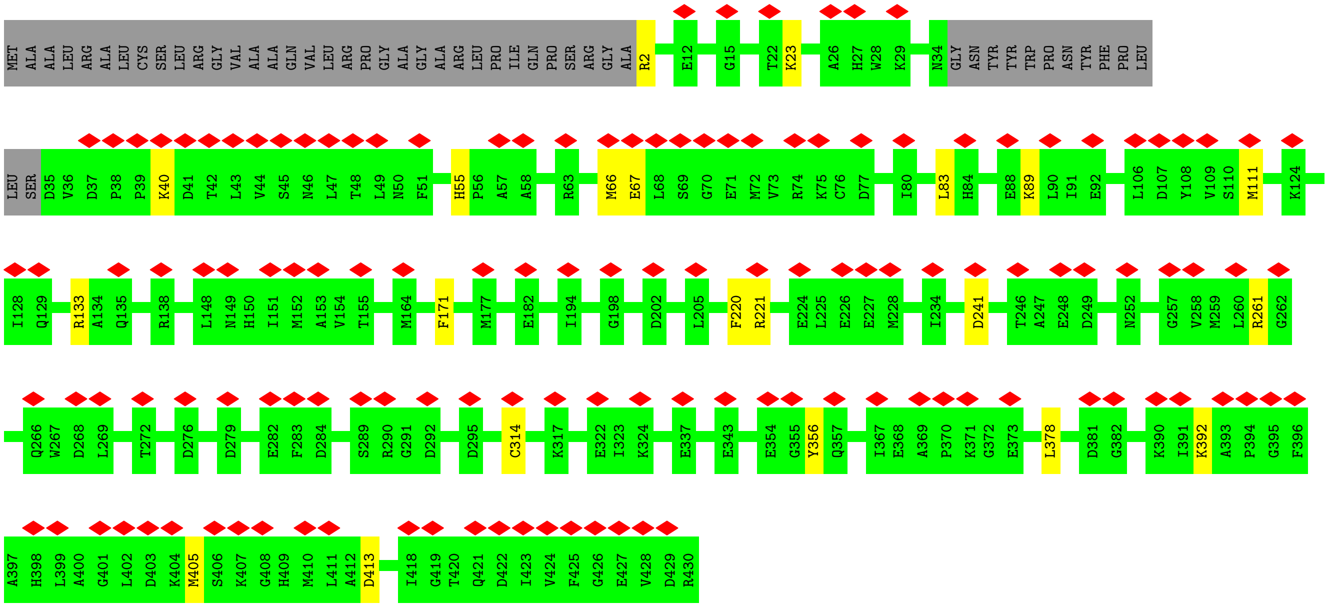
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





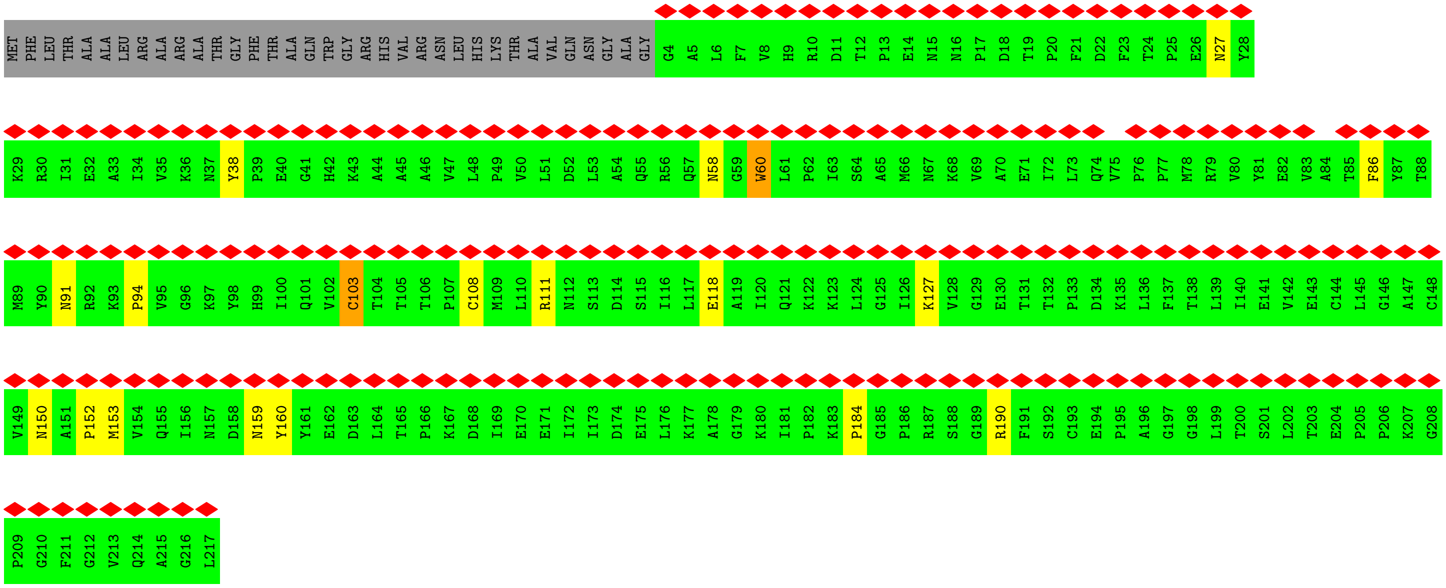
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:

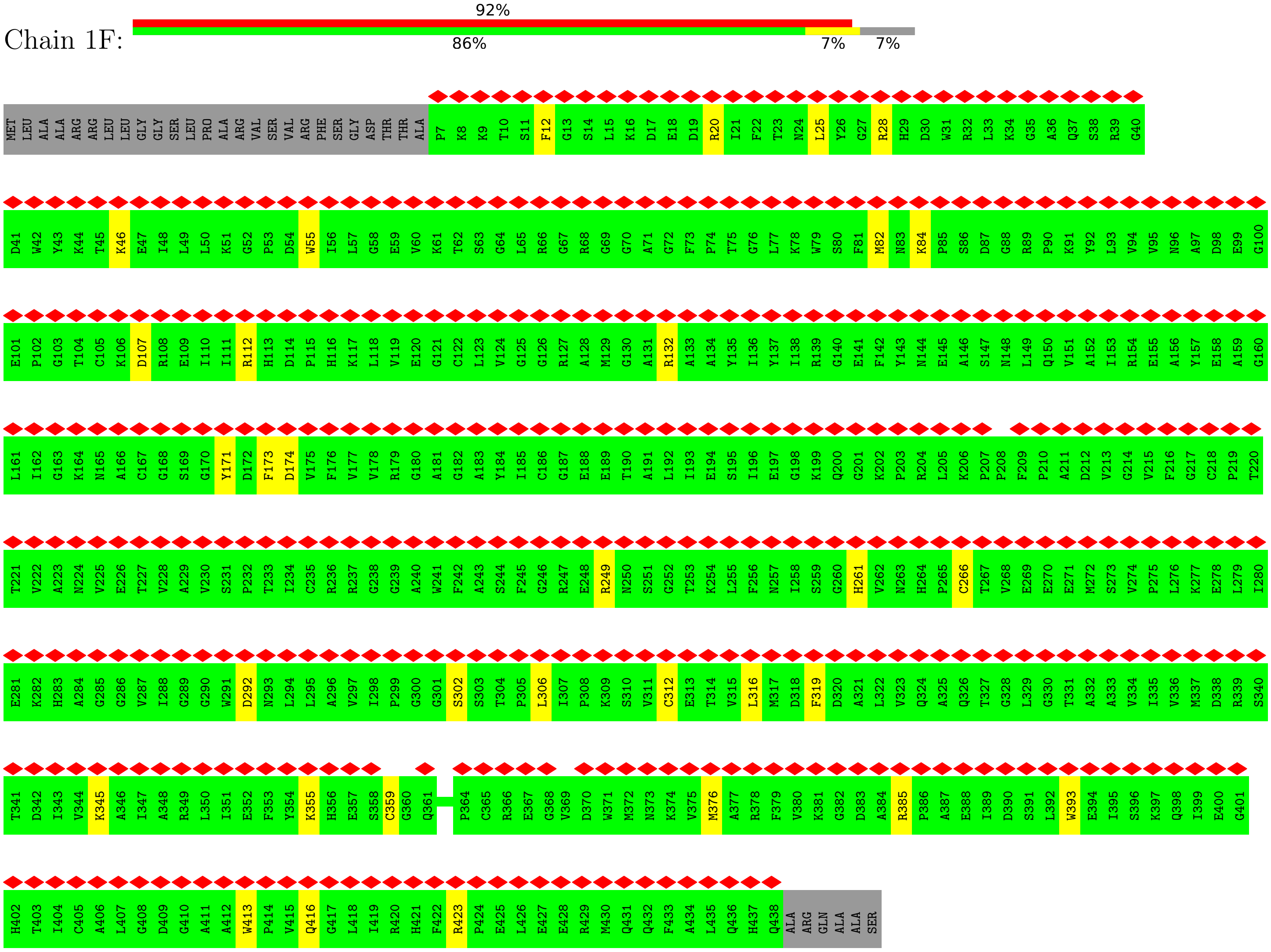


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

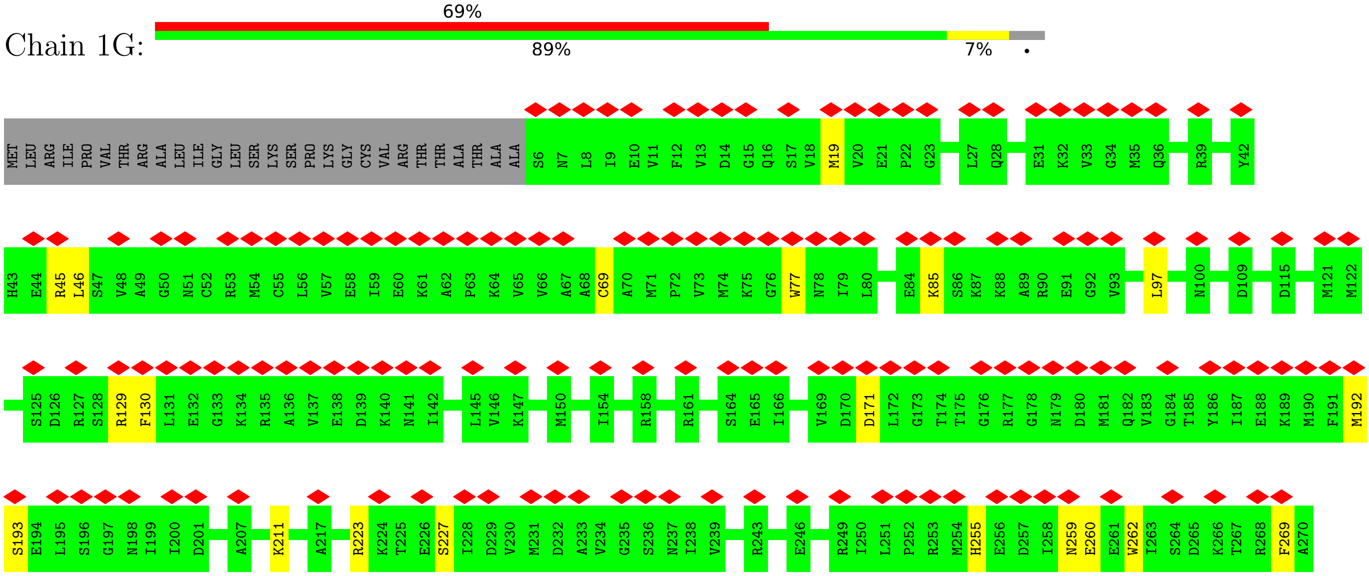
Chain 1E:

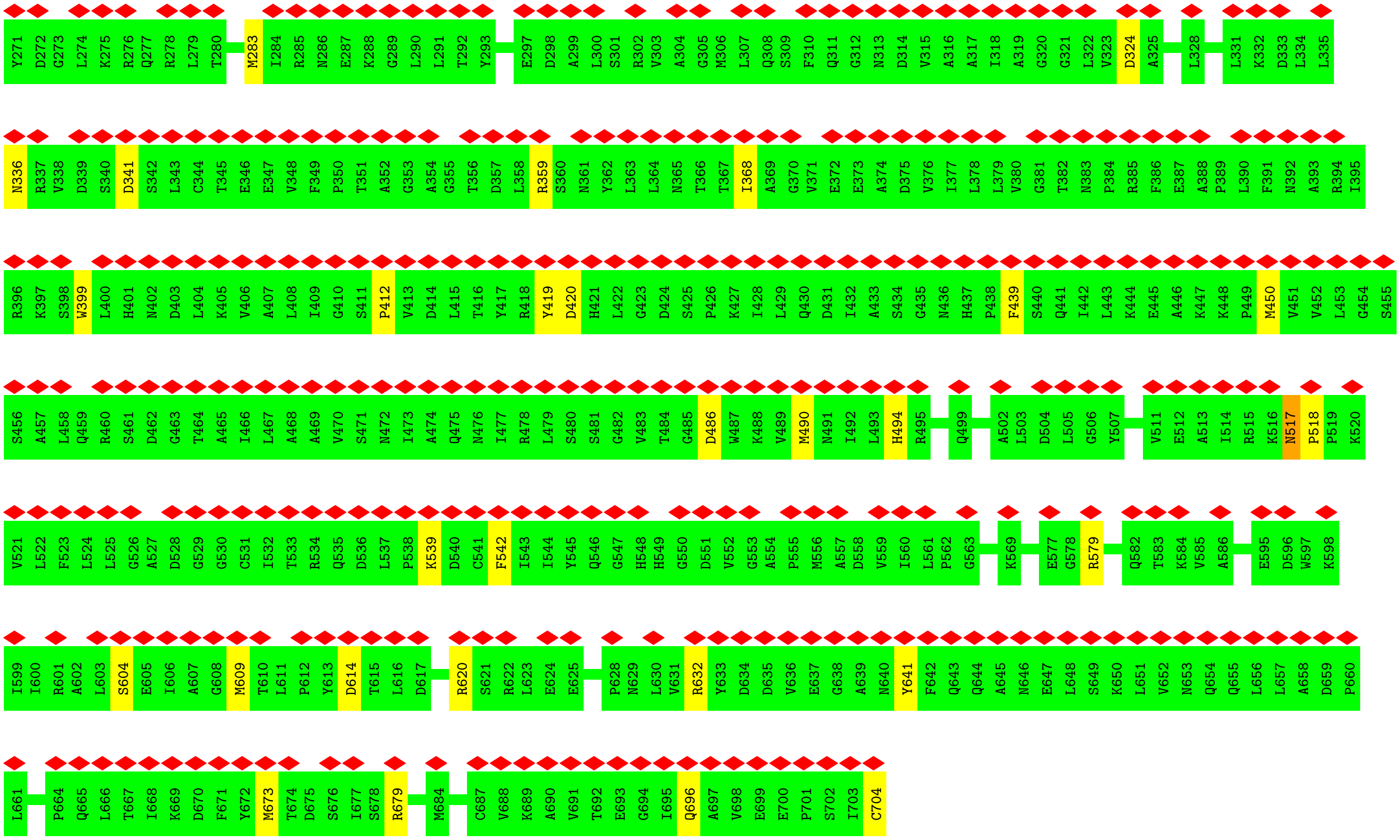


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



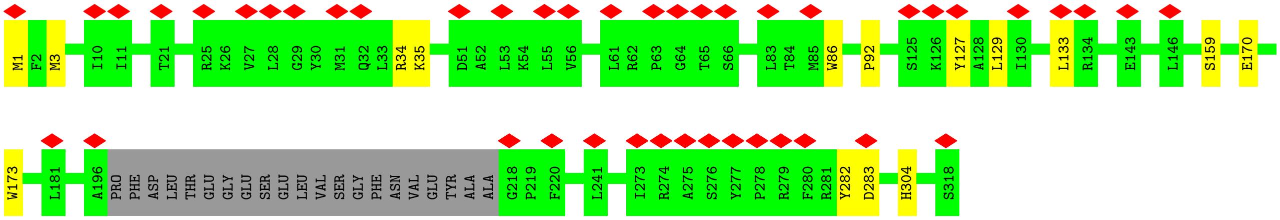
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





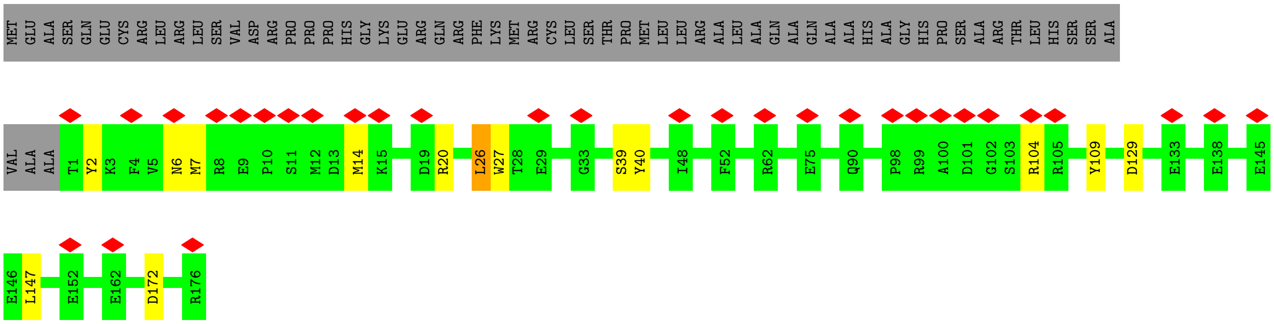
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:

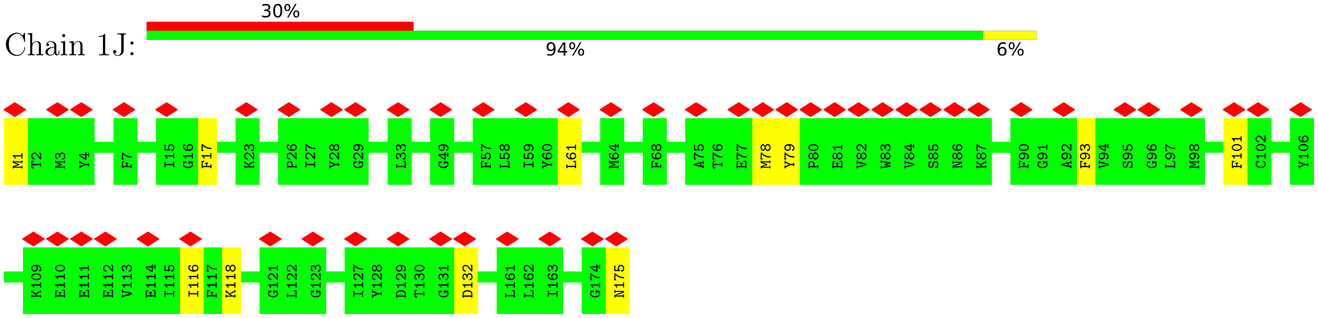
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:

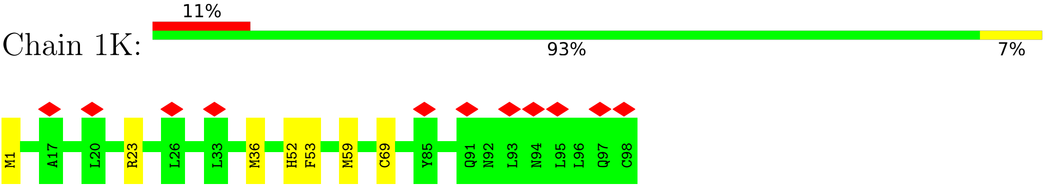
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:



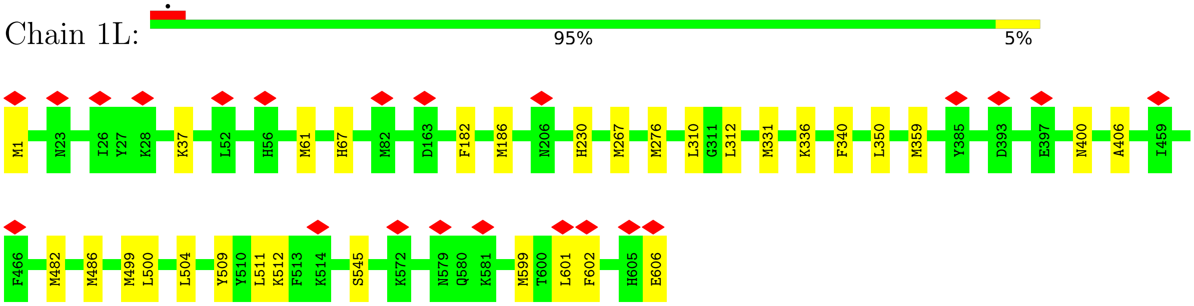
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:



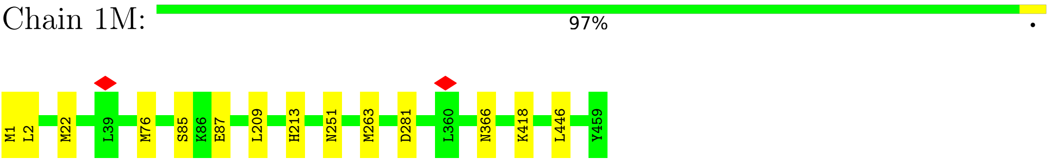
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:



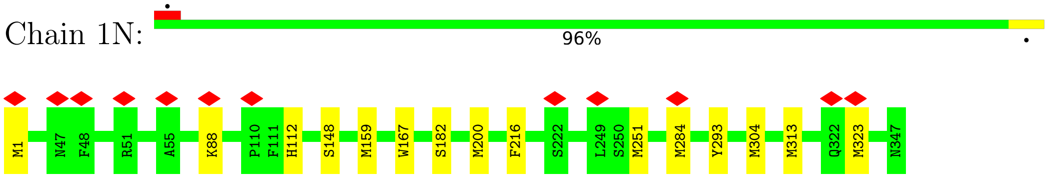
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:



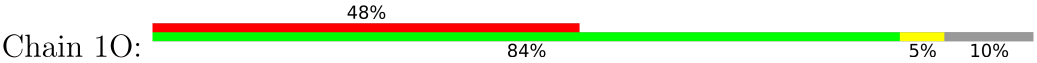
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

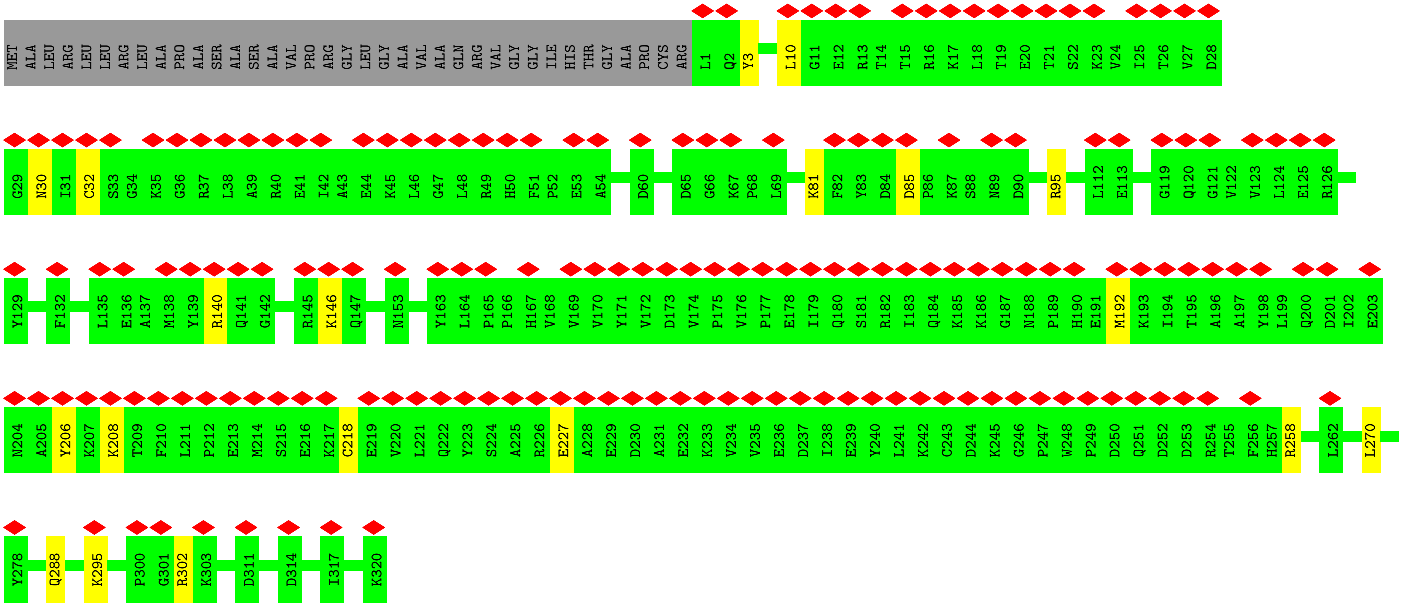
Chain 1N:



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

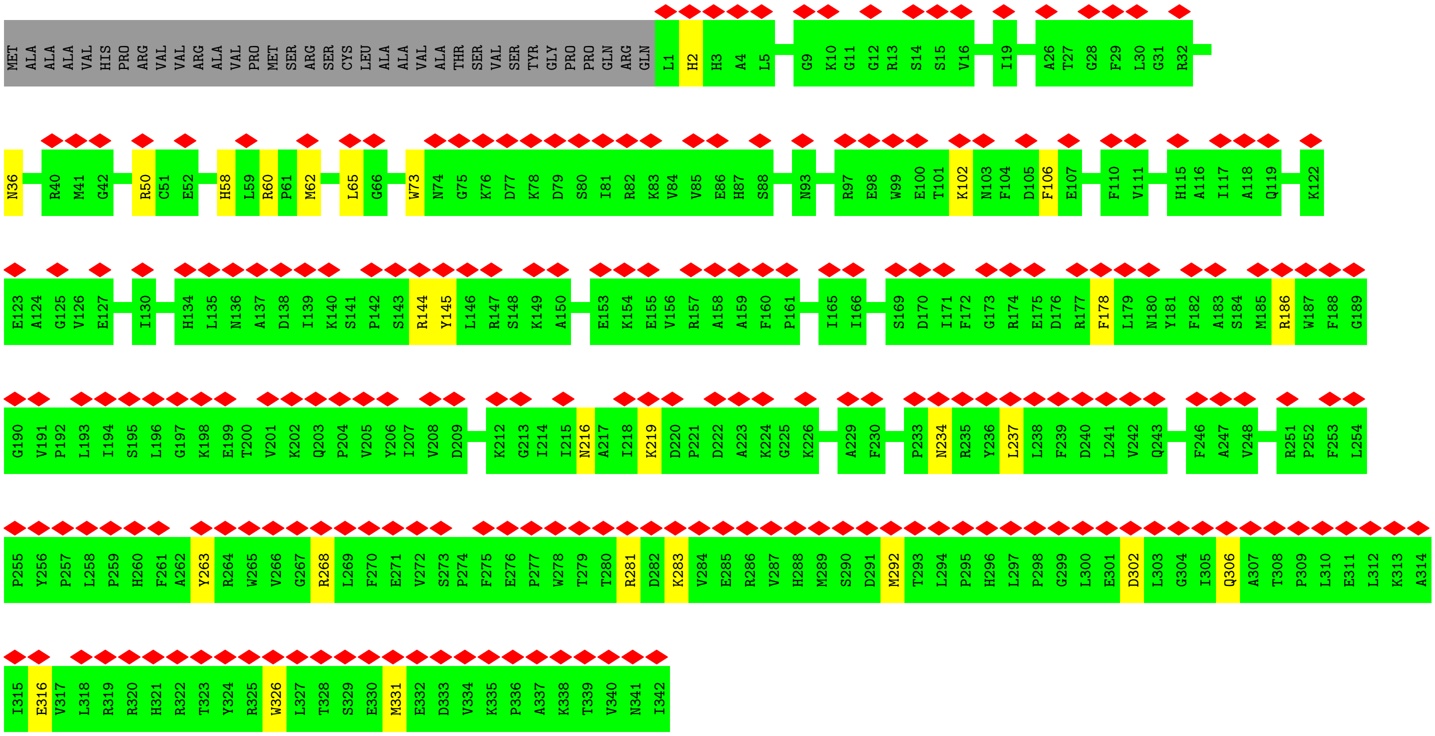
Chain 1O:





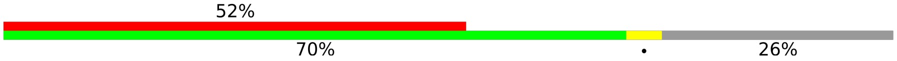
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

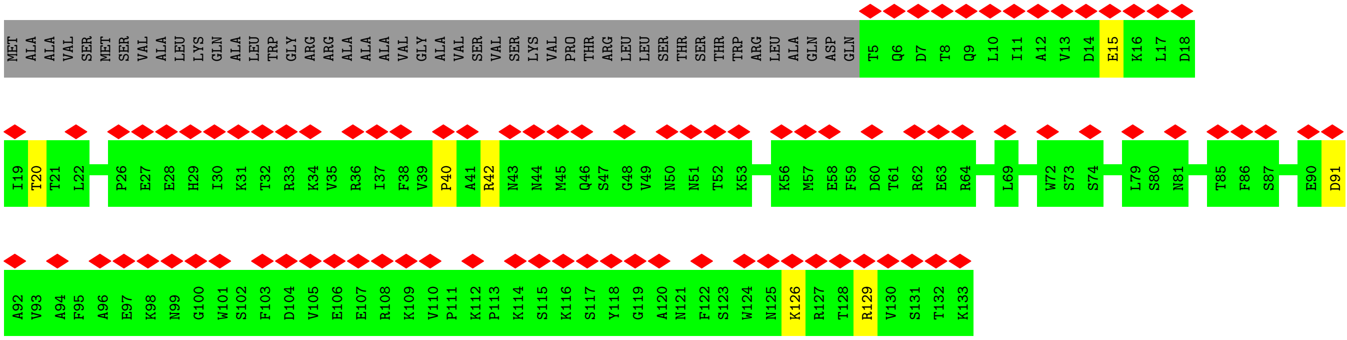
Chain 1P:



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

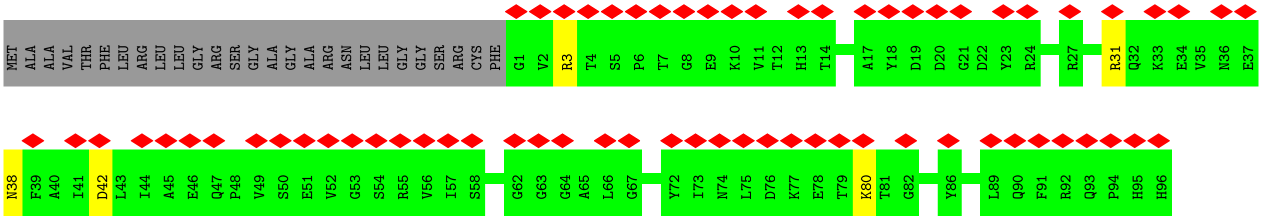
Chain 1Q:





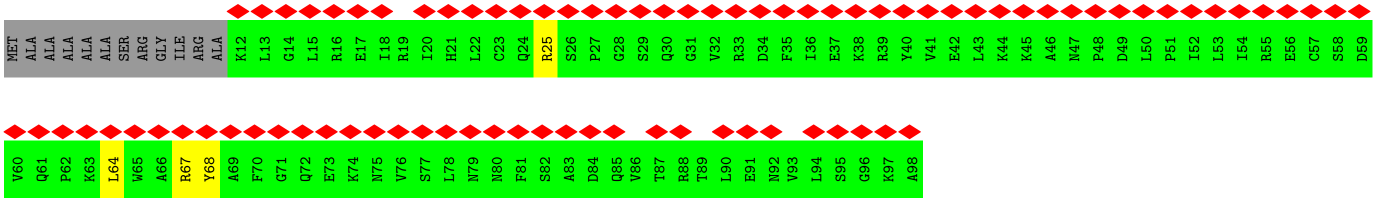
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



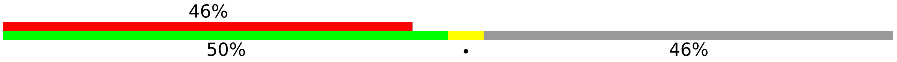
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

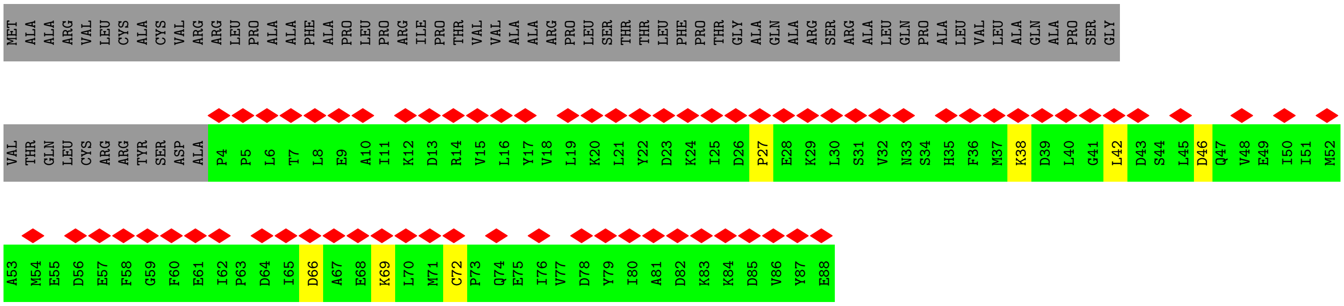
Chain 1S:



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

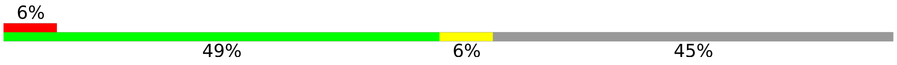
Chain 1T:

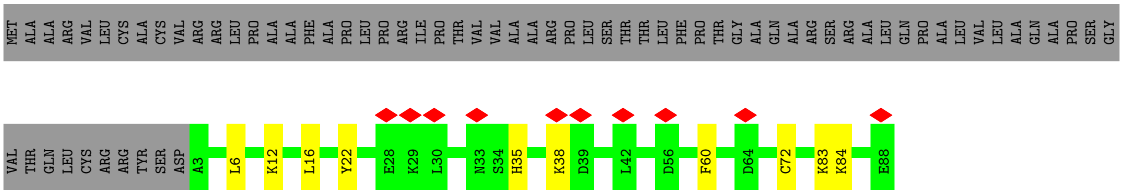




- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

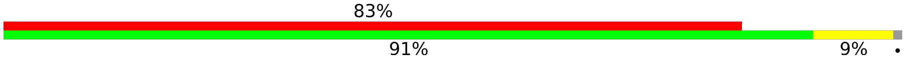
Chain 1U:

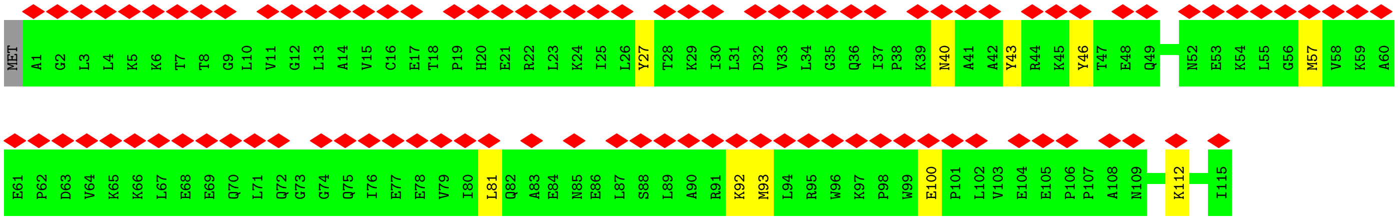




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

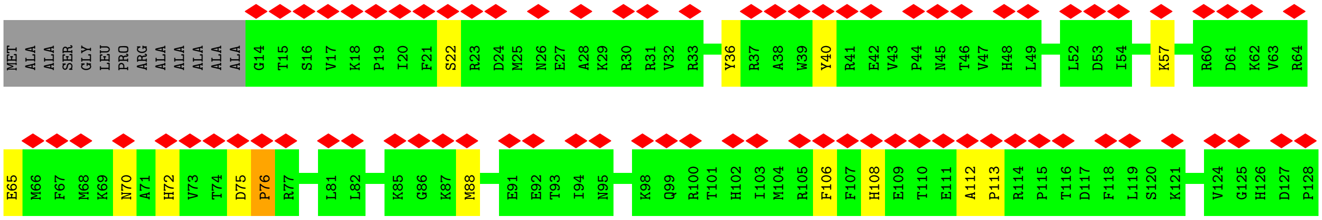
Chain 1V:





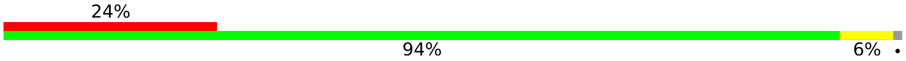
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

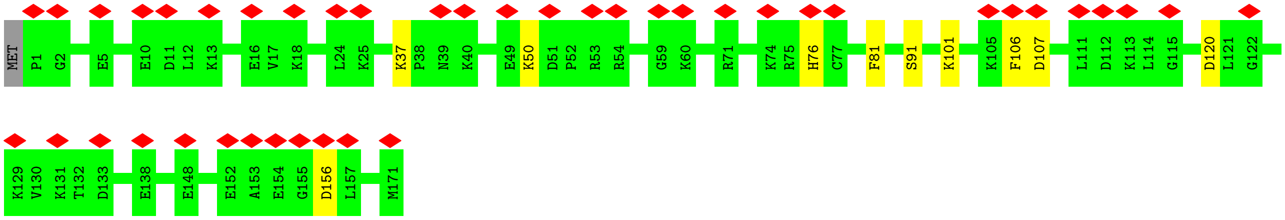
Chain 1W:



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

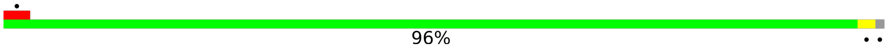
Chain 1X:

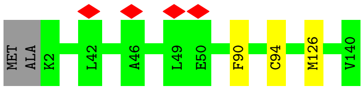




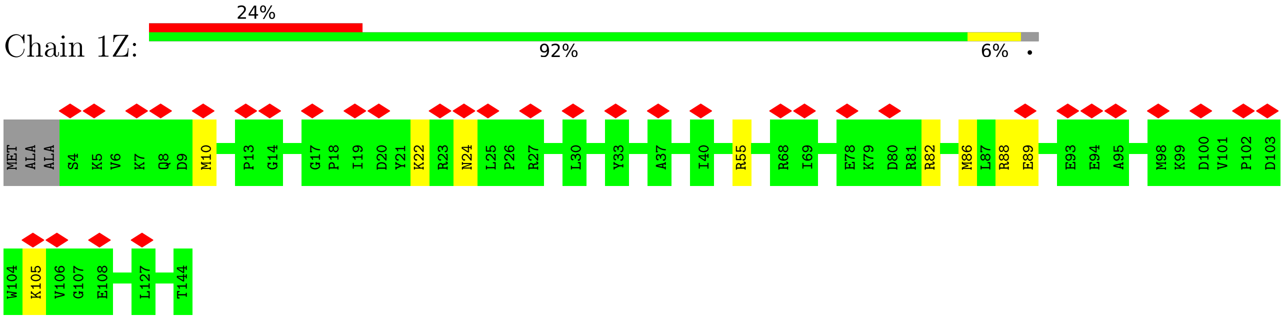
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:

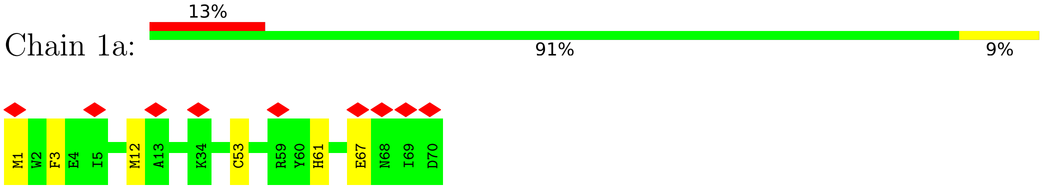




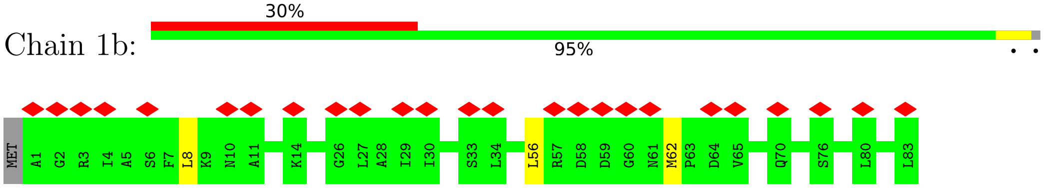
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



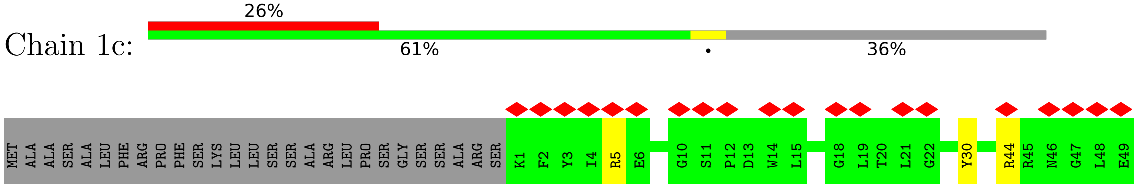
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



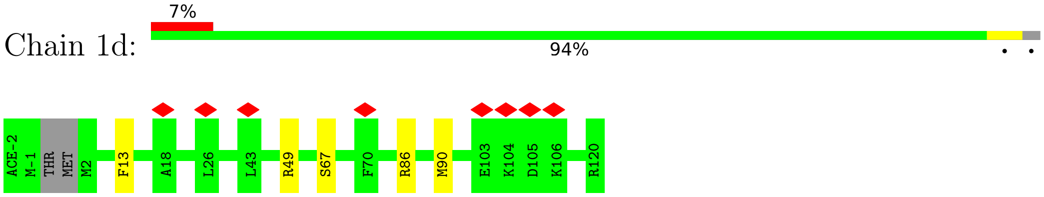
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



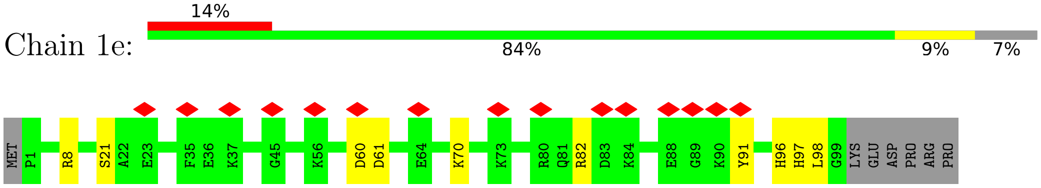
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

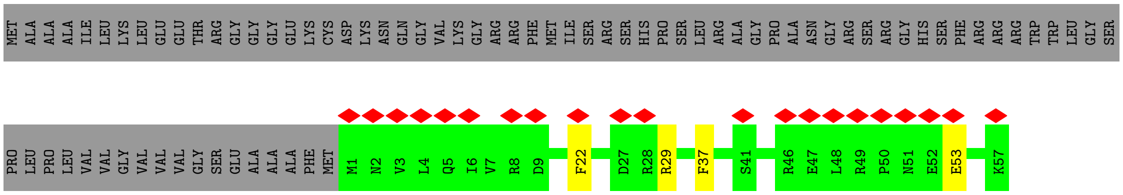


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



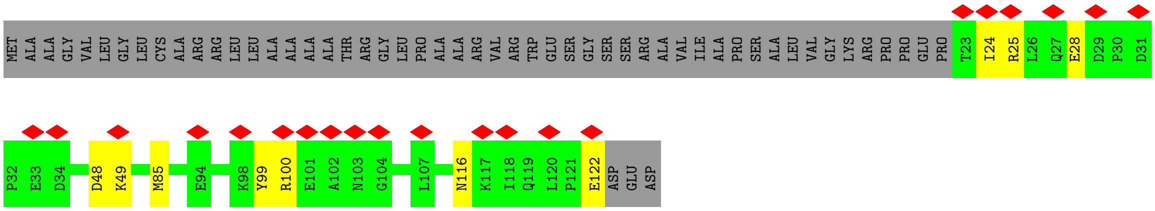
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f:



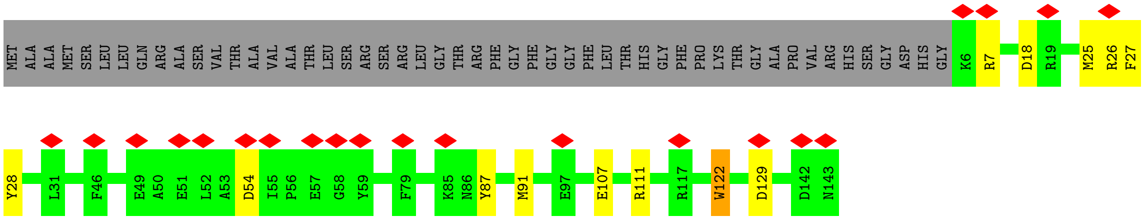
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



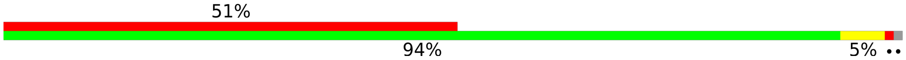
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



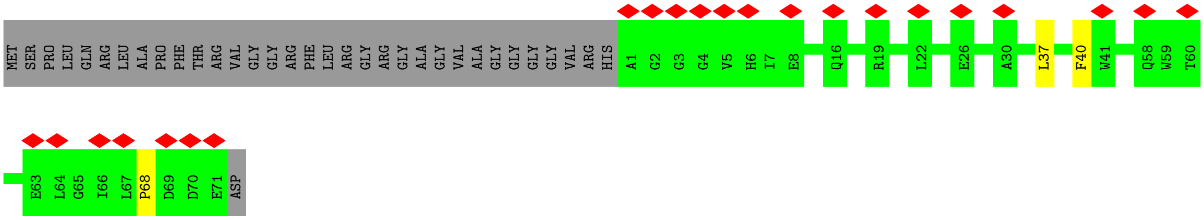
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



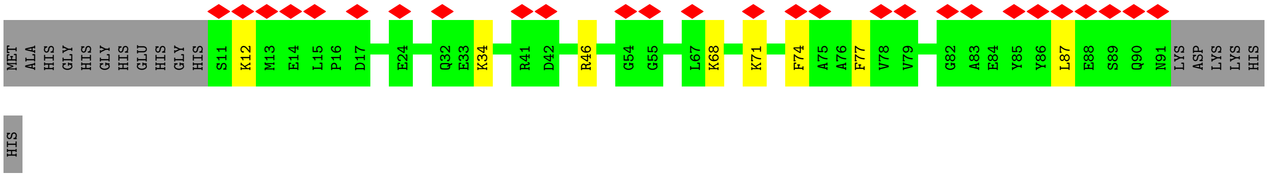
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



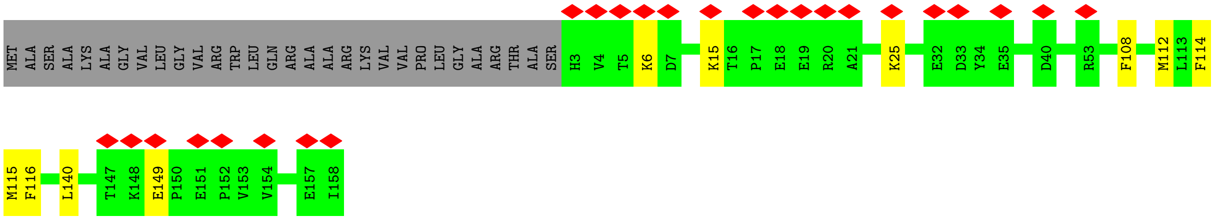
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



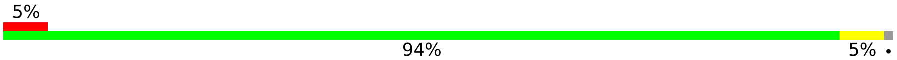
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

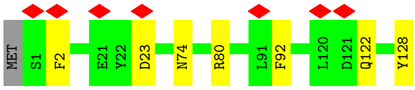
Chain 1l:



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

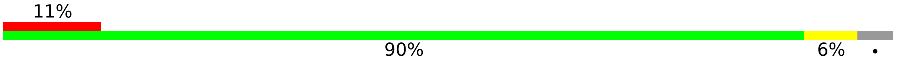
Chain 1m:

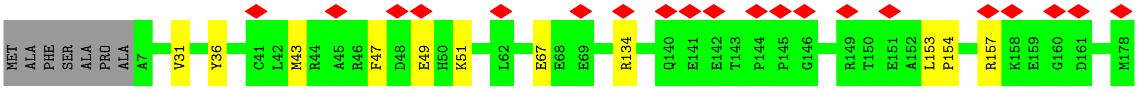




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

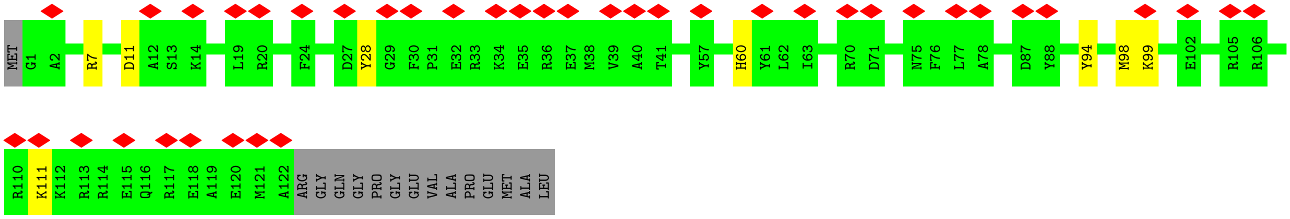
Chain 1n:



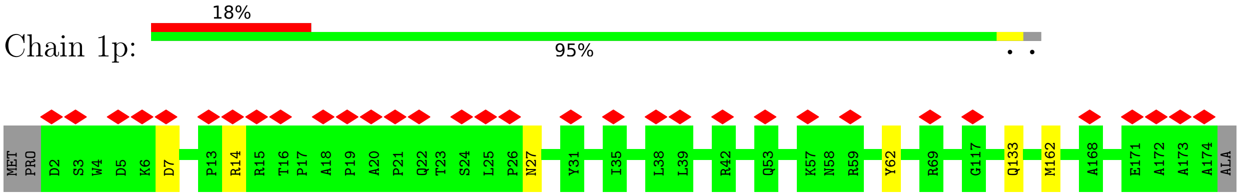


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

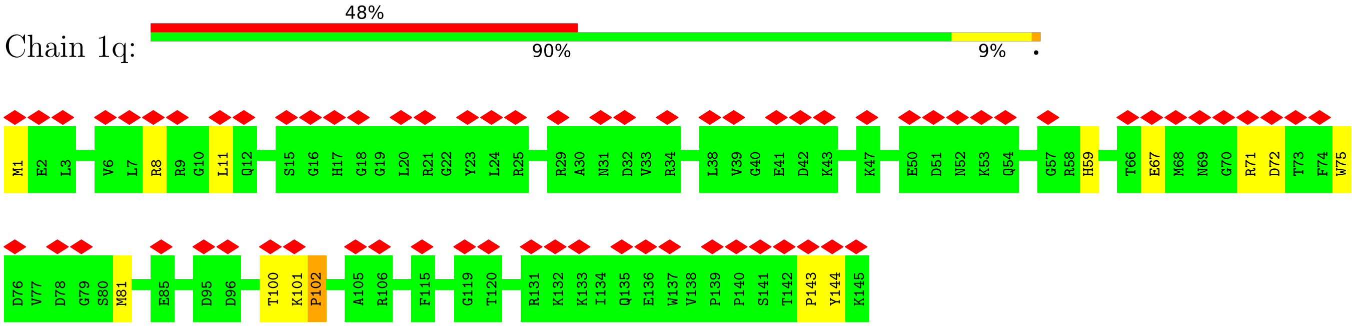
Chain 1o:



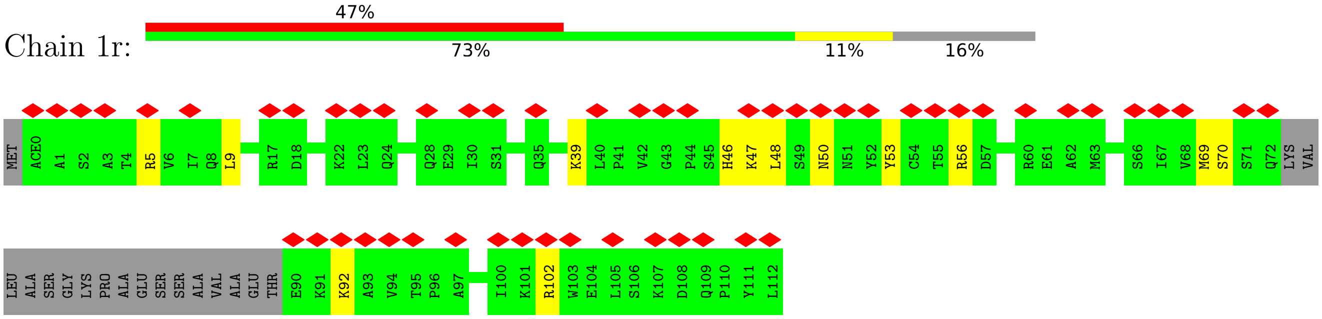
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



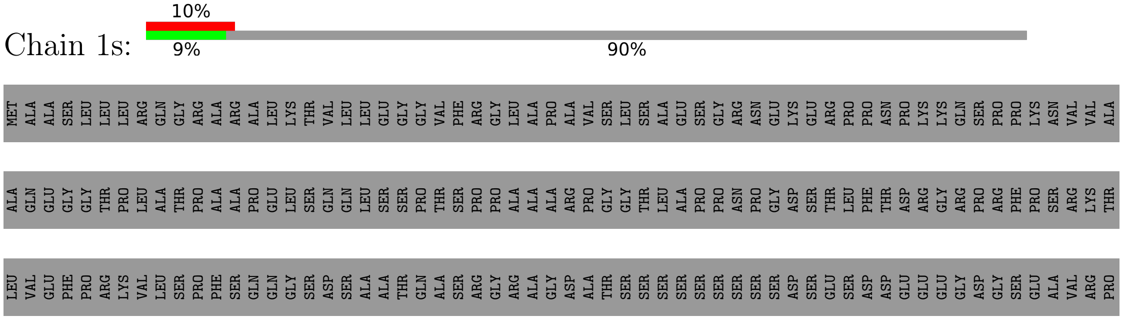
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

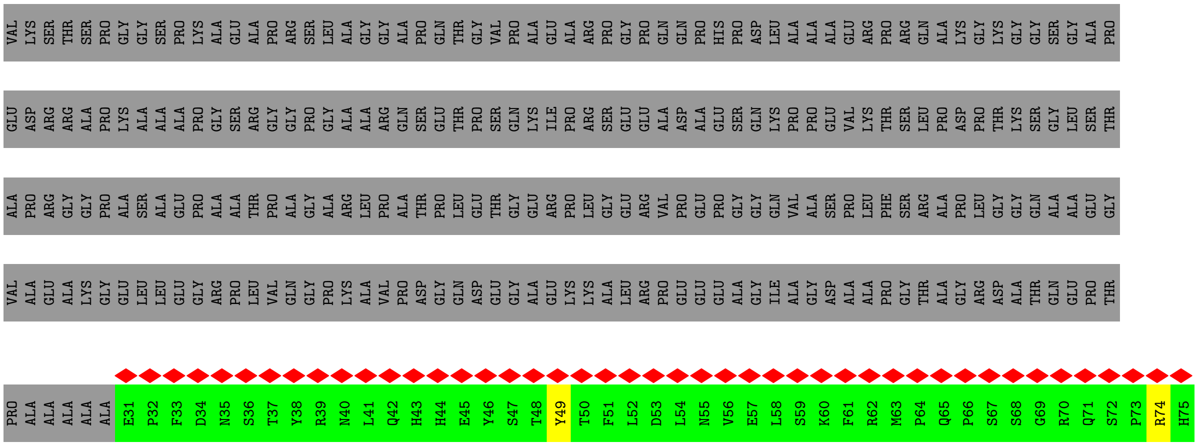


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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




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 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	37000	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	0.909	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1A	0.30	0/713	0.53	0/975
2	1B	0.45	2/1273 (0.2%)	0.66	1/1722 (0.1%)
3	1C	0.29	0/1791	0.57	0/2439
4	1D	0.30	0/3545	0.54	1/4806 (0.0%)
5	1E	0.44	3/1698 (0.2%)	0.72	5/2311 (0.2%)
6	1F	0.32	0/3401	0.58	1/4595 (0.0%)
7	1G	0.42	4/5451 (0.1%)	0.66	10/7387 (0.1%)
8	1H	0.28	0/2401	0.50	0/3282
9	1I	0.31	0/1443	0.63	1/1952 (0.1%)
10	1J	0.31	0/1364	0.52	0/1850
11	1K	0.31	0/751	0.59	0/1018
12	1L	0.27	0/4939	0.52	2/6718 (0.0%)
13	1M	0.26	0/3713	0.47	0/5063
14	1N	0.30	0/2765	0.53	0/3758
15	1O	0.35	1/2650 (0.0%)	0.52	0/3588
16	1P	0.30	0/2828	0.54	1/3834 (0.0%)
17	1Q	0.32	0/1070	0.62	1/1446 (0.1%)
18	1R	0.28	0/755	0.57	0/1018
19	1S	0.30	0/711	0.65	1/956 (0.1%)
20	1T	0.50	1/701 (0.1%)	0.78	2/946 (0.2%)
20	1U	0.29	0/706	0.53	1/954 (0.1%)
21	1V	0.27	0/946	0.49	0/1281
22	1W	1.28	5/995 (0.5%)	1.39	7/1340 (0.5%)
23	1X	0.27	0/1436	0.52	0/1938
24	1Y	0.24	0/1037	0.46	0/1404
25	1Z	0.27	0/1199	0.55	0/1617
26	1a	0.39	0/577	1.04	2/777 (0.3%)
27	1b	0.27	0/664	0.53	0/912
28	1c	0.32	0/430	0.61	0/581
29	1d	0.32	0/1024	0.52	0/1383
30	1e	0.25	0/836	0.53	0/1118
31	1f	0.27	0/499	0.58	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.35	0/858	0.65	0/1165
33	1h	0.33	1/1184 (0.1%)	0.52	0/1603
34	1i	1.14	6/1131 (0.5%)	1.31	7/1541 (0.5%)
35	1j	0.28	0/627	0.58	2/858 (0.2%)
36	1k	0.28	0/668	0.55	0/903
37	1l	0.27	0/1365	0.47	0/1867
38	1m	0.27	0/1092	0.50	0/1481
39	1n	0.37	2/1549 (0.1%)	0.69	2/2098 (0.1%)
40	1o	0.26	0/1069	0.55	0/1430
41	1p	0.27	0/1481	0.54	0/1997
42	1q	0.32	0/1253	0.65	2/1704 (0.1%)
43	1r	0.34	0/782	0.62	0/1057
44	1s	0.27	0/394	0.54	0/533
All	All	0.38	25/67765 (0.0%)	0.61	49/91879 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	1E	0	1
13	1M	0	1
34	1i	0	1
42	1q	0	1
All	All	0	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1W	76	PRO	CG-CD	-24.74	0.69	1.50
34	1i	54	ALA	C-N	23.84	1.79	1.34
22	1W	75	ASP	C-N	19.93	1.72	1.34
34	1i	55	PRO	CG-CD	-19.67	0.85	1.50
22	1W	76	PRO	N-CD	13.94	1.67	1.47
34	1i	55	PRO	CB-CG	13.62	2.18	1.50
22	1W	76	PRO	CB-CG	12.90	2.14	1.50
7	1G	518	PRO	CG-CD	-12.63	1.08	1.50
7	1G	518	PRO	N-CD	11.49	1.64	1.47
7	1G	518	PRO	N-CA	-10.37	1.29	1.47
34	1i	55	PRO	CA-CB	-10.26	1.33	1.53
2	1B	125	TYR	CE1-CZ	-7.90	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1i	55	PRO	N-CD	7.87	1.58	1.47
15	1O	208	LYS	CD-CE	-7.33	1.32	1.51
39	1n	154	PRO	N-CA	-7.12	1.35	1.47
22	1W	76	PRO	CA-CB	-7.02	1.39	1.53
7	1G	412	PRO	CG-CD	-7.02	1.27	1.50
2	1B	125	TYR	CG-CD1	-6.24	1.31	1.39
20	1T	27	PRO	CG-CD	-5.92	1.31	1.50
34	1i	55	PRO	CA-C	5.87	1.64	1.52
39	1n	154	PRO	N-CD	5.79	1.55	1.47
33	1h	122	TRP	CG-CD1	-5.67	1.28	1.36
5	1E	60	TRP	CZ3-CH2	-5.61	1.31	1.40
5	1E	153	MET	CG-SD	-5.48	1.67	1.81
5	1E	160	TYR	CD1-CE1	-5.28	1.31	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1i	55	PRO	CA-N-CD	-27.55	72.92	111.50
34	1i	55	PRO	CB-CG-CD	-27.29	0.05	106.50
22	1W	76	PRO	CB-CG-CD	-25.73	6.17	106.50
26	1a	1	MET	CG-SD-CE	-23.03	63.36	100.20
22	1W	76	PRO	CA-N-CD	-21.45	81.47	111.50
7	1G	518	PRO	CA-N-CD	-19.96	83.55	111.50
22	1W	75	ASP	C-N-CD	18.80	167.89	128.40
39	1n	154	PRO	CA-N-CD	-18.36	85.80	111.50
34	1i	54	ALA	C-N-CD	17.05	164.20	128.40
20	1T	27	PRO	CA-N-CD	-14.19	91.64	111.50
22	1W	113	PRO	CA-N-CD	-13.44	92.68	111.50
34	1i	55	PRO	N-CA-CB	-12.74	88.02	103.30
7	1G	450	MET	CG-SD-CE	-11.48	81.83	100.20
5	1E	94	PRO	CA-N-CD	-11.35	95.61	111.50
42	1q	102	PRO	CA-N-CD	-11.12	95.94	111.50
7	1G	517	ASN	C-N-CD	11.11	151.74	128.40
5	1E	184	PRO	CA-N-CD	-10.42	96.92	111.50
5	1E	103	CYS	CA-CB-SG	10.26	132.47	114.00
2	1B	125	TYR	CD1-CE1-CZ	10.01	128.81	119.80
26	1a	1	MET	CA-CB-CG	9.56	129.56	113.30
22	1W	76	PRO	N-CD-CG	-9.46	89.01	103.20
7	1G	412	PRO	N-CD-CG	-9.14	89.49	103.20
34	1i	55	PRO	CA-CB-CG	-9.05	86.80	104.00
39	1n	153	LEU	C-N-CD	8.90	147.09	128.40
35	1j	68	PRO	CA-N-CD	-8.54	99.55	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1W	76	PRO	CA-CB-CG	-8.50	87.84	104.00
17	1Q	40	PRO	CA-N-CD	-8.32	99.86	111.50
7	1G	518	PRO	CA-CB-CG	-6.93	90.84	104.00
9	1I	26	LEU	CA-CB-CG	6.71	130.74	115.30
5	1E	153	MET	CG-SD-CE	6.61	110.77	100.20
12	1L	350	LEU	CA-CB-CG	6.18	129.52	115.30
7	1G	518	PRO	N-CD-CG	-6.00	94.20	103.20
7	1G	412	PRO	CA-N-CD	-5.95	103.17	111.50
22	1W	112	ALA	C-N-CD	5.81	140.60	128.40
7	1G	412	PRO	CA-CB-CG	-5.78	93.01	104.00
5	1E	108	CYS	CA-CB-SG	5.71	124.27	114.00
7	1G	97	LEU	CA-CB-CG	5.63	128.25	115.30
16	1P	237	LEU	CA-CB-CG	5.63	128.25	115.30
35	1j	37	LEU	CA-CB-CG	5.54	128.05	115.30
4	1D	83	LEU	CA-CB-CG	5.50	127.95	115.30
20	1U	6	LEU	CA-CB-CG	5.46	127.86	115.30
42	1q	11	LEU	CA-CB-CG	5.46	127.85	115.30
34	1i	36	PRO	CA-N-CD	-5.31	104.06	111.50
6	1F	316	LEU	CA-CB-CG	5.29	127.46	115.30
19	1S	64	LEU	CA-CB-CG	5.19	127.23	115.30
34	1i	55	PRO	CA-C-N	5.16	128.54	117.20
7	1G	46	LEU	CA-CB-CG	5.15	127.14	115.30
20	1T	27	PRO	N-CD-CG	-5.11	95.54	103.20
12	1L	511	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1E	152	PRO	Peptide
13	1M	251	ASN	Peptide
34	1i	55	PRO	Mainchain
42	1q	143	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles ⓘ

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	84/115 (73%)	80 (95%)	4 (5%)	0	100	100
2	1B	153/258 (59%)	137 (90%)	16 (10%)	0	100	100
3	1C	207/264 (78%)	194 (94%)	13 (6%)	0	100	100
4	1D	427/476 (90%)	394 (92%)	33 (8%)	0	100	100
5	1E	212/249 (85%)	191 (90%)	21 (10%)	0	100	100
6	1F	430/464 (93%)	398 (93%)	31 (7%)	1 (0%)	47	78
7	1G	697/727 (96%)	643 (92%)	50 (7%)	4 (1%)	25	62
8	1H	293/318 (92%)	279 (95%)	12 (4%)	2 (1%)	22	59
9	1I	174/239 (73%)	163 (94%)	11 (6%)	0	100	100
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	25	62
11	1K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	1L	604/606 (100%)	556 (92%)	45 (8%)	3 (0%)	29	66
13	1M	457/459 (100%)	440 (96%)	16 (4%)	1 (0%)	47	78
14	1N	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
15	1O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	305 (90%)	35 (10%)	0	100	100
17	1Q	127/175 (73%)	111 (87%)	15 (12%)	1 (1%)	19	56
18	1R	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	1U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	17	54
22	1W	113/128 (88%)	103 (91%)	9 (8%)	1 (1%)	17	54
23	1X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	7 (7%)	1 (1%)	15	51
33	1h	136/189 (72%)	128 (94%)	8 (6%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	72 (91%)	7 (9%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	25	62
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
42	1q	143/145 (99%)	129 (90%)	11 (8%)	3 (2%)	7	38
43	1r	90/114 (79%)	83 (92%)	7 (8%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8142/9744 (84%)	7572 (93%)	550 (7%)	20 (0%)	50	78

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	259	ASN
8	1H	92	PRO
12	1L	406	ALA
13	1M	2	LEU
17	1Q	20	THR
32	1g	24	ILE
39	1n	31	VAL
6	1F	302	SER
7	1G	260	GLU
10	1J	116	ILE

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Mol	Chain	Res	Type
12	1L	230	HIS
12	1L	601	LEU
22	1W	76	PRO
7	1G	696	GLN
42	1q	75	TRP
8	1H	170	GLU
21	1V	112	LYS
42	1q	100	THR
42	1q	102	PRO
7	1G	368	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	76/99 (77%)	70 (92%)	6 (8%)	12	42
2	1B	131/212 (62%)	117 (89%)	14 (11%)	6	30
3	1C	190/227 (84%)	178 (94%)	12 (6%)	18	49
4	1D	371/405 (92%)	351 (95%)	20 (5%)	22	54
5	1E	183/207 (88%)	170 (93%)	13 (7%)	14	45
6	1F	346/368 (94%)	316 (91%)	30 (9%)	10	38
7	1G	588/610 (96%)	547 (93%)	41 (7%)	15	45
8	1H	257/274 (94%)	245 (95%)	12 (5%)	26	56
9	1I	151/201 (75%)	137 (91%)	14 (9%)	9	35
10	1J	140/140 (100%)	131 (94%)	9 (6%)	17	48
11	1K	84/84 (100%)	78 (93%)	6 (7%)	14	45
12	1L	539/539 (100%)	514 (95%)	25 (5%)	27	57
13	1M	408/408 (100%)	397 (97%)	11 (3%)	44	68
14	1N	310/310 (100%)	296 (96%)	14 (4%)	27	57
15	1O	283/307 (92%)	265 (94%)	18 (6%)	17	48
16	1P	296/323 (92%)	269 (91%)	27 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	1Q	117/152 (77%)	112 (96%)	5 (4%)	29	58
18	1R	79/97 (81%)	74 (94%)	5 (6%)	18	49
19	1S	77/82 (94%)	74 (96%)	3 (4%)	32	60
20	1T	79/133 (59%)	73 (92%)	6 (8%)	13	43
20	1U	79/133 (59%)	70 (89%)	9 (11%)	5	27
21	1V	100/101 (99%)	91 (91%)	9 (9%)	9	37
22	1W	107/112 (96%)	97 (91%)	10 (9%)	9	35
23	1X	153/154 (99%)	143 (94%)	10 (6%)	17	48
24	1Y	101/102 (99%)	98 (97%)	3 (3%)	41	66
25	1Z	123/124 (99%)	114 (93%)	9 (7%)	14	44
26	1a	58/58 (100%)	53 (91%)	5 (9%)	10	39
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	58
28	1c	45/66 (68%)	42 (93%)	3 (7%)	16	47
29	1d	107/109 (98%)	102 (95%)	5 (5%)	26	56
30	1e	87/94 (93%)	77 (88%)	10 (12%)	5	27
31	1f	54/113 (48%)	50 (93%)	4 (7%)	13	44
32	1g	92/129 (71%)	83 (90%)	9 (10%)	8	33
33	1h	121/158 (77%)	108 (89%)	13 (11%)	6	30
34	1i	119/120 (99%)	115 (97%)	4 (3%)	37	64
35	1j	62/84 (74%)	61 (98%)	1 (2%)	62	80
36	1k	63/76 (83%)	55 (87%)	8 (13%)	4	23
37	1l	141/161 (88%)	131 (93%)	10 (7%)	14	45
38	1m	113/114 (99%)	106 (94%)	7 (6%)	18	49
39	1n	156/160 (98%)	148 (95%)	8 (5%)	24	55
40	1o	110/120 (92%)	102 (93%)	8 (7%)	14	44
41	1p	154/156 (99%)	148 (96%)	6 (4%)	32	60
42	1q	131/131 (100%)	122 (93%)	9 (7%)	15	46
43	1r	85/98 (87%)	72 (85%)	13 (15%)	2	17
44	1s	44/351 (12%)	42 (96%)	2 (4%)	27	57
All	All	7179/8272 (87%)	6710 (94%)	469 (6%)	21	48

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
1	1A	23	TRP
1	1A	54	LYS
1	1A	55	PHE
1	1A	62	PHE
1	1A	104	TYR
2	1B	35	ASP
2	1B	42	ARG
2	1B	45	LEU
2	1B	50	PHE
2	1B	59	MET
2	1B	60	MET
2	1B	69	MET
2	1B	77	ARG
2	1B	81	ARG
2	1B	82	GLN
2	1B	94	ASN
2	1B	105	ASP
2	1B	129	SER
2	1B	174	ARG
3	1C	8	ARG
3	1C	12	ARG
3	1C	14	ARG
3	1C	28	TYR
3	1C	45	PHE
3	1C	69	ASN
3	1C	73	LYS
3	1C	82	ASP
3	1C	89	ARG
3	1C	94	TYR
3	1C	125	LYS
3	1C	182	ARG
4	1D	2	ARG
4	1D	23	LYS
4	1D	40	LYS
4	1D	55	HIS
4	1D	66	MET
4	1D	67	GLU
4	1D	89	LYS
4	1D	111	MET
4	1D	133	ARG
4	1D	171	PHE
4	1D	220	PHE

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Mol	Chain	Res	Type
4	1D	221	ARG
4	1D	241	ASP
4	1D	261	ARG
4	1D	314	CYS
4	1D	356	TYR
4	1D	378	LEU
4	1D	392	LYS
4	1D	405	MET
4	1D	413	ASP
5	1E	27	ASN
5	1E	38	TYR
5	1E	58	ASN
5	1E	60	TRP
5	1E	86	PHE
5	1E	91	ASN
5	1E	103	CYS
5	1E	111	ARG
5	1E	118	GLU
5	1E	127	LYS
5	1E	150	ASN
5	1E	159	ASN
5	1E	190	ARG
6	1F	12	PHE
6	1F	20	ARG
6	1F	25	LEU
6	1F	28	ARG
6	1F	46	LYS
6	1F	55	TRP
6	1F	82	MET
6	1F	84	LYS
6	1F	107	ASP
6	1F	112	ARG
6	1F	132	ARG
6	1F	171	TYR
6	1F	173	PHE
6	1F	174	ASP
6	1F	249	ARG
6	1F	261	HIS
6	1F	266	CYS
6	1F	292	ASP
6	1F	306	LEU
6	1F	312	CYS

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Mol	Chain	Res	Type
6	1F	319	PHE
6	1F	345	LYS
6	1F	355	LYS
6	1F	359	CYS
6	1F	376	MET
6	1F	385	ARG
6	1F	393	TRP
6	1F	413	TRP
6	1F	416	GLN
6	1F	423	ARG
7	1G	19	MET
7	1G	45	ARG
7	1G	69	CYS
7	1G	77	TRP
7	1G	85	LYS
7	1G	129	ARG
7	1G	130	PHE
7	1G	171	ASP
7	1G	192	MET
7	1G	193	SER
7	1G	211	LYS
7	1G	223	ARG
7	1G	227	SER
7	1G	255	HIS
7	1G	262	TRP
7	1G	269	PHE
7	1G	283	MET
7	1G	324	ASP
7	1G	336	ASN
7	1G	341	ASP
7	1G	359	ARG
7	1G	399	TRP
7	1G	419	TYR
7	1G	420	ASP
7	1G	439	PHE
7	1G	486	ASP
7	1G	490	MET
7	1G	494	HIS
7	1G	517	ASN
7	1G	539	LYS
7	1G	542	PHE
7	1G	579	ARG

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Mol	Chain	Res	Type
7	1G	604	SER
7	1G	609	MET
7	1G	614	ASP
7	1G	620	ARG
7	1G	632	ARG
7	1G	641	TYR
7	1G	673	MET
7	1G	679	ARG
7	1G	704	CYS
8	1H	3	MET
8	1H	34	ARG
8	1H	35	LYS
8	1H	86	TRP
8	1H	127	TYR
8	1H	129	LEU
8	1H	133	LEU
8	1H	159	SER
8	1H	173	TRP
8	1H	282	TYR
8	1H	283	ASP
8	1H	304	HIS
9	1I	2	TYR
9	1I	6	ASN
9	1I	7	MET
9	1I	14	MET
9	1I	20	ARG
9	1I	26	LEU
9	1I	27	TRP
9	1I	39	SER
9	1I	40	TYR
9	1I	104	ARG
9	1I	109	TYR
9	1I	129	ASP
9	1I	147	LEU
9	1I	172	ASP
10	1J	17	PHE
10	1J	61	LEU
10	1J	78	MET
10	1J	79	TYR
10	1J	93	PHE
10	1J	101	PHE
10	1J	118	LYS

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Mol	Chain	Res	Type
10	1J	132	ASP
10	1J	175	ASN
11	1K	23	ARG
11	1K	36	MET
11	1K	52	HIS
11	1K	53	PHE
11	1K	59	MET
11	1K	69	CYS
12	1L	37	LYS
12	1L	61	MET
12	1L	67	HIS
12	1L	182	PHE
12	1L	186	MET
12	1L	267	MET
12	1L	276	MET
12	1L	310	LEU
12	1L	312	LEU
12	1L	331	MET
12	1L	336	LYS
12	1L	340	PHE
12	1L	359	MET
12	1L	400	ASN
12	1L	482	MET
12	1L	486	MET
12	1L	499	MET
12	1L	500	LEU
12	1L	504	LEU
12	1L	509	TYR
12	1L	512	LYS
12	1L	545	SER
12	1L	599	MET
12	1L	602	PHE
12	1L	606	GLU
13	1M	22	MET
13	1M	76	MET
13	1M	85	SER
13	1M	87	GLU
13	1M	209	LEU
13	1M	213	HIS
13	1M	263	MET
13	1M	281	ASP
13	1M	366	ASN

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Mol	Chain	Res	Type
13	1M	418	LYS
13	1M	446	LEU
14	1N	88	LYS
14	1N	112	HIS
14	1N	148	SER
14	1N	159	MET
14	1N	167	TRP
14	1N	182	SER
14	1N	200	MET
14	1N	216	PHE
14	1N	251	MET
14	1N	284	MET
14	1N	293	TYR
14	1N	304	MET
14	1N	313	MET
14	1N	323	MET
15	1O	3	TYR
15	1O	10	LEU
15	1O	30	ASN
15	1O	32	CYS
15	1O	81	LYS
15	1O	85	ASP
15	1O	95	ARG
15	1O	140	ARG
15	1O	146	LYS
15	1O	192	MET
15	1O	206	TYR
15	1O	218	CYS
15	1O	227	GLU
15	1O	258	ARG
15	1O	270	LEU
15	1O	288	GLN
15	1O	295	LYS
15	1O	302	ARG
16	1P	2	HIS
16	1P	36	ASN
16	1P	50	ARG
16	1P	58	HIS
16	1P	60	ARG
16	1P	62	MET
16	1P	65	LEU
16	1P	73	TRP

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Mol	Chain	Res	Type
16	1P	102	LYS
16	1P	106	PHE
16	1P	144	ARG
16	1P	145	TYR
16	1P	178	PHE
16	1P	186	ARG
16	1P	216	ASN
16	1P	219	LYS
16	1P	234	ASN
16	1P	263	TYR
16	1P	268	ARG
16	1P	281	ARG
16	1P	283	LYS
16	1P	292	MET
16	1P	302	ASP
16	1P	306	GLN
16	1P	316	GLU
16	1P	326	TRP
16	1P	331	MET
17	1Q	15	GLU
17	1Q	42	ARG
17	1Q	91	ASP
17	1Q	126	LYS
17	1Q	129	ARG
18	1R	3	ARG
18	1R	31	ARG
18	1R	38	ASN
18	1R	42	ASP
18	1R	80	LYS
19	1S	25	ARG
19	1S	67	ARG
19	1S	68	TYR
20	1T	38	LYS
20	1T	42	LEU
20	1T	46	ASP
20	1T	66	ASP
20	1T	69	LYS
20	1T	72	CYS
20	1U	12	LYS
20	1U	16	LEU
20	1U	22	TYR
20	1U	35	HIS

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Mol	Chain	Res	Type
20	1U	38	LYS
20	1U	60	PHE
20	1U	72	CYS
20	1U	83	LYS
20	1U	84	LYS
21	1V	27	TYR
21	1V	40	ASN
21	1V	43	TYR
21	1V	46	TYR
21	1V	57	MET
21	1V	81	LEU
21	1V	92	LYS
21	1V	93	MET
21	1V	100	GLU
22	1W	22	SER
22	1W	36	TYR
22	1W	40	TYR
22	1W	57	LYS
22	1W	65	GLU
22	1W	70	ASN
22	1W	72	HIS
22	1W	88	MET
22	1W	106	PHE
22	1W	108	HIS
23	1X	37	LYS
23	1X	50	LYS
23	1X	76	HIS
23	1X	81	PHE
23	1X	91	SER
23	1X	101	LYS
23	1X	106	PHE
23	1X	107	ASP
23	1X	120	ASP
23	1X	156	ASP
24	1Y	90	PHE
24	1Y	94	CYS
24	1Y	126	MET
25	1Z	10	MET
25	1Z	22	LYS
25	1Z	24	ASN
25	1Z	55	ARG
25	1Z	82	ARG

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Mol	Chain	Res	Type
25	1Z	86	MET
25	1Z	88	ARG
25	1Z	89	GLU
25	1Z	105	LYS
26	1a	3	PHE
26	1a	12	MET
26	1a	53	CYS
26	1a	61	HIS
26	1a	67	GLU
27	1b	8	LEU
27	1b	56	LEU
27	1b	62	MET
28	1c	5	ARG
28	1c	30	TYR
28	1c	44	ARG
29	1d	13	PHE
29	1d	49	ARG
29	1d	67	SER
29	1d	86	ARG
29	1d	90	MET
30	1e	8	ARG
30	1e	21	SER
30	1e	60	ASP
30	1e	61	ASP
30	1e	70	LYS
30	1e	82	ARG
30	1e	91	TYR
30	1e	96	HIS
30	1e	97	HIS
30	1e	98	LEU
31	1f	22	PHE
31	1f	29	ARG
31	1f	37	PHE
31	1f	53	GLU
32	1g	25	ARG
32	1g	28	GLU
32	1g	48	ASP
32	1g	49	LYS
32	1g	85	MET
32	1g	99	TYR
32	1g	100	ARG
32	1g	116	ASN

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Mol	Chain	Res	Type
32	1g	122	GLU
33	1h	7	ARG
33	1h	18	ASP
33	1h	25	MET
33	1h	26	ARG
33	1h	27	PHE
33	1h	28	TYR
33	1h	54	ASP
33	1h	87	TYR
33	1h	91	MET
33	1h	107	GLU
33	1h	111	ARG
33	1h	122	TRP
33	1h	129	ASP
34	1i	3	TYR
34	1i	10	ARG
34	1i	55	PRO
34	1i	69	PHE
35	1j	40	PHE
36	1k	12	LYS
36	1k	34	LYS
36	1k	46	ARG
36	1k	68	LYS
36	1k	71	LYS
36	1k	74	PHE
36	1k	77	PHE
36	1k	87	LEU
37	1l	6	LYS
37	1l	15	LYS
37	1l	25	LYS
37	1l	108	PHE
37	1l	112	MET
37	1l	114	PHE
37	1l	115	MET
37	1l	116	PHE
37	1l	140	LEU
37	1l	149	GLU
38	1m	2	PHE
38	1m	23	ASP
38	1m	74	ASN
38	1m	80	ARG
38	1m	92	PHE

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Mol	Chain	Res	Type
38	1m	122	GLN
38	1m	128	TYR
39	1n	36	TYR
39	1n	43	MET
39	1n	47	PHE
39	1n	49	GLU
39	1n	51	LYS
39	1n	67	GLU
39	1n	134	ARG
39	1n	157	ARG
40	1o	7	ARG
40	1o	11	ASP
40	1o	28	TYR
40	1o	60	HIS
40	1o	94	TYR
40	1o	98	MET
40	1o	99	LYS
40	1o	111	LYS
41	1p	7	ASP
41	1p	14	ARG
41	1p	27	ASN
41	1p	62	TYR
41	1p	133	GLN
41	1p	162	MET
42	1q	1	MET
42	1q	8	ARG
42	1q	59	HIS
42	1q	67	GLU
42	1q	71	ARG
42	1q	72	ASP
42	1q	81	MET
42	1q	101	LYS
42	1q	144	TYR
43	1r	5	ARG
43	1r	9	LEU
43	1r	39	LYS
43	1r	46	HIS
43	1r	47	LYS
43	1r	48	LEU
43	1r	50	ASN
43	1r	53	TYR
43	1r	56	ARG

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Mol	Chain	Res	Type
43	1r	69	MET
43	1r	70	SER
43	1r	92	LYS
43	1r	102	ARG
44	1s	49	TYR
44	1s	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	80	GLN
2	1B	164	GLN
3	1C	192	GLN
4	1D	84	HIS
4	1D	149	ASN
4	1D	150	HIS
4	1D	266	GLN
5	1E	9	HIS
6	1F	83	ASN
6	1F	148	ASN
6	1F	250	ASN
6	1F	257	ASN
7	1G	36	GLN
7	1G	548	HIS
7	1G	549	HIS
7	1G	618	GLN
8	1H	287	HIS
12	1L	175	ASN
12	1L	506	ASN
13	1M	168	GLN
13	1M	415	GLN
14	1N	112	HIS
14	1N	221	HIS
15	1O	30	ASN
15	1O	72	GLN
15	1O	76	ASN
16	1P	67	GLN
17	1Q	81	ASN
19	1S	75	ASN
21	1V	82	GLN
21	1V	85	ASN
24	1Y	88	ASN

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Mol	Chain	Res	Type
26	1a	68	ASN
29	1d	46	ASN
29	1d	61	GLN
29	1d	88	HIS
30	1e	33	HIS
32	1g	57	ASN
34	1i	13	GLN
37	1l	136	ASN
40	1o	3	HIS
40	1o	60	HIS
41	1p	58	ASN
41	1p	99	GLN
41	1p	122	GLN
41	1p	158	GLN
42	1q	13	GLN
42	1q	54	GLN
42	1q	59	HIS
42	1q	69	ASN
42	1q	87	HIS
42	1q	112	ASN
43	1r	24	GLN
43	1r	51	ASN
44	1s	40	ASN
44	1s	43	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	FME	1H	1	8	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
34	SAC	1i	1	-	7,8,9	0.54	0	8,9,11	1.04	1 (12%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	0.94	1 (14%)
14	FME	1N	1	14	8,9,10	0.53	0	7,9,11	1.03	1 (14%)
13	FME	1M	1	13	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
10	FME	1J	1	10	8,9,10	0.53	0	7,9,11	0.97	1 (14%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	1.06	1 (14%)
1	FME	1A	1	1	8,9,10	0.50	0	7,9,11	1.02	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	-
34	SAC	1i	1	-	-	2/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
10	FME	1J	1	10	-	3/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-

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	-2.87	117.26	124.78
12	1L	1	FME	O-C-CA	-2.61	117.93	124.78
13	1M	1	FME	O-C-CA	-2.53	118.15	124.78
10	1J	1	FME	O-C-CA	-2.51	118.20	124.78
1	1A	1	FME	O-C-CA	-2.50	118.23	124.78
14	1N	1	FME	O-C-CA	-2.49	118.26	124.78
8	1H	1	FME	O-C-CA	-2.48	118.28	124.78
11	1K	1	FME	O-C-CA	-2.41	118.47	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	N-CA-CB-CG
10	1J	1	FME	CB-CG-SD-CE
11	1K	1	FME	CB-CG-SD-CE
34	1i	1	SAC	C-CA-N-C1A
34	1i	1	SAC	CB-CA-N-C1A
10	1J	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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	$\#\|Z\| > 2$
56	NDP	1P	501	-	45,52,52	0.62	0	53,80,80	0.87	2 (3%)
48	FMN	1F	501	-	33,33,33	0.58	0	48,50,50	0.64	0
58	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.27	1 (2%)
47	FES	1G	803	7	0,4,4	-	-	-		
46	SF4	1I	201	9	0,12,12	-	-	-		
45	3PE	1Y	202	-	50,50,50	0.26	0	53,55,55	0.31	0
46	SF4	1I	202	9	0,12,12	-	-	-		
50	PC1	1I	203	-	53,53,53	0.26	0	59,61,61	0.32	0
45	3PE	1L	702	-	45,45,50	0.28	0	48,50,55	0.31	0
47	FES	1E	301	5	0,4,4	-	-	-		
46	SF4	1B	201	2	0,12,12	-	-	-		
58	EHZ	1n	201	-	29,36,37	0.18	0	35,44,47	1.20	1 (2%)
50	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.39	0
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	SF4	1G	802	7	0,12,12	-	-	-		
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.44	0
45	3PE	1Y	201	-	30,30,50	0.35	0	33,35,55	0.65	1 (3%)
46	SF4	1F	502	6	0,12,12	-	-	-		
45	3PE	1L	704	-	41,41,50	0.30	0	44,46,55	1.28	5 (11%)
45	3PE	1N	401	-	50,50,50	0.26	0	53,55,55	0.37	0
53	CDL	1r	201	-	60,60,99	0.84	3 (5%)	66,72,111	1.10	4 (6%)
53	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.37	0
51	MYR	1L	701	-	14,14,15	0.34	0	13,13,15	0.41	0
50	PC1	1f	101	-	45,45,53	0.26	0	51,53,61	0.35	0
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.86	1 (3%)
52	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.49	0
50	PC1	1L	703	-	43,43,53	0.29	0	49,51,61	0.38	0
46	SF4	1G	801	7	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	NDP	1P	501	-	-	11/30/77/77	0/5/5/5
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
58	EHZ	1W	201	-	-	8/42/44/45	-
47	FES	1G	803	7	-	-	0/1/1/1
46	SF4	1I	201	9	-	-	0/6/5/5
45	3PE	1Y	202	-	-	8/54/54/54	-
46	SF4	1I	202	9	-	-	0/6/5/5
50	PC1	1I	203	-	-	16/57/57/57	-
45	3PE	1L	702	-	-	4/49/49/54	-
47	FES	1E	301	5	-	-	0/1/1/1
46	SF4	1B	201	2	-	-	0/6/5/5
58	EHZ	1n	201	-	-	8/42/44/45	-
50	PC1	1I	204	-	-	4/47/47/57	-
45	3PE	1A	201	-	-	3/50/50/54	-
50	PC1	1J	201	-	-	3/38/38/57	-
46	SF4	1G	802	7	-	-	0/6/5/5
45	3PE	1Y	201	-	-	9/34/34/54	-
46	SF4	1F	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1L	704	-	-	7/45/45/54	-
45	3PE	1N	401	-	-	10/54/54/54	-
53	CDL	1r	201	-	-	16/71/71/110	-
53	CDL	1N	402	-	-	8/87/87/110	-
51	MYR	1L	701	-	-	1/11/12/13	-
50	PC1	1f	101	-	-	13/49/49/57	-
54	GTP	1O	401	55	-	0/18/38/38	0/3/3/3
52	PGT	1M	501	-	-	23/55/55/55	-
50	PC1	1L	703	-	-	8/47/47/57	-
46	SF4	1G	801	7	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1r	201	CDL	OB5-CB3	4.73	1.63	1.44
54	1O	401	GTP	C5-C6	-2.59	1.42	1.47
53	1r	201	CDL	OB2-CB2	2.19	1.53	1.44
53	1r	201	CDL	PB2-OB4	-2.18	1.45	1.55
54	1O	401	GTP	C8-N7	-2.07	1.31	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1n	201	EHZ	C10-S1-C9	6.79	123.01	101.87
58	1W	201	EHZ	C10-S1-C9	6.74	122.86	101.87
45	1L	704	3PE	O21-C21-C22	6.30	125.08	111.50
53	1r	201	CDL	OB4-PB2-OB2	4.45	128.41	107.75
53	1r	201	CDL	OB5-PB2-OB3	-4.25	92.48	109.07
53	1r	201	CDL	OB2-PB2-OB3	-3.92	93.76	109.07
56	1P	501	NDP	O4D-C1D-C2D	-3.32	99.41	106.64
53	1r	201	CDL	OB4-PB2-OB5	3.30	123.09	107.75
54	1O	401	GTP	O4'-C1'-C2'	-2.72	102.95	106.93
45	1L	704	3PE	O21-C21-O22	-2.68	117.22	123.70
45	1L	704	3PE	C2-O21-C21	2.56	124.10	117.79
45	1Y	201	3PE	O21-C21-C22	2.45	116.79	111.50
45	1L	704	3PE	O21-C2-C1	2.29	116.70	108.40
56	1P	501	NDP	C5A-C6A-N6A	2.25	123.78	120.35
45	1L	704	3PE	O21-C2-C3	2.02	115.73	108.40

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	704	3PE	O22-C21-O21-C2
45	1L	704	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	201	3PE	C1-O11-P-O14
45	1Y	201	3PE	O32-C31-O31-C3
45	1Y	201	3PE	C32-C31-O31-C3
45	1Y	201	3PE	O22-C21-O21-C2
45	1Y	201	3PE	C22-C21-O21-C2
45	1Y	202	3PE	C1-O11-P-O14
50	1I	203	PC1	O13-C11-C12-N
50	1I	204	PC1	C11-O13-P-O14
50	1I	204	PC1	C11-O13-P-O11
50	1J	201	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O13
50	1L	703	PC1	C1-O11-P-O14
52	1M	501	PGT	O31-C31-O2-C2
52	1M	501	PGT	C1-O3P-P-O1P
52	1M	501	PGT	C1-O3P-P-O4P
52	1M	501	PGT	C4-O4P-P-O3P
52	1M	501	PGT	C4-O4P-P-O1P
52	1M	501	PGT	C4-O4P-P-O2P
52	1M	501	PGT	C12-C11-O3-C3
53	1r	201	CDL	CA2-C1-CB2-OB2
53	1r	201	CDL	CA3-OA5-PA1-OA3
53	1r	201	CDL	CB3-OB5-PB2-OB2
53	1r	201	CDL	CB3-OB5-PB2-OB3
56	1P	501	NDP	C5D-O5D-PN-O3
56	1P	501	NDP	C5D-O5D-PN-O1N
58	1W	201	EHZ	N2-C15-C16-C17
58	1W	201	EHZ	N2-C15-C16-O5
58	1W	201	EHZ	O4-C15-C16-C17
58	1n	201	EHZ	C16-C17-C20-O6
58	1n	201	EHZ	O2-C9-S1-C10
58	1n	201	EHZ	C8-C9-S1-C10
52	1M	501	PGT	O11-C11-O3-C3
52	1M	501	PGT	C32-C31-O2-C2
58	1W	201	EHZ	C13-C12-N1-C11
53	1r	201	CDL	O1-C1-CB2-OB2
45	1Y	202	3PE	C2-C1-O11-P
58	1W	201	EHZ	O3-C12-N1-C11
52	1M	501	PGT	C15-C16-C17-C18
58	1W	201	EHZ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
56	1P	501	NDP	C2D-C1D-N1N-C2N
56	1P	501	NDP	C2D-C1D-N1N-C6N
52	1M	501	PGT	C40-C41-C42-C43
52	1M	501	PGT	C14-C15-C16-C17
58	1n	201	EHZ	C18-C17-C20-O6
50	1I	203	PC1	C24-C25-C26-C27
52	1M	501	PGT	C5-C4-O4P-P
50	1f	101	PC1	C25-C26-C27-C28
52	1M	501	PGT	C34-C35-C36-C37
45	1A	201	3PE	O21-C2-C3-O31
53	1N	402	CDL	OA6-CA4-CA6-OA8
50	1I	203	PC1	C11-O13-P-O11
50	1L	703	PC1	C1-O11-P-O13
53	1r	201	CDL	CB4-CB3-OB5-PB2
58	1n	201	EHZ	C1-C21-C22-C23
45	1Y	202	3PE	C3C-C3D-C3E-C3F
52	1M	501	PGT	C21-C22-C23-C24
45	1A	201	3PE	C1-C2-C3-O31
45	1Y	202	3PE	C35-C36-C37-C38
50	1I	203	PC1	O31-C31-C32-C33
58	1W	201	EHZ	O4-C15-C16-O5
50	1f	101	PC1	C31-C32-C33-C34
58	1n	201	EHZ	C19-C17-C20-O6
53	1N	402	CDL	C55-C56-C57-C58
53	1N	402	CDL	C75-C76-C77-C78
53	1r	201	CDL	OB6-CB4-CB6-OB8
52	1M	501	PGT	C44-C45-C46-C47
52	1M	501	PGT	C22-C23-C24-C25
45	1N	401	3PE	O31-C31-C32-C33
50	1f	101	PC1	C1-C2-C3-O31
53	1N	402	CDL	CA3-CA4-CA6-OA8
53	1r	201	CDL	CB3-CB4-CB6-OB8
45	1L	704	3PE	O11-C1-C2-O21
58	1W	201	EHZ	C5-C6-C7-O1
45	1N	401	3PE	C2-C1-O11-P
56	1P	501	NDP	PN-O3-PA-O5B
45	1N	401	3PE	O11-C1-C2-O21
45	1Y	202	3PE	O11-C1-C2-O21
56	1P	501	NDP	O4D-C1D-N1N-C6N
53	1N	402	CDL	C33-C34-C35-C36
50	1I	204	PC1	C34-C35-C36-C37
45	1N	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	1Y	201	3PE	C1-O11-P-O13
45	1Y	202	3PE	C1-O11-P-O13
53	1r	201	CDL	CB2-OB2-PB2-OB5
53	1r	201	CDL	CA4-CA3-OA5-PA1
50	1L	703	PC1	C1-O11-P-O12
53	1r	201	CDL	CB2-OB2-PB2-OB3
53	1r	201	CDL	CB3-OB5-PB2-OB4
56	1P	501	NDP	C5D-O5D-PN-O2N
45	1N	401	3PE	C34-C35-C36-C37
45	1A	201	3PE	C12-C11-O13-P
56	1P	501	NDP	C3B-C2B-O2B-P2B
50	1I	203	PC1	C38-C39-C3A-C3B
50	1J	201	PC1	O13-C11-C12-N
51	1L	701	MYR	C7-C8-C9-C10
52	1M	501	PGT	C16-C17-C18-C19
56	1P	501	NDP	O4D-C1D-N1N-C2N
53	1N	402	CDL	C32-C33-C34-C35
56	1P	501	NDP	C1B-C2B-O2B-P2B
52	1M	501	PGT	C18-C19-C20-C21
45	1Y	202	3PE	O11-C1-C2-C3
45	1N	401	3PE	C39-C3A-C3B-C3C
45	1N	401	3PE	C3A-C3B-C3C-C3D
45	1L	702	3PE	C33-C34-C35-C36
50	1I	204	PC1	O21-C2-C3-O31
50	1f	101	PC1	C11-O13-P-O11
53	1r	201	CDL	CA3-OA5-PA1-OA2
45	1N	401	3PE	C2-C3-O31-C31
50	1I	203	PC1	C11-C12-N-C14
45	1Y	201	3PE	C21-C22-C23-C24
52	1M	501	PGT	C2-C1-O3P-P
50	1f	101	PC1	C21-C22-C23-C24
45	1L	702	3PE	C22-C23-C24-C25
50	1I	203	PC1	C3B-C3C-C3D-C3E
50	1I	203	PC1	O32-C31-C32-C33
58	1n	201	EHZ	S1-C10-C11-N1
53	1r	201	CDL	C12-C13-C14-C15
50	1L	703	PC1	C1-C2-C3-O31
45	1L	704	3PE	C1-C2-O21-C21
50	1f	101	PC1	O21-C2-C3-O31
53	1r	201	CDL	CB2-C1-CA2-OA2
50	1I	203	PC1	C23-C24-C25-C26
52	1M	501	PGT	O3P-C1-C2-O2

Continued on next page...

Continued from previous page...

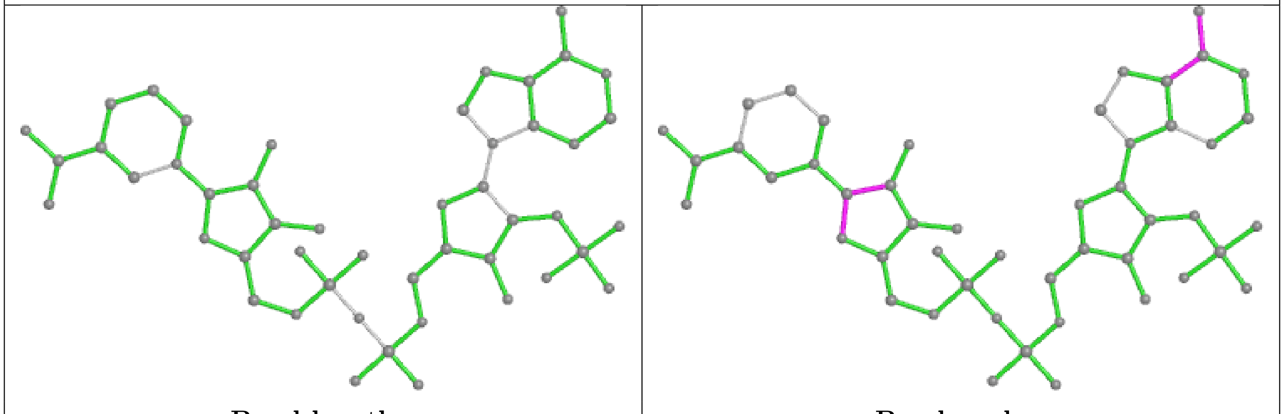
Mol	Chain	Res	Type	Atoms
52	1M	501	PGT	O3P-C1-C2-C3
50	1f	101	PC1	C1-O11-P-O13
50	1L	703	PC1	O31-C31-C32-C33
50	1I	203	PC1	C33-C34-C35-C36
50	1I	203	PC1	C3A-C3B-C3C-C3D
53	1N	402	CDL	C53-C54-C55-C56
45	1L	704	3PE	C1-C2-C3-O31
45	1L	704	3PE	C32-C33-C34-C35
45	1Y	201	3PE	O21-C2-C3-O31
52	1M	501	PGT	C35-C36-C37-C38
50	1I	203	PC1	C11-C12-N-C15
50	1I	203	PC1	C39-C3A-C3B-C3C
50	1f	101	PC1	C27-C28-C29-C2A
45	1L	702	3PE	C37-C38-C39-C3A
58	1n	201	EHZ	C3-C4-C5-C6
45	1N	401	3PE	C11-O13-P-O14
50	1I	203	PC1	C11-O13-P-O14
50	1I	203	PC1	C11-C12-N-C13
50	1L	703	PC1	C11-O13-P-O14
50	1f	101	PC1	C1-O11-P-O14
56	1P	501	NDP	O4B-C4B-C5B-O5B
45	1Y	202	3PE	C12-C11-O13-P
50	1f	101	PC1	O21-C21-C22-C23
50	1L	703	PC1	O32-C31-C32-C33
45	1L	702	3PE	C35-C36-C37-C38
50	1I	203	PC1	C32-C33-C34-C35
48	1F	501	FMN	N10-C1'-C2'-O2'
50	1f	101	PC1	O32-C31-C32-C33
50	1f	101	PC1	O31-C31-C32-C33
53	1r	201	CDL	C12-C11-CA5-OA6
53	1N	402	CDL	C52-C53-C54-C55
50	1f	101	PC1	O22-C21-C22-C23
50	1L	703	PC1	O21-C21-C22-C23
45	1Y	201	3PE	O22-C21-C22-C23
45	1L	704	3PE	C22-C23-C24-C25

There are no ring outliers.

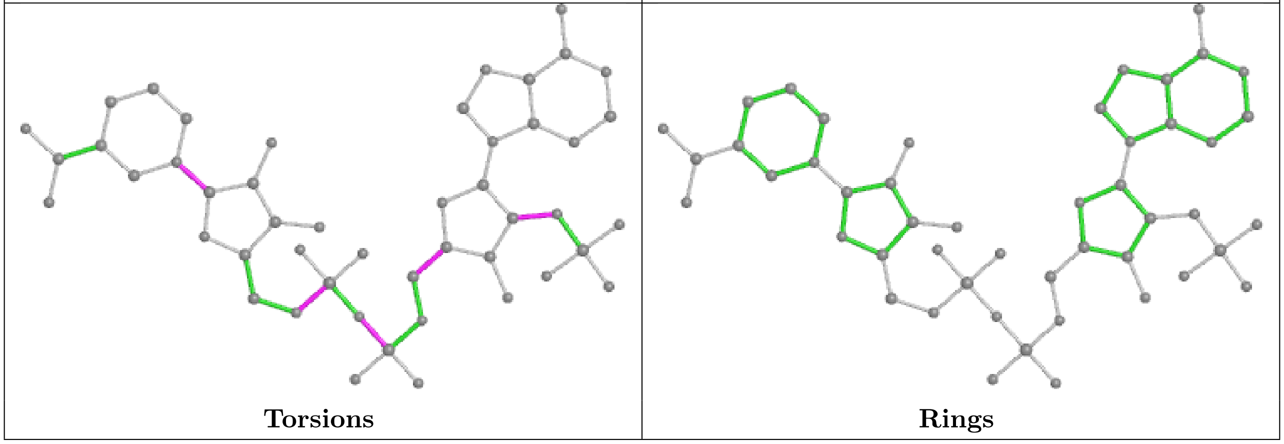
No monomer is involved in short contacts.

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 NDP 1P 501

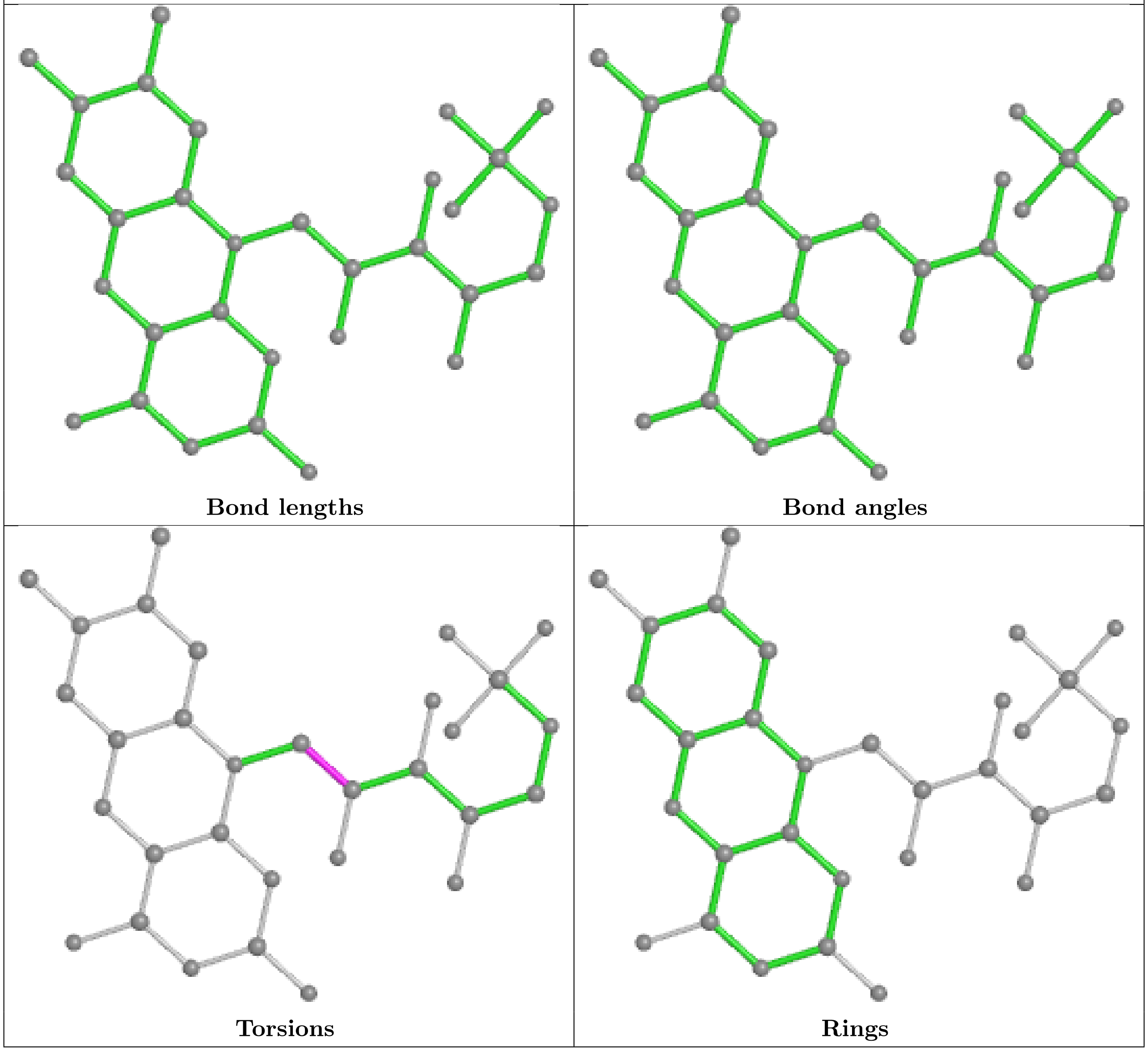


Bond lengths **Bond angles**

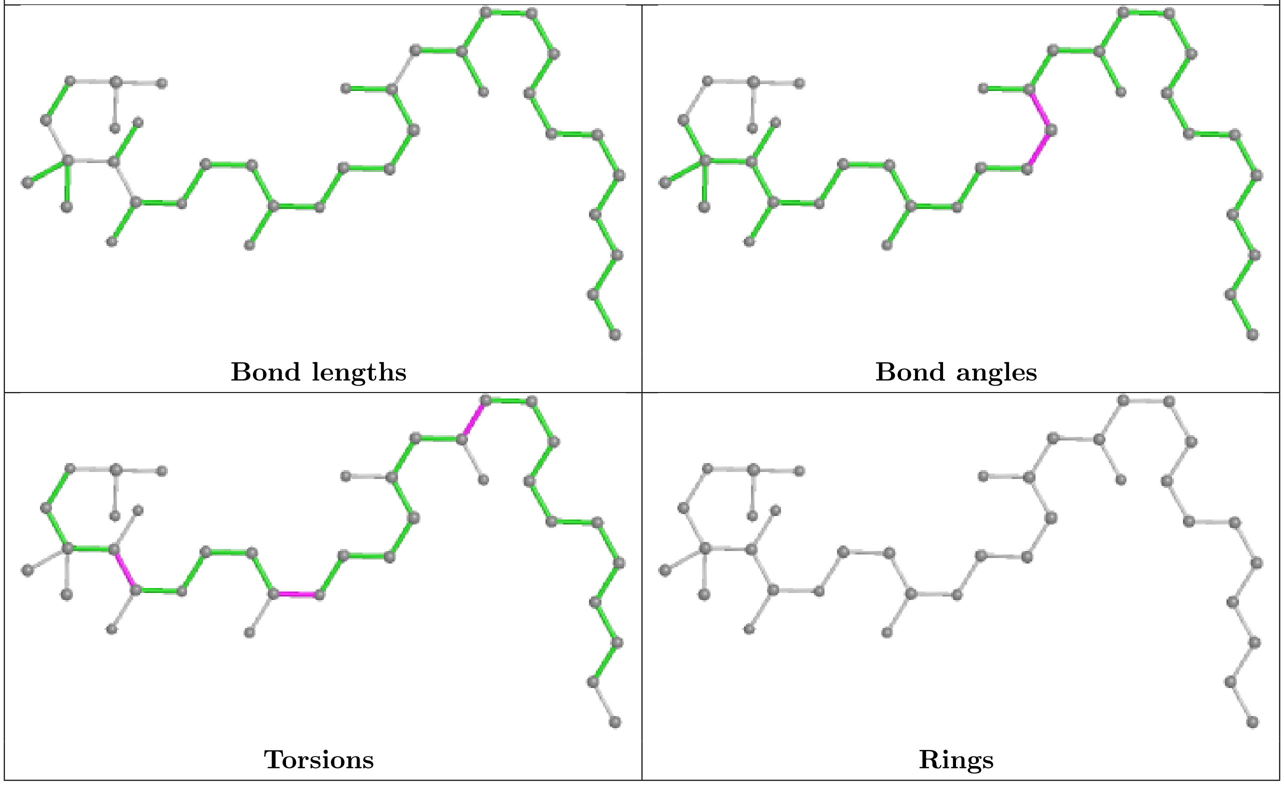


Torsions **Rings**

Ligand FMN 1F 501



Ligand EHZ 1W 201



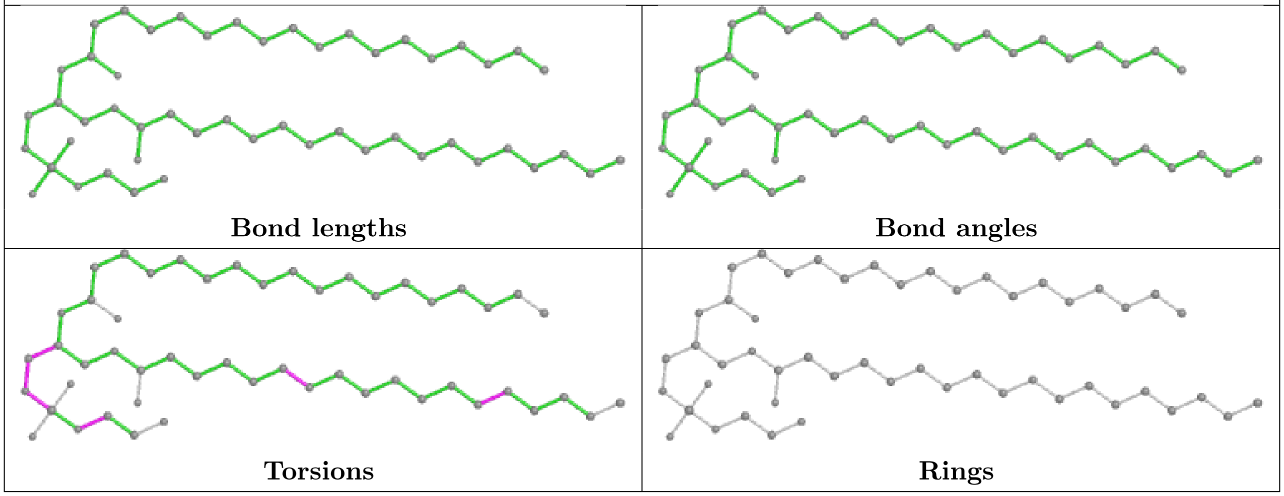
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 1Y 202



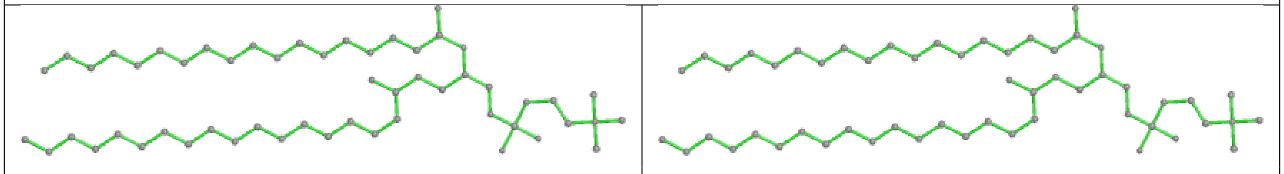
Bond lengths

Bond angles

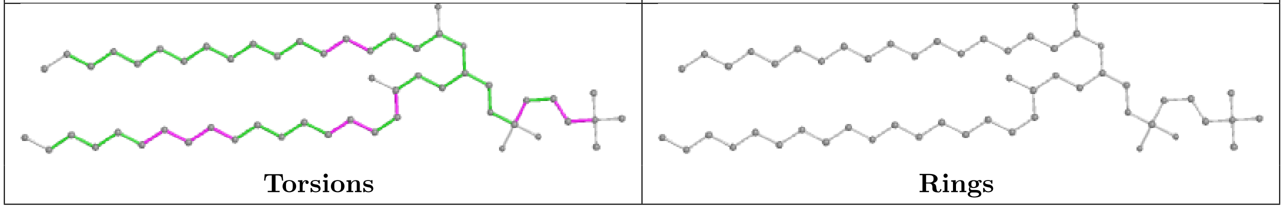
Torsions

Rings

Ligand PC1 1I 203

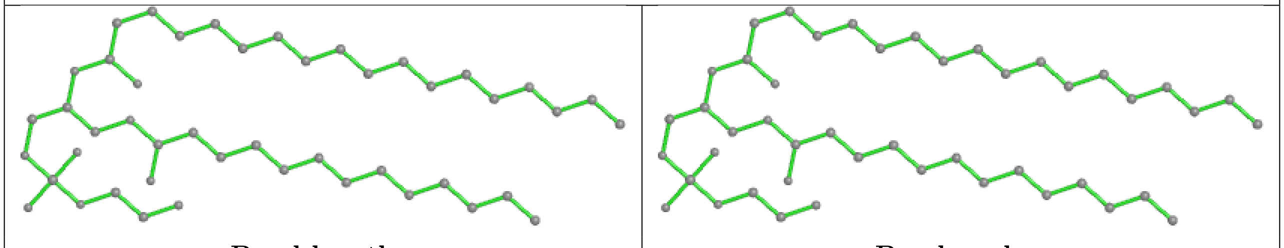


Bond lengths Bond angles

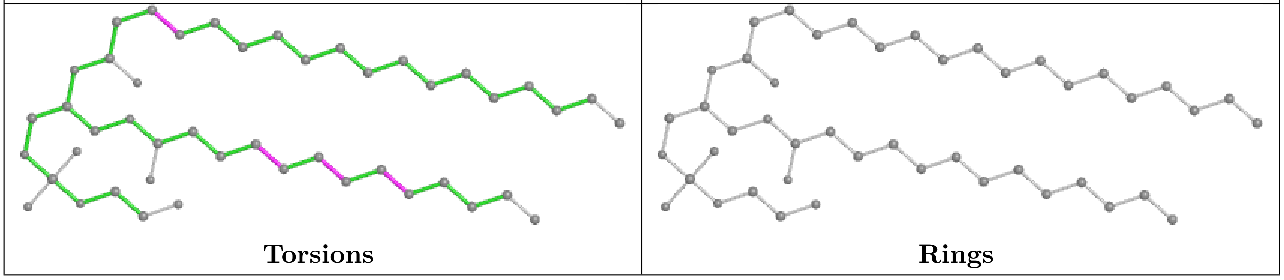


Torsions Rings

Ligand 3PE 1L 702

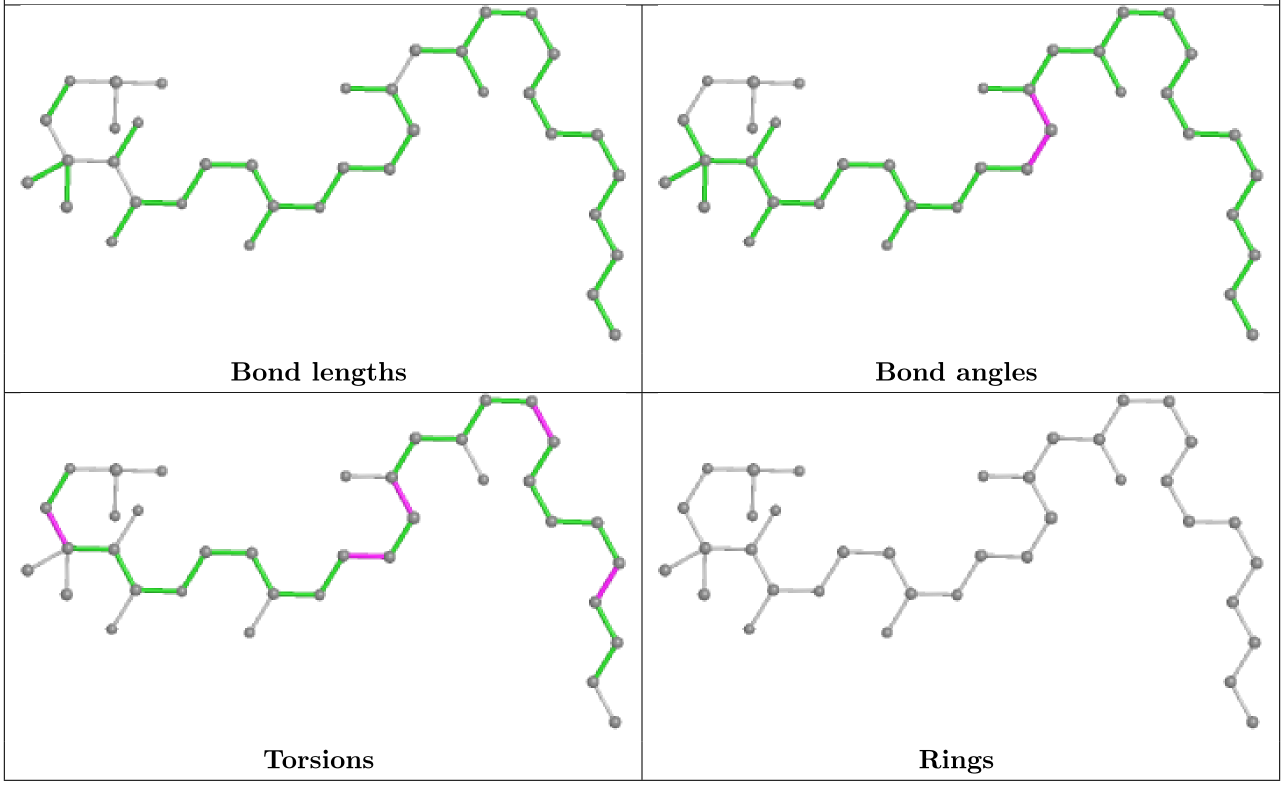


Bond lengths Bond angles



Torsions Rings

Ligand EHZ 1n 201



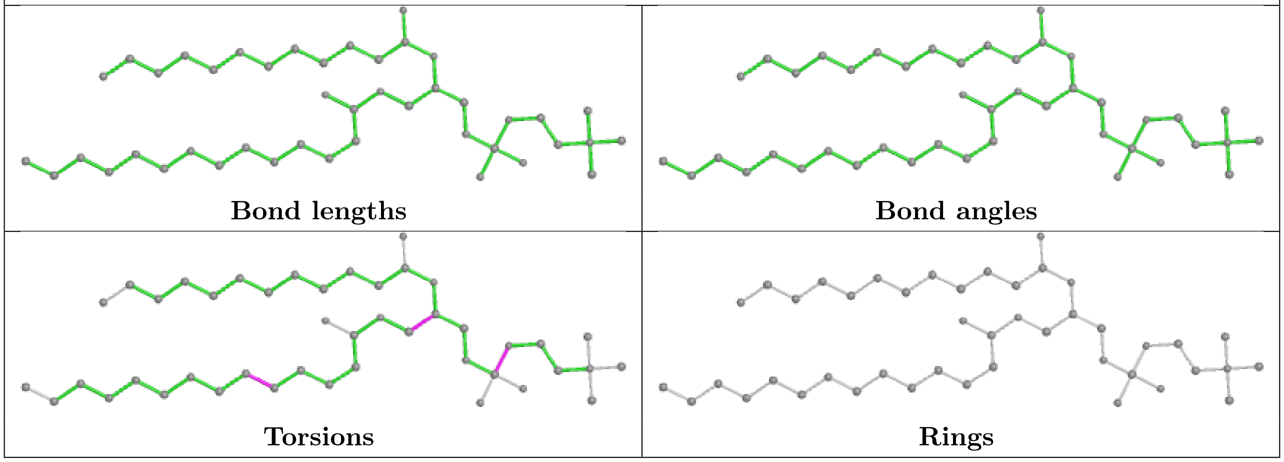
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 1I 204



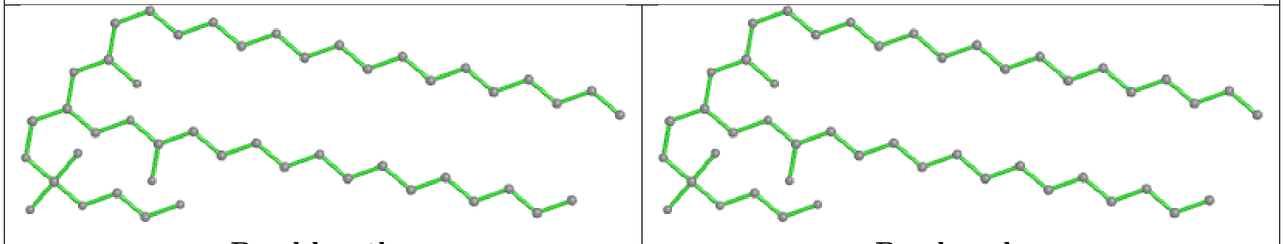
Bond lengths

Bond angles

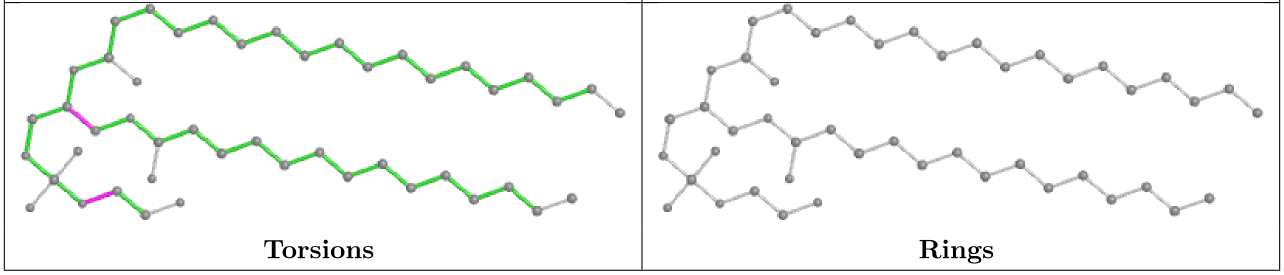
Torsions

Rings

Ligand 3PE 1A 201

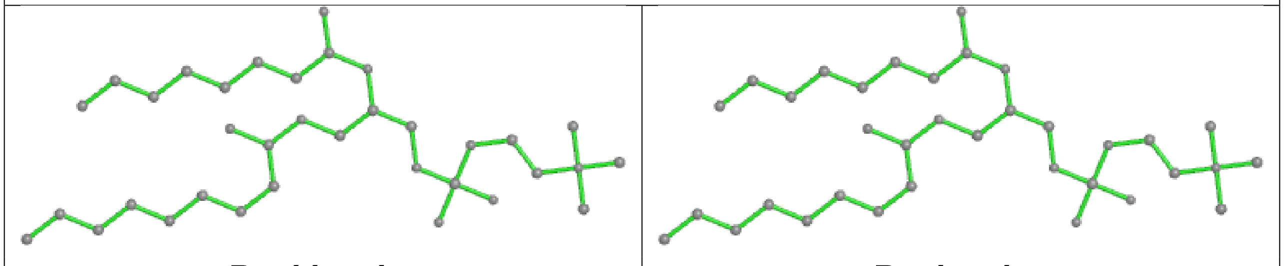


Bond lengths **Bond angles**

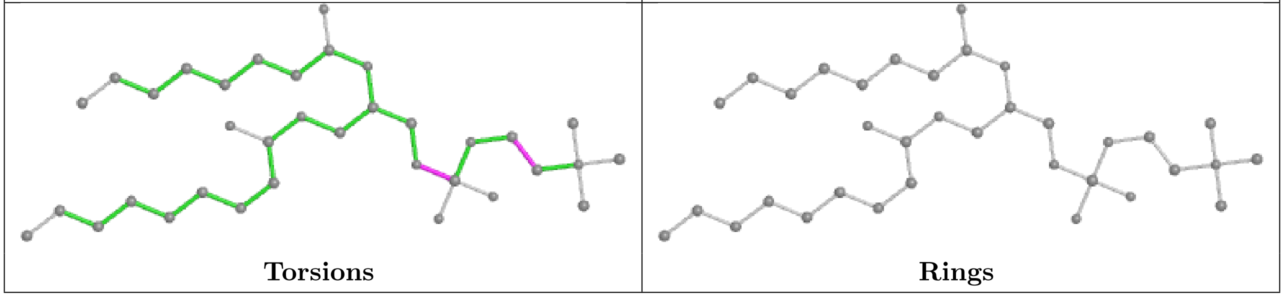


Torsions **Rings**

Ligand PC1 1J 201

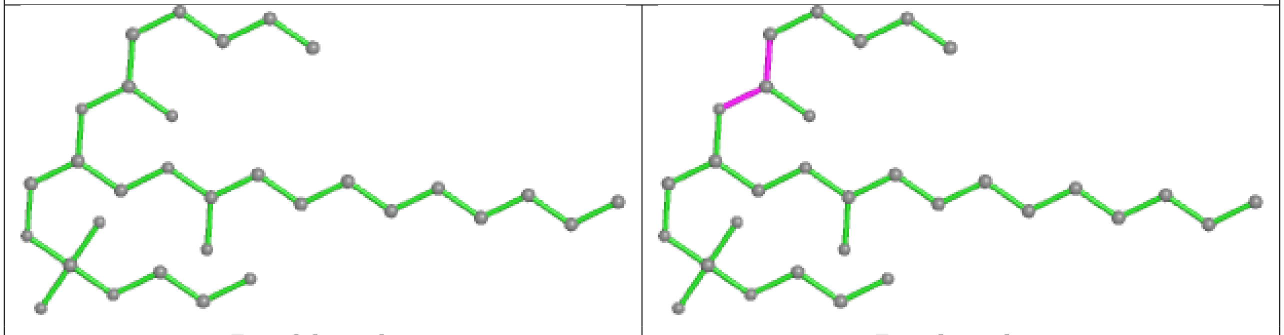


Bond lengths **Bond angles**

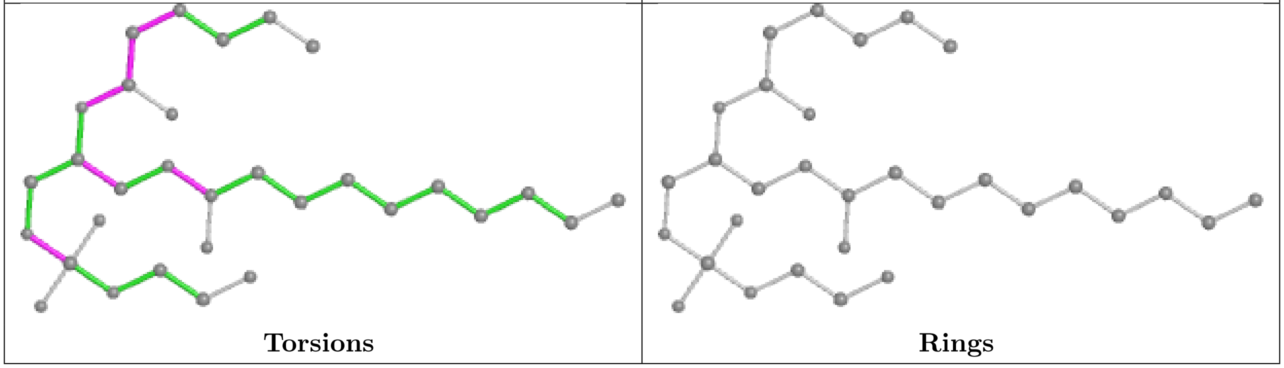


Torsions **Rings**

Ligand 3PE 1Y 201

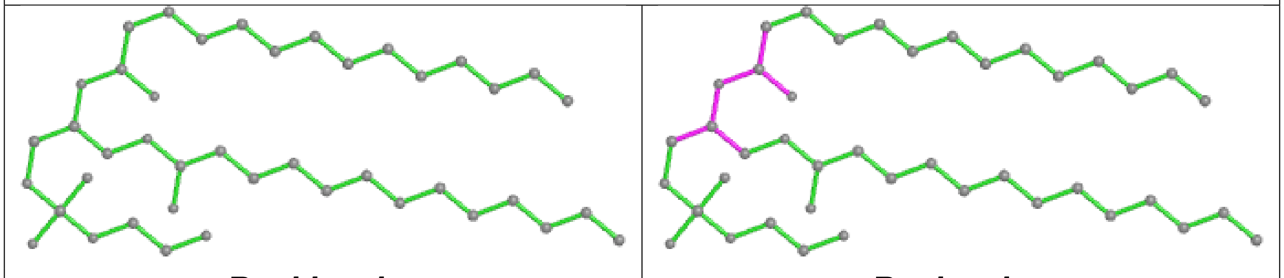


Bond lengths **Bond angles**

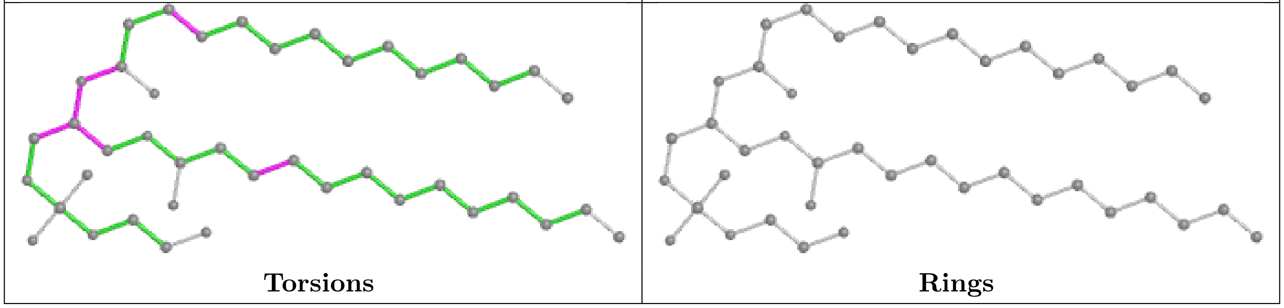


Torsions **Rings**

Ligand 3PE 1L 704

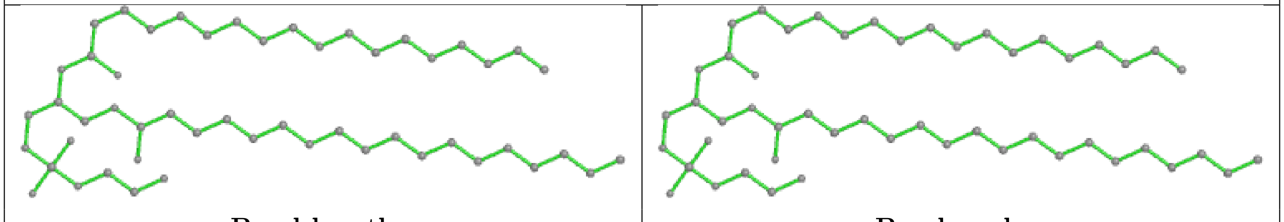


Bond lengths **Bond angles**



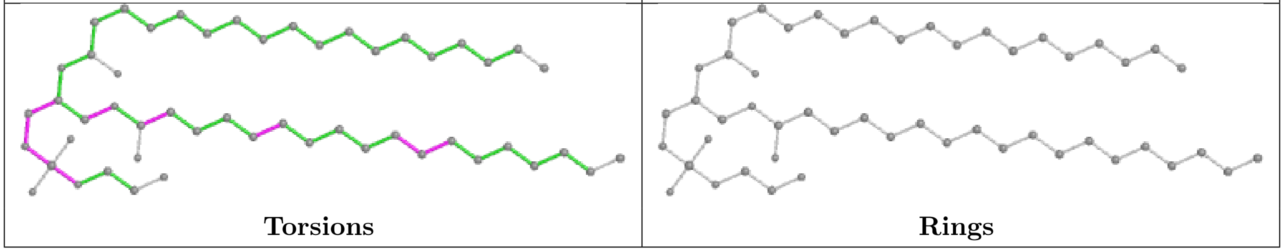
Torsions **Rings**

Ligand 3PE 1N 401



Bond lengths

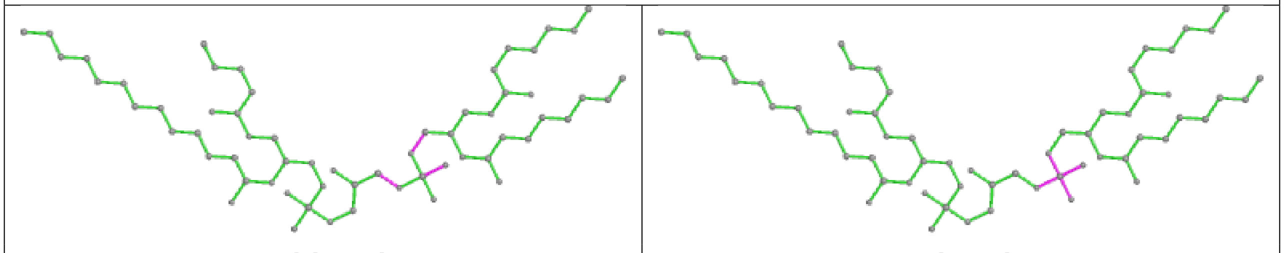
Bond angles



Torsions

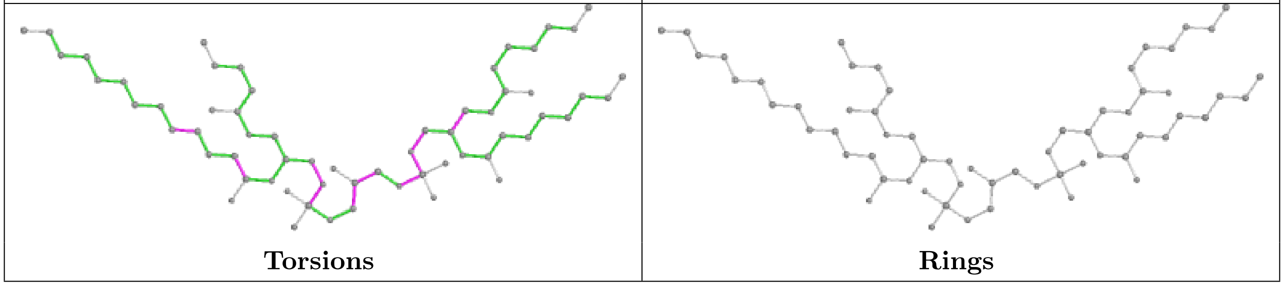
Rings

Ligand CDL 1r 201



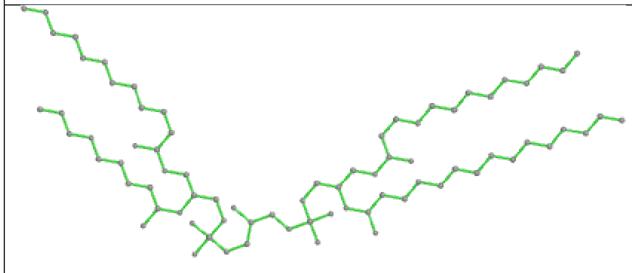
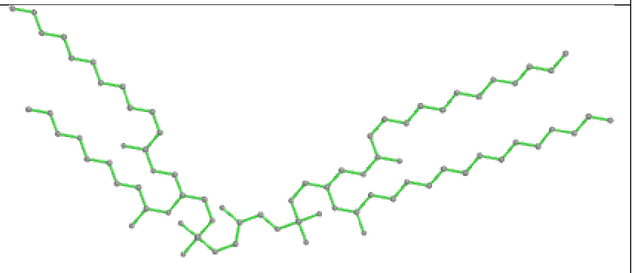
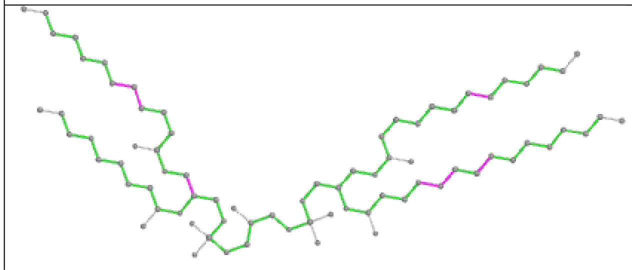
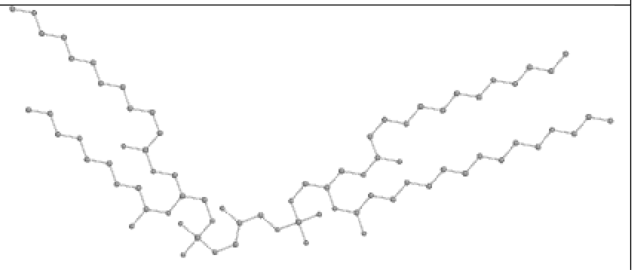
Bond lengths

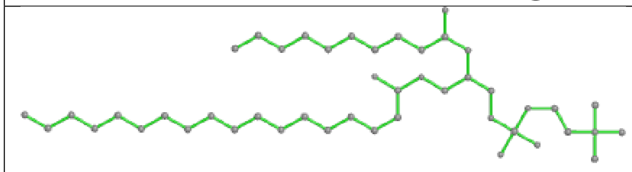
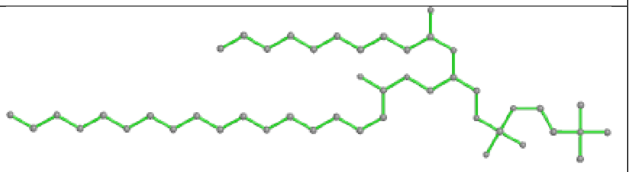
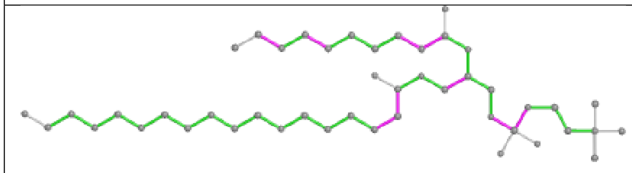
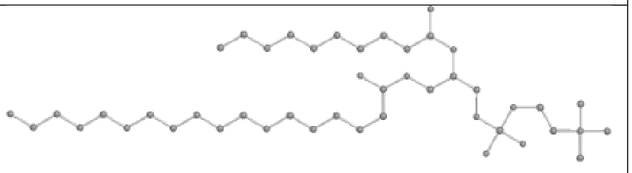
Bond angles



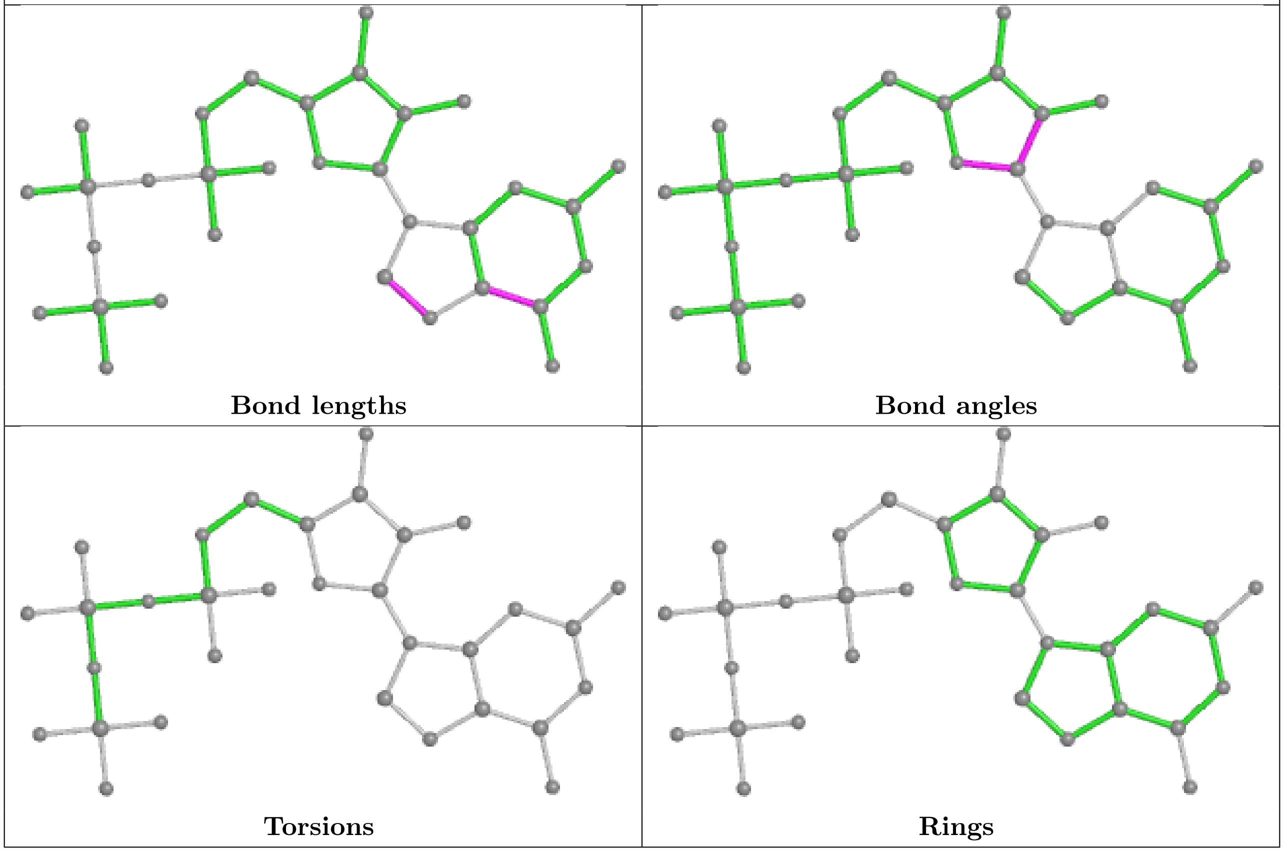
Torsions

Rings

Ligand CDL 1N 402	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand PC1 1f 101	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand GTP 1O 401



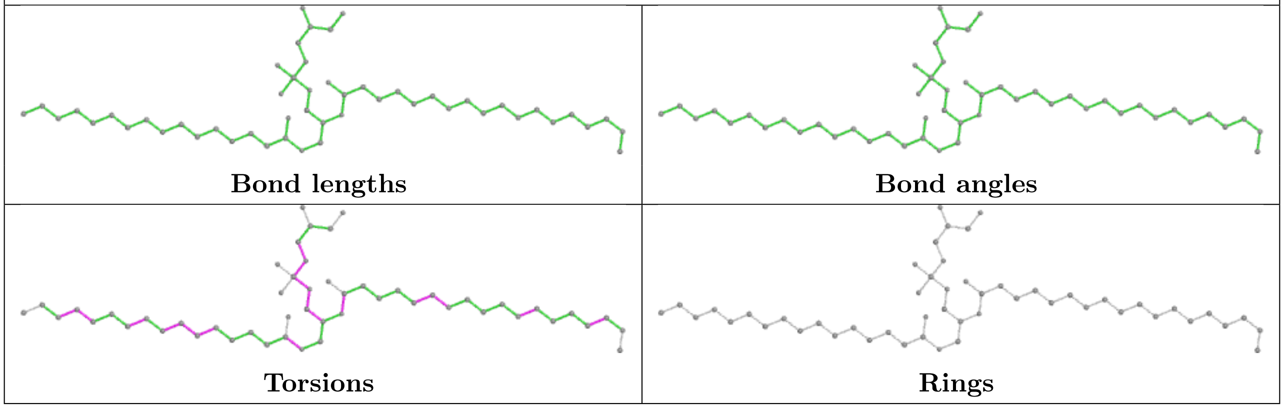
Bond lengths

Bond angles

Torsions

Rings

Ligand PGT 1M 501



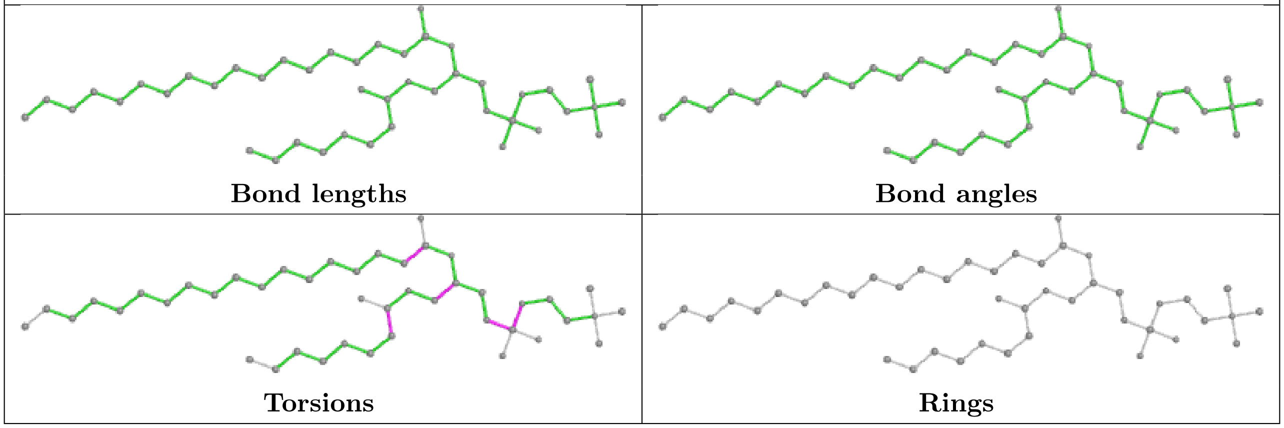
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 1L 703



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	2
43	1r	1
22	1W	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	4.03
1	1r	1:ALA	C	2:SER	N	3.12
1	1i	54:ALA	C	55:PRO	N	1.79
1	1W	75:ASP	C	76:PRO	N	1.72

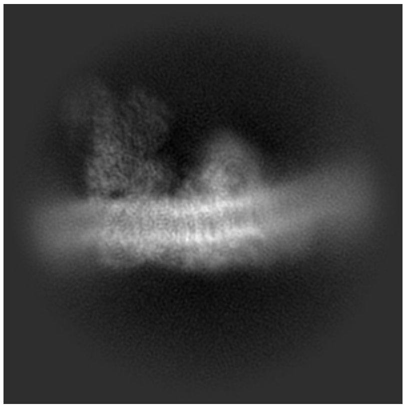
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42172. These allow visual inspection of the internal detail of the map and identification of artifacts.

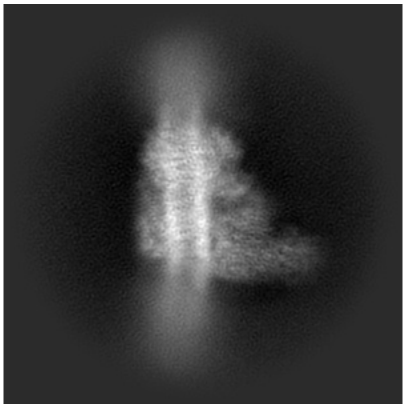
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

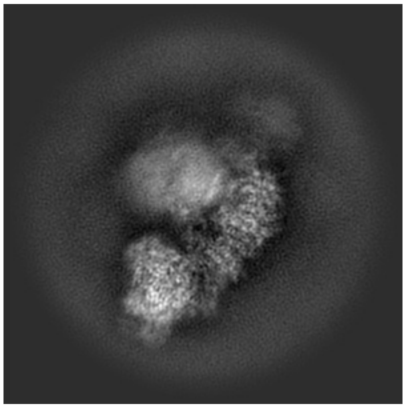
6.1.1 Primary map



X

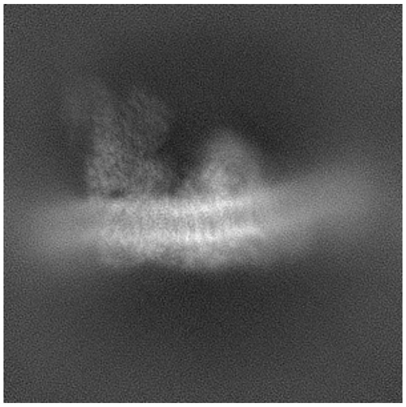


Y

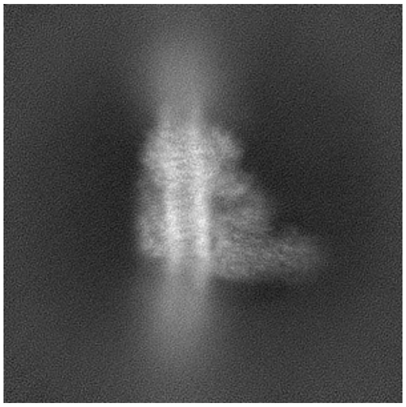


Z

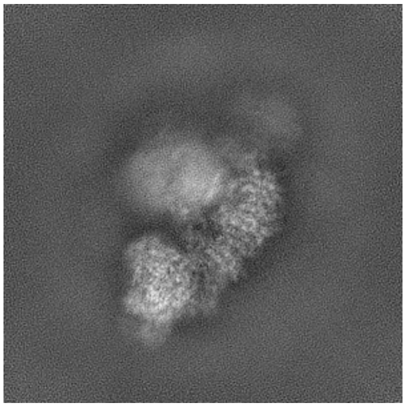
6.1.2 Raw map



X



Y

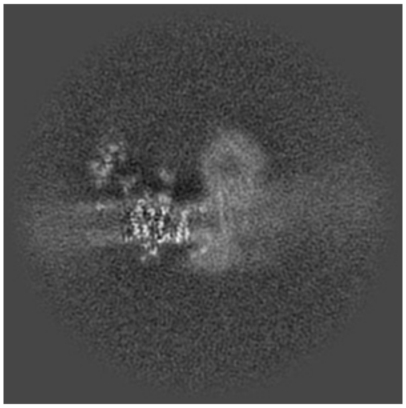


Z

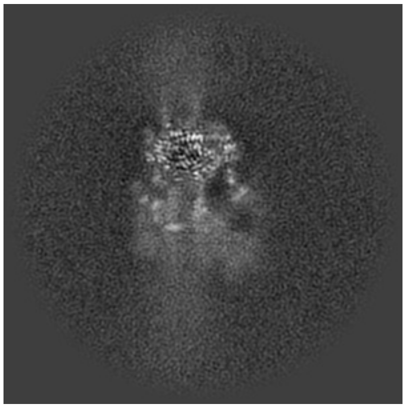
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

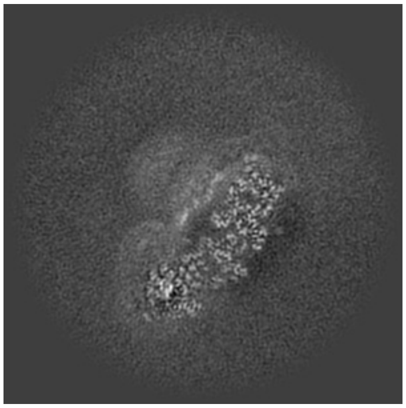
6.2.1 Primary map



X Index: 160

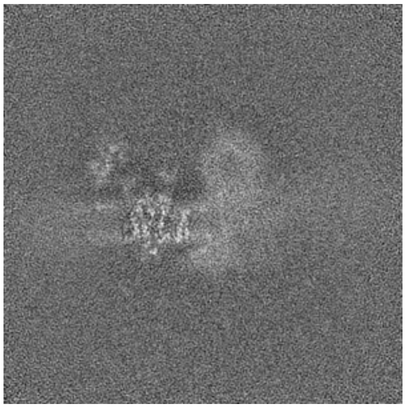


Y Index: 160

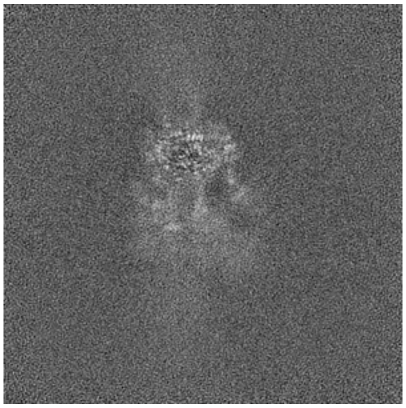


Z Index: 160

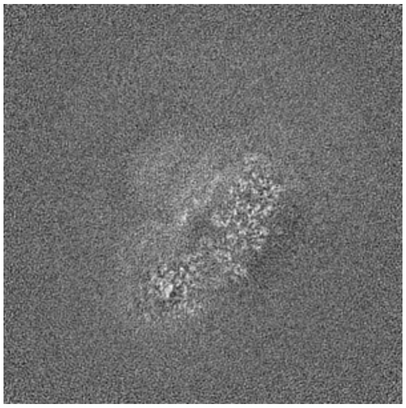
6.2.2 Raw map



X Index: 160



Y Index: 160

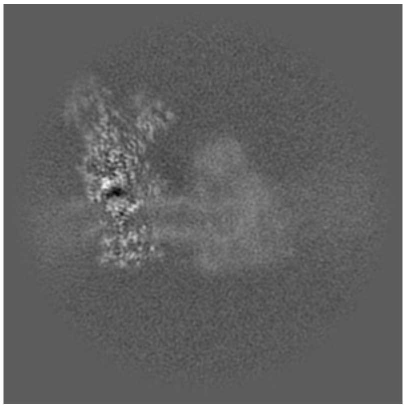


Z Index: 160

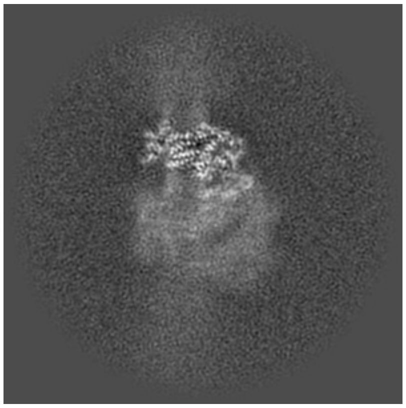
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

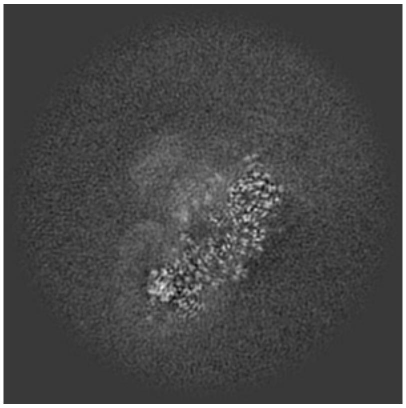
6.3.1 Primary map



X Index: 129

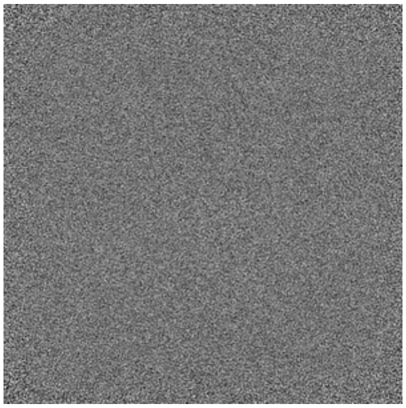


Y Index: 171

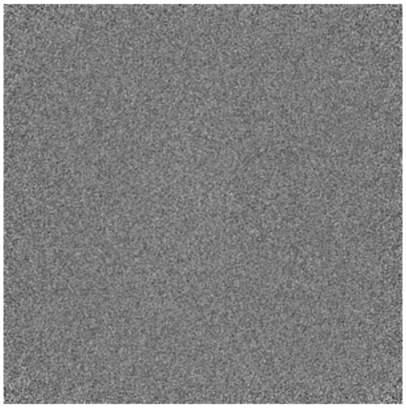


Z Index: 158

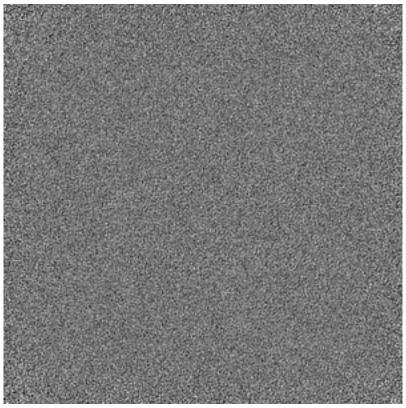
6.3.2 Raw map



X Index: 0



Y Index: 0

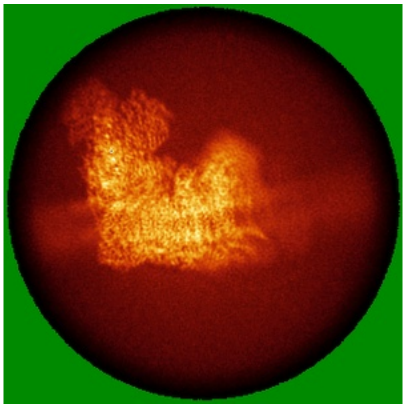


Z Index: 0

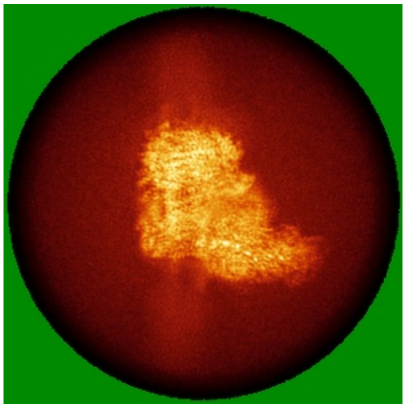
The images above show the largest variance slices of the map in three orthogonal directions.

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

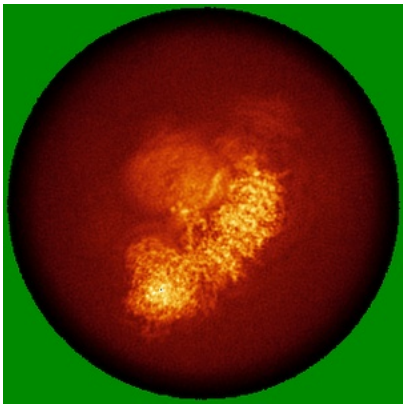
6.4.1 Primary map



X

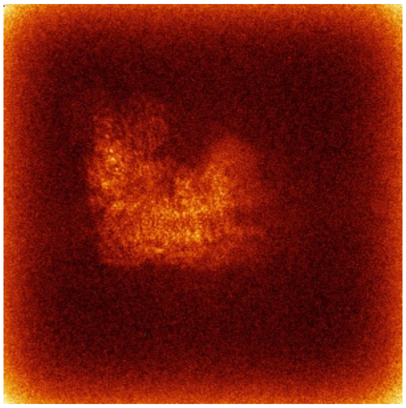


Y

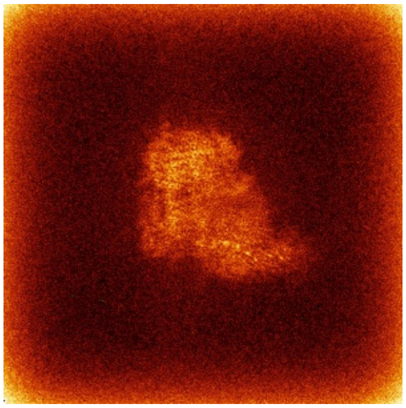


Z

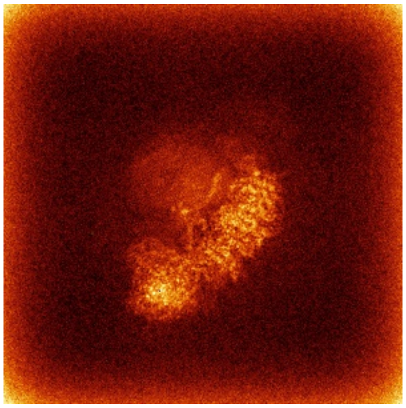
6.4.2 Raw map



X



Y

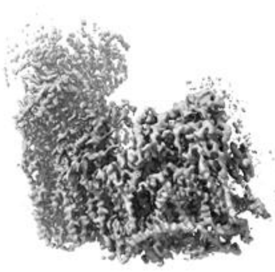


Z

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

6.5 Orthogonal surface views

6.5.1 Primary map


X


Y

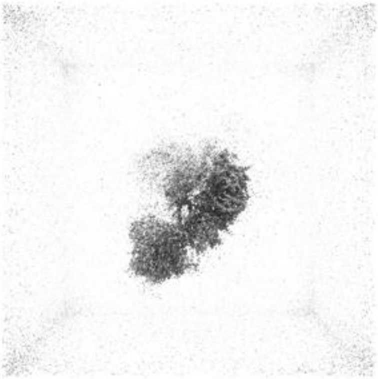

Z

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

6.5.2 Raw map


X


Y


Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

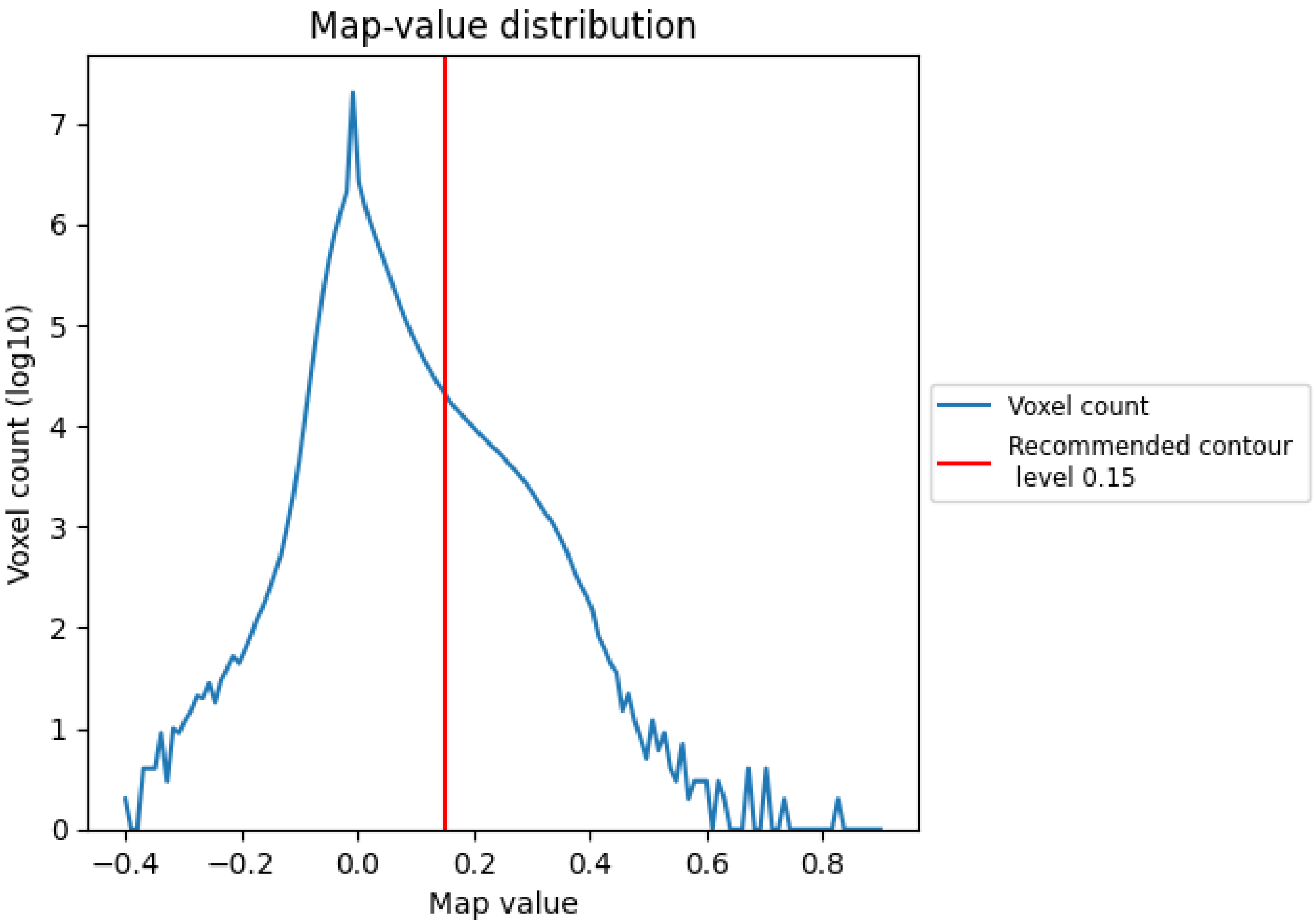
6.6 Mask visualisation

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

7 Map analysis ⓘ

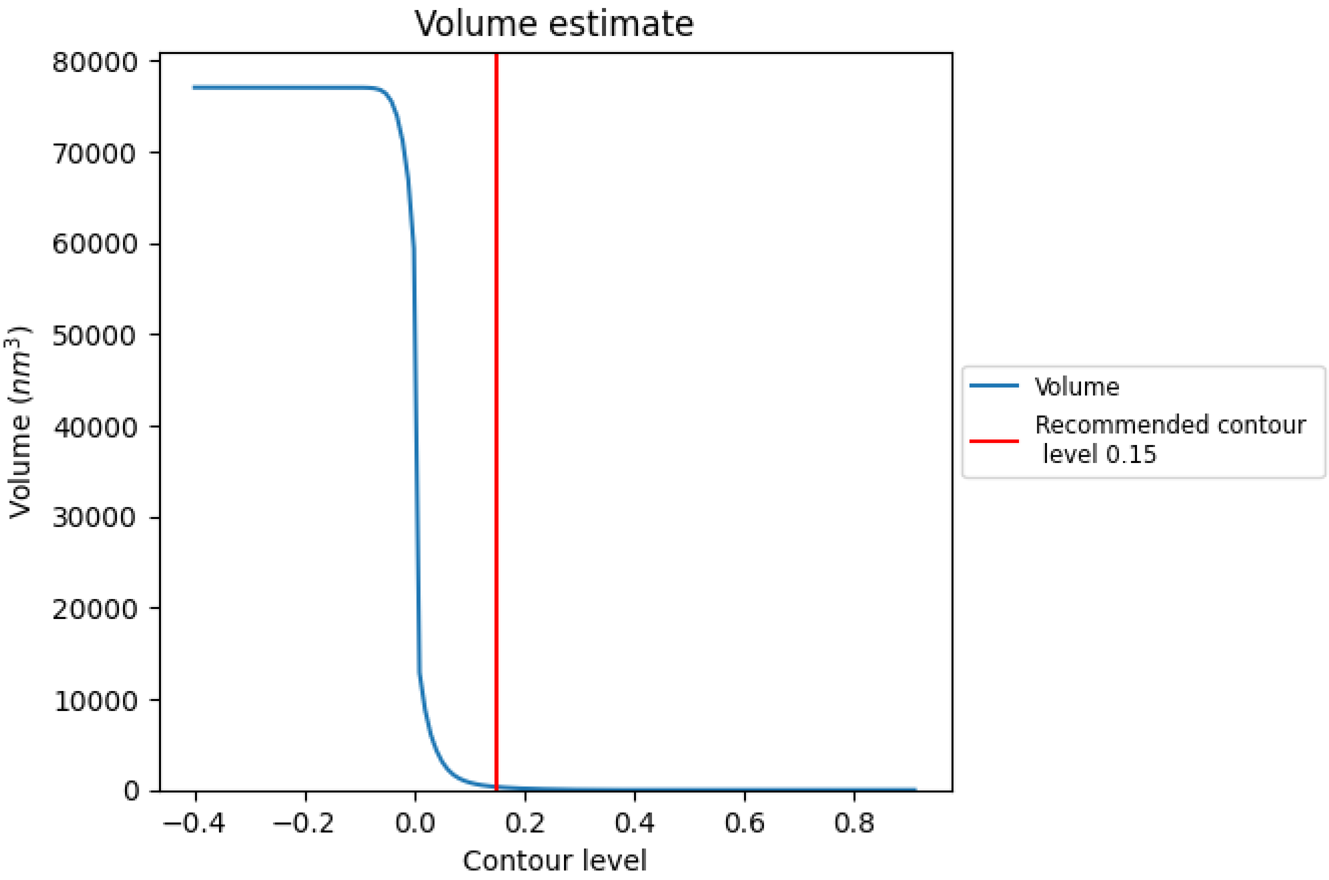
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

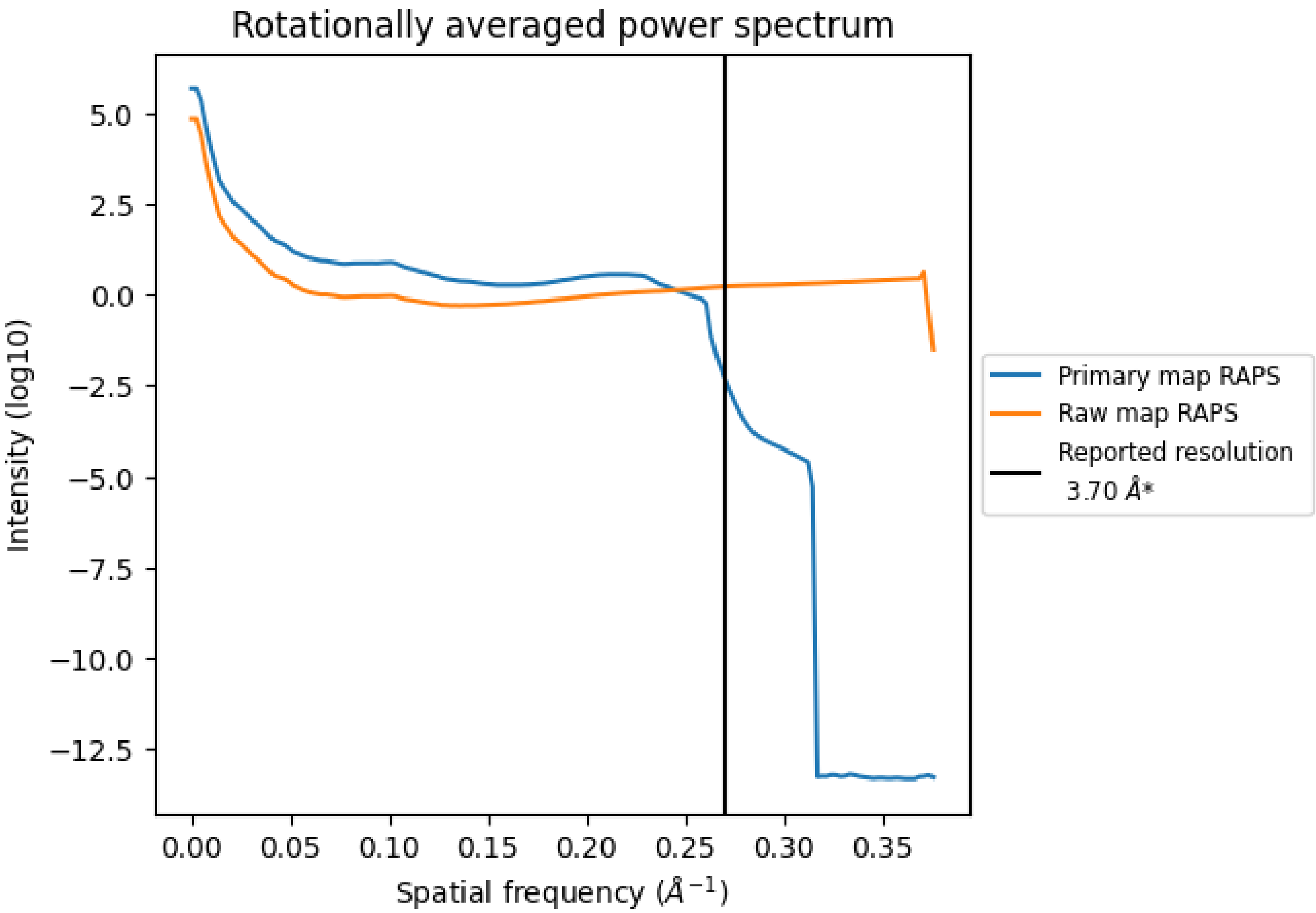
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 329 nm^3; this corresponds to an approximate mass of 297 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

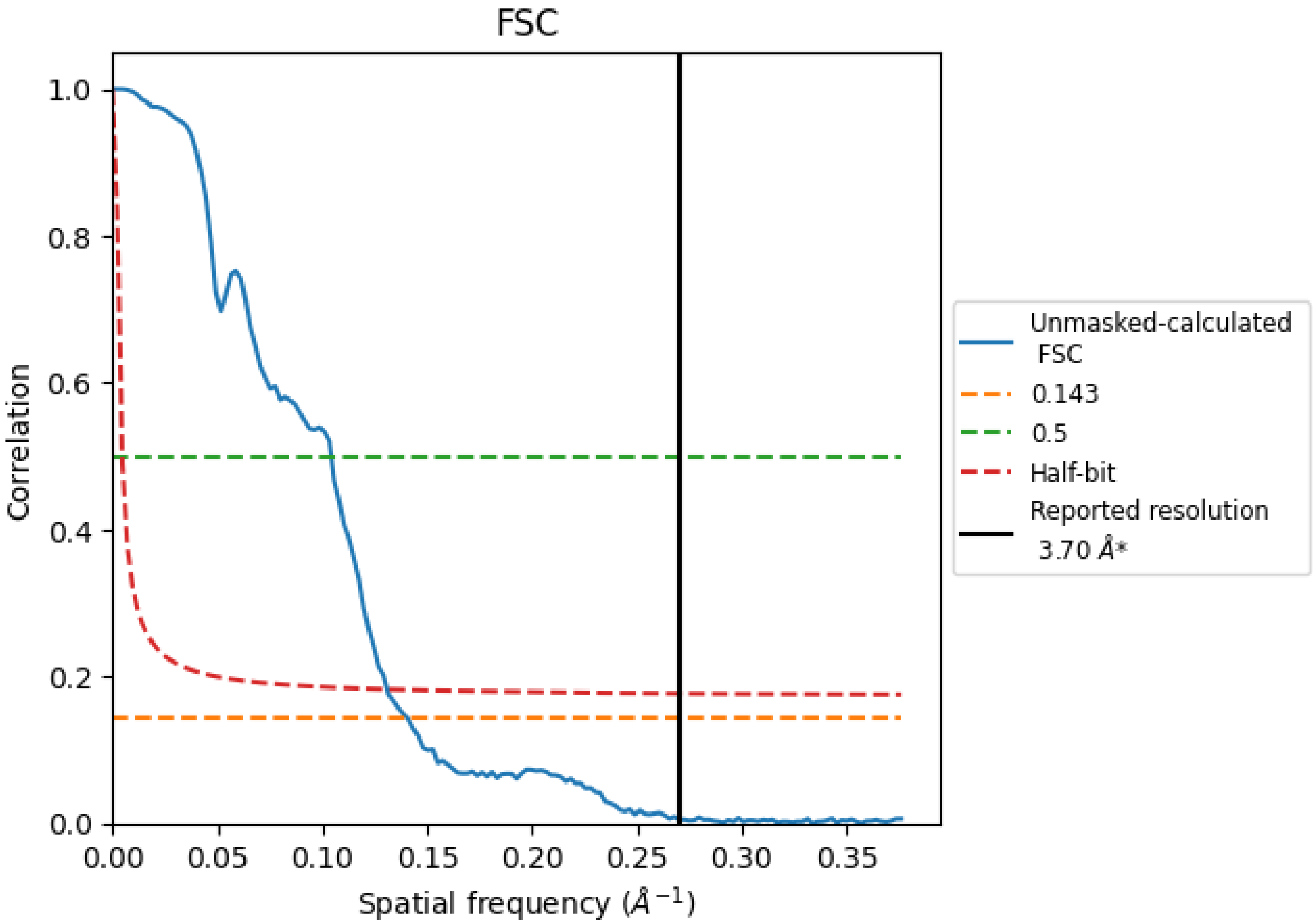


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



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

8.2 Resolution estimates ⓘ

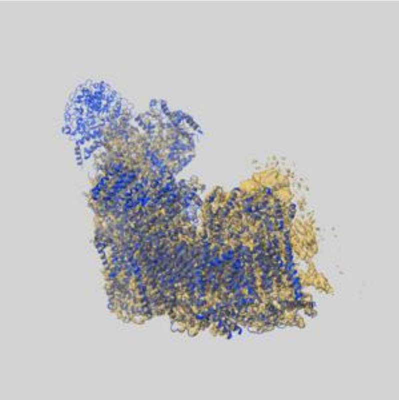
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.11	9.59	7.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.11 differs from the reported value 3.7 by more than 10 %

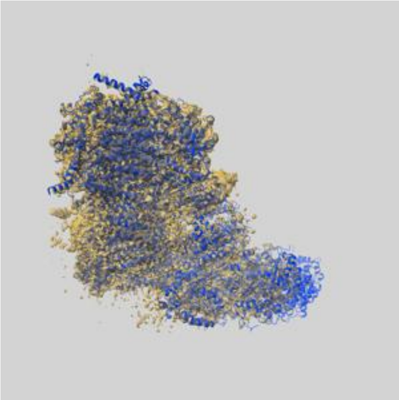
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-42172 and PDB model 8UEV. Per-residue inclusion information can be found in section 3 on page 21.

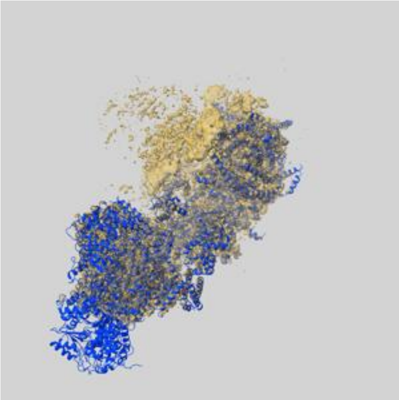
9.1 Map-model overlay ⓘ



X



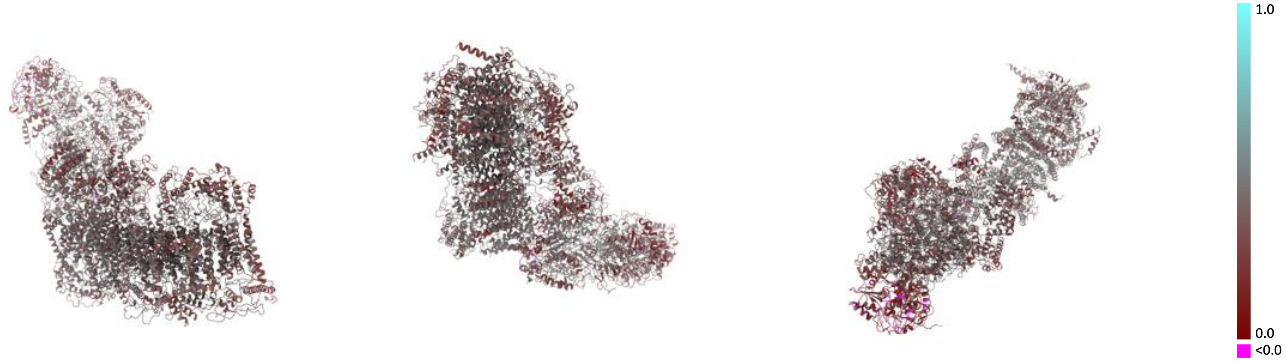
Y



Z

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

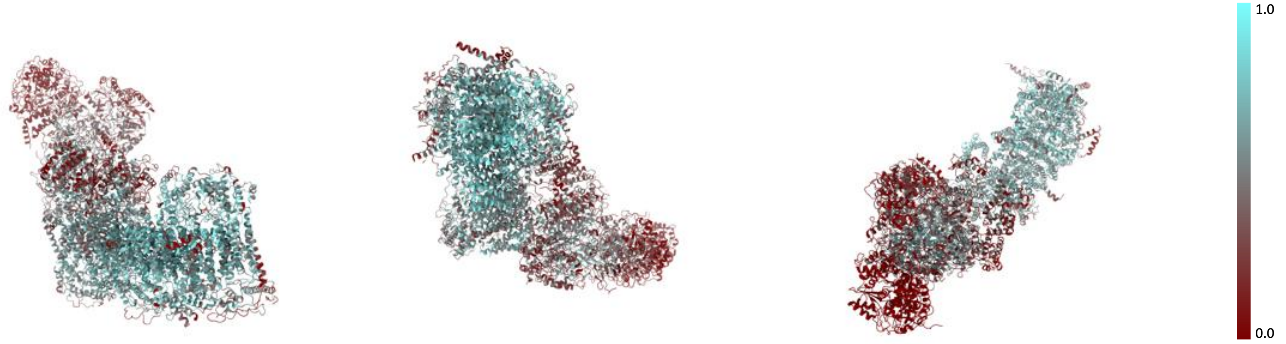
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

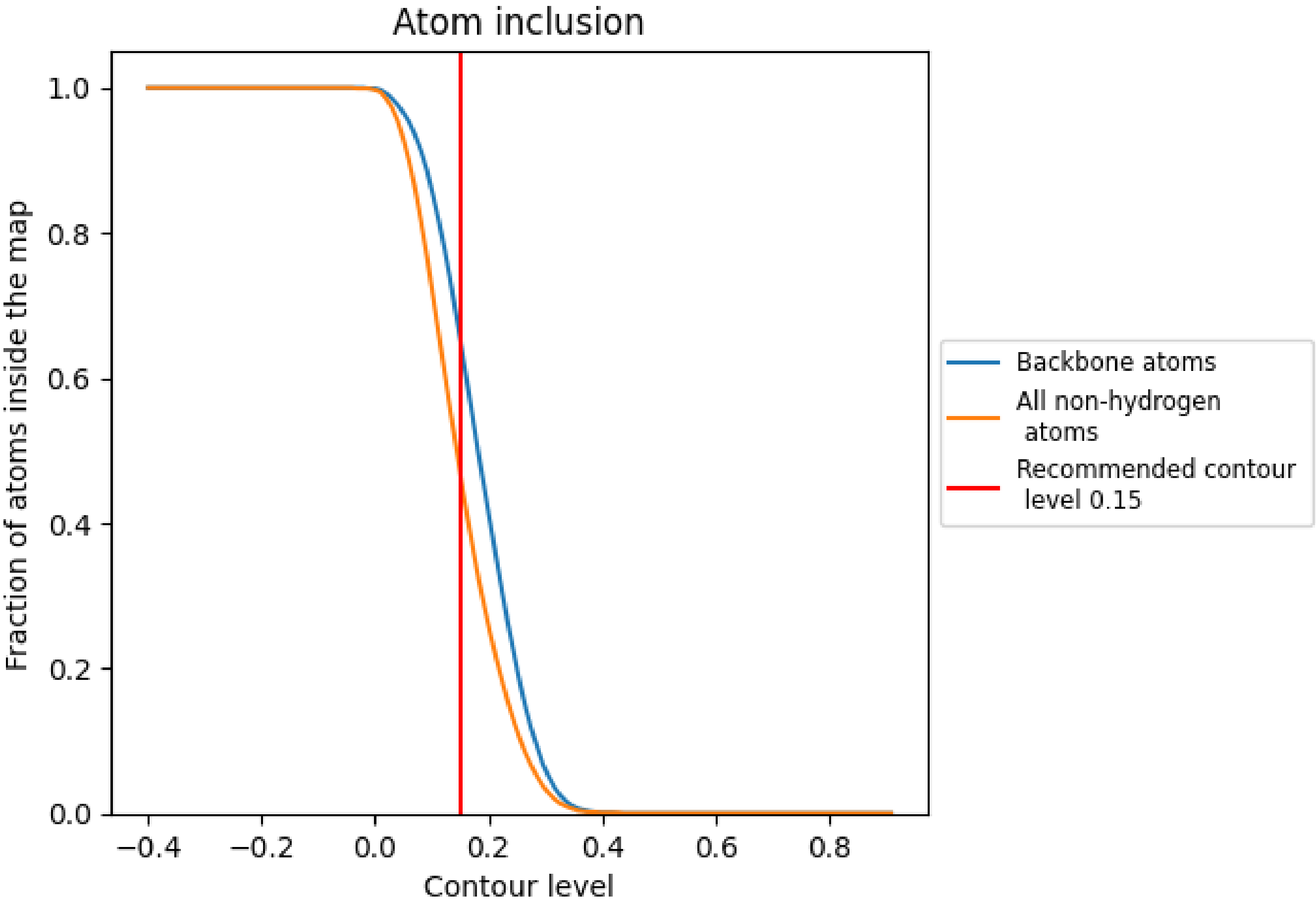
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.4700	0.3720
1A	0.5330	0.3980
1B	0.5360	0.4120
1C	0.3790	0.4050
1D	0.5130	0.3900
1E	0.0170	0.2640
1F	0.0260	0.2420
1G	0.2700	0.3560
1H	0.6000	0.4040
1I	0.5430	0.4040
1J	0.4900	0.3710
1K	0.5900	0.4010
1L	0.7030	0.4000
1M	0.7470	0.4290
1N	0.6660	0.4180
1O	0.3710	0.3540
1P	0.2900	0.3420
1Q	0.2780	0.3820
1R	0.2670	0.4000
1S	0.1250	0.2970
1T	0.2030	0.2660
1U	0.6350	0.3460
1V	0.2070	0.3340
1W	0.2910	0.3410
1X	0.5300	0.4010
1Y	0.6650	0.3700
1Z	0.5480	0.4060
1a	0.6560	0.4080
1b	0.5310	0.4090
1c	0.4360	0.3760
1d	0.6810	0.4150
1e	0.5760	0.4250
1f	0.4550	0.3590
1g	0.6000	0.3840
1h	0.6400	0.3980

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	▬ 0.3950	▬ 0.3490
1j	▬ 0.5200	▬ 0.3690
1k	▬ 0.5260	▬ 0.3480
1l	▬ 0.6480	▬ 0.3910
1m	▬ 0.6980	▬ 0.3850
1n	▬ 0.6530	▬ 0.3660
1o	▬ 0.4940	▬ 0.3250
1p	▬ 0.6120	▬ 0.3770
1q	▬ 0.4190	▬ 0.4040
1r	▬ 0.3430	▬ 0.3900
1s	▬ 0.0000	▬ 0.2230