wwPDB EM Validation Summary Report

Aug 5, 2026 – 04:50 AM EDT

PDB ID	:	8UD1 / pdb_00008ud1
EMDB ID	:	EMD-42143
Title	:	High resolution in-situ structure of complex I in respiratory supercomplex (composite)
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-09-27
Resolution	:	2.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

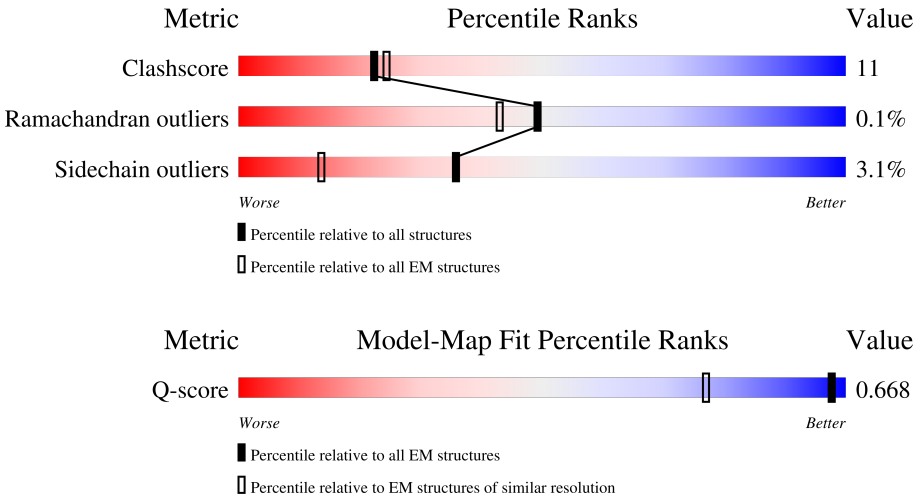
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



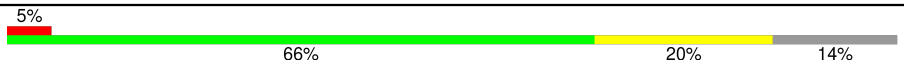
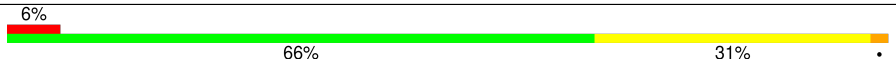
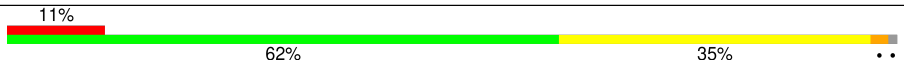
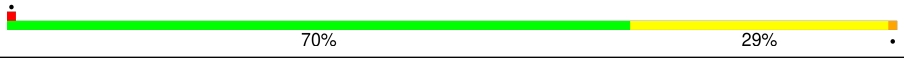
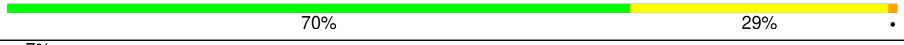
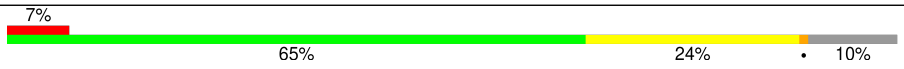
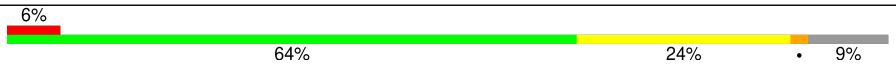
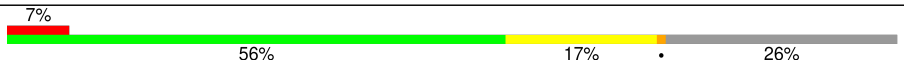
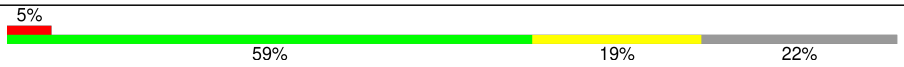
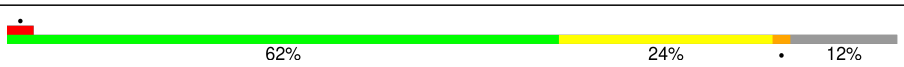
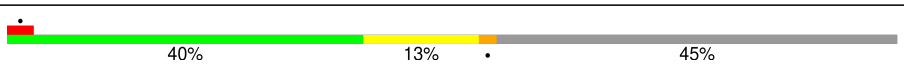
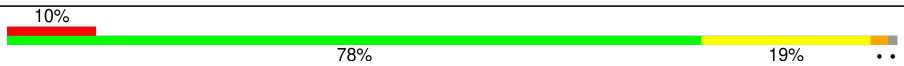
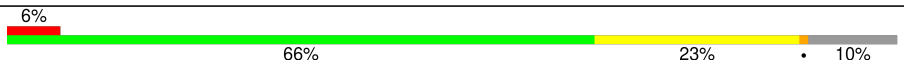
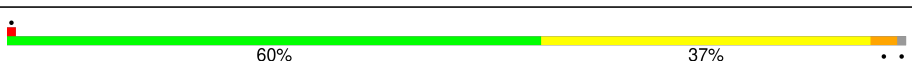
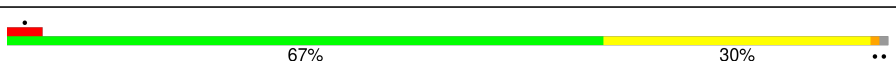
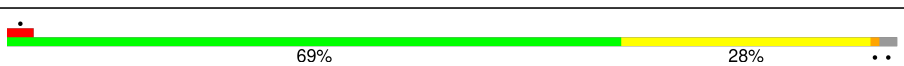
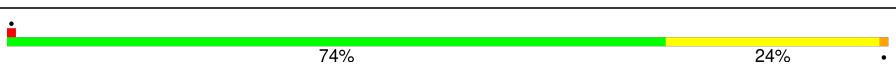
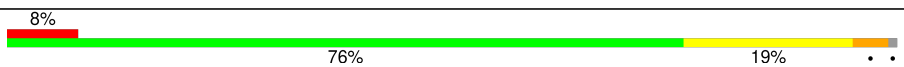
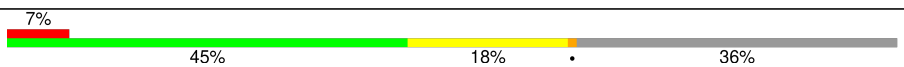
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	23% 64% 34%
2	1B	258	41% 17% 40%
3	1C	264	68% 11% 21%
4	1D	466	5% 69% 22% 8%

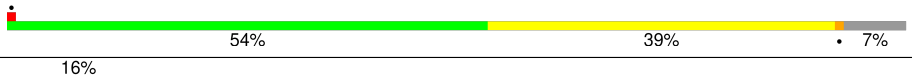
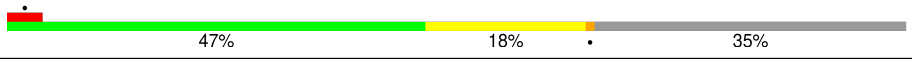
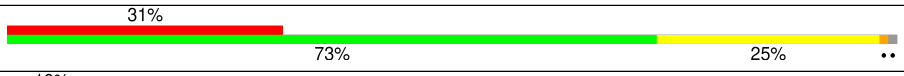
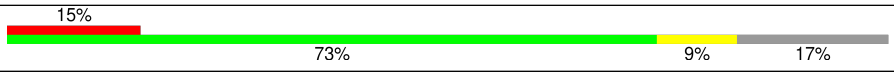
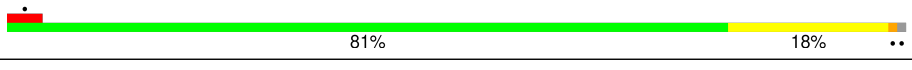
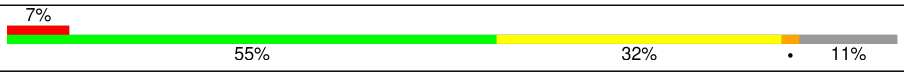
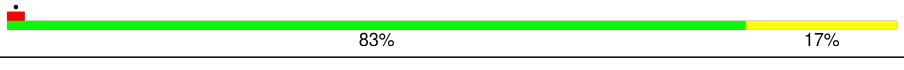
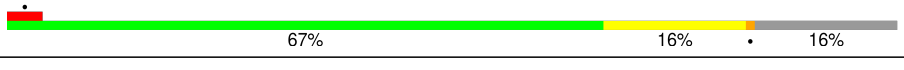
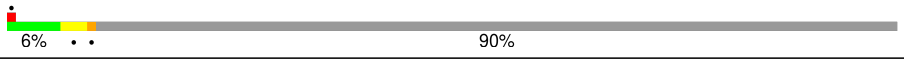
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	

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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	58	
32	1g	154	
33	1h	189	
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	113	
44	1s	471	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	1B	201	-	-	X	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 72881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1746	1128	299	317	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

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

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

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

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

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

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

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

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

- 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	C	N	O	S	0	0
			2590	1649	440	491	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	1	0
			1179	758	206	206	9		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	120	Total	C	N	O	S	0	0
			993	646	172	169	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	1	0
			827	525	155	141	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

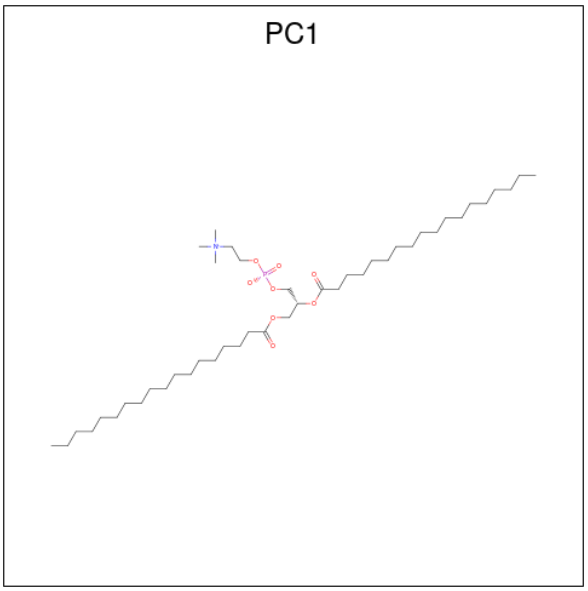
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	95	Total	C	N	O	S	0	0
			767	483	144	137	3		

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

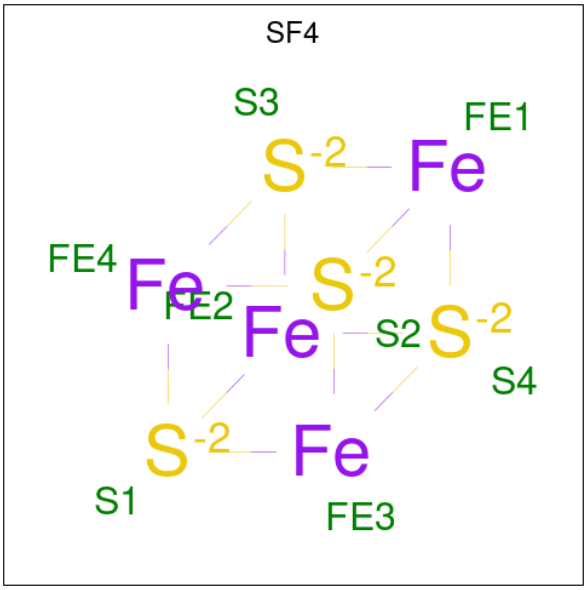
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



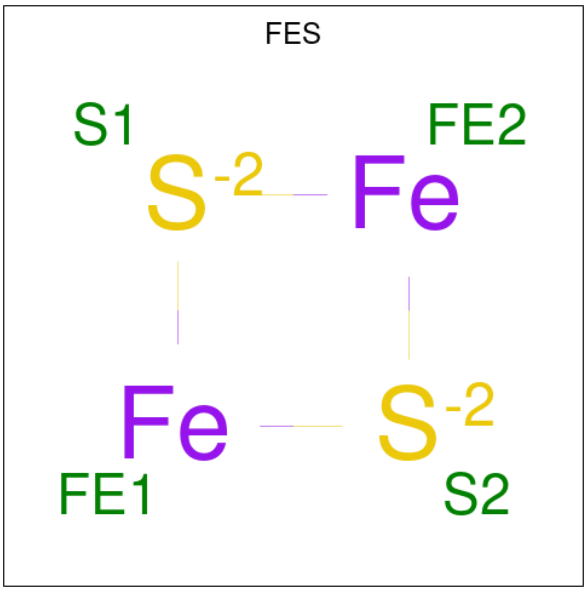
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	1P	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



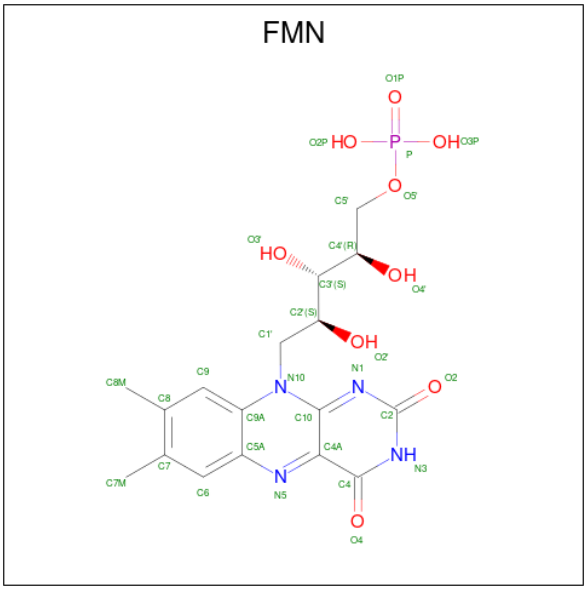
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total Fe S 8 4 4	0
46	1F	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0

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



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

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

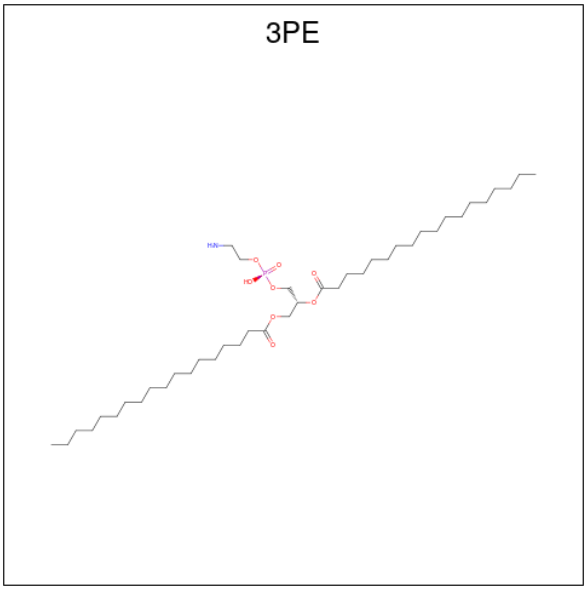


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



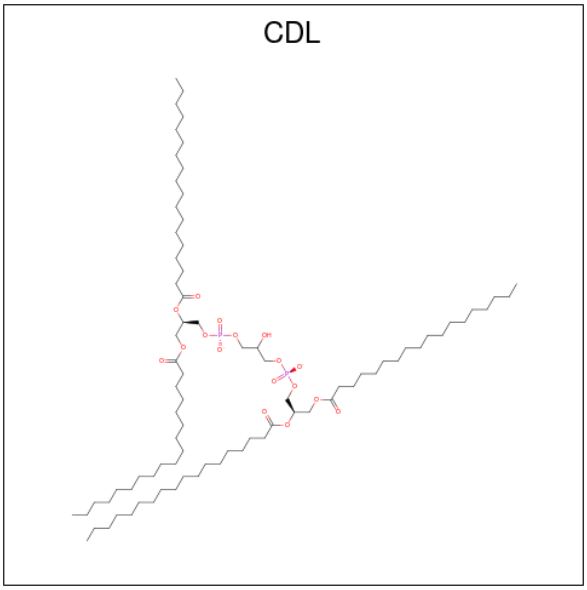
Mol	Chain	Residues	Atoms	AltConf
50	1J	1	Total C N O P 44 34 1 8 1	0
50	1L	1	Total C N O P 46 36 1 8 1	0
50	1L	1	Total C N O P 45 35 1 8 1	0
50	1L	1	Total C N O P 41 31 1 8 1	0
50	1L	1	Total C N O P 42 32 1 8 1	0
50	1M	1	Total C N O P 45 35 1 8 1	0
50	1M	1	Total C N O P 51 41 1 8 1	0
50	1N	1	Total C N O P 49 39 1 8 1	0
50	1N	1	Total C N O P 33 23 1 8 1	0
50	1Y	1	Total C N O P 31 21 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
50	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
50	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
50	1b	1	Total	C	N	O	P	0
			47	37	1	8	1	
50	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
50	1j	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1m	1	Total	C	N	O	P	0
			50	40	1	8	1	
50	1m	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



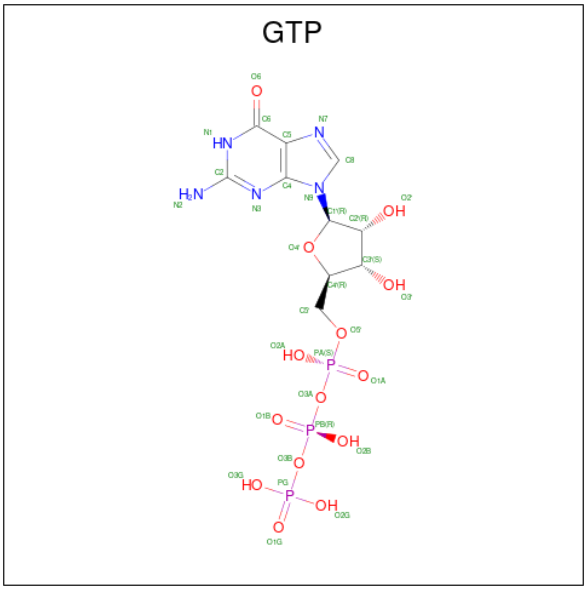
Mol	Chain	Residues	Atoms				AltConf
51	1L	1	Total	C	O	P	0
			87	68	17	2	
51	1N	1	Total	C	O	P	0
			62	43	17	2	
51	1X	1	Total	C	O	P	0
			86	67	17	2	

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Mol	Chain	Residues	Atoms				AltConf
51	1d	1	Total	C	O	P	0
			65	46	17	2	
51	1h	1	Total	C	O	P	0
			80	61	17	2	
51	1q	1	Total	C	O	P	0
			61	42	17	2	

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

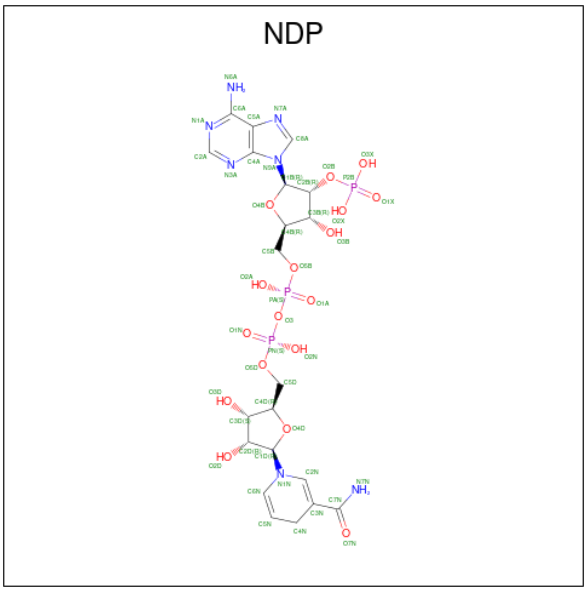


Mol	Chain	Residues	Atoms					AltConf
52	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

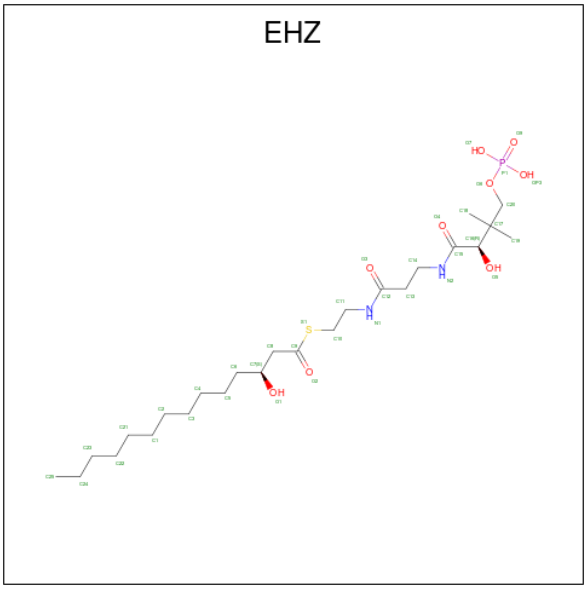


Mol	Chain	Residues	Atoms					AltConf
54	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

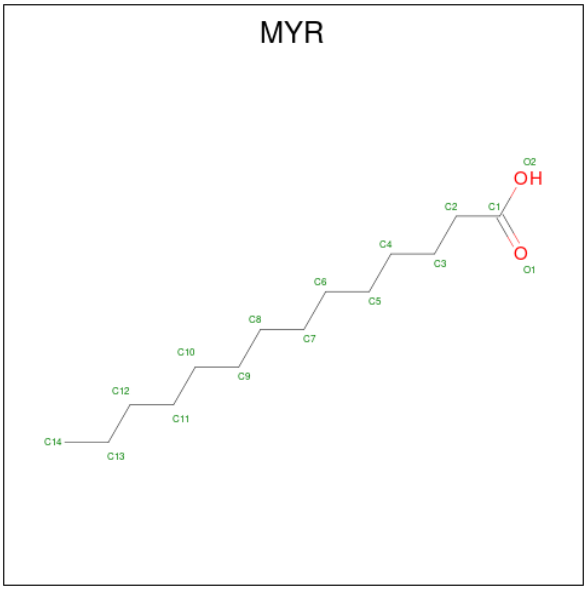
Mol	Chain	Residues	Atoms		AltConf
55	1R	1	Total	Zn	0
			1	1	

- Molecule 56 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



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

- Molecule 57 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	AltConf
57	1l	1	Total C O 15 14 1	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms	AltConf
58	1A	23	Total O 23 23	0
58	1B	68	Total O 68 68	0
58	1C	131	Total O 131 131	0
58	1D	213	Total O 213 213	0
58	1E	50	Total O 50 50	0
58	1F	105	Total O 105 105	0
58	1G	365	Total O 365 365	0

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Mol	Chain	Residues	Atoms	AltConf
58	1H	75	Total O 75 75	0
58	1I	83	Total O 83 83	0
58	1J	40	Total O 40 40	0
58	1K	27	Total O 27 27	0
58	1L	277	Total O 277 277	0
58	1M	221	Total O 221 221	0
58	1N	156	Total O 156 156	0
58	1O	126	Total O 126 126	0
58	1P	207	Total O 207 207	0
58	1Q	110	Total O 110 110	0
58	1R	71	Total O 71 71	0
58	1S	58	Total O 58 58	0
58	1T	24	Total O 24 24	0
58	1U	37	Total O 37 37	0
58	1V	36	Total O 36 36	0
58	1W	64	Total O 64 64	0
58	1X	150	Total O 150 150	0
58	1Y	81	Total O 81 81	0
58	1Z	92	Total O 92 92	0
58	1a	34	Total O 34 34	0
58	1b	42	Total O 42 42	0

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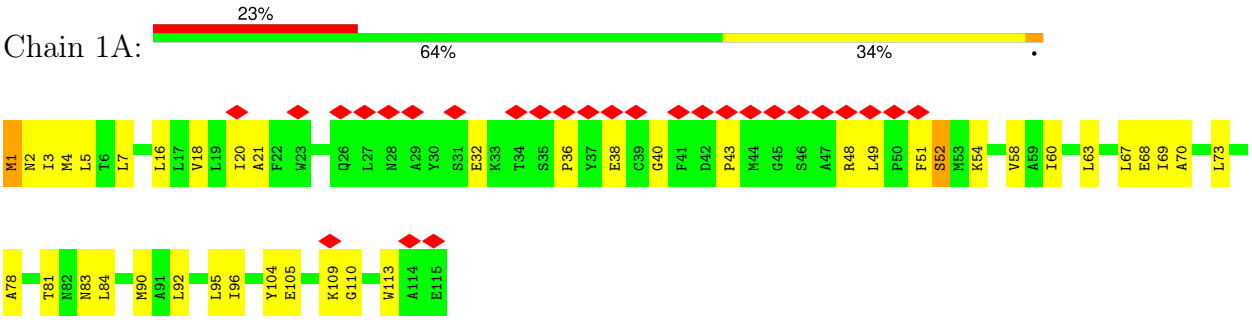
Mol	Chain	Residues	Atoms	AltConf
58	1c	26	Total O 26 26	0
58	1d	93	Total O 93 93	0
58	1e	105	Total O 105 105	0
58	1f	38	Total O 38 38	0
58	1g	80	Total O 80 80	0
58	1h	128	Total O 128 128	0
58	1i	46	Total O 46 46	0
58	1j	32	Total O 32 32	0
58	1k	37	Total O 37 37	0
58	1l	111	Total O 111 111	0
58	1m	105	Total O 105 105	0
58	1n	129	Total O 129 129	0
58	1o	84	Total O 84 84	0
58	1p	153	Total O 153 153	0
58	1q	64	Total O 64 64	0
58	1r	47	Total O 47 47	0
58	1s	21	Total O 21 21	0

3 Residue-property plots (i)

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

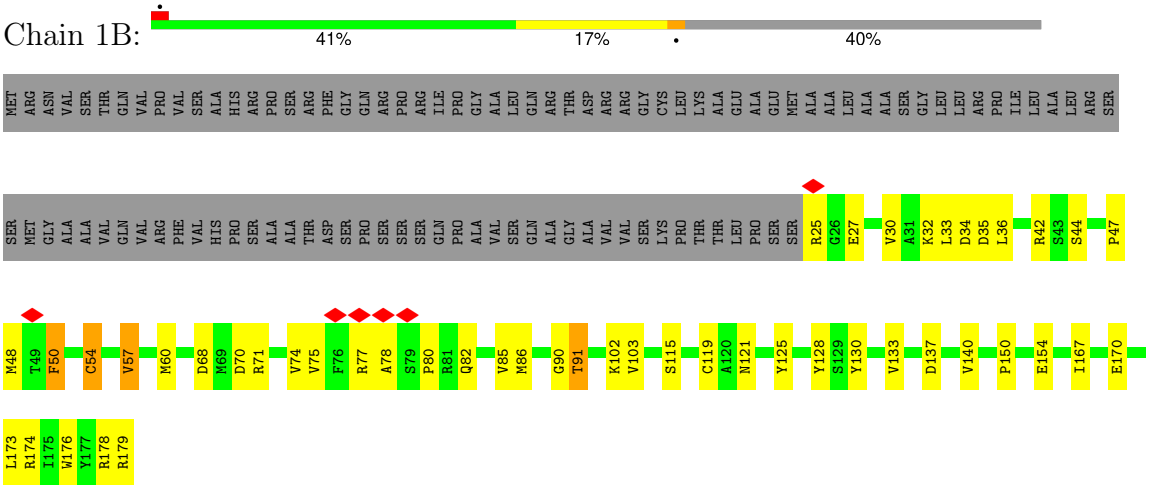
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain 1A:



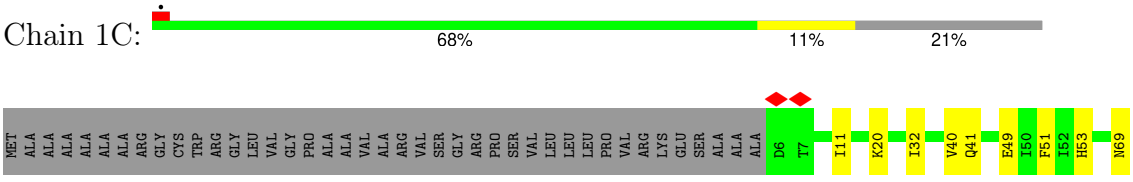
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 1B:



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

Chain 1C:

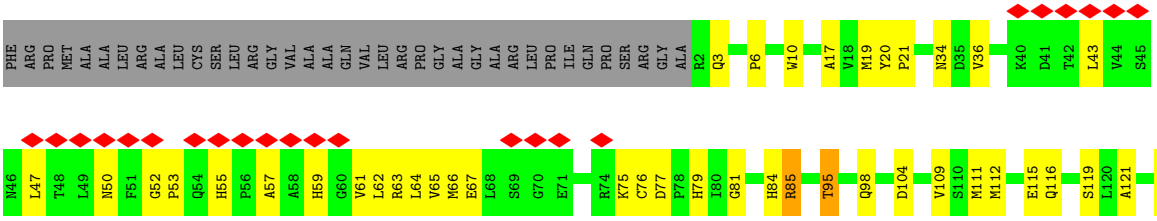




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:

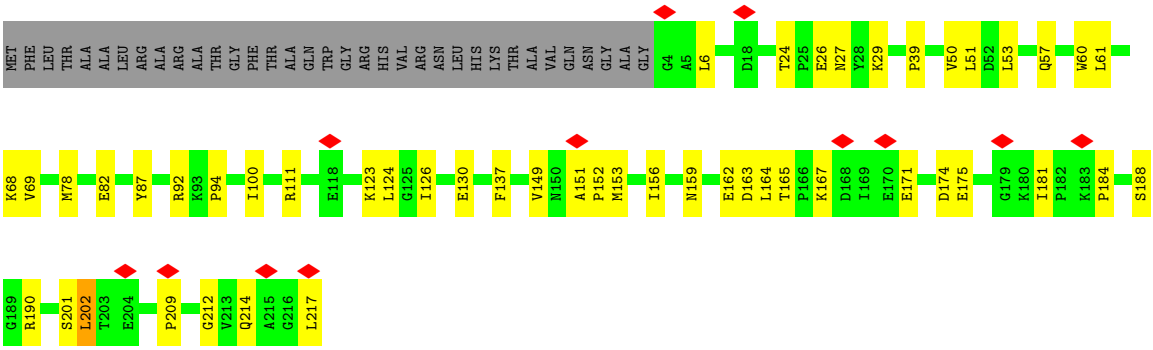




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E:

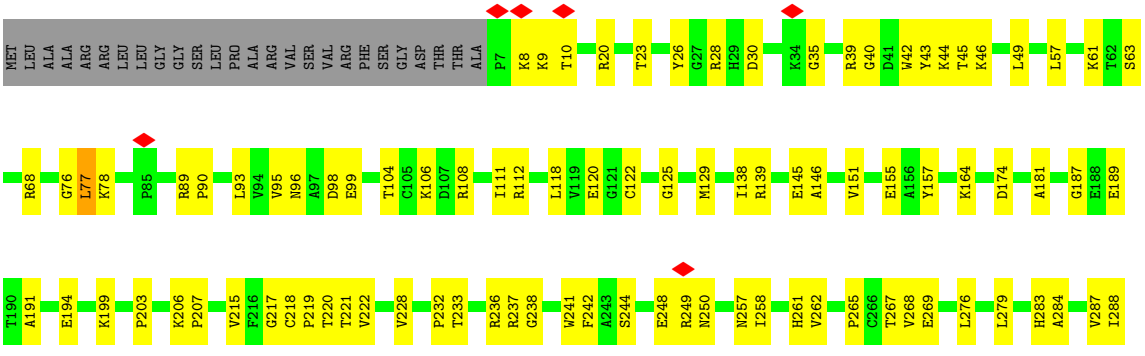


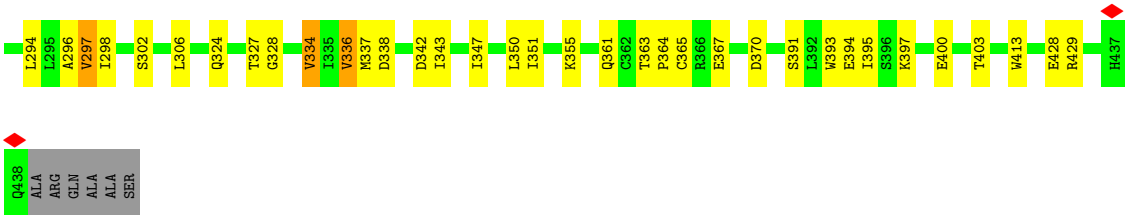


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F:



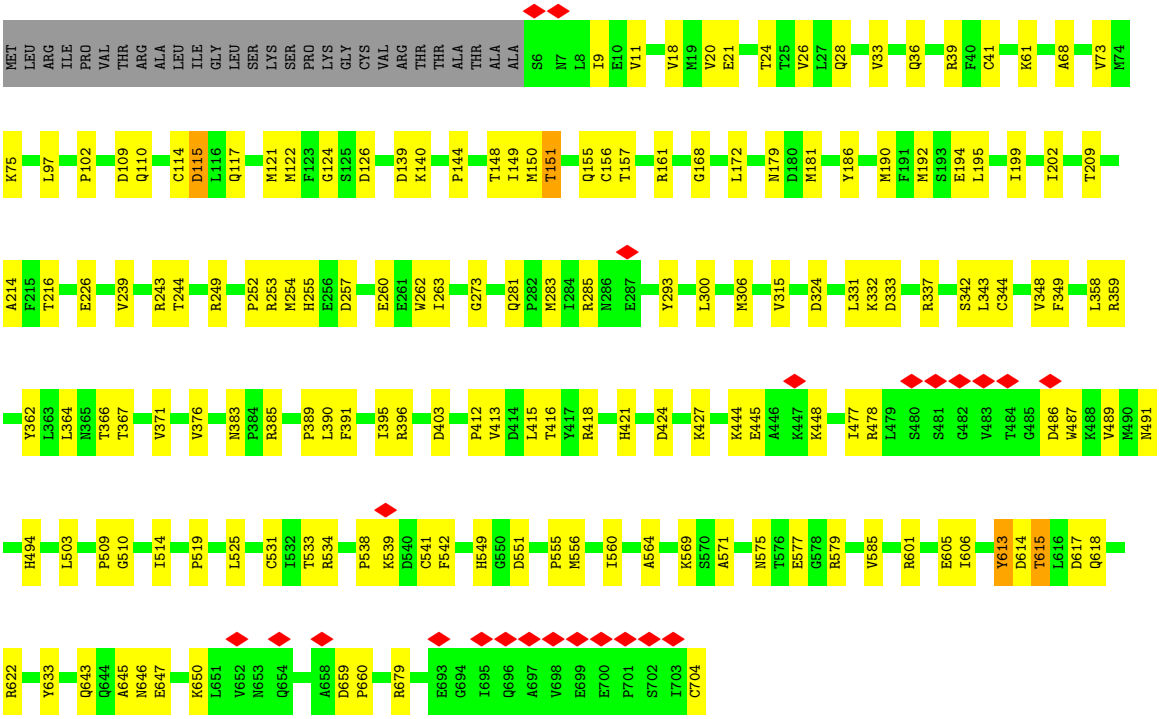




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G:





• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:

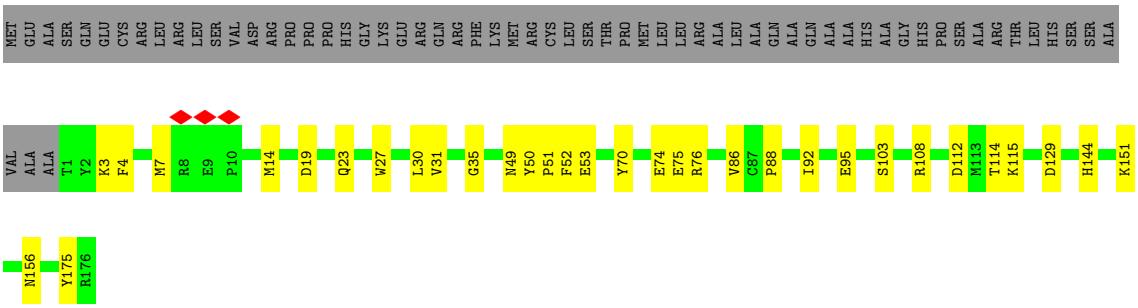




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:

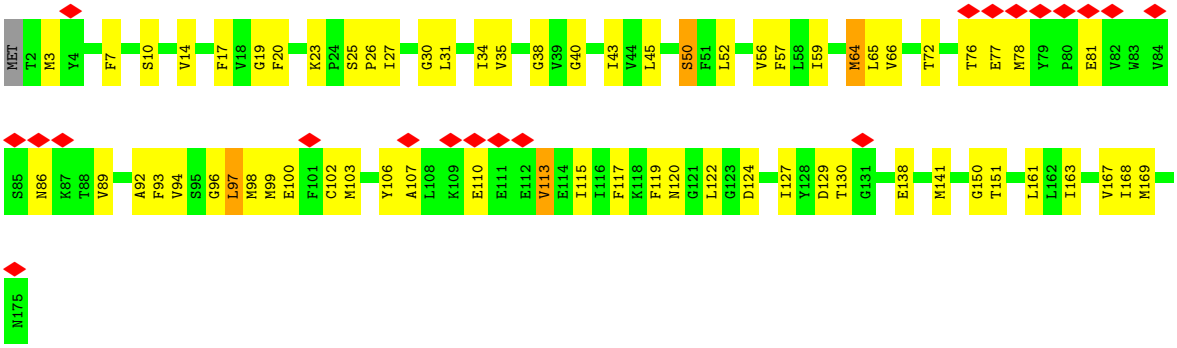




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:

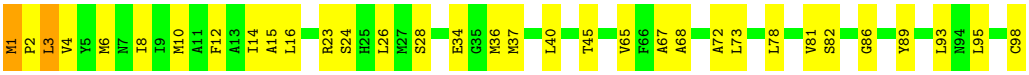




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:

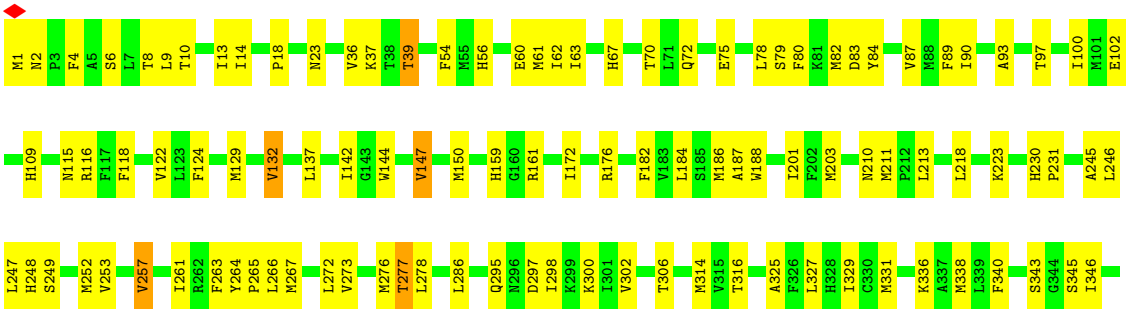


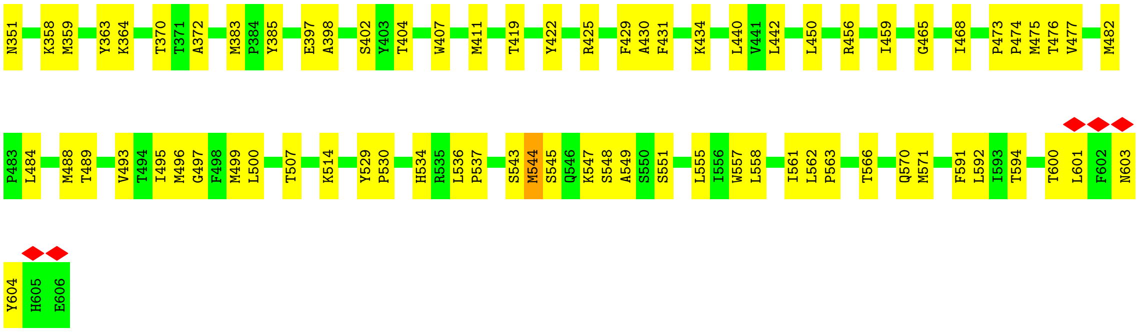


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

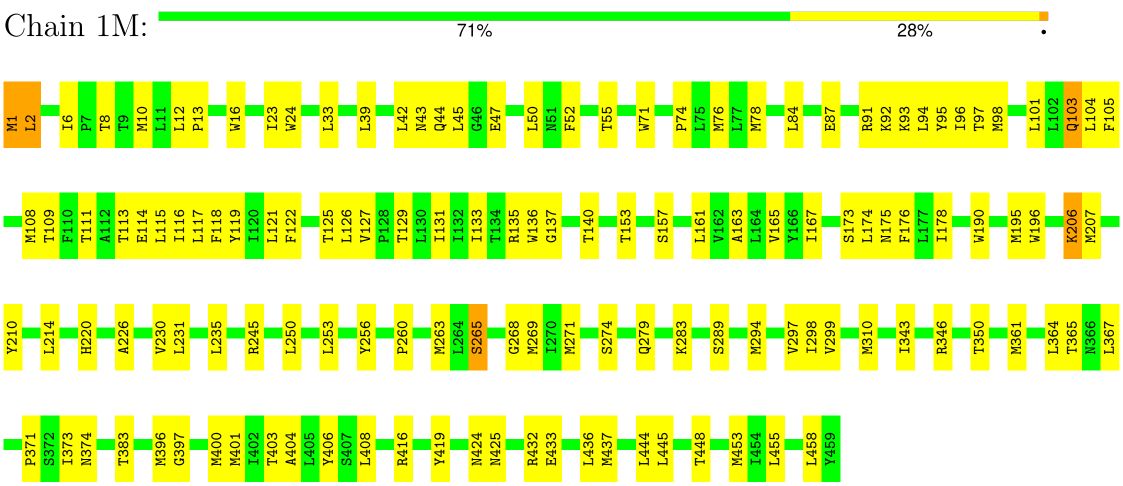
Chain 1L:



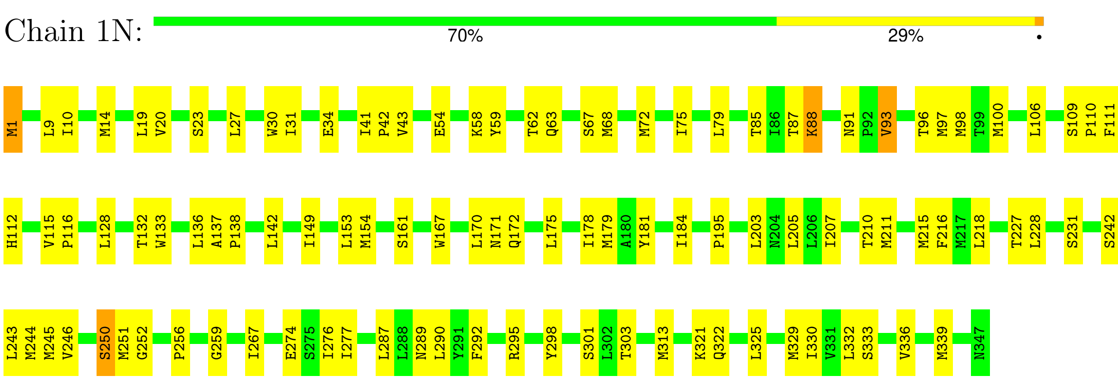




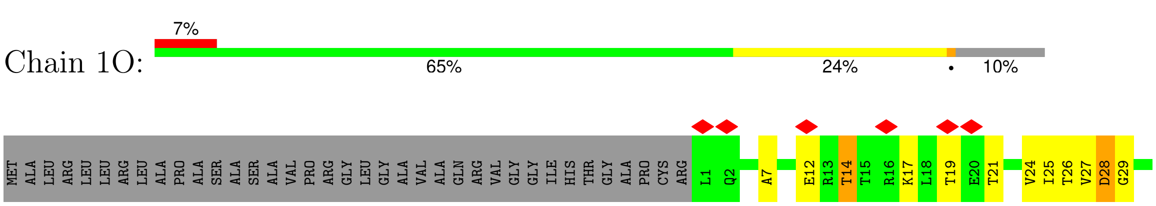
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

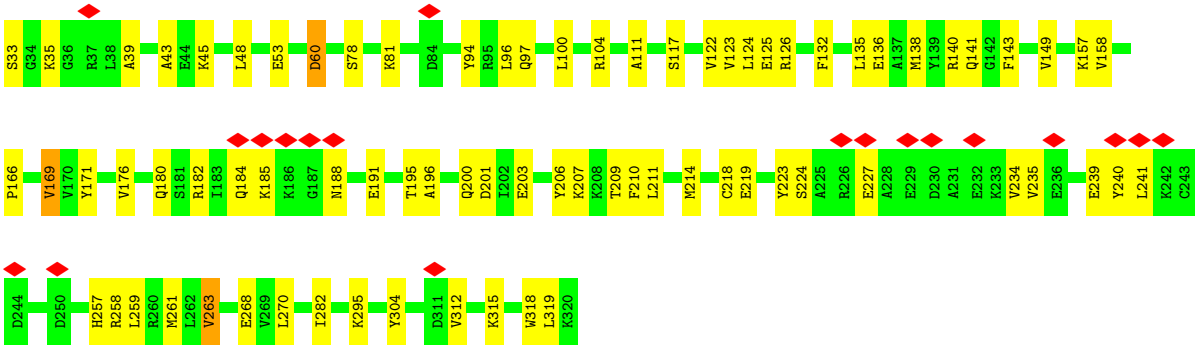


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



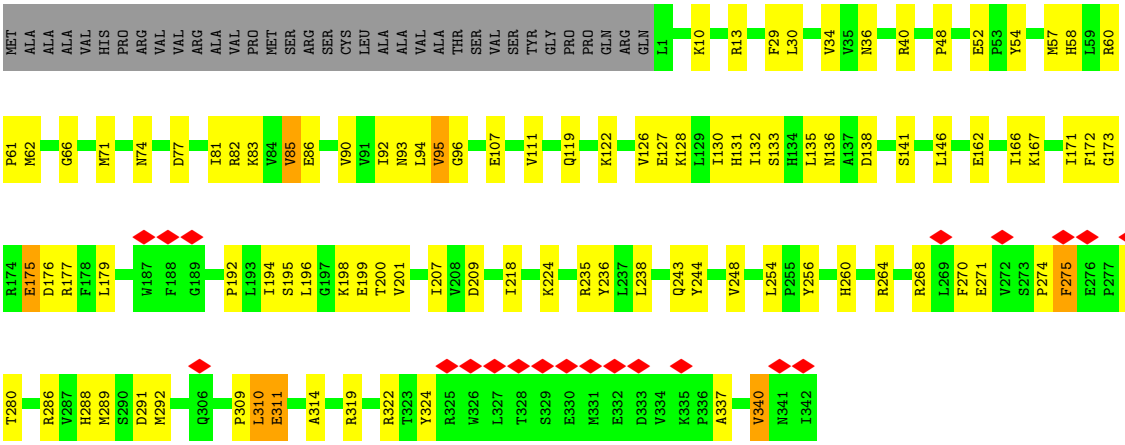
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





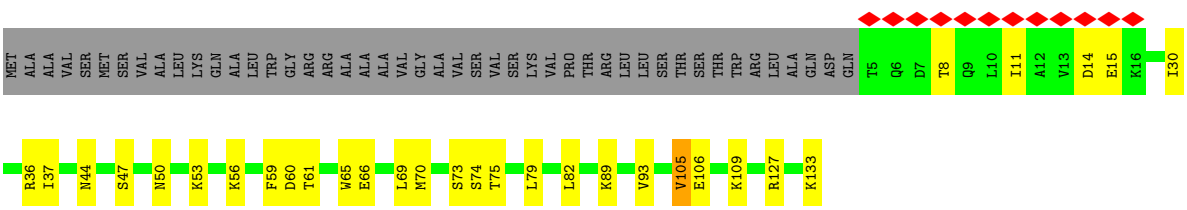
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9





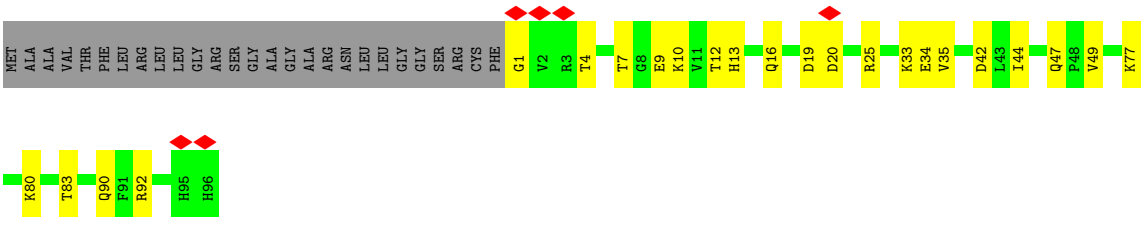
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





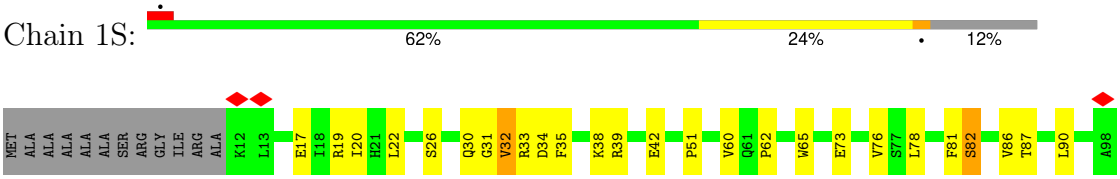
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





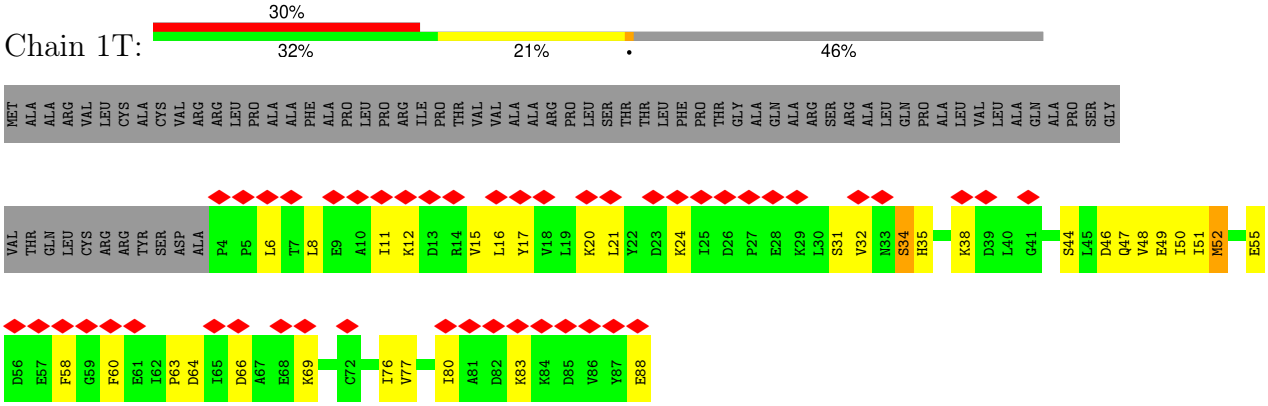
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



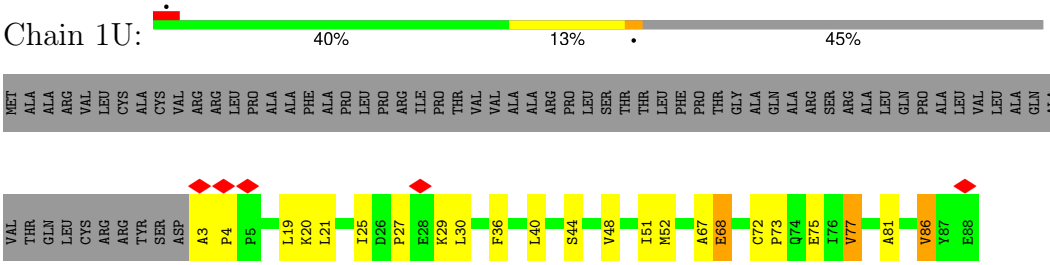
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T:



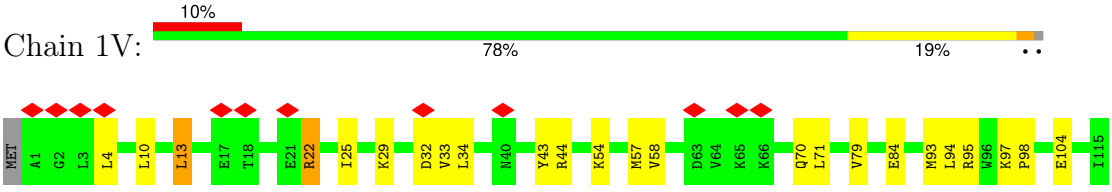
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U:



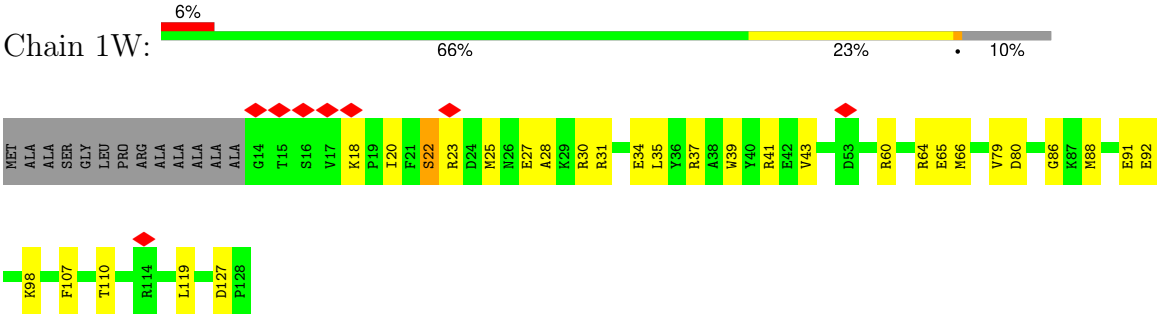
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:



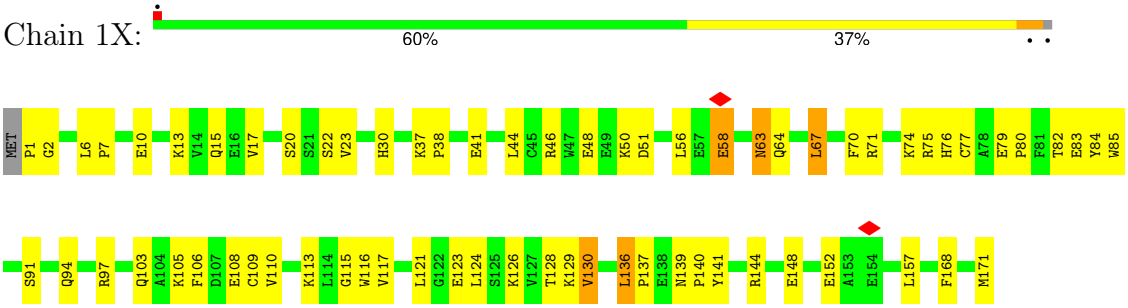
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain 1W:



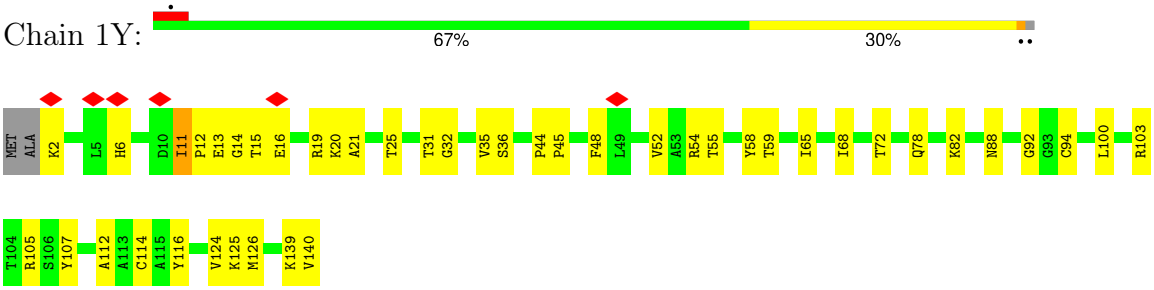
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X:



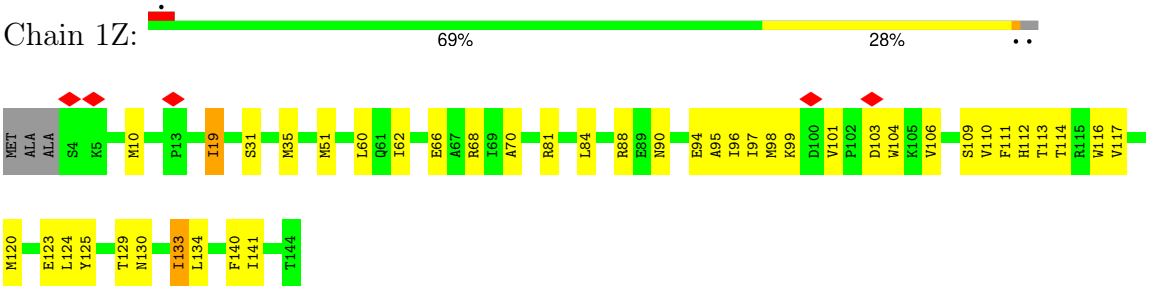
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:



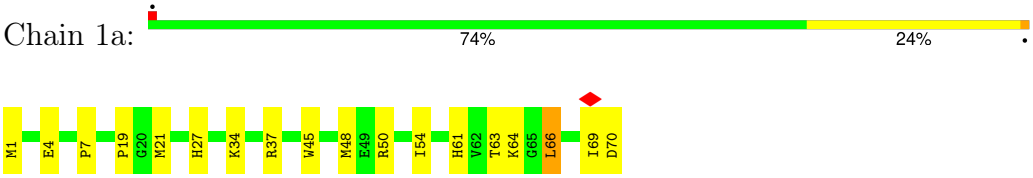
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:



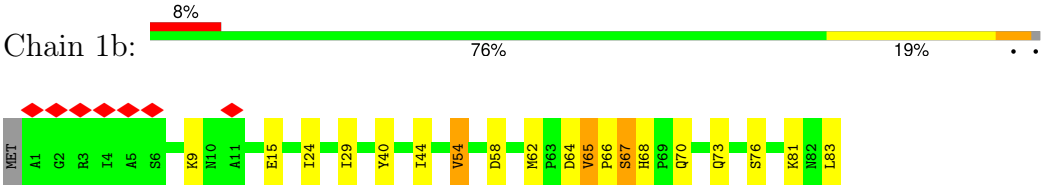
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a:



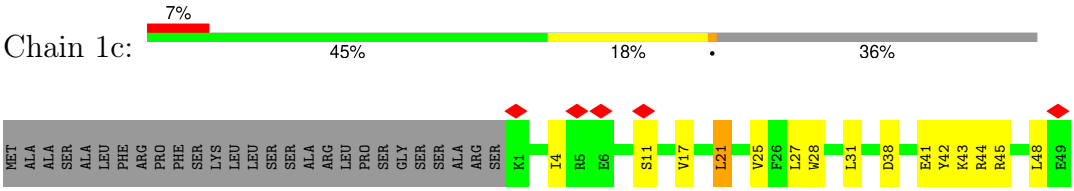
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b:



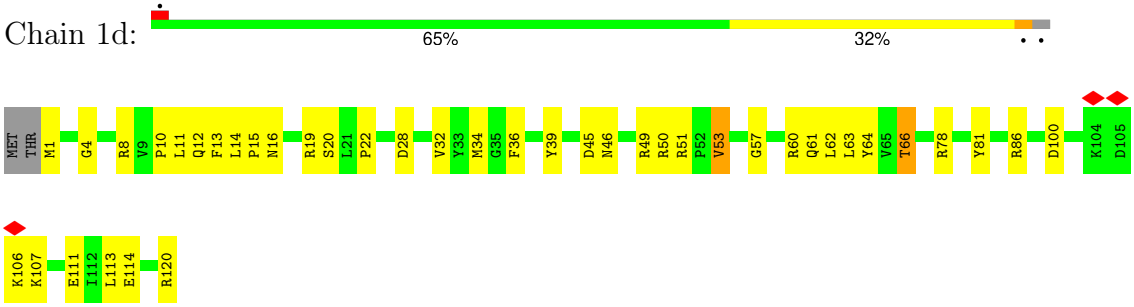
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c:



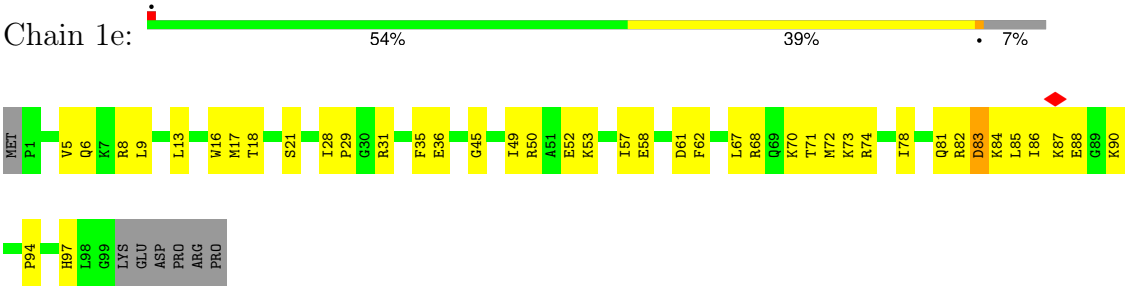
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d:



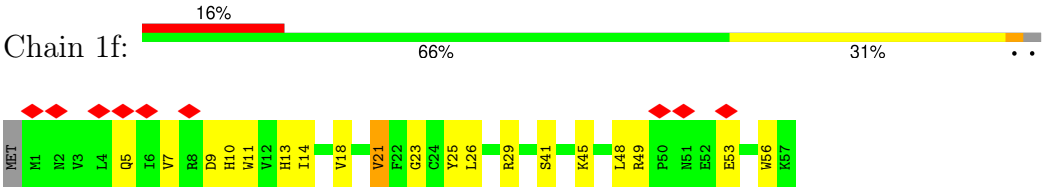
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:



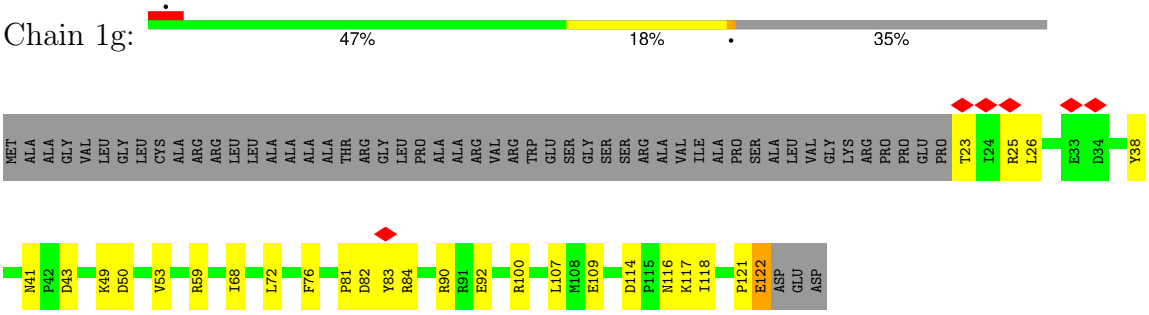
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain 1f:



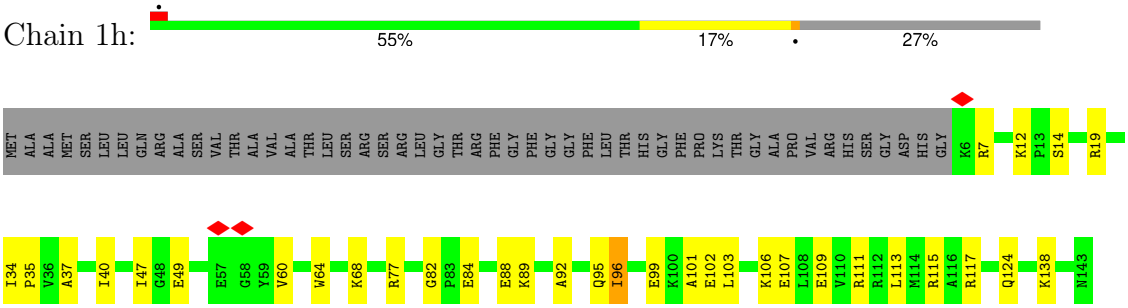
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



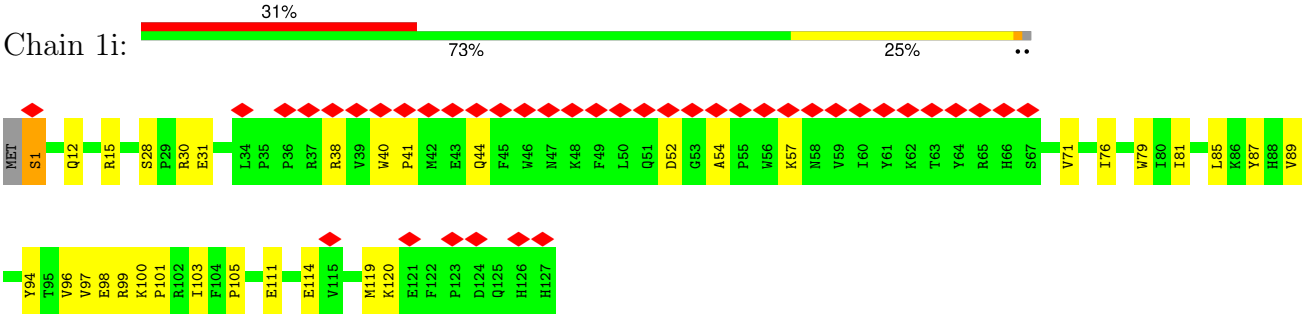
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



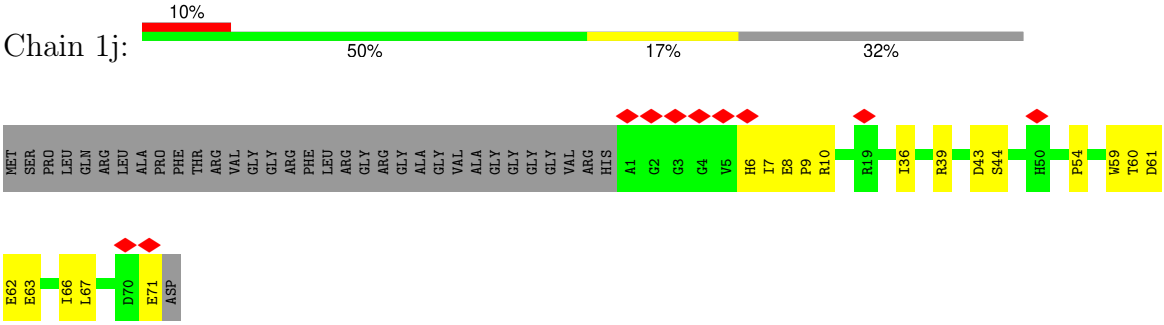
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



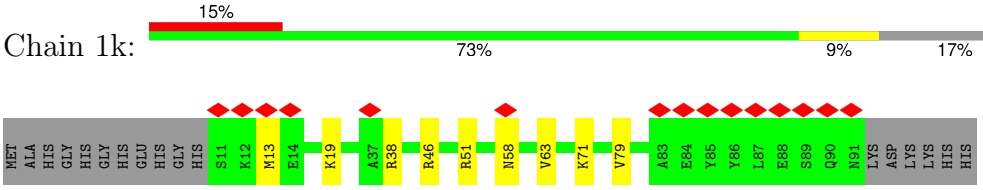
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



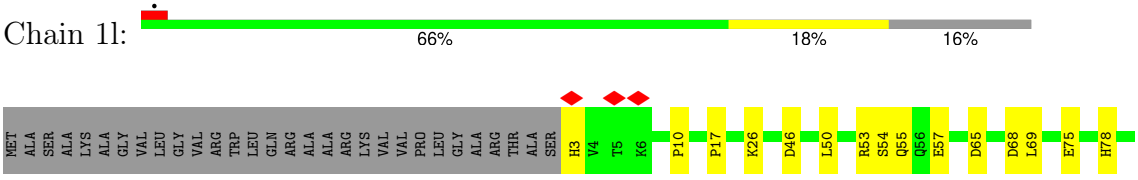
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

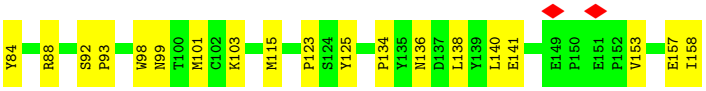
Chain 1k:



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

Chain 1l:

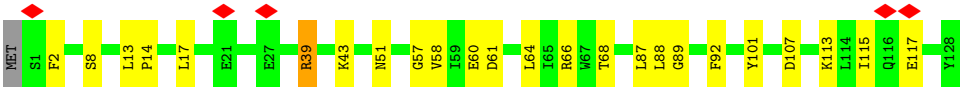




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m:

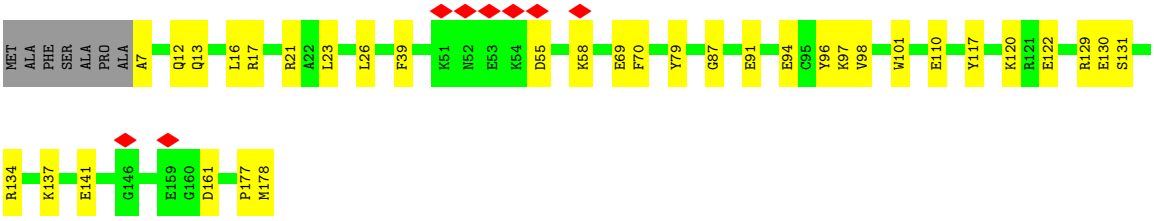




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n:

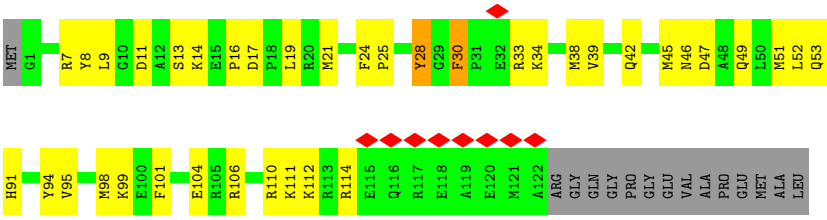




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:

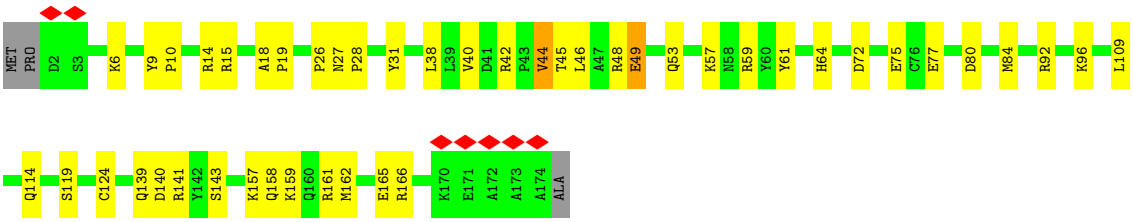




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p:

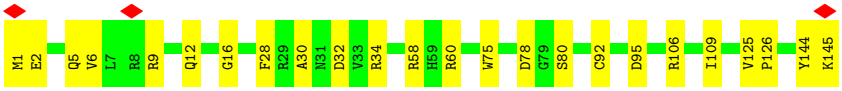




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:

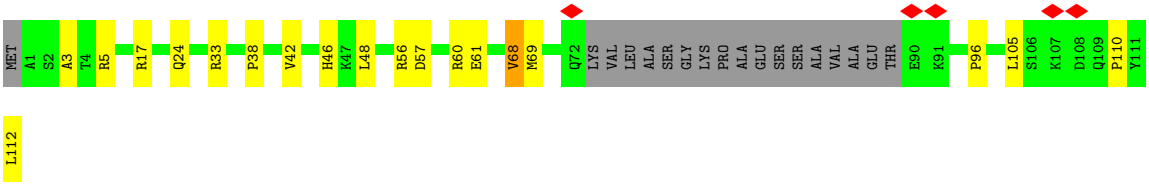




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 1r:

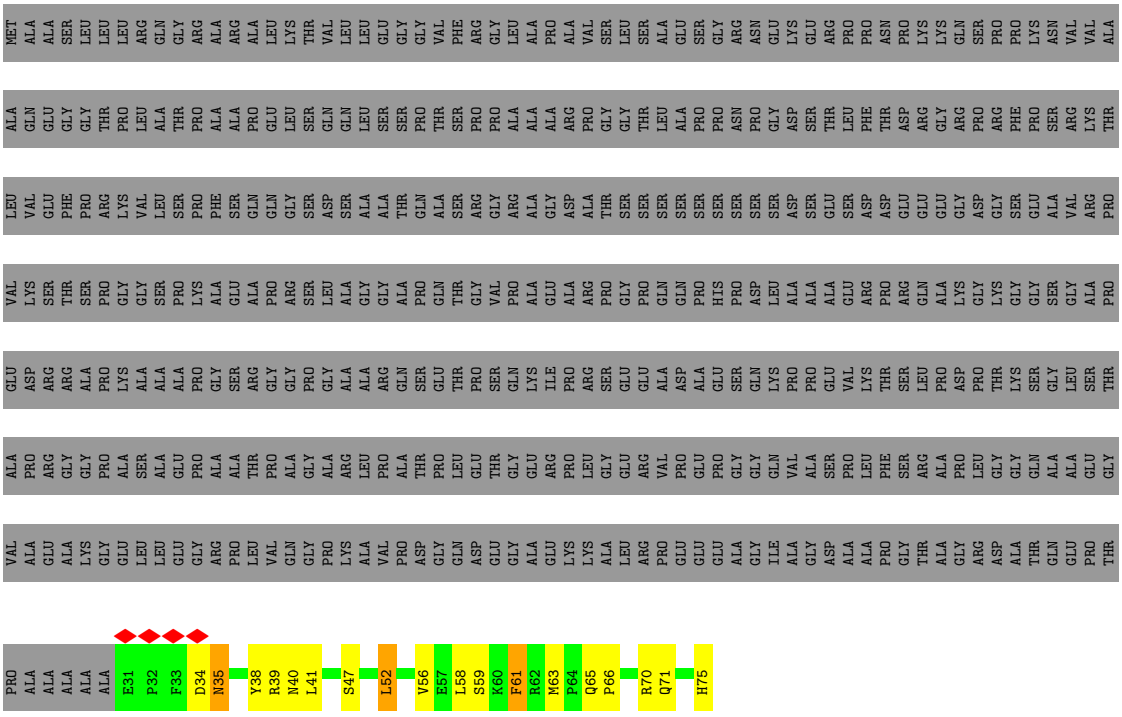




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain 1s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113902	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.780	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	300.24, 300.24, 300.24	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.417, 0.417, 0.417	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: 3PE, MG, FES, SAC, GTP, FME, SF4, FMN, EHZ, CDL, MYR, ZN, PC1, K, NDP, AYA

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	0.17	0/930	0.47	0/1271
2	1B	0.16	0/1273	0.40	0/1722
3	1C	0.14	0/1797	0.34	0/2447
4	1D	0.30	2/3545 (0.1%)	0.58	4/4806 (0.1%)
5	1E	0.18	0/1698	0.43	0/2311
6	1F	0.16	0/3401	0.44	0/4595
7	1G	0.16	0/5451	0.41	0/7387
8	1H	0.17	0/2566	0.45	2/3509 (0.1%)
9	1I	0.13	0/1443	0.38	0/1952
10	1J	0.19	0/1364	0.52	0/1850
11	1K	0.20	0/751	0.41	0/1018
12	1L	0.16	0/4939	0.42	0/6718
13	1M	0.17	0/3713	0.39	0/5063
14	1N	0.17	0/2765	0.40	0/3758
15	1O	0.16	0/2650	0.43	0/3588
16	1P	0.21	1/2828 (0.0%)	0.44	2/3834 (0.1%)
17	1Q	0.13	0/1070	0.35	0/1446
18	1R	0.14	0/755	0.36	0/1018
19	1S	0.15	0/711	0.40	0/956
20	1T	0.20	0/701	0.39	0/946
20	1U	0.14	0/706	0.34	0/954
21	1V	0.13	0/946	0.33	0/1281
22	1W	0.15	0/995	0.34	0/1340
23	1X	0.22	0/1436	0.51	1/1938 (0.1%)
24	1Y	0.17	0/1037	0.36	0/1404
25	1Z	0.16	0/1210	0.40	0/1631
26	1a	0.17	0/577	0.36	0/777
27	1b	0.17	0/664	0.46	0/912
28	1c	0.15	0/430	0.39	0/581
29	1d	0.17	0/1024	0.41	0/1384
30	1e	0.17	0/847	0.43	0/1132
31	1f	0.15	0/499	0.38	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.15	0/858	0.43	0/1165
33	1h	0.15	0/1184	0.40	0/1603
34	1i	0.15	0/1131	0.43	2/1541 (0.1%)
35	1j	0.15	0/627	0.36	0/858
36	1k	0.12	0/668	0.32	0/903
37	1l	0.66	2/1365 (0.1%)	0.82	3/1867 (0.2%)
38	1m	0.13	0/1092	0.34	0/1481
39	1n	0.15	0/1549	0.38	0/2098
40	1o	0.15	0/1069	0.38	0/1430
41	1p	0.42	3/1481 (0.2%)	0.90	4/1997 (0.2%)
42	1q	0.12	0/1253	0.33	0/1704
43	1r	0.14	0/777	0.35	0/1051
44	1s	0.17	0/394	0.46	0/533
All	All	0.20	8/68170 (0.0%)	0.45	18/92433 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1D	0	1
8	1H	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1l	17	PRO	CG-CD	-22.18	0.75	1.50
4	1D	21	PRO	CG-CD	-12.08	1.09	1.50
41	1p	19	PRO	CB-CG	-10.10	0.99	1.49
41	1p	19	PRO	CG-CD	-7.15	1.26	1.50
37	1l	17	PRO	N-CD	7.07	1.57	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	1l	17	PRO	N-CD-CG	-23.98	67.24	103.20
41	1p	19	PRO	CB-CG-CD	23.03	179.78	106.10
4	1D	21	PRO	N-CD-CG	-19.99	73.22	103.20
41	1p	19	PRO	N-CD-CG	-18.35	75.67	103.20
4	1D	21	PRO	CA-CB-CG	-17.70	70.87	104.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1D	421	GLN	Peptide
8	1H	91	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	40	0
2	1B	1242	0	1249	39	0
3	1C	1746	0	1697	24	0
4	1D	3452	0	3389	77	0
5	1E	1658	0	1662	36	0
6	1F	3325	0	3288	93	0
7	1G	5362	0	5388	101	0
8	1H	2504	0	2602	83	0
9	1I	1412	0	1366	30	0
10	1J	1329	0	1326	61	0
11	1K	750	0	798	37	0
12	1L	4818	0	4956	143	0
13	1M	3632	0	3836	108	0
14	1N	2712	0	2873	82	0
15	1O	2590	0	2555	58	0
16	1P	2751	0	2776	69	0
17	1Q	1047	0	1042	23	0
18	1R	741	0	704	15	0
19	1S	700	0	719	19	0
20	1T	689	0	687	27	0
20	1U	694	0	691	14	0
21	1V	927	0	972	16	0
22	1W	971	0	975	31	0
23	1X	1398	0	1378	60	0
24	1Y	1016	0	1020	33	0
25	1Z	1179	0	1173	43	0
26	1a	562	0	557	16	0
27	1b	643	0	645	14	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	1c	417	0	425	12	0
29	1d	993	0	990	41	0
30	1e	827	0	835	38	0
31	1f	487	0	498	14	0
32	1g	835	0	795	27	0
33	1h	1151	0	1164	30	0
34	1i	1100	0	1107	28	0
35	1j	601	0	546	15	0
36	1k	649	0	626	7	0
37	1l	1310	0	1204	25	0
38	1m	1062	0	1075	18	0
39	1n	1495	0	1434	29	0
40	1o	1045	0	1016	40	0
41	1p	1449	0	1416	36	0
42	1q	1212	0	1174	18	0
43	1r	767	0	792	16	0
44	1s	382	0	351	16	0
45	1A	35	0	44	1	0
45	1H	102	0	161	13	0
45	1I	44	0	62	6	0
45	1M	79	0	109	8	0
45	1P	79	0	106	3	0
45	1d	39	0	52	7	0
45	1f	46	0	69	3	0
45	1h	47	0	71	3	0
45	1m	46	0	65	4	0
45	1q	97	0	145	14	0
46	1B	8	0	0	2	0
46	1F	8	0	0	1	0
46	1G	16	0	0	0	0
46	1I	16	0	0	0	0
47	1E	4	0	0	0	0
47	1G	4	0	0	1	0
48	1F	31	0	19	0	0
49	1G	1	0	0	0	0
50	1J	44	0	62	7	0
50	1L	174	0	253	21	0
50	1M	96	0	146	15	0
50	1N	82	0	115	8	0
50	1Y	128	0	155	14	0
50	1b	47	0	71	4	0
50	1d	48	0	73	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	1j	44	0	65	3	0
50	1m	91	0	136	6	0
51	1L	87	0	124	6	0
51	1N	62	0	68	4	0
51	1X	86	0	125	10	0
51	1d	65	0	77	9	0
51	1h	80	0	104	12	0
51	1q	61	0	66	3	0
52	1O	32	0	12	2	0
53	1O	1	0	0	0	0
54	1P	48	0	26	2	0
55	1R	1	0	0	0	0
56	1W	37	0	0	2	0
56	1n	37	0	0	1	0
57	1l	15	0	27	0	0
58	1A	23	0	0	0	0
58	1B	68	0	0	2	0
58	1C	131	0	0	3	0
58	1D	213	0	0	6	0
58	1E	50	0	0	1	0
58	1F	105	0	0	7	0
58	1G	365	0	0	6	0
58	1H	75	0	0	3	0
58	1I	83	0	0	0	0
58	1J	40	0	0	0	0
58	1K	27	0	0	0	0
58	1L	277	0	0	13	0
58	1M	221	0	0	16	0
58	1N	156	0	0	5	0
58	1O	126	0	0	4	0
58	1P	207	0	0	7	0
58	1Q	110	0	0	2	0
58	1R	71	0	0	2	0
58	1S	58	0	0	4	0
58	1T	24	0	0	0	0
58	1U	37	0	0	0	0
58	1V	36	0	0	3	0
58	1W	64	0	0	3	0
58	1X	150	0	0	3	0
58	1Y	81	0	0	0	0
58	1Z	92	0	0	4	0
58	1a	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1b	42	0	0	1	0
58	1c	26	0	0	4	0
58	1d	93	0	0	5	0
58	1e	105	0	0	3	0
58	1f	38	0	0	1	0
58	1g	80	0	0	5	0
58	1h	128	0	0	5	0
58	1i	46	0	0	2	0
58	1j	32	0	0	2	0
58	1k	37	0	0	2	0
58	1l	111	0	0	2	0
58	1m	105	0	0	3	0
58	1n	129	0	0	4	0
58	1o	84	0	0	4	0
58	1p	153	0	0	5	0
58	1q	64	0	0	0	0
58	1r	47	0	0	0	0
58	1s	21	0	0	0	0
All	All	72881	0	69330	1577	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1577 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:77:CYS:HB2	23:1X:80:PRO:HD2	1.50	0.93
12:1L:600:THR:HG22	12:1L:601:LEU:H	1.34	0.92
39:1n:130:GLU:HG3	39:1n:134:ARG:HH22	1.37	0.90
9:1I:14:MET:SD	27:1b:9:LYS:NZ	2.46	0.88
6:1F:215:VAL:HG12	6:1F:220:THR:HG21	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6 3
2	1B	153/258 (59%)	142 (93%)	11 (7%)	0	100 100
3	1C	207/264 (78%)	205 (99%)	2 (1%)	0	100 100
4	1D	427/466 (92%)	409 (96%)	18 (4%)	0	100 100
5	1E	212/249 (85%)	197 (93%)	15 (7%)	0	100 100
6	1F	430/464 (93%)	411 (96%)	17 (4%)	2 (0%)	24 22
7	1G	697/727 (96%)	674 (97%)	20 (3%)	3 (0%)	30 28
8	1H	316/318 (99%)	302 (96%)	12 (4%)	2 (1%)	21 18
9	1I	174/239 (73%)	170 (98%)	4 (2%)	0	100 100
10	1J	172/175 (98%)	162 (94%)	9 (5%)	1 (1%)	21 18
11	1K	96/98 (98%)	95 (99%)	1 (1%)	0	100 100
12	1L	604/606 (100%)	579 (96%)	24 (4%)	1 (0%)	43 44
13	1M	457/459 (100%)	454 (99%)	3 (1%)	0	100 100
14	1N	345/347 (99%)	342 (99%)	3 (1%)	0	100 100
15	1O	318/357 (89%)	303 (95%)	15 (5%)	0	100 100
16	1P	340/377 (90%)	330 (97%)	10 (3%)	0	100 100
17	1Q	127/175 (73%)	124 (98%)	3 (2%)	0	100 100
18	1R	94/123 (76%)	92 (98%)	2 (2%)	0	100 100
19	1S	85/99 (86%)	82 (96%)	3 (4%)	0	100 100
20	1T	83/156 (53%)	81 (98%)	2 (2%)	0	100 100
20	1U	84/156 (54%)	83 (99%)	1 (1%)	0	100 100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
22	1W	113/128 (88%)	109 (96%)	4 (4%)	0	100 100
23	1X	169/172 (98%)	161 (95%)	8 (5%)	0	100 100
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100 100
25	1Z	140/144 (97%)	138 (99%)	2 (1%)	0	100 100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100 100
27	1b	81/84 (96%)	77 (95%)	3 (4%)	1 (1%)	10 7
28	1c	47/76 (62%)	45 (96%)	2 (4%)	0	100 100
29	1d	118/122 (97%)	117 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	98/106 (92%)	95 (97%)	3 (3%)	0	100	100
31	1f	55/58 (95%)	55 (100%)	0	0	100	100
32	1g	98/154 (64%)	92 (94%)	6 (6%)	0	100	100
33	1h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	1i	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	1l	154/186 (83%)	151 (98%)	3 (2%)	0	100	100
38	1m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	1n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	1o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	171 (100%)	0	0	100	100
42	1q	143/145 (99%)	143 (100%)	0	0	100	100
43	1r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	1s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
All	All	8198/9655 (85%)	7944 (97%)	242 (3%)	12 (0%)	49	50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	115	ASP
8	1H	196	ALA
10	1J	66	VAL
27	1b	67	SER
8	1H	208	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	98 (99%)	1 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1B	131/212 (62%)	123 (94%)	8 (6%)	17	15
3	1C	191/228 (84%)	189 (99%)	2 (1%)	68	76
4	1D	371/396 (94%)	362 (98%)	9 (2%)	43	49
5	1E	183/207 (88%)	177 (97%)	6 (3%)	33	37
6	1F	346/368 (94%)	338 (98%)	8 (2%)	44	51
7	1G	588/610 (96%)	571 (97%)	17 (3%)	37	42
8	1H	274/274 (100%)	266 (97%)	8 (3%)	37	42
9	1I	151/201 (75%)	150 (99%)	1 (1%)	76	83
10	1J	140/141 (99%)	132 (94%)	8 (6%)	18	17
11	1K	84/84 (100%)	83 (99%)	1 (1%)	63	72
12	1L	539/539 (100%)	527 (98%)	12 (2%)	45	53
13	1M	408/408 (100%)	395 (97%)	13 (3%)	34	38
14	1N	310/310 (100%)	304 (98%)	6 (2%)	50	58
15	1O	283/307 (92%)	270 (95%)	13 (5%)	24	25
16	1P	296/323 (92%)	282 (95%)	14 (5%)	23	24
17	1Q	117/152 (77%)	113 (97%)	4 (3%)	32	35
18	1R	79/97 (81%)	76 (96%)	3 (4%)	29	32
19	1S	77/82 (94%)	72 (94%)	5 (6%)	15	13
20	1T	79/133 (59%)	77 (98%)	2 (2%)	42	48
20	1U	79/133 (59%)	75 (95%)	4 (5%)	21	21
21	1V	100/101 (99%)	97 (97%)	3 (3%)	36	41
22	1W	107/112 (96%)	106 (99%)	1 (1%)	70	78
23	1X	153/154 (99%)	145 (95%)	8 (5%)	21	20
24	1Y	101/102 (99%)	99 (98%)	2 (2%)	48	56
25	1Z	124/124 (100%)	119 (96%)	5 (4%)	28	29
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	35
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	11
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	12
29	1d	107/109 (98%)	102 (95%)	5 (5%)	23	24
30	1e	88/94 (94%)	84 (96%)	4 (4%)	24	25
31	1f	54/55 (98%)	52 (96%)	2 (4%)	30	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65 74
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33 37
34	1i	119/120 (99%)	117 (98%)	2 (2%)	53 62
35	1j	62/84 (74%)	61 (98%)	1 (2%)	55 64
36	1k	63/76 (83%)	60 (95%)	3 (5%)	23 23
37	1l	141/161 (88%)	141 (100%)	0	100 100
38	1m	113/114 (99%)	108 (96%)	5 (4%)	25 26
39	1n	156/160 (98%)	156 (100%)	0	100 100
40	1o	110/120 (92%)	104 (94%)	6 (6%)	19 18
41	1p	154/156 (99%)	149 (97%)	5 (3%)	34 38
42	1q	131/131 (100%)	130 (99%)	1 (1%)	73 81
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32 35
44	1s	44/351 (12%)	39 (89%)	5 (11%)	5 3
All	All	7222/8207 (88%)	7001 (97%)	221 (3%)	36 39

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	1P	90	VAL
20	1U	77	VAL
44	1s	52	LEU
38	1m	68	THR
16	1P	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
15	1O	180	GLN
20	1T	35	HIS
42	1q	31	ASN
40	1o	46	ASN
15	1O	204	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	1.00	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	1.42	2 (25%)
14	FME	1N	1	14	8,9,10	0.53	0	8,9,11	0.95	1 (12%)
8	FME	1H	1	8	8,9,10	0.56	0	8,9,11	1.00	1 (12%)
1	FME	1A	1	1	8,9,10	0.55	0	8,9,11	0.90	1 (12%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	0.97	1 (12%)
34	SAC	1i	1	34	7,8,9	0.58	0	7,9,11	0.89	1 (14%)
43	AYA	1r	1	43	6,7,8	0.67	0	6,8,10	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	1M	1	13	-	1/7/9/11	-
12	FME	1L	1	12	-	3/7/9/11	-
14	FME	1N	1	14	-	2/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
1	FME	1A	1	1	-	2/7/9/11	-
11	FME	1K	1	11	-	0/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
43	AYA	1r	1	43	-	1/5/6/8	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1L	1	FME	CA-N-CN	2.76	127.06	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1H	1	FME	O-C-CA	-2.64	117.97	124.77
12	1L	1	FME	O-C-CA	-2.64	117.98	124.77
11	1K	1	FME	O-C-CA	-2.61	118.06	124.77
13	1M	1	FME	O-C-CA	-2.58	118.13	124.77

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1L	1	FME	CB-CA-N-CN
12	1L	1	FME	O-C-CA-CB
43	1r	1	AYA	O-C-CA-CB
8	1H	1	FME	CA-CB-CG-SD
1	1A	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1M	1	FME	1	0
14	1N	1	FME	2	0
1	1A	1	FME	1	0
11	1K	1	FME	1	0
34	1i	1	SAC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 3 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	PC1	1d	203	-	38,38,53	0.35	0	44,46,61	0.86	2 (4%)
51	CDL	1L	705	-	86,86,99	0.29	0	92,98,111	0.37	0
45	PC1	1M	504	-	43,43,53	0.33	0	49,51,61	0.35	0
50	3PE	1Y	801	-	30,30,50	0.33	0	33,35,55	0.80	1 (3%)
45	PC1	1q	201	-	47,47,53	0.29	0	53,55,61	0.36	0
50	3PE	1Y	804	-	26,26,50	0.36	0	29,31,55	0.42	0
46	SF4	1G	801	7	0,12,12	-	-	-		
54	NDP	1P	403	-	51,52,52	0.51	0	71,80,80	0.78	2 (2%)
50	3PE	1b	201	-	46,46,50	0.28	0	49,51,55	0.41	0
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.68	1 (2%)
45	PC1	1q	202	-	48,48,53	0.29	0	54,56,61	0.60	1 (1%)
56	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.17	1 (2%)
50	3PE	1L	701	-	45,45,50	0.31	0	48,50,55	0.44	0
46	SF4	1I	201	9	0,12,12	-	-	-		
47	FES	1E	301	5	0,4,4	-	-	-		
45	PC1	1H	402	-	47,47,53	0.29	0	53,55,61	0.41	0
45	PC1	1M	502	-	34,34,53	0.33	0	40,42,61	0.60	1 (2%)
51	CDL	1d	202	-	64,64,99	0.33	0	70,76,111	0.45	0
50	3PE	1Y	803	-	29,29,50	0.35	0	32,34,55	0.61	1 (3%)
51	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.41	0
50	3PE	1L	704	-	41,41,50	0.29	0	44,46,55	0.40	0
56	EHZ	1W	201	-	31,36,37	0.18	0	36,44,47	1.11	1 (2%)
46	SF4	1F	502	6	0,12,12	-	-	-		
46	SF4	1B	201	2	0,12,12	-	-	-		
50	3PE	1L	703	-	40,40,50	0.30	0	43,45,55	0.45	0
46	SF4	1G	802	7	0,12,12	-	-	-		
50	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.40	0
50	3PE	1M	503	-	50,50,50	0.27	0	53,55,55	0.38	0
46	SF4	1I	202	9	0,12,12	-	-	-		
52	GTP	1O	401	53,15	33,34,34	0.60	0	50,54,54	0.62	0
45	PC1	1m	201	38	45,45,53	0.28	0	51,53,61	0.44	0
50	3PE	1d	201	-	47,47,50	0.30	0	50,52,55	0.39	0
51	CDL	1q	203	-	60,60,99	0.34	0	66,72,111	0.45	0
50	3PE	1L	702	-	44,44,50	0.29	0	47,49,55	0.47	0
45	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.35	0
50	3PE	1N	903	-	32,32,50	0.33	0	35,37,55	0.45	0
50	3PE	1Y	802	-	39,39,50	0.30	0	42,44,55	0.41	0
45	PC1	1h	202	-	46,46,53	0.29	0	52,54,61	0.41	0
45	PC1	1f	101	-	45,45,53	0.30	0	51,53,61	0.38	0
45	PC1	1H	401	-	53,53,53	0.27	0	59,61,61	0.36	0
50	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.57	1 (1%)
50	3PE	1J	201	-	43,43,50	0.29	0	46,48,55	0.37	0
50	3PE	1m	202	-	49,49,50	0.27	0	52,54,55	0.39	0
51	CDL	1h	201	-	79,79,99	0.31	0	85,91,111	0.38	0
45	PC1	1P	402	-	45,45,53	0.29	0	51,53,61	0.34	0
50	3PE	1N	901	-	48,48,50	0.29	0	51,53,55	0.43	0
50	3PE	1m	203	-	40,40,50	0.29	0	43,45,55	0.64	1 (2%)
47	FES	1G	803	7	0,4,4	-	-	-		
57	MYR	1l	201	-	13,14,15	0.32	0	12,13,15	0.30	0
45	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.45	0
45	PC1	1A	201	-	34,34,53	0.33	0	40,42,61	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PC1	1d	203	-	-	19/42/42/57	-
51	CDL	1L	705	-	-	15/97/97/110	-
45	PC1	1M	504	-	-	12/47/47/57	-
50	3PE	1Y	801	-	-	7/34/34/54	-
45	PC1	1q	201	-	-	10/51/51/57	-
50	3PE	1Y	804	-	-	5/30/30/54	-
46	SF4	1G	801	7	-	-	0/6/5/5
54	NDP	1P	403	-	-	5/34/77/77	0/5/5/5
50	3PE	1b	201	-	-	9/50/50/54	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
45	PC1	1q	202	-	-	10/52/52/57	-
56	EHZ	1n	201	-	-	4/42/44/45	-
50	3PE	1L	701	-	-	8/49/49/54	-
46	SF4	1I	201	9	-	-	0/6/5/5
47	FES	1E	301	5	-	-	0/1/1/1
45	PC1	1H	402	-	-	12/51/51/57	-
45	PC1	1M	502	-	-	9/38/38/57	-
51	CDL	1d	202	-	-	14/75/75/110	-
50	3PE	1Y	803	-	-	10/33/33/54	-
51	CDL	1X	201	-	-	19/96/96/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	1L	704	-	-	1/45/45/54	-
56	EHZ	1W	201	-	-	11/42/44/45	-
50	3PE	1M	501	-	-	6/48/48/54	-
46	SF4	1B	201	2	-	-	0/6/5/5
50	3PE	1L	703	-	-	8/44/44/54	-
46	SF4	1F	502	6	-	-	0/6/5/5
46	SF4	1G	802	7	-	-	0/6/5/5
50	3PE	1M	503	-	-	10/54/54/54	-
52	GTP	1O	401	53,15	-	6/22/38/38	0/3/3/3
46	SF4	1I	202	9	-	-	0/6/5/5
45	PC1	1m	201	38	-	9/49/49/57	-
50	3PE	1d	201	-	-	15/51/51/54	-
51	CDL	1q	203	-	-	4/71/71/110	-
50	3PE	1L	702	-	-	8/48/48/54	-
45	PC1	1I	203	-	-	1/47/47/57	-
50	3PE	1N	903	-	-	7/36/36/54	-
50	3PE	1Y	802	-	-	7/43/43/54	-
45	PC1	1h	202	-	-	13/50/50/57	-
45	PC1	1f	101	-	-	9/49/49/57	-
45	PC1	1H	401	-	-	11/57/57/57	-
50	3PE	1j	101	-	-	4/47/47/54	-
51	CDL	1N	902	-	-	8/71/71/110	-
50	3PE	1J	201	-	-	8/47/47/54	-
50	3PE	1m	202	-	-	8/53/53/54	-
51	CDL	1h	201	-	-	11/90/90/110	-
45	PC1	1P	402	-	-	4/49/49/57	-
50	3PE	1N	901	-	-	7/52/52/54	-
50	3PE	1m	203	-	-	11/44/44/54	-
47	FES	1G	803	7	-	-	0/1/1/1
57	MYR	1l	201	-	-	0/12/12/13	-
45	PC1	1P	401	-	-	4/36/36/57	-
45	PC1	1A	201	-	-	3/38/38/57	-

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1n	201	EHZ	C10-S1-C9	6.33	120.55	101.84
56	1W	201	EHZ	C10-S1-C9	5.95	119.43	101.84
45	1d	203	PC1	O21-C21-C22	4.30	120.79	111.48
54	1P	403	NDP	P2B-O2B-C2B	-4.17	112.28	123.43
50	1Y	801	3PE	O21-C21-C22	3.18	118.36	111.48

There are no chirality outliers.

5 of 363 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1H	401	PC1	C11-O13-P-O14
45	1H	402	PC1	C11-O13-P-O11
45	1H	402	PC1	C1-O11-P-O14
45	1H	402	PC1	C1-O11-P-O13
45	1H	402	PC1	C12-C11-O13-P

There are no ring outliers.

44 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1d	203	PC1	7	0
51	1L	705	CDL	6	0
45	1M	504	PC1	6	0
50	1Y	801	3PE	3	0
45	1q	201	PC1	6	0
50	1Y	804	3PE	4	0
54	1P	403	NDP	2	0
50	1b	201	3PE	4	0
45	1q	202	PC1	10	0
56	1n	201	EHZ	1	0
50	1L	701	3PE	3	0
45	1H	402	PC1	9	0
45	1M	502	PC1	2	0
51	1d	202	CDL	9	0
50	1Y	803	3PE	3	0
51	1X	201	CDL	10	0
50	1L	704	3PE	3	0
56	1W	201	EHZ	2	0
46	1F	502	SF4	1	0
46	1B	201	SF4	2	0
50	1L	703	3PE	9	0
50	1M	501	3PE	4	0

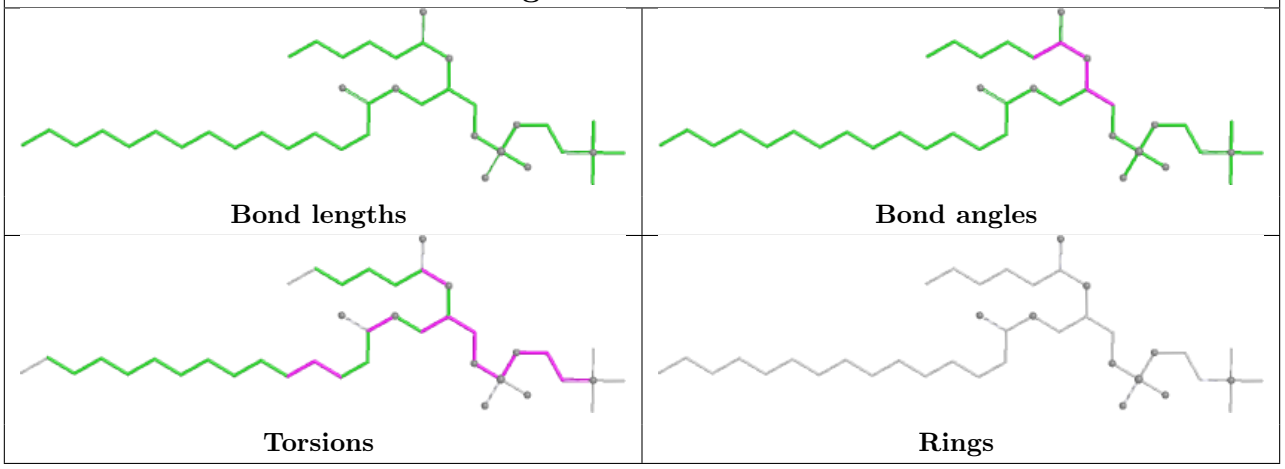
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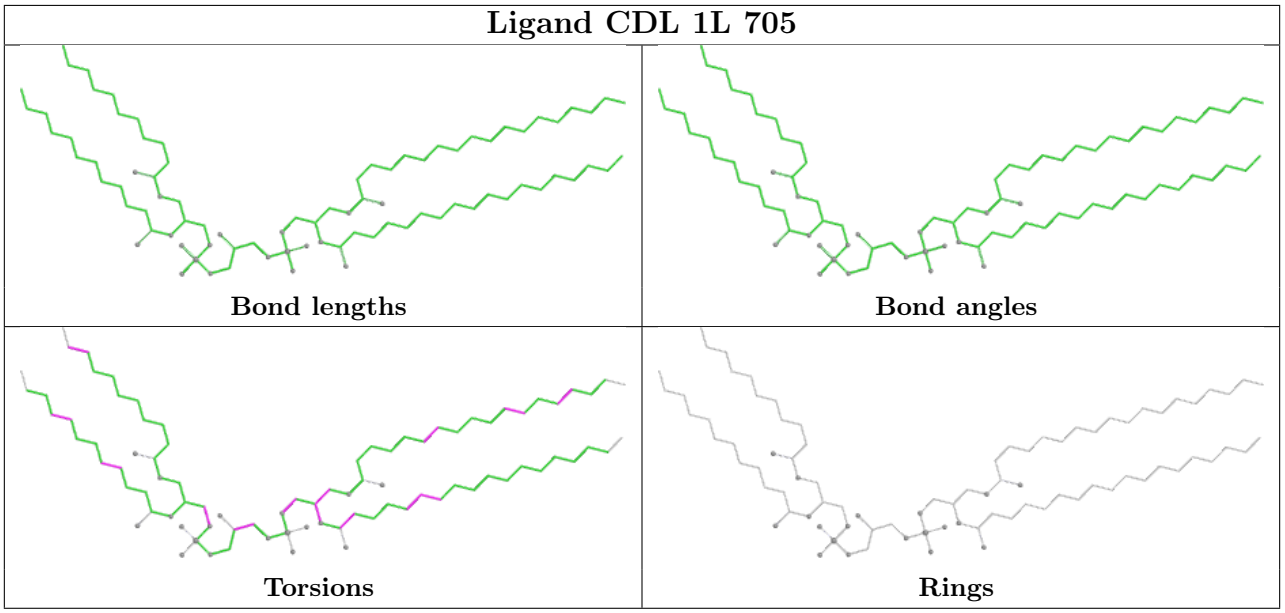
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	1M	503	3PE	11	0
52	1O	401	GTP	2	0
45	1m	201	PC1	4	0
50	1d	201	3PE	7	0
51	1q	203	CDL	3	0
50	1L	702	3PE	6	0
45	1I	203	PC1	6	0
50	1N	903	3PE	3	0
50	1Y	802	3PE	5	0
45	1h	202	PC1	3	0
45	1f	101	PC1	3	0
45	1H	401	PC1	4	0
50	1j	101	3PE	3	0
51	1N	902	CDL	4	0
50	1J	201	3PE	7	0
50	1m	202	3PE	3	0
51	1h	201	CDL	12	0
45	1P	402	PC1	3	0
50	1N	901	3PE	5	0
50	1m	203	3PE	3	0
47	1G	803	FES	1	0
45	1A	201	PC1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

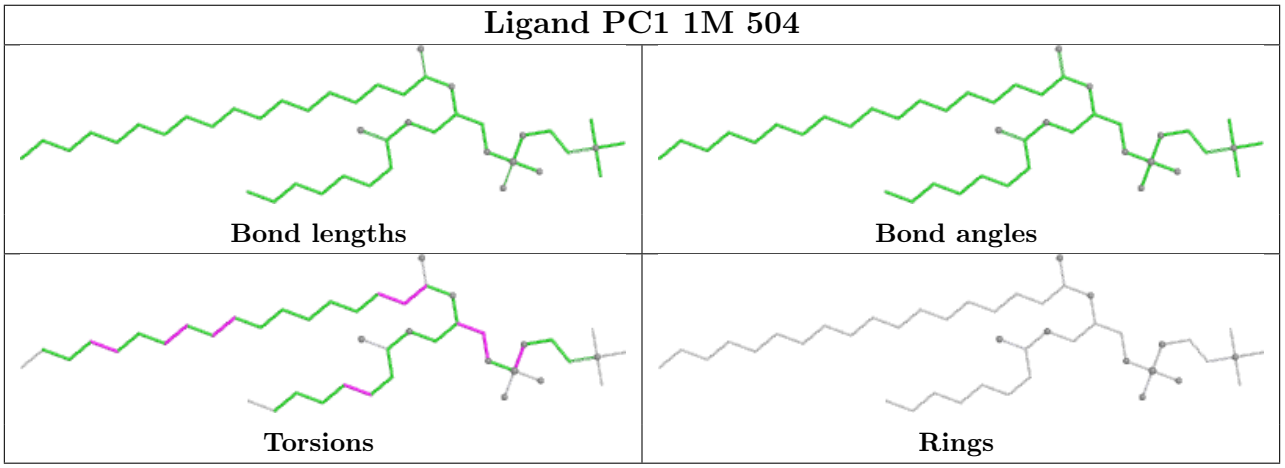
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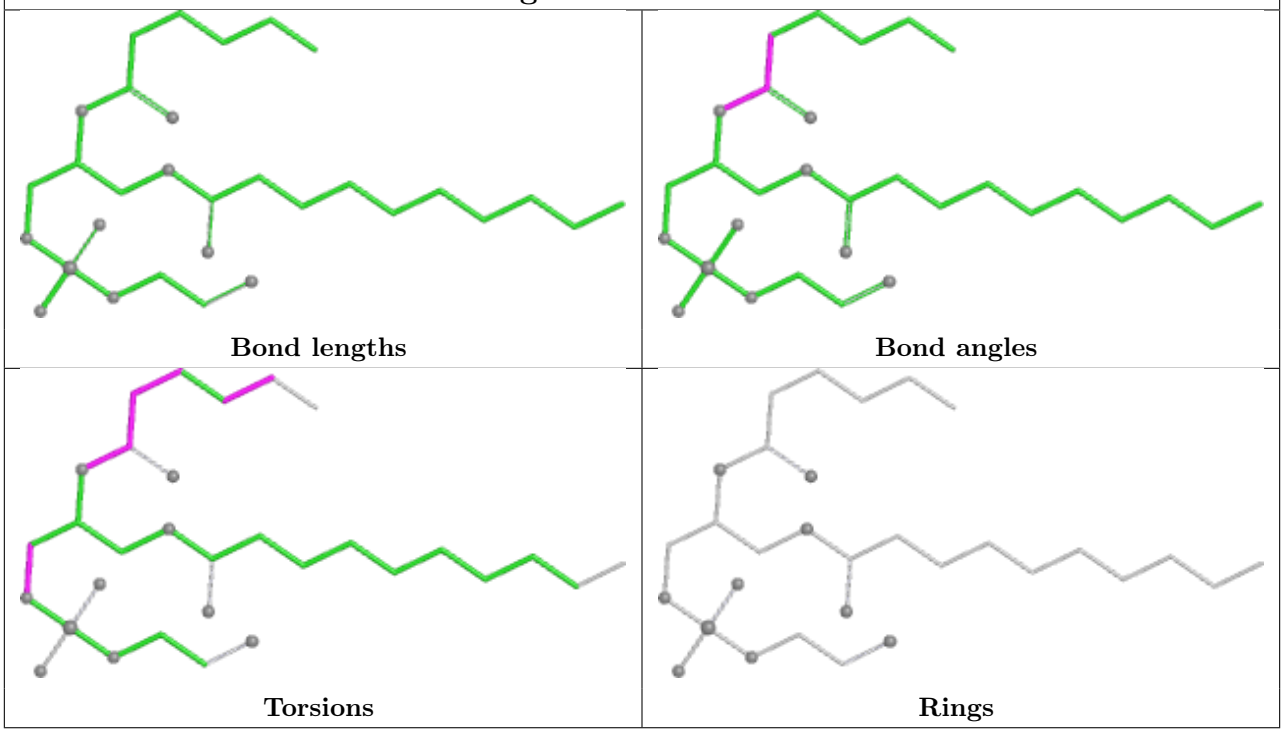
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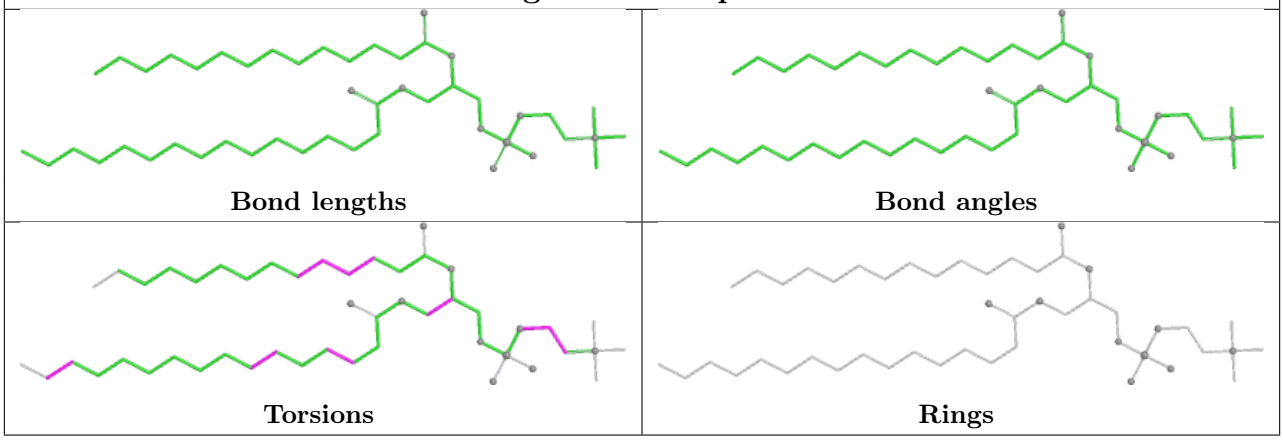
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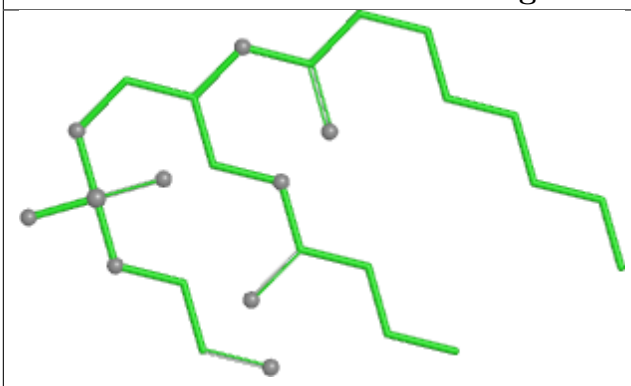
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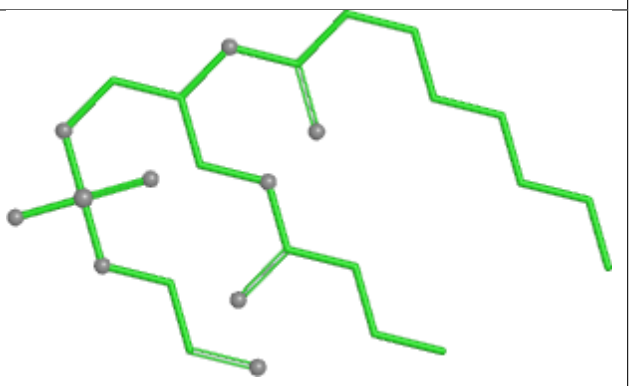
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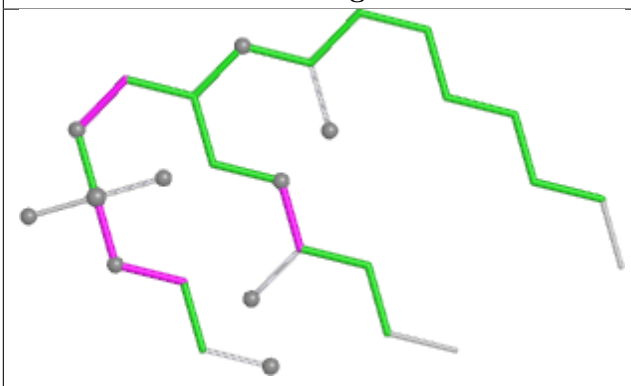
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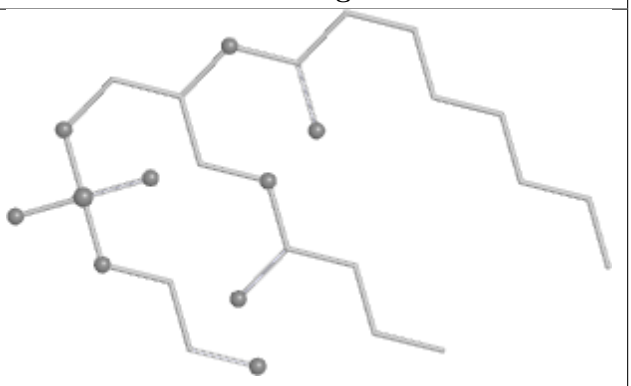
Bond lengths



Bond angles

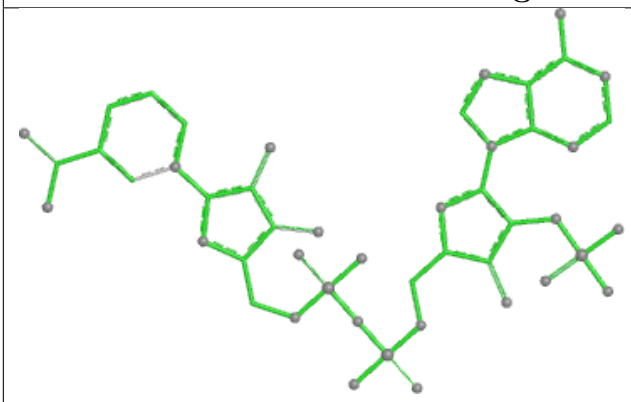


Torsions

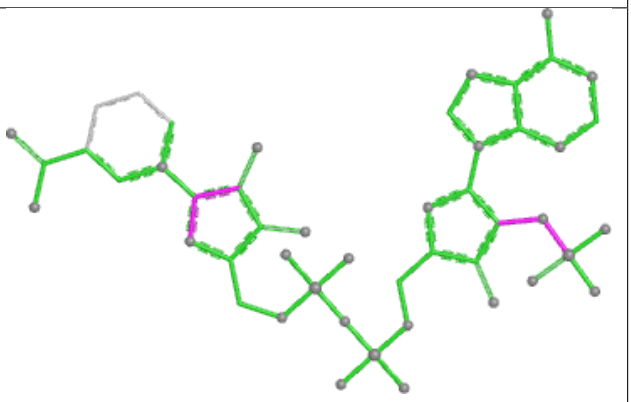


Rings

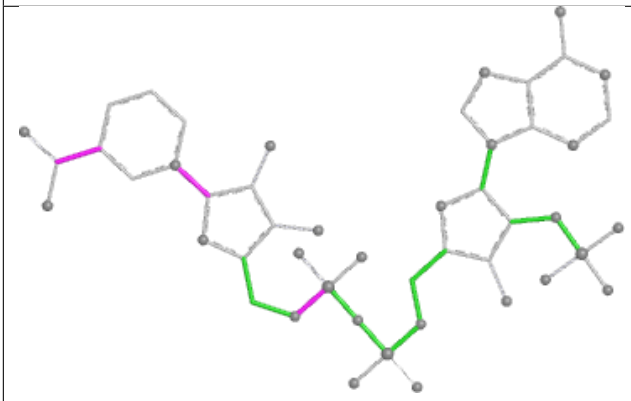
Ligand NDP 1P 403



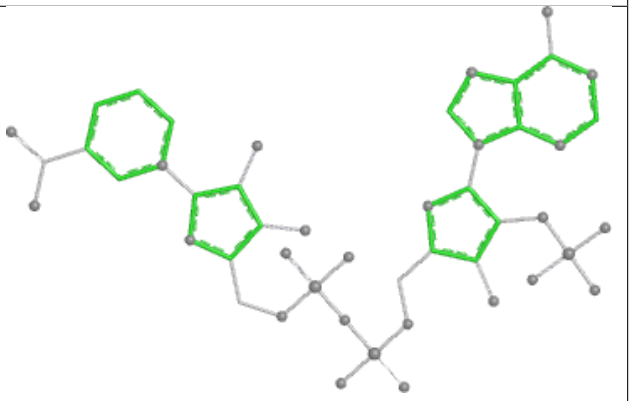
Bond lengths



Bond angles

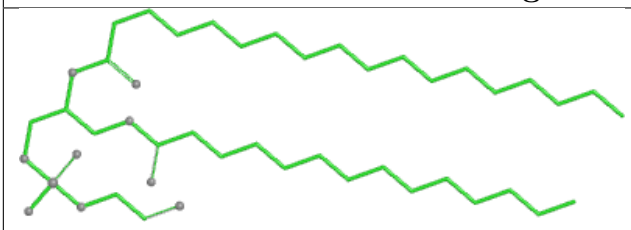


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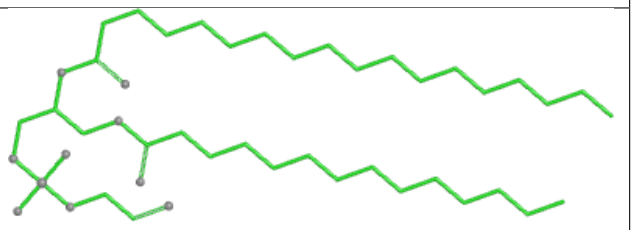


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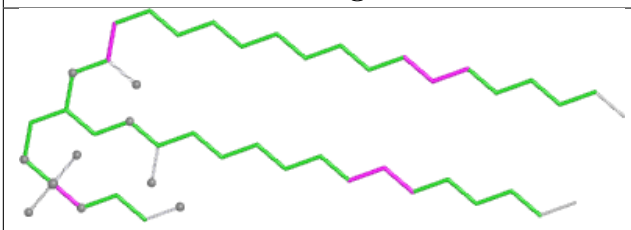
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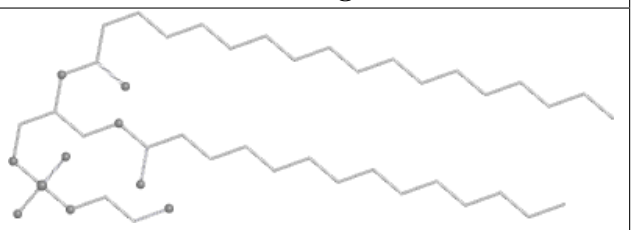
Bond lengths



Bond angles

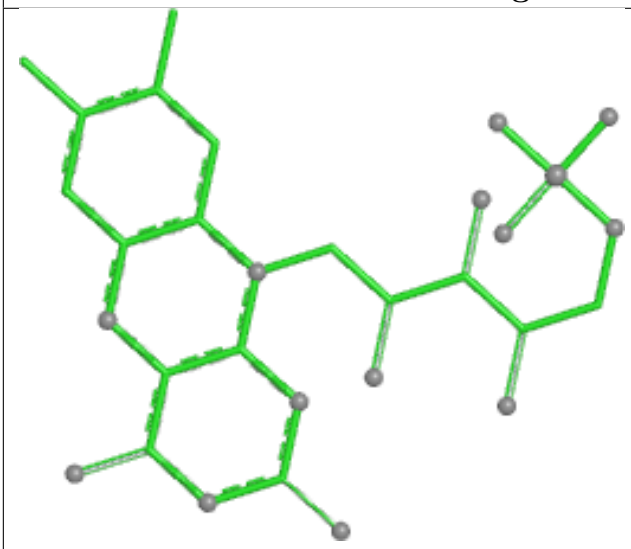


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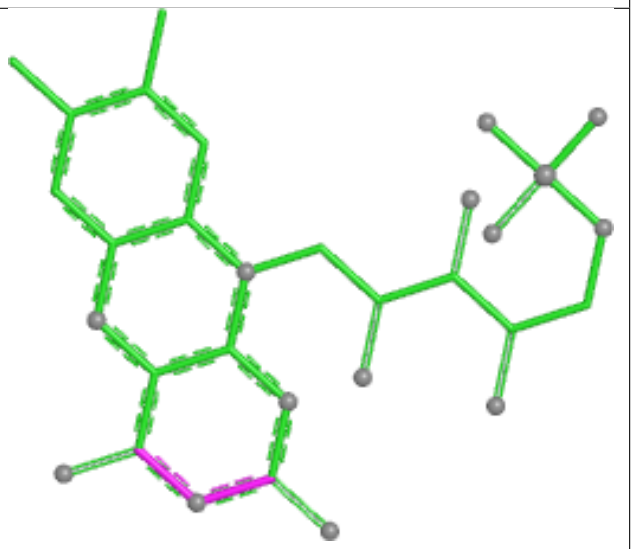


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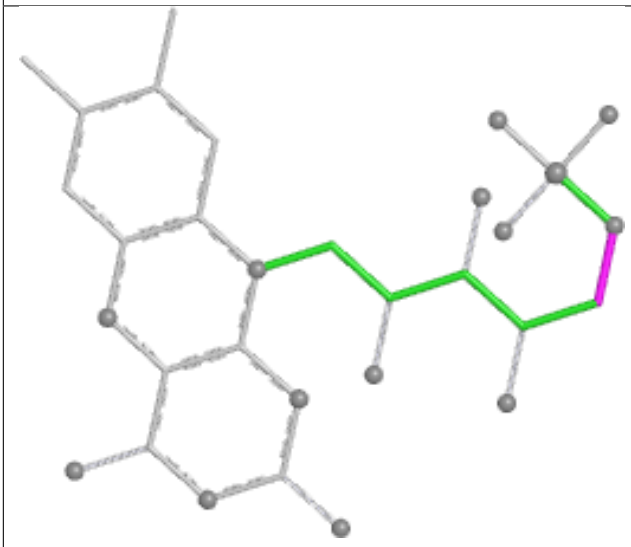
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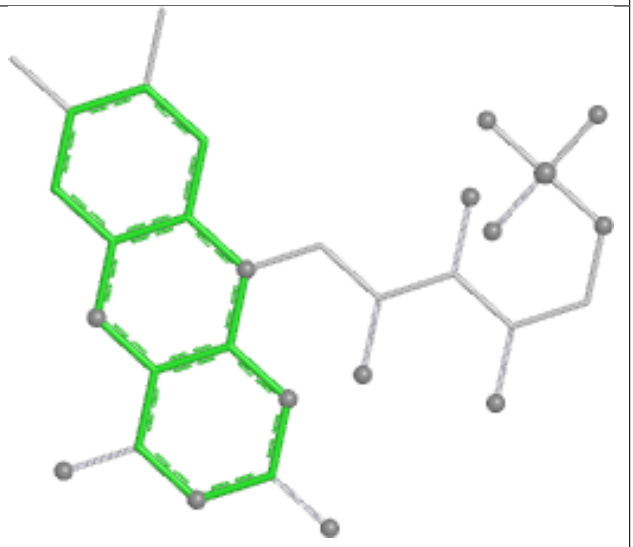
Bond lengths



Bond angles

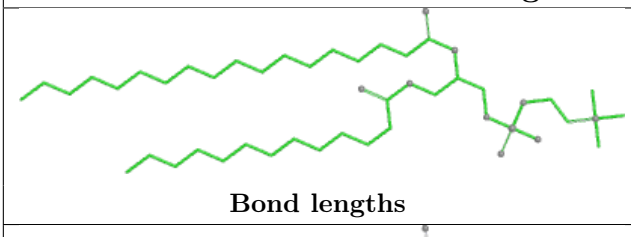


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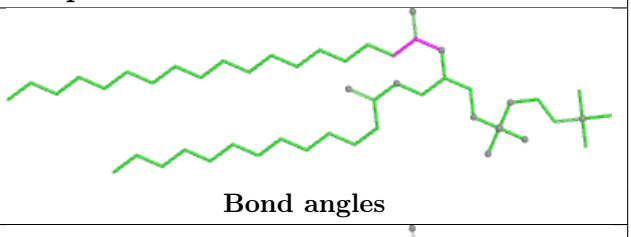


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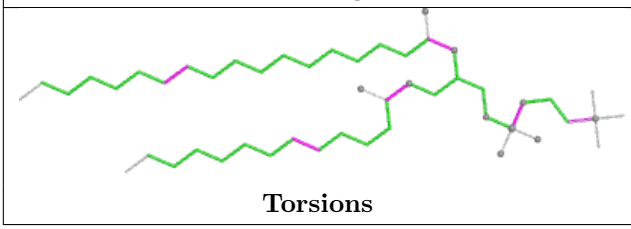
Ligand PC1 1q 202



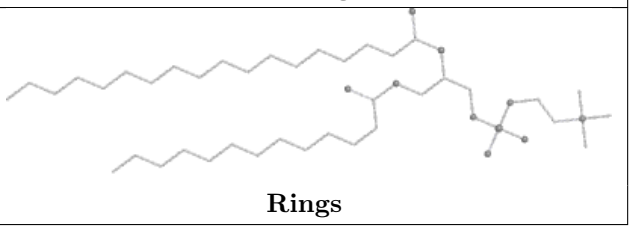
Bond lengths



Bond angles

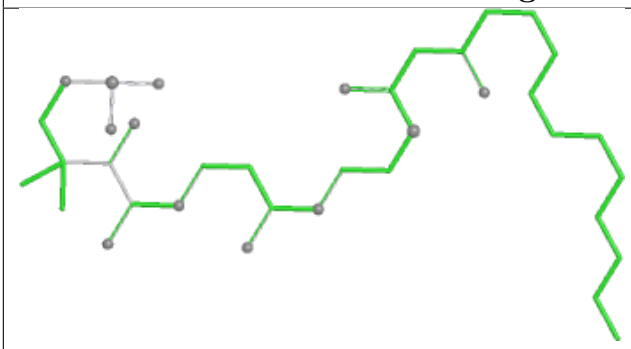


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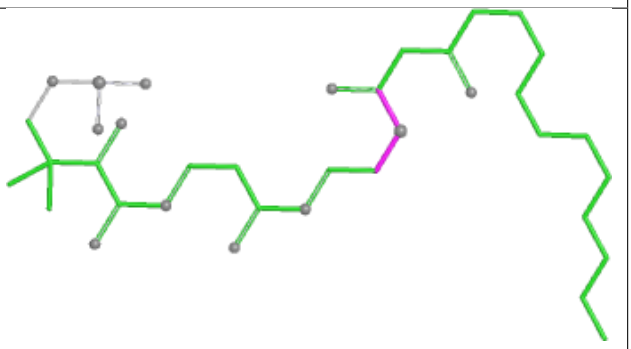


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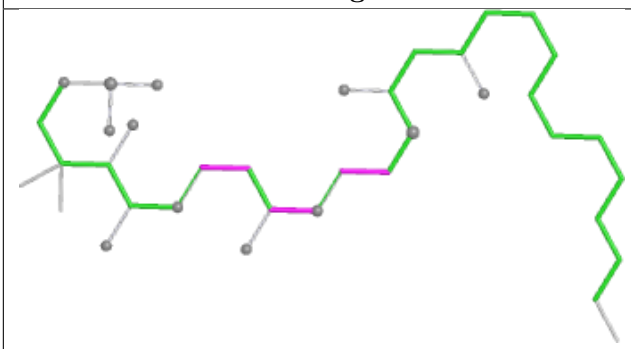
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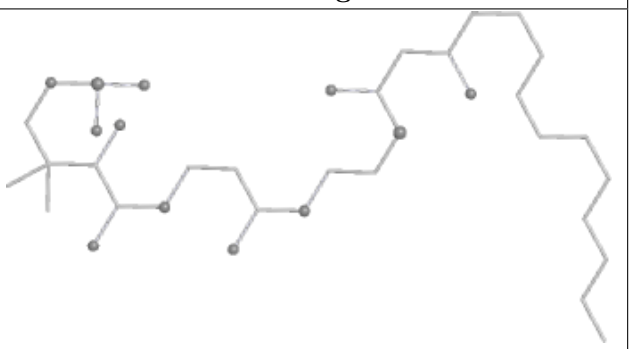
Bond lengths



Bond angles

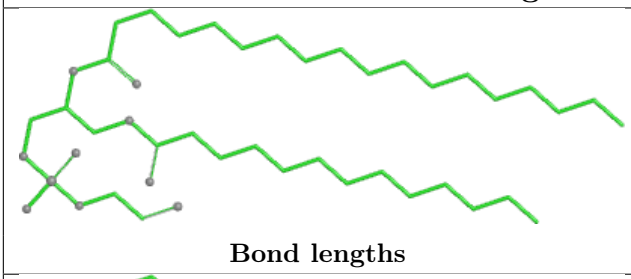


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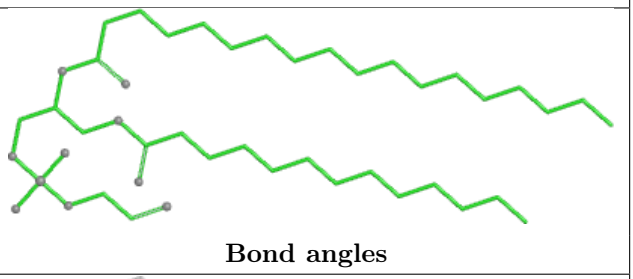


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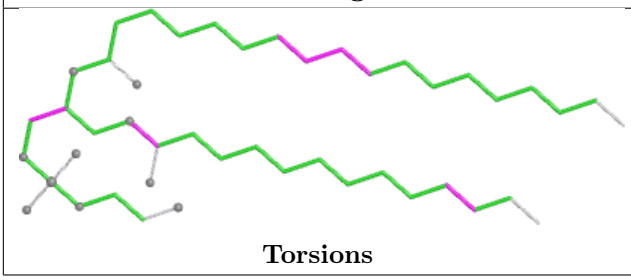
Ligand 3PE 1L 701



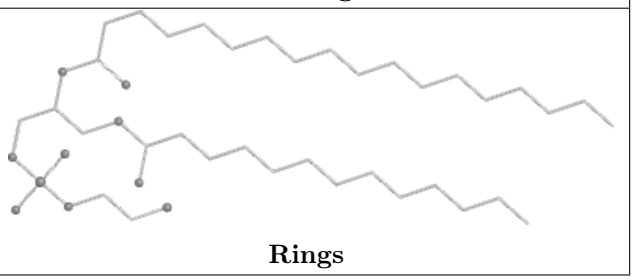
Bond lengths



Bond angles

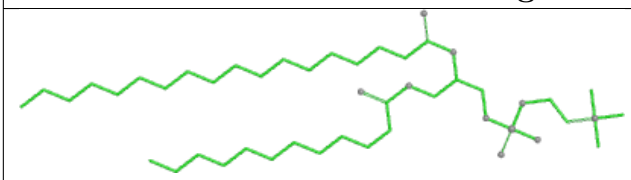


Torsions

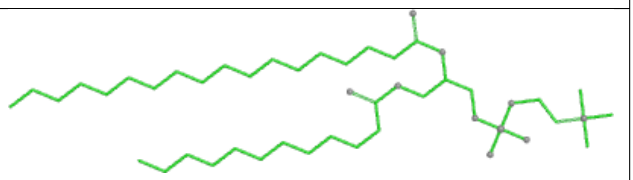


Rings

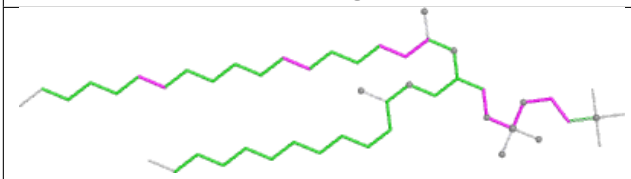
Ligand PC1 1H 402



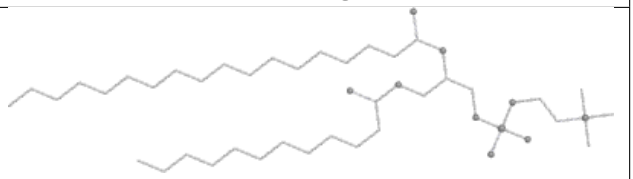
Bond lengths



Bond angles

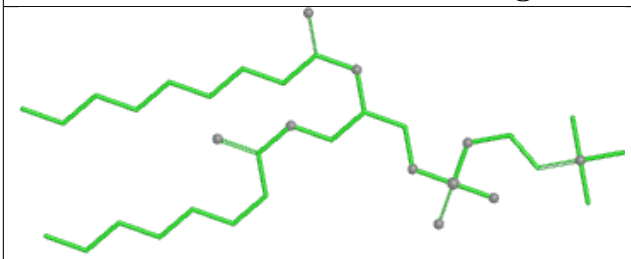


Torsions

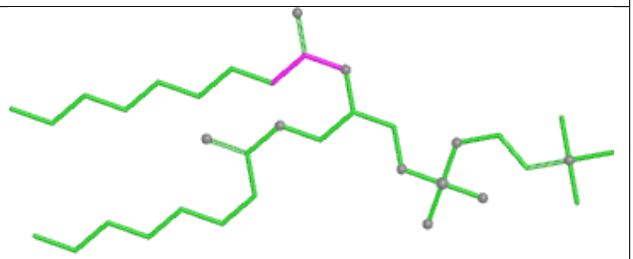


Rings

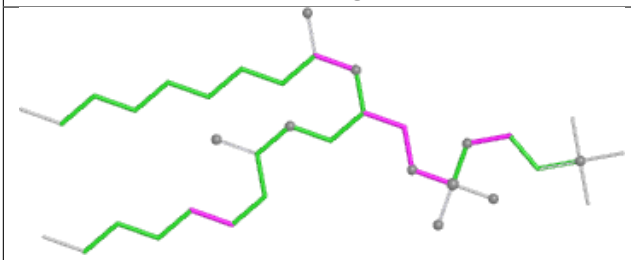
Ligand PC1 1M 502



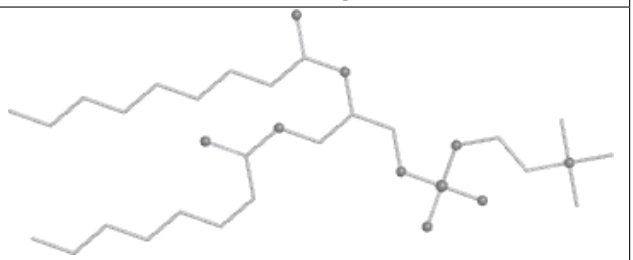
Bond lengths



Bond angles

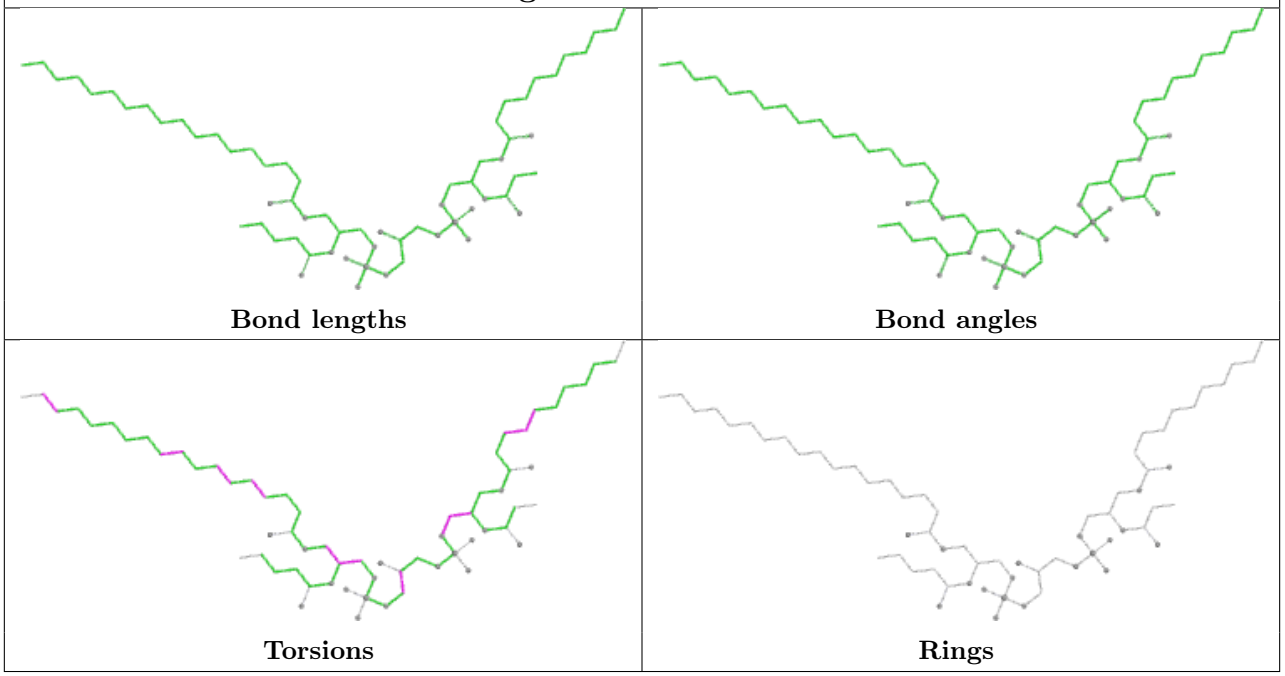


Torsions

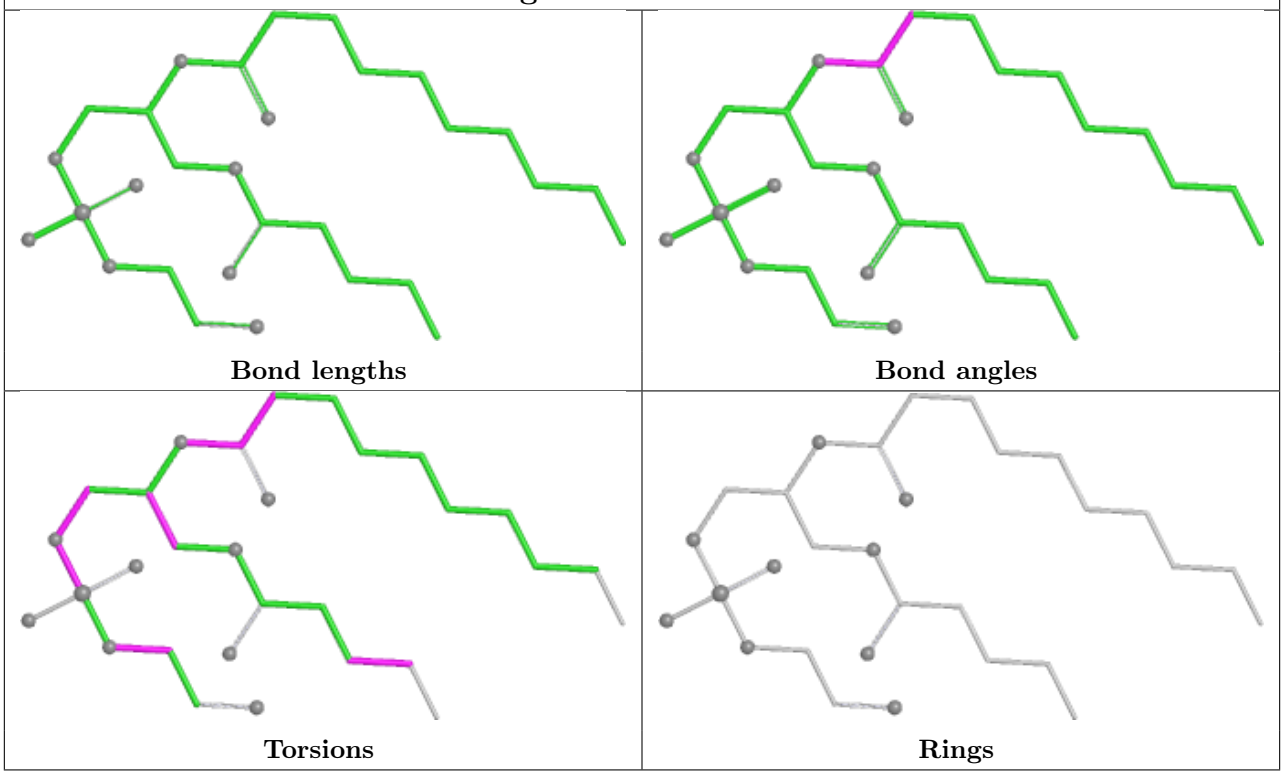


Rings

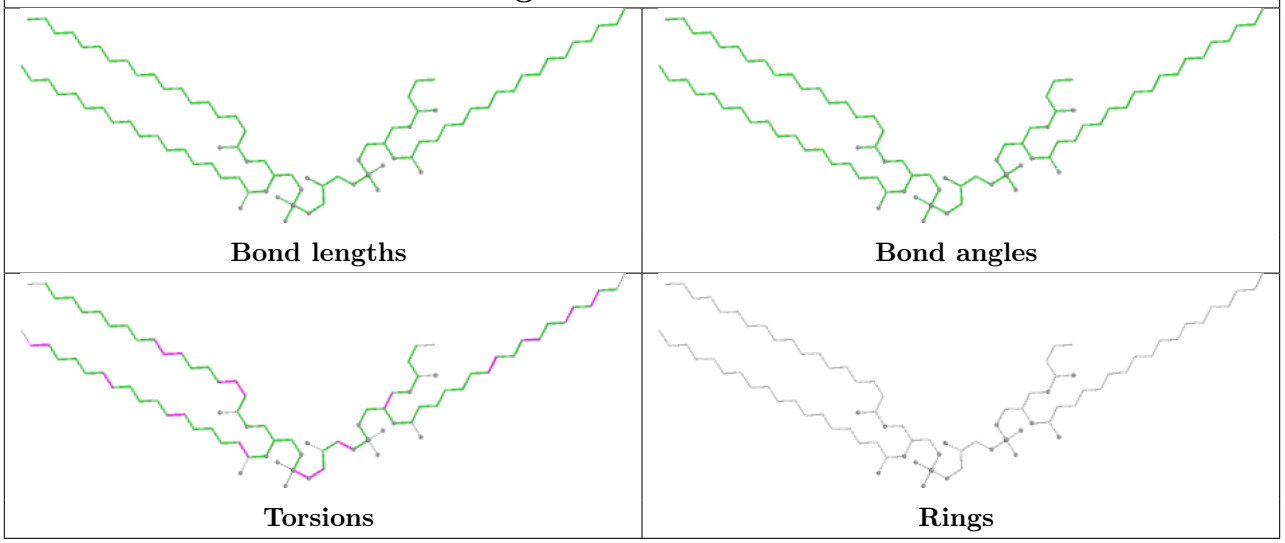
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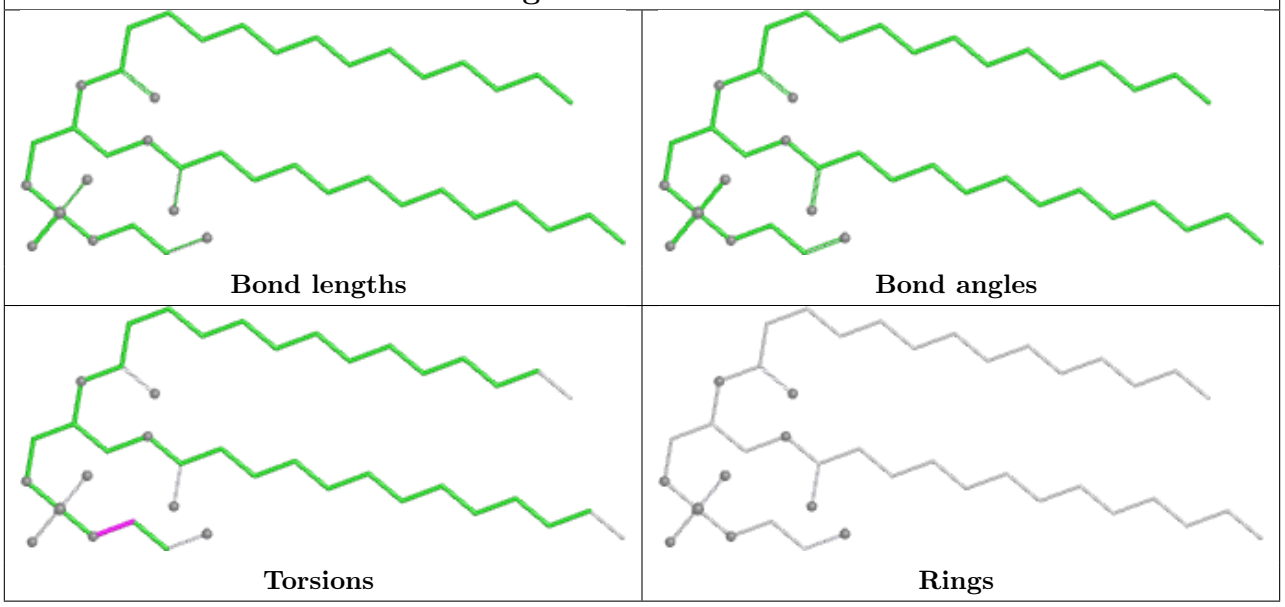
Ligand 3PE 1Y 803



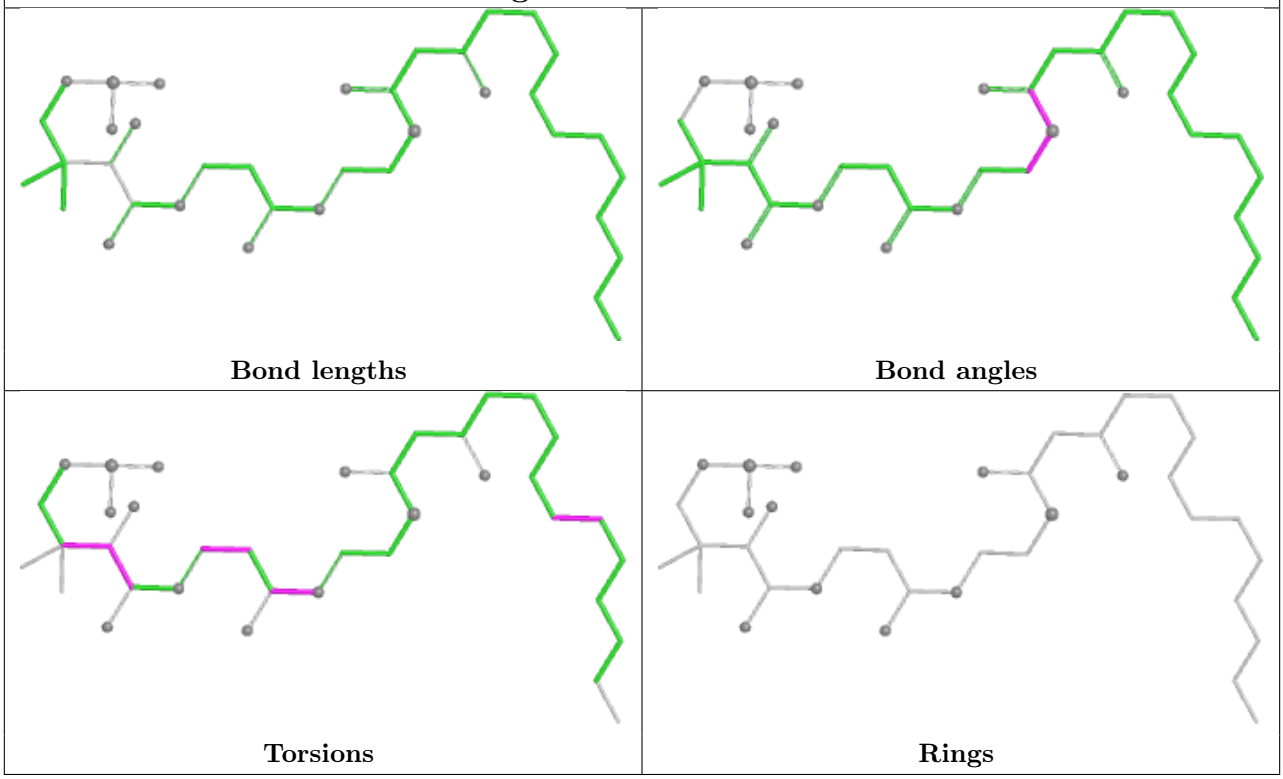
Ligand CDL 1X 201



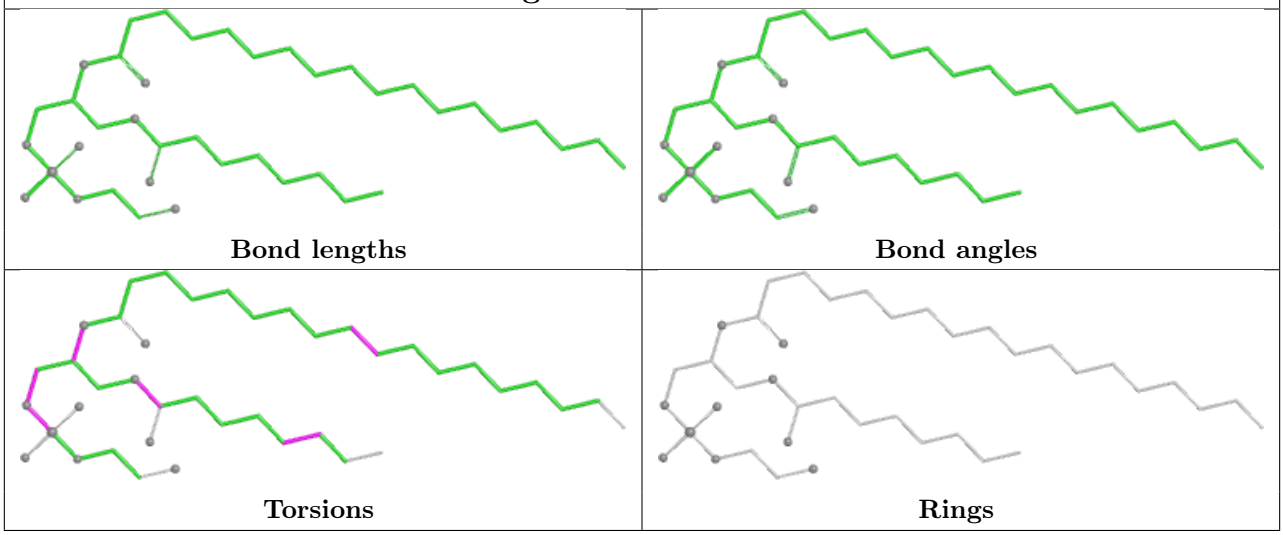
Ligand 3PE 1L 704



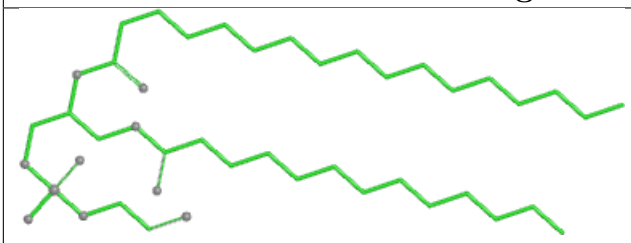
Ligand EHZ 1W 201



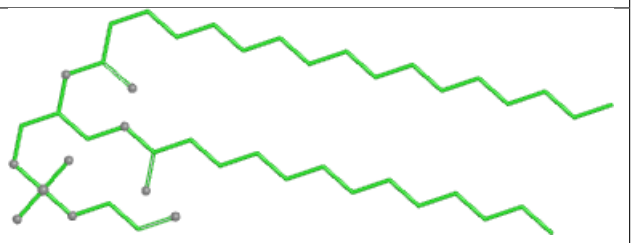
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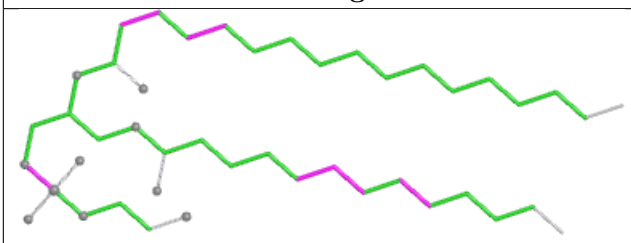
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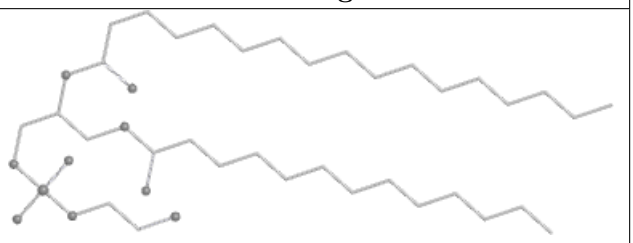
Bond lengths



Bond angles

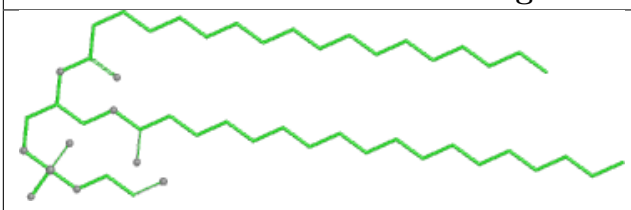


Torsions

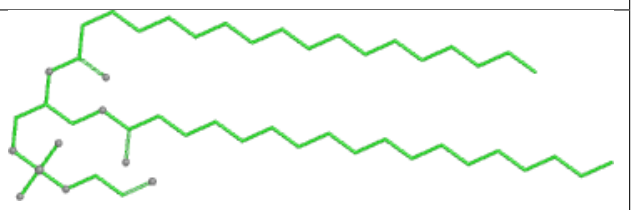


Rings

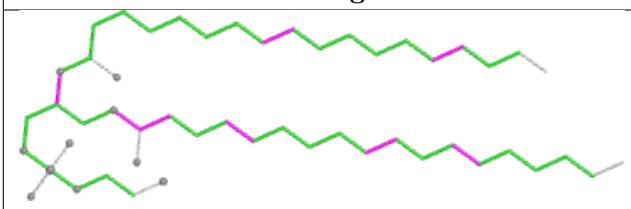
Ligand 3PE 1M 503



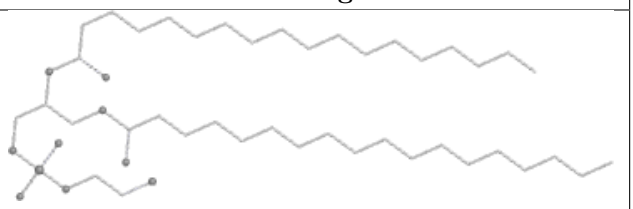
Bond lengths



Bond angles

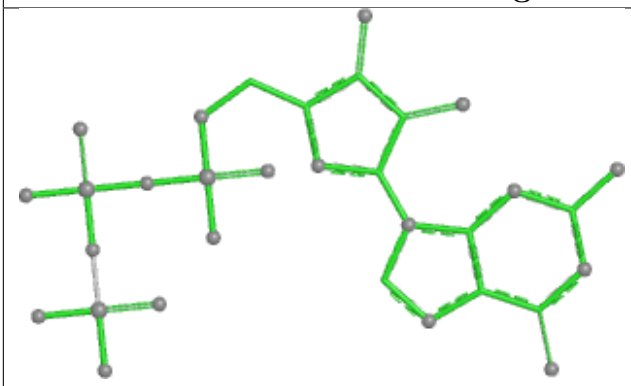


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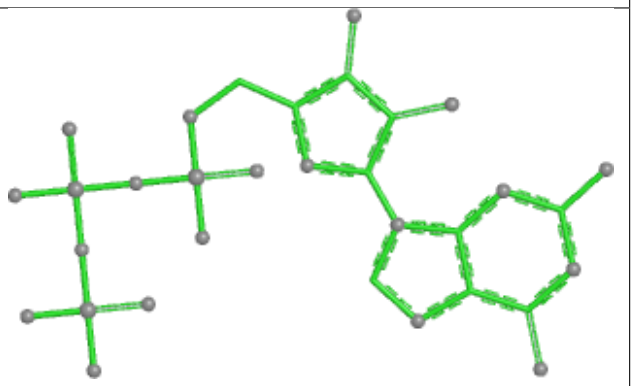


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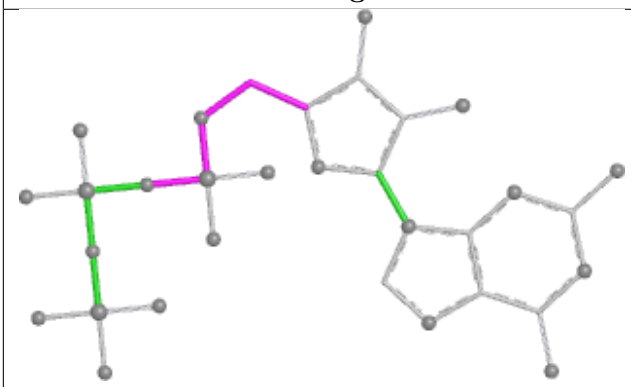
Ligand GTP 1O 401



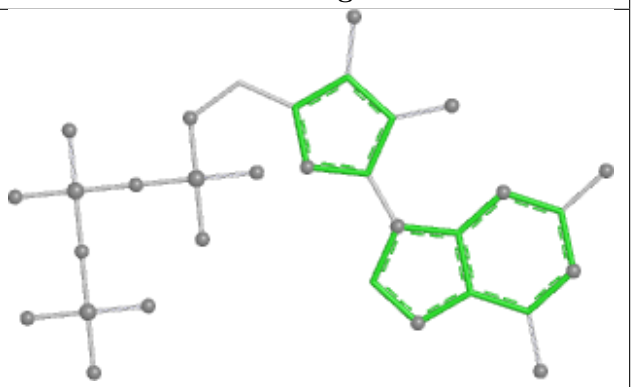
Bond lengths



Bond angles

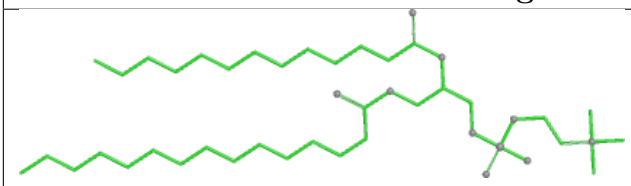


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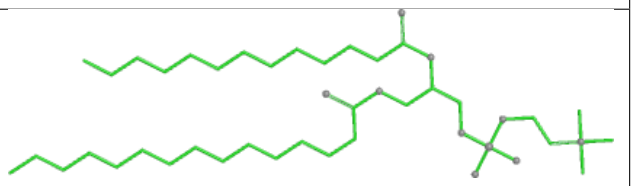


Rings

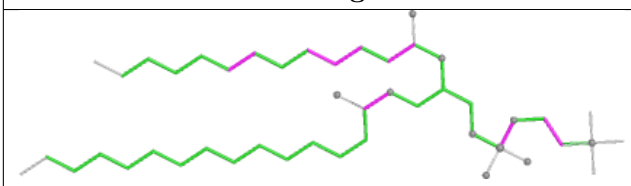
Ligand PC1 1m 201



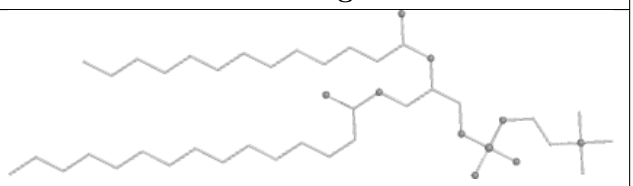
Bond lengths



Bond angles

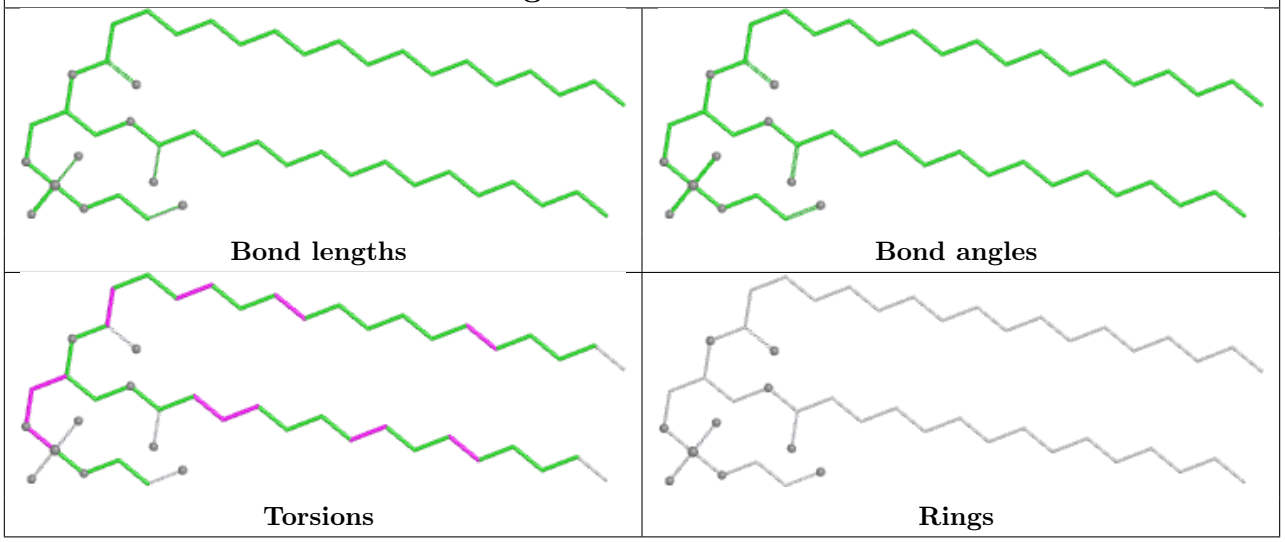


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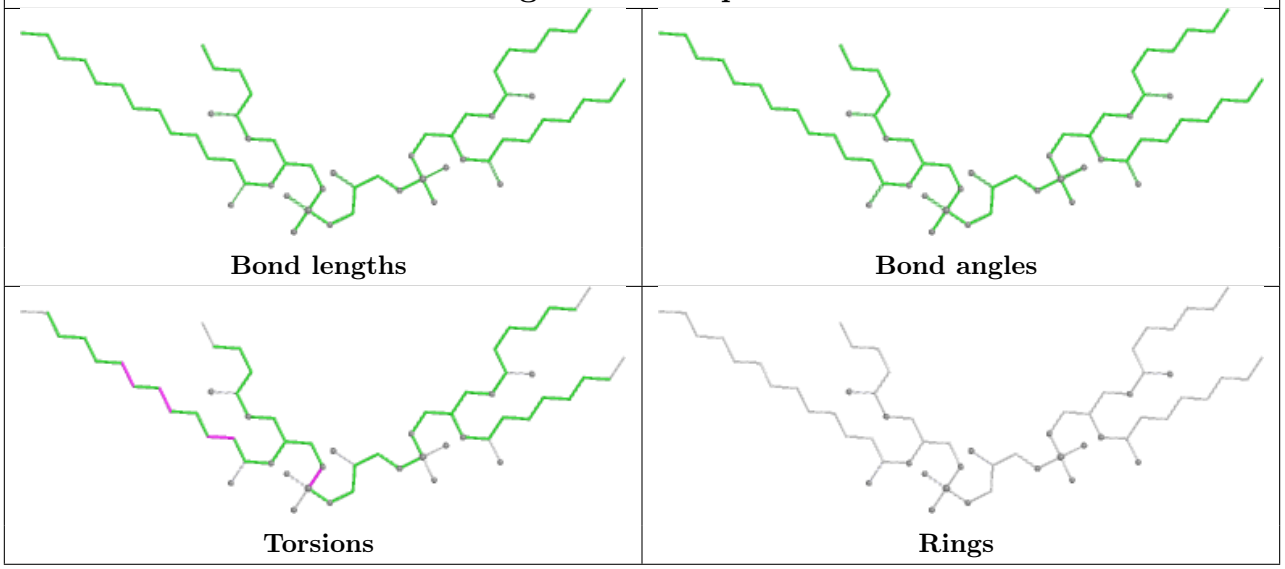


Rings

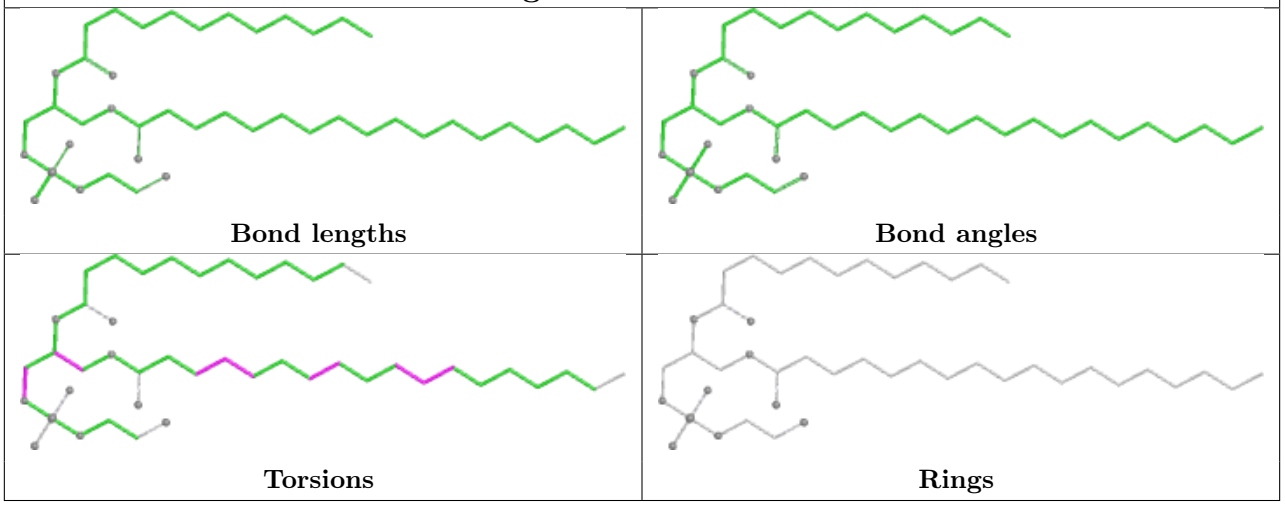
Ligand 3PE 1d 201



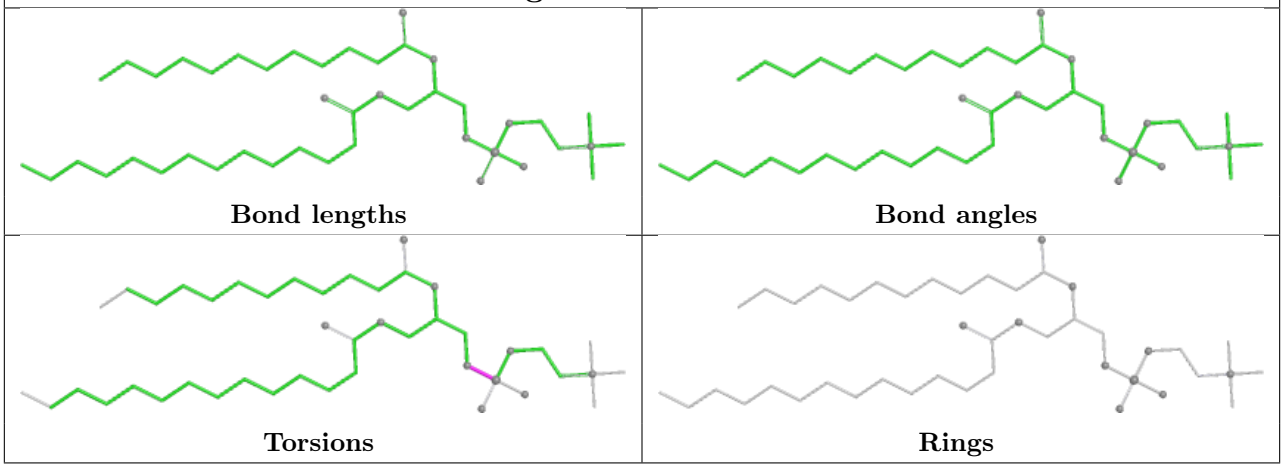
Ligand CDL 1q 203



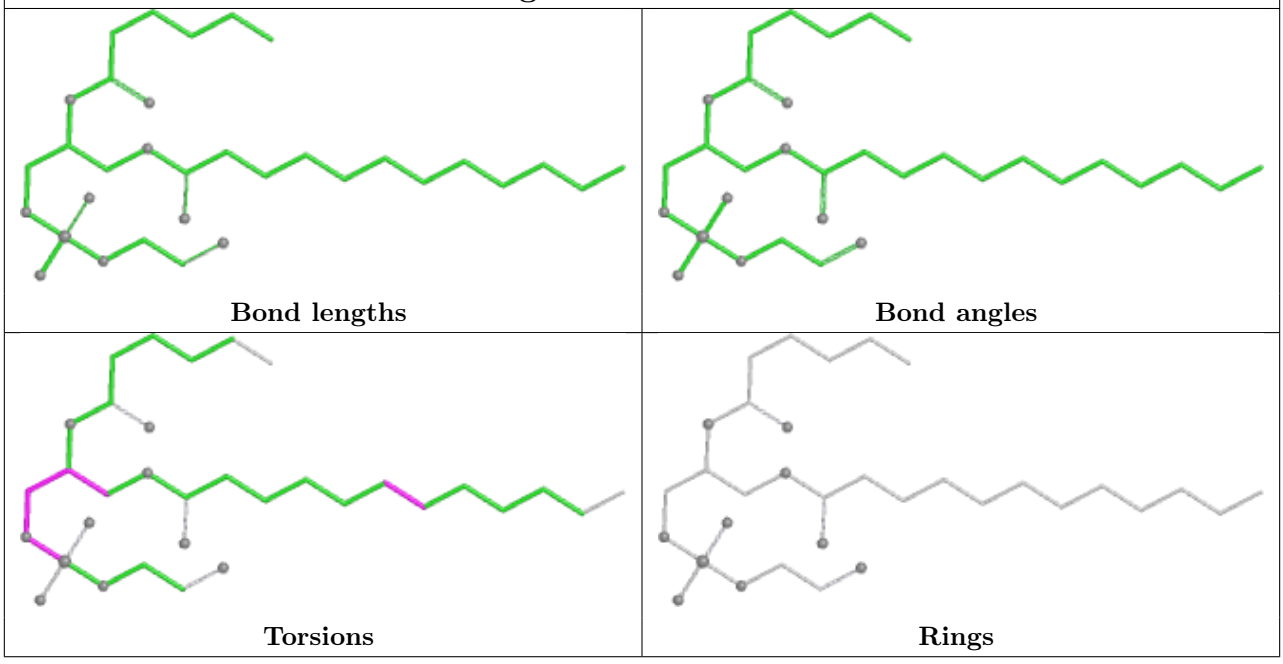
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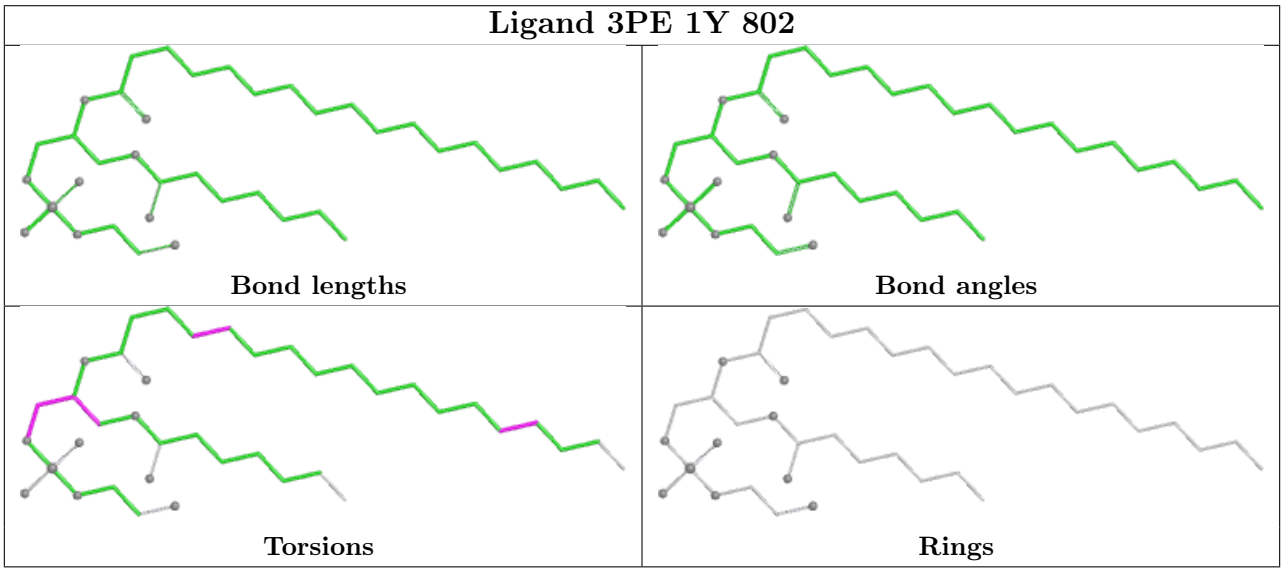
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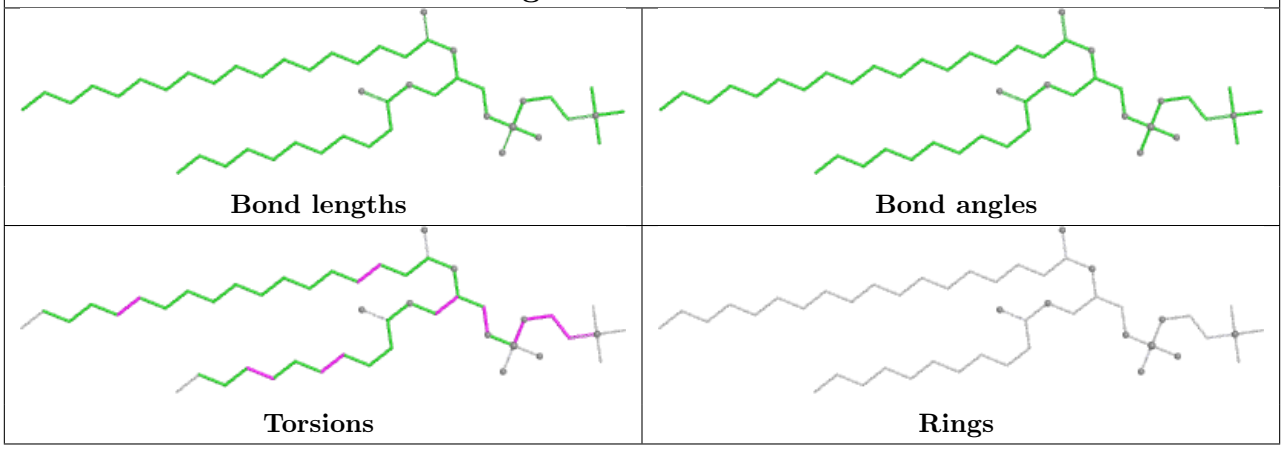
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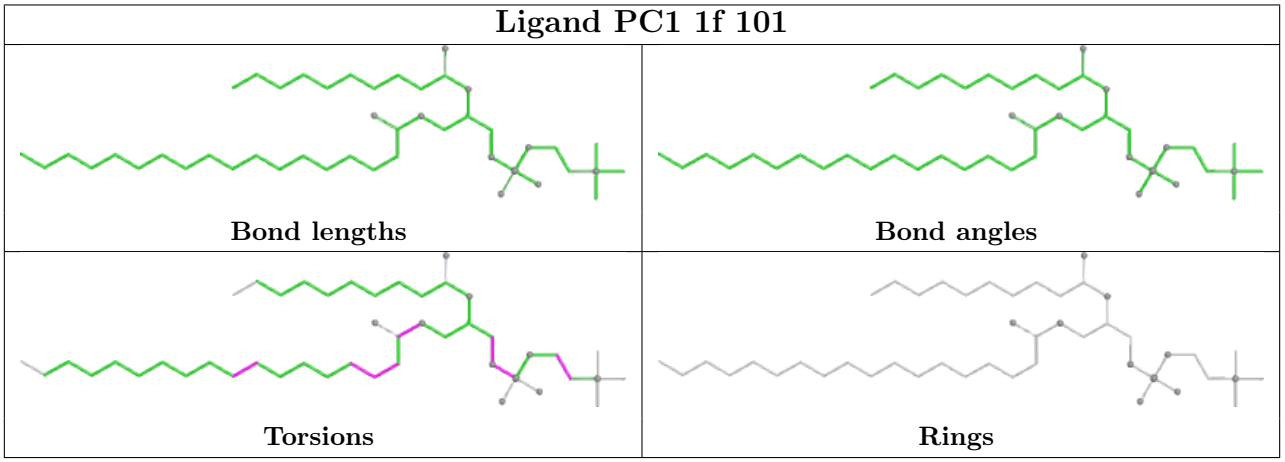
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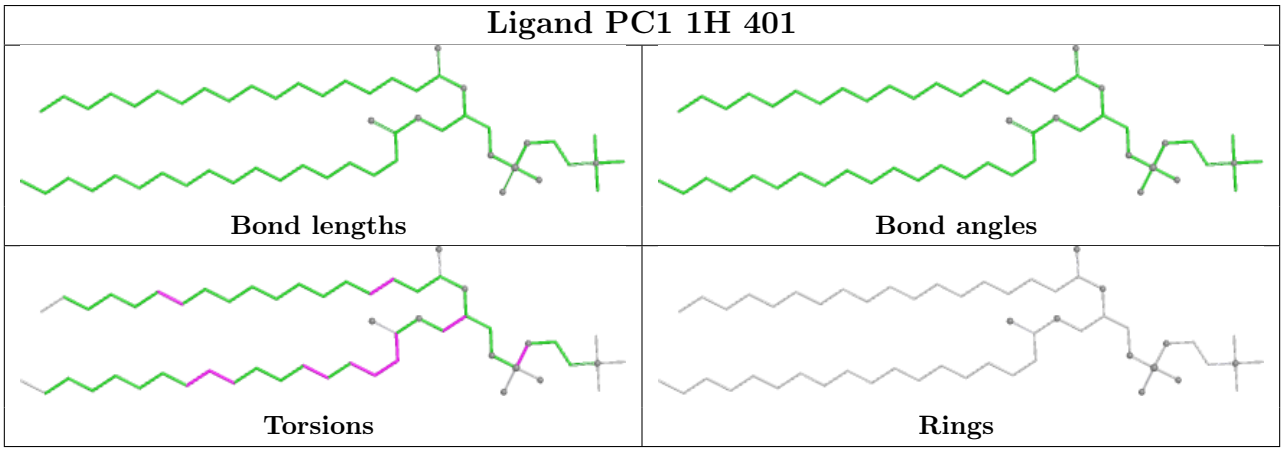
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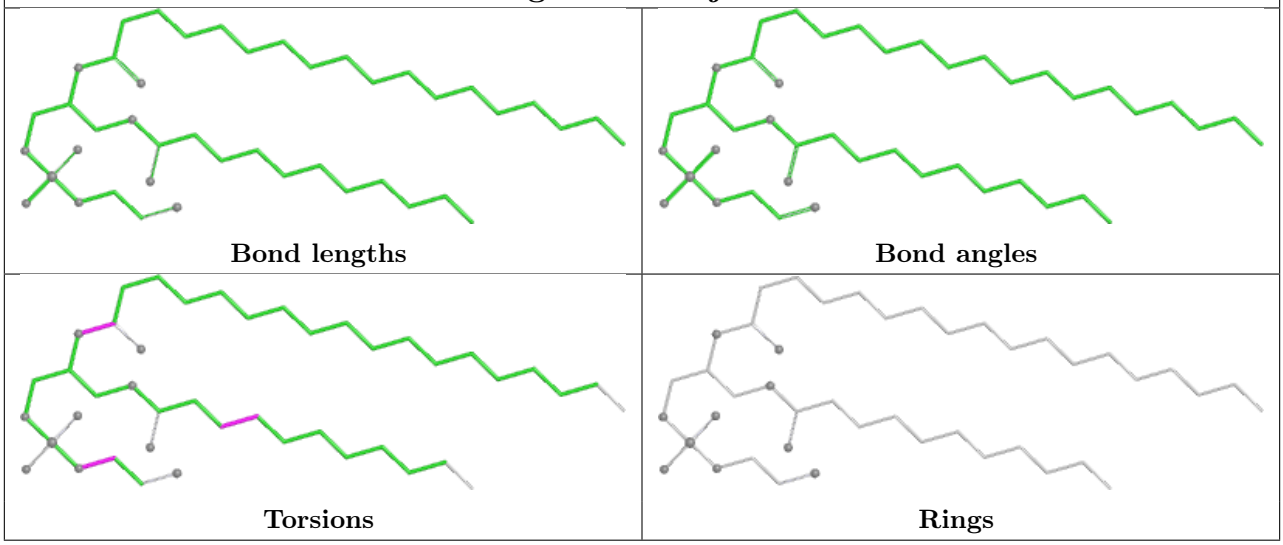
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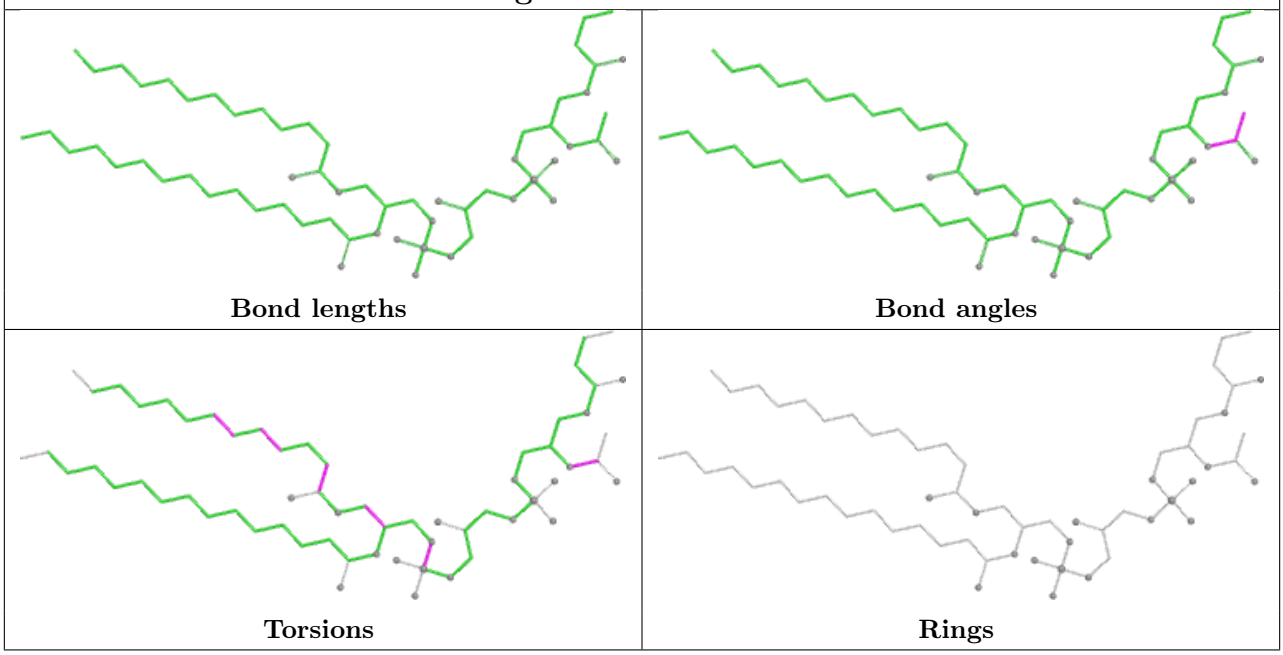
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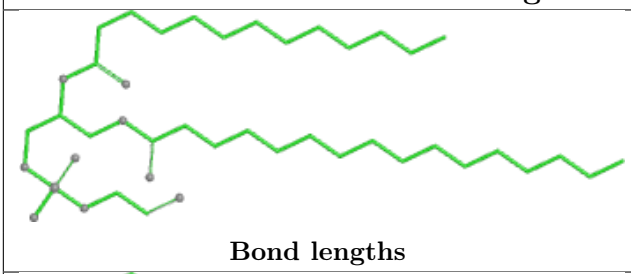
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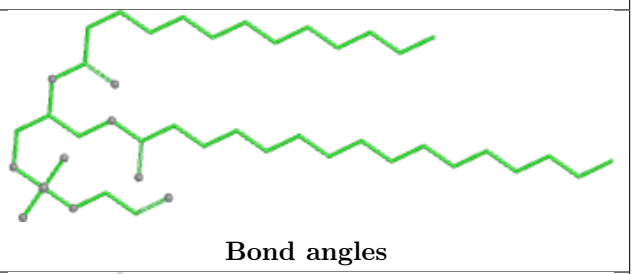
Ligand CDL 1N 902



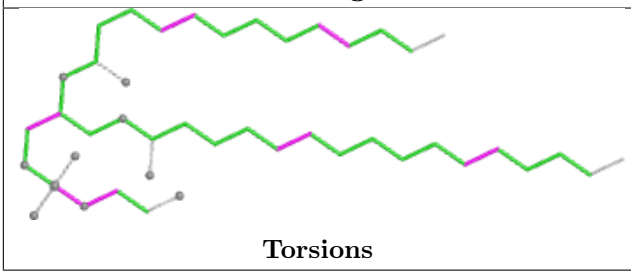
Ligand 3PE 1J 201



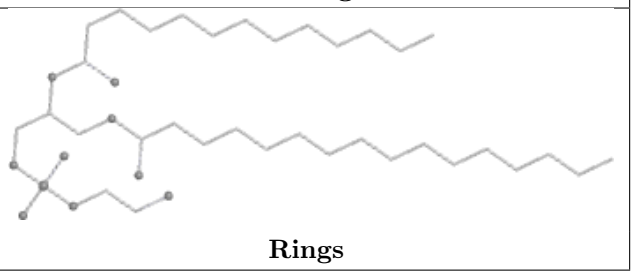
Bond lengths



Bond angles

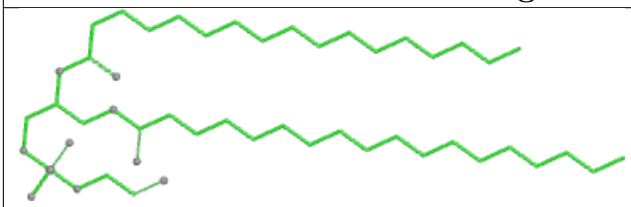


Torsions

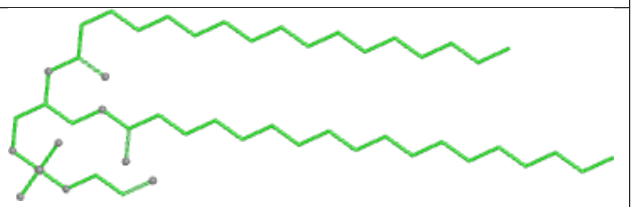


Rings

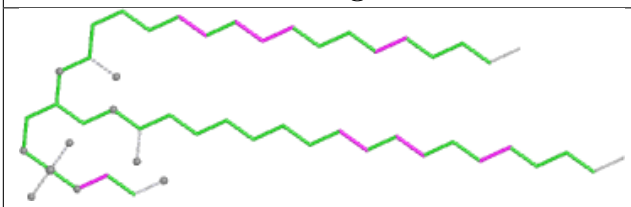
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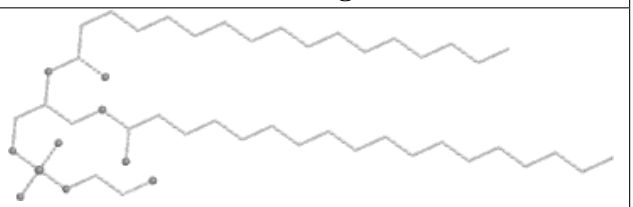
Bond lengths



Bond angles

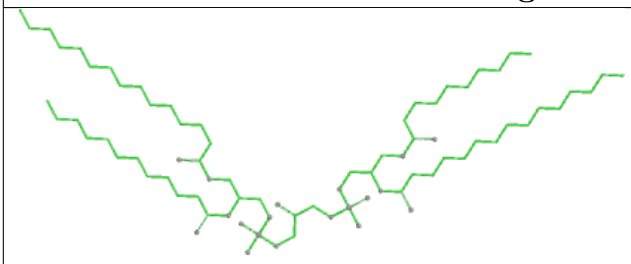


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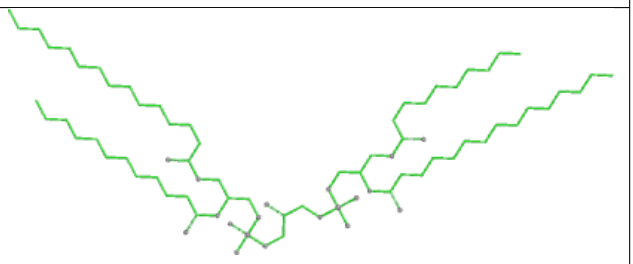


Rings

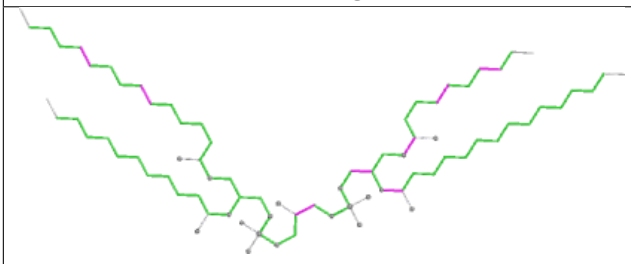
Ligand CDL 1h 201



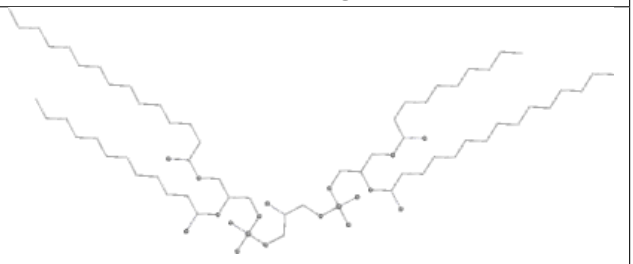
Bond lengths



Bond angles

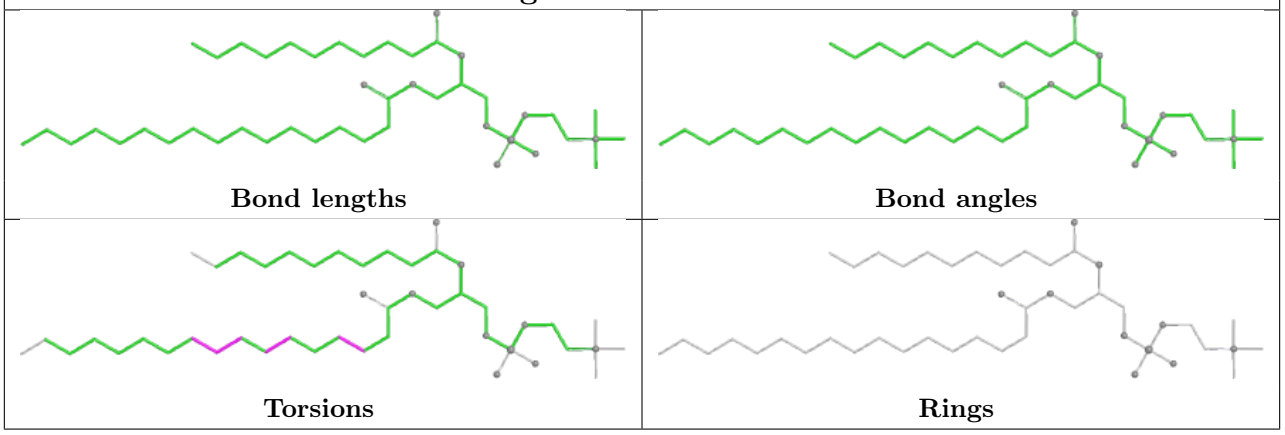


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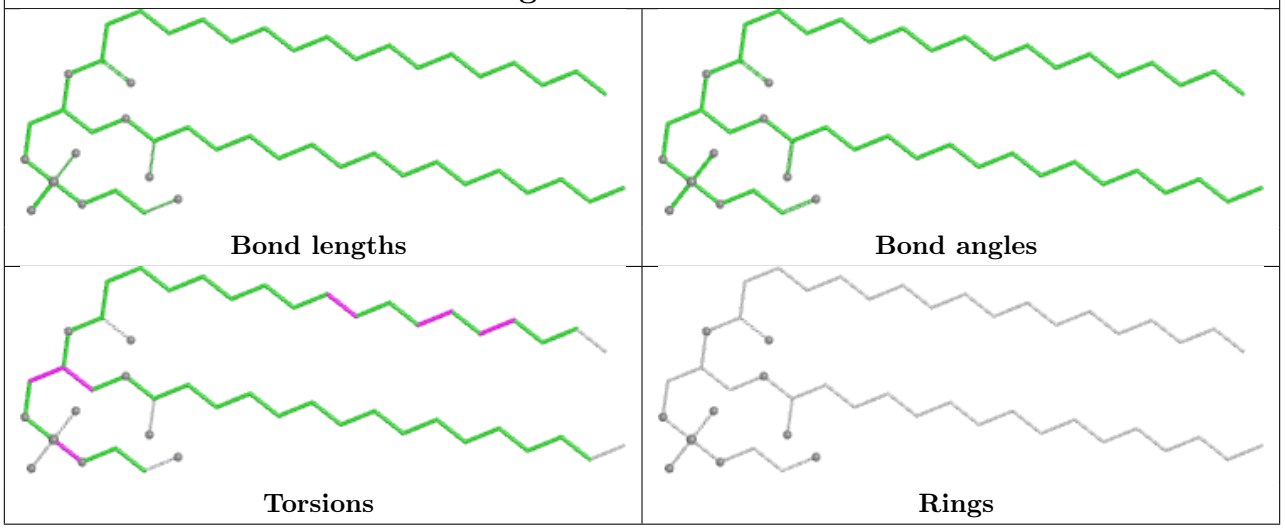


Rings

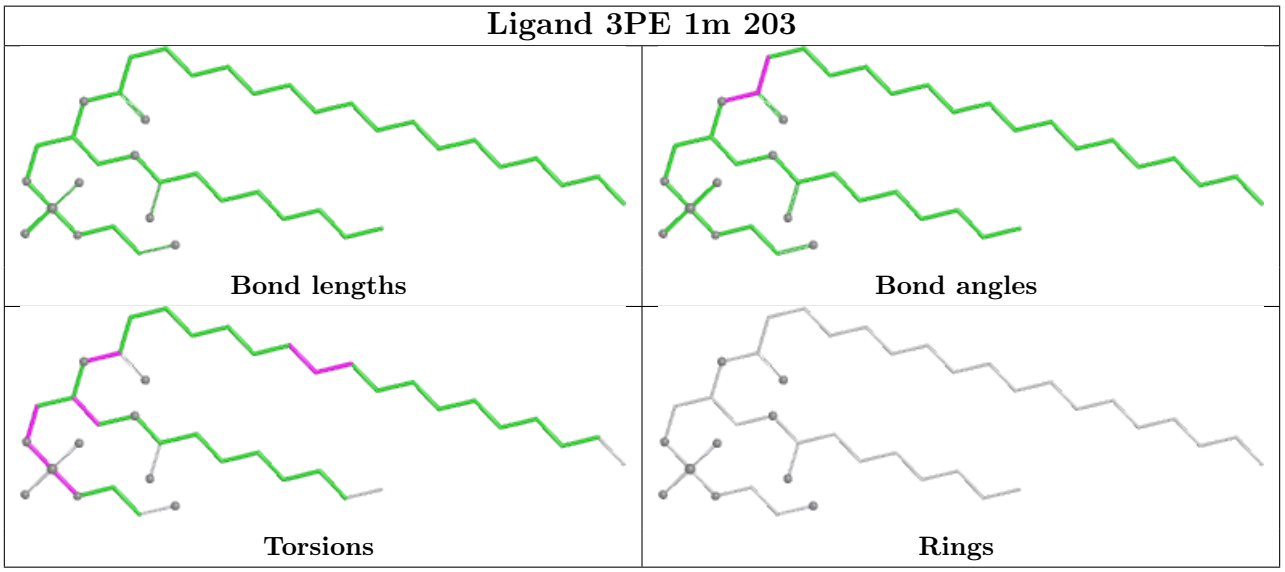
Ligand PC1 1P 402



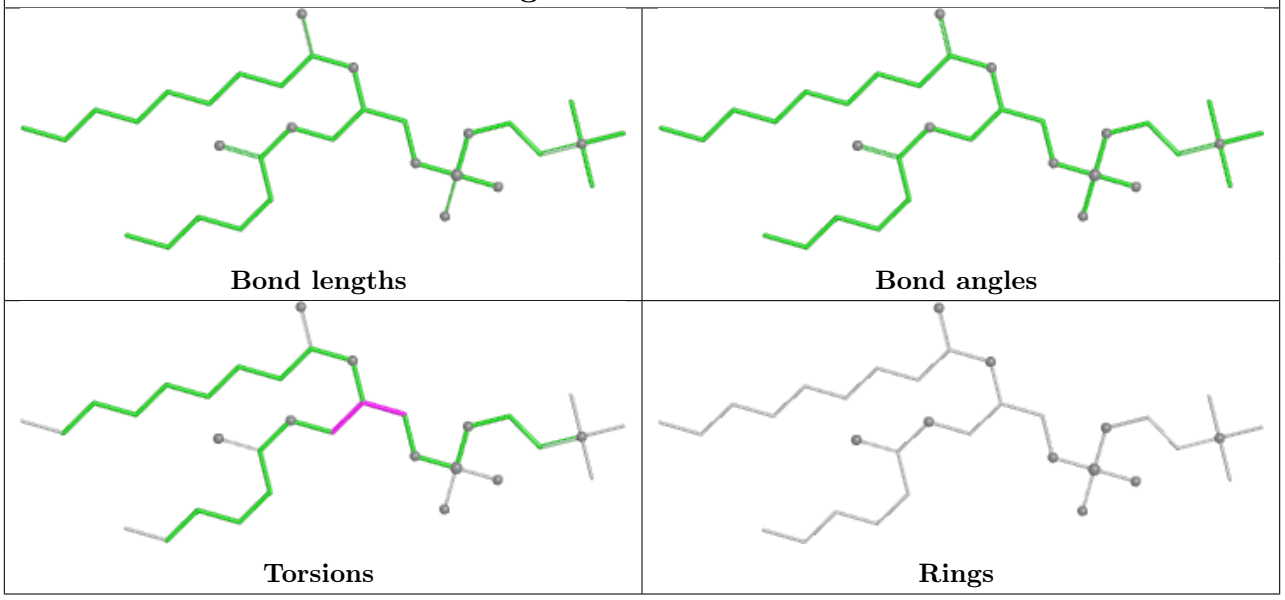
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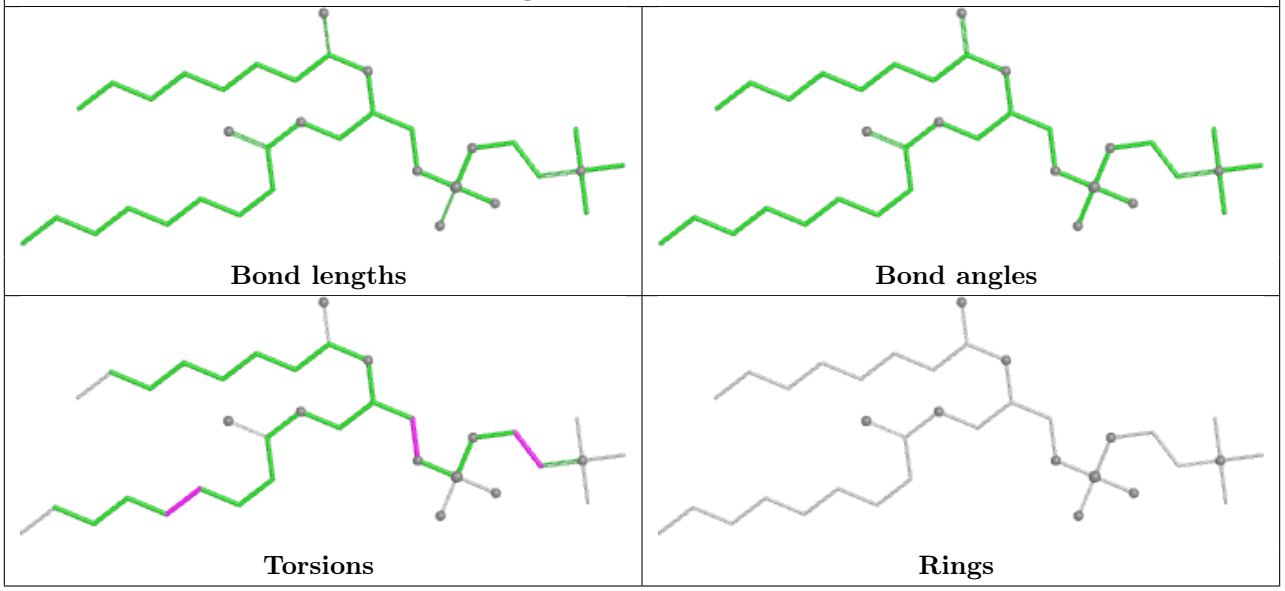
Ligand 3PE 1m 203



Ligand PC1 1P 401



Ligand PC1 1A 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

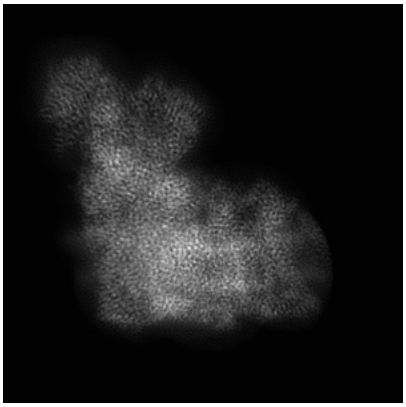
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42143. These allow visual inspection of the internal detail of the map and identification of artifacts.

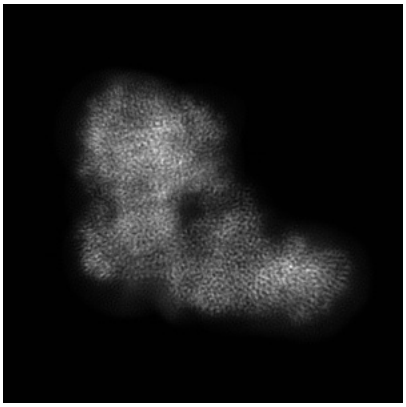
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

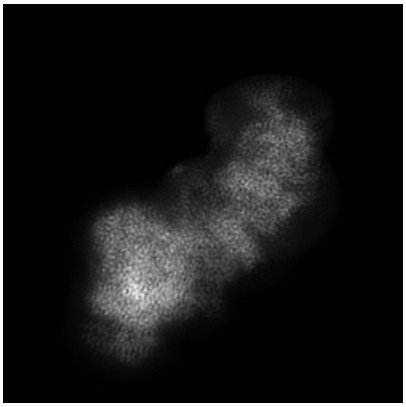
6.1.1 Primary map



X



Y

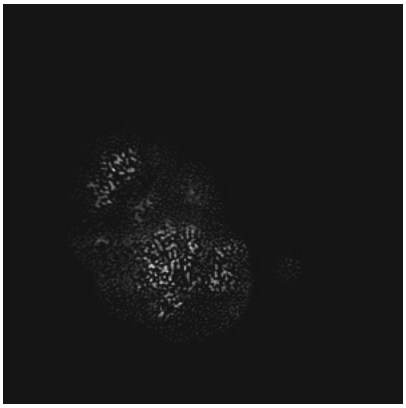


Z

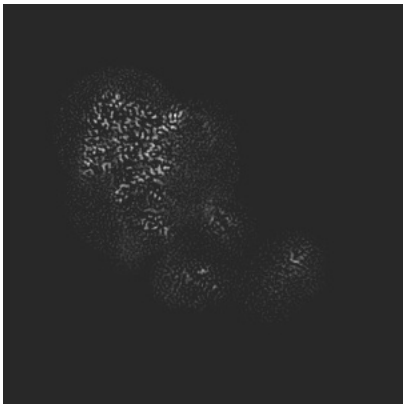
The images above show the map projected in three orthogonal directions.

6.2 Central slices

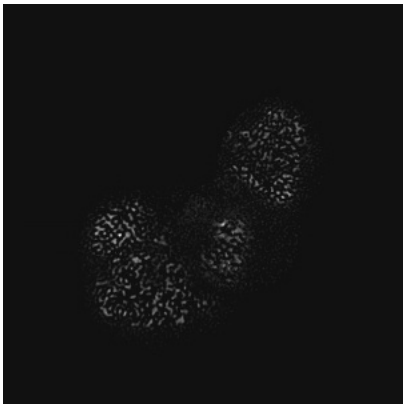
6.2.1 Primary map



X Index: 360



Y Index: 360



Z Index: 360

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 239



Y Index: 196

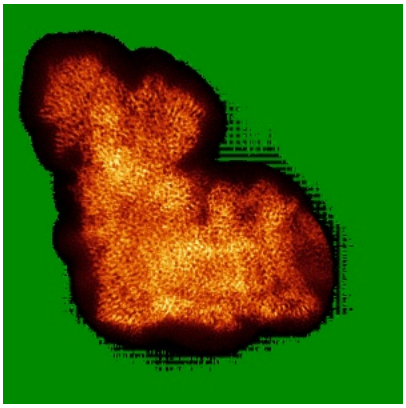


Z Index: 275

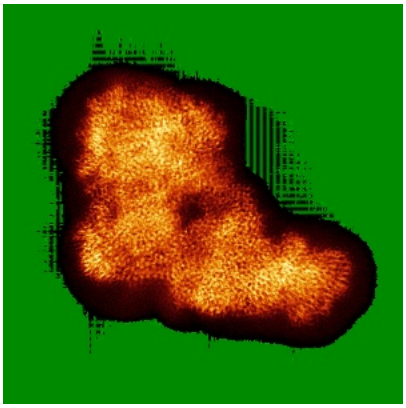
The images above show the largest variance slices of the map in three orthogonal directions.

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

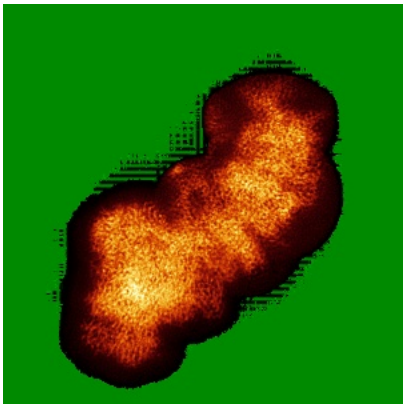
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

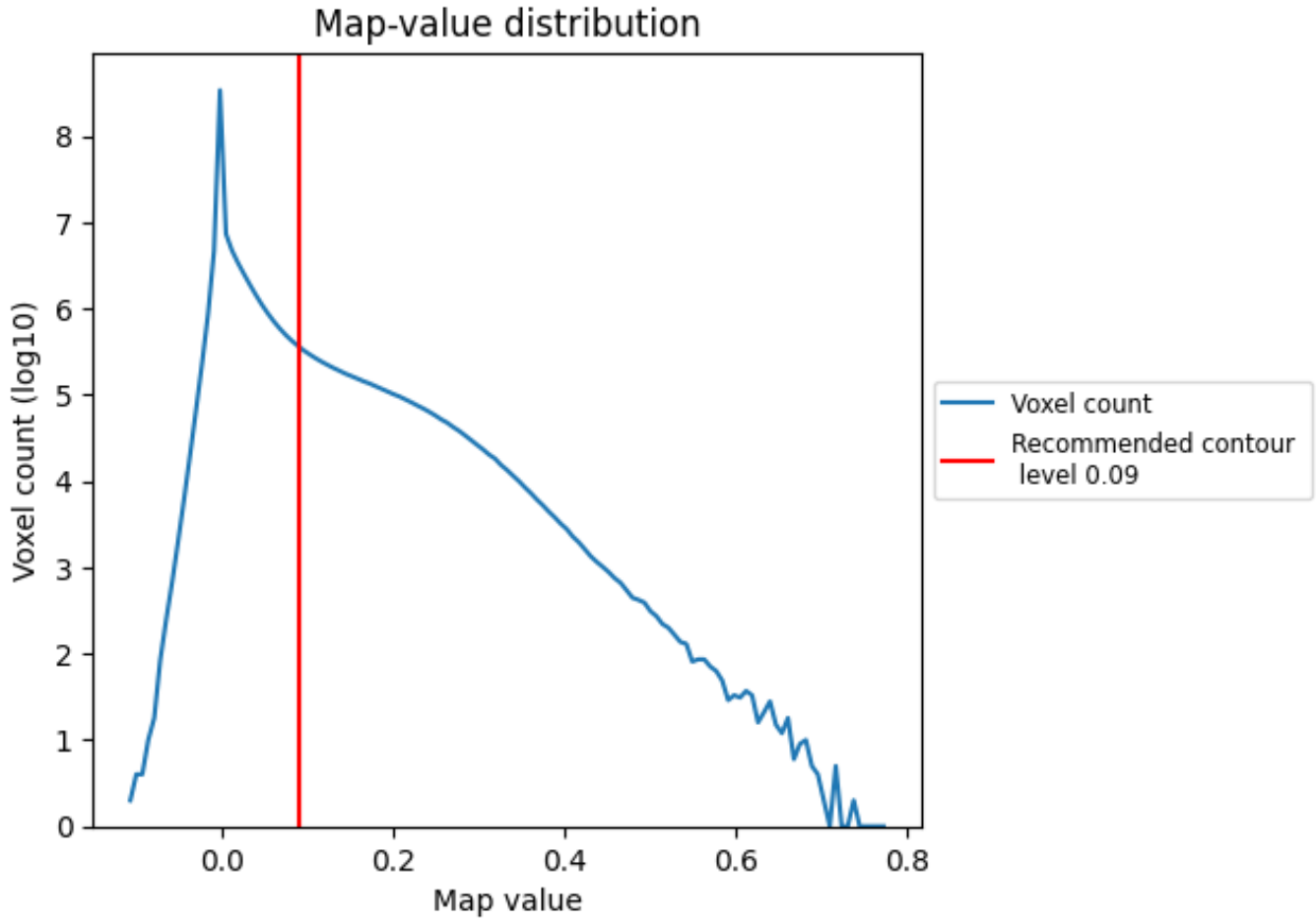
6.6 Mask visualisation (i)

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

7 Map analysis

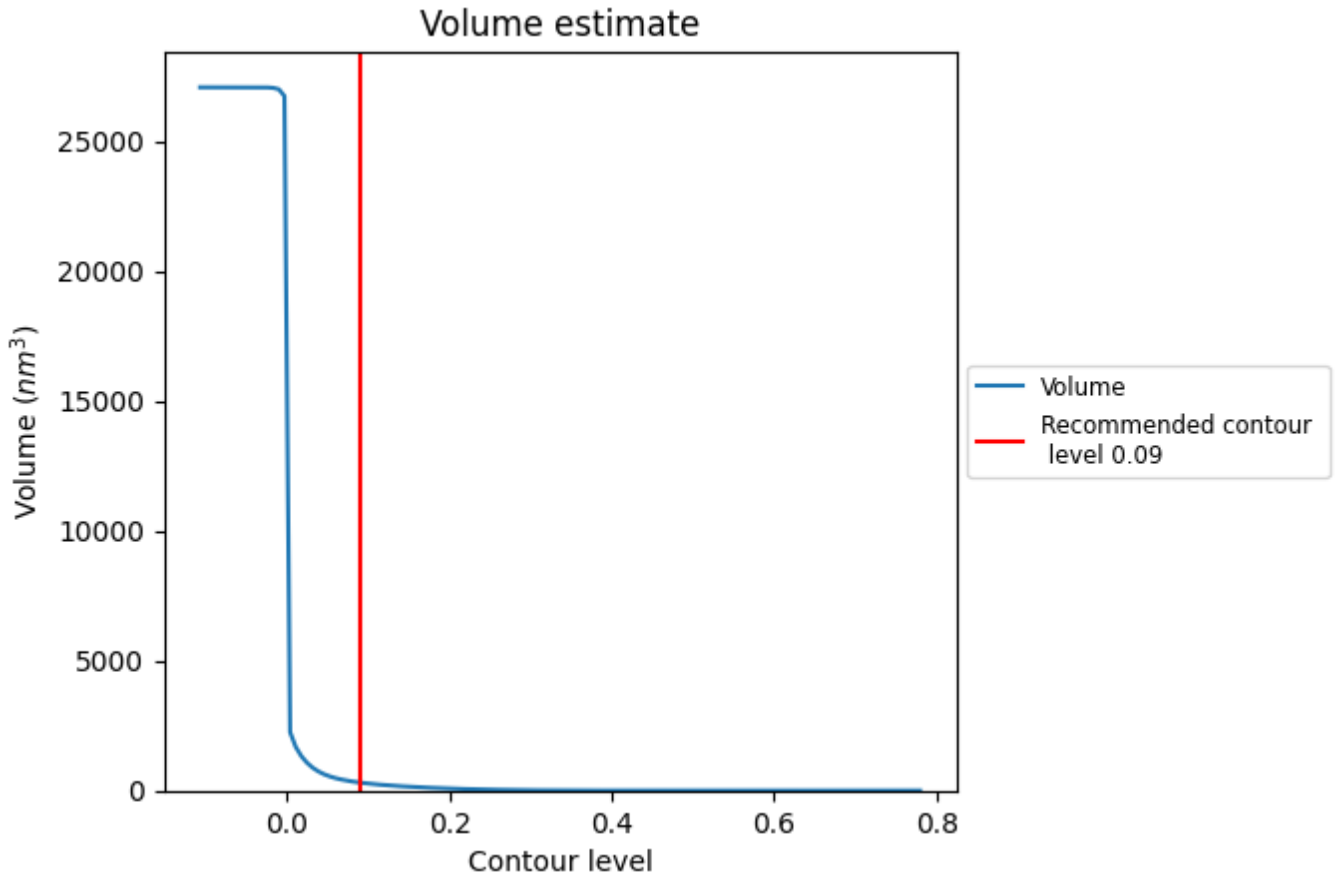
This section contains the results of statistical analysis of the map.

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.

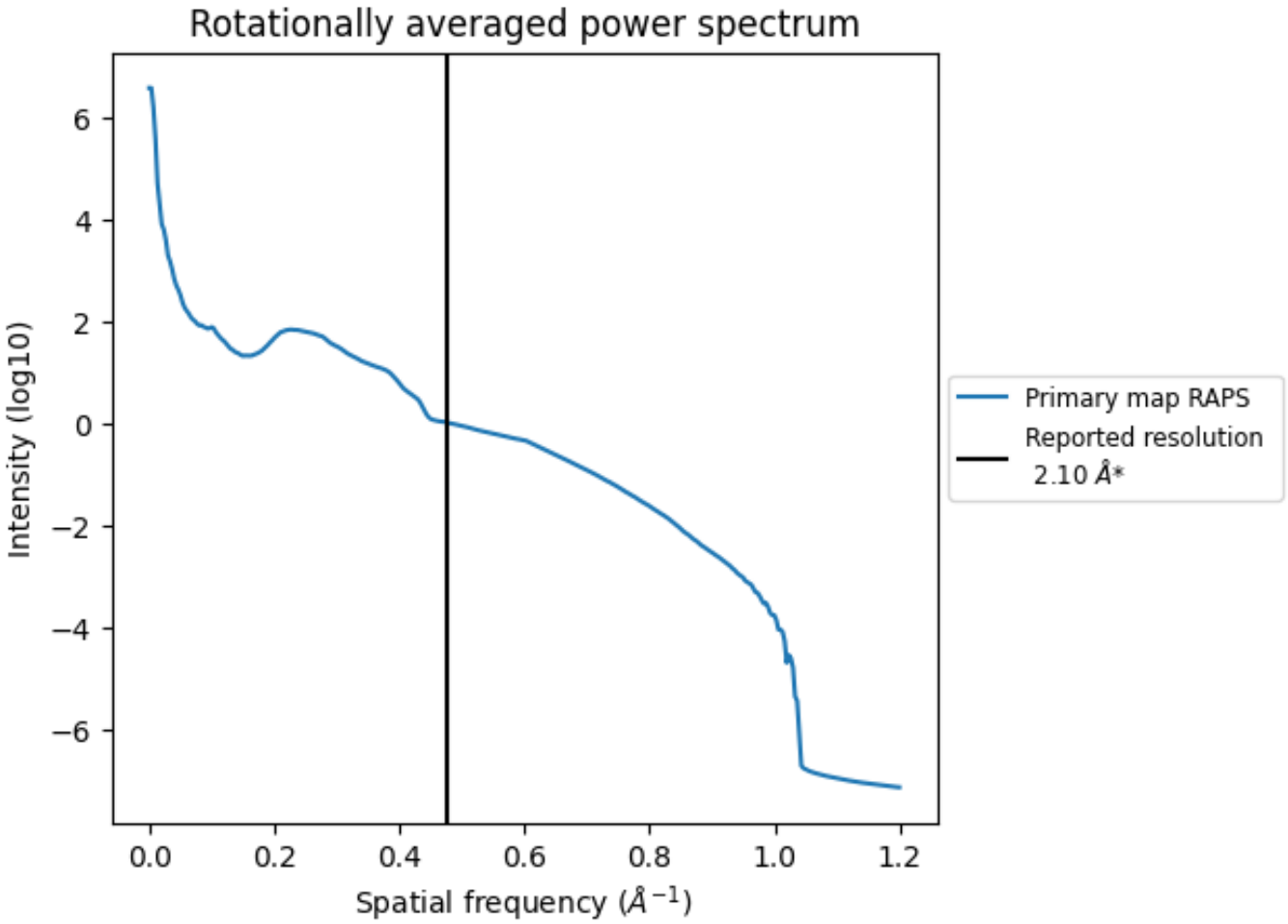
7.2 Volume estimate (i)



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 277 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

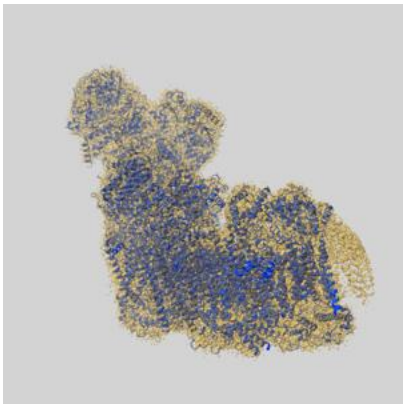
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

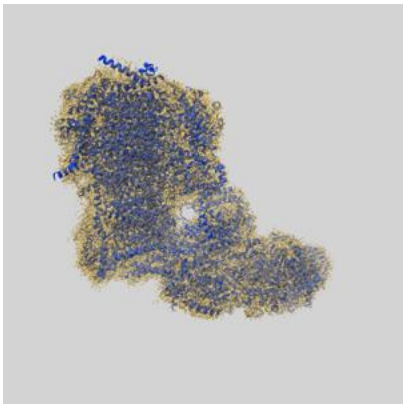
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42143 and PDB model 8UD1. Per-residue inclusion information can be found in section 3 on page 22.

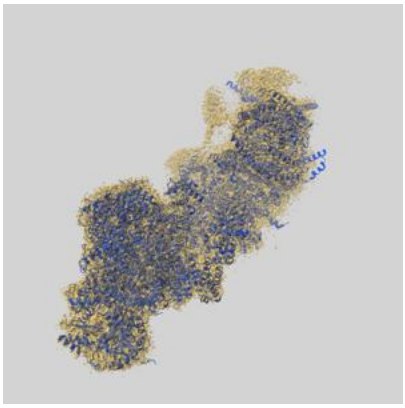
9.1 Map-model overlay



X



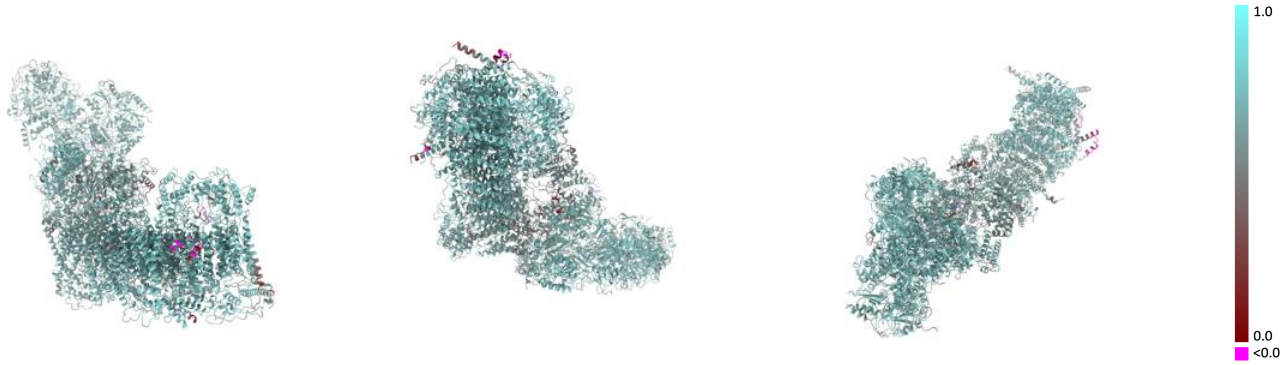
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

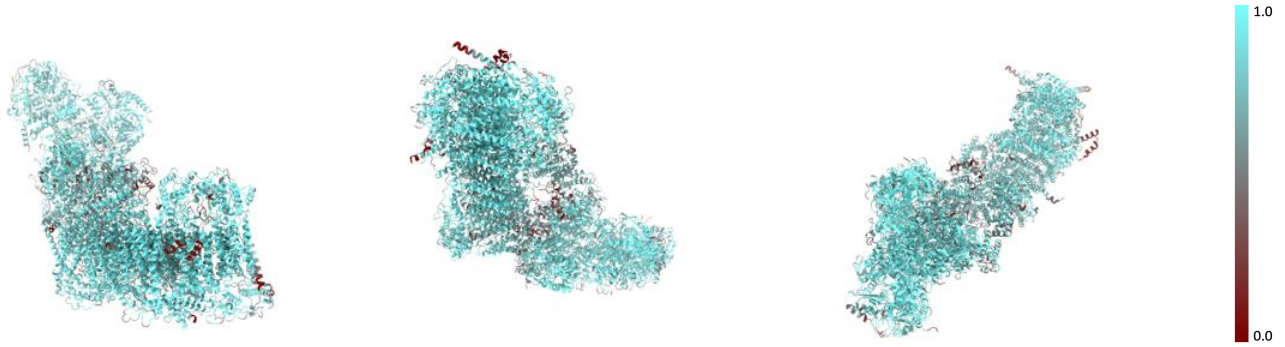
9.2 Q-score mapped to coordinate model



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.

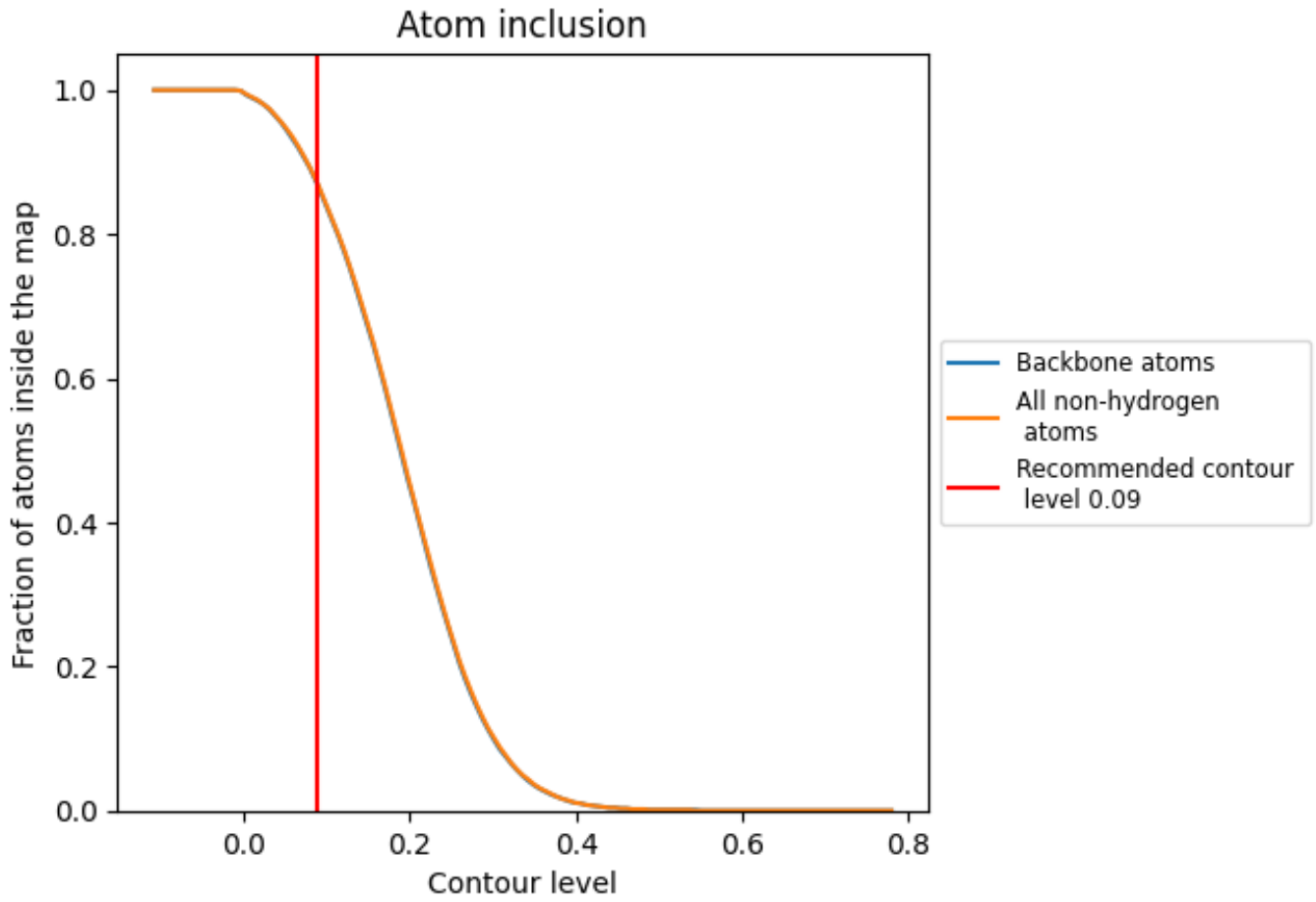
9.3 Atom inclusion mapped to coordinate model



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.6680
1A	0.6800	0.5560
1B	0.9100	0.6920
1C	0.9390	0.7190
1D	0.9040	0.6960
1E	0.8070	0.6470
1F	0.8770	0.6610
1G	0.9120	0.6940
1H	0.8900	0.6440
1I	0.9440	0.7130
1J	0.7800	0.5940
1K	0.9810	0.6960
1L	0.9420	0.7040
1M	0.9680	0.7160
1N	0.9560	0.7100
1O	0.7960	0.6070
1P	0.8300	0.6610
1Q	0.8620	0.6700
1R	0.8550	0.6740
1S	0.8900	0.6630
1T	0.4110	0.4370
1U	0.8180	0.6790
1V	0.7500	0.6390
1W	0.8620	0.6740
1X	0.8840	0.6560
1Y	0.7820	0.6530
1Z	0.8900	0.6660
1a	0.9490	0.6700
1b	0.8150	0.6250
1c	0.7540	0.6260
1d	0.8920	0.6680
1e	0.9350	0.6860
1f	0.7600	0.6210
1g	0.8670	0.6700
1h	0.8950	0.6980



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Continued from previous page...

Chain	Atom inclusion	Q-score
1i	0.6200	0.5180
1j	0.7660	0.6100
1k	0.7470	0.6050
1l	0.8930	0.6980
1m	0.8570	0.6690
1n	0.8850	0.6960
1o	0.8210	0.6400
1p	0.8770	0.6690
1q	0.8420	0.6840
1r	0.8530	0.6840
1s	0.7440	0.6140