Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 03:18 PM EDT

PDB ID	:	8UD1
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 Full wwPDB EM Validation 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:

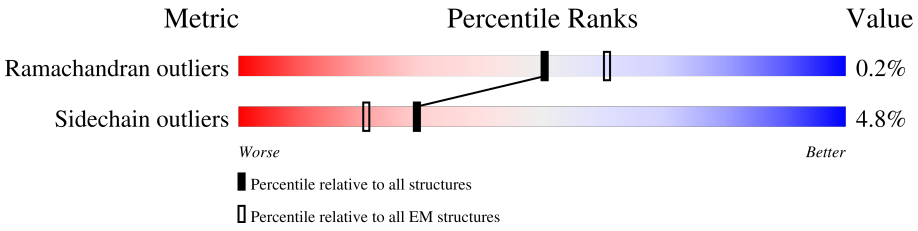
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1A	115	25% 92% 8%
2	1B	258	55% 5% 40%
3	1C	264	78% 21%
4	1D	466	5% 89% 8%
5	1E	249	8% 80% 6% 14%
6	1F	464	89% 7%
7	1G	727	92% 5%
8	1H	318	8% 96%
9	1I	239	72% 26%

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Mol	Chain	Length	Quality of chain
10	1J	175	15% 92% 7%
11	1K	98	97%
12	1L	606	96%
13	1M	459	97%
14	1N	347	96%
15	1O	357	9% 85% 10%
16	1P	377	6% 87% 9%
17	1Q	175	7% 69% 5% 26%
18	1R	123	5% 72% 6% 22%
19	1S	99	5% 86% 12%
20	1T	156	31% 51% 46%
20	1U	156	52% 45%
21	1V	116	15% 94% 5%
22	1W	128	8% 89% 10%
23	1X	172	94% 6%
24	1Y	141	5% 93% 6%
25	1Z	144	94%
26	1a	70	97%
27	1b	84	11% 92% 7%
28	1c	76	8% 64% 36%
29	1d	122	95%
30	1e	106	89% 5% 7%
31	1f	135	7% 39% 58%
32	1g	154	5% 61% 35%
33	1h	189	70% 27%

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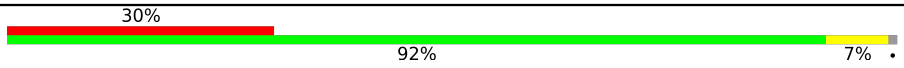
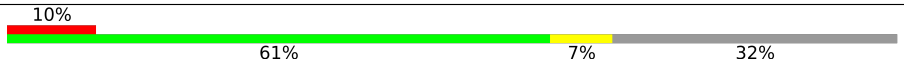
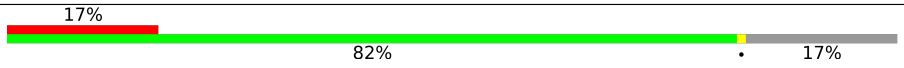
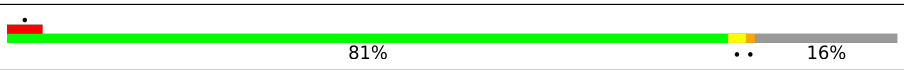
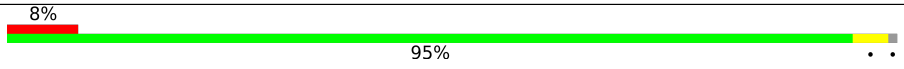
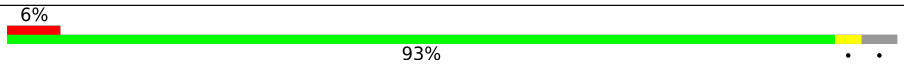
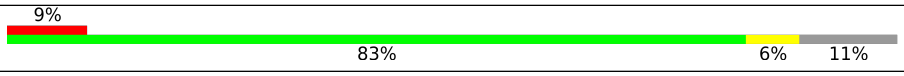
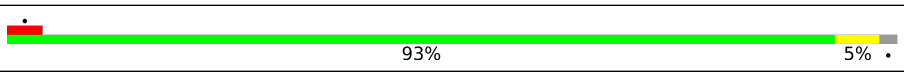
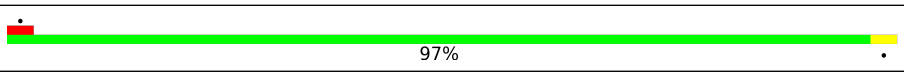
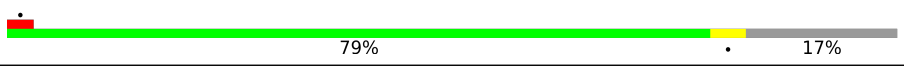
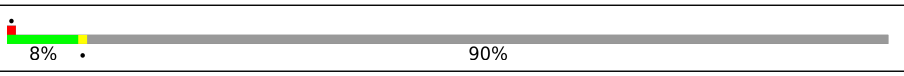
Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 71989 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- 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 sub-

unit 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	0	0
			1168	752	202	205	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	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- 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	0	0
			816	519	151	140	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		

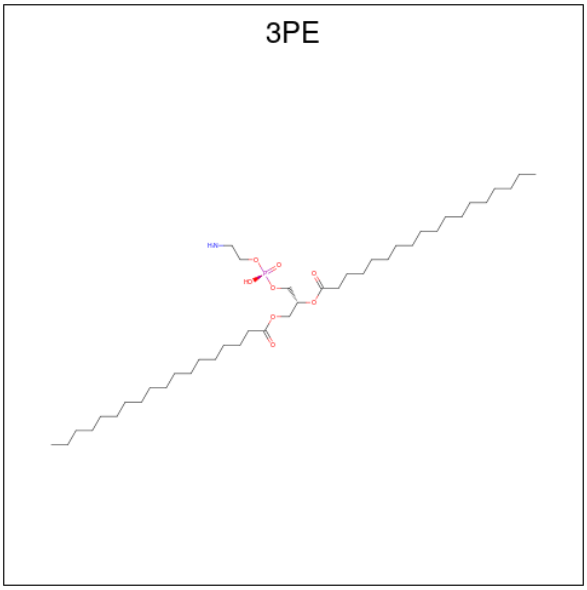
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	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-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	1N	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	1N	1	Total	C	N	O	P	0
			33	23	1	8	1	

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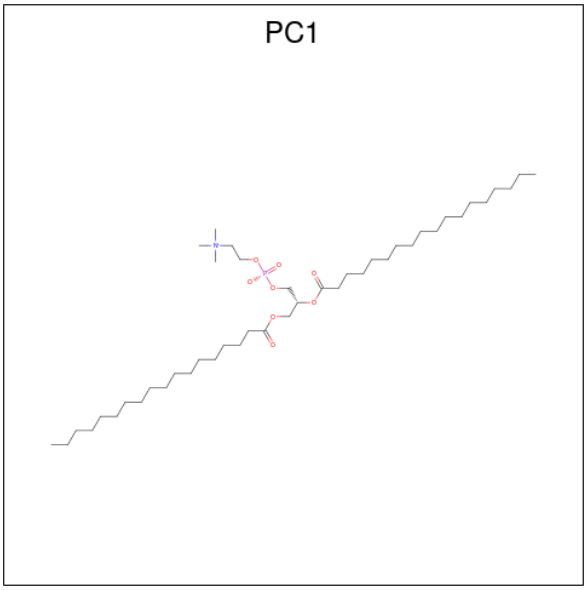
Mol	Chain	Residues	Atoms					AltConf
45	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	1j	1	Total	C	N	O	P	0
			44	34	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf
46	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	

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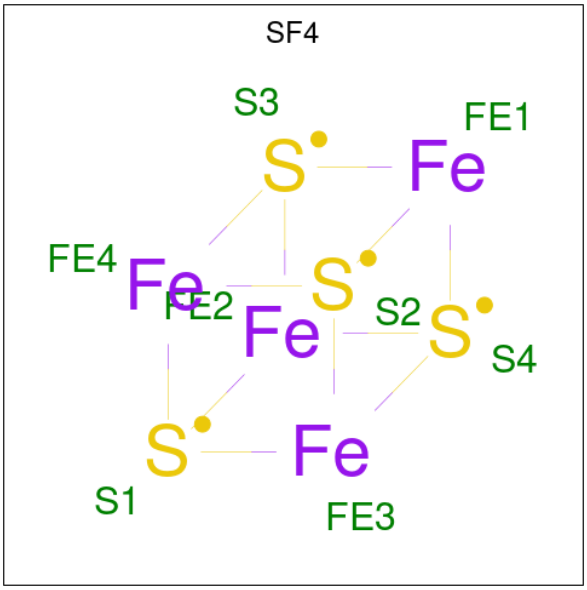
Mol	Chain	Residues	Atoms					AltConf
46	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
47	1B	1	Total	Fe	S	0
			8	4	4	
47	1F	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	

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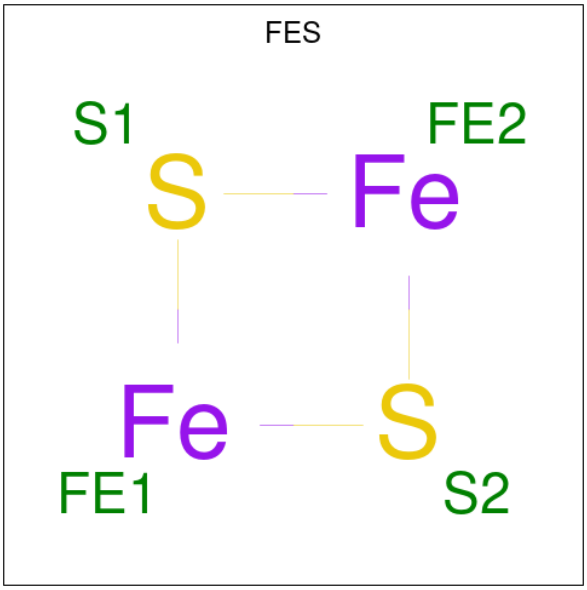
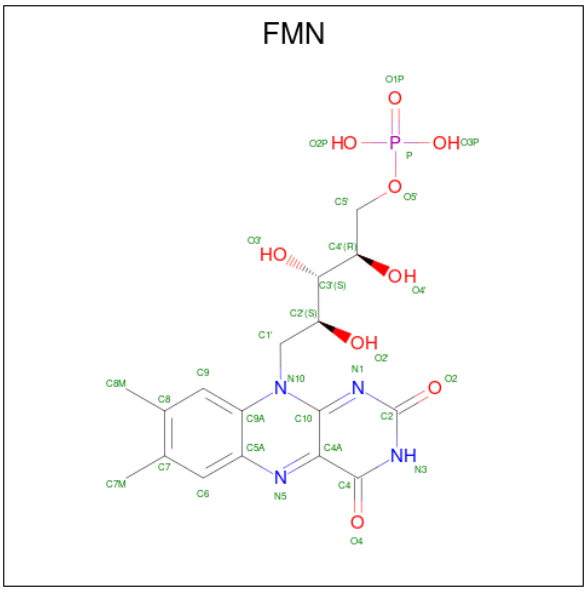
Mol	Chain	Residues	Atoms	AltConf
47	1I	1	Total Fe S 8 4 4	0
47	1I	1	Total Fe S 8 4 4	0

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



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

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

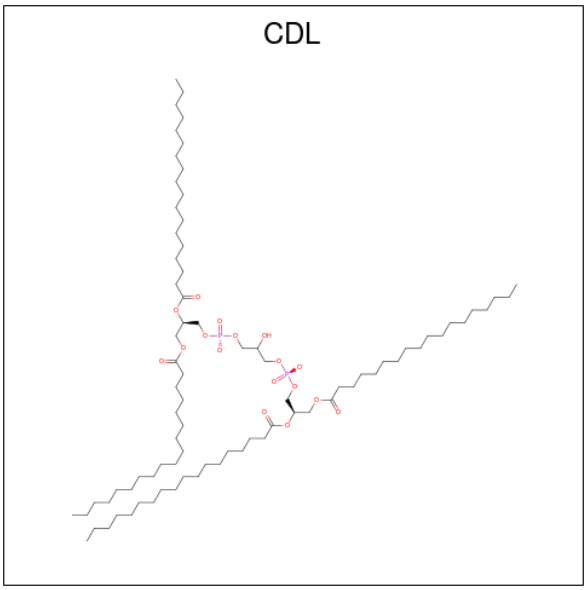


Mol	Chain	Residues	Atoms					AltConf
49	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

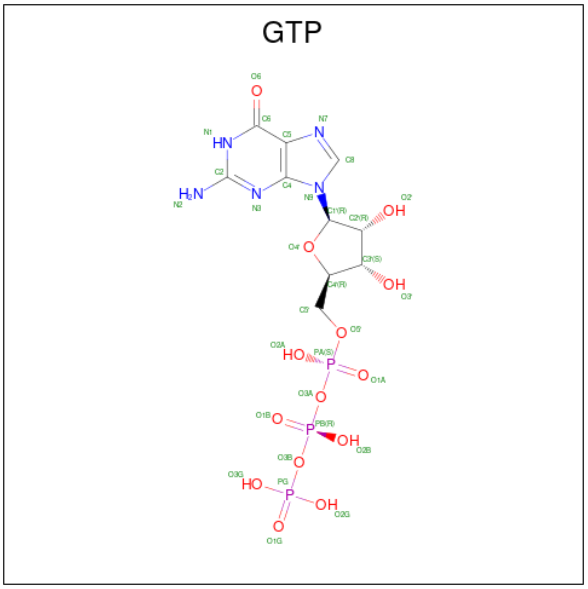
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
51	1L	1	Total	C	O	P	0
			76	57	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	
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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



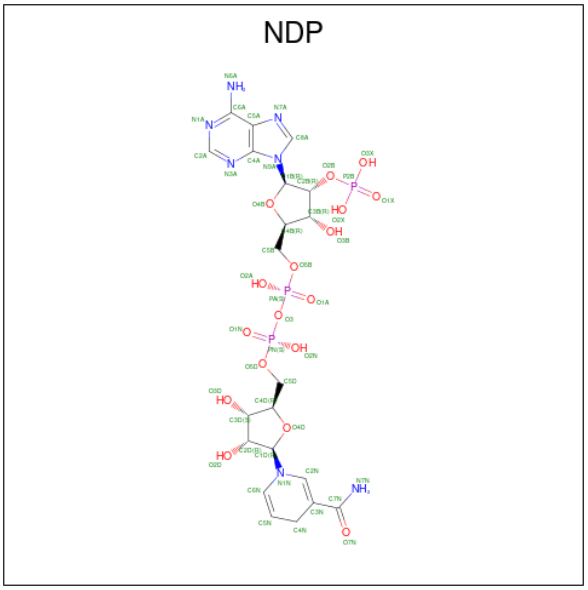
Mol	Chain	Residues	Atoms					AltConf
52	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (three-letter code: 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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

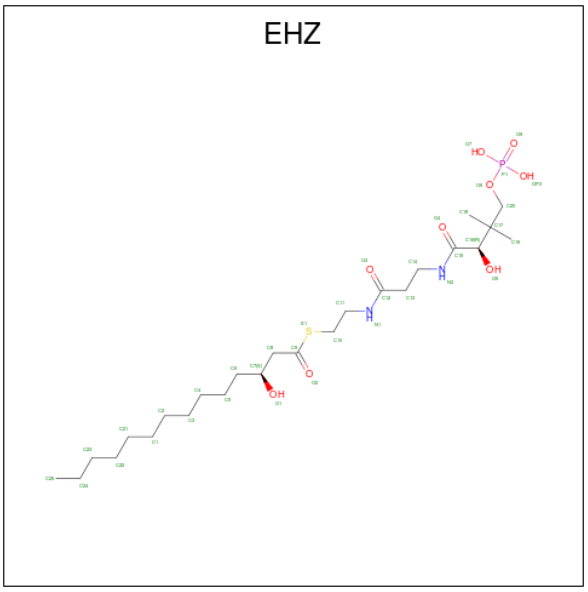


Mol	Chain	Residues	Atoms					AltConf
54	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

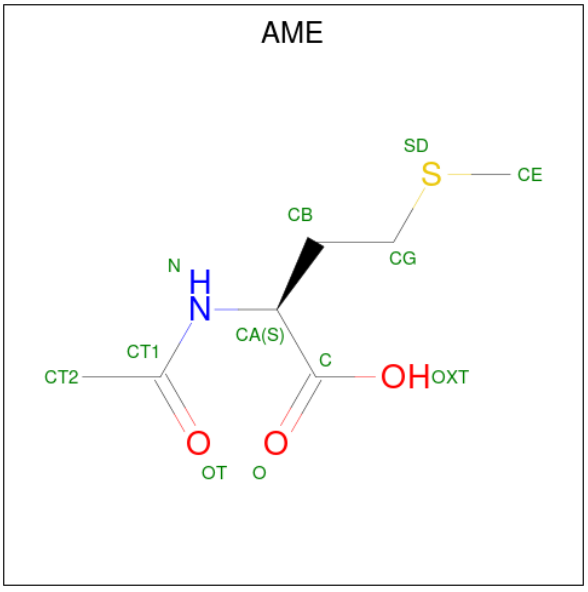
Mol	Chain	Residues	Atoms		AltConf
55	1R	1	Total	Zn	0
			1	1	

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



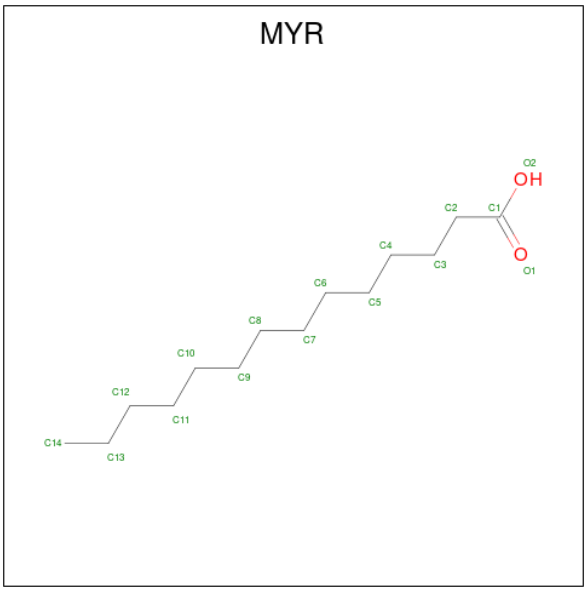
Mol	Chain	Residues	Atoms						AltConf
56	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 57 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: $C_7H_{13}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
57	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	1A	21	Total O 21 21	0
59	1B	53	Total O 53 53	0
59	1C	96	Total O 96 96	0
59	1D	138	Total O 138 138	0
59	1E	55	Total O 55 55	0
59	1F	113	Total O 113 113	0
59	1G	255	Total O 255 255	0
59	1H	80	Total O 80 80	0
59	1I	75	Total O 75 75	0
59	1J	56	Total O 56 56	0
59	1K	38	Total O 38 38	0

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Mol	Chain	Residues	Atoms	AltConf
59	1L	228	Total O 228 228	0
59	1M	201	Total O 201 201	0
59	1N	154	Total O 154 154	0
59	1O	150	Total O 150 150	0
59	1P	118	Total O 118 118	0
59	1Q	63	Total O 63 63	0
59	1R	41	Total O 41 41	0
59	1S	56	Total O 56 56	0
59	1T	12	Total O 12 12	0
59	1U	26	Total O 26 26	0
59	1V	20	Total O 20 20	0
59	1W	37	Total O 37 37	0
59	1X	106	Total O 106 106	0
59	1Y	54	Total O 54 54	0
59	1Z	83	Total O 83 83	0
59	1a	30	Total O 30 30	0
59	1b	35	Total O 35 35	0
59	1c	23	Total O 23 23	0
59	1d	95	Total O 95 95	0
59	1e	91	Total O 91 91	0
59	1f	43	Total O 43 43	0

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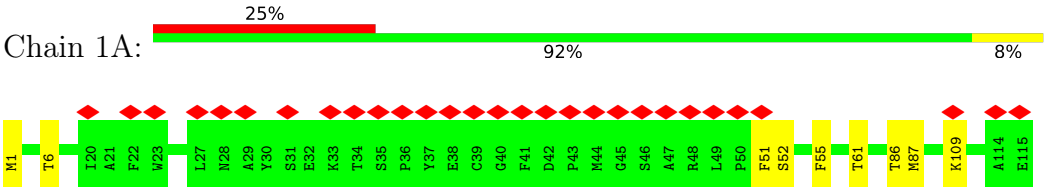
Mol	Chain	Residues	Atoms	AltConf
59	1g	76	Total O 76 76	0
59	1h	116	Total O 116 116	0
59	1i	48	Total O 48 48	0
59	1j	37	Total O 37 37	0
59	1k	35	Total O 35 35	0
59	1l	97	Total O 97 97	0
59	1m	82	Total O 82 82	0
59	1n	120	Total O 120 120	0
59	1o	100	Total O 100 100	0
59	1p	141	Total O 141 141	0
59	1q	47	Total O 47 47	0
59	1r	25	Total O 25 25	0
59	1s	15	Total O 15 15	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.

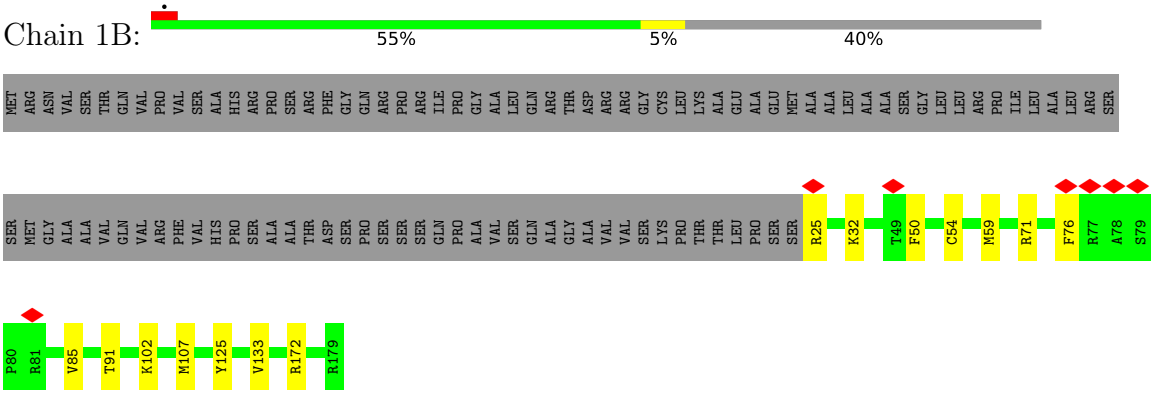
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain 1A:



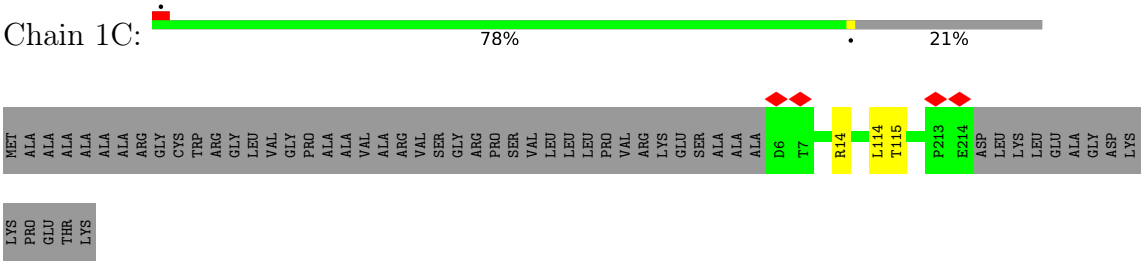
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 1B:



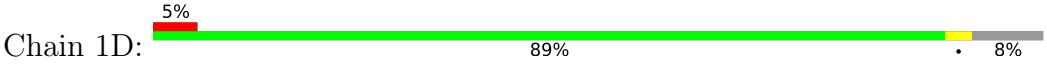
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

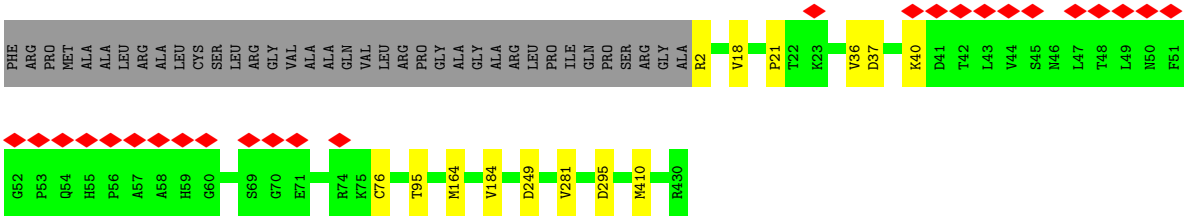
Chain 1C:



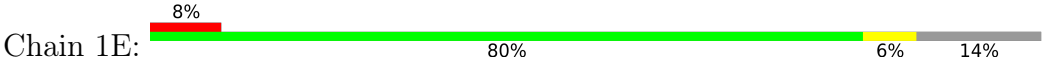
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

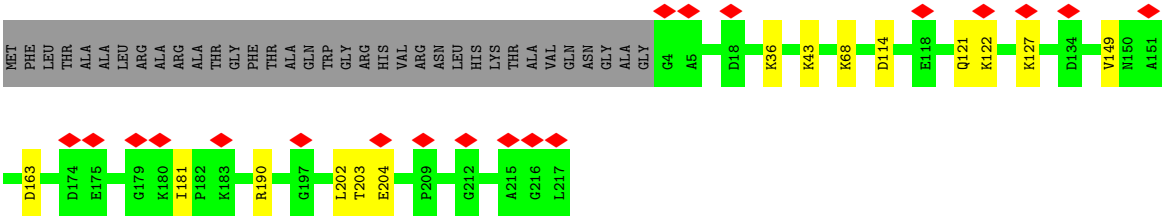
Chain 1D:



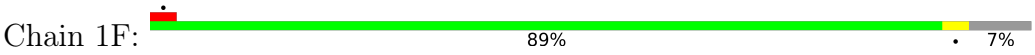


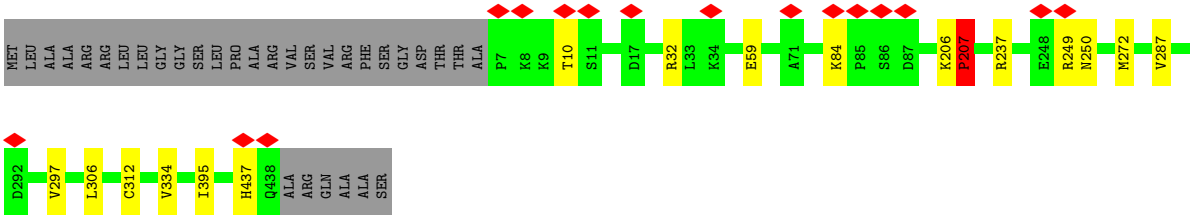
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



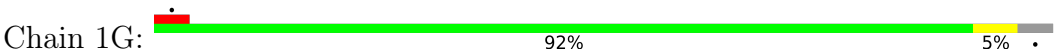


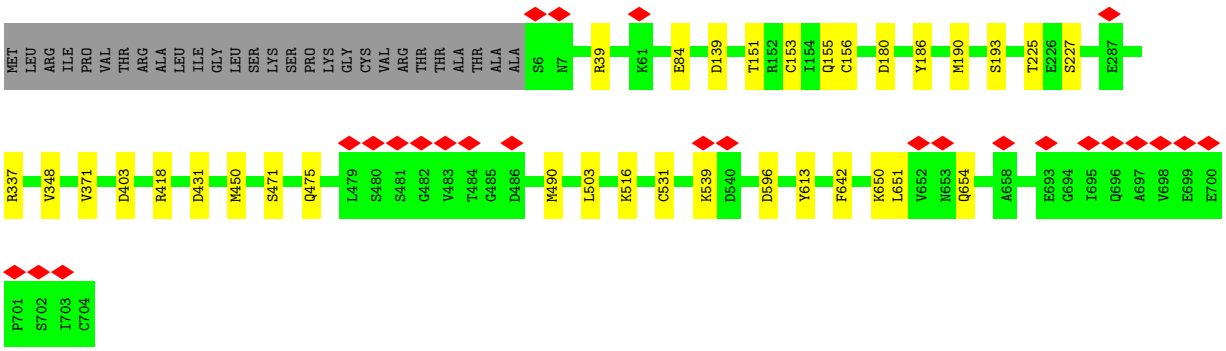
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



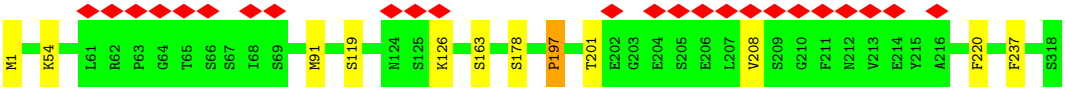


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



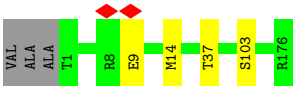


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



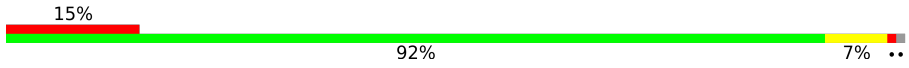
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

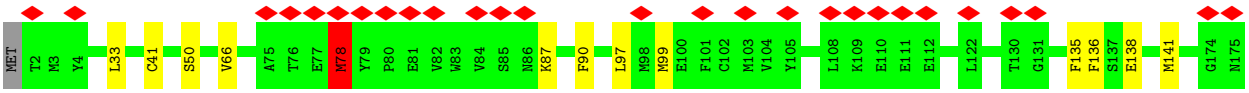
Chain 1I:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

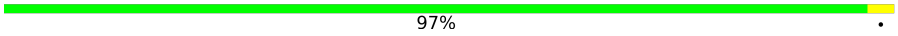
Chain 1J:





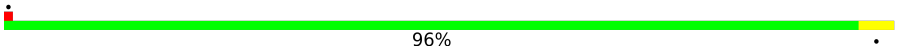
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

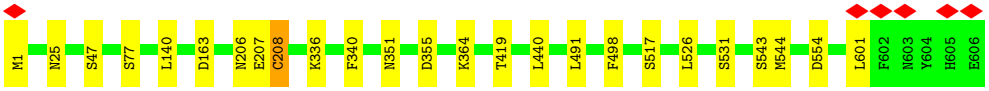
Chain 1K:



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

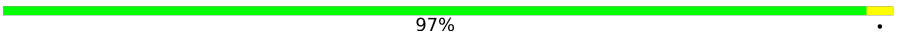
Chain 1L:

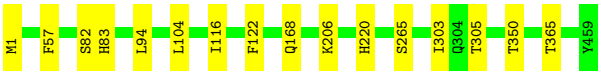




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

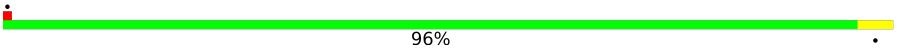
Chain 1M:

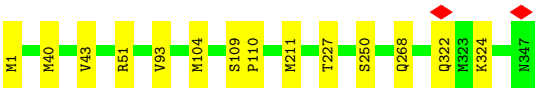




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

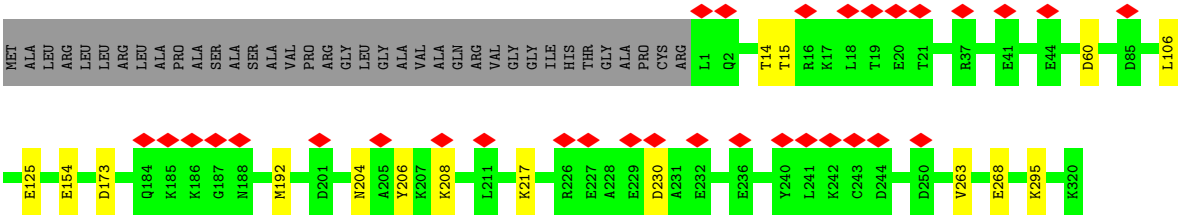
Chain 1N:





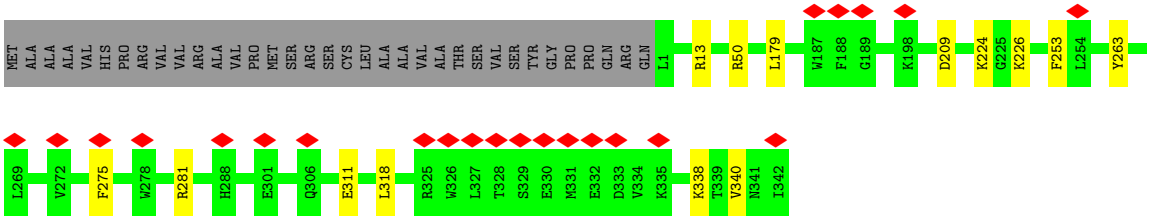
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:



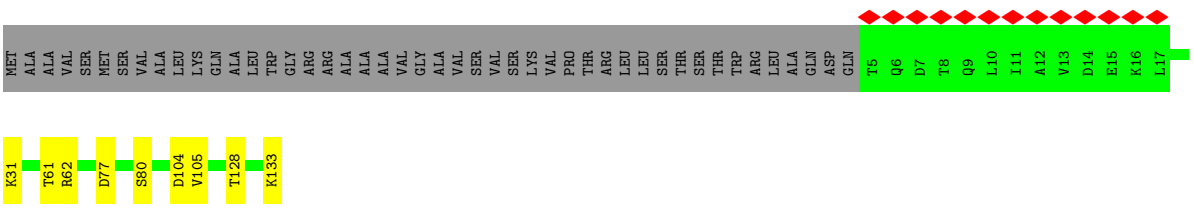
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



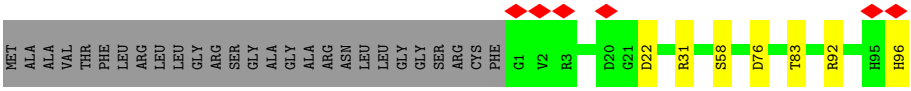
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



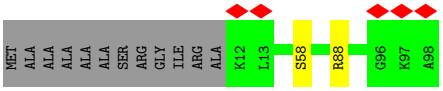
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



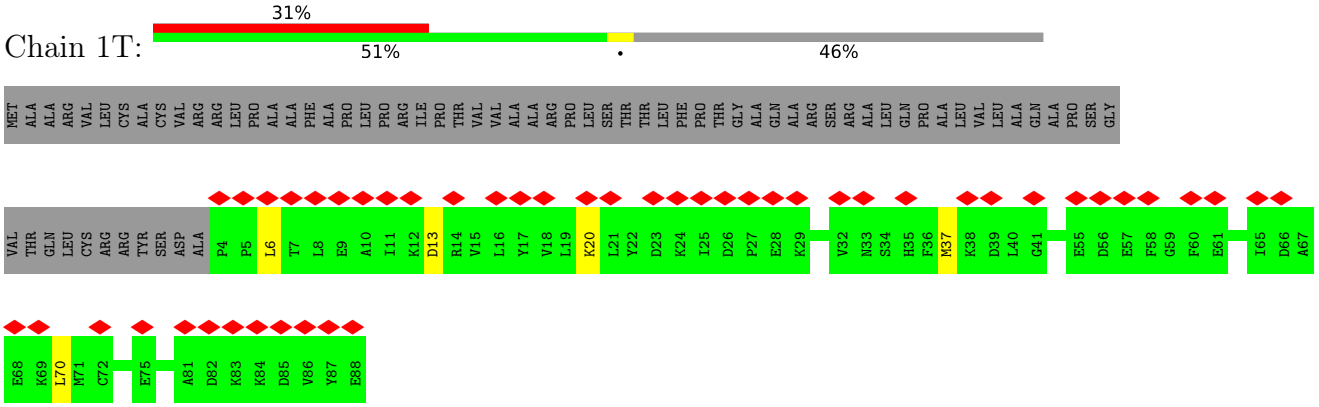
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



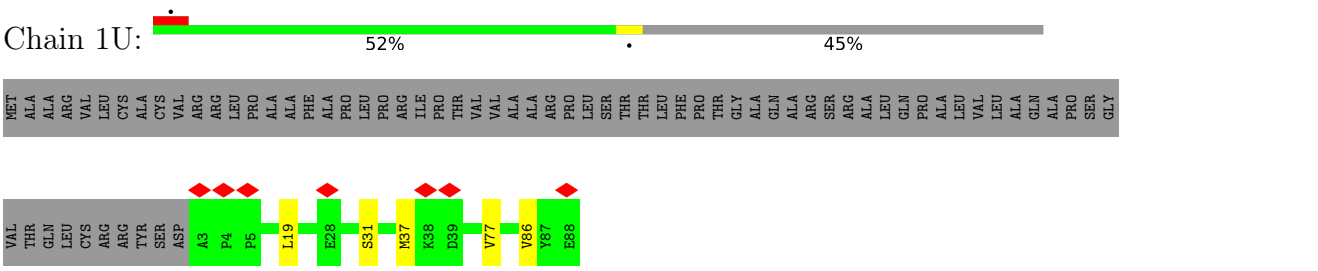
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T:



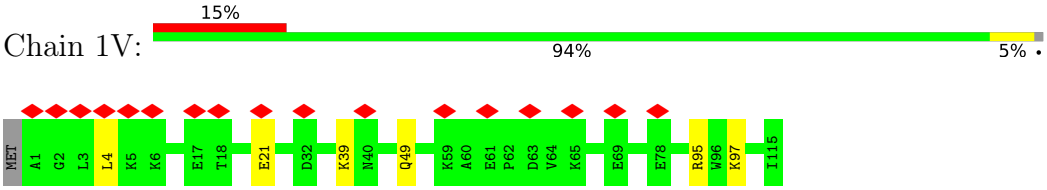
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U:



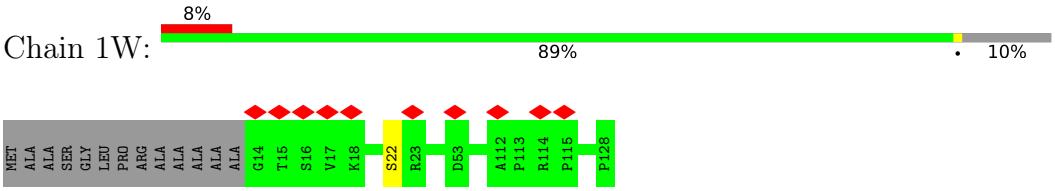
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:



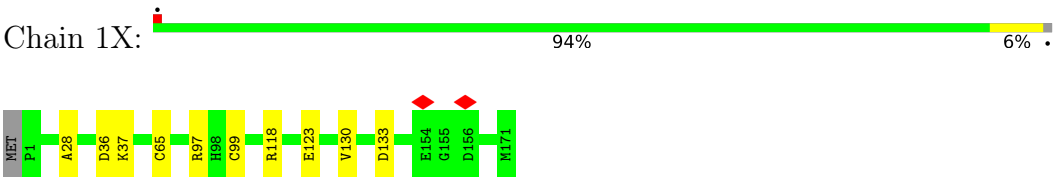
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain 1W:



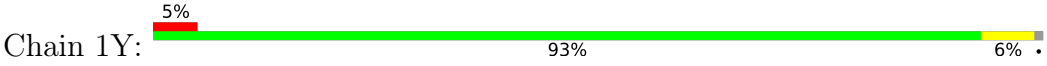
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

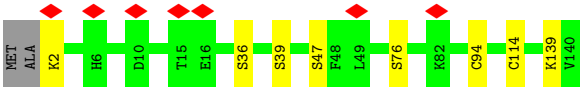
Chain 1X:



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

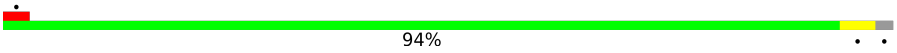
Chain 1Y:

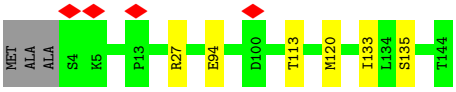




• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

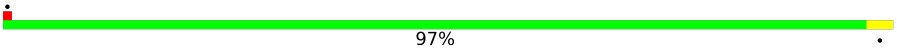
Chain 1Z:

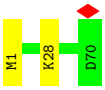




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

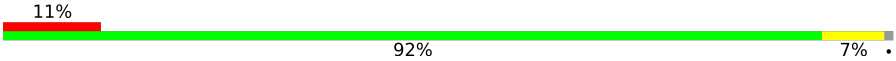
Chain 1a:

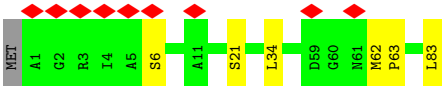




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

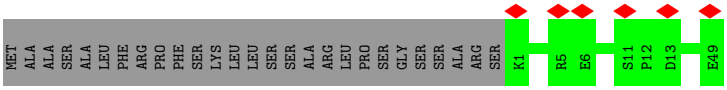
Chain 1b:





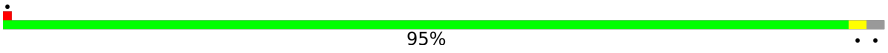
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

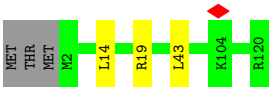
Chain 1c:



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

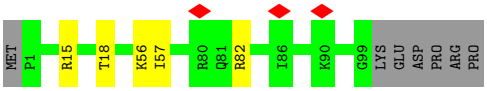
Chain 1d:





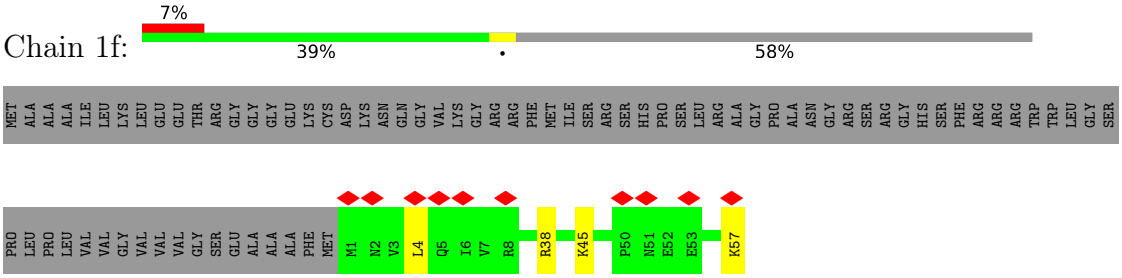
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:



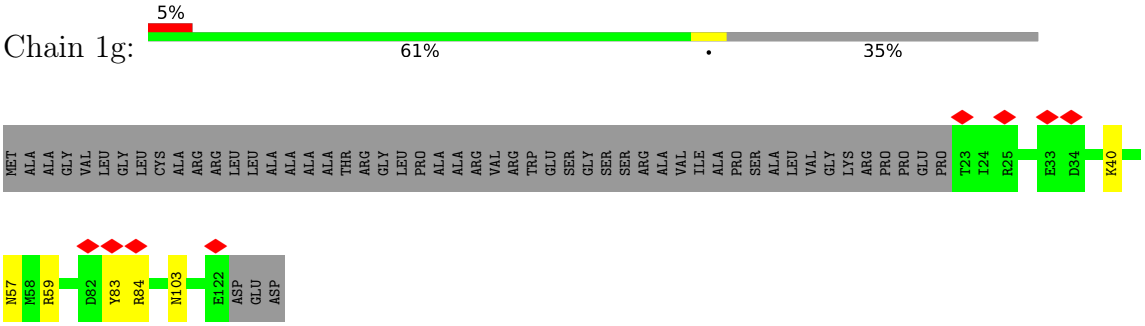
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain 1f:



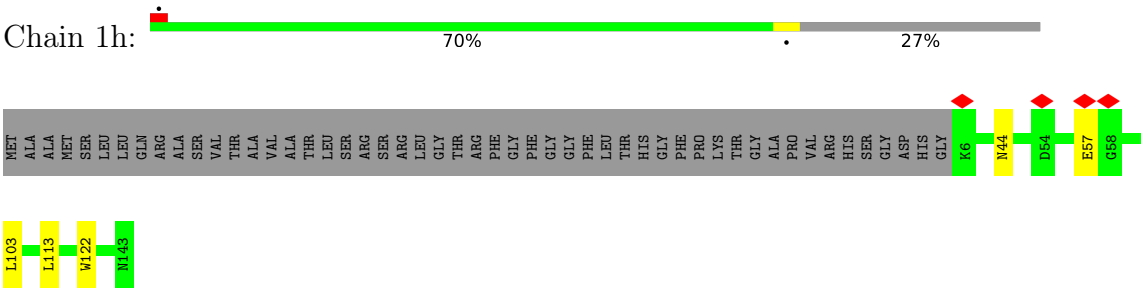
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



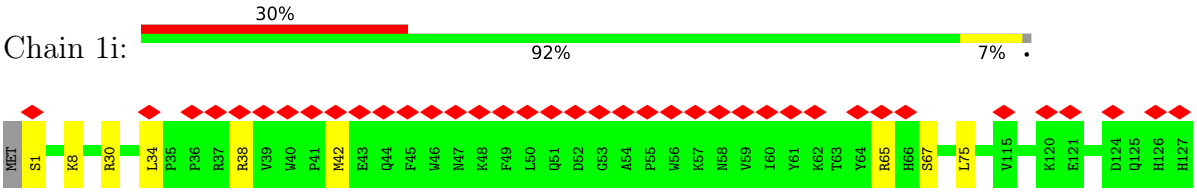
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



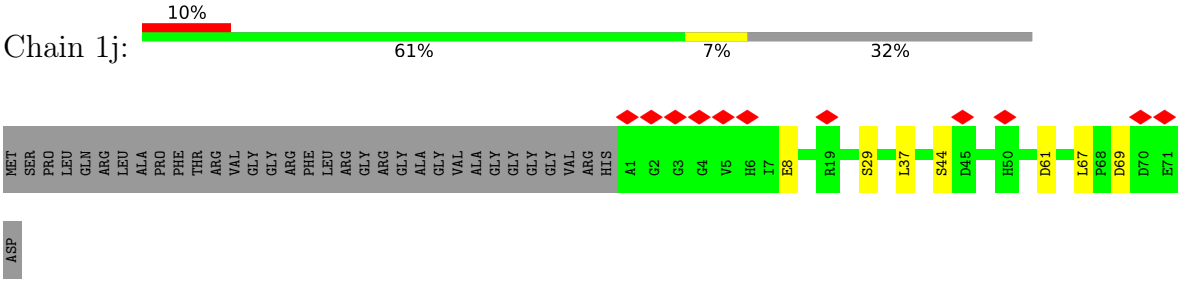
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



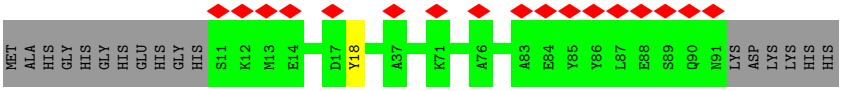
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



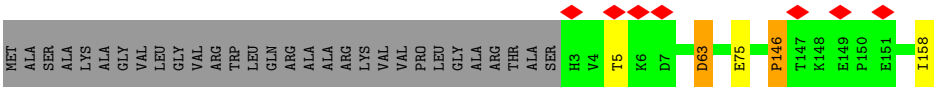
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



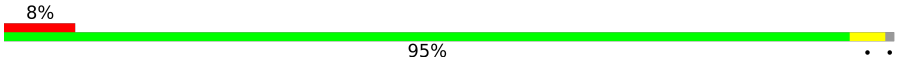
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

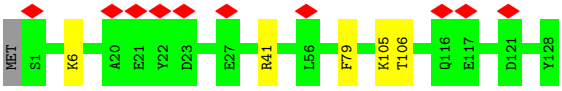
Chain 1l:



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

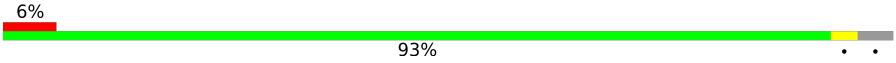
Chain 1m:

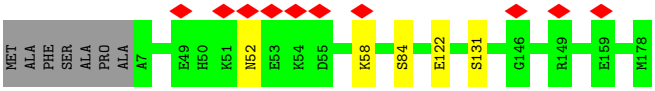




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

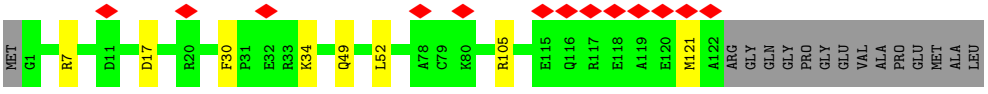
Chain 1n:





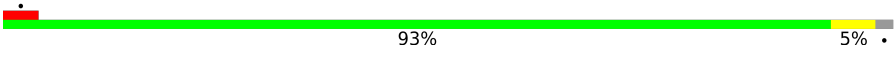
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

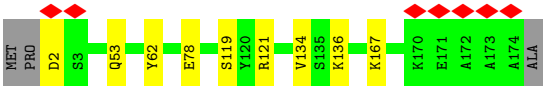
Chain 1o:



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

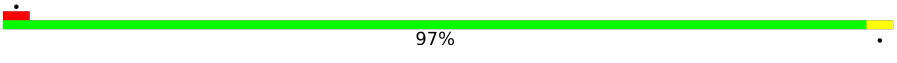
Chain 1p:

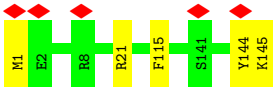




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

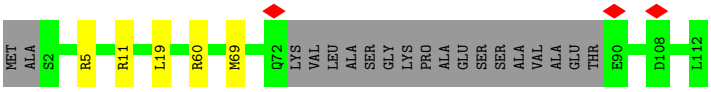
Chain 1q:





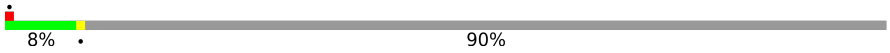
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

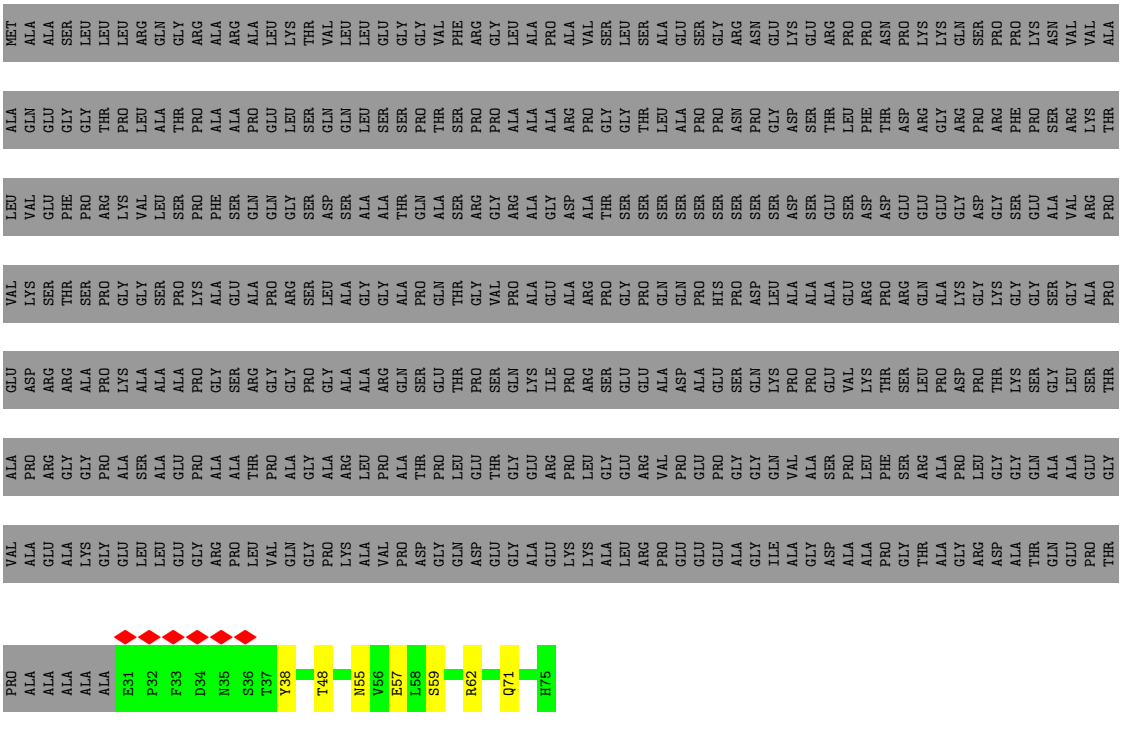
Chain 1r:



• 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: FME, MG, FES, FMN, AME, PC1, CDL, GTP, MYR, EHZ, K, SF4, NDP, ZN, 3PE, SAC

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	0.25	0/930	0.49	0/1271
2	1B	0.27	0/1273	0.54	0/1722
3	1C	0.26	0/1791	0.51	0/2439
4	1D	0.36	2/3545 (0.1%)	0.65	4/4806 (0.1%)
5	1E	0.27	0/1698	0.51	1/2311 (0.0%)
6	1F	0.36	1/3401 (0.0%)	0.62	3/4595 (0.1%)
7	1G	0.26	0/5451	0.51	0/7387
8	1H	0.27	0/2566	0.54	3/3509 (0.1%)
9	1I	0.26	0/1443	0.51	0/1952
10	1J	0.28	0/1364	0.56	1/1850 (0.1%)
11	1K	0.26	0/751	0.47	0/1018
12	1L	0.27	0/4939	0.45	0/6718
13	1M	0.26	0/3713	0.47	0/5063
14	1N	0.26	0/2765	0.46	0/3758
15	1O	0.26	0/2650	0.51	0/3588
16	1P	0.26	0/2828	0.50	0/3834
17	1Q	0.26	0/1070	0.51	0/1446
18	1R	0.25	0/755	0.51	0/1018
19	1S	0.27	0/711	0.54	0/956
20	1T	0.26	0/701	0.45	0/946
20	1U	0.26	0/706	0.42	0/954
21	1V	0.25	0/946	0.43	0/1281
22	1W	0.26	0/995	0.51	0/1340
23	1X	0.27	0/1436	0.51	0/1938
24	1Y	0.41	2/1037 (0.2%)	0.55	1/1404 (0.1%)
25	1Z	0.27	0/1199	0.52	0/1617
26	1a	0.26	0/577	0.45	0/777
27	1b	1.12	3/664 (0.5%)	1.23	6/912 (0.7%)
28	1c	0.25	0/430	0.47	0/581
29	1d	0.28	0/1016	0.49	0/1374
30	1e	0.27	0/836	0.52	0/1118
31	1f	0.25	0/499	0.54	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.27	0/858	0.53	0/1165
33	1h	0.27	0/1184	0.52	0/1603
34	1i	0.24	0/1131	0.49	0/1541
35	1j	0.24	0/627	0.46	0/858
36	1k	0.26	0/668	0.44	0/903
37	1l	0.41	1/1365 (0.1%)	0.72	4/1867 (0.2%)
38	1m	0.27	0/1092	0.54	0/1481
39	1n	0.26	0/1549	0.52	0/2098
40	1o	0.26	0/1069	0.52	0/1430
41	1p	0.26	0/1481	0.52	0/1997
42	1q	0.25	0/1253	0.50	0/1704
43	1r	0.27	0/777	0.51	0/1051
44	1s	0.27	0/394	0.51	0/533
All	All	0.30	9/68134 (0.0%)	0.53	23/92387 (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
6	1F	0	2
8	1H	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1b	63	PRO	CB-CG	20.89	2.54	1.50
27	1b	63	PRO	CG-CD	-17.12	0.94	1.50
6	1F	207	PRO	CG-CD	-12.54	1.09	1.50
4	1D	21	PRO	CG-CD	-11.81	1.11	1.50
37	1l	146	PRO	CG-CD	-10.52	1.16	1.50
24	1Y	114	CYS	CB-SG	7.83	1.95	1.82
27	1b	63	PRO	N-CD	7.04	1.57	1.47
4	1D	21	PRO	CB-CG	-6.96	1.15	1.50
24	1Y	94	CYS	CB-SG	-6.79	1.70	1.82

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1b	63	PRO	CB-CG-CD	-25.44	7.28	106.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1D	21	PRO	N-CD-CG	-19.68	73.68	103.20
6	1F	207	PRO	N-CD-CG	-17.61	76.78	103.20
4	1D	21	PRO	CA-CB-CG	-17.24	71.24	104.00
6	1F	207	PRO	CA-CB-CG	-14.99	75.52	104.00
37	1l	146	PRO	N-CD-CG	-14.82	80.97	103.20
27	1b	63	PRO	N-CA-CB	-12.76	87.99	103.30
27	1b	63	PRO	CA-N-CD	-12.41	94.12	111.50
37	1l	146	PRO	CA-CB-CG	-11.94	81.31	104.00
4	1D	21	PRO	CB-CG-CD	11.10	149.78	106.50
24	1Y	94	CYS	CA-CB-SG	9.36	130.84	114.00
27	1b	62	MET	C-N-CD	9.14	147.60	128.40
27	1b	63	PRO	CA-CB-CG	-8.69	87.48	104.00
8	1H	197	PRO	N-CD-CG	-8.34	90.69	103.20
6	1F	207	PRO	N-CA-CB	-8.24	93.41	103.30
10	1J	78	MET	CA-CB-CG	7.97	126.85	113.30
27	1b	63	PRO	N-CD-CG	-7.82	91.47	103.20
37	1l	146	PRO	N-CA-CB	-7.71	94.05	103.30
8	1H	197	PRO	CA-CB-CG	-7.06	90.59	104.00
8	1H	197	PRO	CA-N-CD	-6.87	101.88	111.50
37	1l	63	ASP	CB-CG-OD1	6.73	124.36	118.30
4	1D	21	PRO	CA-N-CD	-6.17	102.86	111.50
5	1E	163	ASP	CB-CG-OD1	5.67	123.40	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
6	1F	207	PRO	Peptide
8	1H	91	MET	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (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%)	105 (93%)	6 (5%)	2 (2%)	8 4
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100 100
3	1C	207/264 (78%)	204 (99%)	3 (1%)	0	100 100
4	1D	427/466 (92%)	408 (96%)	19 (4%)	0	100 100
5	1E	212/249 (85%)	198 (93%)	14 (7%)	0	100 100
6	1F	430/464 (93%)	410 (95%)	18 (4%)	2 (0%)	29 26
7	1G	697/727 (96%)	672 (96%)	22 (3%)	3 (0%)	34 32
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	41 41
9	1I	174/239 (73%)	169 (97%)	5 (3%)	0	100 100
10	1J	172/175 (98%)	157 (91%)	13 (8%)	2 (1%)	13 8
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100 100
12	1L	604/606 (100%)	572 (95%)	30 (5%)	2 (0%)	41 41
13	1M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	47 49
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	41 41
15	1O	318/357 (89%)	308 (97%)	10 (3%)	0	100 100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100 100
17	1Q	127/175 (73%)	120 (94%)	7 (6%)	0	100 100
18	1R	94/123 (76%)	88 (94%)	6 (6%)	0	100 100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100 100
20	1T	83/156 (53%)	83 (100%)	0	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%)	7 (4%)	1 (1%)	25 21
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100 100
25	1Z	139/144 (96%)	138 (99%)	1 (1%)	0	100 100
26	1a	68/70 (97%)	68 (100%)	0	0	100 100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100 100
28	1c	47/76 (62%)	47 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	87 (89%)	11 (11%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	1i	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	7 (4%)	0	100	100
40	1o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
All	All	8194/9732 (84%)	7881 (96%)	298 (4%)	15 (0%)	50	49

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1J	66	VAL
13	1M	82	SER
23	1X	28	ALA
7	1G	155	GLN
8	1H	208	VAL
1	1A	52	SER
6	1F	249	ARG
6	1F	297	VAL
7	1G	186	TYR
7	1G	654	GLN
10	1J	78	MET
1	1A	109	LYS
12	1L	208	CYS
12	1L	601	LEU
14	1N	110	PRO

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%)	93 (94%)	6 (6%)	18	16
2	1B	131/212 (62%)	117 (89%)	14 (11%)	6	3
3	1C	190/227 (84%)	187 (98%)	3 (2%)	62	69
4	1D	371/396 (94%)	358 (96%)	13 (4%)	36	38
5	1E	183/207 (88%)	170 (93%)	13 (7%)	14	11
6	1F	346/368 (94%)	332 (96%)	14 (4%)	31	32
7	1G	588/610 (96%)	558 (95%)	30 (5%)	24	22
8	1H	274/274 (100%)	265 (97%)	9 (3%)	38	40
9	1I	151/201 (75%)	147 (97%)	4 (3%)	46	50
10	1J	140/141 (99%)	128 (91%)	12 (9%)	10	7
11	1K	84/84 (100%)	82 (98%)	2 (2%)	49	53
12	1L	539/539 (100%)	516 (96%)	23 (4%)	29	29
13	1M	408/408 (100%)	394 (97%)	14 (3%)	37	39
14	1N	310/310 (100%)	298 (96%)	12 (4%)	32	33
15	1O	283/307 (92%)	267 (94%)	16 (6%)	20	18
16	1P	296/323 (92%)	282 (95%)	14 (5%)	26	25
17	1Q	117/152 (77%)	108 (92%)	9 (8%)	13	9
18	1R	79/97 (81%)	72 (91%)	7 (9%)	9	6
19	1S	77/82 (94%)	75 (97%)	2 (3%)	46	50
20	1T	79/133 (59%)	74 (94%)	5 (6%)	18	15
20	1U	79/133 (59%)	74 (94%)	5 (6%)	18	15
21	1V	100/101 (99%)	94 (94%)	6 (6%)	19	16
22	1W	107/112 (96%)	106 (99%)	1 (1%)	78	84
23	1X	153/154 (99%)	144 (94%)	9 (6%)	19	17
24	1Y	101/102 (99%)	95 (94%)	6 (6%)	19	17
25	1Z	123/124 (99%)	117 (95%)	6 (5%)	25	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	1a	58/58 (100%)	56 (97%)	2 (3%)	37 39
27	1b	69/70 (99%)	65 (94%)	4 (6%)	20 17
28	1c	45/66 (68%)	45 (100%)	0	100 100
29	1d	106/109 (97%)	103 (97%)	3 (3%)	43 47
30	1e	87/94 (93%)	82 (94%)	5 (6%)	20 18
31	1f	54/113 (48%)	50 (93%)	4 (7%)	13 10
32	1g	92/129 (71%)	86 (94%)	6 (6%)	17 14
33	1h	121/158 (77%)	116 (96%)	5 (4%)	30 31
34	1i	119/120 (99%)	111 (93%)	8 (7%)	16 13
35	1j	62/84 (74%)	55 (89%)	7 (11%)	6 3
36	1k	63/76 (83%)	62 (98%)	1 (2%)	62 69
37	1l	141/161 (88%)	136 (96%)	5 (4%)	36 38
38	1m	113/114 (99%)	108 (96%)	5 (4%)	28 28
39	1n	156/160 (98%)	151 (97%)	5 (3%)	39 41
40	1o	110/120 (92%)	102 (93%)	8 (7%)	14 11
41	1p	154/156 (99%)	145 (94%)	9 (6%)	20 17
42	1q	131/131 (100%)	126 (96%)	5 (4%)	33 34
43	1r	85/98 (87%)	80 (94%)	5 (6%)	19 17
44	1s	44/351 (12%)	37 (84%)	7 (16%)	2 1
All	All	7218/8264 (87%)	6869 (95%)	349 (5%)	29 24

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	6	THR
1	1A	51	PHE
1	1A	55	PHE
1	1A	61	THR
1	1A	86	THR
1	1A	87	MET
2	1B	25	ARG
2	1B	32	LYS
2	1B	50	PHE
2	1B	54	CYS
2	1B	59	MET

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Mol	Chain	Res	Type
2	1B	71	ARG
2	1B	76	PHE
2	1B	85	VAL
2	1B	91	THR
2	1B	102	LYS
2	1B	107	MET
2	1B	125	TYR
2	1B	133	VAL
2	1B	172	ARG
3	1C	14	ARG
3	1C	114	LEU
3	1C	115	THR
4	1D	2	ARG
4	1D	18	VAL
4	1D	36	VAL
4	1D	37	ASP
4	1D	40	LYS
4	1D	76	CYS
4	1D	95	THR
4	1D	164	MET
4	1D	184	VAL
4	1D	249	ASP
4	1D	281	VAL
4	1D	295	ASP
4	1D	410	MET
5	1E	36	LYS
5	1E	43	LYS
5	1E	68	LYS
5	1E	114	ASP
5	1E	121	GLN
5	1E	122	LYS
5	1E	127	LYS
5	1E	149	VAL
5	1E	181	ILE
5	1E	190	ARG
5	1E	202	LEU
5	1E	203	THR
5	1E	204	GLU
6	1F	10	THR
6	1F	32	ARG
6	1F	59	GLU
6	1F	84	LYS

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Mol	Chain	Res	Type
6	1F	207	PRO
6	1F	237	ARG
6	1F	250	ASN
6	1F	272	MET
6	1F	287	VAL
6	1F	306	LEU
6	1F	312	CYS
6	1F	334	VAL
6	1F	395	ILE
6	1F	437	HIS
7	1G	39	ARG
7	1G	84	GLU
7	1G	139	ASP
7	1G	151	THR
7	1G	153	CYS
7	1G	156	CYS
7	1G	180	ASP
7	1G	190	MET
7	1G	193	SER
7	1G	225	THR
7	1G	227	SER
7	1G	337	ARG
7	1G	348	VAL
7	1G	371	VAL
7	1G	403	ASP
7	1G	418	ARG
7	1G	431	ASP
7	1G	450	MET
7	1G	471	SER
7	1G	475	GLN
7	1G	490	MET
7	1G	503	LEU
7	1G	516	LYS
7	1G	531	CYS
7	1G	539	LYS
7	1G	596	ASP
7	1G	613	TYR
7	1G	642	PHE
7	1G	650	LYS
7	1G	651	LEU
8	1H	54	LYS
8	1H	119	SER

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Mol	Chain	Res	Type
8	1H	126	LYS
8	1H	163	SER
8	1H	178	SER
8	1H	197	PRO
8	1H	201	THR
8	1H	220	PHE
8	1H	237	PHE
9	1I	9	GLU
9	1I	14	MET
9	1I	37	THR
9	1I	103	SER
10	1J	33	LEU
10	1J	41	CYS
10	1J	50	SER
10	1J	78	MET
10	1J	87	LYS
10	1J	90	PHE
10	1J	97	LEU
10	1J	99	MET
10	1J	135	PHE
10	1J	136	PHE
10	1J	138	GLU
10	1J	141	MET
11	1K	53	PHE
11	1K	59	MET
12	1L	25	ASN
12	1L	47	SER
12	1L	77	SER
12	1L	140	LEU
12	1L	163	ASP
12	1L	206	ASN
12	1L	207	GLU
12	1L	208	CYS
12	1L	336	LYS
12	1L	340	PHE
12	1L	351	ASN
12	1L	355	ASP
12	1L	364	LYS
12	1L	419	THR
12	1L	440	LEU
12	1L	491	LEU
12	1L	498	PHE

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Mol	Chain	Res	Type
12	1L	517	SER
12	1L	526	LEU
12	1L	531	SER
12	1L	543	SER
12	1L	544	MET
12	1L	554	ASP
13	1M	57	PHE
13	1M	83	HIS
13	1M	94	LEU
13	1M	104	LEU
13	1M	116	ILE
13	1M	122	PHE
13	1M	168	GLN
13	1M	206	LYS
13	1M	220	HIS
13	1M	265	SER
13	1M	303	ILE
13	1M	305	THR
13	1M	350	THR
13	1M	365	THR
14	1N	40	MET
14	1N	43	VAL
14	1N	51	ARG
14	1N	93	VAL
14	1N	104	MET
14	1N	109	SER
14	1N	211	MET
14	1N	227	THR
14	1N	250	SER
14	1N	268	GLN
14	1N	322	GLN
14	1N	324	LYS
15	1O	14	THR
15	1O	15	THR
15	1O	60	ASP
15	1O	106	LEU
15	1O	125	GLU
15	1O	154	GLU
15	1O	173	ASP
15	1O	192	MET
15	1O	204	ASN
15	1O	206	TYR

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Mol	Chain	Res	Type
15	1O	208	LYS
15	1O	217	LYS
15	1O	230	ASP
15	1O	263	VAL
15	1O	268	GLU
15	1O	295	LYS
16	1P	13	ARG
16	1P	50	ARG
16	1P	179	LEU
16	1P	209	ASP
16	1P	224	LYS
16	1P	226	LYS
16	1P	253	PHE
16	1P	263	TYR
16	1P	275	PHE
16	1P	281	ARG
16	1P	311	GLU
16	1P	318	LEU
16	1P	338	LYS
16	1P	340	VAL
17	1Q	31	LYS
17	1Q	61	THR
17	1Q	62	ARG
17	1Q	77	ASP
17	1Q	80	SER
17	1Q	104	ASP
17	1Q	105	VAL
17	1Q	128	THR
17	1Q	133	LYS
18	1R	22	ASP
18	1R	31	ARG
18	1R	58	SER
18	1R	76	ASP
18	1R	83	THR
18	1R	92	ARG
18	1R	96	HIS
19	1S	58	SER
19	1S	88	ARG
20	1T	6	LEU
20	1T	13	ASP
20	1T	20	LYS
20	1T	37	MET

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Mol	Chain	Res	Type
20	1T	70	LEU
20	1U	19	LEU
20	1U	31	SER
20	1U	37	MET
20	1U	77	VAL
20	1U	86	VAL
21	1V	4	LEU
21	1V	21	GLU
21	1V	39	LYS
21	1V	49	GLN
21	1V	95	ARG
21	1V	97	LYS
22	1W	22	SER
23	1X	36	ASP
23	1X	37	LYS
23	1X	65	CYS
23	1X	97	ARG
23	1X	99	CYS
23	1X	118	ARG
23	1X	123	GLU
23	1X	130	VAL
23	1X	133	ASP
24	1Y	2	LYS
24	1Y	36	SER
24	1Y	39	SER
24	1Y	47	SER
24	1Y	76	SER
24	1Y	139	LYS
25	1Z	27	ARG
25	1Z	94	GLU
25	1Z	113	THR
25	1Z	120	MET
25	1Z	133	ILE
25	1Z	135	SER
26	1a	1	MET
26	1a	28	LYS
27	1b	6	SER
27	1b	21	SER
27	1b	34	LEU
27	1b	83	LEU
29	1d	14	LEU
29	1d	19	ARG

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Mol	Chain	Res	Type
29	1d	43	LEU
30	1e	15	ARG
30	1e	18	THR
30	1e	56	LYS
30	1e	57	ILE
30	1e	82	ARG
31	1f	4	LEU
31	1f	38	ARG
31	1f	45	LYS
31	1f	57	LYS
32	1g	40	LYS
32	1g	57	ASN
32	1g	59	ARG
32	1g	83	TYR
32	1g	84	ARG
32	1g	103	ASN
33	1h	44	ASN
33	1h	57	GLU
33	1h	103	LEU
33	1h	113	LEU
33	1h	122	TRP
34	1i	8	LYS
34	1i	30	ARG
34	1i	34	LEU
34	1i	38	ARG
34	1i	42	MET
34	1i	65	ARG
34	1i	67	SER
34	1i	75	LEU
35	1j	8	GLU
35	1j	29	SER
35	1j	37	LEU
35	1j	44	SER
35	1j	61	ASP
35	1j	67	LEU
35	1j	69	ASP
36	1k	18	TYR
37	1l	5	THR
37	1l	63	ASP
37	1l	75	GLU
37	1l	146	PRO
37	1l	158	ILE

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Mol	Chain	Res	Type
38	1m	6	LYS
38	1m	41	ARG
38	1m	79	PHE
38	1m	105	LYS
38	1m	106	THR
39	1n	52	ASN
39	1n	58	LYS
39	1n	84	SER
39	1n	122	GLU
39	1n	131	SER
40	1o	7	ARG
40	1o	17	ASP
40	1o	30	PHE
40	1o	34	LYS
40	1o	49	GLN
40	1o	52	LEU
40	1o	105	ARG
40	1o	121	MET
41	1p	2	ASP
41	1p	53	GLN
41	1p	62	TYR
41	1p	78	GLU
41	1p	119	SER
41	1p	121	ARG
41	1p	134	VAL
41	1p	136	LYS
41	1p	167	LYS
42	1q	1	MET
42	1q	21	ARG
42	1q	115	PHE
42	1q	144	TYR
42	1q	145	LYS
43	1r	5	ARG
43	1r	11	ARG
43	1r	19	LEU
43	1r	60	ARG
43	1r	69	MET
44	1s	38	TYR
44	1s	48	THR
44	1s	55	ASN
44	1s	57	GLU
44	1s	59	SER

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Mol	Chain	Res	Type
44	1s	62	ARG
44	1s	71	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
6	1F	373	ASN
11	1K	83	ASN
12	1L	296	ASN
12	1L	524	ASN
13	1M	220	HIS
14	1N	322	GLN
15	1O	200	GLN
15	1O	204	ASN
29	1d	12	GLN
29	1d	46	ASN
29	1d	59	HIS
29	1d	61	GLN
29	1d	97	HIS
33	1h	44	ASN
37	1l	99	ASN
39	1n	77	GLN
40	1o	49	GLN
41	1p	130	GLN
43	1r	50	ASN
44	1s	43	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	$\#\|Z\| > 2$
14	FME	1N	1	14	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
13	FME	1M	1	13	8,9,10	0.50	0	7,9,11	1.13	1 (14%)
34	SAC	1i	1	34	7,8,9	0.53	0	8,9,11	0.89	1 (12%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
1	FME	1A	1	1	8,9,10	0.52	0	7,9,11	1.05	1 (14%)
11	FME	1K	1	11	8,9,10	0.49	0	7,9,11	1.02	1 (14%)
12	FME	1L	1	12	8,9,10	0.52	0	7,9,11	0.95	1 (14%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1K	1	FME	O-C-CA	-2.62	117.91	124.78
8	1H	1	FME	O-C-CA	-2.61	117.93	124.78
13	1M	1	FME	O-C-CA	-2.61	117.94	124.78
14	1N	1	FME	O-C-CA	-2.57	118.04	124.78
1	1A	1	FME	O-C-CA	-2.42	118.44	124.78
34	1i	1	SAC	O-C-CA	-2.38	118.53	124.78
12	1L	1	FME	O-C-CA	-2.37	118.57	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
11	1K	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
1	1A	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 3 are monoatomic - leaving 49 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	3PE	1N	903	-	32,32,50	0.33	0	35,37,55	0.43	0
45	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.37	0
45	3PE	1J	201	-	43,43,50	0.28	0	46,48,55	0.39	0
45	3PE	1Y	204	-	26,26,50	0.35	0	29,31,55	0.42	0
46	PC1	1H	401	-	47,47,53	0.29	0	53,55,61	0.37	0
46	PC1	1Z	201	-	43,43,53	0.28	0	49,51,61	0.33	0
47	SF4	1G	802	7	0,12,12	-	-	-		
49	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
46	PC1	1B	203	-	47,47,53	0.28	0	53,55,61	0.44	0
51	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.44	0
46	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.32	0
57	AME	1h	201	-	9,10,11	0.49	0	9,11,13	1.06	1 (11%)
47	SF4	1I	203	9	0,12,12	-	-	-		
46	PC1	1M	503	-	43,43,53	0.31	0	49,51,61	0.37	0
45	3PE	1Y	202	-	39,39,50	0.29	0	42,44,55	0.40	0
47	SF4	1G	801	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.42	0
45	3PE	1d	201	-	47,47,50	0.28	0	50,52,55	0.43	0
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.34	0
46	PC1	1m	201	-	45,45,53	0.30	0	51,53,61	1.09	3 (5%)
46	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.54	1 (1%)
48	FES	1G	803	7	0,4,4	-	-	-		
47	SF4	1B	201	2	0,12,12	-	-	-		
51	CDL	1d	202	-	64,64,99	0.32	0	70,76,111	0.41	0
45	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.45	0
46	PC1	1Y	201	-	34,34,53	0.33	0	40,42,61	0.42	0
45	3PE	1L	701	-	45,45,50	0.30	0	48,50,55	0.46	0
51	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
51	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.39	0
52	GTP	1O	401	53	26,34,34	0.95	2 (7%)	32,54,54	0.89	1 (3%)
47	SF4	1F	502	6	0,12,12	-	-	-		
45	3PE	1N	901	-	48,48,50	0.31	0	51,53,55	0.41	0
45	3PE	1Y	205	-	40,40,50	0.30	0	43,45,55	0.67	1 (2%)
45	3PE	1L	703	-	44,44,50	0.28	0	47,49,55	0.48	0
46	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
56	EHZ	1T	101	-	29,36,37	0.17	0	35,44,47	1.07	1 (2%)
56	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.08	1 (2%)
45	3PE	1Y	203	-	29,29,50	0.34	0	32,34,55	0.70	1 (3%)
54	NDP	1P	402	-	45,52,52	0.60	0	53,80,80	0.75	2 (3%)
48	FES	1E	301	5	0,4,4	-	-	-		
46	PC1	1I	201	-	53,53,53	0.26	0	59,61,61	0.38	0
45	3PE	1L	704	-	30,30,50	0.34	0	33,35,55	0.68	1 (3%)
58	MYR	1l	201	-	14,14,15	0.35	0	13,13,15	0.38	0
46	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
51	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.56	1 (1%)
45	3PE	1M	502	-	50,50,50	0.27	0	53,55,55	0.39	0
46	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.47	0
45	3PE	1M	504	-	49,49,50	0.26	0	52,54,55	0.36	0
47	SF4	1I	202	9	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1N	903	-	-	4/36/36/54	-
45	3PE	1M	501	-	-	9/48/48/54	-
45	3PE	1J	201	-	-	12/47/47/54	-
45	3PE	1Y	204	-	-	6/30/30/54	-
46	PC1	1H	401	-	-	13/51/51/57	-
46	PC1	1Z	201	-	-	2/47/47/57	-
47	SF4	1G	802	7	-	-	0/6/5/5
49	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
46	PC1	1B	203	-	-	13/51/51/57	-
46	PC1	1B	202	-	-	9/49/49/57	-
57	AME	1h	201	-	-	2/9/10/12	-
47	SF4	1I	203	9	-	-	0/6/5/5
46	PC1	1M	503	-	-	8/47/47/57	-
47	SF4	1I	202	9	-	-	0/6/5/5
45	3PE	1Y	202	-	-	9/43/43/54	-
47	SF4	1G	801	7	-	-	0/6/5/5
51	CDL	1q	202	-	-	9/71/71/110	-
45	3PE	1d	201	-	-	18/51/51/54	-
45	3PE	1A	201	-	-	10/50/50/54	-
46	PC1	1m	201	-	-	12/49/49/57	-
46	PC1	1q	201	-	-	9/52/52/57	-
51	CDL	1d	202	-	-	25/75/75/110	-
47	SF4	1B	201	2	-	-	0/6/5/5
48	FES	1G	803	7	-	-	0/1/1/1
45	3PE	1j	101	-	-	5/47/47/54	-
46	PC1	1Y	201	-	-	9/38/38/57	-
45	3PE	1L	701	-	-	6/49/49/54	-
51	CDL	1L	702	-	-	13/86/86/110	-
51	CDL	1X	201	-	-	18/96/96/110	-
52	GTP	1O	401	53	-	4/18/38/38	0/3/3/3
47	SF4	1F	502	6	-	-	0/6/5/5
45	3PE	1N	901	-	-	13/52/52/54	-
45	3PE	1Y	205	-	-	16/44/44/54	-
45	3PE	1L	703	-	-	9/48/48/54	-
46	PC1	1h	203	-	-	14/50/50/57	-
56	EHZ	1T	101	-	-	15/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	EHZ	1n	201	-	-	2/42/44/45	-
45	3PE	1Y	203	-	-	14/33/33/54	-
54	NDP	1P	402	-	-	3/30/77/77	0/5/5/5
48	FES	1E	301	5	-	-	0/1/1/1
46	PC1	1I	201	-	-	10/57/57/57	-
45	3PE	1L	704	-	-	9/34/34/54	-
58	MYR	1l	201	-	-	0/11/12/13	-
46	PC1	1A	202	-	-	5/38/38/57	-
51	CDL	1N	902	-	-	12/71/71/110	-
45	3PE	1M	502	-	-	12/54/54/54	-
46	PC1	1P	401	-	-	10/36/36/57	-
45	3PE	1M	504	-	-	6/53/53/54	-
51	CDL	1h	202	-	-	10/90/90/110	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1O	401	GTP	C5-C6	-2.62	1.42	1.47
52	1O	401	GTP	C8-N7	-2.05	1.31	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1m	201	PC1	O21-C21-C22	5.93	124.29	111.50
56	1n	201	EHZ	C10-S1-C9	5.89	120.20	101.87
56	1T	101	EHZ	C10-S1-C9	5.60	119.29	101.87
45	1Y	205	3PE	O21-C21-C22	3.15	118.28	111.50
51	1N	902	CDL	OB6-CB5-C51	3.12	116.82	111.09
57	1h	201	AME	O-C-CA	-2.99	116.94	124.78
45	1Y	203	3PE	O21-C21-C22	2.88	117.72	111.50
52	1O	401	GTP	O4'-C1'-C2'	-2.80	102.83	106.93
54	1P	402	NDP	O4D-C1D-C2D	-2.76	100.61	106.64
46	1m	201	PC1	O21-C21-O22	-2.70	117.19	123.70
46	1q	201	PC1	O21-C21-C22	2.65	117.22	111.50
45	1L	704	3PE	O21-C21-C22	2.63	117.17	111.50
46	1m	201	PC1	C2-O21-C21	2.39	123.69	117.79
54	1P	402	NDP	C5A-C6A-N6A	2.23	123.75	120.35
49	1F	501	FMN	C4-N3-C2	-2.02	121.91	125.64

There are no chirality outliers.

All (386) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1A	201	3PE	C1-O11-P-O14
45	1J	201	3PE	C1-O11-P-O14
45	1J	201	3PE	C11-O13-P-O12
45	1J	201	3PE	C12-C11-O13-P
45	1L	701	3PE	O32-C31-O31-C3
45	1L	701	3PE	C32-C31-O31-C3
45	1L	704	3PE	O22-C21-O21-C2
45	1L	704	3PE	C22-C21-O21-C2
45	1M	501	3PE	C1-O11-P-O14
45	1M	502	3PE	C2-C1-O11-P
45	1N	901	3PE	C11-O13-P-O14
45	1N	903	3PE	O21-C2-C3-O31
45	1Y	202	3PE	C1-O11-P-O12
45	1Y	202	3PE	C2-C1-O11-P
45	1Y	203	3PE	O22-C21-O21-C2
45	1Y	203	3PE	C22-C21-O21-C2
45	1Y	204	3PE	C11-O13-P-O14
45	1Y	204	3PE	C12-C11-O13-P
45	1Y	204	3PE	O32-C31-O31-C3
45	1Y	204	3PE	C32-C31-O31-C3
45	1Y	205	3PE	C11-O13-P-O12
45	1Y	205	3PE	O32-C31-O31-C3
45	1Y	205	3PE	C32-C31-O31-C3
45	1Y	205	3PE	O22-C21-O21-C2
45	1Y	205	3PE	C22-C21-O21-C2
45	1d	201	3PE	C11-O13-P-O11
45	1d	201	3PE	C11-O13-P-O14
45	1d	201	3PE	C2-C1-O11-P
45	1d	201	3PE	O32-C31-O31-C3
45	1d	201	3PE	C32-C31-O31-C3
45	1j	101	3PE	O22-C21-O21-C2
45	1j	101	3PE	C22-C21-O21-C2
46	1A	202	PC1	C1-O11-P-O14
46	1A	202	PC1	O13-C11-C12-N
46	1B	203	PC1	O13-C11-C12-N
46	1H	401	PC1	C1-O11-P-O14
46	1H	401	PC1	C12-C11-O13-P
46	1H	401	PC1	O13-C11-C12-N
46	1I	201	PC1	C11-O13-P-O14
46	1P	401	PC1	O32-C31-O31-C3
46	1P	401	PC1	C32-C31-O31-C3
46	1Y	201	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	1Z	201	PC1	C1-O11-P-O14
46	1h	203	PC1	C11-O13-P-O14
46	1h	203	PC1	O32-C31-O31-C3
46	1h	203	PC1	C32-C31-O31-C3
46	1m	201	PC1	C11-O13-P-O14
46	1m	201	PC1	C11-O13-P-O11
46	1m	201	PC1	O22-C21-O21-C2
46	1m	201	PC1	C22-C21-O21-C2
46	1q	201	PC1	C11-O13-P-O14
46	1q	201	PC1	O22-C21-O21-C2
46	1q	201	PC1	C22-C21-O21-C2
46	1q	201	PC1	O32-C31-O31-C3
46	1q	201	PC1	C32-C31-O31-C3
51	1L	702	CDL	CB2-OB2-PB2-OB4
51	1N	902	CDL	CA3-OA5-PA1-OA3
51	1X	201	CDL	C1-CA2-OA2-PA1
51	1X	201	CDL	CA2-OA2-PA1-OA5
51	1d	202	CDL	CA2-OA2-PA1-OA4
51	1d	202	CDL	CA3-OA5-PA1-OA2
51	1d	202	CDL	CA3-OA5-PA1-OA4
51	1d	202	CDL	CB3-OB5-PB2-OB2
51	1d	202	CDL	CB3-OB5-PB2-OB3
51	1d	202	CDL	CB3-OB5-PB2-OB4
51	1d	202	CDL	OB5-CB3-CB4-OB6
51	1h	202	CDL	CA2-OA2-PA1-OA5
51	1h	202	CDL	CB3-OB5-PB2-OB2
51	1h	202	CDL	OB7-CB5-OB6-CB4
51	1h	202	CDL	C51-CB5-OB6-CB4
51	1h	202	CDL	OB9-CB7-OB8-CB6
51	1h	202	CDL	C71-CB7-OB8-CB6
52	1O	401	GTP	PB-O3A-PA-O5'
56	1T	101	EHZ	N2-C15-C16-O5
56	1n	201	EHZ	C7-C8-C9-O2
56	1T	101	EHZ	C13-C12-N1-C11
51	1N	902	CDL	C51-CB5-OB6-CB4
51	1N	902	CDL	OB7-CB5-OB6-CB4
52	1O	401	GTP	C3'-C4'-C5'-O5'
56	1T	101	EHZ	O3-C12-N1-C11
46	1H	401	PC1	C22-C23-C24-C25
46	1P	401	PC1	C21-C22-C23-C24
52	1O	401	GTP	O4'-C4'-C5'-O5'
51	1d	202	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	1q	202	CDL	CA5-C11-C12-C13
45	1J	201	3PE	C1-O11-P-O13
45	1Y	202	3PE	C1-O11-P-O13
45	1Y	205	3PE	C1-O11-P-O13
45	1Y	205	3PE	C11-O13-P-O11
46	1H	401	PC1	C11-O13-P-O11
46	1H	401	PC1	C1-O11-P-O13
51	1L	702	CDL	CB2-OB2-PB2-OB5
51	1d	202	CDL	CA2-OA2-PA1-OA5
51	1q	202	CDL	C14-C15-C16-C17
45	1L	703	3PE	C33-C34-C35-C36
51	1d	202	CDL	C42-C43-C44-C45
46	1H	401	PC1	C2-C1-O11-P
46	1h	203	PC1	C2-C1-O11-P
51	1L	702	CDL	C37-C38-C39-C40
46	1I	201	PC1	C31-C32-C33-C34
45	1Y	205	3PE	C2D-C2E-C2F-C2G
45	1L	703	3PE	C39-C3A-C3B-C3C
45	1d	201	3PE	C32-C33-C34-C35
45	1d	201	3PE	C23-C24-C25-C26
46	1Y	201	PC1	C32-C33-C34-C35
54	1P	402	NDP	O4D-C1D-N1N-C6N
46	1B	202	PC1	C38-C39-C3A-C3B
46	1h	203	PC1	C32-C33-C34-C35
46	1q	201	PC1	C2A-C2B-C2C-C2D
45	1M	504	3PE	C2B-C2C-C2D-C2E
56	1T	101	EHZ	C21-C22-C23-C24
46	1M	503	PC1	C21-C22-C23-C24
51	1L	702	CDL	C33-C34-C35-C36
45	1N	901	3PE	C31-C32-C33-C34
46	1M	503	PC1	C32-C33-C34-C35
46	1A	202	PC1	C21-C22-C23-C24
46	1m	201	PC1	C22-C23-C24-C25
46	1B	203	PC1	C32-C33-C34-C35
51	1X	201	CDL	C58-C59-C60-C61
45	1N	901	3PE	O11-C1-C2-O21
46	1M	503	PC1	C2A-C2B-C2C-C2D
45	1Y	202	3PE	O21-C2-C3-O31
51	1N	902	CDL	OA6-CA4-CA6-OA8
45	1M	502	3PE	C2D-C2E-C2F-C2G
51	1X	201	CDL	C19-C20-C21-C22
45	1M	504	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
45	1d	201	3PE	C26-C27-C28-C29
45	1Y	205	3PE	C29-C2A-C2B-C2C
45	1A	201	3PE	C1-O11-P-O13
45	1M	502	3PE	C1-O11-P-O13
51	1L	702	CDL	CA2-OA2-PA1-OA5
45	1L	703	3PE	C2-C1-O11-P
45	1Y	203	3PE	C2-C1-O11-P
51	1h	202	CDL	C1-CB2-OB2-PB2
45	1Y	203	3PE	O11-C1-C2-C3
46	1P	401	PC1	O11-C1-C2-C3
46	1I	201	PC1	C2B-C2C-C2D-C2E
45	1N	901	3PE	C28-C29-C2A-C2B
45	1L	701	3PE	C28-C29-C2A-C2B
45	1Y	203	3PE	C1-C2-C3-O31
46	1P	401	PC1	C1-C2-C3-O31
46	1h	203	PC1	C1-C2-C3-O31
51	1X	201	CDL	CB3-CB4-CB6-OB8
51	1d	202	CDL	CA3-CA4-CA6-OA8
45	1M	504	3PE	C26-C27-C28-C29
56	1T	101	EHZ	O4-C15-C16-O5
46	1M	503	PC1	C23-C24-C25-C26
45	1N	901	3PE	C32-C33-C34-C35
45	1N	903	3PE	C35-C36-C37-C38
46	1h	203	PC1	C2A-C2B-C2C-C2D
46	1m	201	PC1	C23-C24-C25-C26
51	1N	902	CDL	C32-C31-CA7-OA8
46	1Y	201	PC1	O21-C2-C3-O31
45	1J	201	3PE	C34-C35-C36-C37
45	1Y	203	3PE	O31-C31-C32-C33
51	1d	202	CDL	C12-C11-CA5-OA6
51	1X	201	CDL	C18-C19-C20-C21
45	1N	901	3PE	O11-C1-C2-C3
45	1Y	202	3PE	O11-C1-C2-C3
51	1d	202	CDL	OB5-CB3-CB4-CB6
56	1T	101	EHZ	O4-C15-C16-C17
51	1X	201	CDL	CA7-C31-C32-C33
45	1A	201	3PE	O31-C31-C32-C33
45	1A	201	3PE	O21-C21-C22-C23
51	1q	202	CDL	C52-C51-CB5-OB6
49	1F	501	FMN	C4'-C5'-O5'-P
51	1X	201	CDL	C1-CB2-OB2-PB2
51	1d	202	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
51	1d	202	CDL	CA4-CA3-OA5-PA1
51	1X	201	CDL	C61-C62-C63-C64
45	1L	703	3PE	C1-C2-C3-O31
51	1N	902	CDL	CA3-CA4-CA6-OA8
45	1L	703	3PE	C28-C29-C2A-C2B
45	1M	501	3PE	C1-O11-P-O13
46	1P	401	PC1	C11-O13-P-O11
45	1J	201	3PE	C3A-C3B-C3C-C3D
45	1Y	203	3PE	O11-C1-C2-O21
45	1d	201	3PE	O21-C21-C22-C23
46	1B	202	PC1	O31-C31-C32-C33
45	1L	703	3PE	O21-C2-C3-O31
45	1Y	203	3PE	O21-C2-C3-O31
45	1d	201	3PE	O21-C2-C3-O31
51	1X	201	CDL	OB6-CB4-CB6-OB8
51	1N	902	CDL	C12-C13-C14-C15
51	1X	201	CDL	C36-C37-C38-C39
51	1d	202	CDL	CB4-CB3-OB5-PB2
52	1O	401	GTP	C4'-C5'-O5'-PA
45	1Y	202	3PE	C23-C24-C25-C26
45	1d	201	3PE	C2C-C2D-C2E-C2F
51	1L	702	CDL	C11-C12-C13-C14
45	1N	903	3PE	C1-C2-C3-O31
45	1Y	205	3PE	C2-C1-O11-P
46	1B	203	PC1	C1-C2-C3-O31
46	1Y	201	PC1	C1-C2-C3-O31
46	1B	203	PC1	O11-C1-C2-O21
56	1T	101	EHZ	C15-C16-C17-C19
45	1M	502	3PE	O21-C2-C3-O31
46	1B	203	PC1	O21-C2-C3-O31
51	1d	202	CDL	OA6-CA4-CA6-OA8
46	1B	203	PC1	C24-C25-C26-C27
45	1M	502	3PE	C24-C25-C26-C27
46	1h	203	PC1	C2B-C2C-C2D-C2E
46	1I	201	PC1	C32-C33-C34-C35
51	1X	201	CDL	C12-C11-CA5-OA6
45	1A	201	3PE	C36-C37-C38-C39
45	1Y	203	3PE	C23-C24-C25-C26
46	1B	202	PC1	C23-C24-C25-C26
46	1A	202	PC1	C1-O11-P-O13
46	1I	201	PC1	C11-O13-P-O11
46	1Y	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	1Z	201	PC1	C1-O11-P-O13
46	1h	203	PC1	C11-O13-P-O11
46	1q	201	PC1	C11-O13-P-O11
45	1A	201	3PE	C2-C1-O11-P
45	1J	201	3PE	C1-O11-P-O12
45	1N	901	3PE	C11-O13-P-O12
45	1Y	205	3PE	C1-O11-P-O14
46	1H	401	PC1	C11-O13-P-O14
46	1H	401	PC1	C1-O11-P-O12
51	1L	702	CDL	CA2-OA2-PA1-OA4
51	1X	201	CDL	CA2-OA2-PA1-OA4
51	1d	202	CDL	CA2-OA2-PA1-OA3
51	1d	202	CDL	CA3-OA5-PA1-OA3
51	1h	202	CDL	CA2-OA2-PA1-OA4
51	1h	202	CDL	CB3-OB5-PB2-OB4
45	1M	502	3PE	C3F-C3G-C3H-C3I
51	1d	202	CDL	OA5-CA3-CA4-CA6
45	1L	704	3PE	C12-C11-O13-P
45	1M	502	3PE	C12-C11-O13-P
45	1M	504	3PE	C12-C11-O13-P
45	1j	101	3PE	C12-C11-O13-P
46	1B	203	PC1	C12-C11-O13-P
46	1m	201	PC1	C12-C11-O13-P
57	1h	201	AME	CB-CA-N-CT1
51	1X	201	CDL	C31-C32-C33-C34
46	1H	401	PC1	C21-C22-C23-C24
45	1A	201	3PE	C28-C29-C2A-C2B
45	1Y	202	3PE	O11-C1-C2-O21
46	1P	401	PC1	O11-C1-C2-O21
56	1T	101	EHZ	C15-C16-C17-C20
51	1h	202	CDL	C34-C35-C36-C37
45	1M	502	3PE	C1-C2-C3-O31
45	1Y	202	3PE	C1-C2-C3-O31
46	1h	203	PC1	O13-C11-C12-N
46	1m	201	PC1	O13-C11-C12-N
46	1P	401	PC1	O21-C2-C3-O31
46	1h	203	PC1	O21-C2-C3-O31
46	1H	401	PC1	C37-C38-C39-C3A
45	1d	201	3PE	C3C-C3D-C3E-C3F
45	1Y	204	3PE	C2-C1-O11-P
45	1N	901	3PE	C2B-C2C-C2D-C2E
51	1X	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
45	1M	501	3PE	C23-C24-C25-C26
46	1I	201	PC1	C38-C39-C3A-C3B
45	1L	701	3PE	C25-C26-C27-C28
45	1M	501	3PE	C2-C1-O11-P
46	1Y	201	PC1	C2-C1-O11-P
56	1T	101	EHZ	C1-C2-C3-C4
45	1L	704	3PE	C23-C24-C25-C26
45	1L	701	3PE	C11-O13-P-O11
45	1L	704	3PE	C11-O13-P-O11
45	1M	501	3PE	C11-O13-P-O11
45	1M	502	3PE	C11-O13-P-O11
45	1M	504	3PE	C11-O13-P-O11
45	1N	903	3PE	C1-O11-P-O13
45	1Y	203	3PE	C11-O13-P-O11
45	1Y	204	3PE	C11-O13-P-O11
45	1j	101	3PE	C1-O11-P-O13
45	1j	101	3PE	C11-O13-P-O11
46	1B	203	PC1	C1-O11-P-O13
46	1m	201	PC1	C1-O11-P-O13
46	1q	201	PC1	C1-O11-P-O13
51	1N	902	CDL	CA3-OA5-PA1-OA2
51	1d	202	CDL	CB2-OB2-PB2-OB5
51	1q	202	CDL	CA3-OA5-PA1-OA2
51	1q	202	CDL	CB2-OB2-PB2-OB5
45	1M	502	3PE	C21-C22-C23-C24
45	1N	901	3PE	C2D-C2E-C2F-C2G
51	1X	201	CDL	C35-C36-C37-C38
45	1Y	205	3PE	C2A-C2B-C2C-C2D
45	1Y	203	3PE	C21-C22-C23-C24
45	1M	501	3PE	C21-C22-C23-C24
51	1L	702	CDL	CA4-CA3-OA5-PA1
46	1B	202	PC1	C35-C36-C37-C38
46	1M	503	PC1	C2-C1-O11-P
56	1T	101	EHZ	C10-C11-N1-C12
56	1n	201	EHZ	C10-C11-N1-C12
45	1L	704	3PE	C22-C23-C24-C25
45	1A	201	3PE	O32-C31-C32-C33
45	1J	201	3PE	C3D-C3E-C3F-C3G
51	1X	201	CDL	C12-C13-C14-C15
45	1Y	202	3PE	C2D-C2E-C2F-C2G
45	1J	201	3PE	C23-C24-C25-C26
46	1B	203	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
56	1T	101	EHZ	C11-C10-S1-C9
45	1M	501	3PE	C36-C37-C38-C39
45	1d	201	3PE	O22-C21-C22-C23
46	1h	203	PC1	C22-C23-C24-C25
45	1M	502	3PE	C38-C39-C3A-C3B
56	1T	101	EHZ	C1-C21-C22-C23
51	1q	202	CDL	C52-C51-CB5-OB7
46	1I	201	PC1	C34-C35-C36-C37
51	1X	201	CDL	C63-C64-C65-C66
46	1B	202	PC1	O32-C31-C32-C33
45	1L	703	3PE	C29-C2A-C2B-C2C
46	1H	401	PC1	C38-C39-C3A-C3B
46	1M	503	PC1	C28-C29-C2A-C2B
45	1Y	203	3PE	O32-C31-C32-C33
46	1B	203	PC1	C22-C23-C24-C25
46	1Y	201	PC1	C2-C3-O31-C31
45	1J	201	3PE	C28-C29-C2A-C2B
51	1L	702	CDL	C72-C71-CB7-OB8
45	1d	201	3PE	C36-C37-C38-C39
46	1B	202	PC1	C33-C34-C35-C36
45	1L	703	3PE	C34-C35-C36-C37
46	1I	201	PC1	C22-C23-C24-C25
56	1T	101	EHZ	C12-C13-C14-N2
46	1B	202	PC1	C3D-C3E-C3F-C3G
45	1d	201	3PE	C1-C2-C3-O31
51	1N	902	CDL	C32-C31-CA7-OA9
45	1M	504	3PE	C3A-C3B-C3C-C3D
46	1m	201	PC1	O21-C21-C22-C23
51	1d	202	CDL	C12-C11-CA5-OA7
56	1T	101	EHZ	C15-C16-C17-C18
45	1Y	203	3PE	O21-C21-C22-C23
45	1Y	205	3PE	C26-C27-C28-C29
46	1I	201	PC1	O21-C2-C3-O31
51	1N	902	CDL	OB6-CB4-CB6-OB8
46	1P	401	PC1	O21-C21-C22-C23
45	1N	901	3PE	O31-C31-C32-C33
45	1L	703	3PE	C25-C26-C27-C28
46	1q	201	PC1	C34-C35-C36-C37
45	1L	704	3PE	O21-C21-C22-C23
54	1P	402	NDP	O4B-C4B-C5B-O5B
45	1A	201	3PE	O22-C21-C22-C23
45	1M	501	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
45	1L	704	3PE	O22-C21-C22-C23
46	1B	203	PC1	C23-C24-C25-C26
57	1h	201	AME	C-CA-N-CT1
46	1P	401	PC1	O22-C21-C22-C23
51	1N	902	CDL	CB3-CB4-CB6-OB8
45	1J	201	3PE	C11-O13-P-O11
51	1L	702	CDL	C72-C71-CB7-OB9
45	1A	201	3PE	C1-O11-P-O12
45	1J	201	3PE	C11-O13-P-O14
45	1L	701	3PE	C11-O13-P-O14
45	1L	704	3PE	C11-O13-P-O14
46	1B	203	PC1	C1-O11-P-O14
46	1I	201	PC1	C11-O13-P-O12
51	1d	202	CDL	CB2-OB2-PB2-OB3
51	1q	202	CDL	CA3-OA5-PA1-OA3
54	1P	402	NDP	C2N-C3N-C7N-N7N
51	1q	202	CDL	C53-C54-C55-C56
46	1M	503	PC1	O22-C21-C22-C23
45	1Y	203	3PE	O22-C21-C22-C23
46	1Y	201	PC1	O22-C21-C22-C23
46	1m	201	PC1	O22-C21-C22-C23
51	1L	702	CDL	C32-C31-CA7-OA8
46	1H	401	PC1	C2C-C2D-C2E-C2F
46	1B	202	PC1	C37-C38-C39-C3A
45	1N	901	3PE	O32-C31-C32-C33
45	1M	502	3PE	C3-C2-O21-C21
45	1Y	205	3PE	C12-C11-O13-P
45	1d	201	3PE	C12-C11-O13-P
46	1A	202	PC1	C12-C11-O13-P
46	1m	201	PC1	C3-C2-O21-C21
45	1N	901	3PE	C34-C35-C36-C37
46	1M	503	PC1	O21-C21-C22-C23
51	1q	202	CDL	C12-C11-CA5-OA6
45	1N	901	3PE	C23-C24-C25-C26
45	1d	201	3PE	O31-C31-C32-C33
46	1h	203	PC1	O31-C31-C32-C33
51	1L	702	CDL	CA2-C1-CB2-OB2
56	1T	101	EHZ	S1-C10-C11-N1
45	1Y	205	3PE	C23-C24-C25-C26
45	1Y	205	3PE	O31-C31-C32-C33
46	1B	202	PC1	O21-C21-C22-C23
46	1Y	201	PC1	O21-C21-C22-C23

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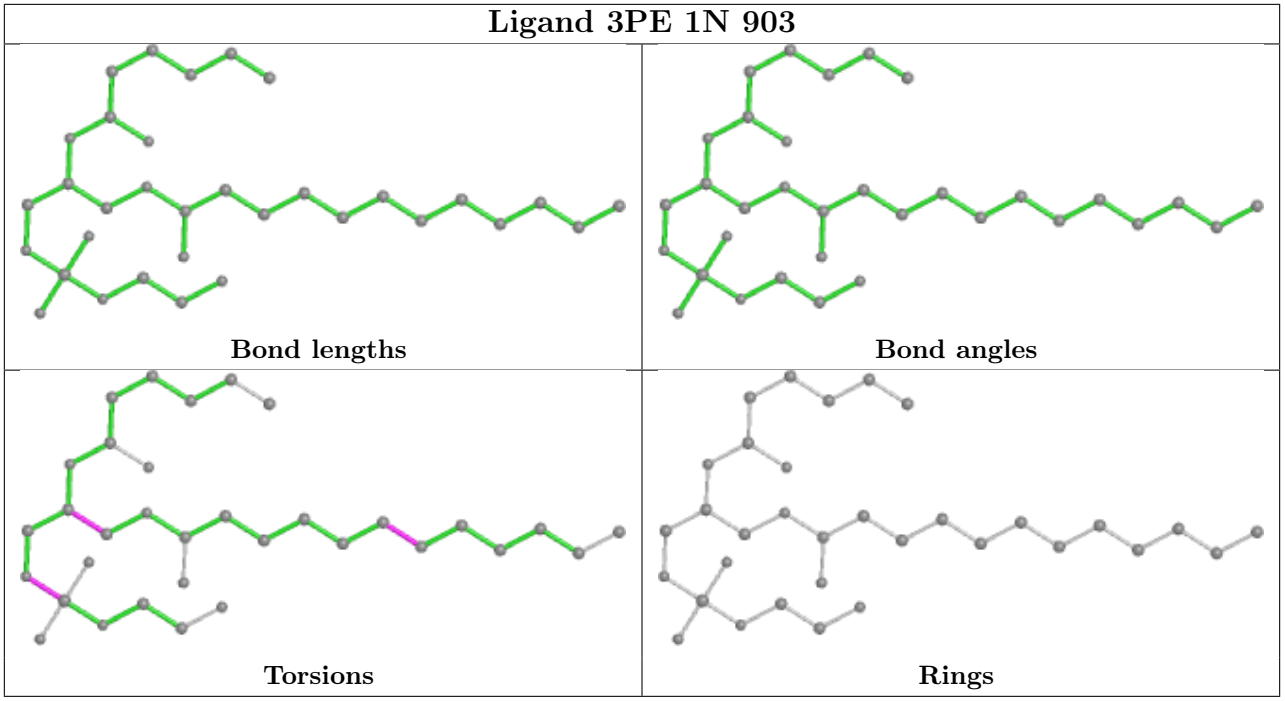
Mol	Chain	Res	Type	Atoms
51	1d	202	CDL	C32-C31-CA7-OA8
51	1L	702	CDL	C36-C37-C38-C39
45	1d	201	3PE	O32-C31-C32-C33
51	1d	202	CDL	C32-C31-CA7-OA9
45	1M	501	3PE	O31-C31-C32-C33
51	1N	902	CDL	C72-C71-CB7-OB8
46	1h	203	PC1	O32-C31-C32-C33
46	1B	203	PC1	C2A-C2B-C2C-C2D

There are no ring outliers.

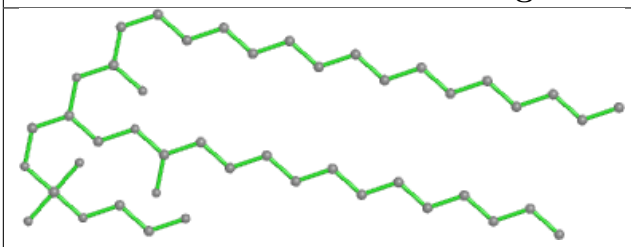
No monomer is involved in short contacts.

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

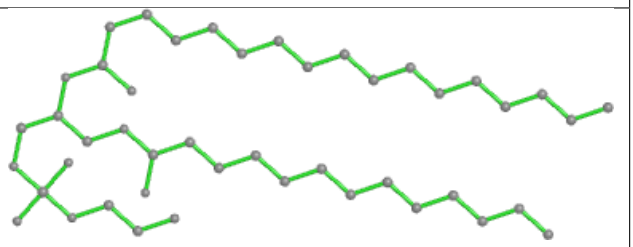
Ligand 3PE 1N 903



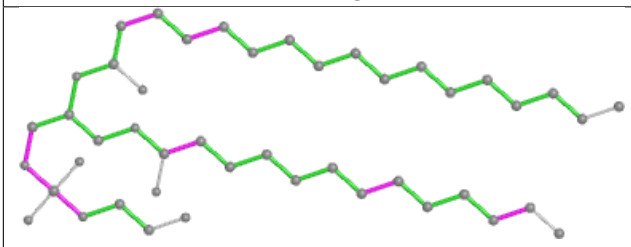
Ligand 3PE 1M 501



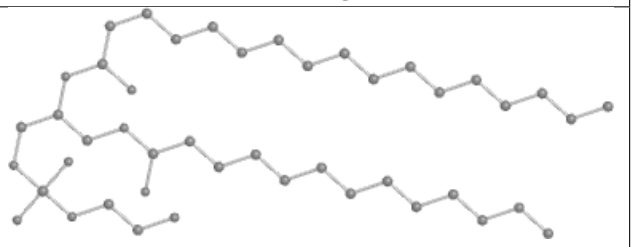
Bond lengths



Bond angles

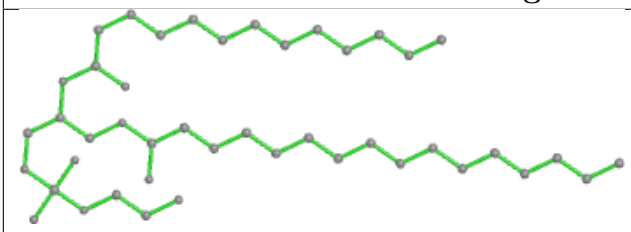


Torsions

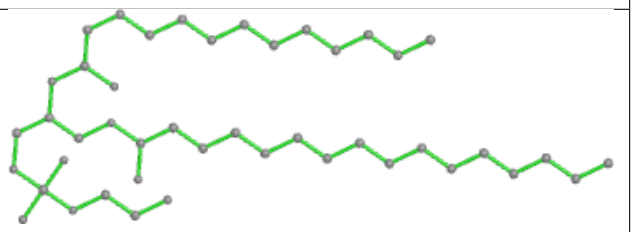


Rings

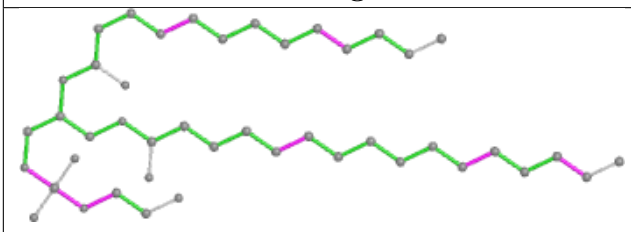
Ligand 3PE 1J 201



Bond lengths



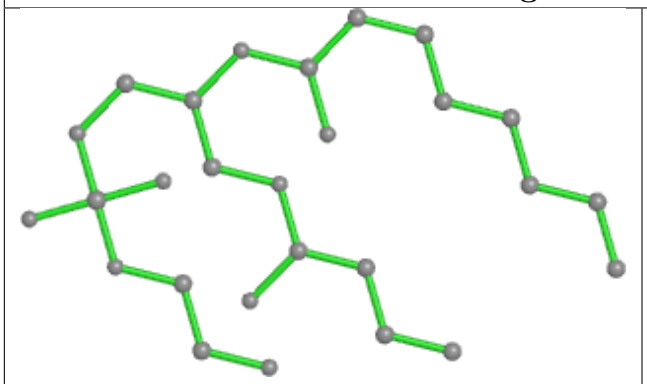
Bond angles



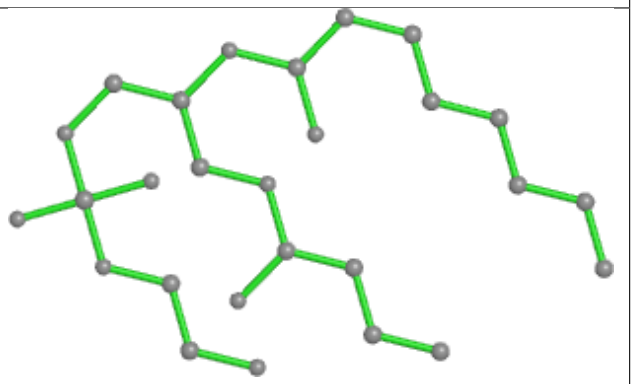
Torsions

Rings

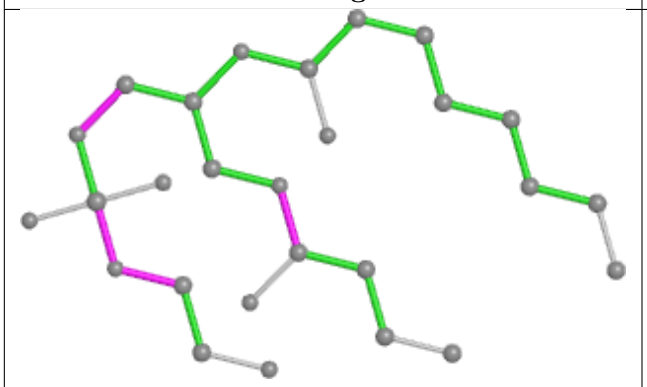
Ligand 3PE 1Y 204



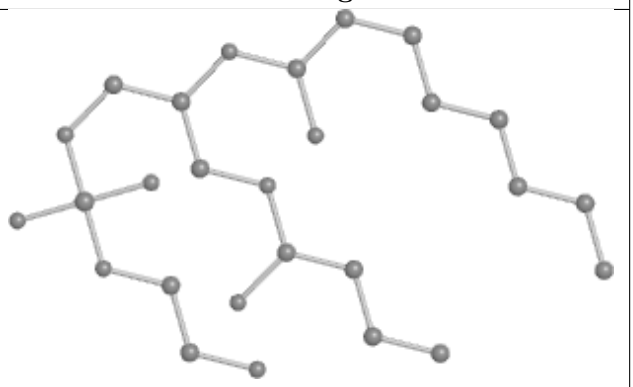
Bond lengths



Bond angles

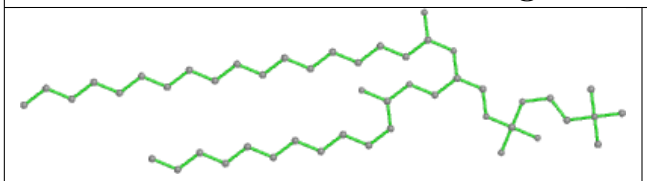


Torsions

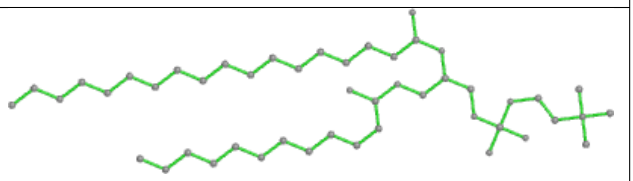


Rings

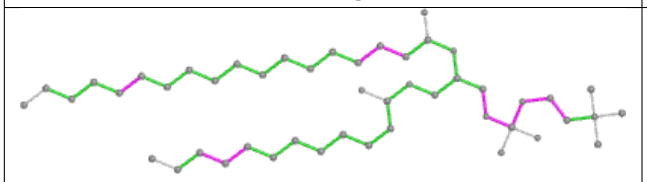
Ligand PC1 1H 401



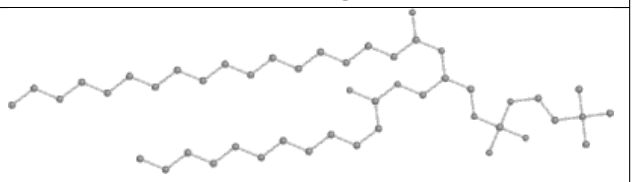
Bond lengths



Bond angles

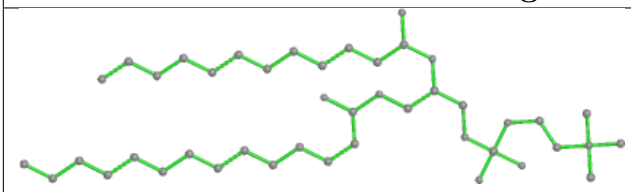


Torsions

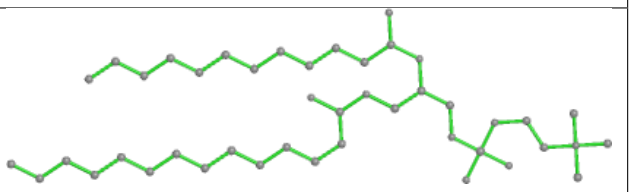


Rings

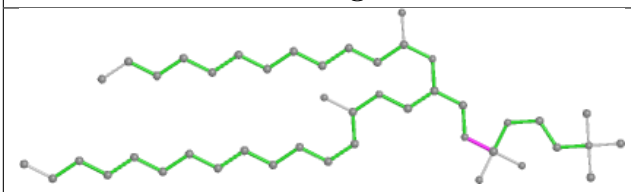
Ligand PC1 1Z 201



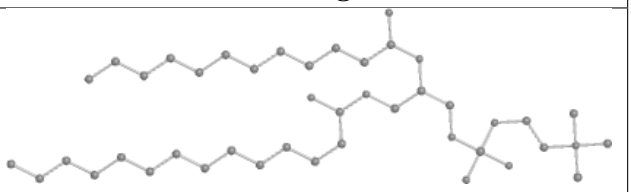
Bond lengths



Bond angles

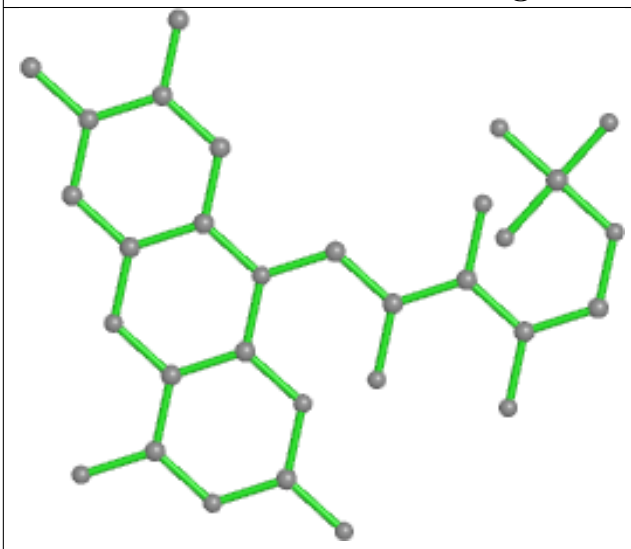


Torsions

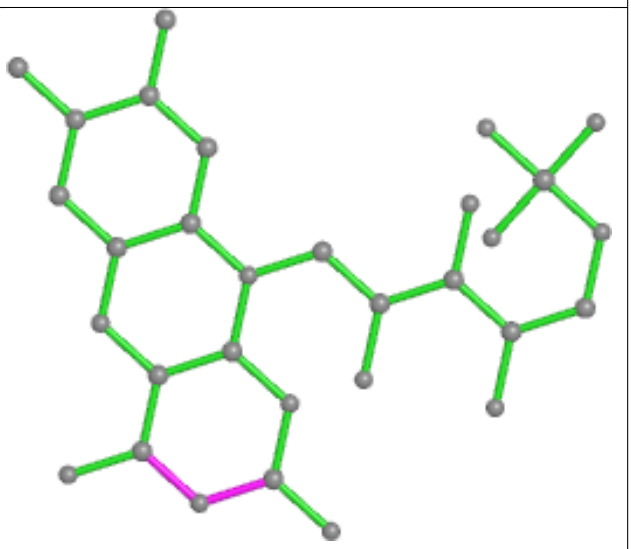


Rings

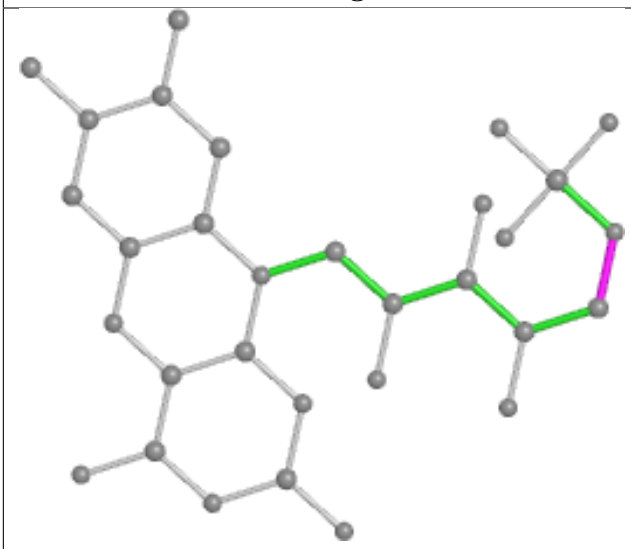
Ligand FMN 1F 501



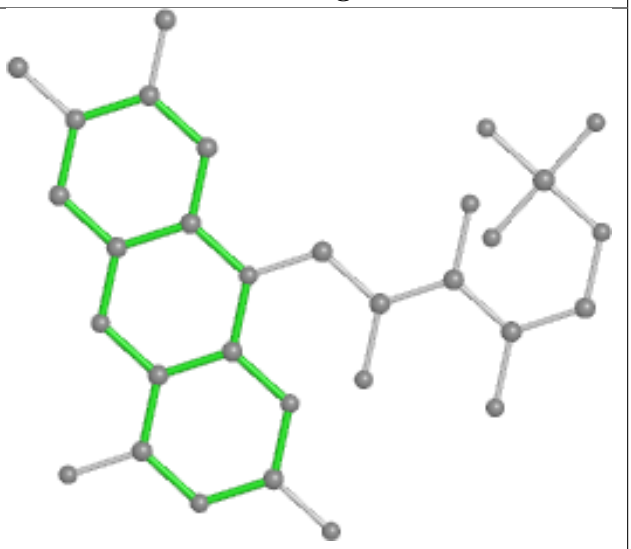
Bond lengths



Bond angles

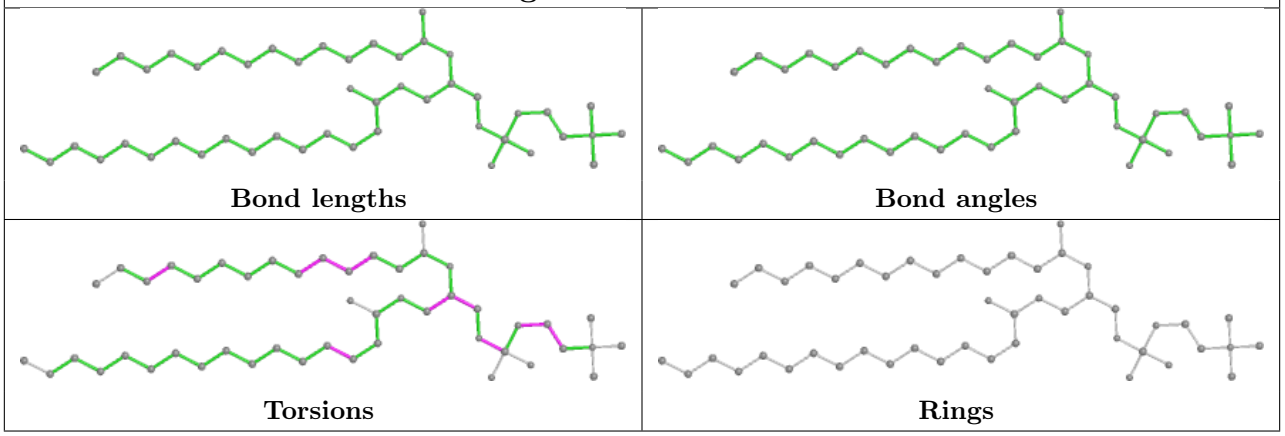


Torsions

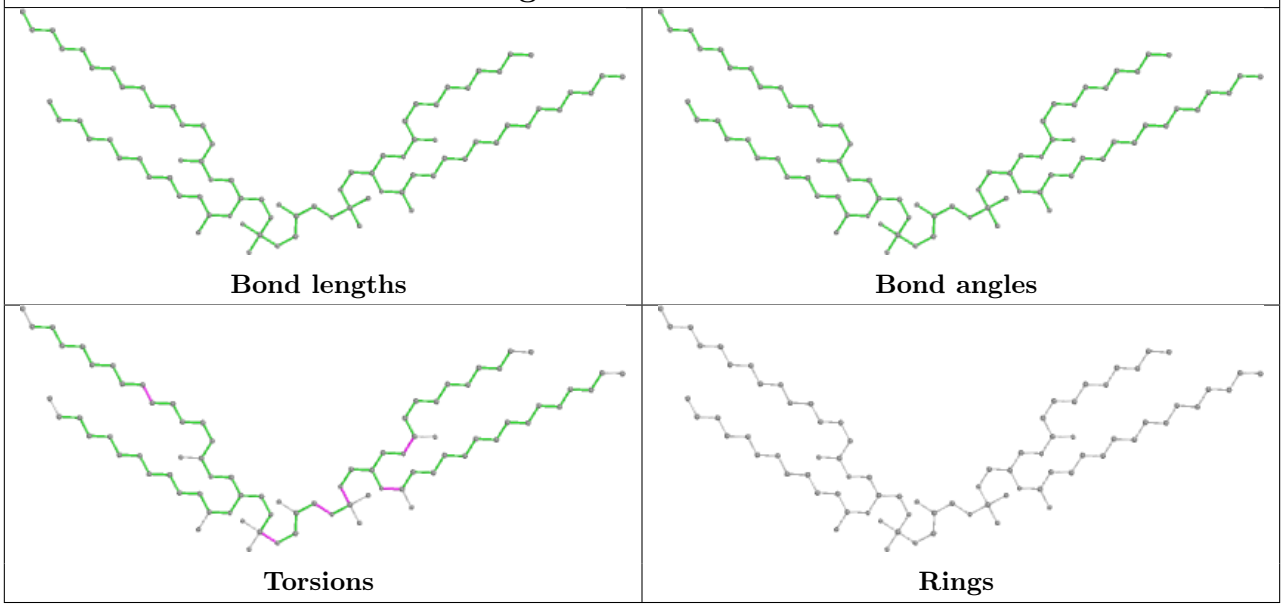


Rings

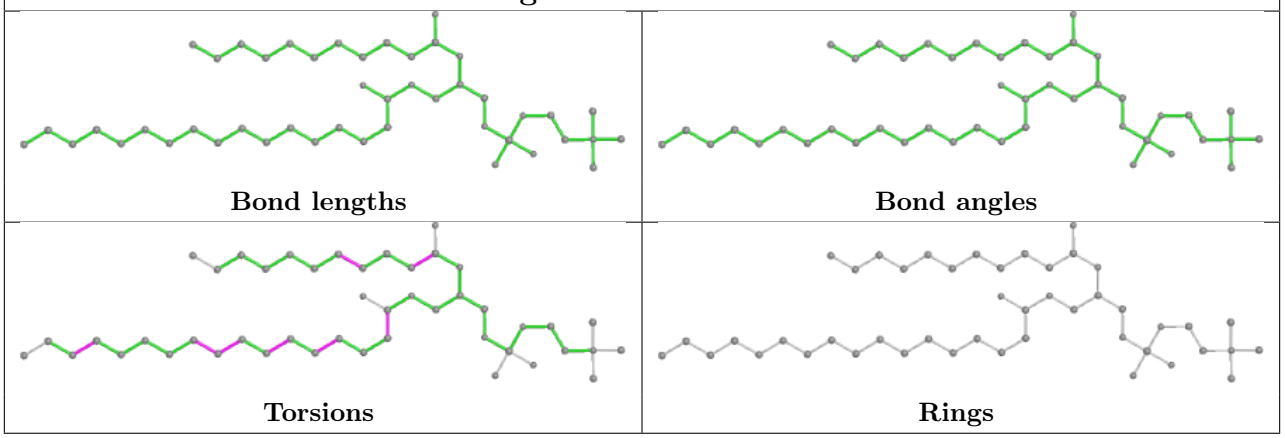
Ligand PC1 1B 203



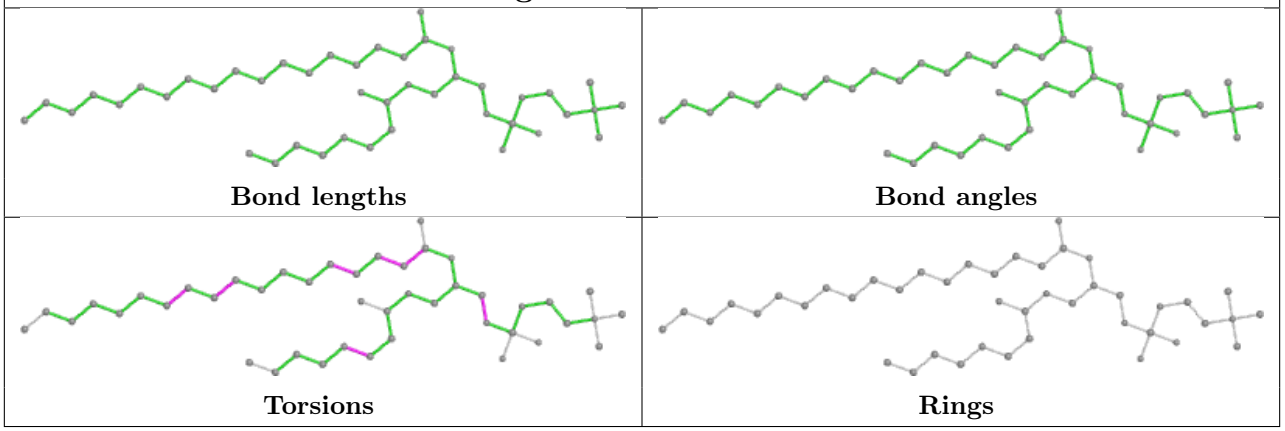
Ligand CDL 1h 202



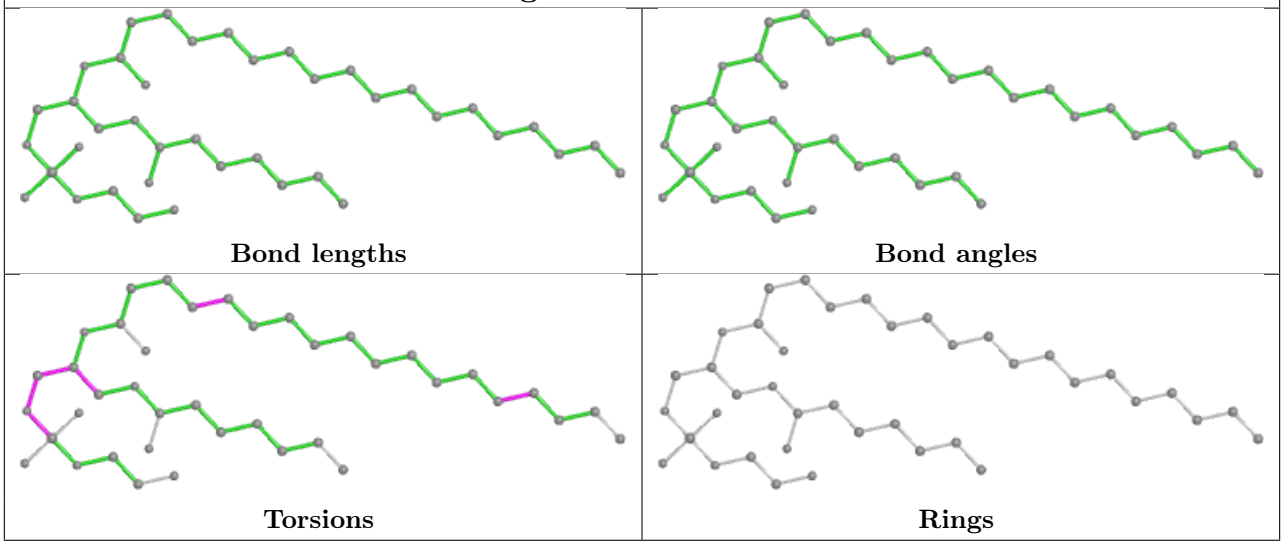
Ligand PC1 1B 202



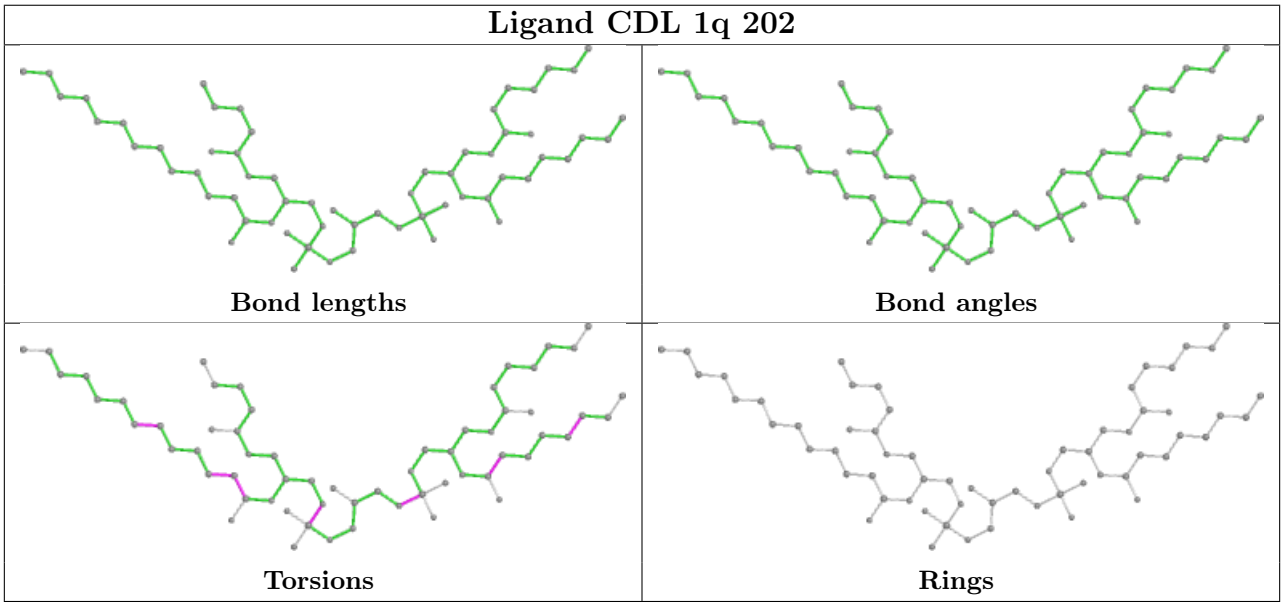
Ligand PC1 1M 503



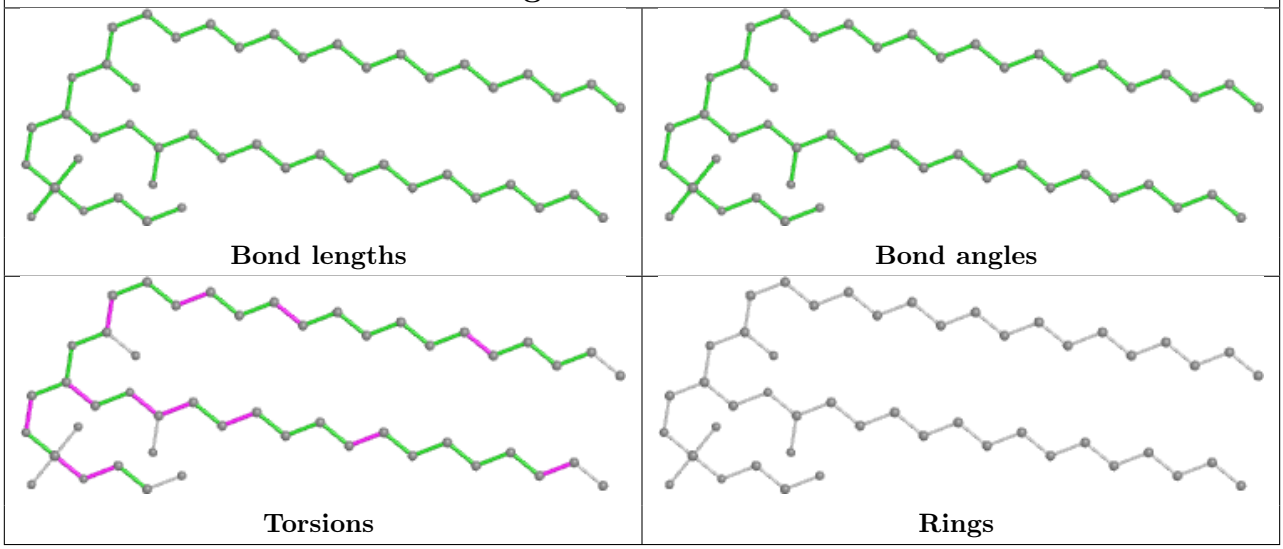
Ligand 3PE 1Y 202



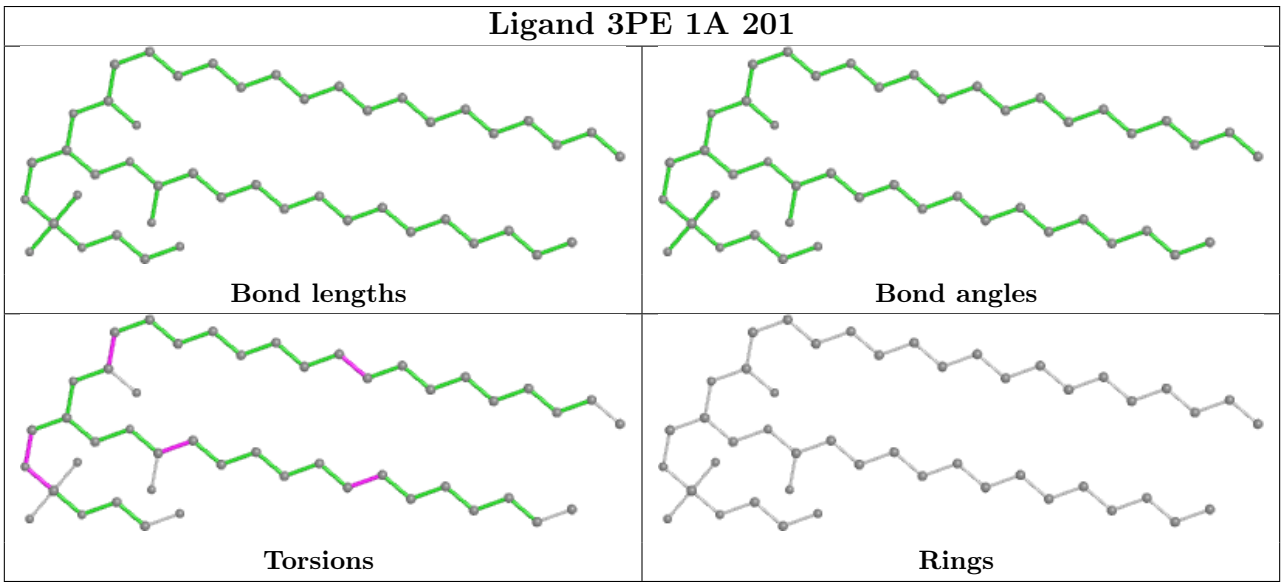
Ligand CDL 1q 202



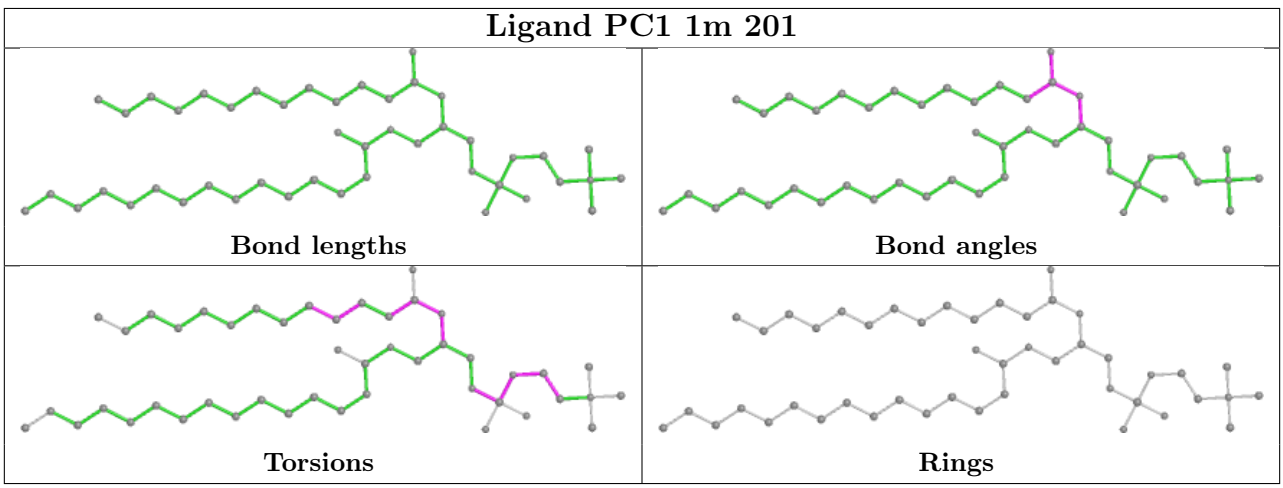
Ligand 3PE 1d 201



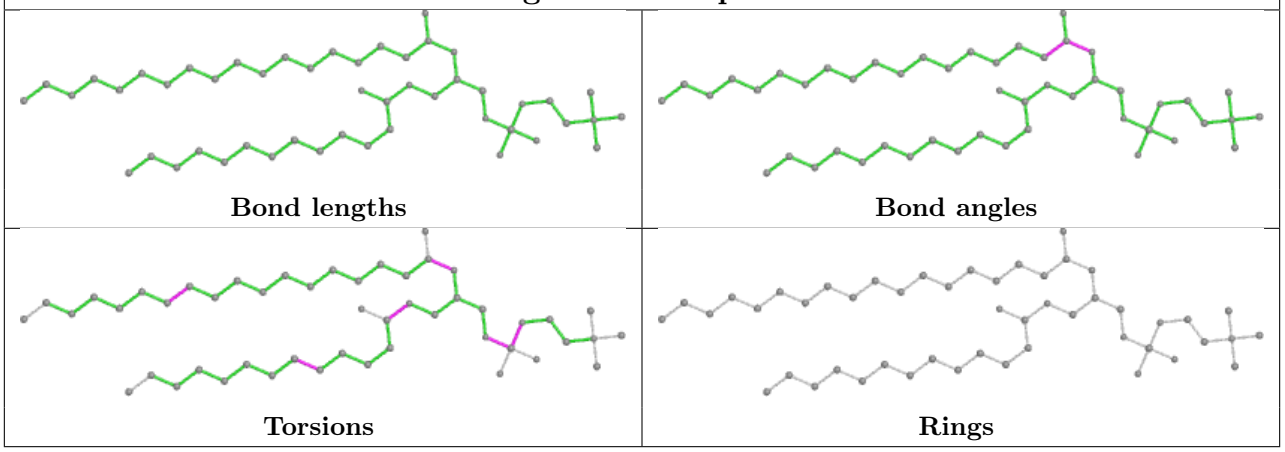
Ligand 3PE 1A 201



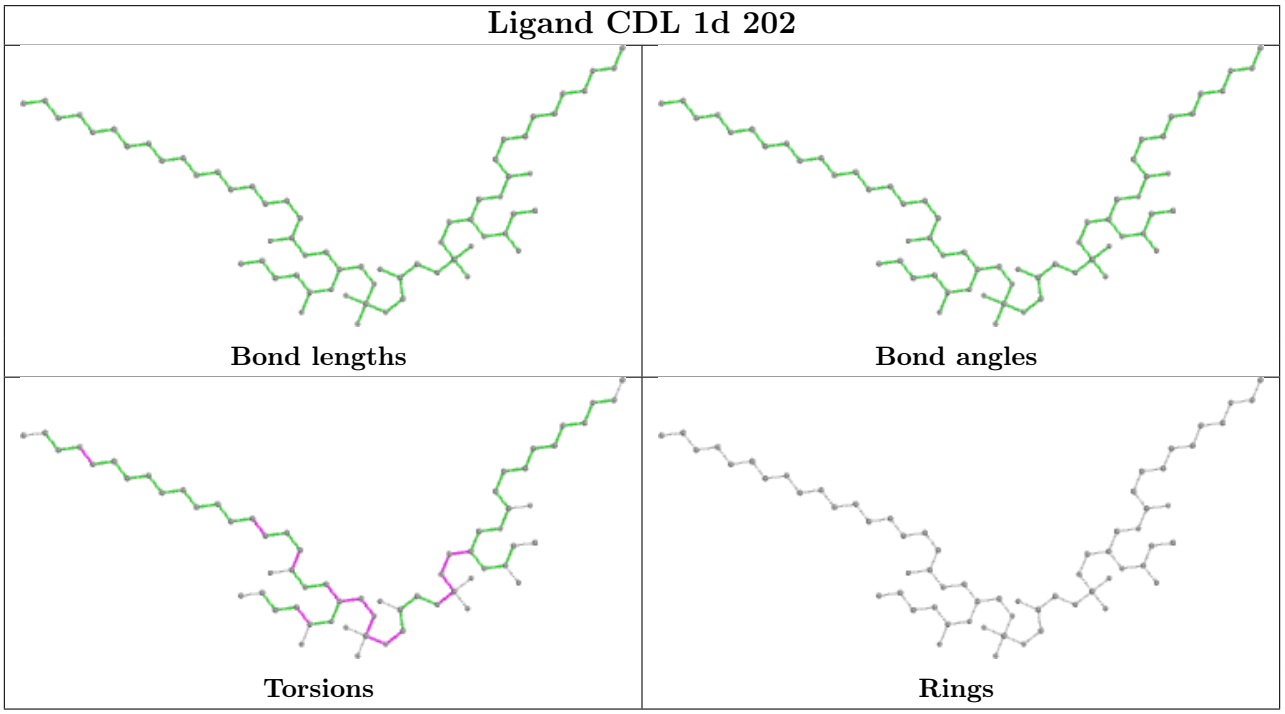
Ligand PC1 1m 201



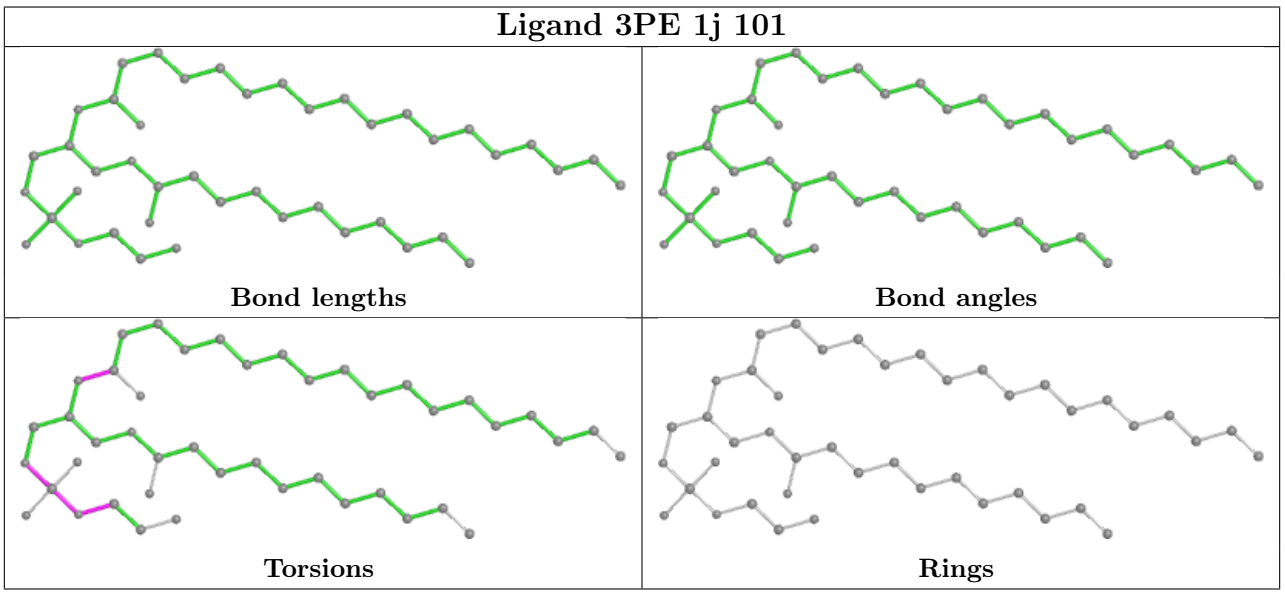
Ligand PC1 1q 201



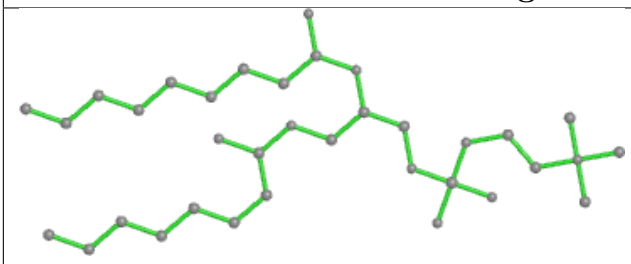
Ligand CDL 1d 202



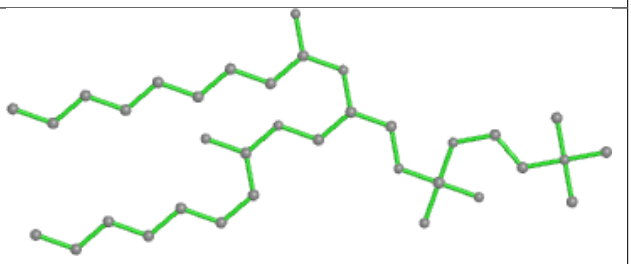
Ligand 3PE 1j 101



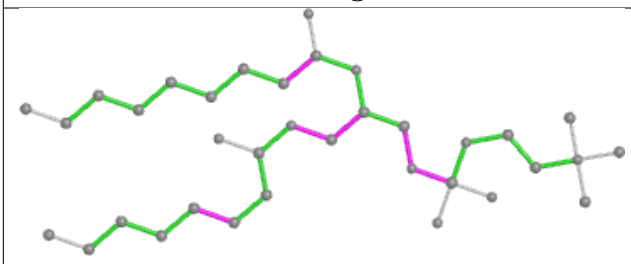
Ligand PC1 1Y 201



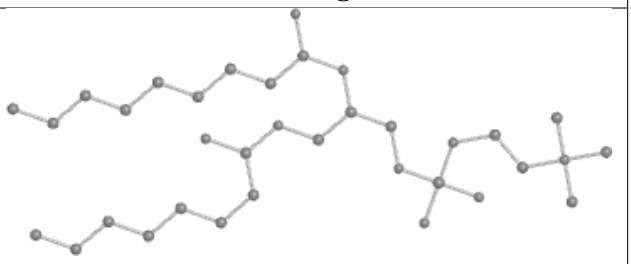
Bond lengths



Bond angles

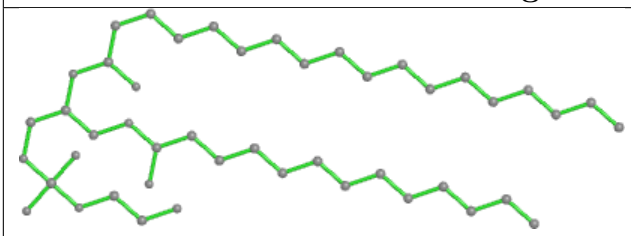


Torsions

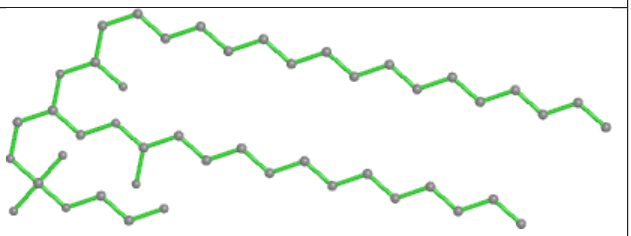


Rings

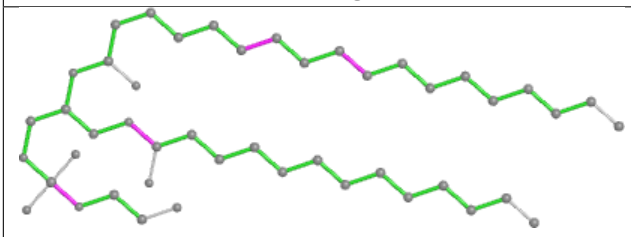
Ligand 3PE 1L 701



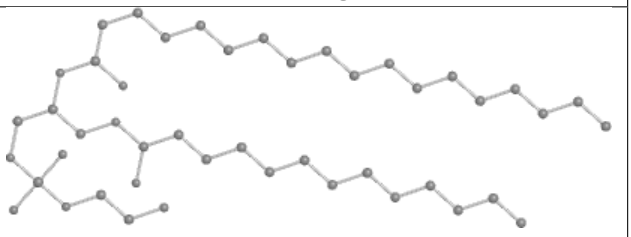
Bond lengths



Bond angles

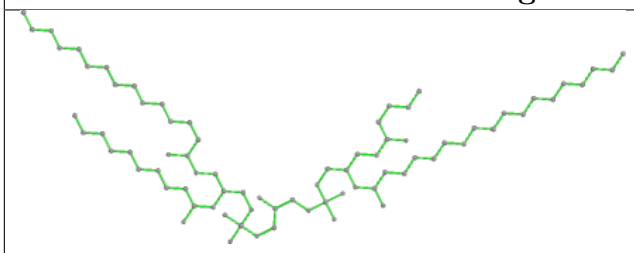


Torsions

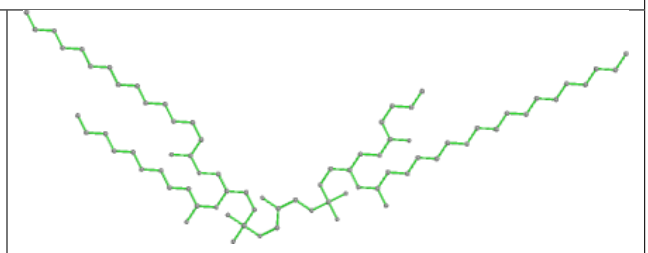


Rings

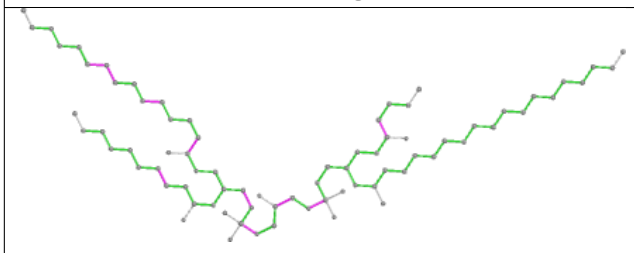
Ligand CDL 1L 702



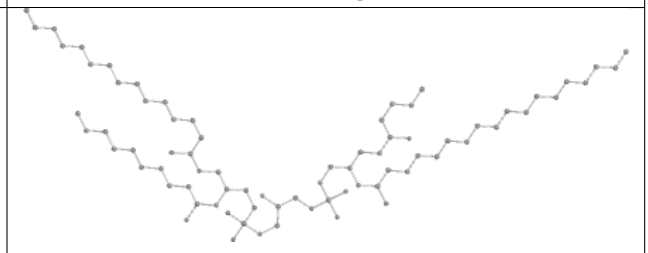
Bond lengths



Bond angles

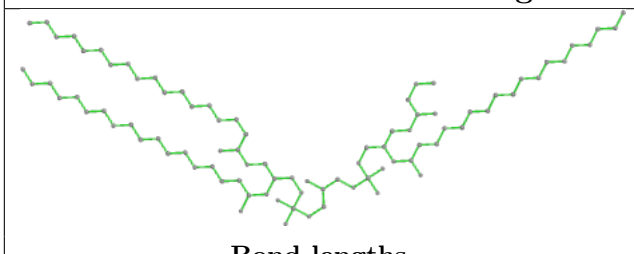


Torsions

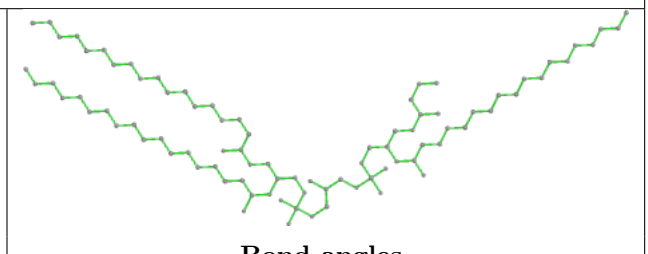


Rings

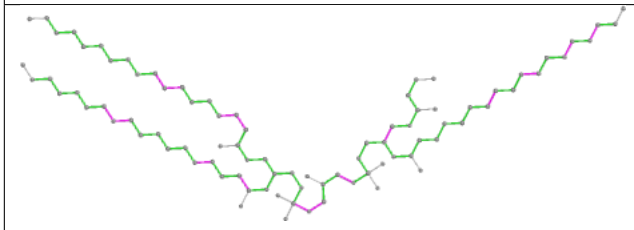
Ligand CDL 1X 201



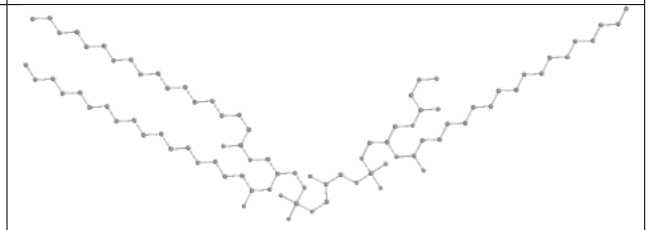
Bond lengths



Bond angles

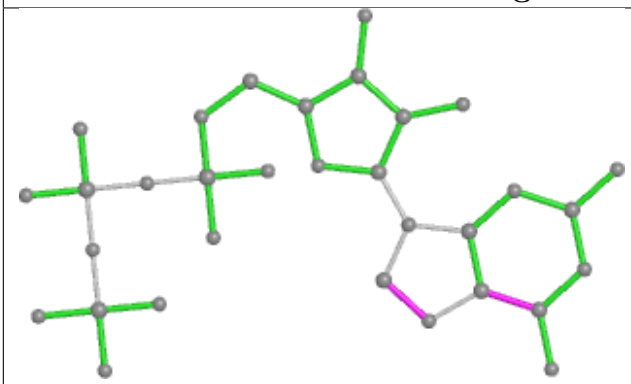


Torsions

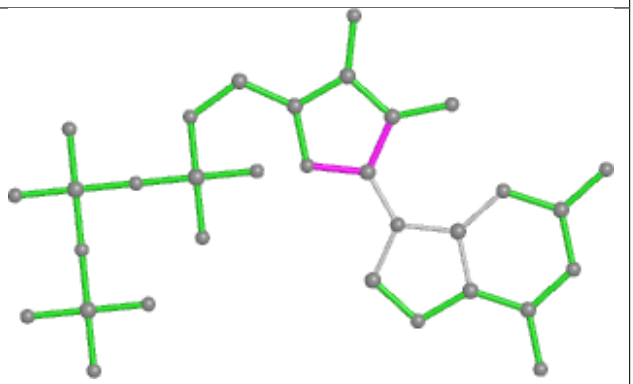


Rings

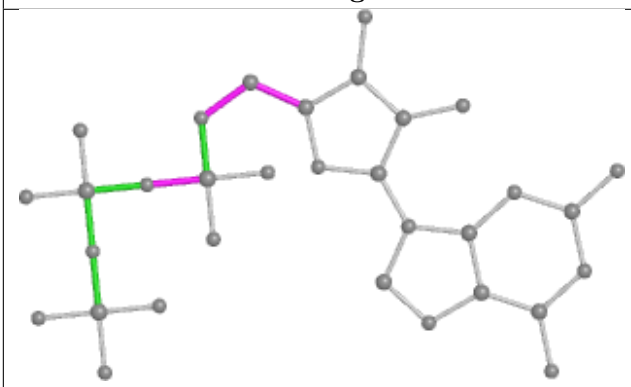
Ligand GTP 1O 401



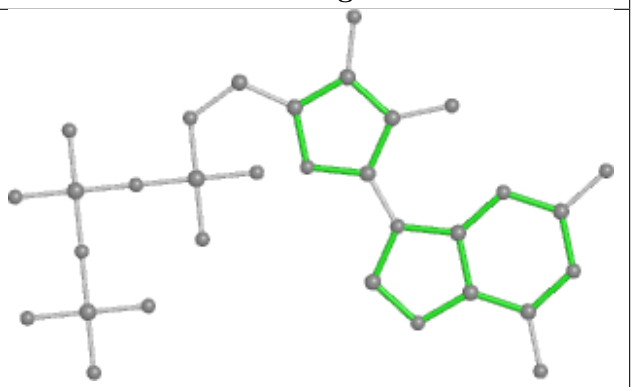
Bond lengths



Bond angles

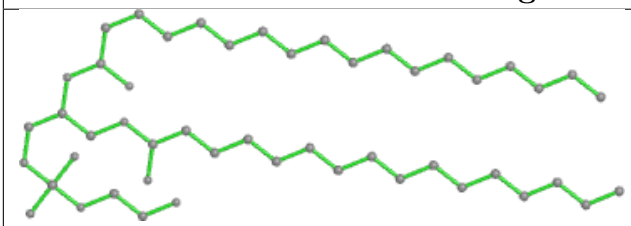


Torsions

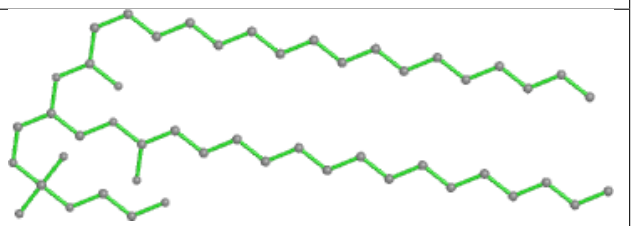


Rings

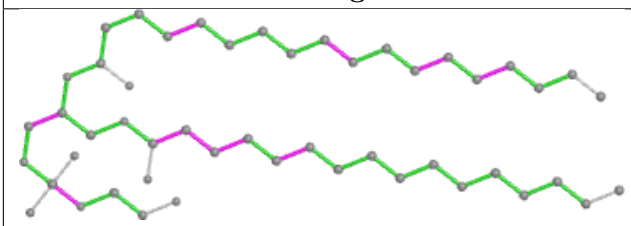
Ligand 3PE 1N 901



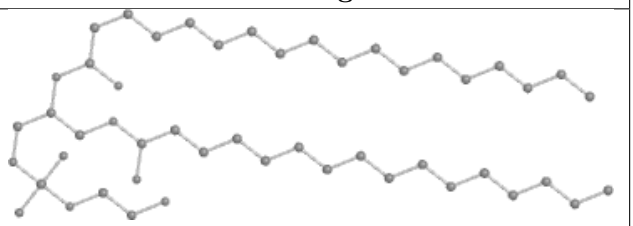
Bond lengths



Bond angles

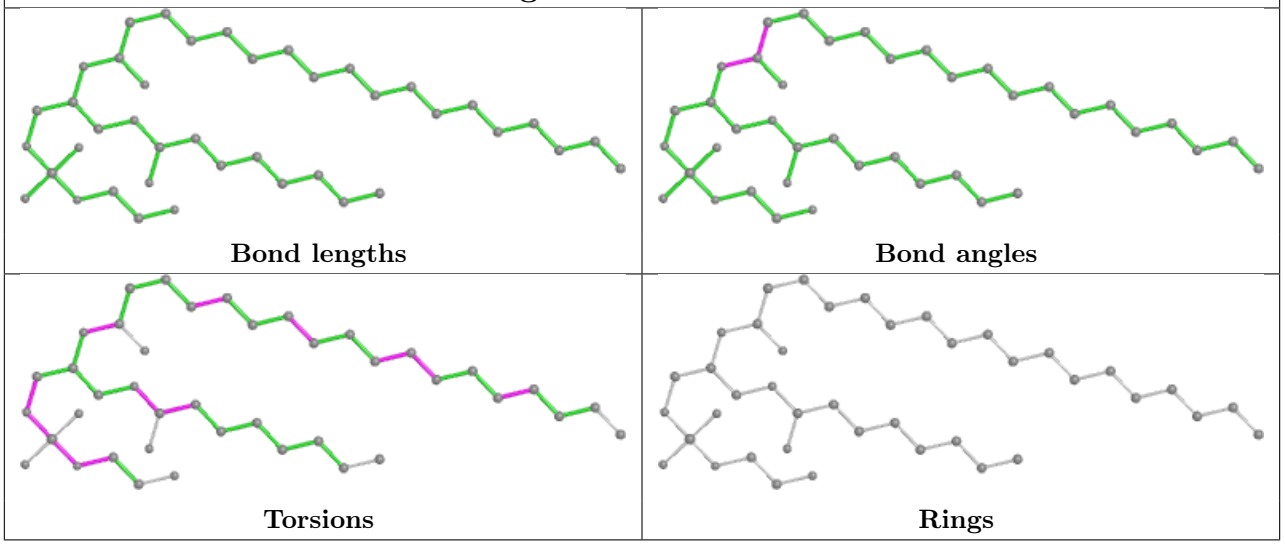


Torsions

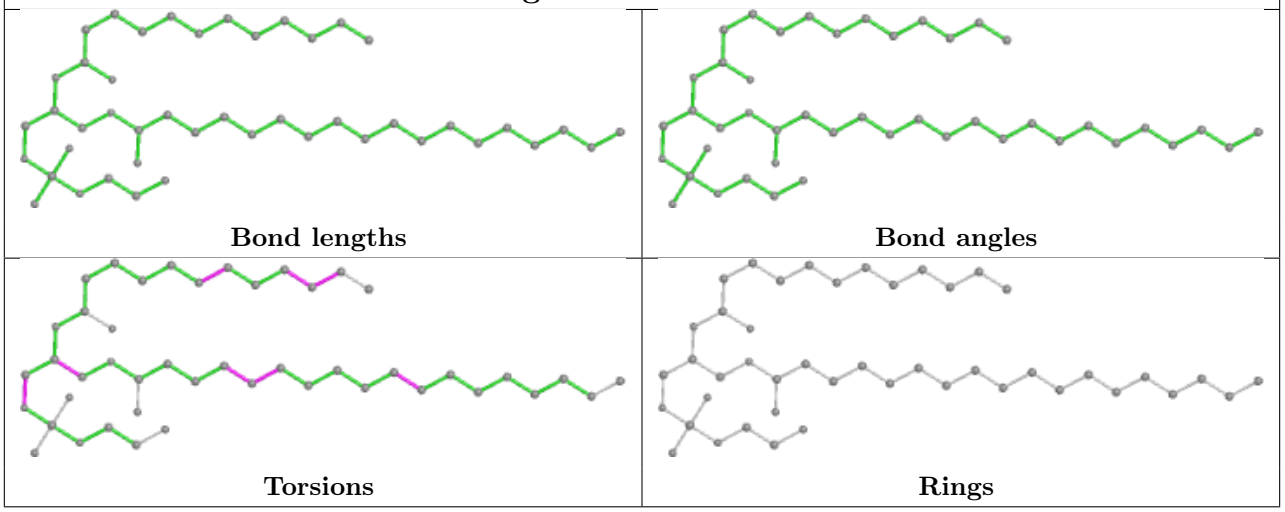


Rings

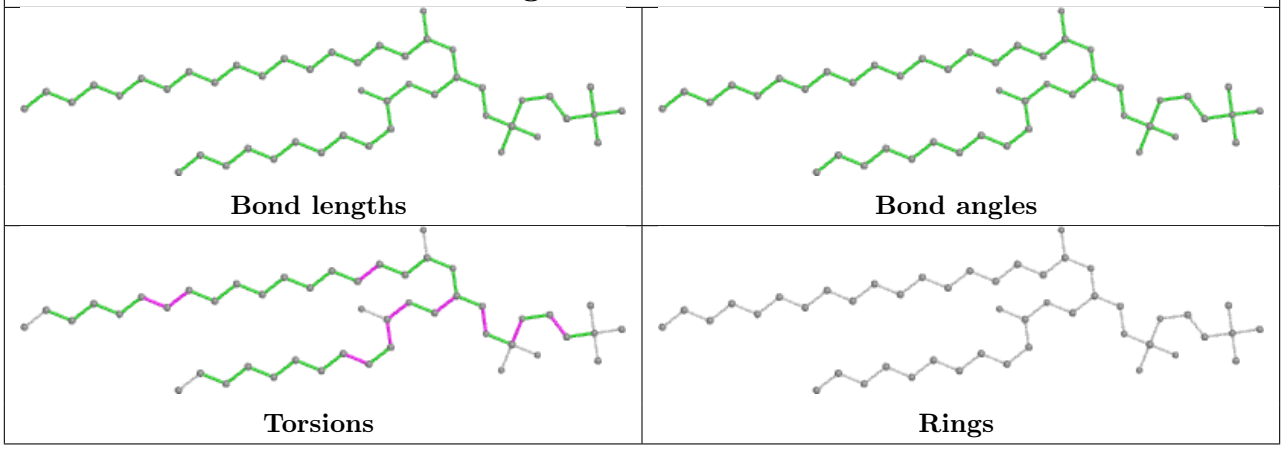
Ligand 3PE 1Y 205



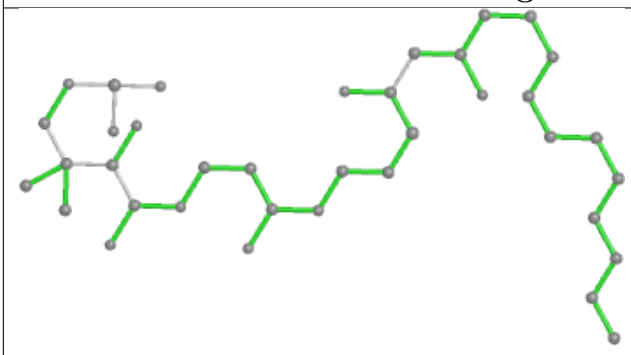
Ligand 3PE 1L 703



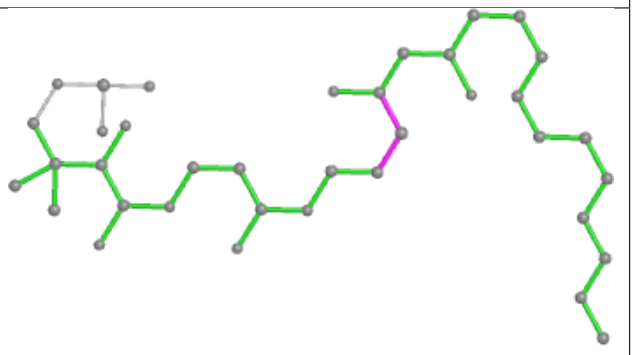
Ligand PC1 1h 203



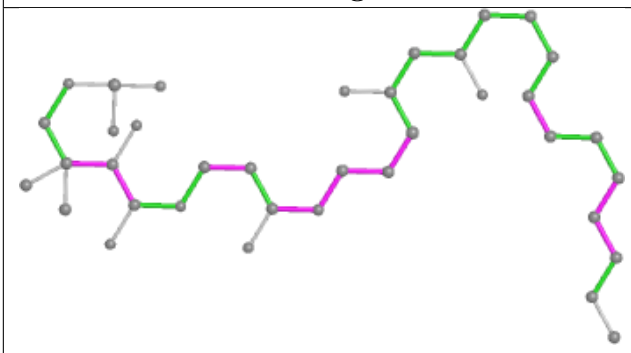
Ligand EHZ 1T 101



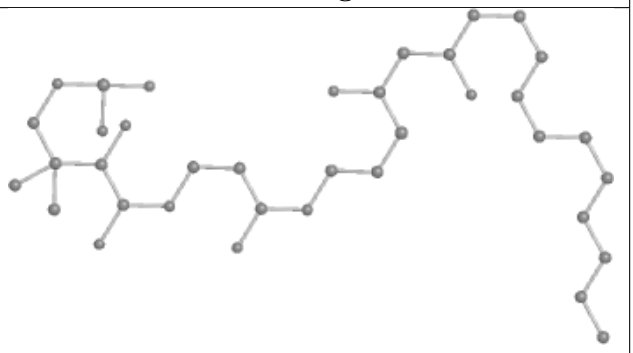
Bond lengths



Bond angles

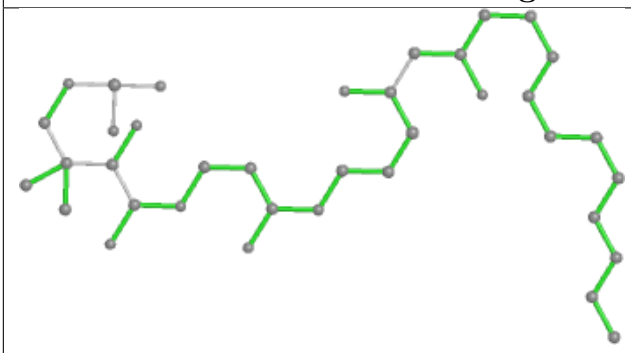


Torsions

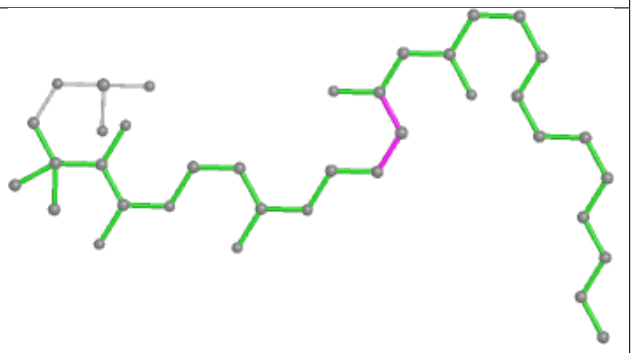


Rings

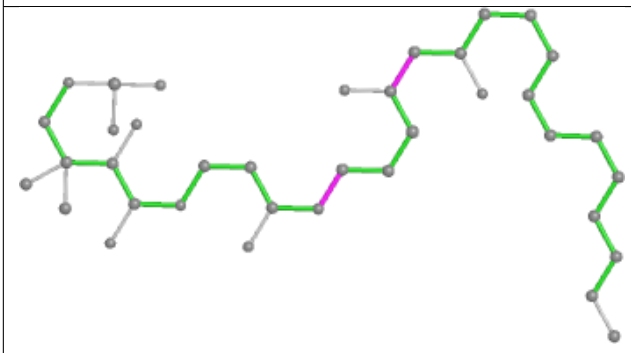
Ligand EHZ 1n 201



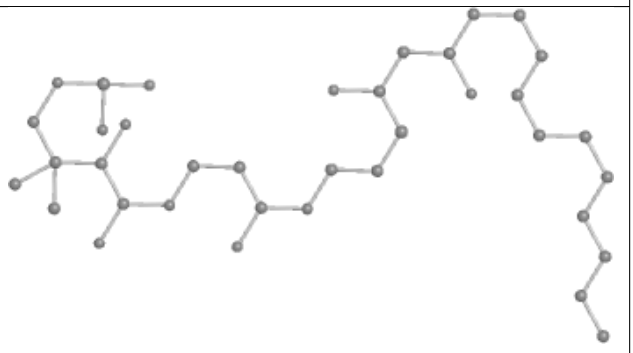
Bond lengths



Bond angles

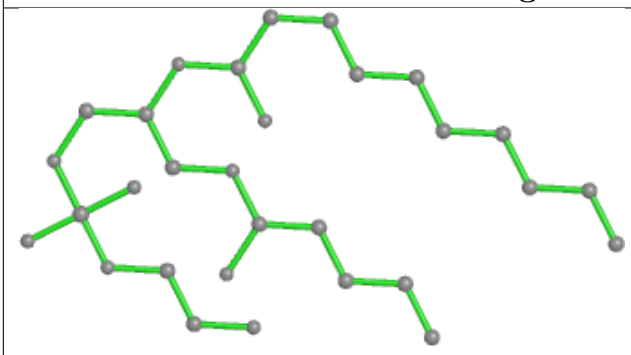


Torsions

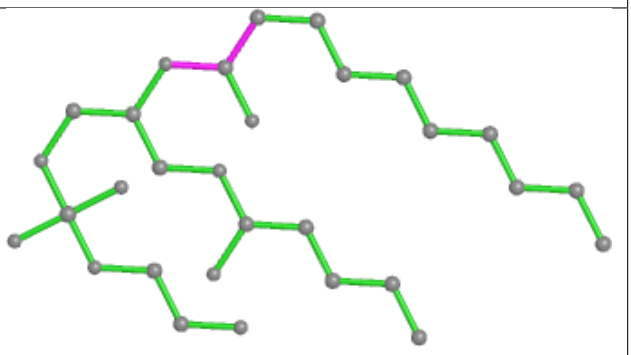


Rings

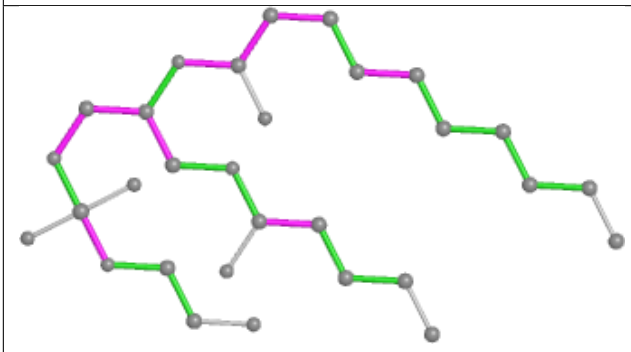
Ligand 3PE 1Y 203



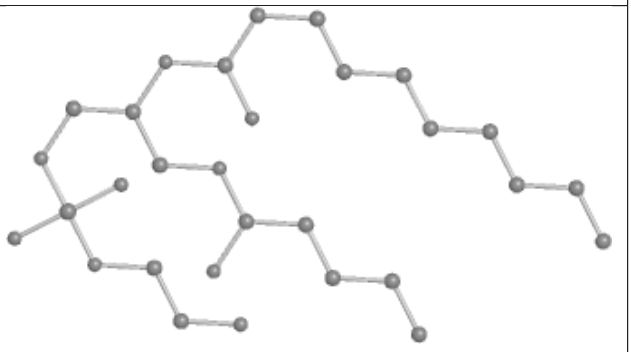
Bond lengths



Bond angles

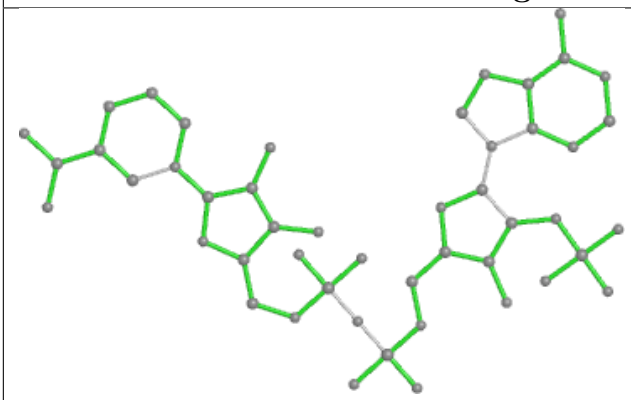


Torsions

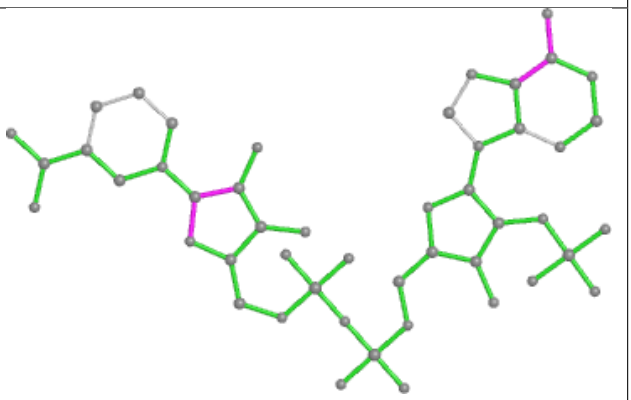


Rings

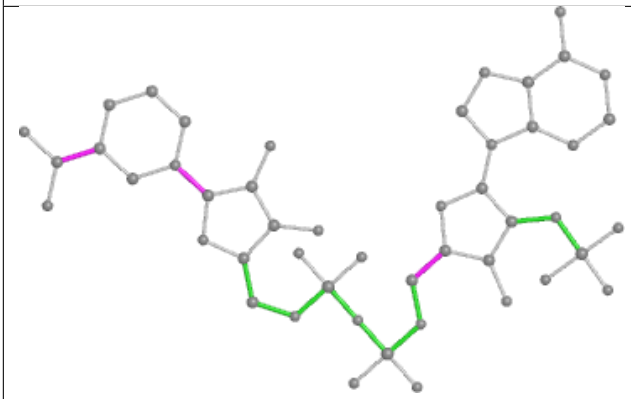
Ligand NDP 1P 402



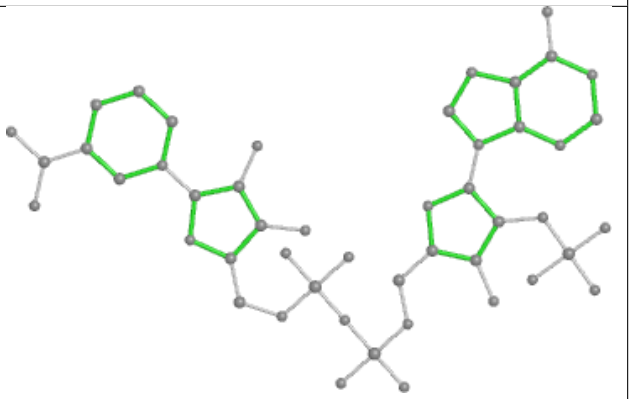
Bond lengths



Bond angles

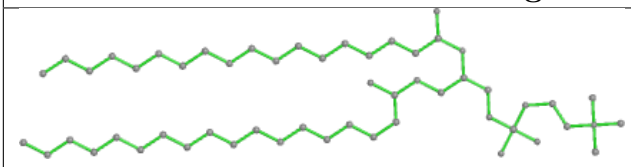


Torsions

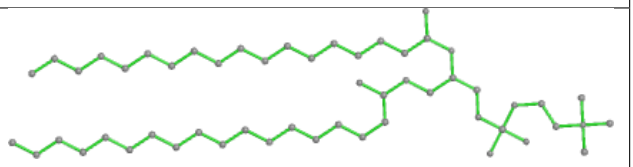


Rings

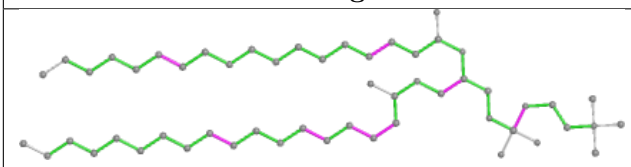
Ligand PC1 1I 201



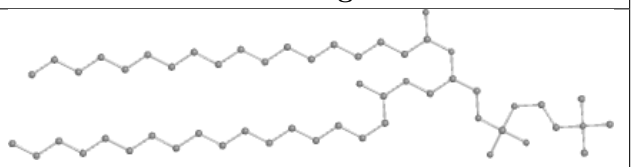
Bond lengths



Bond angles

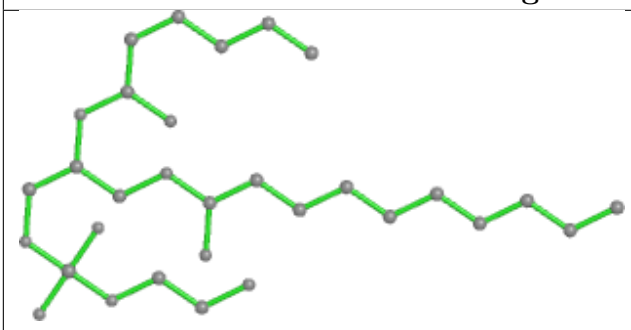


Torsions

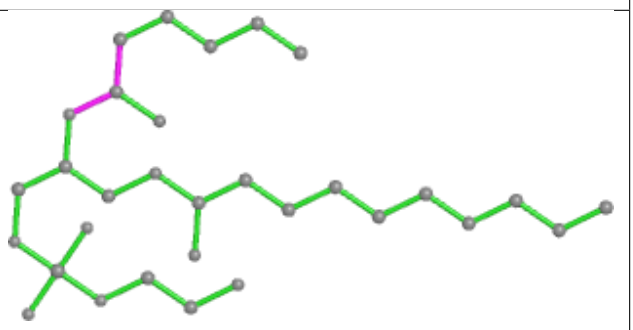


Rings

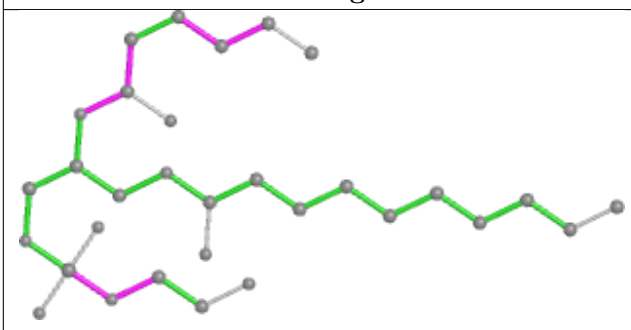
Ligand 3PE 1L 704



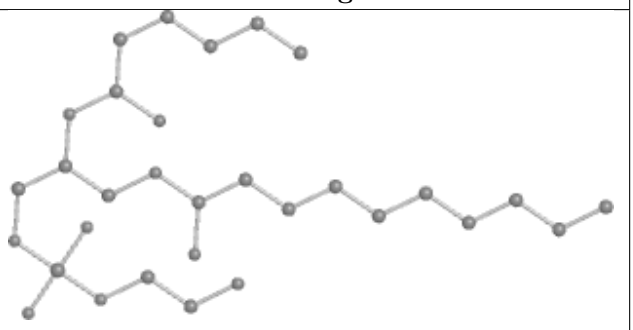
Bond lengths



Bond angles

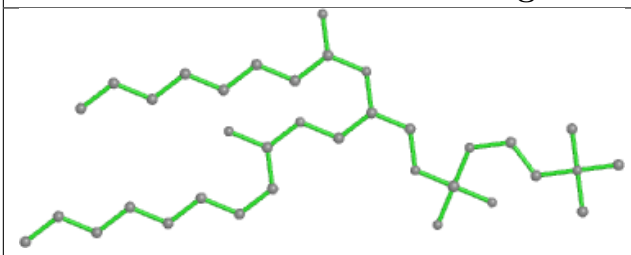


Torsions

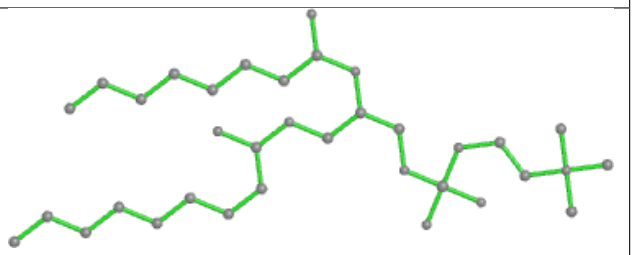


Rings

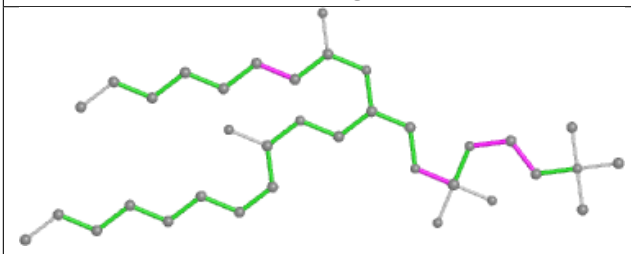
Ligand PC1 1A 202



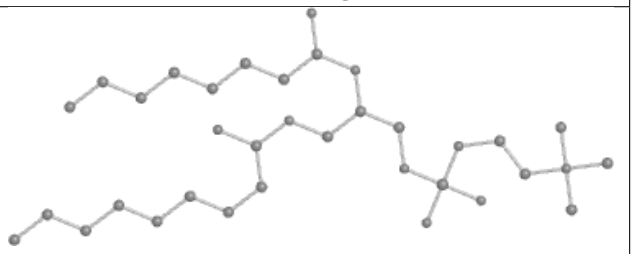
Bond lengths



Bond angles

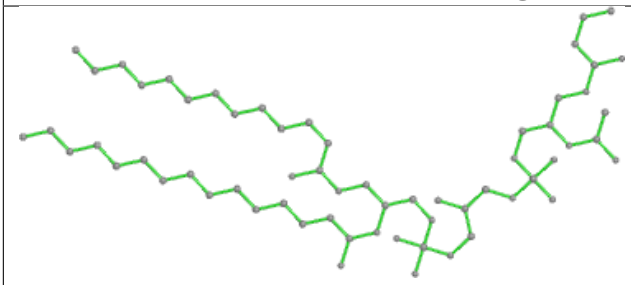


Torsions

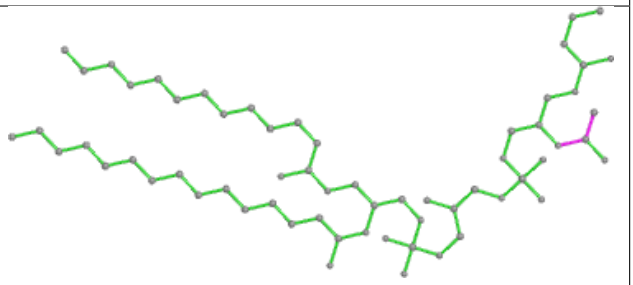


Rings

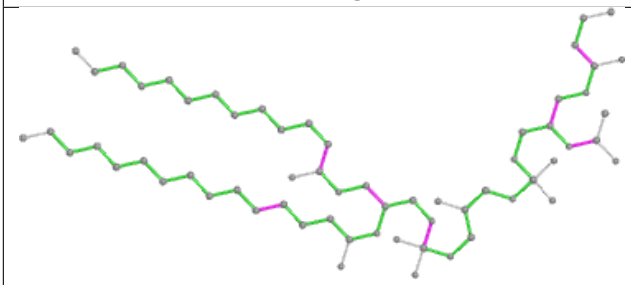
Ligand CDL 1N 902



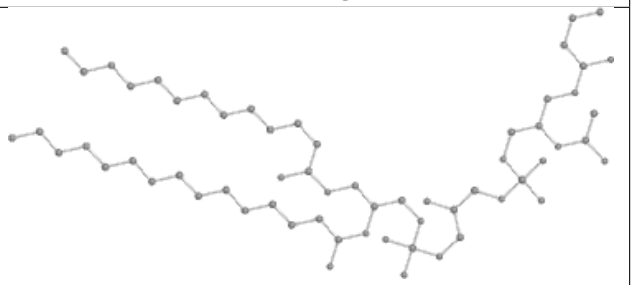
Bond lengths



Bond angles

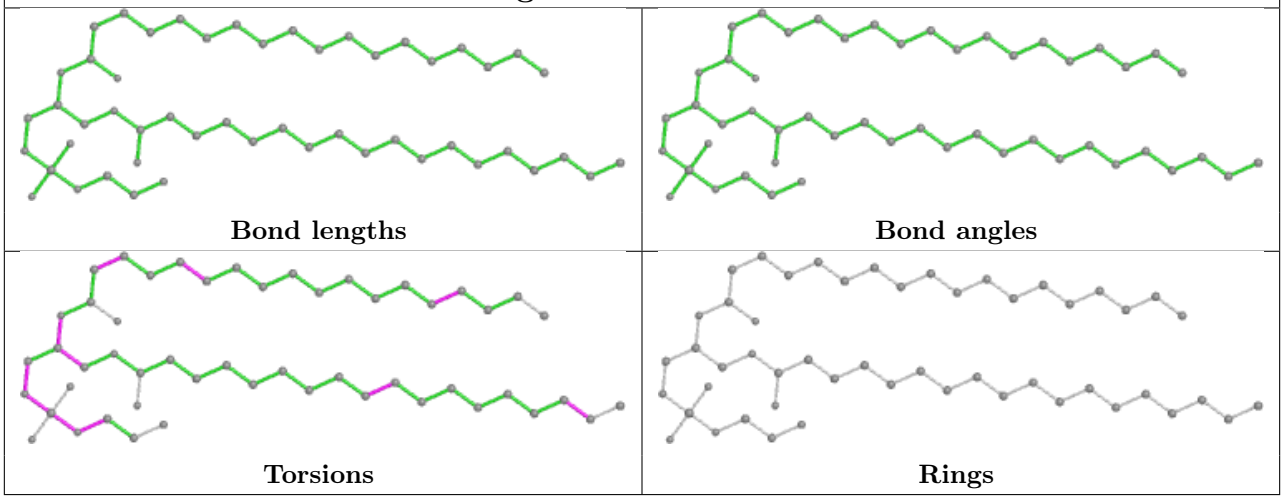


Torsions

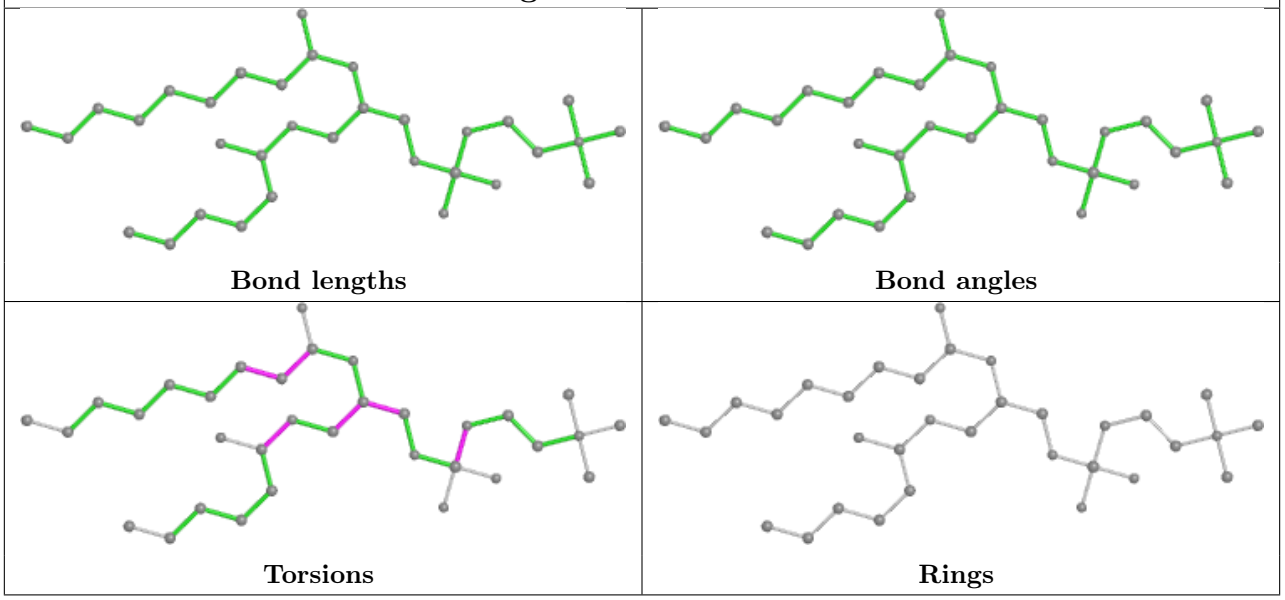


Rings

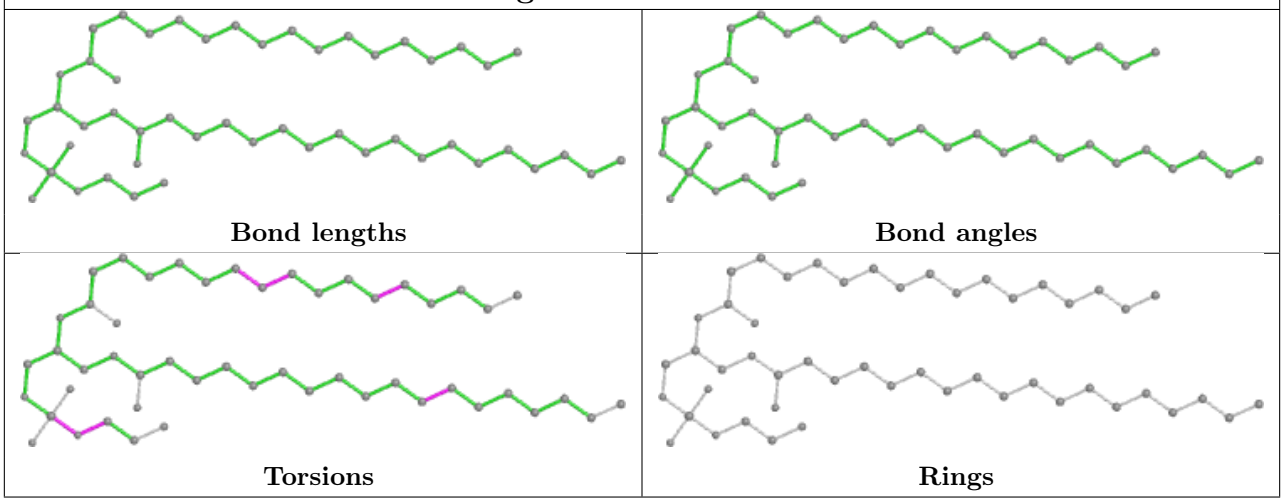
Ligand 3PE 1M 502



Ligand PC1 1P 401



Ligand 3PE 1M 504



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.

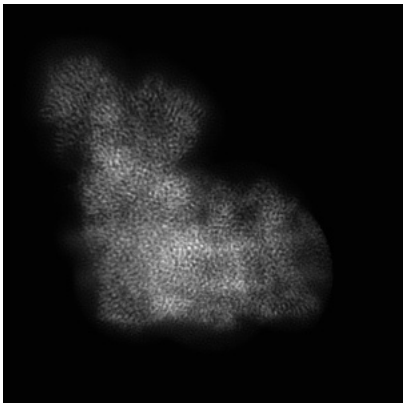
6 Map visualisation

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.

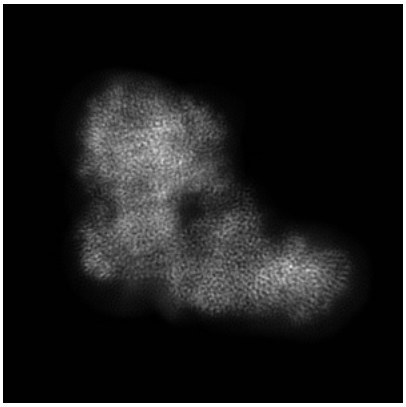
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

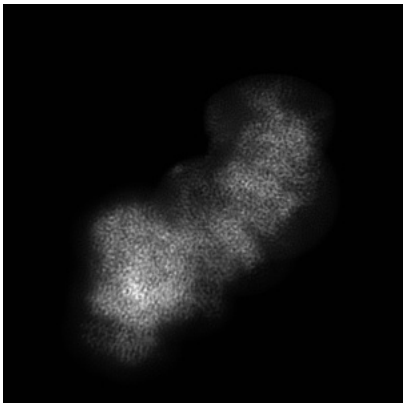
6.1.1 Primary map



X



Y

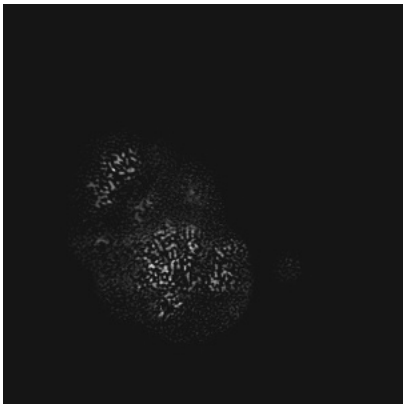


Z

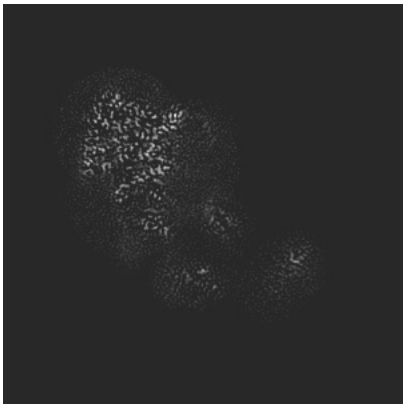
The images above show the map projected in three orthogonal directions.

6.2 Central slices

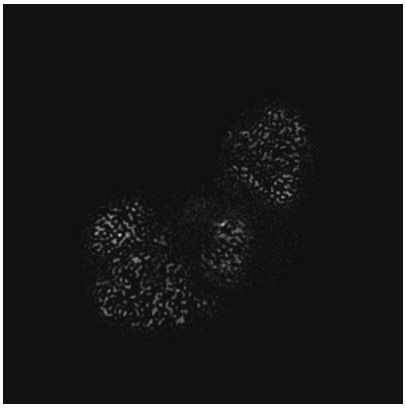
6.2.1 Primary map



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

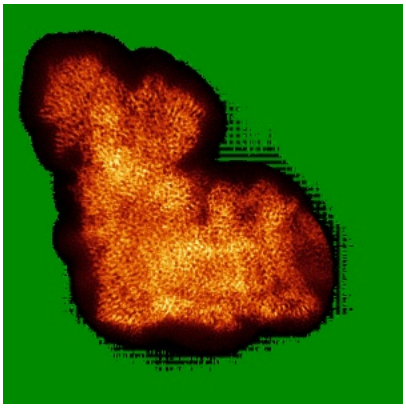
Y Index: 196

Z Index: 275

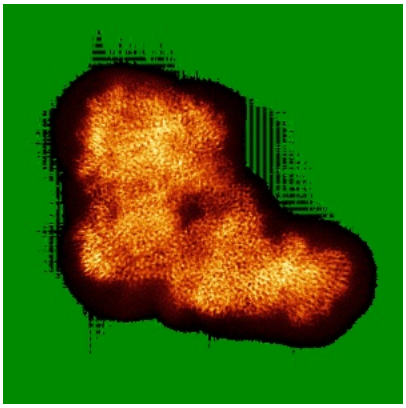
The images above show the largest variance slices of the map in three orthogonal directions.

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

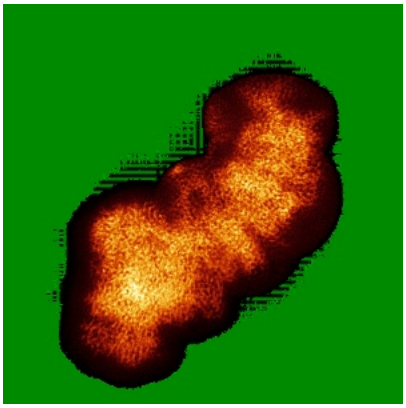
6.4.1 Primary map



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.

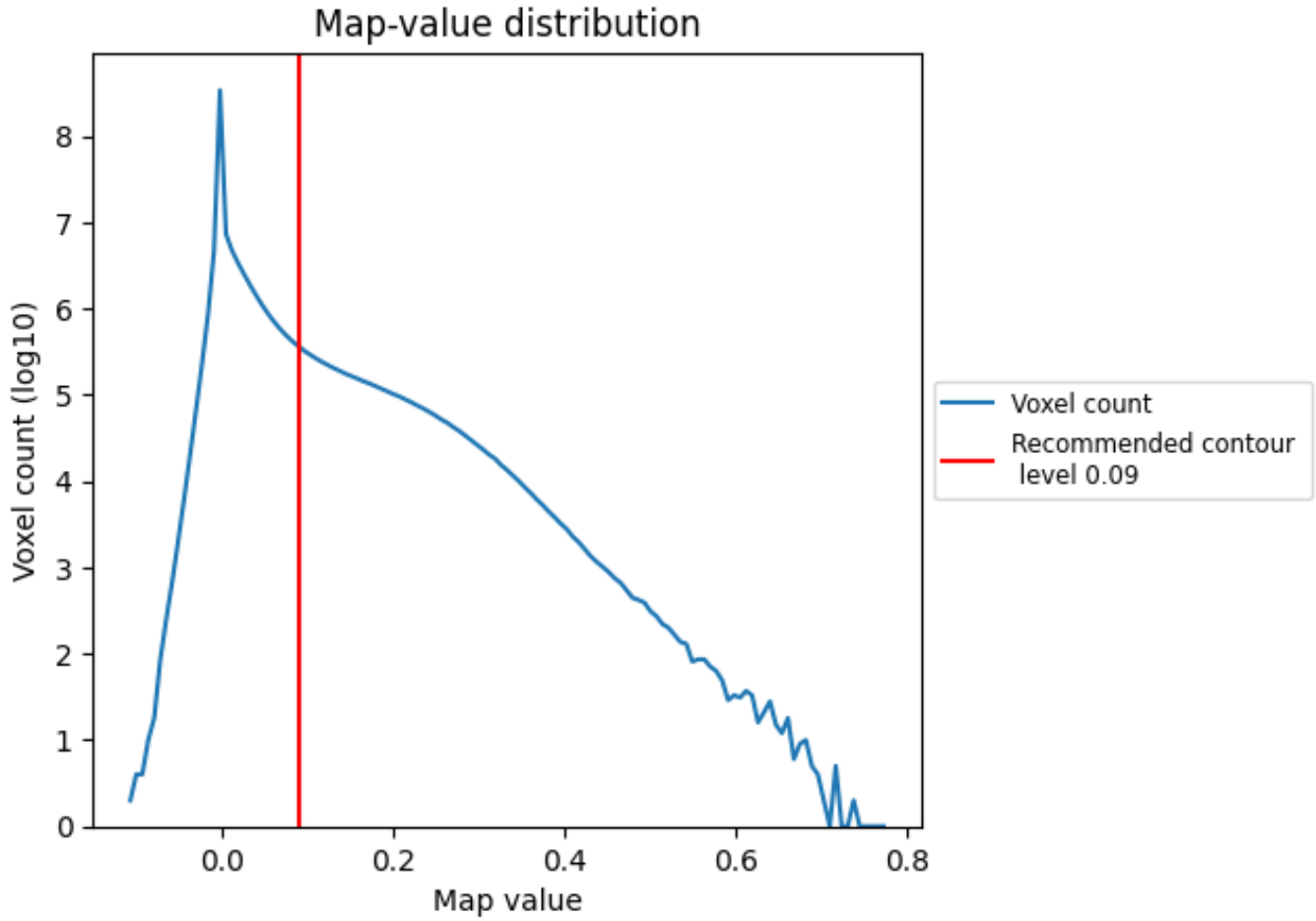
6.6 Mask visualisation (i)

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

7 Map analysis

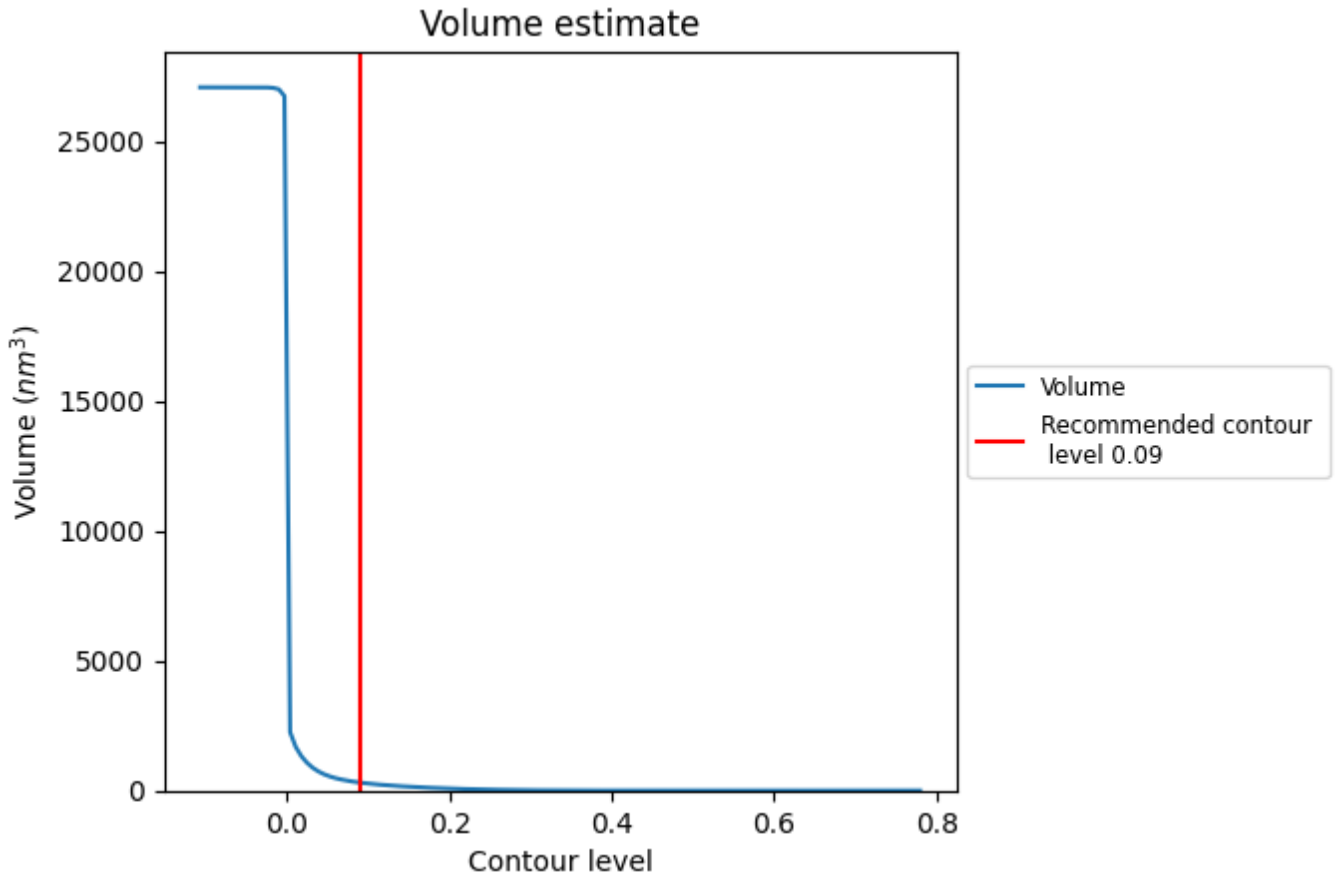
This section contains the results of statistical analysis of the map.

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.

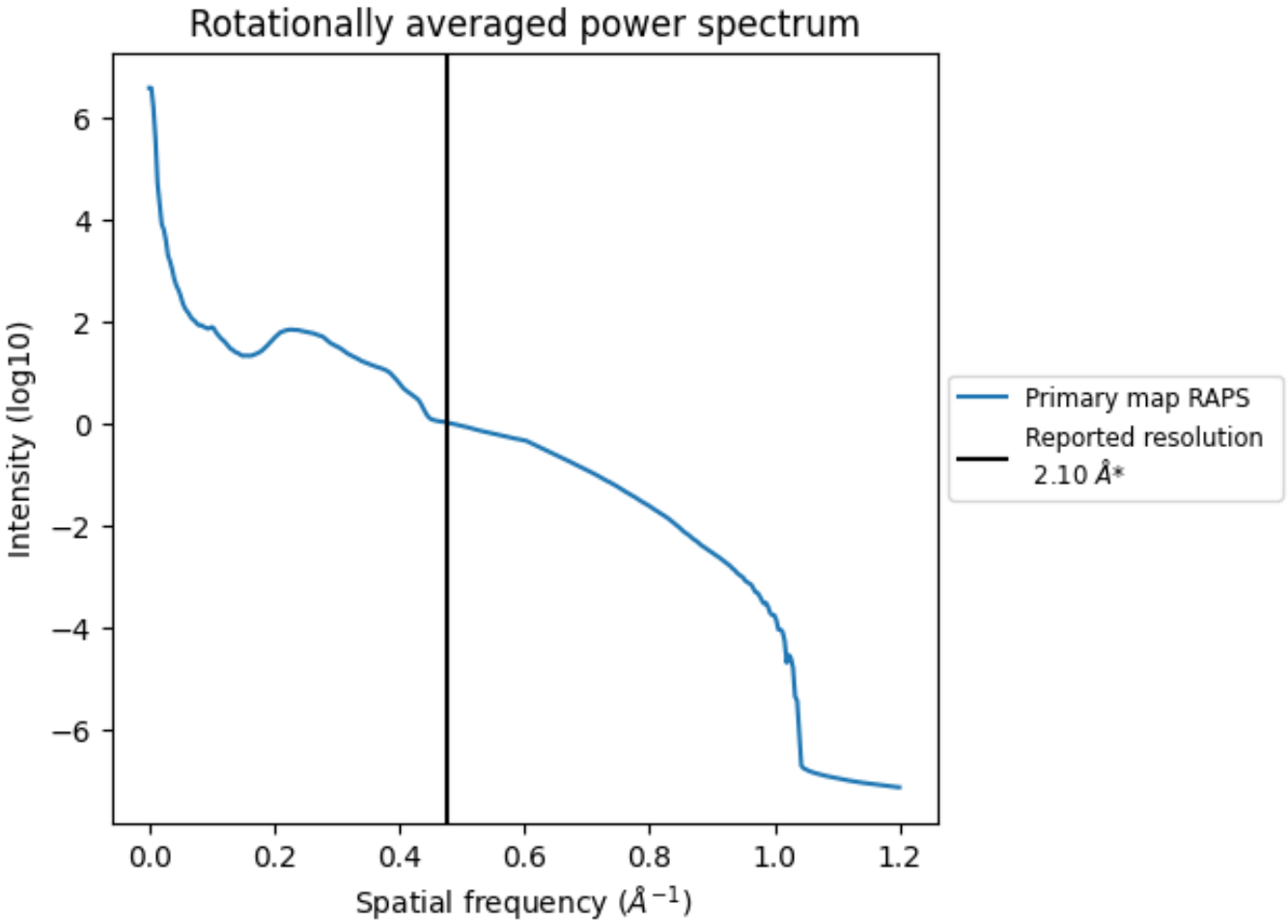
7.2 Volume estimate



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}

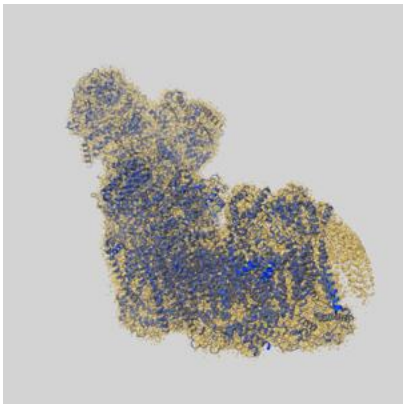
8 Fourier-Shell correlation (i)

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

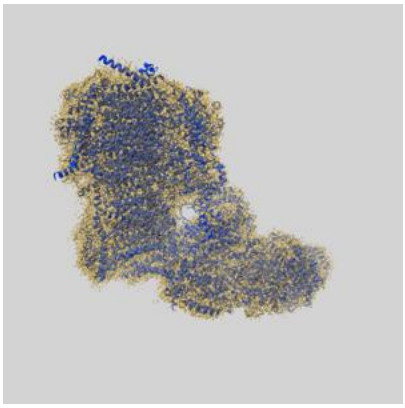
9 Map-model fit

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 23.

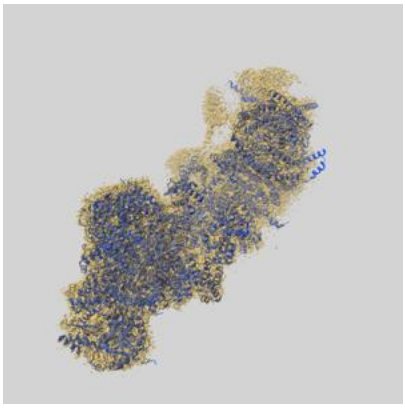
9.1 Map-model overlay



X



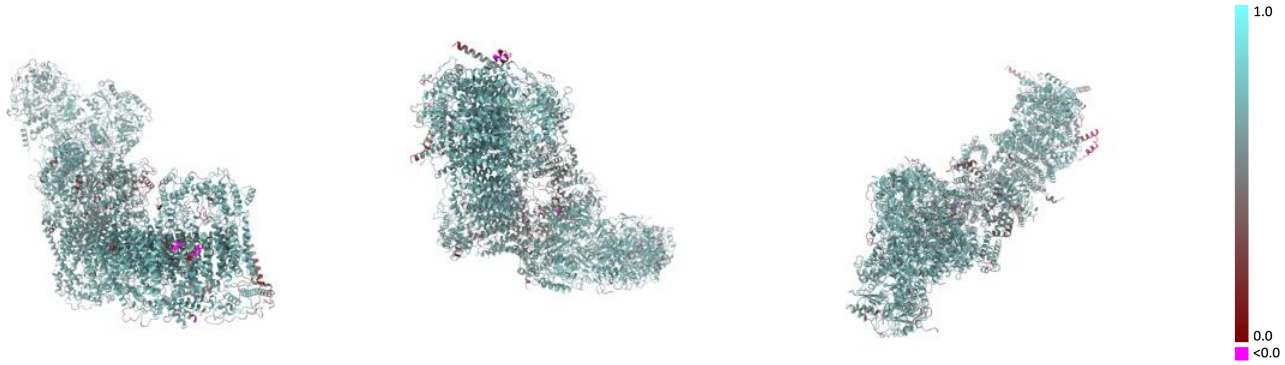
Y



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.

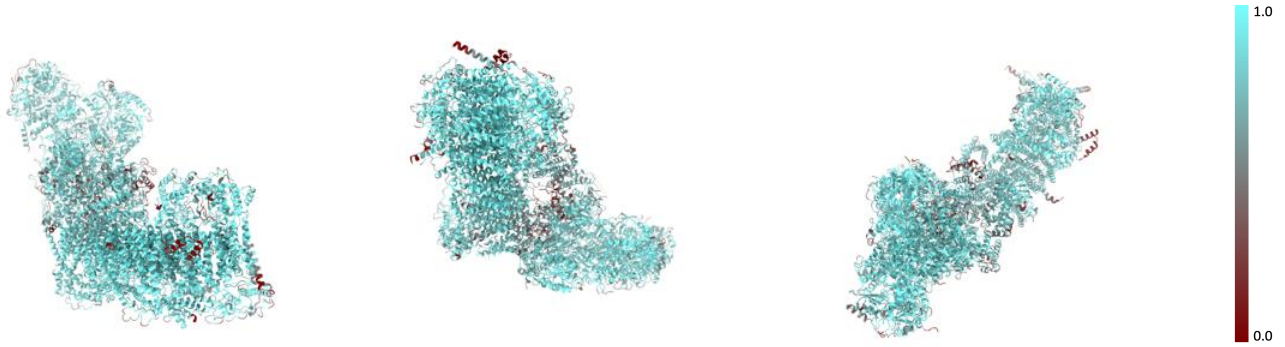
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

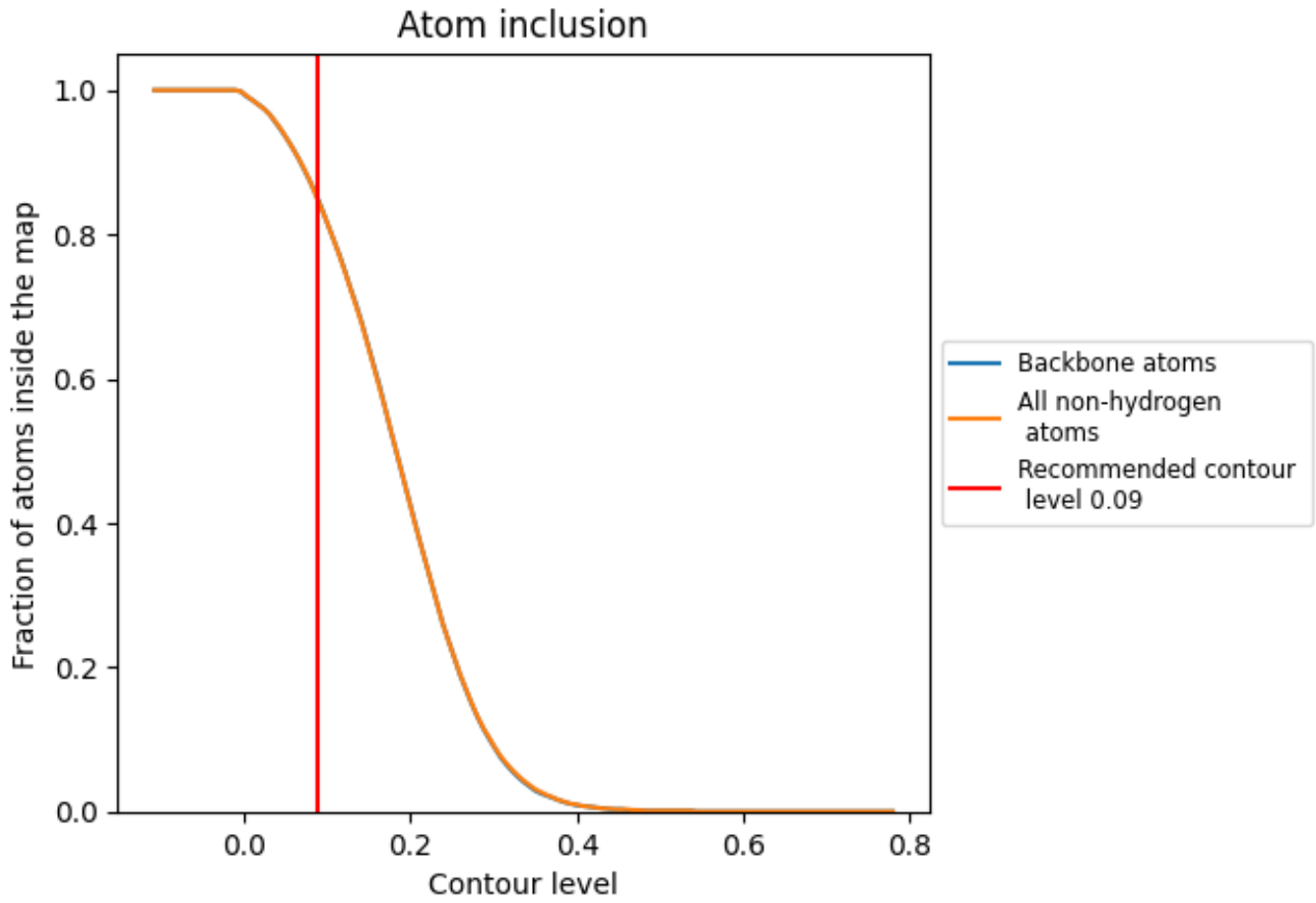
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.8460	0.6360
1A	0.6650	0.5360
1B	0.8760	0.6660
1C	0.9180	0.6910
1D	0.8850	0.6720
1E	0.7590	0.5920
1F	0.8410	0.6220
1G	0.8900	0.6600
1H	0.8730	0.6260
1I	0.9340	0.6930
1J	0.7620	0.5670
1K	0.9580	0.6740
1L	0.9260	0.6680
1M	0.9560	0.6910
1N	0.9480	0.6880
1O	0.7660	0.5680
1P	0.8070	0.6270
1Q	0.8410	0.6280
1R	0.8410	0.6420
1S	0.8530	0.6160
1T	0.4010	0.4190
1U	0.7860	0.6260
1V	0.7200	0.6110
1W	0.8340	0.6520
1X	0.8640	0.6320
1Y	0.7570	0.6180
1Z	0.8690	0.6430
1a	0.9240	0.6580
1b	0.8000	0.6040
1c	0.7240	0.5960
1d	0.8980	0.6640
1e	0.9050	0.6490
1f	0.7350	0.5720
1g	0.8290	0.6170
1h	0.8650	0.6580

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	0.5870	0.4820
1j	0.7250	0.5520
1k	0.7030	0.5800
1l	0.8710	0.6520
1m	0.8390	0.6290
1n	0.8610	0.6470
1o	0.8030	0.6050
1p	0.8530	0.6330
1q	0.8300	0.6660
1r	0.8310	0.6520
1s	0.7060	0.5780