wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 02:22 AM EDT

PDB ID	:	8ESZ
EMDB ID	:	EMD-28582
Title	:	Structure of mitochondrial complex I from Drosophila melanogaster, Helix-locked state
Authors	:	Padavannil, A.; Letts, J.A.
Deposited on	:	2022-10-15
Resolution	:	3.40 Å(reported)

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

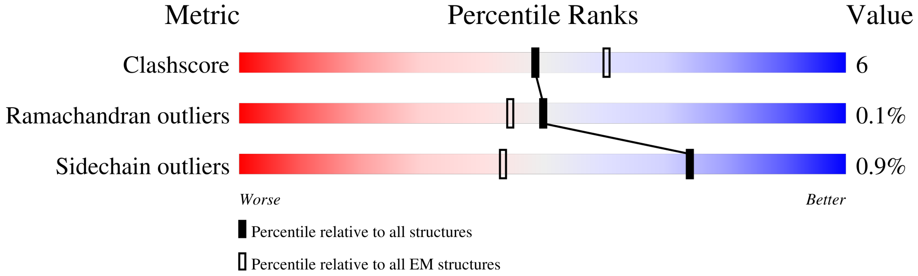
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

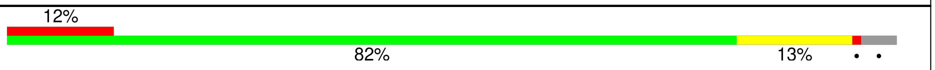
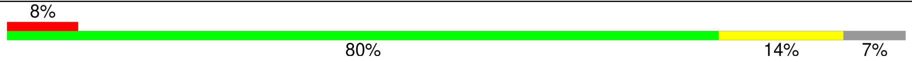
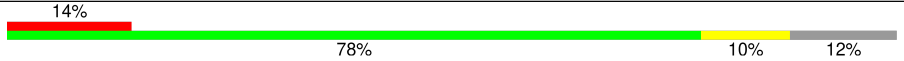
The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AN	142	
2	S6	126	
3	S1	731	
4	S3	265	
5	V2	242	
6	S7	221	
7	S8	217	
8	1	315	

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Mol	Chain	Length	Quality of chain
9	4	446	77% 23%
10	5	577	5% 80% 18% •
11	A8	175	9% 87% 10% • •
12	A1	123	• 43% 14% 43%
13	AO	154	6% 87% 7% • 5%
14	S5	101	• 85% 13% • •
15	AM	170	18% 84% 15% • •
16	BL	159	• 91% • 5%
17	B6	167	11% 88% 8% •
18	B4	113	• 84% 11% 5%
19	B7	117	25% 85% 15%
20	B5	186	• 73% • 23%
21	B9	144	10% 81% 12% 7%
22	BM	150	7% 67% • 29%
23	B8	175	8% 75% 5% • 18%
24	B3	110	19% 68% 5% 26%
25	AB	152	39% 47% 8% • 45%
25	AC	152	12% 47% 8% • 44%
26	C2	116	• 93% 6% •
27	B1	56	21% 86% 12% •
28	S4	183	9% 75% 8% 17%
29	A9	416	6% 78% 13% 9%
30	B2	94	17% 56% 6% • 36%
31	S2	468	• 73% 18% • 8%
32	V3	37	70% 70% • 27%

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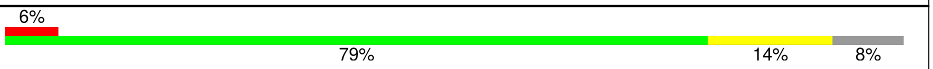
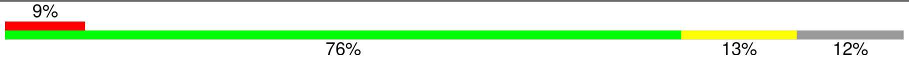
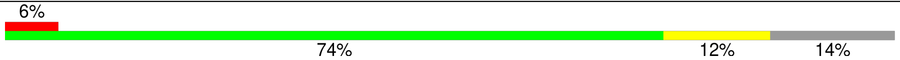
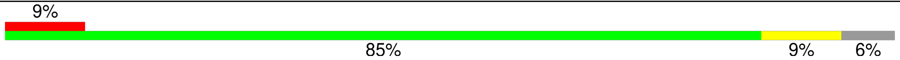
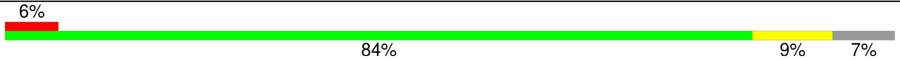
Mol	Chain	Length	Quality of chain
33	V1	474	
34	2	341	
35	A7	103	
36	A3	77	
37	4L	96	
38	6	174	
39	3	117	
40	A5	124	
41	AL	407	
42	A6	124	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	S7	301	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 67757 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 dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AN	136	1145	747	191	202	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S6	89	716	453	130	129	4	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	683	5181	3246	919	987	29	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S3	205	1699	1086	298	310	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	V2	214	1680	1062	285	321	12	0	0

- Molecule 6 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S7	182	1435	920	251	250	14	0	0

- Molecule 7 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	S8	186	1485	935	251	287	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1	315	2571	1764	367	418	22	0	0

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	4	446	3606	2450	533	581	42	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	5	577	4606	3092	680	774	60	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A8	174	1384	867	240	267	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A1	70	581	375	97	103	6	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AO	146	Total	C	N	O	S	0	0
			1202	787	203	210	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S5	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	168	Total	C	N	O	S	0	0
			1281	832	212	230	7		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	151	Total	C	N	O	S	0	0
			1266	794	232	230	10		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B6	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B4	107	Total	C	N	O	S	0	0
			884	566	162	155	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B7	117	Total	C	N	O	S	0	0
			972	617	170	175	10		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B5	143	Total	C	N	O	S	0	0
			1221	787	209	222	3		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B9	134	Total	C	N	O	S	0	0
			1148	732	217	196	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BM	106	Total	C	N	O	S	0	0
			871	560	140	170	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B8	144	Total	C	N	O	S	0	0
			1201	783	191	223	4		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B3	81	Total	C	N	O	S	0	0
			646	421	113	111	1		

- Molecule 25 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AC	85	Total	C	N	O	S	0	0
			680	438	103	137	2		
25	AB	84	Total	C	N	O	S	0	0
			670	433	102	133	2		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	C2	115	908	590	159	158	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	B1	55	430	278	76	74	2	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	S4	151	1214	756	227	227	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	A9	377	3030	1931	546	543	10	0	0

- Molecule 30 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	B2	60	495	323	88	83	1	0	0

- Molecule 31 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	S2	429	3427	2197	578	629	23	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	V3	27	135	81	27	27	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	V1	438	3361	2121	599	615	26	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	2	341	2797	1893	411	459	34	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	A7	91	736	463	138	134	1	0	0

- Molecule 36 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	A3	66	519	327	95	96	1	0	0

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	4L	96	794	540	113	128	13	0	0

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	6	174	1404	949	202	236	17	0	0

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	3	117	956	652	141	156	7	0	0

- Molecule 40 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A5	117	Total 914	C 584	N 161	O 165	S 4	0	0

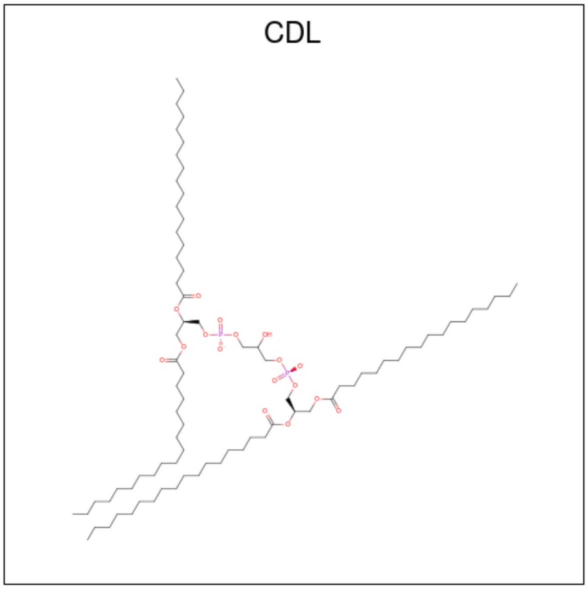
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AL	368	Total 3008	C 1927	N 504	O 561	S 16	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A6	115	Total 977	C 624	N 174	O 173	S 6	0	0

- Molecule 43 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
43	AN	1	Total 67	C 48	O 17	P 2	0
43	AM	1	Total 76	C 57	O 17	P 2	0
43	B6	1	Total 47	C 28	O 17	P 2	0

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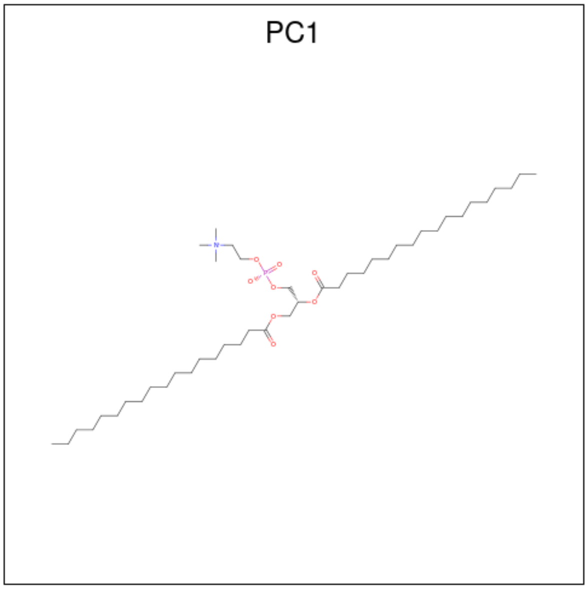
Mol	Chain	Residues	Atoms	AltConf
43	B5	1	Total C O P 76 57 17 2	0
43	B5	1	Total C O P 66 47 17 2	0
43	2	1	Total C O P 45 27 16 2	0
43	6	1	Total C O P 86 67 17 2	0
43	3	1	Total C O P 54 35 17 2	0

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



Mol	Chain	Residues	Atoms	AltConf
44	AN	1	Total C N O P 44 34 1 8 1	0
44	S7	1	Total C N O P 46 36 1 8 1	0
44	1	1	Total C N O P 54 44 1 8 1	0
44	4	1	Total C N O P 39 29 1 8 1	0
44	4	1	Total C N O P 39 29 1 8 1	0
44	5	1	Total C N O P 34 24 1 8 1	0

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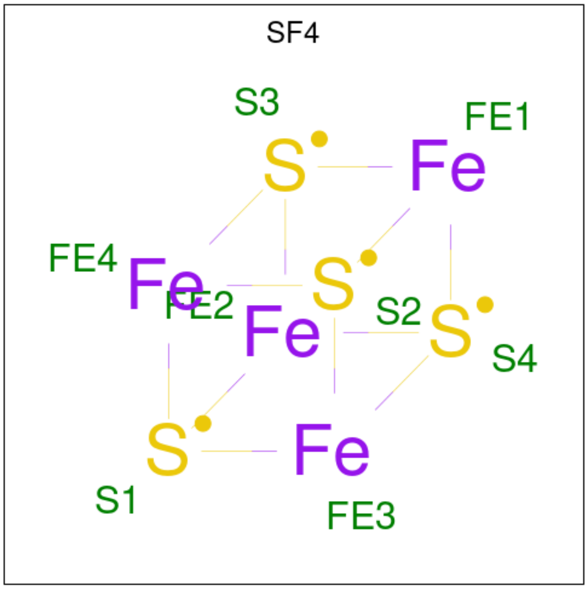
Mol	Chain	Residues	Atoms	AltConf
44	AM	1	Total C N O P 37 27 1 8 1	0
44	AM	1	Total C N O P 44 34 1 8 1	0
44	AM	1	Total C N O P 32 22 1 8 1	0
44	B6	1	Total C N O P 37 27 1 8 1	0
44	A9	1	Total C N O P 44 34 1 8 1	0
44	2	1	Total C N O P 45 35 1 8 1	0

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
45	S6	1	Total Zn 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
46	S1	1	Total Fe S 8 4 4	0
46	S1	1	Total Fe S 8 4 4	0

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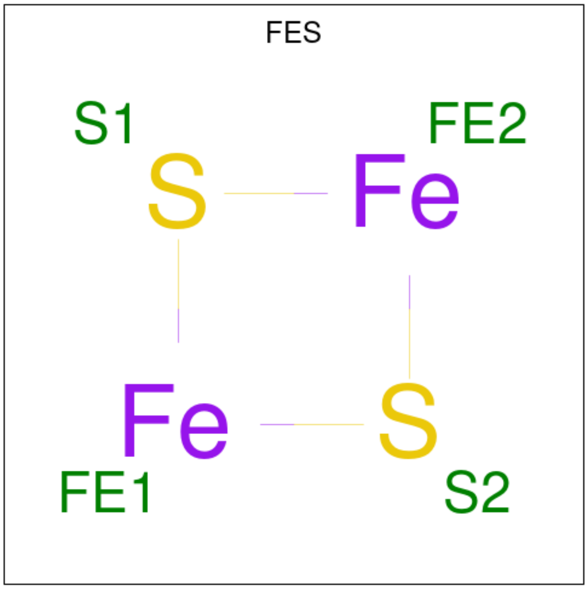
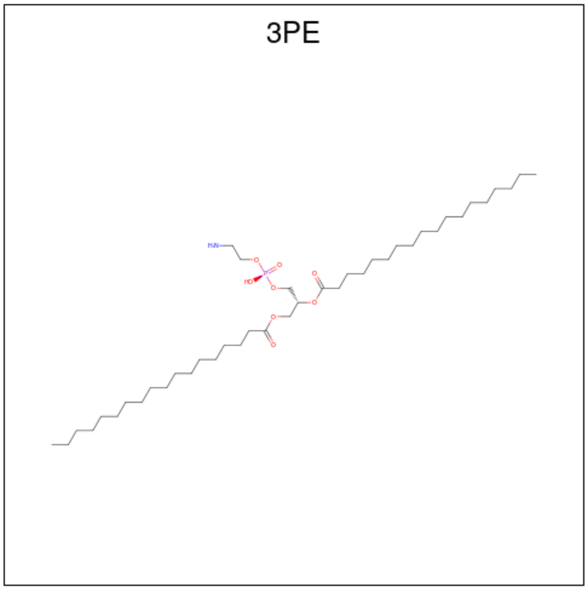
Mol	Chain	Residues	Atoms	AltConf
46	S7	1	Total Fe S 8 4 4	0
46	S8	1	Total Fe S 8 4 4	0
46	S8	1	Total Fe S 8 4 4	0
46	V1	1	Total Fe S 8 4 4	0

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



Mol	Chain	Residues	Atoms	AltConf
47	S1	1	Total Fe S 4 2 2	0
47	V2	1	Total Fe S 4 2 2	0

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
48	S7	1	Total C N O P 33 23 1 8 1	0
48	S7	1	Total C N O P 33 23 1 8 1	0
48	1	1	Total C N O P 51 41 1 8 1	0
48	4	1	Total C N O P 32 22 1 8 1	0
48	4	1	Total C N O P 45 35 1 8 1	0
48	4	1	Total C N O P 36 26 1 8 1	0
48	4	1	Total C N O P 39 29 1 8 1	0
48	5	1	Total C O P 32 23 8 1	0
48	5	1	Total C N O P 51 41 1 8 1	0
48	5	1	Total C N O P 33 23 1 8 1	0
48	5	1	Total C N O P 30 20 1 8 1	0
48	5	1	Total C N O P 33 23 1 8 1	0
48	5	1	Total C N O P 51 41 1 8 1	0
48	5	1	Total C N O P 45 35 1 8 1	0

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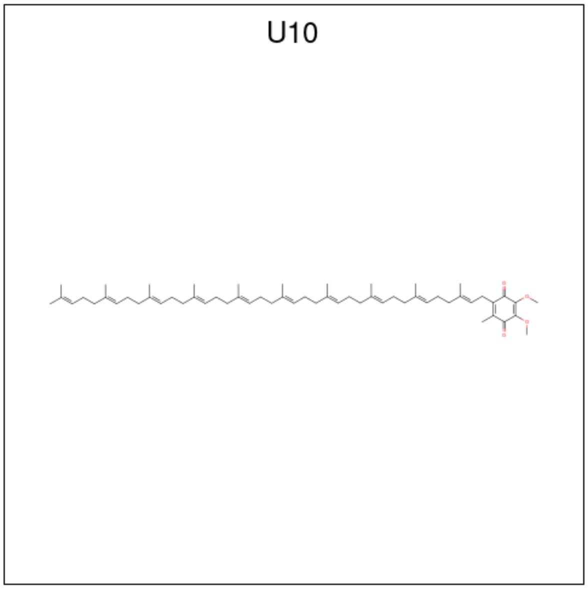
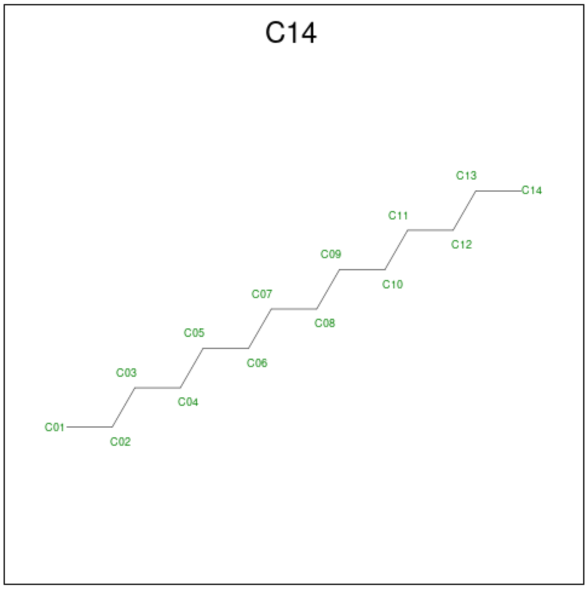
Mol	Chain	Residues	Atoms	AltConf
48	AM	1	Total C N O P 41 31 1 8 1	0
48	AM	1	Total C N O P 31 21 1 8 1	0
48	B6	1	Total C O P 48 39 8 1	0
48	B4	1	Total C N O P 47 37 1 8 1	0
48	C2	1	Total C N O P 45 35 1 8 1	0
48	B1	1	Total C N O P 37 27 1 8 1	0
48	2	1	Total C N O P 30 20 1 8 1	0
48	6	1	Total C N O P 35 25 1 8 1	0
48	3	1	Total C N O P 51 41 1 8 1	0
48	3	1	Total C N O P 41 31 1 8 1	0

- Molecule 49 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



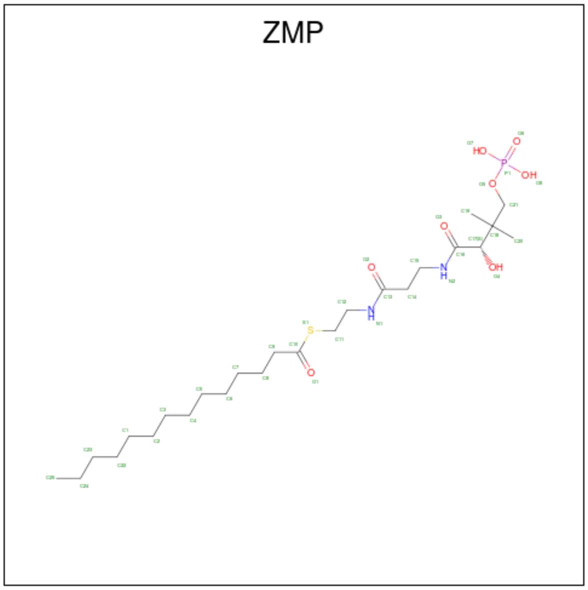
Mol	Chain	Residues	Atoms	AltConf
49	1	1	Total C O 63 59 4	0

- Molecule 50 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



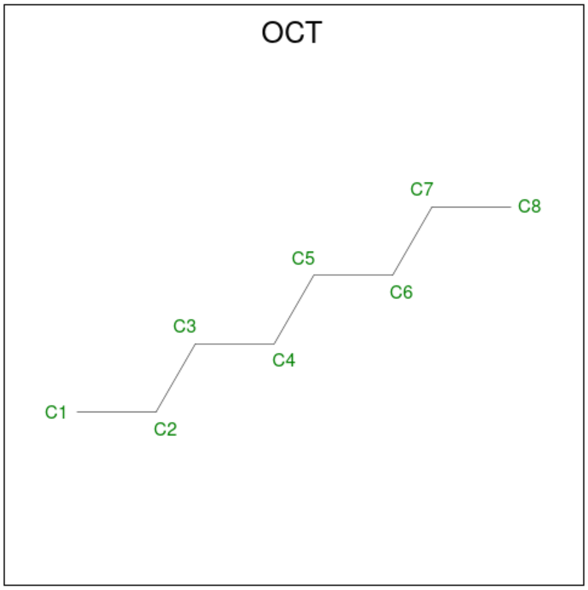
Mol	Chain	Residues	Atoms	AltConf
50	AO	1	Total C 14 14	0
50	B5	1	Total C 14 14	0
50	C2	1	Total C 14 14	0

- Molecule 51 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



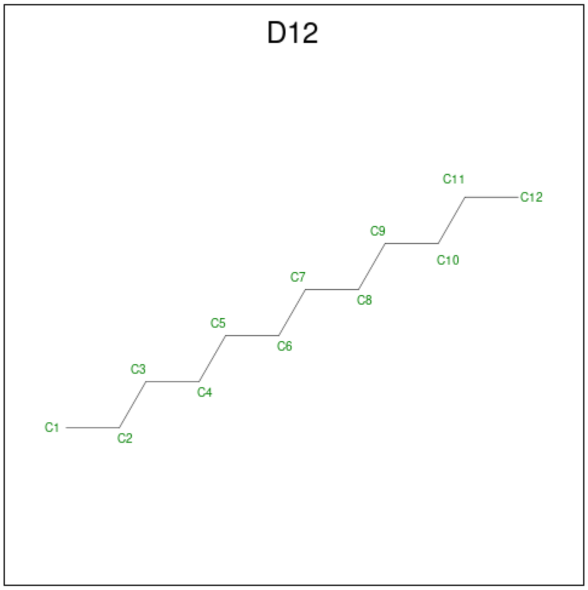
Mol	Chain	Residues	Atoms						AltConf
51	AC	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
51	AB	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 52 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



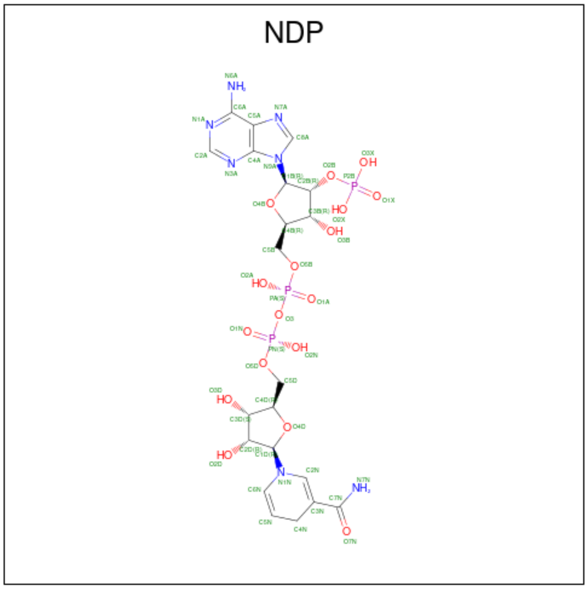
Mol	Chain	Residues	Atoms		AltConf
52	B1	1	Total	C	0
			8	8	

- Molecule 53 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



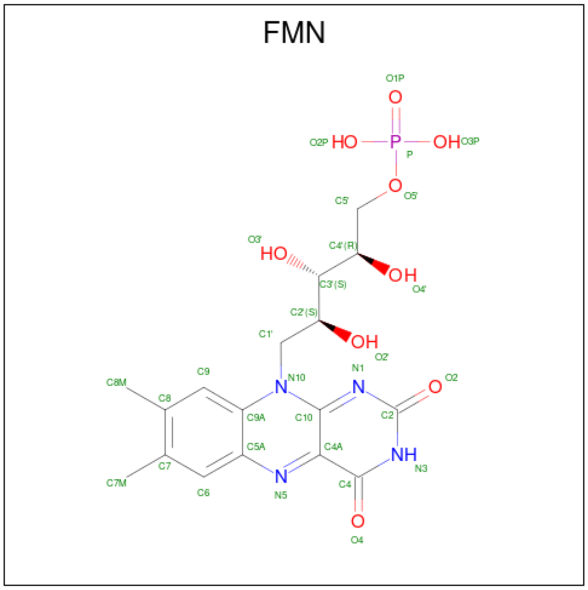
Mol	Chain	Residues	Atoms		AltConf
53	B1	1	Total 12	C 12	0
53	A9	1	Total 12	C 12	0
53	A9	1	Total 12	C 12	0
53	A3	1	Total 12	C 12	0

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



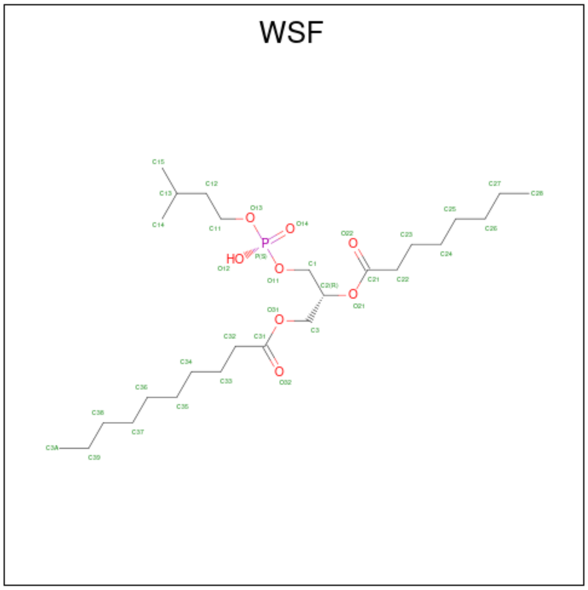
Mol	Chain	Residues	Atoms					AltConf
54	A9	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 55 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



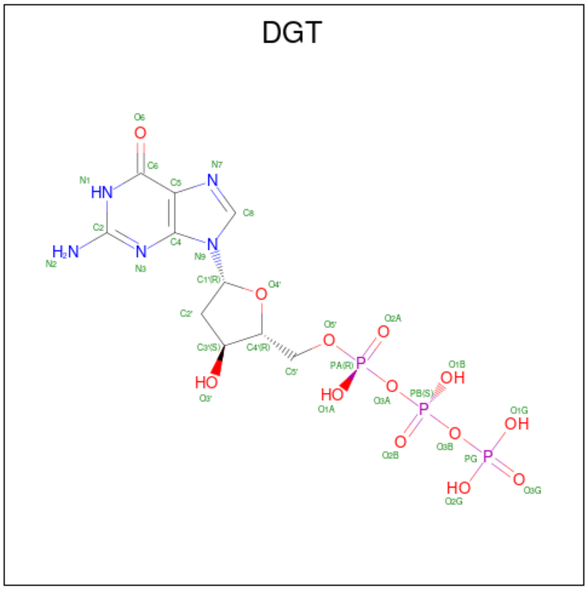
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	V1	1	31	17	4	9	1	0

- Molecule 56 is (2R)-3-{[(S)-hydroxy(3-methylbutoxy)phosphoryl]oxy}-2-(octanoyloxy)propyl decanoate (three-letter code: WSF) (formula: $C_{26}H_{51}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
56	6	1	35	26	8	1	0

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

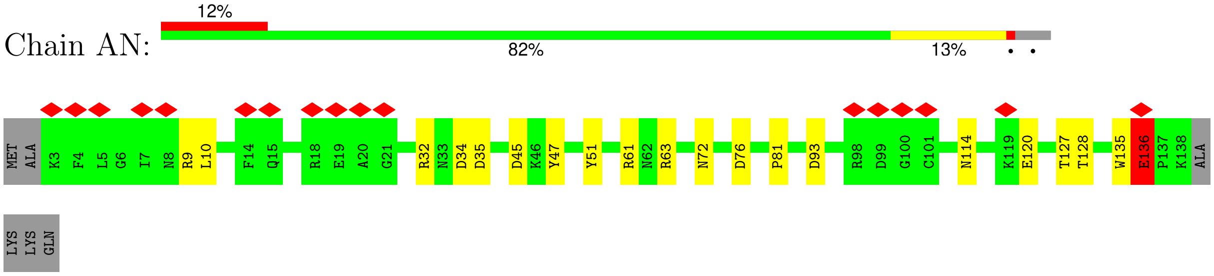


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	AL	1	31	10	5	13	3	0

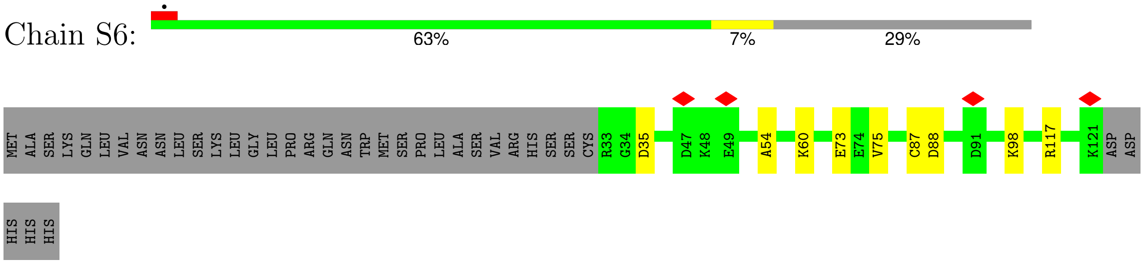
3 Residue-property plots ⓘ

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

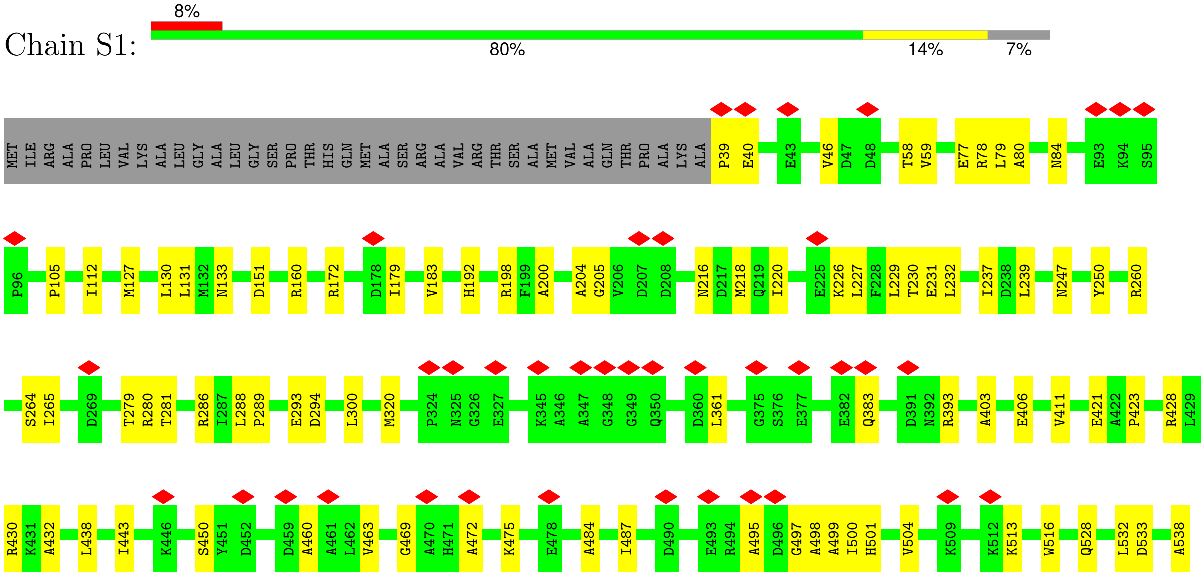
- Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

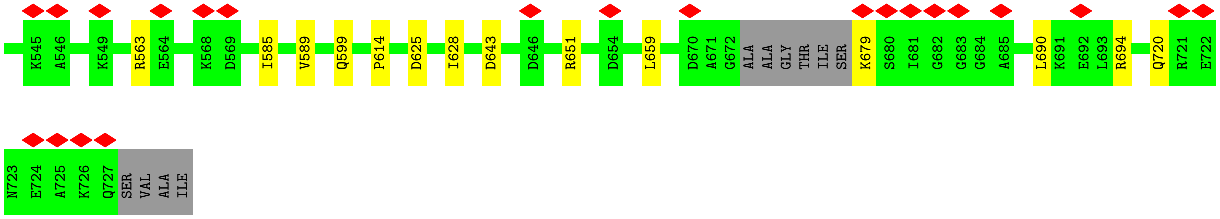


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



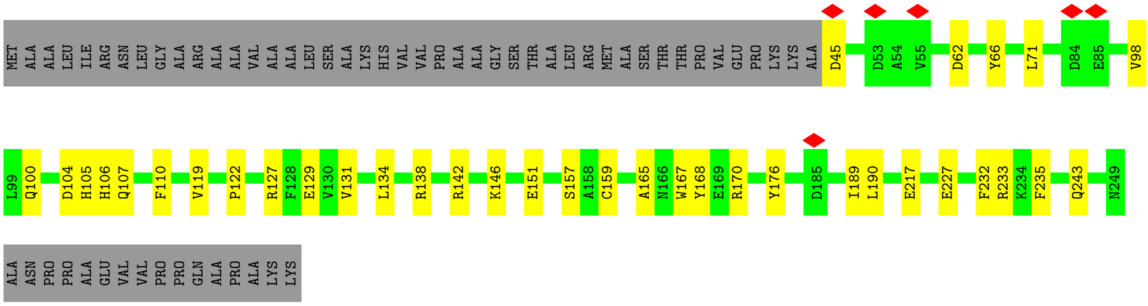
- Molecule 3: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





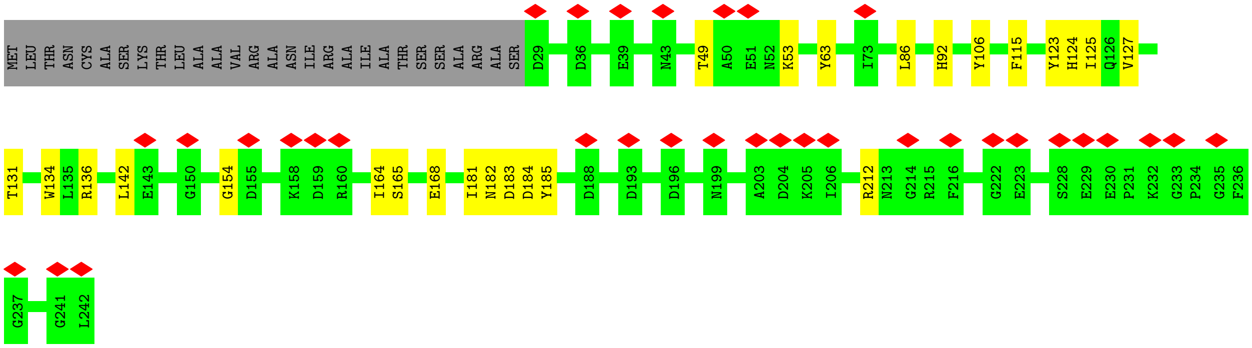
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain S3:



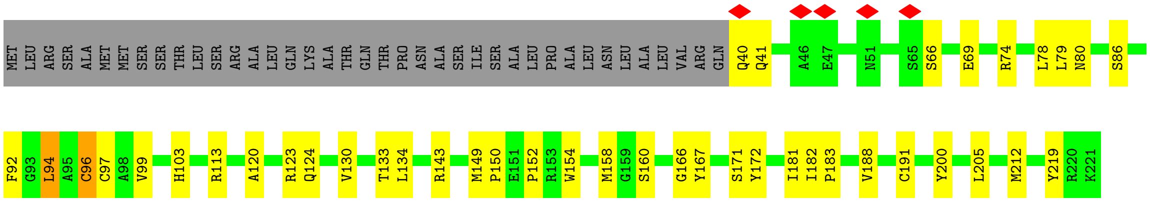
- Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

Chain V2:



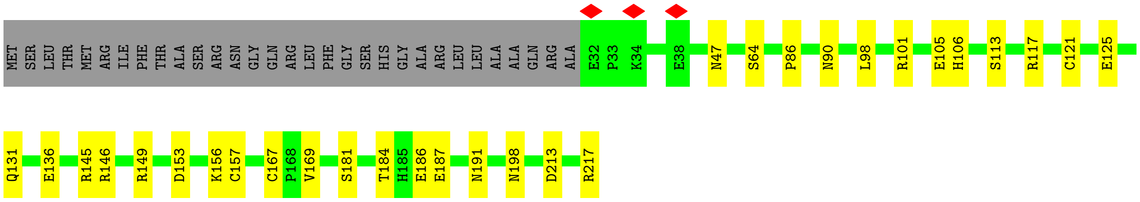
- Molecule 6: LD31474p

Chain S7:



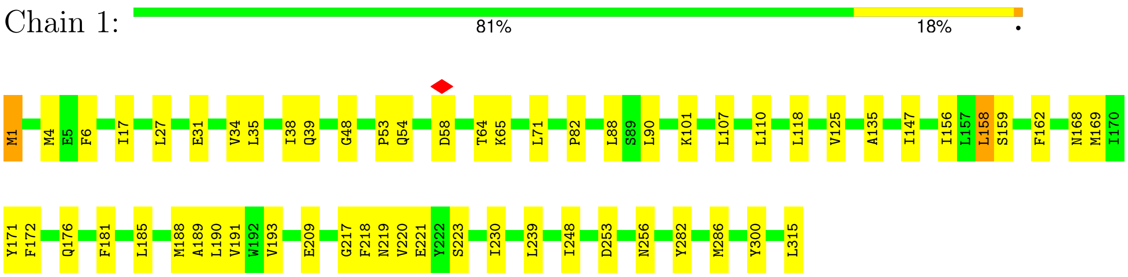
- Molecule 7: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain S8:



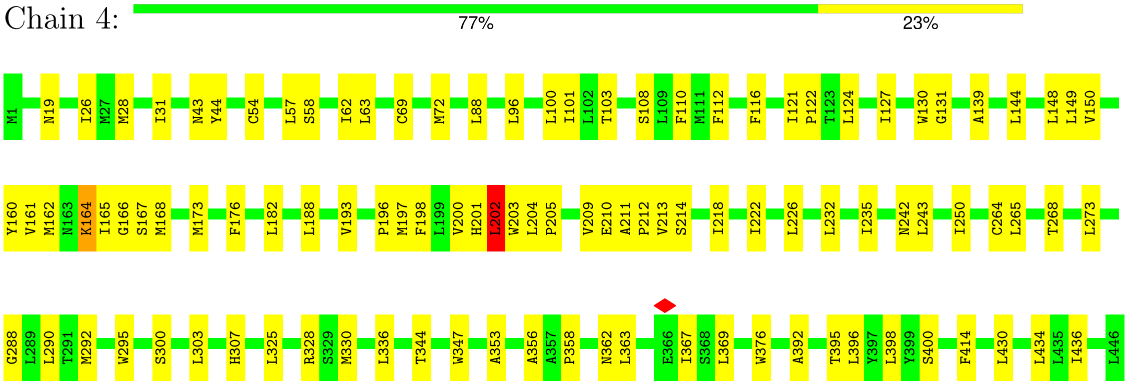
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



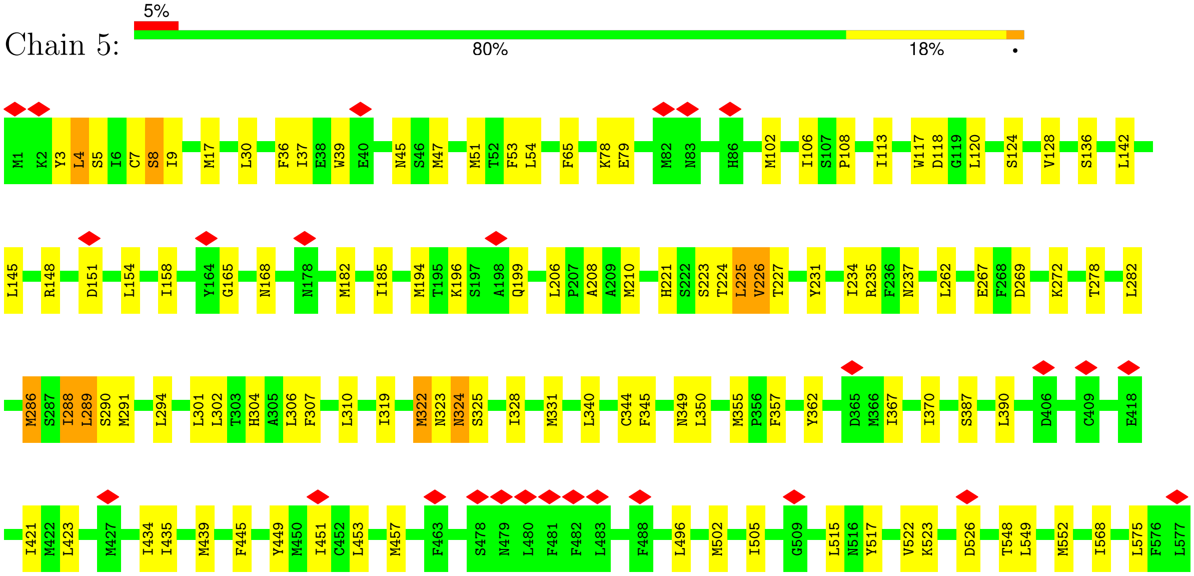
- Molecule 9: NADH-ubiquinone oxidoreductase chain 4

Chain 4:



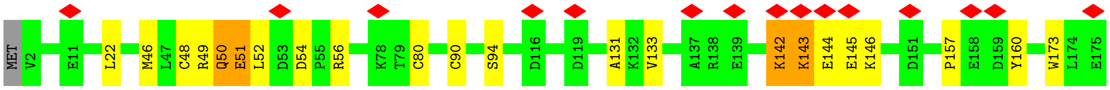
- Molecule 10: NADH-ubiquinone oxidoreductase chain 5

Chain 5:



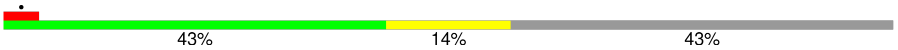
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

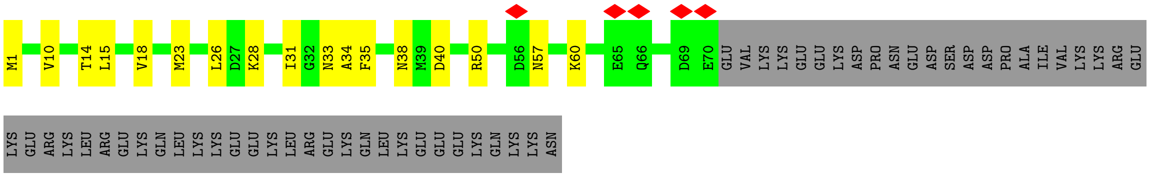
Chain A8:



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

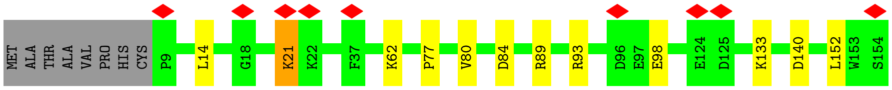
Chain A1:





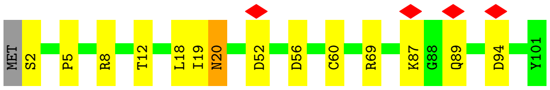
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AO:



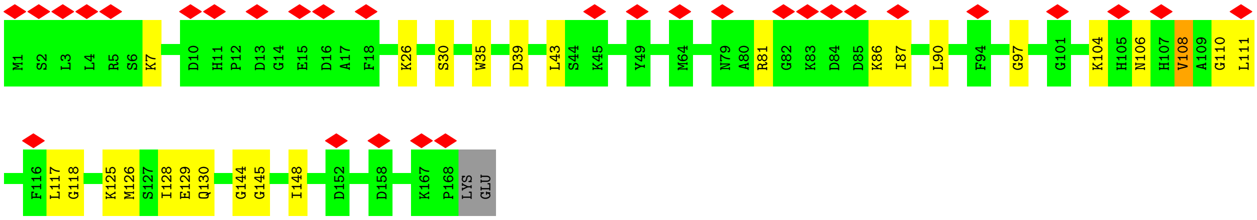
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:



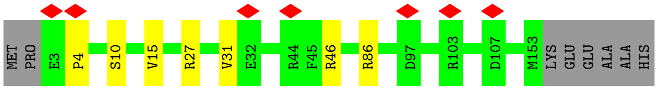
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AM:



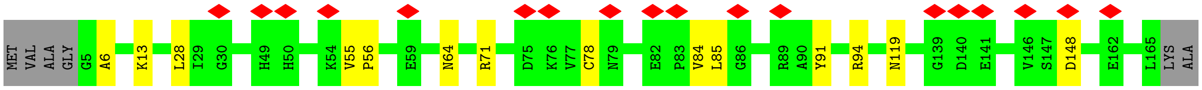
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BL:



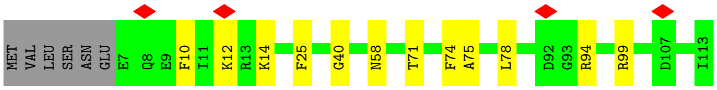
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



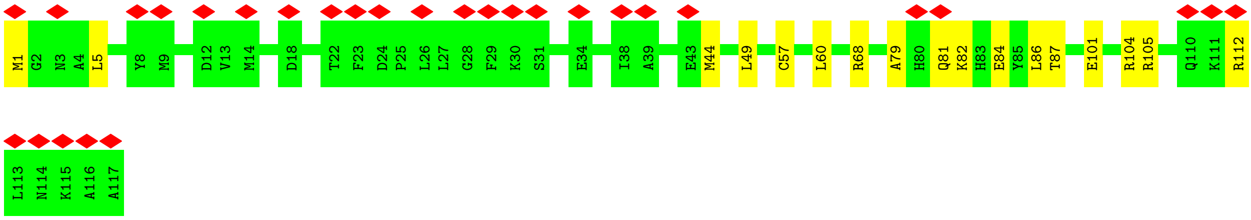
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:



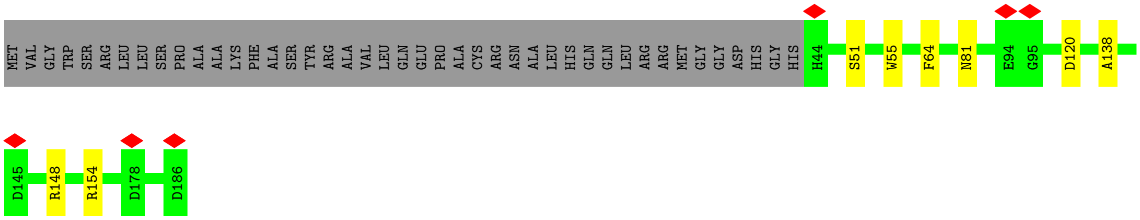
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



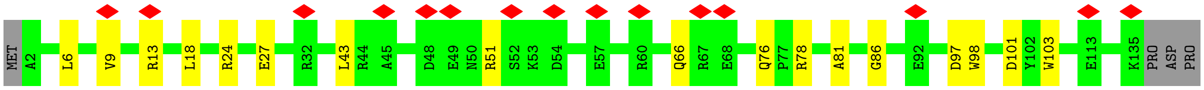
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:



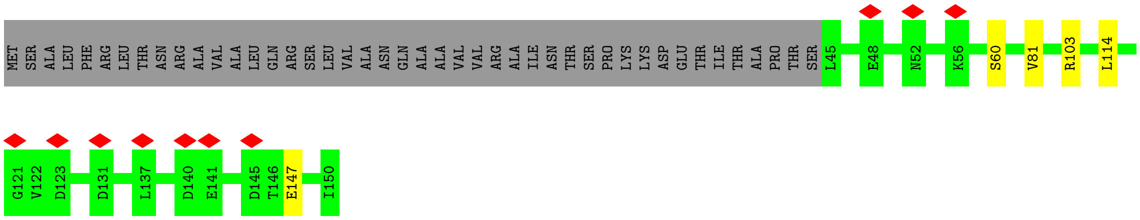
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



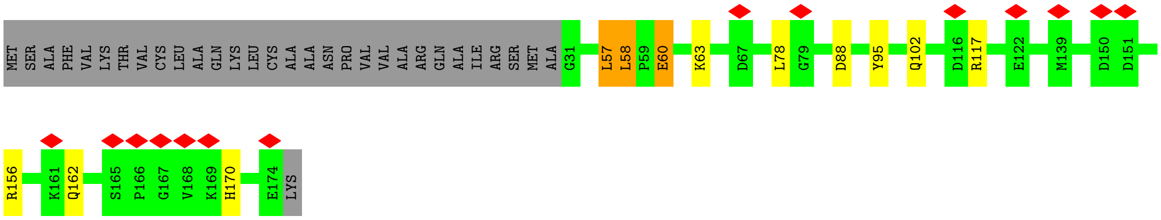
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BM:



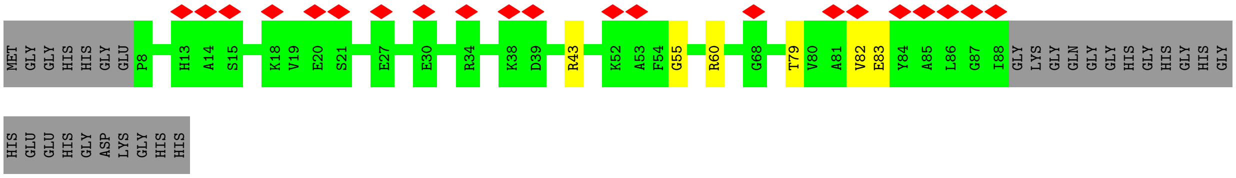
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



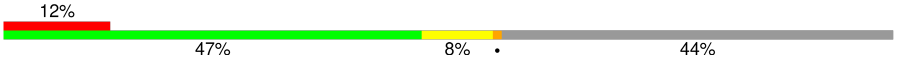
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

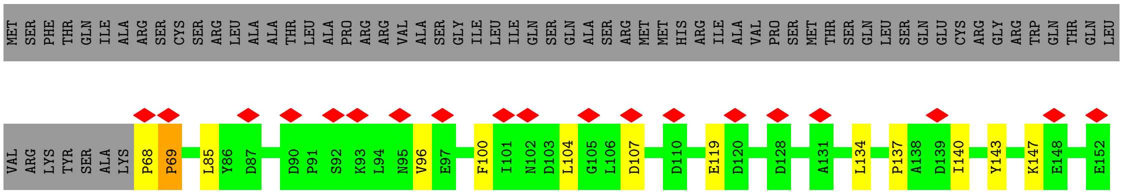
Chain B3:



- Molecule 25: Acyl carrier protein, mitochondrial

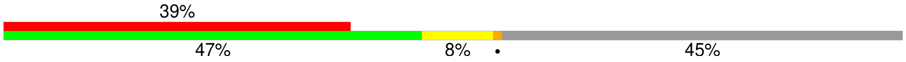
Chain AC:

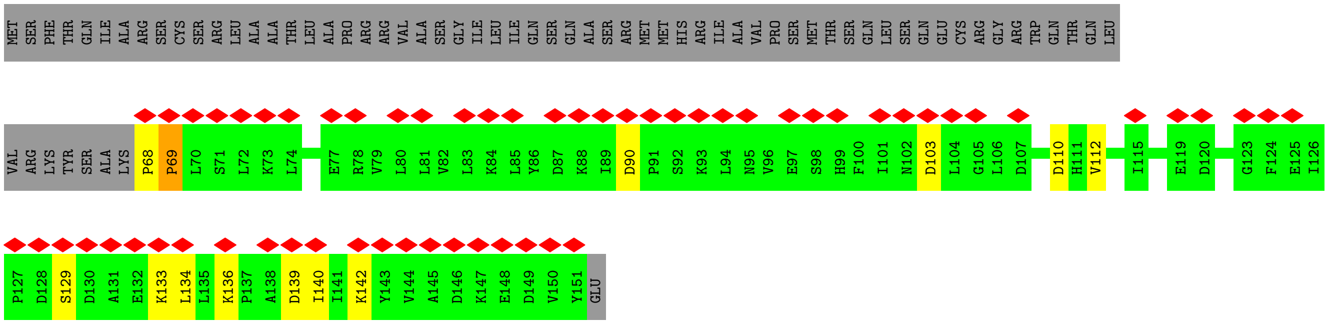




- Molecule 25: Acyl carrier protein, mitochondrial

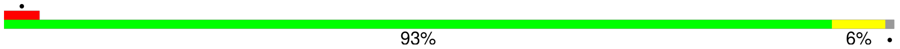
Chain AB:

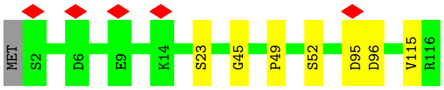




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C2

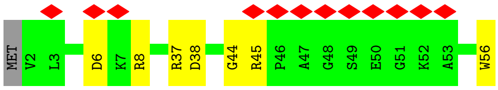
Chain C2:





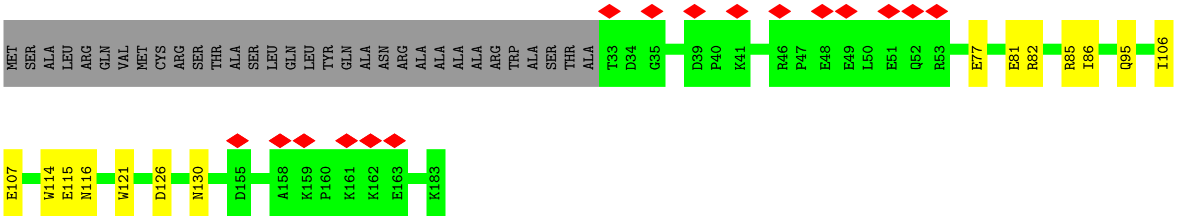
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:



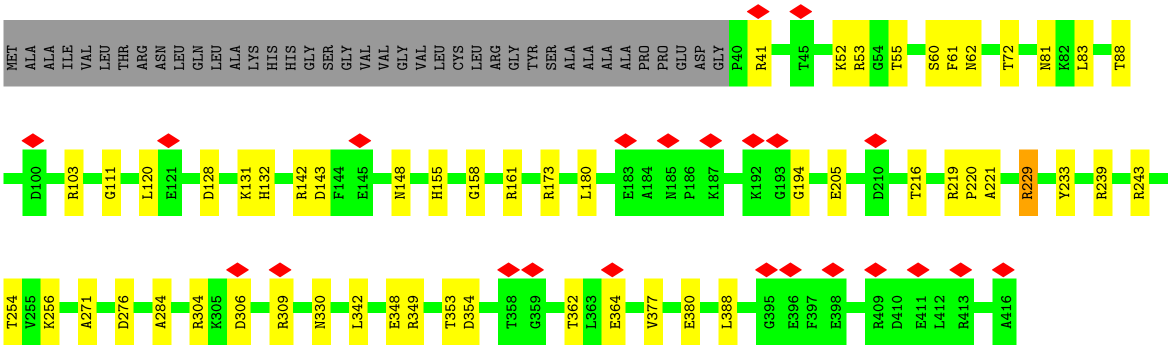
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:



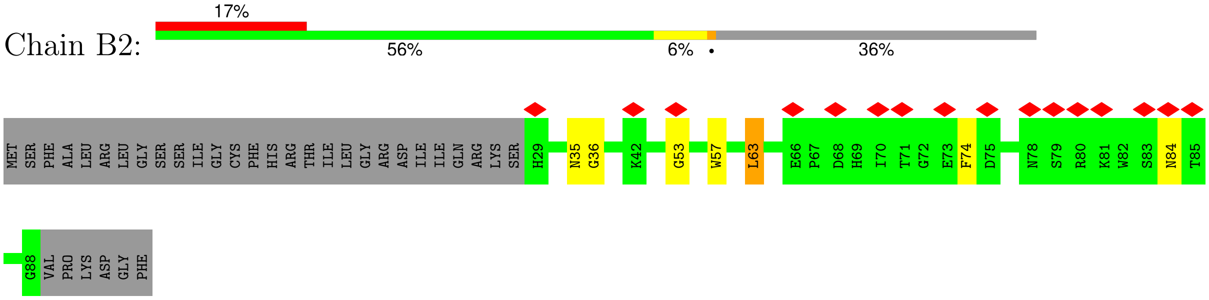
- Molecule 29: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A

Chain A9:



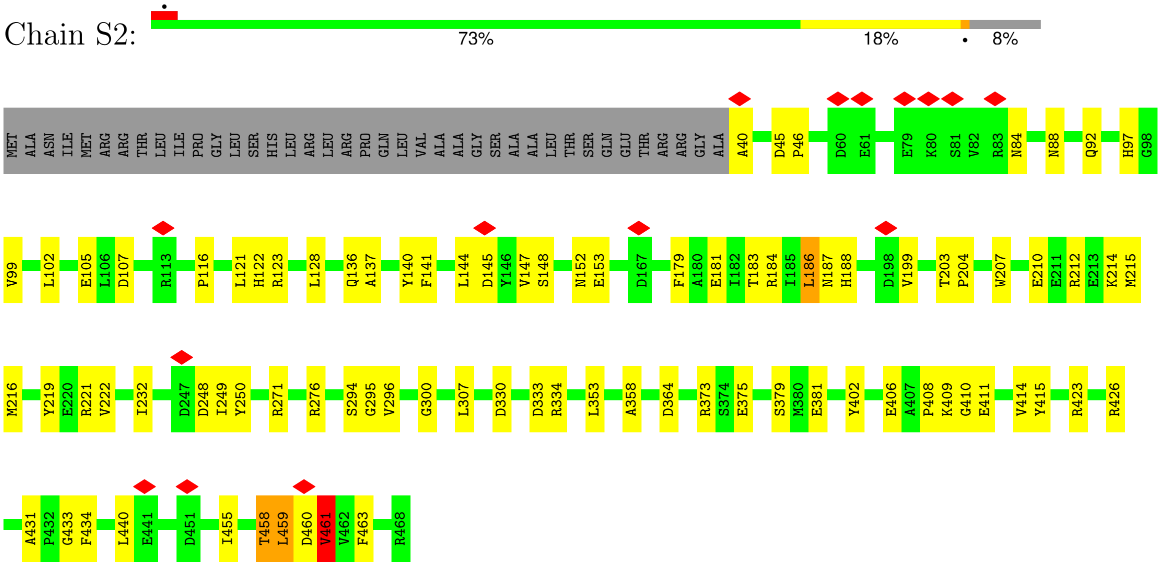
- Molecule 30: GEO11417p1

Chain B2:



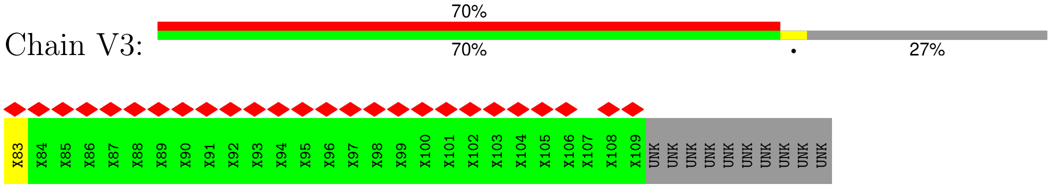
- Molecule 31: Complex I-49kD

Chain S2:



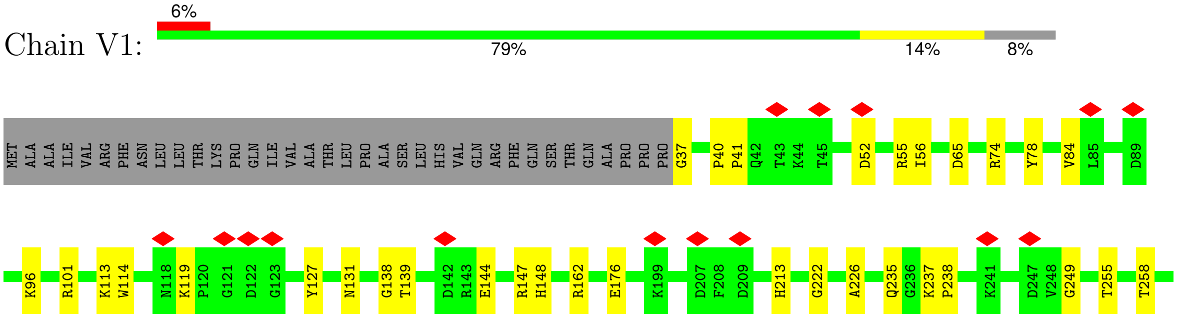
- Molecule 32: NADH dehydrogenase [ubiquinone] flavoprotein 3

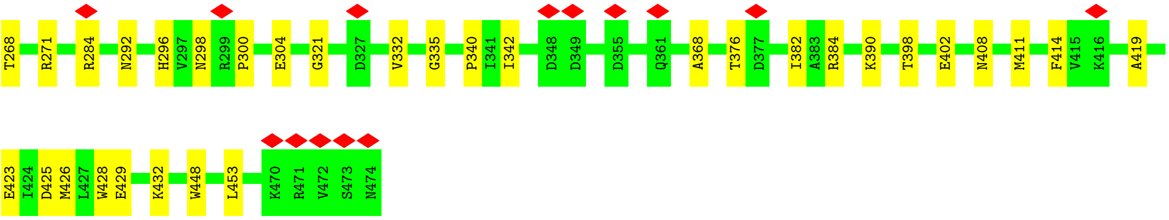
Chain V3:



- Molecule 33: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

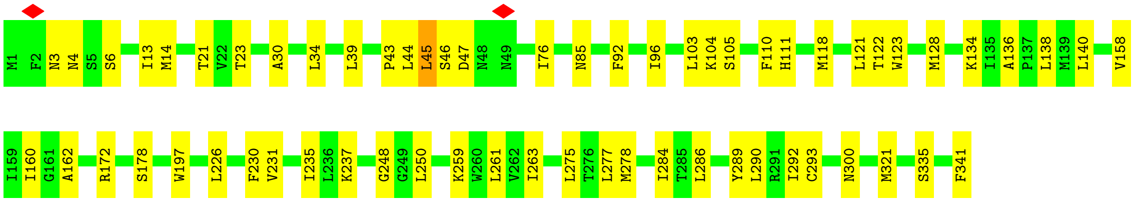
Chain V1:





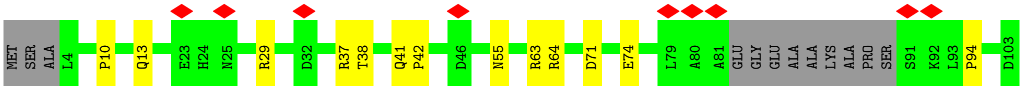
- Molecule 34: NADH-ubiquinone oxidoreductase chain 2

Chain 2:



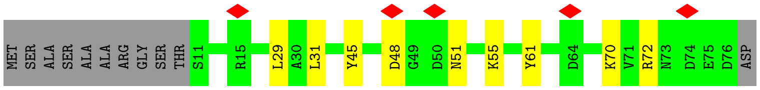
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7:



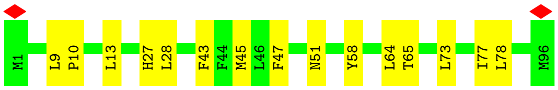
- Molecule 36: RH45008p

Chain A3:



- Molecule 37: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:

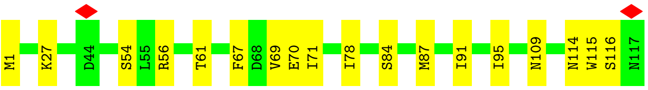


- Molecule 38: NADH-ubiquinone oxidoreductase chain 6

Chain 6:

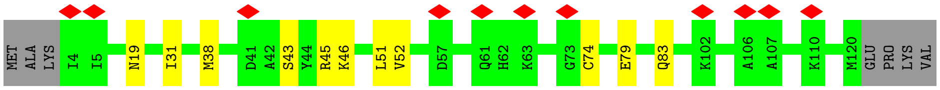
- Molecule 39: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



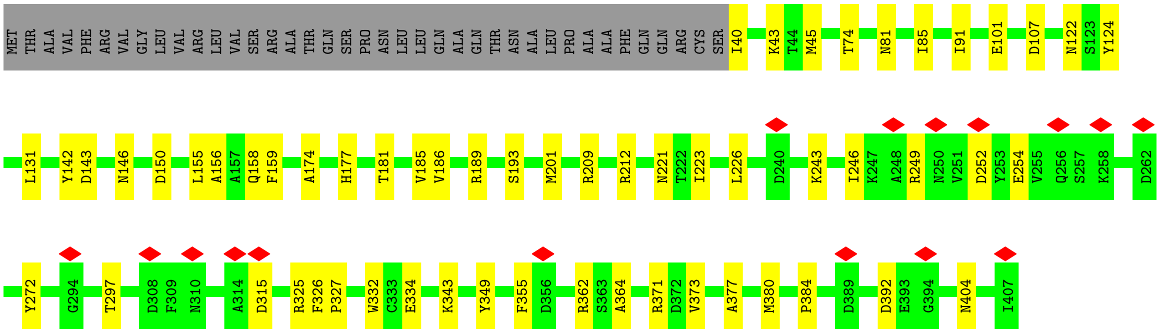
- Molecule 40: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain A5:



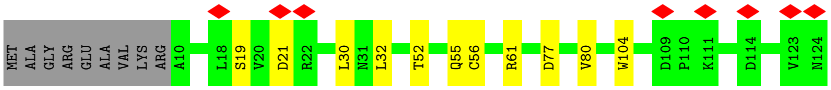
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AL:



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.876	Depositor
Minimum map value	-1.949	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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: C14, WSF, ZN, FMN, FES, 3PE, SF4, CDL, NDP, U10, ZMP, D12, PC1, OCT, DGT

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	AN	0.31	0/1185	0.61	0/1605
2	S6	0.27	0/733	0.51	0/987
3	S1	0.28	0/5264	0.58	0/7133
4	S3	0.30	0/1745	0.59	0/2370
5	V2	0.30	0/1719	0.55	0/2328
6	S7	0.35	0/1473	0.62	0/1997
7	S8	0.31	0/1518	0.57	0/2050
8	1	0.34	0/2651	0.60	0/3593
9	4	0.35	0/3711	0.63	0/5029
10	5	0.36	0/4726	0.62	0/6396
11	A8	0.35	0/1417	0.58	1/1911 (0.1%)
12	A1	0.30	0/594	0.58	0/801
13	AO	0.31	0/1240	0.55	0/1682
14	S5	0.32	0/846	0.58	0/1128
15	AM	0.31	0/1318	0.56	0/1790
16	BL	0.33	0/1299	0.64	0/1754
17	B6	0.29	0/1338	0.63	0/1808
18	B4	0.30	0/905	0.57	0/1210
19	B7	0.32	0/995	0.59	0/1336
20	B5	0.27	0/1255	0.52	0/1694
21	B9	0.29	0/1181	0.57	0/1593
22	BM	0.28	0/896	0.54	0/1222
23	B8	0.30	0/1250	0.55	0/1701
24	B3	0.27	0/665	0.54	0/903
25	AB	0.29	0/680	0.69	3/919 (0.3%)
25	AC	0.31	0/690	0.65	2/931 (0.2%)
26	C2	0.30	0/936	0.54	0/1271
27	B1	0.26	0/441	0.55	0/590
28	S4	0.30	0/1245	0.60	0/1687
29	A9	0.29	0/3105	0.58	0/4200
30	B2	0.27	0/519	0.47	0/713
31	S2	0.33	0/3512	0.63	0/4761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	V1	0.31	0/3438	0.59	0/4643
34	2	0.32	0/2876	0.59	0/3890
35	A7	0.28	0/752	0.62	0/1018
36	A3	0.25	0/528	0.57	0/714
37	4L	0.34	0/815	0.62	0/1095
38	6	0.33	0/1431	0.63	0/1933
39	3	0.33	0/979	0.66	0/1325
40	A5	0.26	0/933	0.54	0/1265
41	AL	0.28	0/3083	0.55	0/4168
42	A6	0.28	0/997	0.60	0/1340
All	All	0.31	0/66884	0.59	6/90484 (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	S7	0	1
16	BL	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AC	69	PRO	N-CA-CB	6.45	111.04	103.30
25	AB	69	PRO	N-CA-CB	6.29	110.85	103.30
25	AB	103	ASP	CB-CG-OD1	6.15	123.83	118.30
25	AC	68	PRO	N-CA-CB	5.93	110.42	103.30
25	AB	68	PRO	N-CA-CB	5.93	110.42	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	BL	86	ARG	Sidechain
6	S7	191	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1145	0	1102	18	0
2	S6	716	0	700	7	0
3	S1	5181	0	5227	60	0
4	S3	1699	0	1648	26	0
5	V2	1680	0	1657	15	0
6	S7	1435	0	1448	38	0
7	S8	1485	0	1422	24	0
8	1	2571	0	2628	42	0
9	4	3606	0	3740	73	0
10	5	4606	0	4742	84	0
11	A8	1384	0	1324	13	0
12	A1	581	0	582	11	0
13	AO	1202	0	1211	10	0
14	S5	828	0	807	10	0
15	AM	1281	0	1267	19	0
16	BL	1266	0	1205	4	0
17	B6	1302	0	1295	11	0
18	B4	884	0	879	13	0
19	B7	972	0	959	10	0
20	B5	1221	0	1186	8	0
21	B9	1148	0	1113	12	0
22	BM	871	0	822	5	0
23	B8	1201	0	1107	11	0
24	B3	646	0	641	4	0
25	AB	670	0	669	7	0
25	AC	680	0	675	8	0
26	C2	908	0	896	7	0
27	B1	430	0	436	5	0
28	S4	1214	0	1186	10	0
29	A9	3030	0	3032	37	0
30	B2	495	0	457	5	0
31	S2	3427	0	3399	71	0
32	V3	135	0	30	1	0
33	V1	3361	0	3339	39	0
34	2	2797	0	2879	45	0
35	A7	736	0	737	9	0
36	A3	519	0	517	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4L	794	0	818	14	0
38	6	1404	0	1517	28	0
39	3	956	0	1030	16	0
40	A5	914	0	944	8	0
41	AL	3008	0	2945	39	0
42	A6	977	0	997	7	0
43	2	45	0	34	0	0
43	3	54	0	52	0	0
43	6	86	0	122	3	0
43	AM	76	0	96	5	0
43	AN	67	0	78	3	0
43	B5	142	0	172	7	0
43	B6	47	0	38	1	0
44	1	54	0	88	2	0
44	2	45	0	67	1	0
44	4	78	0	104	4	0
44	5	34	0	41	3	0
44	A9	44	0	62	3	0
44	AM	113	0	151	5	0
44	AN	44	0	62	2	0
44	B6	37	0	48	1	0
44	S7	46	0	69	0	0
45	S6	1	0	0	0	0
46	S1	16	0	0	0	0
46	S7	8	0	0	6	0
46	S8	16	0	0	0	0
46	V1	8	0	0	0	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	1	51	0	82	1	0
48	2	30	0	34	2	0
48	3	92	0	141	3	0
48	4	152	0	203	2	0
48	5	275	0	377	9	0
48	6	35	0	43	2	0
48	AM	72	0	95	3	0
48	B1	37	0	48	0	0
48	B4	47	0	71	0	0
48	B6	48	0	75	2	0
48	C2	45	0	67	1	0
48	S7	66	0	80	3	0
49	1	63	0	87	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	AO	14	0	30	0	0
50	B5	14	0	30	0	0
50	C2	14	0	30	0	0
51	AB	32	0	36	0	0
51	AC	34	0	40	1	0
52	B1	8	0	18	0	0
53	A3	12	0	26	0	0
53	A9	24	0	52	0	0
53	B1	12	0	26	0	0
54	A9	48	0	26	0	0
55	V1	31	0	19	2	0
56	6	35	0	0	7	0
57	AL	31	0	12	5	0
All	All	67757	0	68247	764	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 764 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:97:CYS:SG	46:S7:301:SF4:FE1	1.46	1.06
31:S2:186:LEU:HD12	31:S2:212:ARG:HG3	1.42	1.02
56:6:201:WSF:C13	56:6:201:WSF:C15	2.43	0.96
56:6:201:WSF:C15	56:6:201:WSF:C14	2.44	0.96
56:6:201:WSF:C13	56:6:201:WSF:C14	2.43	0.96

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	134/142 (94%)	130 (97%)	3 (2%)	1 (1%)	19	47
2	S6	87/126 (69%)	87 (100%)	0	0	100	100
3	S1	679/731 (93%)	660 (97%)	19 (3%)	0	100	100
4	S3	203/265 (77%)	196 (97%)	7 (3%)	0	100	100
5	V2	212/242 (88%)	208 (98%)	4 (2%)	0	100	100
6	S7	180/221 (81%)	168 (93%)	12 (7%)	0	100	100
7	S8	184/217 (85%)	179 (97%)	5 (3%)	0	100	100
8	1	313/315 (99%)	300 (96%)	13 (4%)	0	100	100
9	4	444/446 (100%)	421 (95%)	21 (5%)	2 (0%)	25	54
10	5	575/577 (100%)	552 (96%)	22 (4%)	1 (0%)	44	72
11	A8	172/175 (98%)	164 (95%)	8 (5%)	0	100	100
12	A1	68/123 (55%)	68 (100%)	0	0	100	100
13	AO	144/154 (94%)	140 (97%)	4 (3%)	0	100	100
14	S5	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	AM	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
16	BL	149/159 (94%)	148 (99%)	1 (1%)	0	100	100
17	B6	159/167 (95%)	155 (98%)	4 (2%)	0	100	100
18	B4	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
19	B7	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
20	B5	141/186 (76%)	139 (99%)	2 (1%)	0	100	100
21	B9	132/144 (92%)	131 (99%)	1 (1%)	0	100	100
22	BM	104/150 (69%)	100 (96%)	4 (4%)	0	100	100
23	B8	142/175 (81%)	134 (94%)	8 (6%)	0	100	100
24	B3	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
25	AB	82/152 (54%)	78 (95%)	3 (4%)	1 (1%)	11	35
25	AC	83/152 (55%)	79 (95%)	3 (4%)	1 (1%)	11	35
26	C2	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
27	B1	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
28	S4	149/183 (81%)	145 (97%)	4 (3%)	0	100	100
29	A9	375/416 (90%)	366 (98%)	9 (2%)	0	100	100
30	B2	58/94 (62%)	57 (98%)	1 (2%)	0	100	100
31	S2	427/468 (91%)	418 (98%)	8 (2%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	V1	436/474 (92%)	421 (97%)	15 (3%)	0	100	100
34	2	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
35	A7	87/103 (84%)	85 (98%)	2 (2%)	0	100	100
36	A3	64/77 (83%)	64 (100%)	0	0	100	100
37	4L	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
38	6	172/174 (99%)	172 (100%)	0	0	100	100
39	3	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
40	A5	115/124 (93%)	114 (99%)	1 (1%)	0	100	100
41	AL	366/407 (90%)	354 (97%)	12 (3%)	0	100	100
42	A6	113/124 (91%)	107 (95%)	6 (5%)	0	100	100
All	All	8026/9000 (89%)	7779 (97%)	240 (3%)	7 (0%)	50	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	4	43	ASN
9	4	202	LEU
10	5	324	ASN
25	AB	69	PRO
25	AC	69	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AN	118/122 (97%)	117 (99%)	1 (1%)	79	87
2	S6	77/111 (69%)	77 (100%)	0	100	100
3	S1	549/582 (94%)	545 (99%)	4 (1%)	81	88
4	S3	184/225 (82%)	184 (100%)	0	100	100
5	V2	185/205 (90%)	183 (99%)	2 (1%)	70	81
6	S7	152/184 (83%)	150 (99%)	2 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	S8	159/182 (87%)	159 (100%)	0	100	100
8	1	282/282 (100%)	277 (98%)	5 (2%)	54	73
9	4	403/404 (100%)	399 (99%)	4 (1%)	73	83
10	5	518/518 (100%)	505 (98%)	13 (2%)	42	65
11	A8	150/151 (99%)	144 (96%)	6 (4%)	27	52
12	A1	63/115 (55%)	63 (100%)	0	100	100
13	AO	128/134 (96%)	127 (99%)	1 (1%)	79	87
14	S5	88/89 (99%)	87 (99%)	1 (1%)	70	81
15	AM	129/131 (98%)	128 (99%)	1 (1%)	79	87
16	BL	135/141 (96%)	135 (100%)	0	100	100
17	B6	133/136 (98%)	132 (99%)	1 (1%)	79	87
18	B4	88/94 (94%)	88 (100%)	0	100	100
19	B7	104/104 (100%)	103 (99%)	1 (1%)	73	83
20	B5	129/162 (80%)	129 (100%)	0	100	100
21	B9	116/126 (92%)	116 (100%)	0	100	100
22	BM	95/131 (72%)	95 (100%)	0	100	100
23	B8	121/145 (83%)	117 (97%)	4 (3%)	33	58
24	B3	66/84 (79%)	66 (100%)	0	100	100
25	AB	76/136 (56%)	76 (100%)	0	100	100
25	AC	77/136 (57%)	77 (100%)	0	100	100
26	C2	93/94 (99%)	93 (100%)	0	100	100
27	B1	42/43 (98%)	42 (100%)	0	100	100
28	S4	131/154 (85%)	131 (100%)	0	100	100
29	A9	319/346 (92%)	318 (100%)	1 (0%)	91	95
30	B2	51/80 (64%)	50 (98%)	1 (2%)	50	70
31	S2	368/398 (92%)	364 (99%)	4 (1%)	70	81
33	V1	350/381 (92%)	349 (100%)	1 (0%)	91	95
34	2	317/317 (100%)	314 (99%)	3 (1%)	75	86
35	A7	79/86 (92%)	78 (99%)	1 (1%)	65	78
36	A3	52/59 (88%)	52 (100%)	0	100	100
37	4L	91/91 (100%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	6	167/167 (100%)	164 (98%)	3 (2%)	54	73
39	3	110/110 (100%)	109 (99%)	1 (1%)	75	86
40	A5	96/102 (94%)	96 (100%)	0	100	100
41	AL	324/356 (91%)	324 (100%)	0	100	100
42	A6	108/114 (95%)	108 (100%)	0	100	100
All	All	7023/7728 (91%)	6962 (99%)	61 (1%)	74	86

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	5	291	MET
34	2	47	ASP
11	A8	145	GLU
34	2	46	SER
38	6	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
11	A8	50	GLN
17	B6	119	ASN
37	4L	51	ASN
31	S2	152	ASN
10	5	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 1 is monoatomic - leaving 67 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	$\#\|Z\| > 2$
48	3PE	C2	201	-	44,44,50	0.32	0	47,49,55	0.35	0
57	DGT	AL	501	-	29,33,33	0.96	3 (10%)	37,52,52	0.70	1 (2%)
50	C14	AO	201	-	13,13,13	0.11	0	12,12,12	0.07	0
51	ZMP	AB	201	-	26,31,36	0.77	1 (3%)	30,38,45	3.45	6 (20%)
44	PC1	AM	205	-	43,43,53	0.32	0	49,51,61	0.44	0
46	SF4	V1	502	33	0,12,12	-	-	-		
43	CDL	B5	202	-	65,65,99	0.36	0	71,77,111	0.31	0
43	CDL	6	203	-	85,85,99	0.32	0	91,97,111	0.29	0
48	3PE	4	506	-	38,38,50	0.36	0	41,43,55	0.63	1 (2%)
48	3PE	4	503	-	44,44,50	0.31	0	47,49,55	0.27	0
48	3PE	B1	103	-	36,36,50	0.37	0	39,41,55	0.64	1 (2%)
48	3PE	S7	303	-	32,32,50	0.37	0	35,37,55	0.34	0
44	PC1	B6	202	-	36,36,53	0.36	0	42,44,61	0.64	1 (2%)
48	3PE	5	604	-	29,29,50	0.39	0	32,34,55	0.35	0
48	3PE	5	605	-	32,32,50	0.37	0	35,37,55	0.32	0
48	3PE	2	401	-	29,29,50	0.38	0	32,34,55	0.36	0
48	3PE	5	608	-	44,44,50	0.34	0	47,49,55	0.59	1 (2%)
53	D12	A3	101	-	11,11,11	0.11	0	10,10,10	0.06	0
44	PC1	2	402	-	44,44,53	0.31	0	50,52,61	0.32	0
44	PC1	4	501	-	38,38,53	0.35	0	44,46,61	0.37	0
46	SF4	S1	802	3	0,12,12	-	-	-		
48	3PE	4	502	-	31,31,50	0.37	0	34,36,55	0.33	0
48	3PE	3	203	-	40,40,50	0.36	0	43,45,55	0.60	1 (2%)
52	OCT	B1	101	-	7,7,7	0.12	0	6,6,6	0.05	0
44	PC1	A9	501	-	43,43,53	0.31	0	49,51,61	0.30	0
44	PC1	1	401	-	53,53,53	0.33	0	59,61,61	0.55	1 (1%)
48	3PE	5	601	-	31,31,50	0.38	0	34,36,55	0.34	0
48	3PE	5	602	-	50,50,50	0.31	0	53,55,55	0.32	0
48	3PE	B4	201	-	46,46,50	0.31	0	49,51,55	0.28	0
43	CDL	2	403	-	43,43,99	0.60	1 (2%)	47,54,111	0.63	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	FES	V2	301	5	0,4,4	-	-	-		
44	PC1	AM	201	-	36,36,53	0.34	0	42,44,61	0.36	0
43	CDL	AM	204	-	75,75,99	0.36	0	81,87,111	0.49	1 (1%)
44	PC1	AN	202	-	43,43,53	0.33	0	49,51,61	0.30	0
50	C14	C2	202	-	13,13,13	0.10	0	12,12,12	0.07	0
44	PC1	4	505	-	38,38,53	0.33	0	44,46,61	0.34	0
43	CDL	3	201	-	53,53,99	0.40	0	59,65,111	0.35	0
46	SF4	S7	301	6	0,12,12	-	-	-		
48	3PE	5	603	-	32,32,50	0.40	0	35,37,55	0.69	1 (2%)
48	3PE	3	202	-	50,50,50	0.30	0	53,55,55	0.37	0
48	3PE	B6	201	-	47,47,50	0.38	0	50,52,55	0.39	1 (2%)
46	SF4	S1	801	3	0,12,12	-	-	-		
56	WSF	6	201	-	34,34,34	4.99	3 (8%)	37,40,40	2.85	4 (10%)
43	CDL	AN	201	-	66,66,99	0.36	0	72,78,111	0.38	0
43	CDL	B6	203	-	46,46,99	0.41	0	52,58,111	0.39	0
44	PC1	5	606	-	33,33,53	0.38	0	39,41,61	0.39	0
51	ZMP	AC	201	-	28,33,36	0.81	1 (3%)	32,40,45	3.27	6 (18%)
46	SF4	S8	301	7	0,12,12	-	-	-		
48	3PE	S7	302	-	32,32,50	0.37	0	35,37,55	0.31	0
50	C14	B5	203	-	13,13,13	0.11	0	12,12,12	0.07	0
44	PC1	S7	304	-	45,45,53	0.33	0	51,53,61	0.33	0
48	3PE	6	202	-	34,34,50	0.37	0	37,39,55	0.34	0
48	3PE	AM	203	-	30,30,50	0.38	0	33,35,55	0.35	0
44	PC1	AM	206	-	31,31,53	0.39	0	37,39,61	0.41	0
54	NDP	A9	502	-	47,52,52	0.54	0	61,80,80	0.54	1 (1%)
55	FMN	V1	501	-	33,33,33	0.31	0	48,50,50	0.43	0
43	CDL	B5	201	-	75,75,99	0.34	0	81,87,111	0.31	0
48	3PE	1	403	-	50,50,50	0.30	0	53,55,55	0.31	0
49	U10	1	402	-	63,63,63	2.26	25 (39%)	78,79,79	1.48	19 (24%)
48	3PE	4	504	-	35,35,50	0.35	0	38,40,55	0.34	0
46	SF4	S8	302	7	0,12,12	-	-	-		
53	D12	B1	102	-	11,11,11	0.10	0	10,10,10	0.06	0
48	3PE	AM	202	-	40,40,50	0.33	0	43,45,55	0.35	0
53	D12	A9	504	-	11,11,11	0.11	0	10,10,10	0.07	0
47	FES	S1	803	3	0,4,4	-	-	-		
53	D12	A9	503	-	11,11,11	0.11	0	10,10,10	0.05	0
48	3PE	5	607	-	50,50,50	0.29	0	53,55,55	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	3PE	C2	201	-	-	8/48/48/54	-
57	DGT	AL	501	-	-	3/18/34/34	0/3/3/3
50	C14	AO	201	-	-	0/11/11/11	-
51	ZMP	AB	201	-	-	5/36/38/43	-
44	PC1	AM	205	-	-	9/47/47/57	-
46	SF4	V1	502	33	-	-	0/6/5/5
43	CDL	B5	202	-	-	16/76/76/110	-
43	CDL	6	203	-	-	16/96/96/110	-
48	3PE	4	506	-	-	11/42/42/54	-
48	3PE	4	503	-	-	5/48/48/54	-
48	3PE	B1	103	-	-	7/40/40/54	-
48	3PE	S7	303	-	-	6/36/36/54	-
44	PC1	B6	202	-	-	10/40/40/57	-
48	3PE	5	604	-	-	8/33/33/54	-
48	3PE	5	605	-	-	7/36/36/54	-
48	3PE	2	401	-	-	8/33/33/54	-
48	3PE	5	608	-	-	11/48/48/54	-
53	D12	A3	101	-	-	0/9/9/9	-
44	PC1	2	402	-	-	6/48/48/57	-
44	PC1	4	501	-	-	17/42/42/57	-
48	3PE	4	502	-	-	8/35/35/54	-
46	SF4	S1	802	3	-	-	0/6/5/5
48	3PE	3	203	-	-	12/44/44/54	-
52	OCT	B1	101	-	-	0/5/5/5	-
44	PC1	A9	501	-	-	6/47/47/57	-
44	PC1	1	401	-	-	13/57/57/57	-
48	3PE	B4	201	-	-	9/50/50/54	-
48	3PE	5	602	-	-	5/54/54/54	-
43	CDL	2	403	-	-	20/53/53/110	-
47	FES	V2	301	5	-	-	0/1/1/1
44	PC1	AM	201	-	-	5/40/40/57	-
43	CDL	AM	204	-	-	23/86/86/110	-
47	FES	S1	803	3	-	-	0/1/1/1
44	PC1	AN	202	-	-	6/47/47/57	-
50	C14	C2	202	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	PC1	4	505	-	-	6/42/42/57	-
43	CDL	3	201	-	-	17/64/64/110	-
48	3PE	5	603	-	-	9/36/36/54	-
46	SF4	S7	301	6	-	-	0/6/5/5
48	3PE	3	202	-	-	12/54/54/54	-
48	3PE	B6	201	-	-	6/49/49/54	-
56	WSF	6	201	-	-	5/38/38/38	-
46	SF4	S1	801	3	-	-	0/6/5/5
43	CDL	AN	201	-	-	28/77/77/110	-
43	CDL	B6	203	-	-	21/56/56/110	-
44	PC1	5	606	-	-	9/37/37/57	-
51	ZMP	AC	201	-	-	13/38/40/43	-
46	SF4	S8	301	7	-	-	0/6/5/5
48	3PE	S7	302	-	-	6/36/36/54	-
50	C14	B5	203	-	-	0/11/11/11	-
44	PC1	S7	304	-	-	14/49/49/57	-
48	3PE	6	202	-	-	11/38/38/54	-
48	3PE	AM	203	-	-	6/34/34/54	-
44	PC1	AM	206	-	-	14/35/35/57	-
54	NDP	A9	502	-	-	2/30/77/77	0/5/5/5
55	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
43	CDL	B5	201	-	-	18/86/86/110	-
48	3PE	1	403	-	-	9/54/54/54	-
49	U10	1	402	-	-	19/63/87/87	0/1/1/1
48	3PE	4	504	-	-	12/39/39/54	-
53	D12	B1	102	-	-	0/9/9/9	-
46	SF4	S8	302	7	-	-	0/6/5/5
48	3PE	AM	202	-	-	6/44/44/54	-
53	D12	A9	504	-	-	0/9/9/9	-
48	3PE	5	601	-	-	8/35/35/54	-
53	D12	A9	503	-	-	0/9/9/9	-
48	3PE	5	607	-	-	12/54/54/54	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	6	201	WSF	C14-C13	17.63	2.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	6	201	WSF	C15-C13	17.59	2.43	1.51
56	6	201	WSF	C12-C13	14.87	2.46	1.51
49	1	402	U10	C6-C1	10.61	1.54	1.35
49	1	402	U10	C4-C3	4.81	1.53	1.36

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	6	201	WSF	C15-C13-C14	-11.30	60.13	110.53
51	AB	201	ZMP	C19-C18-C17	-10.47	90.92	108.77
51	AC	201	ZMP	C20-C18-C17	-9.61	92.38	108.77
51	AC	201	ZMP	C19-C18-C17	-9.44	92.67	108.77
51	AB	201	ZMP	C20-C18-C17	-9.25	92.99	108.77

There are no chirality outliers.

5 of 534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	CA2-OA2-PA1-OA3
43	AN	201	CDL	CA2-OA2-PA1-OA4
43	AN	201	CDL	CA2-OA2-PA1-OA5
43	AN	201	CDL	CA3-OA5-PA1-OA2
43	AN	201	CDL	OA5-CA3-CA4-OA6

There are no ring outliers.

42 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	C2	201	3PE	1	0
57	AL	501	DGT	5	0
44	AM	205	PC1	4	0
43	B5	202	CDL	1	0
43	6	203	CDL	3	0
48	S7	303	3PE	2	0
44	B6	202	PC1	1	0
48	5	604	3PE	1	0
48	5	605	3PE	1	0
48	2	401	3PE	2	0
48	5	608	3PE	2	0
44	2	402	PC1	1	0
44	4	501	PC1	2	0

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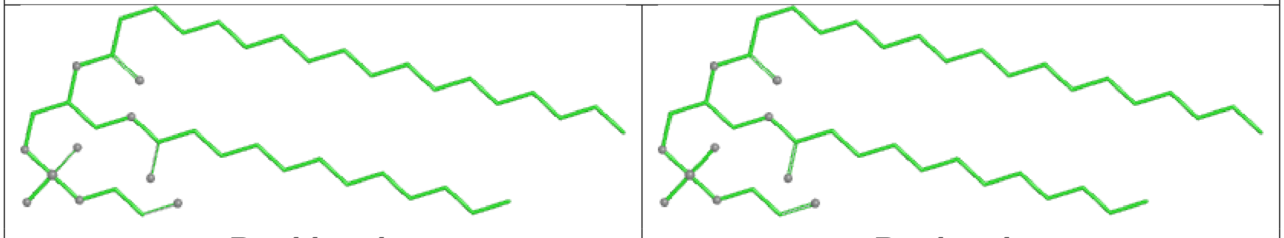
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	4	502	3PE	1	0
48	3	203	3PE	2	0
44	A9	501	PC1	3	0
44	1	401	PC1	2	0
48	5	601	3PE	1	0
48	5	602	3PE	1	0
43	AM	204	CDL	5	0
44	AN	202	PC1	2	0
44	4	505	PC1	2	0
46	S7	301	SF4	6	0
48	5	603	3PE	1	0
48	3	202	3PE	1	0
48	B6	201	3PE	2	0
56	6	201	WSF	7	0
43	AN	201	CDL	3	0
43	B6	203	CDL	1	0
44	5	606	PC1	3	0
51	AC	201	ZMP	1	0
48	S7	302	3PE	1	0
48	6	202	3PE	2	0
48	AM	203	3PE	1	0
44	AM	206	PC1	1	0
55	V1	501	FMN	2	0
43	B5	201	CDL	6	0
48	1	403	3PE	1	0
49	1	402	U10	3	0
48	4	504	3PE	1	0
48	AM	202	3PE	2	0
48	5	607	3PE	2	0

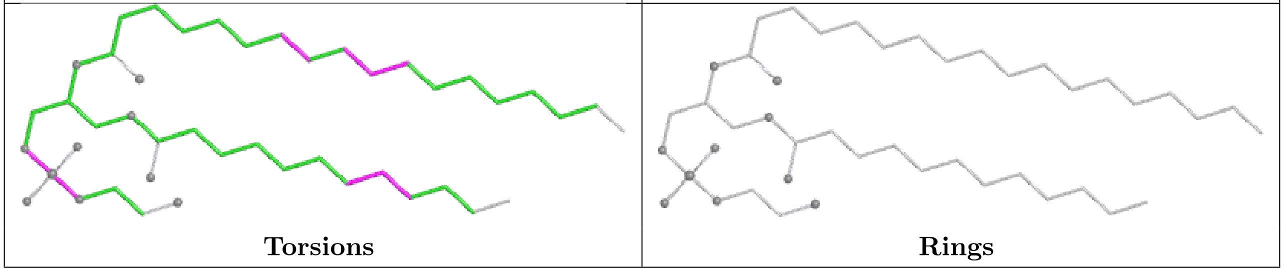
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 3PE C2 201



Bond lengths

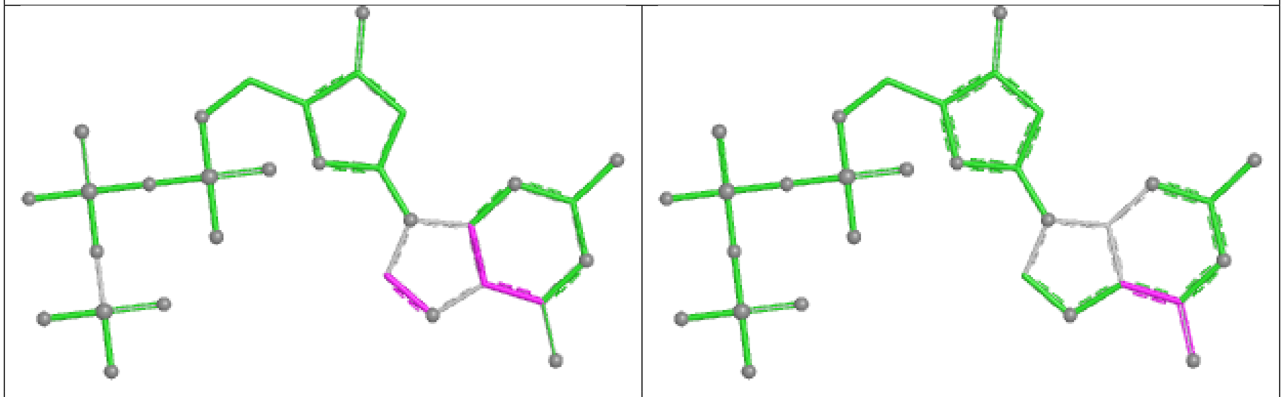
Bond angles



Torsions

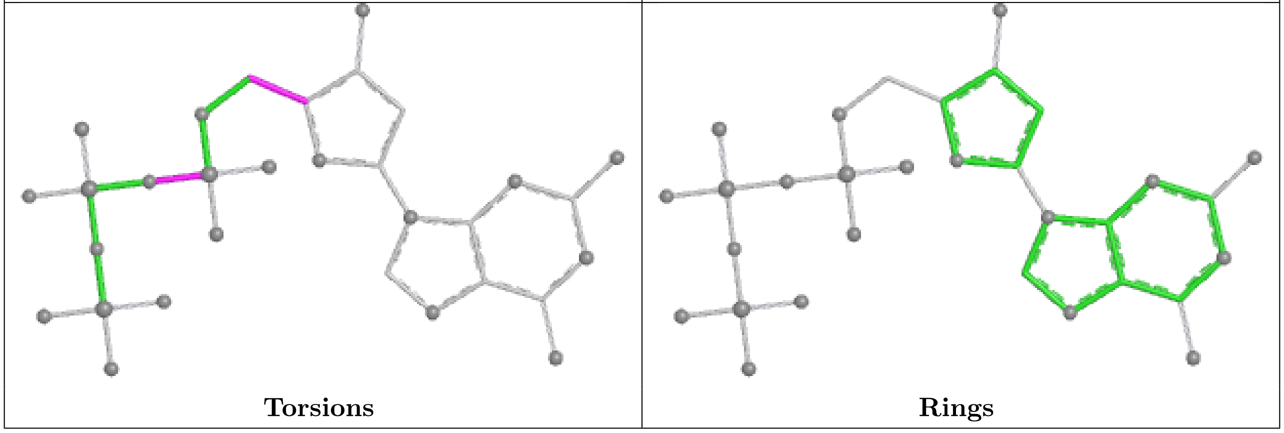
Rings

Ligand DGT AL 501



Bond lengths

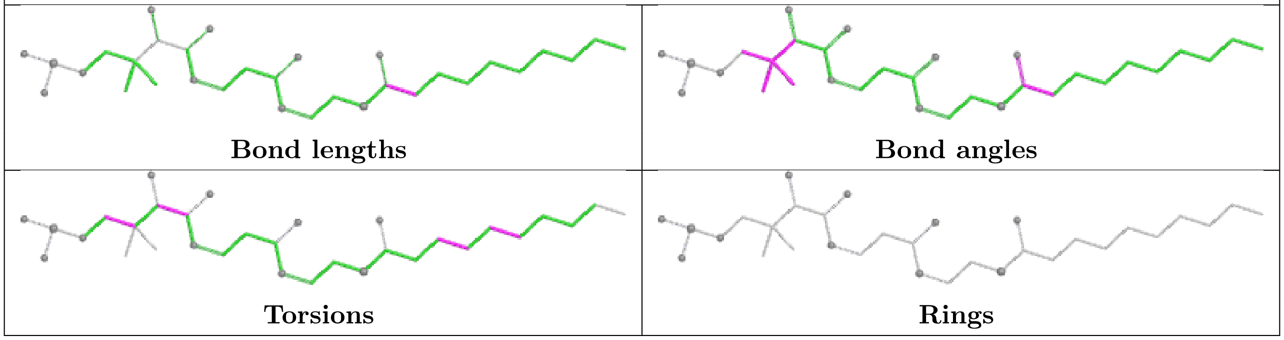
Bond angles



Torsions

Rings

Ligand ZMP AB 201



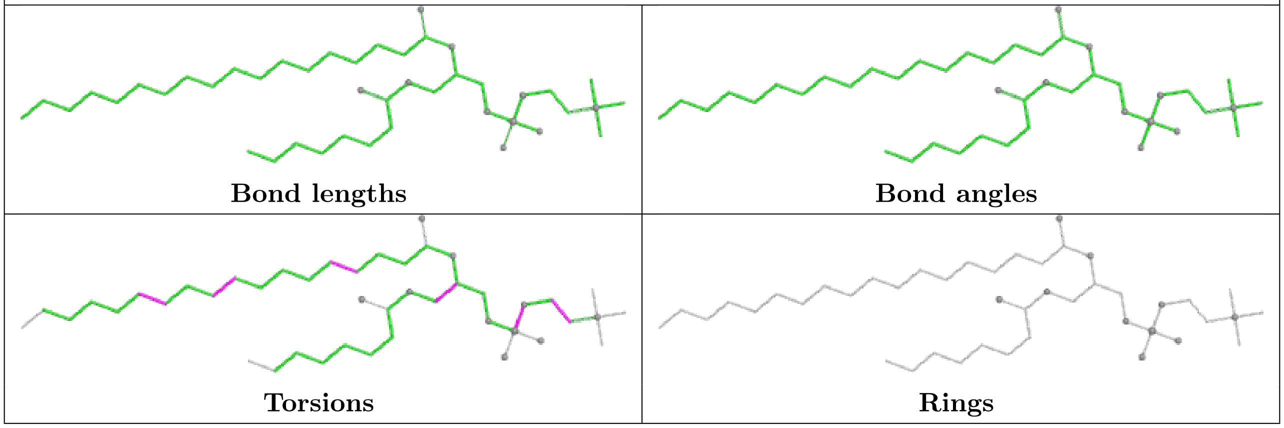
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 AM 205



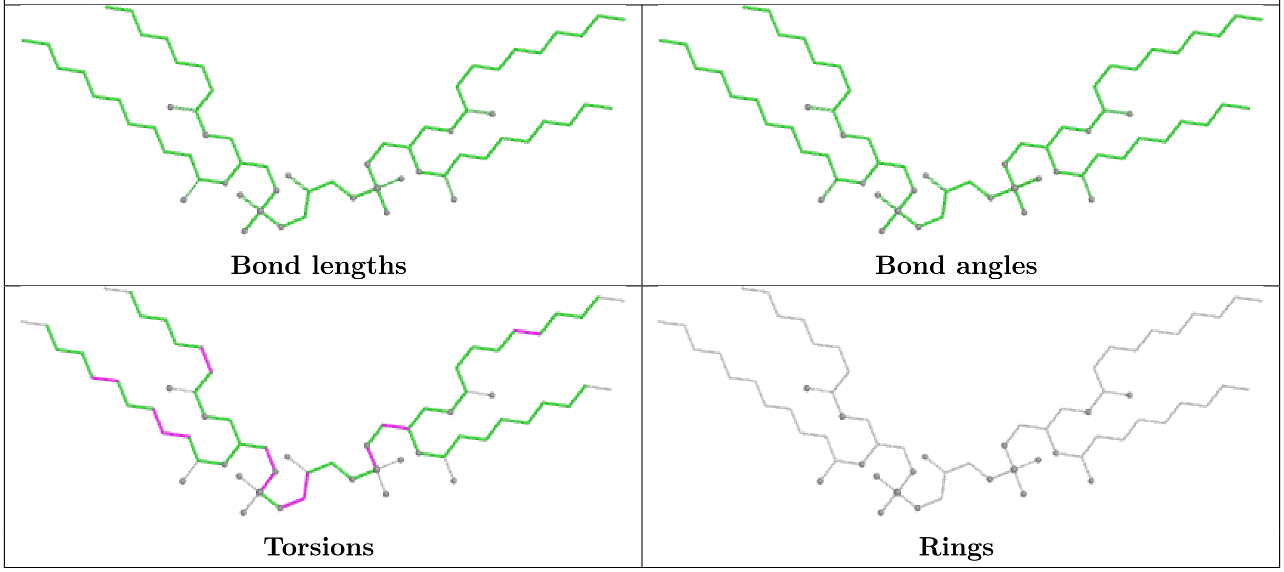
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL B5 202



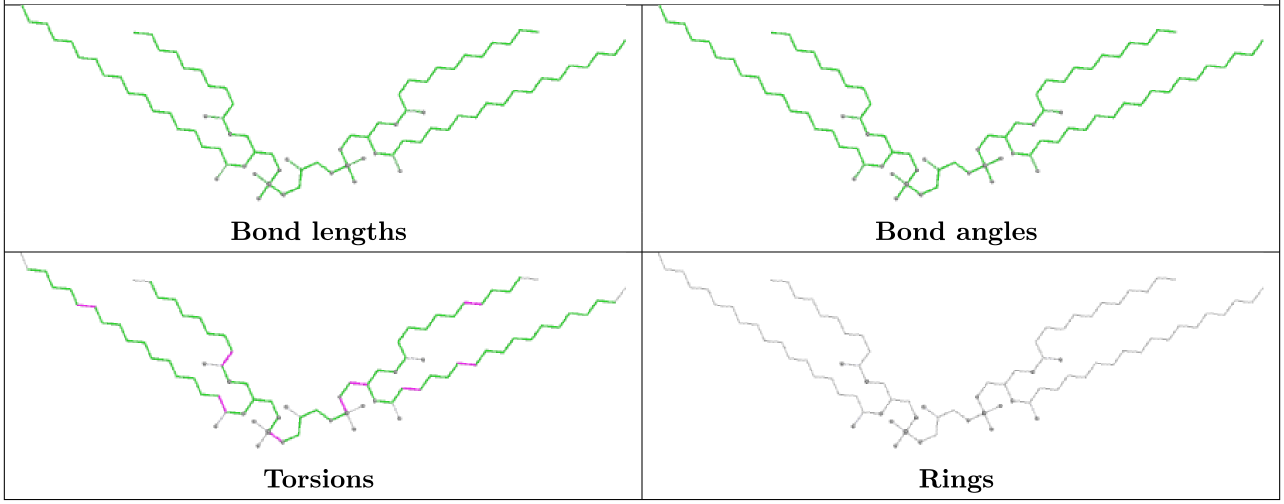
Bond lengths

Bond angles

Torsions

Rings

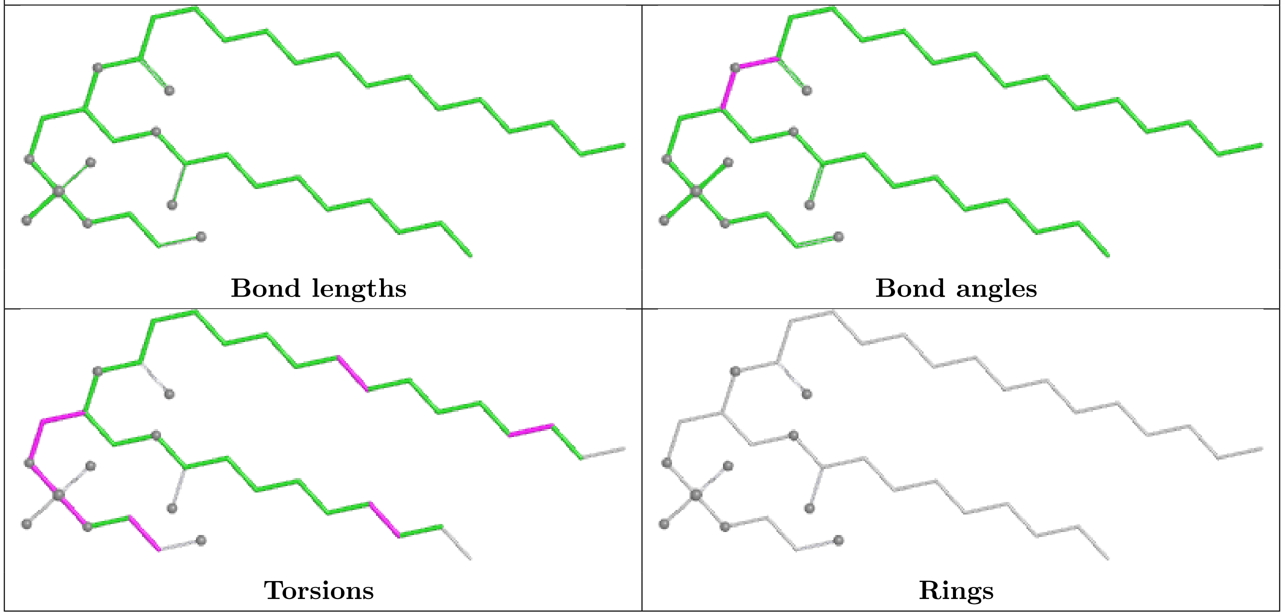
Ligand CDL 6 203



Bond lengths Bond angles

Torsions Rings

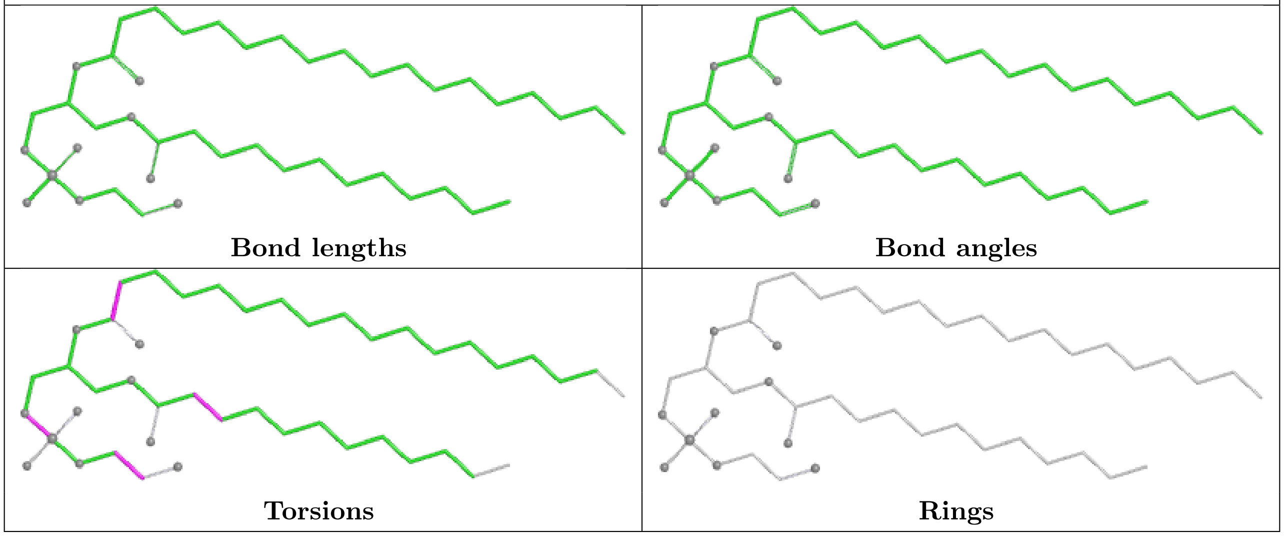
Ligand 3PE 4 506



Bond lengths Bond angles

Torsions Rings

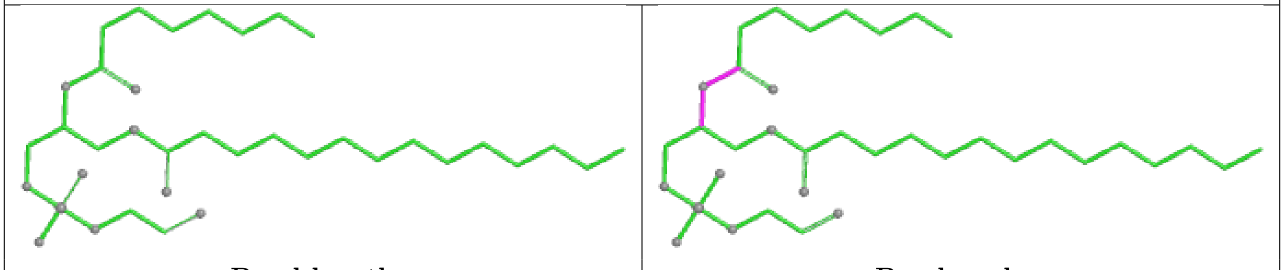
Ligand 3PE 4 503



Bond lengths Bond angles

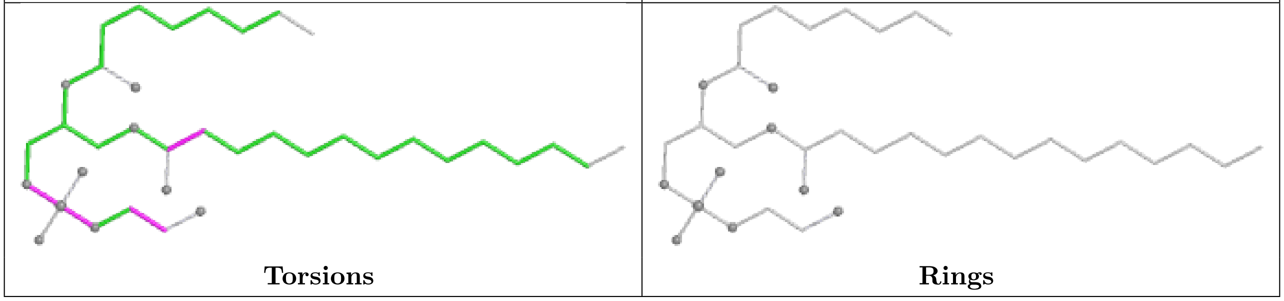
Torsions Rings

Ligand 3PE B1 103



Bond lengths

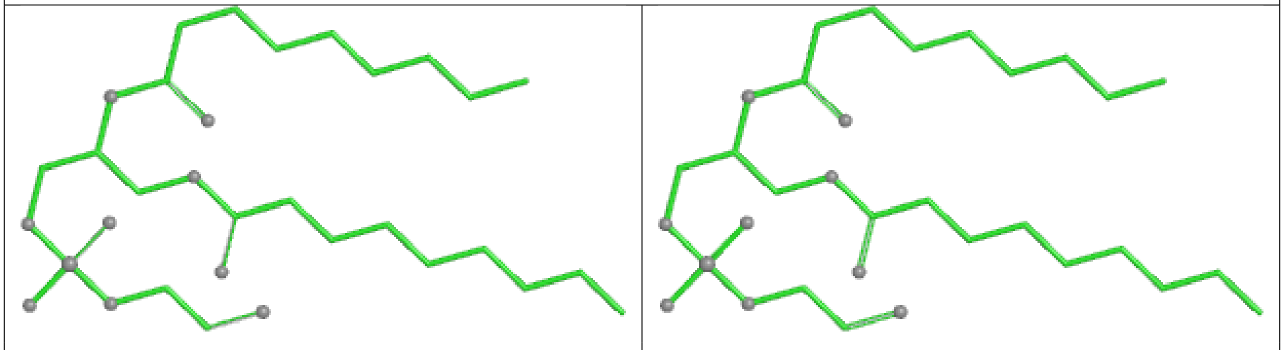
Bond angles



Torsions

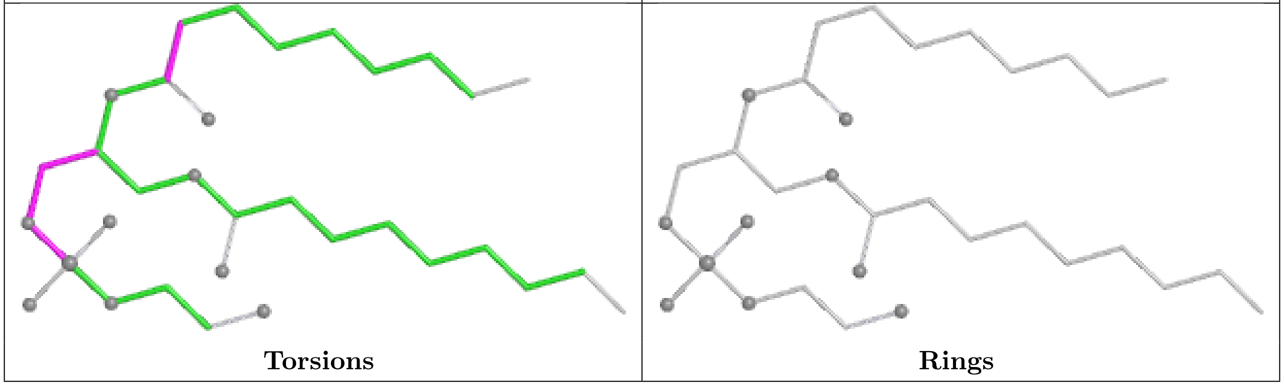
Rings

Ligand 3PE S7 303



Bond lengths

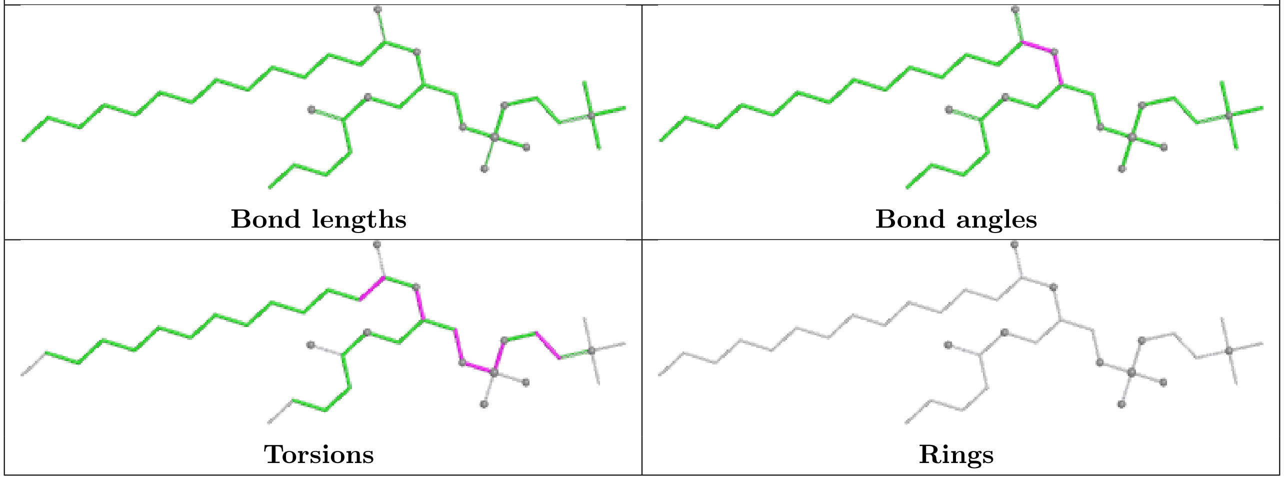
Bond angles



Torsions

Rings

Ligand PC1 B6 202



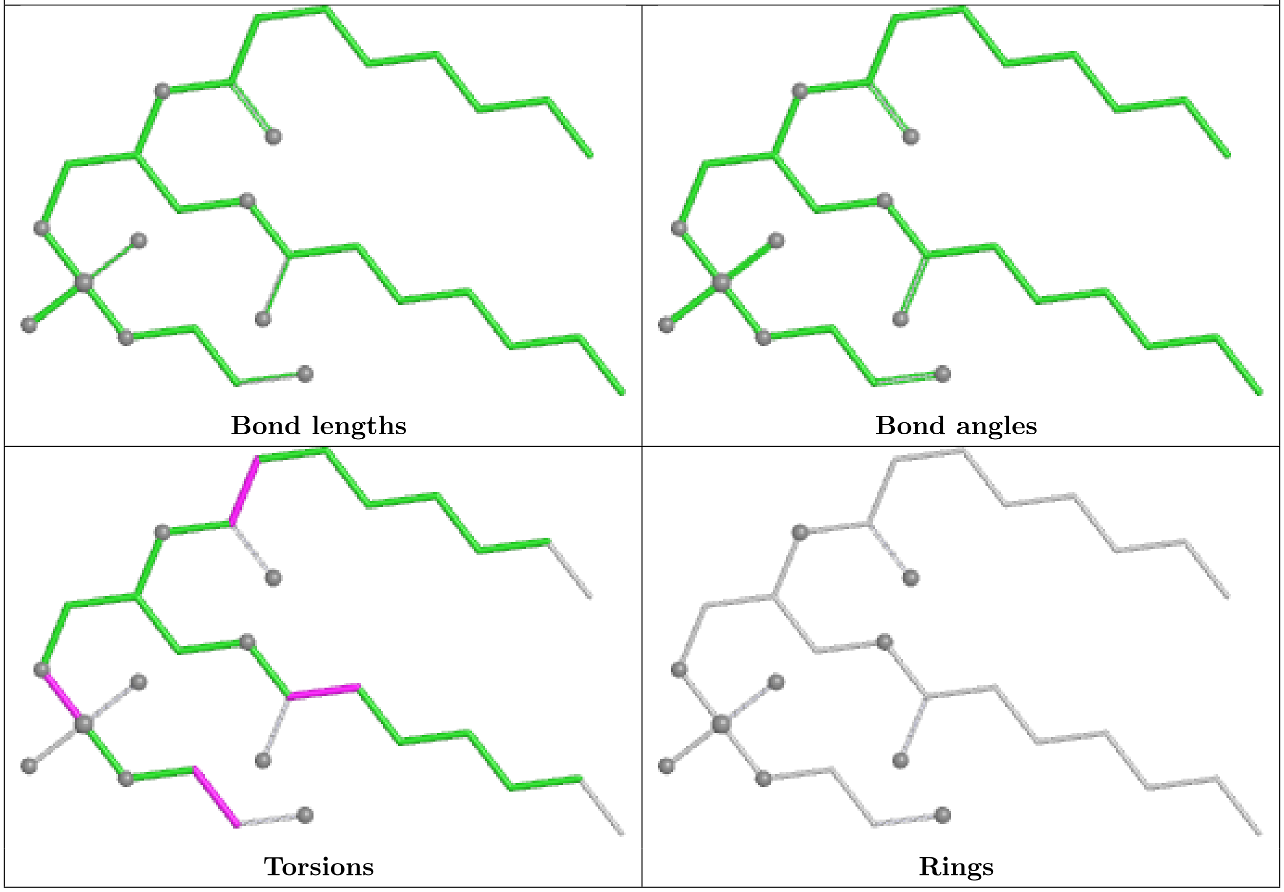
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 5 604



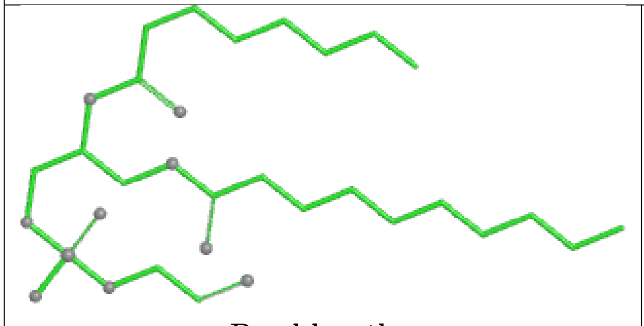
Bond lengths

Bond angles

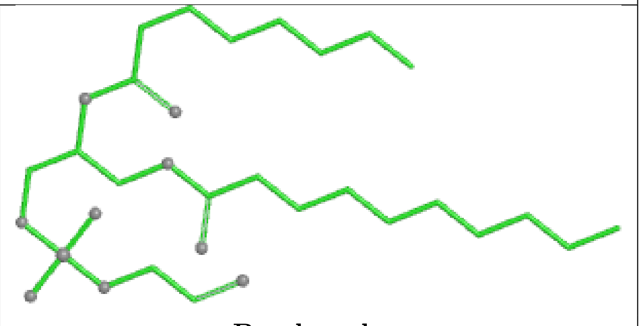
Torsions

Rings

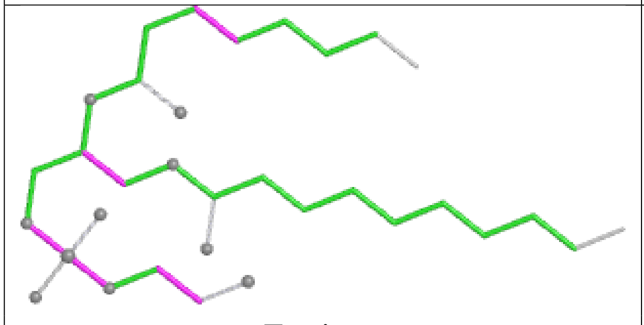
Ligand 3PE 5 605



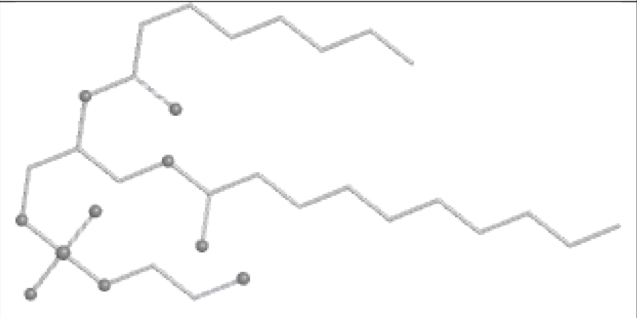
Bond lengths



Bond angles

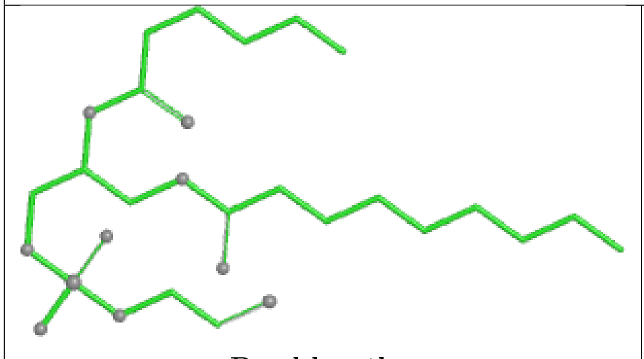


Torsions



Rings

Ligand 3PE 2 401



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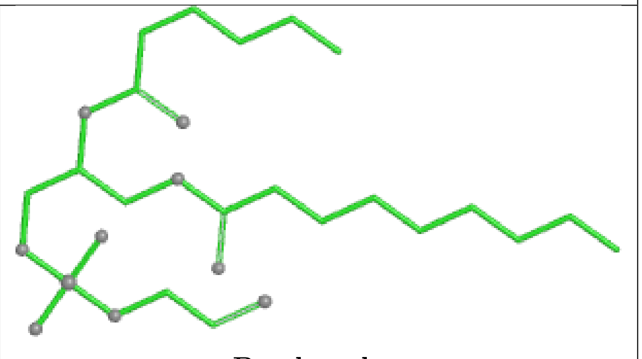
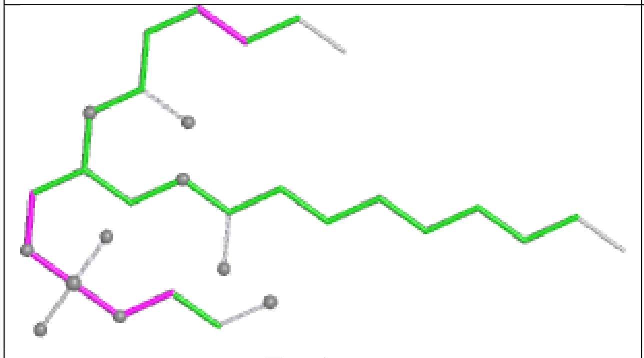
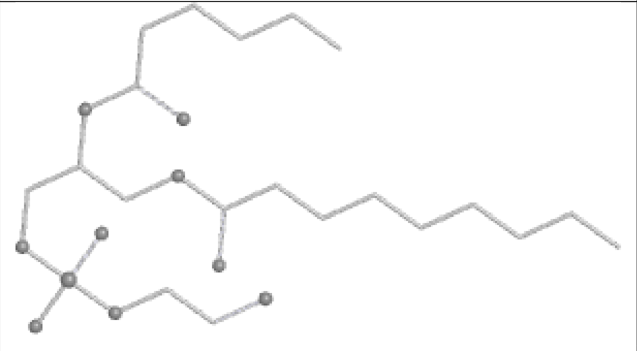


Bond angles

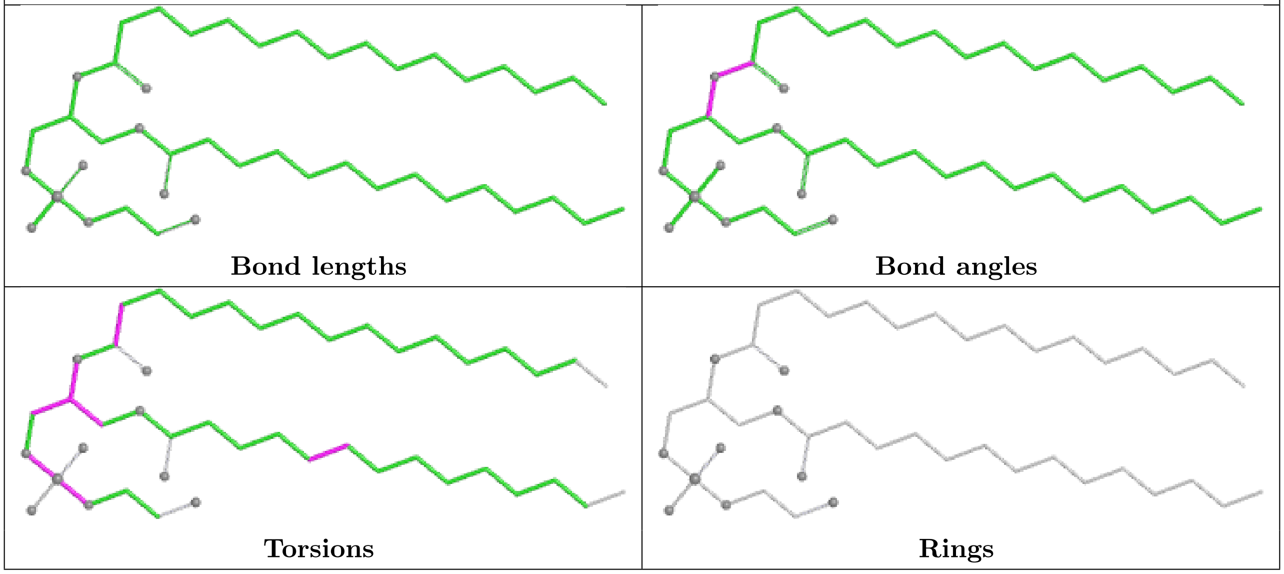


Torsions

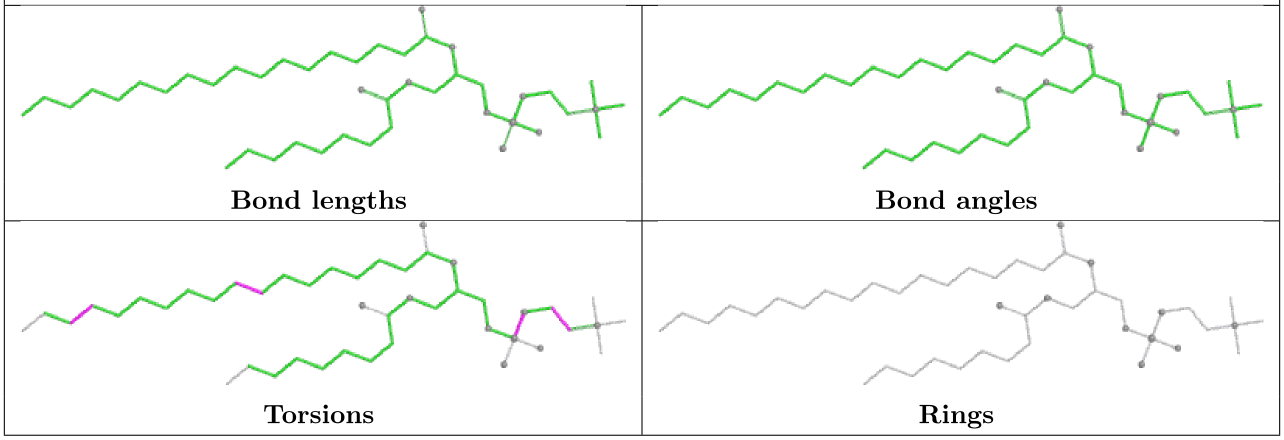


Rings

Ligand 3PE 5 608



Ligand PC1 2 402



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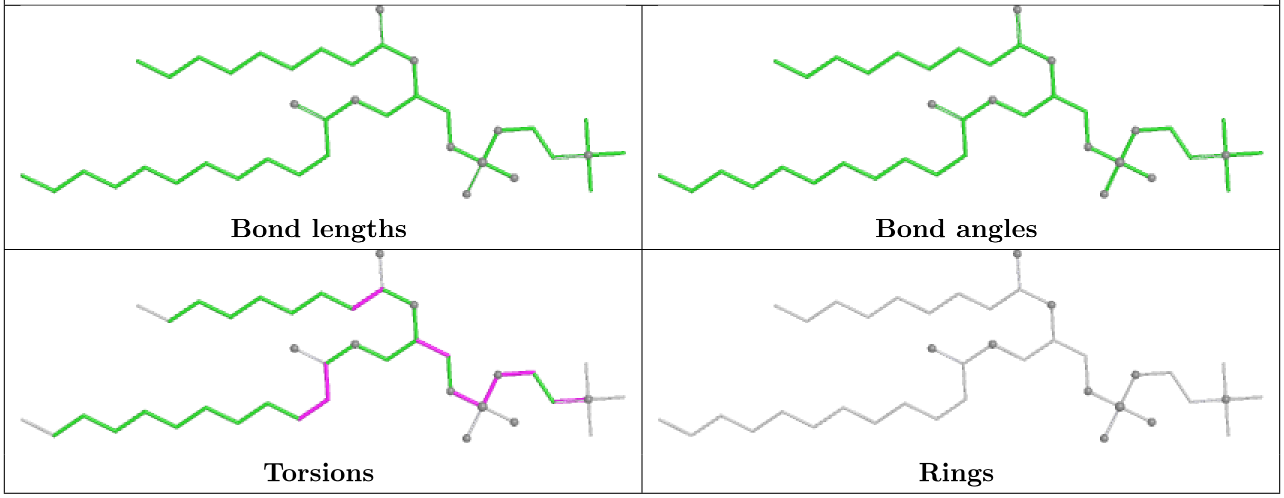

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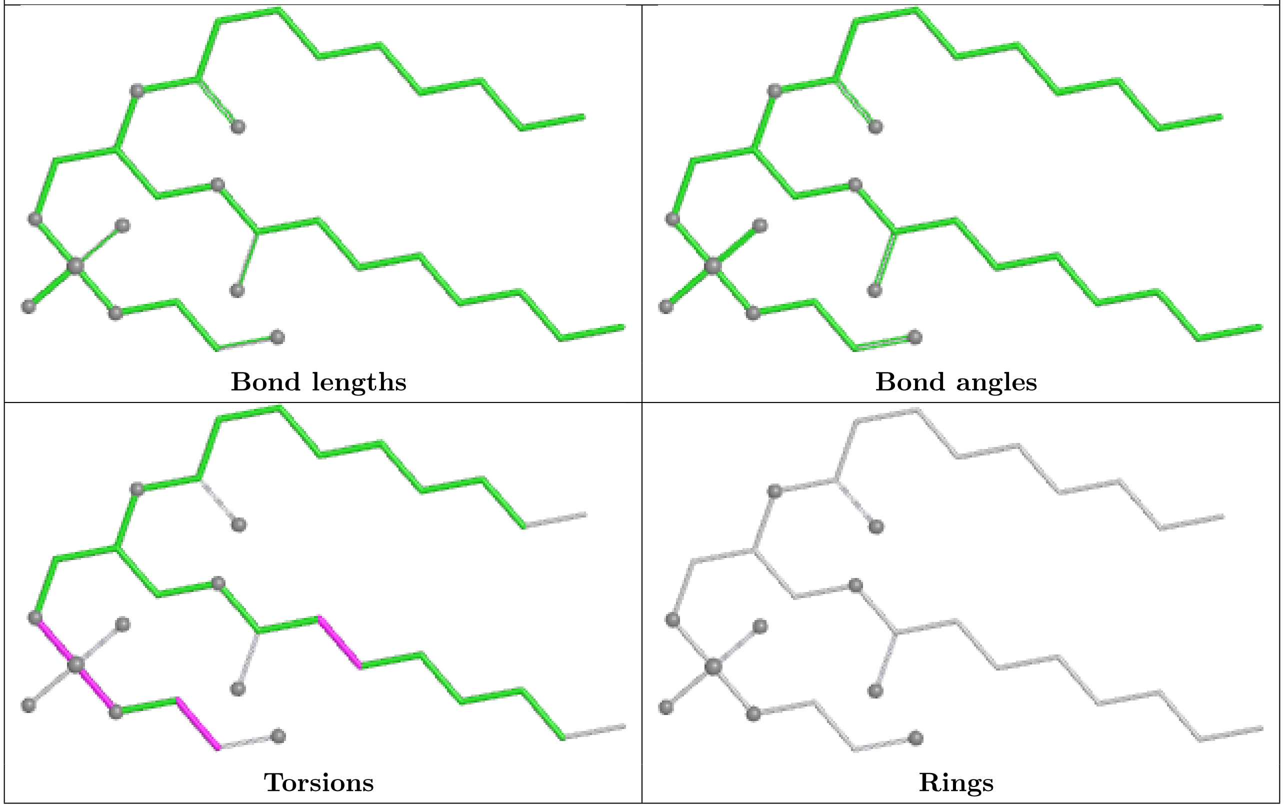


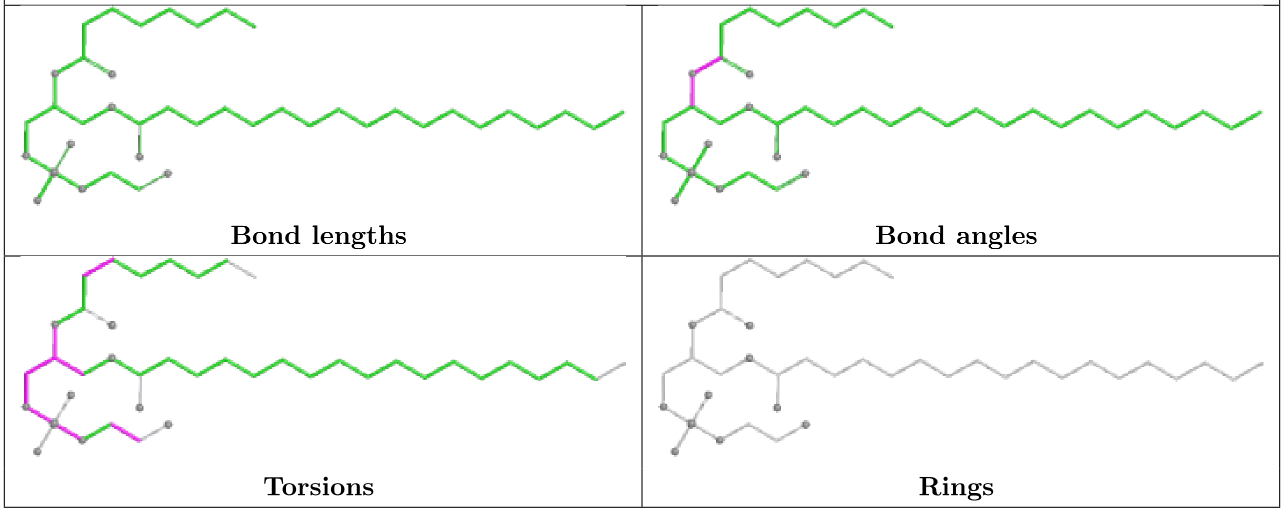
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 3 203



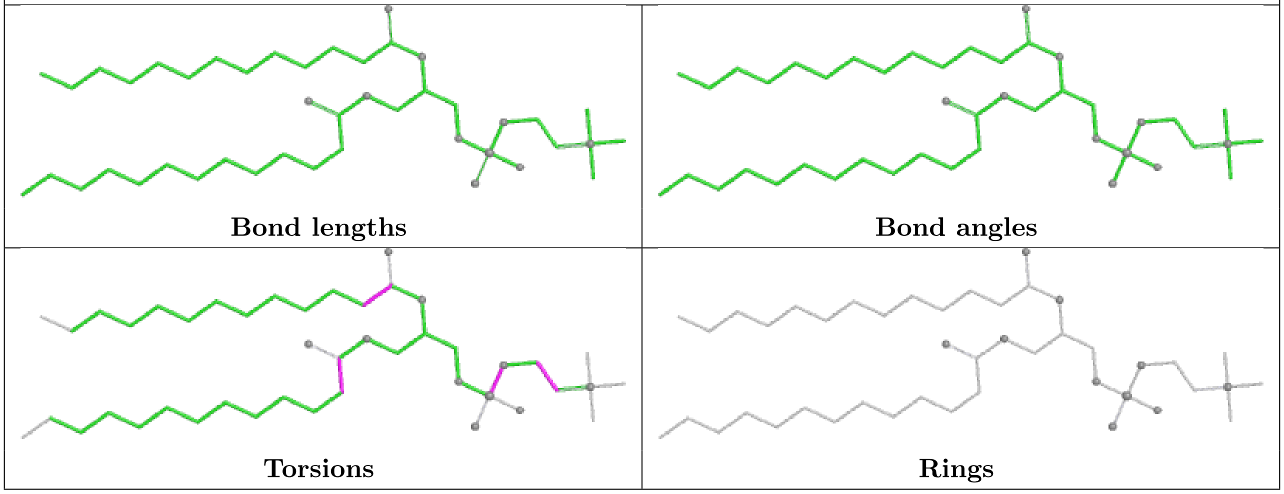
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A9 501



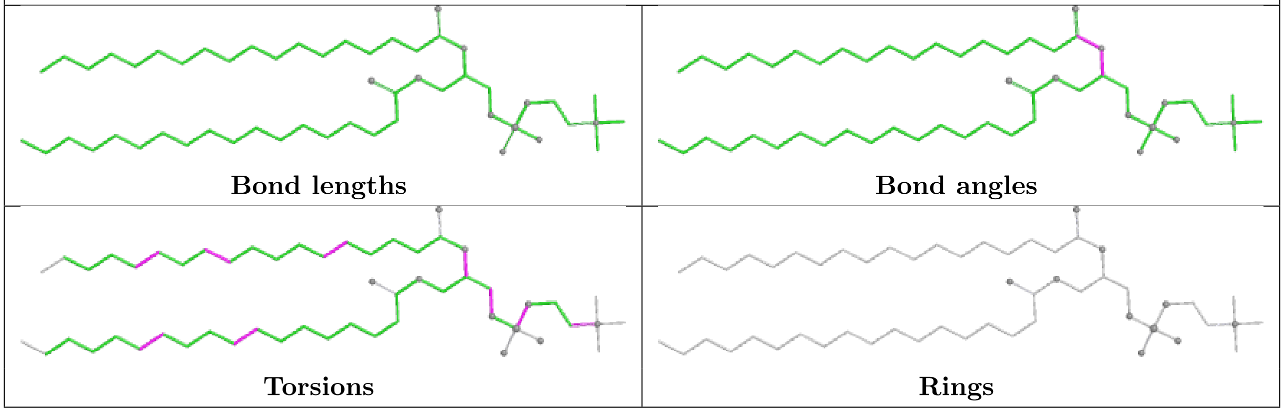
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 1 401



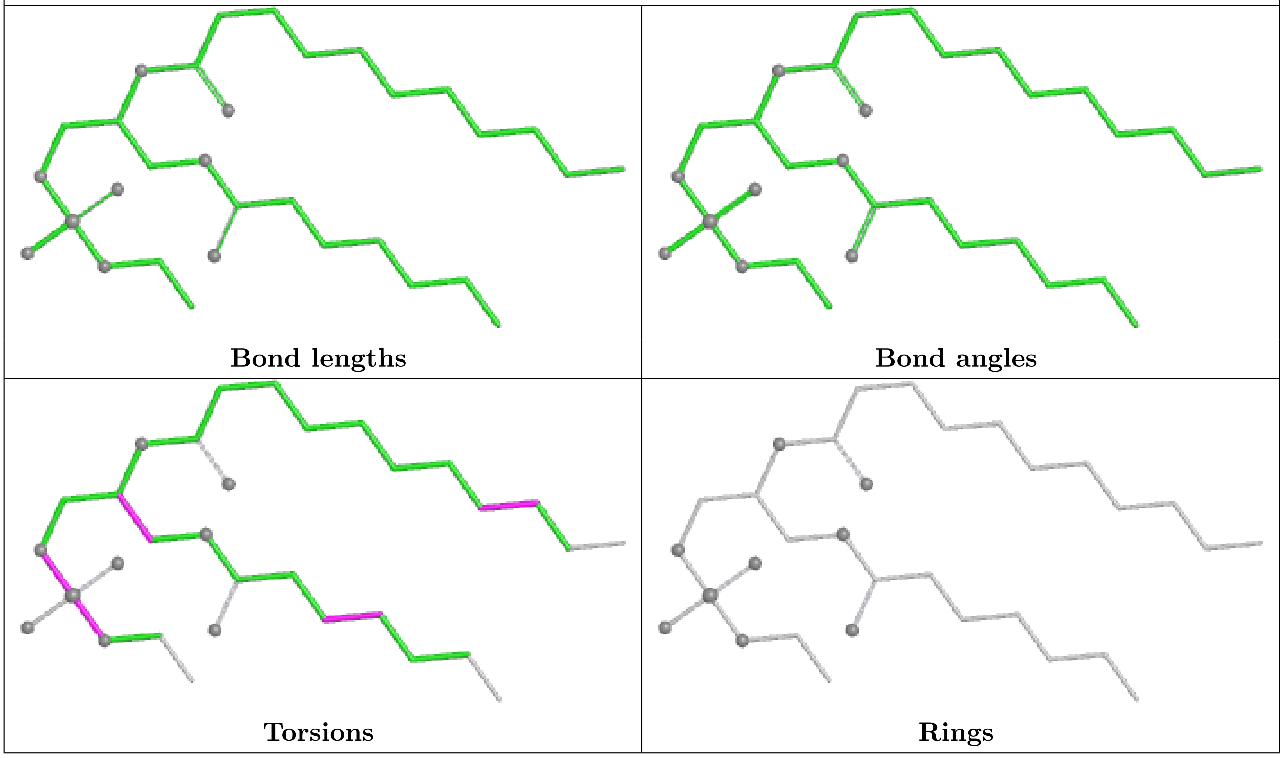
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 5 601



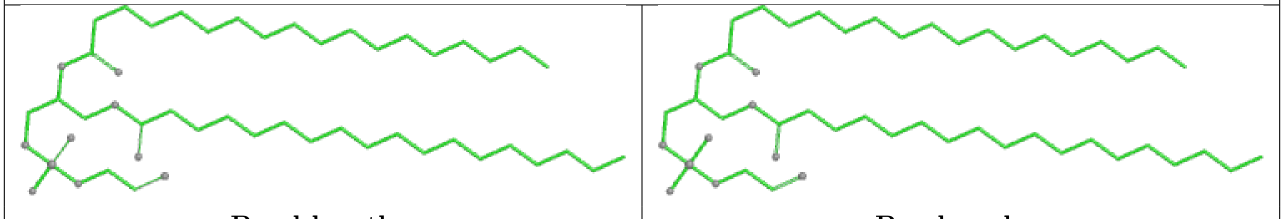
Bond lengths

Bond angles

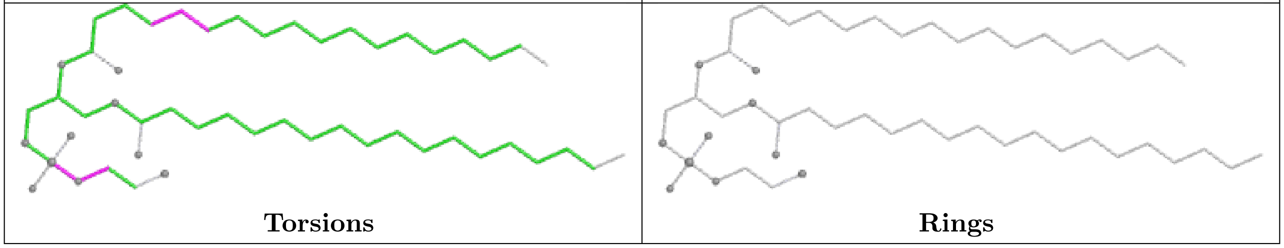
Torsions

Rings

Ligand 3PE 5 602

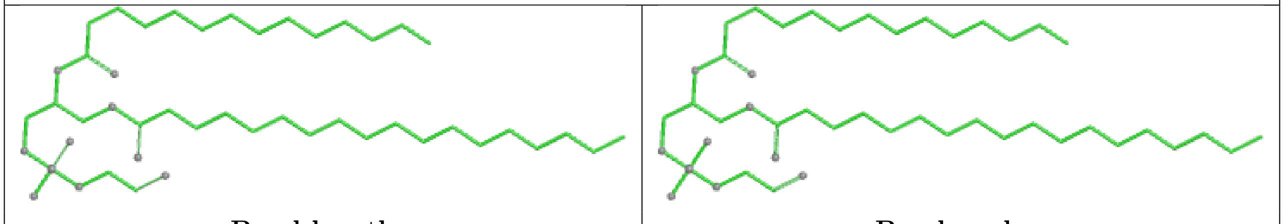


Bond lengths Bond angles

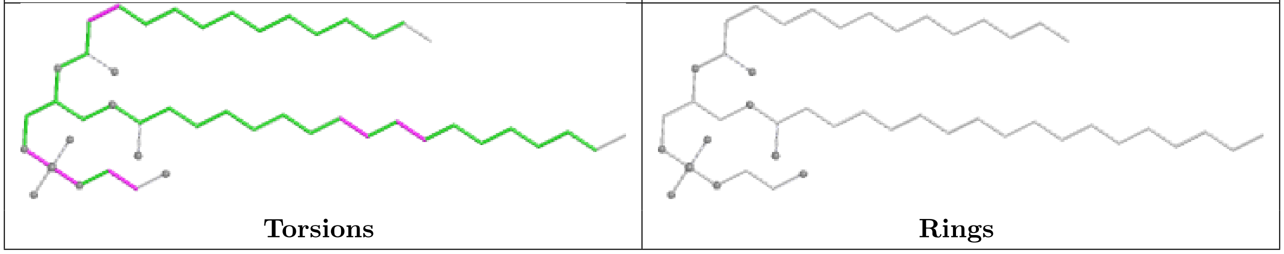


Torsions Rings

Ligand 3PE B4 201

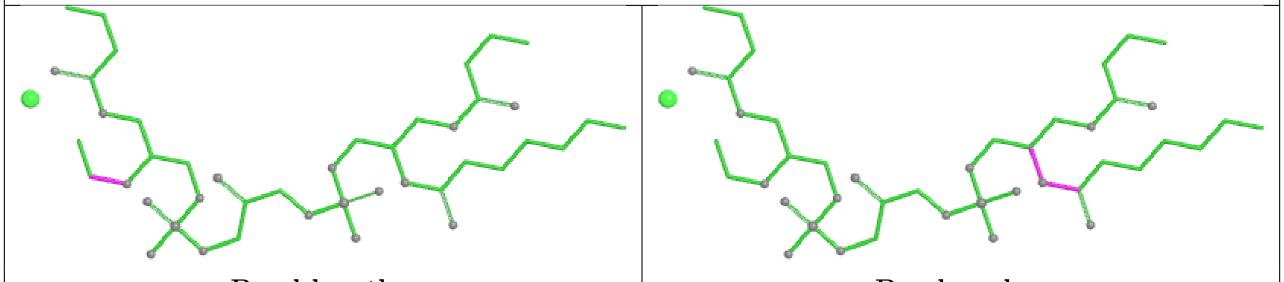


Bond lengths Bond angles

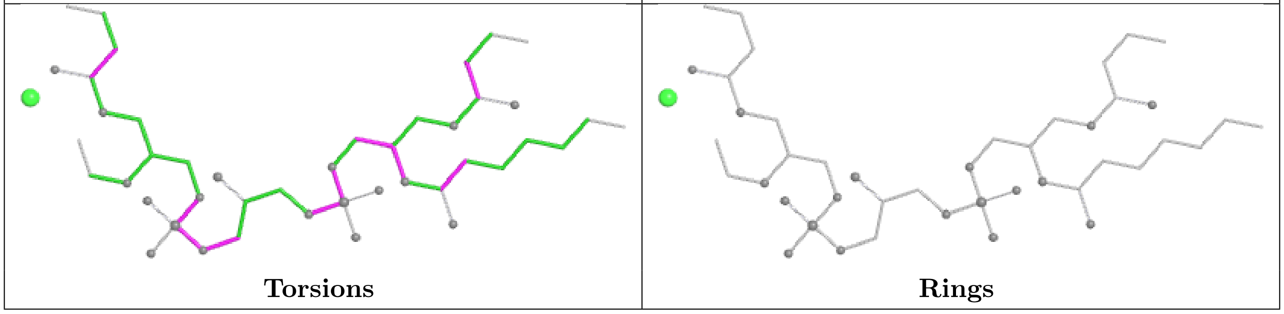


Torsions Rings

Ligand CDL 2 403

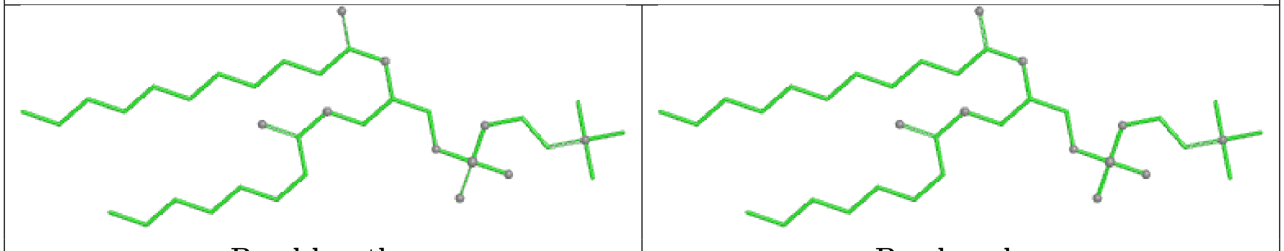


Bond lengths Bond angles



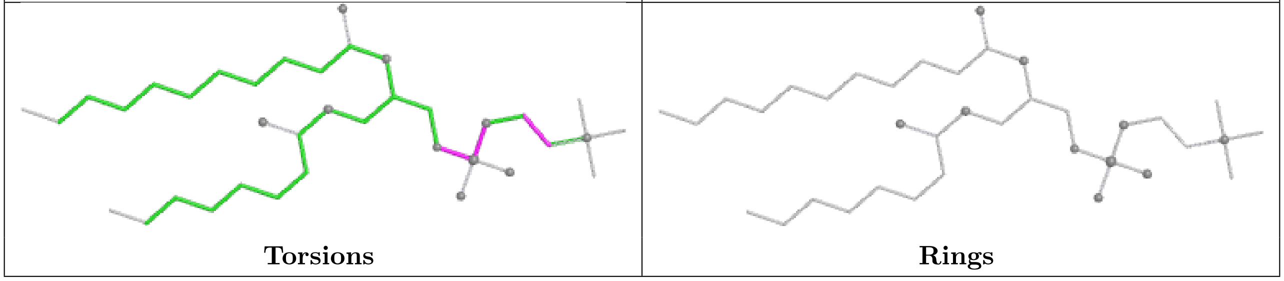
Torsions Rings

Ligand PC1 AM 201



Bond lengths

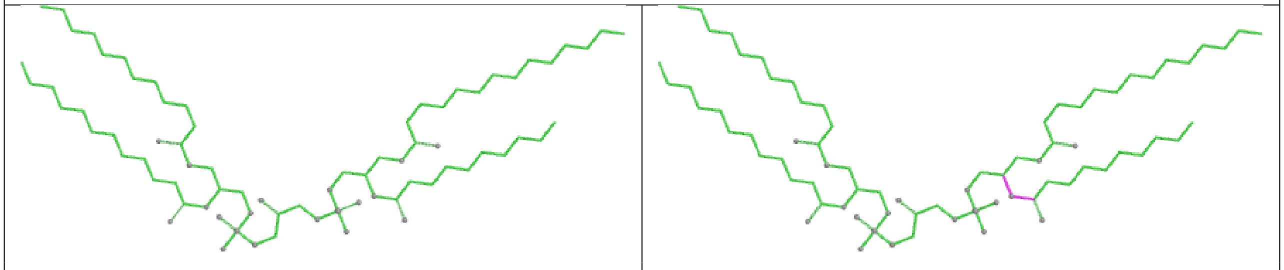
Bond angles



Torsions

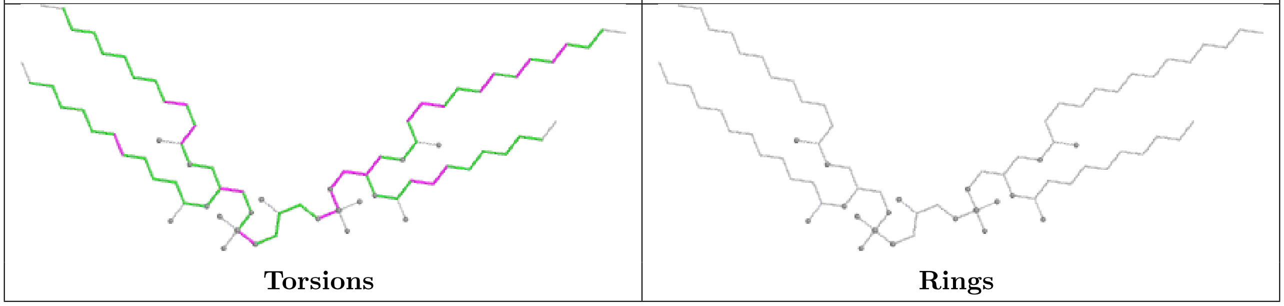
Rings

Ligand CDL AM 204



Bond lengths

Bond angles



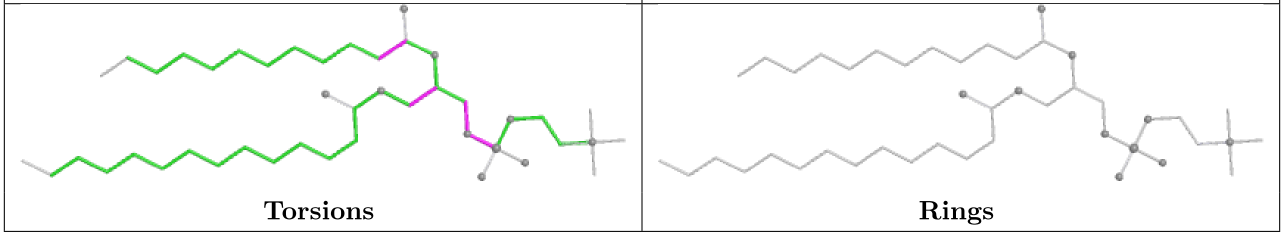
Torsions

Rings

Ligand PC1 AN 202

Bond lengths

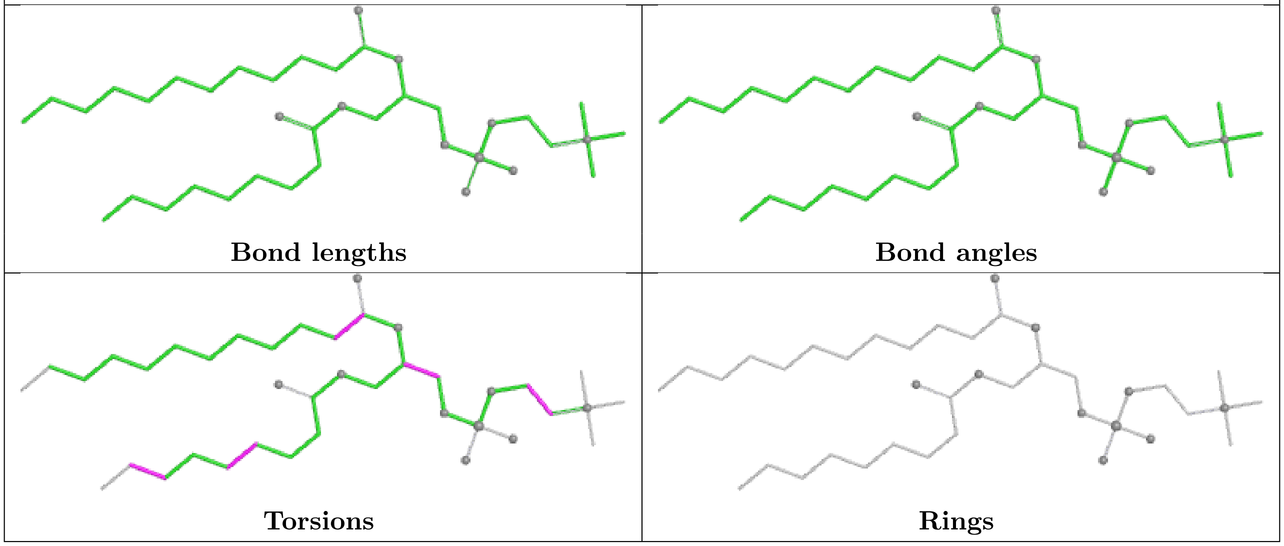
Bond angles



Torsions

Rings

Ligand PC1 4 505



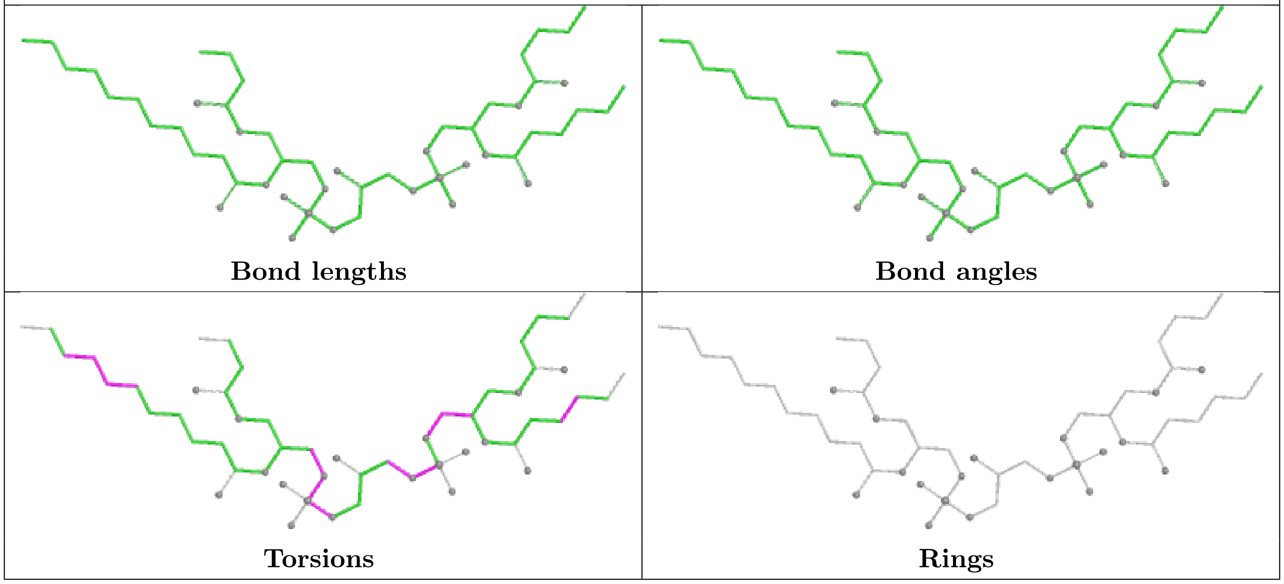
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL 3 201



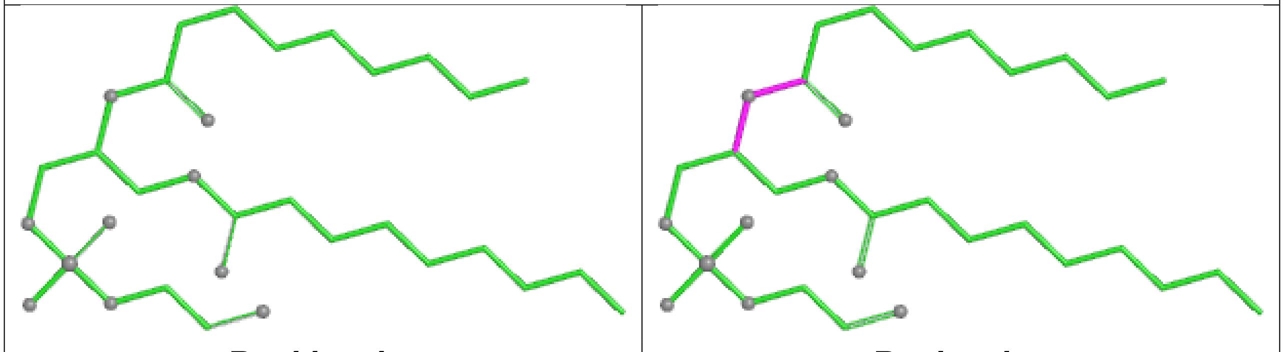
Bond lengths

Bond angles

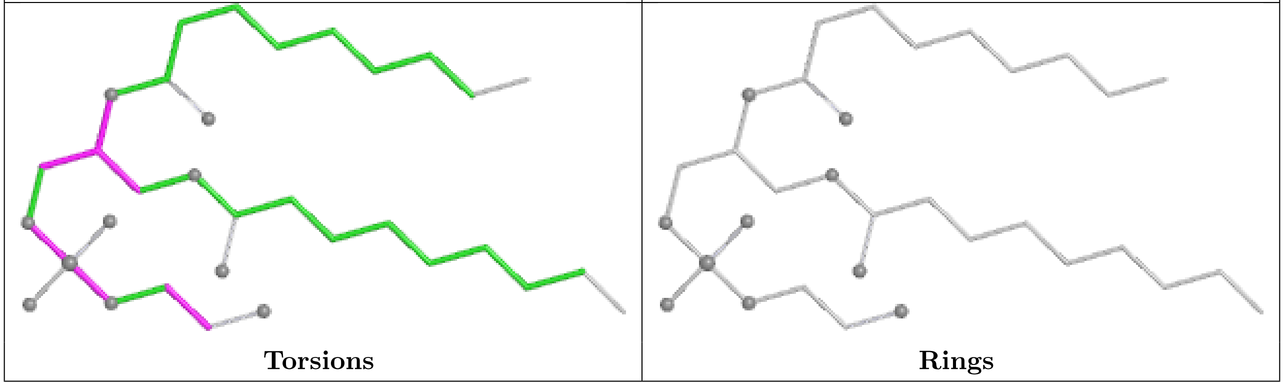
Torsions

Rings

Ligand 3PE 5 603

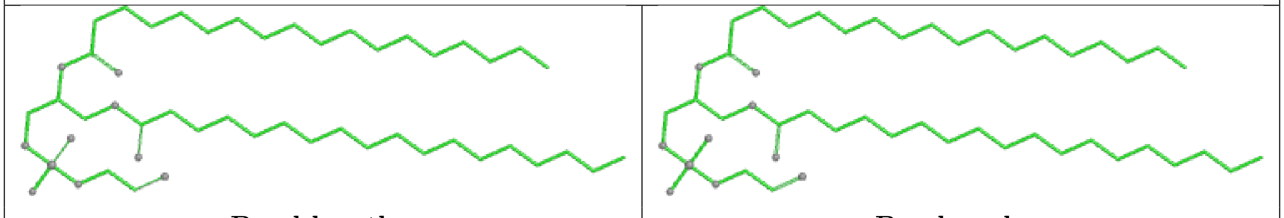


Bond lengths Bond angles

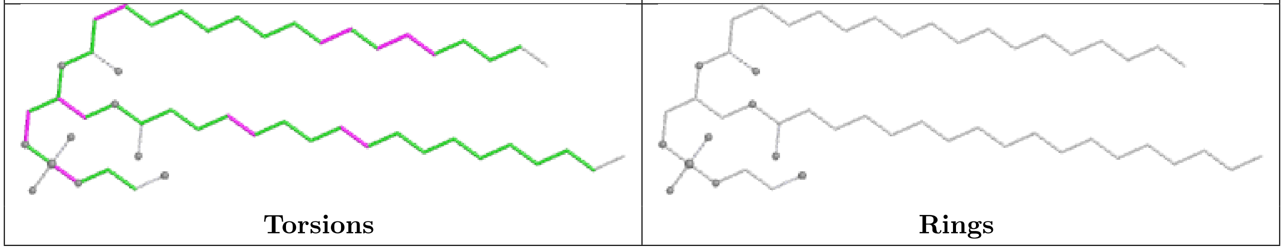


Torsions Rings

Ligand 3PE 3 202

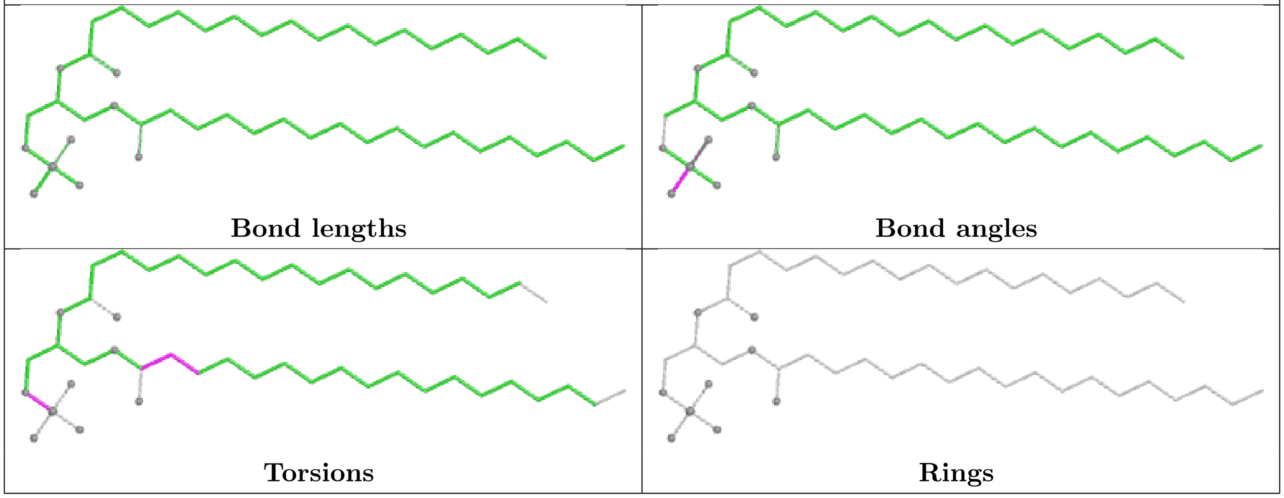


Bond lengths Bond angles

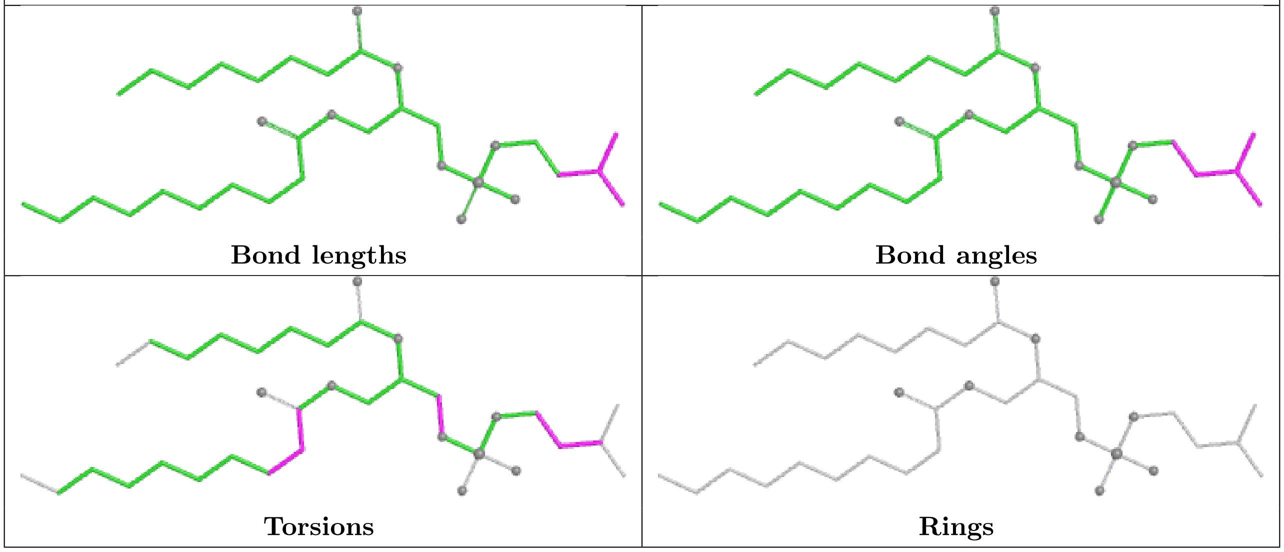


Torsions Rings

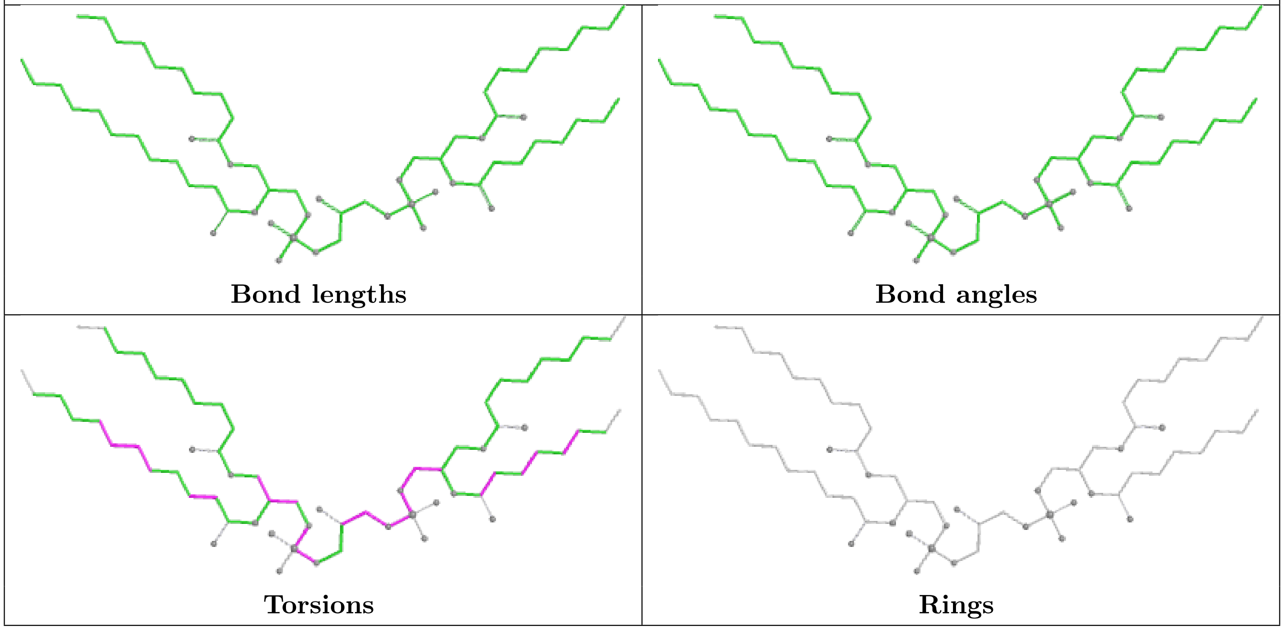
Ligand 3PE B6 201



Ligand WSF 6 201



Ligand CDL AN 201



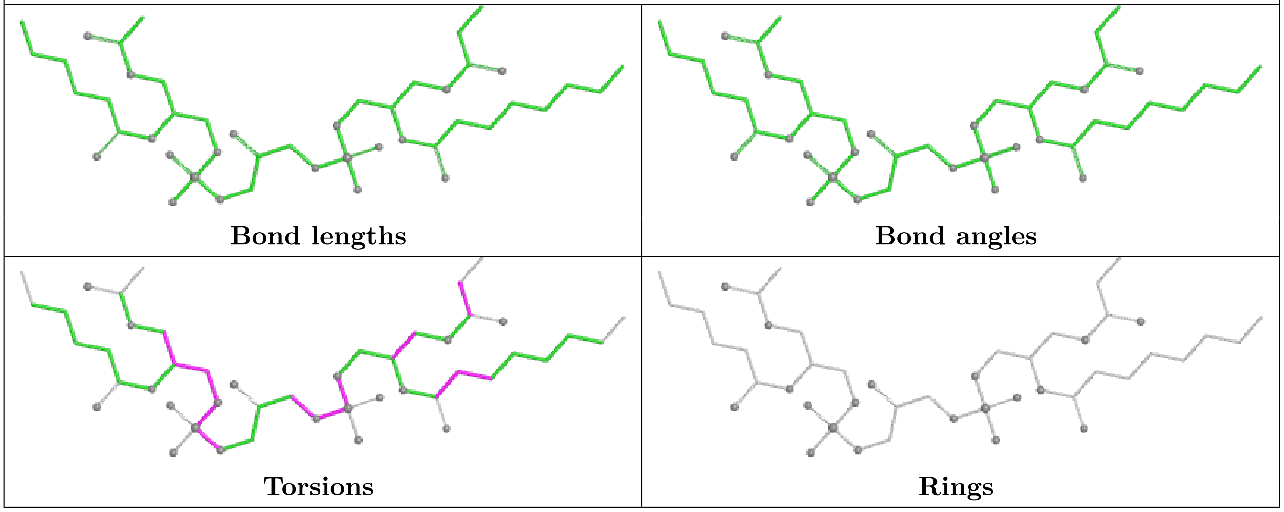
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL B6 203



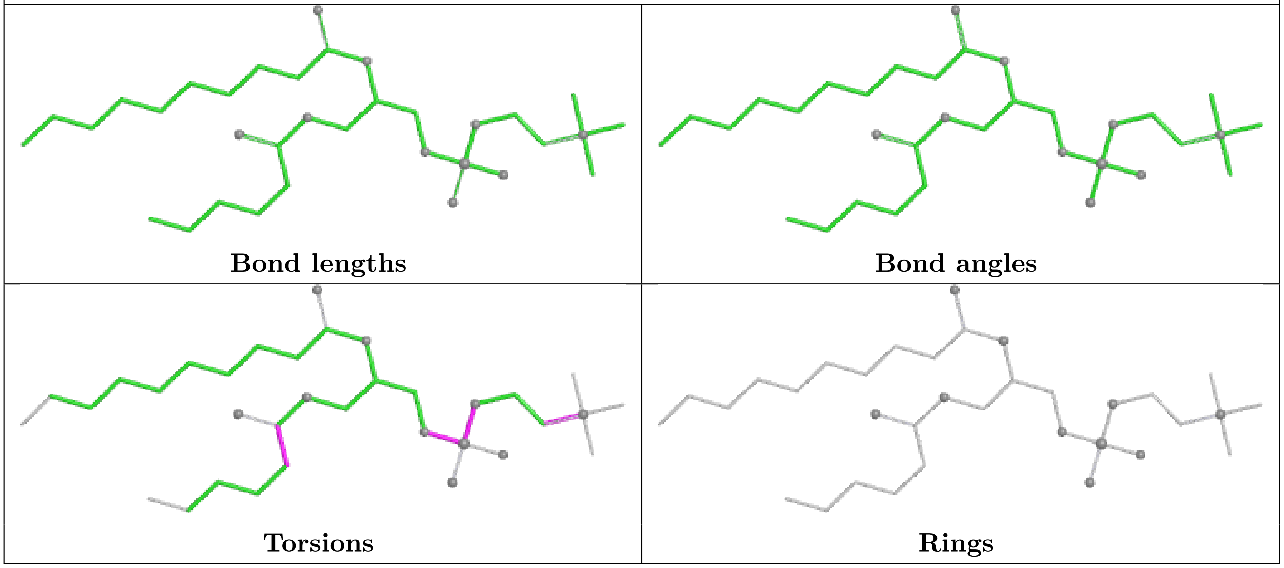
Bond lengths

Bond angles

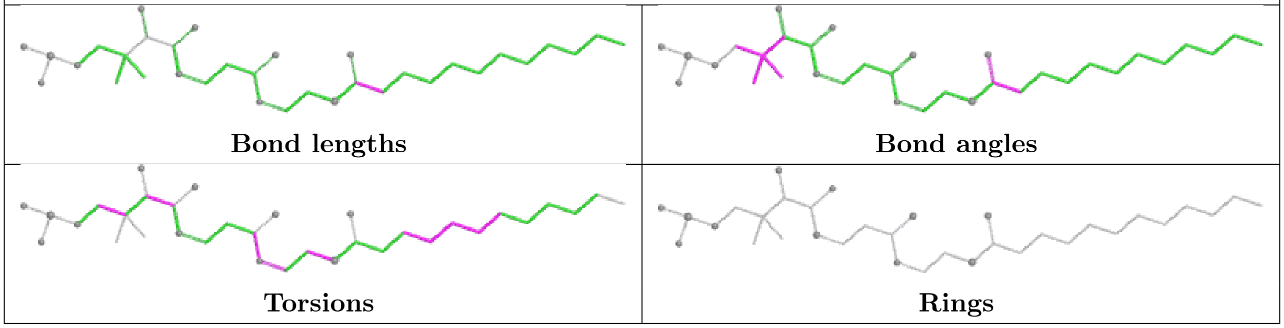
Torsions

Rings

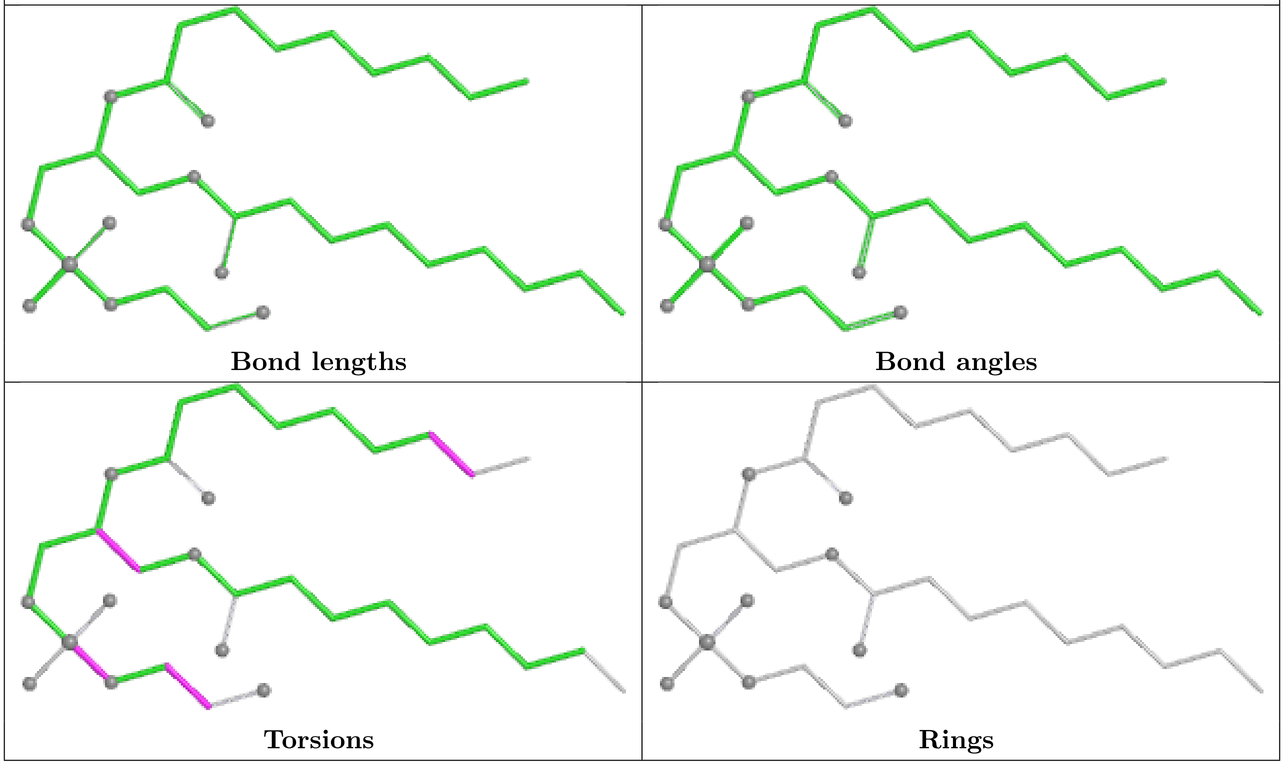
Ligand PC1 5 606



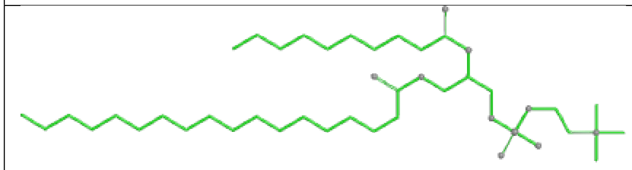
Ligand ZMP AC 201



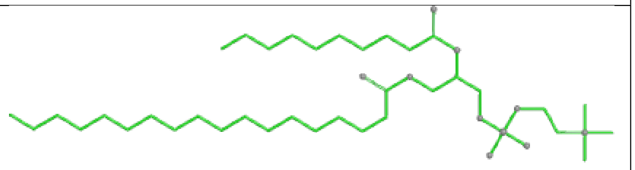
Ligand 3PE S7 302



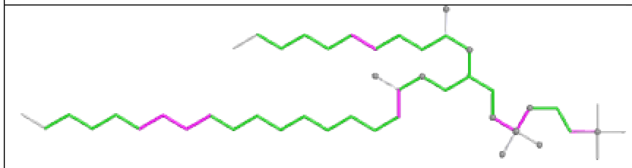
Ligand PC1 S7 304



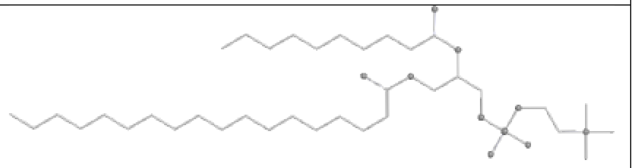
Bond lengths



Bond angles

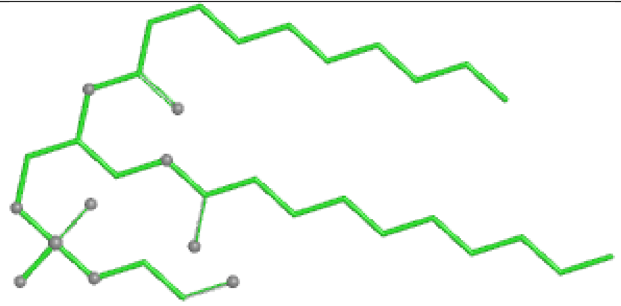


Torsions

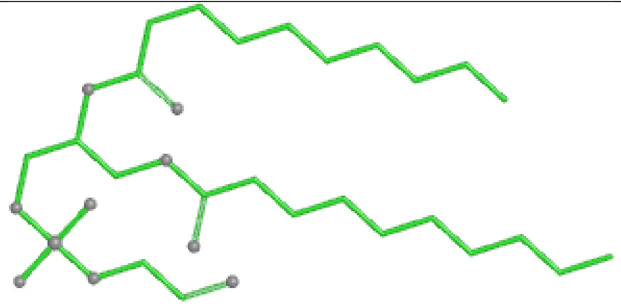


Rings

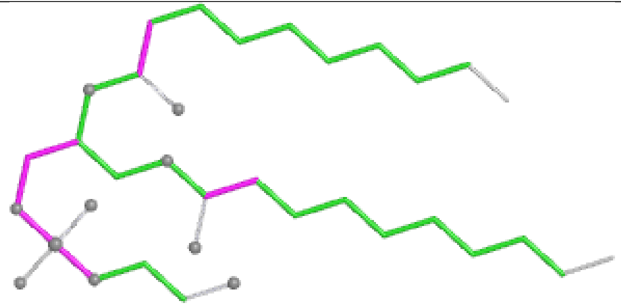
Ligand 3PE 6 202



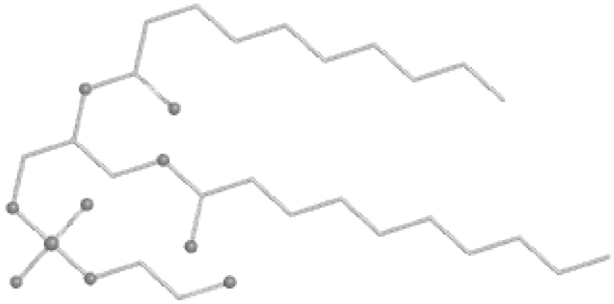
Bond lengths



Bond angles

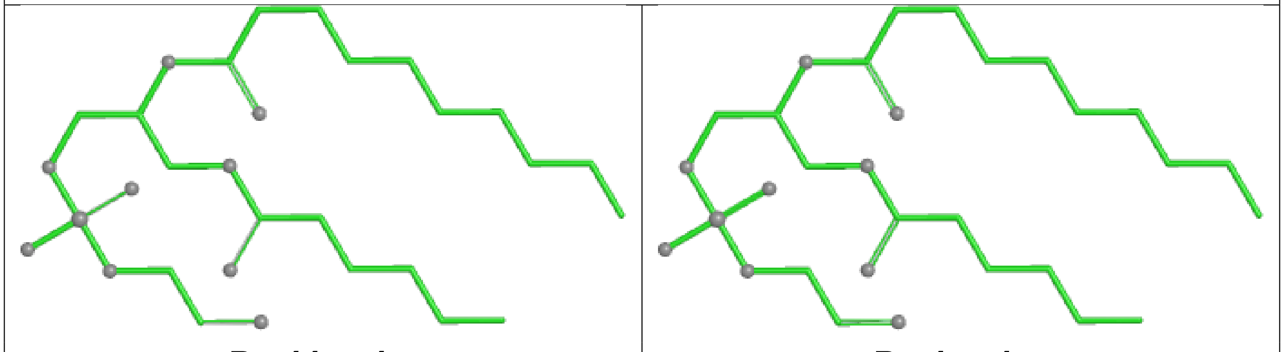


Torsions



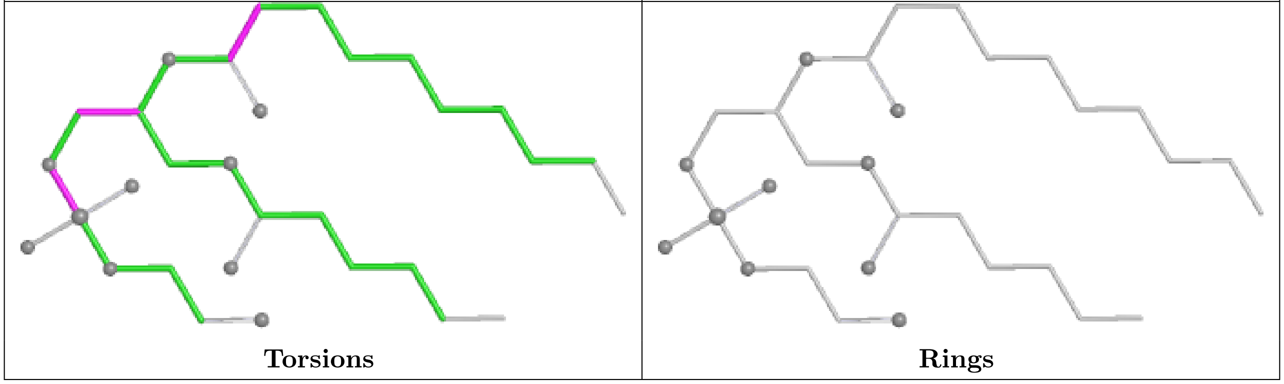
Rings

Ligand 3PE AM 203



Bond lengths

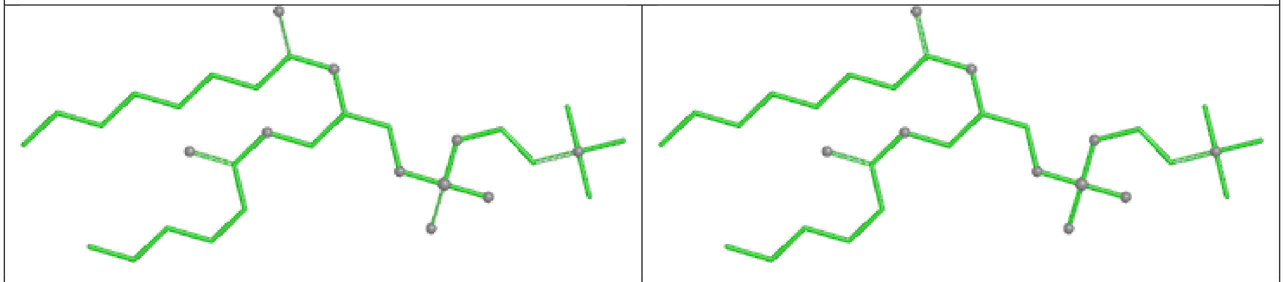
Bond angles



Torsions

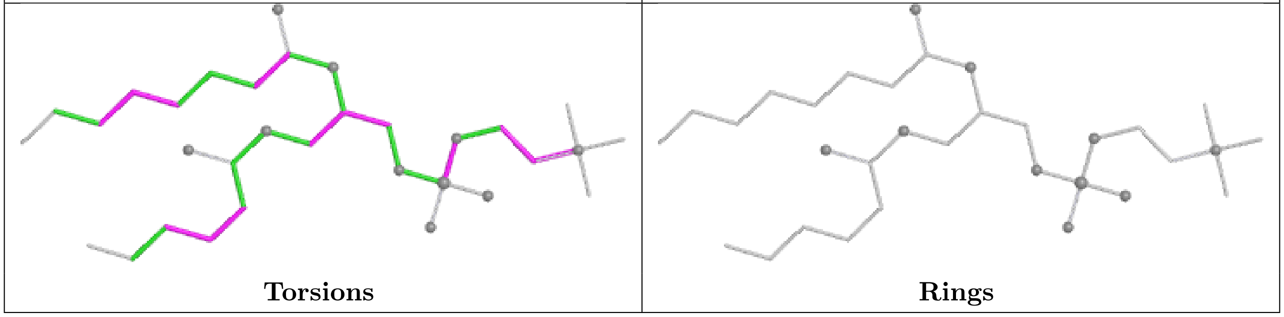
Rings

Ligand PC1 AM 206



Bond lengths

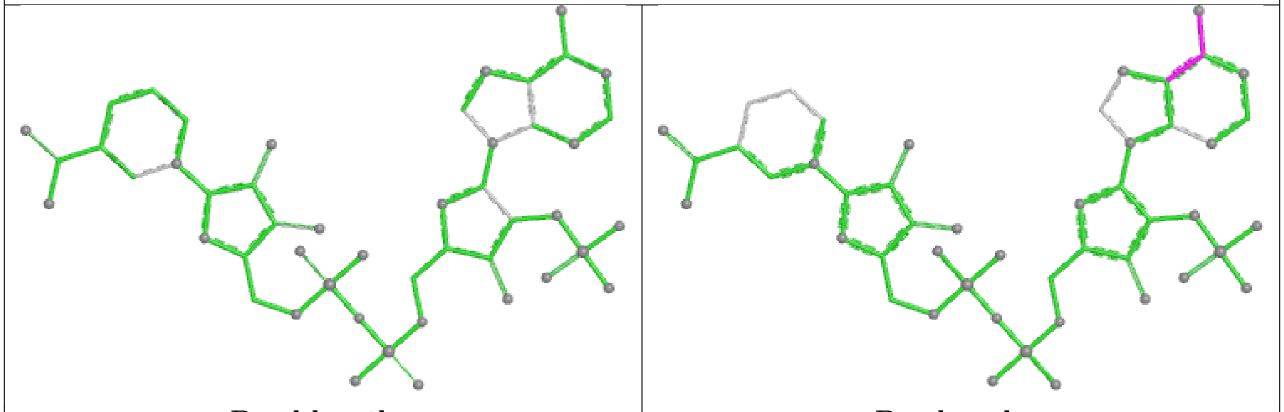
Bond angles



Torsions

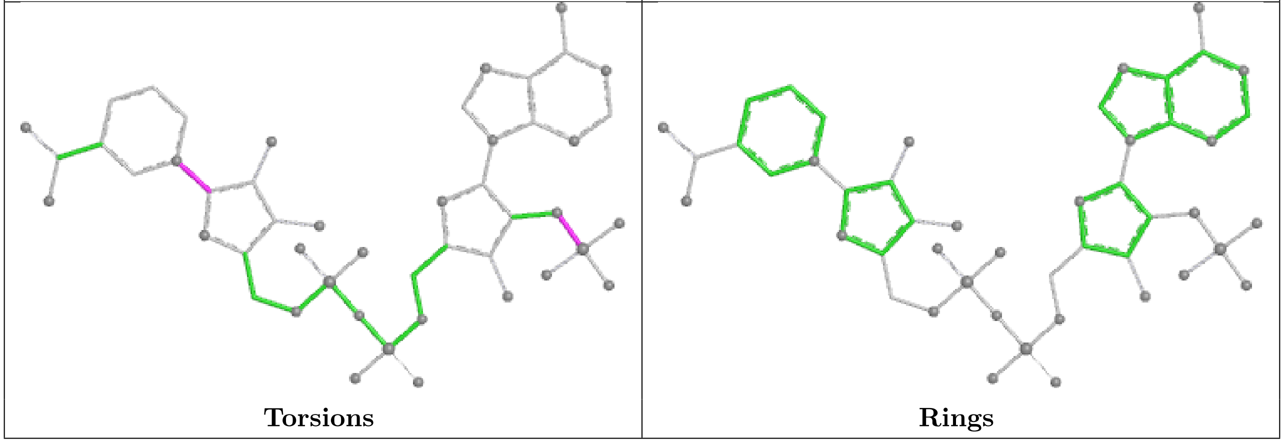
Rings

Ligand NDP A9 502



Bond lengths

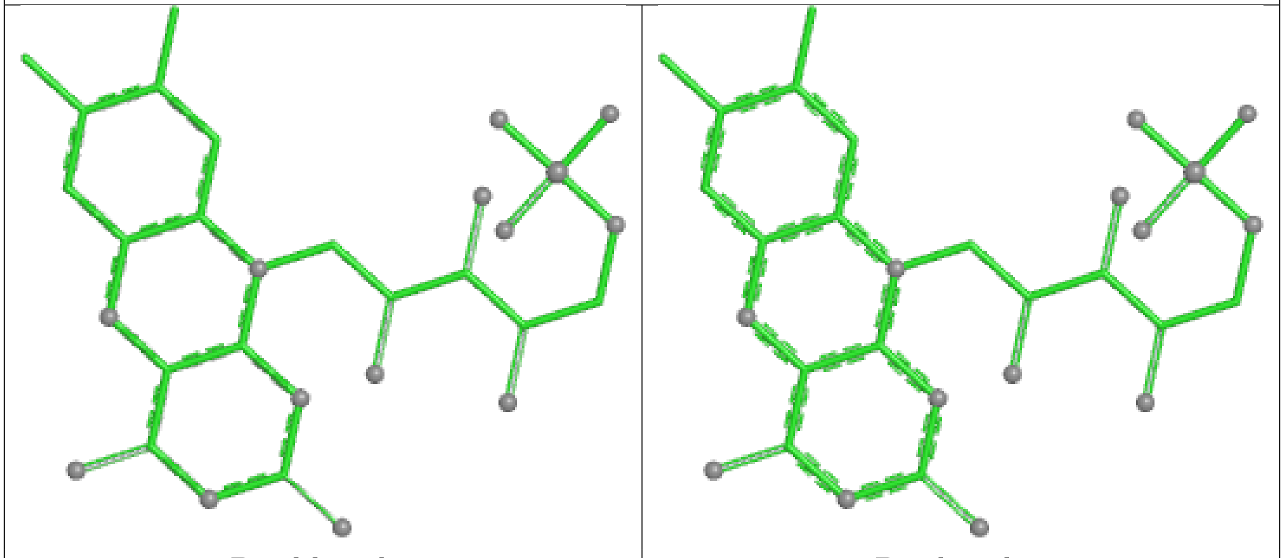
Bond angles



Torsions

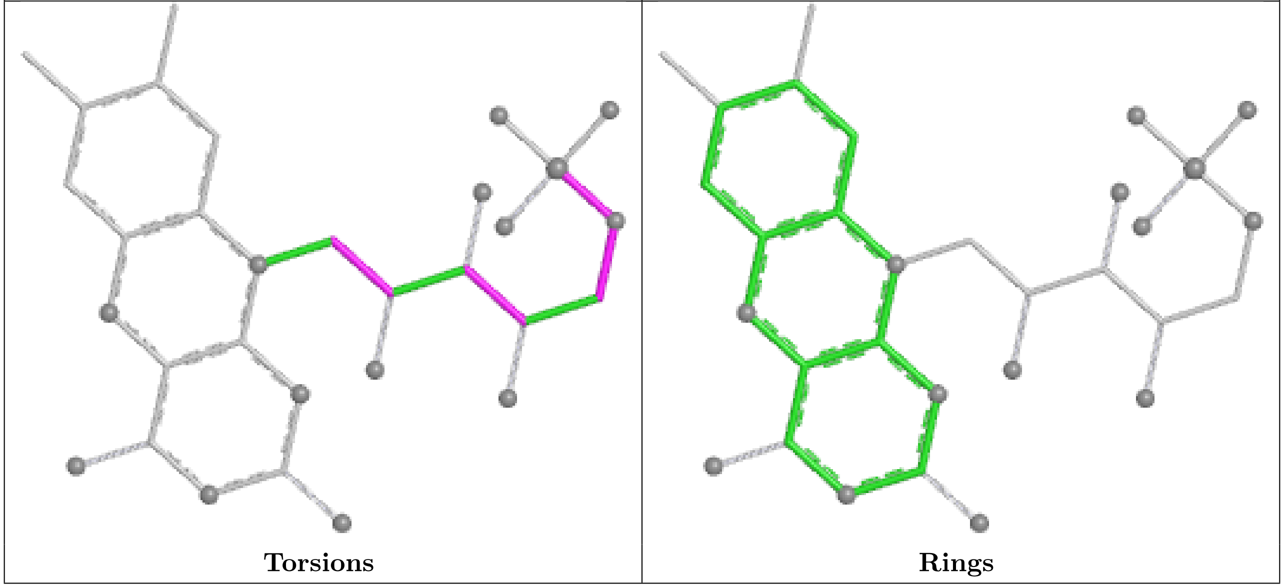
Rings

Ligand FMN V1 501



Bond lengths

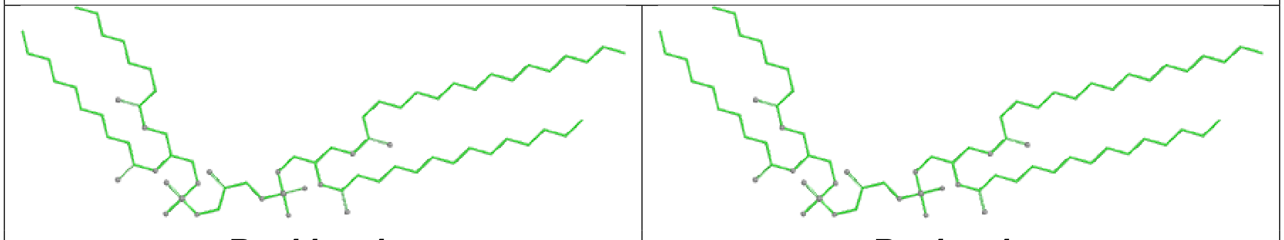
Bond angles



Torsions

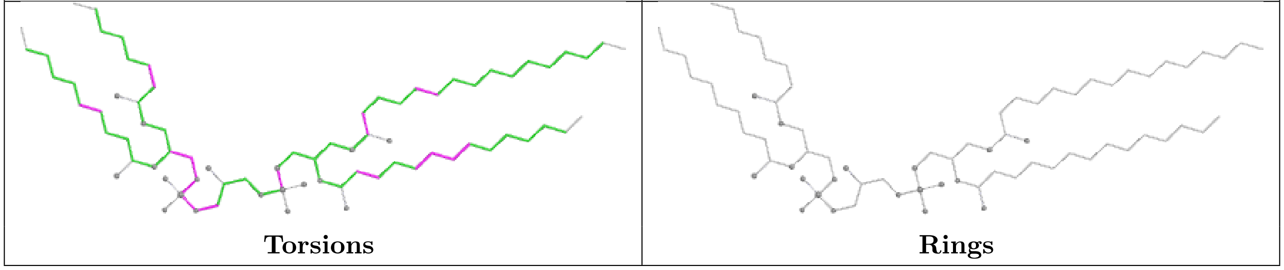
Rings

Ligand CDL B5 201



Bond lengths

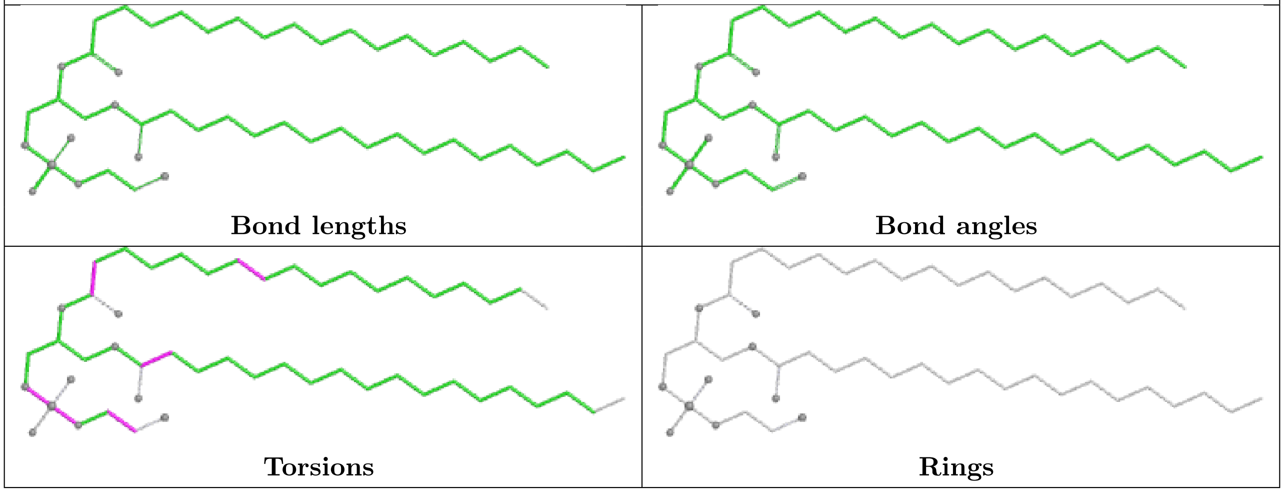
Bond angles



Torsions

Rings

Ligand 3PE 1 403



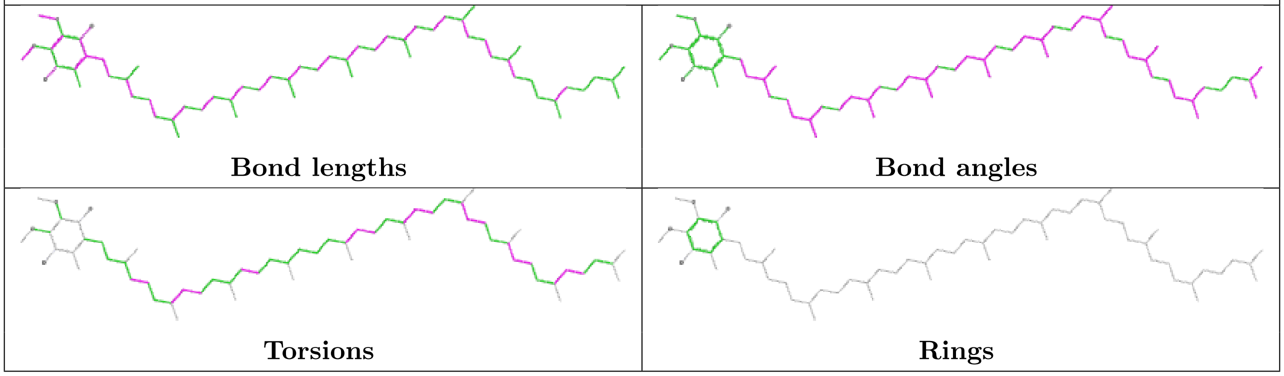
Bond lengths

Bond angles

Torsions

Rings

Ligand U10 1 402



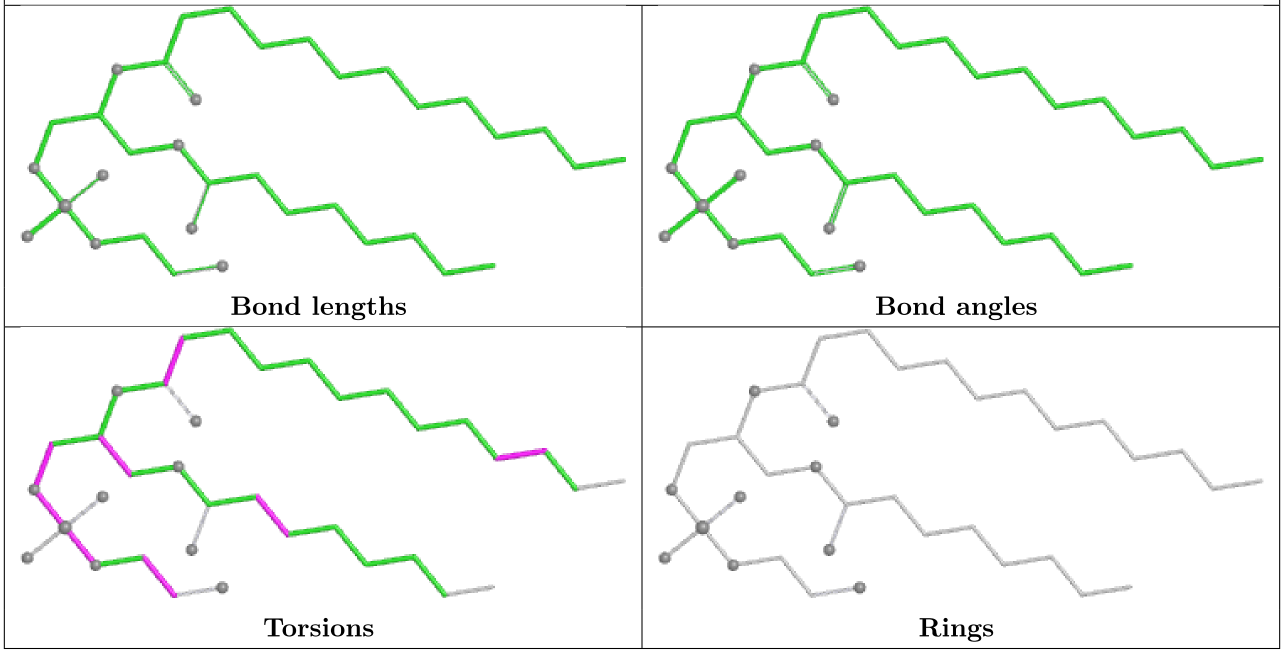
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE 4 504



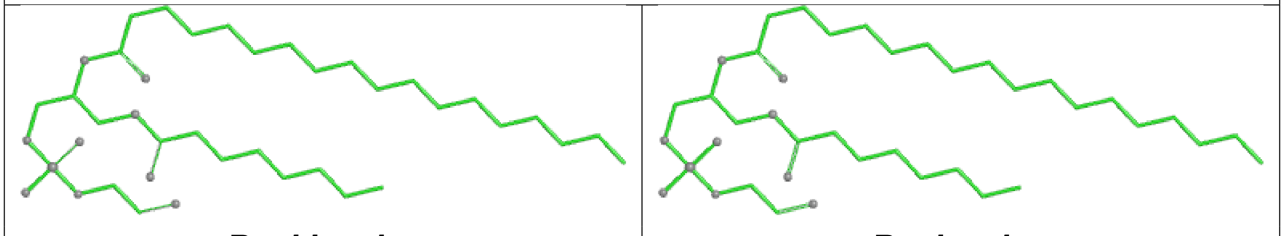
Bond lengths

Bond angles

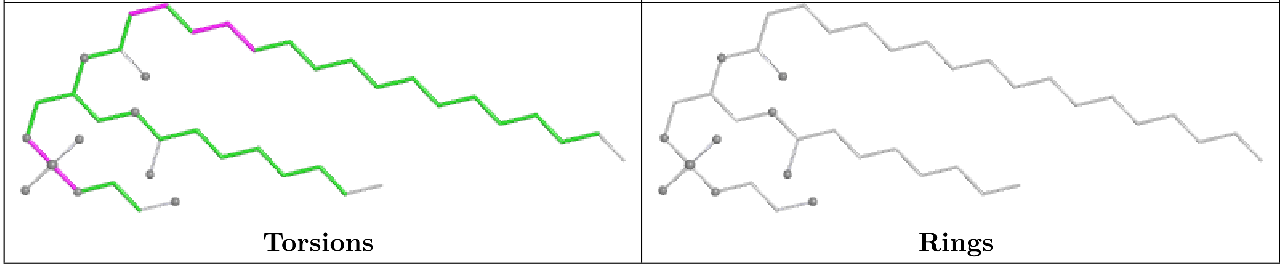
Torsions

Rings

Ligand 3PE AM 202

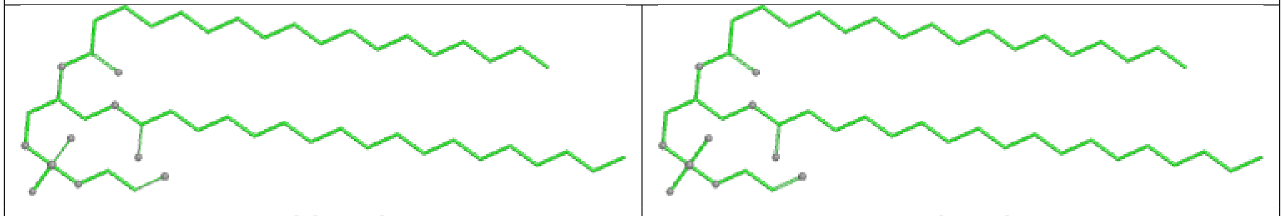


Bond lengths Bond angles

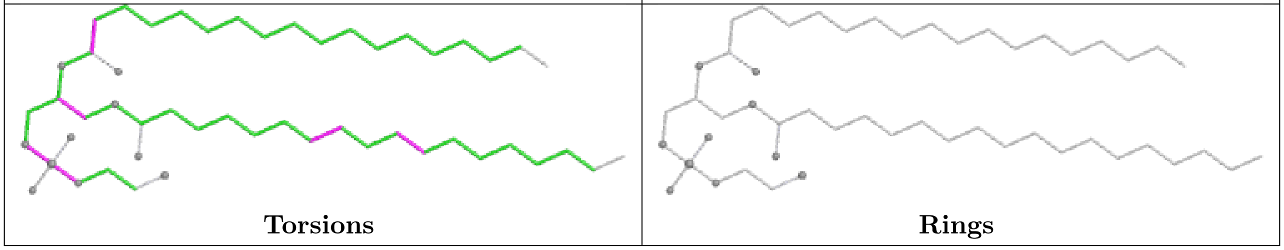


Torsions Rings

Ligand 3PE 5 607



Bond lengths Bond angles



Torsions Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

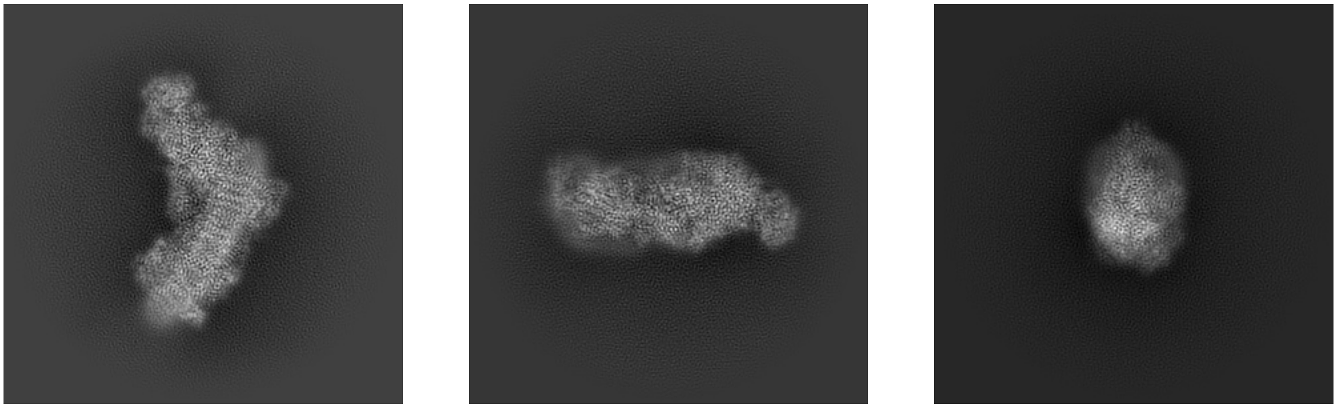
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-28582. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

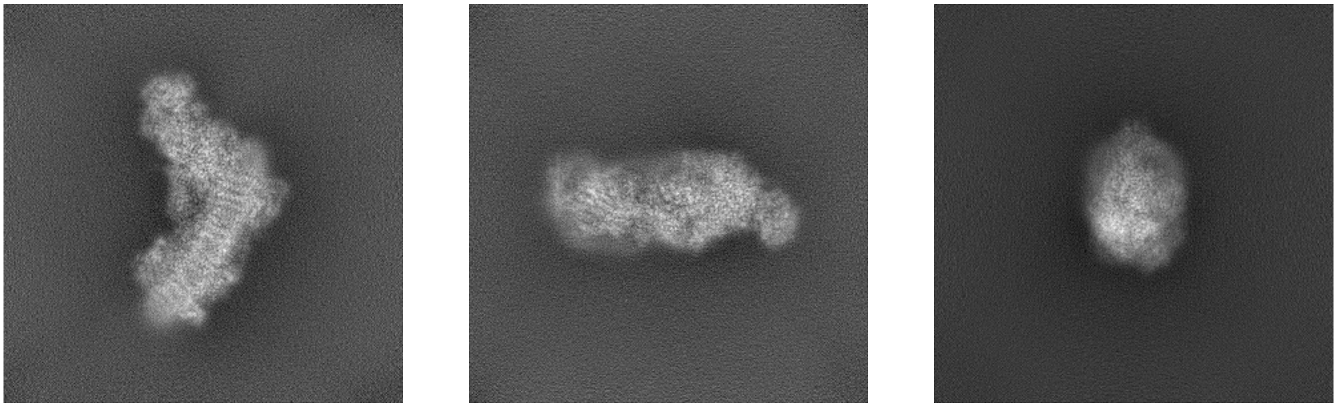
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

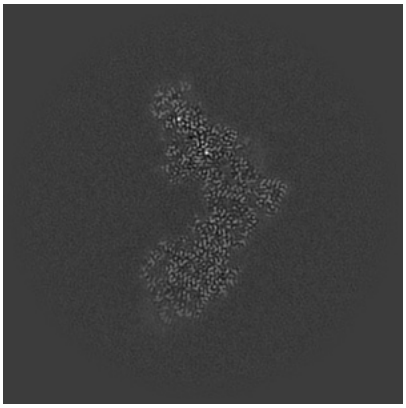


X Y Z

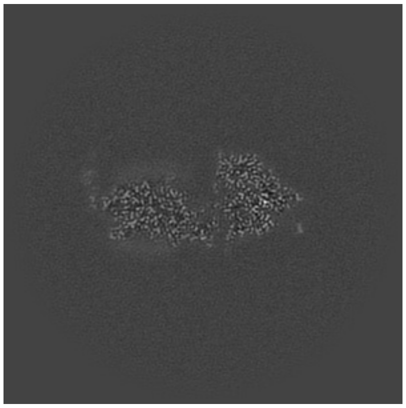
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

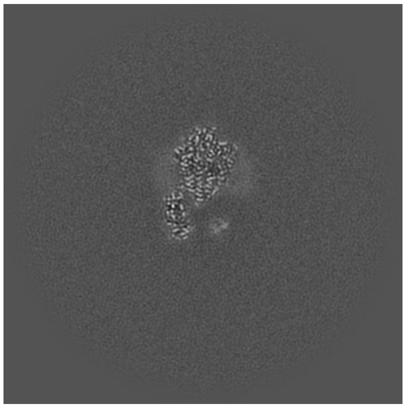
6.2.1 Primary map



X Index: 256

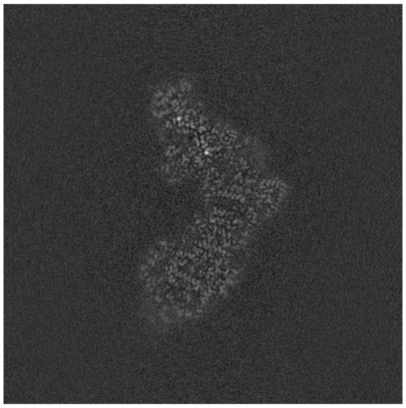


Y Index: 256

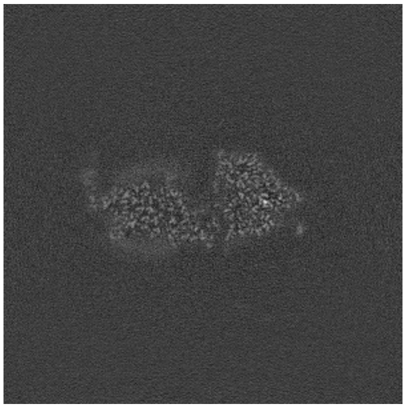


Z Index: 256

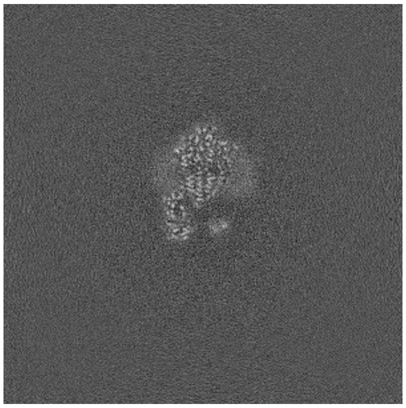
6.2.2 Raw map



X Index: 256



Y Index: 256

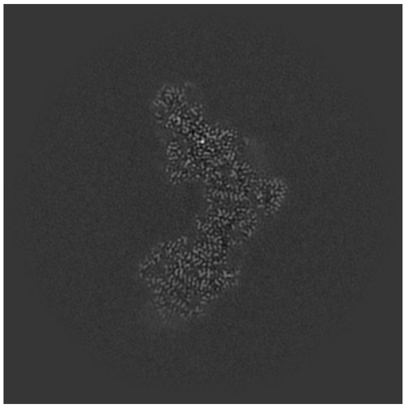


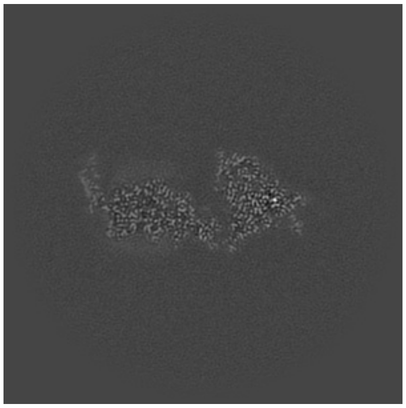
Z Index: 256

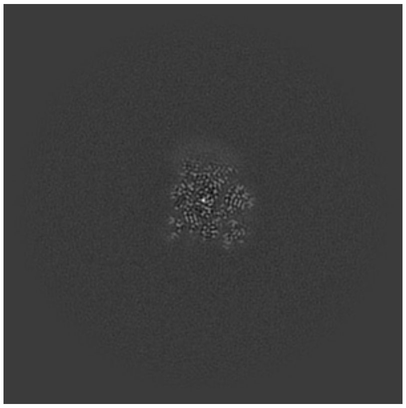
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

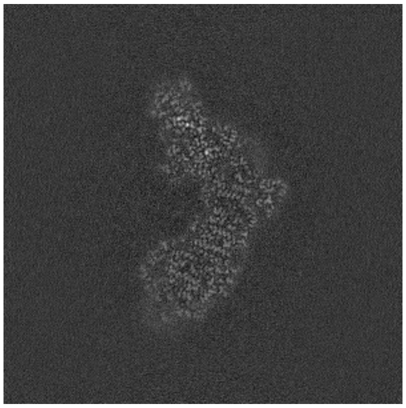
6.3.1 Primary map

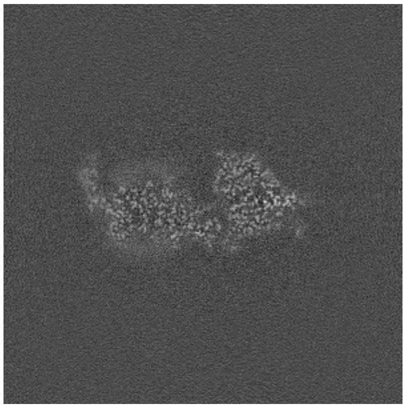

X Index: 258

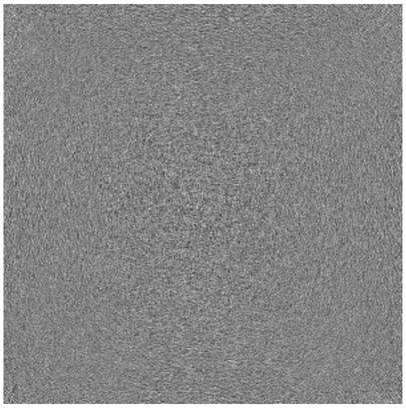

Y Index: 251


Z Index: 321

6.3.2 Raw map


X Index: 255

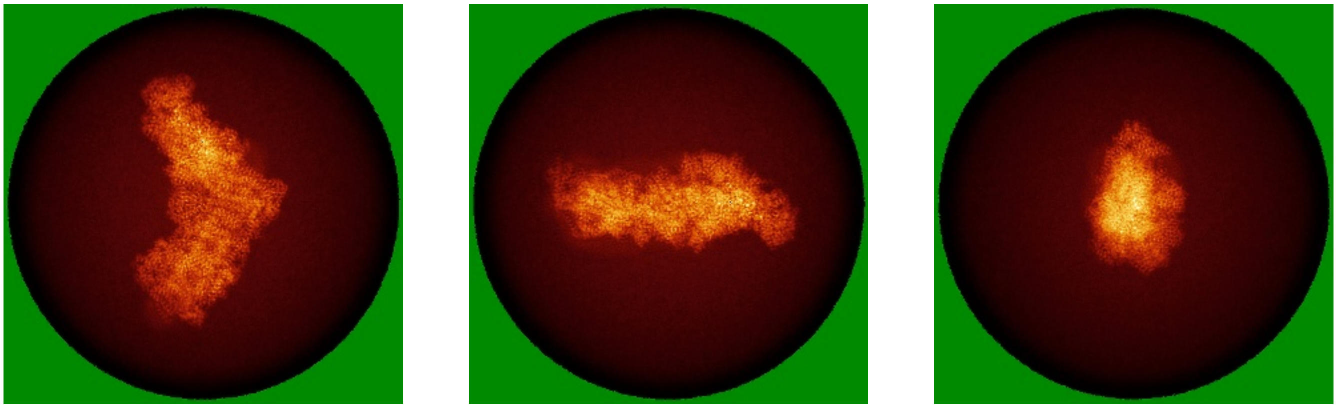

Y Index: 253


Z Index: 0

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

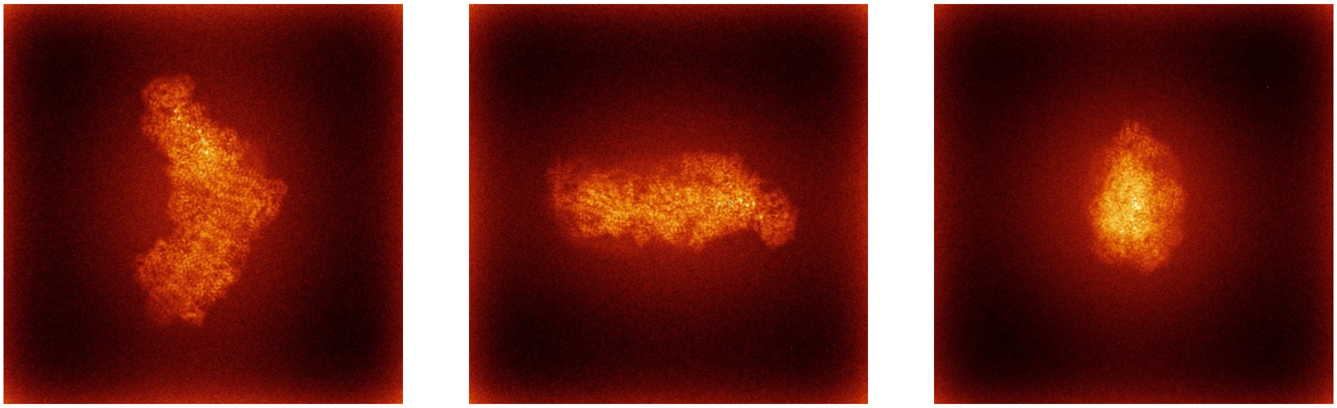
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

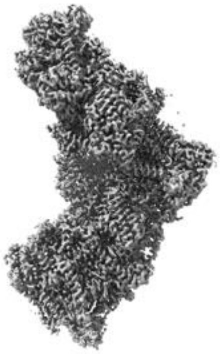


X Y Z

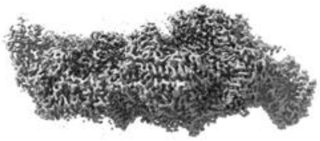
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

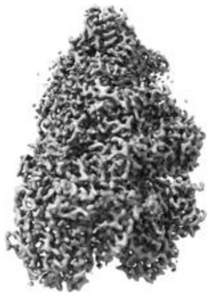
6.5.1 Primary map



X



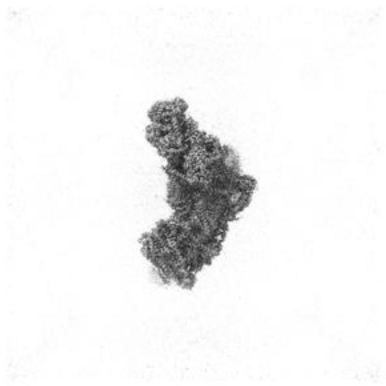
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y

Z

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

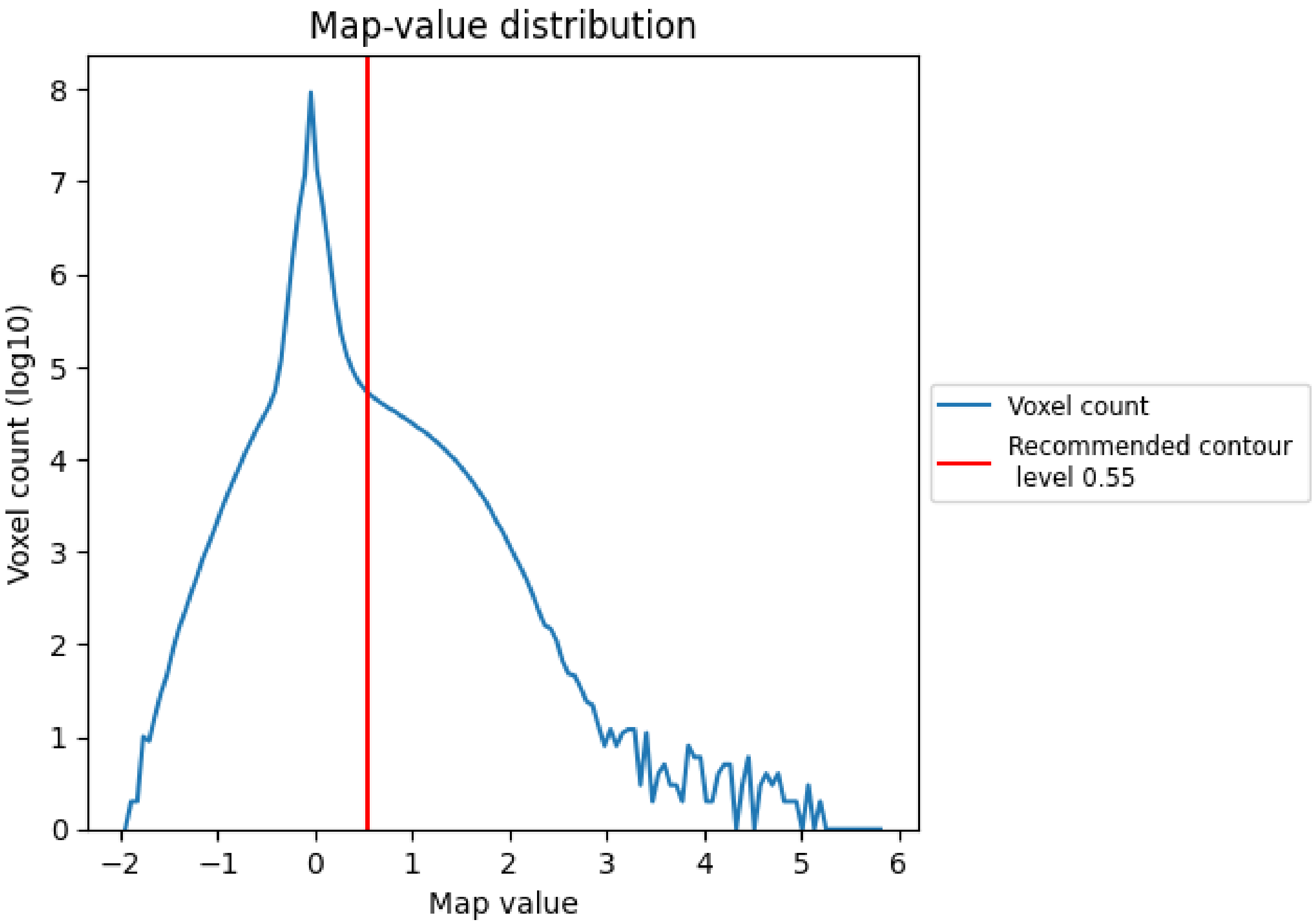
6.6 Mask visualisation

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

7 Map analysis ⓘ

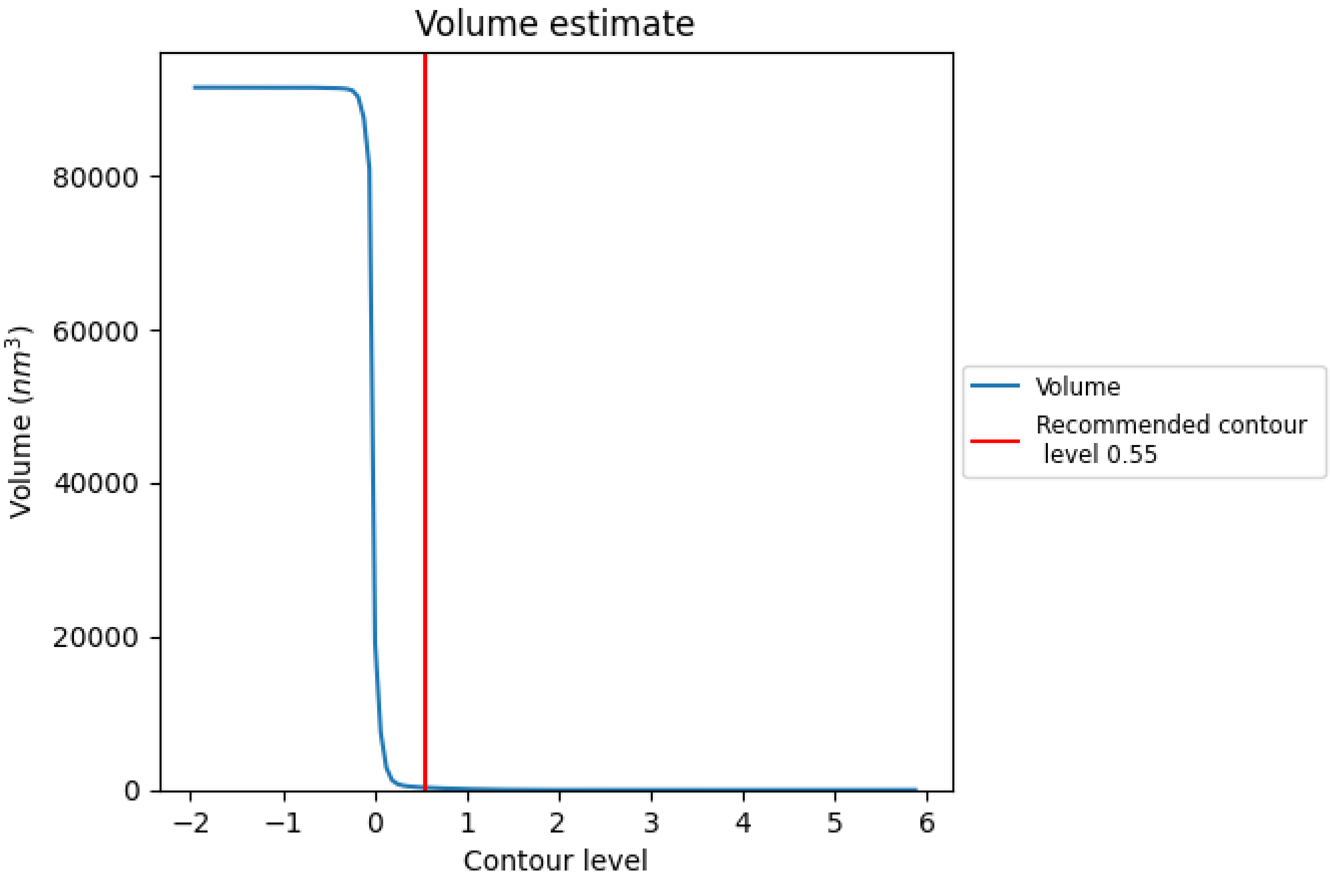
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

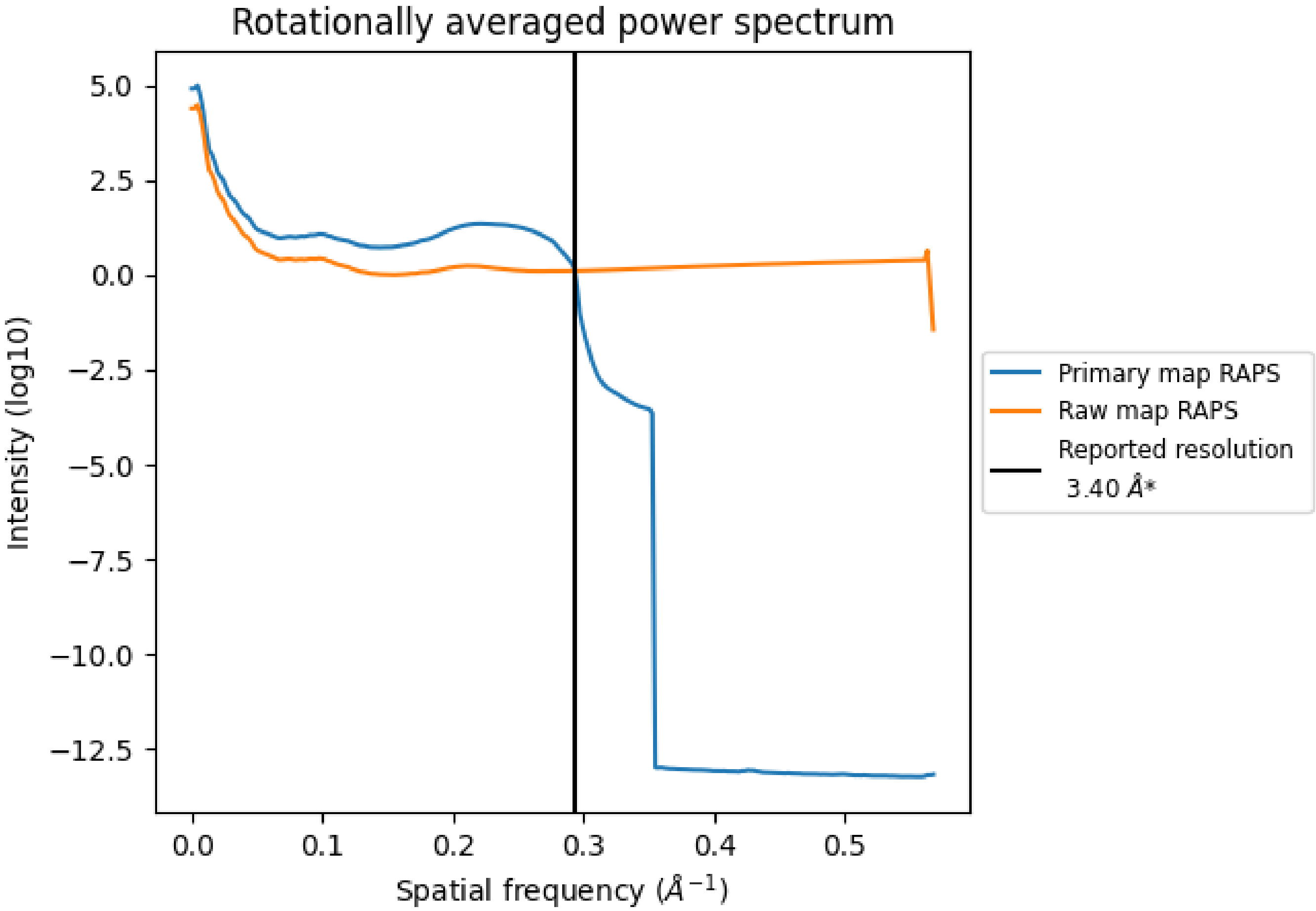
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 311 nm^3; this corresponds to an approximate mass of 281 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

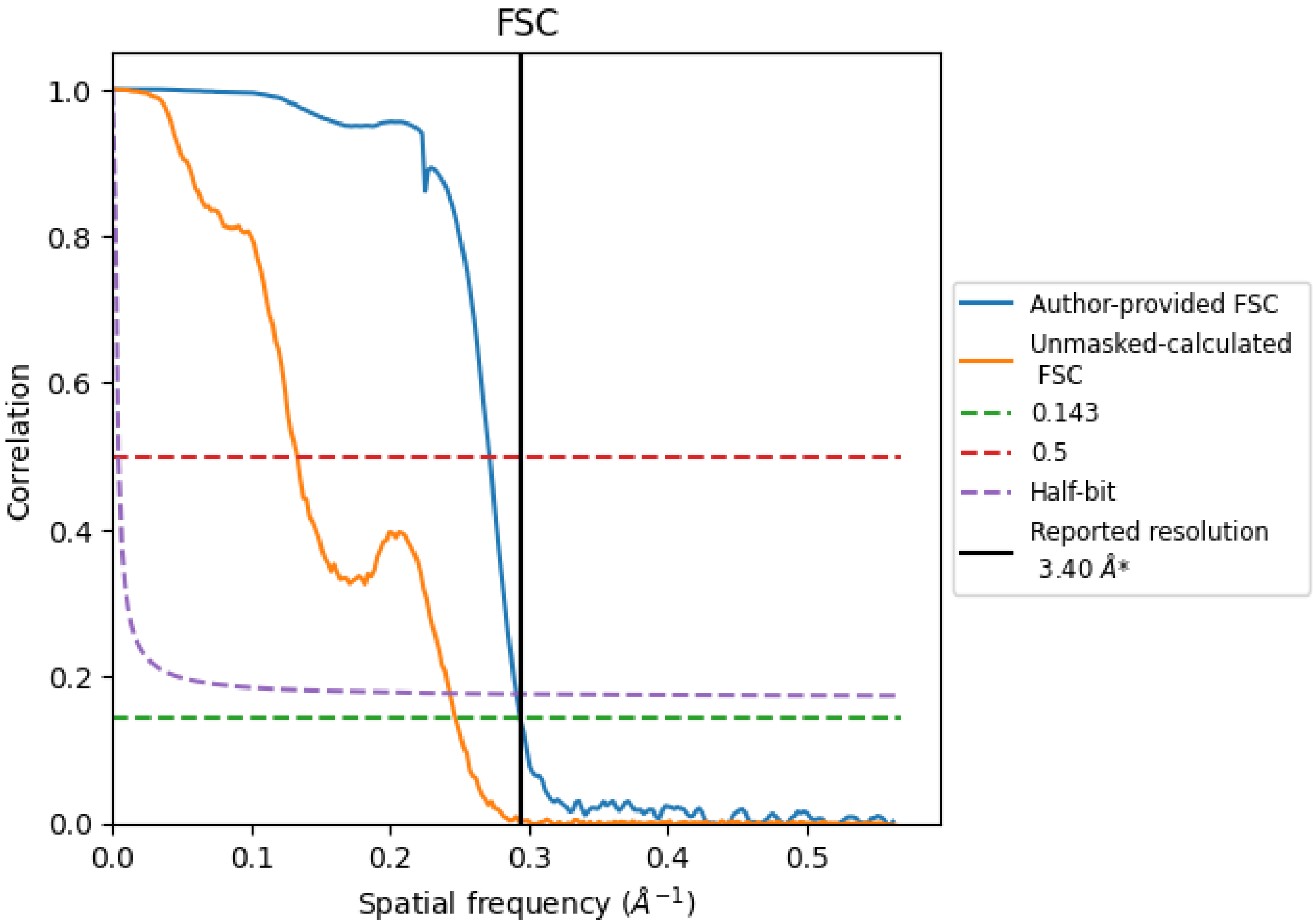


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates ⓘ

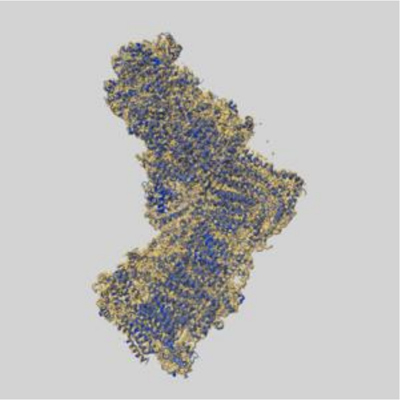
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.68	3.44
Unmasked-calculated*	4.05	7.52	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

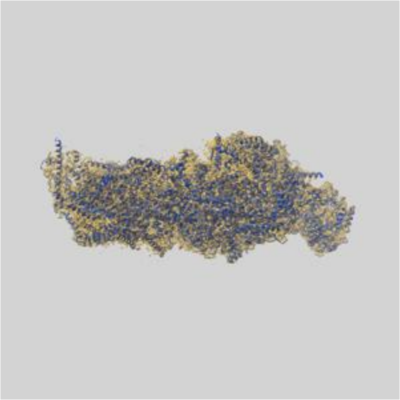
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-28582 and PDB model 8ESZ. Per-residue inclusion information can be found in section 3 on page 22.

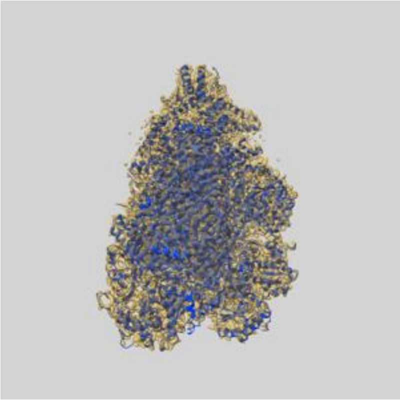
9.1 Map-model overlay ⓘ



X



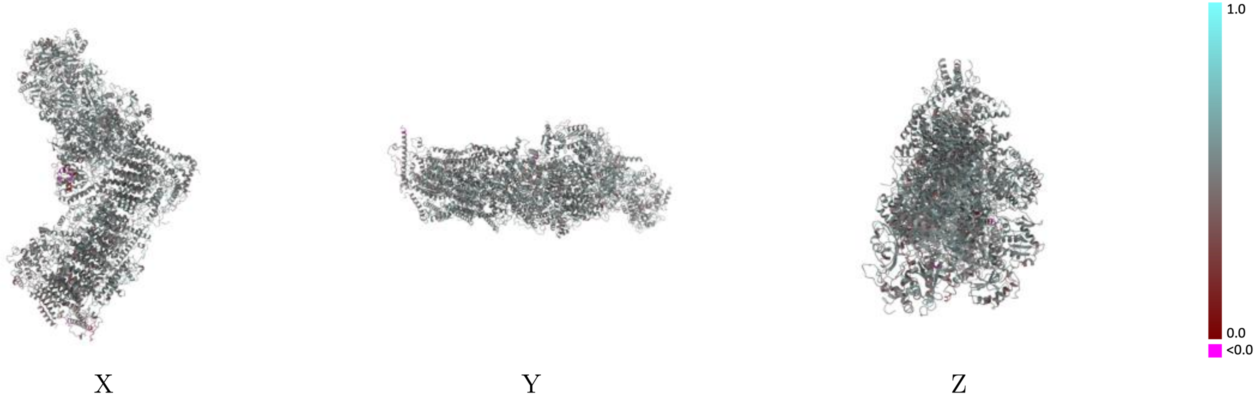
Y



Z

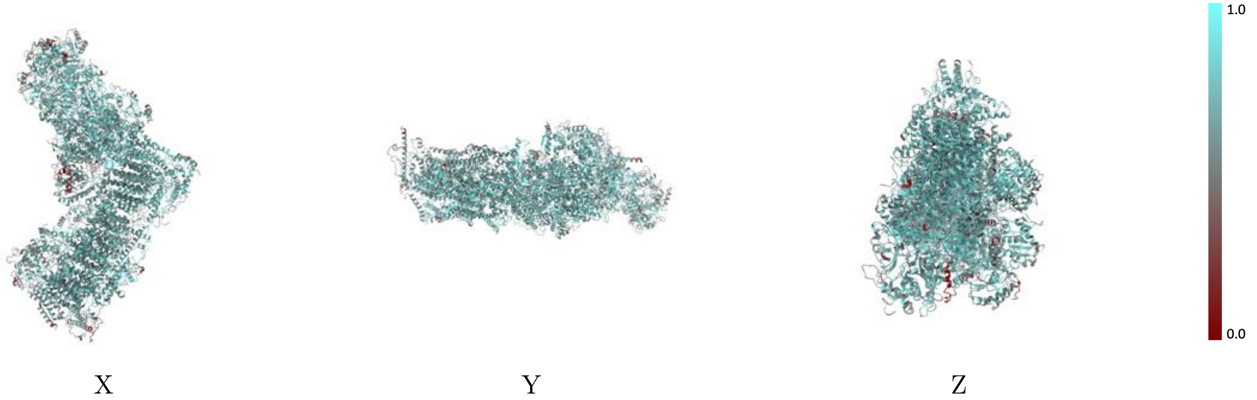
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



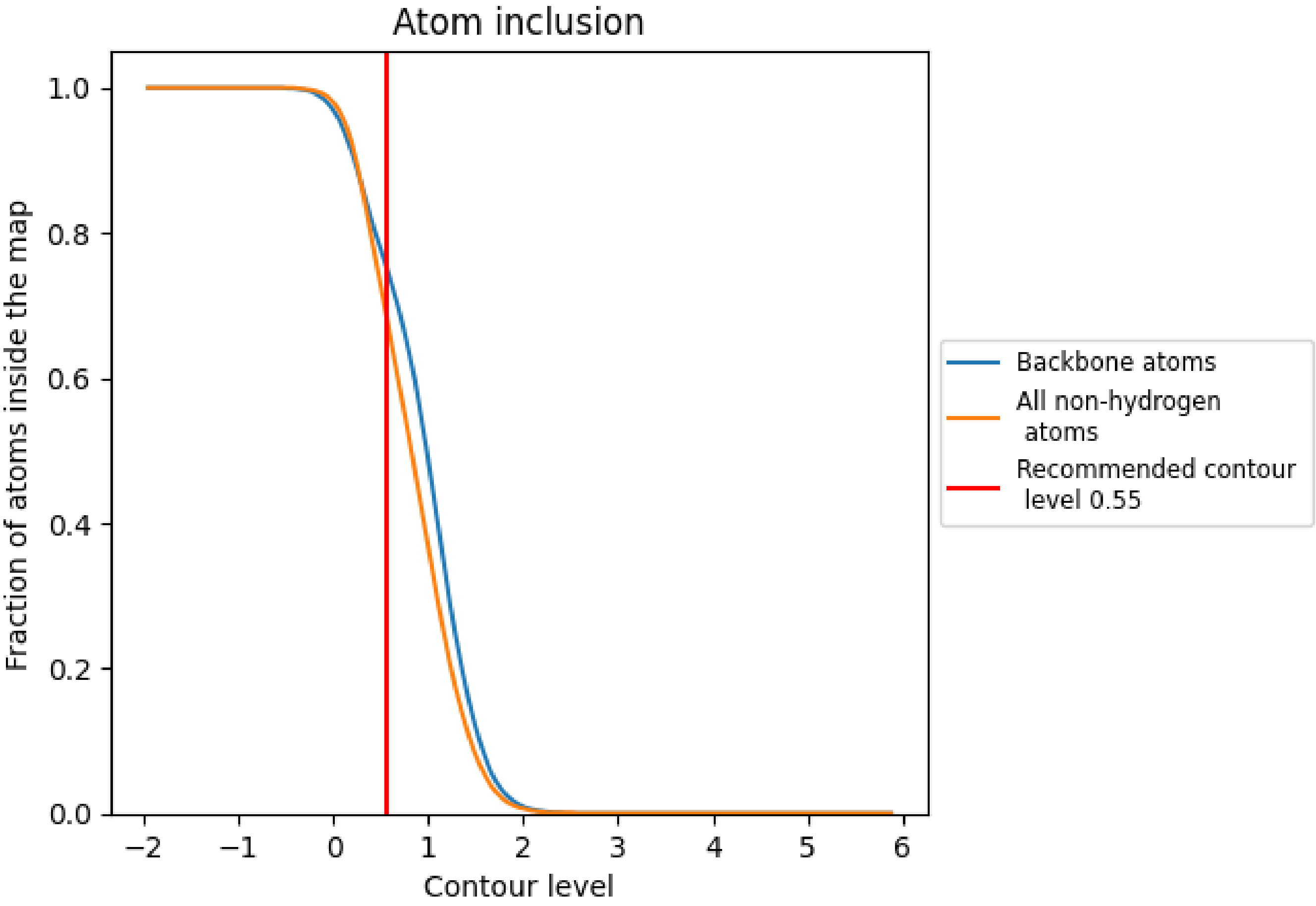
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.55).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 69% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4980
1	0.7330	0.5050
2	0.7390	0.5110
3	0.6850	0.4990
4	0.7440	0.5130
4L	0.7090	0.4980
5	0.6680	0.4840
6	0.6760	0.4990
A1	0.7160	0.4930
A3	0.6920	0.5070
A5	0.6810	0.5030
A6	0.6790	0.4900
A7	0.6730	0.5000
A8	0.6810	0.4930
A9	0.7240	0.5140
AB	0.3060	0.3330
AC	0.5680	0.4610
AL	0.7260	0.5090
AM	0.5800	0.4840
AN	0.6500	0.4960
AO	0.7240	0.5040
B1	0.5950	0.4860
B2	0.5740	0.4560
B3	0.5400	0.4410
B4	0.6930	0.4910
B5	0.7390	0.5250
B6	0.6420	0.4920
B7	0.5390	0.4190
B8	0.6740	0.4870
B9	0.6740	0.4870
BL	0.7320	0.5060
BM	0.6830	0.4900
C2	0.7030	0.5130
S1	0.7020	0.5040
S2	0.7440	0.5120

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Chain	Atom inclusion	Q-score
S3	0.7680	0.5300
S4	0.6750	0.5070
S5	0.7370	0.5150
S6	0.7240	0.5330
S7	0.7450	0.5060
S8	0.7760	0.5190
V1	0.6850	0.4880
V2	0.6370	0.4870
V3	0.1480	0.3400