wwPDB EM Validation Summary Report

Sep 22, 2022 – 03:44 am BST

PDB ID	:	7QSN
EMDB ID	:	EMD-14139
Title	:	Bovine complex I in lipid nanodisc, Deactive-apo
Authors	:	Chung, I.; Bridges, H.R.; Hirst, J.
Deposited on	:	2022-01-13
Resolution	:	2.81 Å(reported)

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

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

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

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

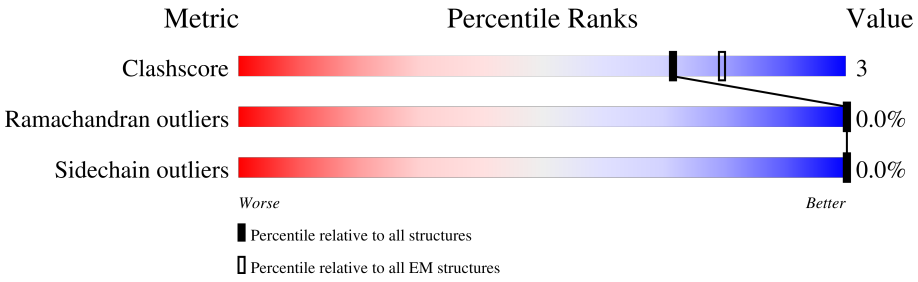
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.81 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	158937	4297
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	A	115	18% 77% 15% 8%
2	B	216	63% 9% 28%
3	C	266	72% 6% 22%
4	D	463	81% 6% 13%
5	E	249	78% 8% 14%
6	F	464	84% 9% 7%
7	G	727	87% 8% 5%
8	H	318	9% 79% 12% 8%

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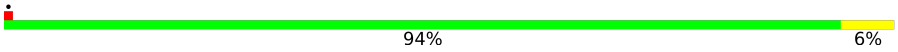
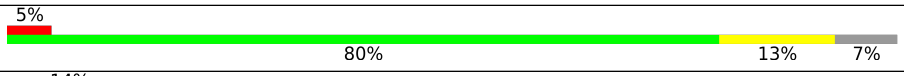
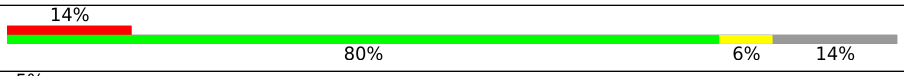
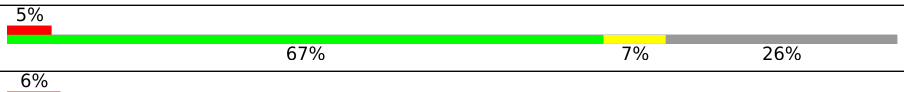
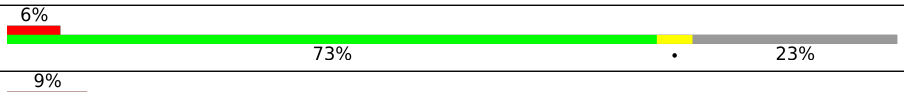
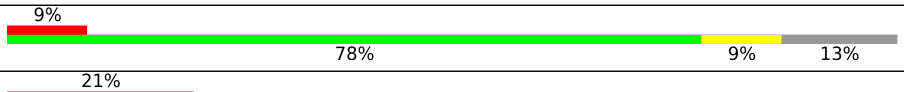
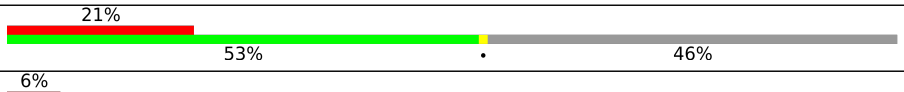
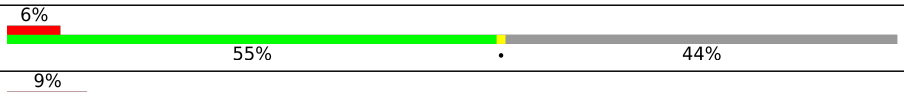
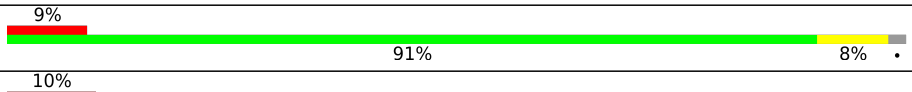
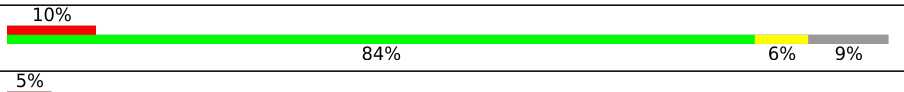
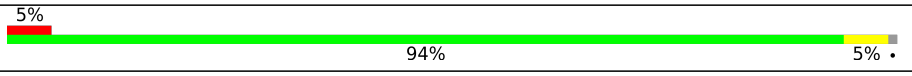
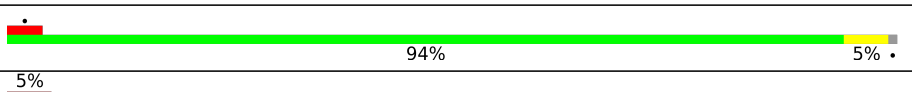
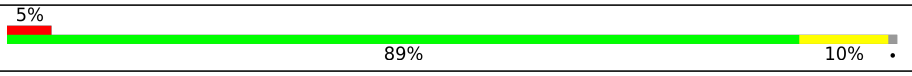
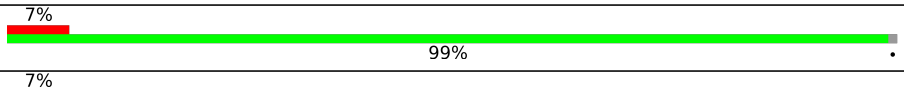
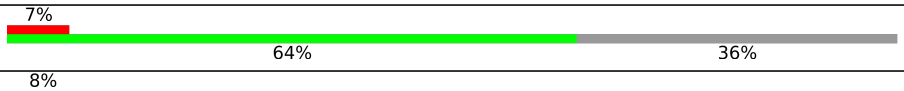
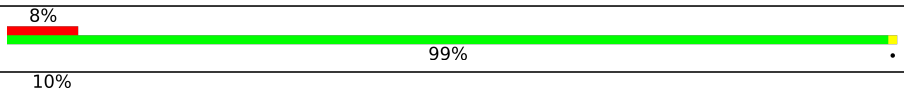
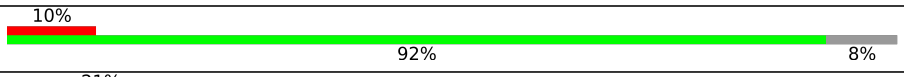
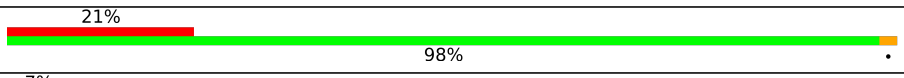
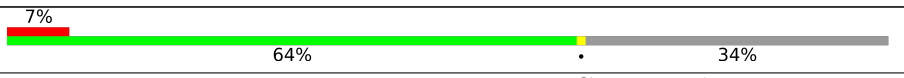
Mol	Chain	Length	Quality of chain
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	

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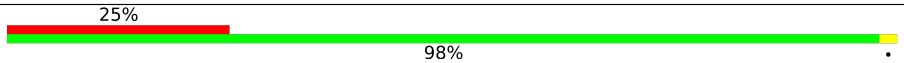
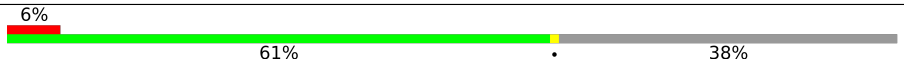
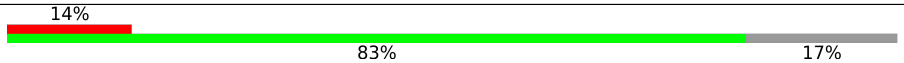
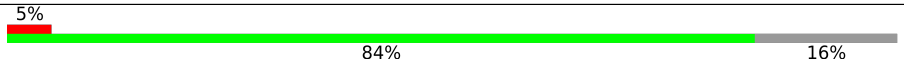
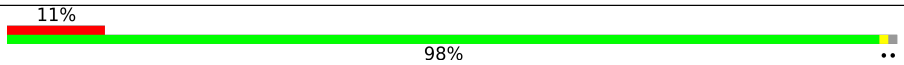
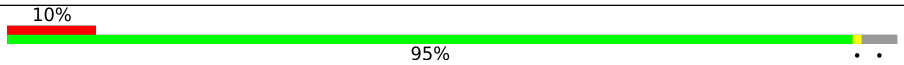
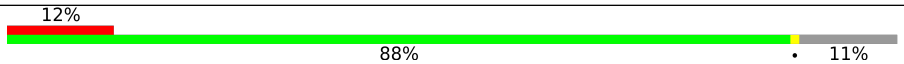
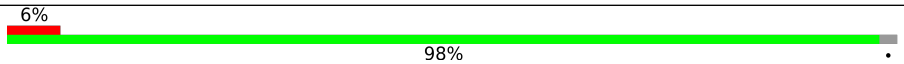
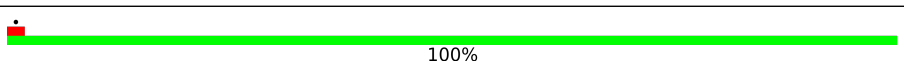
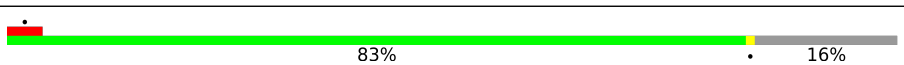
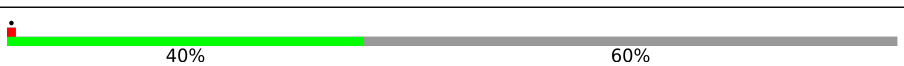
Mol	Chain	Length	Quality of chain
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 69319 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	A	106	852	578	124	145	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	795	225	213	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	C	207	1721	1111	296	311	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	404	3262	2083	560	595	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	1	0
			3336	2102	597	617	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	691	Total	C	N	O	S	0	0
			5298	3318	925	1016	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	291	Total	C	N	O	S	1	0
			2316	1555	357	381	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	327	Total	C	N	O	S	0	0
			2623	1695	464	459	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total	C	N	O	S	0	0
			982	628	182	168	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	98	Total	C	N	O	S	0	0
			825	521	157	141	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			846	544	140	158	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	128	Total	C	N	O	0	0
			1067	684	188	195		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	1	0
			1498	958	276	257	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1450	909	268	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

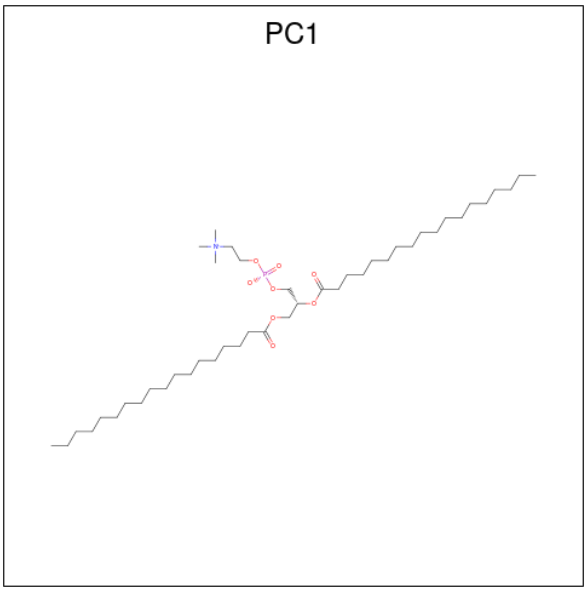
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

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

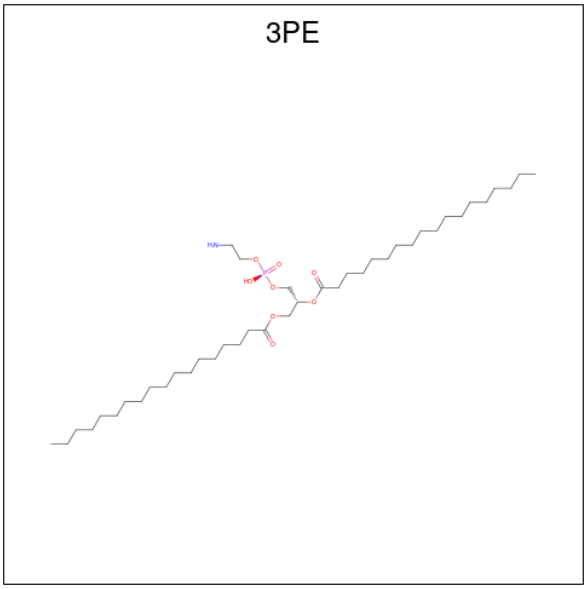
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

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



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	M	1	Total	C	N	O	P	0
			95	75	2	16	2	
45	M	1	Total	C	N	O	P	0
			95	75	2	16	2	
45	N	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	d	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	I	1	Total	C	N	O	P	0
			102	82	2	16	2	
46	I	1	Total	C	N	O	P	0
			102	82	2	16	2	
46	K	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	L	1	Total	C	N	O	P	0
			121	91	3	24	3	
46	L	1	Total	C	N	O	P	0
			121	91	3	24	3	
46	L	1	Total	C	N	O	P	0
			121	91	3	24	3	
46	M	1	Total	C	N	O	P	0
			145	115	3	24	3	
46	M	1	Total	C	N	O	P	0
			145	115	3	24	3	
46	M	1	Total	C	N	O	P	0
			145	115	3	24	3	
46	N	1	Total	C	N	O	P	0
			90	70	2	16	2	

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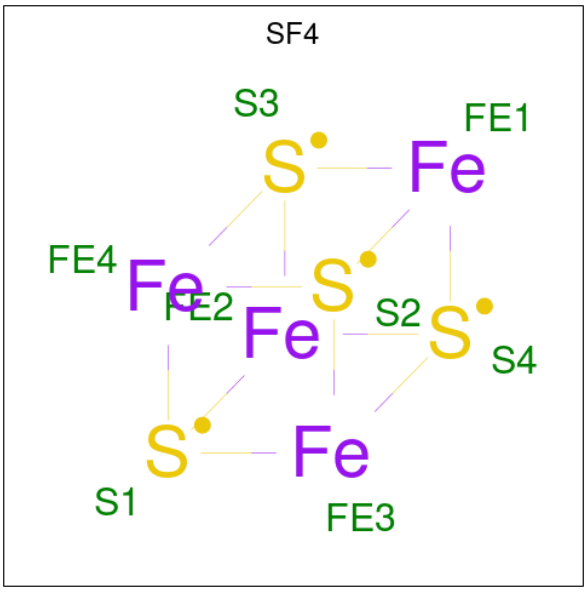
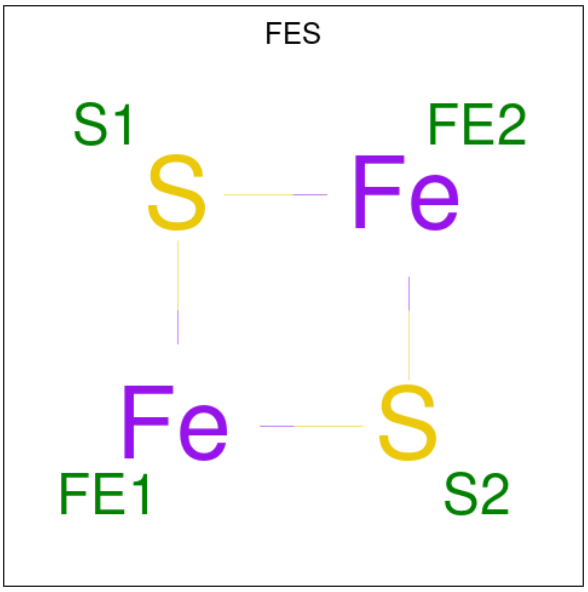
Mol	Chain	Residues	Atoms					AltConf
46	N	1	Total	C	N	O	P	0
			90	70	2	16	2	
46	O	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	Y	1	Total	C	N	O	P	0
			211	161	5	40	5	
46	Y	1	Total	C	N	O	P	0
			211	161	5	40	5	
46	Y	1	Total	C	N	O	P	0
			211	161	5	40	5	
46	Y	1	Total	C	N	O	P	0
			211	161	5	40	5	
46	Y	1	Total	C	N	O	P	0
			211	161	5	40	5	
46	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	b	1	Total	C	N	O	P	0
			88	68	2	16	2	
46	b	1	Total	C	N	O	P	0
			88	68	2	16	2	
46	d	1	Total	C	N	O	P	0
			90	70	2	16	2	
46	d	1	Total	C	N	O	P	0
			90	70	2	16	2	
46	f	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	g	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	h	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	m	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



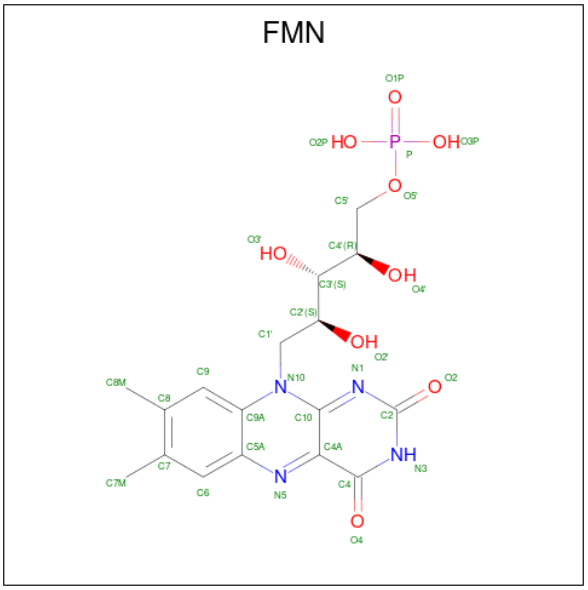
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			16	8	8	
47	G	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	

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



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

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

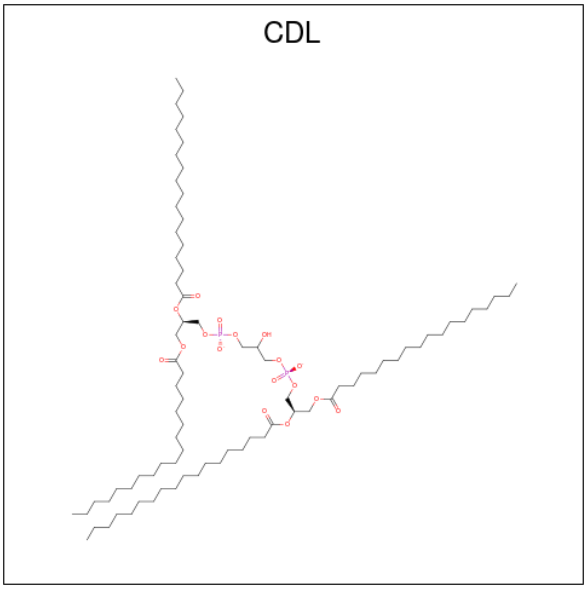


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

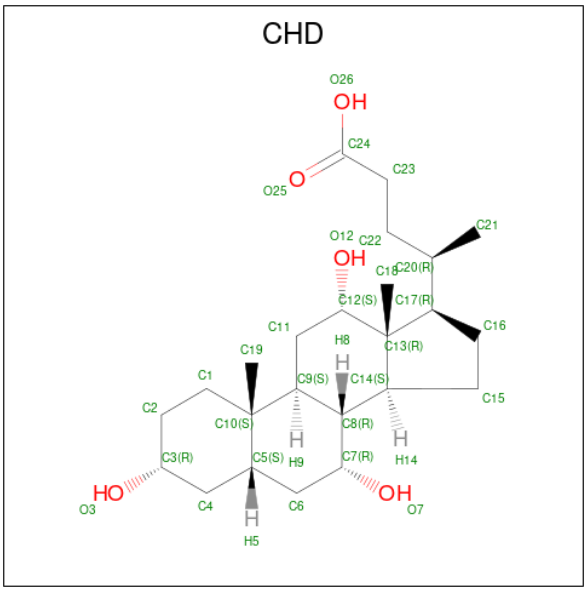
Mol	Chain	Residues	Atoms	AltConf
50	G	1	Total K 1 1	0

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



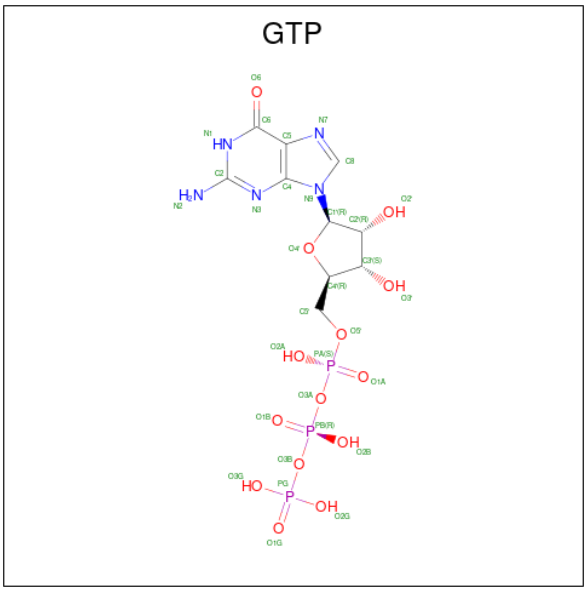
Mol	Chain	Residues	Atoms	AltConf
51	L	1	Total C O P 79 60 17 2	0
51	N	1	Total C O P 85 66 17 2	0
51	X	1	Total C O P 86 67 17 2	0
51	d	1	Total C O P 65 46 17 2	0
51	h	1	Total C O P 68 49 17 2	0
51	r	1	Total C O P 64 45 17 2	0

- Molecule 52 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
52	L	1	Total	C	O	0
			29	24	5	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

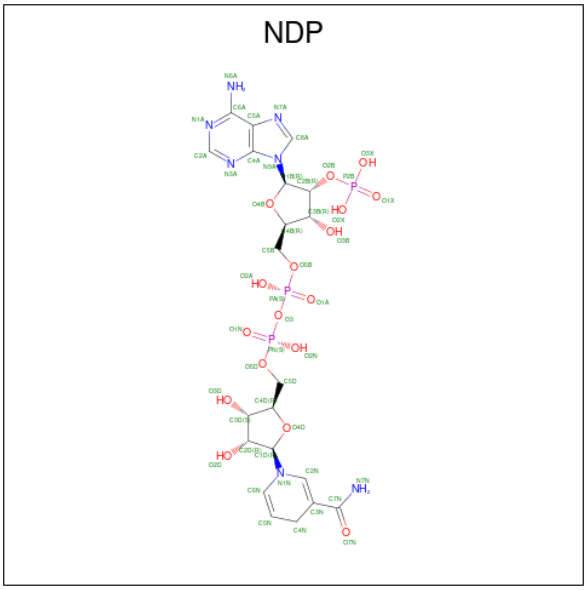


Mol	Chain	Residues	Atoms					AltConf
53	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

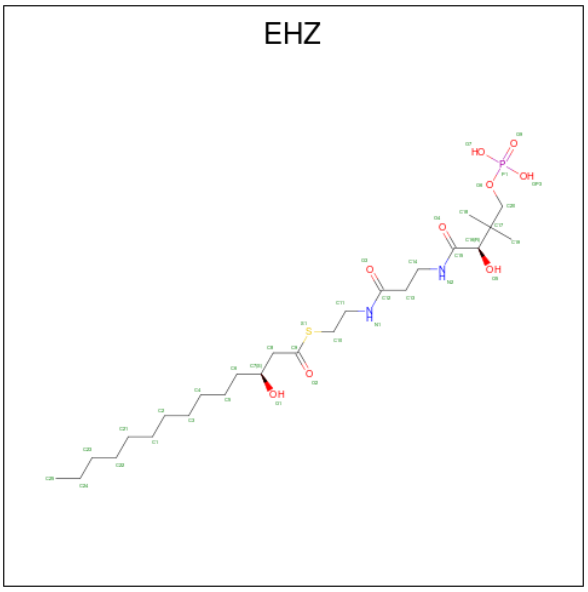


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

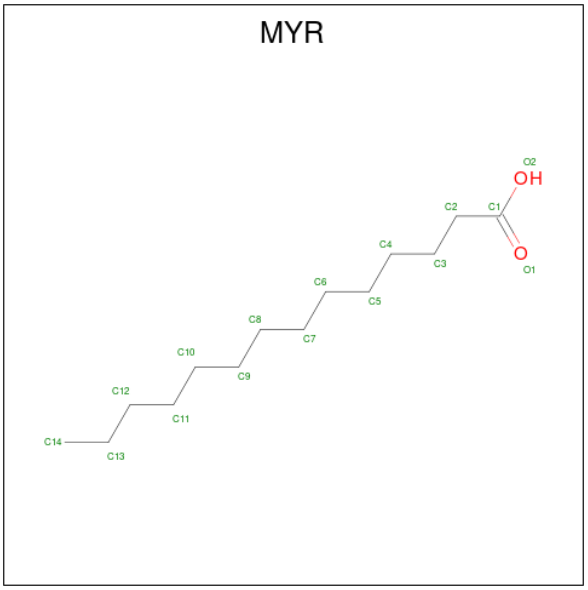
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

- Molecule 57 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
57	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	A	5	Total O 5 5	0
59	B	37	Total O 37 37	0
59	C	58	Total O 58 58	0
59	D	113	Total O 113 113	0
59	E	8	Total O 8 8	0
59	F	30	Total O 30 30	0
59	G	157	Total O 157 157	0
59	H	39	Total O 39 39	0
59	I	65	Total O 65 65	0
59	J	18	Total O 18 18	0
59	K	10	Total O 10 10	0
59	L	64	Total O 64 64	0
59	M	80	Total O 80 80	0
59	N	48	Total O 48 48	0
59	O	8	Total O 8 8	0
59	P	29	Total O 29 29	0
59	Q	63	Total O 63 63	0
59	R	12	Total O 12 12	0
59	S	1	Total O 1 1	0
59	U	8	Total O 8 8	0
59	V	5	Total O 5 5	0
59	W	3	Total O 3 3	0

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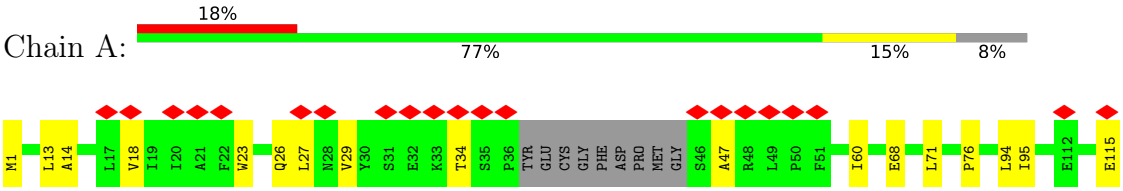
Mol	Chain	Residues	Atoms	AltConf
59	X	13	Total O 13 13	0
59	Y	1	Total O 1 1	0
59	Z	23	Total O 23 23	0
59	a	13	Total O 13 13	0
59	b	2	Total O 2 2	0
59	c	1	Total O 1 1	0
59	d	16	Total O 16 16	0
59	e	14	Total O 14 14	0
59	f	1	Total O 1 1	0
59	g	12	Total O 12 12	0
59	h	26	Total O 26 26	0
59	i	5	Total O 5 5	0
59	j	2	Total O 2 2	0
59	l	13	Total O 13 13	0
59	m	10	Total O 10 10	0
59	n	23	Total O 23 23	0
59	o	3	Total O 3 3	0
59	p	22	Total O 22 22	0
59	q	19	Total O 19 19	0
59	r	14	Total O 14 14	0
59	s	2	Total O 2 2	0

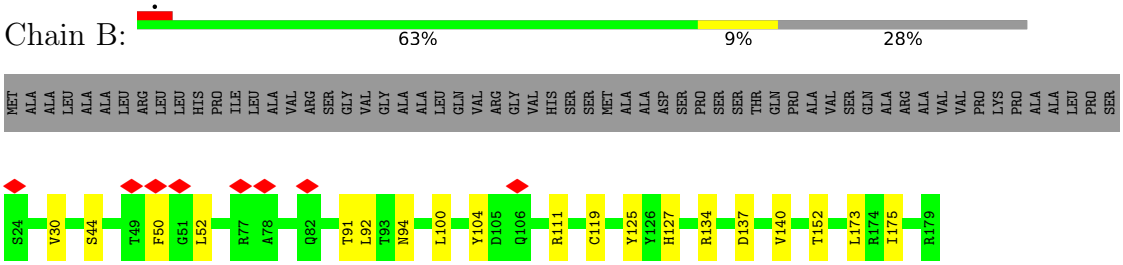
3 Residue-property plots (i)

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.

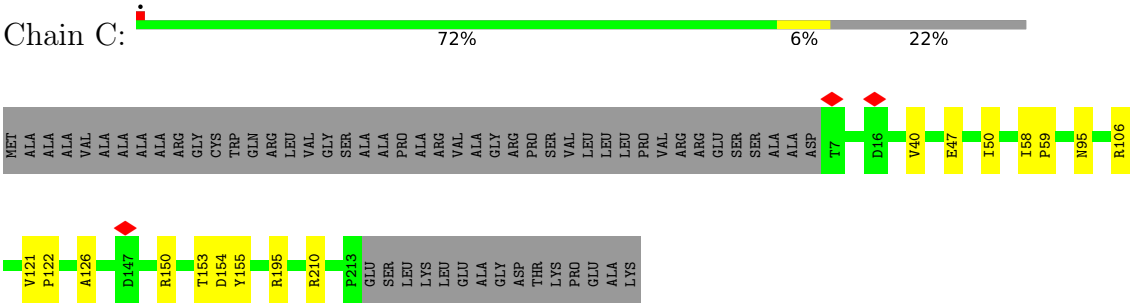
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



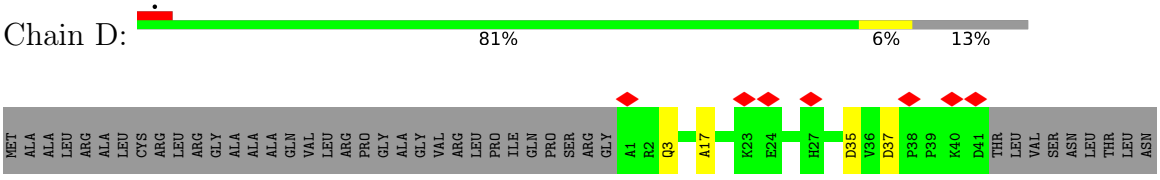
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

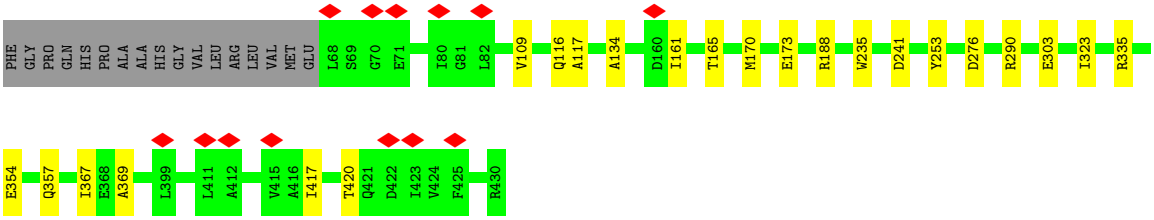


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



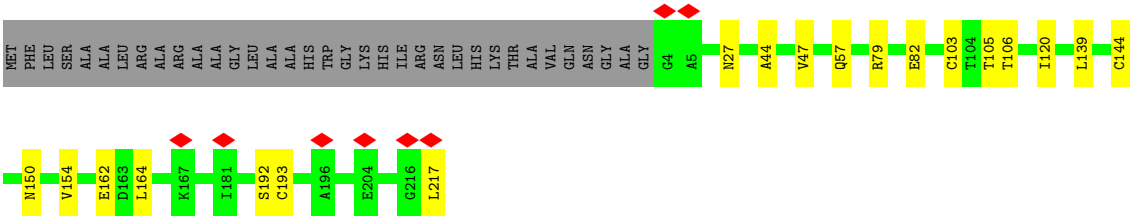
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





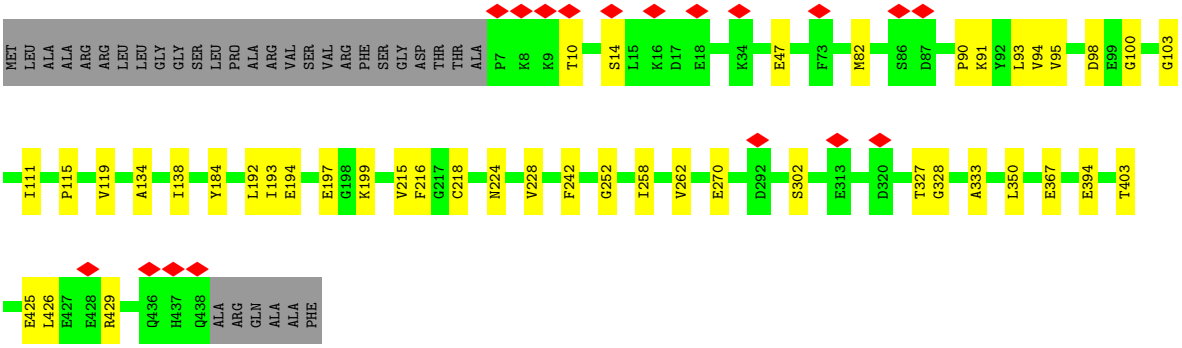
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



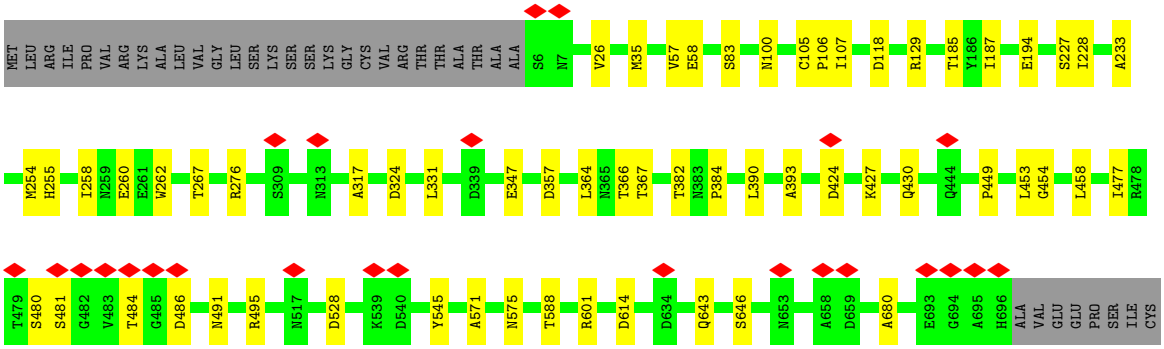
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

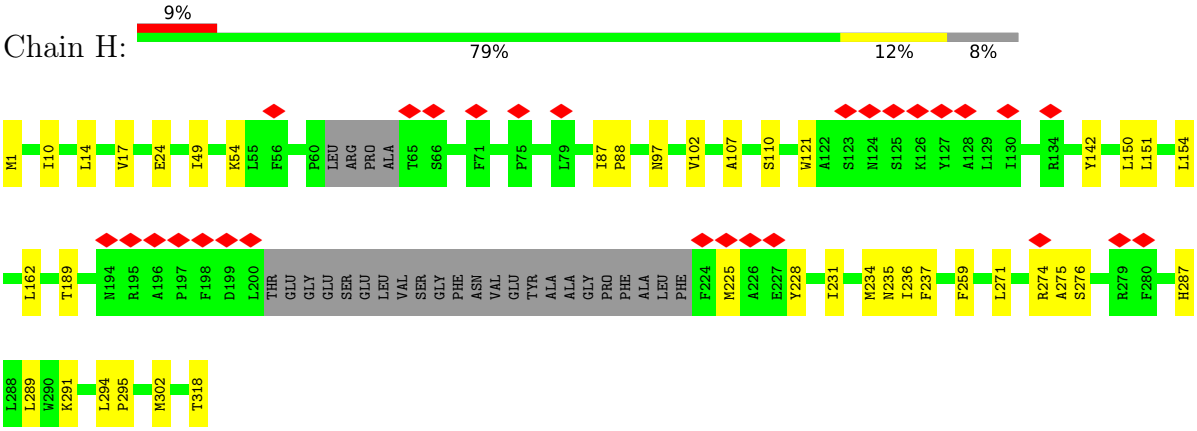


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

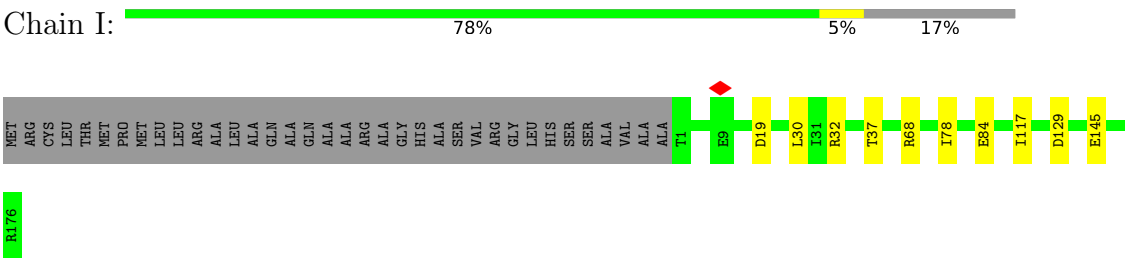
Chain G:



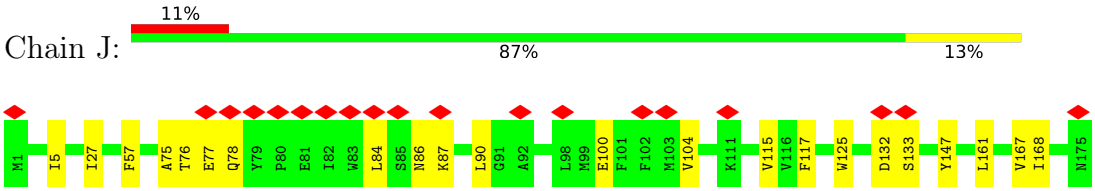
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



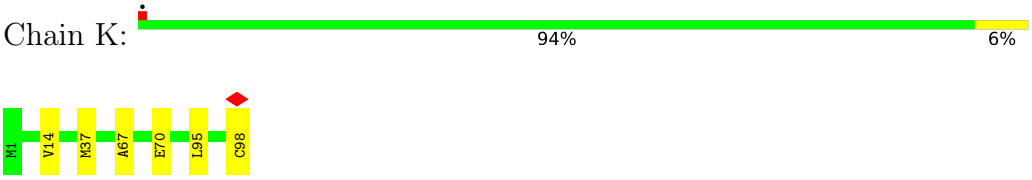
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



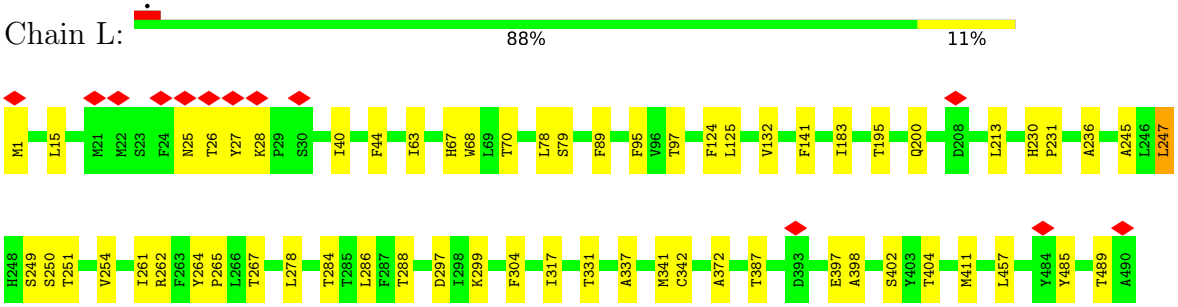
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

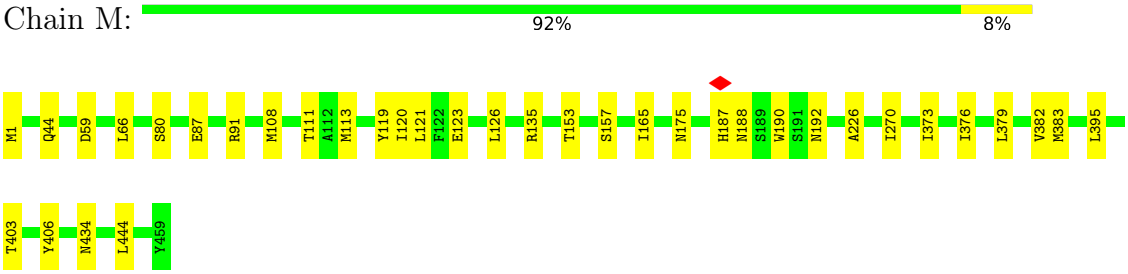


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



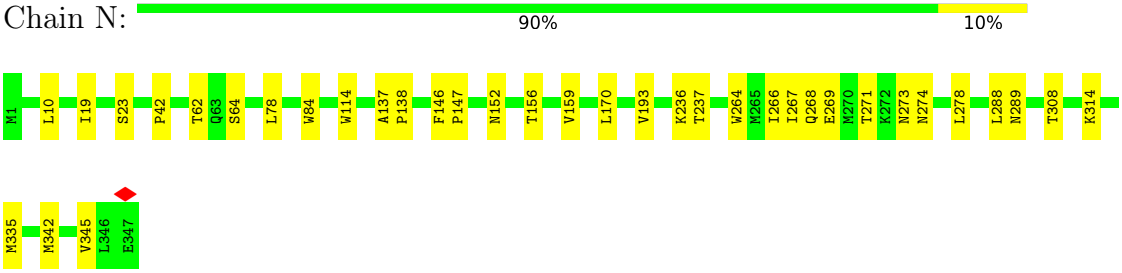
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



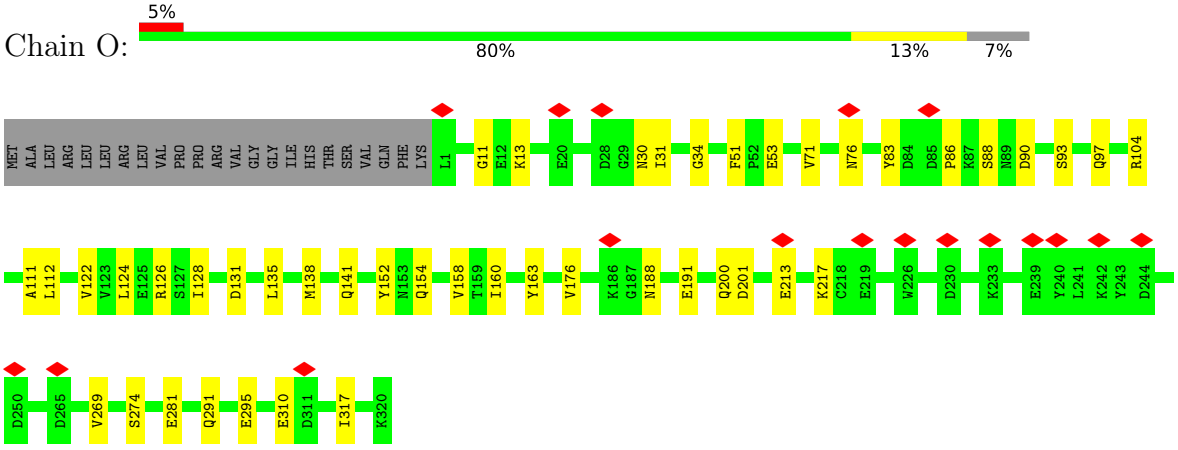
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



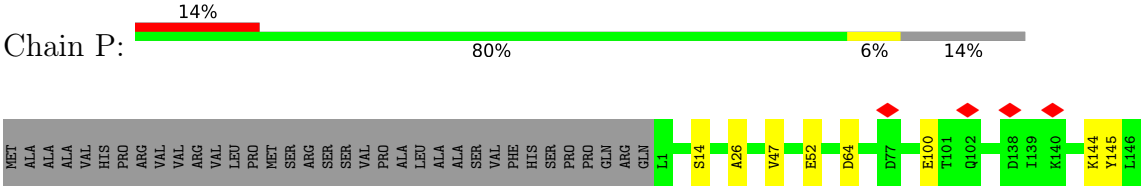
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

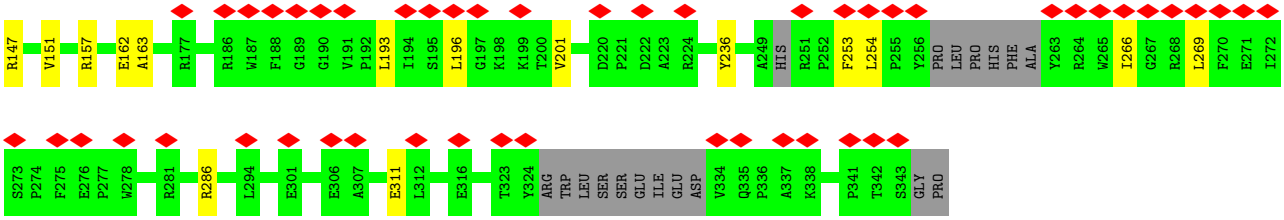
Chain O:



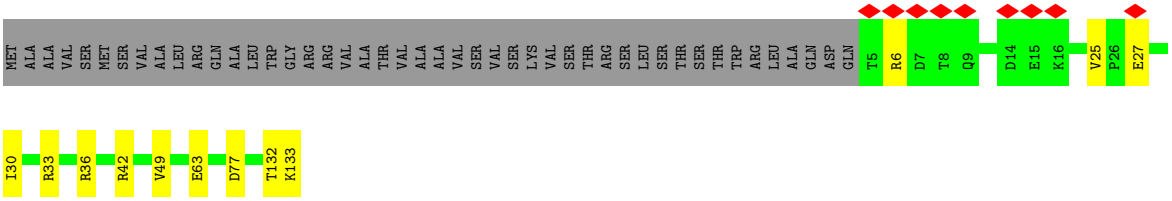
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

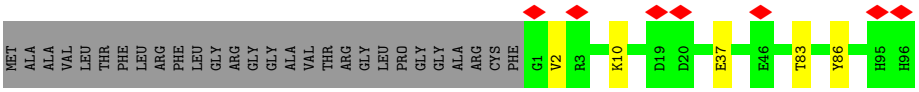




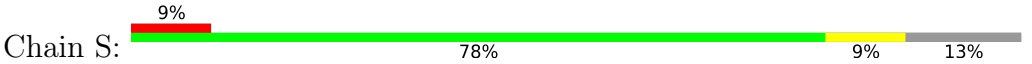
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

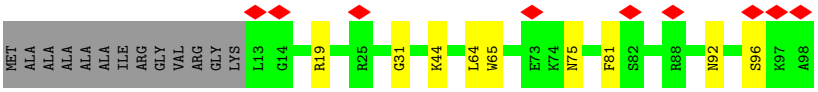


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

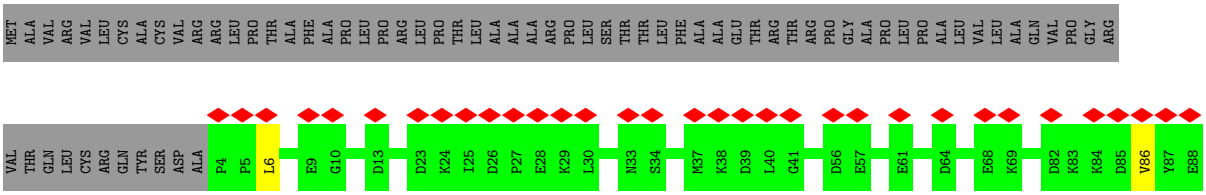


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

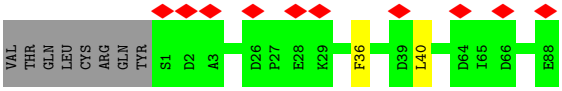




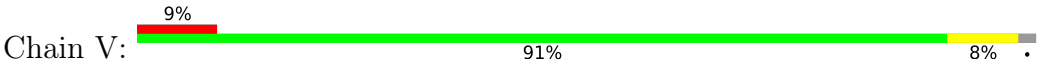
• Molecule 20: Acyl carrier protein, mitochondrial

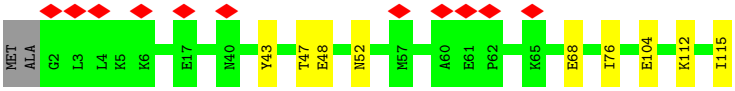


• Molecule 20: Acyl carrier protein, mitochondrial

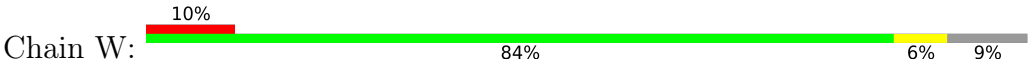


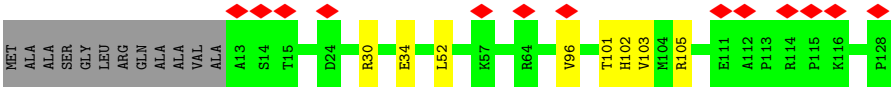
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



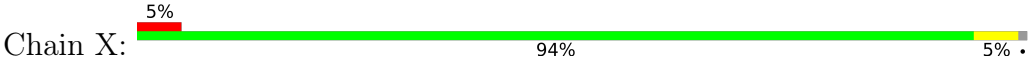


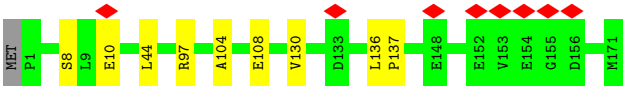
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



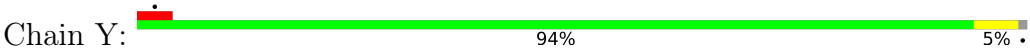


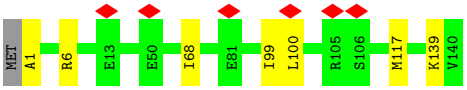
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



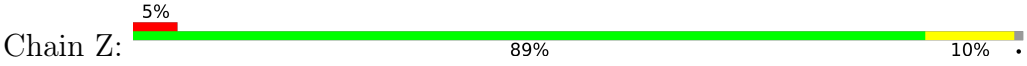


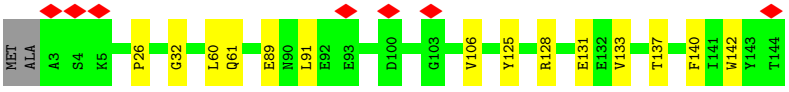
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

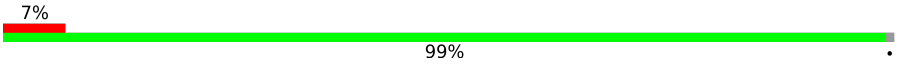


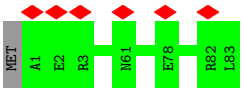


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

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

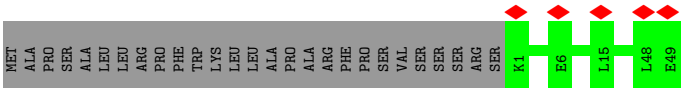
Chain b:





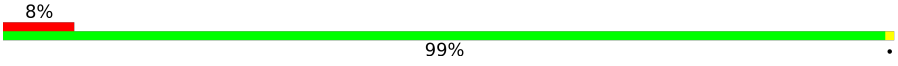
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

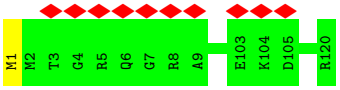
Chain c:



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

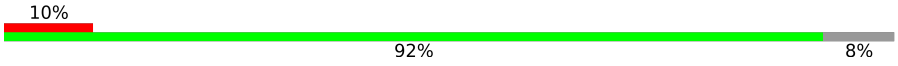
Chain d:

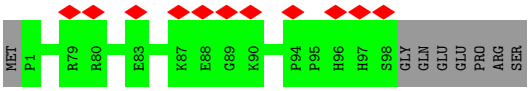




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

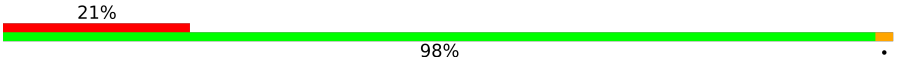
Chain e:

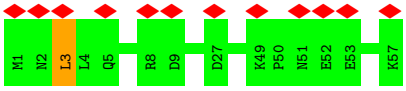




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

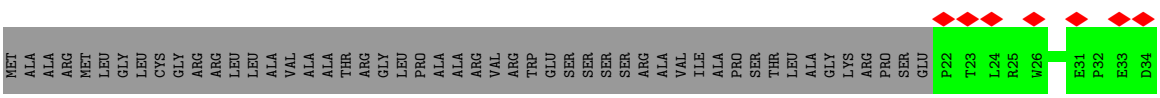
Chain f:

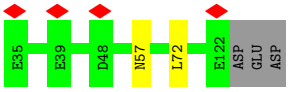




• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

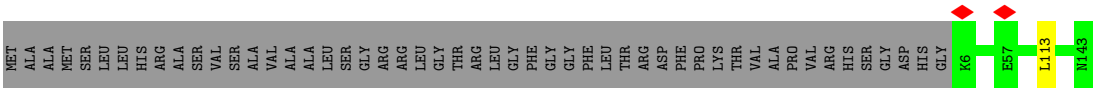
Chain g:





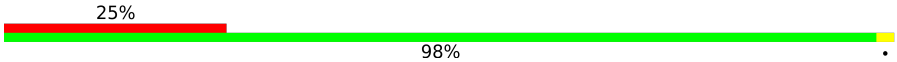
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

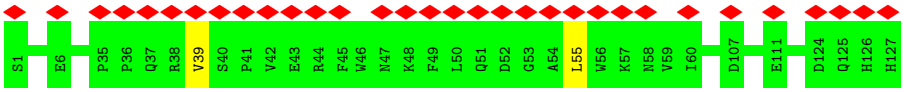
Chain h:



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

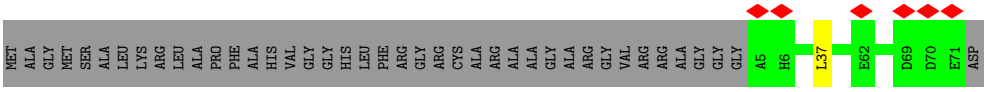
Chain i:





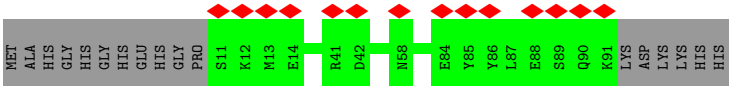
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



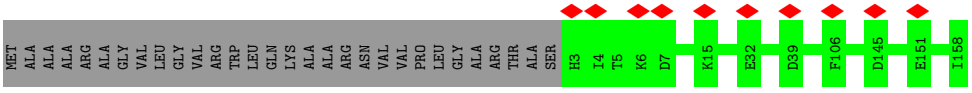
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



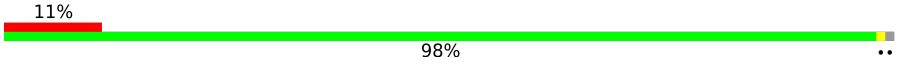
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

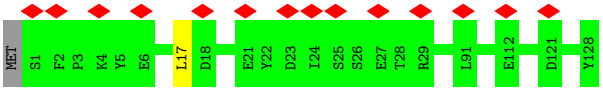
Chain l:



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

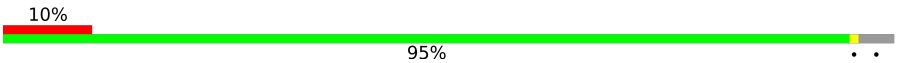
Chain m:

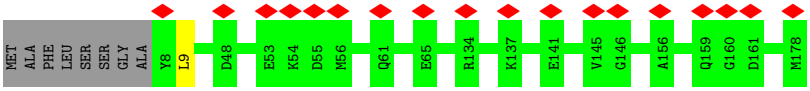




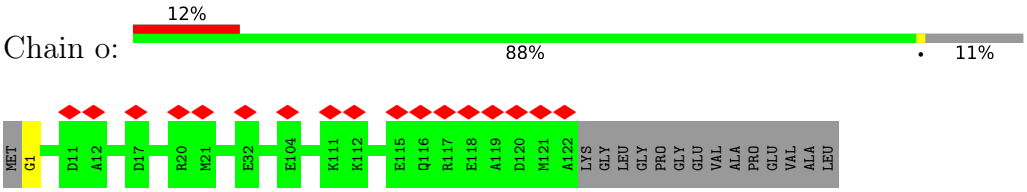
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

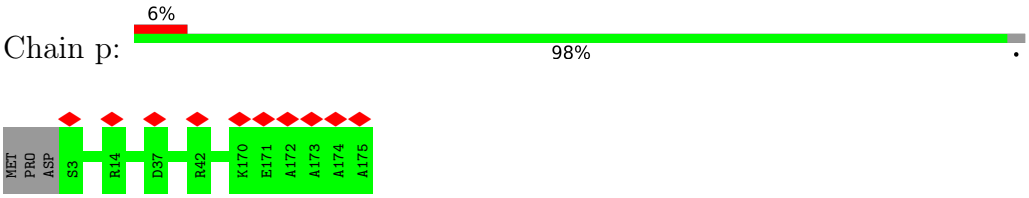




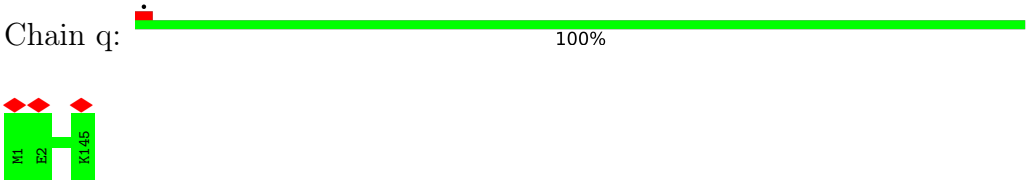
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



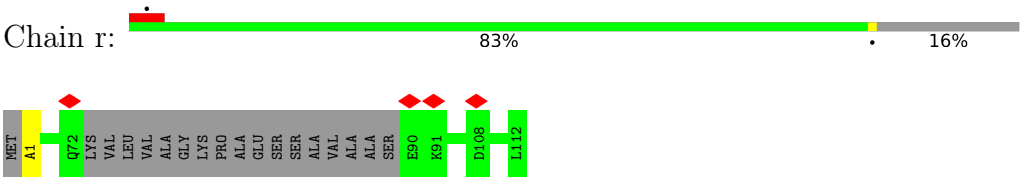
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



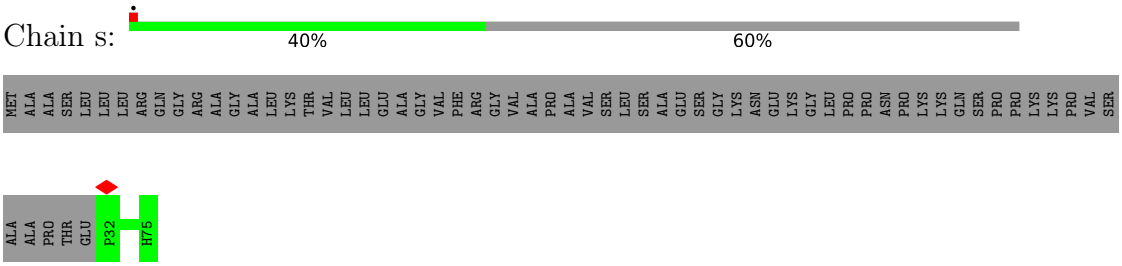
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23583	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 ($e^-/Å^2$)	40.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	29.852	Depositor
Minimum map value	-10.648	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.943	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	479.744, 479.744, 479.744	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7496, 0.7496, 0.7496	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EHZ, K, PC1, 2MR, ZN, 3PE, FME, FES, CHD, SAC, CDL, NDP, MYR, MG, FMN, GTP, SF4, AYA, AME

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	A	0.31	0/863	0.43	0/1181
2	B	0.42	0/1278	0.46	0/1728
3	C	0.39	0/1772	0.46	0/2413
4	D	0.38	0/3334	0.45	0/4514
5	E	0.35	0/1699	0.48	2/2312 (0.1%)
6	F	0.36	0/3412	0.48	2/4610 (0.0%)
7	G	0.34	0/5387	0.47	0/7301
8	H	0.33	0/2371	0.43	0/3237
9	I	0.40	0/1445	0.48	0/1956
10	J	0.37	0/1370	0.44	0/1859
11	K	0.33	0/745	0.44	0/1008
12	L	0.34	0/4920	0.45	4/6694 (0.1%)
13	M	0.34	0/3738	0.43	0/5097
14	N	0.33	0/2792	0.44	0/3800
15	O	0.37	0/2651	0.45	2/3587 (0.1%)
16	P	0.33	0/2690	0.50	6/3642 (0.2%)
17	Q	0.34	0/1072	0.45	0/1449
18	R	0.38	0/753	0.45	0/1014
19	S	0.30	0/702	0.48	0/945
20	T	0.32	0/700	0.55	2/944 (0.2%)
20	U	0.36	0/719	0.42	0/971
21	V	0.32	0/943	0.39	0/1277
22	W	0.34	0/1006	0.42	0/1352
23	X	0.35	0/1439	0.43	0/1942
24	Y	0.32	0/1042	0.41	0/1414
25	Z	0.37	0/1186	0.45	0/1599
26	a	0.36	0/584	0.41	0/786
27	b	0.34	0/672	0.43	0/923
28	c	0.37	0/427	0.38	0/579
29	d	0.41	0/1018	0.44	0/1375
30	e	0.33	0/846	0.41	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.36	0/505	0.52	2/681 (0.3%)
32	g	0.37	0/873	0.48	2/1186 (0.2%)
33	h	0.38	0/1188	0.47	2/1607 (0.1%)
34	i	0.35	0/1127	0.52	3/1534 (0.2%)
35	j	0.37	0/607	0.48	2/833 (0.2%)
36	k	0.34	0/672	0.41	0/906
37	l	0.39	0/1369	0.42	0/1873
38	m	0.37	0/1094	0.48	2/1480 (0.1%)
39	n	0.36	0/1551	0.44	2/2099 (0.1%)
40	o	0.37	1/1073 (0.1%)	0.41	0/1437
41	p	0.36	0/1483	0.43	0/2000
42	q	0.39	0/1250	0.45	0/1698
43	r	0.36	0/789	0.43	0/1068
44	s	0.34	0/383	0.45	0/518
All	All	0.35	1/67540 (0.0%)	0.45	33/91560 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	o	1	GLY	CA-C	5.00	1.59	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	T	86	VAL	CG1-CB-CG2	6.69	121.60	110.90
34	i	39	VAL	CG1-CB-CG2	6.63	121.51	110.90
12	L	247	LEU	CB-CG-CD2	6.39	121.86	111.00
39	n	9	LEU	CB-CG-CD2	6.25	121.62	111.00
33	h	113	LEU	CB-CG-CD2	6.14	121.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	852	0	896	14	0
2	B	1247	0	1256	12	0
3	C	1721	0	1675	11	0
4	D	3262	0	3201	21	0
5	E	1659	0	1664	11	0
6	F	3336	0	3288	28	0
7	G	5298	0	5316	42	0
8	H	2316	0	2435	31	0
9	I	1414	0	1370	13	0
10	J	1345	0	1352	20	0
11	K	745	0	785	5	0
12	L	4802	0	4960	43	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	25	0
15	O	2589	0	2566	28	0
16	P	2623	0	2651	13	0
17	Q	1049	0	1045	9	0
18	R	740	0	714	4	0
19	S	691	0	706	5	0
20	T	688	0	684	0	0
20	U	707	0	700	1	0
21	V	923	0	964	5	0
22	W	982	0	999	5	0
23	X	1402	0	1381	6	0
24	Y	1030	0	1039	4	0
25	Z	1157	0	1156	11	0
26	a	569	0	568	0	0
27	b	651	0	662	0	0
28	c	414	0	415	0	0
29	d	999	0	988	0	0
30	e	825	0	826	0	0
31	f	492	0	501	0	0
32	g	846	0	798	0	0
33	h	1154	0	1168	0	0
34	i	1097	0	1108	0	0
35	j	580	0	519	0	0
36	k	653	0	639	0	0
37	l	1314	0	1210	0	0
38	m	1067	0	1067	0	0
39	n	1498	0	1445	0	0
40	o	1048	0	1018	0	0
41	p	1450	0	1426	0	0
42	q	1209	0	1182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	776	0	782	0	0
44	s	371	0	344	0	0
45	A	50	0	77	0	0
45	B	51	0	79	1	0
45	J	46	0	69	3	0
45	M	95	0	144	4	0
45	N	30	0	34	0	0
45	d	40	0	54	0	0
46	A	47	0	71	0	0
46	H	36	0	49	0	0
46	I	102	0	164	2	0
46	K	43	0	60	1	0
46	L	121	0	170	1	0
46	M	145	0	224	6	0
46	N	90	0	137	2	0
46	O	36	0	46	0	0
46	Y	211	0	304	1	0
46	Z	43	0	63	0	0
46	b	88	0	130	0	0
46	d	90	0	131	0	0
46	f	31	0	36	0	0
46	g	36	0	46	0	0
46	h	39	0	52	0	0
46	m	40	0	57	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	G	1	0	0	0	0
51	L	79	0	108	1	0
51	N	85	0	117	1	0
51	X	86	0	125	0	0
51	d	65	0	77	0	0
51	h	68	0	80	0	0
51	r	64	0	72	0	0
52	L	29	0	37	2	0
53	O	32	0	12	5	0
54	O	1	0	0	0	0
55	P	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R	1	0	0	0	0
57	T	37	0	0	1	0
57	U	37	0	0	0	0
58	o	15	0	27	0	0
59	A	5	0	0	0	0
59	B	37	0	0	1	0
59	C	58	0	0	3	0
59	D	113	0	0	5	0
59	E	8	0	0	0	0
59	F	30	0	0	3	0
59	G	157	0	0	5	0
59	H	39	0	0	1	0
59	I	65	0	0	1	0
59	J	18	0	0	0	0
59	K	10	0	0	0	0
59	L	64	0	0	3	0
59	M	80	0	0	4	0
59	N	48	0	0	3	0
59	O	8	0	0	1	0
59	P	29	0	0	2	0
59	Q	63	0	0	3	0
59	R	12	0	0	1	0
59	S	1	0	0	0	0
59	U	8	0	0	0	0
59	V	5	0	0	0	0
59	W	3	0	0	0	0
59	X	13	0	0	0	0
59	Y	1	0	0	0	0
59	Z	23	0	0	0	0
59	a	13	0	0	0	0
59	b	2	0	0	0	0
59	c	1	0	0	0	0
59	d	16	0	0	0	0
59	e	14	0	0	0	0
59	f	1	0	0	0	0
59	g	12	0	0	0	0
59	h	26	0	0	0	0
59	i	5	0	0	0	0
59	j	2	0	0	0	0
59	l	13	0	0	0	0
59	m	10	0	0	0	0
59	n	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	o	3	0	0	0	0
59	p	22	0	0	0	0
59	q	19	0	0	0	0
59	r	14	0	0	0	0
59	s	2	0	0	0	0
All	All	69319	0	69130	356	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 3.

The worst 5 of 356 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)
17:Q:133:LYS:O	59:Q:201:HOH:O	1.87	0.93
6:F:98:ASP:OD2	59:F:601:HOH:O	1.90	0.89
7:G:484:THR:OG1	7:G:486:ASP:OD1	1.92	0.87
15:O:83:TYR:OH	53:O:401:GTP:O2'	1.92	0.86
13:M:44:GLN:OE1	59:M:701:HOH:O	1.94	0.86

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	A	102/115 (89%)	101 (99%)	1 (1%)	0	100	100
2	B	154/216 (71%)	148 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	198 (97%)	7 (3%)	0	100	100
4	D	399/463 (86%)	382 (96%)	17 (4%)	0	100	100
5	E	212/249 (85%)	205 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	431/464 (93%)	416 (96%)	15 (4%)	0	100	100
7	G	689/727 (95%)	664 (96%)	25 (4%)	0	100	100
8	H	286/318 (90%)	277 (97%)	9 (3%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	572 (95%)	31 (5%)	1 (0%)	47	76
13	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	319/380 (84%)	304 (95%)	15 (5%)	0	100	100
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
19	S	84/99 (85%)	80 (95%)	4 (5%)	0	100	100
20	T	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	114/128 (89%)	110 (96%)	4 (4%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	8	26
32	g	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	n	170/179 (95%)	167 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	87 (96%)	4 (4%)	0	100	100
44	s	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
All	All	8097/9212 (88%)	7827 (97%)	268 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
31	f	3	LEU

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	A	93/100 (93%)	93 (100%)	0	100	100
2	B	132/175 (75%)	132 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	348/392 (89%)	348 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	347/368 (94%)	347 (100%)	0	100	100
7	G	579/608 (95%)	579 (100%)	0	100	100
8	H	255/274 (93%)	255 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	141/141 (100%)	141 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	282/327 (86%)	282 (100%)	0	100	100
17	Q	116/153 (76%)	116 (100%)	0	100	100
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	79/135 (58%)	79 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	105 (100%)	0	100	100
30	e	89/96 (93%)	89 (100%)	0	100	100
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	92/131 (70%)	91 (99%)	1 (1%)	73	91
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	120/120 (100%)	120 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	63/76 (83%)	63 (100%)	0	100	100
37	l	140/159 (88%)	140 (100%)	0	100	100
38	m	114/115 (99%)	114 (100%)	0	100	100
39	n	157/161 (98%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7156/7892 (91%)	7155 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	g	57	ASN

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

Mol	Chain	Res	Type
14	N	289	ASN
30	e	26	HIS
42	q	91	HIS
41	p	133	GLN
13	M	44	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\|>2$
11	FME	K	1	11	8,9,10	0.85	0	7,9,11	0.95	0
14	FME	N	1	14	8,9,10	0.95	0	7,9,11	0.98	0
43	AYA	r	1	43	6,7,8	1.29	1 (16%)	5,8,10	1.19	1 (20%)
4	2MR	D	85	4	10,12,13	0.37	0	5,13,15	1.06	0
12	FME	L	1	12	8,9,10	0.92	0	7,9,11	1.05	1 (14%)
8	FME	H	1	8	8,9,10	1.04	1 (12%)	7,9,11	0.68	0
10	FME	J	1	10	8,9,10	0.95	0	7,9,11	0.73	0
13	FME	M	1	13	8,9,10	1.01	1 (12%)	7,9,11	0.94	0
24	AYA	Y	1	24	6,7,8	1.26	1 (16%)	5,8,10	1.27	1 (20%)
1	FME	A	1	1	8,9,10	1.01	1 (12%)	7,9,11	0.69	0
29	AME	d	1	29	9,10,11	1.45	1 (11%)	9,11,13	1.63	2 (22%)
34	SAC	i	1	34	7,8,9	1.00	0	8,9,11	1.07	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
11	FME	K	1	11	-	2/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	1/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
24	AYA	Y	1	24	-	2/4/6/8	-
1	FME	A	1	1	-	0/7/9/11	-
29	AME	d	1	29	-	2/9/10/12	-
34	SAC	i	1	34	-	6/7/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	1	AME	CT1-N	3.17	1.45	1.34
43	r	1	AYA	CA-N	-2.68	1.43	1.46
24	Y	1	AYA	CA-N	-2.58	1.43	1.46
8	H	1	FME	CA-N	-2.23	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	FME	CA-N	-2.16	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	1	AME	CE-SD-CG	3.07	110.93	100.40
29	d	1	AME	CG-CB-CA	-2.56	105.84	112.95
24	Y	1	AYA	CB-CA-N	2.54	112.44	109.61
43	r	1	AYA	CB-CA-N	2.30	112.17	109.61
12	L	1	FME	C-CA-N	2.19	113.69	109.73

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	C-CA-CB-CG

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 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 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	$\#\|Z\|>2$
47	SF4	F	502	6	0,12,12	-	-	-		
45	PC1	J	201	-	45,45,53	0.38	0	51,53,61	0.39	0
48	FES	E	301	5	0,4,4	-	-	-		
46	3PE	b	102	-	50,50,50	0.88	4 (8%)	53,55,55	1.02	2 (3%)
45	PC1	B	202	-	50,50,53	0.96	4 (8%)	56,58,61	1.04	2 (3%)
46	3PE	L	701	-	38,38,50	0.96	3 (7%)	41,43,55	1.12	2 (4%)
46	3PE	L	704	-	38,38,50	0.97	3 (7%)	41,43,55	1.16	2 (4%)
46	3PE	M	604	-	50,50,50	0.87	4 (8%)	53,55,55	0.98	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-		
57	EHZ	T	101	20	29,36,37	1.66	4 (13%)	35,44,47	1.52	3 (8%)
46	3PE	d	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.14	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-		
46	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.02	2 (3%)
46	3PE	I	204	-	50,50,50	0.86	4 (8%)	53,55,55	0.94	2 (3%)
46	3PE	M	601	-	42,42,50	0.93	3 (7%)	45,47,55	1.15	2 (4%)
51	CDL	L	702	-	78,78,99	0.97	6 (7%)	84,90,111	1.14	4 (4%)
57	EHZ	U	101	20	29,36,37	1.65	5 (17%)	35,44,47	1.41	2 (5%)
58	MYR	o	201	40	14,14,15	0.85	0	13,13,15	0.68	0
46	3PE	Z	201	-	42,42,50	0.94	4 (9%)	45,47,55	1.04	2 (4%)
46	3PE	d	202	-	48,48,50	0.88	3 (6%)	51,53,55	1.06	2 (3%)
55	NDP	P	501	-	45,52,52	2.17	7 (15%)	53,80,80	1.71	10 (18%)
46	3PE	Y	204	-	31,31,50	1.07	4 (12%)	34,36,55	1.11	2 (5%)
45	PC1	d	203	-	39,39,53	1.11	4 (10%)	45,47,61	1.08	2 (4%)
51	CDL	h	201	-	67,67,99	1.06	7 (10%)	73,79,111	1.22	4 (5%)
46	3PE	L	703	-	42,42,50	0.92	3 (7%)	45,47,55	1.12	2 (4%)
46	3PE	m	201	-	39,39,50	0.96	4 (10%)	42,44,55	1.05	2 (4%)
52	CHD	L	705	-	32,32,32	3.21	10 (31%)	51,51,51	2.88	24 (47%)
45	PC1	N	903	-	29,29,53	1.20	3 (10%)	35,37,61	1.04	1 (2%)
45	PC1	A	301	-	49,49,53	0.99	4 (8%)	55,57,61	1.03	2 (3%)
46	3PE	Y	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
46	3PE	N	904	-	38,38,50	0.99	3 (7%)	41,43,55	1.13	2 (4%)
46	3PE	Y	205	-	44,44,50	0.92	3 (6%)	47,49,55	1.03	2 (4%)
45	PC1	M	603	-	45,45,53	1.03	3 (6%)	51,53,61	0.99	2 (3%)
46	3PE	Y	203	-	38,38,50	1.00	4 (10%)	41,43,55	1.13	2 (4%)
49	FMN	F	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.22	6 (12%)
46	3PE	H	601	-	35,35,50	1.01	4 (11%)	38,40,55	1.17	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	3PE	Y	202	-	43,43,50	0.92	4 (9%)	46,48,55	1.04	2 (4%)
46	3PE	h	202	-	38,38,50	0.97	4 (10%)	41,43,55	1.06	2 (4%)
51	CDL	N	902	-	84,84,99	0.95	8 (9%)	90,96,111	1.08	4 (4%)
45	PC1	M	605	-	48,48,53	1.01	4 (8%)	54,56,61	1.02	2 (3%)
46	3PE	b	101	-	36,36,50	1.03	4 (11%)	39,41,55	1.11	2 (5%)
51	CDL	r	201	-	63,63,99	1.09	7 (11%)	69,75,111	1.15	4 (5%)
46	3PE	g	201	-	35,35,50	1.02	4 (11%)	38,40,55	1.14	2 (5%)
46	3PE	A	302	-	46,46,50	0.88	4 (8%)	49,51,55	0.99	2 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
53	GTP	O	401	54	26,34,34	2.91	10 (38%)	32,54,54	1.75	11 (34%)
46	3PE	O	403	-	35,35,50	1.03	4 (11%)	38,40,55	1.17	2 (5%)
46	3PE	K	101	-	42,42,50	0.91	4 (9%)	45,47,55	1.16	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-		
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	f	101	-	30,30,50	1.12	4 (13%)	33,35,55	1.13	2 (6%)
51	CDL	X	201	-	85,85,99	0.93	6 (7%)	91,97,111	1.10	4 (4%)
46	3PE	M	602	-	50,50,50	0.86	3 (6%)	53,55,55	1.08	2 (3%)
47	SF4	I	203	9	0,12,12	-	-	-		
51	CDL	d	204	-	64,64,99	1.07	8 (12%)	70,76,111	1.10	4 (5%)
46	3PE	N	901	-	50,50,50	0.85	4 (8%)	53,55,55	1.06	2 (3%)

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
47	SF4	F	502	6	-	-	0/6/5/5
45	PC1	J	201	-	-	6/49/49/57	-
48	FES	E	301	5	-	-	0/1/1/1
46	3PE	b	102	-	-	25/54/54/54	-
45	PC1	B	202	-	-	19/54/54/57	-
46	3PE	L	701	-	-	16/42/42/54	-
46	3PE	L	704	-	-	16/42/42/54	-
46	3PE	M	604	-	-	26/54/54/54	-
57	EHZ	T	101	20	-	10/42/44/45	-
58	MYR	o	201	40	-	4/11/12/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	d	201	-	-	18/44/44/54	-
47	SF4	I	202	9	-	-	0/6/5/5
46	3PE	I	201	-	-	26/54/54/54	-
46	3PE	I	204	-	-	25/54/54/54	-
46	3PE	M	601	-	-	25/46/46/54	-
51	CDL	L	702	-	-	39/89/89/110	-
57	EHZ	U	101	20	-	5/42/44/45	-
48	FES	G	803	7	-	-	0/1/1/1
46	3PE	Z	201	-	-	20/46/46/54	-
46	3PE	d	202	-	-	23/52/52/54	-
46	3PE	Y	204	-	-	20/35/35/54	-
45	PC1	d	203	-	-	18/43/43/57	-
51	CDL	h	201	-	-	38/78/78/110	-
47	SF4	I	203	9	-	-	0/6/5/5
46	3PE	L	703	-	-	23/46/46/54	-
46	3PE	m	201	-	-	23/43/43/54	-
52	CHD	L	705	-	-	3/9/74/74	0/4/4/4
45	PC1	N	903	-	-	15/32/32/57	-
45	PC1	A	301	-	-	19/53/53/57	-
46	3PE	Y	201	-	-	22/54/54/54	-
46	3PE	N	904	-	-	21/42/42/54	-
46	3PE	Y	205	-	-	29/48/48/54	-
45	PC1	M	603	-	-	20/49/49/57	-
46	3PE	Y	203	-	-	20/42/42/54	-
49	FMN	F	501	-	-	4/18/18/18	0/3/3/3
46	3PE	H	601	-	-	20/39/39/54	-
46	3PE	Y	202	-	-	18/47/47/54	-
46	3PE	h	202	-	-	21/42/42/54	-
51	CDL	N	902	-	-	43/95/95/110	-
45	PC1	M	605	-	-	18/52/52/57	-
46	3PE	b	101	-	-	17/40/40/54	-
51	CDL	r	201	-	-	28/74/74/110	-
46	3PE	g	201	-	-	17/39/39/54	-
46	3PE	A	302	-	-	19/50/50/54	-
47	SF4	G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GTP	O	401	54	-	3/18/38/38	0/3/3/3
46	3PE	O	403	-	-	22/39/39/54	-
46	3PE	K	101	-	-	22/46/46/54	-
47	SF4	B	201	2	-	-	0/6/5/5
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	f	101	-	-	17/34/34/54	-
51	CDL	X	201	-	-	48/96/96/110	-
46	3PE	M	602	-	-	29/54/54/54	-
55	NDP	P	501	-	-	10/30/77/77	0/5/5/5
51	CDL	d	204	-	-	36/75/75/110	-
46	3PE	N	901	-	-	17/54/54/54	-

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	11.90	1.81	1.59
52	L	705	CHD	C11-C12	8.33	1.67	1.53
53	O	401	GTP	O6-C6	8.17	1.39	1.23
52	L	705	CHD	C16-C15	6.86	1.72	1.54
52	L	705	CHD	C8-C9	5.86	1.65	1.53

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	L	705	CHD	C4-C5-C10	9.32	122.56	112.66
55	P	501	NDP	PN-O3-PA	-6.89	109.17	132.83
52	L	705	CHD	C11-C9-C8	6.45	120.31	110.88
57	T	101	EHZ	C8-C9-S1	6.18	121.27	113.63
52	L	705	CHD	C11-C9-C10	5.62	119.52	113.73

There are no chirality outliers.

5 of 983 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	PC1	O21-C2-C3-O31
45	B	202	PC1	C22-C21-O21-C2
45	M	603	PC1	C11-O13-P-O12
45	M	603	PC1	C11-O13-P-O14
45	M	603	PC1	C2-C1-O11-P

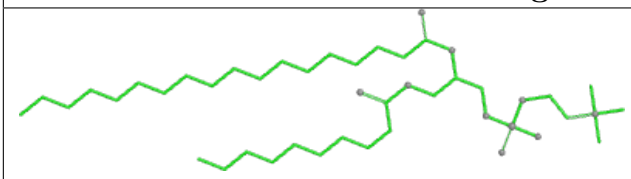
There are no ring outliers.

18 monomers are involved in 31 short contacts:

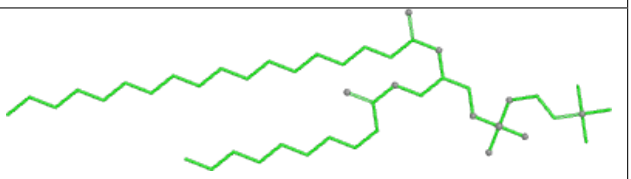
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	F	502	SF4	1	0
45	J	201	PC1	3	0
45	B	202	PC1	1	0
46	L	704	3PE	1	0
46	M	604	3PE	2	0
57	T	101	EHZ	1	0
46	I	201	3PE	2	0
46	M	601	3PE	3	0
51	L	702	CDL	1	0
52	L	705	CHD	2	0
46	Y	205	3PE	1	0
49	F	501	FMN	2	0
51	N	902	CDL	1	0
45	M	605	PC1	4	0
53	O	401	GTP	5	0
46	K	101	3PE	1	0
46	M	602	3PE	1	0
46	N	901	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.

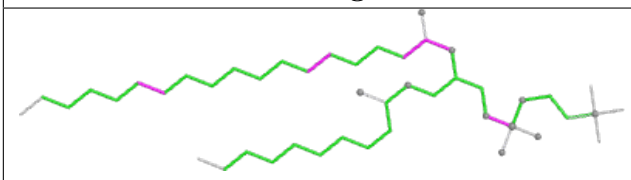
Ligand PC1 J 201



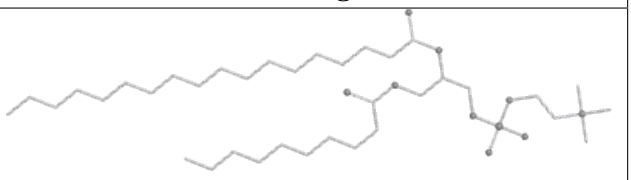
Bond lengths



Bond angles

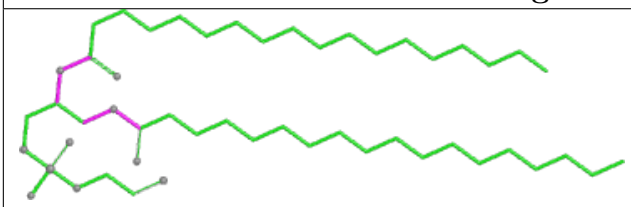


Torsions

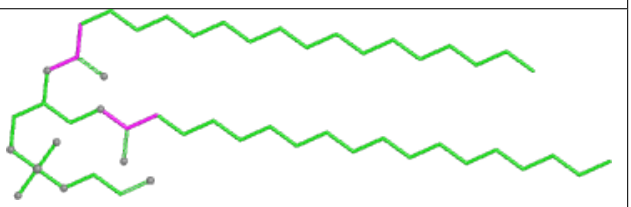


Rings

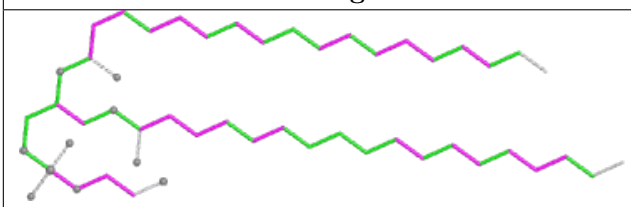
Ligand 3PE b 102



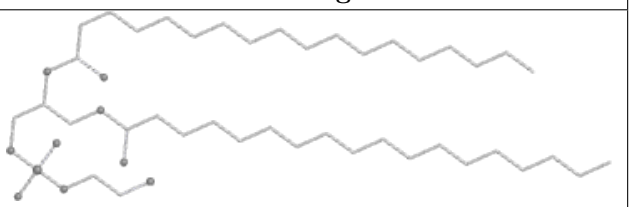
Bond lengths



Bond angles

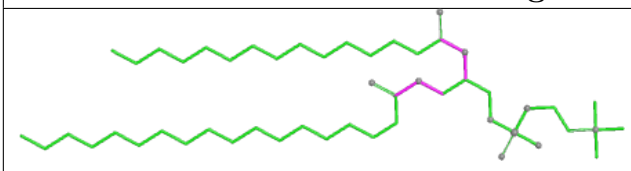


Torsions

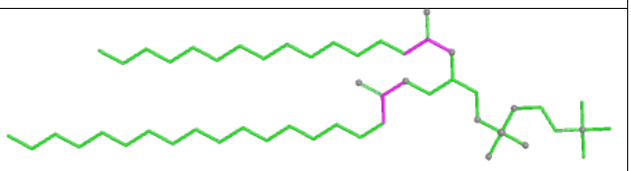


Rings

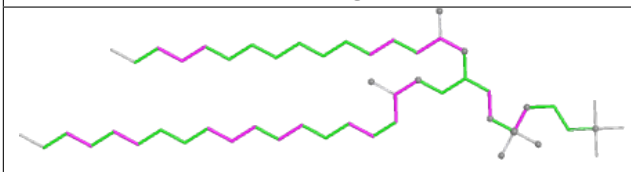
Ligand PC1 B 202



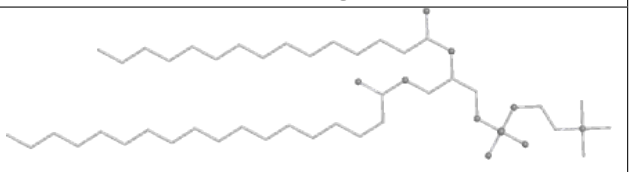
Bond lengths



Bond angles

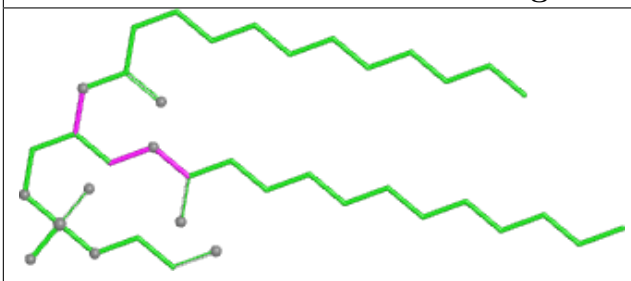


Torsions

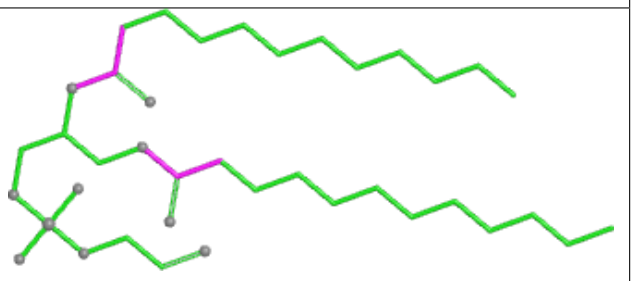


Rings

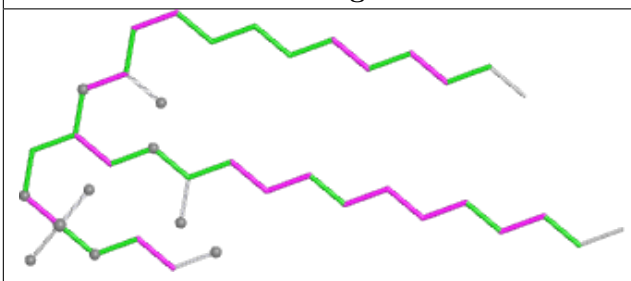
Ligand 3PE L 701



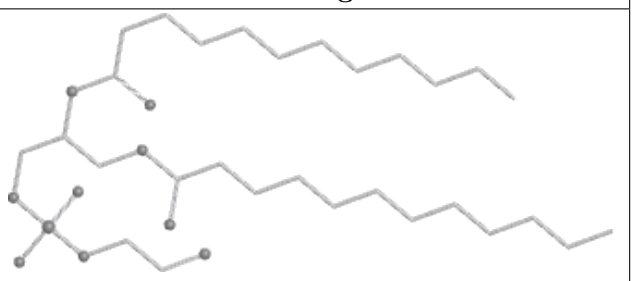
Bond lengths



Bond angles

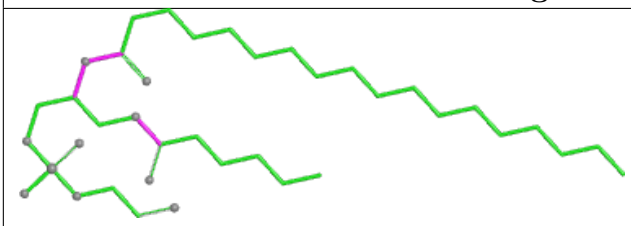


Torsions

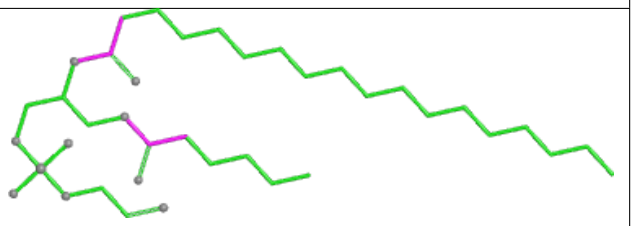


Rings

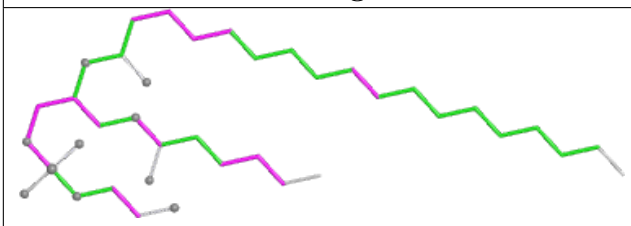
Ligand 3PE L 704



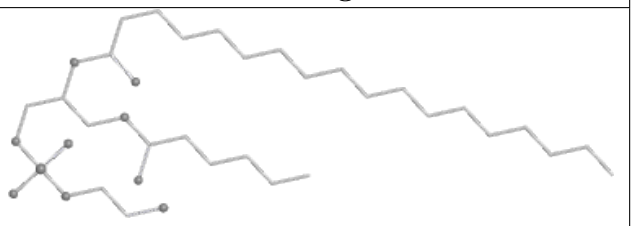
Bond lengths



Bond angles



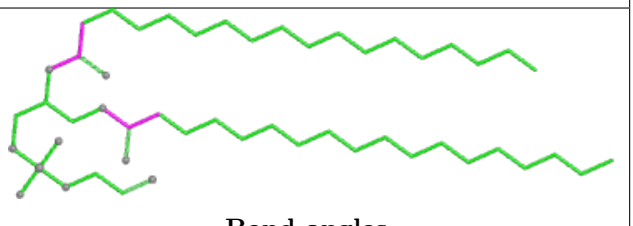
Torsions



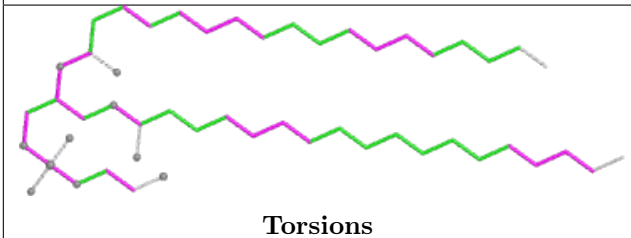
Rings

Ligand 3PE M 604

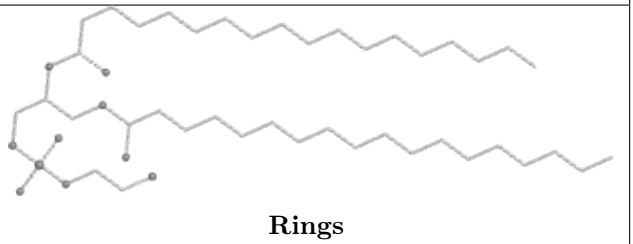
Bond lengths



Bond angles

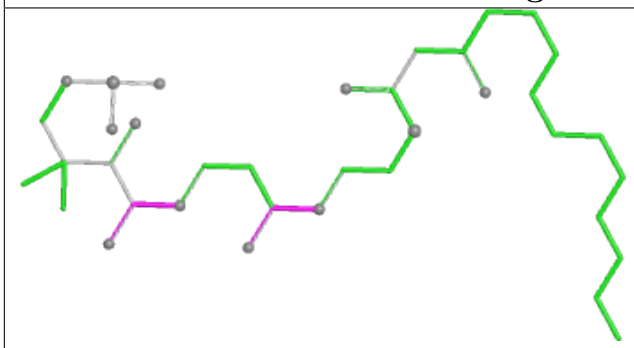


Torsions

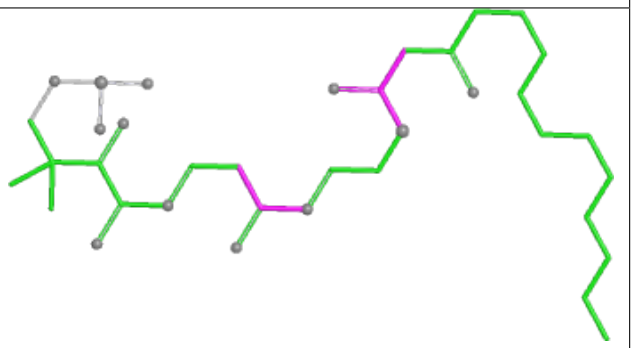


Rings

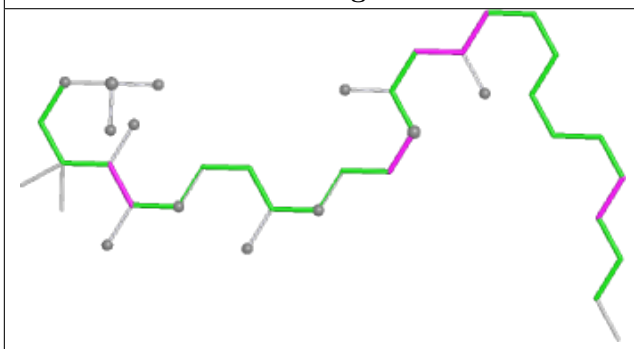
Ligand EHZ T 101



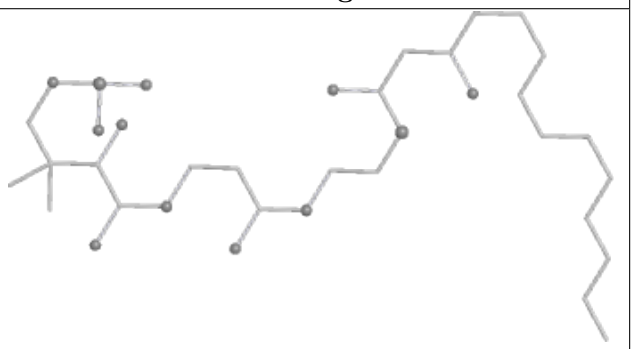
Bond lengths



Bond angles

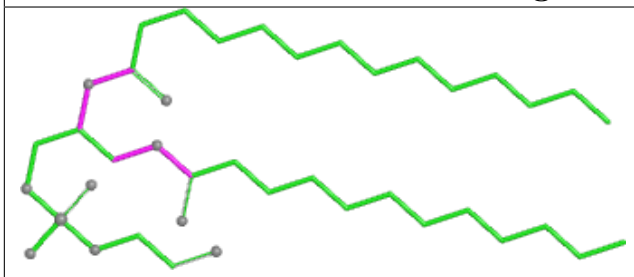


Torsions



Rings

Ligand 3PE d 201



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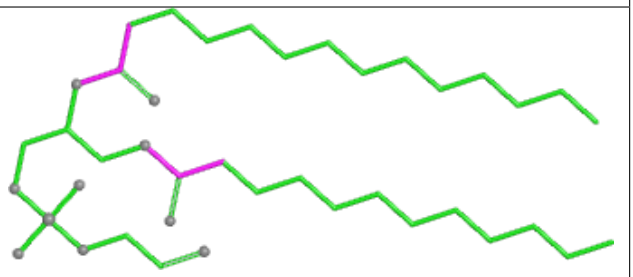

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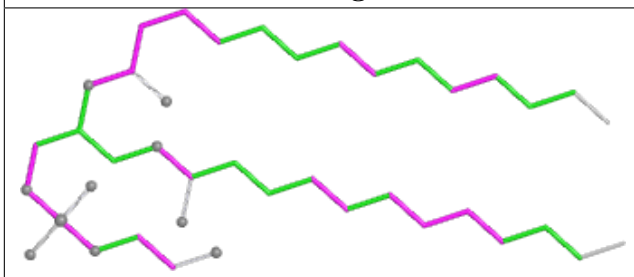

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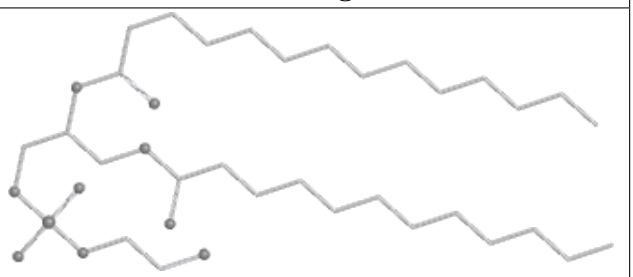
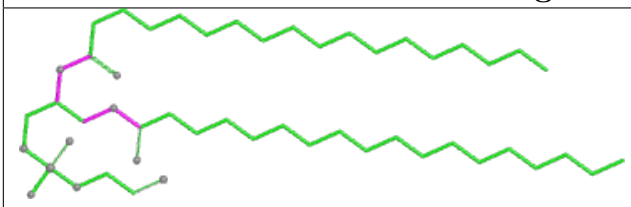


Rings

Ligand 3PE I 201



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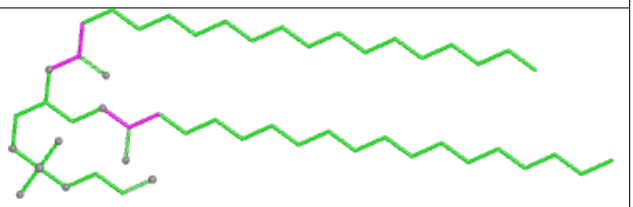

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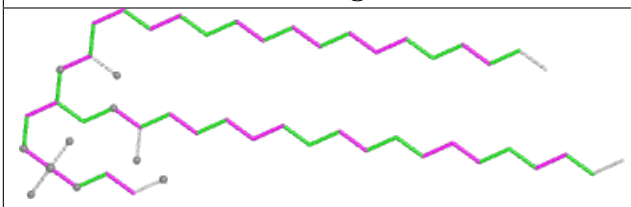

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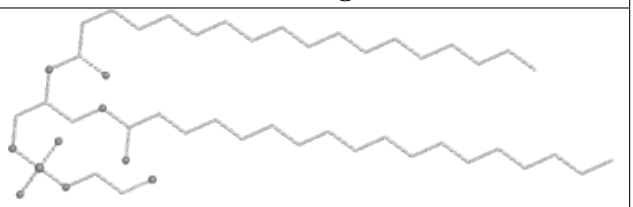

Rings

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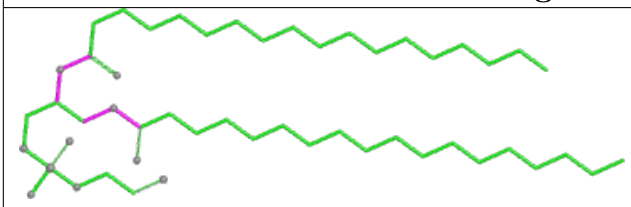

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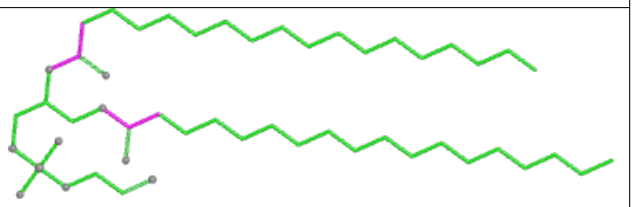

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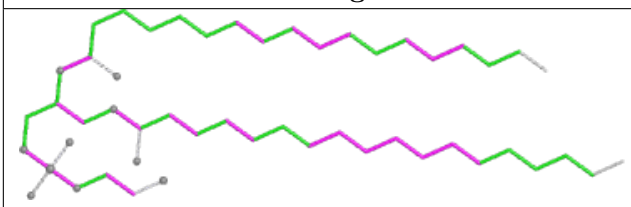

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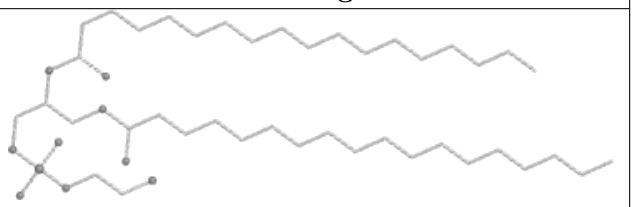
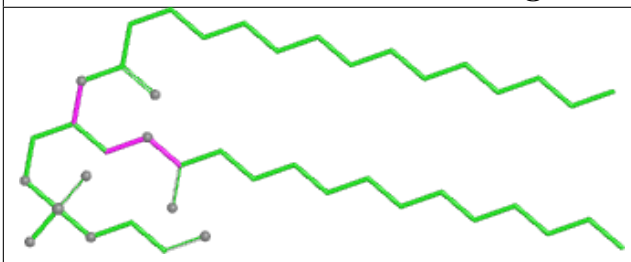


Rings

Ligand 3PE M 601



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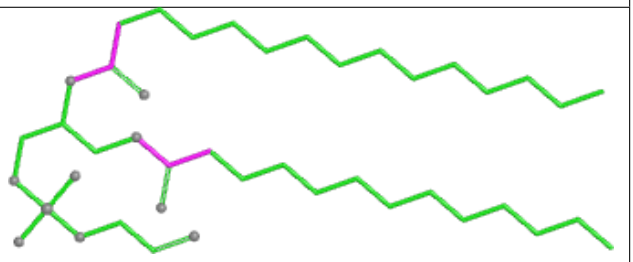
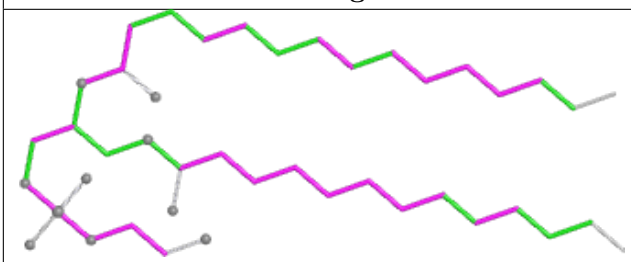


Bond angles



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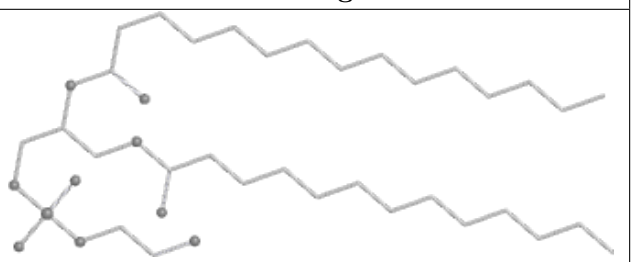
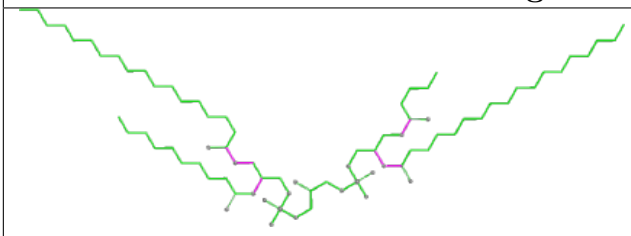


Rings

Ligand CDL L 702



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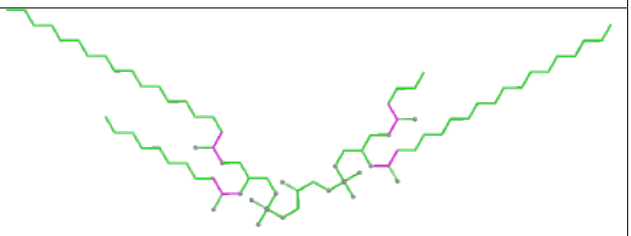

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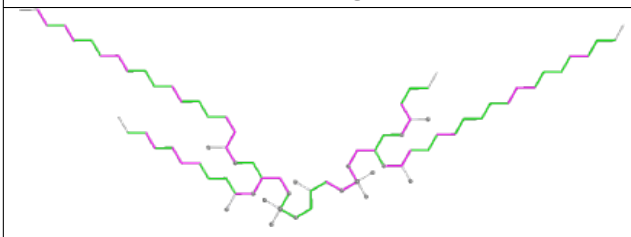

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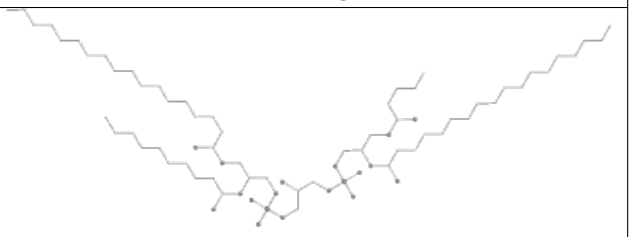
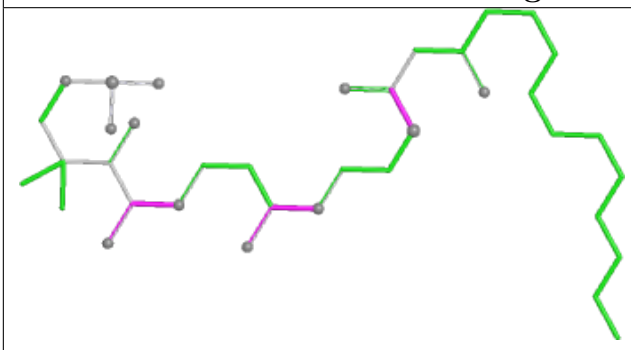


Rings

Ligand EHZ U 101



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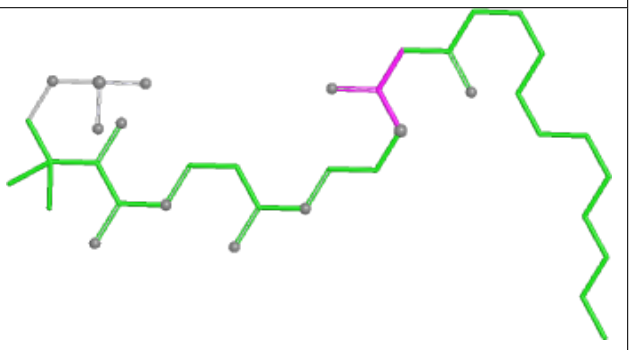
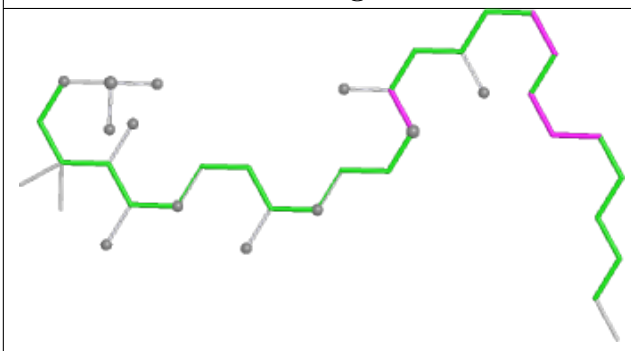


Bond angles



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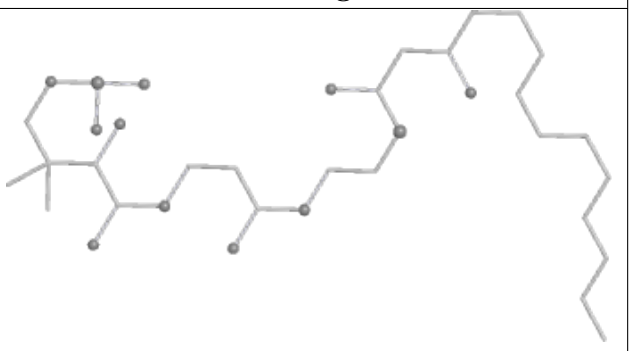

Rings

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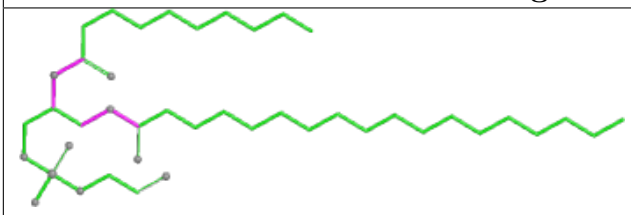
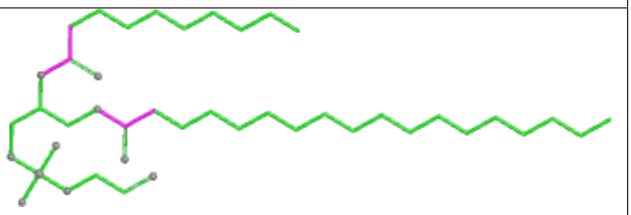
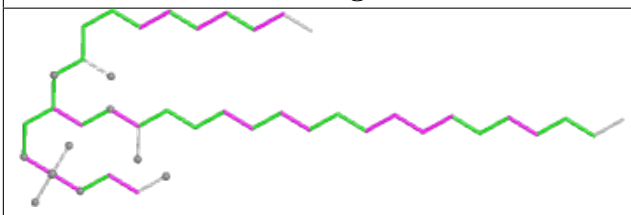
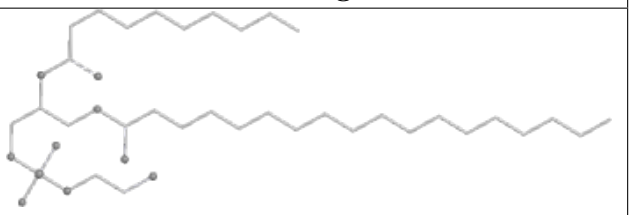
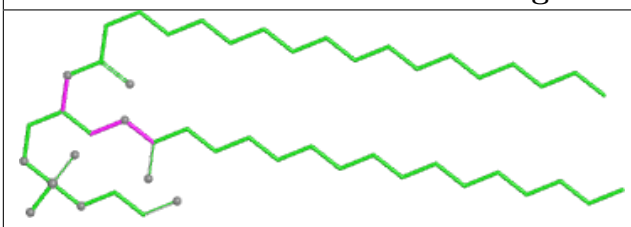
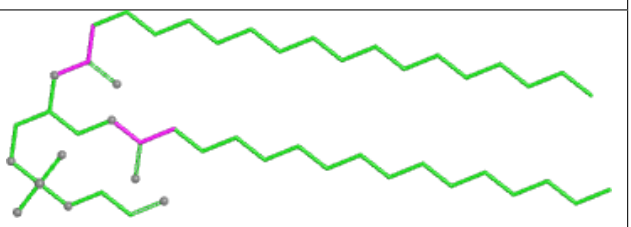
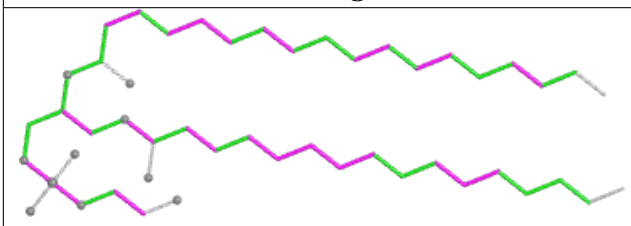
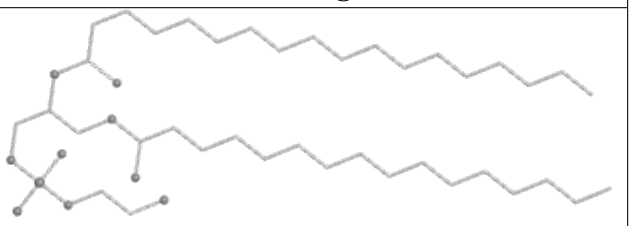
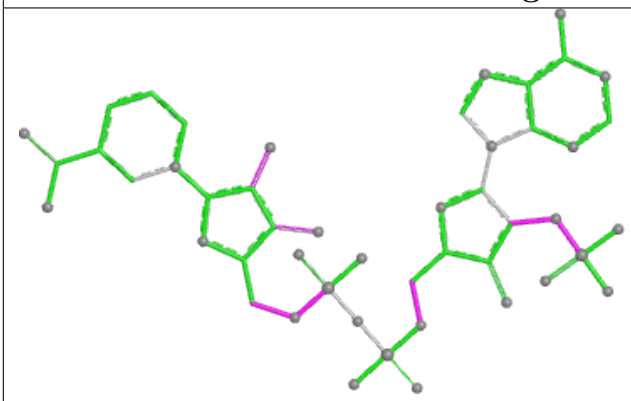
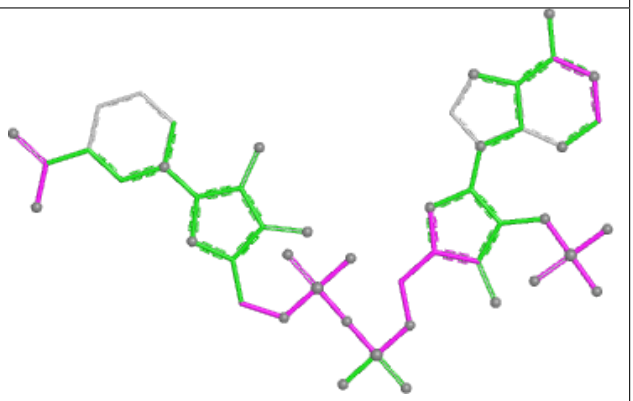
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE d 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

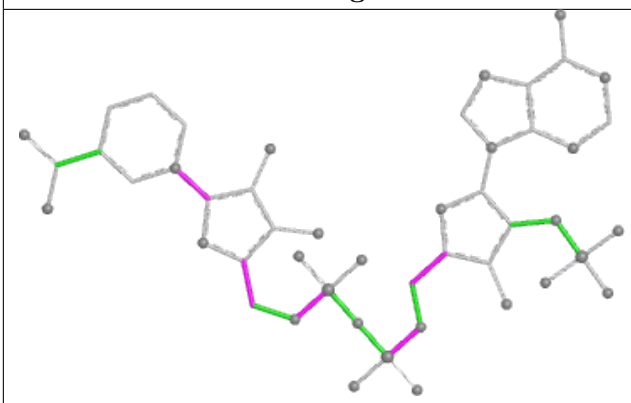
Ligand NDP P 501



Bond lengths



Bond angles



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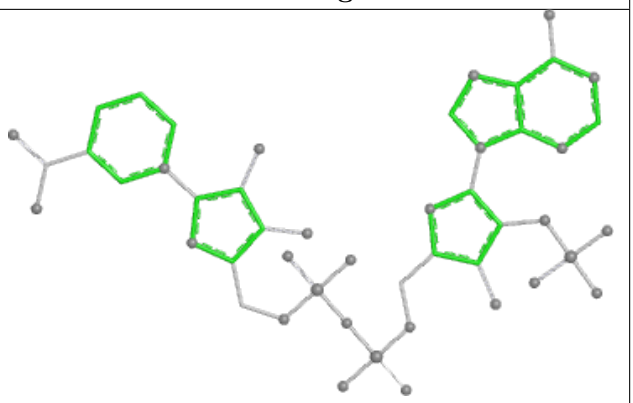
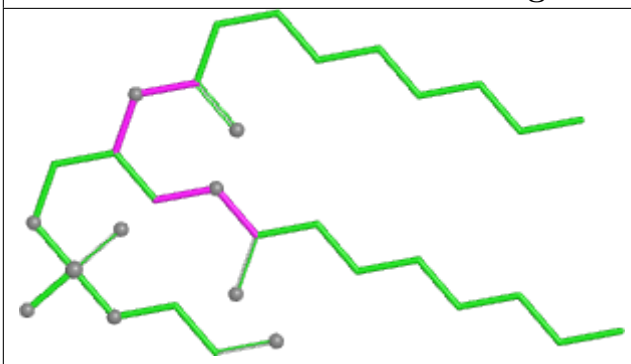
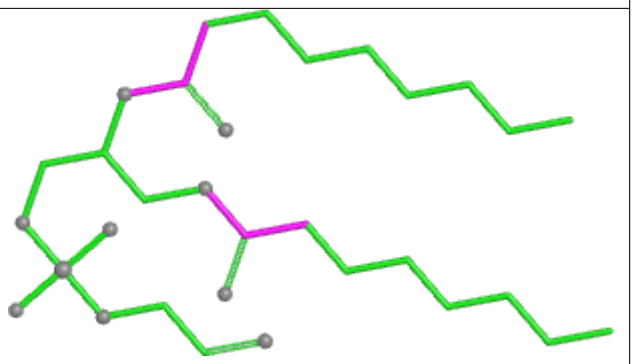


Rings

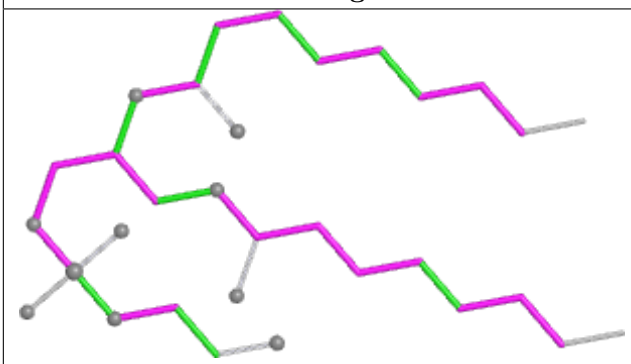
Ligand 3PE Y 204



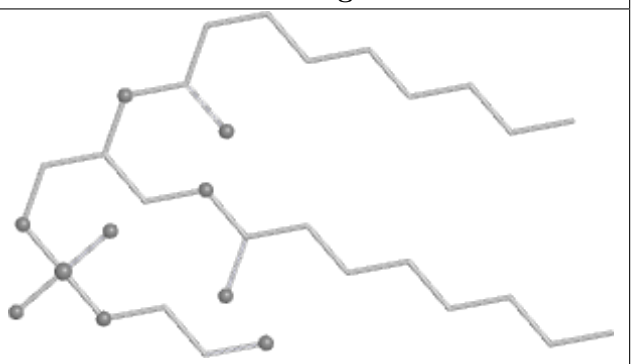
Bond lengths



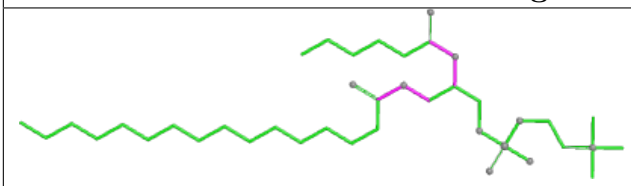
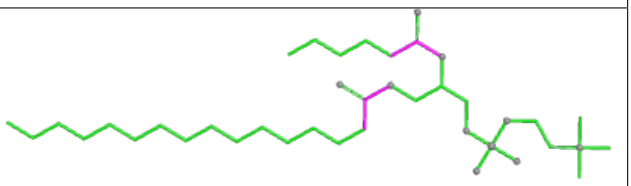
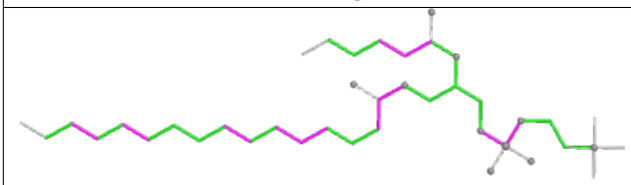
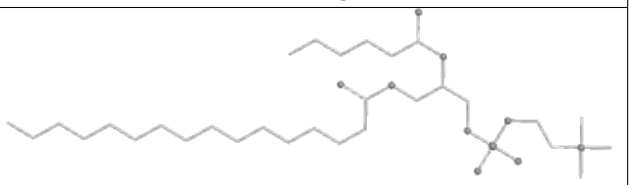
Bond angles

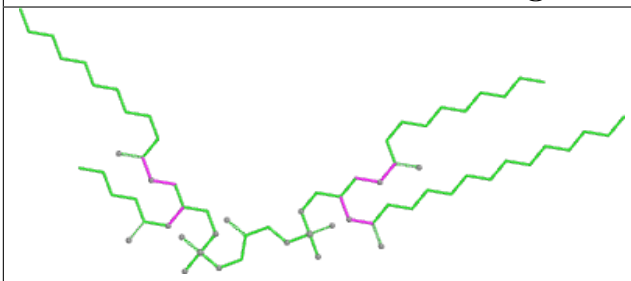
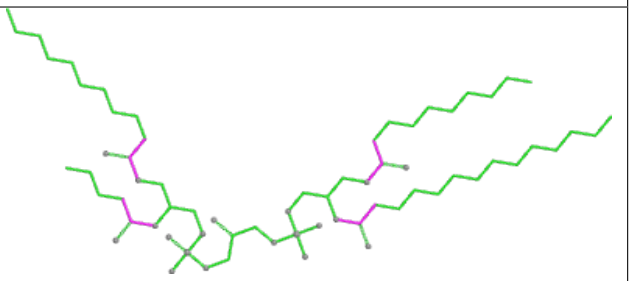
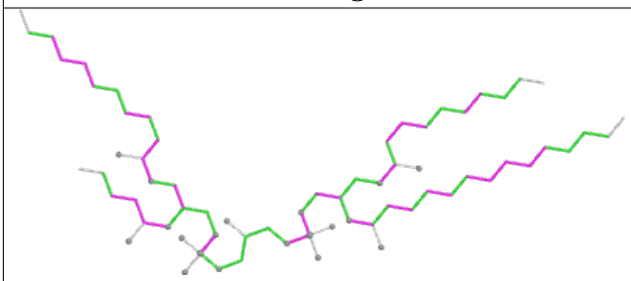
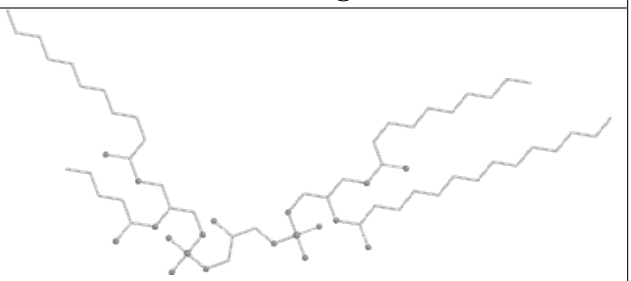


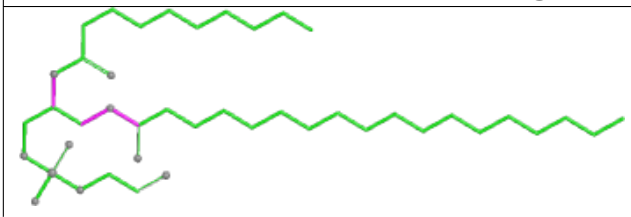
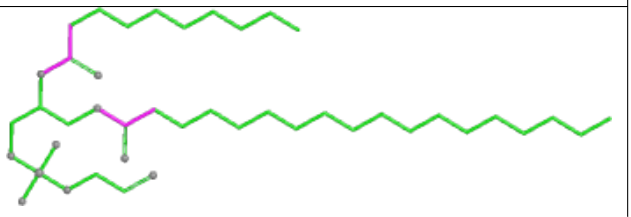
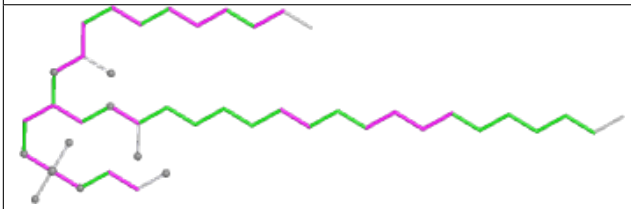
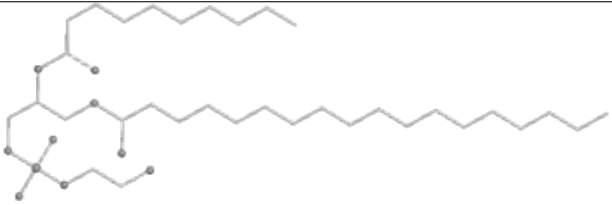
Torsions



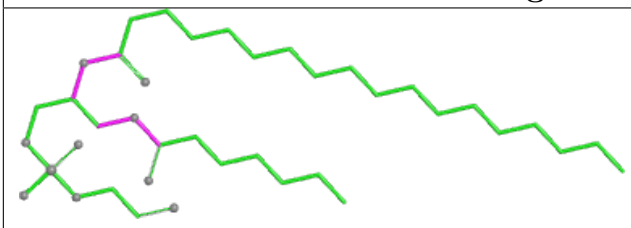
Rings

Ligand PC1 d 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

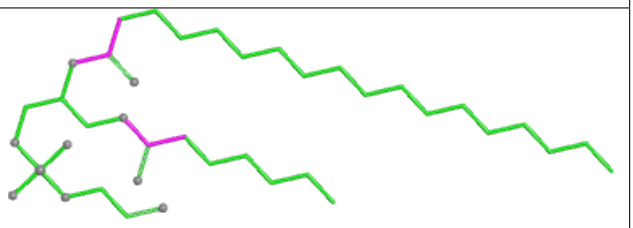
Ligand CDL h 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

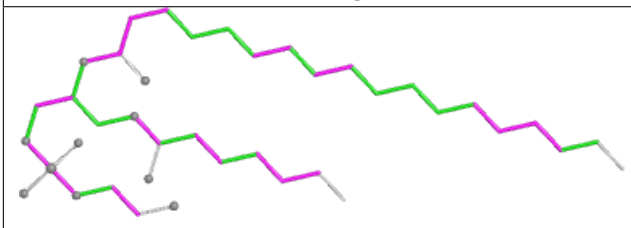
Ligand 3PE m 201



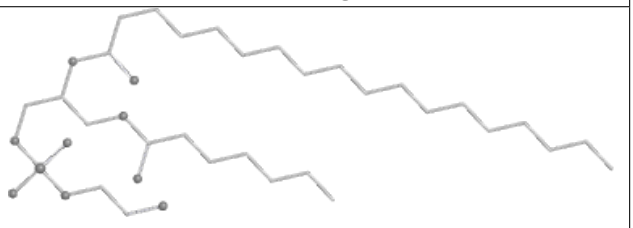
Bond lengths



Bond angles

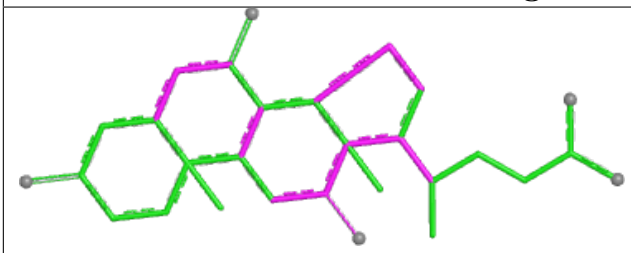


Torsions

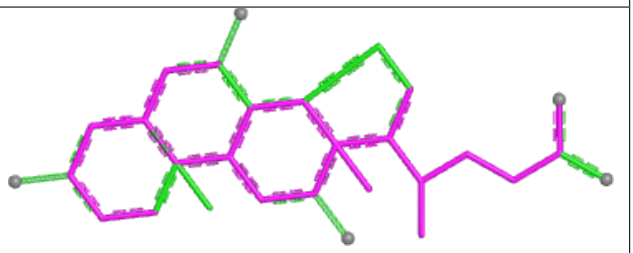


Rings

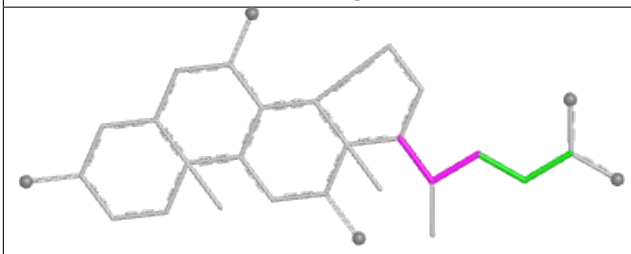
Ligand CHD L 705



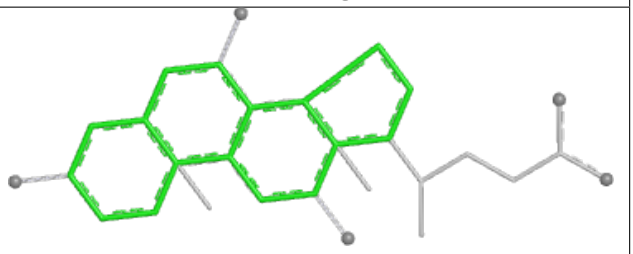
Bond lengths



Bond angles

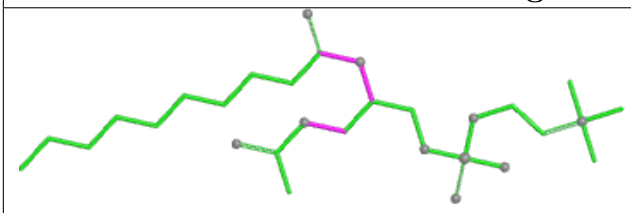


Torsions

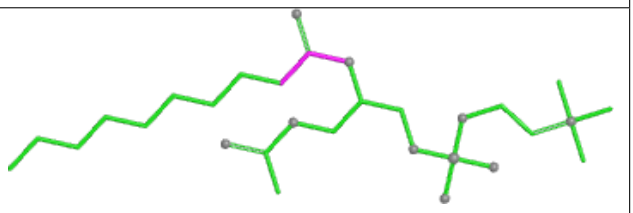


Rings

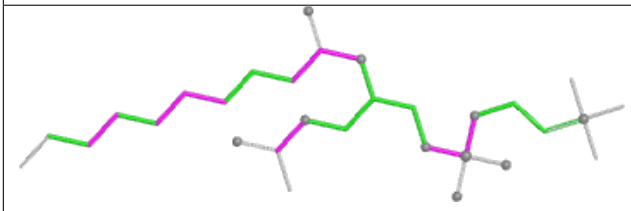
Ligand PC1 N 903



Bond lengths



Bond angles



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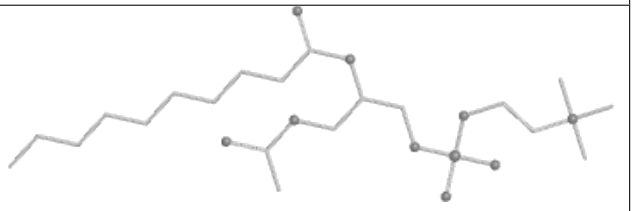
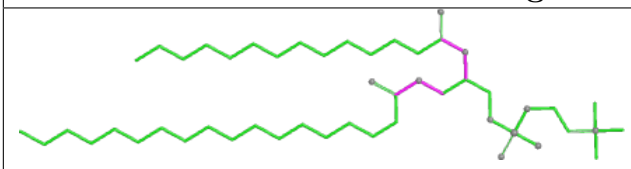
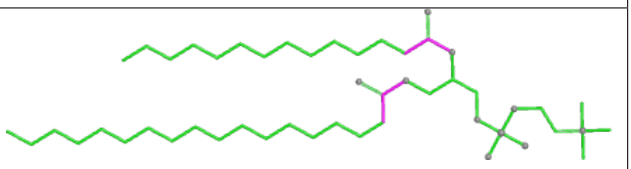
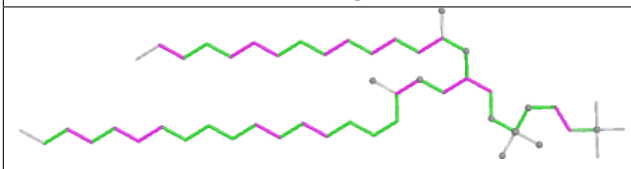
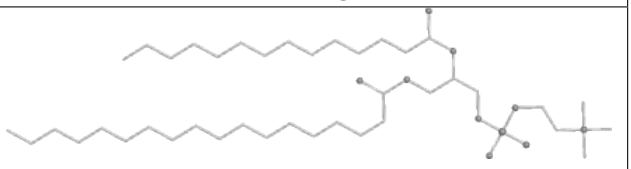
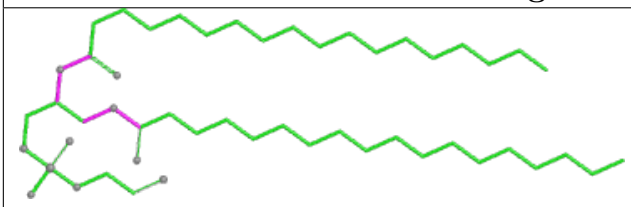
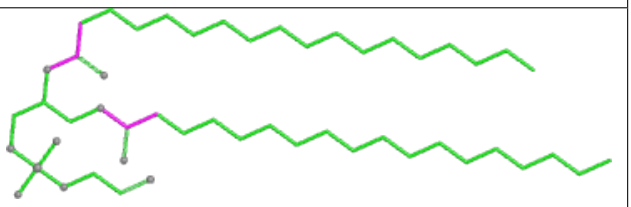
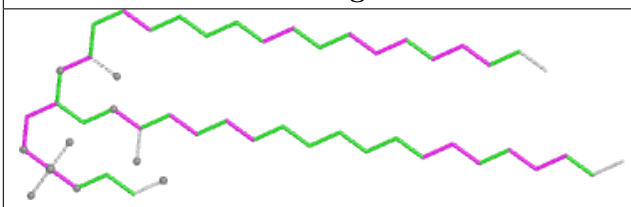
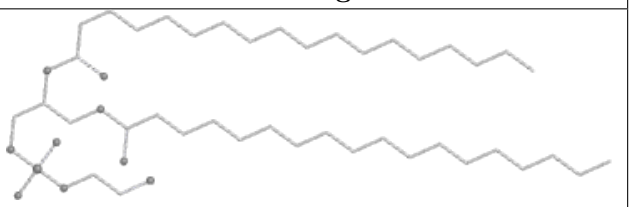
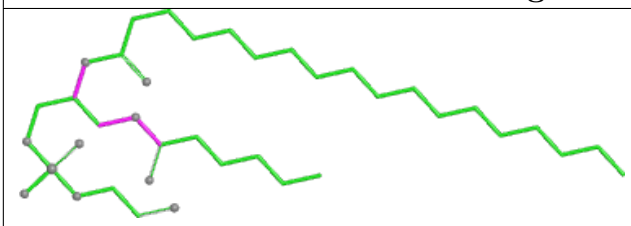
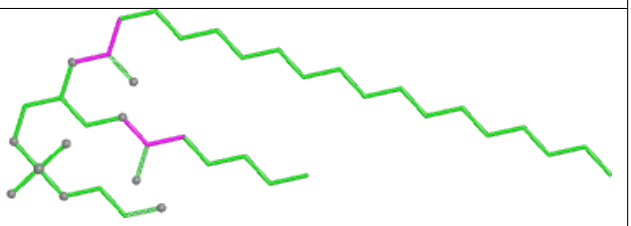
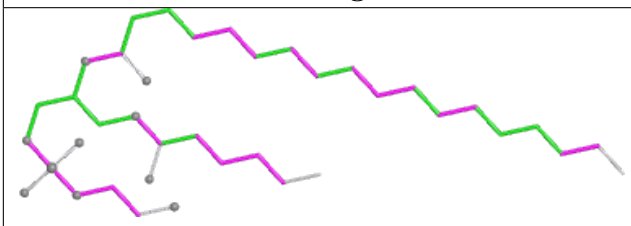
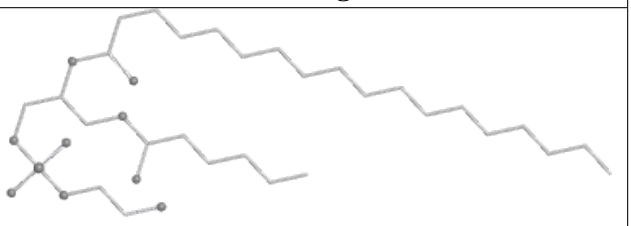


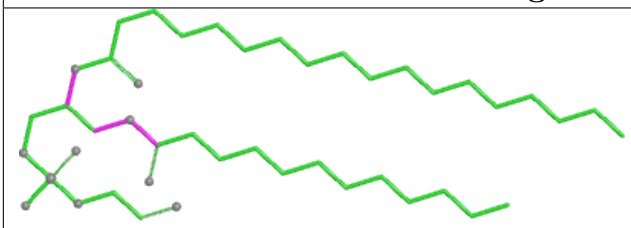
Rings

Ligand PC1 A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

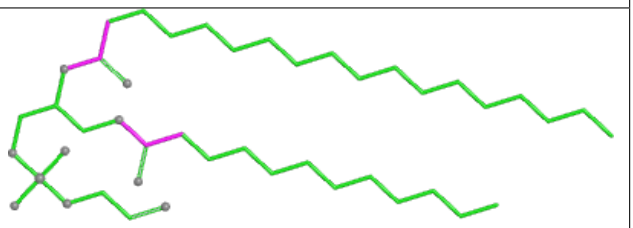
Ligand 3PE Y 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE N 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

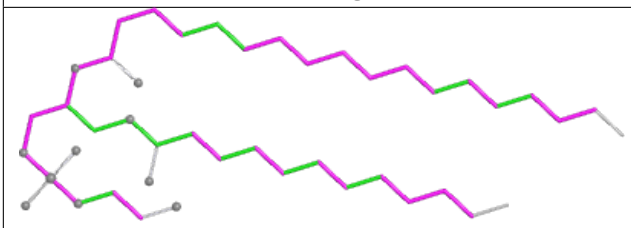
Ligand 3PE Y 205



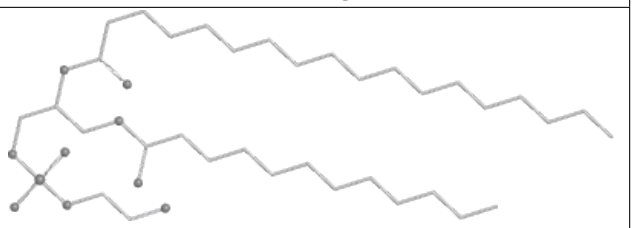
Bond lengths



Bond angles

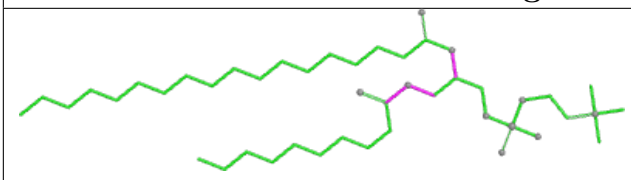


Torsions



Rings

Ligand PC1 M 603



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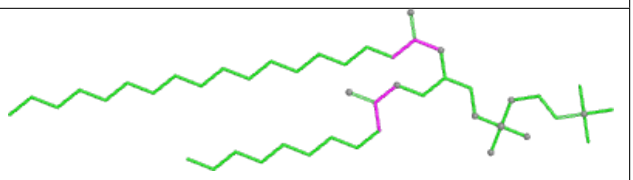
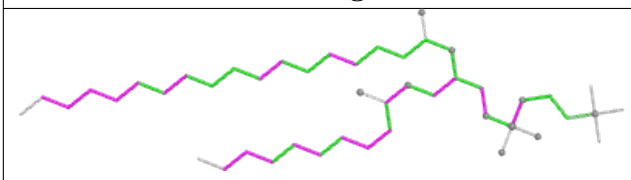


Bond angles



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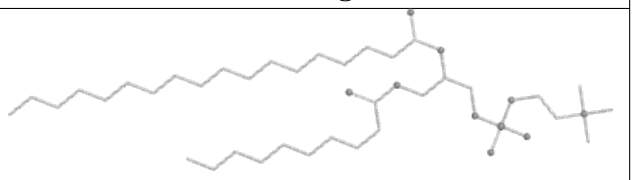
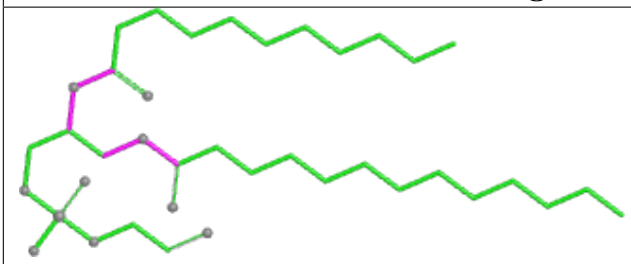
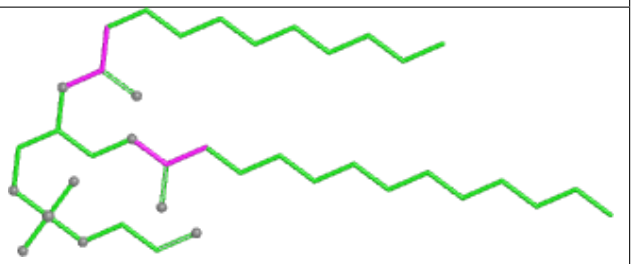


Rings

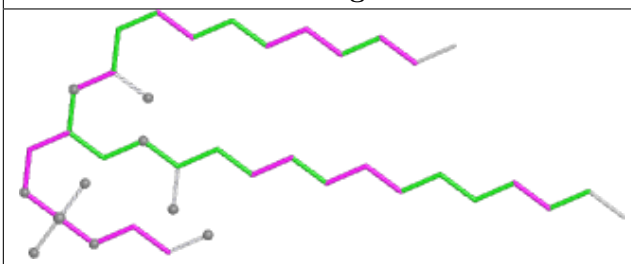
Ligand 3PE Y 203



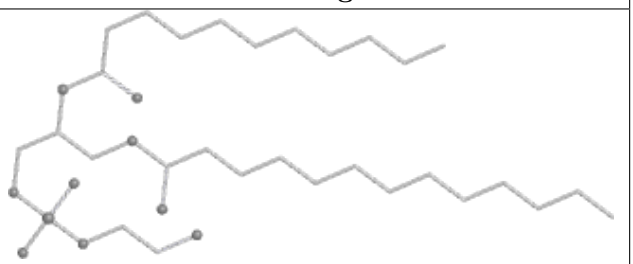
Bond lengths



Bond angles

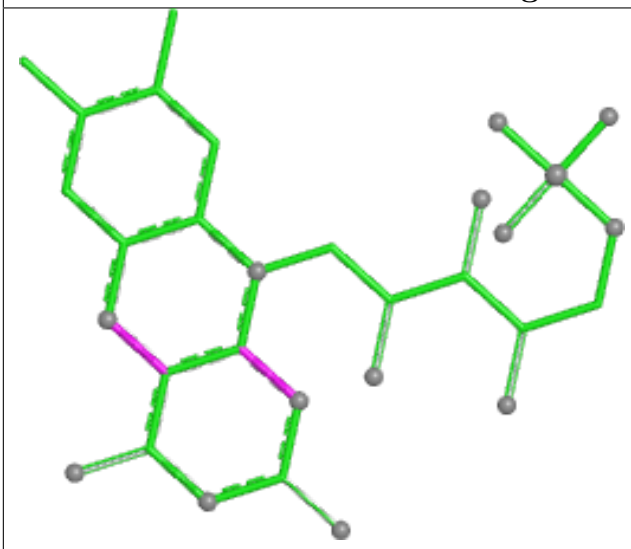


Torsions

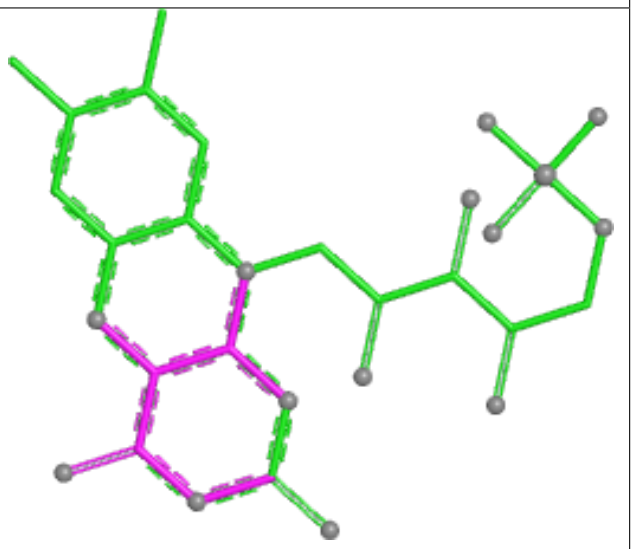


Rings

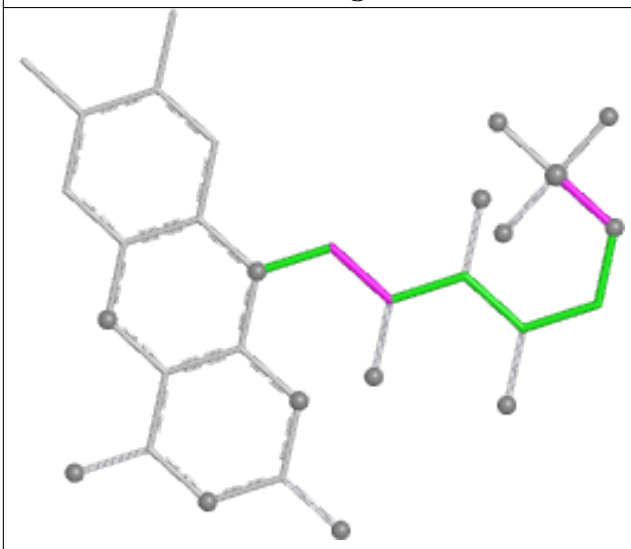
Ligand FMN F 501



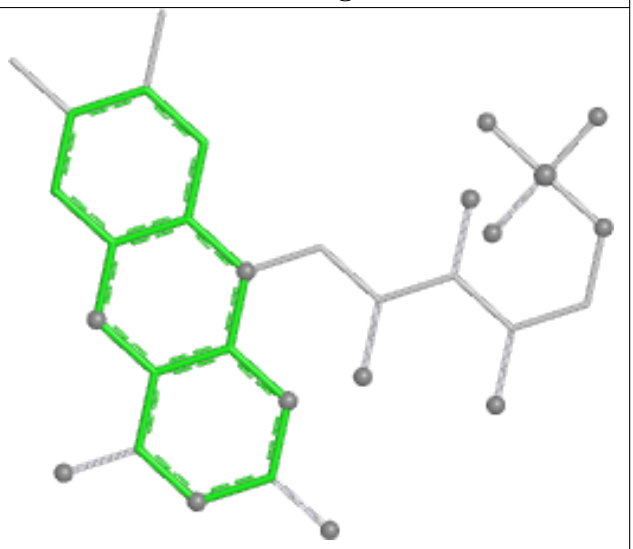
Bond lengths



Bond angles

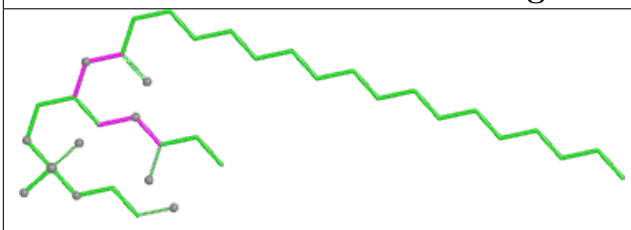


Torsions

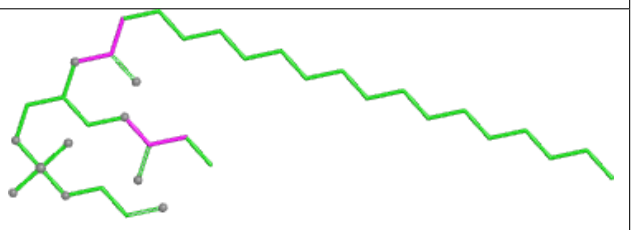


Rings

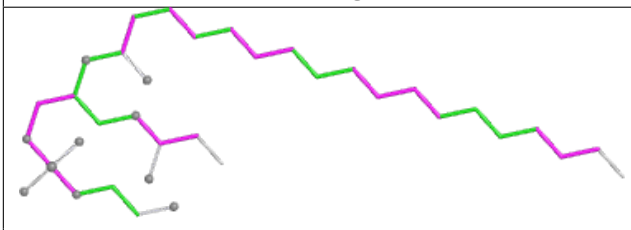
Ligand 3PE H 601



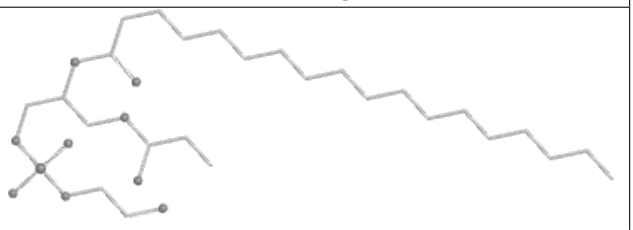
Bond lengths



Bond angles

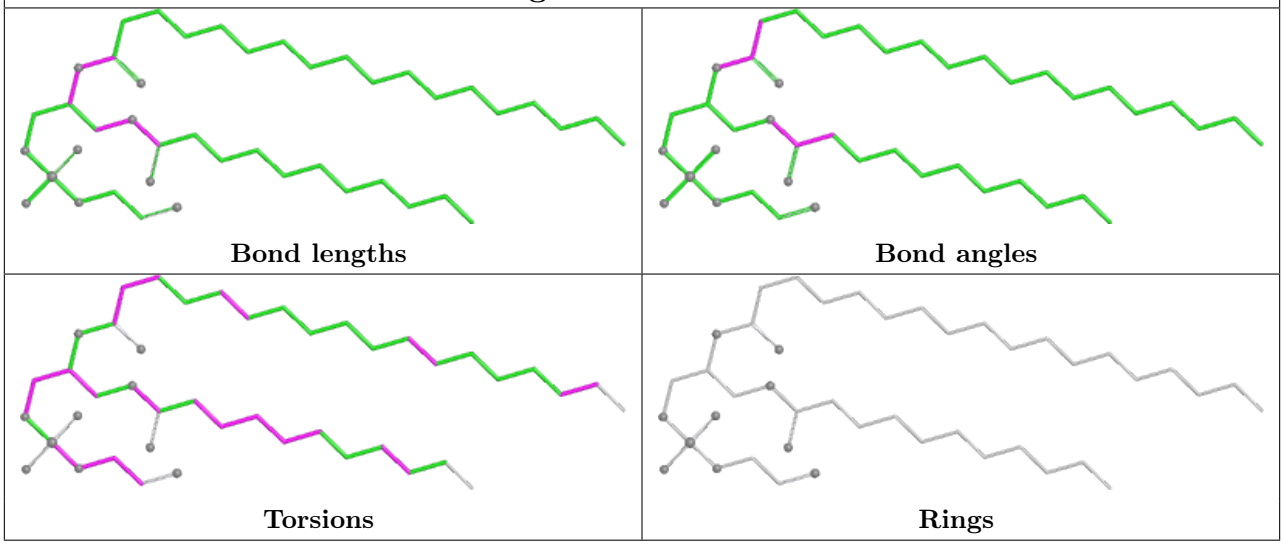


Torsions

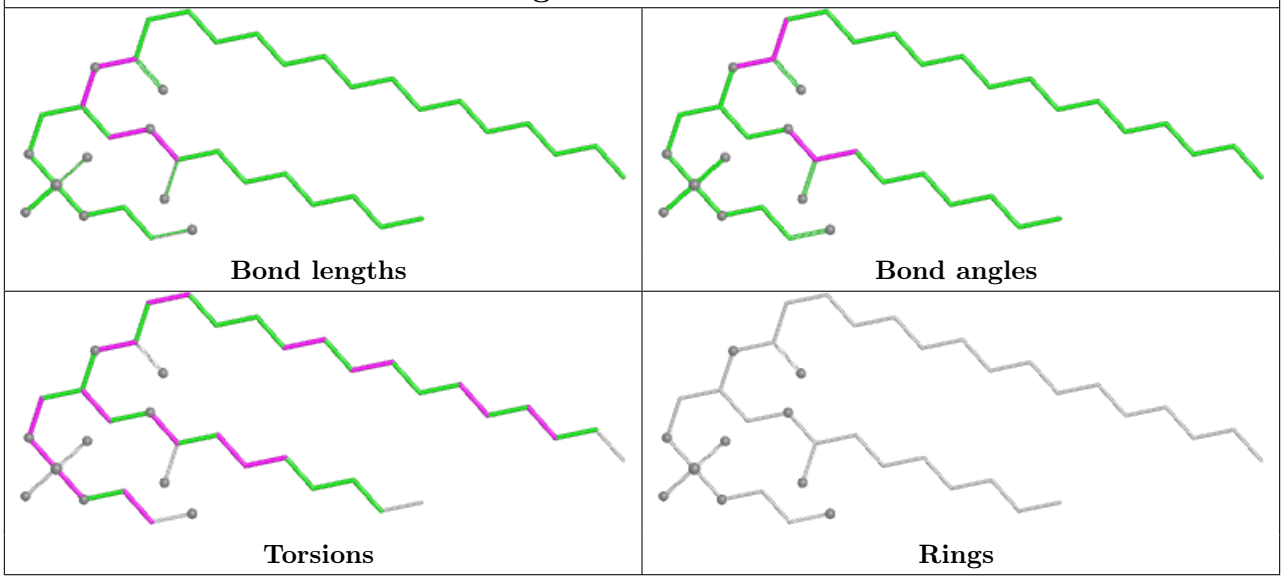


Rings

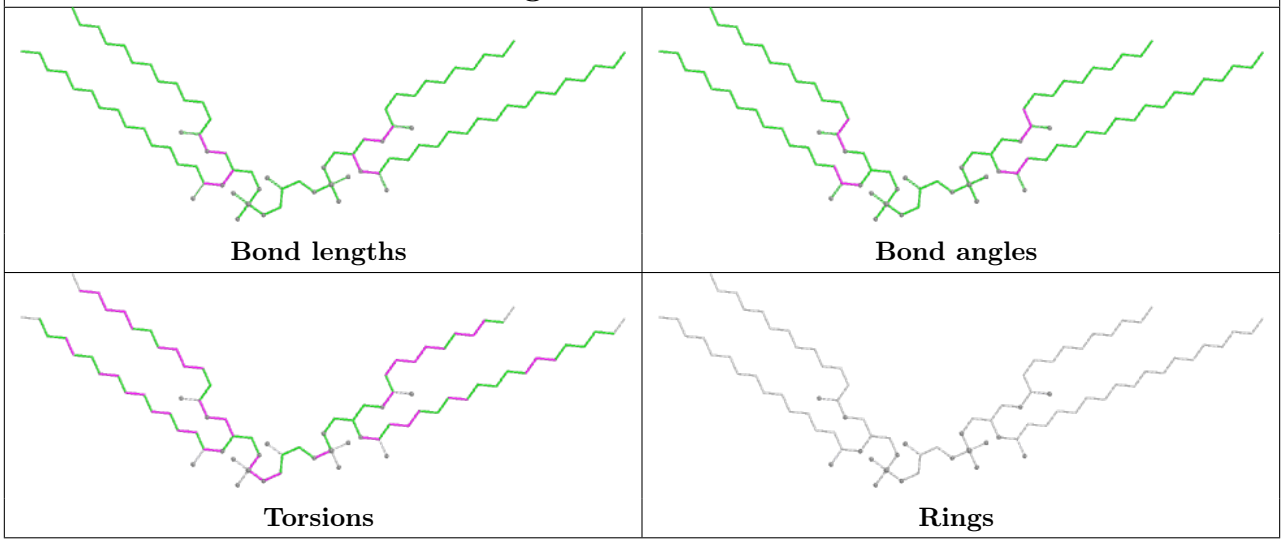
Ligand 3PE Y 202



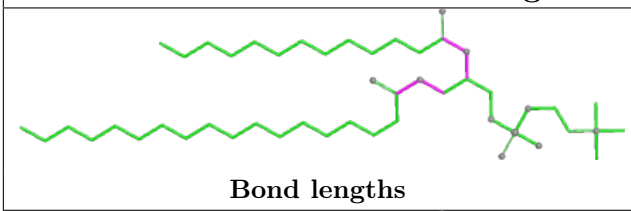
Ligand 3PE h 202



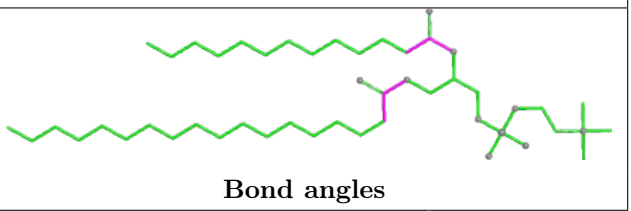
Ligand CDL N 902



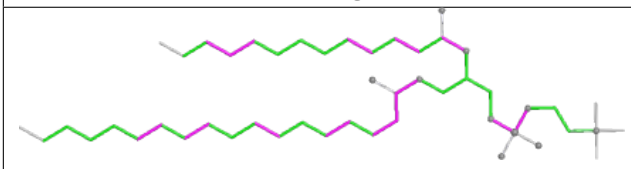
Ligand PC1 M 605



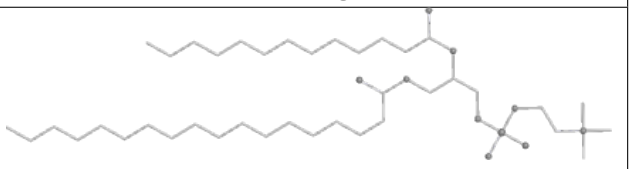
Bond lengths



Bond angles

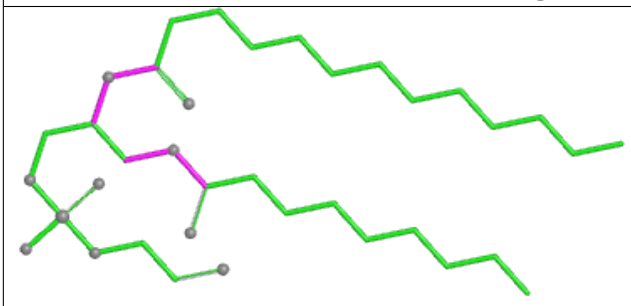


Torsions

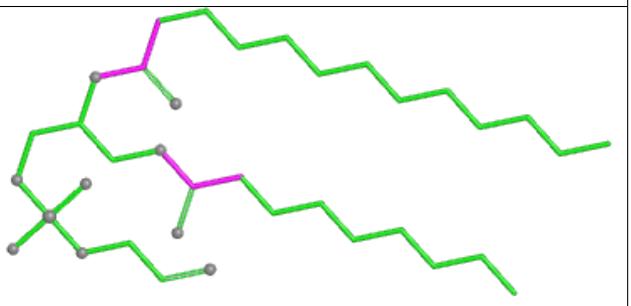


Rings

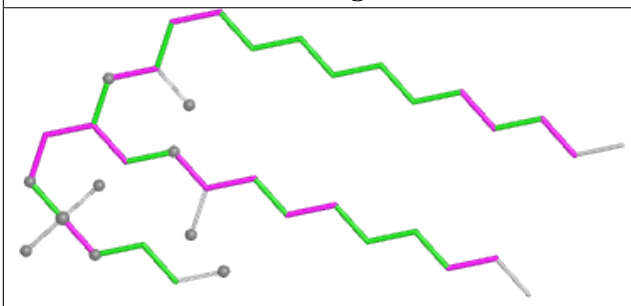
Ligand 3PE b 101



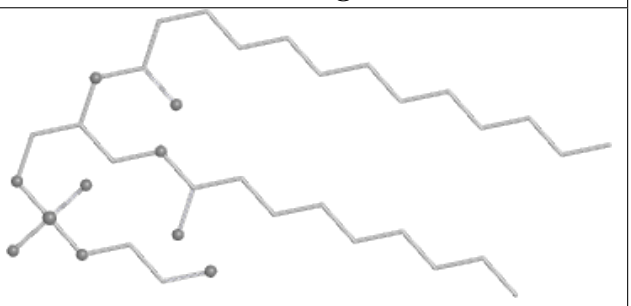
Bond lengths



Bond angles

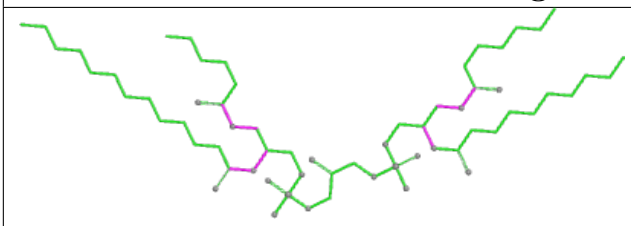


Torsions

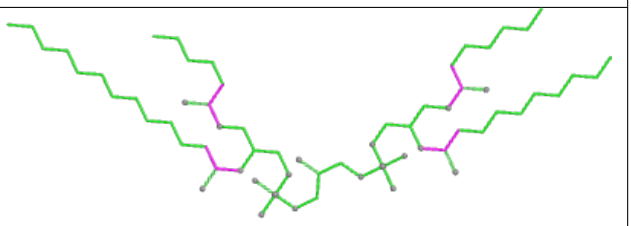


Rings

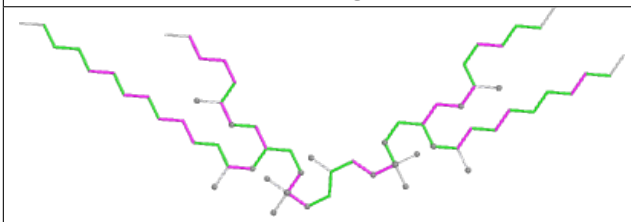
Ligand CDL r 201



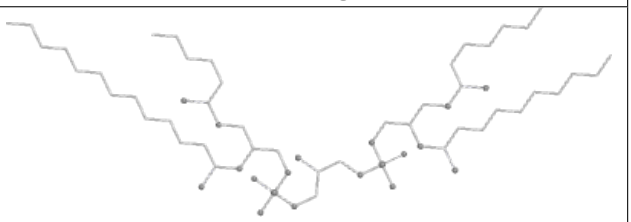
Bond lengths



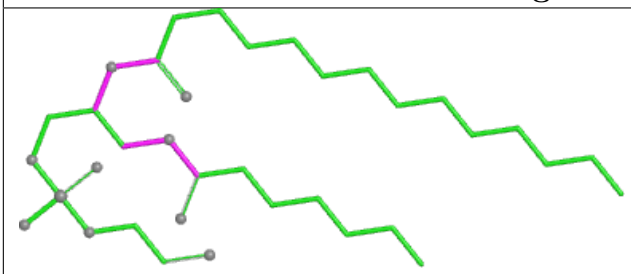
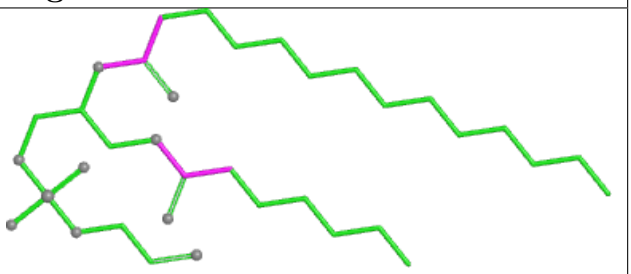
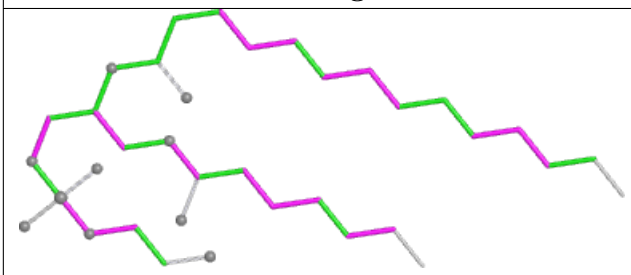
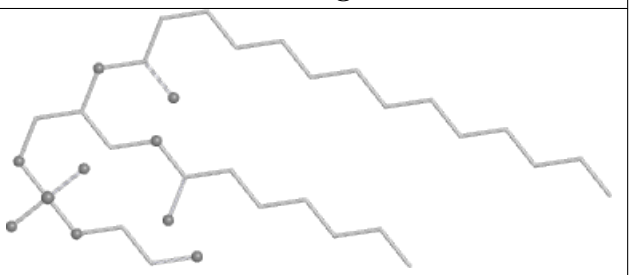
Bond angles

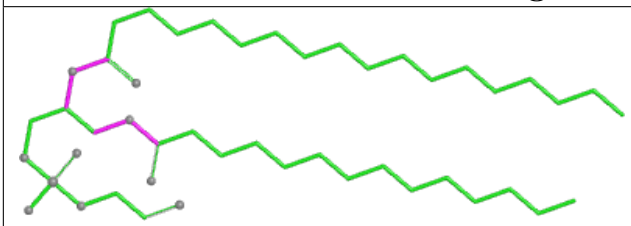
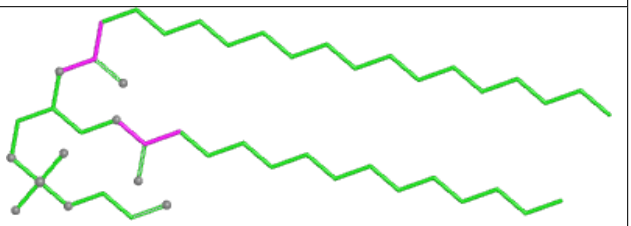
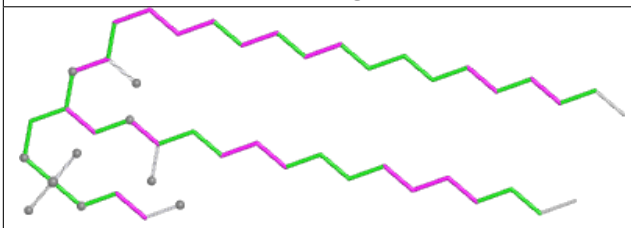
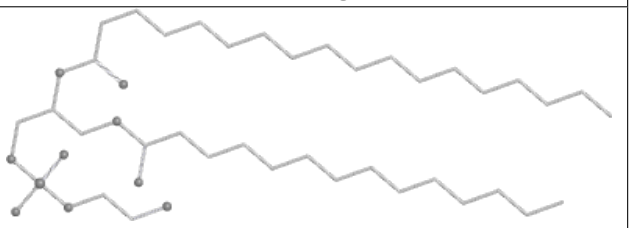


Torsions

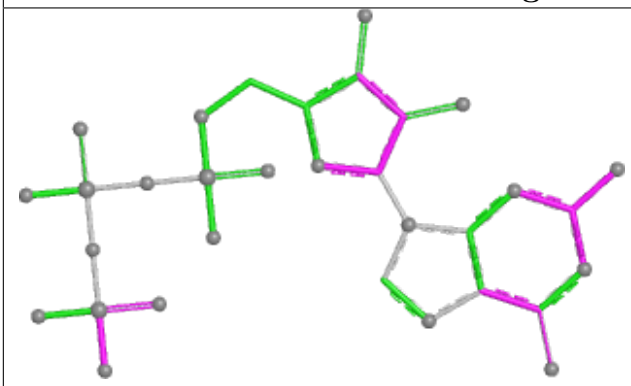


Rings

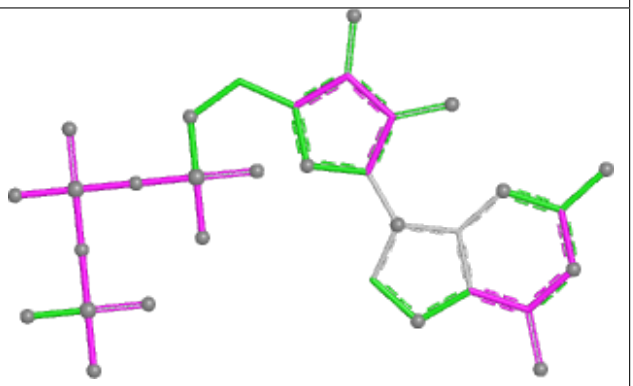
Ligand 3PE g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

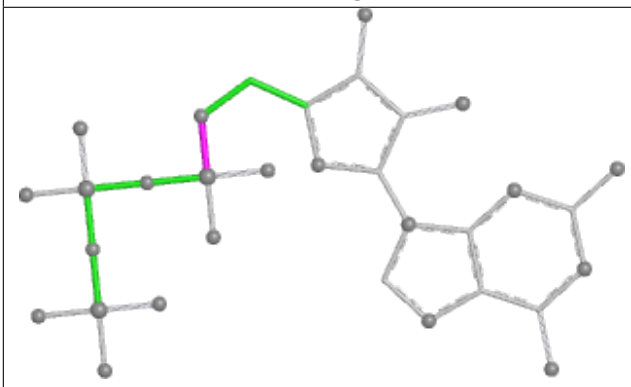
Ligand GTP O 401



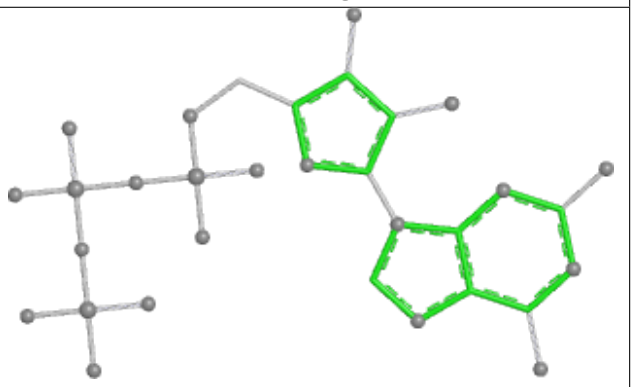
Bond lengths



Bond angles

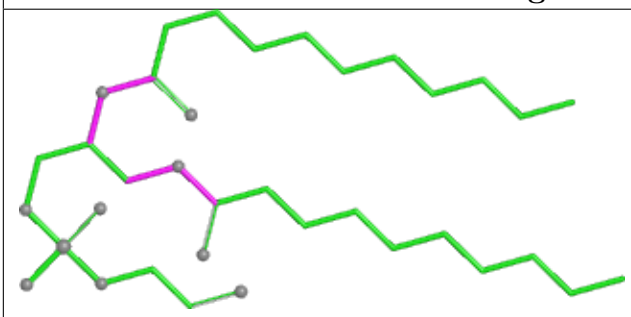


Torsions

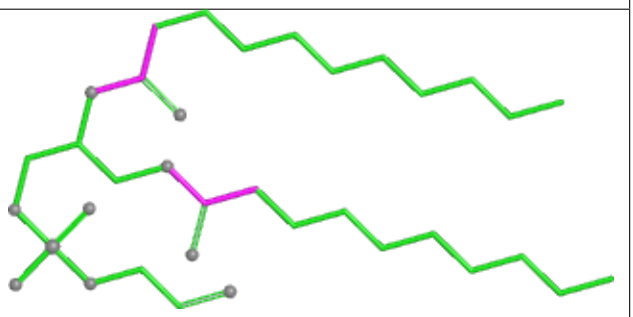


Rings

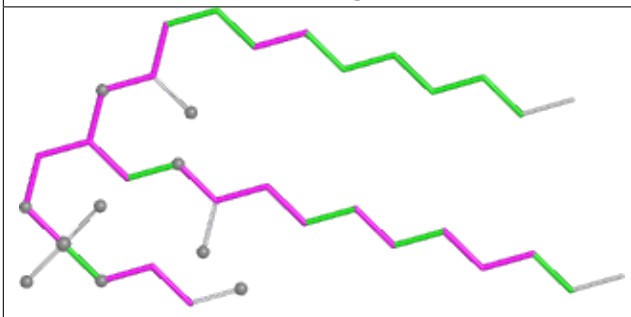
Ligand 3PE O 403



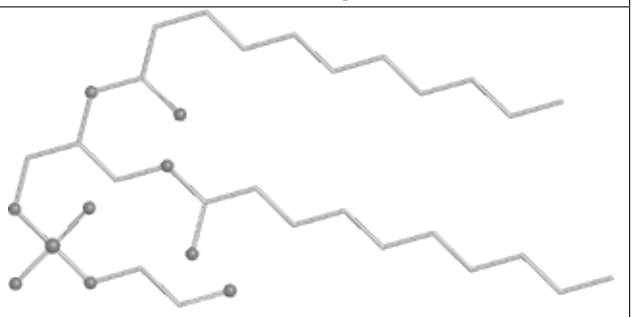
Bond lengths



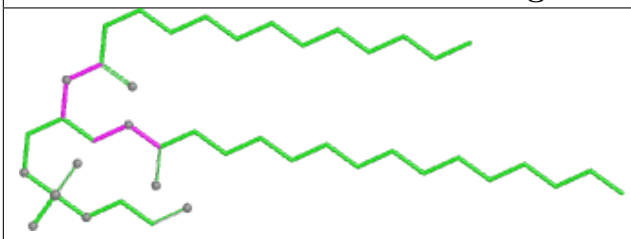
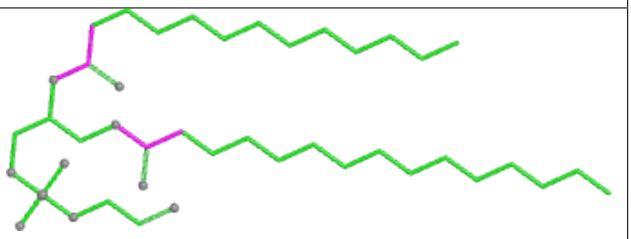
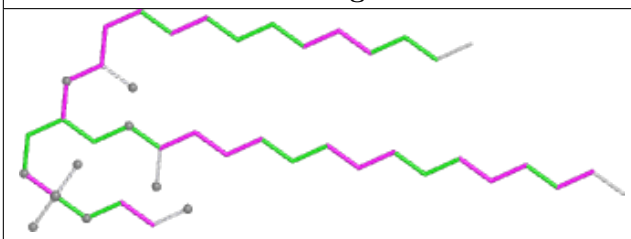
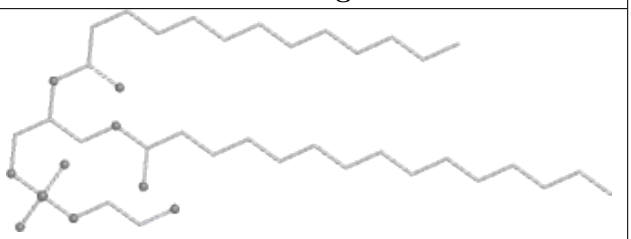
Bond angles

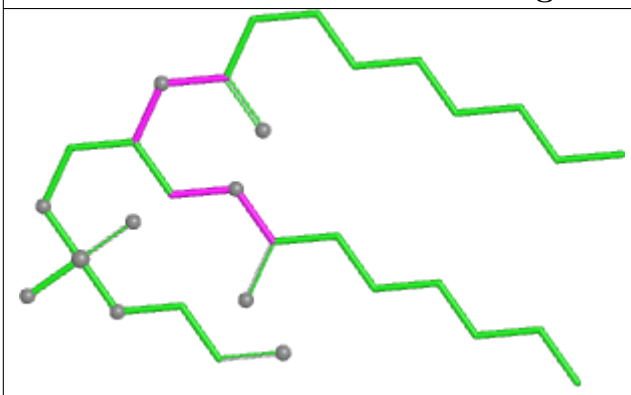
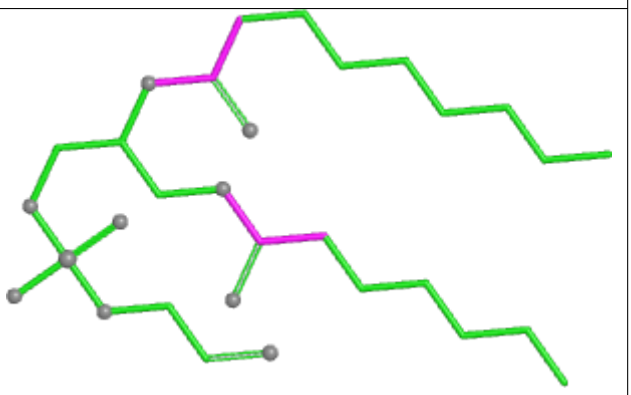
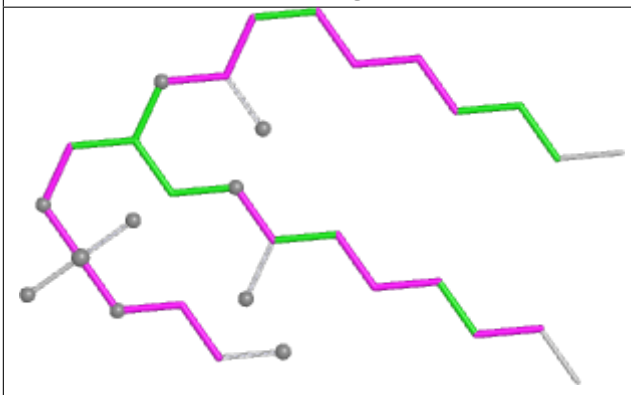
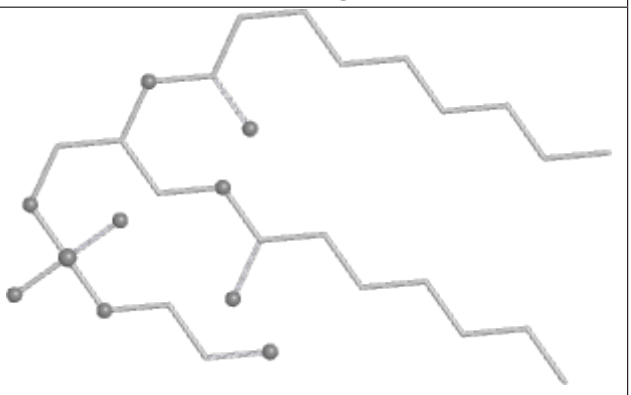


Torsions

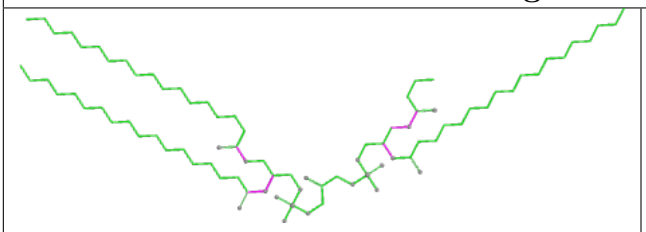


Rings

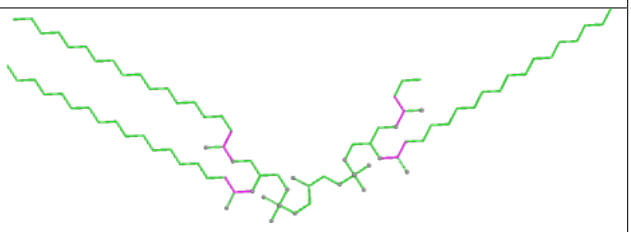
Ligand 3PE K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE f 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

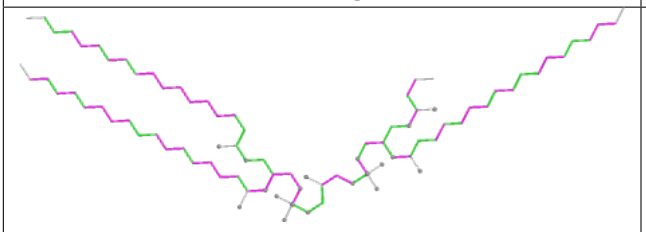
Ligand CDL X 201



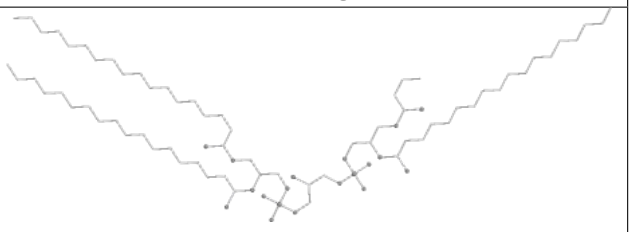
Bond lengths



Bond angles

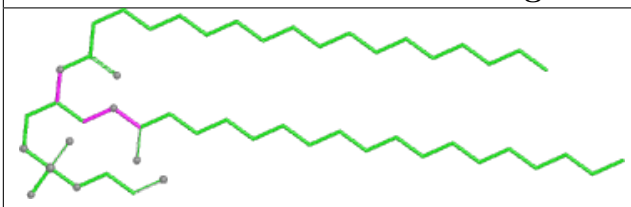


Torsions

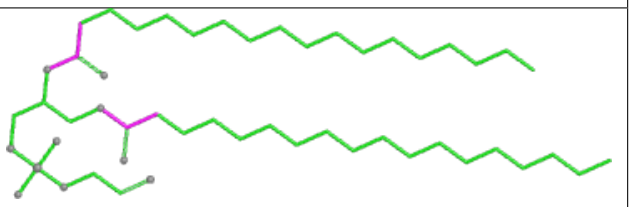


Rings

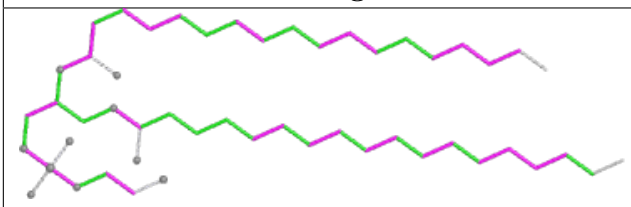
Ligand 3PE M 602



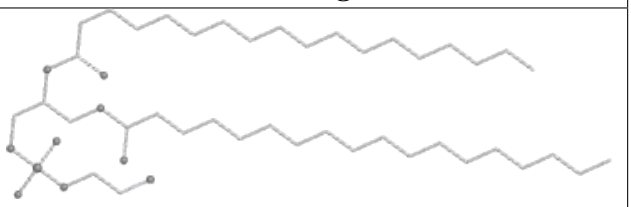
Bond lengths



Bond angles

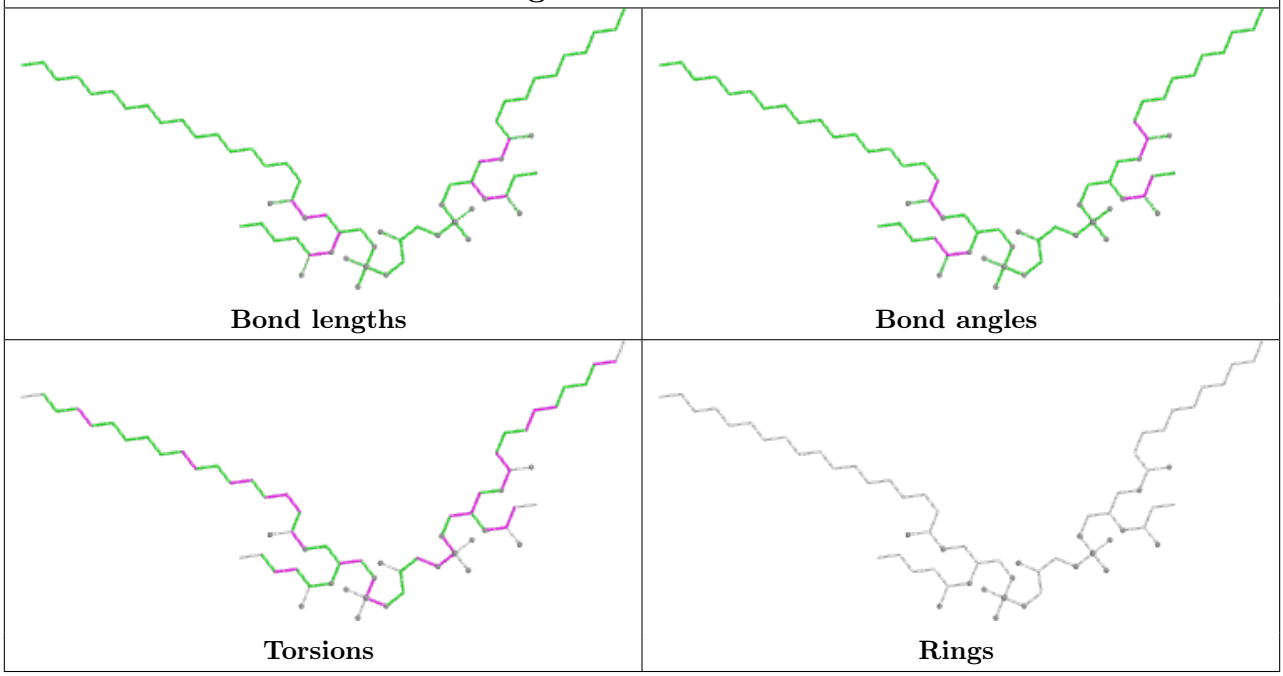


Torsions

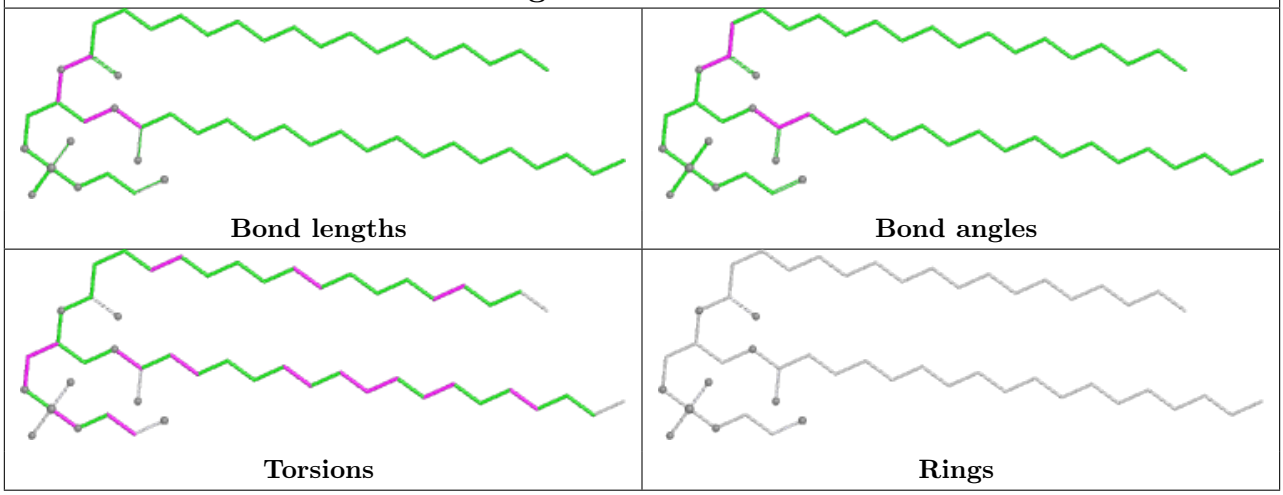


Rings

Ligand CDL d 204



Ligand 3PE N 901



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.

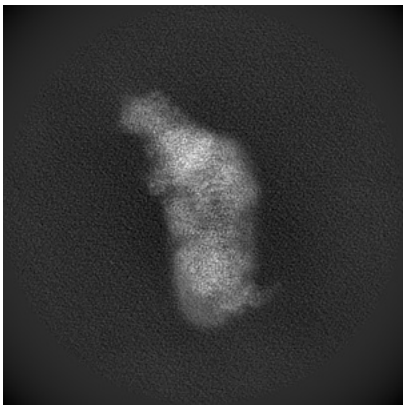
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14139. These allow visual inspection of the internal detail of the map and identification of artifacts.

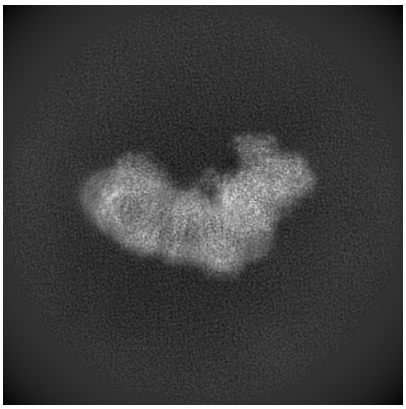
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

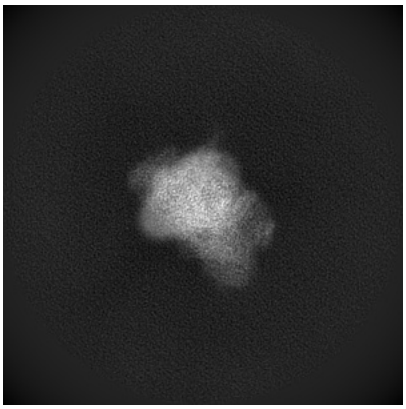
6.1.1 Primary map



X

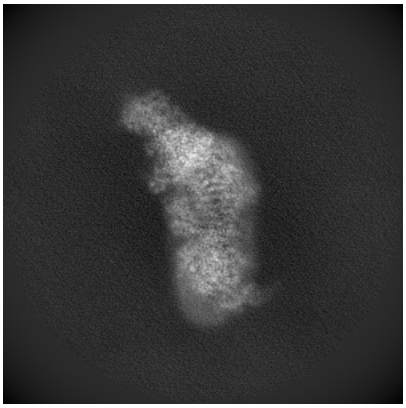


Y

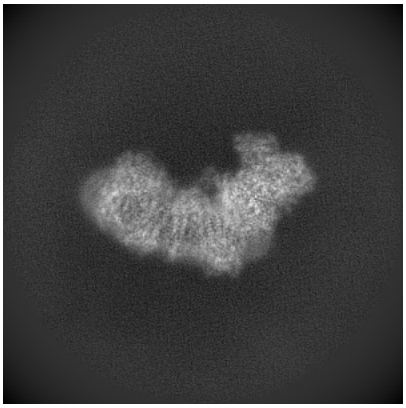


Z

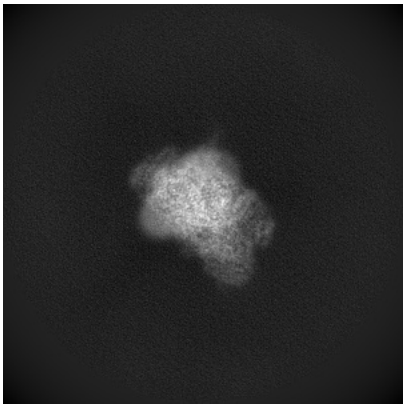
6.1.2 Raw map



X



Y

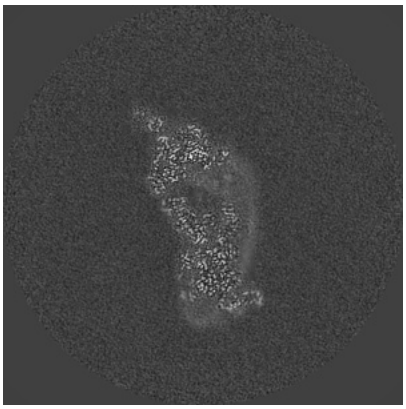


Z

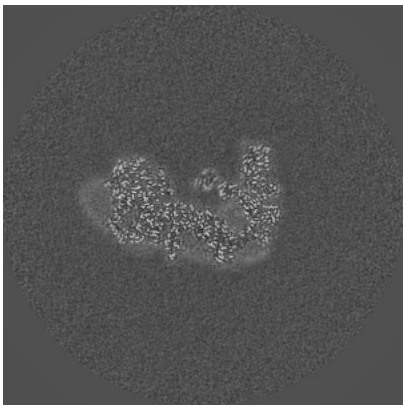
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

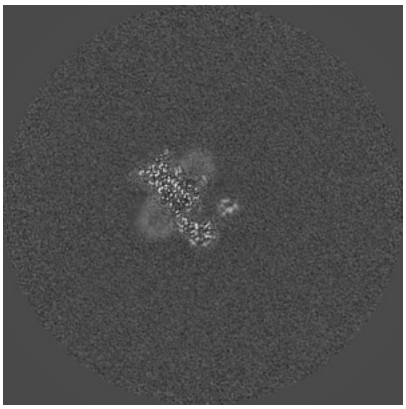
6.2.1 Primary map



X Index: 320

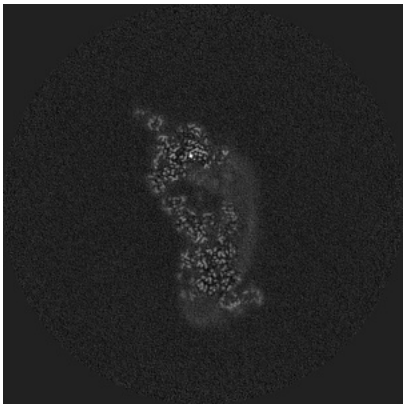


Y Index: 320

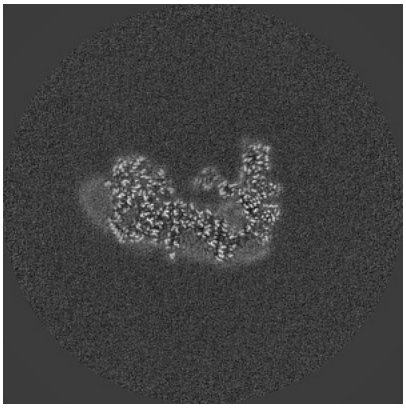


Z Index: 320

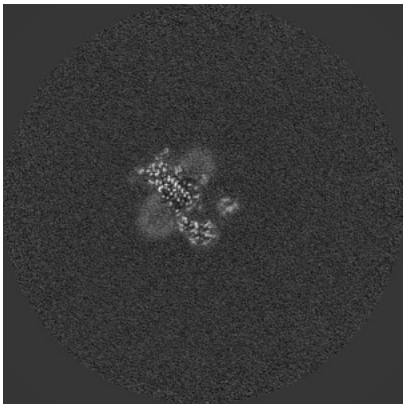
6.2.2 Raw map



X Index: 320



Y Index: 320

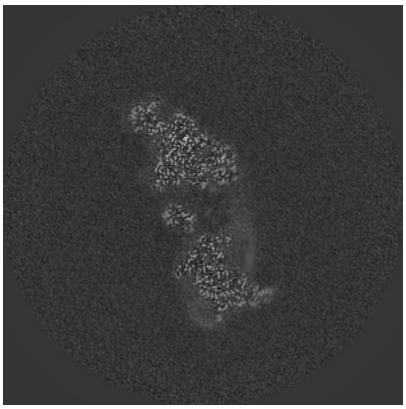


Z Index: 320

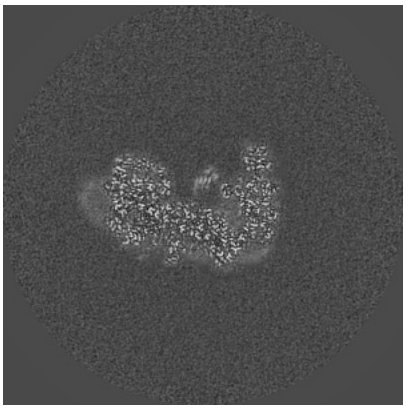
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

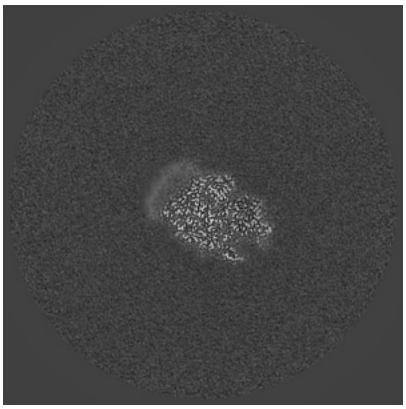
6.3.1 Primary map



X Index: 337

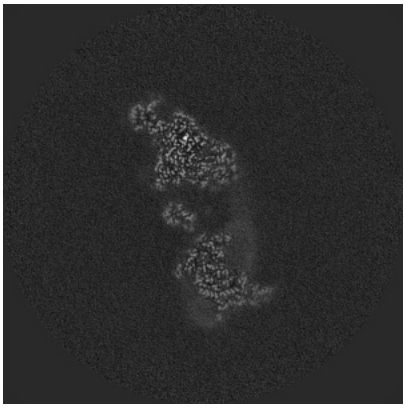


Y Index: 324

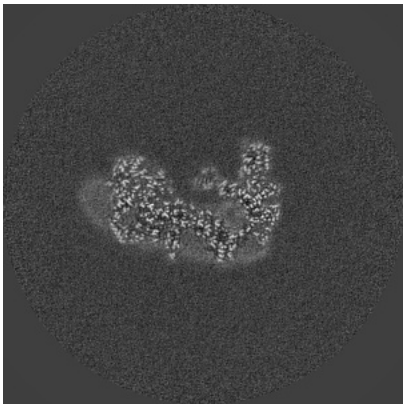


Z Index: 404

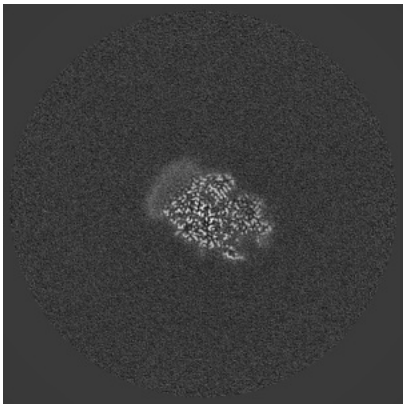
6.3.2 Raw map



X Index: 337



Y Index: 319

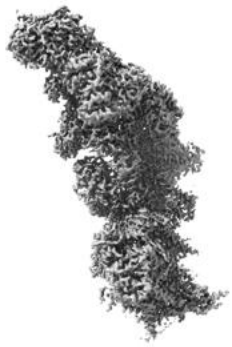


Z Index: 404

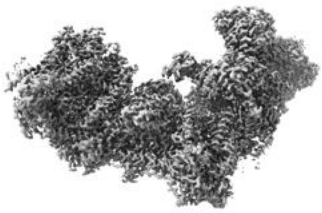
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

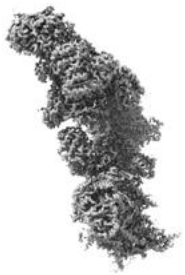


Y

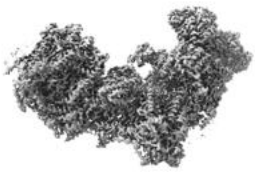
Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

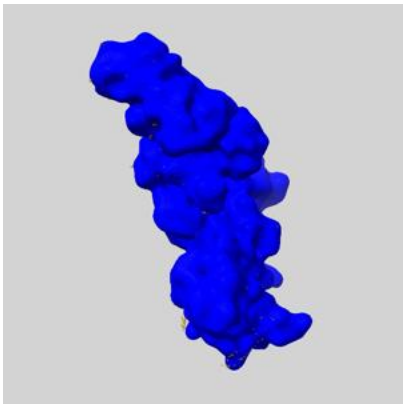
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

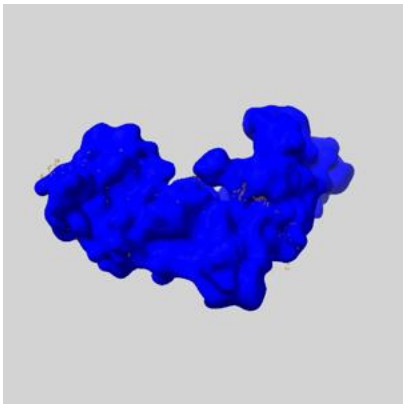
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

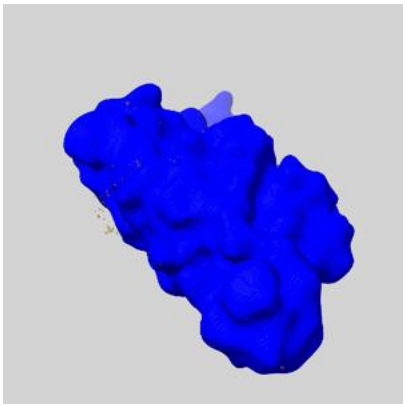
6.5.1 emd_14139_msk_1.map (i)



X



Y

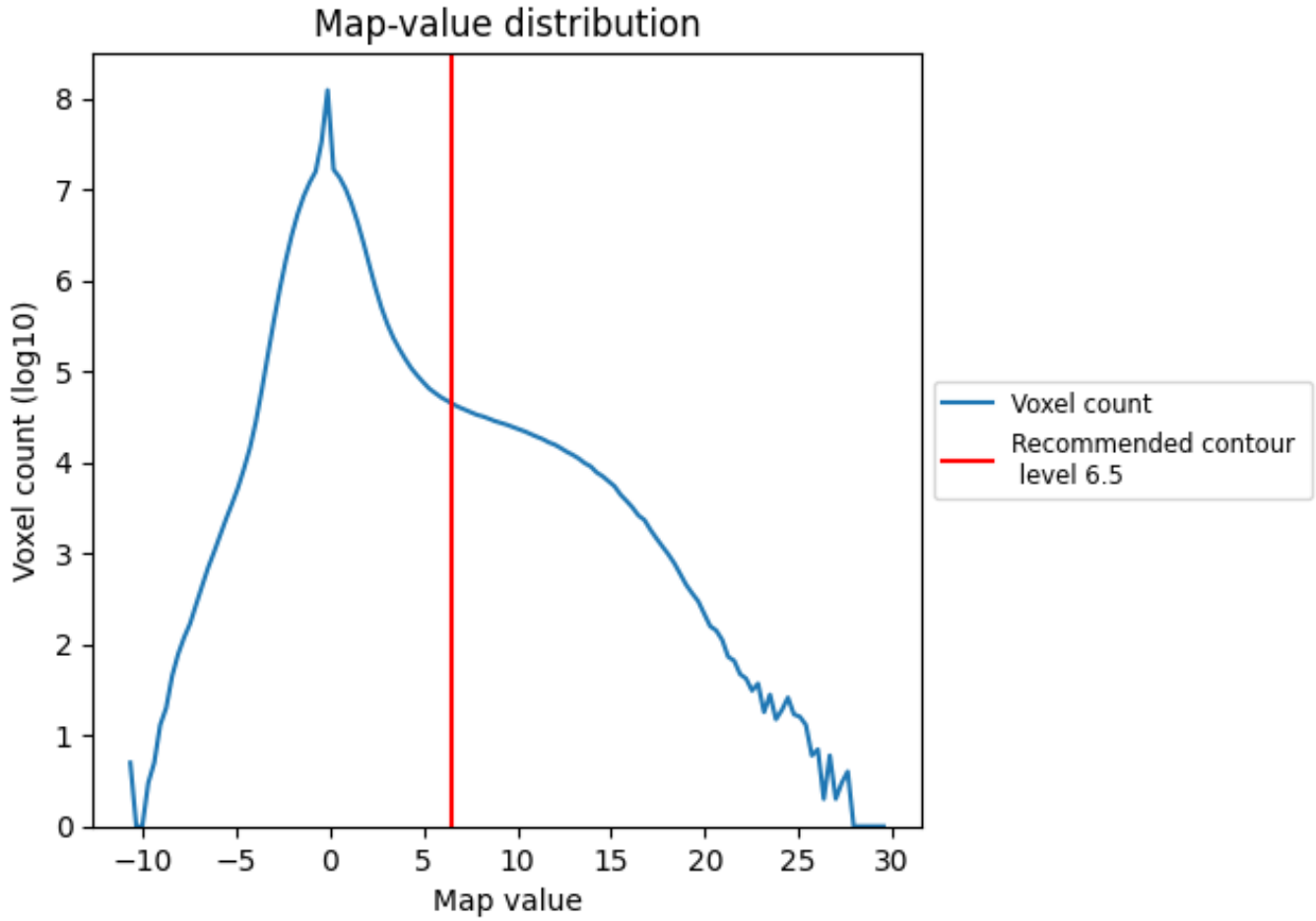


Z

7 Map analysis

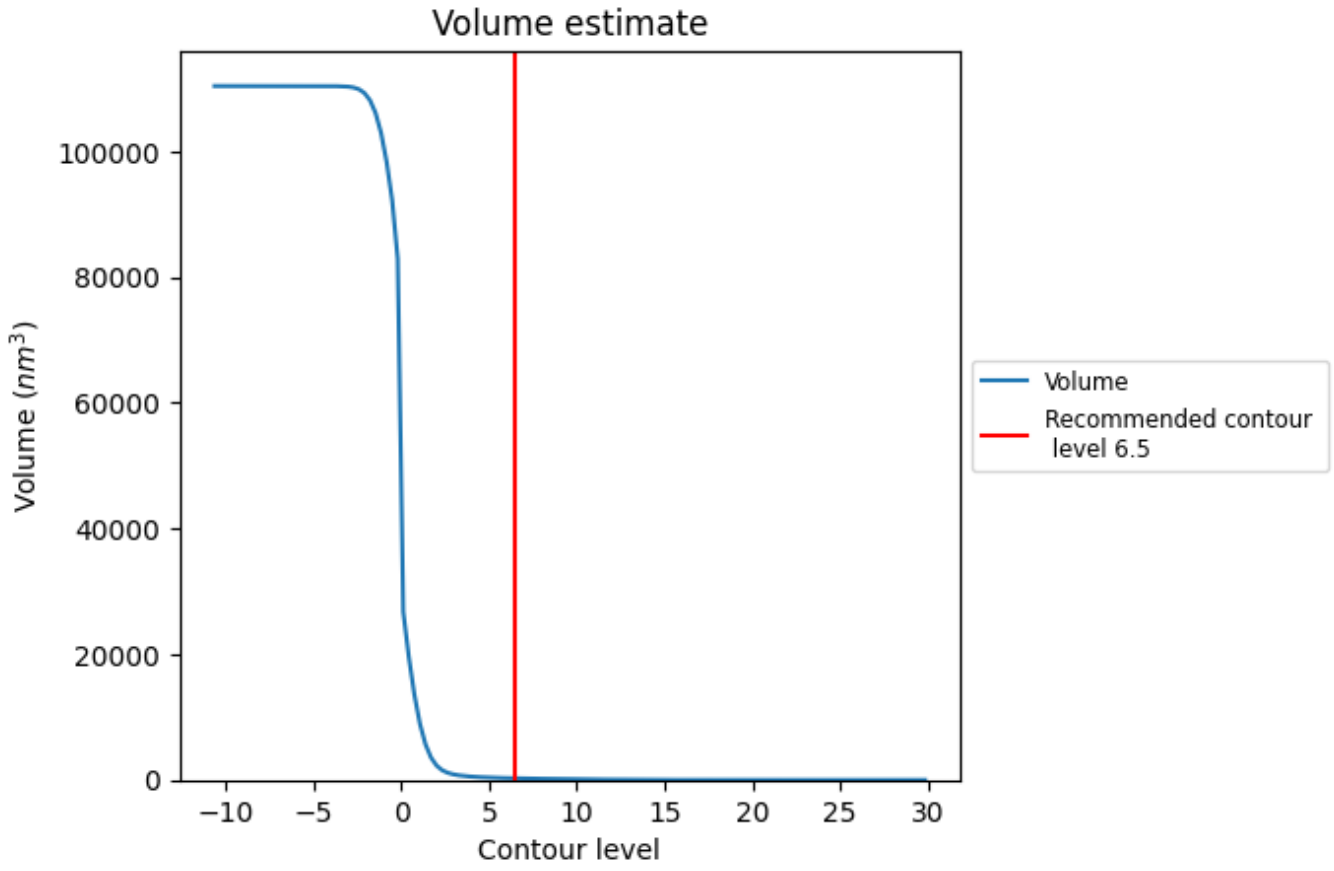
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

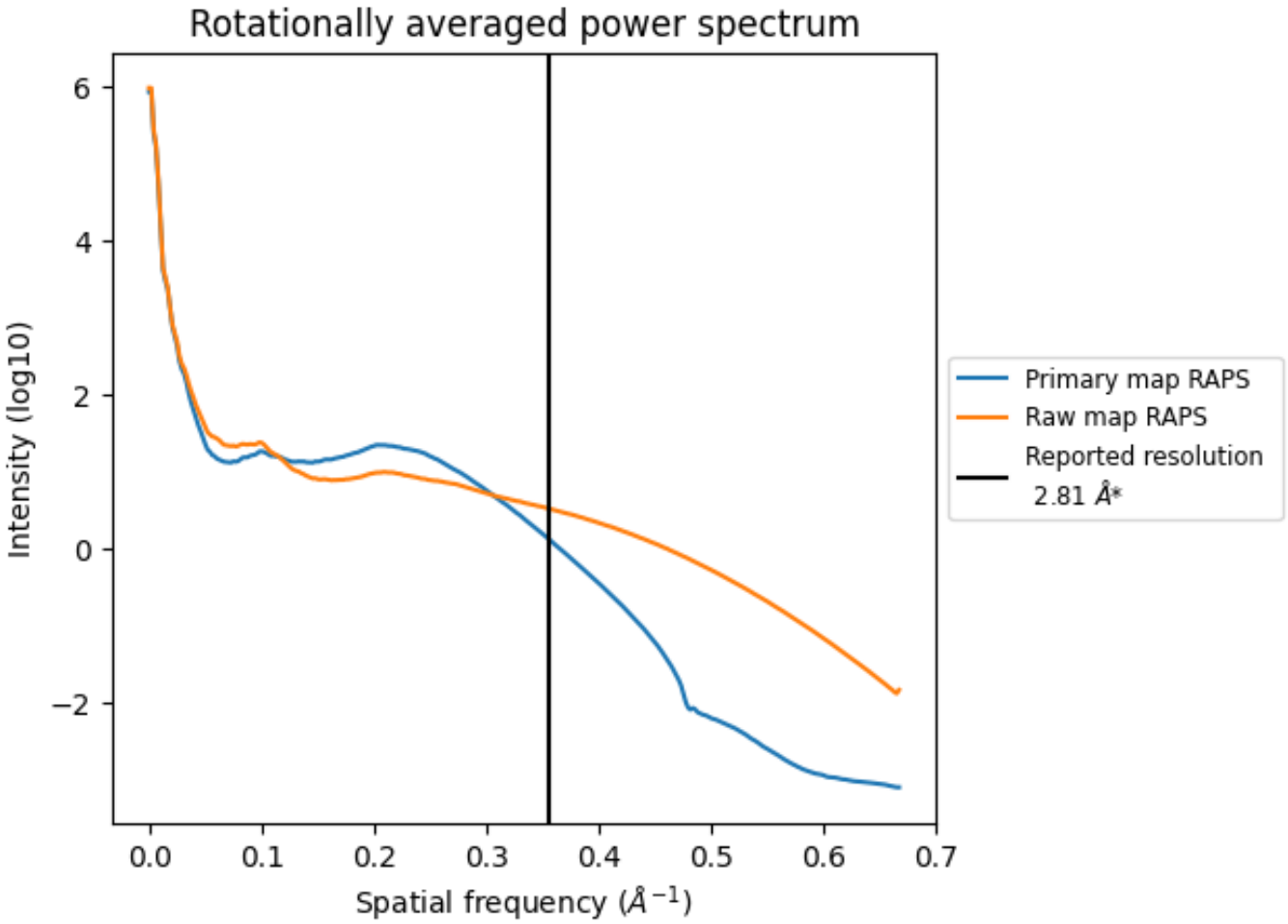
7.2 Volume estimate (i)



The volume at the recommended contour level is 263 nm^3; this corresponds to an approximate mass of 237 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)

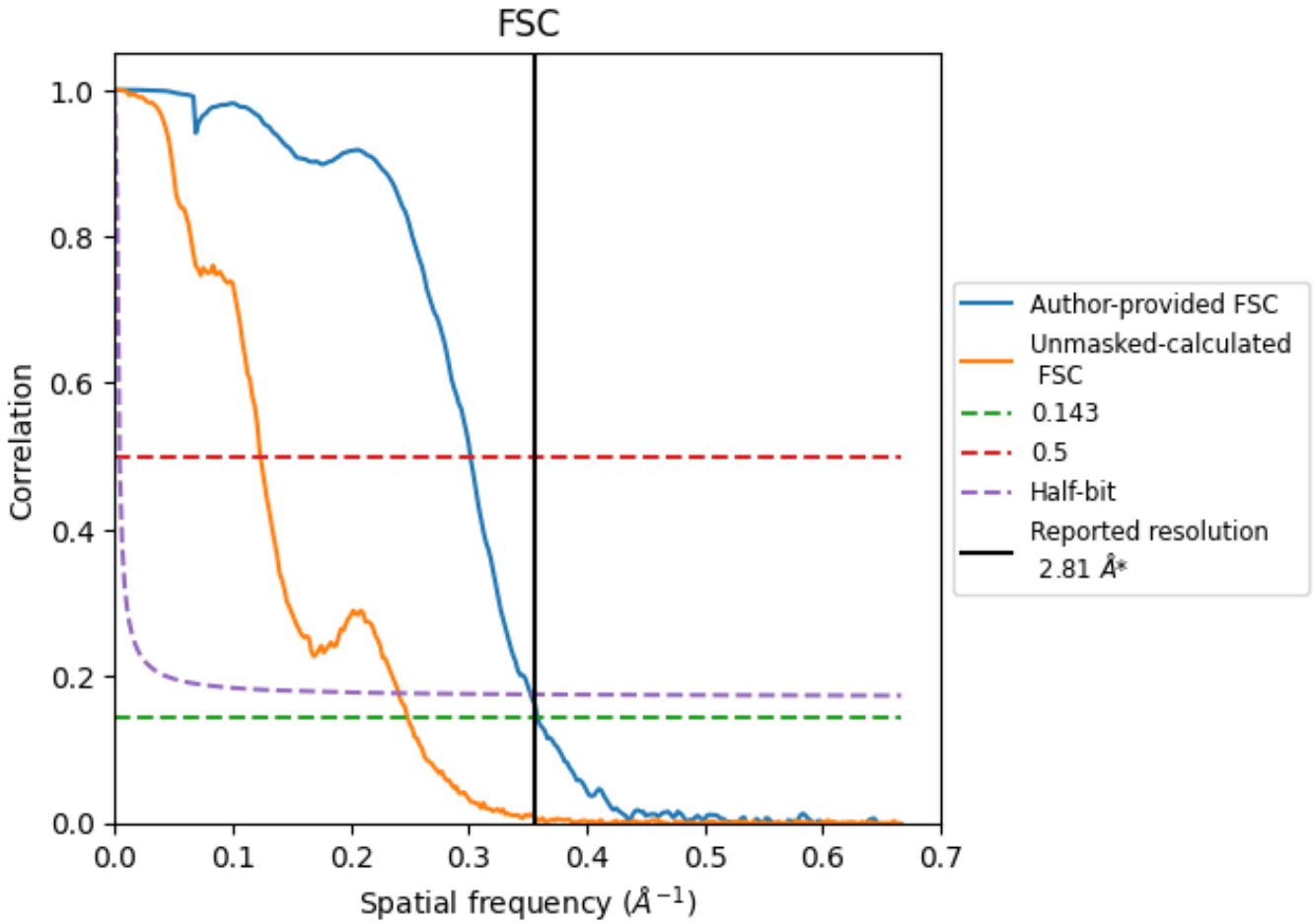


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

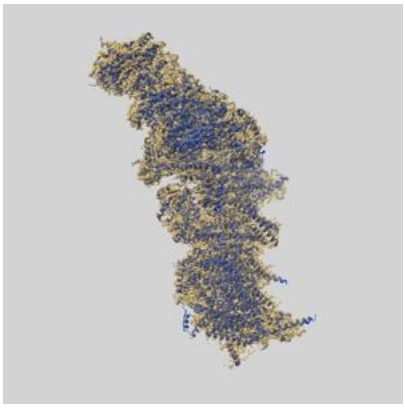
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.32	2.84
Unmasked-calculated*	4.03	8.10	4.15

*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 4.03 differs from the reported value 2.81 by more than 10 %

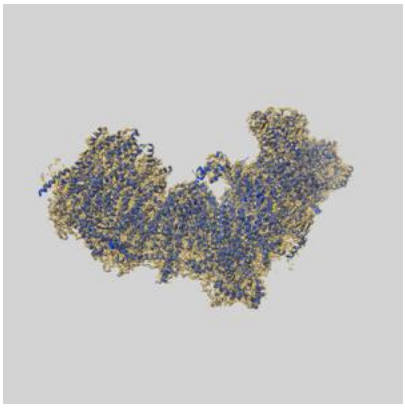
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14139 and PDB model 7QSN. Per-residue inclusion information can be found in section 3 on page 23.

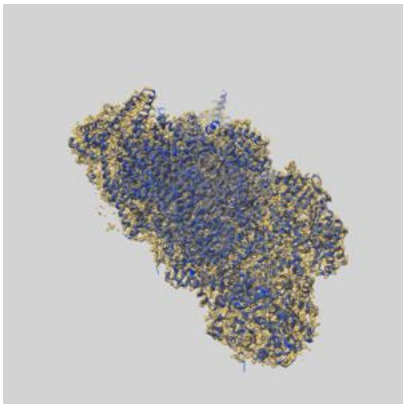
9.1 Map-model overlay



X



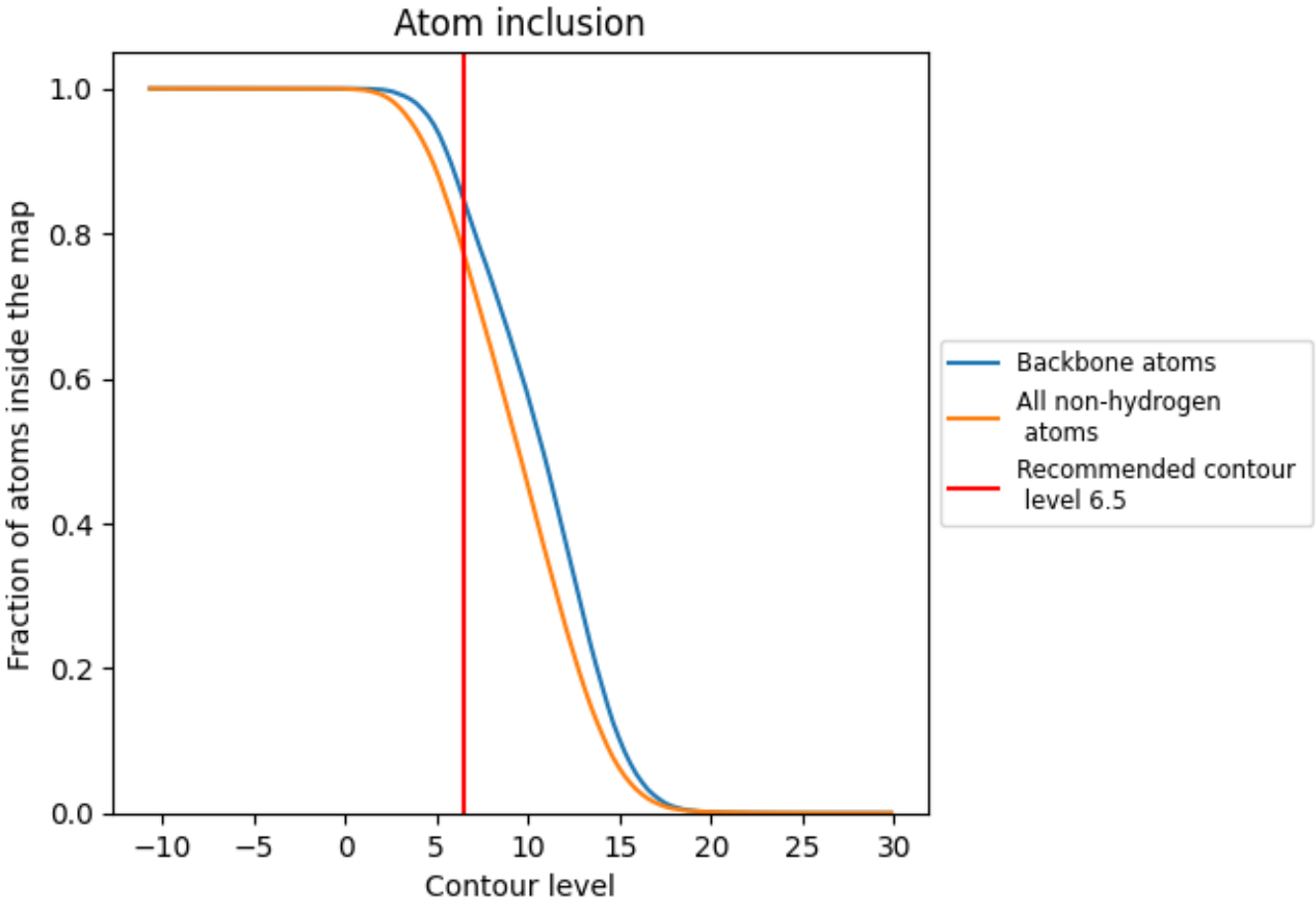
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5 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 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.