Full wwPDB EM Validation Report ⓘ

Aug 3, 2023 – 02:34 pm BST

PDB ID	:	8OLT
EMDB ID	:	EMD-16962
Title	:	Mitochondrial complex I from Mus musculus in the active state bound with piericidin A
Authors	:	Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on	:	2023-03-30
Resolution	:	2.84 Å(reported)
Based on initial model	:	6ZR2

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

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

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

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

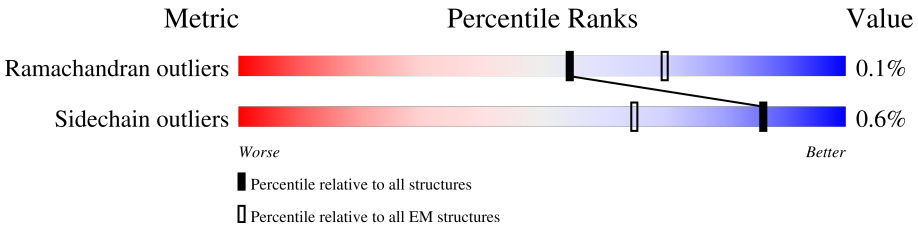
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 Å.

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



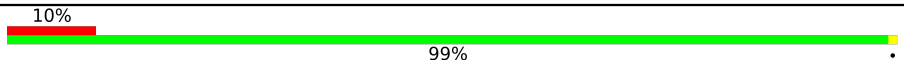
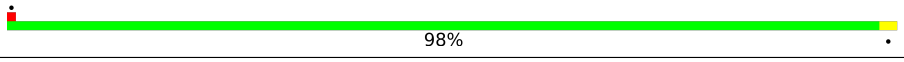
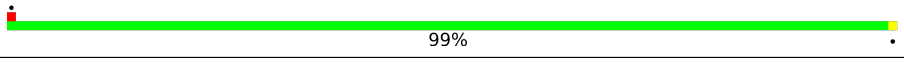
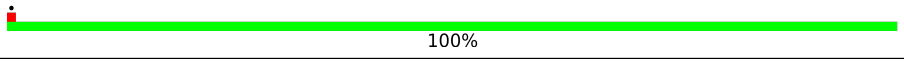
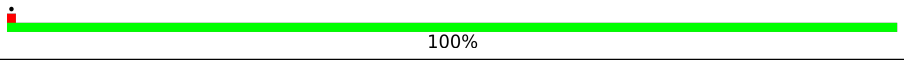
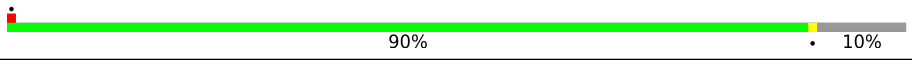
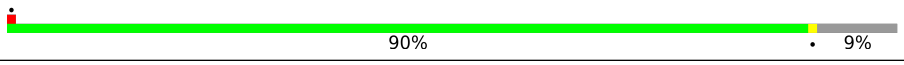
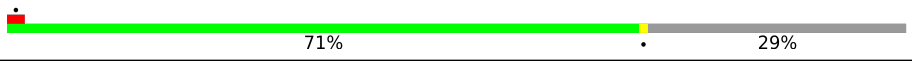
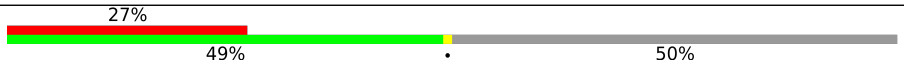
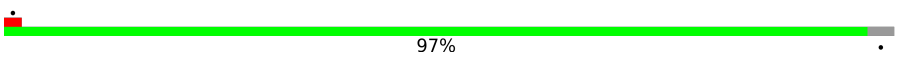
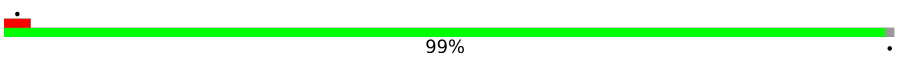
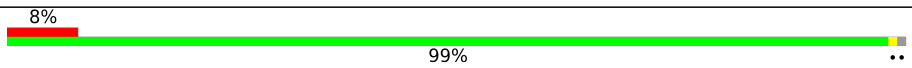
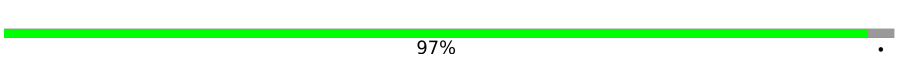
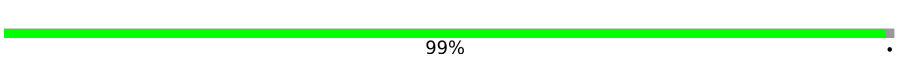
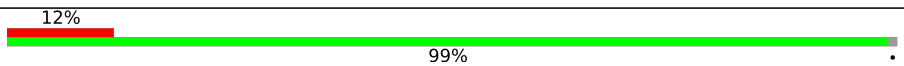
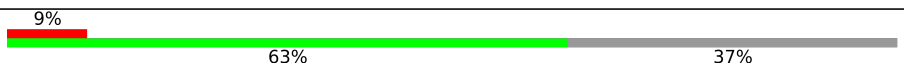
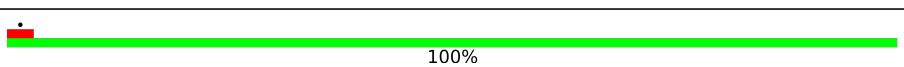
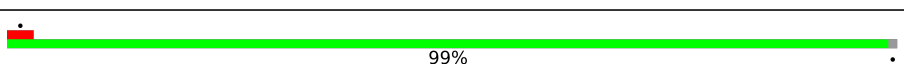
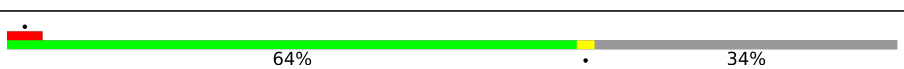
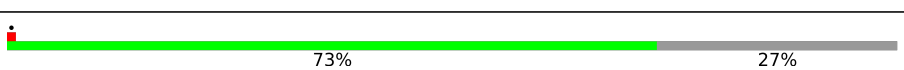
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	115	100%
2	B	224	68% 30%
3	C	263	79% 21%
4	D	463	92% 7%
5	E	248	7% 86% 14%
6	F	464	92% 7%
7	G	727	94% 5%
8	H	318	98%
9	I	212	83% 16%

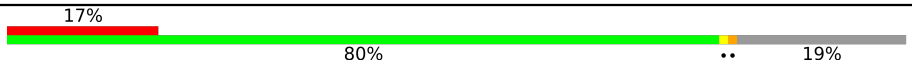
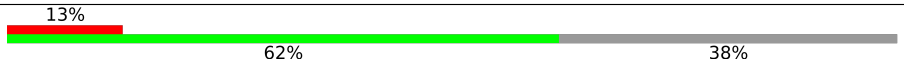
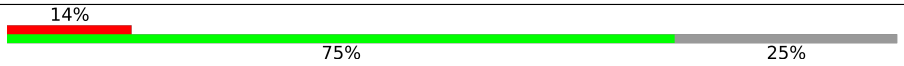
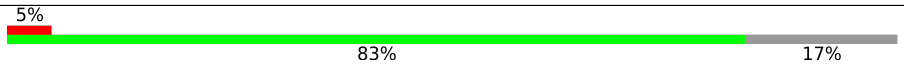
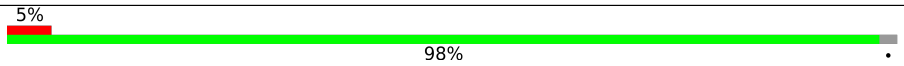
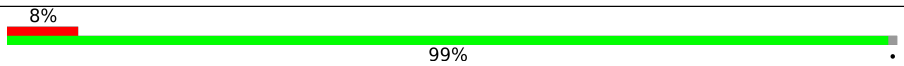
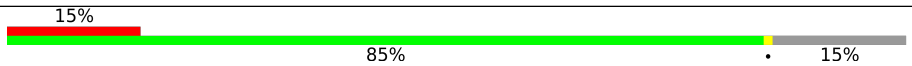
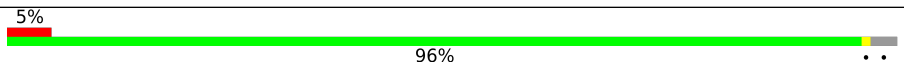
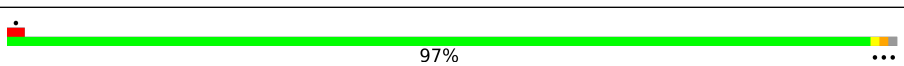
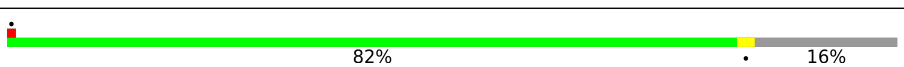
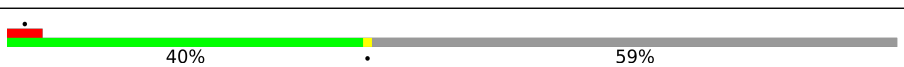
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 68075 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	115	933	633	133	160	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	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	208	1730	1116	297	314	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	430	3464	2215	595	630	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1660	1056	279	314	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5296	3321	919	1015	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- 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
			737	477	112	137	11		

- 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
			4800	3182	746	827	45		

- 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
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- 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
			2607	1674	431	492	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1015	642	179	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			663	415	126	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
20	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- 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
			1396	889	250	247	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	142	Total	C	N	O	S	0	0
			1050	670	177	194	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	69	Total	C	N	O	S	0	0
			564	366	100	94	4		

- 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
			648	425	105	114	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- 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
			996	651	171	165	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	100	Total	C	N	O	S	0	0
			842	545	135	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
			1162	762	194	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	104	Total	C	N	O	S	0	0
			869	565	152	149	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	78	Total	C	N	O	S	0	0
			630	416	107	105	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	126	Total	C	N	O	0	0
			1050	676	189	185		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLYOXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	117	Total	C	N	O	S	0	0
			1005	634	189	174	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1439	904	258	269	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1203	773	213	212	5		

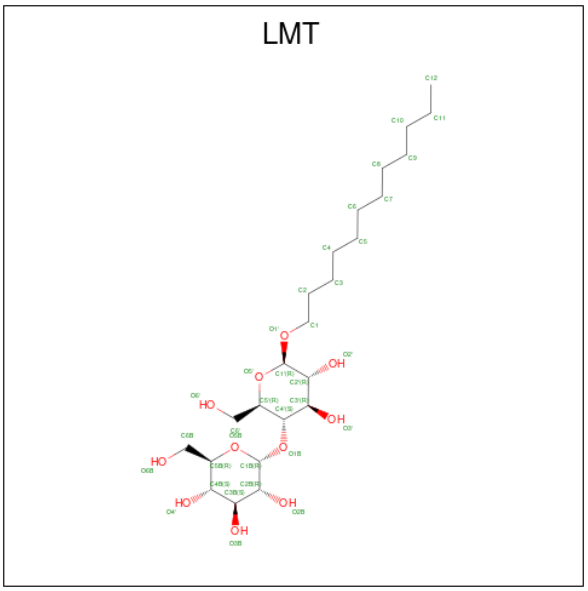
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			767	484	143	137	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	43	Total	C	N	O	0	0
			361	225	65	71		

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



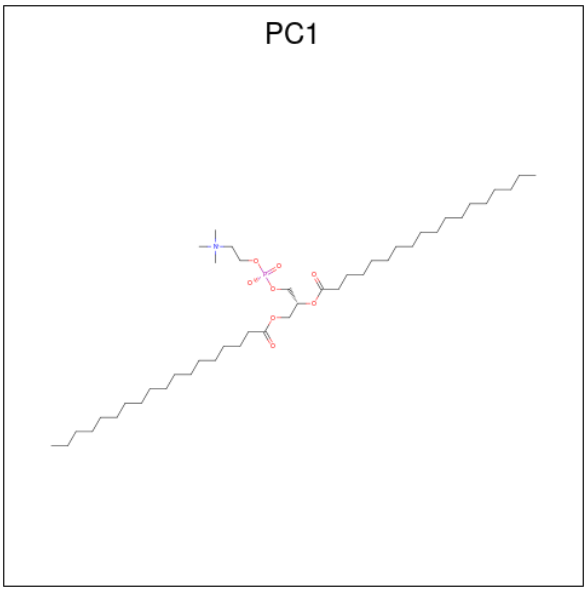
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	K	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	O	1	Total	C	O	0
			35	24	11	
45	P	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

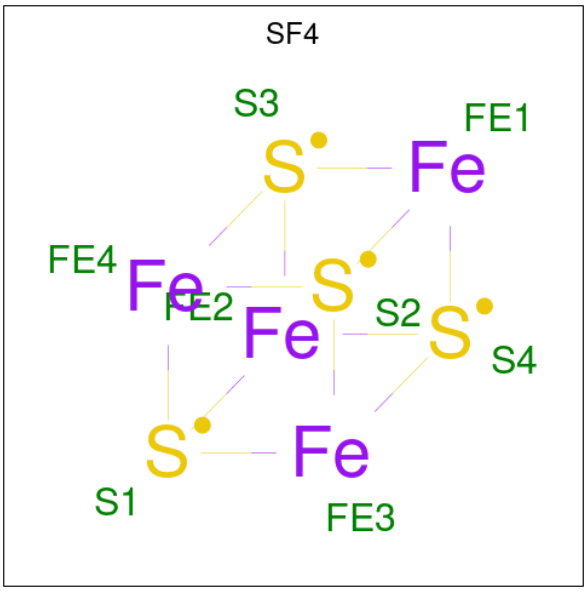
Mol	Chain	Residues	Atoms	AltConf
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0

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



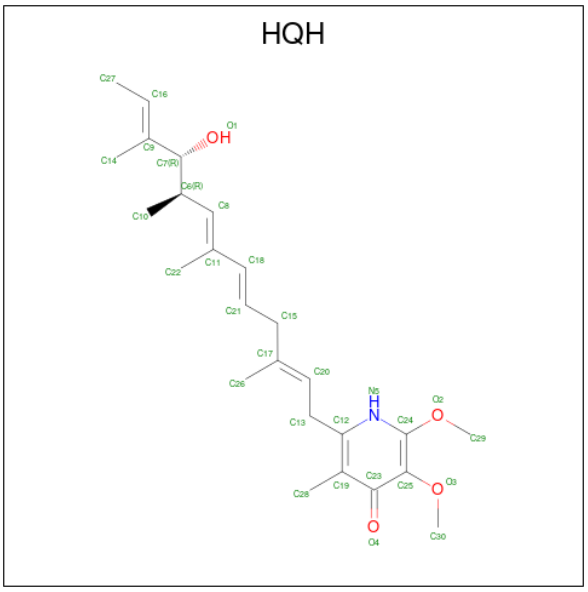
Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 29 19 1 8 1	0
46	B	1	Total C N O P 38 28 1 8 1	0
46	B	1	Total C N O P 41 31 1 8 1	0

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



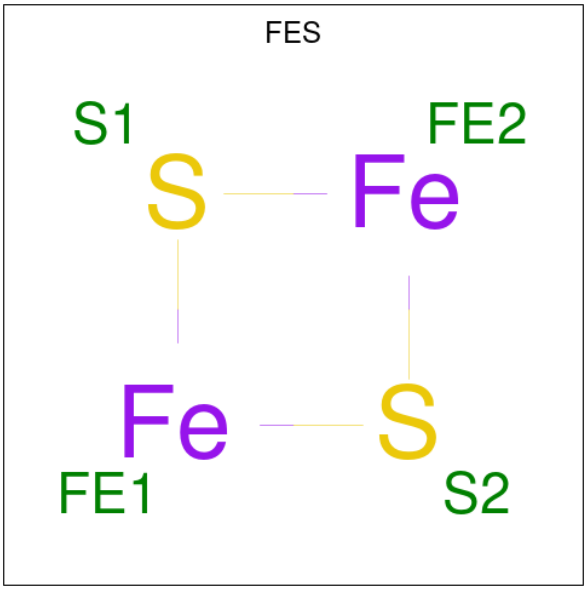
Mol	Chain	Residues	Atoms	AltConf
47	B	1	Total Fe S 8 4 4	0
47	F	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0

- Molecule 48 is Piericidin A (three-letter code: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



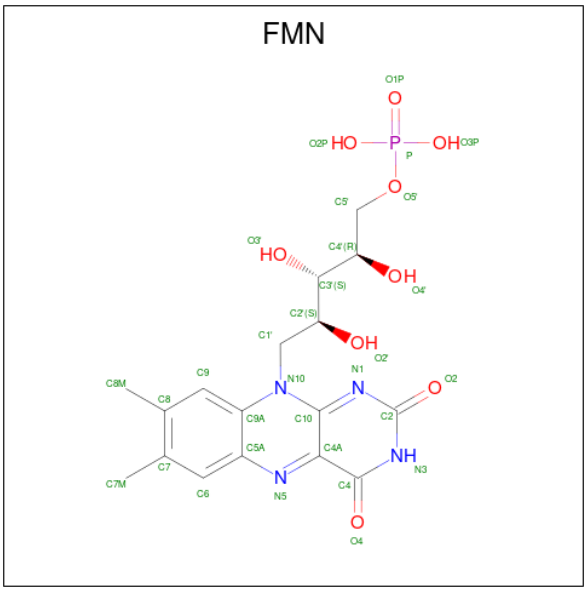
Mol	Chain	Residues	Atoms				AltConf
48	D	1	Total	C	N	O	0
			30	25	1	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

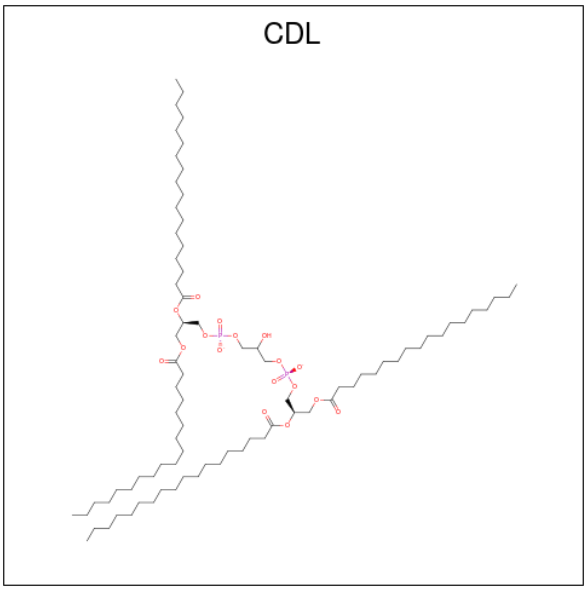


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is SODIUM ION (three-letter code: NA) (formula: Na).

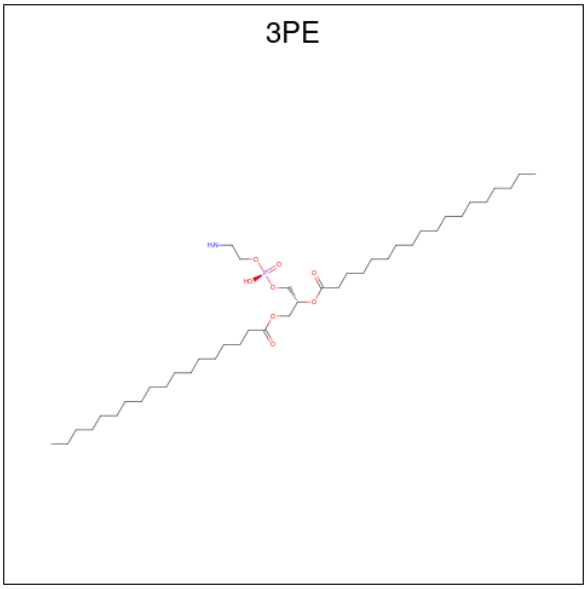
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	Na	0
			1	1	

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	H	1	Total 48	C 29	O 17	P 2	0
52	L	1	Total 64	C 45	O 17	P 2	0
52	h	1	Total 57	C 39	O 16	P 2	0
52	h	1	Total 48	C 29	O 17	P 2	0
52	q	1	Total 64	C 45	O 17	P 2	0

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	I	1	Total 44	C 34	N 1	O 8	P 1	0
53	L	1	Total 41	C 31	N 1	O 8	P 1	0
53	L	1	Total 44	C 34	N 1	O 8	P 1	0
53	M	1	Total 36	C 26	N 1	O 8	P 1	0
53	M	1	Total 36	C 26	N 1	O 8	P 1	0
53	N	1	Total 34	C 24	N 1	O 8	P 1	0

Continued on next page...

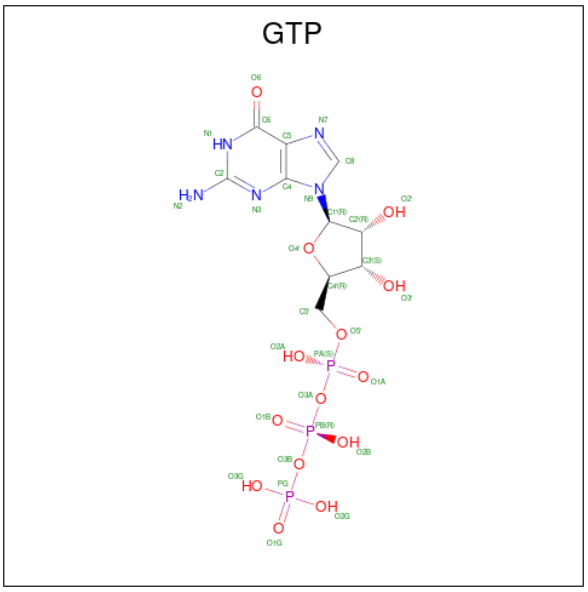
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
53	N	1	Total	C	N	O	P	0
			33	23	1	8	1	
53	O	1	Total	C	N	O	P	0
			30	20	1	8	1	
53	X	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	Z	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	Z	1	Total	C	N	O	P	0
			41	31	1	8	1	
53	d	1	Total	C	N	O	P	0
			33	23	1	8	1	
53	i	1	Total	C	N	O	P	0
			30	20	1	8	1	
53	r	1	Total	C	N	O	P	0
			45	35	1	8	1	

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

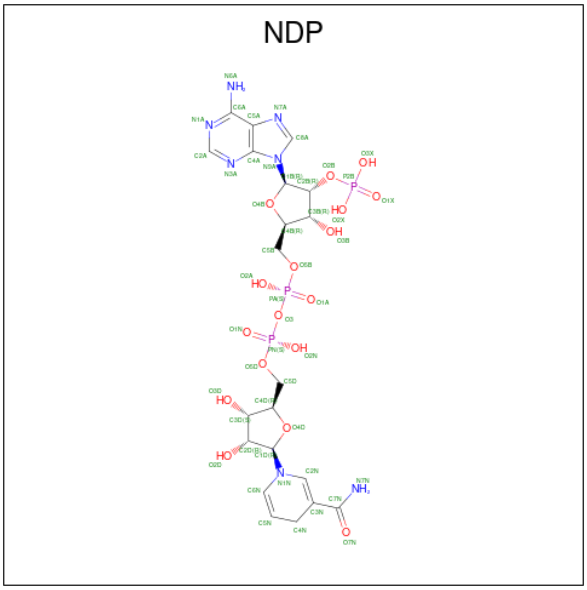
Mol	Chain	Residues	Atoms		AltConf
54	O	1	Total	Mg	0
			1	1	

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

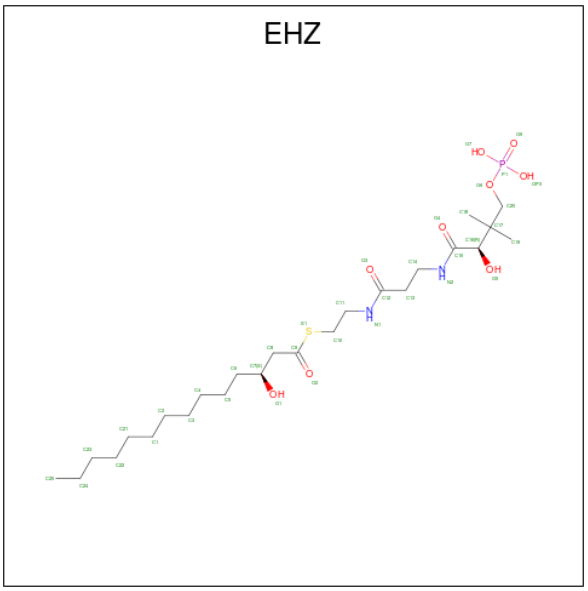


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

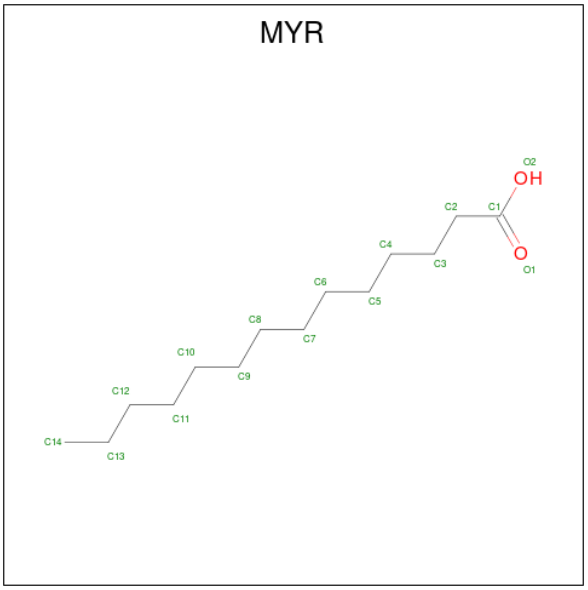
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

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



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

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	1	Total O 1 1	0
60	B	33	Total O 33 33	0
60	C	25	Total O 25 25	0
60	D	46	Total O 46 46	0
60	E	1	Total O 1 1	0
60	F	3	Total O 3 3	0
60	G	43	Total O 43 43	0
60	H	8	Total O 8 8	0
60	I	40	Total O 40 40	0
60	J	3	Total O 3 3	0
60	K	1	Total O 1 1	0
60	L	3	Total O 3 3	0
60	M	3	Total O 3 3	0
60	N	4	Total O 4 4	0
60	O	5	Total O 5 5	0
60	P	13	Total O 13 13	0
60	Q	9	Total O 9 9	0
60	R	5	Total O 5 5	0
60	W	1	Total O 1 1	0
60	X	4	Total O 4 4	0
60	Z	5	Total O 5 5	0
60	a	2	Total O 2 2	0

Continued on next page...

Continued from previous page...

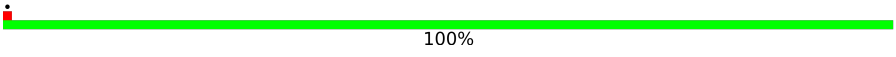
Mol	Chain	Residues	Atoms	AltConf
60	d	1	Total O 1 1	0
60	e	2	Total O 2 2	0
60	g	1	Total O 1 1	0
60	h	3	Total O 3 3	0
60	i	1	Total O 1 1	0
60	l	3	Total O 3 3	0
60	m	1	Total O 1 1	0
60	n	1	Total O 1 1	0
60	p	1	Total O 1 1	0
60	q	5	Total O 5 5	0
60	r	3	Total O 3 3	0

3 Residue-property plots (i)

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

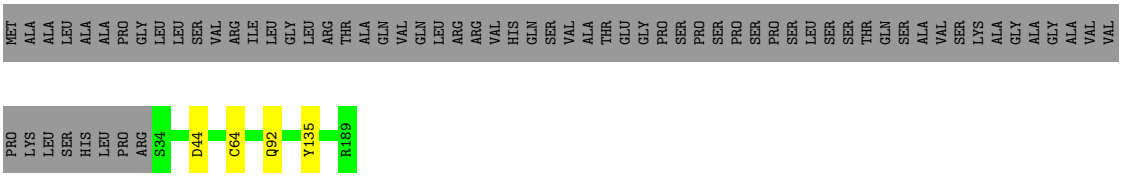
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



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

Chain B:

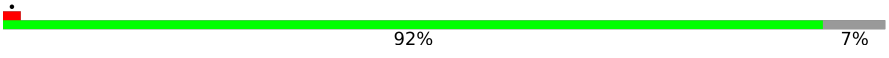


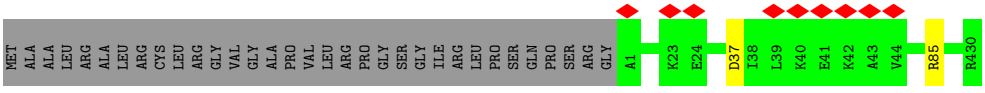
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

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

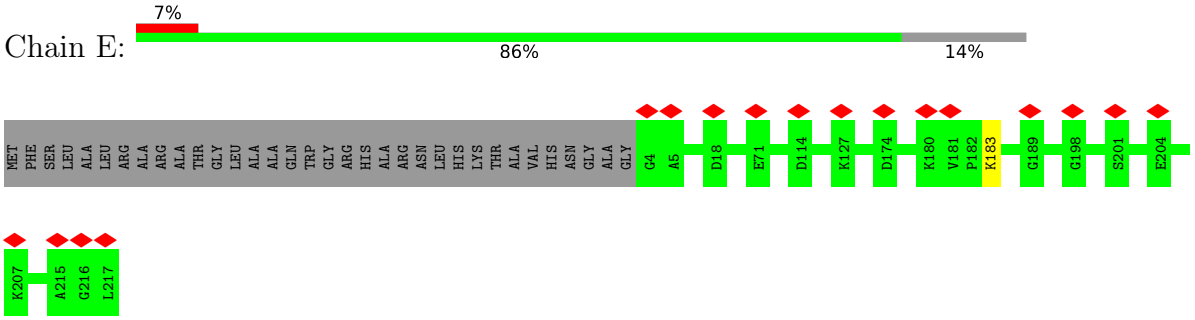
Chain D:





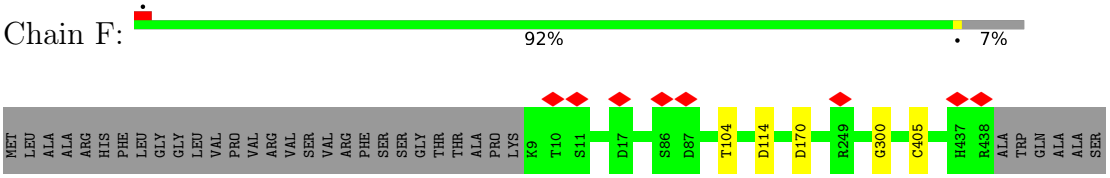
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



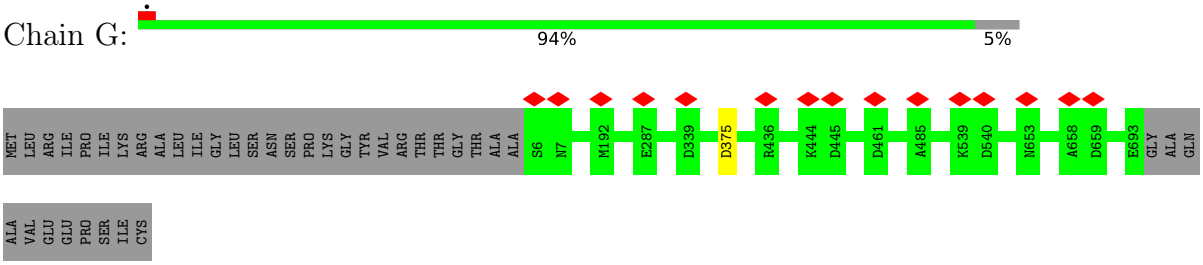
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



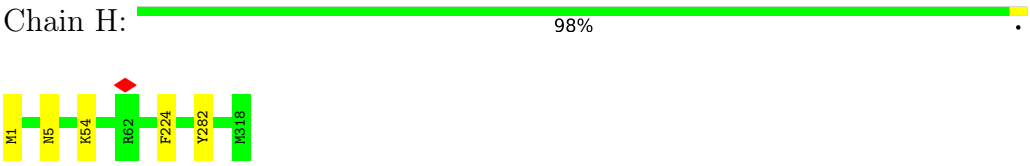
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



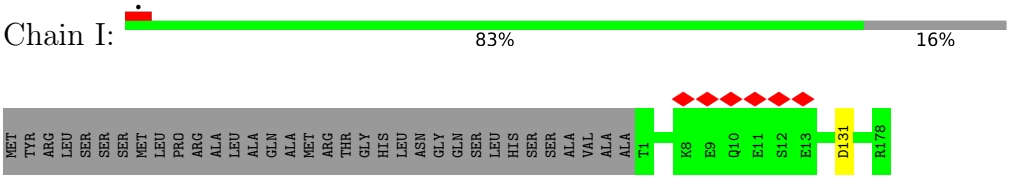
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



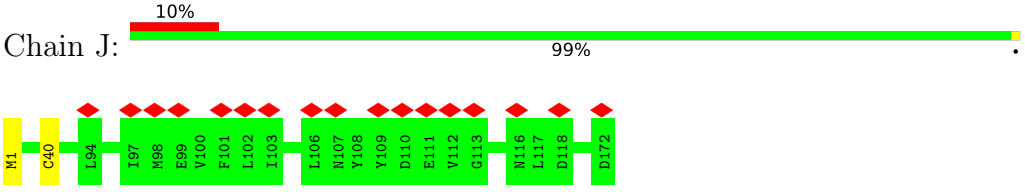
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



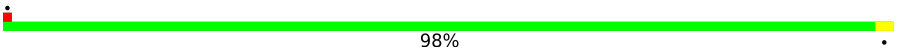
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

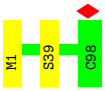
Chain J:



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

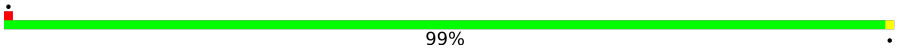
Chain K:

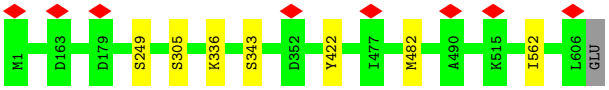




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

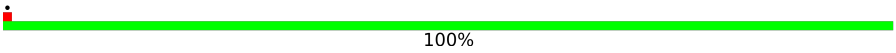
Chain L:

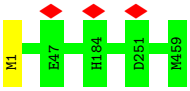




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

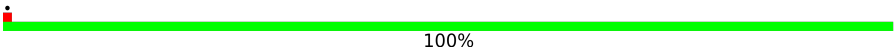
Chain M:

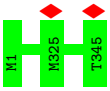




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

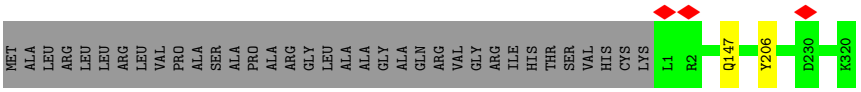
Chain N:





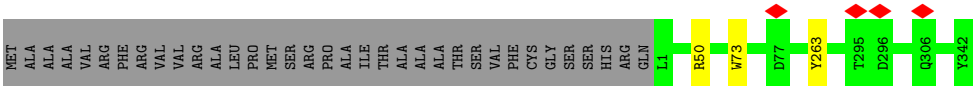
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



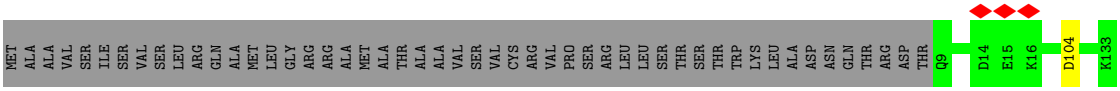
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



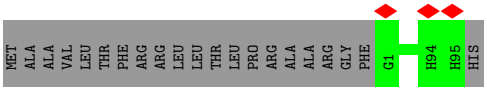
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



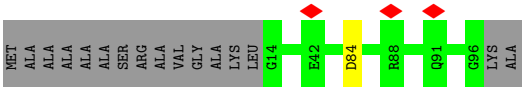
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



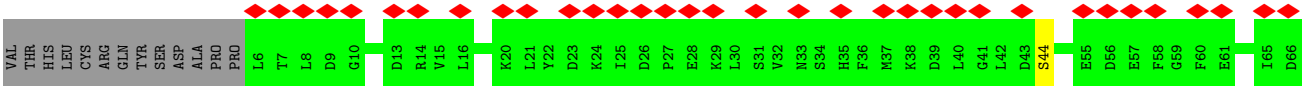
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

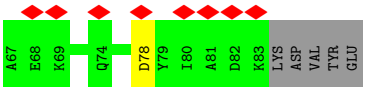
Chain S:



• Molecule 20: Acyl carrier protein, mitochondrial

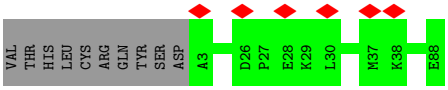
Chain T:





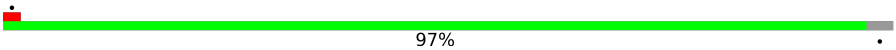
• Molecule 20: Acyl carrier protein, mitochondrial

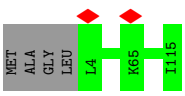
Chain U:



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

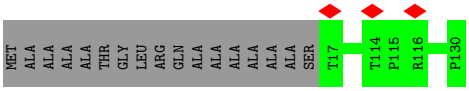
Chain V:





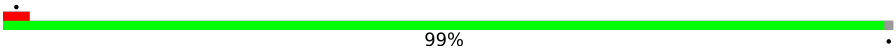
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

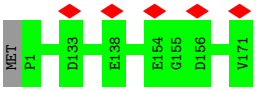
Chain W:



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

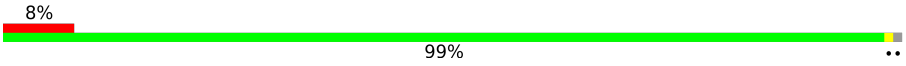
Chain X:

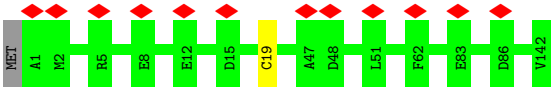




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

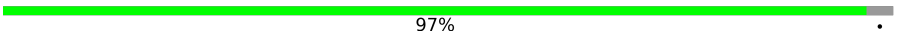
Chain Y:

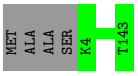




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

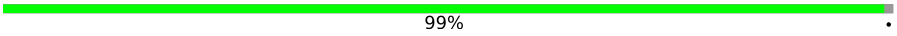
Chain Z:





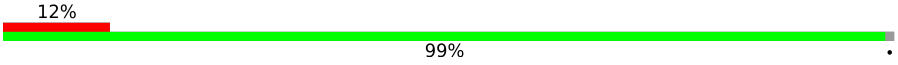
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

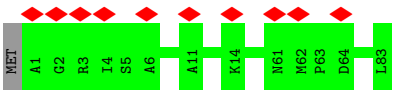
Chain a:



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

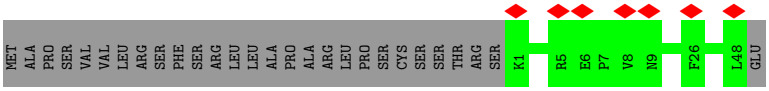
Chain b:





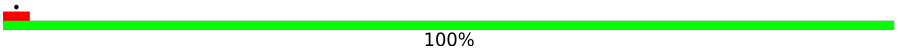
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

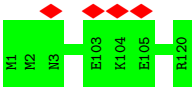
Chain c:



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

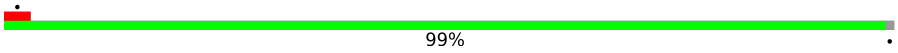
Chain d:

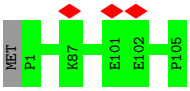




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

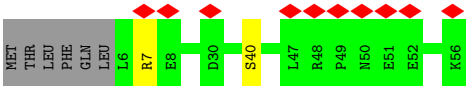
Chain e:





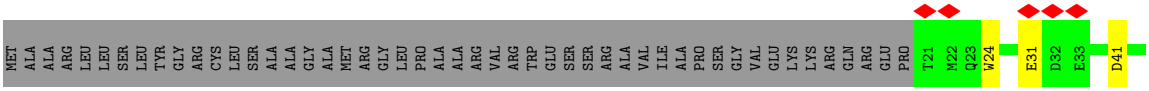
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

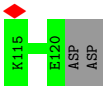
Chain f:



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

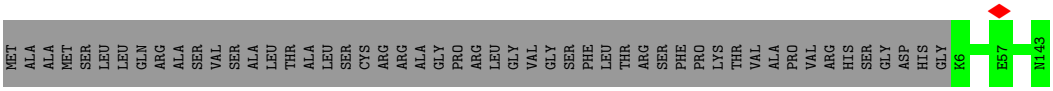
Chain g:





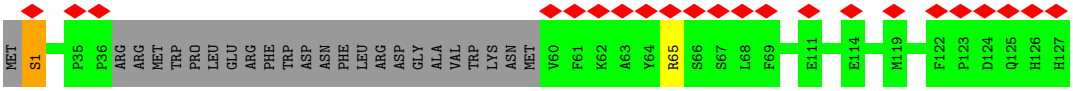
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



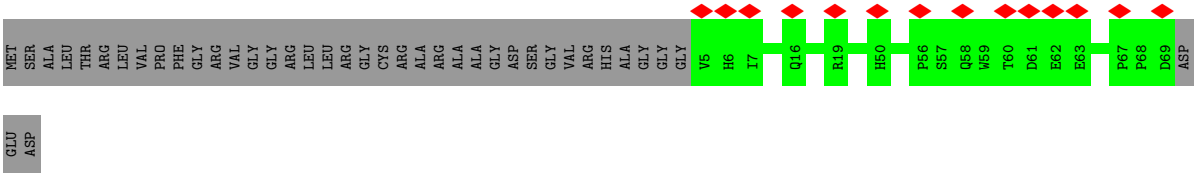
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



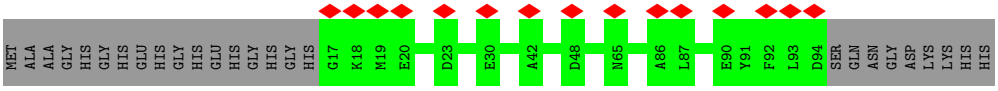
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



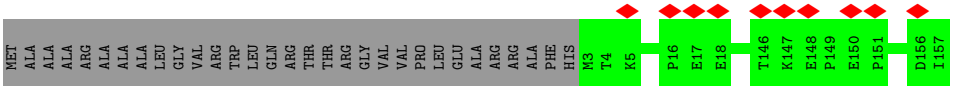
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



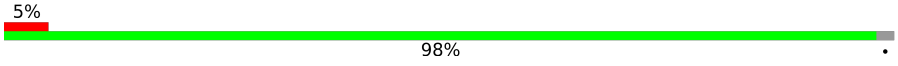
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

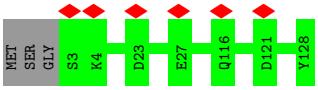
Chain l:



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

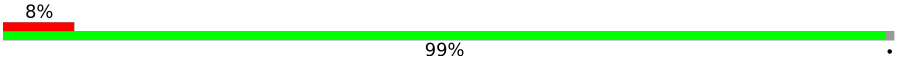
Chain m:

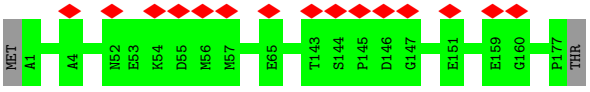




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

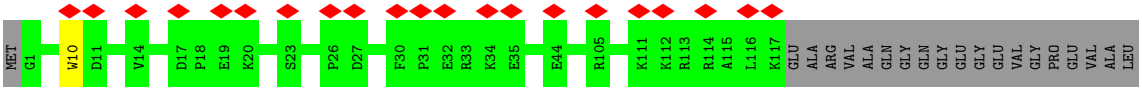
Chain n:





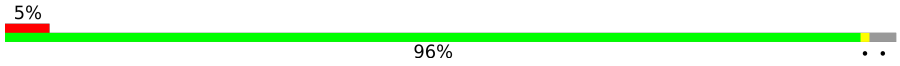
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7, METHYLGLYOXAL BIS-(GUANYLHYDRAZONE), NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

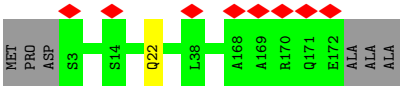
Chain o:



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

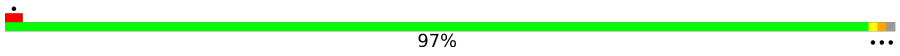
Chain p:

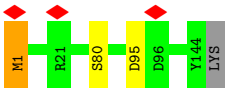




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

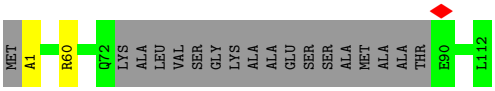
Chain q:





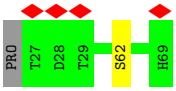
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50, 46	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	535.5, 535.5, 535.5	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0625, 1.0625, 1.0625	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.41	0/949	0.46	0/1297
2	B	0.56	0/1278	0.47	0/1730
3	C	0.49	0/1780	0.48	0/2424
4	D	0.47	0/3540	0.47	0/4795
5	E	0.43	0/1700	0.47	0/2316
6	F	0.44	0/3396	0.48	0/4586
7	G	0.43	0/5383	0.48	0/7293
8	H	0.44	0/2607	0.45	0/3564
9	I	0.54	0/1461	0.50	0/1974
10	J	0.44	0/1330	0.45	0/1810
11	K	0.41	0/738	0.44	0/1002
12	L	0.40	0/4913	0.45	0/6686
13	M	0.41	0/3709	0.46	0/5052
14	N	0.40	0/2755	0.45	0/3751
15	O	0.49	0/2674	0.46	0/3626
16	P	0.44	0/2823	0.47	0/3828
17	Q	0.42	0/1038	0.48	0/1401
18	R	0.48	0/762	0.46	0/1026
19	S	0.39	0/674	0.47	0/909
20	T	0.37	0/637	0.42	0/858
20	U	0.46	0/704	0.44	0/951
21	V	0.43	0/937	0.41	0/1270
22	W	0.45	0/993	0.45	0/1335
23	X	0.44	0/1434	0.44	0/1937
24	Y	0.42	0/1074	0.45	0/1456
25	Z	0.44	0/1192	0.46	0/1608
26	a	0.50	0/577	0.45	0/777
27	b	0.42	0/671	0.43	0/921
28	c	0.47	0/409	0.42	0/555
29	d	0.47	0/1028	0.43	0/1387
30	e	0.43	0/900	0.43	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	f	0.38	0/451	0.44	0/607
32	g	0.50	0/870	0.44	0/1185
33	h	0.49	0/1197	0.42	0/1621
34	i	0.45	0/889	0.46	0/1210
35	j	0.44	0/587	0.42	0/804
36	k	0.41	0/650	0.46	0/878
37	l	0.49	0/1356	0.44	0/1851
38	m	0.46	0/1079	0.45	0/1463
39	n	0.47	0/1589	0.43	0/2152
40	o	0.41	0/1030	0.43	0/1382
41	p	0.46	0/1472	0.42	0/1989
42	q	0.47	0/1234	0.48	0/1681
43	r	0.45	0/777	0.47	0/1051
44	s	0.40	0/371	0.48	0/504
All	All	0.45	0/67618	0.46	0/91702

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

Mol	Chain	#Chirality outliers	#Planarity outliers
34	i	0	1
42	q	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain
42	q	1	AME	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	206/263 (78%)	196 (95%)	10 (5%)	0	100	100
4	D	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
5	E	212/248 (86%)	192 (91%)	19 (9%)	1 (0%)	29	51
6	F	428/464 (92%)	410 (96%)	16 (4%)	2 (0%)	29	51
7	G	686/727 (94%)	652 (95%)	34 (5%)	0	100	100
8	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	604/607 (100%)	568 (94%)	34 (6%)	2 (0%)	41	61
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
15	O	318/355 (90%)	310 (98%)	8 (2%)	0	100	100
16	P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100
18	R	93/116 (80%)	84 (90%)	9 (10%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	76/156 (49%)	64 (84%)	12 (16%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	Y	140/143 (98%)	138 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
31	f	49/57 (86%)	45 (92%)	4 (8%)	0	100	100
32	g	98/151 (65%)	98 (100%)	0	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	100/128 (78%)	90 (90%)	10 (10%)	0	100	100
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	76/104 (73%)	74 (97%)	2 (3%)	0	100	100
37	l	153/186 (82%)	145 (95%)	8 (5%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
40	o	115/137 (84%)	105 (91%)	9 (8%)	1 (1%)	17	34
41	p	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
42	q	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
43	r	91/113 (80%)	84 (92%)	7 (8%)	0	100	100
44	s	41/104 (39%)	38 (93%)	3 (7%)	0	100	100
All	All	8118/9214 (88%)	7731 (95%)	381 (5%)	6 (0%)	54	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	170	ASP
12	L	562	ILE
40	o	10	TRP
12	L	249	SER
5	E	183	LYS
6	F	300	GLY

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	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	128 (97%)	4 (3%)	41	65
3	C	190/227 (84%)	189 (100%)	1 (0%)	88	94
4	D	370/394 (94%)	369 (100%)	1 (0%)	92	96
5	E	184/206 (89%)	184 (100%)	0	100	100
6	F	345/370 (93%)	342 (99%)	3 (1%)	78	89
7	G	580/610 (95%)	579 (100%)	1 (0%)	93	97
8	H	279/279 (100%)	275 (99%)	4 (1%)	67	83
9	I	152/178 (85%)	151 (99%)	1 (1%)	84	91
10	J	137/137 (100%)	136 (99%)	1 (1%)	84	91
11	K	87/87 (100%)	86 (99%)	1 (1%)	73	86
12	L	548/549 (100%)	543 (99%)	5 (1%)	78	89
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	307/307 (100%)	307 (100%)	0	100	100
15	O	284/309 (92%)	282 (99%)	2 (1%)	84	91
16	P	299/325 (92%)	296 (99%)	3 (1%)	76	88
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78	89
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	73/80 (91%)	72 (99%)	1 (1%)	67	83
20	T	72/135 (53%)	70 (97%)	2 (3%)	43	68
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	106/107 (99%)	105 (99%)	1 (1%)	78	89
25	Z	121/123 (98%)	121 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	59/60 (98%)	59 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	47/53 (89%)	45 (96%)	2 (4%)	29	54
32	g	91/129 (70%)	88 (97%)	3 (3%)	38	63
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	95/119 (80%)	94 (99%)	1 (1%)	73	86
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	60/78 (77%)	60 (100%)	0	100	100
37	l	140/161 (87%)	140 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	108/121 (89%)	108 (100%)	0	100	100
41	p	155/158 (98%)	154 (99%)	1 (1%)	86	93
42	q	129/130 (99%)	127 (98%)	2 (2%)	62	81
43	r	85/96 (88%)	84 (99%)	1 (1%)	71	85
44	s	42/95 (44%)	41 (98%)	1 (2%)	49	72
All	All	7198/7947 (91%)	7155 (99%)	43 (1%)	86	93

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	44	ASP
2	B	64	CYS
2	B	92	GLN
2	B	135	TYR
3	C	74	SER
4	D	37	ASP
6	F	104	THR
6	F	114	ASP
6	F	405	CYS
7	G	375	ASP
8	H	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	54	LYS
8	H	224	PHE
8	H	282	TYR
9	I	131	ASP
10	J	40	CYS
11	K	39	SER
12	L	305	SER
12	L	336	LYS
12	L	343	SER
12	L	422	TYR
12	L	482	MET
15	O	147	GLN
15	O	206	TYR
16	P	50	ARG
16	P	73	TRP
16	P	263	TYR
17	Q	104	ASP
19	S	84	ASP
20	T	44	SER
20	T	78	ASP
24	Y	19	CYS
31	f	7	ARG
31	f	40	SER
32	g	24	TRP
32	g	31	GLU
32	g	41	ASP
34	i	65	ARG
41	p	22	GLN
42	q	80	SER
42	q	95	ASP
43	r	60	ARG
44	s	62	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	257	ASN
7	G	491	ASN
12	L	109	HIS
13	M	184	HIS
30	e	97	HIS
32	g	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	m	85	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.92	0	7,9,11	0.86	0
34	SAC	i	1	34	7,8,9	1.83	1 (14%)	8,9,11	1.88	2 (25%)
42	AME	q	1	42	9,10,11	1.50	1 (11%)	9,11,13	1.88	2 (22%)
8	FME	H	1	8	8,9,10	1.02	1 (12%)	7,9,11	1.08	0
4	2MR	D	85	4	10,12,13	2.25	2 (20%)	5,13,15	1.23	1 (20%)
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.65	0
11	FME	K	1	11	8,9,10	1.02	1 (12%)	7,9,11	1.21	1 (14%)
13	FME	M	1	13	8,9,10	1.10	1 (12%)	7,9,11	0.71	0
43	AYA	r	1	43	6,7,8	1.41	1 (16%)	5,8,10	1.17	1 (20%)
10	FME	J	1	10	8,9,10	0.97	1 (12%)	7,9,11	0.91	0
14	FME	N	1	14	8,9,10	0.88	0	7,9,11	0.83	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
1	FME	A	1	1	-	1/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	q	1	42	-	5/9/10/12	-
8	FME	H	1	8	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	2/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	3/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.62	1.43	1.33
4	D	85	2MR	CZ-NE	4.48	1.43	1.34
34	i	1	SAC	O-C	4.21	1.36	1.19
42	q	1	AME	CT1-N	3.41	1.46	1.34
43	r	1	AYA	CA-N	-3.03	1.43	1.46
13	M	1	FME	CA-N	-2.49	1.42	1.46
8	H	1	FME	CA-N	-2.14	1.43	1.46
11	K	1	FME	CA-N	-2.13	1.43	1.46
10	J	1	FME	CA-N	-2.04	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.52	112.94	124.78
42	q	1	AME	CT2-CT1-N	3.67	122.31	116.10
42	q	1	AME	CE-SD-CG	2.74	109.81	100.40
34	i	1	SAC	OG-CB-CA	-2.57	104.41	110.97
11	K	1	FME	C-CA-N	2.34	113.95	109.73
4	D	85	2MR	NE-CZ-NH2	-2.28	117.39	119.48
43	r	1	AYA	CB-CA-N	2.26	112.12	109.61

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
42	q	1	AME	C-CA-CB-CG
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	CA-CB-CG-SD
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
10	J	1	FME	N-CA-CB-CG
11	K	1	FME	N-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	CA-CB-CG-SD
42	q	1	AME	CB-CG-SD-CE
14	N	1	FME	CB-CA-N-CN
42	q	1	AME	N-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 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	LMT	Y	202	-	36,36,36	1.22	6 (16%)	47,47,47	0.96	2 (4%)
45	LMT	h	203	-	36,36,36	1.22	5 (13%)	47,47,47	1.02	2 (4%)
53	3PE	L	702	-	40,40,50	0.96	3 (7%)	43,45,55	1.12	2 (4%)
45	LMT	J	202	-	36,36,36	1.19	6 (16%)	47,47,47	1.00	0
53	3PE	N	401	-	33,33,50	1.07	4 (12%)	36,38,55	1.05	2 (5%)
53	3PE	L	703	-	43,43,50	0.91	4 (9%)	46,48,55	1.07	3 (6%)
45	LMT	j	101	-	36,36,36	1.15	4 (11%)	47,47,47	0.95	1 (2%)
46	PC1	B	202	-	37,37,53	1.12	4 (10%)	43,45,61	1.15	2 (4%)
58	EHZ	U	201	20	29,36,37	1.62	5 (17%)	35,44,47	1.72	8 (22%)
59	MYR	o	201	40	14,14,15	0.75	0	13,13,15	0.63	0
52	CDL	h	201	-	56,56,99	1.05	5 (8%)	61,67,111	1.18	4 (6%)
45	LMT	M	501	-	36,36,36	1.27	7 (19%)	47,47,47	1.19	3 (6%)
52	CDL	L	705	-	63,63,99	1.08	7 (11%)	69,75,111	1.20	4 (5%)
45	LMT	L	701	-	36,36,36	1.25	6 (16%)	47,47,47	0.94	1 (2%)
53	3PE	r	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.08	2 (4%)
53	3PE	M	502	-	35,35,50	1.00	3 (8%)	38,40,55	1.13	2 (5%)
45	LMT	P	502	-	36,36,36	1.18	5 (13%)	47,47,47	1.19	4 (8%)
47	SF4	F	501	6	0,12,12	-	-	-		
53	3PE	Z	201	-	30,30,50	1.09	3 (10%)	33,35,55	1.10	2 (6%)
45	LMT	Y	204	-	36,36,36	1.22	6 (16%)	47,47,47	1.05	3 (6%)
52	CDL	H	401	-	47,47,99	1.16	6 (12%)	51,58,111	1.26	3 (5%)
53	3PE	N	402	-	32,32,50	1.06	4 (12%)	35,37,55	1.11	2 (5%)
53	3PE	i	201	34	29,29,50	1.14	3 (10%)	32,34,55	1.25	2 (6%)
56	NDP	P	501	-	45,52,52	2.07	8 (17%)	53,80,80	1.68	9 (16%)
49	FES	G	803	7	0,4,4	-	-	-		
53	3PE	Z	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.05	2 (4%)
45	LMT	A	401	-	36,36,36	1.23	6 (16%)	47,47,47	1.01	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
47	SF4	I	202	9	0,12,12	-	-	-		
45	LMT	J	201	-	36,36,36	1.22	5 (13%)	47,47,47	1.15	2 (4%)
45	LMT	Y	203	-	36,36,36	1.15	5 (13%)	47,47,47	1.07	2 (4%)
58	EHZ	T	201	20	29,36,37	1.67	5 (17%)	35,44,47	1.63	9 (25%)
47	SF4	G	802	7	0,12,12	-	-	-		
52	CDL	h	202	-	46,46,99	1.53	8 (17%)	50,57,111	1.36	4 (8%)
53	3PE	d	201	-	32,32,50	1.06	3 (9%)	35,37,55	1.11	2 (5%)
45	LMT	L	704	-	36,36,36	1.23	7 (19%)	47,47,47	1.12	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	FMN	F	502	-	33,33,33	2.51	6 (18%)	48,50,50	1.51	10 (20%)
49	FES	E	301	5	0,4,4	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
53	3PE	O	504	-	29,29,50	1.10	4 (13%)	32,34,55	1.04	2 (6%)
55	GTP	O	502	-	26,34,34	2.95	11 (42%)	32,54,54	1.91	10 (31%)
45	LMT	O	503	-	36,36,36	1.15	5 (13%)	47,47,47	1.48	4 (8%)
45	LMT	A	403	-	36,36,36	1.18	4 (11%)	47,47,47	1.06	2 (4%)
47	SF4	I	201	9	0,12,12	-	-	-		
46	PC1	B	203	-	40,40,53	1.09	2 (5%)	46,48,61	1.14	2 (4%)
53	3PE	X	201	-	35,35,50	1.00	4 (11%)	38,40,55	1.22	2 (5%)
52	CDL	q	501	-	63,63,99	1.06	5 (7%)	69,75,111	1.03	4 (5%)
45	LMT	K	201	-	36,36,36	1.33	7 (19%)	47,47,47	1.07	2 (4%)
45	LMT	Y	201	-	36,36,36	1.29	6 (16%)	47,47,47	1.02	1 (2%)
53	3PE	I	203	-	43,43,50	0.92	3 (6%)	46,48,55	1.08	2 (4%)
46	PC1	A	402	-	28,28,53	1.29	3 (10%)	34,36,61	0.98	2 (5%)
53	3PE	M	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.11	2 (5%)
48	HQH	D	601	-	29,30,30	0.83	2 (6%)	28,40,40	1.40	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	Y	202	-	-	9/21/61/61	0/2/2/2
45	LMT	h	203	-	-	7/21/61/61	0/2/2/2
53	3PE	L	702	-	-	20/44/44/54	-
45	LMT	J	202	-	-	8/21/61/61	0/2/2/2
53	3PE	N	401	-	-	19/37/37/54	-
53	3PE	L	703	-	-	24/47/47/54	-
45	LMT	j	101	-	-	11/21/61/61	0/2/2/2
46	PC1	B	202	-	-	19/41/41/57	-
58	EHZ	U	201	20	-	16/42/44/45	-
59	MYR	o	201	40	-	6/11/12/13	-
52	CDL	h	201	-	-	31/65/65/110	-
45	LMT	M	501	-	-	14/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	L	705	-	-	36/74/74/110	-
45	LMT	L	701	-	-	7/21/61/61	0/2/2/2
53	3PE	r	201	-	-	16/48/48/54	-
53	3PE	M	502	-	-	19/39/39/54	-
45	LMT	P	502	-	-	13/21/61/61	0/2/2/2
47	SF4	F	501	6	-	-	0/6/5/5
53	3PE	Z	201	-	-	21/34/34/54	-
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
52	CDL	H	401	-	-	24/57/57/110	-
53	3PE	N	402	-	-	16/36/36/54	-
53	3PE	i	201	34	-	19/33/33/54	-
56	NDP	P	501	-	-	3/30/77/77	0/5/5/5
49	FES	G	803	7	-	-	0/1/1/1
53	3PE	Z	202	-	-	20/44/44/54	-
45	LMT	A	401	-	-	10/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	J	201	-	-	10/21/61/61	0/2/2/2
45	LMT	Y	203	-	-	15/21/61/61	0/2/2/2
58	EHZ	T	201	20	-	17/42/44/45	-
47	SF4	G	802	7	-	-	0/6/5/5
52	CDL	h	202	-	-	32/56/56/110	-
53	3PE	d	201	-	-	18/36/36/54	-
45	LMT	L	704	-	-	11/21/61/61	0/2/2/2
50	FMN	F	502	-	-	9/18/18/18	0/3/3/3
55	GTP	O	502	-	-	7/18/38/38	0/3/3/3
53	3PE	O	504	-	-	14/33/33/54	-
47	SF4	B	201	2	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
45	LMT	O	503	-	-	9/21/61/61	0/2/2/2
45	LMT	A	403	-	-	10/21/61/61	0/2/2/2
47	SF4	I	201	9	-	-	0/6/5/5
46	PC1	B	203	-	-	20/44/44/57	-
53	3PE	X	201	-	-	16/39/39/54	-
52	CDL	q	501	-	-	36/73/73/110	-
45	LMT	K	201	-	-	6/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
53	3PE	I	203	-	-	16/47/47/54	-
46	PC1	A	402	-	-	15/32/32/57	-
53	3PE	M	503	-	-	17/39/39/54	-
48	HQH	D	601	-	-	10/27/29/29	0/1/1/1

All (217) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	10.62	1.79	1.59
50	F	502	FMN	O4-C4	8.42	1.39	1.23
55	O	502	GTP	O6-C6	8.17	1.39	1.23
50	F	502	FMN	O2-C2	8.16	1.39	1.24
52	h	202	CDL	OA6-CA4	-6.08	1.39	1.46
58	T	201	EHZ	C15-N2	5.62	1.45	1.33
55	O	502	GTP	O4'-C1'	5.41	1.48	1.41
58	U	201	EHZ	C15-N2	4.92	1.44	1.33
58	U	201	EHZ	C12-N1	4.77	1.44	1.33
58	T	201	EHZ	C12-N1	4.77	1.44	1.33
55	O	502	GTP	C2-N1	4.58	1.49	1.37
55	O	502	GTP	C2-N3	4.46	1.44	1.33
55	O	502	GTP	C2-N2	4.42	1.44	1.34
50	F	502	FMN	C2-N1	3.89	1.46	1.36
55	O	502	GTP	C5-C6	-3.61	1.40	1.47
55	O	502	GTP	C2'-C1'	-3.47	1.48	1.53
56	P	501	NDP	O2B-C2B	-3.33	1.32	1.44
56	P	501	NDP	PN-O5D	3.26	1.72	1.59
45	M	501	LMT	O3'-C3'	-3.14	1.35	1.43
45	K	201	LMT	O2B-C2B	-3.07	1.35	1.43
52	h	202	CDL	OA6-CA5	3.03	1.40	1.33
45	A	401	LMT	O3'-C3'	-3.00	1.35	1.43
45	J	201	LMT	O3'-C3'	-2.97	1.36	1.43
45	M	501	LMT	O2'-C2'	-2.96	1.36	1.43
45	Y	203	LMT	O3'-C3'	-2.94	1.36	1.43
45	L	704	LMT	O3'-C3'	-2.90	1.36	1.43
45	Y	202	LMT	O3'-C3'	-2.90	1.36	1.43
52	h	201	CDL	OB6-CB4	-2.89	1.39	1.46
53	I	203	3PE	O21-C2	-2.89	1.39	1.46
45	Y	201	LMT	O3'-C3'	-2.87	1.36	1.43
45	Y	202	LMT	O2'-C2'	-2.87	1.36	1.43
52	q	501	CDL	OA6-CA4	-2.87	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	Z	202	3PE	O21-C2	-2.87	1.39	1.46
46	B	203	PC1	O21-C2	-2.85	1.39	1.46
45	J	202	LMT	O3'-C3'	-2.84	1.36	1.43
45	Y	204	LMT	O3'-C3'	-2.82	1.36	1.43
53	L	702	3PE	O21-C2	-2.82	1.39	1.46
45	j	101	LMT	O3'-C3'	-2.81	1.36	1.43
45	K	201	LMT	O3'-C3'	-2.77	1.36	1.43
45	Y	201	LMT	O2'-C2'	-2.77	1.36	1.43
52	h	202	CDL	OB6-CB4	-2.77	1.39	1.46
52	L	705	CDL	OB6-CB4	-2.76	1.39	1.46
52	q	501	CDL	OB6-CB4	-2.75	1.39	1.46
53	i	201	3PE	O31-C31	2.74	1.41	1.33
46	A	402	PC1	O21-C2	-2.74	1.39	1.46
45	L	701	LMT	O3'-C3'	-2.73	1.36	1.43
45	Y	204	LMT	O2'-C2'	-2.73	1.36	1.43
45	K	201	LMT	O2'-C2'	-2.72	1.36	1.43
52	h	201	CDL	OA6-CA4	-2.72	1.39	1.46
53	X	201	3PE	O21-C2	-2.69	1.39	1.46
53	i	201	3PE	O21-C2	-2.68	1.39	1.46
45	L	701	LMT	O2B-C2B	-2.67	1.36	1.43
45	Y	201	LMT	O2B-C2B	-2.66	1.36	1.43
45	A	403	LMT	O2'-C2'	-2.66	1.36	1.43
53	Z	201	3PE	O21-C2	-2.65	1.40	1.46
45	O	503	LMT	O3'-C3'	-2.65	1.36	1.43
53	N	401	3PE	O31-C31	2.65	1.41	1.33
53	r	201	3PE	O21-C2	-2.64	1.40	1.46
53	N	401	3PE	O21-C2	-2.64	1.40	1.46
45	A	403	LMT	O3'-C3'	-2.63	1.36	1.43
58	U	201	EHZ	O3-C12	-2.63	1.17	1.23
52	L	705	CDL	OA6-CA4	-2.63	1.40	1.46
45	J	201	LMT	O2B-C2B	-2.63	1.36	1.43
45	h	203	LMT	O3'-C3'	-2.61	1.36	1.43
45	M	501	LMT	O2B-C2B	-2.61	1.36	1.43
56	P	501	NDP	O4B-C4B	-2.61	1.39	1.45
45	P	502	LMT	O3'-C3'	-2.60	1.36	1.43
45	P	502	LMT	O2'-C2'	-2.60	1.36	1.43
53	d	201	3PE	O21-C2	-2.59	1.40	1.46
50	F	502	FMN	P-O2P	-2.58	1.44	1.54
46	B	202	PC1	O21-C2	-2.57	1.40	1.46
45	M	501	LMT	O4'-C4B	-2.57	1.36	1.43
45	O	503	LMT	O2'-C2'	-2.56	1.36	1.43
53	N	402	3PE	O21-C2	-2.56	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	701	LMT	O2'-C2'	-2.55	1.37	1.43
55	O	502	GTP	C2'-C3'	-2.54	1.46	1.53
46	B	203	PC1	O31-C3	-2.53	1.39	1.45
45	h	203	LMT	O3B-C3B	-2.52	1.37	1.43
53	r	201	3PE	O31-C31	2.52	1.40	1.33
53	O	504	3PE	O31-C31	2.51	1.40	1.33
45	K	201	LMT	O1'-C1'	-2.50	1.35	1.40
45	J	202	LMT	O3B-C3B	-2.49	1.37	1.43
58	T	201	EHZ	O3-C12	-2.48	1.18	1.23
45	O	503	LMT	O2B-C2B	-2.48	1.37	1.43
45	J	202	LMT	O2B-C2B	-2.47	1.37	1.43
58	U	201	EHZ	O4-C15	-2.47	1.18	1.23
45	Y	201	LMT	O4'-C4B	-2.47	1.37	1.43
52	h	201	CDL	OB8-CB7	2.47	1.40	1.33
53	M	502	3PE	O31-C31	2.46	1.40	1.33
50	F	502	FMN	P-O3P	-2.46	1.45	1.54
52	L	705	CDL	OA8-CA7	2.45	1.40	1.33
53	M	503	3PE	O21-C2	-2.44	1.40	1.46
52	q	501	CDL	OB8-CB7	2.43	1.40	1.33
48	D	601	HQH	C12-C19	2.43	1.40	1.37
45	P	502	LMT	O2B-C2B	-2.42	1.37	1.43
52	H	401	CDL	OB6-CB4	-2.42	1.40	1.46
53	X	201	3PE	O31-C3	-2.42	1.39	1.45
58	T	201	EHZ	O4-C15	-2.42	1.18	1.23
55	O	502	GTP	PG-O2G	-2.42	1.45	1.54
55	O	502	GTP	PG-O3G	-2.41	1.45	1.54
45	P	502	LMT	O3B-C3B	-2.41	1.37	1.43
53	Z	201	3PE	O31-C31	2.41	1.40	1.33
46	B	202	PC1	O31-C31	2.41	1.40	1.33
52	h	202	CDL	OB8-CB7	2.41	1.40	1.33
53	M	502	3PE	O21-C2	-2.40	1.40	1.46
45	L	701	LMT	O4'-C4B	-2.39	1.37	1.43
50	F	502	FMN	C4A-N5	2.39	1.35	1.30
45	J	202	LMT	O2'-C2'	-2.39	1.37	1.43
45	A	401	LMT	O3B-C3B	-2.39	1.37	1.43
45	K	201	LMT	O3B-C3B	-2.39	1.37	1.43
46	A	402	PC1	O31-C3	-2.39	1.39	1.45
45	j	101	LMT	O3B-C3B	-2.38	1.37	1.43
45	L	704	LMT	O2B-C2B	-2.38	1.37	1.43
53	L	702	3PE	O31-C31	2.38	1.40	1.33
53	O	504	3PE	O21-C2	-2.37	1.40	1.46
53	M	503	3PE	O31-C3	-2.36	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	O	503	LMT	O3B-C3B	-2.36	1.37	1.43
45	Y	204	LMT	O3B-C3B	-2.35	1.37	1.43
45	Y	203	LMT	O3B-C3B	-2.35	1.37	1.43
45	A	403	LMT	O2B-C2B	-2.35	1.37	1.43
45	Y	202	LMT	O2B-C2B	-2.34	1.37	1.43
53	d	201	3PE	O31-C3	-2.33	1.39	1.45
45	J	201	LMT	O3B-C3B	-2.33	1.37	1.43
45	A	403	LMT	O3B-C3B	-2.33	1.37	1.43
45	A	401	LMT	O2'-C2'	-2.32	1.37	1.43
53	N	402	3PE	O31-C31	2.32	1.40	1.33
45	Y	204	LMT	O2B-C2B	-2.31	1.37	1.43
45	h	203	LMT	O2'-C2'	-2.31	1.37	1.43
52	h	202	CDL	OA8-CA7	2.30	1.40	1.33
45	L	701	LMT	O3B-C3B	-2.29	1.37	1.43
52	H	401	CDL	OB8-CB7	2.28	1.40	1.33
45	h	203	LMT	O2B-C2B	-2.28	1.37	1.43
45	K	201	LMT	O5'-C5'	-2.28	1.38	1.44
45	Y	201	LMT	O1'-C1'	-2.28	1.36	1.40
53	Z	202	3PE	O31-C31	2.28	1.40	1.33
45	A	401	LMT	O4'-C4B	-2.27	1.37	1.43
45	j	101	LMT	O2'-C2'	-2.27	1.37	1.43
52	h	202	CDL	OB8-CB6	-2.27	1.40	1.45
56	P	501	NDP	C7N-C3N	-2.26	1.43	1.48
46	B	202	PC1	O31-C3	-2.26	1.40	1.45
56	P	501	NDP	O3B-C3B	-2.26	1.37	1.43
45	j	101	LMT	O2B-C2B	-2.25	1.37	1.43
53	O	504	3PE	O21-C21	2.25	1.40	1.34
53	I	203	3PE	O31-C3	-2.24	1.40	1.45
45	Y	203	LMT	O2B-C2B	-2.24	1.37	1.43
52	h	202	CDL	OA8-CA6	-2.24	1.40	1.45
45	L	704	LMT	O2'-C2'	-2.24	1.37	1.43
53	d	201	3PE	O31-C31	2.23	1.39	1.33
45	P	502	LMT	O1'-C1'	-2.23	1.36	1.40
45	Y	204	LMT	O1'-C1'	-2.23	1.36	1.40
45	J	202	LMT	O1'-C1'	-2.22	1.36	1.40
45	L	701	LMT	O1'-C1'	-2.22	1.36	1.40
45	Y	201	LMT	O3B-C3B	-2.22	1.37	1.43
45	A	401	LMT	O2B-C2B	-2.21	1.37	1.43
53	L	703	3PE	O31-C31	2.21	1.39	1.33
45	Y	203	LMT	O2'-C2'	-2.21	1.37	1.43
56	P	501	NDP	O2D-C2D	-2.21	1.37	1.43
52	L	705	CDL	OB8-CB7	2.20	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	501	LMT	O3B-C3B	-2.20	1.37	1.43
52	H	401	CDL	OA6-CA4	-2.20	1.41	1.46
45	h	203	LMT	O4'-C4B	-2.20	1.37	1.43
53	I	203	3PE	O31-C31	2.20	1.39	1.33
53	Z	202	3PE	O31-C3	-2.19	1.40	1.45
52	L	705	CDL	OB8-CB6	-2.19	1.40	1.45
45	Y	203	LMT	O4'-C4B	-2.19	1.37	1.43
45	J	201	LMT	O4'-C4B	-2.19	1.37	1.43
53	L	703	3PE	O21-C2	-2.18	1.41	1.46
45	Y	202	LMT	O3B-C3B	-2.18	1.37	1.43
45	Y	204	LMT	O4'-C4B	-2.18	1.37	1.43
46	A	402	PC1	O31-C31	2.17	1.39	1.33
53	N	402	3PE	O21-C21	2.17	1.40	1.34
45	M	501	LMT	O5'-C5'	-2.17	1.39	1.44
52	H	401	CDL	OA6-CA5	2.17	1.40	1.34
45	L	704	LMT	O4'-C4B	-2.17	1.37	1.43
53	L	702	3PE	O31-C3	-2.16	1.40	1.45
53	L	703	3PE	O21-C21	2.16	1.40	1.34
45	J	201	LMT	O2'-C2'	-2.16	1.37	1.43
45	L	704	LMT	O3B-C3B	-2.16	1.37	1.43
58	U	201	EHZ	C9-S1	2.15	1.81	1.76
56	P	501	NDP	O5D-C5D	-2.15	1.36	1.44
52	H	401	CDL	OB8-CB6	-2.15	1.40	1.45
45	L	704	LMT	O1'-C1'	-2.13	1.36	1.40
45	A	401	LMT	O1'-C1'	-2.13	1.36	1.40
45	L	704	LMT	O5'-C5'	-2.12	1.39	1.44
52	q	501	CDL	OB6-CB5	2.12	1.40	1.34
46	B	202	PC1	O21-C21	2.11	1.40	1.34
45	O	503	LMT	O4'-C4B	-2.11	1.38	1.43
52	H	401	CDL	OB6-CB5	2.11	1.40	1.34
53	Z	201	3PE	O31-C3	-2.10	1.40	1.45
53	L	703	3PE	O31-C3	-2.10	1.40	1.45
53	X	201	3PE	O31-C31	2.10	1.39	1.33
45	M	501	LMT	O1'-C1'	-2.09	1.36	1.40
53	M	503	3PE	O21-C21	2.09	1.40	1.34
45	K	201	LMT	O4'-C4B	-2.09	1.38	1.43
52	h	201	CDL	OA6-CA5	2.09	1.39	1.35
53	N	402	3PE	O31-C3	-2.09	1.40	1.45
53	r	201	3PE	O31-C3	-2.09	1.40	1.45
52	h	201	CDL	OB8-CB6	-2.08	1.40	1.45
58	T	201	EHZ	O6-C20	-2.08	1.39	1.44
53	N	401	3PE	O21-C21	2.07	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	M	503	3PE	O31-C31	2.06	1.39	1.33
48	D	601	HQH	C22-C11	-2.06	1.46	1.50
53	r	201	3PE	O21-C21	2.06	1.40	1.34
53	i	201	3PE	O21-C21	2.04	1.40	1.34
52	L	705	CDL	OA6-CA5	2.04	1.40	1.34
53	M	502	3PE	O21-C21	2.04	1.40	1.34
53	Z	202	3PE	O21-C21	2.04	1.40	1.34
45	Y	202	LMT	O4'-C4B	-2.03	1.38	1.43
52	q	501	CDL	OB8-CB6	-2.03	1.40	1.45
52	L	705	CDL	OA8-CA6	-2.03	1.40	1.45
55	O	502	GTP	PB-O2B	-2.03	1.45	1.55
45	Y	202	LMT	O1'-C1'	-2.02	1.36	1.40
53	O	504	3PE	O31-C3	-2.02	1.40	1.45
45	J	202	LMT	O4'-C4B	-2.01	1.38	1.43
53	X	201	3PE	O21-C21	2.00	1.40	1.34
53	N	401	3PE	O31-C3	-2.00	1.40	1.45
52	h	202	CDL	OB6-CB5	2.00	1.40	1.34

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	P	501	NDP	PN-O3-PA	-6.41	110.84	132.83
45	O	503	LMT	C1-O1'-C1'	5.12	122.33	113.84
45	O	503	LMT	O1'-C1'-C2'	4.97	116.06	108.30
52	H	401	CDL	OB6-CB5-C51	4.79	121.83	111.50
52	L	705	CDL	OA6-CA5-C11	4.57	121.35	111.50
52	h	201	CDL	OA6-CA5-C11	4.51	119.39	111.09
52	h	202	CDL	OB6-CB5-C51	4.51	121.22	111.50
45	M	501	LMT	O5B-C5B-C4B	4.42	117.72	109.69
58	U	201	EHZ	C8-C9-S1	4.36	119.03	113.63
52	h	202	CDL	OA6-CA5-OA7	-4.25	120.17	125.57
55	O	502	GTP	PB-O3B-PG	-4.24	118.27	132.83
55	O	502	GTP	C3'-C2'-C1'	4.21	107.32	100.98
46	B	202	PC1	O21-C21-C22	4.21	120.57	111.50
46	B	203	PC1	O21-C21-C22	4.18	120.52	111.50
53	X	201	3PE	O21-C21-C22	4.17	120.48	111.50
58	T	201	EHZ	C8-C9-S1	4.17	118.78	113.63
53	M	502	3PE	O21-C21-C22	4.13	120.41	111.50
52	H	401	CDL	OA6-CA5-C11	4.10	120.33	111.50
58	U	201	EHZ	C14-C13-C12	-4.08	105.56	112.36
53	L	702	3PE	O21-C21-C22	4.07	120.28	111.50
52	L	705	CDL	OB6-CB5-C51	3.98	120.08	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	M	503	3PE	O21-C21-C22	3.96	120.04	111.50
53	N	401	3PE	O21-C21-C22	3.92	119.95	111.50
53	r	201	3PE	O21-C21-C22	3.91	119.93	111.50
52	h	201	CDL	OB6-CB5-C51	3.86	119.83	111.50
53	i	201	3PE	O21-C21-C22	3.86	119.83	111.50
53	Z	201	3PE	O21-C21-C22	3.85	119.80	111.50
53	N	402	3PE	O21-C21-C22	3.78	119.66	111.50
55	O	502	GTP	PA-O3A-PB	-3.75	119.96	132.83
52	q	501	CDL	OB6-CB5-C51	3.74	119.56	111.50
53	d	201	3PE	O21-C21-C22	3.69	119.46	111.50
52	q	501	CDL	OA6-CA5-C11	3.68	119.42	111.50
53	Z	202	3PE	O21-C21-C22	3.67	119.41	111.50
53	i	201	3PE	O31-C31-C32	3.65	123.37	111.91
53	I	203	3PE	O21-C21-C22	3.65	119.37	111.50
53	O	504	3PE	O21-C21-C22	3.58	119.22	111.50
53	L	703	3PE	O21-C21-C22	3.55	119.16	111.50
50	F	502	FMN	C4-N3-C2	-3.54	119.10	125.64
50	F	502	FMN	C9-C9A-N10	3.49	126.56	121.84
56	P	501	NDP	O2B-P2B-O1X	-3.34	96.49	109.39
58	U	201	EHZ	C13-C12-N1	3.34	122.04	116.42
58	T	201	EHZ	C11-N1-C12	-3.29	116.73	122.84
52	H	401	CDL	OB8-CB7-C71	3.28	119.98	111.38
55	O	502	GTP	C2-N1-C6	-3.24	119.13	125.10
45	J	201	LMT	C3'-C4'-C5'	-3.22	103.54	110.93
46	A	402	PC1	O21-C21-C22	3.21	119.76	110.80
58	T	201	EHZ	C13-C12-N1	3.19	121.80	116.42
48	D	601	HQH	O2-C24-N5	3.18	123.05	113.49
53	M	502	3PE	O31-C31-C32	3.17	119.70	111.38
55	O	502	GTP	C5-C6-N1	3.15	119.51	113.95
50	F	502	FMN	O5'-P-O1P	3.13	115.24	106.47
52	h	202	CDL	OB8-CB7-C71	3.11	121.68	111.91
45	K	201	LMT	C2'-C3'-C4'	3.11	116.79	109.68
45	A	403	LMT	C3B-C4B-C5B	-3.08	104.74	110.24
46	B	202	PC1	O31-C31-C32	3.06	121.50	111.91
45	Y	203	LMT	C3'-C4'-C5'	-2.98	104.08	110.93
45	L	704	LMT	C3'-C4'-C5'	-2.97	104.12	110.93
55	O	502	GTP	O3G-PG-O3B	2.96	114.56	104.64
48	D	601	HQH	O3-C25-C23	2.95	126.53	116.56
45	Y	204	LMT	C1'-O5'-C5'	-2.94	107.92	113.69
56	P	501	NDP	PA-O5B-C5B	-2.93	104.50	121.68
45	K	201	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
53	Z	202	3PE	O31-C31-C32	2.86	120.88	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	P	502	LMT	C1'-O5'-C5'	-2.84	108.11	113.69
45	Y	202	LMT	C1'-O5'-C5'	-2.81	108.18	113.69
53	L	703	3PE	O31-C31-C32	2.81	120.71	111.91
53	d	201	3PE	O31-C31-C32	2.79	120.67	111.91
50	F	502	FMN	C4A-C4-N3	2.78	120.26	113.19
52	L	705	CDL	OA8-CA7-C31	2.77	120.60	111.91
50	F	502	FMN	C6-C5A-N5	-2.75	113.71	118.51
53	r	201	3PE	O31-C31-C32	2.74	120.52	111.91
50	F	502	FMN	O2P-P-O5'	2.69	113.90	106.73
45	h	203	LMT	C1'-O5'-C5'	-2.69	108.40	113.69
46	B	203	PC1	O31-C31-C32	2.68	120.31	111.91
55	O	502	GTP	C2'-C3'-C4'	2.65	107.79	102.64
56	P	501	NDP	PN-O5D-C5D	-2.64	106.19	121.68
52	L	705	CDL	OB8-CB7-C71	2.64	120.19	111.91
52	q	501	CDL	OB8-CB7-C71	2.62	120.12	111.91
53	X	201	3PE	O31-C31-C32	2.61	120.10	111.91
58	T	201	EHZ	C7-C8-C9	-2.60	107.95	113.89
52	h	201	CDL	OB8-CB7-C71	2.60	120.08	111.91
45	L	704	LMT	C1'-O5'-C5'	-2.59	108.60	113.69
53	Z	201	3PE	O31-C31-C32	2.59	120.03	111.91
48	D	601	HQH	C15-C21-C18	2.58	128.19	124.18
50	F	502	FMN	O3P-P-O5'	2.54	113.49	106.73
53	N	402	3PE	O31-C31-C32	2.54	119.88	111.91
48	D	601	HQH	C10-C6-C8	-2.54	105.83	110.05
56	P	501	NDP	O3X-P2B-O2X	2.53	117.32	107.64
45	J	201	LMT	C1'-O5'-C5'	-2.52	108.75	113.69
52	h	202	CDL	OA8-CA7-C31	2.50	119.75	111.91
56	P	501	NDP	O5D-PN-O1N	-2.49	99.33	109.07
53	I	203	3PE	O31-C31-C32	2.49	119.72	111.91
52	h	201	CDL	CA4-OA6-CA5	-2.47	113.29	117.90
45	A	401	LMT	C3'-C4'-C5'	-2.47	105.27	110.93
53	L	702	3PE	O31-C31-C32	2.46	119.64	111.91
53	O	504	3PE	O31-C31-C32	2.45	119.60	111.91
50	F	502	FMN	O4-C4-C4A	-2.45	120.10	126.60
45	P	502	LMT	O1'-C1'-C2'	2.44	112.12	108.30
56	P	501	NDP	C2A-N1A-C6A	-2.43	114.60	118.75
45	A	403	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
45	P	502	LMT	O5B-C5B-C4B	2.40	114.06	109.69
53	N	401	3PE	O31-C31-C32	2.39	119.42	111.91
53	M	503	3PE	O31-C31-C32	2.39	119.40	111.91
58	U	201	EHZ	C11-N1-C12	-2.38	118.42	122.84
45	j	101	LMT	C3'-C4'-C5'	-2.36	105.51	110.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	O	503	LMT	O5'-C1'-C2'	-2.35	105.37	110.35
58	U	201	EHZ	C10-S1-C9	2.35	109.18	101.87
45	h	203	LMT	O1'-C1'-C2'	2.30	111.90	108.30
58	T	201	EHZ	C19-C17-C16	2.30	112.81	108.82
58	U	201	EHZ	C7-C8-C9	-2.29	108.66	113.89
45	O	503	LMT	C1'-O5'-C5'	-2.29	109.20	113.69
58	T	201	EHZ	O2-C9-S1	-2.27	119.67	122.61
45	M	501	LMT	C1'-O5'-C5'	-2.26	109.25	113.69
45	Y	204	LMT	C3'-C4'-C5'	-2.25	105.77	110.93
45	L	701	LMT	O5B-C5B-C4B	2.23	113.74	109.69
45	Y	204	LMT	C3B-C4B-C5B	-2.23	106.27	110.24
50	F	502	FMN	C5'-C4'-C3'	-2.22	107.92	112.20
45	P	502	LMT	O5B-C5B-C6B	2.21	111.93	106.44
45	Y	201	LMT	C1-O1'-C1'	2.20	117.48	113.84
55	O	502	GTP	O6-C6-C5	-2.18	120.11	124.37
53	L	703	3PE	O31-C31-O32	-2.17	118.11	123.59
56	P	501	NDP	O2N-PN-O1N	2.14	122.82	112.24
56	P	501	NDP	O3X-P2B-O2B	-2.14	96.41	105.99
45	A	401	LMT	O5'-C1'-O1'	-2.11	104.97	109.97
58	U	201	EHZ	C10-C11-N1	-2.10	108.00	112.42
45	Y	202	LMT	O5B-C5B-C4B	2.10	113.50	109.69
50	F	502	FMN	C9A-C5A-N5	2.10	124.71	122.43
46	A	402	PC1	O31-C31-C32	2.09	118.48	111.91
58	T	201	EHZ	C14-C13-C12	-2.09	108.87	112.36
58	U	201	EHZ	C13-C14-N2	-2.09	107.68	111.90
45	M	501	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
45	Y	203	LMT	C3B-C4B-C5B	-2.06	106.57	110.24
55	O	502	GTP	O2A-PA-O1A	-2.05	102.11	112.24
55	O	502	GTP	O2B-PB-O1B	-2.04	102.15	112.24
45	L	704	LMT	O5B-C5B-C4B	2.02	113.36	109.69
45	L	704	LMT	O5'-C1'-O1'	-2.02	105.20	109.97
52	q	501	CDL	OA8-CA7-C31	2.01	121.16	112.38
58	T	201	EHZ	C13-C14-N2	2.01	115.95	111.90
58	T	201	EHZ	C10-S1-C9	2.00	108.10	101.87

There are no chirality outliers.

All (699) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	401	LMT	O5'-C1'-O1'-C1
45	A	401	LMT	C2-C1-O1'-C1'
45	K	201	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	701	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	O5'-C1'-O1'-C1
45	M	501	LMT	C2-C1-O1'-C1'
45	O	503	LMT	C2'-C1'-O1'-C1
45	O	503	LMT	C2-C1-O1'-C1'
45	Y	201	LMT	C2'-C1'-O1'-C1
45	Y	201	LMT	O5'-C1'-O1'-C1
45	Y	202	LMT	C2'-C1'-O1'-C1
45	Y	202	LMT	O5'-C1'-O1'-C1
45	Y	203	LMT	C2'-C1'-O1'-C1
45	Y	203	LMT	O5'-C1'-O1'-C1
45	Y	203	LMT	C2-C1-O1'-C1'
45	j	101	LMT	O5'-C1'-O1'-C1
46	A	402	PC1	C11-O13-P-O14
46	A	402	PC1	C11-O13-P-O11
46	A	402	PC1	C1-O11-P-O12
46	A	402	PC1	C1-O11-P-O13
46	A	402	PC1	O13-C11-C12-N
46	A	402	PC1	O22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	O22-C21-O21-C2
46	B	202	PC1	C22-C21-O21-C2
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	O11-C1-C2-O21
46	B	203	PC1	C22-C21-O21-C2
48	D	601	HQH	C22-C11-C8-C6
48	D	601	HQH	C18-C11-C8-C6
48	D	601	HQH	C19-C12-C13-C20
48	D	601	HQH	N5-C12-C13-C20
50	F	502	FMN	C1'-C2'-C3'-O3'
50	F	502	FMN	C1'-C2'-C3'-C4'
50	F	502	FMN	C5'-O5'-P-O2P
50	F	502	FMN	C5'-O5'-P-O3P
52	H	401	CDL	CA4-CA3-OA5-PA1
52	H	401	CDL	OA9-CA7-OA8-CA6
52	H	401	CDL	CB3-OB5-PB2-OB2
52	H	401	CDL	CB3-OB5-PB2-OB4
52	L	705	CDL	C11-CA5-OA6-CA4
52	L	705	CDL	CB2-OB2-PB2-OB3
52	L	705	CDL	CB2-OB2-PB2-OB4
52	L	705	CDL	CB2-OB2-PB2-OB5
52	h	201	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	h	201	CDL	CA3-OA5-PA1-OA4
52	h	201	CDL	OA7-CA5-OA6-CA4
52	h	201	CDL	C11-CA5-OA6-CA4
52	h	201	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	OB6-CB4-CB6-OB8
52	h	202	CDL	CA2-C1-CB2-OB2
52	h	202	CDL	CA3-CA4-OA6-CA5
52	h	202	CDL	CA6-CA4-OA6-CA5
52	h	202	CDL	OA7-CA5-OA6-CA4
52	h	202	CDL	CB2-OB2-PB2-OB4
52	h	202	CDL	CB3-OB5-PB2-OB3
52	h	202	CDL	CB3-OB5-PB2-OB4
52	h	202	CDL	C51-CB5-OB6-CB4
52	q	501	CDL	CA2-OA2-PA1-OA4
52	q	501	CDL	CA3-OA5-PA1-OA3
52	q	501	CDL	CB3-OB5-PB2-OB2
52	q	501	CDL	CB3-OB5-PB2-OB3
53	I	203	3PE	O13-C11-C12-N
53	I	203	3PE	O11-C1-C2-O21
53	L	702	3PE	C1-O11-P-O14
53	L	702	3PE	O21-C2-C3-O31
53	L	703	3PE	C11-O13-P-O11
53	L	703	3PE	C11-O13-P-O14
53	L	703	3PE	O13-C11-C12-N
53	M	502	3PE	C1-O11-P-O12
53	M	503	3PE	C1-O11-P-O12
53	M	503	3PE	C1-O11-P-O14
53	N	401	3PE	C12-C11-O13-P
53	N	401	3PE	O13-C11-C12-N
53	N	401	3PE	O22-C21-O21-C2
53	N	402	3PE	C11-O13-P-O14
53	N	402	3PE	C12-C11-O13-P
53	N	402	3PE	O13-C11-C12-N
53	N	402	3PE	C22-C21-O21-C2
53	O	504	3PE	O21-C2-C3-O31
53	X	201	3PE	C12-C11-O13-P
53	X	201	3PE	O13-C11-C12-N
53	X	201	3PE	O22-C21-O21-C2
53	X	201	3PE	C22-C21-O21-C2
53	Z	201	3PE	C1-O11-P-O12
53	Z	201	3PE	C1-O11-P-O14
53	Z	201	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	Z	201	3PE	C11-O13-P-O14
53	Z	201	3PE	O13-C11-C12-N
53	Z	202	3PE	C12-C11-O13-P
53	Z	202	3PE	O13-C11-C12-N
53	d	201	3PE	C11-O13-P-O14
53	d	201	3PE	C22-C21-O21-C2
53	i	201	3PE	C11-O13-P-O12
53	i	201	3PE	C11-O13-P-O14
53	i	201	3PE	C12-C11-O13-P
53	i	201	3PE	O32-C31-O31-C3
53	i	201	3PE	C32-C31-O31-C3
53	i	201	3PE	C22-C21-O21-C2
55	O	502	GTP	PB-O3B-PG-O2G
55	O	502	GTP	C5'-O5'-PA-O3A
55	O	502	GTP	C5'-O5'-PA-O1A
58	T	201	EHZ	S1-C10-C11-N1
58	T	201	EHZ	C11-C10-S1-C9
58	T	201	EHZ	C15-C16-C17-C20
58	T	201	EHZ	O5-C16-C17-C19
58	T	201	EHZ	O5-C16-C17-C20
58	U	201	EHZ	C15-C16-C17-C19
58	U	201	EHZ	C15-C16-C17-C20
59	o	201	MYR	C1-C2-C3-C4
46	B	202	PC1	O32-C31-O31-C3
45	P	502	LMT	O5B-C1B-O1B-C4'
58	T	201	EHZ	C13-C14-N2-C15
46	B	202	PC1	C32-C31-O31-C3
52	H	401	CDL	C71-CB7-OB8-CB6
52	H	401	CDL	OB9-CB7-OB8-CB6
52	L	705	CDL	OA9-CA7-OA8-CA6
52	h	202	CDL	OA9-CA7-OA8-CA6
52	h	202	CDL	OB9-CB7-OB8-CB6
53	Z	201	3PE	O32-C31-O31-C3
45	O	503	LMT	O5B-C5B-C6B-O6B
46	B	203	PC1	O22-C21-O21-C2
52	L	705	CDL	OA7-CA5-OA6-CA4
52	h	202	CDL	OB7-CB5-OB6-CB4
53	N	402	3PE	O22-C21-O21-C2
53	d	201	3PE	O22-C21-O21-C2
53	i	201	3PE	O22-C21-O21-C2
52	L	705	CDL	C31-CA7-OA8-CA6
52	h	202	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	h	202	CDL	C71-CB7-OB8-CB6
53	Z	201	3PE	C32-C31-O31-C3
45	A	403	LMT	O5'-C5'-C6'-O6'
46	A	402	PC1	C22-C21-O21-C2
53	N	401	3PE	C22-C21-O21-C2
46	B	203	PC1	C32-C31-O31-C3
45	Y	203	LMT	O5B-C5B-C6B-O6B
45	J	202	LMT	O5'-C5'-C6'-O6'
45	Y	201	LMT	O5'-C5'-C6'-O6'
52	h	202	CDL	O1-C1-CB2-OB2
45	J	201	LMT	O5'-C5'-C6'-O6'
45	L	701	LMT	O5B-C5B-C6B-O6B
45	L	701	LMT	C4B-C5B-C6B-O6B
45	O	503	LMT	C4B-C5B-C6B-O6B
45	Y	202	LMT	O5B-C1B-O1B-C4'
45	M	501	LMT	O5'-C5'-C6'-O6'
45	J	202	LMT	O5B-C5B-C6B-O6B
45	A	403	LMT	C4'-C5'-C6'-O6'
45	J	201	LMT	C3'-C4'-O1B-C1B
45	h	203	LMT	O5B-C5B-C6B-O6B
45	j	101	LMT	O5B-C5B-C6B-O6B
46	B	203	PC1	O32-C31-O31-C3
45	Y	204	LMT	O5'-C5'-C6'-O6'
45	P	502	LMT	C4'-C5'-C6'-O6'
52	q	501	CDL	OA9-CA7-OA8-CA6
45	j	101	LMT	O5'-C5'-C6'-O6'
45	Y	203	LMT	C4B-C5B-C6B-O6B
45	M	501	LMT	O5B-C5B-C6B-O6B
45	J	201	LMT	C4'-C5'-C6'-O6'
45	Y	201	LMT	C4B-C5B-C6B-O6B
52	q	501	CDL	C31-CA7-OA8-CA6
45	O	503	LMT	O5B-C1B-O1B-C4'
52	L	705	CDL	CB2-C1-CA2-OA2
52	L	705	CDL	CA2-C1-CB2-OB2
52	q	501	CDL	C71-CB7-OB8-CB6
53	Z	202	3PE	C32-C31-O31-C3
53	r	201	3PE	C32-C31-O31-C3
45	j	101	LMT	C4'-C5'-C6'-O6'
45	L	701	LMT	O5'-C5'-C6'-O6'
45	O	503	LMT	C2B-C1B-O1B-C4'
53	N	401	3PE	O11-C1-C2-O21
45	L	704	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	Z	202	3PE	C31-C32-C33-C34
45	J	201	LMT	C2'-C1'-O1'-C1
45	K	201	LMT	C2'-C1'-O1'-C1
45	j	101	LMT	C2'-C1'-O1'-C1
53	Z	202	3PE	O21-C2-C3-O31
53	Z	202	3PE	O32-C31-O31-C3
45	J	202	LMT	C4'-C5'-C6'-O6'
45	M	501	LMT	O5B-C1B-O1B-C4'
48	D	601	HQH	C22-C11-C18-C21
48	D	601	HQH	C8-C11-C18-C21
45	Y	202	LMT	O5'-C5'-C6'-O6'
45	M	501	LMT	C4'-C5'-C6'-O6'
53	L	702	3PE	C21-C22-C23-C24
53	d	201	3PE	C21-C22-C23-C24
53	r	201	3PE	O32-C31-O31-C3
45	L	704	LMT	O5B-C5B-C6B-O6B
45	P	502	LMT	O5'-C5'-C6'-O6'
45	Y	204	LMT	C4'-C5'-C6'-O6'
52	L	705	CDL	CA7-C31-C32-C33
45	A	403	LMT	O5B-C5B-C6B-O6B
52	h	202	CDL	CB5-C51-C52-C53
52	H	401	CDL	CB5-C51-C52-C53
52	L	705	CDL	CB5-C51-C52-C53
52	q	501	CDL	CB7-C71-C72-C73
53	N	401	3PE	C21-C22-C23-C24
56	P	501	NDP	O4D-C4D-C5D-O5D
58	T	201	EHZ	C5-C6-C7-O1
53	M	503	3PE	C32-C31-O31-C3
45	j	101	LMT	C5'-C4'-O1B-C1B
45	j	101	LMT	C4B-C5B-C6B-O6B
46	A	402	PC1	C31-C32-C33-C34
53	X	201	3PE	C31-C32-C33-C34
52	q	501	CDL	OB9-CB7-OB8-CB6
52	L	705	CDL	O1-C1-CA2-OA2
52	L	705	CDL	O1-C1-CB2-OB2
45	Y	201	LMT	C4'-C5'-C6'-O6'
53	L	703	3PE	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O13
52	H	401	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CA3-OA5-PA1-OA2
52	h	202	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	h	202	CDL	CB3-OB5-PB2-OB2
52	q	501	CDL	CA2-OA2-PA1-OA5
52	q	501	CDL	CA3-OA5-PA1-OA2
53	L	702	3PE	C1-O11-P-O13
53	M	502	3PE	C1-O11-P-O13
53	M	503	3PE	C1-O11-P-O13
53	M	503	3PE	C11-O13-P-O11
53	N	401	3PE	C11-O13-P-O11
53	N	402	3PE	C11-O13-P-O11
53	O	504	3PE	C11-O13-P-O11
53	Z	201	3PE	C1-O11-P-O13
53	Z	201	3PE	C11-O13-P-O11
53	i	201	3PE	C1-O11-P-O13
53	X	201	3PE	C32-C31-O31-C3
53	L	703	3PE	O22-C21-O21-C2
45	j	101	LMT	C3'-C4'-O1B-C1B
50	F	502	FMN	O2'-C2'-C3'-O3'
53	M	503	3PE	C22-C21-O21-C2
52	h	201	CDL	C57-C58-C59-C60
53	N	402	3PE	C34-C35-C36-C37
45	Y	204	LMT	C4B-C5B-C6B-O6B
53	L	702	3PE	C37-C38-C39-C3A
58	U	201	EHZ	C3-C4-C5-C6
59	o	201	MYR	C9-C10-C11-C12
45	M	501	LMT	O1'-C1-C2-C3
58	U	201	EHZ	C2-C1-C21-C22
45	P	502	LMT	C6-C7-C8-C9
45	h	203	LMT	C2-C3-C4-C5
46	B	203	PC1	C3A-C3B-C3C-C3D
53	I	203	3PE	C29-C2A-C2B-C2C
53	r	201	3PE	C26-C27-C28-C29
45	L	704	LMT	O1'-C1-C2-C3
46	B	203	PC1	C33-C34-C35-C36
45	A	401	LMT	C2'-C1'-O1'-C1
53	L	703	3PE	C32-C31-O31-C3
45	Y	202	LMT	C4-C5-C6-C7
45	Y	204	LMT	C6-C7-C8-C9
46	B	203	PC1	C37-C38-C39-C3A
52	L	705	CDL	C52-C53-C54-C55
53	O	504	3PE	C24-C25-C26-C27
53	d	201	3PE	C34-C35-C36-C37
53	r	201	3PE	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	X	201	3PE	O32-C31-O31-C3
45	A	403	LMT	C11-C10-C9-C8
46	B	202	PC1	C34-C35-C36-C37
46	B	202	PC1	C36-C37-C38-C39
52	H	401	CDL	C11-C12-C13-C14
53	M	502	3PE	C29-C2A-C2B-C2C
45	Y	201	LMT	O5B-C5B-C6B-O6B
53	M	503	3PE	O32-C31-O31-C3
45	P	502	LMT	C5'-C4'-O1B-C1B
52	q	501	CDL	C79-C80-C81-C82
53	i	201	3PE	C24-C25-C26-C27
53	M	503	3PE	O22-C21-O21-C2
52	H	401	CDL	C11-CA5-OA6-CA4
53	L	702	3PE	C22-C21-O21-C2
53	r	201	3PE	C22-C21-O21-C2
46	B	202	PC1	C24-C25-C26-C27
53	Z	201	3PE	C24-C25-C26-C27
45	J	201	LMT	C5'-C4'-O1B-C1B
45	Y	201	LMT	C5-C6-C7-C8
52	L	705	CDL	C71-C72-C73-C74
59	o	201	MYR	C3-C4-C5-C6
45	A	403	LMT	C1-C2-C3-C4
45	O	503	LMT	O5'-C1'-O1'-C1
52	H	401	CDL	C52-C53-C54-C55
53	M	502	3PE	O13-C11-C12-N
53	M	503	3PE	O13-C11-C12-N
52	h	202	CDL	C31-C32-C33-C34
58	U	201	EHZ	C1-C2-C3-C4
45	h	203	LMT	C4B-C5B-C6B-O6B
45	J	201	LMT	C3-C4-C5-C6
53	Z	202	3PE	C34-C35-C36-C37
45	K	201	LMT	C2-C1-O1'-C1'
45	P	502	LMT	C2-C1-O1'-C1'
45	Y	204	LMT	C2-C1-O1'-C1'
46	B	203	PC1	C24-C25-C26-C27
45	Y	203	LMT	C4-C5-C6-C7
53	M	503	3PE	C24-C25-C26-C27
52	H	401	CDL	OA7-CA5-OA6-CA4
53	r	201	3PE	O22-C21-O21-C2
45	O	503	LMT	O1'-C1-C2-C3
45	J	202	LMT	C11-C10-C9-C8
52	h	201	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	L	703	3PE	C3C-C3D-C3E-C3F
52	q	501	CDL	CA5-C11-C12-C13
45	P	502	LMT	O5B-C5B-C6B-O6B
53	L	702	3PE	C26-C27-C28-C29
53	X	201	3PE	C33-C34-C35-C36
52	h	201	CDL	OB7-CB5-OB6-CB4
53	L	702	3PE	O22-C21-O21-C2
45	J	201	LMT	C1-C2-C3-C4
50	F	502	FMN	O2'-C2'-C3'-C4'
53	I	203	3PE	C26-C27-C28-C29
53	N	401	3PE	C35-C36-C37-C38
45	Y	204	LMT	O1'-C1-C2-C3
53	I	203	3PE	C32-C31-O31-C3
46	B	202	PC1	C33-C34-C35-C36
53	L	703	3PE	O32-C31-O31-C3
52	q	501	CDL	OA7-CA5-OA6-CA4
52	q	501	CDL	C75-C76-C77-C78
53	M	502	3PE	C2D-C2E-C2F-C2G
45	L	704	LMT	C6-C7-C8-C9
52	L	705	CDL	C18-C19-C20-C21
52	h	201	CDL	C59-C60-C61-C62
53	r	201	3PE	C28-C29-C2A-C2B
52	L	705	CDL	CA4-CA6-OA8-CA7
53	Z	202	3PE	C26-C27-C28-C29
52	q	501	CDL	C11-CA5-OA6-CA4
53	N	402	3PE	O11-C1-C2-O21
53	i	201	3PE	O11-C1-C2-O21
46	B	203	PC1	C23-C24-C25-C26
52	q	501	CDL	OB6-CB4-CB6-OB8
53	Z	201	3PE	O21-C2-C3-O31
53	d	201	3PE	C32-C31-O31-C3
45	J	201	LMT	C11-C10-C9-C8
53	Z	201	3PE	C23-C24-C25-C26
53	d	201	3PE	C36-C37-C38-C39
45	Y	203	LMT	O5'-C5'-C6'-O6'
52	L	705	CDL	C12-C13-C14-C15
53	I	203	3PE	O32-C31-O31-C3
53	N	401	3PE	C34-C35-C36-C37
52	h	201	CDL	CB3-OB5-PB2-OB2
53	L	702	3PE	C11-O13-P-O11
53	X	201	3PE	C11-O13-P-O11
53	i	201	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	203	LMT	C3-C4-C5-C6
52	h	201	CDL	OA5-CA3-CA4-CA6
53	I	203	3PE	O11-C1-C2-C3
53	N	401	3PE	O11-C1-C2-C3
53	N	402	3PE	O11-C1-C2-C3
45	A	401	LMT	C5-C6-C7-C8
45	A	403	LMT	O1'-C1-C2-C3
45	M	501	LMT	C5'-C4'-O1B-C1B
45	A	401	LMT	O5B-C5B-C6B-O6B
53	M	502	3PE	C24-C25-C26-C27
45	M	501	LMT	C6-C7-C8-C9
45	L	704	LMT	C4-C5-C6-C7
52	q	501	CDL	C78-C79-C80-C81
53	d	201	3PE	C31-C32-C33-C34
45	Y	202	LMT	C11-C10-C9-C8
52	q	501	CDL	CA3-CA4-CA6-OA8
52	q	501	CDL	CB3-CB4-CB6-OB8
53	O	504	3PE	C23-C24-C25-C26
48	D	601	HQH	C24-C25-O3-C30
53	d	201	3PE	C39-C3A-C3B-C3C
45	L	704	LMT	O5'-C5'-C6'-O6'
53	M	503	3PE	C34-C35-C36-C37
45	Y	204	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C9-C10-C11-C12
45	Y	203	LMT	C2-C3-C4-C5
52	L	705	CDL	C22-C23-C24-C25
53	N	401	3PE	C36-C37-C38-C39
53	L	703	3PE	C25-C26-C27-C28
58	T	201	EHZ	C18-C17-C20-O6
58	T	201	EHZ	C19-C17-C20-O6
45	K	201	LMT	C9-C10-C11-C12
52	L	705	CDL	C55-C56-C57-C58
45	P	502	LMT	C11-C10-C9-C8
53	O	504	3PE	C27-C28-C29-C2A
50	F	502	FMN	C5'-O5'-P-O1P
53	L	703	3PE	C34-C35-C36-C37
53	d	201	3PE	C33-C34-C35-C36
52	h	202	CDL	OB5-CB3-CB4-OB6
52	q	501	CDL	OA5-CA3-CA4-OA6
53	d	201	3PE	O11-C1-C2-O21
53	r	201	3PE	C21-C22-C23-C24
45	J	202	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	d	201	3PE	O32-C31-O31-C3
45	L	704	LMT	C7-C8-C9-C10
45	P	502	LMT	C3'-C4'-O1B-C1B
46	A	402	PC1	C35-C36-C37-C38
52	q	501	CDL	OA6-CA4-CA6-OA8
53	M	502	3PE	O21-C2-C3-O31
58	T	201	EHZ	O5-C16-C17-C18
58	U	201	EHZ	O5-C16-C17-C18
58	U	201	EHZ	O5-C16-C17-C19
45	A	401	LMT	O1'-C1-C2-C3
46	B	202	PC1	C31-C32-C33-C34
45	O	503	LMT	C4-C5-C6-C7
58	T	201	EHZ	C5-C6-C7-C8
53	M	502	3PE	C22-C23-C24-C25
53	N	402	3PE	C36-C37-C38-C39
53	Z	201	3PE	C35-C36-C37-C38
45	M	501	LMT	C4B-C5B-C6B-O6B
45	h	203	LMT	C9-C10-C11-C12
45	j	101	LMT	C9-C10-C11-C12
45	P	502	LMT	C1-C2-C3-C4
52	L	705	CDL	OA5-CA3-CA4-CA6
53	Z	202	3PE	O11-C1-C2-C3
53	i	201	3PE	O11-C1-C2-C3
45	L	701	LMT	C2-C3-C4-C5
52	q	501	CDL	C71-C72-C73-C74
59	o	201	MYR	C7-C8-C9-C10
53	L	702	3PE	O13-C11-C12-N
52	h	202	CDL	CB7-C71-C72-C73
52	h	201	CDL	CA4-CA3-OA5-PA1
52	L	705	CDL	C72-C73-C74-C75
53	M	502	3PE	C2C-C2D-C2E-C2F
53	N	402	3PE	C31-C32-C33-C34
46	B	203	PC1	C1-C2-C3-O31
52	h	202	CDL	CA3-CA4-CA6-OA8
53	L	702	3PE	C1-C2-C3-O31
53	L	703	3PE	C1-C2-C3-O31
53	N	402	3PE	C1-C2-C3-O31
53	X	201	3PE	C1-C2-C3-O31
53	Z	201	3PE	C1-C2-C3-O31
53	Z	202	3PE	C1-C2-C3-O31
53	d	201	3PE	C1-C2-C3-O31
53	i	201	3PE	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	I	203	3PE	C32-C33-C34-C35
53	r	201	3PE	C33-C34-C35-C36
45	h	203	LMT	C4'-C5'-C6'-O6'
53	Z	201	3PE	C25-C26-C27-C28
45	P	502	LMT	C5-C6-C7-C8
52	h	201	CDL	C61-C62-C63-C64
45	P	502	LMT	C4-C5-C6-C7
52	q	501	CDL	OB5-CB3-CB4-OB6
53	Z	201	3PE	O11-C1-C2-O21
53	Z	202	3PE	O11-C1-C2-O21
52	H	401	CDL	C54-C55-C56-C57
52	h	201	CDL	C74-C75-C76-C77
48	D	601	HQH	C23-C25-O3-C30
52	h	201	CDL	C77-C78-C79-C80
52	h	202	CDL	OA6-CA4-CA6-OA8
45	h	203	LMT	O5'-C1'-O1'-C1
46	B	202	PC1	C22-C23-C24-C25
53	Z	202	3PE	C2A-C2B-C2C-C2D
53	Z	202	3PE	C24-C25-C26-C27
52	H	401	CDL	C1-CA2-OA2-PA1
52	H	401	CDL	CB4-CB3-OB5-PB2
52	L	705	CDL	C1-CB2-OB2-PB2
52	L	705	CDL	CB4-CB3-OB5-PB2
45	J	202	LMT	C4-C5-C6-C7
53	Z	202	3PE	C27-C28-C29-C2A
58	T	201	EHZ	C21-C22-C23-C24
58	U	201	EHZ	O2-C9-S1-C10
45	K	201	LMT	O1'-C1-C2-C3
53	O	504	3PE	C32-C33-C34-C35
45	Y	202	LMT	C5-C6-C7-C8
46	B	203	PC1	O11-C1-C2-C3
53	M	503	3PE	O11-C1-C2-C3
45	L	704	LMT	C3-C4-C5-C6
53	L	702	3PE	C23-C24-C25-C26
45	Y	202	LMT	C4'-C5'-C6'-O6'
53	I	203	3PE	C24-C25-C26-C27
53	N	401	3PE	C33-C34-C35-C36
52	H	401	CDL	CA6-CA4-OA6-CA5
58	U	201	EHZ	C8-C9-S1-C10
46	B	202	PC1	C25-C26-C27-C28
46	A	402	PC1	C1-C2-C3-O31
52	h	201	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	O	504	3PE	C1-C2-C3-O31
53	X	201	3PE	C2-C1-O11-P
45	A	403	LMT	C4B-C5B-C6B-O6B
45	M	501	LMT	C3'-C4'-O1B-C1B
46	B	202	PC1	O11-C1-C2-O21
45	M	501	LMT	C1-C2-C3-C4
58	T	201	EHZ	C15-C16-C17-C19
45	Y	201	LMT	C3'-C4'-O1B-C1B
52	q	501	CDL	C55-C56-C57-C58
53	L	703	3PE	C3B-C3C-C3D-C3E
46	B	203	PC1	O21-C2-C3-O31
53	L	703	3PE	O21-C2-C3-O31
53	i	201	3PE	O21-C2-C3-O31
53	L	703	3PE	C3A-C3B-C3C-C3D
53	Z	202	3PE	C2B-C2C-C2D-C2E
45	A	401	LMT	C11-C10-C9-C8
52	h	201	CDL	C76-C77-C78-C79
45	M	501	LMT	C2-C3-C4-C5
45	M	501	LMT	C9-C10-C11-C12
53	M	502	3PE	C25-C26-C27-C28
53	M	502	3PE	C11-O13-P-O11
53	N	401	3PE	C1-O11-P-O13
56	P	501	NDP	O4D-C1D-N1N-C6N
52	h	202	CDL	CA4-CA3-OA5-PA1
46	A	402	PC1	C1-O11-P-O14
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O14
52	H	401	CDL	CA2-OA2-PA1-OA4
52	H	401	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	CB2-OB2-PB2-OB4
52	h	202	CDL	CB2-OB2-PB2-OB3
52	q	501	CDL	CA2-OA2-PA1-OA3
53	L	702	3PE	C1-O11-P-O12
53	M	502	3PE	C1-O11-P-O14
53	M	503	3PE	C11-O13-P-O14
53	N	401	3PE	C1-O11-P-O12
53	N	401	3PE	C11-O13-P-O12
53	O	504	3PE	C11-O13-P-O12
53	O	504	3PE	C11-O13-P-O14
53	i	201	3PE	C1-O11-P-O14
53	I	203	3PE	C22-C23-C24-C25
45	A	403	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	704	LMT	O5'-C1'-O1'-C1
46	B	202	PC1	O11-C1-C2-C3
52	q	501	CDL	OB5-CB3-CB4-CB6
53	Z	201	3PE	O11-C1-C2-C3
53	d	201	3PE	O11-C1-C2-C3
46	B	202	PC1	C27-C28-C29-C2A
53	i	201	3PE	C33-C34-C35-C36
52	q	501	CDL	C54-C55-C56-C57
45	Y	203	LMT	C11-C10-C9-C8
53	r	201	3PE	C22-C23-C24-C25
53	I	203	3PE	C12-C11-O13-P
53	L	703	3PE	C12-C11-O13-P
53	L	703	3PE	C3D-C3E-C3F-C3G
52	L	705	CDL	C53-C54-C55-C56
53	i	201	3PE	C31-C32-C33-C34
52	L	705	CDL	OA5-CA3-CA4-OA6
53	M	503	3PE	O11-C1-C2-O21
53	M	502	3PE	O31-C31-C32-C33
45	A	401	LMT	C2-C3-C4-C5
58	U	201	EHZ	C10-C11-N1-C12
53	M	502	3PE	C1-C2-C3-O31
58	T	201	EHZ	C16-C17-C20-O6
58	U	201	EHZ	O5-C16-C17-C20
46	A	402	PC1	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
53	N	402	3PE	O21-C2-C3-O31
53	X	201	3PE	O21-C2-C3-O31
53	d	201	3PE	O21-C2-C3-O31
53	X	201	3PE	C3C-C3D-C3E-C3F
53	r	201	3PE	C36-C37-C38-C39
45	j	101	LMT	C1-C2-C3-C4
45	Y	204	LMT	C7-C8-C9-C10
53	N	401	3PE	C32-C31-O31-C3
53	L	703	3PE	C37-C38-C39-C3A
45	P	502	LMT	C7-C8-C9-C10
45	Y	203	LMT	C6-C7-C8-C9
59	o	201	MYR	C5-C6-C7-C8
53	N	401	3PE	O32-C31-O31-C3
45	Y	203	LMT	O1'-C1-C2-C3
45	Y	204	LMT	O5B-C5B-C6B-O6B
53	L	702	3PE	C28-C29-C2A-C2B
45	L	704	LMT	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	L	703	3PE	C33-C34-C35-C36
53	L	703	3PE	C1-C2-O21-C21
53	X	201	3PE	C3-C2-O21-C21
52	h	202	CDL	OB5-CB3-CB4-CB6
45	Y	202	LMT	C2-C3-C4-C5
52	H	401	CDL	C51-C52-C53-C54
52	q	501	CDL	C1-CB2-OB2-PB2
52	H	401	CDL	OB5-CB3-CB4-OB6
52	h	201	CDL	OA5-CA3-CA4-OA6
53	M	502	3PE	C2B-C2C-C2D-C2E
45	A	401	LMT	C7-C8-C9-C10
45	M	501	LMT	O5'-C1'-O1'-C1
45	L	704	LMT	C2'-C1'-O1'-C1
45	h	203	LMT	C2'-C1'-O1'-C1
45	J	202	LMT	C2-C3-C4-C5
52	L	705	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CA2-OA2-PA1-OA5
52	h	202	CDL	CA2-OA2-PA1-OA5
53	Z	202	3PE	C1-O11-P-O13
53	d	201	3PE	C1-O11-P-O13
53	d	201	3PE	C11-O13-P-O11
53	L	703	3PE	C39-C3A-C3B-C3C
58	U	201	EHZ	C21-C22-C23-C24
53	M	502	3PE	C2A-C2B-C2C-C2D
45	Y	201	LMT	C2-C3-C4-C5
59	o	201	MYR	C2-C3-C4-C5
55	O	502	GTP	PA-O3A-PB-O2B
53	X	201	3PE	C22-C23-C24-C25
53	Z	202	3PE	C32-C33-C34-C35
53	r	201	3PE	C3C-C3D-C3E-C3F
50	F	502	FMN	C4'-C5'-O5'-P
53	M	503	3PE	C2-C1-O11-P
52	H	401	CDL	OB7-CB5-OB6-CB4
46	B	203	PC1	C31-C32-C33-C34
53	i	201	3PE	O13-C11-C12-N
46	B	203	PC1	C35-C36-C37-C38
52	q	501	CDL	C76-C77-C78-C79
53	M	502	3PE	O32-C31-C32-C33
53	Z	201	3PE	C2-C1-O11-P
53	O	504	3PE	C25-C26-C27-C28
45	Y	203	LMT	C9-C10-C11-C12
53	M	503	3PE	C37-C38-C39-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	J	201	LMT	O5'-C1'-O1'-C1
52	q	501	CDL	C56-C57-C58-C59
52	h	201	CDL	CB2-OB2-PB2-OB5
52	h	201	CDL	C79-C80-C81-C82
53	N	401	3PE	C27-C28-C29-C2A
52	q	501	CDL	CB4-CB3-OB5-PB2
53	N	402	3PE	C2-C1-O11-P
53	I	203	3PE	C28-C29-C2A-C2B
58	U	201	EHZ	C1-C21-C22-C23
52	q	501	CDL	OA5-CA3-CA4-CA6
45	Y	201	LMT	C5'-C4'-O1B-C1B
58	U	201	EHZ	C11-C10-S1-C9
52	H	401	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	C52-C53-C54-C55
53	r	201	3PE	C3A-C3B-C3C-C3D
58	U	201	EHZ	C22-C23-C24-C25
53	L	702	3PE	C24-C25-C26-C27
45	K	201	LMT	C6-C7-C8-C9
45	Y	201	LMT	C7-C8-C9-C10
52	L	705	CDL	C31-C32-C33-C34
45	Y	203	LMT	C7-C8-C9-C10
53	Z	202	3PE	C35-C36-C37-C38
53	r	201	3PE	O11-C1-C2-O21
45	A	401	LMT	O5'-C5'-C6'-O6'
45	Y	204	LMT	O5B-C1B-O1B-C4'
52	L	705	CDL	C17-C18-C19-C20
52	h	201	CDL	C51-C52-C53-C54
52	h	201	CDL	C60-C61-C62-C63
52	h	201	CDL	OA6-CA4-CA6-OA8
53	Z	202	3PE	O21-C21-C22-C23
45	A	403	LMT	C2'-C1'-O1'-C1
58	T	201	EHZ	C2-C1-C21-C22
53	N	401	3PE	O21-C2-C3-O31
52	h	201	CDL	C58-C59-C60-C61
52	h	202	CDL	C72-C73-C74-C75
58	T	201	EHZ	C1-C21-C22-C23
52	L	705	CDL	C52-C51-CB5-OB6
56	P	501	NDP	C3D-C4D-C5D-O5D
52	h	202	CDL	C52-C51-CB5-OB6
53	L	703	3PE	O21-C21-C22-C23
53	L	702	3PE	C39-C3A-C3B-C3C
52	L	705	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	Z	202	3PE	C11-O13-P-O11
53	I	203	3PE	C37-C38-C39-C3A
52	L	705	CDL	C32-C31-CA7-OA8
48	D	601	HQH	C21-C15-C17-C26
52	h	201	CDL	C75-C76-C77-C78
45	J	202	LMT	C3-C4-C5-C6
52	h	202	CDL	C72-C71-CB7-OB8
53	L	702	3PE	O21-C21-C22-C23
53	Z	201	3PE	C34-C35-C36-C37
46	B	202	PC1	C1-C2-C3-O31
48	D	601	HQH	C17-C15-C21-C18
45	Y	203	LMT	C5'-C4'-O1B-C1B
45	A	403	LMT	C9-C10-C11-C12
53	L	703	3PE	C35-C36-C37-C38
55	O	502	GTP	PB-O3B-PG-O3G
58	U	201	EHZ	C15-C16-C17-C18
52	q	501	CDL	C59-C60-C61-C62
52	H	401	CDL	OB5-CB3-CB4-CB6
53	r	201	3PE	O11-C1-C2-C3
53	r	201	3PE	O21-C2-C3-O31
46	B	203	PC1	C21-C22-C23-C24
53	I	203	3PE	C33-C34-C35-C36
53	L	703	3PE	C38-C39-C3A-C3B
45	J	201	LMT	C6-C7-C8-C9
45	j	101	LMT	C4-C5-C6-C7
53	L	702	3PE	C32-C33-C34-C35
46	A	402	PC1	O21-C21-C22-C23
55	O	502	GTP	O4'-C4'-C5'-O5'
53	O	504	3PE	C22-C23-C24-C25
52	L	705	CDL	C51-CB5-OB6-CB4
53	L	702	3PE	C34-C35-C36-C37
52	h	202	CDL	C52-C51-CB5-OB7
52	H	401	CDL	CB2-C1-CA2-OA2
52	h	202	CDL	C72-C71-CB7-OB9
53	N	402	3PE	O31-C31-C32-C33
53	L	703	3PE	O22-C21-C22-C23
52	L	705	CDL	C52-C51-CB5-OB7
45	Y	204	LMT	C2B-C1B-O1B-C4'
55	O	502	GTP	C4'-C5'-O5'-PA
52	h	202	CDL	CA2-OA2-PA1-OA3
53	I	203	3PE	C1-O11-P-O14
53	I	203	3PE	C11-O13-P-O14

Continued on next page...

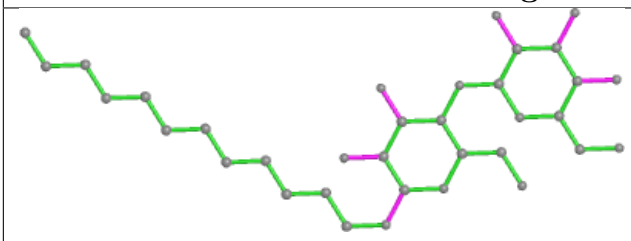
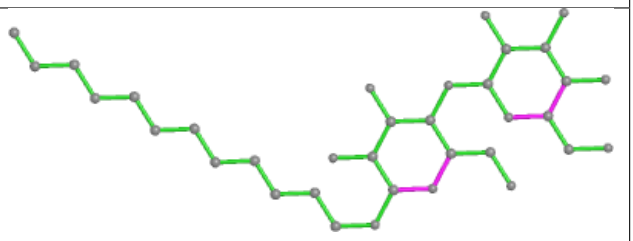
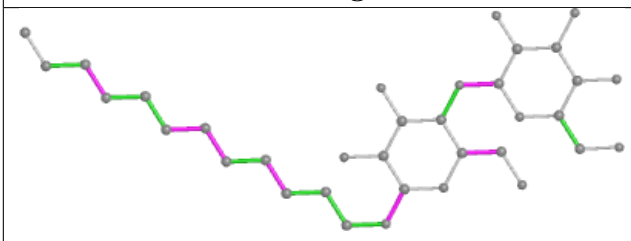
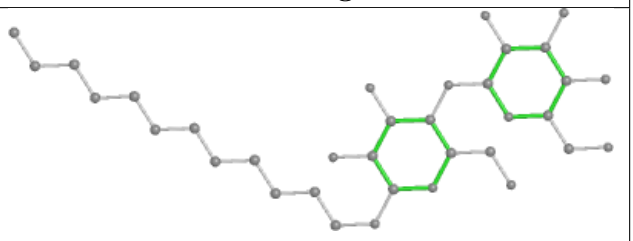
Continued from previous page...

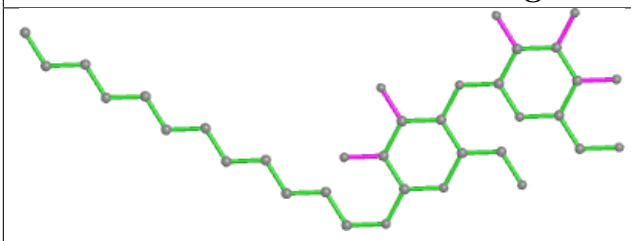
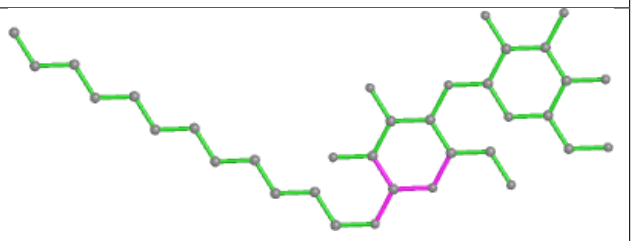
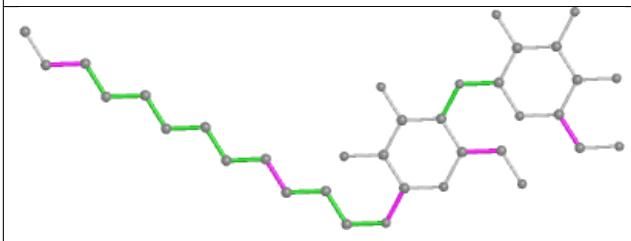
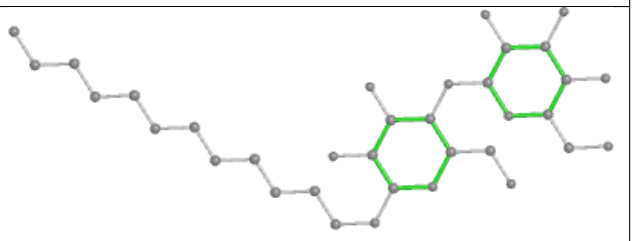
Mol	Chain	Res	Type	Atoms
53	X	201	3PE	C11-O13-P-O12
53	i	201	3PE	C1-O11-P-O12
53	M	503	3PE	O31-C31-C32-C33
53	M	502	3PE	O11-C1-C2-C3
46	B	202	PC1	C26-C27-C28-C29
52	q	501	CDL	C58-C59-C60-C61
53	L	702	3PE	O22-C21-C22-C23
46	A	402	PC1	O31-C31-C32-C33
53	M	502	3PE	O22-C21-O21-C2
52	L	705	CDL	C32-C31-CA7-OA9
53	N	402	3PE	C32-C33-C34-C35
53	Z	201	3PE	C12-C11-O13-P
52	q	501	CDL	C52-C53-C54-C55
53	d	201	3PE	C35-C36-C37-C38
53	Z	201	3PE	O21-C21-C22-C23
46	A	402	PC1	O32-C31-C32-C33
58	T	201	EHZ	O3-C12-C13-C14
50	F	502	FMN	N10-C1'-C2'-O2'
52	h	201	CDL	C52-C51-CB5-OB6
53	O	504	3PE	O31-C31-C32-C33
45	Y	201	LMT	C2-C1-O1'-C1'
53	O	504	3PE	O21-C21-C22-C23
52	L	705	CDL	OB7-CB5-OB6-CB4
53	O	504	3PE	O32-C31-C32-C33

There are no ring outliers.

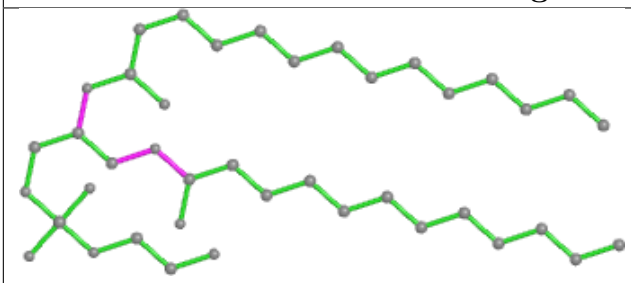
No monomer is involved in short contacts.

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

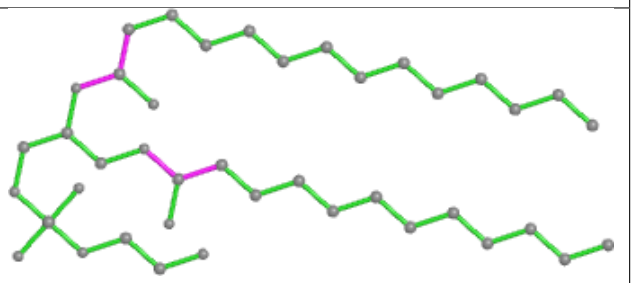
Ligand LMT Y 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT h 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

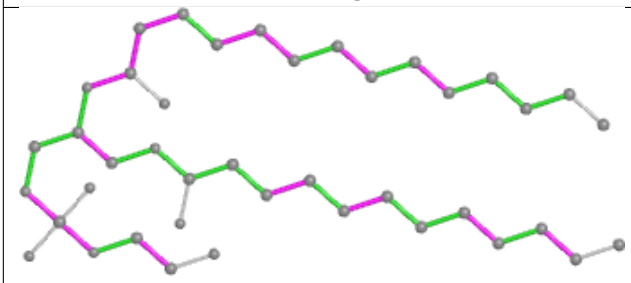
Ligand 3PE L 702



Bond lengths



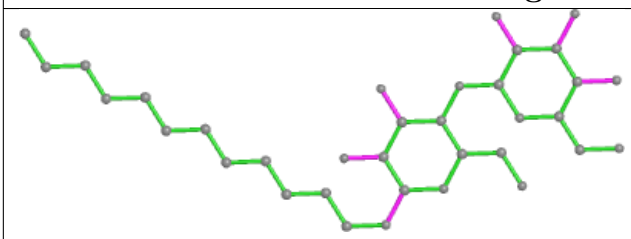
Bond angles



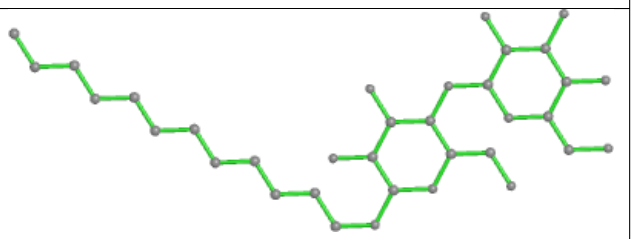
Torsions

Rings

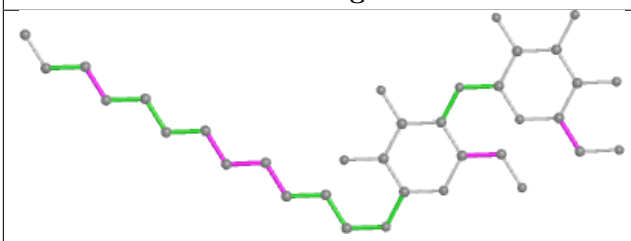
Ligand LMT J 202



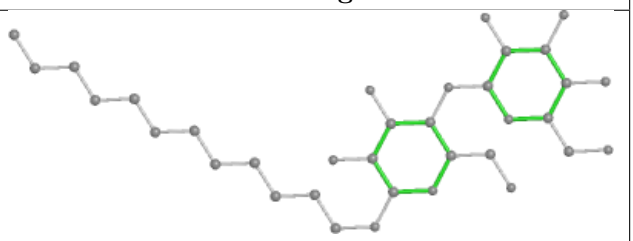
Bond lengths



Bond angles

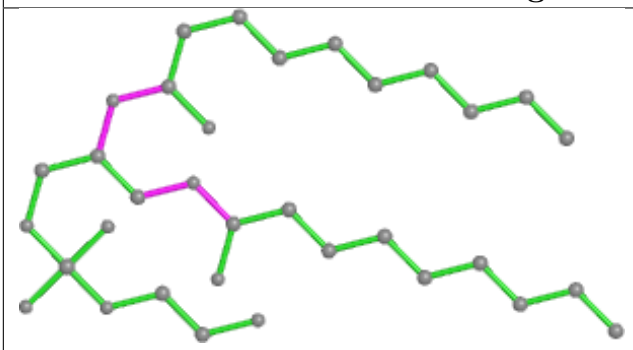


Torsions

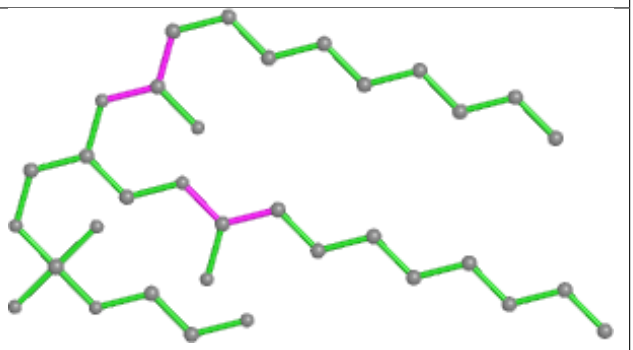


Rings

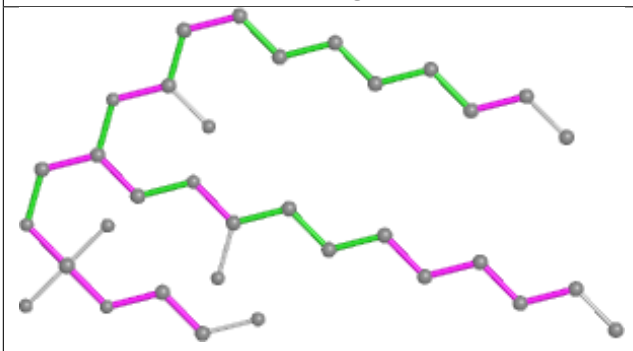
Ligand 3PE N 401



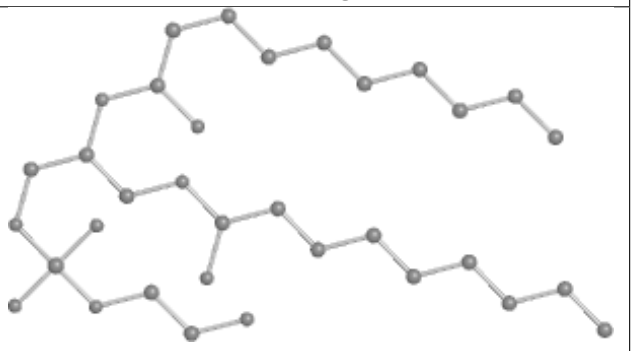
Bond lengths



Bond angles

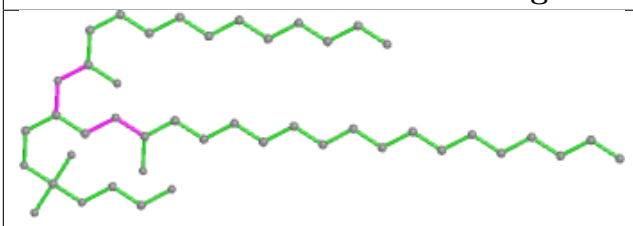


Torsions

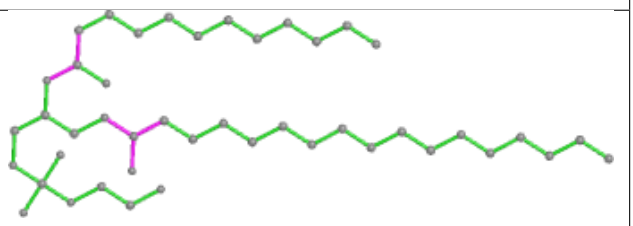


Rings

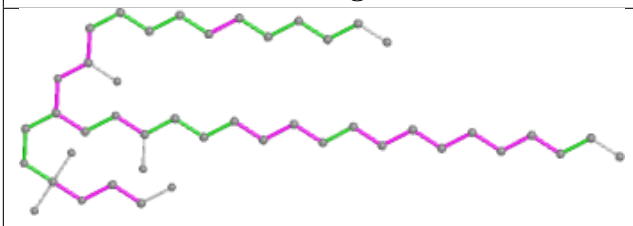
Ligand 3PE L 703



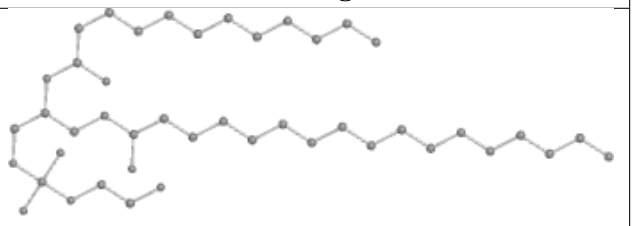
Bond lengths



Bond angles

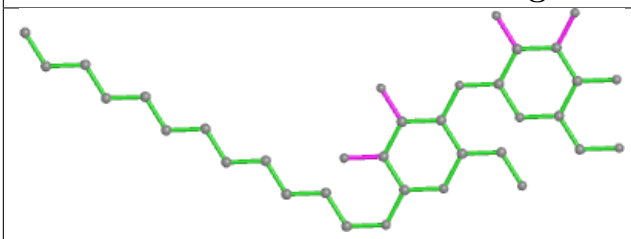


Torsions

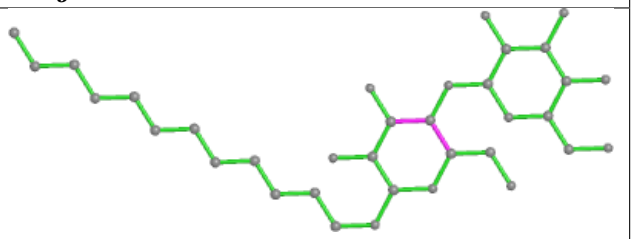


Rings

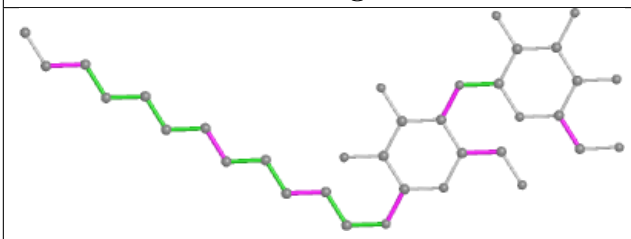
Ligand LMT j 101



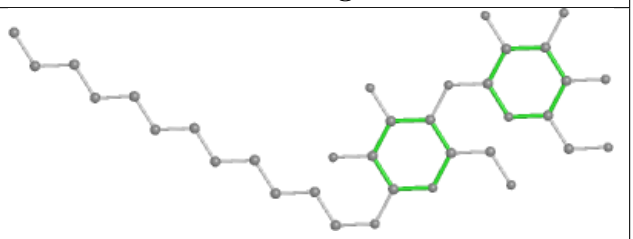
Bond lengths



Bond angles

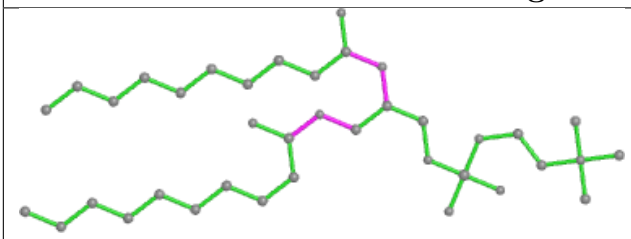


Torsions

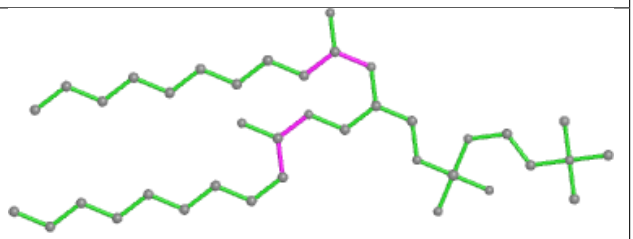


Rings

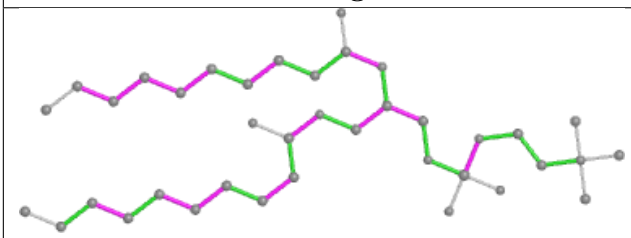
Ligand PC1 B 202



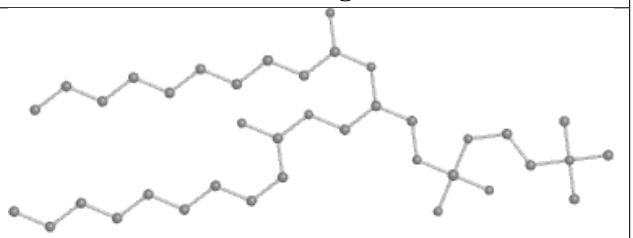
Bond lengths



Bond angles

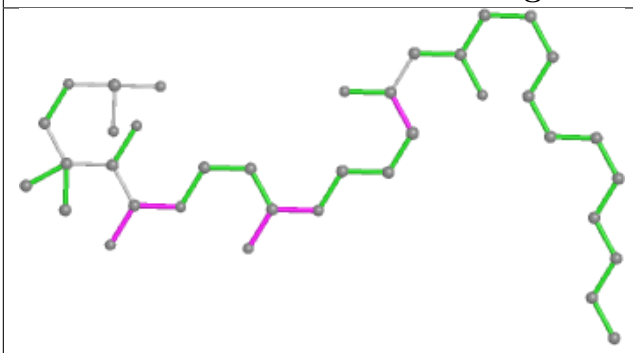


Torsions

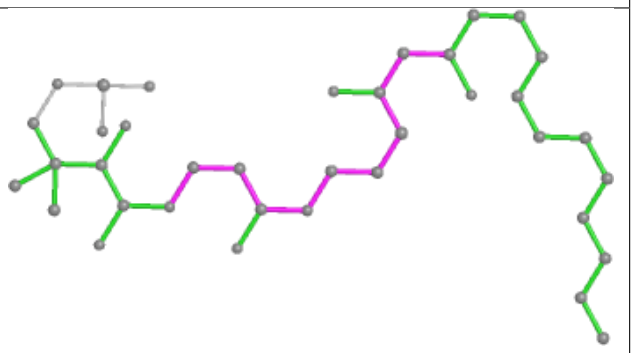


Rings

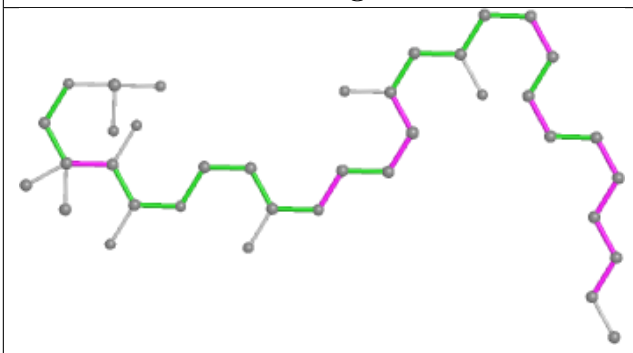
Ligand EHZ U 201



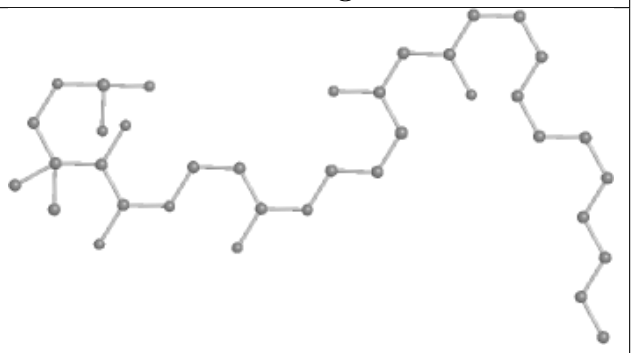
Bond lengths



Bond angles

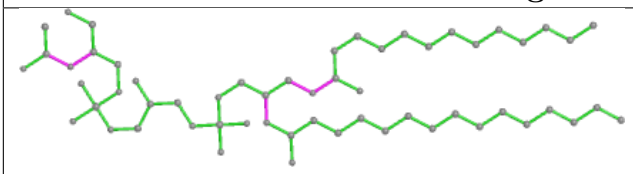


Torsions

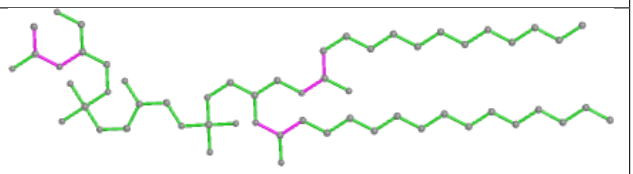


Rings

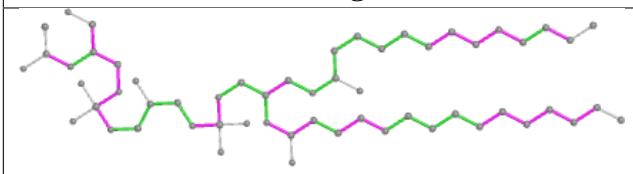
Ligand CDL h 201



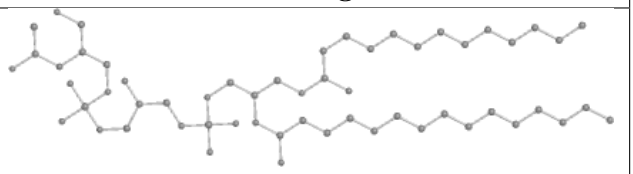
Bond lengths



Bond angles

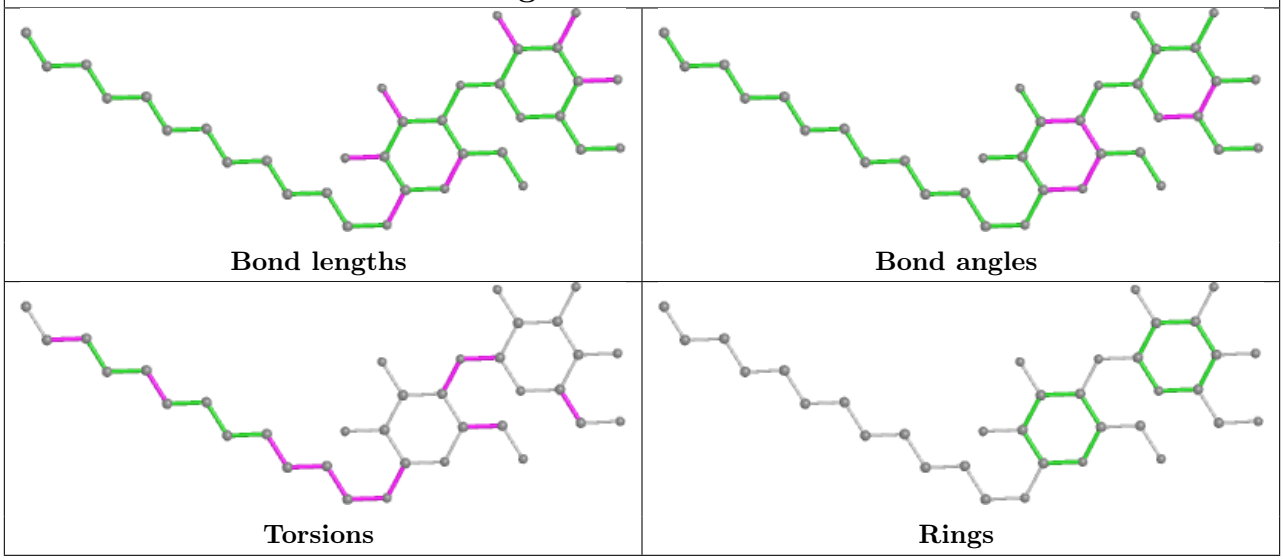


Torsions

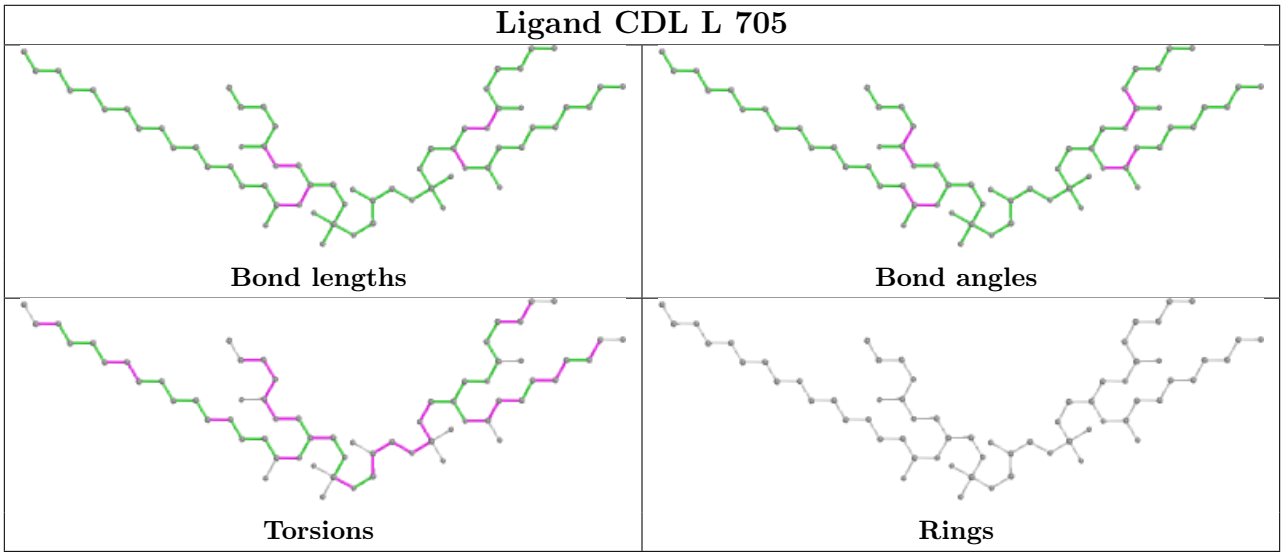


Rings

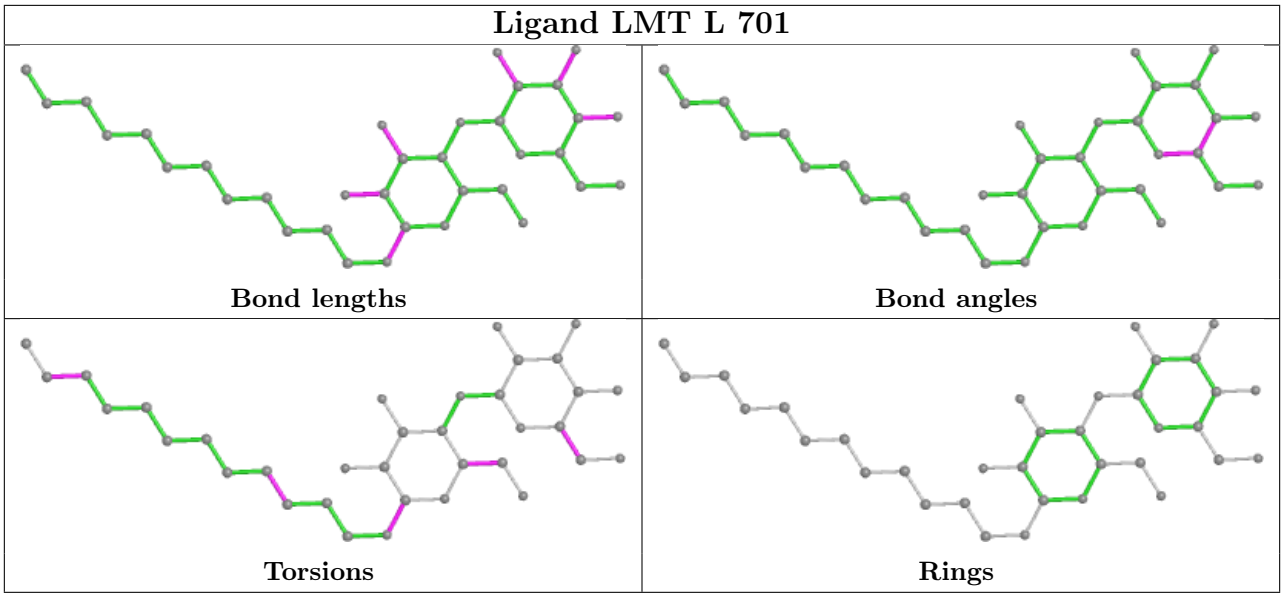
Ligand LMT M 501



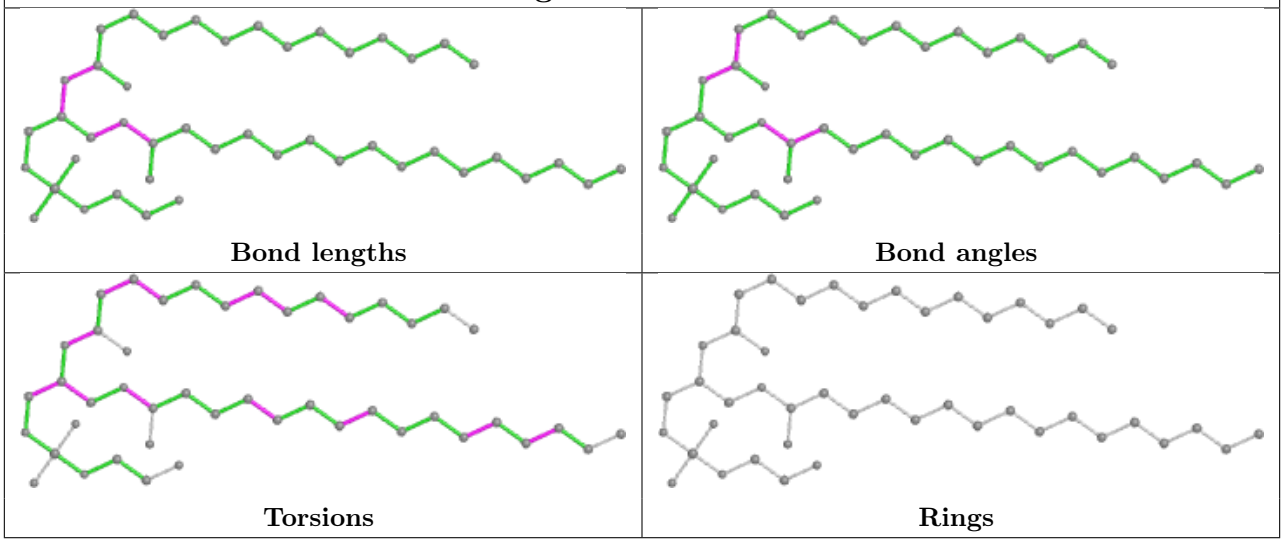
Ligand CDL L 705



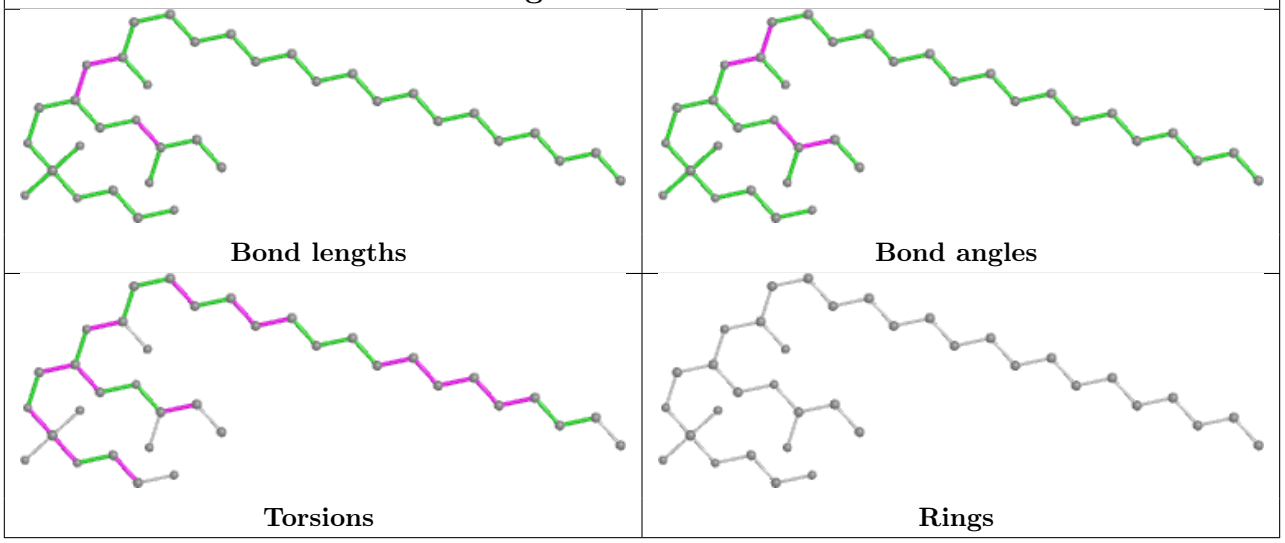
Ligand LMT L 701



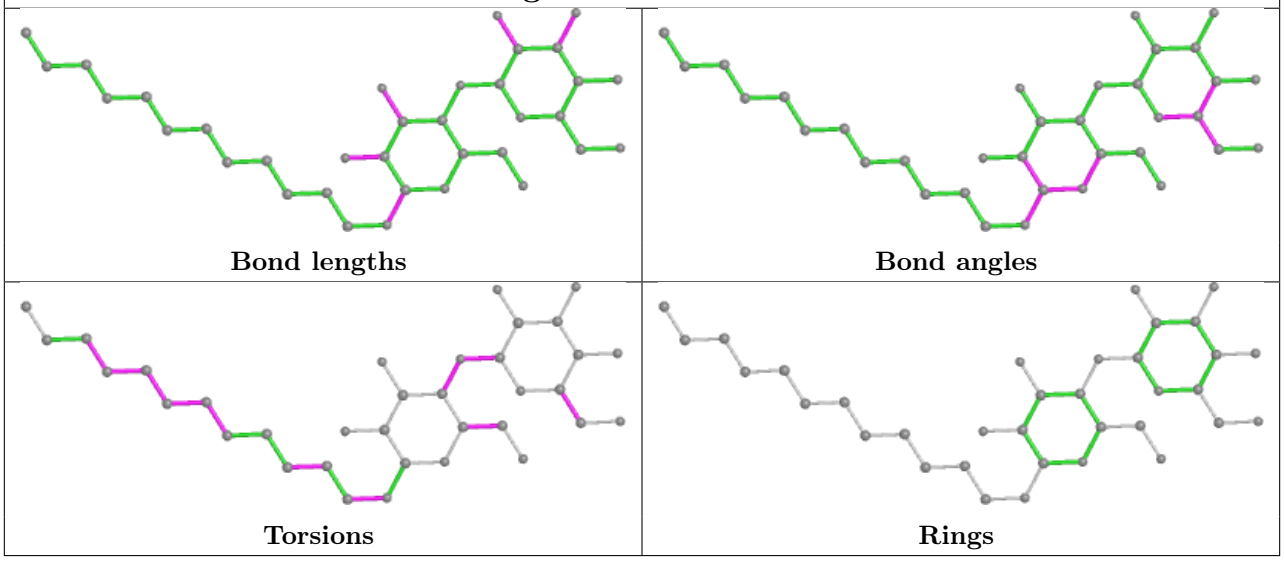
Ligand 3PE r 201



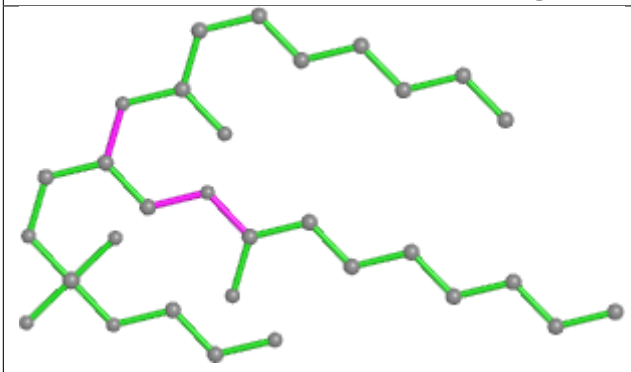
Ligand 3PE M 502



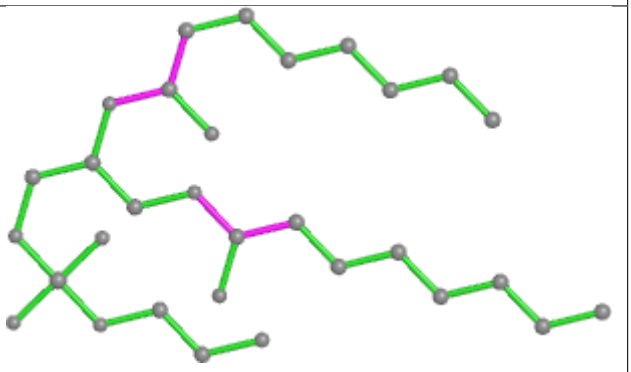
Ligand LMT P 502



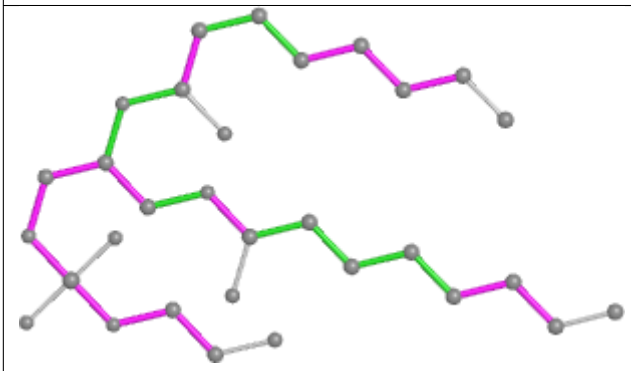
Ligand 3PE Z 201



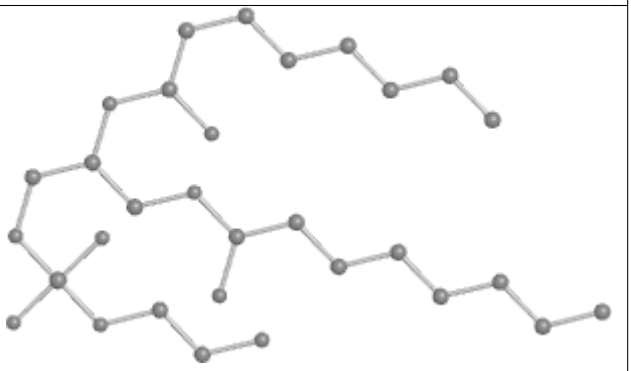
Bond lengths



Bond angles

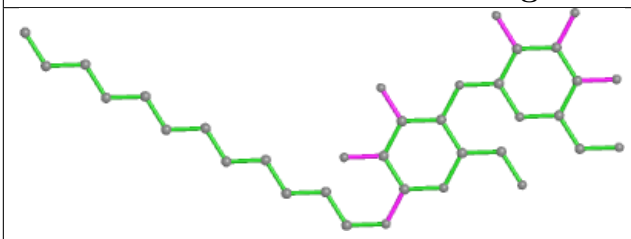


Torsions

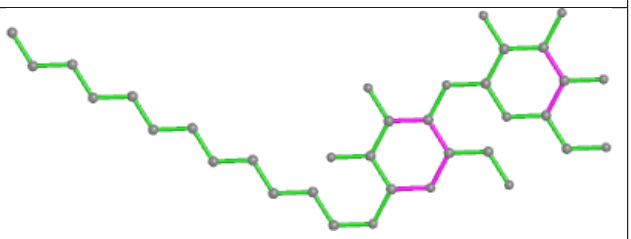


Rings

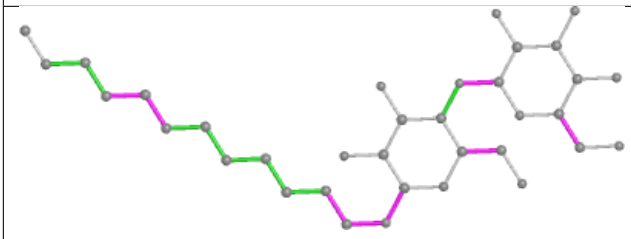
Ligand LMT Y 204



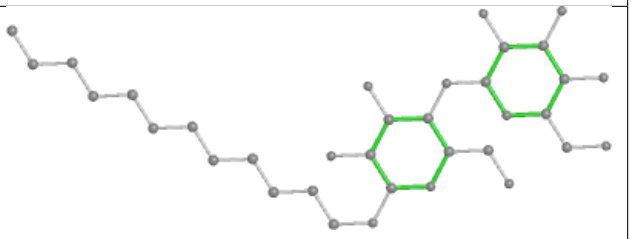
Bond lengths



Bond angles

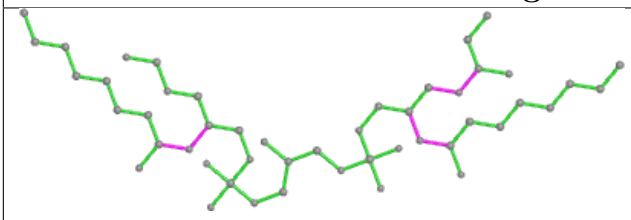


Torsions

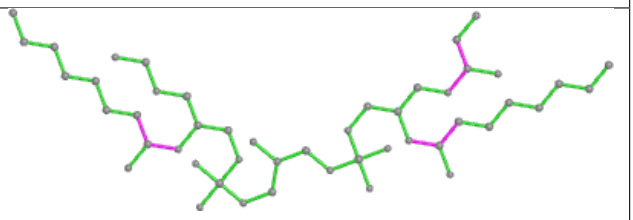


Rings

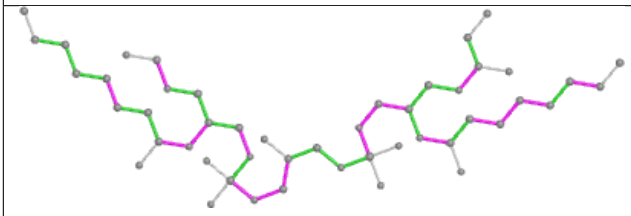
Ligand CDL H 401



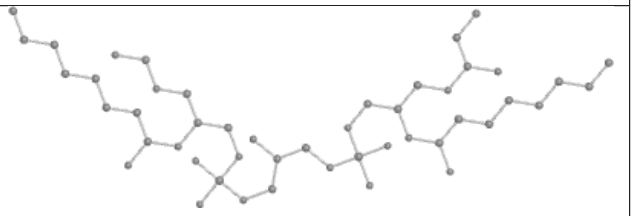
Bond lengths



Bond angles

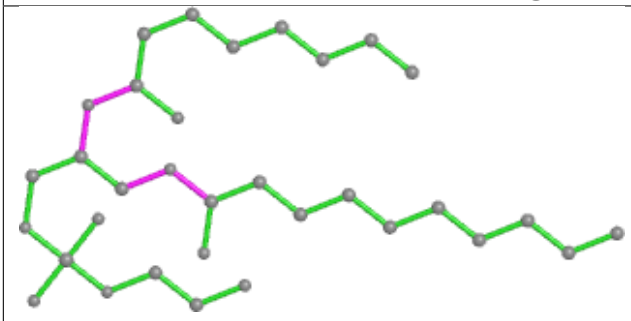


Torsions

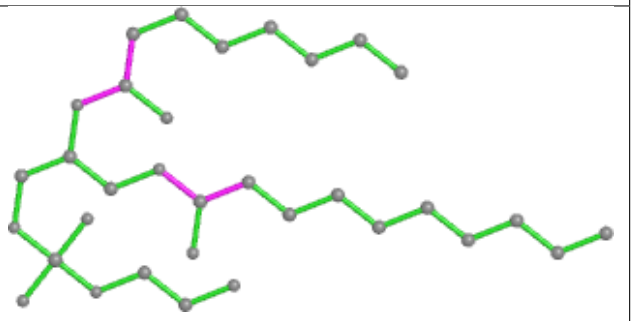


Rings

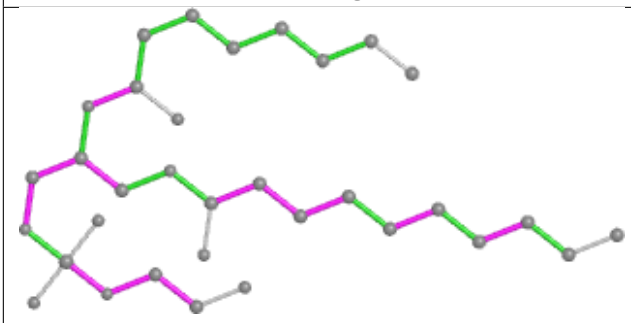
Ligand 3PE N 402



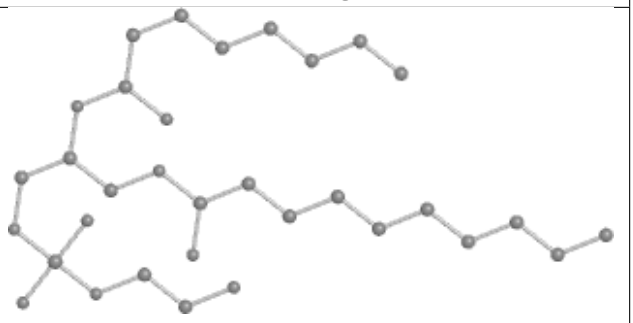
Bond lengths



Bond angles

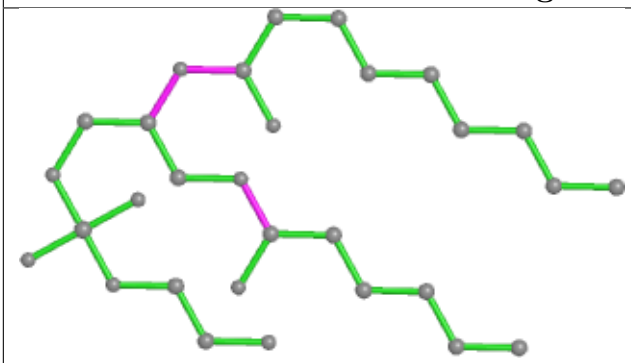


Torsions

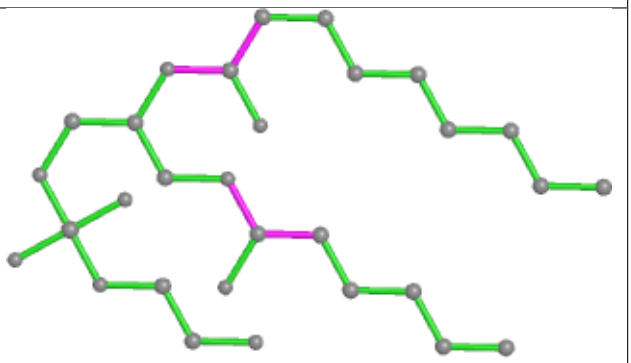


Rings

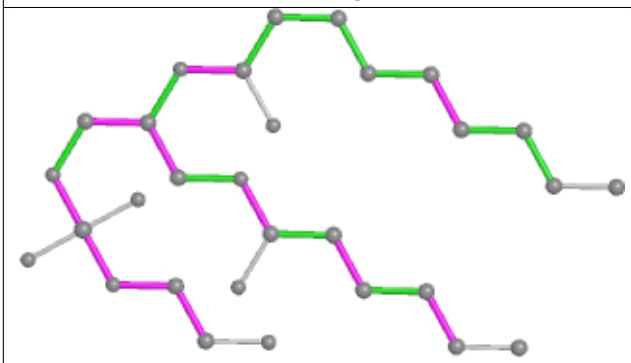
Ligand 3PE i 201



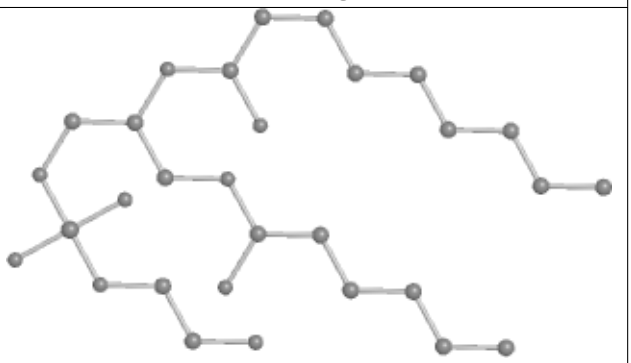
Bond lengths



Bond angles

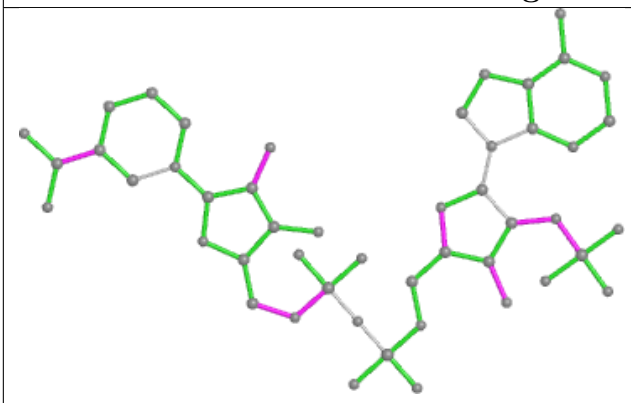


Torsions

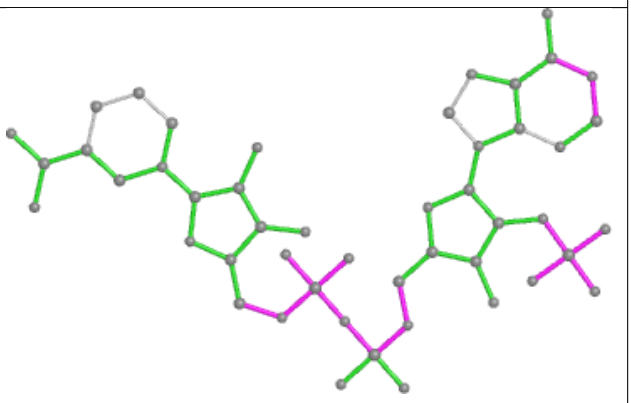


Rings

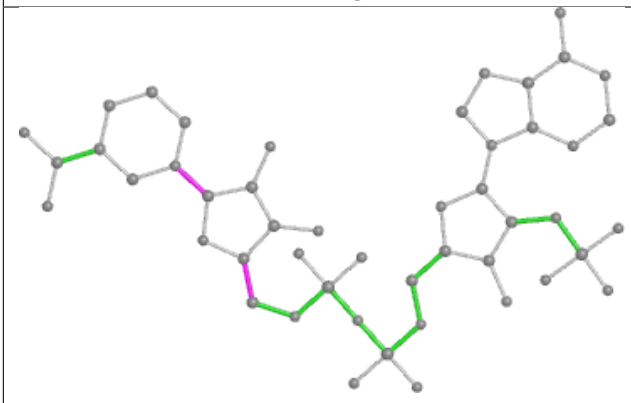
Ligand NDP P 501



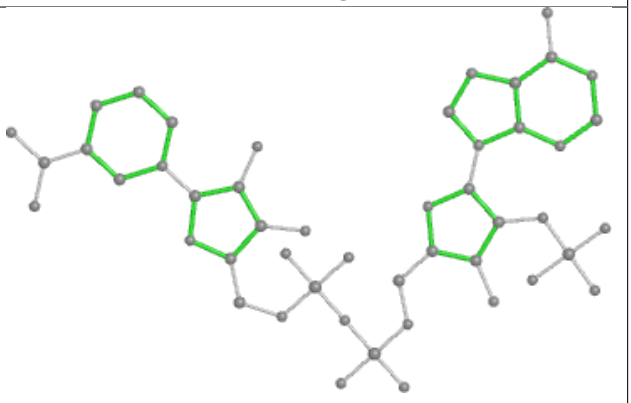
Bond lengths



Bond angles

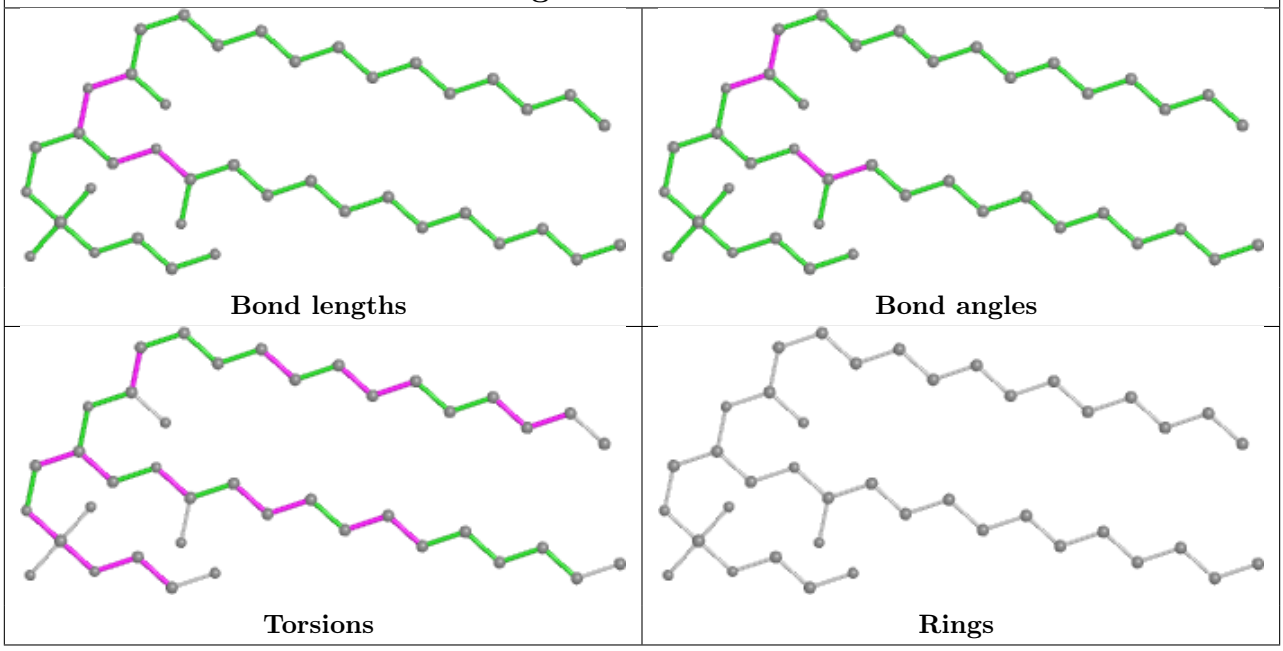


Torsions

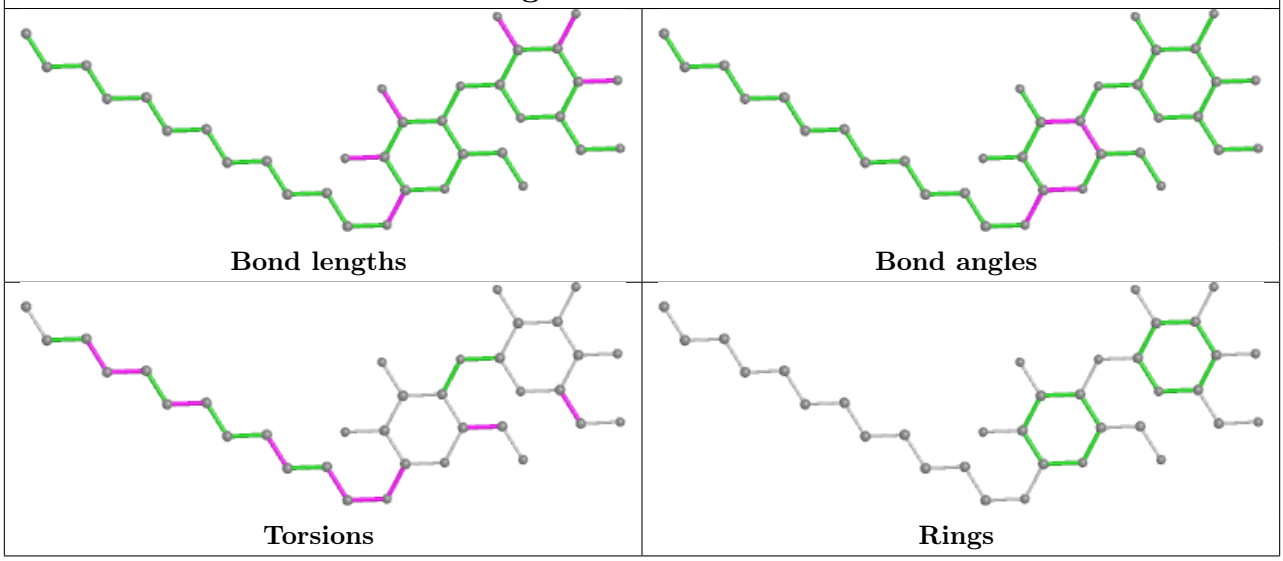


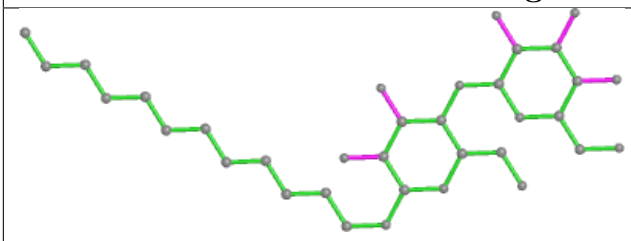
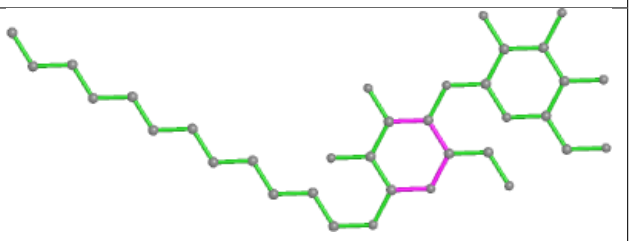
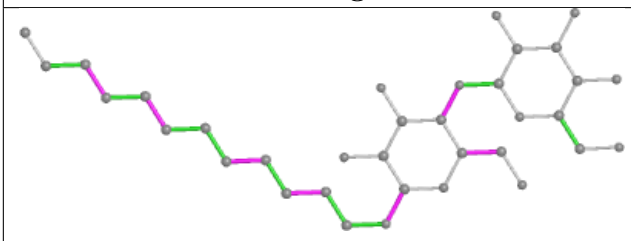
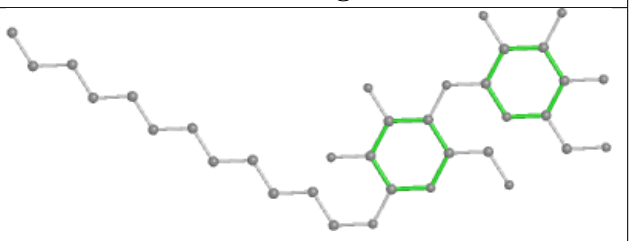
Rings

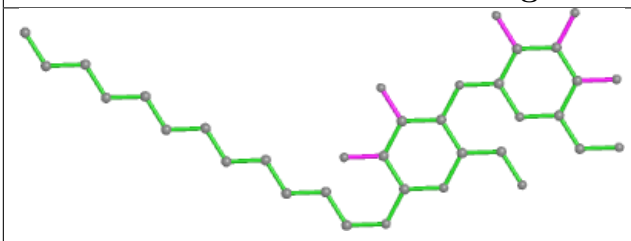
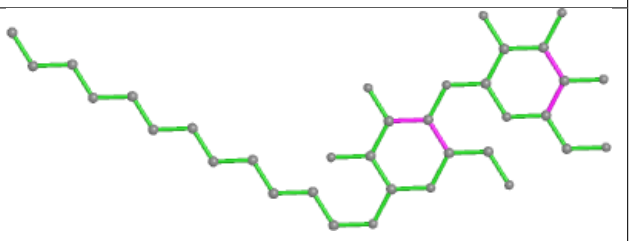
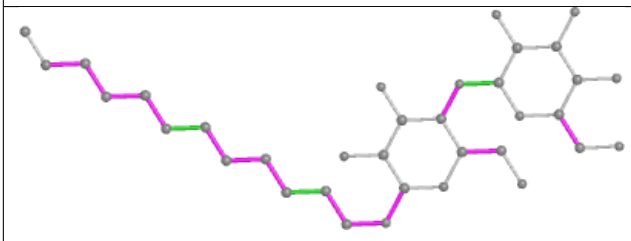
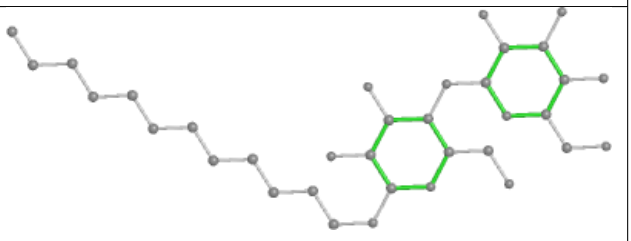
Ligand 3PE Z 202



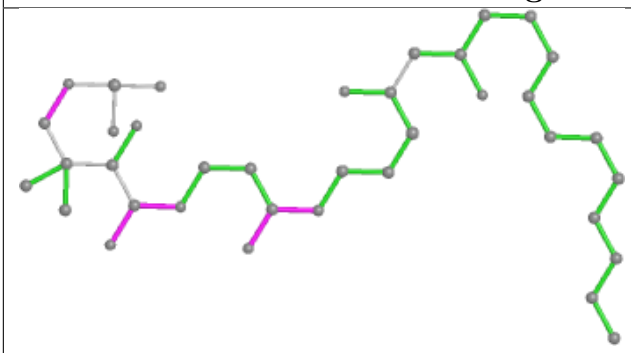
Ligand LMT A 401



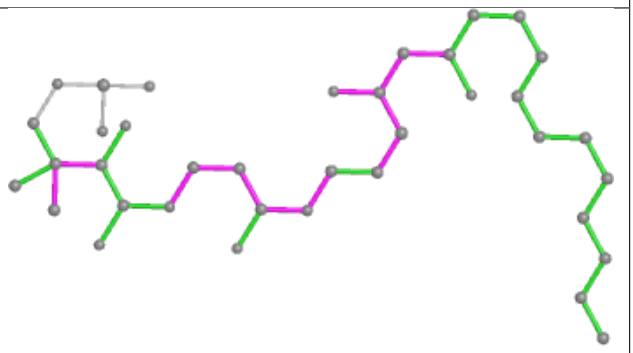
Ligand LMT J 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT Y 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

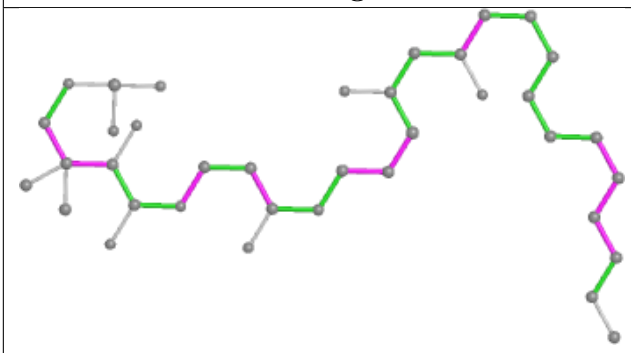
Ligand EHZ T 201



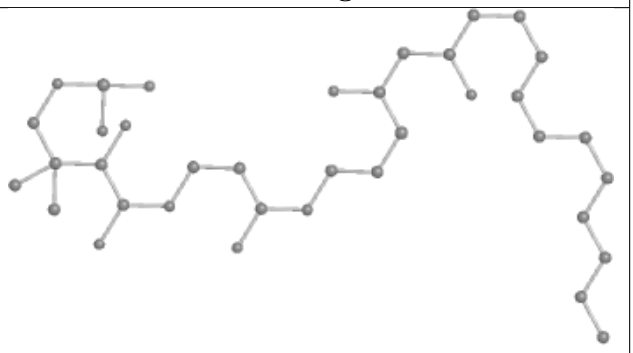
Bond lengths



Bond angles

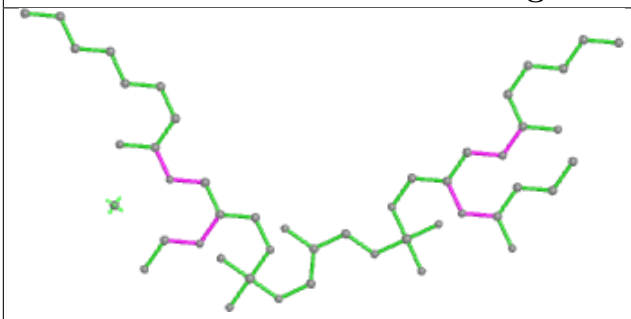


Torsions

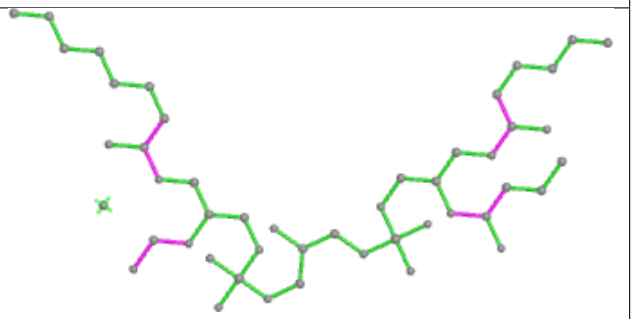


Rings

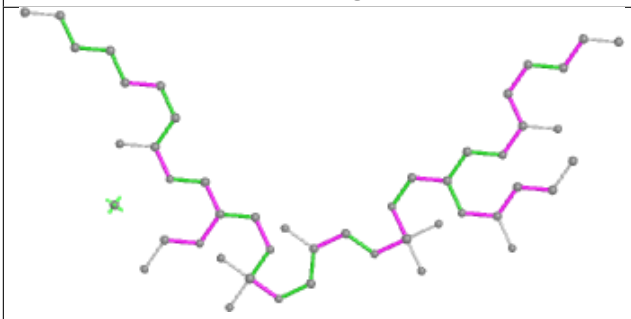
Ligand CDL h 202



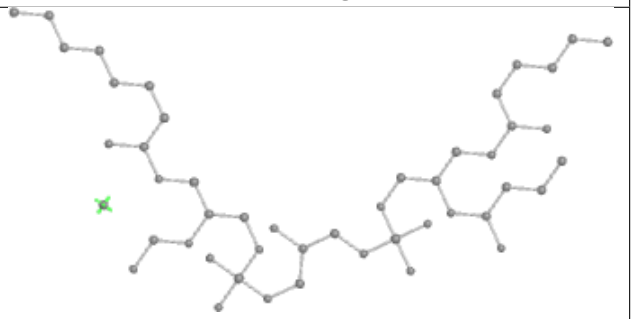
Bond lengths



Bond angles

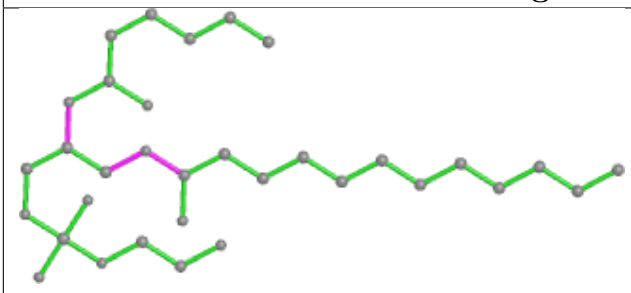


Torsions

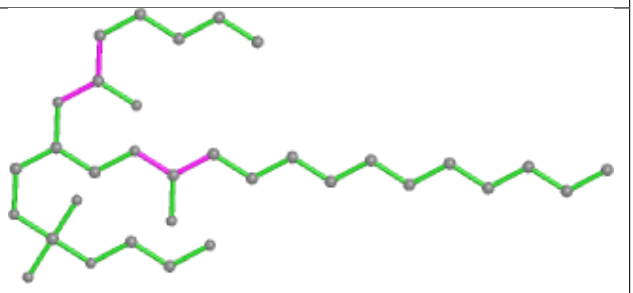


Rings

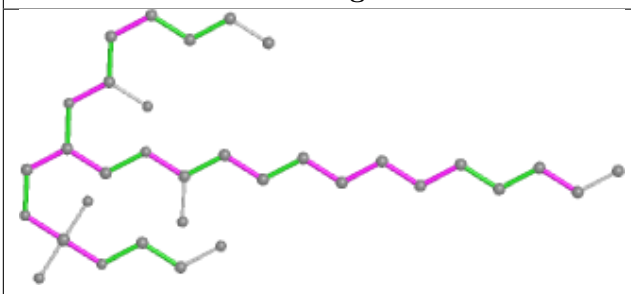
Ligand 3PE d 201



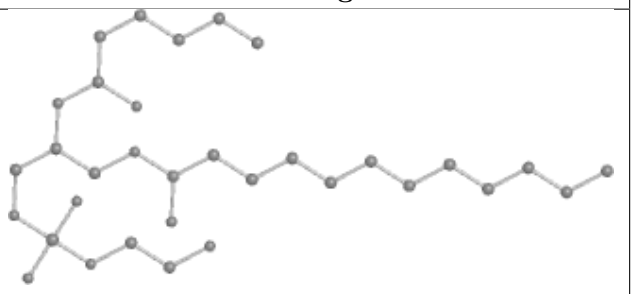
Bond lengths



Bond angles

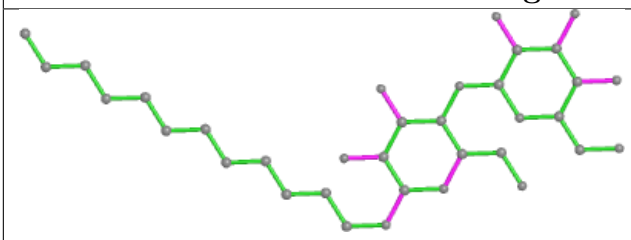


Torsions

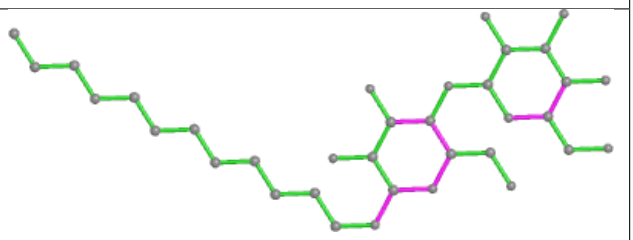


Rings

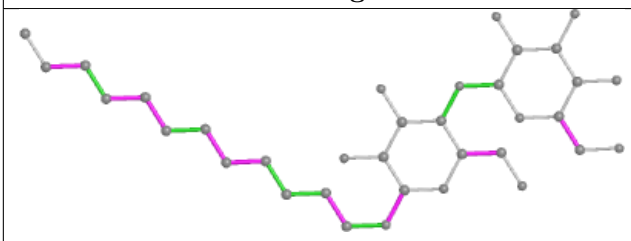
Ligand LMT L 704



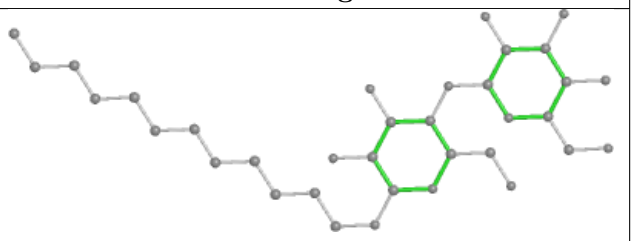
Bond lengths



Bond angles

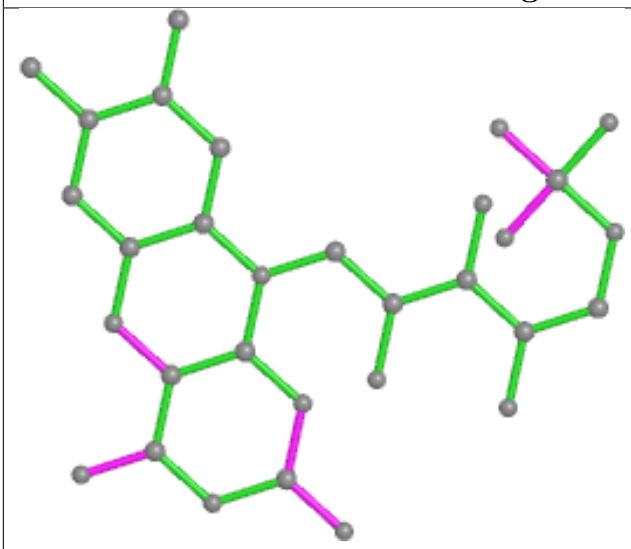


Torsions

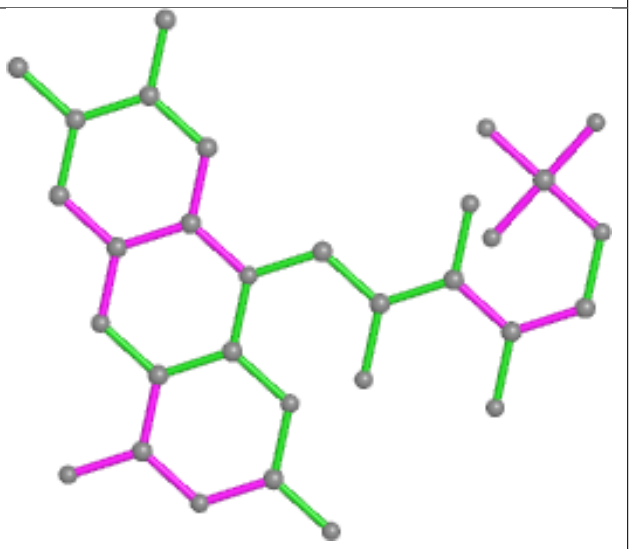


Rings

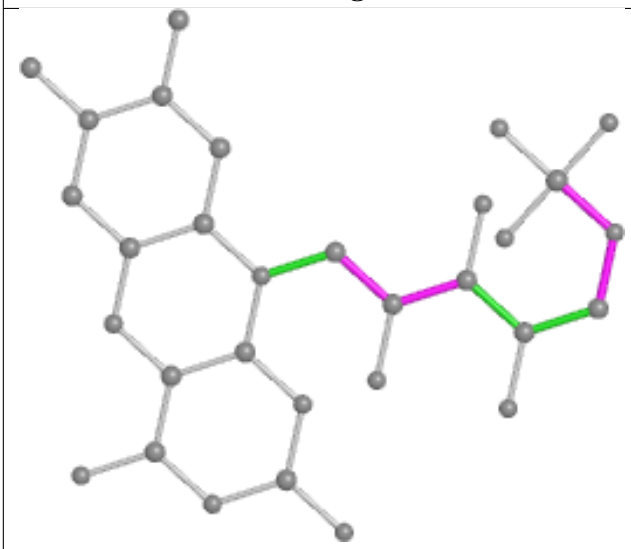
Ligand FMN F 502



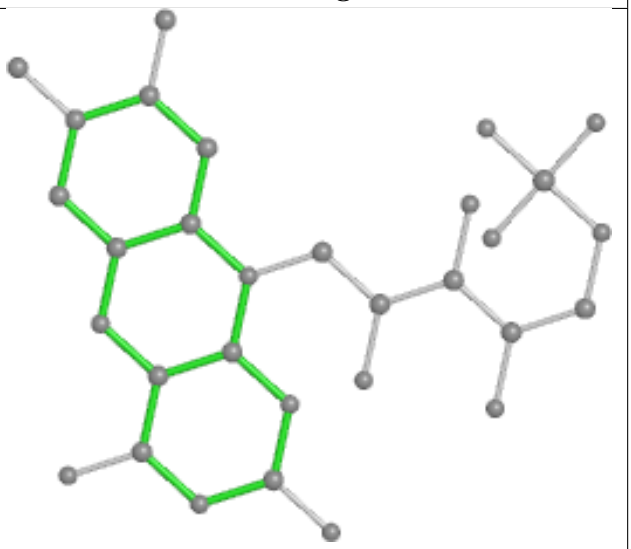
Bond lengths



Bond angles

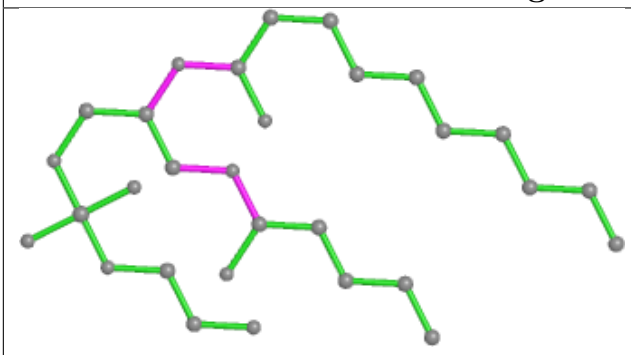


Torsions

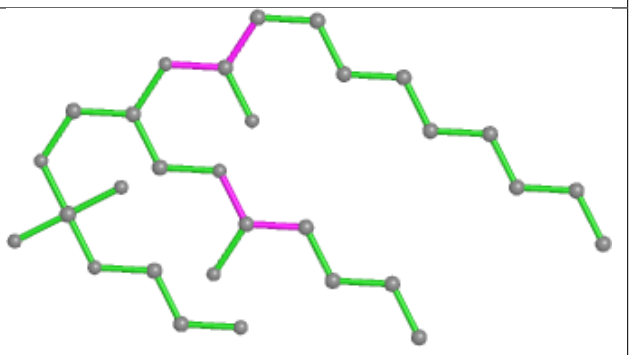


Rings

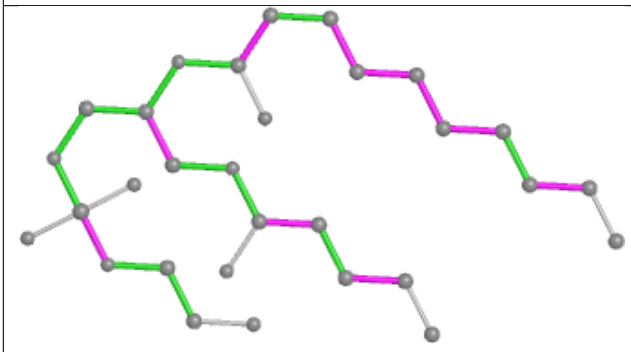
Ligand 3PE O 504



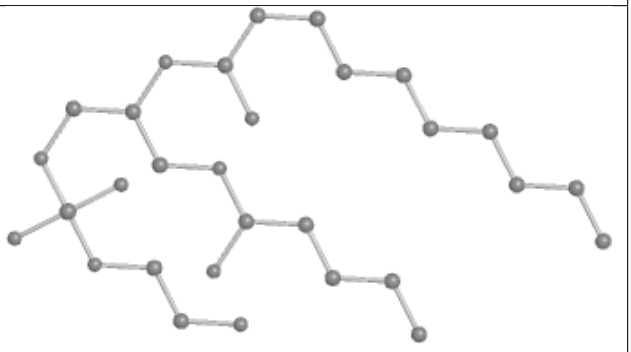
Bond lengths



Bond angles

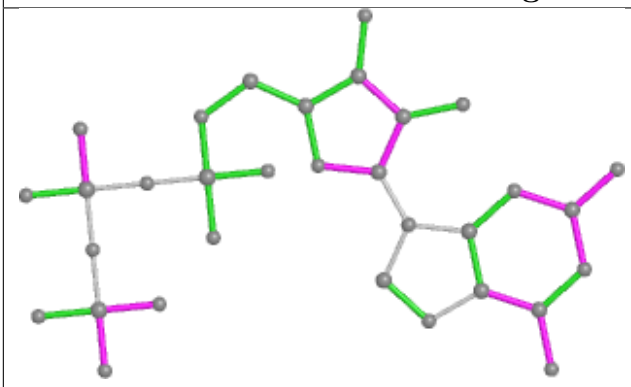


Torsions

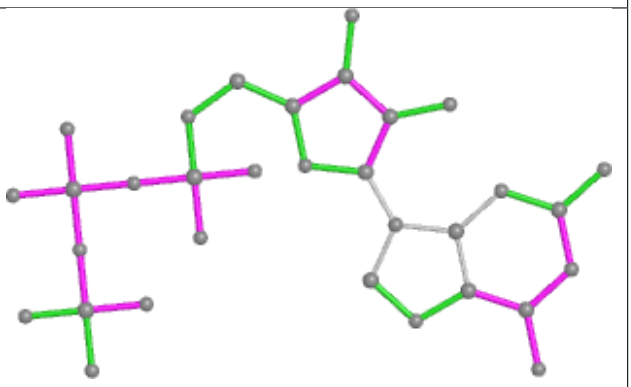


Rings

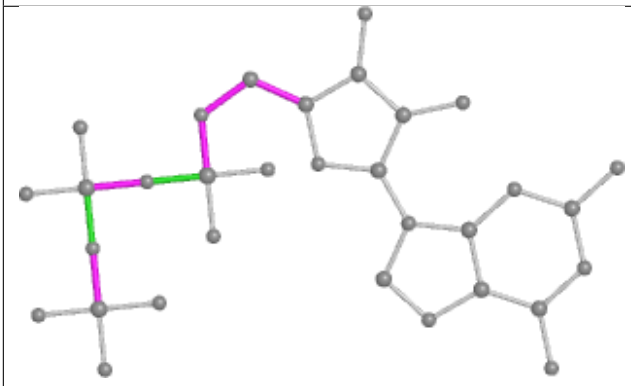
Ligand GTP O 502



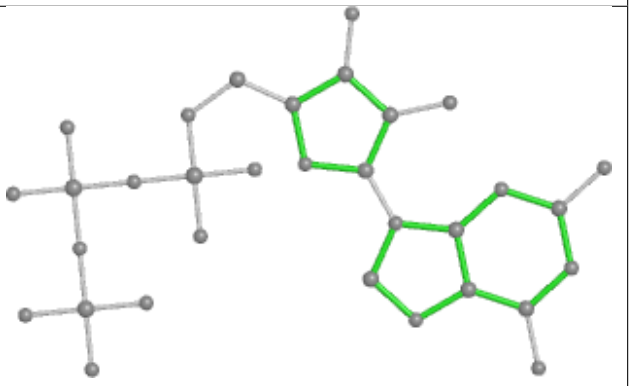
Bond lengths



Bond angles

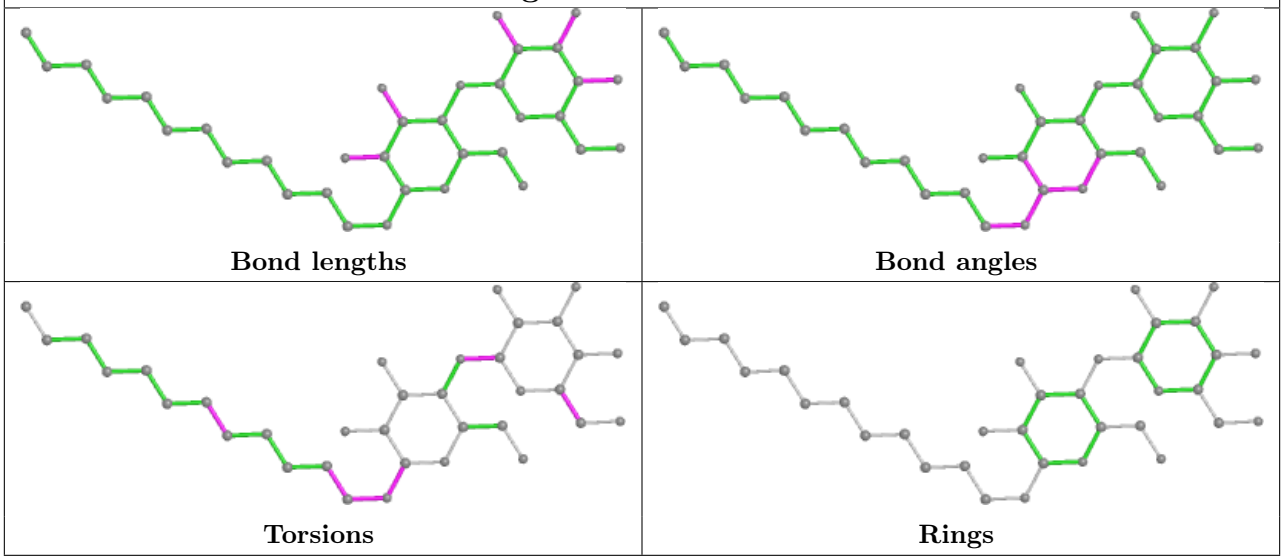


Torsions

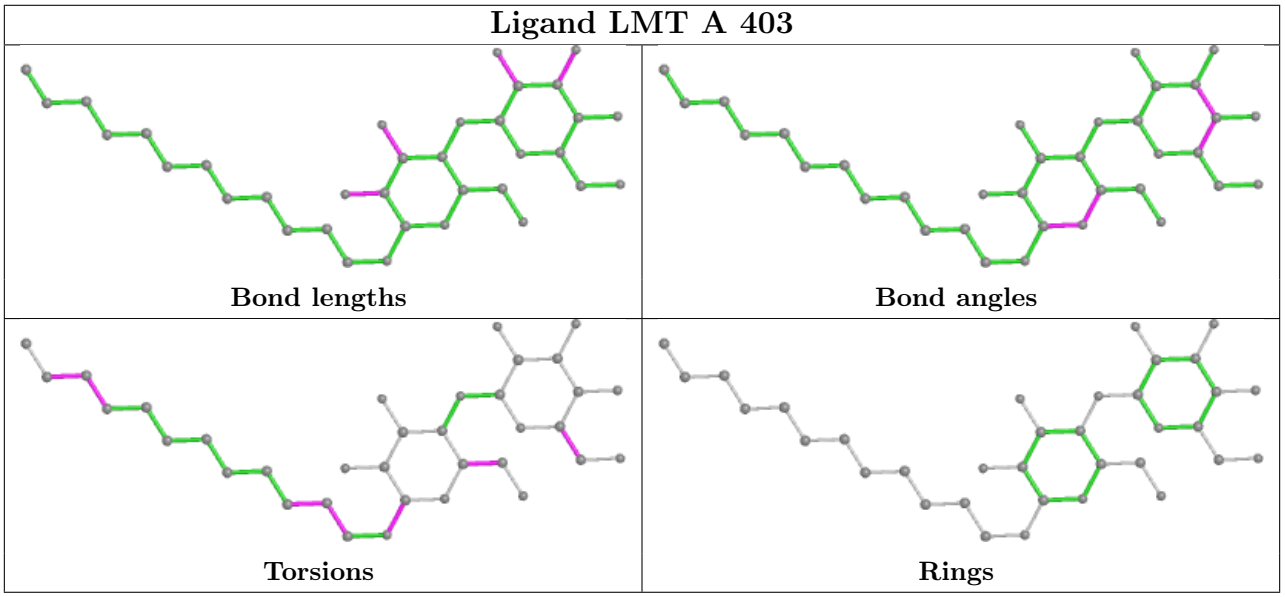


Rings

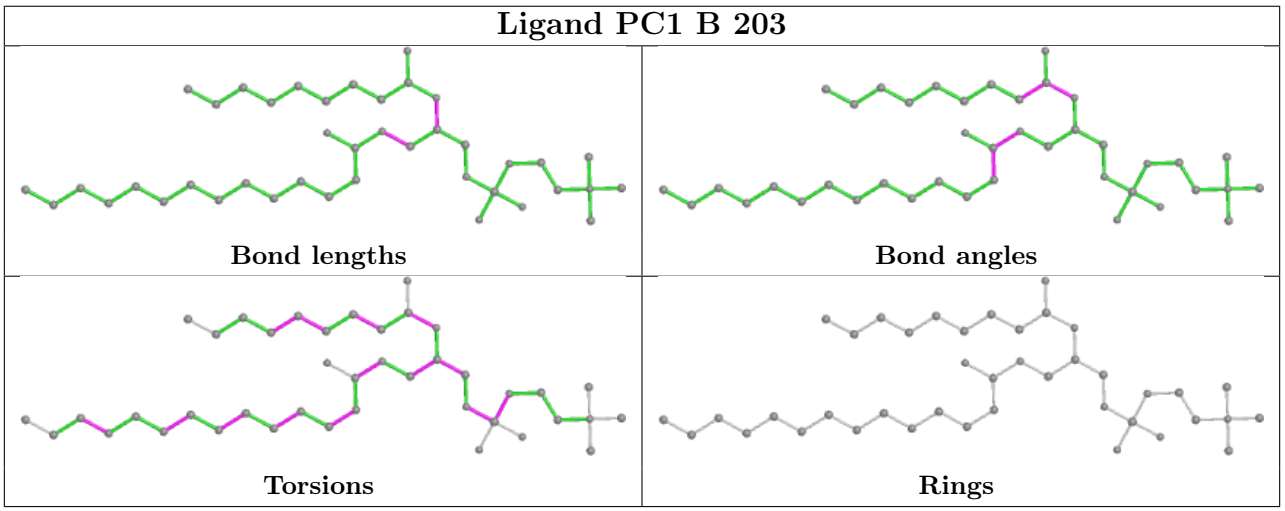
Ligand LMT O 503



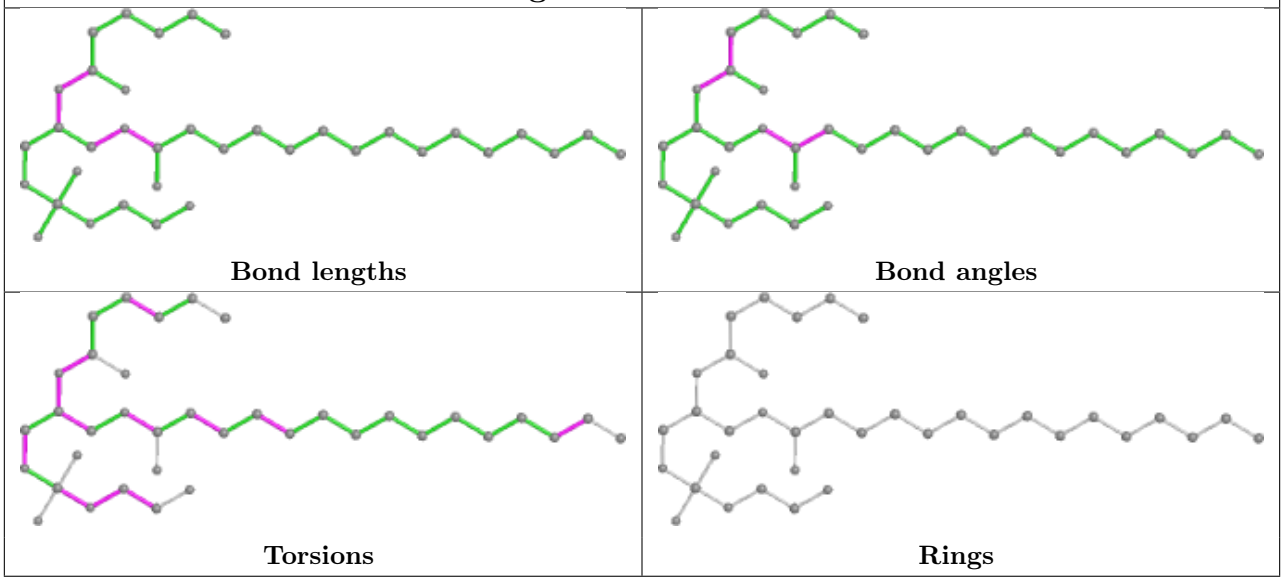
Ligand LMT A 403



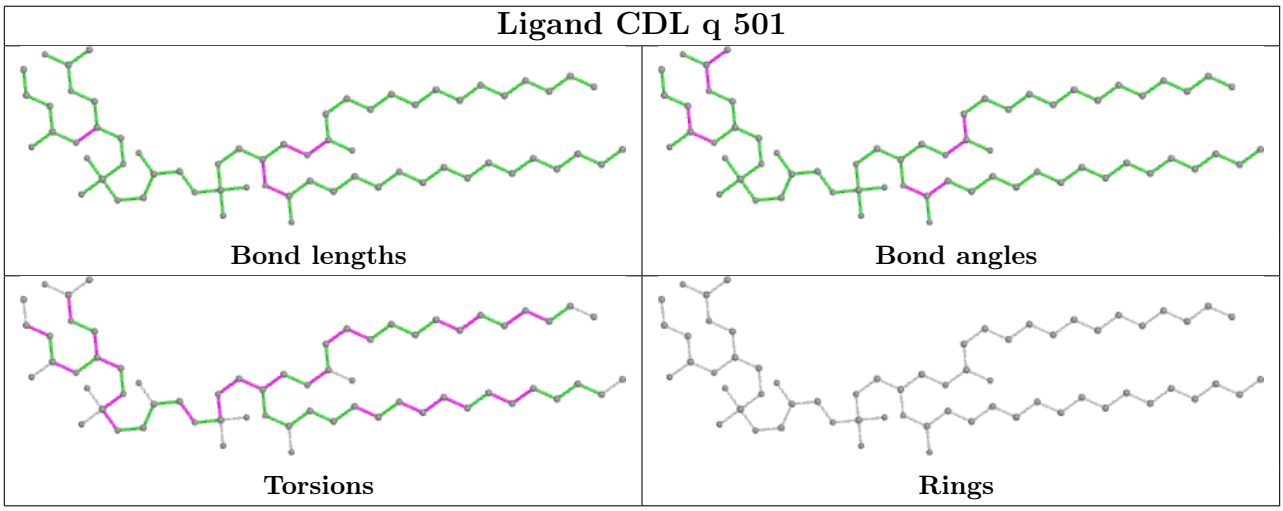
Ligand PC1 B 203



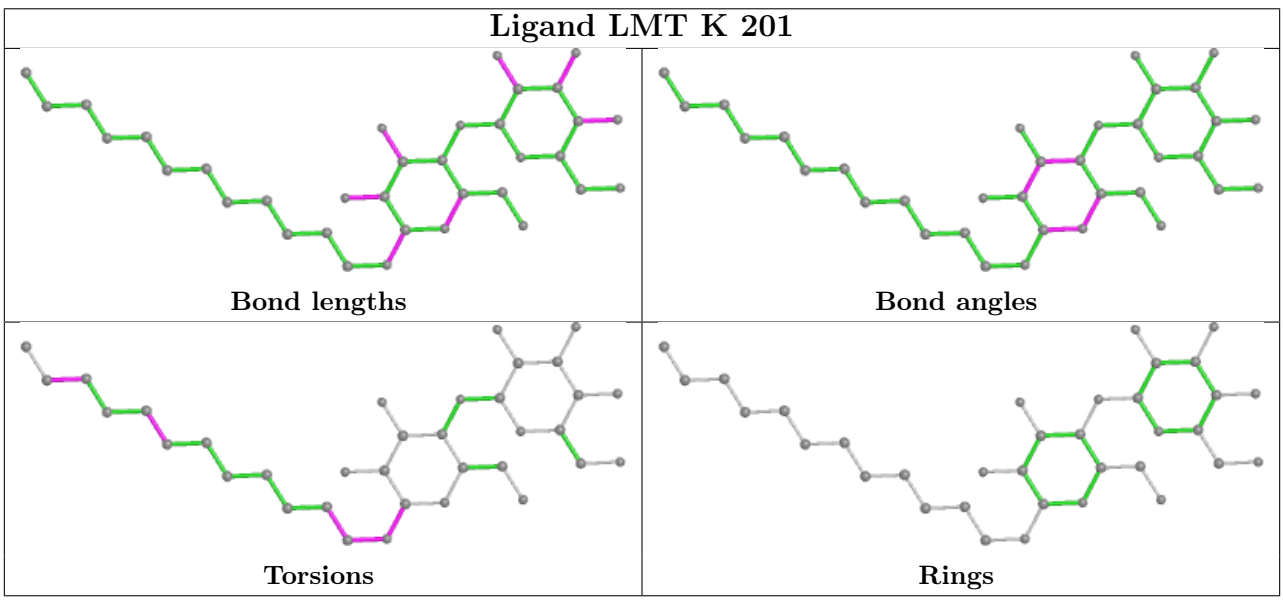
Ligand 3PE X 201



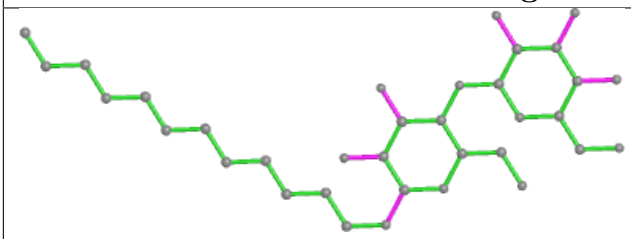
Ligand CDL q 501



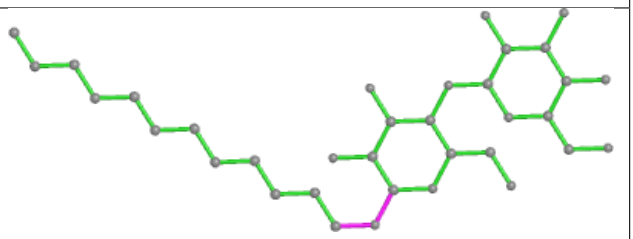
Ligand LMT K 201



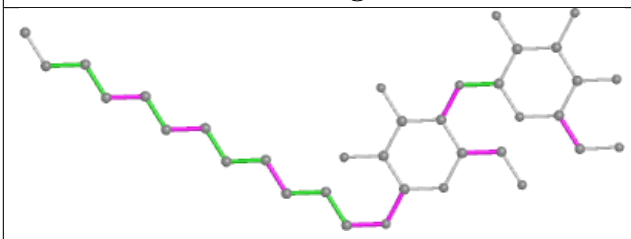
Ligand LMT Y 201



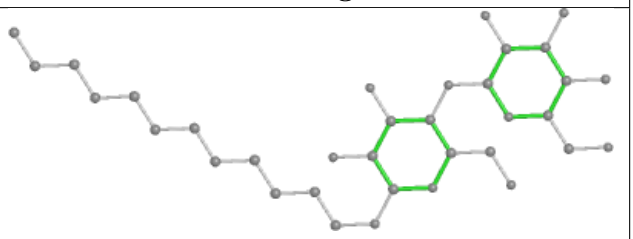
Bond lengths



Bond angles

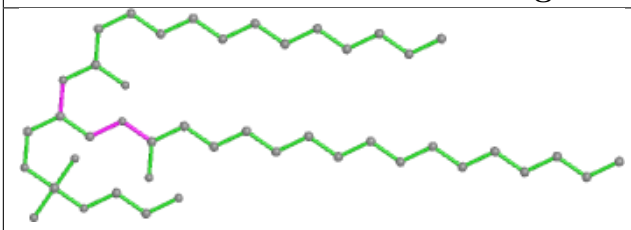


Torsions

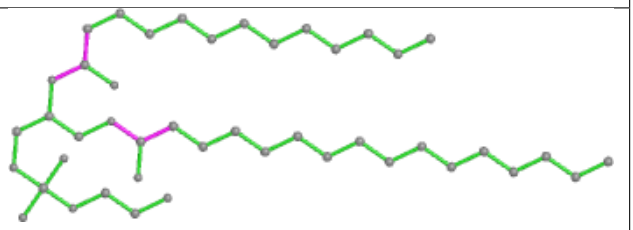


Rings

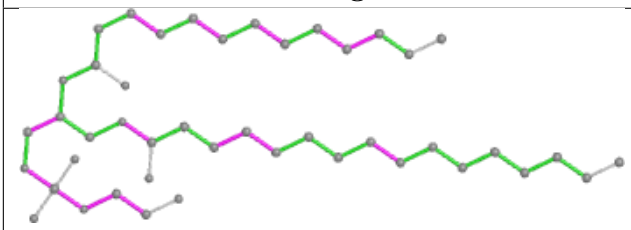
Ligand 3PE I 203



Bond lengths



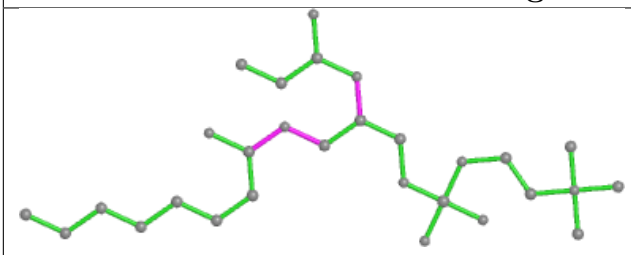
Bond angles



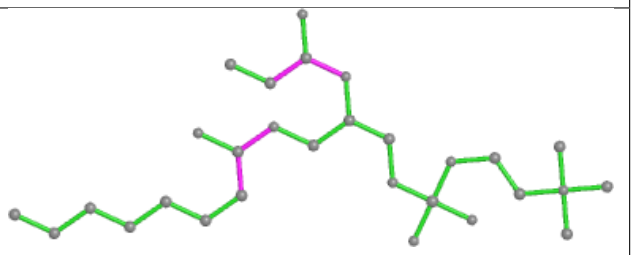
Torsions

Rings

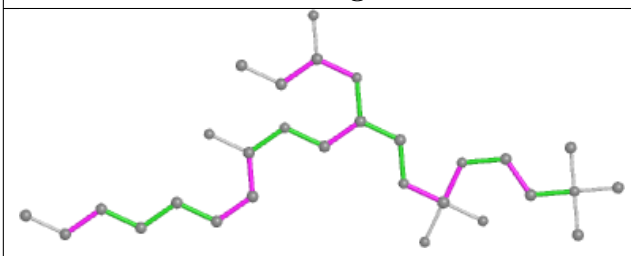
Ligand PC1 A 402



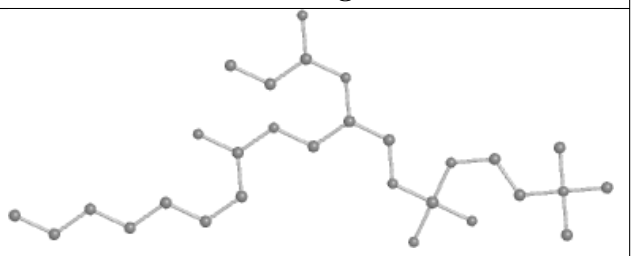
Bond lengths



Bond angles

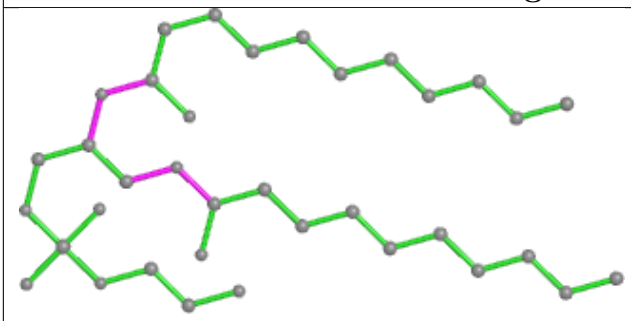


Torsions

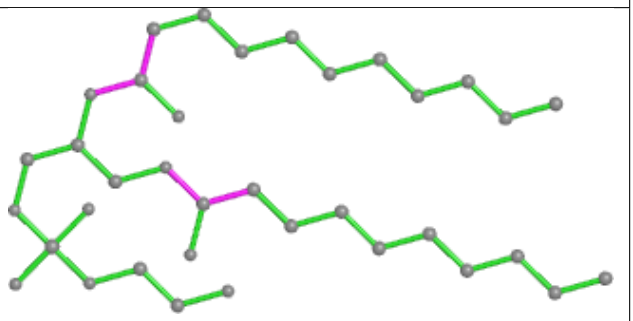


Rings

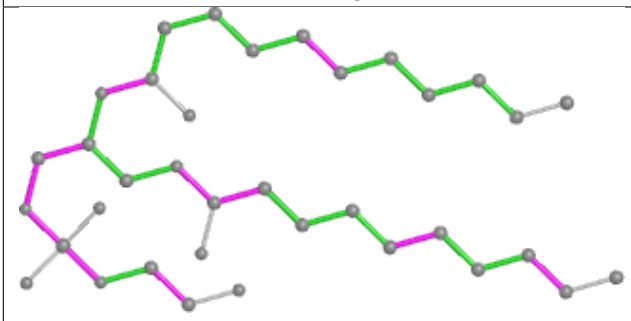
Ligand 3PE M 503



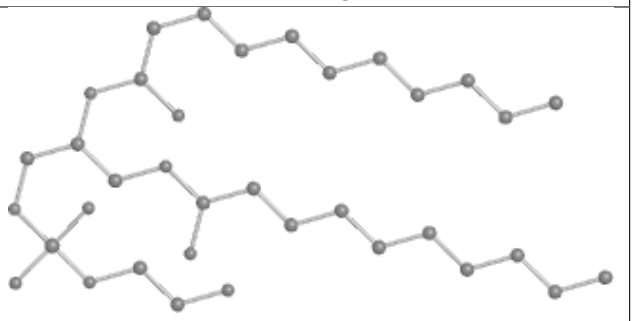
Bond lengths



Bond angles

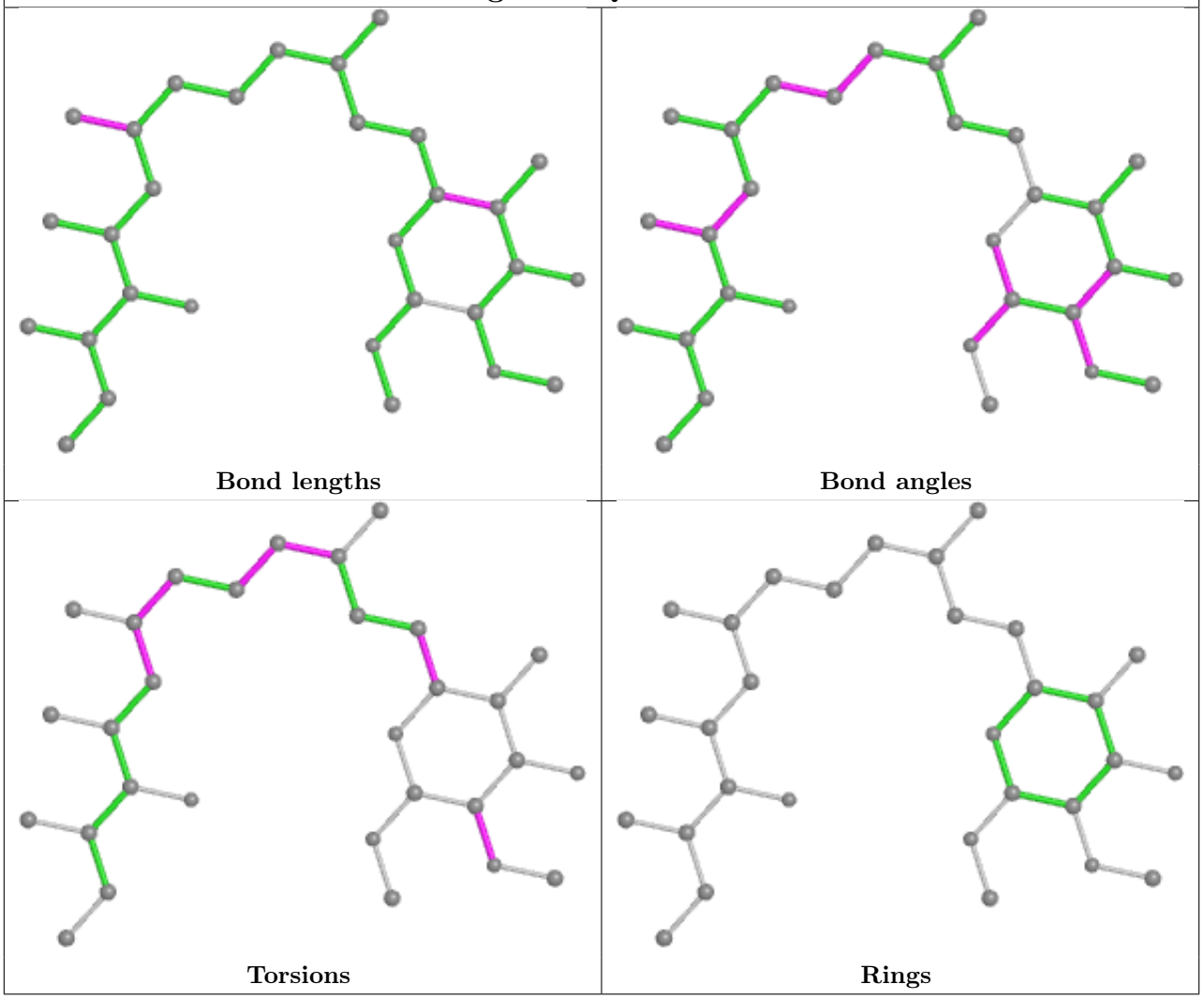


Torsions



Rings

Ligand HQH D 601



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.

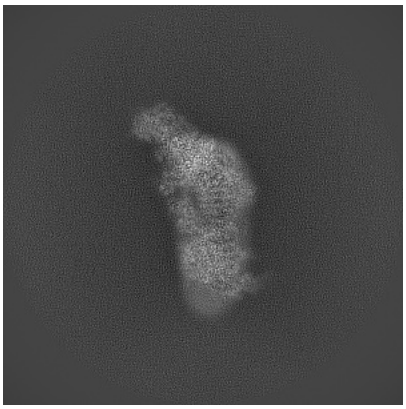
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16962. These allow visual inspection of the internal detail of the map and identification of artifacts.

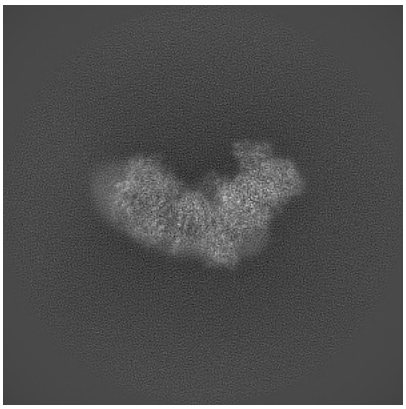
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

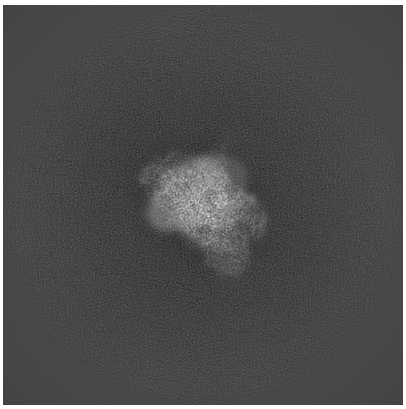
6.1.1 Primary map



X

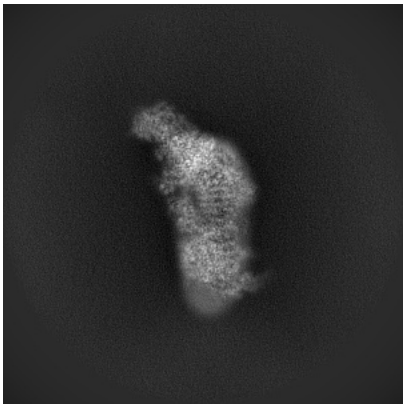


Y

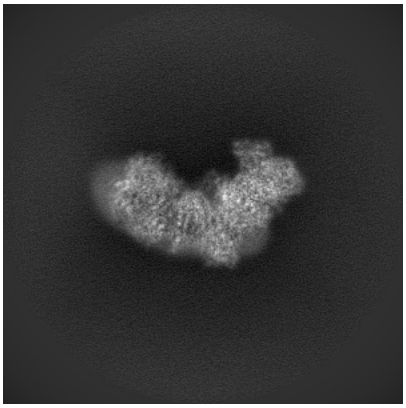


Z

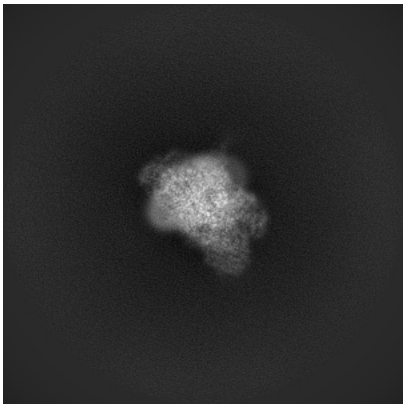
6.1.2 Raw map



X



Y

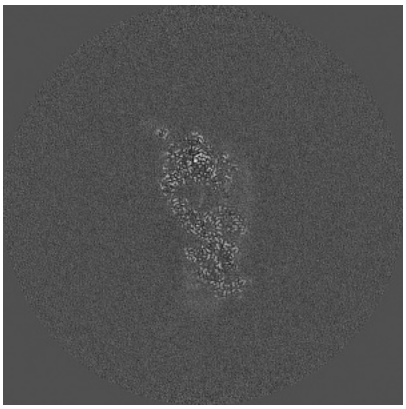


Z

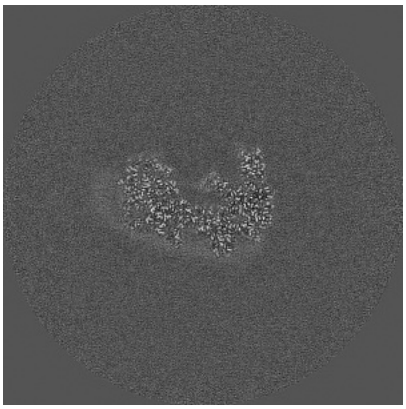
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

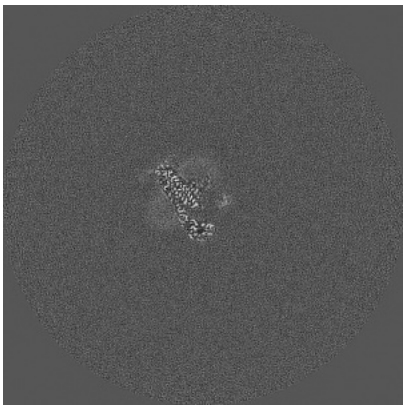
6.2.1 Primary map



X Index: 252

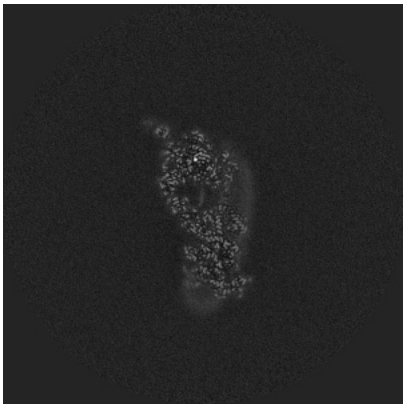


Y Index: 252

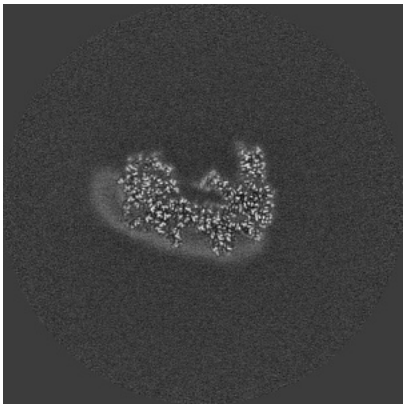


Z Index: 252

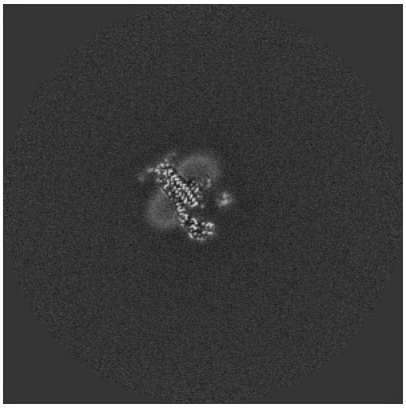
6.2.2 Raw map



X Index: 252



Y Index: 252

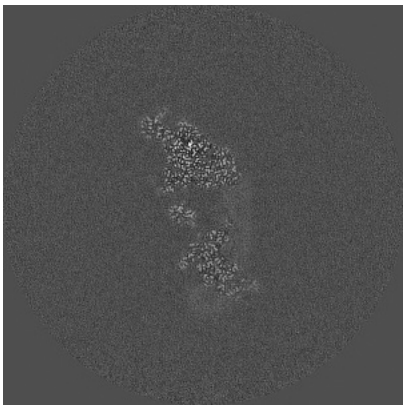


Z Index: 252

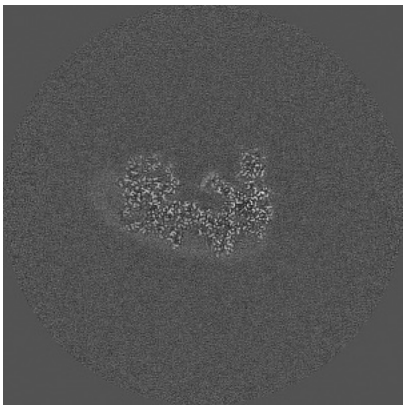
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

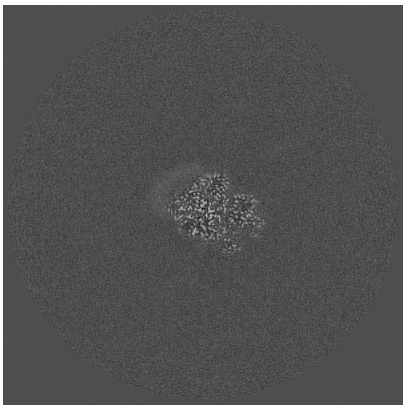
6.3.1 Primary map



X Index: 264

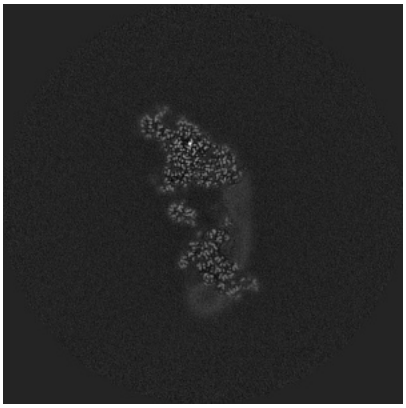


Y Index: 254

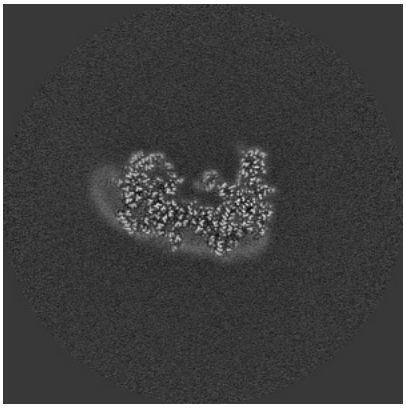


Z Index: 313

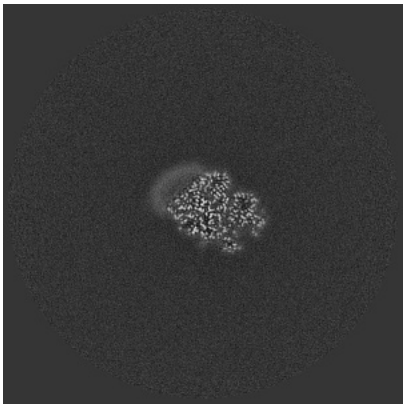
6.3.2 Raw map



X Index: 264



Y Index: 257

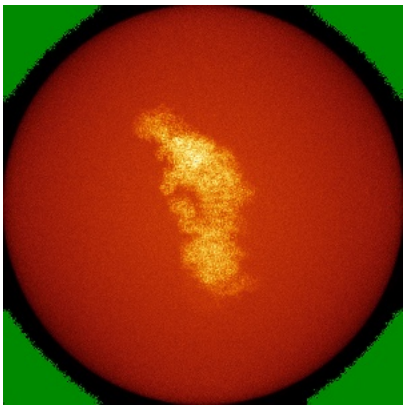


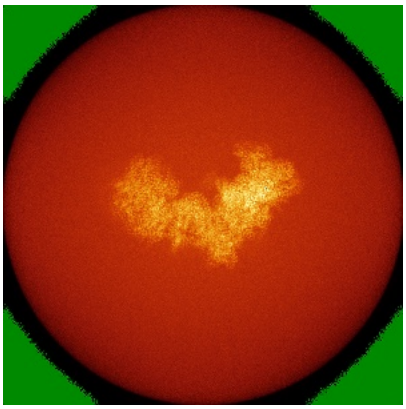
Z Index: 313

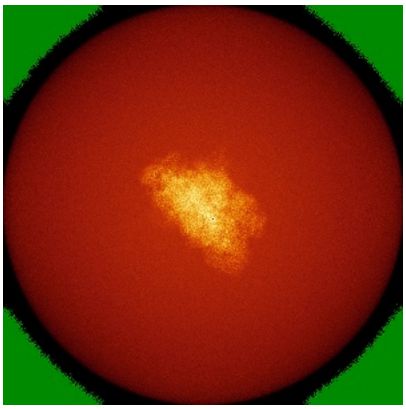
The images above show the largest variance slices of the map in three orthogonal directions.

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

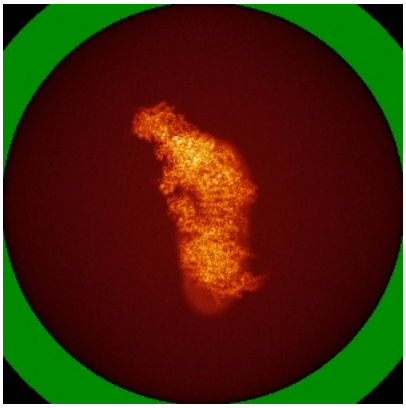
6.4.1 Primary map

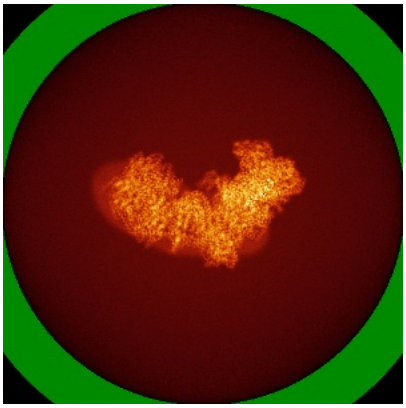

X

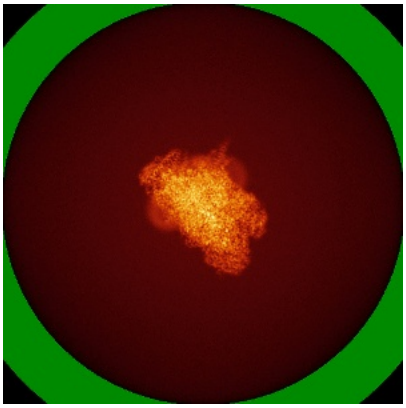

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

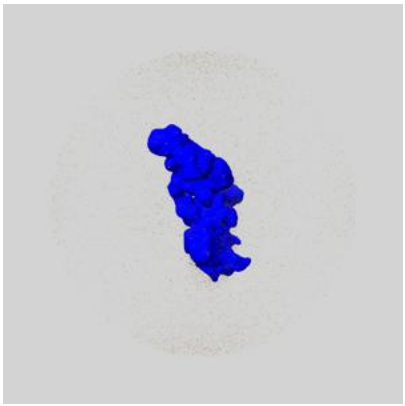
6.6 Mask visualisation

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

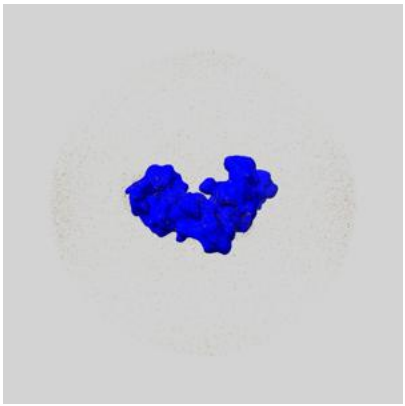
A mask typically either:

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

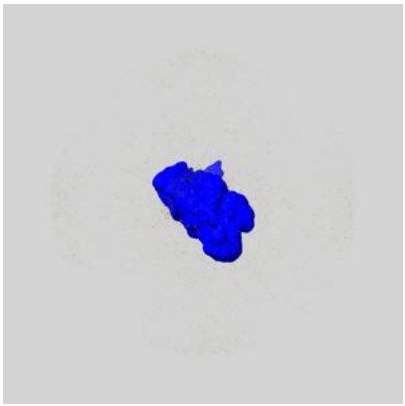
6.6.1 emd_16962_msk_1.map



X



Y

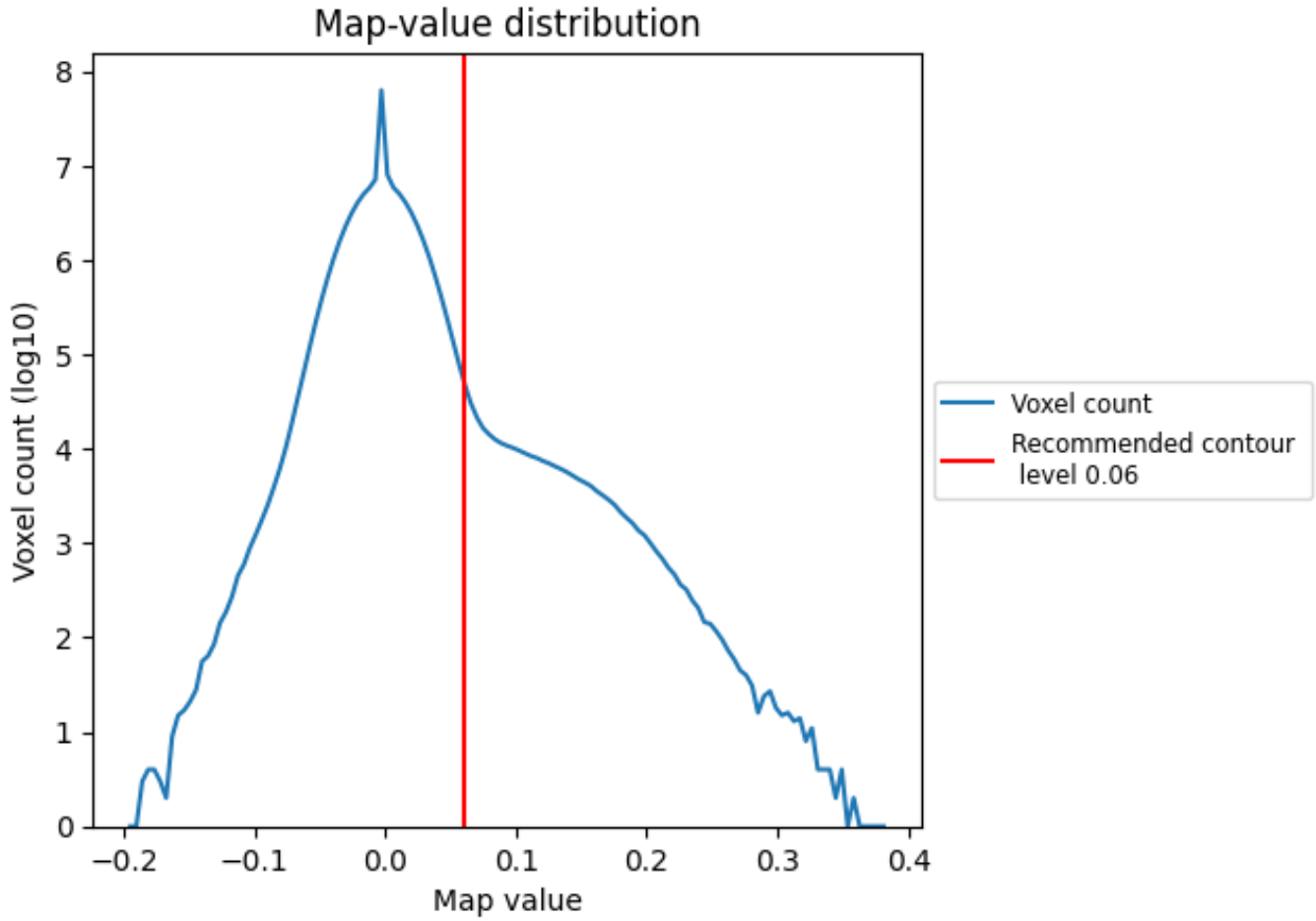


Z

7 Map analysis

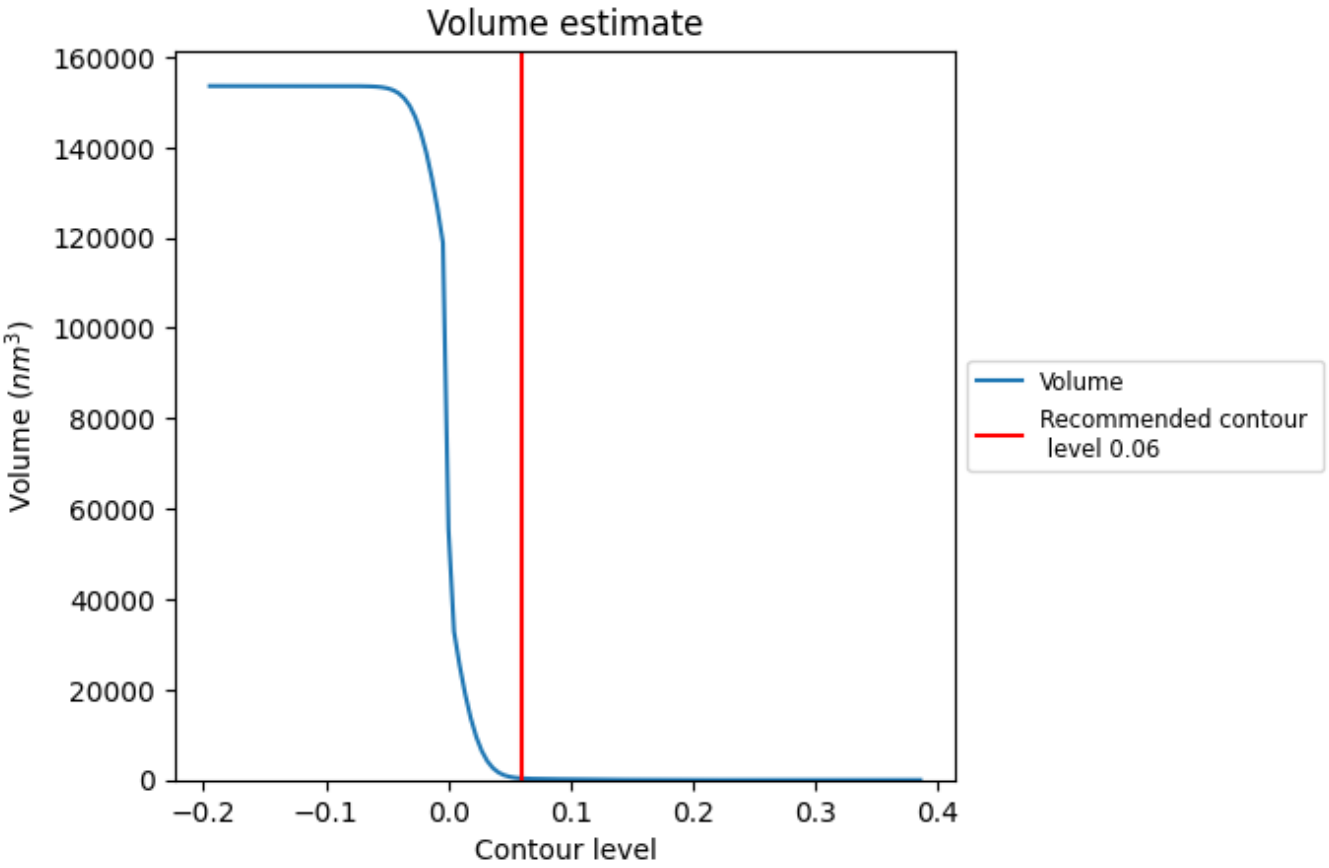
This section contains the results of statistical analysis of the map.

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.

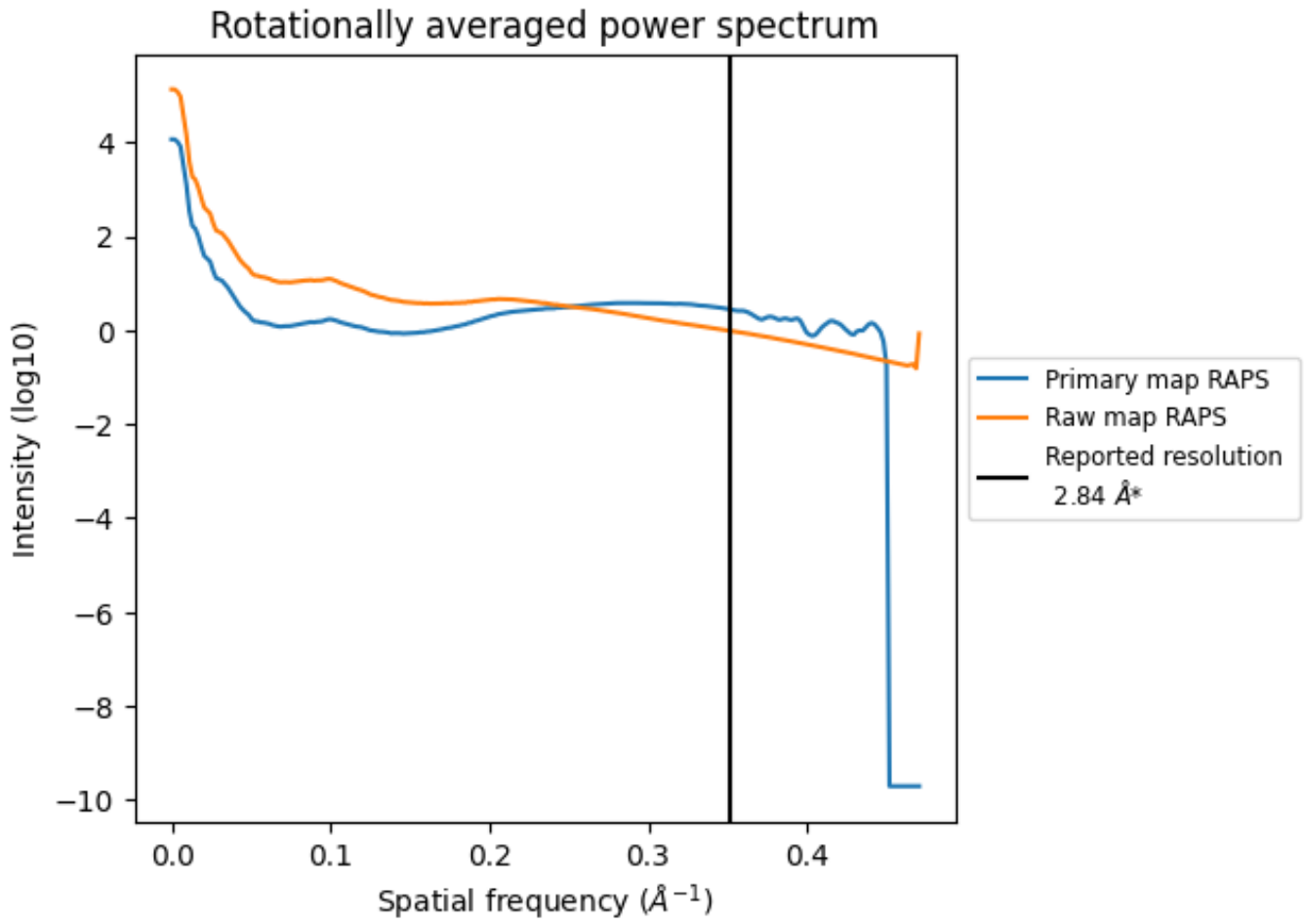
7.2 Volume estimate



The volume at the recommended contour level is 366 nm^3; this corresponds to an approximate mass of 331 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)

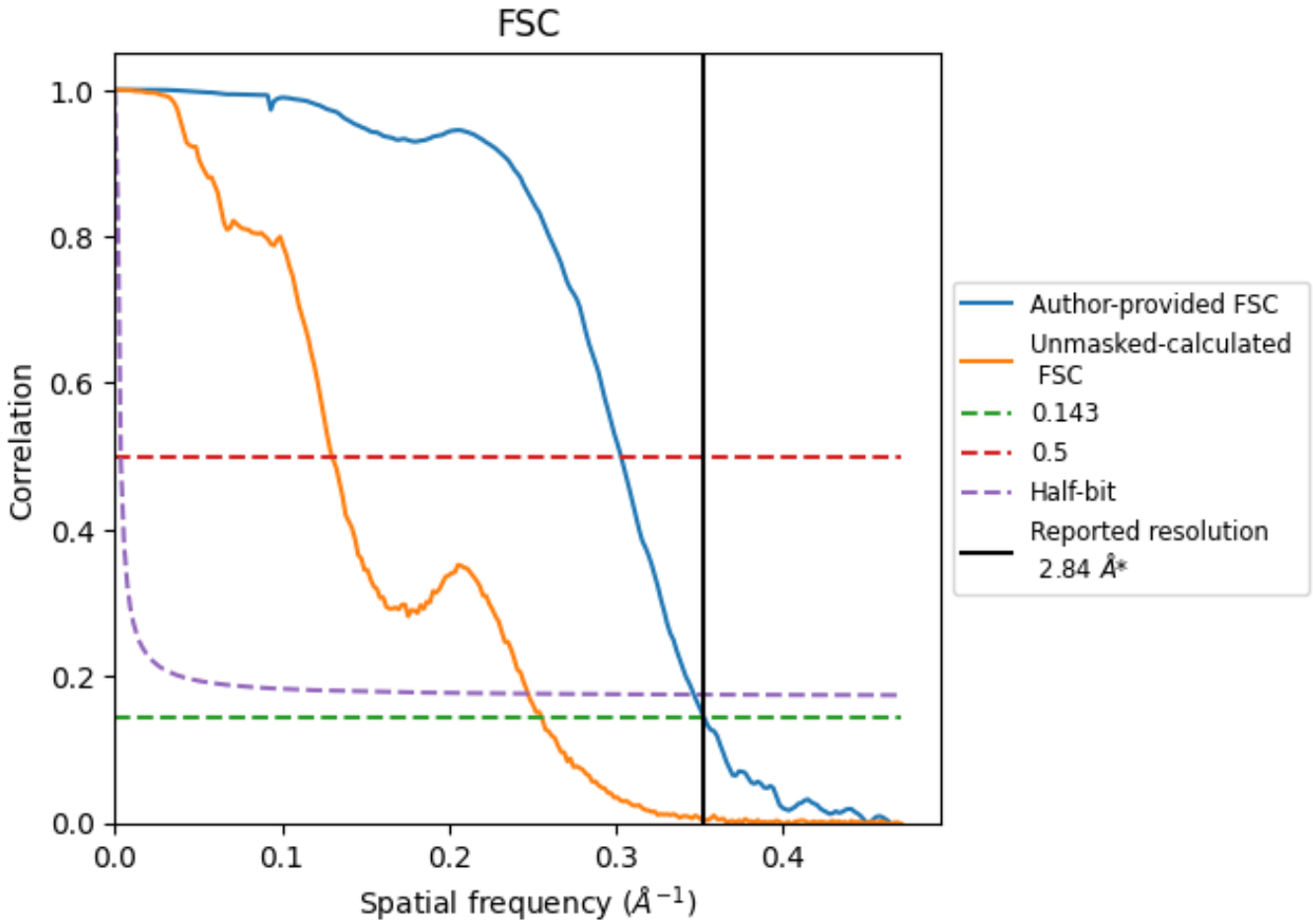


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

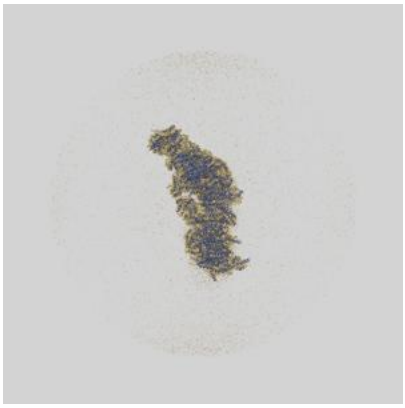
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.30	2.89
Unmasked-calculated*	3.91	7.69	4.04

*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 3.91 differs from the reported value 2.84 by more than 10 %

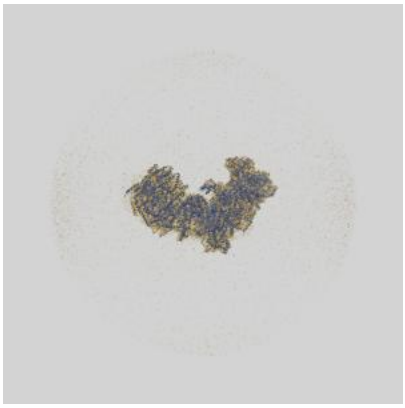
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16962 and PDB model 8OLT. Per-residue inclusion information can be found in section 3 on page 23.

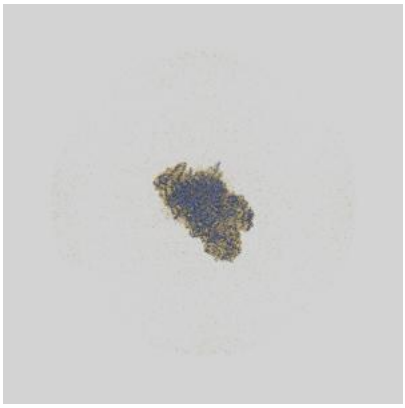
9.1 Map-model overlay



X



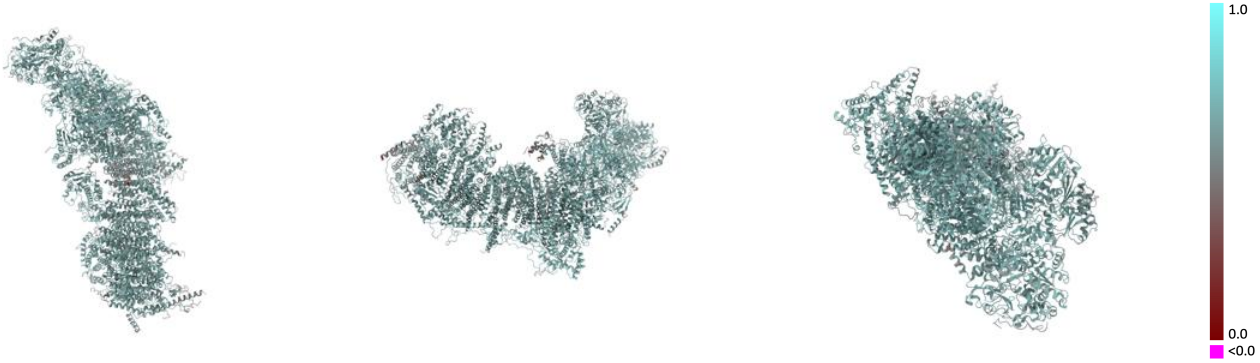
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

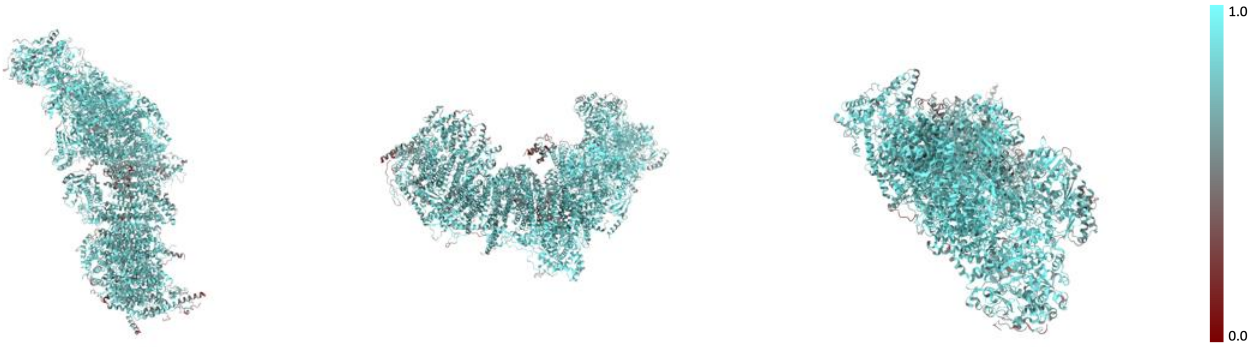
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

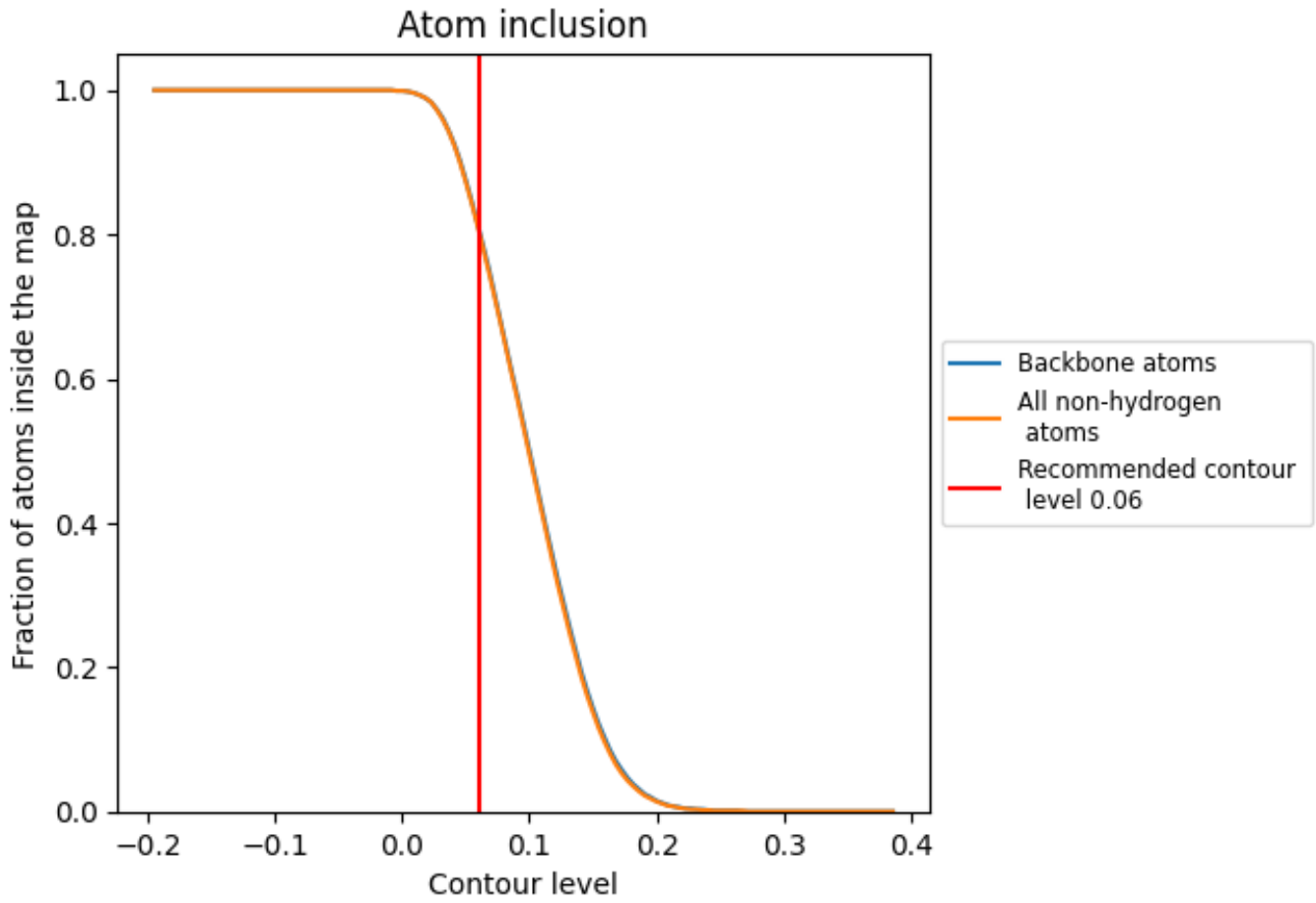
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.6280
A	0.7870	0.6350
B	0.9050	0.6610
C	0.9000	0.6610
D	0.8880	0.6560
E	0.7650	0.6010
F	0.8080	0.6180
G	0.8310	0.6320
H	0.8680	0.6510
I	0.8960	0.6550
J	0.7490	0.6110
K	0.8410	0.6450
L	0.8020	0.6270
M	0.8610	0.6470
N	0.8660	0.6520
O	0.8270	0.6390
P	0.8480	0.6380
Q	0.8560	0.6450
R	0.8460	0.6370
S	0.7190	0.5950
T	0.4240	0.4780
U	0.7080	0.6040
V	0.8160	0.6390
W	0.8190	0.6290
X	0.8150	0.6280
Y	0.6600	0.5890
Z	0.8270	0.6370
a	0.8790	0.6460
b	0.7520	0.6120
c	0.6980	0.5950
d	0.8170	0.6300
e	0.8260	0.6310
f	0.7140	0.5950
g	0.8060	0.6230
h	0.7960	0.6290

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6630	0.5830
j	0.6320	0.5570
k	0.6220	0.5620
l	0.7790	0.6140
m	0.7690	0.6120
n	0.7680	0.6090
o	0.6330	0.5550
p	0.7710	0.6090
q	0.8410	0.6370
r	0.8130	0.6310
s	0.7440	0.5980