Full wwPDB EM Validation Report ⓘ

Feb 4, 2023 – 09:04 am GMT

PDB ID	:	7R4C
EMDB ID	:	EMD-14292
Title	:	Bovine complex I in the presence of IM1761092, deactive class v (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.30 Å(reported)

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

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

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

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

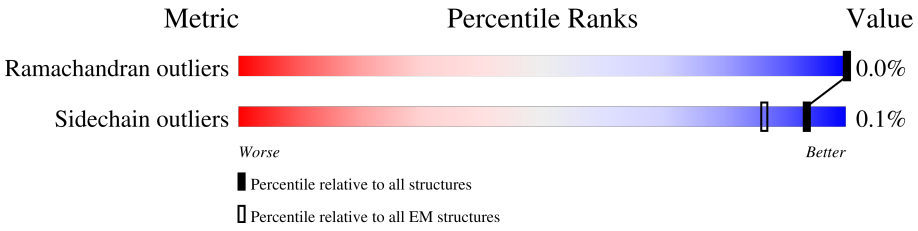
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.30 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	86% 14%
2	B	216	71% 29%
3	C	266	77% 23%
4	D	463	89% 11%
5	E	249	85% 15%
6	F	464	92% 8%
7	G	727	94% 5%
8	H	318	97%
9	I	212	83% 17%

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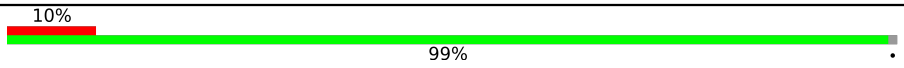
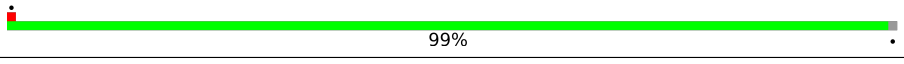
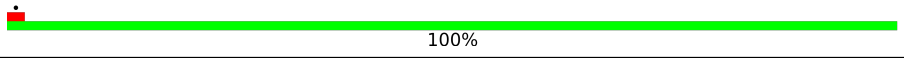
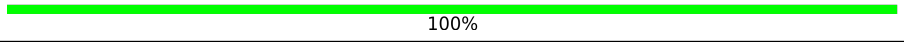
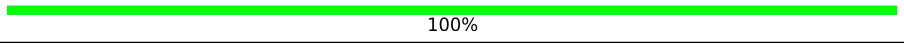
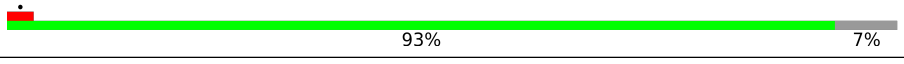
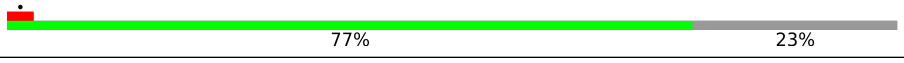
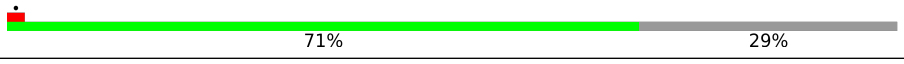
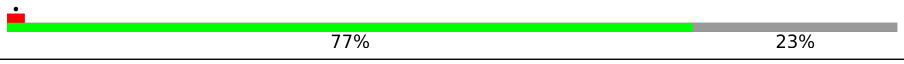
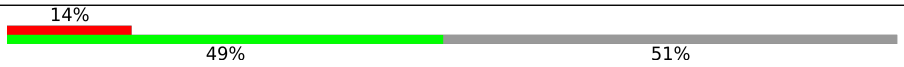
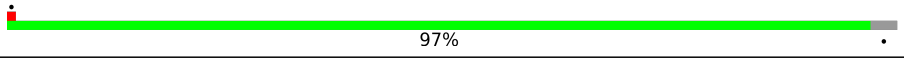
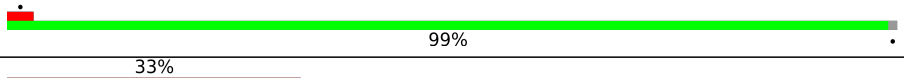
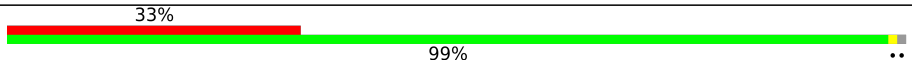
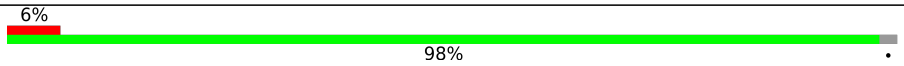
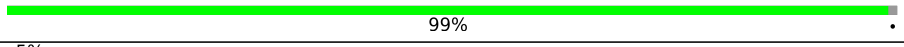
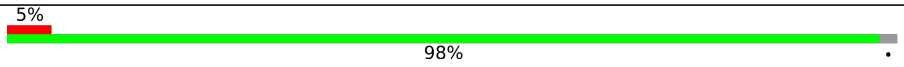
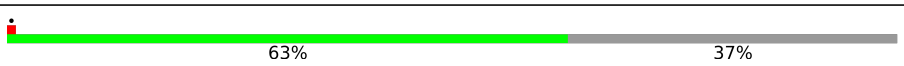
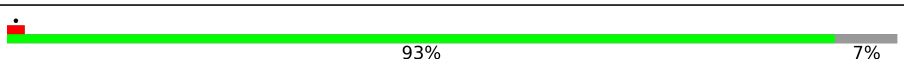
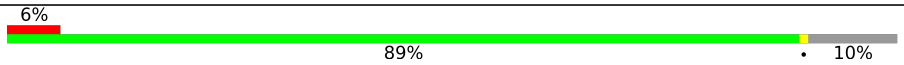
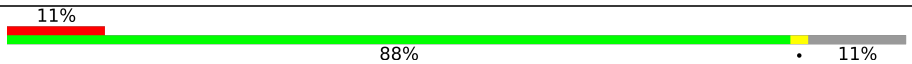
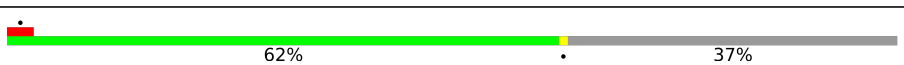
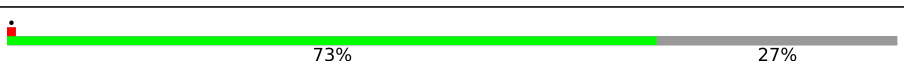
Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	

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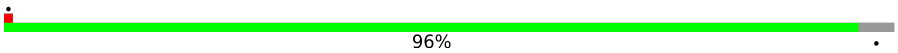
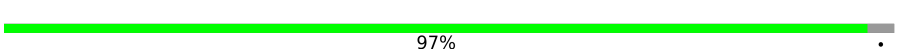
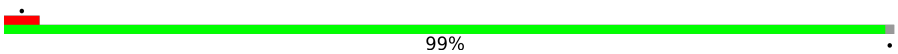
Mol	Chain	Length	Quality of chain
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 68045 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	99	799	547	116	131	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	154	1230	786	220	210	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	206	1714	1107	295	309	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	412	3327	2124	572	606	25	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1650	1054	276	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3301	2080	589	612	20		

- 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
			5279	3307	920	1013	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	308	Total	C	N	O	S	0	0
			2428	1628	374	403	23		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			739	483	111	130	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	604	Total	C	N	O	S	0	0
			4765	3169	732	821	43		

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	292	Total	C	N	O	S	0	0
			2323	1487	418	413	5		

- 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
			1016	641	181	191	3		

- 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
			730	448	137	142	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
			669	419	125	123	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	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
			911	589	154	165	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
			971	622	180	165	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- 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
			561	361	103	92	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			646	422	108	114	2		

- 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	0	0
			405	268	69	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	112	Total	C	N	O	S	0	0
			934	613	157	161	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	95	Total	C	N	O	S	0	0
			799	506	150	137	6		

- 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
			444	291	78	74	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	97	Total	C	N	O	S	0	0
			813	523	133	153	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	103	Total	C	N	O	S	0	0
			884	584	149	150	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	79	Total	C	N	O	S	0	0
			638	418	107	111	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
			1304	844	213	239	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	113	Total	C	N	O	0	0
			948	608	167	173		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1043	650	200	184	9		

- 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
			1435	900	265	262	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
			1201	773	215	209	4		

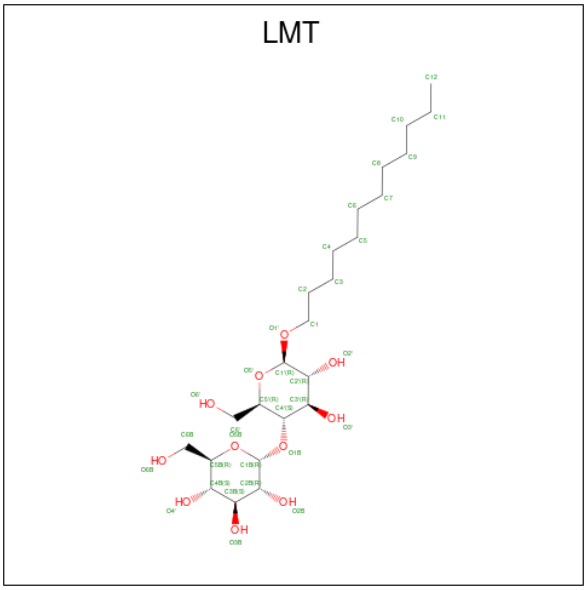
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	42	Total	C	N	O	S	0	0
			353	219	64	69	1		

- 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	B	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	N	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	b	1	Total	C	O	0
			35	24	11	

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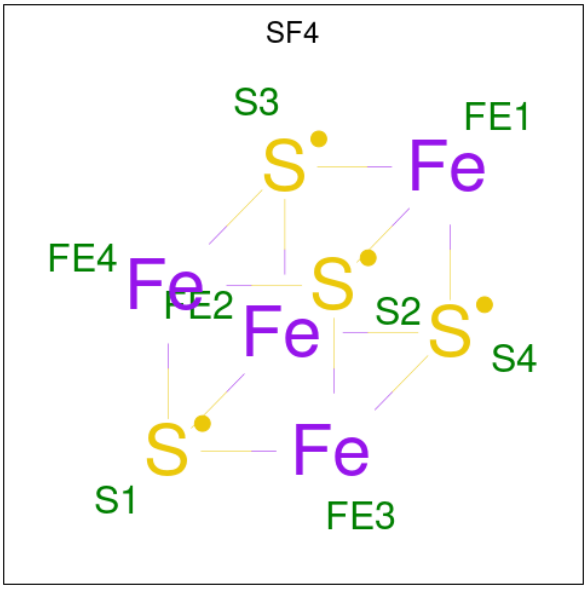
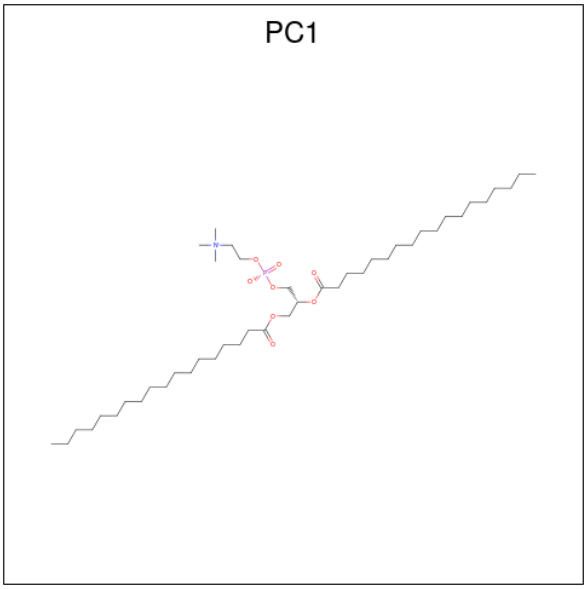
Mol	Chain	Residues	Atoms	AltConf
45	d	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	h	1	Total C O 35 24 11	0
45	j	1	Total C O 35 24 11	0
45	l	1	Total C O 35 24 11	0

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



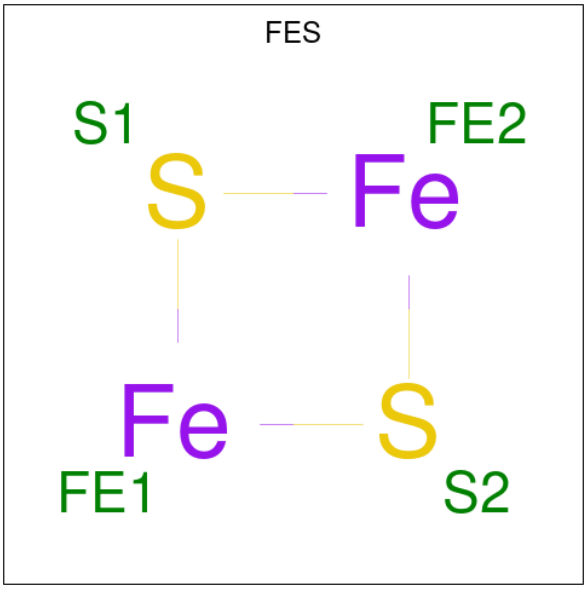
Mol	Chain	Residues	Atoms	AltConf
46	B	1	Total Fe S 8 4 4	0
46	F	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



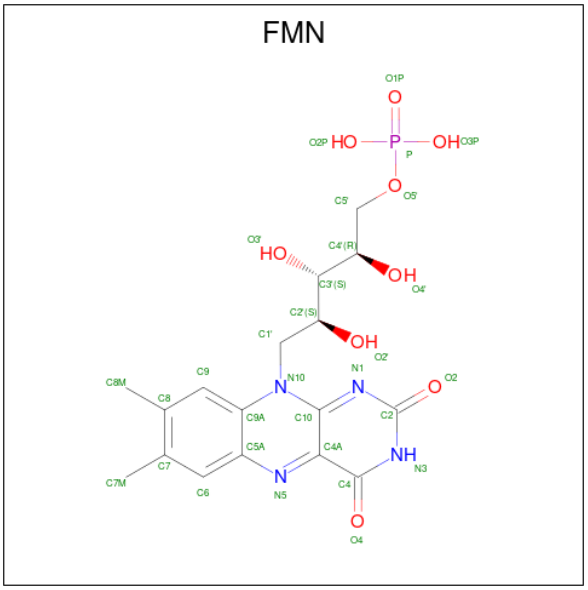
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	M	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



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

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

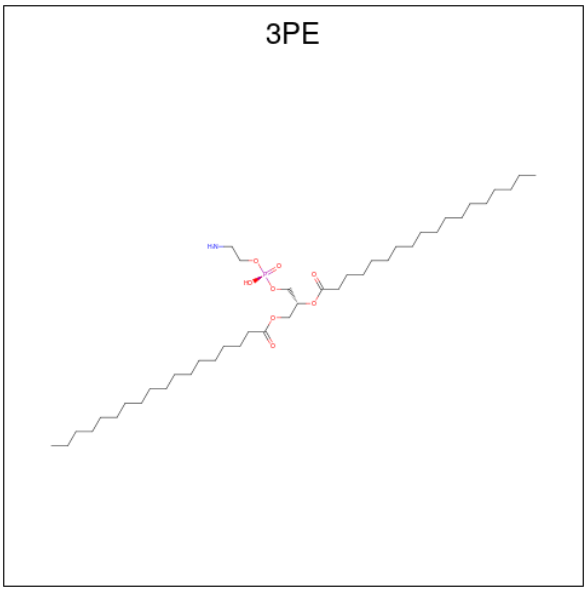


Mol	Chain	Residues	Atoms	AltConf
49	F	1	Total C N O P 31 17 4 9 1	0

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

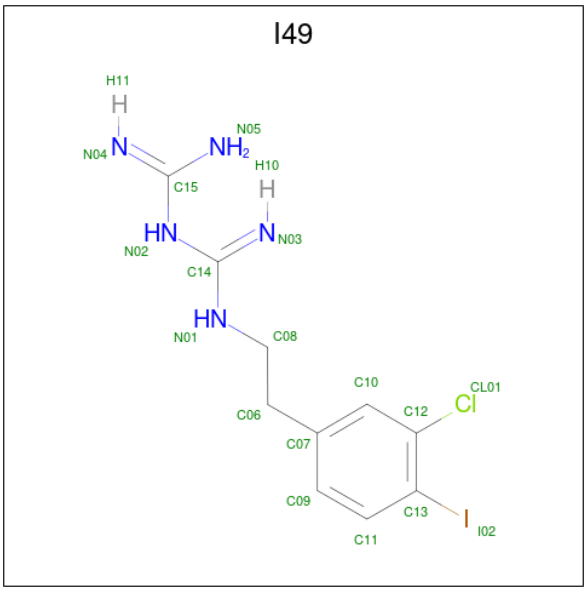
Mol	Chain	Residues	Atoms	AltConf
50	G	1	Total K 1 1	0

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



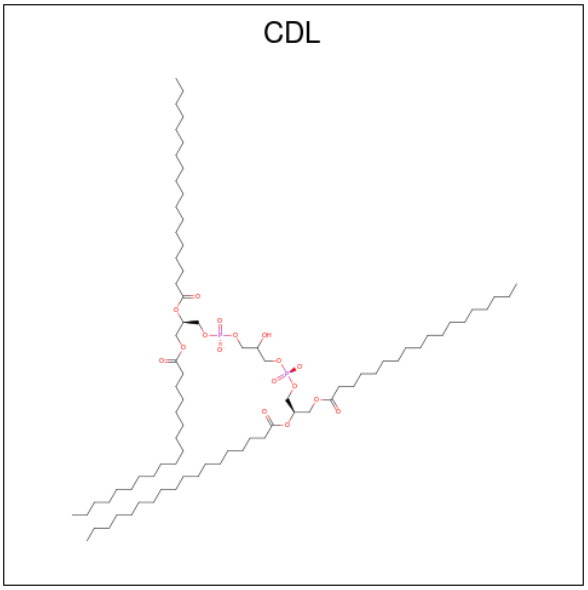
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	N	O	P	0
			25	15	1	8	1	
51	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	J	1	Total	C	N	O	P	0
			38	28	1	8	1	
51	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
51	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
51	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
51	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
51	e	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	
52	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			63	44	17	2	
53	X	1	Total	C	O	P	0
			71	52	17	2	

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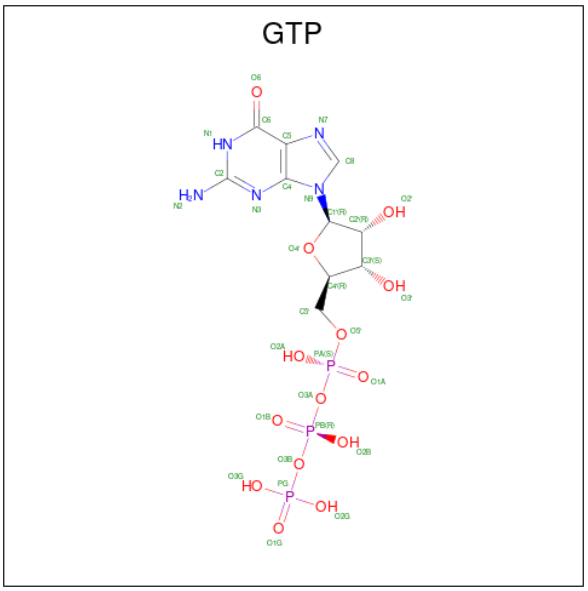
Mol	Chain	Residues	Atoms				AltConf
53	Y	1	Total	C	O	P	0
			71	52	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

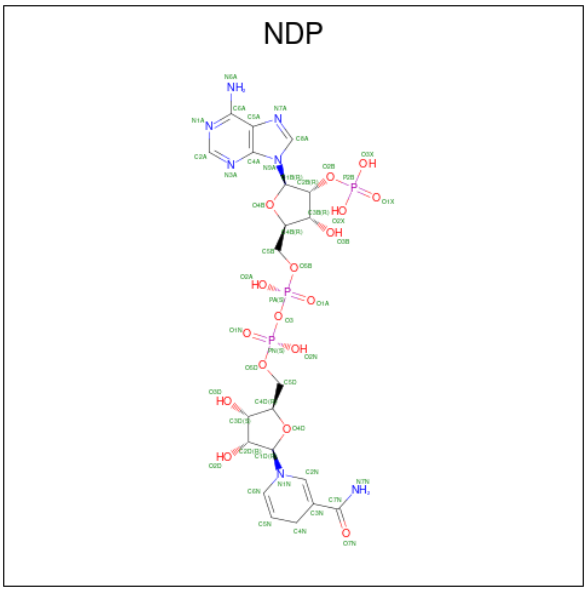


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

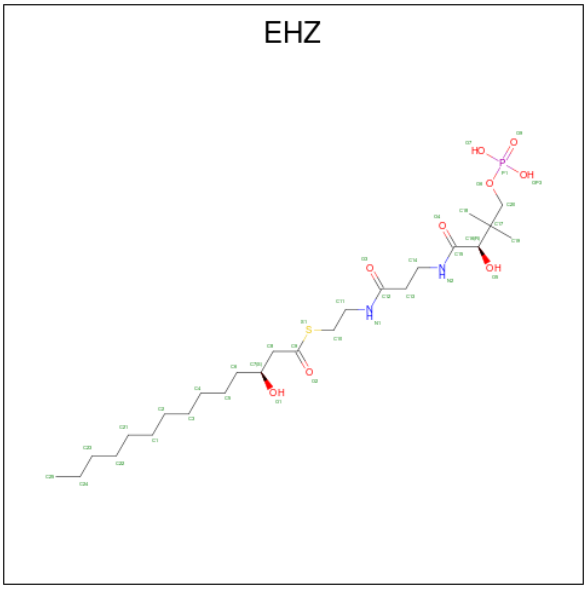


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

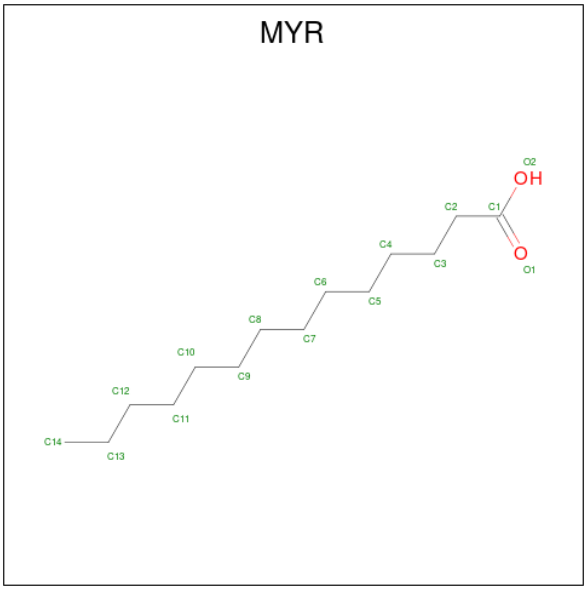
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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
			7	6	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	10	Total	O	0
			10	10	
60	B	62	Total	O	0
			62	62	
60	C	100	Total	O	0
			100	100	
60	D	155	Total	O	0
			155	155	
60	E	20	Total	O	0
			20	20	
60	F	68	Total	O	0
			68	68	
60	G	208	Total	O	0
			208	208	

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Mol	Chain	Residues	Atoms	AltConf
60	H	52	Total O 52 52	0
60	I	99	Total O 99 99	0
60	J	7	Total O 7 7	0
60	K	10	Total O 10 10	0
60	L	63	Total O 63 63	0
60	M	68	Total O 68 68	0
60	N	38	Total O 38 38	0
60	O	20	Total O 20 20	0
60	P	49	Total O 49 49	0
60	Q	66	Total O 66 66	0
60	R	41	Total O 41 41	0
60	S	2	Total O 2 2	0
60	U	13	Total O 13 13	0
60	V	16	Total O 16 16	0
60	W	13	Total O 13 13	0
60	X	26	Total O 26 26	0
60	Y	1	Total O 1 1	0
60	Z	22	Total O 22 22	0
60	a	15	Total O 15 15	0
60	b	6	Total O 6 6	0
60	d	10	Total O 10 10	0

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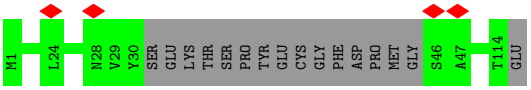
Mol	Chain	Residues	Atoms	AltConf
60	e	18	Total O 18 18	0
60	f	4	Total O 4 4	0
60	g	13	Total O 13 13	0
60	h	23	Total O 23 23	0
60	i	6	Total O 6 6	0
60	j	3	Total O 3 3	0
60	k	8	Total O 8 8	0
60	l	33	Total O 33 33	0
60	m	15	Total O 15 15	0
60	n	31	Total O 31 31	0
60	o	13	Total O 13 13	0
60	p	38	Total O 38 38	0
60	q	24	Total O 24 24	0
60	r	28	Total O 28 28	0
60	s	8	Total O 8 8	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.

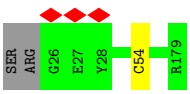
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



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

Chain B:

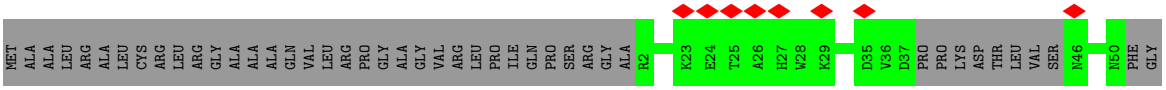


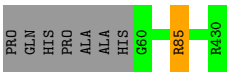
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

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

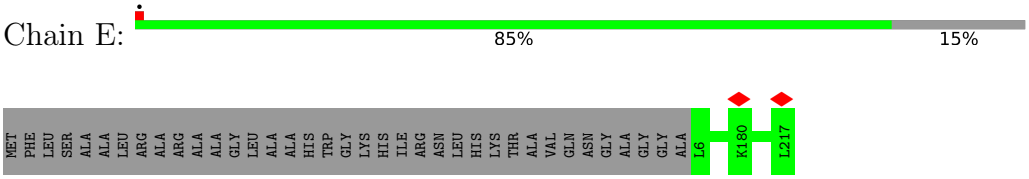
Chain D:





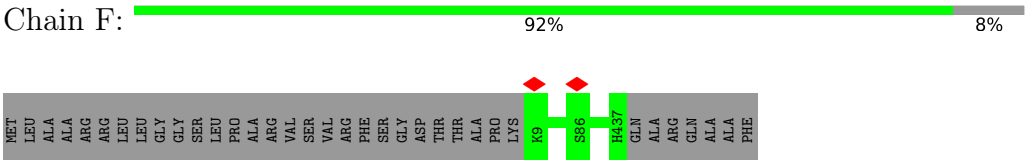
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



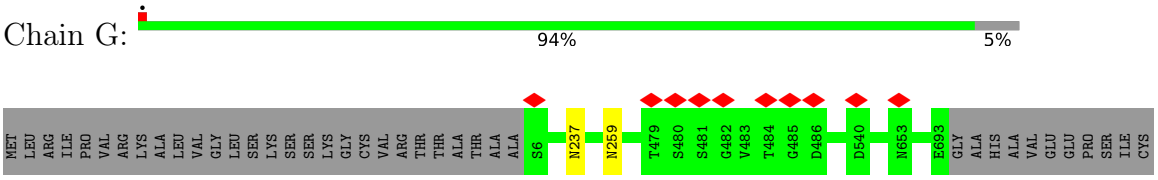
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



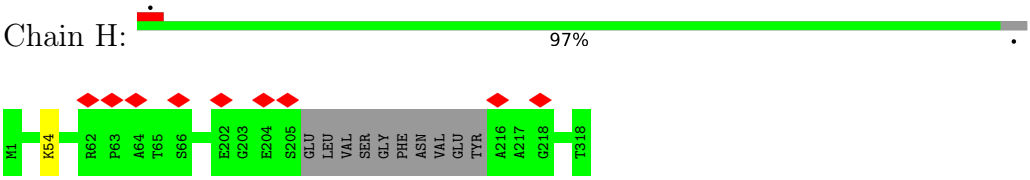
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



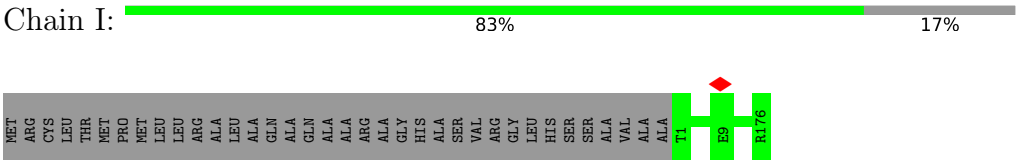
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



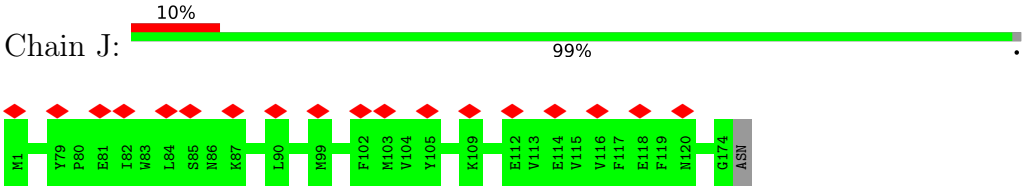
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

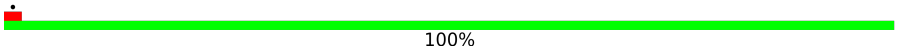


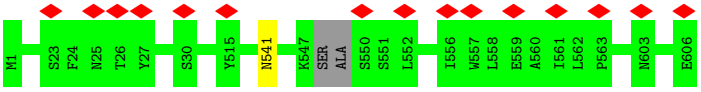
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

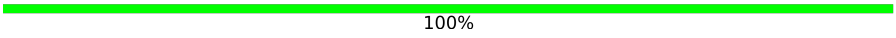
Chain L:





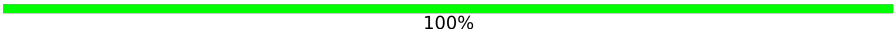
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



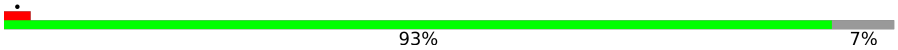
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

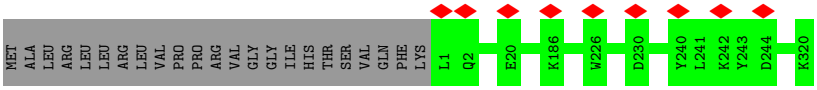
Chain N:



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

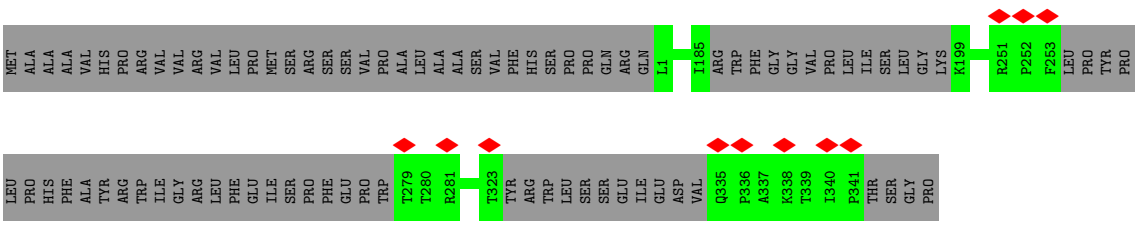
Chain O:





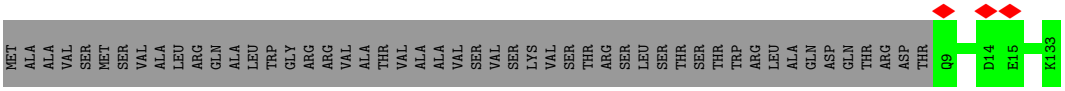
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

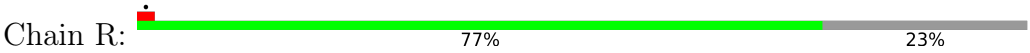


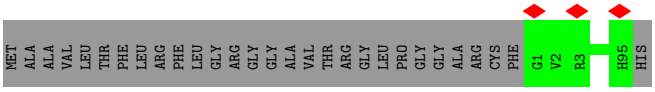
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

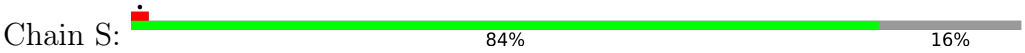


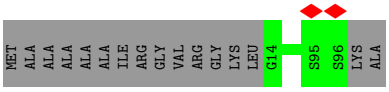
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



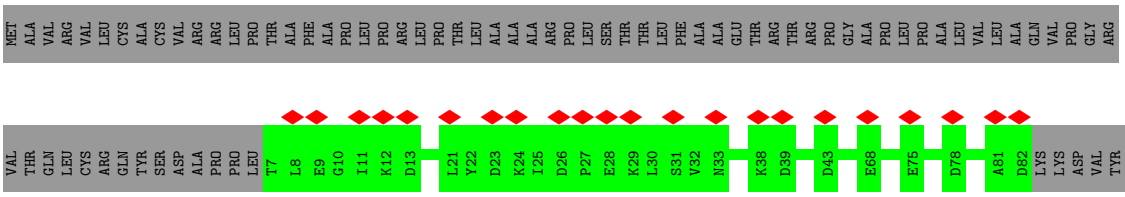


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

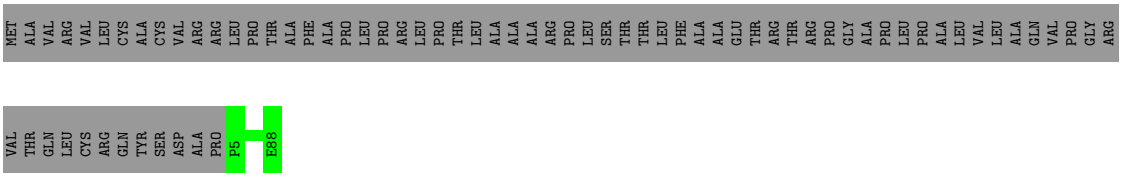




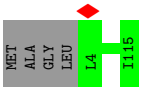
• Molecule 20: Acyl carrier protein, mitochondrial



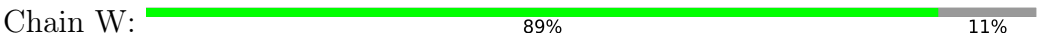
• Molecule 20: Acyl carrier protein, mitochondrial

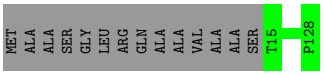


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



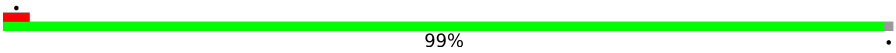
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

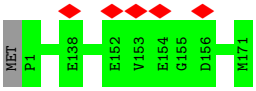




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

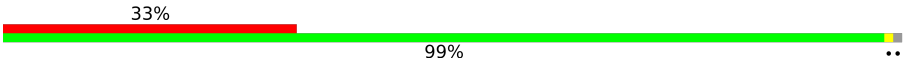
Chain X:

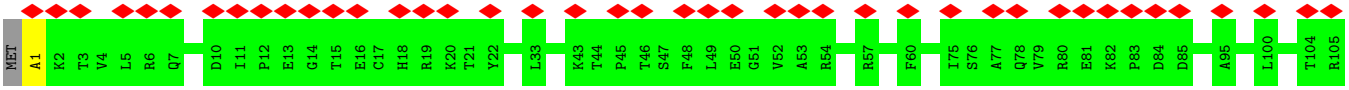


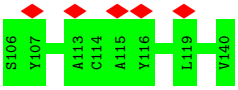


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

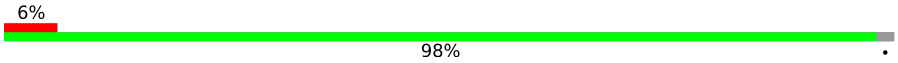


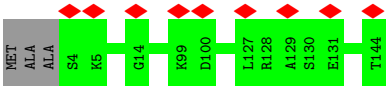




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

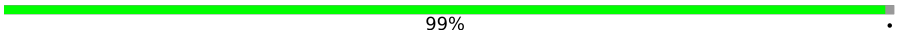
Chain Z:





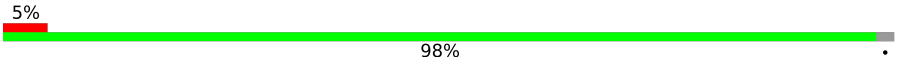
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

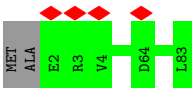
Chain a:



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

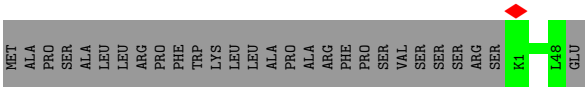
Chain b:





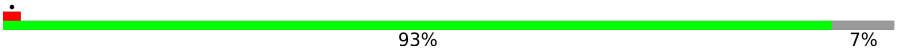
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

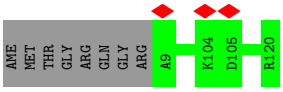
Chain c:



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

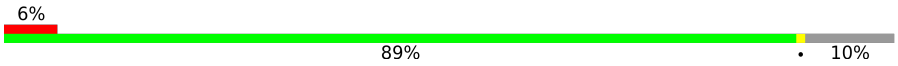
Chain d:

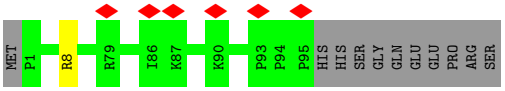




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

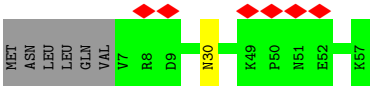
Chain e:





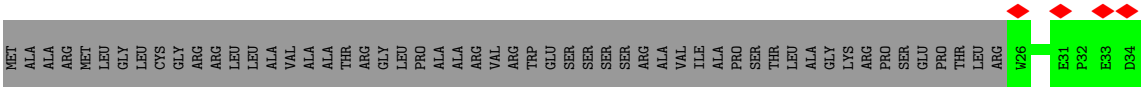
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

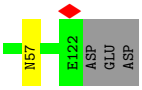
Chain f:



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

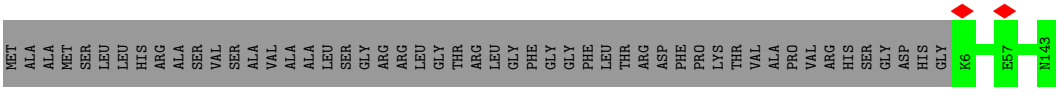
Chain g:





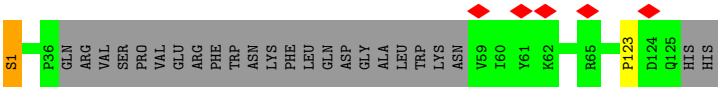
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



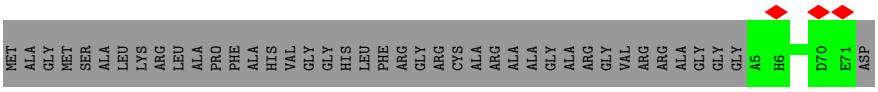
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



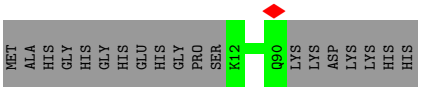
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



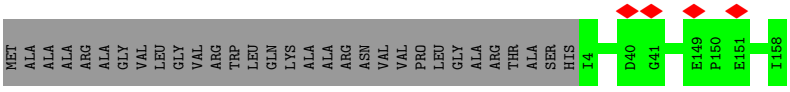
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



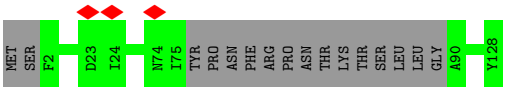
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



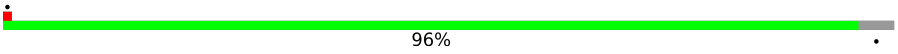
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

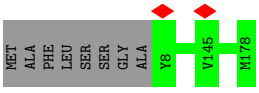
Chain m:



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

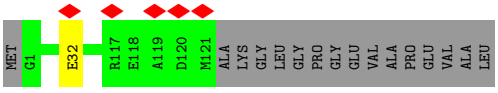
Chain n:





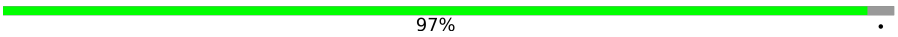
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

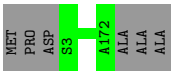
Chain o:



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

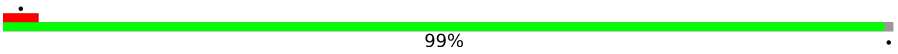
Chain p:

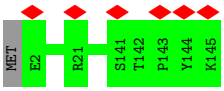




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

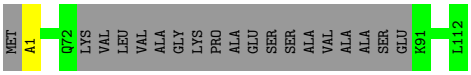
Chain q:





• 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	91673	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	42.630	Depositor
Minimum map value	-15.720	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.072	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, K, LMT, FES, GTP, MG, FMN, MYR, SAC, FME, CDL, NDP, AYA, 2MR, SF4, EHZ, 3PE, ZN, I49

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	0.29	0/809	0.41	0/1108
2	B	0.39	1/1261 (0.1%)	0.49	1/1706 (0.1%)
3	C	0.34	0/1765	0.45	0/2403
4	D	0.33	0/3396	0.45	0/4595
5	E	0.32	0/1690	0.43	0/2300
6	F	0.33	0/3375	0.45	0/4561
7	G	0.31	0/5367	0.47	0/7274
8	H	0.33	0/2487	0.45	0/3397
9	I	0.36	0/1445	0.48	0/1956
10	J	0.32	0/1362	0.44	0/1848
11	K	0.29	0/739	0.42	0/1000
12	L	0.33	0/4880	0.43	0/6641
13	M	0.32	0/3738	0.43	0/5097
14	N	0.30	0/2792	0.43	0/3800
15	O	0.33	0/2651	0.42	0/3587
16	P	0.31	0/2375	0.45	0/3210
17	Q	0.32	0/1039	0.46	0/1404
18	R	0.34	0/742	0.46	0/999
19	S	0.30	0/680	0.45	0/916
20	T	0.29	0/621	0.38	0/837
20	U	0.37	0/692	0.41	0/932
21	V	0.28	0/931	0.38	0/1261
22	W	0.29	0/995	0.42	0/1337
23	X	0.32	0/1439	0.42	0/1942
24	Y	0.27	0/1042	0.41	0/1414
25	Z	0.31	0/1181	0.43	0/1592
26	a	0.34	0/576	0.41	0/775
27	b	0.30	0/667	0.40	0/916
28	c	0.31	0/418	0.36	0/567
29	d	0.35	0/964	0.40	0/1305
30	e	0.30	0/818	0.43	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.32	0/457	0.41	0/616
32	g	0.35	0/839	0.40	0/1140
33	h	0.33	0/1188	0.41	0/1607
34	i	0.36	0/904	0.42	0/1230
35	j	0.35	0/607	0.39	0/833
36	k	0.34	0/657	0.41	0/887
37	l	0.37	0/1358	0.41	0/1858
38	m	0.36	0/970	0.42	0/1309
39	n	0.36	0/1540	0.40	0/2085
40	o	0.38	0/1068	0.40	0/1430
41	p	0.35	0/1468	0.42	0/1979
42	q	0.31	0/1242	0.44	0/1688
43	r	0.33	0/780	0.44	0/1056
44	s	0.30	0/363	0.41	0/491
All	All	0.33	1/66378 (0.0%)	0.43	1/89982 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
7	G	0	1
34	i	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	CYS	CB-SG	-5.32	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	54	CYS	CA-CB-SG	5.00	123.01	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
7	G	259	ASN	Peptide
34	i	1	SAC	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	95/115 (83%)	92 (97%)	3 (3%)	0	100	100
2	B	152/216 (70%)	146 (96%)	6 (4%)	0	100	100
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	405/463 (88%)	396 (98%)	9 (2%)	0	100	100
5	E	210/249 (84%)	205 (98%)	5 (2%)	0	100	100
6	F	427/464 (92%)	419 (98%)	8 (2%)	0	100	100
7	G	686/727 (94%)	668 (97%)	18 (3%)	0	100	100
8	H	304/318 (96%)	296 (97%)	8 (3%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
12	L	600/606 (99%)	585 (98%)	15 (2%)	0	100	100
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	284/380 (75%)	276 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
19	S	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	110 (100%)	0	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	110 (100%)	0	0	100	100
30	e	93/106 (88%)	89 (96%)	4 (4%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	95/154 (62%)	90 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	96 (97%)	2 (2%)	1 (1%)	15	17
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
38	m	109/129 (84%)	106 (97%)	3 (3%)	0	100	100
39	n	169/179 (94%)	167 (99%)	2 (1%)	0	100	100
40	o	119/137 (87%)	117 (98%)	1 (1%)	1 (1%)	19	23
41	p	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	40/109 (37%)	37 (92%)	3 (8%)	0	100	100
All	All	7956/9212 (86%)	7776 (98%)	178 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	i	123	PRO
40	o	32	GLU

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	86/100 (86%)	86 (100%)	0	100 100
2	B	130/175 (74%)	130 (100%)	0	100 100
3	C	187/228 (82%)	187 (100%)	0	100 100
4	D	356/392 (91%)	356 (100%)	0	100 100
5	E	183/205 (89%)	183 (100%)	0	100 100
6	F	343/368 (93%)	343 (100%)	0	100 100
7	G	578/608 (95%)	577 (100%)	1 (0%)	93 97
8	H	265/274 (97%)	264 (100%)	1 (0%)	91 96
9	I	151/175 (86%)	151 (100%)	0	100 100
10	J	140/141 (99%)	140 (100%)	0	100 100
11	K	84/85 (99%)	84 (100%)	0	100 100
12	L	526/533 (99%)	525 (100%)	1 (0%)	93 97
13	M	412/412 (100%)	412 (100%)	0	100 100
14	N	315/315 (100%)	315 (100%)	0	100 100
15	O	283/303 (93%)	283 (100%)	0	100 100
16	P	251/327 (77%)	251 (100%)	0	100 100
17	Q	112/153 (73%)	112 (100%)	0	100 100
18	R	78/97 (80%)	78 (100%)	0	100 100
19	S	74/82 (90%)	74 (100%)	0	100 100
20	T	70/135 (52%)	70 (100%)	0	100 100
20	U	78/135 (58%)	78 (100%)	0	100 100
21	V	100/102 (98%)	100 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	85 (99%)	1 (1%)	71	84
31	f	48/54 (89%)	47 (98%)	1 (2%)	53	70
32	g	88/131 (67%)	87 (99%)	1 (1%)	73	86
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	98 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	100/115 (87%)	100 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	41/92 (45%)	41 (100%)	0	100	100
All	All	7034/7892 (89%)	7028 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	237	ASN
8	H	54	LYS
12	L	541	ASN
30	e	8	ARG
31	f	30	ASN
32	g	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
12	L	541	ASN
17	Q	44	ASN
38	m	47	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.85	0
14	FME	N	1	14	8,9,10	1.03	1 (12%)	7,9,11	0.87	0
4	2MR	D	85	4	10,12,13	2.65	3 (30%)	5,13,15	1.40	1 (20%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.34	1 (20%)
34	SAC	i	1	34	7,8,9	1.87	1 (14%)	8,9,11	1.69	2 (25%)
10	FME	J	1	10	8,9,10	0.93	0	7,9,11	0.84	0
24	AYA	Y	1	24	6,7,8	1.80	2 (33%)	5,8,10	1.30	1 (20%)
11	FME	K	1	11	8,9,10	0.91	0	7,9,11	0.96	0
1	FME	A	1	1	8,9,10	0.93	0	7,9,11	0.77	0
13	FME	M	1	13	8,9,10	0.98	0	7,9,11	1.01	1 (14%)
8	FME	H	1	8	8,9,10	0.95	0	7,9,11	0.80	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
12	FME	L	1	12	-	3/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
34	SAC	i	1	34	-	1/7/8/10	-
10	FME	J	1	10	-	3/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
11	FME	K	1	11	-	1/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.06	1.44	1.33
4	D	85	2MR	CZ-NE	4.61	1.44	1.34
34	i	1	SAC	O-C	4.23	1.36	1.19
4	D	85	2MR	O-C	3.94	1.35	1.19
24	Y	1	AYA	CT-N	3.28	1.45	1.34
43	r	1	AYA	CT-N	3.21	1.45	1.34
14	N	1	FME	CA-N	-2.11	1.43	1.46
43	r	1	AYA	OT-CT	-2.08	1.18	1.23
24	Y	1	AYA	OT-CT	-2.02	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.14	113.93	124.78
4	D	85	2MR	NE-CZ-NH2	-2.85	116.87	119.48
43	r	1	AYA	CM-CT-N	2.46	120.26	116.10
24	Y	1	AYA	CM-CT-N	2.30	120.00	116.10
13	M	1	FME	C-CA-N	2.24	113.77	109.73
34	i	1	SAC	OG-CB-CA	-2.01	105.84	110.97

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
34	i	1	SAC	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	CB-CG-SD-CE
13	M	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CA-N-CN
8	H	1	FME	C-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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	$\#\|Z\| > 2$
46	SF4	G	801	7	0,12,12	-	-	-		
47	PC1	B	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.12	2 (5%)
45	LMT	B	202	-	36,36,36	1.19	2 (5%)	47,47,47	0.95	1 (2%)
48	FES	E	301	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	GTP	O	401	55	26,34,34	2.90	10 (38%)	32,54,54	1.71	10 (31%)
46	SF4	I	202	9	0,12,12	-	-	-		
51	3PE	e	801	-	40,40,50	0.94	3 (7%)	43,45,55	1.05	2 (4%)
45	LMT	J	402	-	36,36,36	1.18	3 (8%)	47,47,47	0.99	1 (2%)
51	3PE	d	1201	-	38,38,50	0.99	4 (10%)	41,43,55	1.11	2 (4%)
51	3PE	L	701	-	48,48,50	0.88	4 (8%)	51,53,55	1.15	2 (3%)
45	LMT	h	1002	-	36,36,36	1.18	3 (8%)	47,47,47	1.00	2 (4%)
45	LMT	b	301	-	36,36,36	1.19	2 (5%)	47,47,47	0.84	1 (2%)
51	3PE	b	302	-	39,39,50	0.95	4 (10%)	42,44,55	1.11	2 (4%)
45	LMT	A	1001	-	36,36,36	1.20	3 (8%)	47,47,47	1.03	2 (4%)
59	MYR	o	201	40	6,6,15	1.02	0	5,5,15	0.96	0
53	CDL	L	702	-	62,62,99	1.03	6 (9%)	66,73,111	1.11	3 (4%)
48	FES	G	803	7	0,4,4	-	-	-		
53	CDL	X	1701	-	70,70,99	0.99	6 (8%)	76,82,111	1.13	3 (3%)
58	EHZ	T	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.53	4 (11%)
45	LMT	N	901	-	36,36,36	1.18	3 (8%)	47,47,47	0.83	0
53	CDL	d	1202	-	64,64,99	1.07	8 (12%)	70,76,111	1.13	4 (5%)
51	3PE	H	601	-	24,24,50	1.69	4 (16%)	25,28,55	1.22	2 (8%)
51	3PE	J	401	-	37,37,50	0.97	4 (10%)	40,42,55	1.08	2 (5%)
49	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.23	6 (12%)
45	LMT	l	201	-	36,36,36	1.19	3 (8%)	47,47,47	0.99	1 (2%)
56	NDP	P	501	-	45,52,52	2.17	4 (8%)	53,80,80	1.65	10 (18%)
53	CDL	Y	403	-	70,70,99	1.03	8 (11%)	76,82,111	1.07	4 (5%)
51	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.06	2 (4%)
51	3PE	Y	401	-	30,30,50	1.10	4 (13%)	33,35,55	1.20	2 (6%)
46	SF4	B	201	2	0,12,12	-	-	-		
53	CDL	q	201	-	56,56,99	1.14	8 (14%)	62,68,111	1.08	4 (6%)
51	3PE	M	601	-	42,42,50	0.93	4 (9%)	45,47,55	1.07	2 (4%)
45	LMT	d	1203	-	36,36,36	1.19	3 (8%)	47,47,47	1.09	4 (8%)
45	LMT	h	1003	-	36,36,36	1.13	2 (5%)	47,47,47	1.06	4 (8%)
51	3PE	N	902	-	40,40,50	0.96	4 (10%)	43,45,55	1.10	2 (4%)
51	3PE	I	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.01	2 (3%)
52	I49	H	602	-	15,17,17	1.53	2 (13%)	21,22,22	2.05	4 (19%)
53	CDL	h	1001	-	66,66,99	1.05	7 (10%)	72,78,111	1.28	5 (6%)
45	LMT	K	501	-	36,36,36	1.20	3 (8%)	47,47,47	0.87	1 (2%)
46	SF4	F	502	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	I49	N	903	-	15,17,17	1.54	2 (13%)	21,22,22	1.66	4 (19%)
47	PC1	M	603	-	39,39,53	1.08	3 (7%)	45,47,61	1.00	2 (4%)
46	SF4	G	802	7	0,12,12	-	-	-		
51	3PE	M	602	-	50,50,50	0.86	3 (6%)	53,55,55	1.11	2 (3%)
46	SF4	I	203	9	0,12,12	-	-	-		
45	LMT	j	101	-	36,36,36	1.19	3 (8%)	47,47,47	0.97	1 (2%)
45	LMT	Y	402	-	36,36,36	1.21	3 (8%)	47,47,47	0.96	2 (4%)
58	EHZ	U	101	20	29,36,37	1.66	6 (20%)	35,44,47	1.44	2 (5%)

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
46	SF4	G	801	7	-	-	0/6/5/5
47	PC1	B	203	-	-	13/38/38/57	-
45	LMT	B	202	-	-	8/21/61/61	0/2/2/2
54	GTP	O	401	55	-	7/18/38/38	0/3/3/3
48	FES	E	301	5	-	-	0/1/1/1
46	SF4	I	202	9	-	-	0/6/5/5
51	3PE	e	801	-	-	25/44/44/54	-
45	LMT	J	402	-	-	11/21/61/61	0/2/2/2
51	3PE	d	1201	-	-	23/42/42/54	-
51	3PE	L	701	-	-	19/52/52/54	-
45	LMT	h	1002	-	-	10/21/61/61	0/2/2/2
45	LMT	b	301	-	-	8/21/61/61	0/2/2/2
51	3PE	b	302	-	-	25/43/43/54	-
45	LMT	A	1001	-	-	11/21/61/61	0/2/2/2
59	MYR	o	201	40	-	3/3/4/13	-
53	CDL	L	702	-	-	27/72/72/110	-
53	CDL	X	1701	-	-	38/80/80/110	-
58	EHZ	T	101	20	-	13/42/44/45	-
48	FES	G	803	7	-	-	0/1/1/1
45	LMT	N	901	-	-	11/21/61/61	0/2/2/2
53	CDL	d	1202	-	-	39/75/75/110	-
51	3PE	H	601	-	-	10/27/27/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	J	401	-	-	16/41/41/54	-
49	FMN	F	501	-	-	0/18/18/18	0/3/3/3
45	LMT	l	201	-	-	10/21/61/61	0/2/2/2
56	NDP	P	501	-	-	5/30/77/77	0/5/5/5
53	CDL	Y	403	-	-	26/81/81/110	-
51	3PE	L	703	-	-	14/48/48/54	-
51	3PE	Y	401	-	-	18/33/33/54	-
53	CDL	q	201	-	-	31/67/67/110	-
46	SF4	B	201	2	-	-	0/6/5/5
51	3PE	M	601	-	-	18/46/46/54	-
45	LMT	d	1203	-	-	7/21/61/61	0/2/2/2
45	LMT	h	1003	-	-	5/21/61/61	0/2/2/2
51	3PE	N	902	-	-	21/44/44/54	-
51	3PE	I	201	-	-	27/54/54/54	-
52	I49	H	602	-	-	4/10/10/10	0/1/1/1
53	CDL	h	1001	-	-	35/77/77/110	-
45	LMT	K	501	-	-	7/21/61/61	0/2/2/2
46	SF4	F	502	6	-	-	0/6/5/5
52	I49	N	903	-	-	6/10/10/10	0/1/1/1
47	PC1	M	603	-	-	16/43/43/57	-
51	3PE	M	602	-	-	23/54/54/54	-
46	SF4	G	802	7	-	-	0/6/5/5
46	SF4	I	203	9	-	-	0/6/5/5
45	LMT	j	101	-	-	5/21/61/61	0/2/2/2
45	LMT	Y	402	-	-	9/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	11/42/44/45	-

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.04	1.82	1.59
54	O	401	GTP	O6-C6	8.26	1.40	1.23
51	H	601	3PE	O21-C2	-5.92	1.40	1.46
58	U	101	EHZ	C15-N2	5.36	1.45	1.33
54	O	401	GTP	O4'-C1'	5.28	1.48	1.41
58	T	101	EHZ	C12-N1	5.28	1.45	1.33
58	T	101	EHZ	C15-N2	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	U	101	EHZ	C12-N1	4.96	1.44	1.33
52	N	903	I49	C15-N02	-4.78	1.31	1.37
54	O	401	GTP	C2-N1	4.75	1.49	1.37
52	H	602	I49	C15-N02	-4.72	1.31	1.37
54	O	401	GTP	C2-N2	4.54	1.45	1.34
54	O	401	GTP	C2-N3	4.47	1.44	1.33
45	A	1001	LMT	O5B-C1B	3.61	1.51	1.41
49	F	501	FMN	C4A-N5	3.58	1.37	1.30
45	Y	402	LMT	O5B-C1B	3.58	1.51	1.41
45	K	501	LMT	O5B-C1B	3.55	1.50	1.41
45	j	101	LMT	O5B-C1B	3.54	1.50	1.41
45	J	402	LMT	O5B-C1B	3.53	1.50	1.41
45	l	201	LMT	O5B-C1B	3.52	1.50	1.41
45	B	202	LMT	O5B-C1B	3.51	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.47	1.50	1.41
45	N	901	LMT	O5B-C1B	3.43	1.50	1.41
45	b	301	LMT	O5B-C1B	3.42	1.50	1.41
45	d	1203	LMT	O5B-C1B	3.38	1.50	1.41
56	P	501	NDP	PN-O5D	3.37	1.72	1.59
54	O	401	GTP	C2'-C1'	-3.19	1.48	1.53
45	b	301	LMT	O5'-C1'	3.18	1.49	1.41
45	K	501	LMT	O5'-C1'	3.13	1.49	1.41
51	H	601	3PE	O21-C21	3.12	1.40	1.33
54	O	401	GTP	C5-C6	-3.11	1.41	1.47
52	N	903	I49	C14-N03	3.11	1.38	1.29
56	P	501	NDP	O2B-C2B	-3.09	1.32	1.44
45	h	1003	LMT	O5B-C1B	3.07	1.49	1.41
45	j	101	LMT	O5'-C1'	3.07	1.49	1.41
45	l	201	LMT	O5'-C1'	3.05	1.49	1.41
45	Y	402	LMT	O5'-C1'	3.03	1.49	1.41
52	H	602	I49	C14-N03	3.02	1.38	1.29
45	B	202	LMT	O5'-C1'	2.96	1.49	1.41
45	A	1001	LMT	O5'-C1'	2.92	1.49	1.41
45	N	901	LMT	O5'-C1'	2.91	1.49	1.41
45	d	1203	LMT	O5'-C1'	2.90	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.86	1.49	1.41
45	J	402	LMT	O5'-C1'	2.83	1.49	1.41
45	h	1003	LMT	O5'-C1'	2.78	1.48	1.41
51	M	602	3PE	O21-C2	-2.73	1.39	1.46
53	X	1701	CDL	OB6-CB4	-2.71	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.69	1.39	1.46
51	L	703	3PE	O21-C2	-2.69	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	h	1001	CDL	OB6-CB4	-2.68	1.39	1.46
58	T	101	EHZ	O4-C15	-2.67	1.18	1.23
47	M	603	PC1	O21-C2	-2.66	1.39	1.46
51	I	201	3PE	O21-C2	-2.66	1.39	1.46
51	e	801	3PE	O21-C2	-2.66	1.39	1.46
53	Y	403	CDL	OA6-CA4	-2.65	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.64	1.40	1.46
53	L	702	CDL	OA6-CA4	-2.63	1.40	1.46
51	L	701	3PE	O21-C2	-2.62	1.40	1.46
53	h	1001	CDL	OA6-CA4	-2.60	1.40	1.46
51	L	701	3PE	O31-C3	-2.59	1.39	1.45
51	d	1201	3PE	O21-C2	-2.59	1.40	1.46
53	d	1202	CDL	OA6-CA4	-2.58	1.40	1.46
53	X	1701	CDL	OA6-CA4	-2.57	1.40	1.46
58	U	101	EHZ	O4-C15	-2.56	1.18	1.23
53	L	702	CDL	OB6-CB4	-2.56	1.40	1.46
53	Y	403	CDL	OB8-CB7	2.54	1.40	1.33
53	X	1701	CDL	OB8-CB7	2.53	1.40	1.33
51	J	401	3PE	O21-C2	-2.51	1.40	1.46
53	Y	403	CDL	OB6-CB4	-2.50	1.40	1.46
51	M	601	3PE	O21-C2	-2.50	1.40	1.46
53	d	1202	CDL	OB6-CB4	-2.48	1.40	1.46
51	N	902	3PE	O21-C2	-2.45	1.40	1.46
51	H	601	3PE	O31-C31	2.45	1.40	1.33
51	I	201	3PE	O31-C3	-2.44	1.39	1.45
54	O	401	GTP	C2'-C3'	-2.44	1.46	1.53
47	B	203	PC1	O21-C2	-2.42	1.40	1.46
53	q	201	CDL	OA8-CA6	-2.40	1.39	1.45
58	T	101	EHZ	O3-C12	-2.40	1.18	1.23
51	b	302	3PE	O31-C31	2.40	1.40	1.33
53	d	1202	CDL	OB8-CB7	2.40	1.40	1.33
53	h	1001	CDL	OB8-CB6	-2.40	1.39	1.45
53	L	702	CDL	OA8-CA7	2.39	1.40	1.33
51	Y	401	3PE	O31-C31	2.39	1.40	1.33
51	Y	401	3PE	O21-C21	2.38	1.40	1.35
53	Y	403	CDL	OA8-CA7	2.37	1.40	1.33
51	Y	401	3PE	O21-C2	-2.37	1.40	1.46
51	J	401	3PE	O31-C3	-2.36	1.39	1.45
53	q	201	CDL	OB8-CB7	2.36	1.40	1.33
51	d	1201	3PE	O31-C31	2.35	1.40	1.33
51	b	302	3PE	O21-C2	-2.35	1.40	1.46
51	N	902	3PE	O31-C3	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	d	1202	CDL	OA8-CA7	2.32	1.40	1.33
45	h	1002	LMT	O5B-C5B	2.32	1.50	1.44
47	M	603	PC1	O31-C3	-2.31	1.39	1.45
53	d	1202	CDL	OB8-CB6	-2.30	1.39	1.45
51	M	602	3PE	O31-C31	2.30	1.40	1.33
51	M	602	3PE	O31-C3	-2.30	1.39	1.45
51	M	601	3PE	O31-C31	2.30	1.40	1.33
47	B	203	PC1	O31-C31	2.29	1.40	1.33
51	N	902	3PE	O31-C31	2.28	1.40	1.33
58	U	101	EHZ	O3-C12	-2.27	1.18	1.23
51	e	801	3PE	O31-C3	-2.26	1.40	1.45
53	Y	403	CDL	OA8-CA6	-2.26	1.40	1.45
47	B	203	PC1	O21-C21	2.26	1.40	1.34
54	O	401	GTP	PG-O3G	-2.26	1.46	1.54
53	d	1202	CDL	OA8-CA6	-2.25	1.40	1.45
54	O	401	GTP	PG-O2G	-2.24	1.46	1.54
53	q	201	CDL	OB8-CB6	-2.24	1.40	1.45
51	L	703	3PE	O31-C31	2.22	1.39	1.33
53	L	702	CDL	OA8-CA6	-2.22	1.40	1.45
53	h	1001	CDL	OA8-CA7	2.22	1.39	1.33
51	L	703	3PE	O31-C3	-2.22	1.40	1.45
56	P	501	NDP	O5D-C5D	-2.21	1.36	1.44
51	e	801	3PE	O31-C31	2.20	1.39	1.33
47	M	603	PC1	O31-C31	2.20	1.39	1.33
45	Y	402	LMT	O5B-C5B	2.18	1.49	1.44
58	T	101	EHZ	C9-S1	2.17	1.81	1.76
51	M	601	3PE	O31-C3	-2.17	1.40	1.45
51	Y	401	3PE	O31-C3	-2.17	1.40	1.45
51	b	302	3PE	O21-C21	2.16	1.40	1.34
53	Y	403	CDL	OB6-CB5	2.16	1.40	1.34
53	L	702	CDL	OB6-CB5	2.16	1.40	1.34
45	d	1203	LMT	O5B-C5B	2.16	1.49	1.44
53	h	1001	CDL	OA8-CA6	-2.16	1.40	1.45
51	I	201	3PE	O31-C31	2.15	1.39	1.33
51	L	701	3PE	O21-C21	2.15	1.40	1.34
51	M	601	3PE	O21-C21	2.15	1.40	1.34
53	d	1202	CDL	OA6-CA5	2.14	1.40	1.34
53	X	1701	CDL	OB8-CB6	-2.14	1.40	1.45
47	B	203	PC1	O31-C3	-2.14	1.40	1.45
51	N	902	3PE	O21-C21	2.13	1.40	1.34
51	H	601	3PE	O31-C3	-2.12	1.40	1.45
51	J	401	3PE	O21-C21	2.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	d	1202	CDL	OB6-CB5	2.12	1.40	1.34
49	F	501	FMN	C10-N1	2.12	1.37	1.33
53	Y	403	CDL	OB8-CB6	-2.11	1.40	1.45
51	d	1201	3PE	O21-C21	2.11	1.40	1.34
45	K	501	LMT	O5B-C5B	2.10	1.49	1.44
53	q	201	CDL	OA8-CA7	2.10	1.39	1.33
51	J	401	3PE	O31-C31	2.10	1.39	1.33
53	h	1001	CDL	OB8-CB7	2.09	1.39	1.33
45	A	1001	LMT	O5B-C5B	2.08	1.49	1.44
45	j	101	LMT	O5B-C5B	2.08	1.49	1.44
53	q	201	CDL	OB6-CB5	2.08	1.40	1.34
53	X	1701	CDL	OA8-CA6	-2.08	1.40	1.45
45	l	201	LMT	O5B-C5B	2.07	1.49	1.44
51	d	1201	3PE	O31-C3	-2.07	1.40	1.45
53	h	1001	CDL	OB6-CB5	2.06	1.40	1.34
53	X	1701	CDL	OA6-CA5	2.06	1.40	1.34
45	J	402	LMT	O5B-C5B	2.05	1.49	1.44
45	N	901	LMT	O5B-C5B	2.05	1.49	1.44
51	b	302	3PE	O31-C3	-2.04	1.40	1.45
58	U	101	EHZ	O6-C20	-2.04	1.39	1.44
53	q	201	CDL	OA6-CA5	2.03	1.40	1.34
58	U	101	EHZ	C9-S1	2.02	1.81	1.76
53	Y	403	CDL	OA6-CA5	2.02	1.40	1.34
53	L	702	CDL	OA6-CA5	2.01	1.40	1.34
51	L	701	3PE	O31-C31	2.00	1.39	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	H	602	I49	C14-N02-C15	-6.64	114.14	125.21
56	P	501	NDP	PN-O3-PA	-6.48	110.60	132.83
58	T	101	EHZ	C8-C9-S1	6.07	121.14	113.63
58	U	101	EHZ	C8-C9-S1	5.96	121.00	113.63
52	N	903	I49	N01-C14-N03	5.10	129.82	120.26
51	H	601	3PE	O21-C21-O22	-4.70	119.59	125.57
51	Y	401	3PE	O21-C21-C22	4.57	119.50	111.09
53	h	1001	CDL	OB6-CB5-C51	4.54	121.29	111.50
51	L	701	3PE	O21-C21-C22	4.43	121.04	111.50
47	B	203	PC1	O21-C21-C22	4.29	120.74	111.50
53	L	702	CDL	OA6-CA5-C11	4.20	120.56	111.50
53	d	1202	CDL	OA6-CA5-C11	4.19	120.53	111.50
51	b	302	3PE	O21-C21-C22	4.14	120.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	N	902	3PE	O21-C21-C22	4.10	120.33	111.50
51	M	601	3PE	O21-C21-C22	4.06	120.25	111.50
53	h	1001	CDL	OA6-CA5-C11	4.06	120.25	111.50
51	d	1201	3PE	O21-C21-C22	4.00	120.13	111.50
53	X	1701	CDL	OA6-CA5-C11	3.98	120.08	111.50
51	M	602	3PE	O21-C21-C22	3.94	119.98	111.50
53	L	702	CDL	OB6-CB5-C51	3.77	119.63	111.50
51	L	703	3PE	O21-C21-C22	3.73	119.53	111.50
53	Y	403	CDL	OA6-CA5-C11	3.72	119.51	111.50
51	J	401	3PE	O21-C21-C22	3.67	119.41	111.50
53	d	1202	CDL	OB6-CB5-C51	3.63	120.91	110.80
47	M	603	PC1	O21-C21-C22	3.59	119.25	111.50
53	X	1701	CDL	OB6-CB5-C51	3.59	119.25	111.50
51	I	201	3PE	O21-C21-C22	3.56	119.16	111.50
56	P	501	NDP	O2B-P2B-O1X	-3.53	95.76	109.39
53	X	1701	CDL	OB8-CB7-C71	3.46	122.77	111.91
53	q	201	CDL	OA6-CA5-C11	3.44	118.91	111.50
53	Y	403	CDL	OB6-CB5-C51	3.43	118.90	111.50
53	q	201	CDL	OB6-CB5-C51	3.38	118.78	111.50
54	O	401	GTP	PA-O3A-PB	-3.20	121.85	132.83
45	h	1003	LMT	O5'-C5'-C4'	3.19	116.48	109.75
51	e	801	3PE	O21-C21-C22	3.19	118.38	111.50
53	h	1001	CDL	OA8-CA7-C31	3.14	121.75	111.91
49	F	501	FMN	C4-N3-C2	-3.13	119.86	125.64
52	H	602	I49	N01-C14-N03	3.10	126.06	120.26
54	O	401	GTP	C2-N1-C6	-3.09	119.41	125.10
54	O	401	GTP	O3G-PG-O3B	3.08	114.95	104.64
54	O	401	GTP	C5-C6-N1	3.05	119.34	113.95
49	F	501	FMN	C4A-C10-N10	2.97	120.82	116.48
58	T	101	EHZ	C13-C12-N1	2.92	121.34	116.42
45	A	1001	LMT	C2'-C3'-C4'	2.87	116.23	109.68
51	d	1201	3PE	O31-C31-C32	2.86	120.89	111.91
56	P	501	NDP	PA-O5B-C5B	-2.82	105.12	121.68
51	Y	401	3PE	O31-C31-C32	2.80	120.69	111.91
58	T	101	EHZ	O2-C9-S1	-2.78	119.00	122.61
53	Y	403	CDL	OA8-CA7-C31	2.77	120.61	111.91
53	h	1001	CDL	OB8-CB7-C71	2.74	120.51	111.91
54	O	401	GTP	O2G-PG-O3B	2.71	113.71	104.64
51	M	602	3PE	O31-C31-C32	2.70	120.37	111.91
47	B	203	PC1	O31-C31-C32	2.69	120.36	111.91
52	H	602	I49	N05-C15-N04	-2.65	112.09	120.26
49	F	501	FMN	C4A-C4-N3	2.65	119.92	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	M	603	PC1	O31-C31-C32	2.63	120.17	111.91
56	P	501	NDP	PN-O5D-C5D	-2.63	106.28	121.68
51	J	401	3PE	O31-C31-C32	2.62	120.14	111.91
52	N	903	I49	N05-C15-N04	-2.59	112.30	120.26
51	L	701	3PE	O31-C31-C32	2.58	120.01	111.91
53	q	201	CDL	OB8-CB7-C71	2.58	120.00	111.91
53	d	1202	CDL	OB8-CB7-C71	2.57	119.98	111.91
51	N	902	3PE	O31-C31-C32	2.57	119.97	111.91
45	j	101	LMT	C1B-O1B-C4'	-2.53	111.71	117.96
51	L	703	3PE	O31-C31-C32	2.53	119.84	111.91
56	P	501	NDP	O5D-PN-O1N	-2.52	99.23	109.07
56	P	501	NDP	O3X-P2B-O2X	2.52	117.26	107.64
54	O	401	GTP	C3'-C2'-C1'	2.51	104.75	100.98
51	H	601	3PE	O31-C31-C32	2.50	119.76	111.91
53	d	1202	CDL	OA8-CA7-C31	2.50	119.75	111.91
51	e	801	3PE	O31-C31-C32	2.50	119.74	111.91
54	O	401	GTP	PB-O3B-PG	-2.47	124.35	132.83
51	M	601	3PE	O31-C31-C32	2.47	119.65	111.91
51	I	201	3PE	O31-C31-C32	2.43	119.55	111.91
49	F	501	FMN	O4-C4-C4A	-2.43	120.17	126.60
52	N	903	I49	N05-C15-N02	2.42	127.38	117.44
52	H	602	I49	N05-C15-N02	2.41	127.36	117.44
56	P	501	NDP	O4B-C4B-C3B	2.41	109.88	105.11
53	L	702	CDL	OA8-CA7-C31	2.40	119.43	111.91
45	d	1203	LMT	O5B-C5B-C4B	2.40	114.05	109.69
53	Y	403	CDL	OB8-CB7-C71	2.39	119.40	111.91
58	T	101	EHZ	C13-C14-N2	-2.37	107.11	111.90
45	A	1001	LMT	C1'-C2'-C3'	2.36	114.90	110.00
51	b	302	3PE	O31-C31-C32	2.35	119.28	111.91
45	d	1203	LMT	C3B-C4B-C5B	2.34	114.42	110.24
56	P	501	NDP	C2A-N1A-C6A	-2.34	114.75	118.75
45	h	1002	LMT	O5B-C5B-C4B	2.31	113.88	109.69
49	F	501	FMN	C10-C4A-N5	-2.30	119.98	124.86
53	q	201	CDL	OA8-CA7-C31	2.29	119.10	111.91
54	O	401	GTP	O2A-PA-O1A	-2.28	100.95	112.24
45	K	501	LMT	O1B-C4'-C3'	2.27	113.31	107.28
58	U	101	EHZ	C13-C12-N1	2.26	120.23	116.42
45	h	1003	LMT	C1B-O5B-C5B	-2.25	109.28	113.69
54	O	401	GTP	O2B-PB-O1B	-2.24	101.19	112.24
49	F	501	FMN	C4A-C10-N1	-2.23	119.55	124.73
45	h	1003	LMT	C1B-O1B-C4'	-2.22	112.47	117.96
45	d	1203	LMT	C2'-C3'-C4'	2.21	114.73	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	401	GTP	C2'-C3'-C4'	2.21	106.94	102.64
56	P	501	NDP	O2N-PN-O1N	2.20	123.11	112.24
56	P	501	NDP	O7N-C7N-N7N	-2.17	117.80	122.88
45	l	201	LMT	C2'-C3'-C4'	2.16	114.62	109.68
45	B	202	LMT	O1'-C1'-C2'	2.13	111.63	108.30
45	b	301	LMT	O1B-C4'-C3'	2.10	112.87	107.28
45	h	1003	LMT	C3'-C4'-C5'	2.09	115.71	110.93
45	Y	402	LMT	C6B-C5B-C4B	-2.07	108.16	113.00
45	d	1203	LMT	O5'-C5'-C4'	2.04	114.05	109.75
53	h	1001	CDL	CB6-CB4-CB3	-2.02	107.02	111.79
45	Y	402	LMT	C1B-O1B-C4'	-2.01	112.99	117.96
52	N	903	I49	N02-C14-N01	-2.00	112.92	118.08
45	J	402	LMT	O5'-C5'-C4'	2.00	113.97	109.75
45	h	1002	LMT	O1B-C4'-C3'	2.00	112.61	107.28

There are no chirality outliers.

All (615) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	K	501	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
51	H	601	3PE	C11-O13-P-O12
51	H	601	3PE	C11-O13-P-O14
51	H	601	3PE	O13-C11-C12-N
51	H	601	3PE	O22-C21-O21-C2
51	J	401	3PE	C1-O11-P-O14
51	J	401	3PE	O13-C11-C12-N
51	L	701	3PE	C22-C21-O21-C2
51	L	703	3PE	C1-O11-P-O12
51	L	703	3PE	C1-O11-P-O13
51	L	703	3PE	C1-O11-P-O14
51	M	601	3PE	C1-O11-P-O12
51	M	601	3PE	C1-O11-P-O14
51	M	601	3PE	O13-C11-C12-N
51	M	602	3PE	C1-O11-P-O14
51	M	602	3PE	O13-C11-C12-N
51	M	602	3PE	O11-C1-C2-O21
51	N	902	3PE	O13-C11-C12-N
51	Y	401	3PE	O13-C11-C12-N
51	b	302	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
51	b	302	3PE	C11-O13-P-O12
51	b	302	3PE	C11-O13-P-O14
51	b	302	3PE	C12-C11-O13-P
51	b	302	3PE	O13-C11-C12-N
51	b	302	3PE	O21-C2-C3-O31
51	b	302	3PE	C1-C2-O21-C21
51	b	302	3PE	O22-C21-O21-C2
51	d	1201	3PE	C1-O11-P-O12
51	d	1201	3PE	C22-C21-O21-C2
51	e	801	3PE	C11-O13-P-O12
51	e	801	3PE	C11-O13-P-O14
51	e	801	3PE	O13-C11-C12-N
52	H	602	I49	N01-C14-N02-C15
52	H	602	I49	N03-C14-N02-C15
52	N	903	I49	C07-C06-C08-N01
52	N	903	I49	N05-C15-N02-C14
53	L	702	CDL	C11-CA5-OA6-CA4
53	L	702	CDL	CB2-OB2-PB2-OB3
53	L	702	CDL	CB2-OB2-PB2-OB4
53	L	702	CDL	CB3-OB5-PB2-OB3
53	X	1701	CDL	C11-CA5-OA6-CA4
53	X	1701	CDL	CB2-OB2-PB2-OB4
53	Y	403	CDL	C11-CA5-OA6-CA4
53	Y	403	CDL	CB2-OB2-PB2-OB4
53	Y	403	CDL	CB3-OB5-PB2-OB2
53	Y	403	CDL	CB3-OB5-PB2-OB4
53	d	1202	CDL	C11-CA5-OA6-CA4
53	d	1202	CDL	CB3-OB5-PB2-OB2
53	d	1202	CDL	CB3-OB5-PB2-OB3
53	d	1202	CDL	CB3-OB5-PB2-OB4
53	d	1202	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	CB3-OB5-PB2-OB4
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB2-OB2-PB2-OB5
54	O	401	GTP	PB-O3B-PG-O2G
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A
56	P	501	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
58	T	101	EHZ	C5-C6-C7-C8
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
59	o	201	MYR	C1-C2-C3-C4
45	K	501	LMT	C3'-C4'-O1B-C1B
45	d	1203	LMT	O5B-C1B-O1B-C4'
53	X	1701	CDL	OB9-CB7-OB8-CB6
45	d	1203	LMT	C2B-C1B-O1B-C4'
53	X	1701	CDL	C71-CB7-OB8-CB6
45	K	501	LMT	C4'-C5'-C6'-O6'
51	J	401	3PE	O32-C31-O31-C3
51	M	602	3PE	O32-C31-O31-C3
51	d	1201	3PE	O32-C31-O31-C3
45	b	301	LMT	C3'-C4'-O1B-C1B
51	L	701	3PE	O22-C21-O21-C2
51	d	1201	3PE	O22-C21-O21-C2
53	L	702	CDL	OA7-CA5-OA6-CA4
53	X	1701	CDL	OA7-CA5-OA6-CA4
53	Y	403	CDL	OA7-CA5-OA6-CA4
53	d	1202	CDL	OA7-CA5-OA6-CA4
53	d	1202	CDL	OB7-CB5-OB6-CB4
51	J	401	3PE	C32-C31-O31-C3
51	M	602	3PE	C32-C31-O31-C3
51	d	1201	3PE	C32-C31-O31-C3
45	h	1002	LMT	C3'-C4'-O1B-C1B
51	b	302	3PE	C22-C21-O21-C2
53	h	1001	CDL	C51-CB5-OB6-CB4
45	A	1001	LMT	O5B-C5B-C6B-O6B
45	K	501	LMT	O5'-C5'-C6'-O6'
51	N	902	3PE	C32-C31-O31-C3
51	e	801	3PE	C32-C31-O31-C3
53	L	702	CDL	C31-CA7-OA8-CA6
45	J	402	LMT	C4B-C5B-C6B-O6B
45	l	201	LMT	C4'-C5'-C6'-O6'
53	L	702	CDL	OA9-CA7-OA8-CA6
53	Y	403	CDL	OA9-CA7-OA8-CA6
45	A	1001	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
45	d	1203	LMT	O5'-C5'-C6'-O6'
53	L	702	CDL	O1-C1-CA2-OA2
51	L	701	3PE	C32-C31-O31-C3
53	Y	403	CDL	C31-CA7-OA8-CA6
53	X	1701	CDL	OA9-CA7-OA8-CA6
51	e	801	3PE	O32-C31-O31-C3
45	b	301	LMT	O5B-C5B-C6B-O6B
45	B	202	LMT	C3'-C4'-O1B-C1B
45	b	301	LMT	C2-C3-C4-C5
45	N	901	LMT	O5'-C5'-C6'-O6'
53	Y	403	CDL	CB4-CB3-OB5-PB2
51	N	902	3PE	O32-C31-O31-C3
45	J	402	LMT	O5B-C5B-C6B-O6B
45	l	201	LMT	O5'-C5'-C6'-O6'
45	A	1001	LMT	C4B-C5B-C6B-O6B
45	d	1203	LMT	C4'-C5'-C6'-O6'
51	L	701	3PE	O32-C31-O31-C3
45	B	202	LMT	O5'-C1'-O1'-C1
47	B	203	PC1	C32-C31-O31-C3
53	h	1001	CDL	C71-CB7-OB8-CB6
45	b	301	LMT	C4B-C5B-C6B-O6B
53	L	702	CDL	CB2-C1-CA2-OA2
47	B	203	PC1	O32-C31-O31-C3
53	h	1001	CDL	OB9-CB7-OB8-CB6
47	M	603	PC1	C32-C31-O31-C3
51	Y	401	3PE	C32-C31-O31-C3
53	d	1202	CDL	C71-CB7-OB8-CB6
45	N	901	LMT	C4'-C5'-C6'-O6'
45	b	301	LMT	C2'-C1'-O1'-C1
45	N	901	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	C31-CA7-OA8-CA6
47	B	203	PC1	C31-C32-C33-C34
47	M	603	PC1	O32-C31-O31-C3
51	Y	401	3PE	O32-C31-O31-C3
53	d	1202	CDL	OB9-CB7-OB8-CB6
45	j	101	LMT	O5'-C5'-C6'-O6'
53	X	1701	CDL	CB7-C71-C72-C73
51	J	401	3PE	C31-C32-C33-C34
53	Y	403	CDL	CA5-C11-C12-C13
53	d	1202	CDL	C31-CA7-OA8-CA6
45	Y	402	LMT	O5B-C1B-O1B-C4'
51	M	602	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	CA5-C11-C12-C13
53	X	1701	CDL	CB5-C51-C52-C53
53	q	201	CDL	C31-CA7-OA8-CA6
45	h	1003	LMT	C4B-C5B-C6B-O6B
45	J	402	LMT	O5'-C1'-O1'-C1
45	A	1001	LMT	C4'-C5'-C6'-O6'
45	J	402	LMT	C4'-C5'-C6'-O6'
53	d	1202	CDL	OA9-CA7-OA8-CA6
51	H	601	3PE	C11-O13-P-O11
51	I	201	3PE	C11-O13-P-O11
51	M	601	3PE	C1-O11-P-O13
51	d	1201	3PE	C1-O11-P-O13
51	e	801	3PE	C11-O13-P-O11
53	L	702	CDL	CB2-OB2-PB2-OB5
53	L	702	CDL	CB3-OB5-PB2-OB2
53	X	1701	CDL	CB2-OB2-PB2-OB5
53	Y	403	CDL	CB2-OB2-PB2-OB5
53	d	1202	CDL	CA2-OA2-PA1-OA5
53	d	1202	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB3-OB5-PB2-OB2
45	b	301	LMT	O5'-C5'-C6'-O6'
45	j	101	LMT	C2B-C1B-O1B-C4'
53	h	1001	CDL	C31-CA7-OA8-CA6
45	J	402	LMT	O5'-C5'-C6'-O6'
47	B	203	PC1	C22-C21-O21-C2
47	M	603	PC1	C23-C24-C25-C26
51	L	703	3PE	C33-C34-C35-C36
51	M	602	3PE	C3A-C3B-C3C-C3D
53	L	702	CDL	C34-C35-C36-C37
53	d	1202	CDL	C33-C34-C35-C36
53	q	201	CDL	C51-C52-C53-C54
51	L	701	3PE	C2E-C2F-C2G-C2H
51	M	602	3PE	C3D-C3E-C3F-C3G
51	M	602	3PE	C2D-C2E-C2F-C2G
51	b	302	3PE	C2A-C2B-C2C-C2D
53	X	1701	CDL	C11-C12-C13-C14
53	h	1001	CDL	C16-C17-C18-C19
47	B	203	PC1	O22-C21-O21-C2
51	d	1201	3PE	C21-C22-C23-C24
51	I	201	3PE	C3A-C3B-C3C-C3D
51	I	201	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
51	Y	401	3PE	C22-C21-O21-C2
45	A	1001	LMT	C6-C7-C8-C9
45	N	901	LMT	C6-C7-C8-C9
53	L	702	CDL	C56-C57-C58-C59
53	d	1202	CDL	O1-C1-CA2-OA2
51	I	201	3PE	C33-C34-C35-C36
53	X	1701	CDL	C74-C75-C76-C77
53	q	201	CDL	CA5-C11-C12-C13
45	A	1001	LMT	C2'-C1'-O1'-C1
53	L	702	CDL	C52-C53-C54-C55
53	X	1701	CDL	C53-C54-C55-C56
45	A	1001	LMT	C5-C6-C7-C8
51	Y	401	3PE	C35-C36-C37-C38
51	d	1201	3PE	C33-C34-C35-C36
51	L	703	3PE	C38-C39-C3A-C3B
51	b	302	3PE	C26-C27-C28-C29
53	X	1701	CDL	C15-C16-C17-C18
59	o	201	MYR	C2-C3-C4-C5
53	q	201	CDL	OA9-CA7-OA8-CA6
53	h	1001	CDL	C31-C32-C33-C34
45	J	402	LMT	C5-C6-C7-C8
45	N	901	LMT	C5-C6-C7-C8
51	b	302	3PE	C28-C29-C2A-C2B
51	e	801	3PE	C21-C22-C23-C24
51	L	701	3PE	C29-C2A-C2B-C2C
51	N	902	3PE	C29-C2A-C2B-C2C
47	M	603	PC1	C29-C2A-C2B-C2C
53	h	1001	CDL	OA9-CA7-OA8-CA6
45	d	1203	LMT	C5-C6-C7-C8
51	M	601	3PE	C32-C33-C34-C35
51	I	201	3PE	C38-C39-C3A-C3B
51	L	701	3PE	C23-C24-C25-C26
53	q	201	CDL	C15-C16-C17-C18
51	L	703	3PE	C3C-C3D-C3E-C3F
51	N	902	3PE	C23-C24-C25-C26
51	N	902	3PE	C21-C22-C23-C24
53	L	702	CDL	CB5-C51-C52-C53
53	L	702	CDL	C51-CB5-OB6-CB4
51	N	902	3PE	C32-C33-C34-C35
51	M	602	3PE	C33-C34-C35-C36
51	N	902	3PE	C33-C34-C35-C36
45	j	101	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
45	B	202	LMT	C3-C4-C5-C6
45	K	501	LMT	C1-C2-C3-C4
58	U	101	EHZ	C5-C6-C7-O1
51	L	701	3PE	C21-C22-C23-C24
45	l	201	LMT	O5B-C1B-O1B-C4'
51	M	601	3PE	C2C-C2D-C2E-C2F
51	e	801	3PE	C24-C25-C26-C27
53	L	702	CDL	OB7-CB5-OB6-CB4
51	M	602	3PE	C35-C36-C37-C38
45	Y	402	LMT	C2-C3-C4-C5
45	Y	402	LMT	O5B-C5B-C6B-O6B
47	M	603	PC1	C2B-C2C-C2D-C2E
51	L	703	3PE	C22-C21-O21-C2
45	l	201	LMT	C5'-C4'-O1B-C1B
51	M	601	3PE	C36-C37-C38-C39
51	I	201	3PE	O22-C21-O21-C2
47	B	203	PC1	C21-C22-C23-C24
51	Y	401	3PE	C37-C38-C39-C3A
51	M	601	3PE	C26-C27-C28-C29
52	N	903	I49	N04-C15-N02-C14
53	X	1701	CDL	C57-C58-C59-C60
53	d	1202	CDL	C73-C74-C75-C76
45	A	1001	LMT	O5'-C1'-O1'-C1
51	J	401	3PE	C38-C39-C3A-C3B
51	L	701	3PE	C3A-C3B-C3C-C3D
51	M	602	3PE	C39-C3A-C3B-C3C
51	I	201	3PE	C22-C21-O21-C2
51	M	602	3PE	C22-C21-O21-C2
51	e	801	3PE	C22-C21-O21-C2
53	q	201	CDL	C11-CA5-OA6-CA4
53	q	201	CDL	OA7-CA5-OA6-CA4
45	N	901	LMT	C2'-C1'-O1'-C1
47	M	603	PC1	O21-C2-C3-O31
45	h	1003	LMT	O5B-C5B-C6B-O6B
45	l	201	LMT	C3'-C4'-O1B-C1B
53	q	201	CDL	C11-C12-C13-C14
56	P	501	NDP	O4D-C4D-C5D-O5D
51	I	201	3PE	C2B-C2C-C2D-C2E
51	L	701	3PE	C2D-C2E-C2F-C2G
45	h	1002	LMT	O5B-C5B-C6B-O6B
47	M	603	PC1	C2C-C2D-C2E-C2F
51	L	703	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
51	M	602	3PE	O22-C21-O21-C2
51	e	801	3PE	O22-C21-O21-C2
53	Y	403	CDL	C36-C37-C38-C39
51	N	902	3PE	C11-O13-P-O11
53	X	1701	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB2-OB2-PB2-OB5
51	e	801	3PE	C33-C34-C35-C36
51	I	201	3PE	C21-C22-C23-C24
45	N	901	LMT	C4B-C5B-C6B-O6B
45	Y	402	LMT	C4'-C5'-C6'-O6'
53	q	201	CDL	C71-CB7-OB8-CB6
53	X	1701	CDL	OB5-CB3-CB4-CB6
53	d	1202	CDL	OA5-CA3-CA4-CA6
51	Y	401	3PE	C31-C32-C33-C34
53	Y	403	CDL	C15-C16-C17-C18
51	b	302	3PE	C2C-C2D-C2E-C2F
45	A	1001	LMT	C11-C10-C9-C8
51	N	902	3PE	C1-C2-C3-O31
51	Y	401	3PE	C1-C2-C3-O31
51	d	1201	3PE	C1-C2-C3-O31
53	X	1701	CDL	CB3-CB4-CB6-OB8
51	b	302	3PE	C21-C22-C23-C24
58	T	101	EHZ	O4-C15-C16-O5
45	b	301	LMT	O1'-C1-C2-C3
58	U	101	EHZ	C1-C2-C3-C4
53	h	1001	CDL	C20-C21-C22-C23
45	B	202	LMT	O5'-C5'-C6'-O6'
45	K	501	LMT	O5B-C5B-C6B-O6B
58	T	101	EHZ	C5-C6-C7-O1
51	I	201	3PE	C23-C24-C25-C26
51	e	801	3PE	C2B-C2C-C2D-C2E
51	M	601	3PE	C32-C31-O31-C3
45	d	1203	LMT	C5'-C4'-O1B-C1B
51	e	801	3PE	O11-C1-C2-O21
53	X	1701	CDL	OA5-CA3-CA4-OA6
53	q	201	CDL	OA5-CA3-CA4-OA6
51	I	201	3PE	C3E-C3F-C3G-C3H
47	B	203	PC1	O21-C2-C3-O31
51	N	902	3PE	O21-C2-C3-O31
53	q	201	CDL	OB9-CB7-OB8-CB6
51	e	801	3PE	C32-C33-C34-C35
53	q	201	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
51	e	801	3PE	C38-C39-C3A-C3B
53	Y	403	CDL	C11-C12-C13-C14
51	L	701	3PE	C25-C26-C27-C28
51	L	703	3PE	C36-C37-C38-C39
54	O	401	GTP	PG-O3B-PB-O1B
45	B	202	LMT	C7-C8-C9-C10
51	Y	401	3PE	C33-C34-C35-C36
58	T	101	EHZ	C1-C21-C22-C23
45	K	501	LMT	C5-C6-C7-C8
53	Y	403	CDL	C13-C14-C15-C16
53	q	201	CDL	CA7-C31-C32-C33
45	d	1203	LMT	C3'-C4'-O1B-C1B
51	Y	401	3PE	O11-C1-C2-C3
51	e	801	3PE	O11-C1-C2-C3
53	h	1001	CDL	OB5-CB3-CB4-CB6
51	Y	401	3PE	O22-C21-O21-C2
51	I	201	3PE	C35-C36-C37-C38
51	d	1201	3PE	C31-C32-C33-C34
45	J	402	LMT	C2-C1-O1'-C1'
45	Y	402	LMT	C2-C1-O1'-C1'
53	d	1202	CDL	C76-C77-C78-C79
53	h	1001	CDL	CA5-C11-C12-C13
45	h	1002	LMT	C5'-C4'-O1B-C1B
51	M	601	3PE	C33-C34-C35-C36
53	h	1001	CDL	C24-C25-C26-C27
53	q	201	CDL	C52-C53-C54-C55
53	L	702	CDL	CB3-CB4-CB6-OB8
53	Y	403	CDL	CA3-CA4-CA6-OA8
53	d	1202	CDL	CB3-CB4-CB6-OB8
52	H	602	I49	C08-C06-C07-C09
45	Y	402	LMT	C3'-C4'-O1B-C1B
51	J	401	3PE	C35-C36-C37-C38
53	q	201	CDL	CA2-OA2-PA1-OA5
45	Y	402	LMT	C3-C4-C5-C6
51	L	701	3PE	O11-C1-C2-O21
51	Y	401	3PE	O11-C1-C2-O21
53	X	1701	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	OA5-CA3-CA4-OA6
53	h	1001	CDL	OA5-CA3-CA4-OA6
53	h	1001	CDL	OB5-CB3-CB4-OB6
53	q	201	CDL	CB7-C71-C72-C73
51	M	601	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	M	603	PC1	C2E-C2F-C2G-C2H
51	J	401	3PE	O21-C2-C3-O31
51	d	1201	3PE	O21-C2-C3-O31
53	X	1701	CDL	OB6-CB4-CB6-OB8
53	h	1001	CDL	OA6-CA4-CA6-OA8
51	I	201	3PE	C2C-C2D-C2E-C2F
45	N	901	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	O1'-C1-C2-C3
51	d	1201	3PE	C25-C26-C27-C28
58	U	101	EHZ	C1-C21-C22-C23
47	M	603	PC1	C2-C1-O11-P
51	N	902	3PE	C2-C1-O11-P
51	b	302	3PE	C2-C1-O11-P
53	X	1701	CDL	CB4-CB3-OB5-PB2
53	q	201	CDL	CA4-CA3-OA5-PA1
52	H	602	I49	C08-C06-C07-C10
51	L	701	3PE	C38-C39-C3A-C3B
53	d	1202	CDL	CA7-C31-C32-C33
45	Y	402	LMT	C5'-C4'-O1B-C1B
51	L	701	3PE	O11-C1-C2-C3
51	M	602	3PE	O11-C1-C2-C3
51	H	601	3PE	C33-C34-C35-C36
53	h	1001	CDL	C18-C19-C20-C21
45	B	202	LMT	C5'-C4'-O1B-C1B
53	d	1202	CDL	C32-C33-C34-C35
54	O	401	GTP	PB-O3B-PG-O1G
53	Y	403	CDL	C53-C54-C55-C56
53	X	1701	CDL	C19-C20-C21-C22
51	e	801	3PE	C3-C2-O21-C21
47	B	203	PC1	C2-C1-O11-P
47	M	603	PC1	C1-C2-C3-O31
51	b	302	3PE	C1-C2-C3-O31
51	e	801	3PE	C1-C2-C3-O31
52	N	903	I49	N01-C14-N02-C15
53	q	201	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	C31-C32-C33-C34
45	J	402	LMT	C2B-C1B-O1B-C4'
58	T	101	EHZ	O1-C7-C8-C9
51	J	401	3PE	C32-C33-C34-C35
51	L	703	3PE	C26-C27-C28-C29
51	Y	401	3PE	O21-C2-C3-O31
53	L	702	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
53	Y	403	CDL	OA6-CA4-CA6-OA8
53	d	1202	CDL	OB6-CB4-CB6-OB8
45	N	901	LMT	C1-C2-C3-C4
53	d	1202	CDL	C38-C39-C40-C41
51	M	602	3PE	C1-O11-P-O13
51	Y	401	3PE	C11-O13-P-O11
53	d	1202	CDL	CA3-OA5-PA1-OA2
51	d	1201	3PE	C35-C36-C37-C38
51	I	201	3PE	C1-O11-P-O14
51	I	201	3PE	C11-O13-P-O12
51	M	602	3PE	C1-O11-P-O12
51	M	602	3PE	C11-O13-P-O14
51	N	902	3PE	C11-O13-P-O12
51	Y	401	3PE	C11-O13-P-O12
51	d	1201	3PE	C1-O11-P-O14
51	d	1201	3PE	C11-O13-P-O14
53	L	702	CDL	CB3-OB5-PB2-OB4
53	X	1701	CDL	CA2-OA2-PA1-OA4
53	X	1701	CDL	CB2-OB2-PB2-OB3
53	Y	403	CDL	CB2-OB2-PB2-OB3
53	Y	403	CDL	CB3-OB5-PB2-OB3
53	d	1202	CDL	CA2-OA2-PA1-OA3
53	d	1202	CDL	CA2-OA2-PA1-OA4
53	d	1202	CDL	CA3-OA5-PA1-OA3
53	d	1202	CDL	CB2-OB2-PB2-OB4
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CB2-OB2-PB2-OB3
53	h	1001	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CA2-OA2-PA1-OA3
53	q	201	CDL	CB2-OB2-PB2-OB4
58	T	101	EHZ	C6-C7-C8-C9
53	d	1202	CDL	CB7-C71-C72-C73
51	I	201	3PE	C2E-C2F-C2G-C2H
45	b	301	LMT	O5'-C1'-O1'-C1
53	Y	403	CDL	OB5-CB3-CB4-CB6
53	h	1001	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	OA5-CA3-CA4-CA6
53	L	702	CDL	C60-C61-C62-C63
45	A	1001	LMT	C9-C10-C11-C12
51	d	1201	3PE	C12-C11-O13-P
58	U	101	EHZ	C2-C3-C4-C5
51	H	601	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
45	B	202	LMT	O5B-C5B-C6B-O6B
51	M	601	3PE	C23-C24-C25-C26
56	P	501	NDP	O4D-C1D-N1N-C6N
45	h	1003	LMT	C7-C8-C9-C10
53	d	1202	CDL	CA5-C11-C12-C13
47	B	203	PC1	C1-C2-C3-O31
51	J	401	3PE	C1-C2-C3-O31
53	L	702	CDL	OB9-CB7-OB8-CB6
53	X	1701	CDL	C56-C57-C58-C59
53	h	1001	CDL	CA3-CA4-CA6-OA8
51	Y	401	3PE	C34-C35-C36-C37
51	I	201	3PE	C28-C29-C2A-C2B
51	I	201	3PE	C27-C28-C29-C2A
53	h	1001	CDL	C73-C74-C75-C76
51	M	602	3PE	C23-C24-C25-C26
51	I	201	3PE	C36-C37-C38-C39
53	q	201	CDL	C17-C18-C19-C20
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
53	h	1001	CDL	CB3-CB4-OB6-CB5
53	X	1701	CDL	OA5-CA3-CA4-CA6
45	j	101	LMT	C4'-C5'-C6'-O6'
53	h	1001	CDL	OA7-CA5-OA6-CA4
53	X	1701	CDL	C76-C77-C78-C79
45	J	402	LMT	O5B-C1B-O1B-C4'
45	h	1002	LMT	O5B-C1B-O1B-C4'
51	M	601	3PE	C2-C1-O11-P
53	q	201	CDL	C1-CB2-OB2-PB2
51	b	302	3PE	C23-C24-C25-C26
53	Y	403	CDL	OB5-CB3-CB4-OB6
45	h	1002	LMT	C4-C5-C6-C7
53	h	1001	CDL	C11-C12-C13-C14
51	L	701	3PE	C33-C34-C35-C36
53	X	1701	CDL	C55-C56-C57-C58
58	U	101	EHZ	C3-C4-C5-C6
51	M	602	3PE	C22-C23-C24-C25
58	T	101	EHZ	C21-C22-C23-C24
51	b	302	3PE	C2B-C2C-C2D-C2E
51	I	201	3PE	C32-C31-O31-C3
51	e	801	3PE	C2-C1-O11-P
53	d	1202	CDL	C44-C45-C46-C47
51	M	601	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
51	I	201	3PE	O32-C31-O31-C3
51	b	302	3PE	C31-C32-C33-C34
51	b	302	3PE	C27-C28-C29-C2A
51	b	302	3PE	C33-C34-C35-C36
53	X	1701	CDL	C13-C14-C15-C16
47	M	603	PC1	C27-C28-C29-C2A
45	h	1002	LMT	C2B-C1B-O1B-C4'
51	M	601	3PE	C34-C35-C36-C37
51	M	601	3PE	O21-C2-C3-O31
51	L	703	3PE	C34-C35-C36-C37
53	h	1001	CDL	C72-C73-C74-C75
51	H	601	3PE	C2-C1-O11-P
53	h	1001	CDL	C52-C53-C54-C55
51	M	602	3PE	C26-C27-C28-C29
51	J	401	3PE	C33-C34-C35-C36
51	I	201	3PE	C1-O11-P-O13
53	X	1701	CDL	C75-C76-C77-C78
47	B	203	PC1	O11-C1-C2-O21
51	H	601	3PE	O11-C1-C2-C3
53	Y	403	CDL	C18-C19-C20-C21
53	h	1001	CDL	C11-CA5-OA6-CA4
51	d	1201	3PE	C34-C35-C36-C37
53	X	1701	CDL	C71-C72-C73-C74
51	e	801	3PE	C39-C3A-C3B-C3C
51	M	601	3PE	C21-C22-C23-C24
51	N	902	3PE	O22-C21-O21-C2
45	h	1002	LMT	C5-C6-C7-C8
51	M	601	3PE	C25-C26-C27-C28
59	o	201	MYR	C3-C4-C5-C6
45	l	201	LMT	C1-C2-C3-C4
47	M	603	PC1	C2F-C2G-C2H-C2I
53	Y	403	CDL	C38-C39-C40-C41
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	A	1001	LMT	O1'-C1-C2-C3
52	N	903	I49	C06-C08-N01-C14
53	L	702	CDL	C39-C40-C41-C42
51	I	201	3PE	C2D-C2E-C2F-C2G
51	N	902	3PE	C31-C32-C33-C34
47	B	203	PC1	C24-C25-C26-C27
53	q	201	CDL	OB5-CB3-CB4-CB6
51	J	401	3PE	C34-C35-C36-C37
47	M	603	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	d	1201	3PE	C2-C1-O11-P
45	l	201	LMT	C11-C10-C9-C8
51	e	801	3PE	C34-C35-C36-C37
51	e	801	3PE	O21-C2-C3-O31
45	Y	402	LMT	O5'-C5'-C6'-O6'
53	Y	403	CDL	C52-C53-C54-C55
51	Y	401	3PE	C39-C3A-C3B-C3C
51	J	401	3PE	C1-O11-P-O13
51	b	302	3PE	C22-C23-C24-C25
51	e	801	3PE	O21-C21-C22-C23
53	h	1001	CDL	CB6-CB4-OB6-CB5
45	h	1003	LMT	C6-C7-C8-C9
51	M	602	3PE	C3C-C3D-C3E-C3F
45	l	201	LMT	C2B-C1B-O1B-C4'
51	L	701	3PE	C3C-C3D-C3E-C3F
51	b	302	3PE	O21-C21-C22-C23
51	N	902	3PE	C22-C23-C24-C25
53	L	702	CDL	CA3-CA4-CA6-OA8
53	d	1202	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	C72-C71-CB7-OB8
56	P	501	NDP	C3D-C4D-C5D-O5D
58	U	101	EHZ	C21-C1-C2-C3
51	N	902	3PE	C24-C25-C26-C27
51	e	801	3PE	C27-C28-C29-C2A
53	Y	403	CDL	C41-C42-C43-C44
51	I	201	3PE	C34-C35-C36-C37
51	J	401	3PE	O21-C21-C22-C23
45	B	202	LMT	C5-C6-C7-C8
51	I	201	3PE	O21-C2-C3-O31
47	B	203	PC1	O21-C21-C22-C23
51	L	701	3PE	C26-C27-C28-C29
51	d	1201	3PE	O21-C21-C22-C23
56	P	501	NDP	O4B-C4B-C5B-O5B
51	e	801	3PE	O22-C21-C22-C23
54	O	401	GTP	PB-O3A-PA-O2A
51	N	902	3PE	C22-C21-O21-C2
51	L	703	3PE	O21-C21-C22-C23
45	J	402	LMT	C11-C10-C9-C8
52	N	903	I49	N03-C14-N02-C15
53	d	1202	CDL	C75-C76-C77-C78
53	X	1701	CDL	C16-C17-C18-C19
51	d	1201	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	C31-C32-C33-C34
51	L	703	3PE	C1-C2-C3-O31
45	l	201	LMT	C4B-C5B-C6B-O6B
53	d	1202	CDL	C72-C71-CB7-OB9
53	L	702	CDL	C54-C55-C56-C57
51	H	601	3PE	C1-O11-P-O14
51	I	201	3PE	C11-O13-P-O14
51	N	902	3PE	C11-O13-P-O14
53	L	702	CDL	CA2-OA2-PA1-OA3
53	X	1701	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	CB3-OB5-PB2-OB3
53	Y	403	CDL	CA3-OA5-PA1-OA3
53	d	1202	CDL	CB2-OB2-PB2-OB3
53	h	1001	CDL	CA3-OA5-PA1-OA3
51	J	401	3PE	O22-C21-C22-C23
51	b	302	3PE	O22-C21-C22-C23
51	d	1201	3PE	O13-C11-C12-N
51	d	1201	3PE	O22-C21-C22-C23
51	M	602	3PE	C36-C37-C38-C39
53	q	201	CDL	C14-C15-C16-C17
51	I	201	3PE	C12-C11-O13-P
53	h	1001	CDL	CA6-CA4-OA6-CA5
58	T	101	EHZ	O4-C15-C16-C17
51	Y	401	3PE	C3B-C3C-C3D-C3E
45	J	402	LMT	C3-C4-C5-C6
47	B	203	PC1	O22-C21-C22-C23
45	N	901	LMT	C3-C4-C5-C6
53	X	1701	CDL	C21-C22-C23-C24
51	L	701	3PE	O21-C21-C22-C23
51	b	302	3PE	O32-C31-O31-C3
51	d	1201	3PE	C29-C2A-C2B-C2C
47	M	603	PC1	O31-C31-C32-C33
51	N	902	3PE	O21-C21-C22-C23
47	M	603	PC1	C26-C27-C28-C29
47	M	603	PC1	O32-C31-C32-C33
51	L	701	3PE	O22-C21-C22-C23
45	N	901	LMT	C2-C1-O1'-C1'
45	h	1003	LMT	C2-C1-O1'-C1'
51	J	401	3PE	O31-C31-C32-C33
51	L	703	3PE	C3F-C3G-C3H-C3I
53	q	201	CDL	C32-C31-CA7-OA8
58	U	101	EHZ	C10-C11-N1-C12

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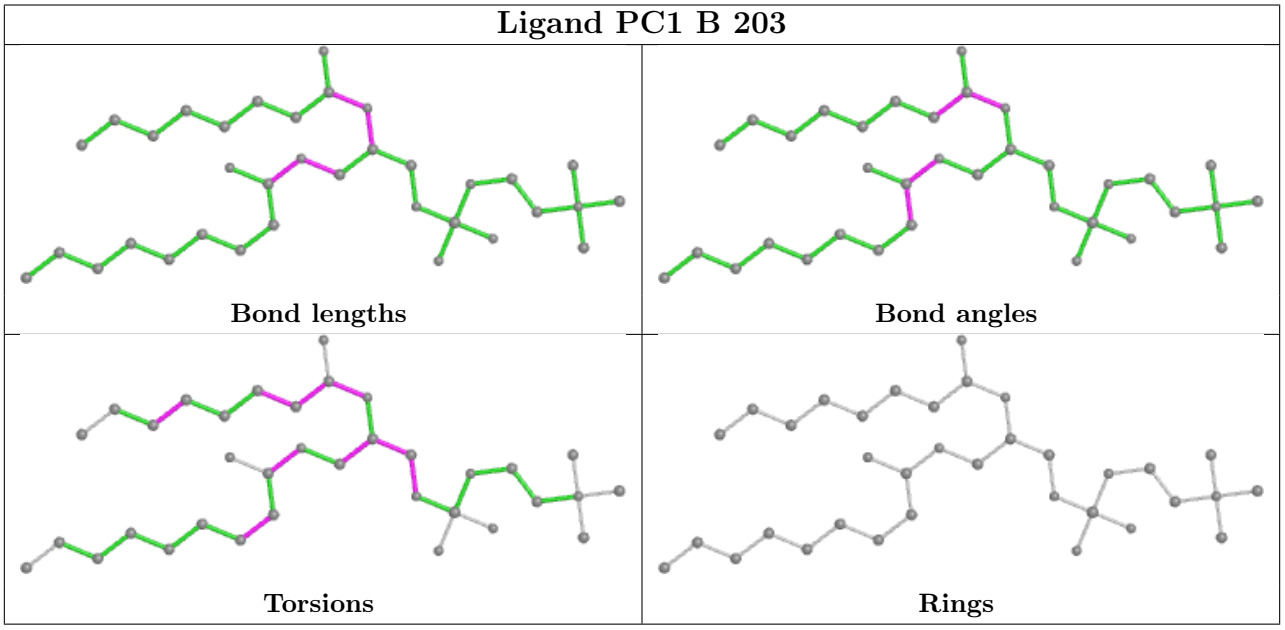
Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	C77-C78-C79-C80
53	d	1202	CDL	C34-C35-C36-C37
53	L	702	CDL	C38-C39-C40-C41
51	N	902	3PE	C26-C27-C28-C29

There are no ring outliers.

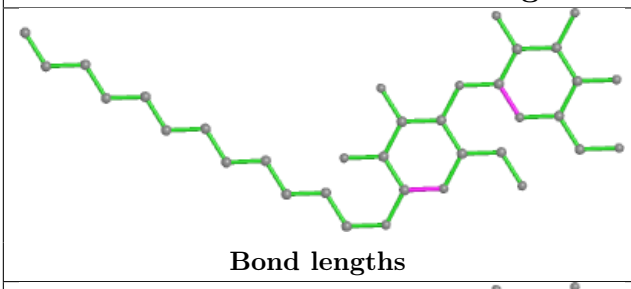
No monomer is involved in short contacts.

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.

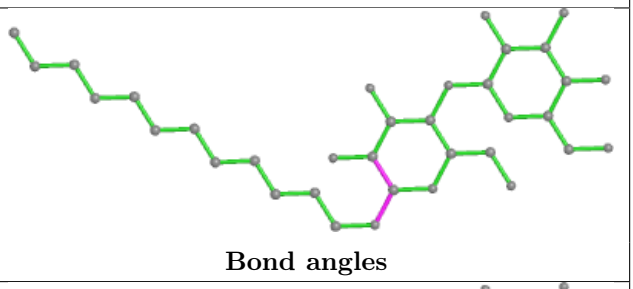
Ligand PC1 B 203



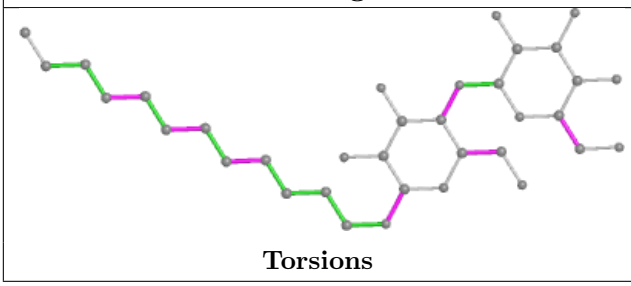
Ligand LMT B 202



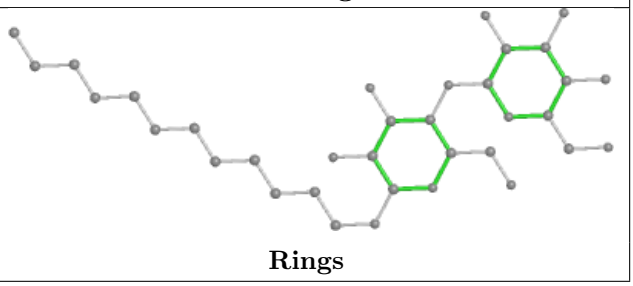
Bond lengths



Bond angles

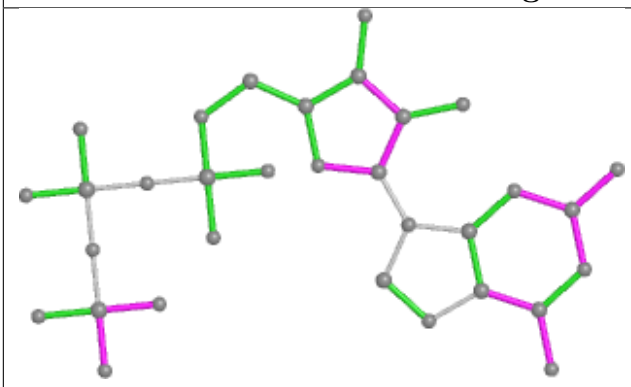


Torsions

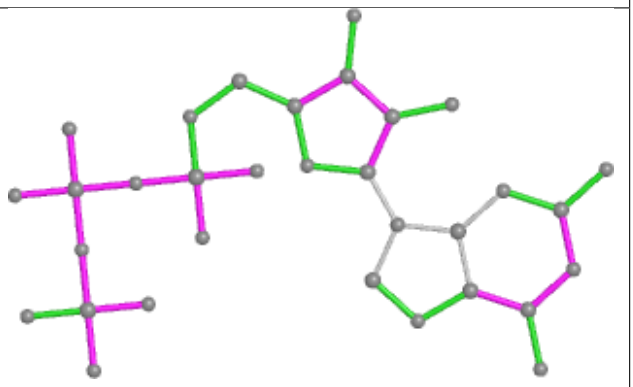


Rings

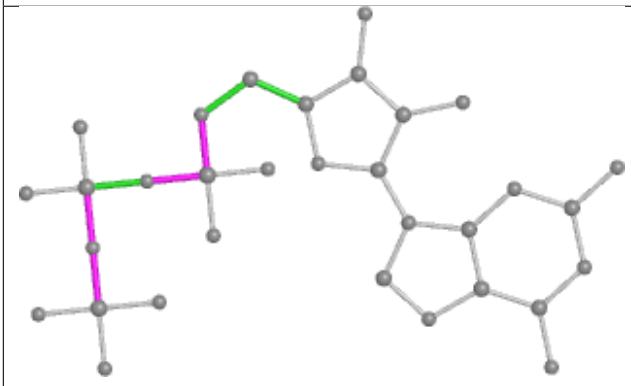
Ligand GTP O 401



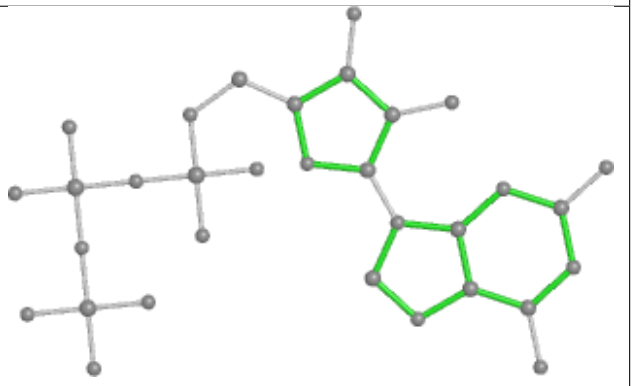
Bond lengths



Bond angles

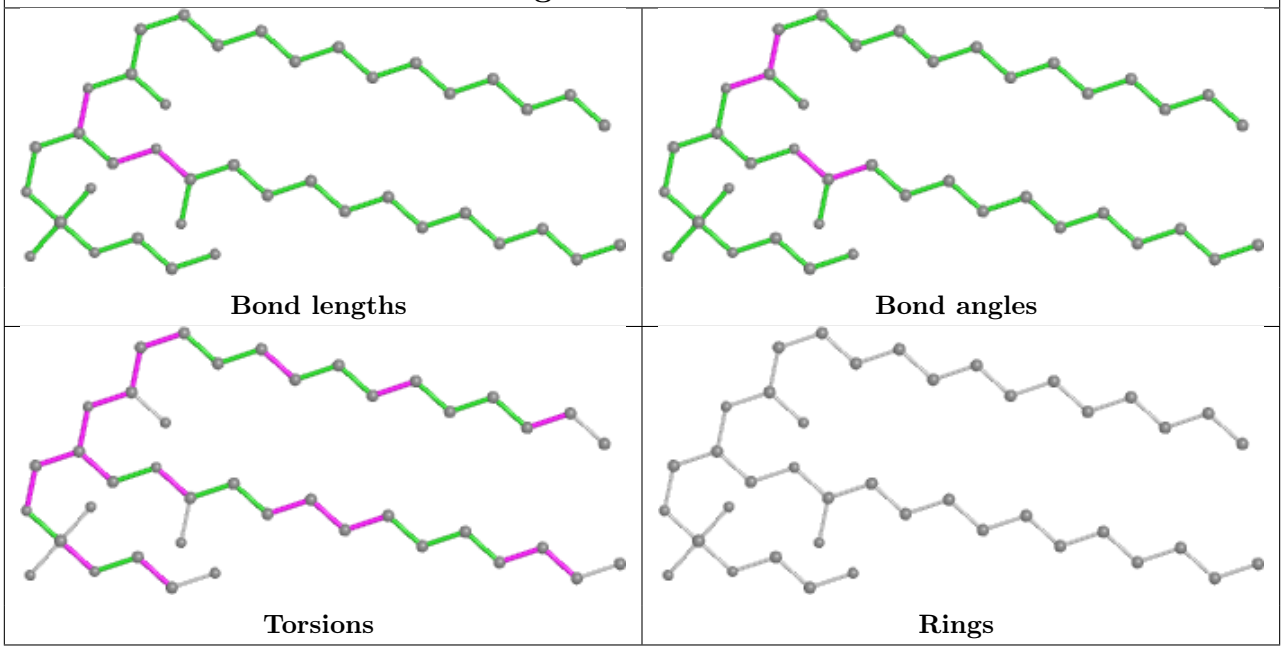


Torsions

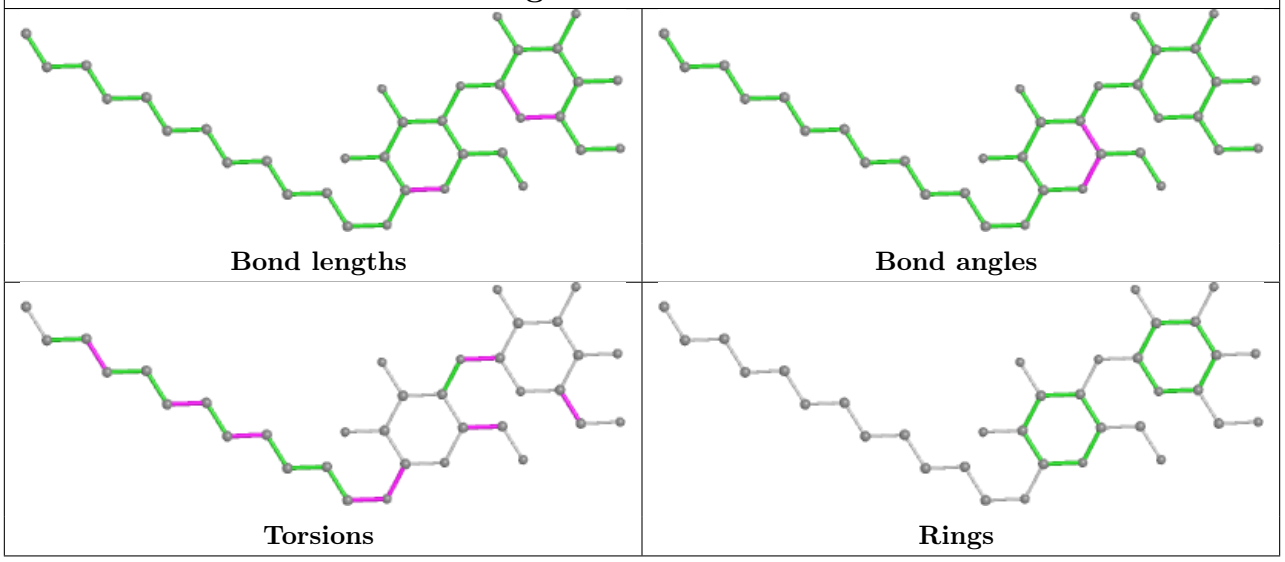


Rings

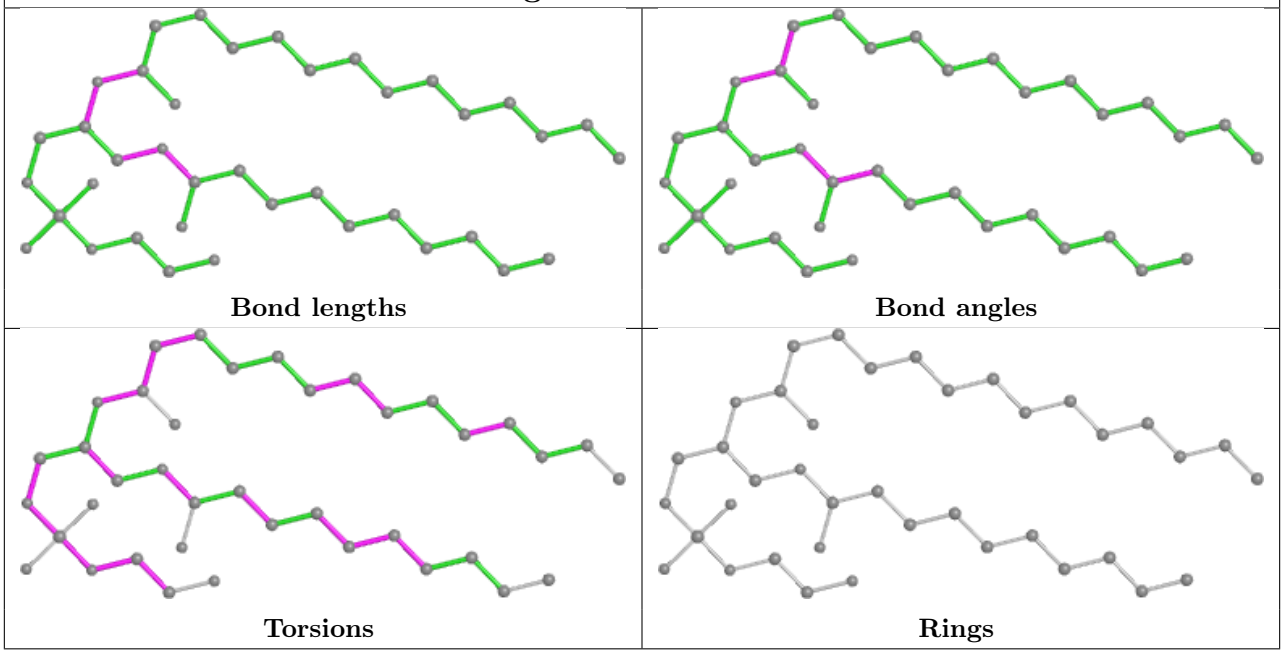
Ligand 3PE e 801



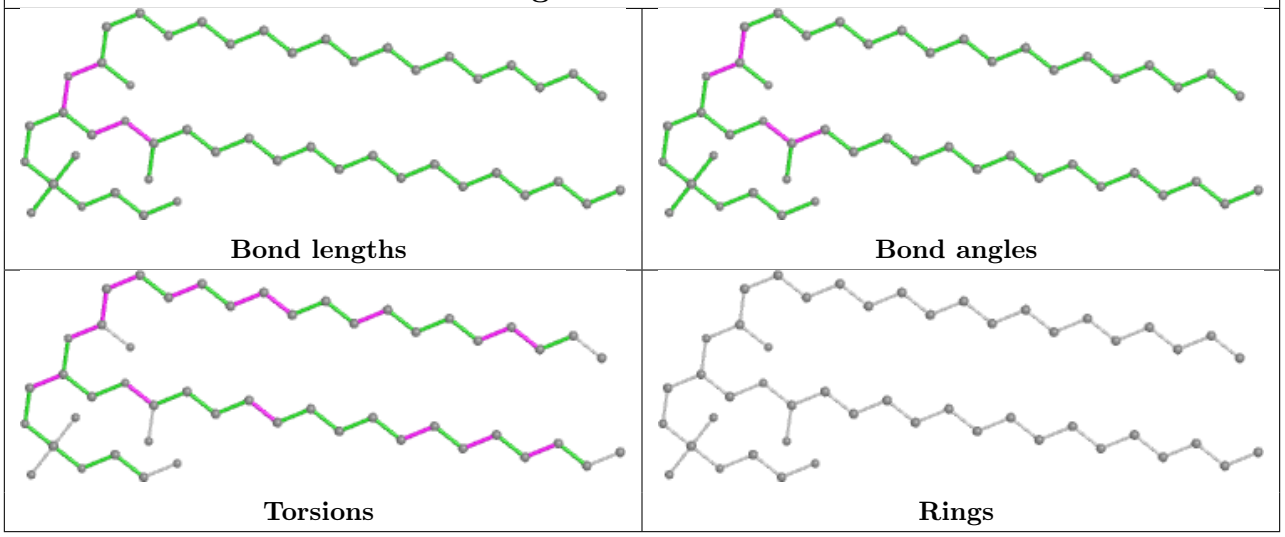
Ligand LMT J 402

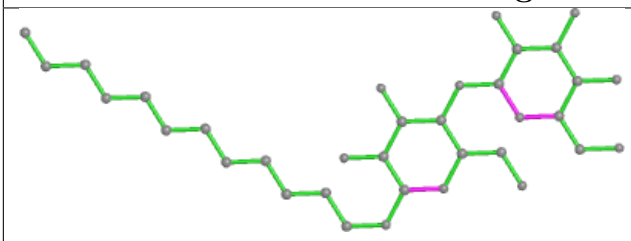
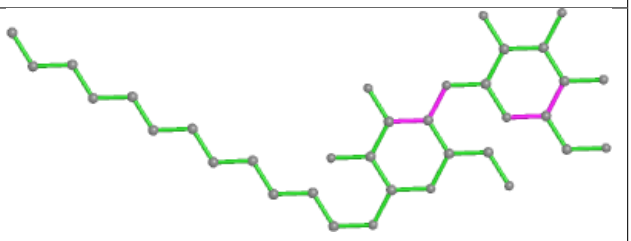
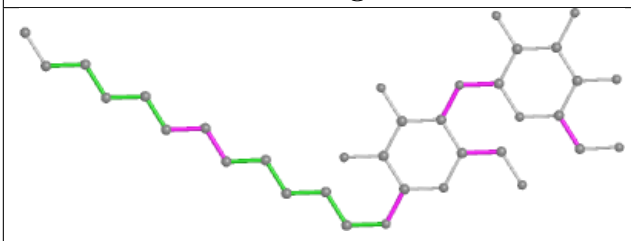
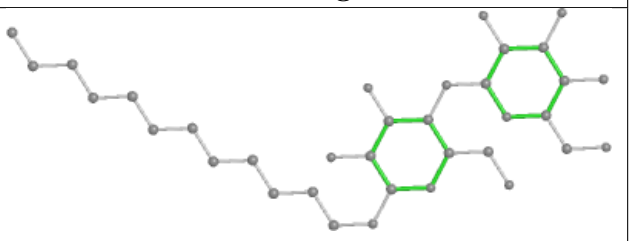


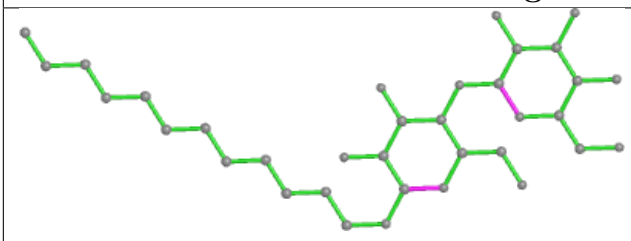
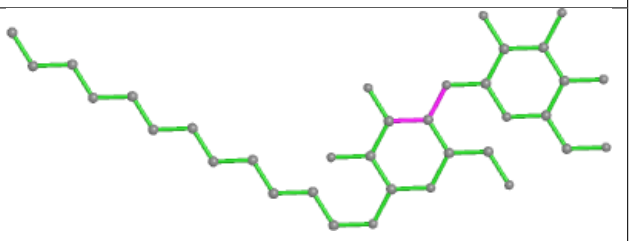
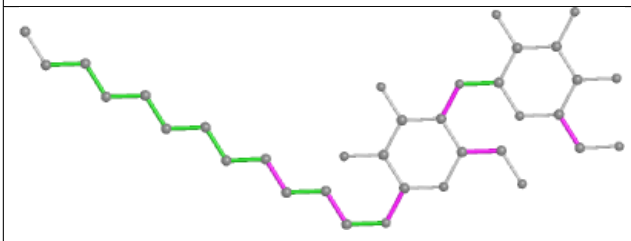
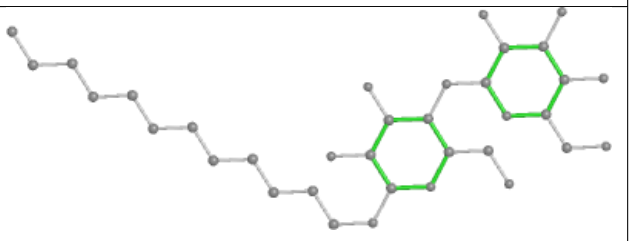
Ligand 3PE d 1201



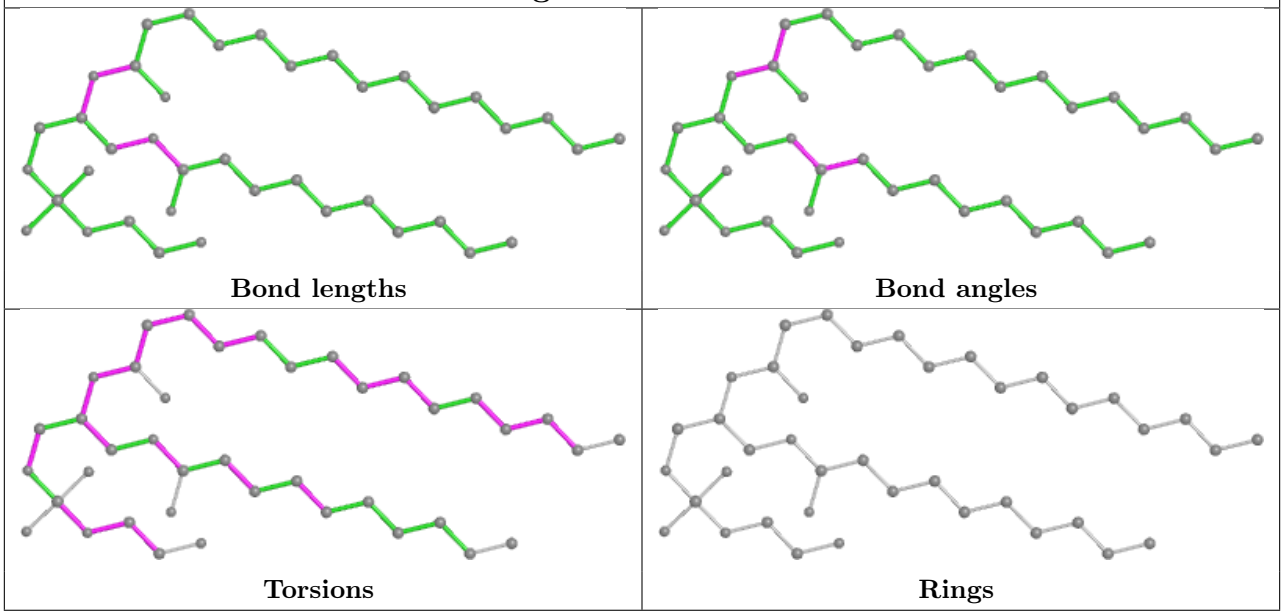
Ligand 3PE L 701



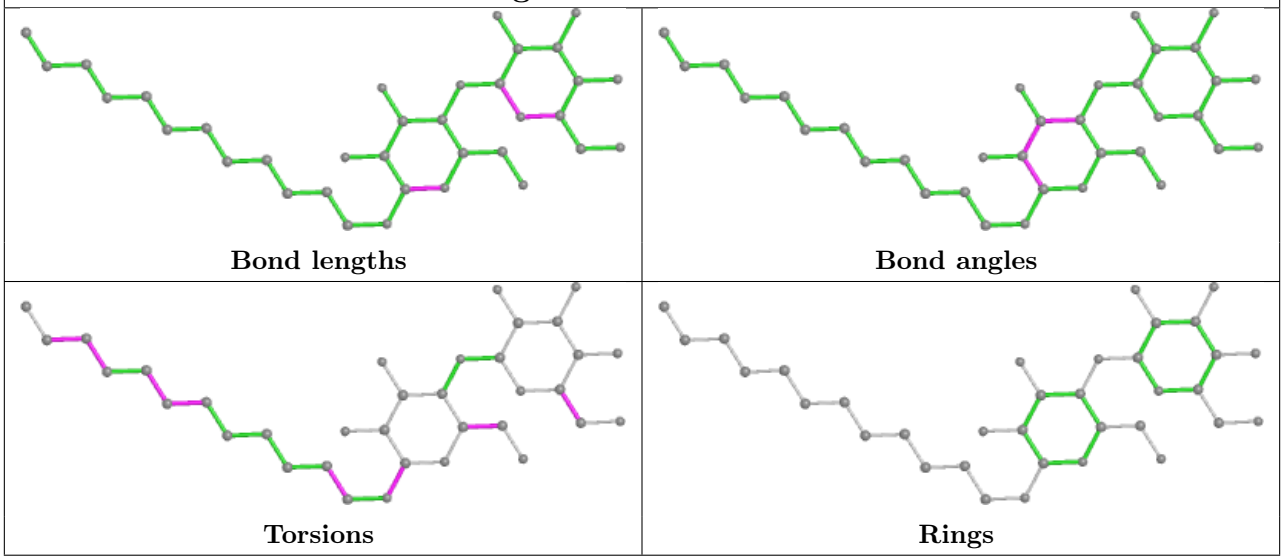
Ligand LMT h 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT b 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

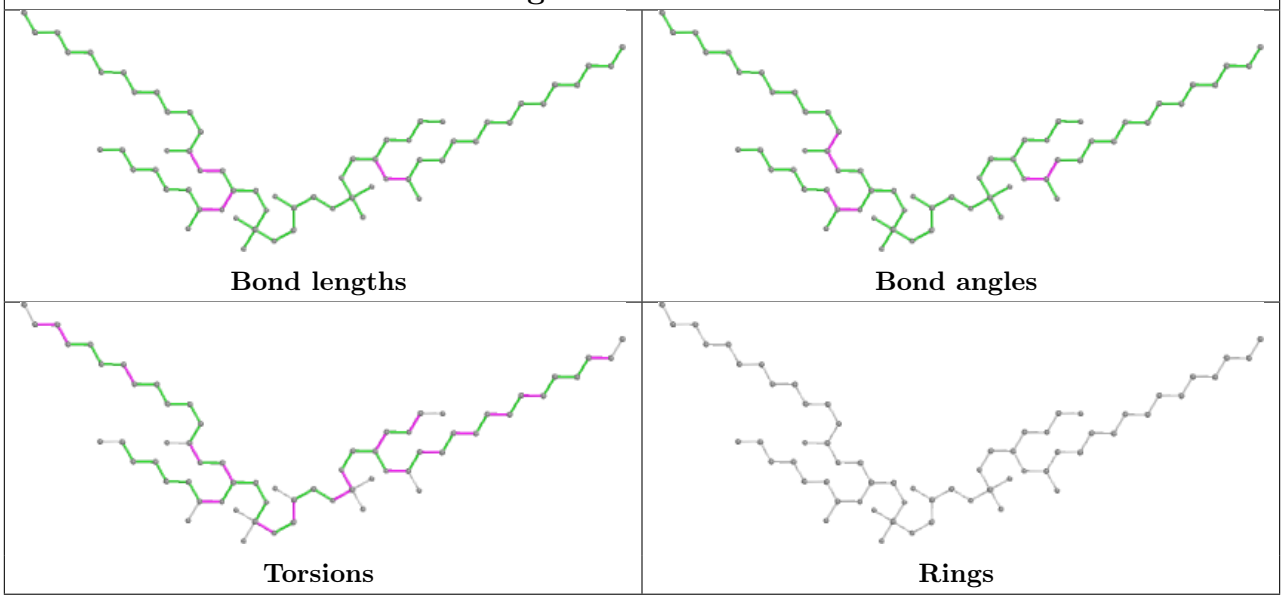
Ligand 3PE b 302



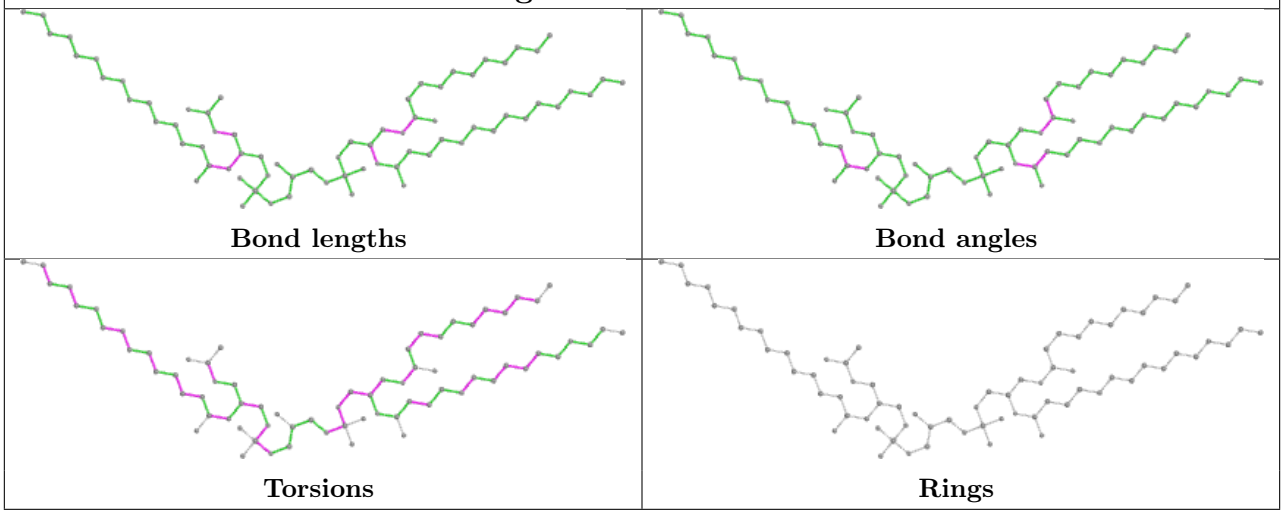
Ligand LMT A 1001



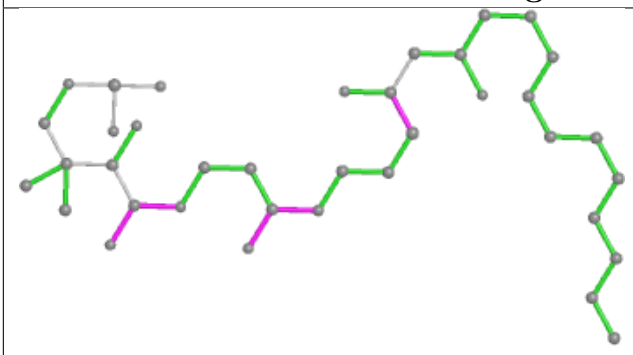
Ligand CDL L 702



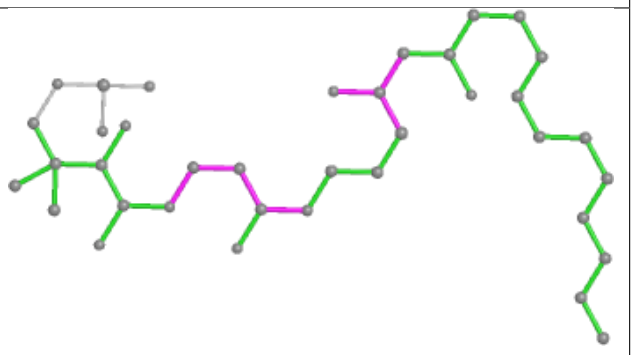
Ligand CDL X 1701



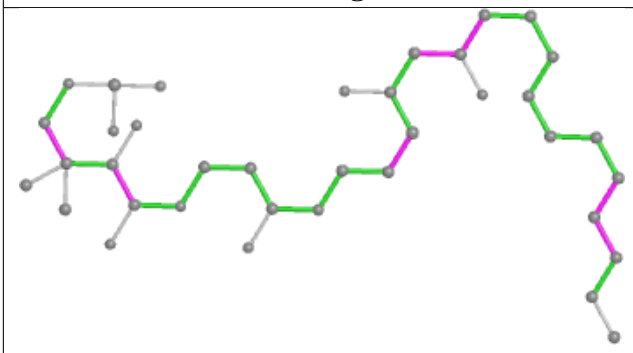
Ligand EHZ T 101



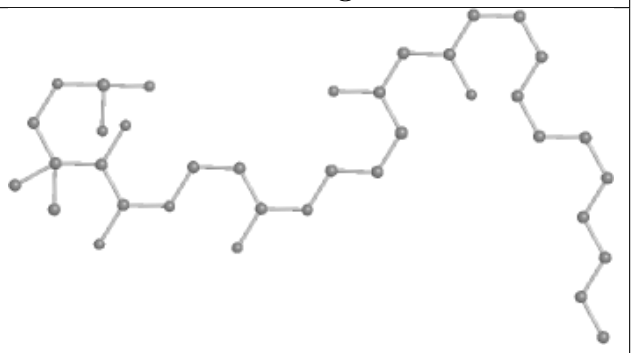
Bond lengths



Bond angles

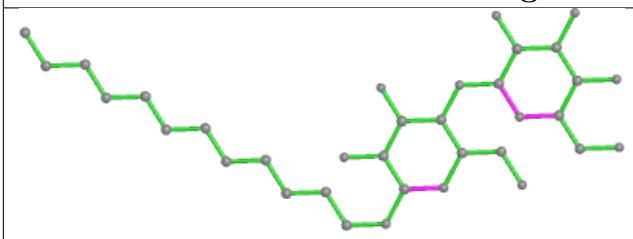


Torsions

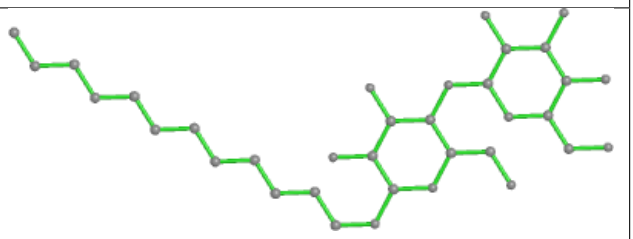


Rings

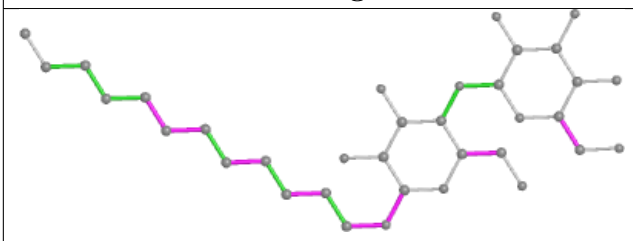
Ligand LMT N 901



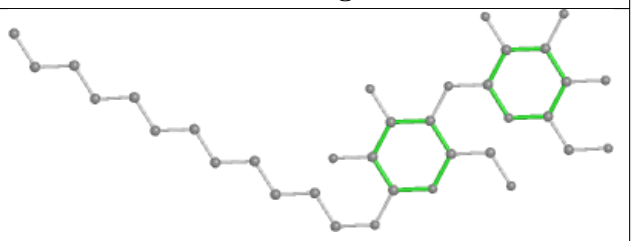
Bond lengths



Bond angles

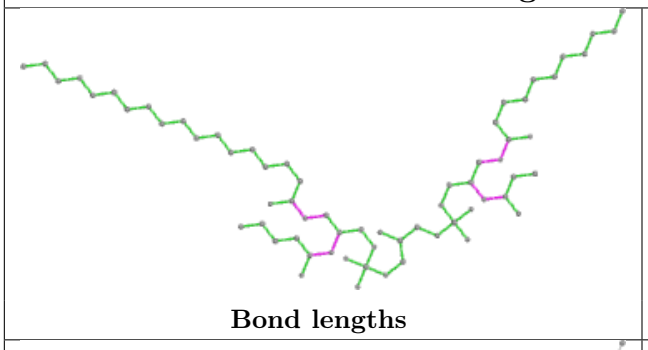


Torsions

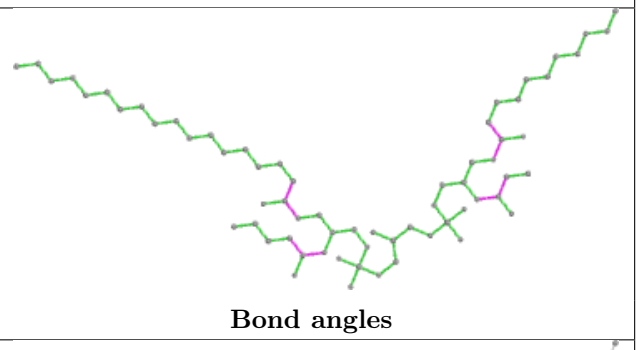


Rings

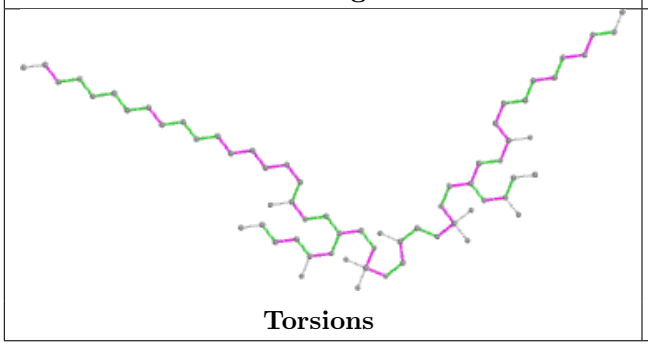
Ligand CDL d 1202



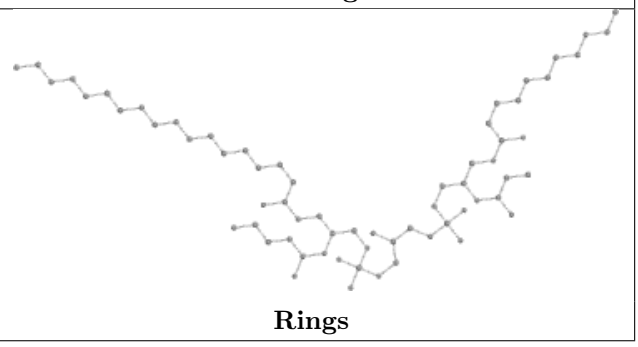
Bond lengths



Bond angles

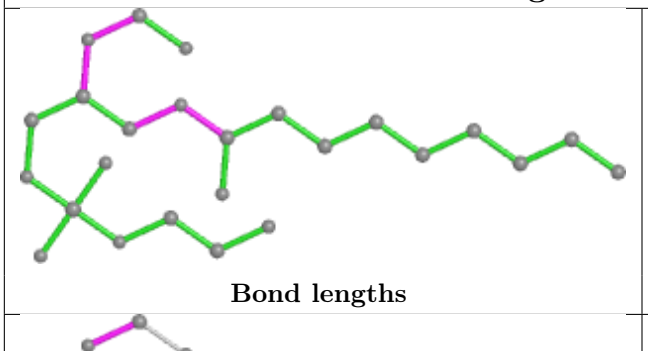


Torsions

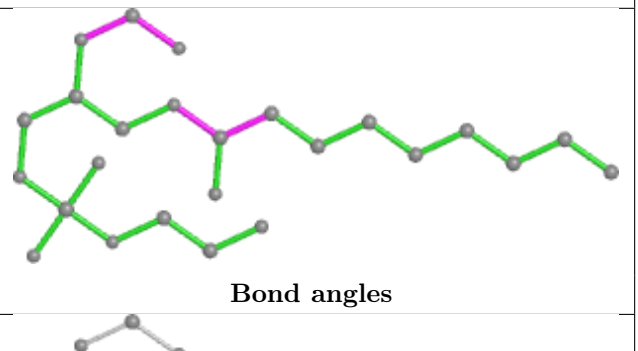


Rings

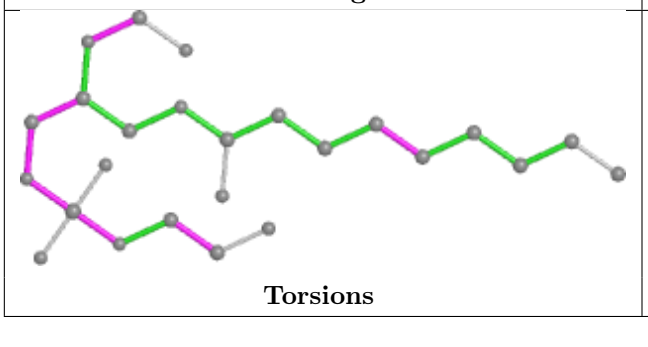
Ligand 3PE H 601



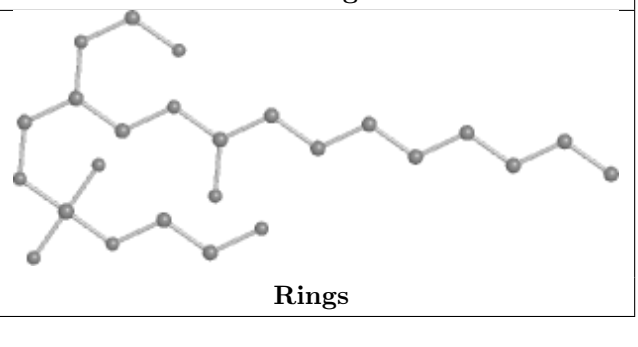
Bond lengths



Bond angles

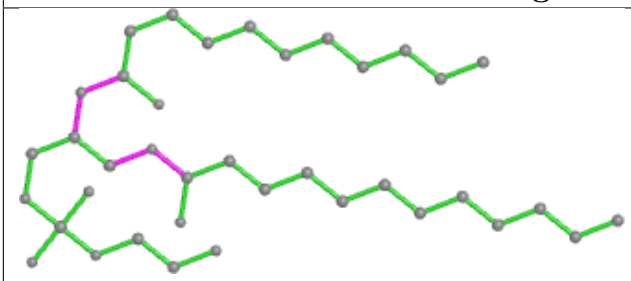


Torsions

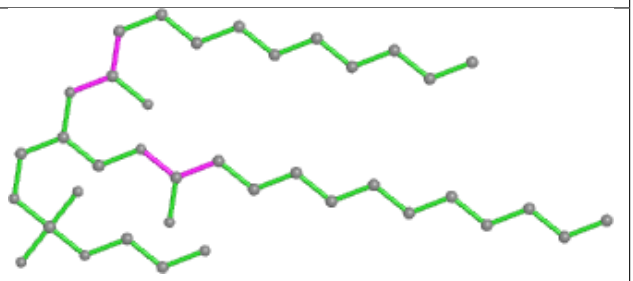


Rings

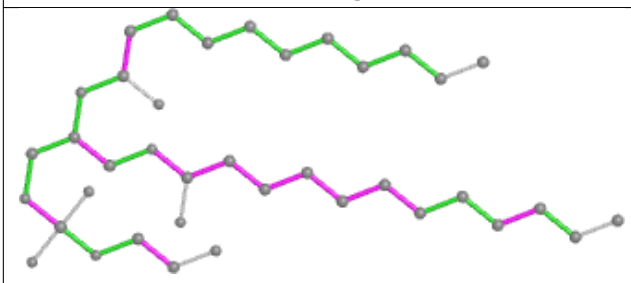
Ligand 3PE J 401



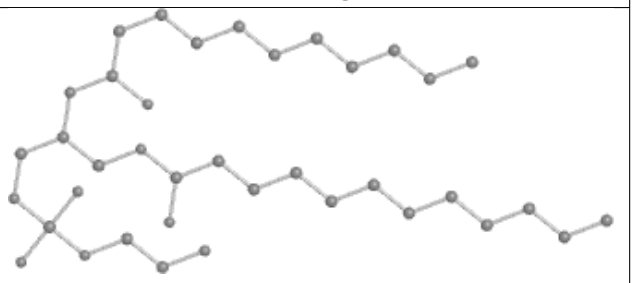
Bond lengths



Bond angles

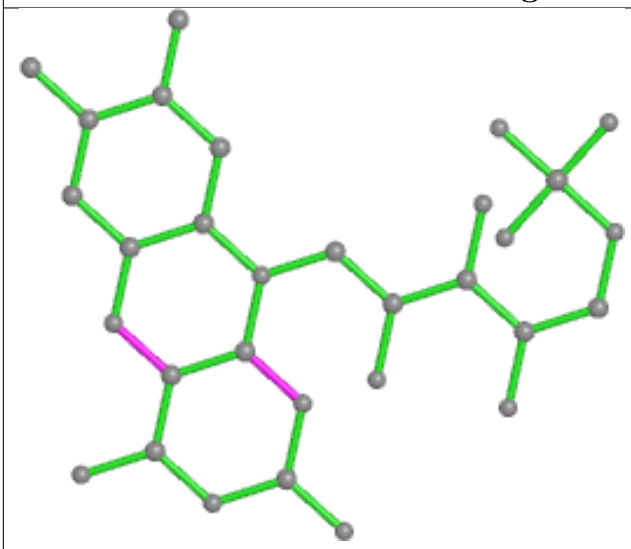


Torsions

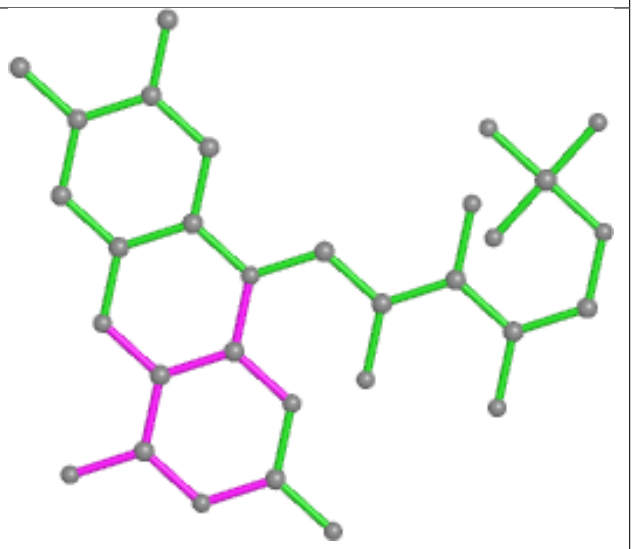


Rings

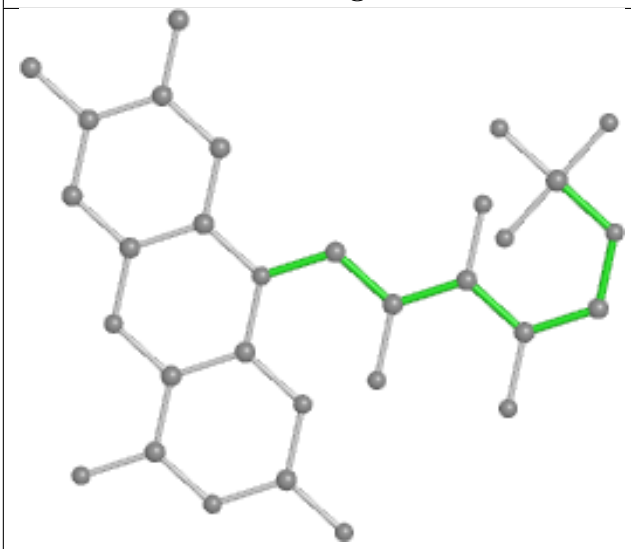
Ligand FMN F 501



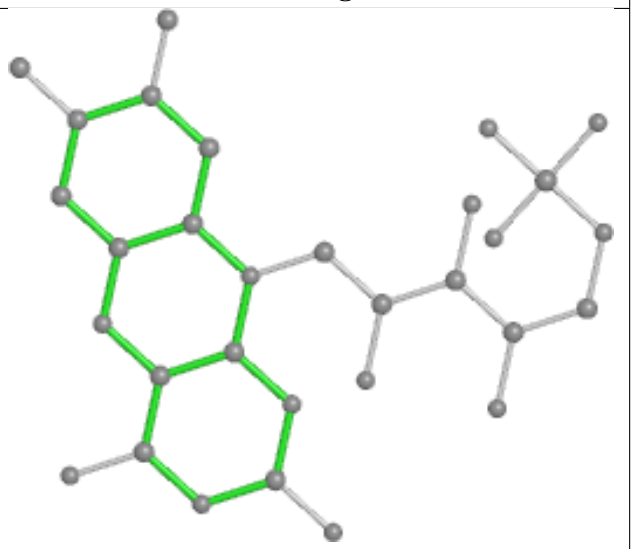
Bond lengths



Bond angles

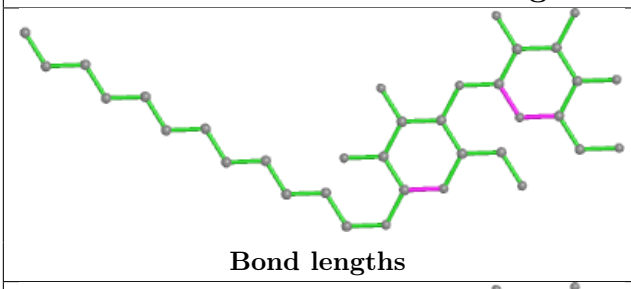


Torsions

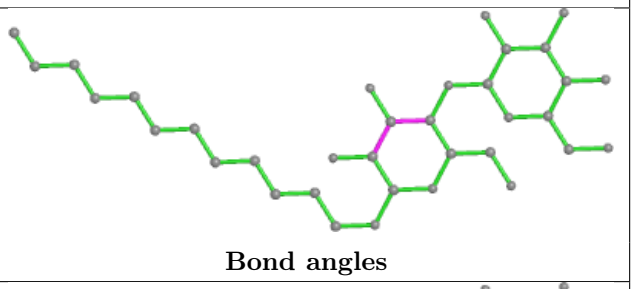


Rings

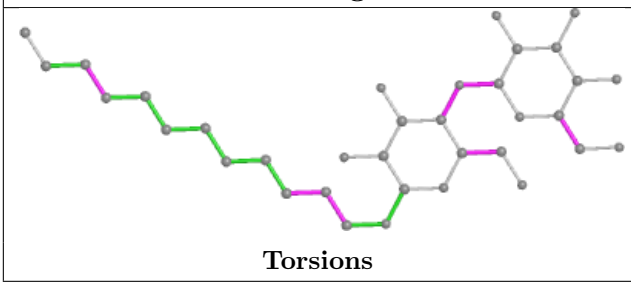
Ligand LMT l 201



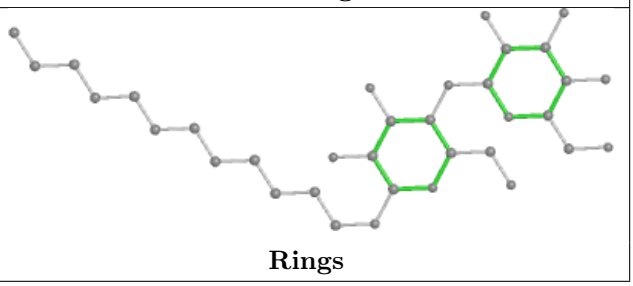
Bond lengths



Bond angles

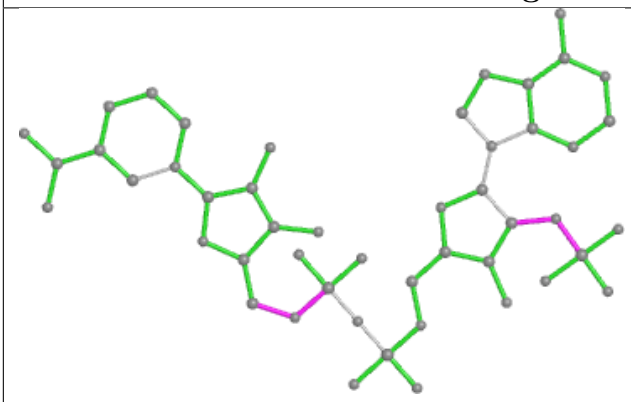


Torsions

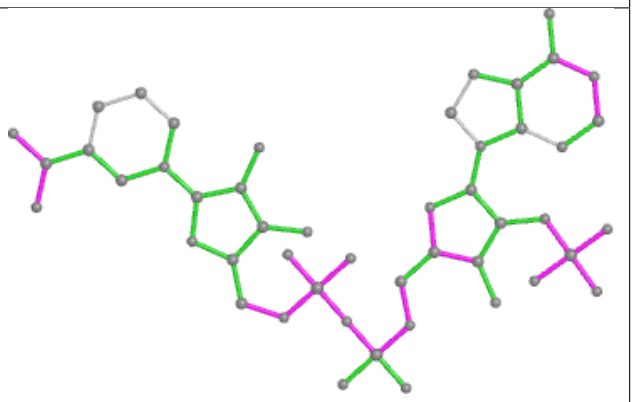


Rings

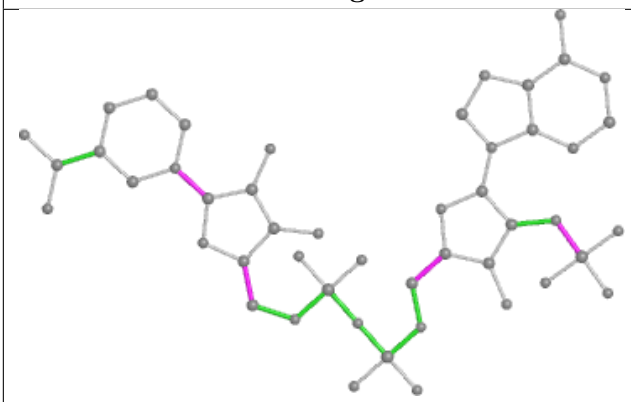
Ligand NDP P 501



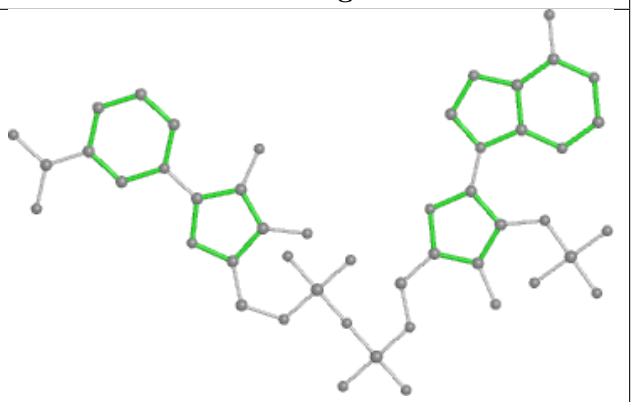
Bond lengths



Bond angles

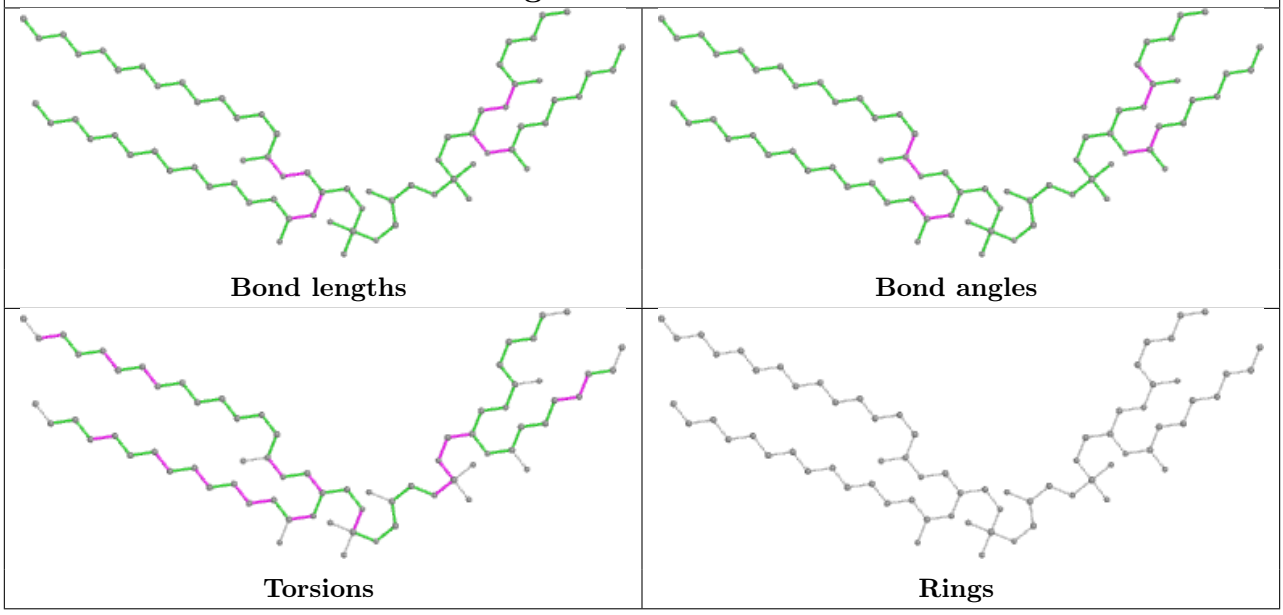


Torsions

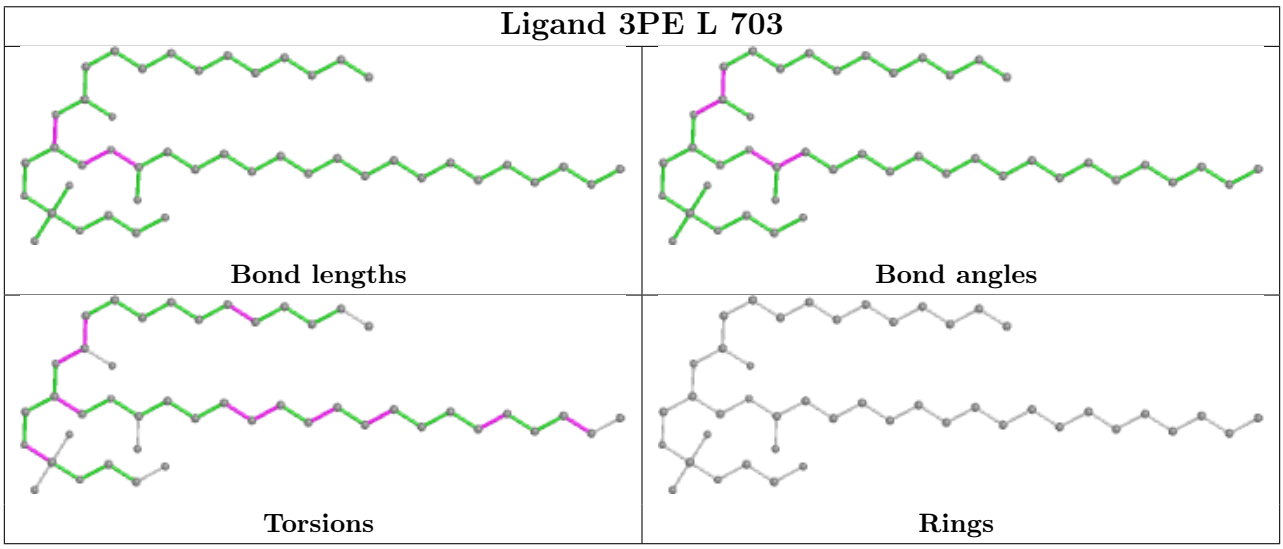


Rings

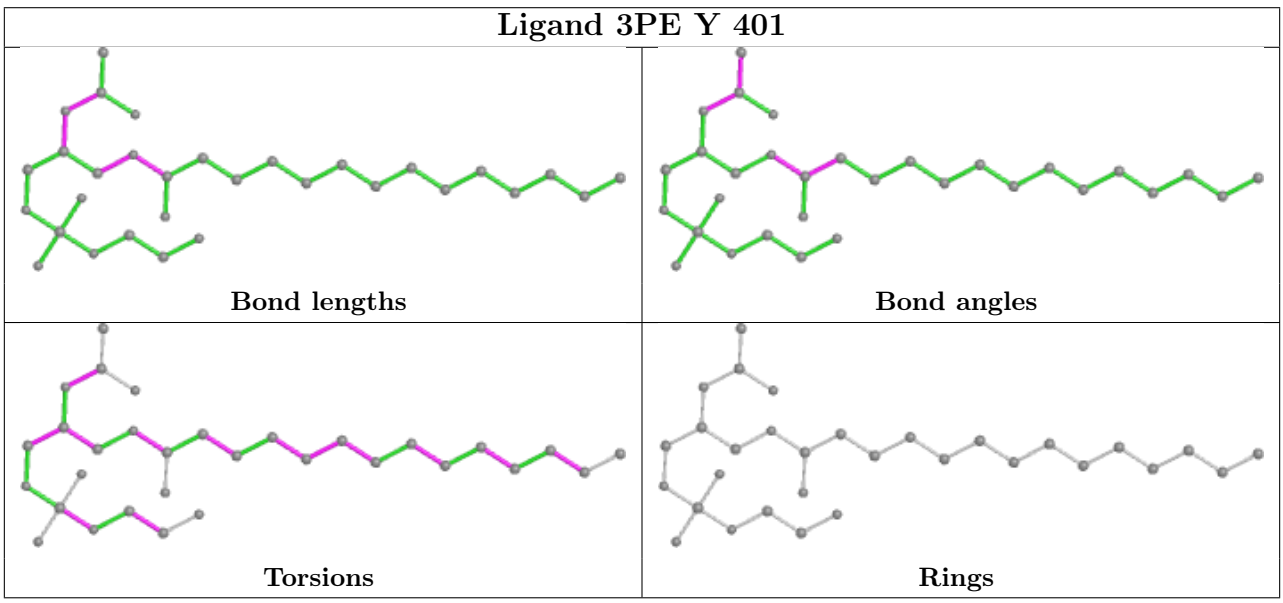
Ligand CDL Y 403



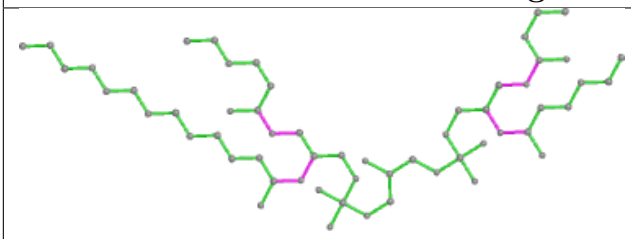
Ligand 3PE L 703



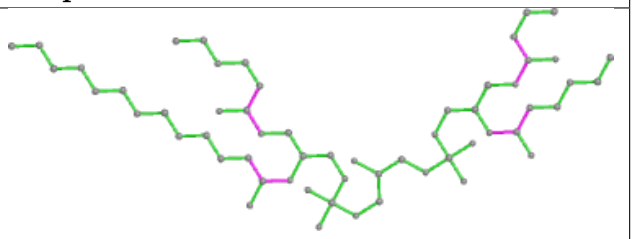
Ligand 3PE Y 401



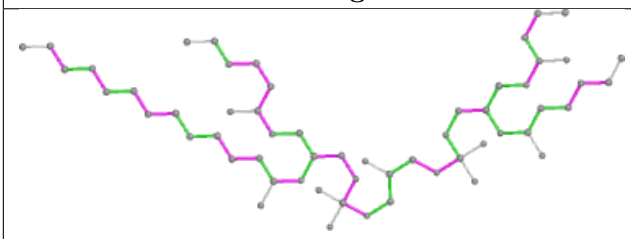
Ligand CDL q 201



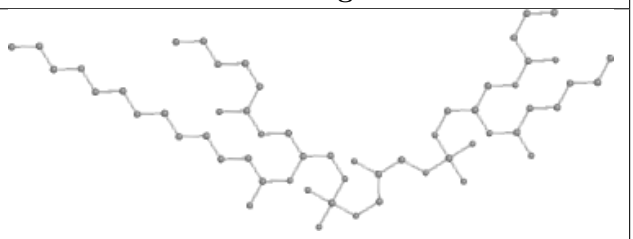
Bond lengths



Bond angles

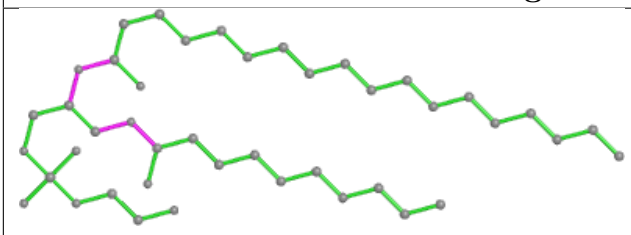


Torsions

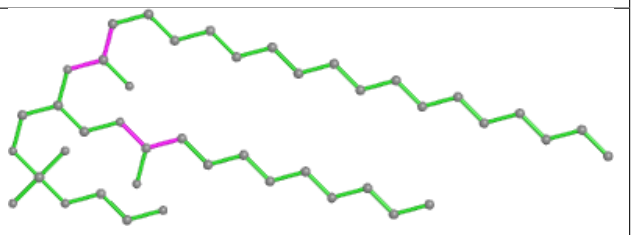


Rings

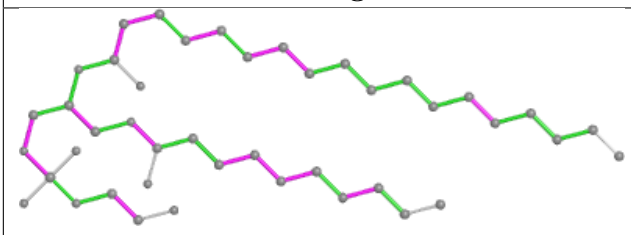
Ligand 3PE M 601



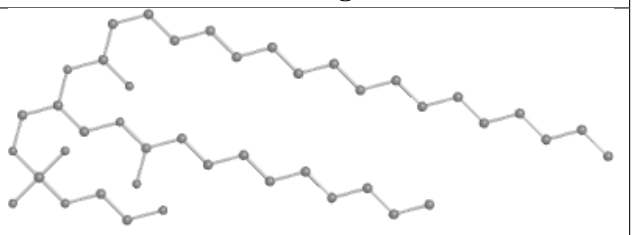
Bond lengths



Bond angles

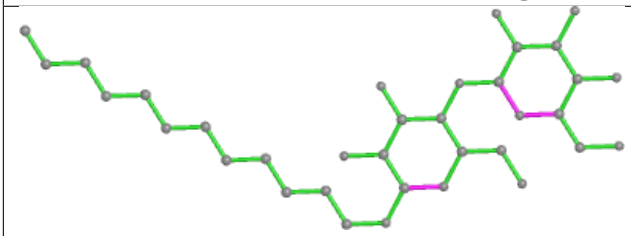


Torsions

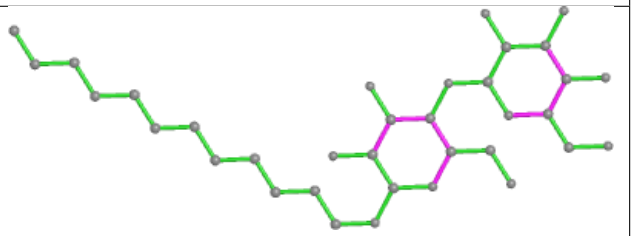


Rings

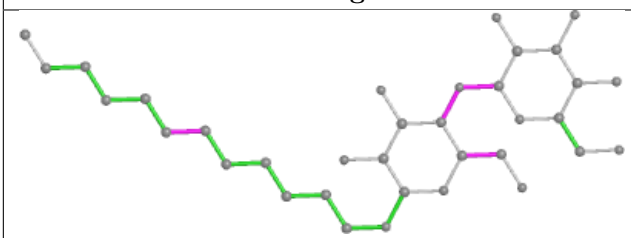
Ligand LMT d 1203



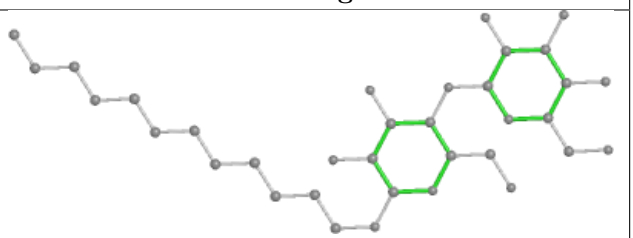
Bond lengths



Bond angles

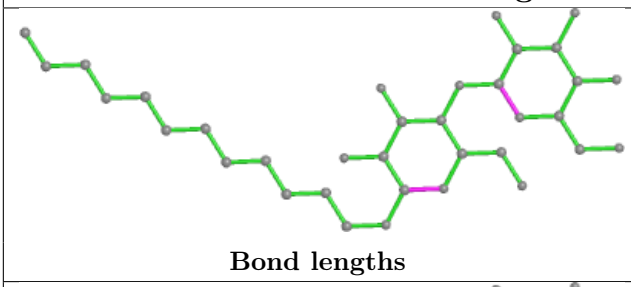


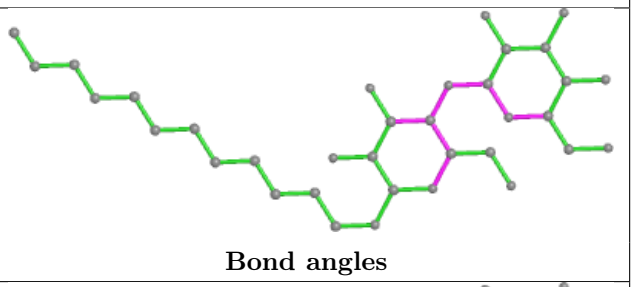
Torsions

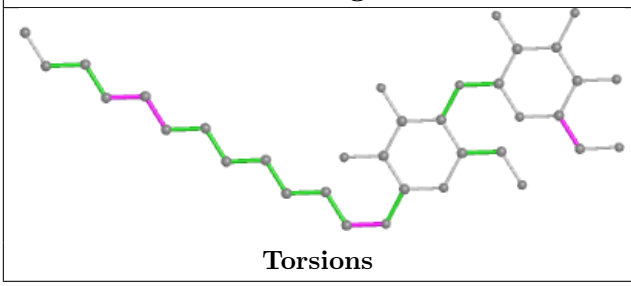


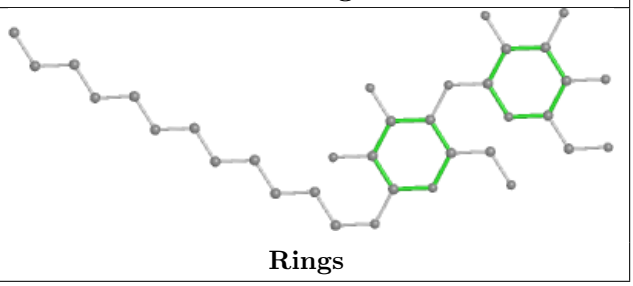
Rings

Ligand LMT h 1003

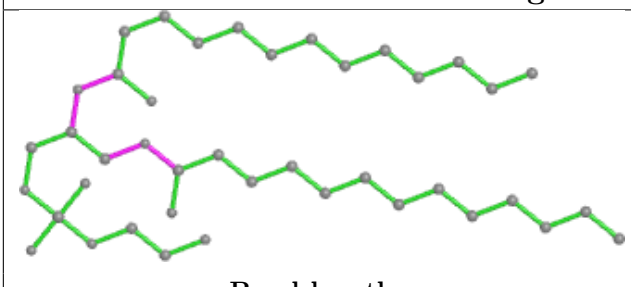

Bond lengths

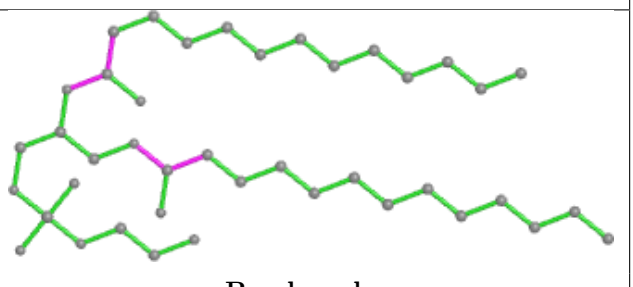

Bond angles

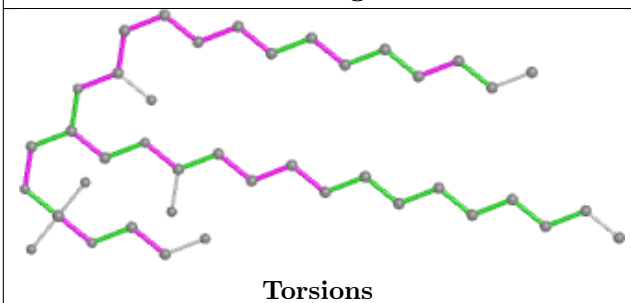

Torsions

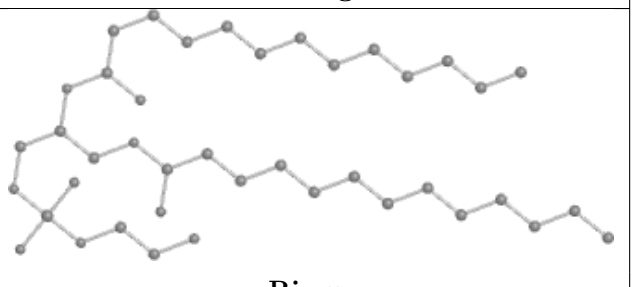

Rings

Ligand 3PE N 902

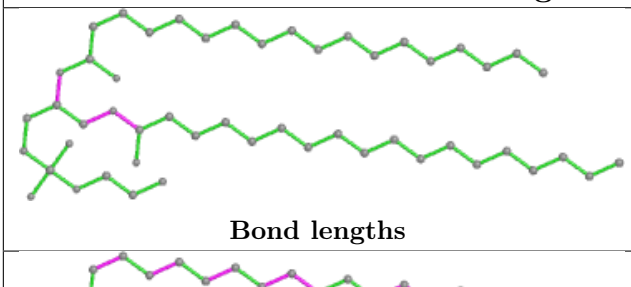

Bond lengths

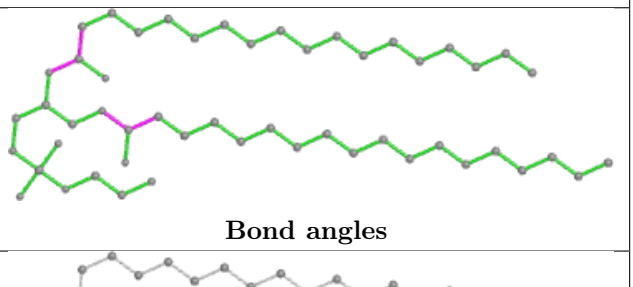

Bond angles

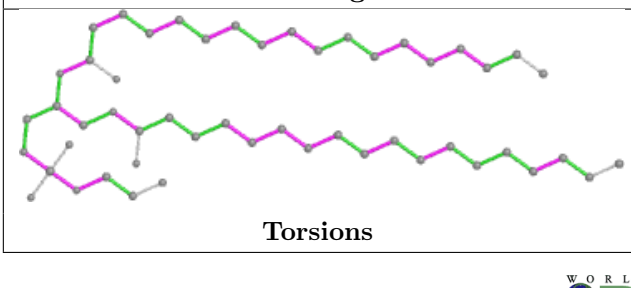

Torsions

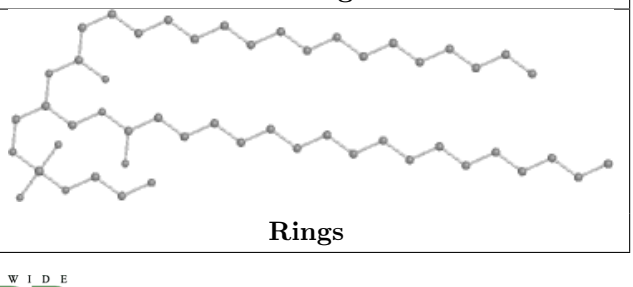

Rings

Ligand 3PE I 201

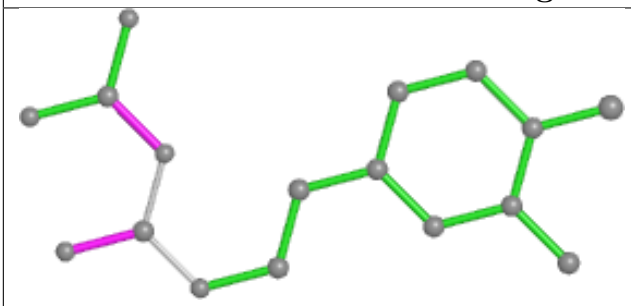

Bond lengths


Bond angles

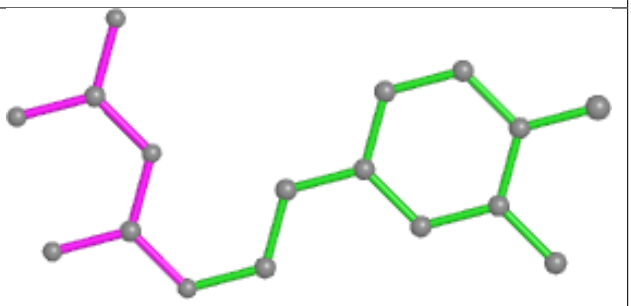

Torsions


Rings

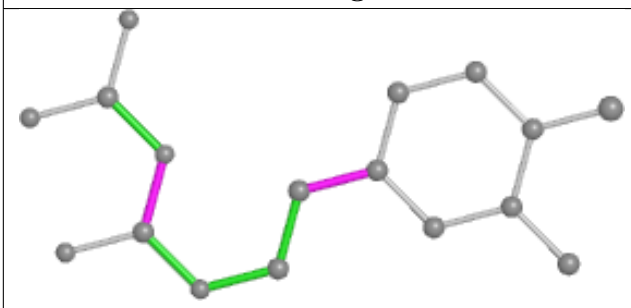
Ligand I49 H 602



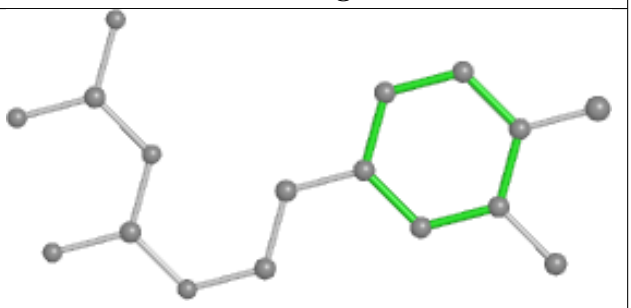
Bond lengths



Bond angles

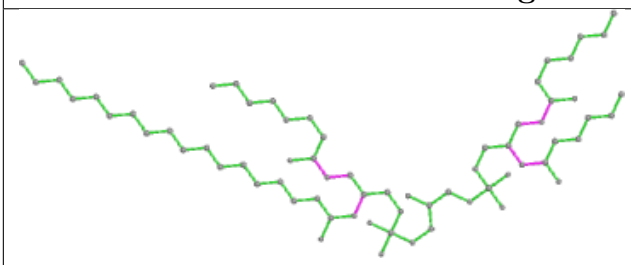


Torsions

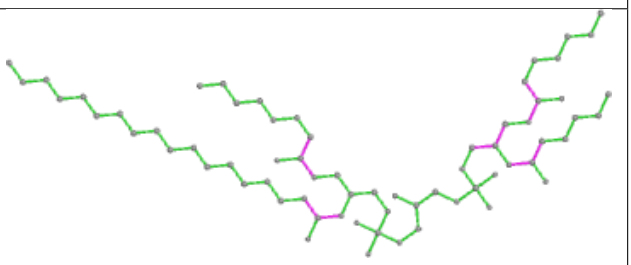


Rings

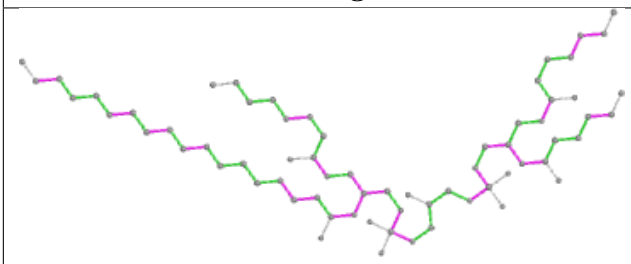
Ligand CDL h 1001



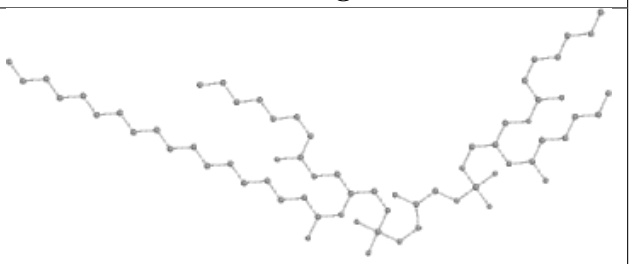
Bond lengths



Bond angles

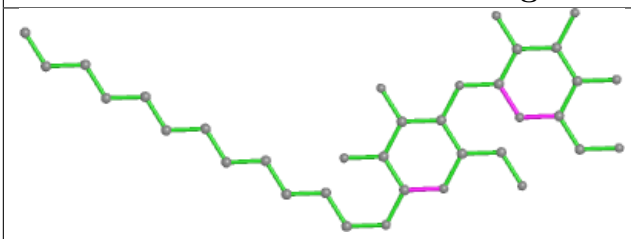


Torsions

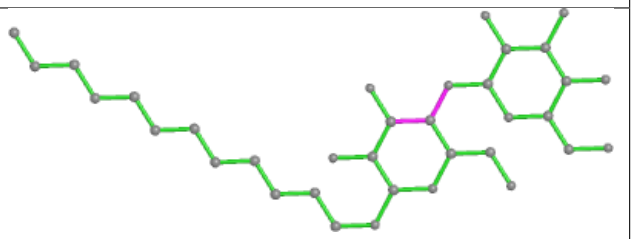


Rings

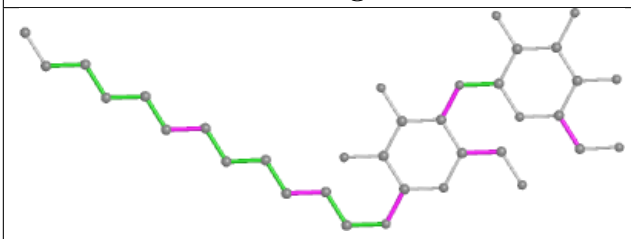
Ligand LMT K 501



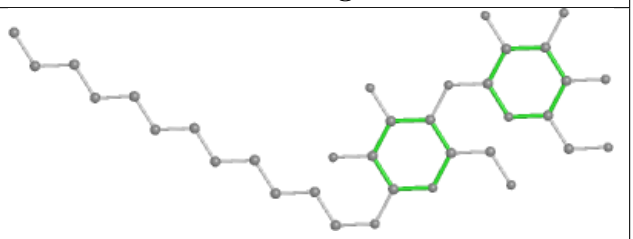
Bond lengths



Bond angles

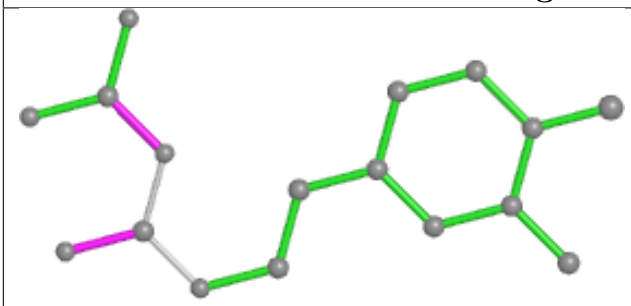


Torsions

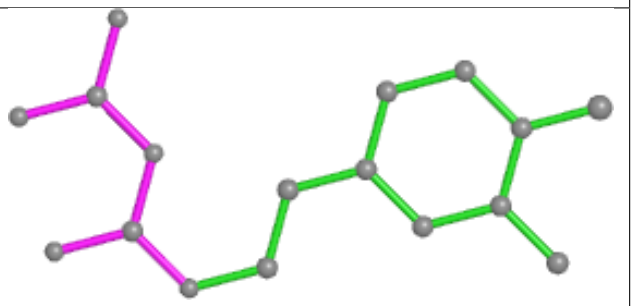


Rings

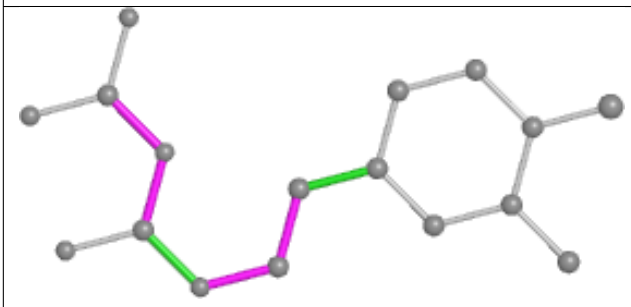
Ligand I49 N 903



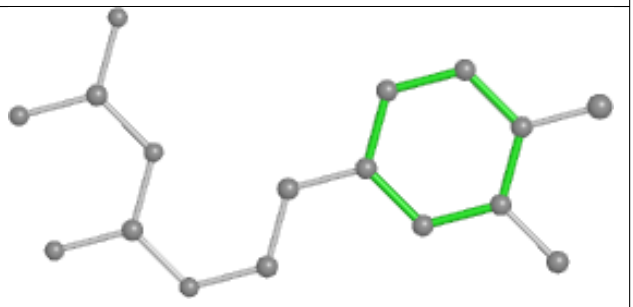
Bond lengths



Bond angles

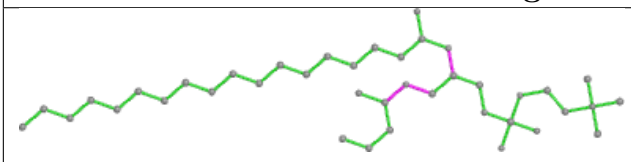


Torsions

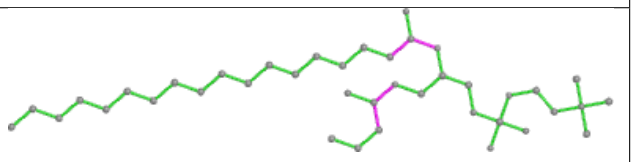


Rings

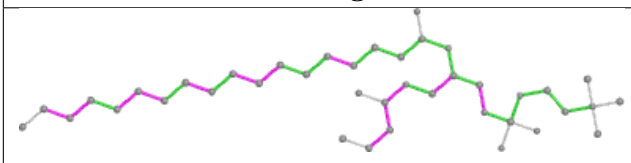
Ligand PC1 M 603



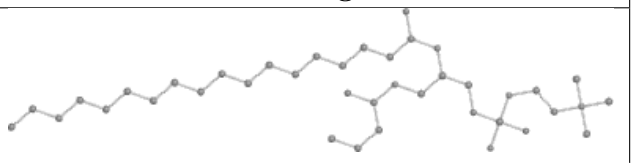
Bond lengths



Bond angles

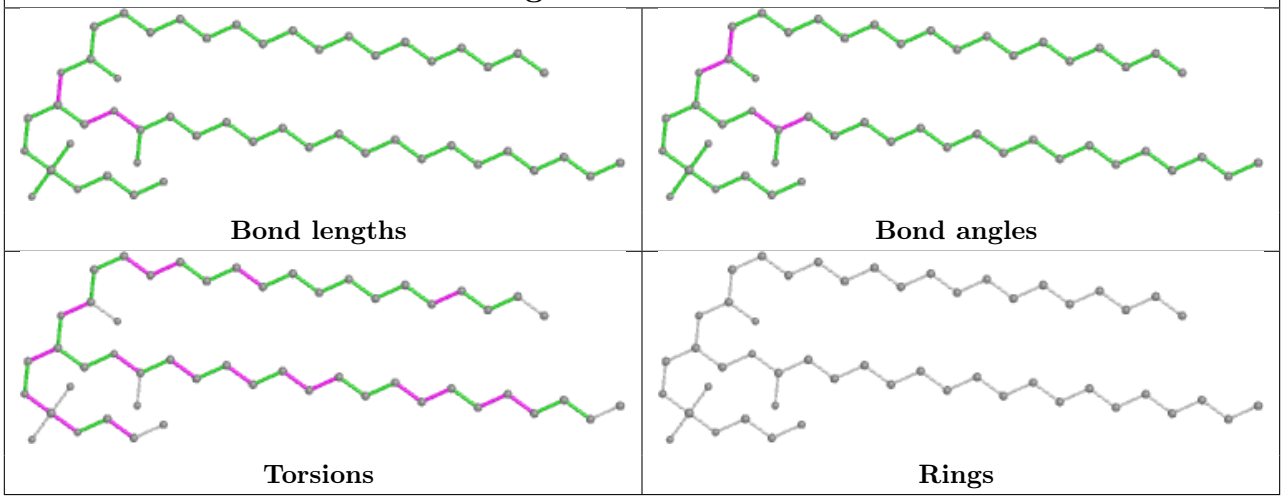


Torsions

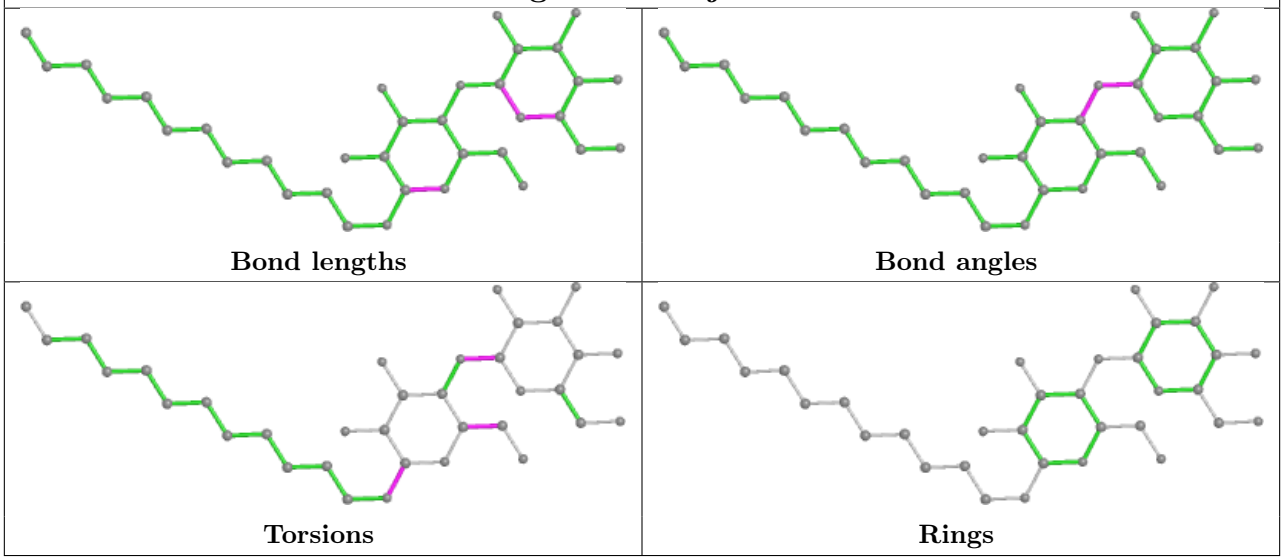


Rings

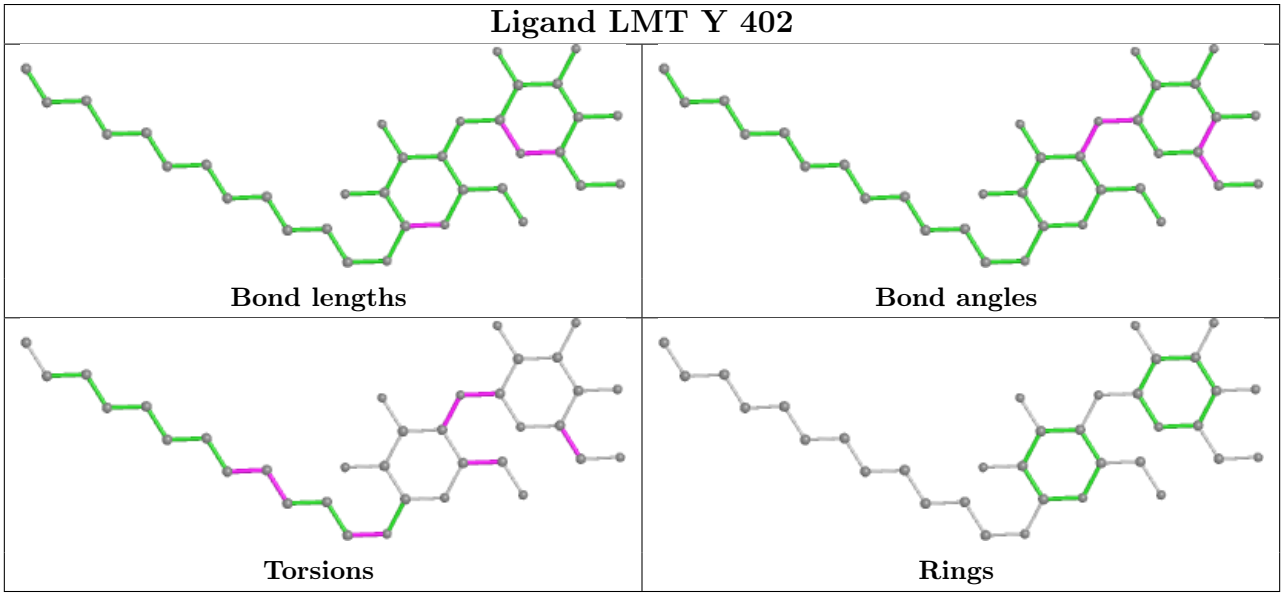
Ligand 3PE M 602



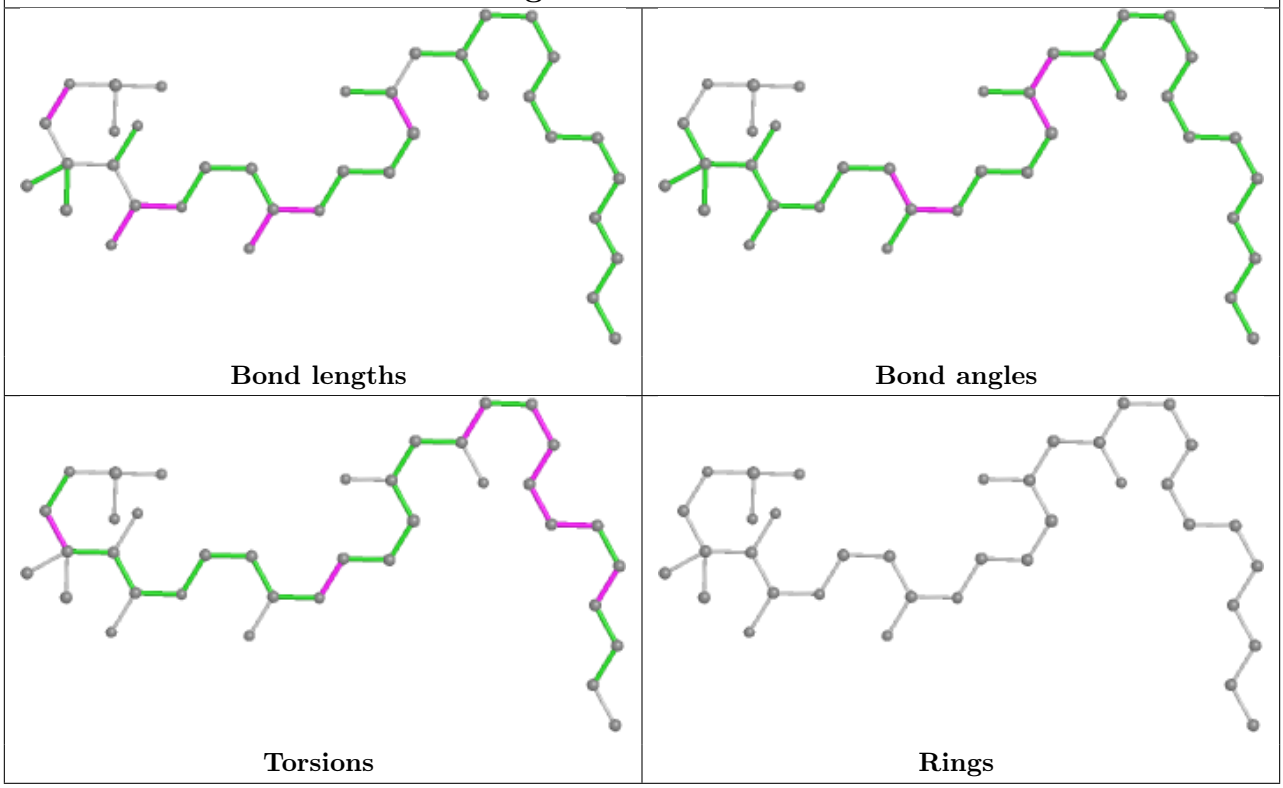
Ligand LMT j 101



Ligand LMT Y 402



Ligand EHZ U 101



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.

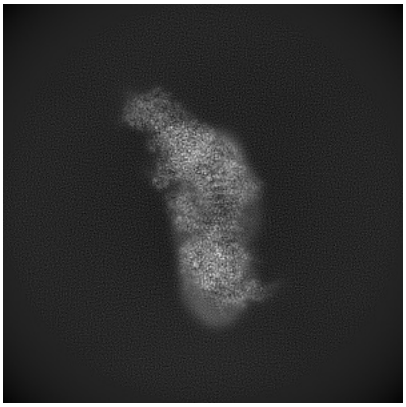
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14292. These allow visual inspection of the internal detail of the map and identification of artifacts.

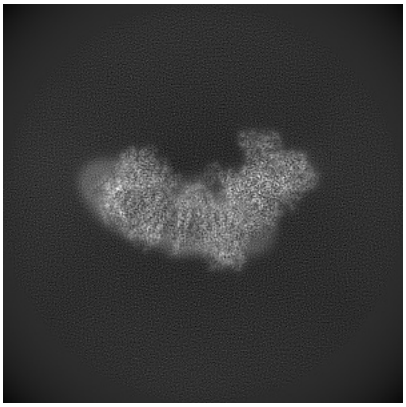
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

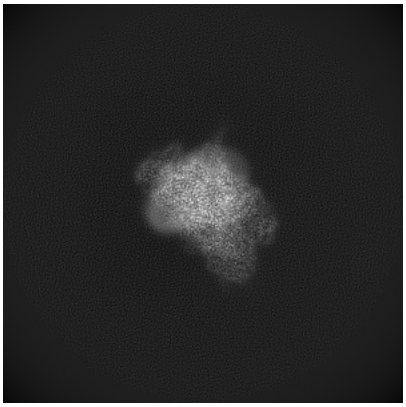
6.1.1 Primary map



X



Y

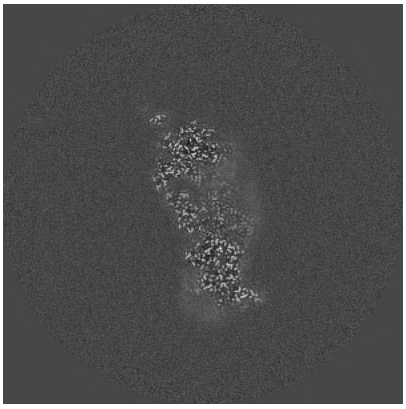


Z

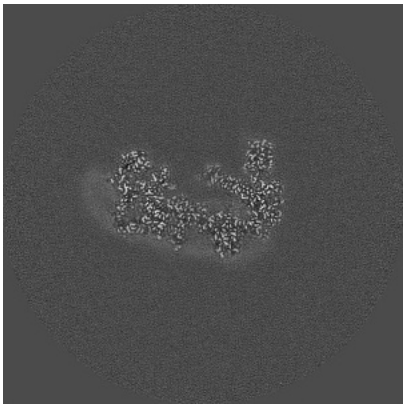
The images above show the map projected in three orthogonal directions.

6.2 Central slices

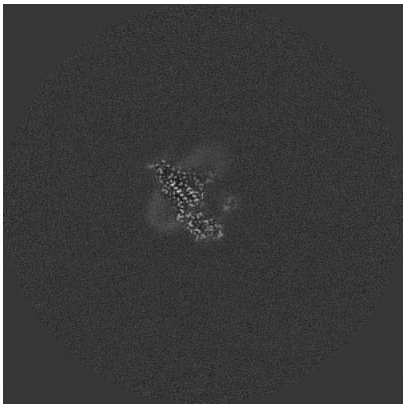
6.2.1 Primary map



X Index: 330



Y Index: 330

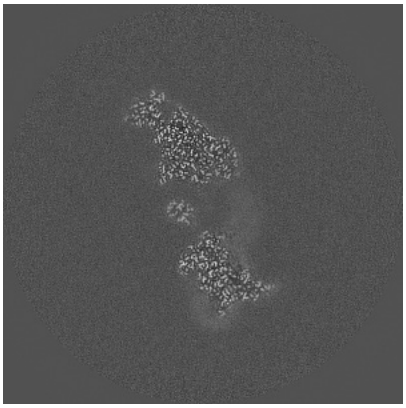


Z Index: 330

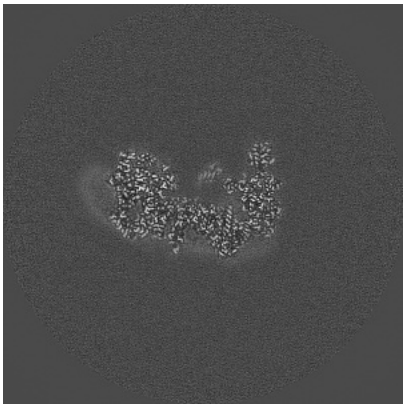
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

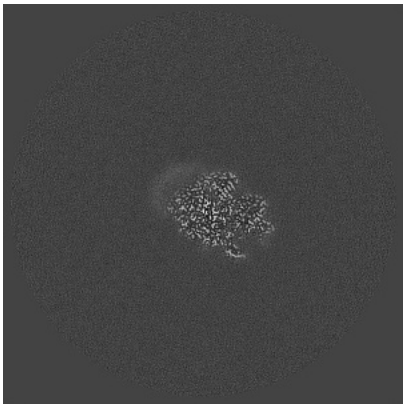
6.3.1 Primary map



X Index: 357



Y Index: 337



Z Index: 422

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

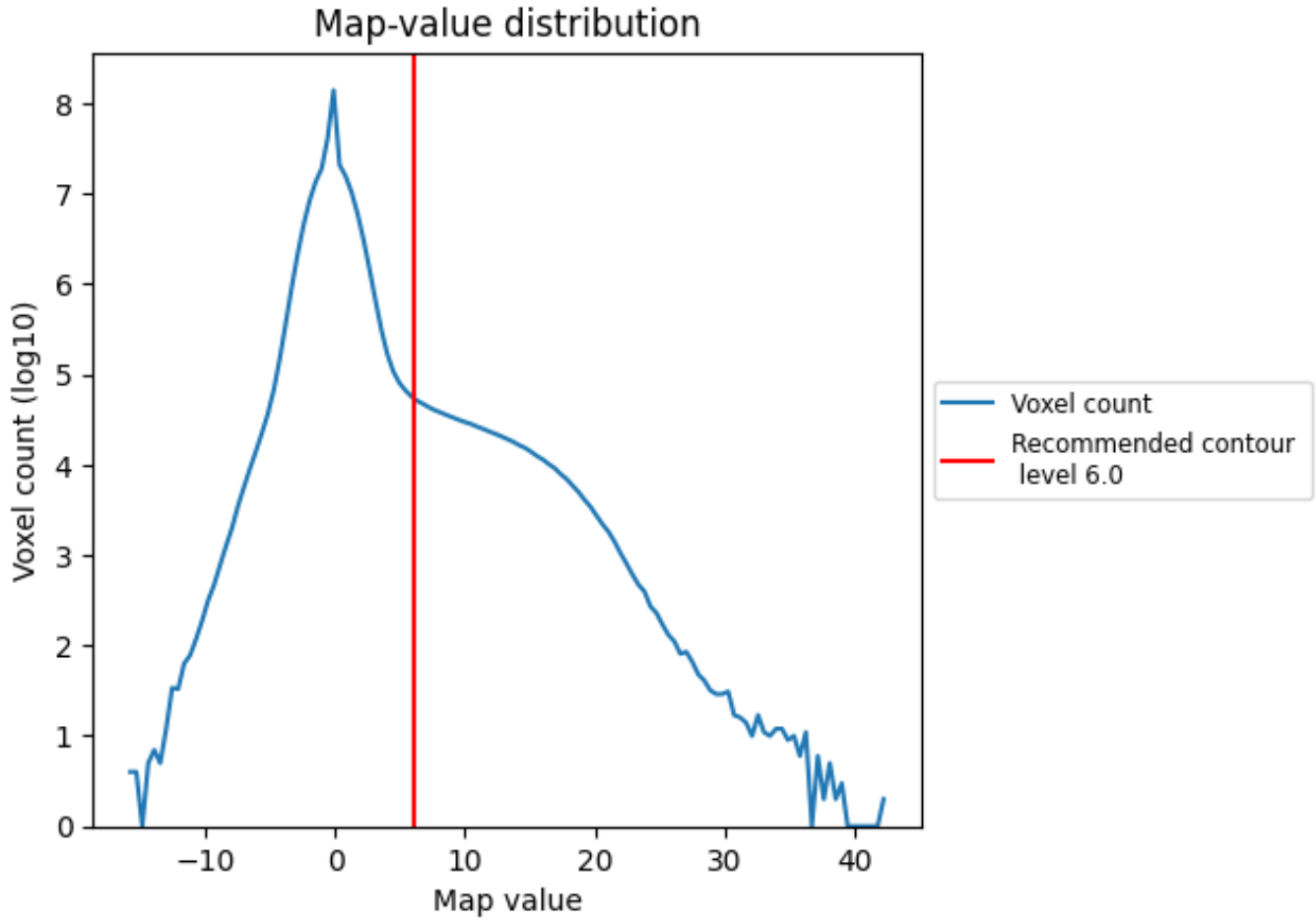
6.5 Mask visualisation (i)

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

7 Map analysis

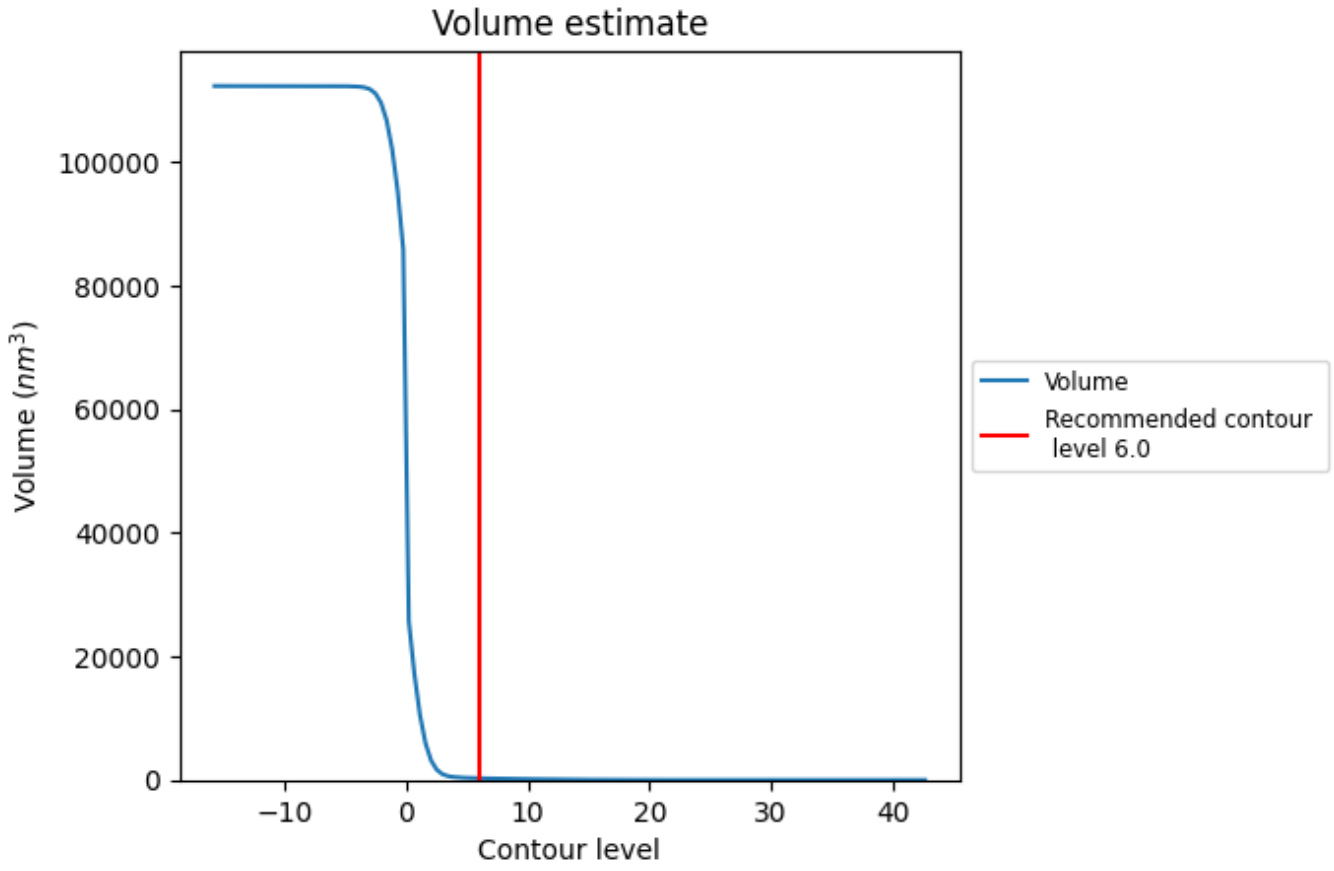
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

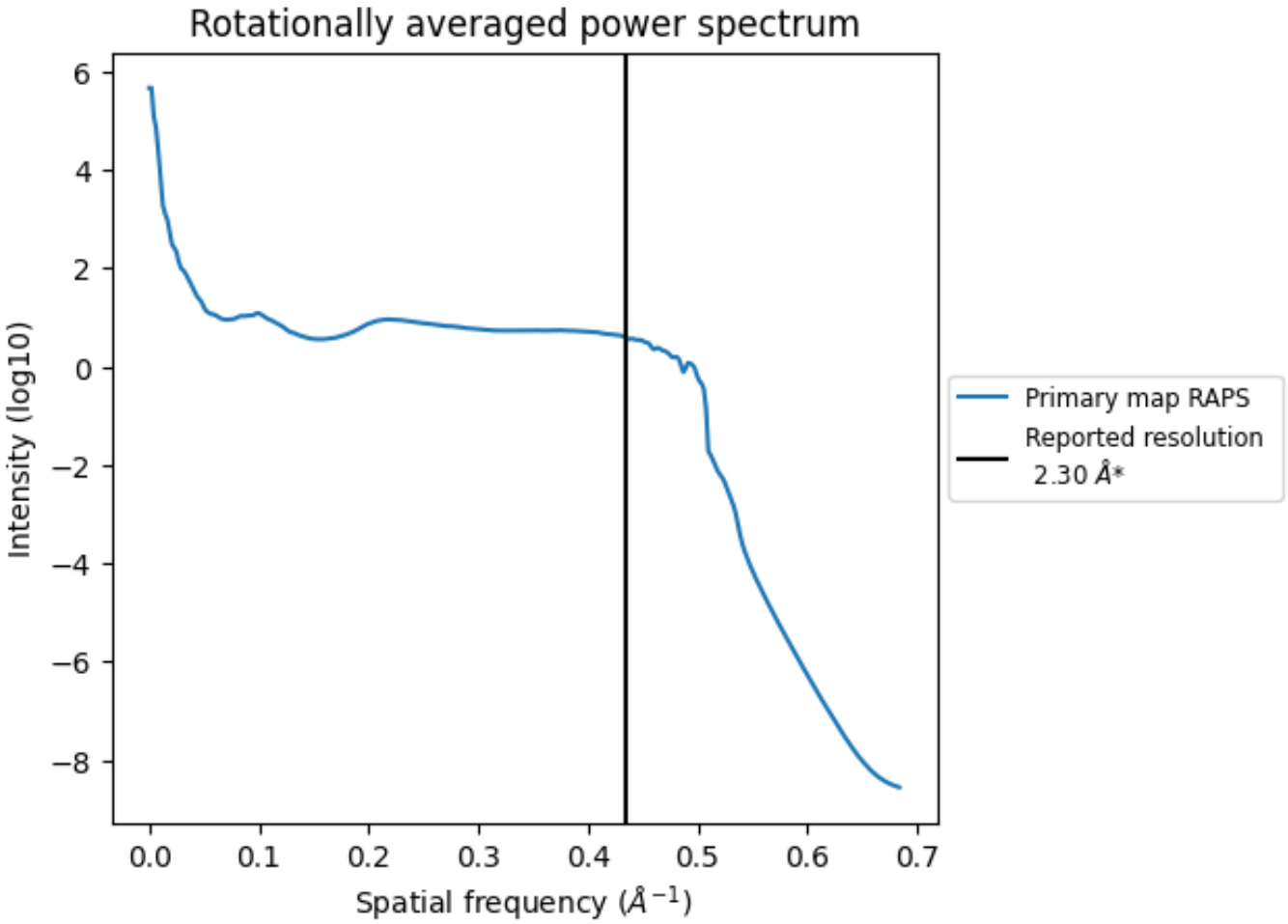
7.2 Volume estimate



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 249 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 0.435 Å^{-1}

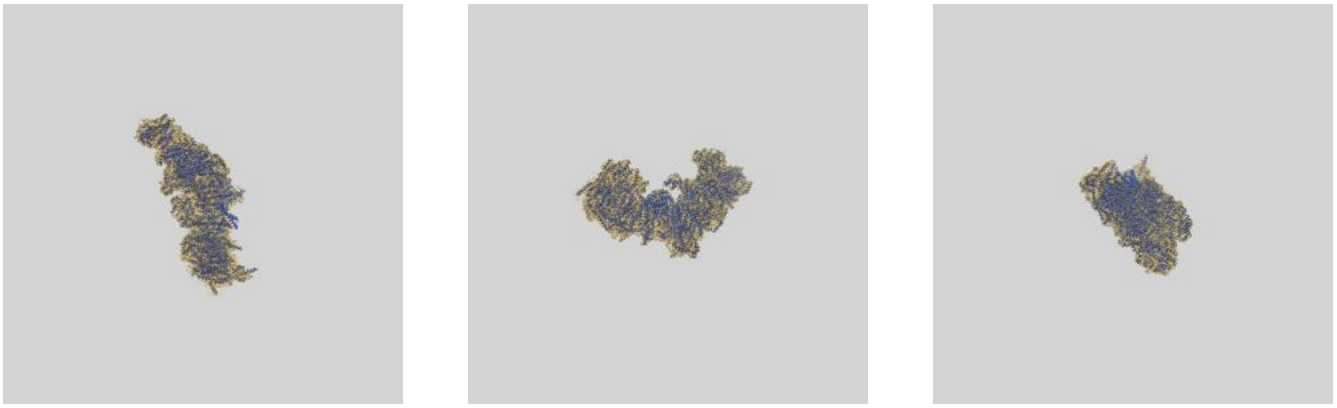
8 Fourier-Shell correlation

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14292 and PDB model 7R4C. Per-residue inclusion information can be found in section 3 on page 23.

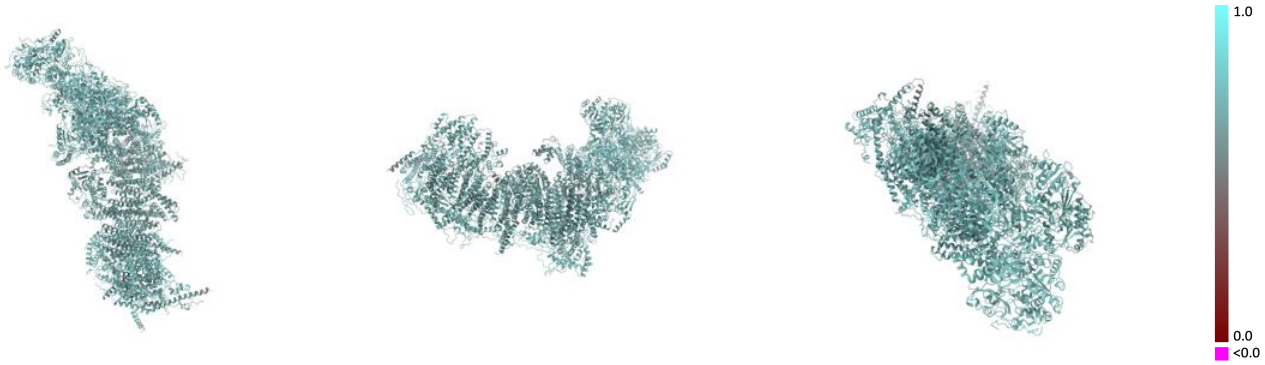
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

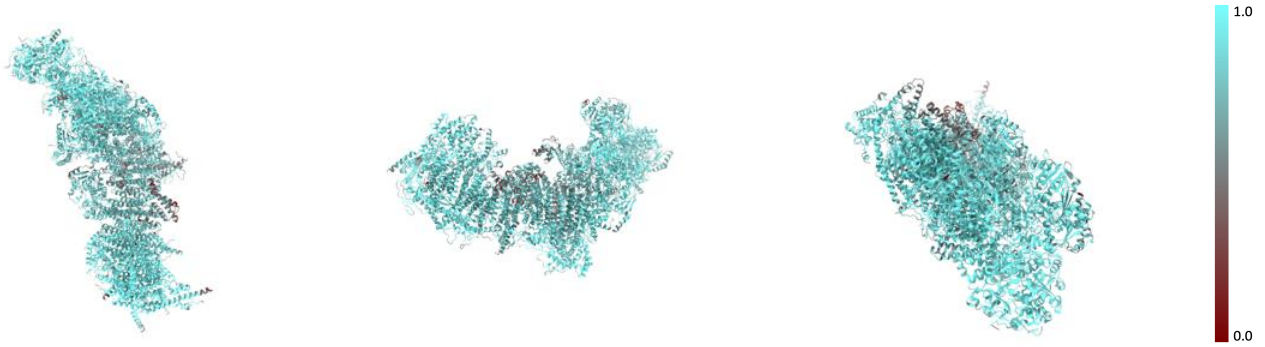
9.2 Q-score mapped to coordinate model (i)



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.

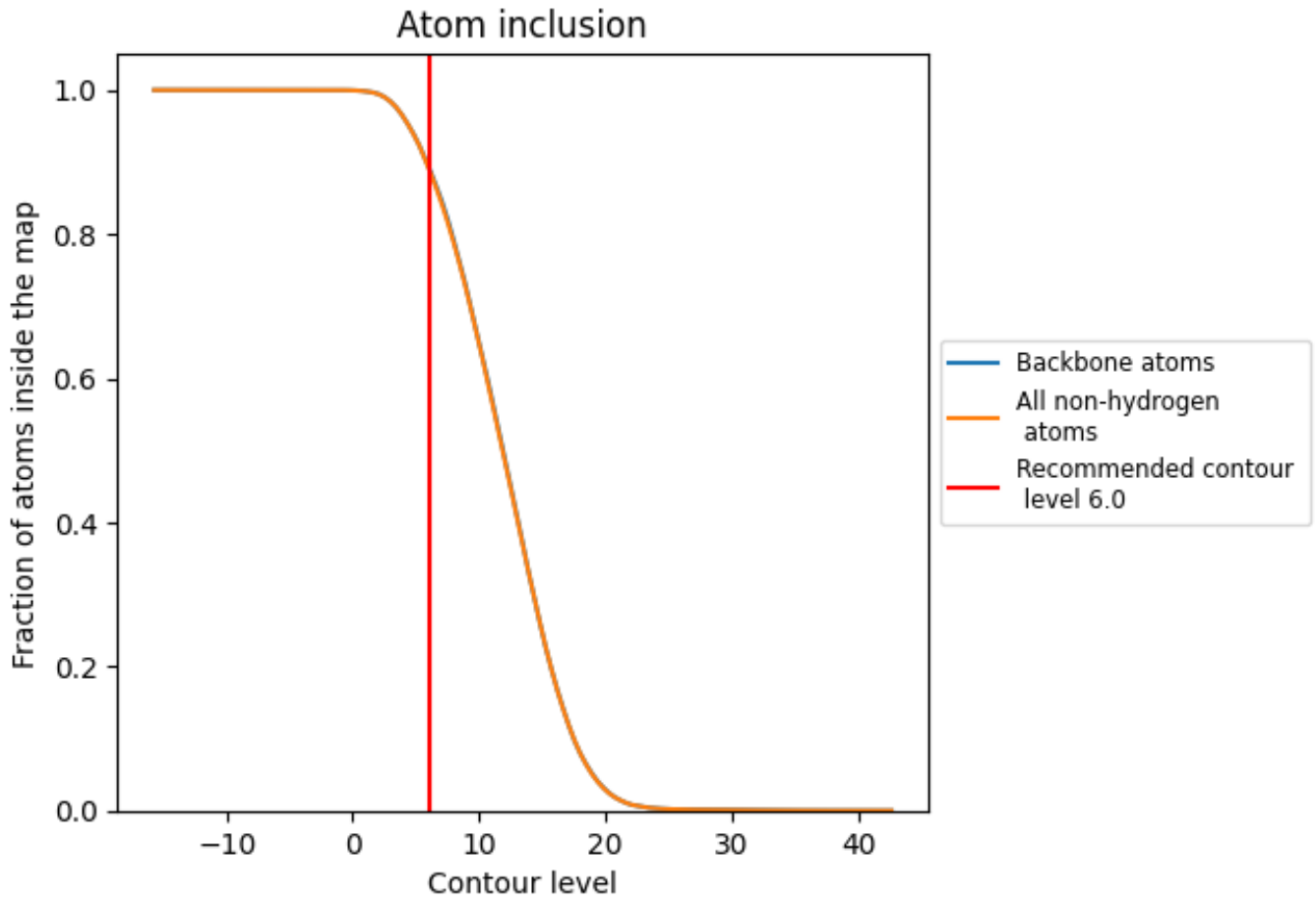
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8919	0.6990
A	0.8257	0.6800
B	0.9130	0.7240
C	0.9658	0.7420
D	0.9371	0.7370
E	0.9061	0.6980
F	0.9391	0.7120
G	0.9268	0.7190
H	0.9290	0.7100
I	0.9673	0.7450
J	0.7690	0.6690
K	0.9036	0.7060
L	0.9217	0.6940
M	0.9663	0.7170
N	0.9540	0.7170
O	0.8564	0.6700
P	0.8707	0.7000
Q	0.9114	0.7260
R	0.8962	0.7220
S	0.8554	0.6760
T	0.6165	0.6260
U	0.9326	0.6940
V	0.8783	0.7050
W	0.8811	0.7040
X	0.8671	0.6810
Y	0.4747	0.6290
Z	0.8501	0.6820
a	0.9519	0.7060
b	0.8317	0.6560
c	0.7727	0.6550
d	0.8290	0.6800
e	0.8140	0.6700
f	0.8097	0.6620
g	0.8802	0.6880
h	0.8905	0.6910

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Chain	Atom inclusion	Q-score
i	0.8859	0.6700
j	0.8683	0.6590
k	0.8875	0.6610
l	0.9033	0.6820
m	0.8804	0.6780
n	0.9218	0.6920
o	0.8900	0.6630
p	0.9165	0.6910
q	0.8693	0.7070
r	0.9084	0.7130
s	0.8983	0.6990