wwPDB EM Validation Summary Report (i)

Feb 4, 2023 – 09:04 am GMT

PDB ID	:	7R4G
EMDB ID	:	EMD-14307
Title	:	Bovine complex I in the presence of IM1761092, slack class ii (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

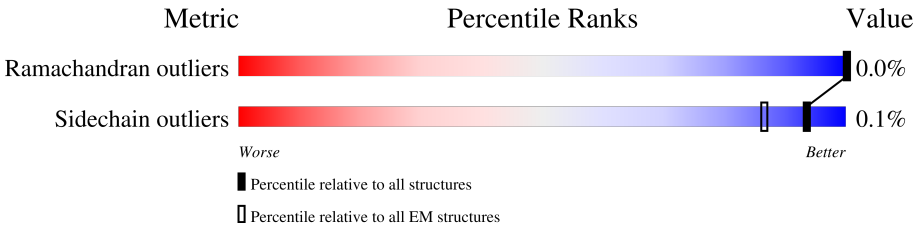
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	6%, 80%, 19%
2	B	216	70%, 29%
3	C	266	77%, 23%
4	D	463	83%, 17%
5	E	249	86%, 14%
6	F	464	93%, 7%
7	G	727	94%, 5%
8	H	318	98%
9	I	212	83%, 17%

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Mol	Chain	Length	Quality of chain
10	J	175	7% 73% 27%
11	K	98	99%
12	L	606	90% 10%
13	M	459	100%
14	N	347	5% 100%
15	O	343	39% 93% 7%
16	P	380	76% 24%
17	Q	175	71% 29%
18	R	124	76% 24%
19	S	99	83% 17%
20	T	156	23% 48% 51%
20	U	156	54% 46%
21	V	116	97%
22	W	128	5% 89% 11%
23	X	172	99%
24	Y	141	6% 14% 86%
25	Z	144	15% 97%
26	a	70	99%
27	b	84	7% 99%
28	c	76	11% 63% 37%
29	d	120	93% 7%
30	e	106	8% 90% 10%
31	f	57	9% 91% 9%
32	g	154	56% 43%
33	h	189	73% 27%

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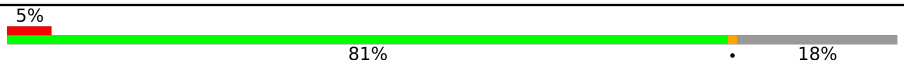
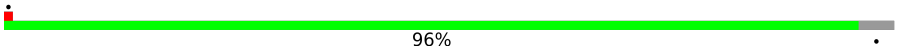
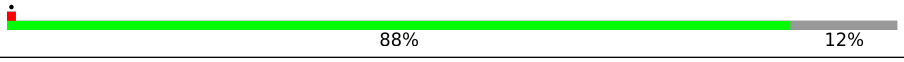
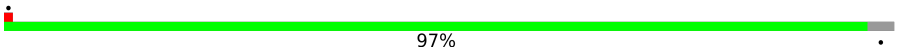
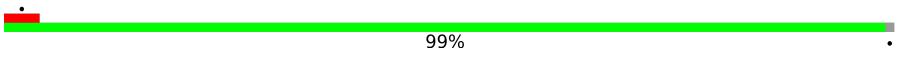
Mol	Chain	Length	Quality of chain
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 65153 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	93	748	513	108	122	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	386	3095	1973	536	562	24	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3310	2085	591	614	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	313	Total	C	N	O	S	0	0
			2468	1655	379	411	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	127	Total	C	N	O	S	0	0
			946	635	135	167	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	547	Total	C	N	O	S	0	0
			4318	2869	665	743	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2424	565	604	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	288	Total	C	N	O	S	0	0
			2289	1464	413	407	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	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			663	416	124	121	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	20	Total	C	N	O	S	0	0
			154	102	25	26	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	140	Total	C	N	O	S	0	0
			1145	736	200	200	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	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	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	52	Total	C	N	O	S	0	0
			451	296	79	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	88	Total	C	N	O	S	0	0
			733	474	122	133	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	104	Total	C	N	O	S	0	0
			892	588	151	152	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	108	Total	C	N	O	0	0
			908	580	161	167		

- 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	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			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	143	Total	C	N	O	S	0	0
			1192	768	214	206	4		

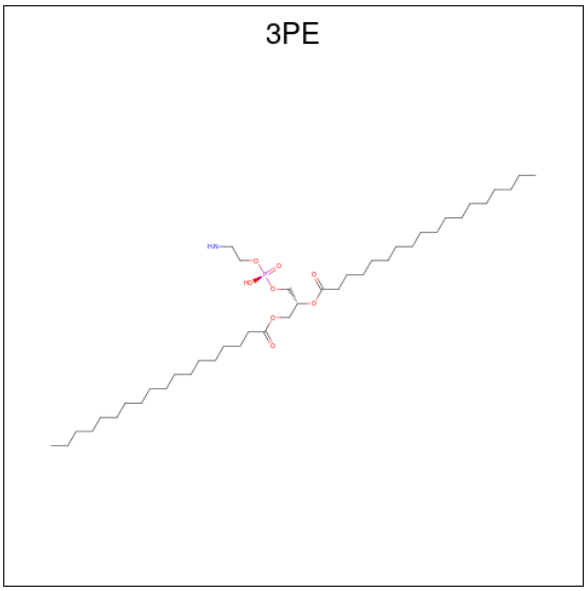
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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	43	Total	C	N	O	S	0	0
			364	228	65	70	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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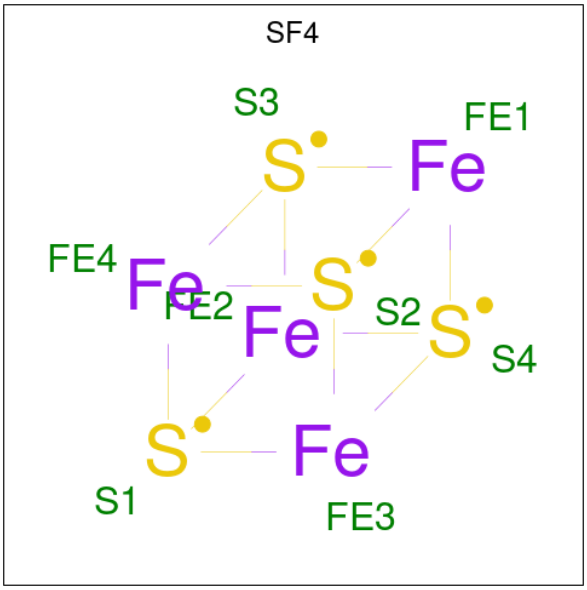
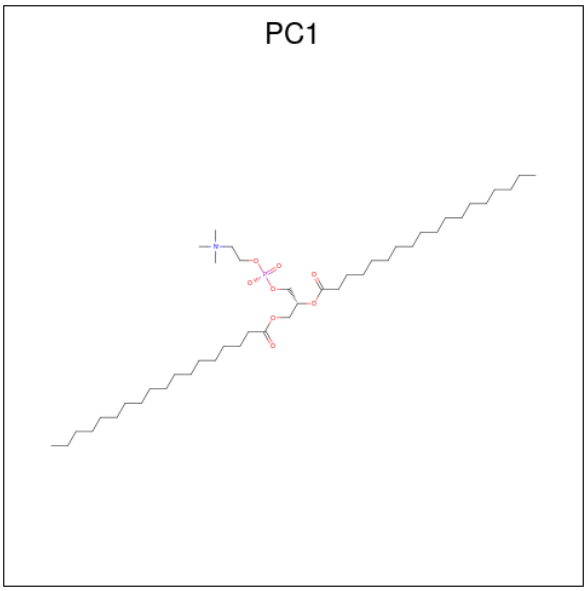
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	O	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



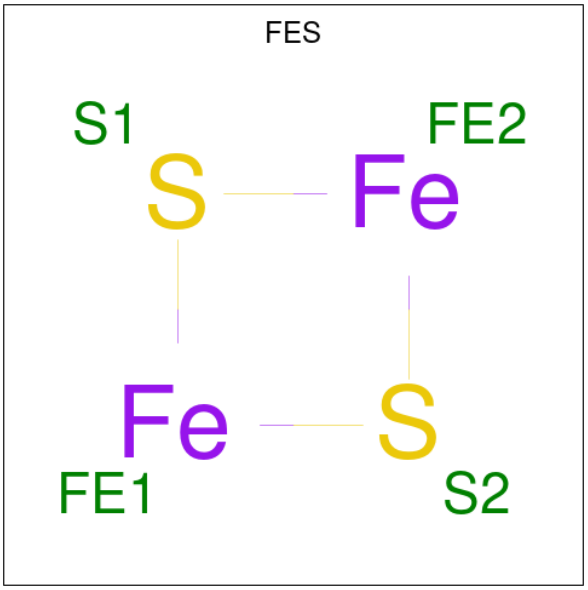
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

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



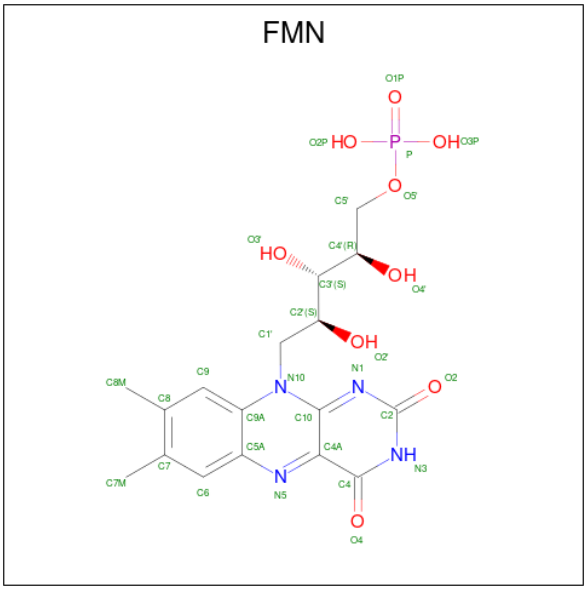
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	M	1	Total	C	N	O	P	0
			49	39	1	8	1	

- 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	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

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

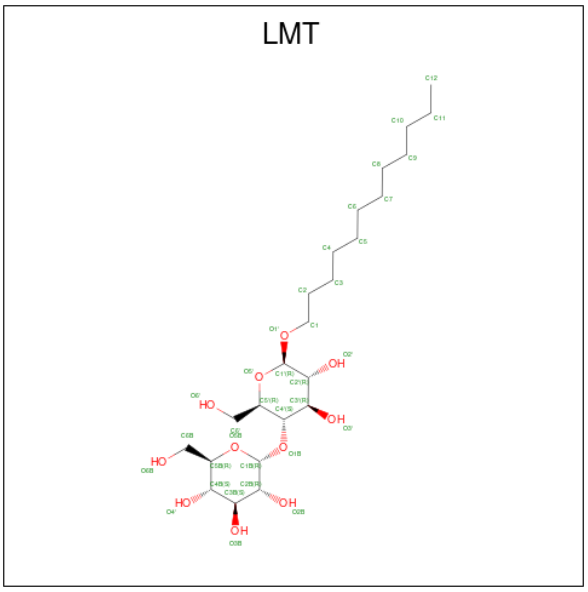


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

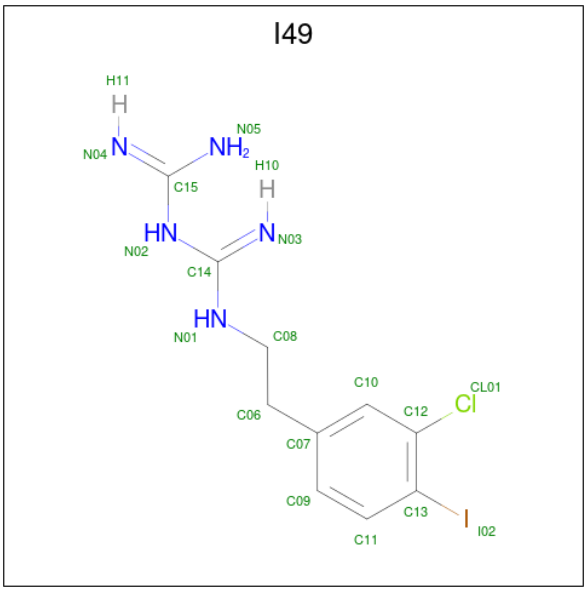
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



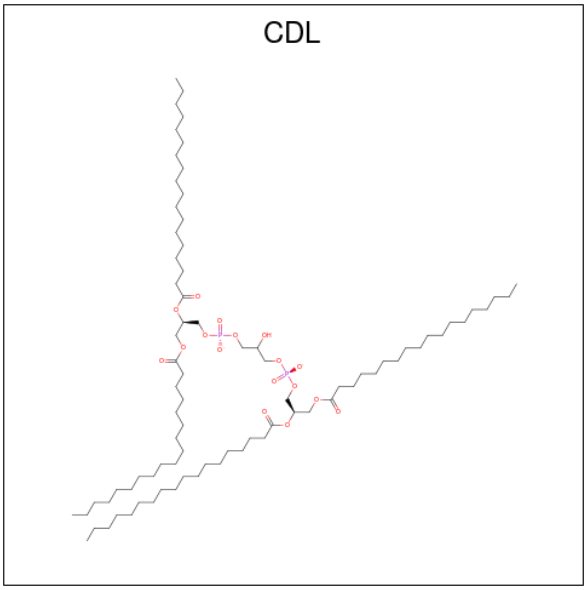
Mol	Chain	Residues	Atoms	AltConf
51	H	1	Total C O 35 24 11	0
51	J	1	Total C O 35 24 11	0
51	K	1	Total C O 35 24 11	0
51	L	1	Total C O 35 24 11	0
51	N	1	Total C O 35 24 11	0
51	b	1	Total C O 35 24 11	0
51	g	1	Total C O 35 24 11	0
51	h	1	Total C O 35 24 11	0
51	l	1	Total C O 35 24 11	0
51	p	1	Total C O 35 24 11	0

- 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
			69	50	17	2	
53	N	1	Total	C	O	P	0
			67	48	17	2	

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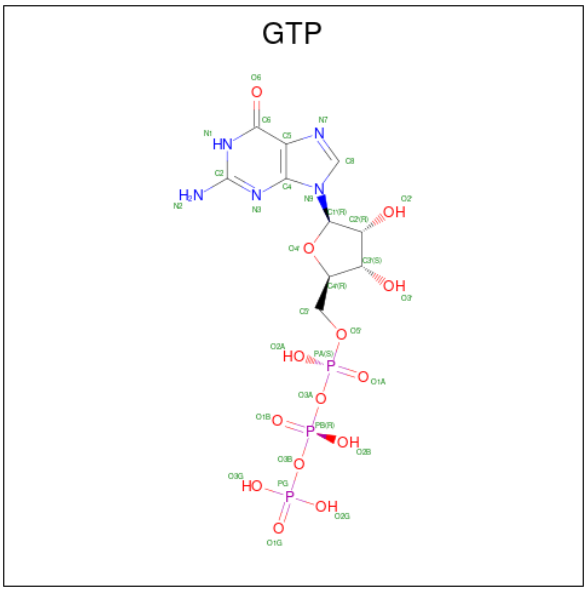
Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			65	46	17	2	
53	X	1	Total	C	O	P	0
			52	33	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			76	57	17	2	

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

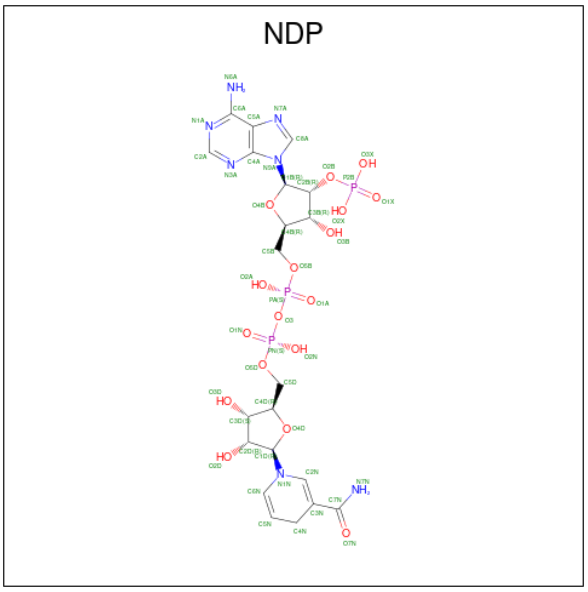


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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: $C_{21}H_{30}N_7O_{17}P_3$).

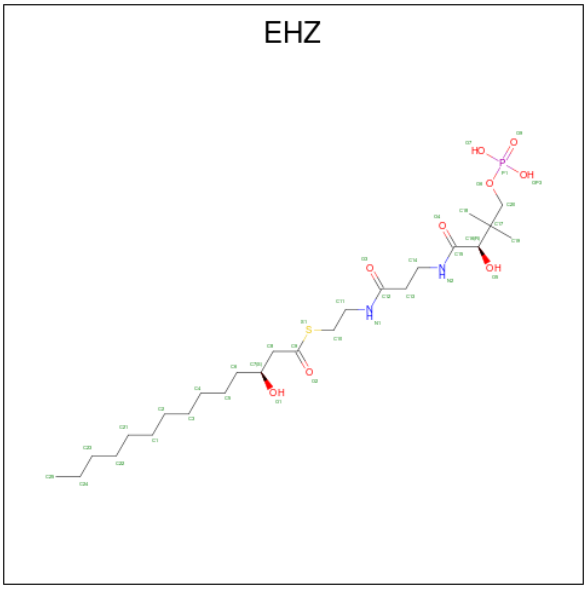


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

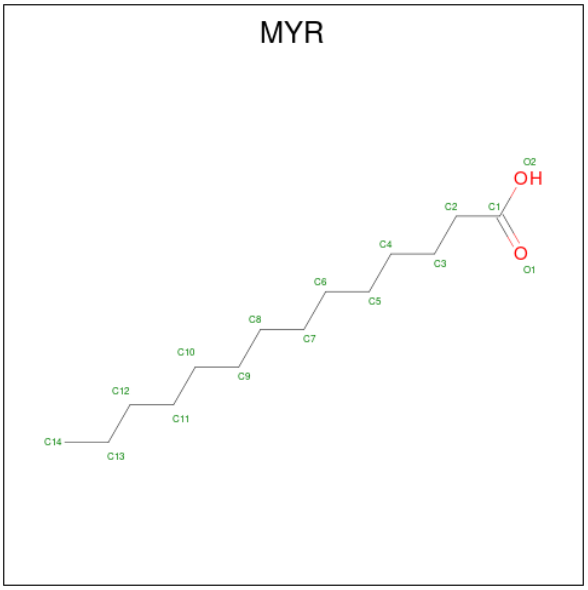
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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 37 25 2 8 1 1	0
58	U	1	Total C N O P S 37 25 2 8 1 1	0

- 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 15 14 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	6	Total O 6 6	0
60	B	36	Total O 36 36	0
60	C	55	Total O 55 55	0
60	D	104	Total O 104 104	0
60	E	8	Total O 8 8	0
60	F	38	Total O 38 38	0
60	G	139	Total O 139 139	0

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Mol	Chain	Residues	Atoms	AltConf
60	H	25	Total O 25 25	0
60	I	76	Total O 76 76	0
60	J	1	Total O 1 1	0
60	K	1	Total O 1 1	0
60	L	32	Total O 32 32	0
60	M	25	Total O 25 25	0
60	N	7	Total O 7 7	0
60	P	25	Total O 25 25	0
60	Q	54	Total O 54 54	0
60	R	25	Total O 25 25	0
60	U	5	Total O 5 5	0
60	V	3	Total O 3 3	0
60	W	7	Total O 7 7	0
60	X	12	Total O 12 12	0
60	Y	1	Total O 1 1	0
60	Z	13	Total O 13 13	0
60	a	4	Total O 4 4	0
60	b	5	Total O 5 5	0
60	d	2	Total O 2 2	0
60	e	4	Total O 4 4	0
60	f	6	Total O 6 6	0

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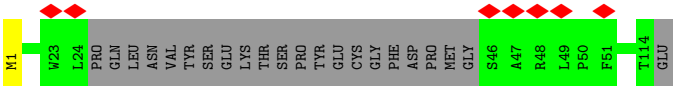
Mol	Chain	Residues	Atoms	AltConf
60	g	5	Total O 5 5	0
60	h	9	Total O 9 9	0
60	i	1	Total O 1 1	0
60	j	3	Total O 3 3	0
60	k	4	Total O 4 4	0
60	l	11	Total O 11 11	0
60	m	9	Total O 9 9	0
60	n	16	Total O 16 16	0
60	o	5	Total O 5 5	0
60	p	18	Total O 18 18	0
60	q	22	Total O 22 22	0
60	r	26	Total O 26 26	0
60	s	3	Total O 3 3	0

3 Residue-property plots (i)

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

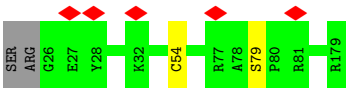
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



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

Chain B:

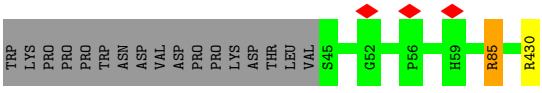


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

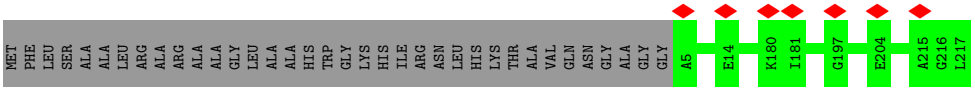
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



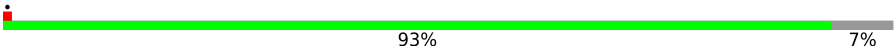
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

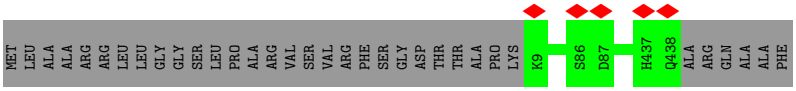
Chain E:



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

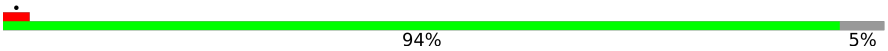
Chain F:

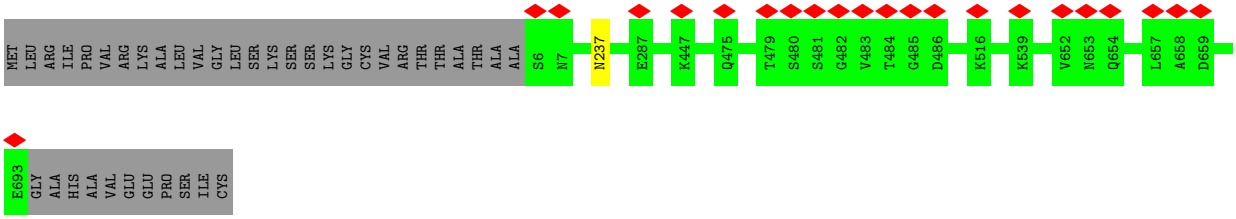




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

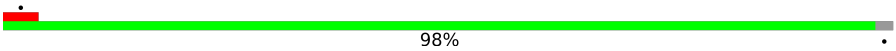
Chain G:

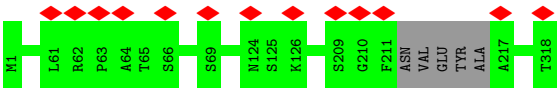




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

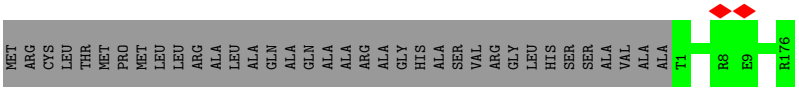
Chain H:





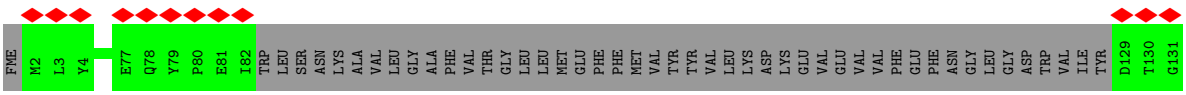
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



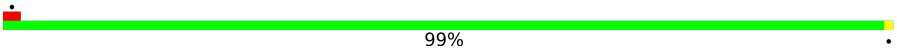
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



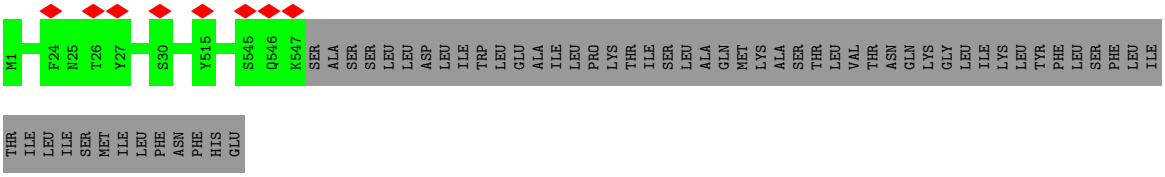
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



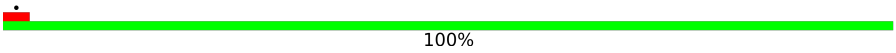
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

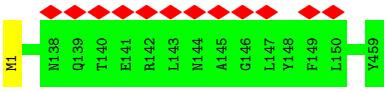
Chain L:



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

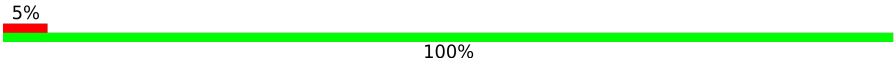
Chain M:

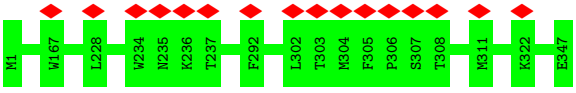




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

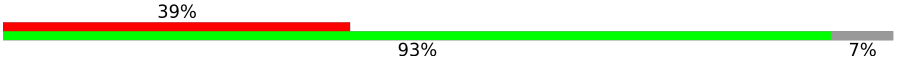
Chain N:

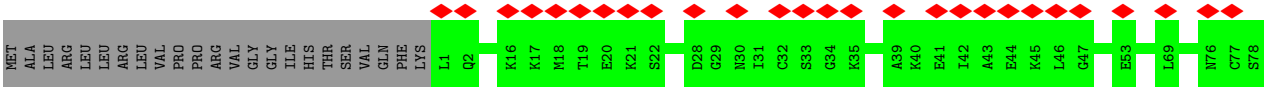


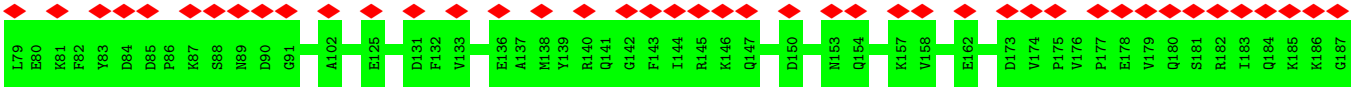


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:

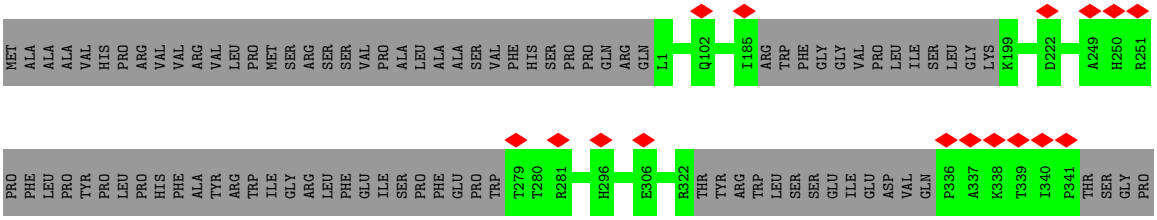






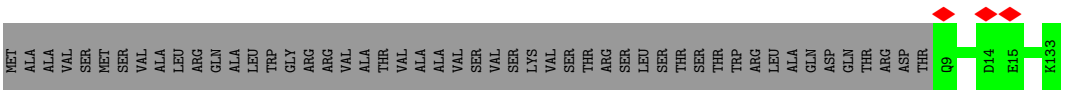
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



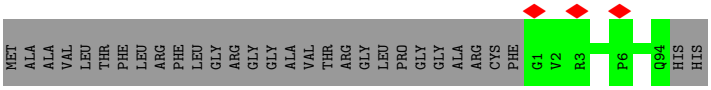
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



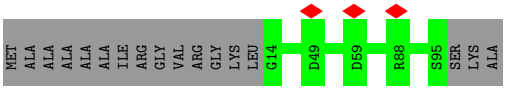
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



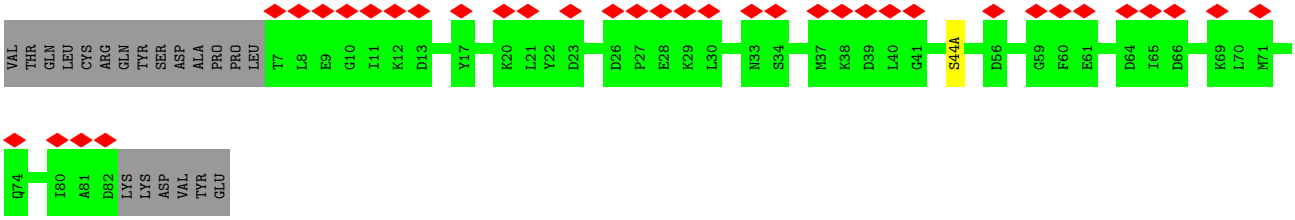
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:

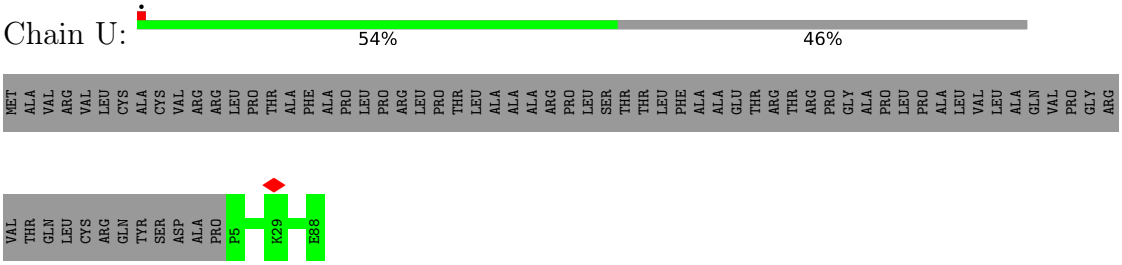


• Molecule 20: Acyl carrier protein, mitochondrial

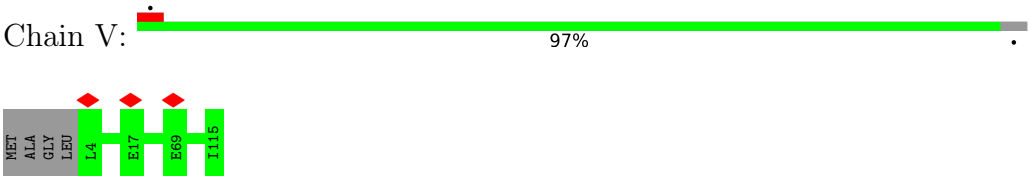
Chain T:



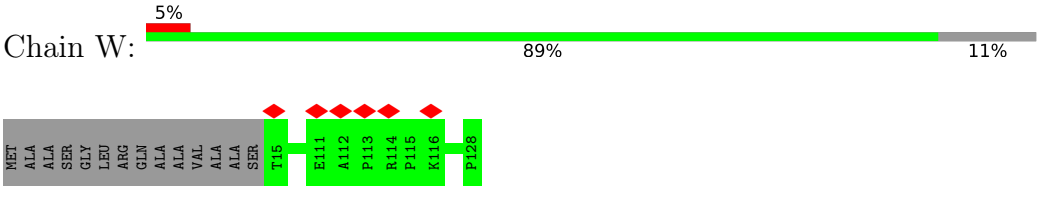
• Molecule 20: Acyl carrier protein, mitochondrial



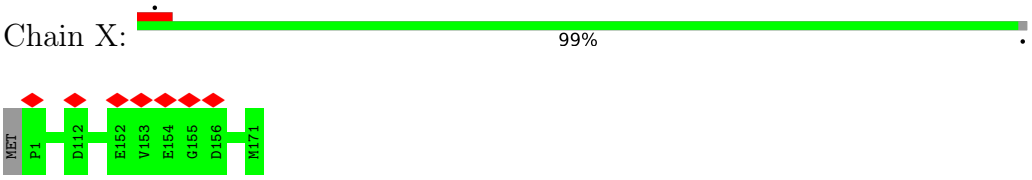
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



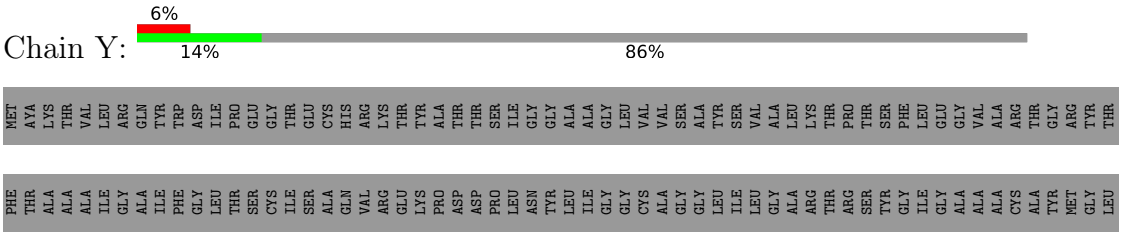
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

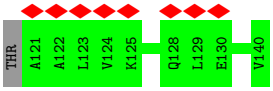


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



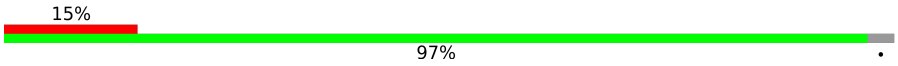
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

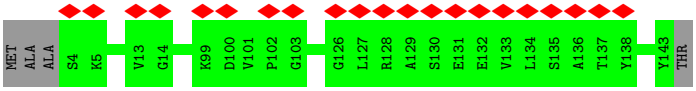




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

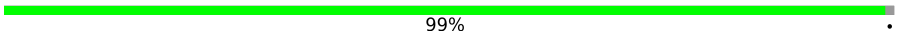
Chain Z:





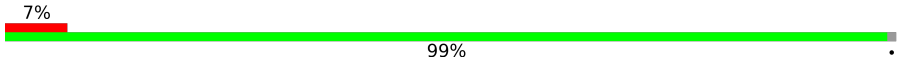
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

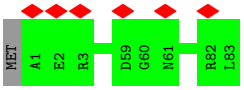
Chain a:



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

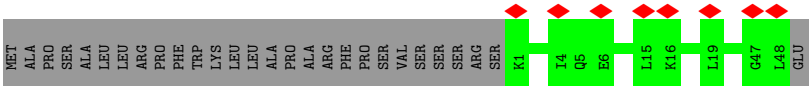
Chain b:





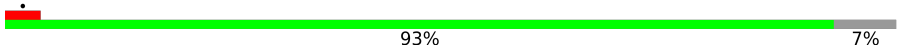
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

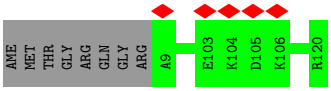
Chain c:



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

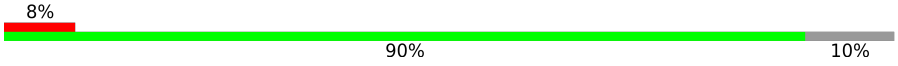
Chain d:

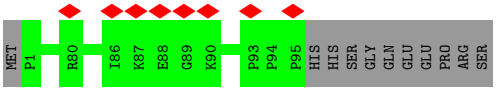




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

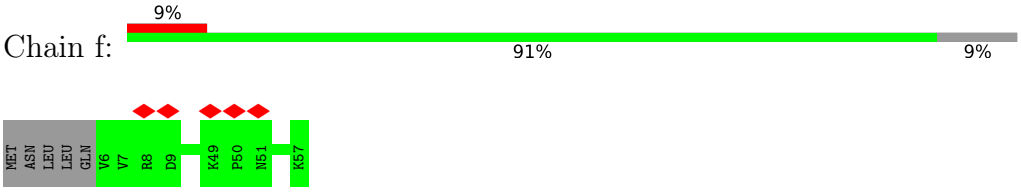
Chain e:





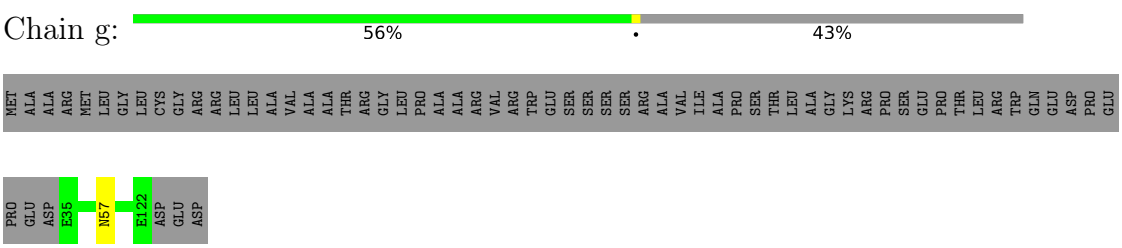
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



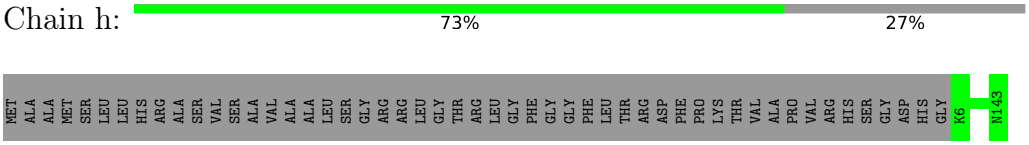
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



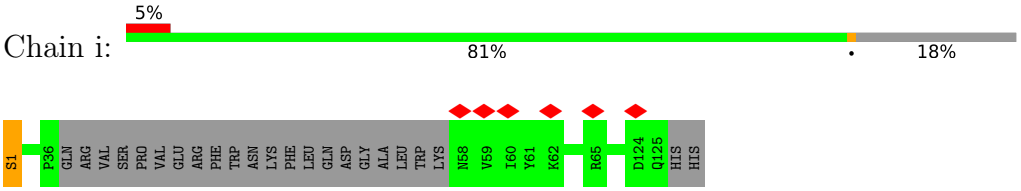
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



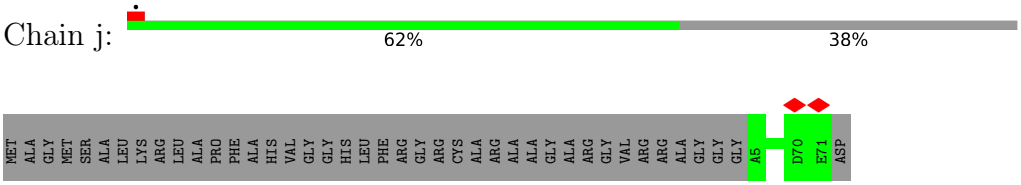
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



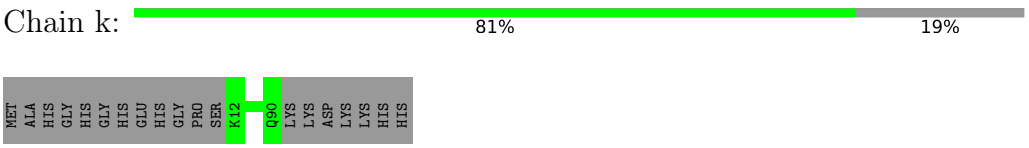
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



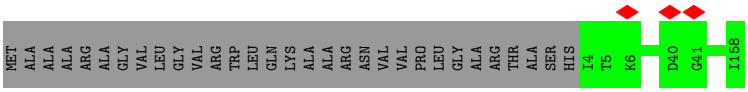
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



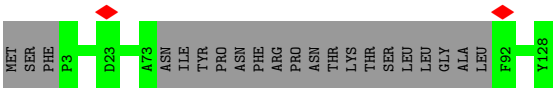
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



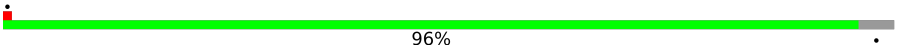
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

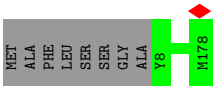
Chain m:



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

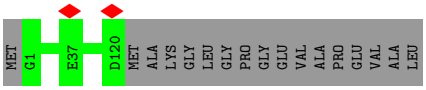
Chain n:





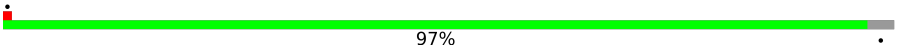
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

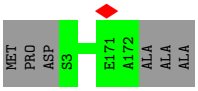
Chain o:



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

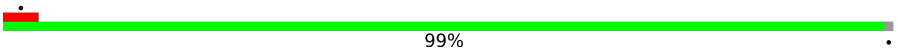
Chain p:

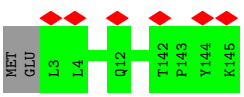




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

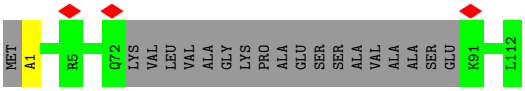
Chain q:





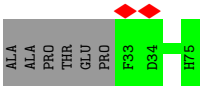
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

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	40154	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	33.163	Depositor
Minimum map value	-13.512	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.066	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 (i)

5.1 Standard geometry (i)

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

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	0.34	0/756	0.43	0/1034
2	B	0.43	1/1261 (0.1%)	0.49	0/1706
3	C	0.37	0/1765	0.46	0/2403
4	D	0.36	0/3155	0.46	0/4264
5	E	0.32	0/1695	0.44	0/2307
6	F	0.34	0/3384	0.45	0/4573
7	G	0.33	0/5367	0.46	0/7274
8	H	0.34	0/2528	0.43	0/3452
9	I	0.38	0/1445	0.46	0/1956
10	J	0.36	0/968	0.44	0/1311
11	K	0.31	0/745	0.44	0/1008
12	L	0.37	0/4426	0.43	0/6025
13	M	0.35	0/3716	0.43	0/5069
14	N	0.31	0/2792	0.42	0/3800
15	O	0.29	0/2651	0.42	0/3587
16	P	0.32	0/2339	0.45	0/3159
17	Q	0.33	0/1039	0.45	0/1404
18	R	0.36	0/731	0.45	0/984
19	S	0.30	0/674	0.44	0/908
20	T	0.29	0/621	0.39	0/837
20	U	0.42	0/692	0.41	0/932
21	V	0.30	0/931	0.38	0/1261
22	W	0.31	0/995	0.41	0/1337
23	X	0.33	0/1439	0.43	0/1942
24	Y	0.26	0/157	0.38	0/211
25	Z	0.34	0/1174	0.43	0/1582
26	a	0.36	0/576	0.41	0/775
27	b	0.33	0/672	0.40	0/923
28	c	0.30	0/418	0.36	0/567
29	d	0.35	0/964	0.41	0/1305
30	e	0.31	0/818	0.45	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.36	0/464	0.41	0/626
32	g	0.40	0/755	0.40	0/1023
33	h	0.35	0/1188	0.42	0/1607
34	i	0.39	0/912	0.42	0/1241
35	j	0.38	0/607	0.39	0/833
36	k	0.39	0/657	0.41	0/887
37	l	0.41	0/1358	0.41	0/1858
38	m	0.37	0/929	0.42	0/1252
39	n	0.41	0/1540	0.41	0/2085
40	o	0.41	0/1060	0.41	0/1420
41	p	0.38	0/1468	0.42	0/1979
42	q	0.33	0/1233	0.44	0/1676
43	r	0.33	0/780	0.47	0/1056
44	s	0.31	0/375	0.45	0/507
All	All	0.35	1/64220 (0.0%)	0.44	0/87039

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
34	i	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	CYS	CB-SG	-5.24	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
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	89/115 (77%)	87 (98%)	2 (2%)	0	100	100
2	B	152/216 (70%)	140 (92%)	11 (7%)	1 (1%)	22	39
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	383/463 (83%)	370 (97%)	13 (3%)	0	100	100
5	E	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
6	F	428/464 (92%)	411 (96%)	17 (4%)	0	100	100
7	G	686/727 (94%)	663 (97%)	23 (3%)	0	100	100
8	H	309/318 (97%)	294 (95%)	15 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	123/175 (70%)	115 (94%)	8 (6%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	545/606 (90%)	522 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	O	318/343 (93%)	302 (95%)	16 (5%)	0	100	100
16	P	280/380 (74%)	276 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	92/124 (74%)	89 (97%)	3 (3%)	0	100	100
19	S	80/99 (81%)	79 (99%)	1 (1%)	0	100	100
20	T	74/156 (47%)	71 (96%)	3 (4%)	0	100	100
20	U	82/156 (53%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	18/141 (13%)	16 (89%)	2 (11%)	0	100	100
25	Z	138/144 (96%)	129 (94%)	9 (6%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	43 (94%)	3 (6%)	0	100	100
29	d	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	86/154 (56%)	83 (96%)	3 (4%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	63 (97%)	2 (3%)	0	100	100
36	k	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
38	m	104/129 (81%)	100 (96%)	4 (4%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	118/137 (86%)	112 (95%)	6 (5%)	0	100	100
41	p	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
42	q	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	39 (95%)	2 (5%)	0	100	100
All	All	7693/9212 (84%)	7447 (97%)	245 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	79	SER

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	80/100 (80%)	80 (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	332/392 (85%)	331 (100%)	1 (0%)	92 97
5	E	183/205 (89%)	183 (100%)	0	100 100
6	F	344/368 (94%)	344 (100%)	0	100 100
7	G	578/608 (95%)	577 (100%)	1 (0%)	93 98
8	H	270/274 (98%)	270 (100%)	0	100 100
9	I	151/175 (86%)	151 (100%)	0	100 100
10	J	100/141 (71%)	100 (100%)	0	100 100
11	K	85/85 (100%)	85 (100%)	0	100 100
12	L	475/533 (89%)	475 (100%)	0	100 100
13	M	406/412 (98%)	406 (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	247/327 (76%)	247 (100%)	0	100 100
17	Q	112/153 (73%)	112 (100%)	0	100 100
18	R	77/97 (79%)	77 (100%)	0	100 100
19	S	73/82 (89%)	73 (100%)	0	100 100
20	T	70/135 (52%)	69 (99%)	1 (1%)	67 86
20	U	78/135 (58%)	78 (100%)	0	100 100
21	V	100/102 (98%)	100 (100%)	0	100 100
22	W	107/114 (94%)	107 (100%)	0	100 100
23	X	154/155 (99%)	154 (100%)	0	100 100
24	Y	15/102 (15%)	15 (100%)	0	100 100
25	Z	119/121 (98%)	119 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86 (100%)	0	100	100
31	f	49/54 (91%)	49 (100%)	0	100	100
32	g	79/131 (60%)	78 (99%)	1 (1%)	69	87
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	99/120 (82%)	99 (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	96/115 (84%)	96 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	6809/7892 (86%)	6805 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	430	ARG
7	G	237	ASN
20	T	44(A)	SER
32	g	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
4	D	55	HIS

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Mol	Chain	Res	Type
8	H	304	HIS
12	L	199	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)

9 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	$\#\|Z\| > 2$
4	2MR	D	85	4	10,12,13	2.68	4 (40%)	5,13,15	1.01	0
14	FME	N	1	14	8,9,10	0.97	0	7,9,11	0.85	0
1	FME	A	1	1	8,9,10	0.91	0	7,9,11	1.15	1 (14%)
34	SAC	i	1	34	7,8,9	1.85	1 (14%)	8,9,11	1.97	1 (12%)
8	FME	H	1	8	8,9,10	0.96	0	7,9,11	1.02	0
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	1.05	1 (14%)
13	FME	M	1	13	8,9,10	0.98	1 (12%)	7,9,11	0.97	1 (14%)
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.79	0
43	AYA	r	1	43	6,7,8	1.82	2 (33%)	5,8,10	1.35	1 (20%)

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
4	2MR	D	85	4	-	0/10/13/15	-
14	FME	N	1	14	-	2/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SAC	i	1	34	-	5/7/8/10	-
8	FME	H	1	8	-	0/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
12	FME	L	1	12	-	5/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.14	1.44	1.33
4	D	85	2MR	CZ-NE	4.65	1.44	1.34
34	i	1	SAC	O-C	4.23	1.36	1.19
4	D	85	2MR	O-C	3.97	1.35	1.19
43	r	1	AYA	CT-N	3.27	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.67	112.53	124.78
1	A	1	FME	C-CA-N	2.45	114.16	109.73
43	r	1	AYA	CM-CT-N	2.42	120.19	116.10
13	M	1	FME	C-CA-N	2.14	113.59	109.73
11	K	1	FME	C-CA-N	2.05	113.43	109.73

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	O1-CN-N-CA

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 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
53	CDL	L	702	-	68,68,99	1.04	7 (10%)	74,80,111	1.09	4 (5%)
53	CDL	h	1001	-	66,66,99	1.06	8 (12%)	72,78,111	1.19	4 (5%)
45	3PE	L	701	-	48,48,50	0.88	3 (6%)	51,53,55	1.16	3 (5%)
46	SF4	F	502	6	0,12,12	-	-	-		
46	SF4	G	802	7	0,12,12	-	-	-		
54	GTP	O	1202	55	26,34,34	2.92	10 (38%)	32,54,54	1.81	11 (34%)
51	LMT	L	704	-	36,36,36	1.22	2 (5%)	47,47,47	0.80	1 (2%)
45	3PE	M	601	-	42,42,50	0.92	4 (9%)	45,47,55	1.02	2 (4%)
51	LMT	g	1101	-	36,36,36	1.22	4 (11%)	47,47,47	0.85	0
51	LMT	h	1002	-	36,36,36	1.14	2 (5%)	47,47,47	1.29	8 (17%)
48	FES	E	301	5	0,4,4	-	-	-		
45	3PE	I	204	-	32,32,50	1.07	4 (12%)	35,37,55	1.08	2 (5%)
51	LMT	l	201	-	36,36,36	1.23	3 (8%)	47,47,47	0.89	0
53	CDL	X	201	-	51,51,99	1.18	7 (13%)	57,63,111	1.29	4 (7%)
46	SF4	G	801	7	0,12,12	-	-	-		
47	PC1	M	602	-	48,48,53	1.00	3 (6%)	54,56,61	1.01	2 (3%)
46	SF4	I	202	9	0,12,12	-	-	-		
53	CDL	N	1304	-	64,64,99	1.06	8 (12%)	70,76,111	1.15	4 (5%)
53	CDL	q	201	-	75,75,99	1.00	7 (9%)	81,87,111	1.12	4 (4%)
58	EHZ	T	101	20	29,36,37	1.79	5 (17%)	35,44,47	1.77	7 (20%)
51	LMT	K	901	-	36,36,36	1.15	2 (5%)	47,47,47	1.11	4 (8%)
56	NDP	P	501	-	45,52,52	2.16	6 (13%)	53,80,80	1.69	10 (18%)
45	3PE	O	1201	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	3PE	N	1301	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2 (3%)
46	SF4	I	203	9	0,12,12	-	-	-		
49	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.24	6 (12%)
51	LMT	N	1303	-	36,36,36	1.18	3 (8%)	47,47,47	1.05	4 (8%)
52	I49	N	1305	-	15,17,17	1.49	2 (13%)	21,22,22	1.85	5 (23%)
52	I49	H	403	-	15,17,17	1.55	2 (13%)	21,22,22	1.92	7 (33%)
46	SF4	B	201	2	0,12,12	-	-	-		
45	3PE	H	402	-	33,33,50	1.35	4 (12%)	34,37,55	1.21	2 (5%)
47	PC1	B	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.10	2 (5%)
45	3PE	A	902	-	43,43,50	0.93	3 (6%)	46,48,55	1.12	2 (4%)
45	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.07	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-		
53	CDL	N	1302	-	66,66,99	1.05	7 (10%)	72,78,111	1.15	4 (5%)
51	LMT	J	201	-	36,36,36	1.18	3 (8%)	47,47,47	0.93	2 (4%)
51	LMT	p	201	-	36,36,36	1.17	3 (8%)	47,47,47	1.12	5 (10%)
45	3PE	A	901	-	47,47,50	0.88	4 (8%)	50,52,55	1.20	3 (6%)
51	LMT	H	401	-	36,36,36	1.23	4 (11%)	47,47,47	1.02	2 (4%)
51	LMT	b	301	-	36,36,36	1.20	2 (5%)	47,47,47	0.95	1 (2%)
58	EHZ	U	101	20	29,36,37	1.64	4 (13%)	35,44,47	1.47	3 (8%)
59	MYR	o	201	40	14,14,15	0.85	0	13,13,15	0.70	0
45	3PE	L	703	-	44,44,50	0.90	3 (6%)	47,49,55	1.25	3 (6%)

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
53	CDL	L	702	-	-	21/79/79/110	-
53	CDL	h	1001	-	-	36/77/77/110	-
45	3PE	L	701	-	-	23/52/52/54	-
46	SF4	F	502	6	-	-	0/6/5/5
54	GTP	O	1202	55	-	6/18/38/38	0/3/3/3
46	SF4	G	802	7	-	-	0/6/5/5
51	LMT	L	704	-	-	8/21/61/61	0/2/2/2
45	3PE	M	601	-	-	18/46/46/54	-
51	LMT	g	1101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	LMT	h	1002	-	-	4/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
45	3PE	I	204	-	-	16/36/36/54	-
51	LMT	l	201	-	-	9/21/61/61	0/2/2/2
53	CDL	X	201	-	-	18/61/61/110	-
46	SF4	G	801	7	-	-	0/6/5/5
47	PC1	M	602	-	-	25/52/52/57	-
46	SF4	I	202	9	-	-	0/6/5/5
53	CDL	N	1304	-	-	28/75/75/110	-
53	CDL	q	201	-	-	41/86/86/110	-
58	EHZ	T	101	20	-	15/42/44/45	-
51	LMT	K	901	-	-	7/21/61/61	0/2/2/2
56	NDP	P	501	-	-	7/30/77/77	0/5/5/5
45	3PE	O	1201	-	-	29/54/54/54	-
45	3PE	N	1301	-	-	18/54/54/54	-
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
51	LMT	N	1303	-	-	3/21/61/61	0/2/2/2
46	SF4	I	203	9	-	-	0/6/5/5
52	I49	N	1305	-	-	4/10/10/10	0/1/1/1
52	I49	H	403	-	-	5/10/10/10	0/1/1/1
46	SF4	B	201	2	-	-	0/6/5/5
45	3PE	H	402	-	-	19/36/36/54	-
47	PC1	B	202	-	-	20/38/38/57	-
45	3PE	A	902	-	-	23/47/47/54	-
45	3PE	I	201	-	-	18/54/54/54	-
53	CDL	N	1302	-	-	40/77/77/110	-
48	FES	G	803	7	-	-	0/1/1/1
51	LMT	J	201	-	-	7/21/61/61	0/2/2/2
51	LMT	p	201	-	-	10/21/61/61	0/2/2/2
45	3PE	A	901	-	-	26/51/51/54	-
51	LMT	H	401	-	-	9/21/61/61	0/2/2/2
51	LMT	b	301	-	-	8/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	14/42/44/45	-
59	MYR	o	201	40	-	7/11/12/13	-
45	3PE	L	703	-	-	19/48/48/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.86	1.81	1.59
54	O	1202	GTP	O6-C6	8.25	1.40	1.23
58	T	101	EHZ	C15-N2	5.94	1.46	1.33
58	T	101	EHZ	C12-N1	5.35	1.45	1.33
54	O	1202	GTP	O4'-C1'	5.26	1.48	1.41

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	P	501	NDP	PN-O3-PA	-6.82	109.42	132.83
58	U	101	EHZ	C8-C9-S1	6.18	121.27	113.63
58	T	101	EHZ	C16-C15-N2	5.58	127.68	116.58
58	T	101	EHZ	C8-C9-S1	5.38	120.28	113.63
45	A	901	3PE	O21-C21-C22	4.97	122.22	111.50

There are no chirality outliers.

5 of 570 torsion outliers are listed below:

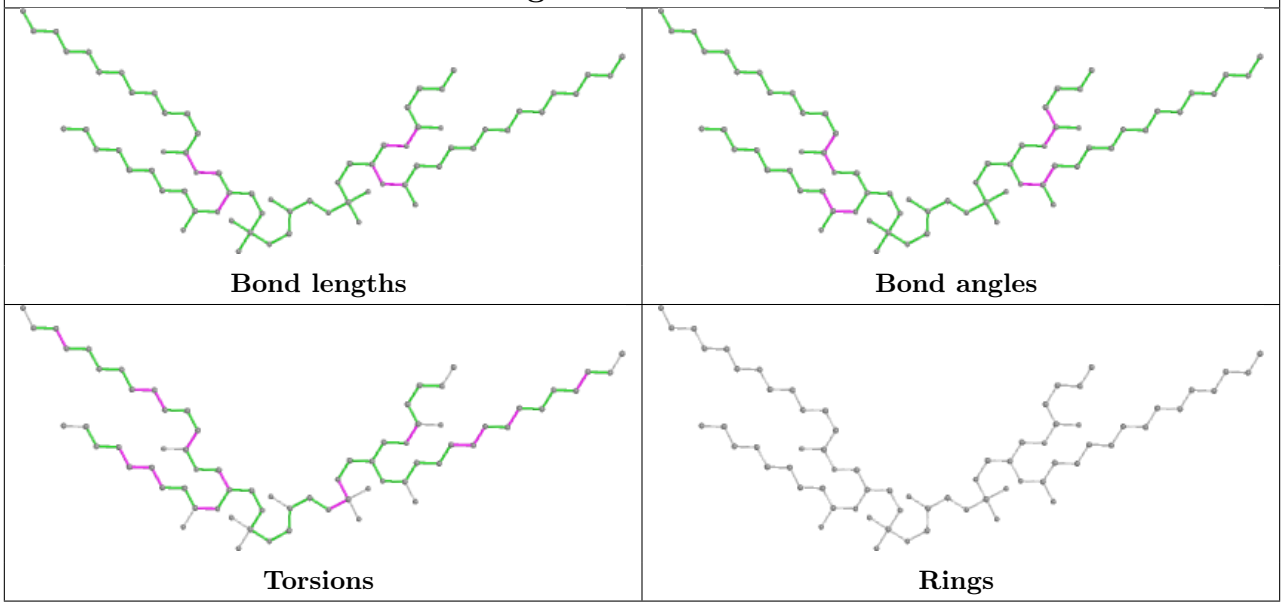
Mol	Chain	Res	Type	Atoms
45	A	901	3PE	C11-O13-P-O14
45	A	901	3PE	C12-C11-O13-P
45	A	901	3PE	O13-C11-C12-N
45	A	901	3PE	O22-C21-O21-C2
45	A	902	3PE	C1-O11-P-O12

There are no ring outliers.

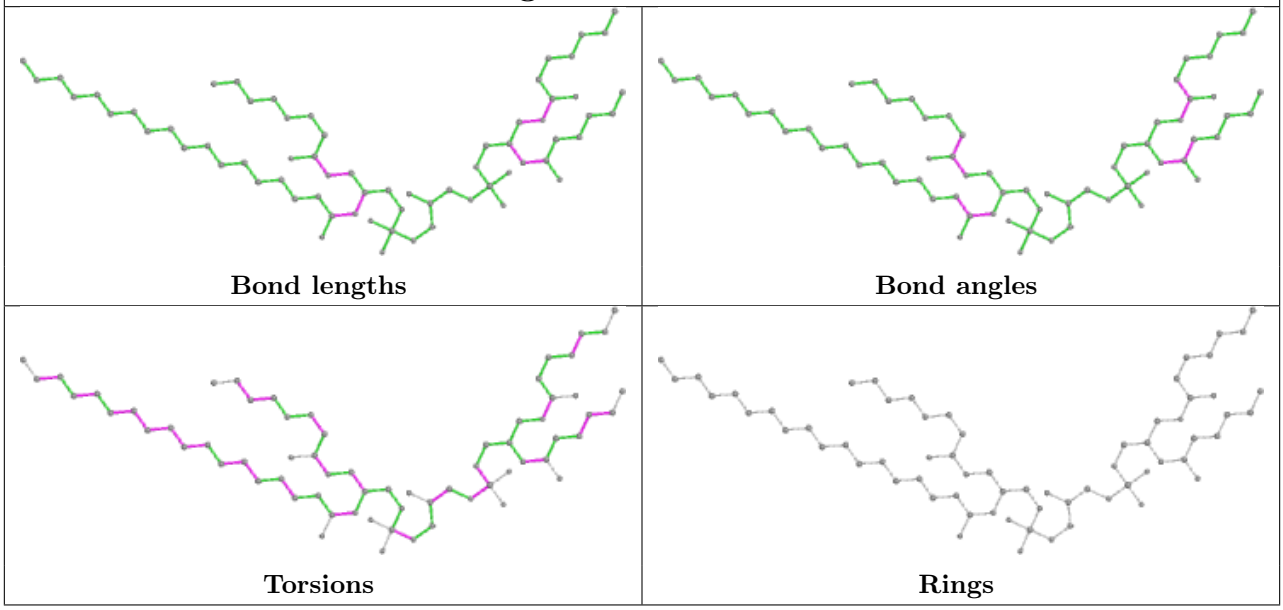
No monomer is involved in short contacts.

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.

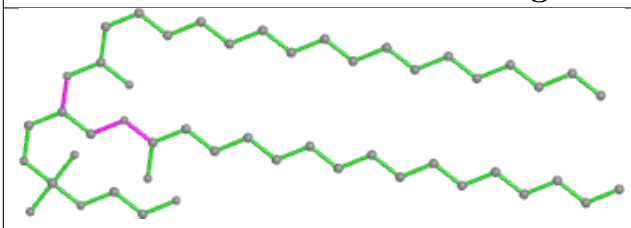
Ligand CDL L 702



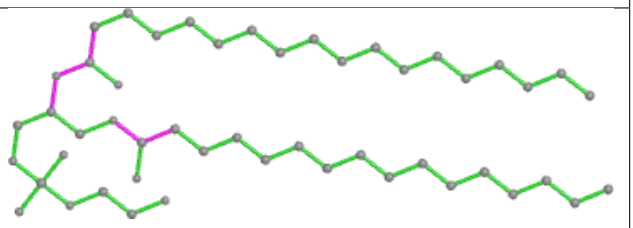
Ligand CDL h 1001



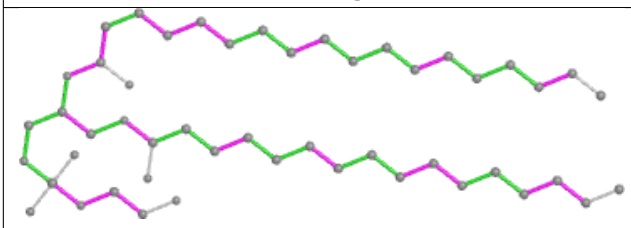
Ligand 3PE L 701



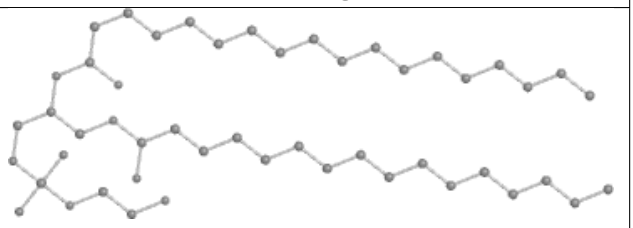
Bond lengths



Bond angles

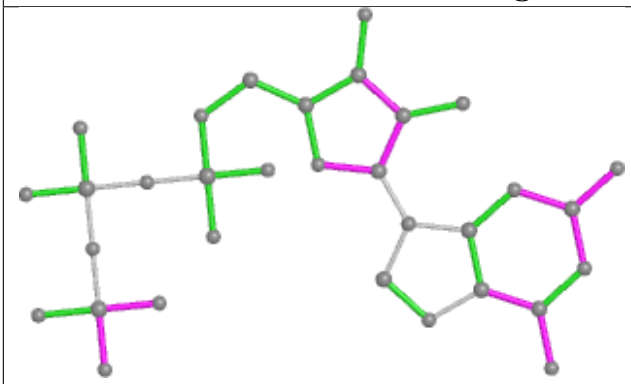


Torsions

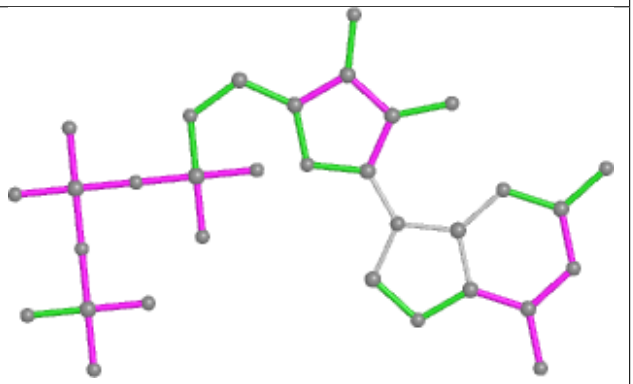


Rings

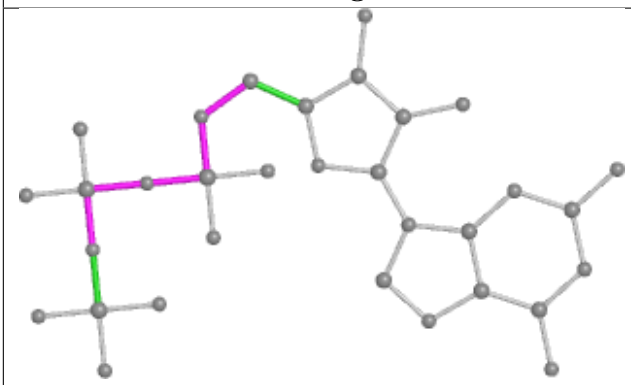
Ligand GTP O 1202



Bond lengths



Bond angles



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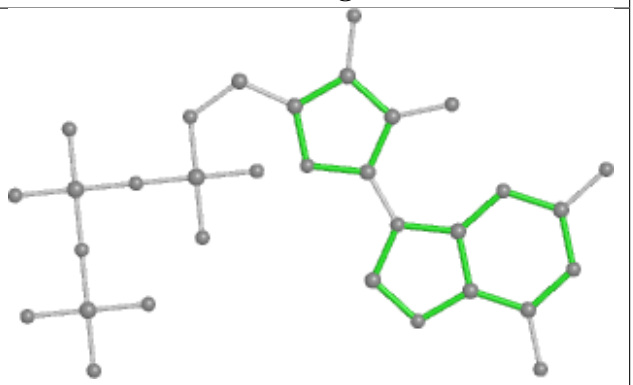
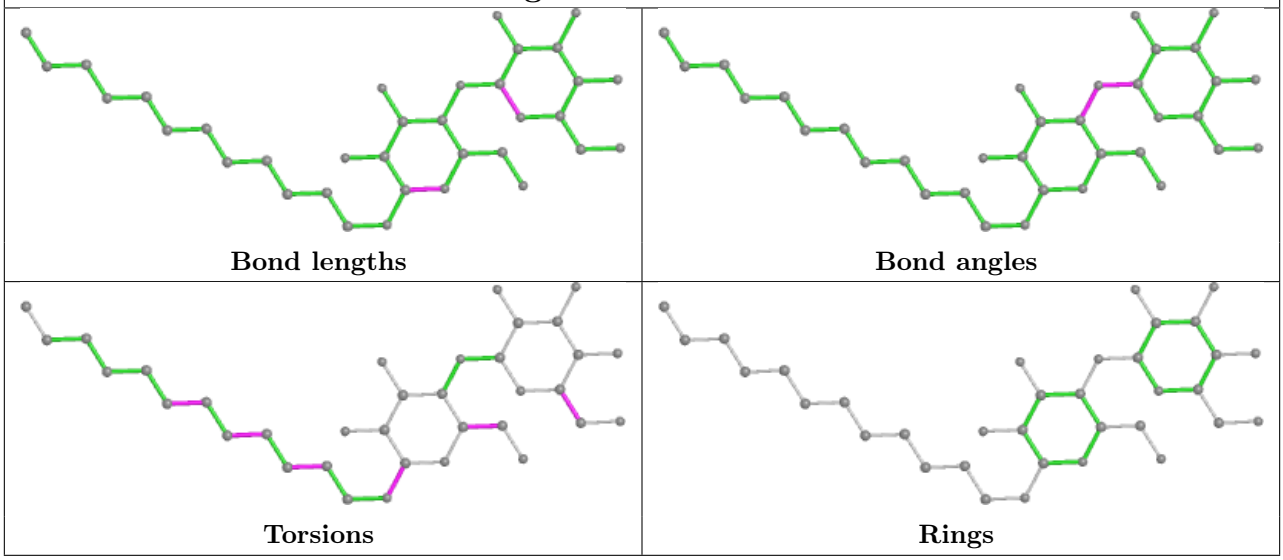
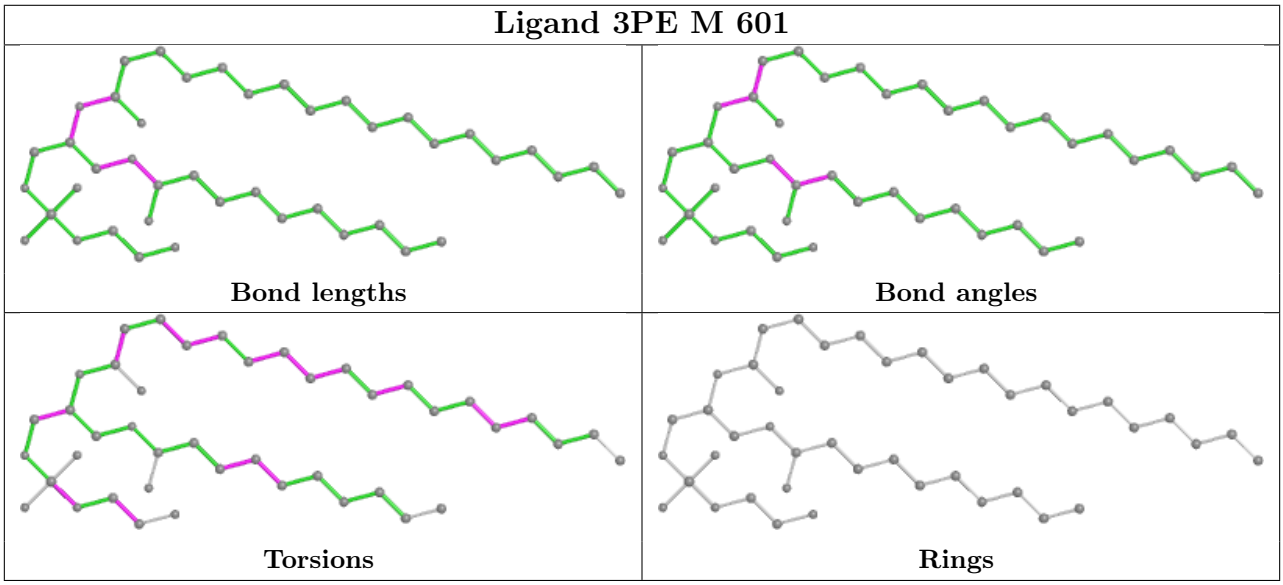


Rings

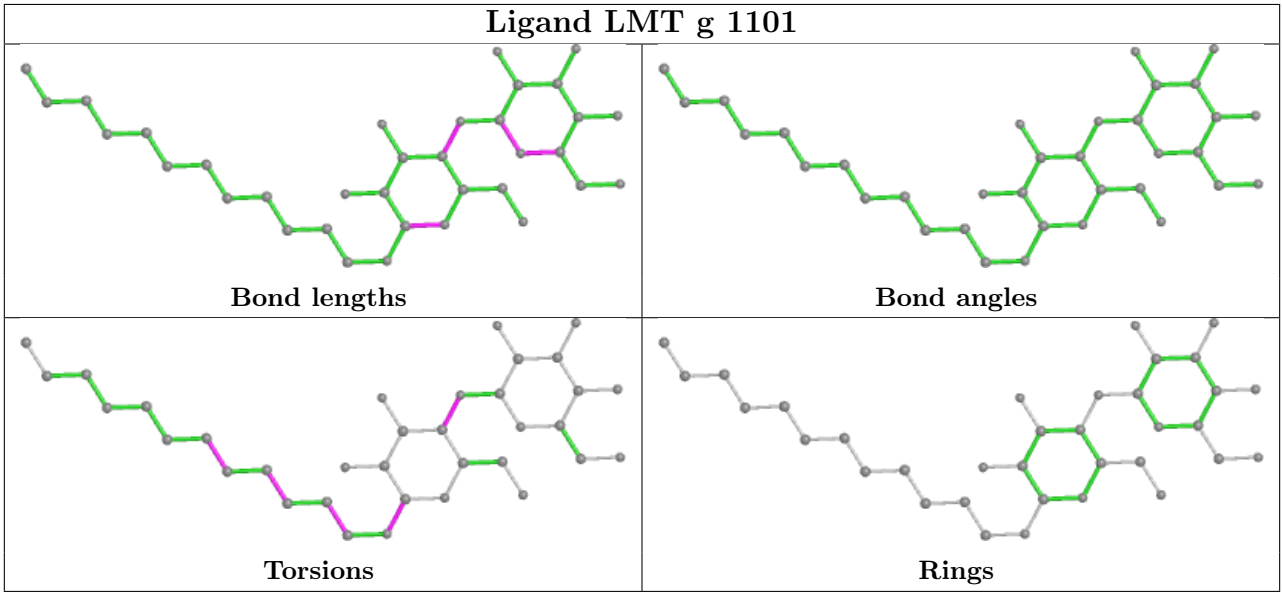
Ligand LMT L 704



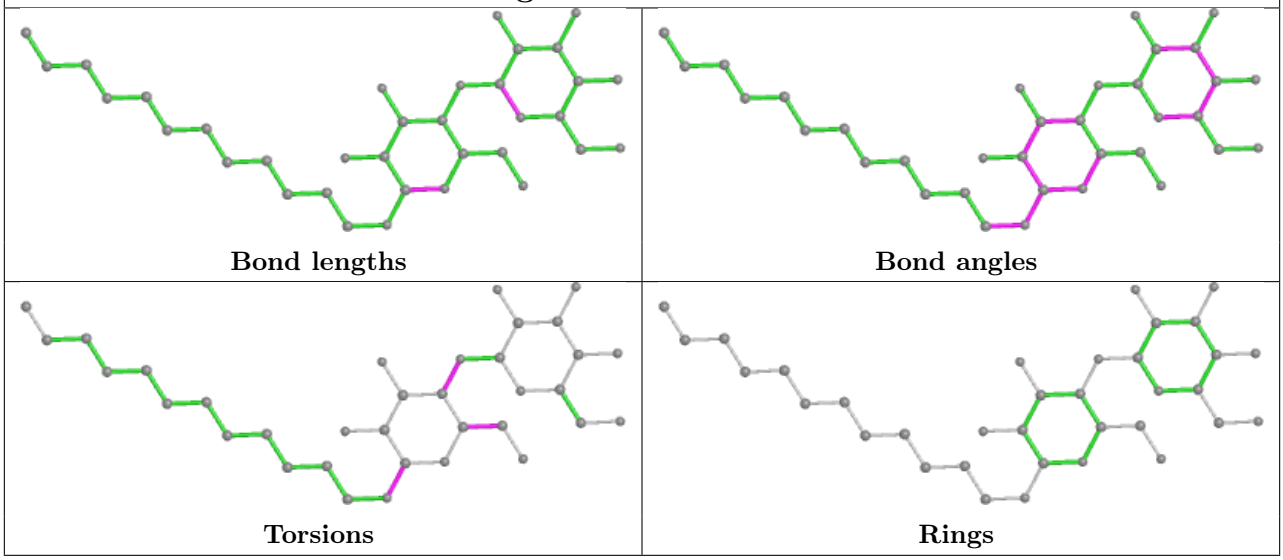
Ligand 3PE M 601



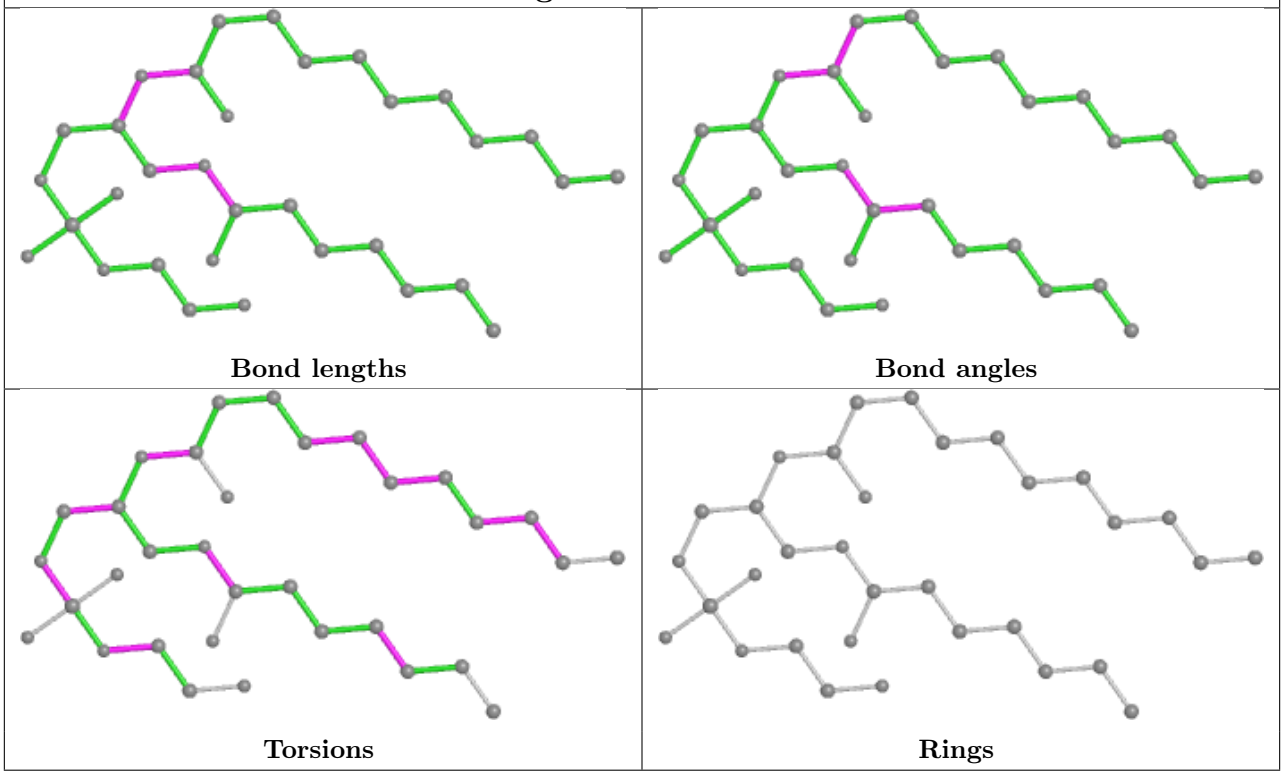
Ligand LMT g 1101



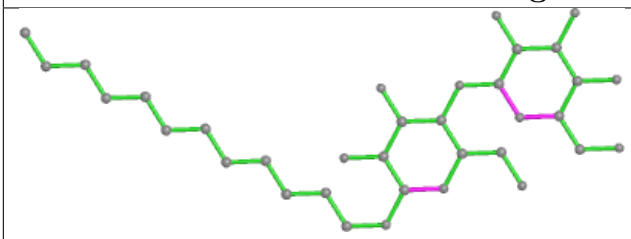
Ligand LMT h 1002



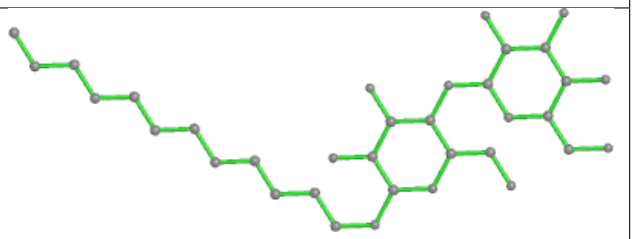
Ligand 3PE I 204



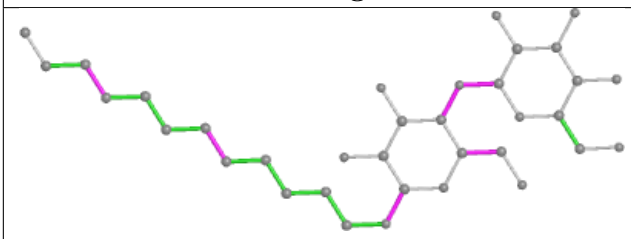
Ligand LMT l 201



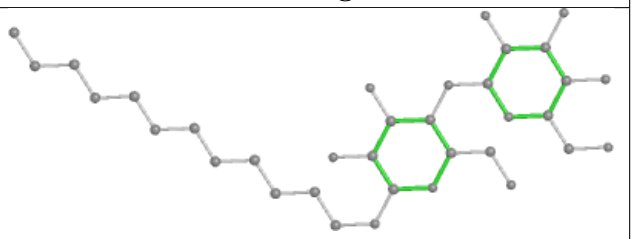
Bond lengths



Bond angles

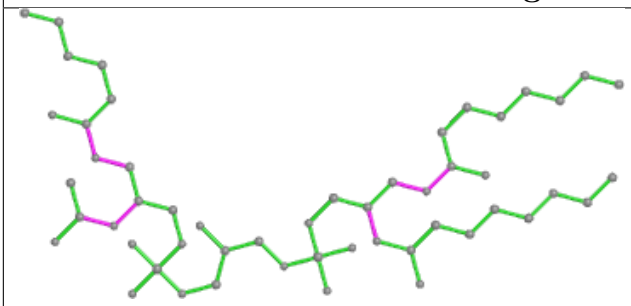


Torsions

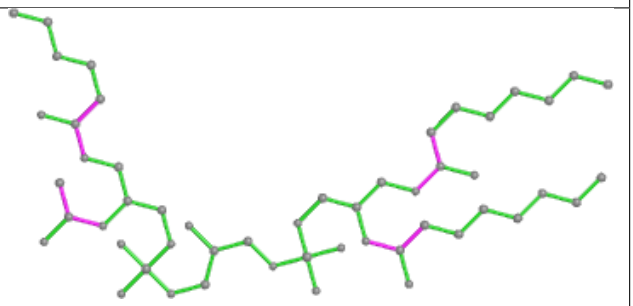


Rings

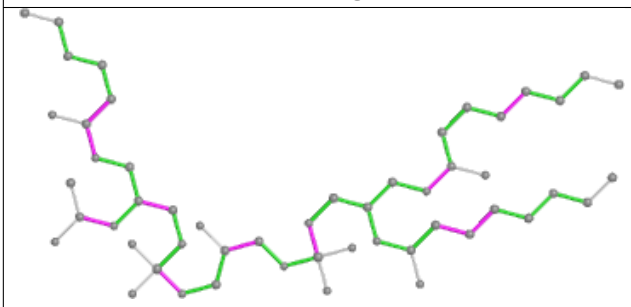
Ligand CDL X 201



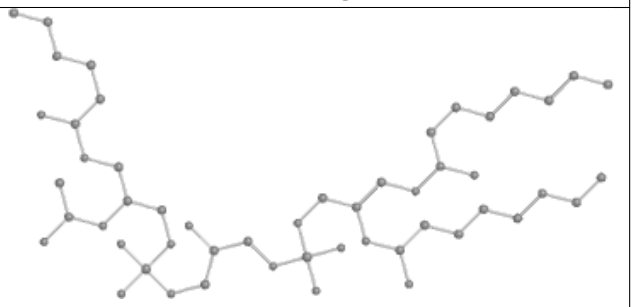
Bond lengths



Bond angles

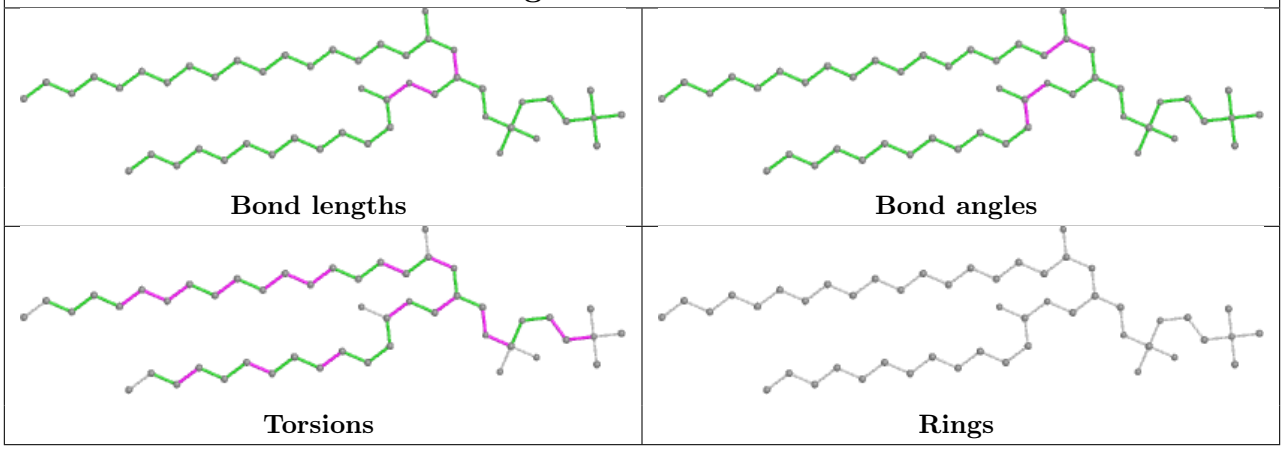


Torsions

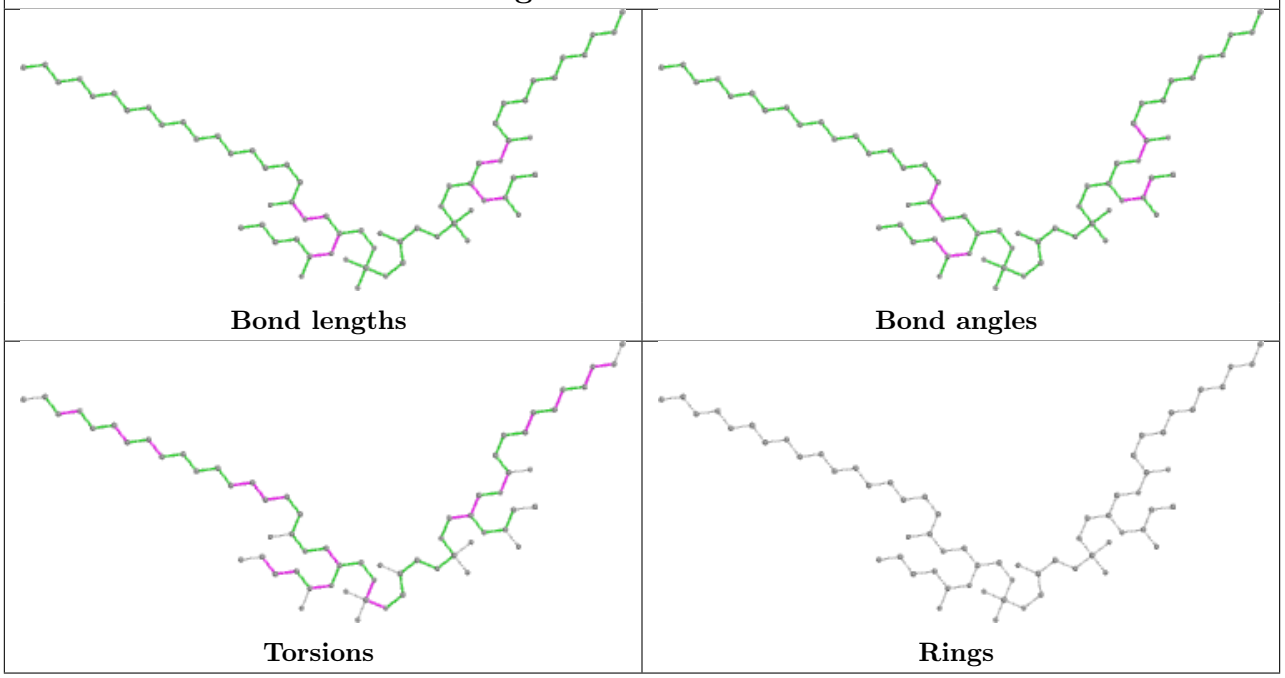


Rings

Ligand PC1 M 602



Ligand CDL N 1304



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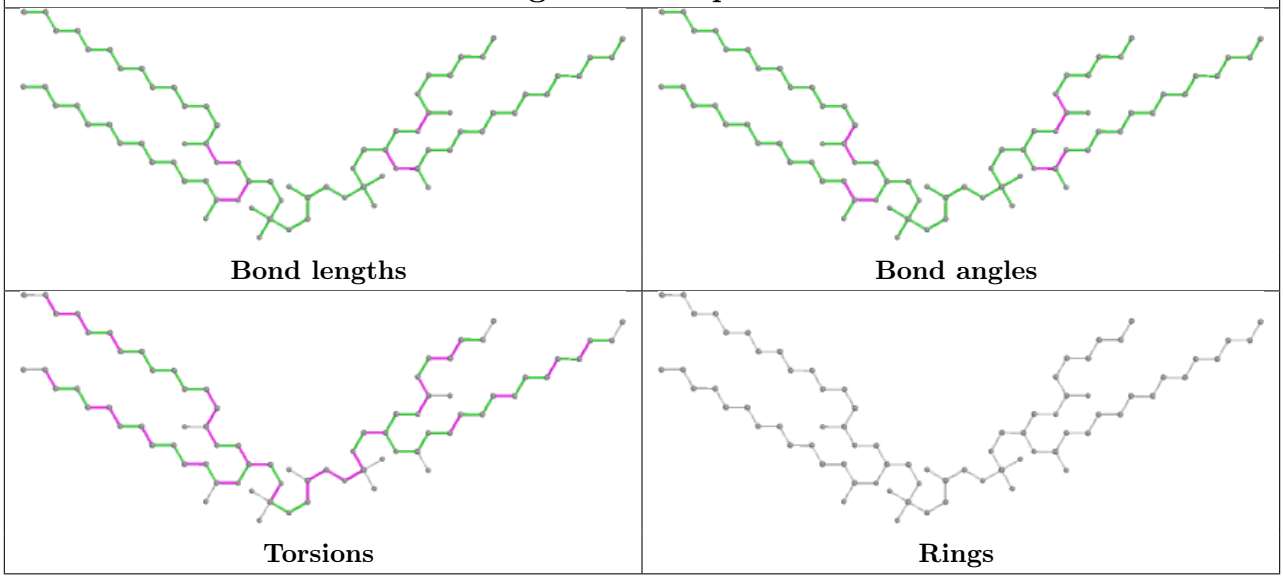
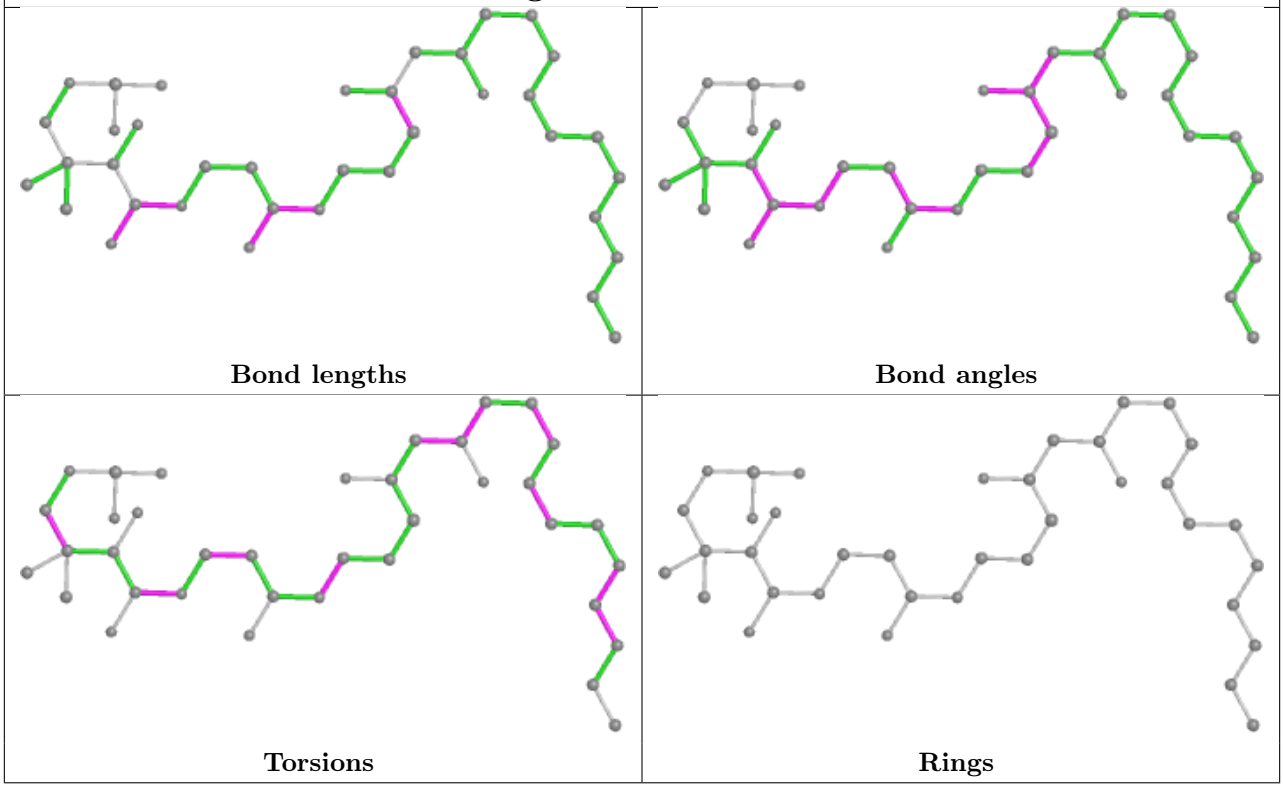
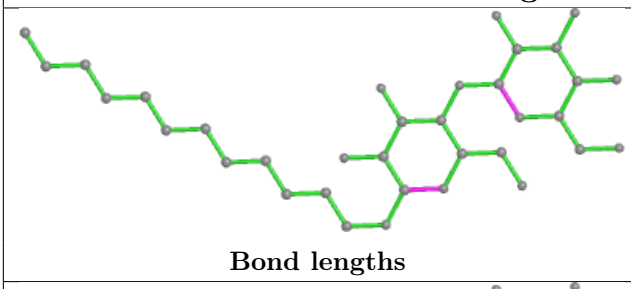


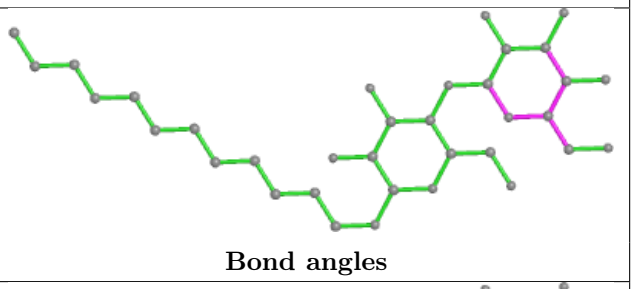
Ligand EHZ T 101



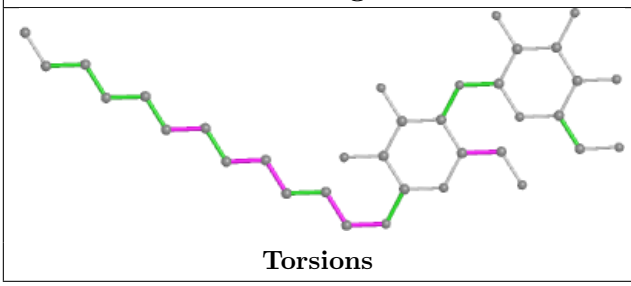
Ligand LMT K 901



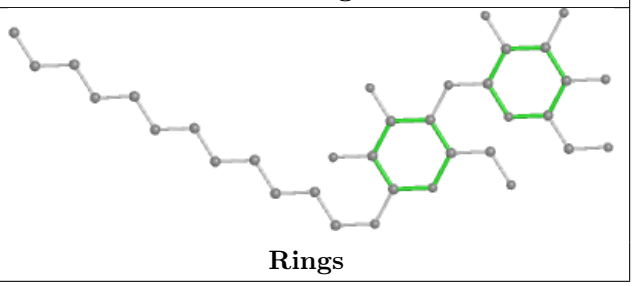
Bond lengths



Bond angles

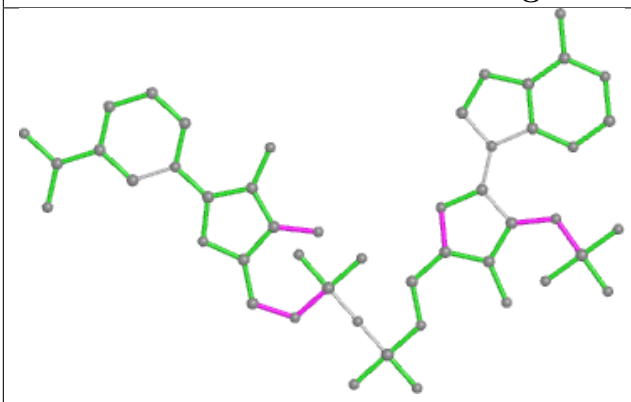


Torsions



Rings

Ligand NDP P 501



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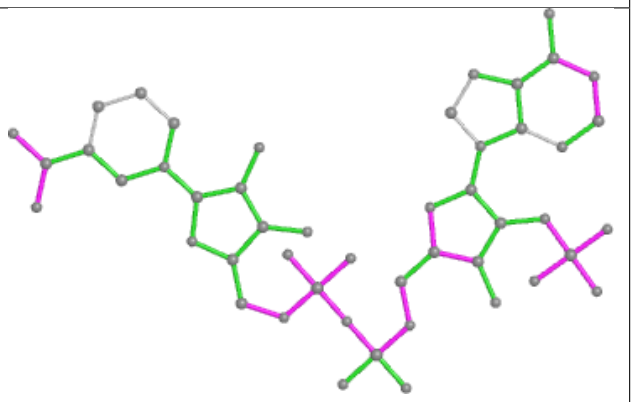
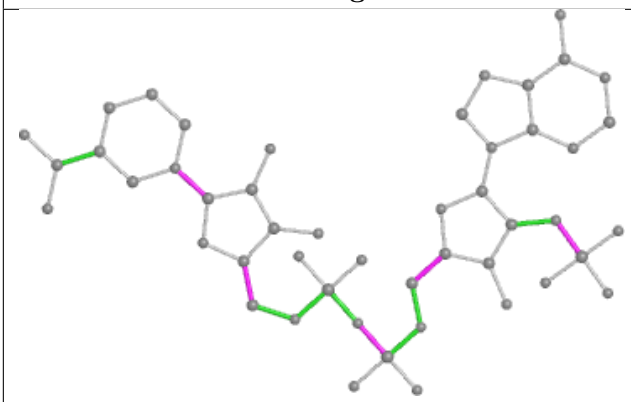


Bond angles



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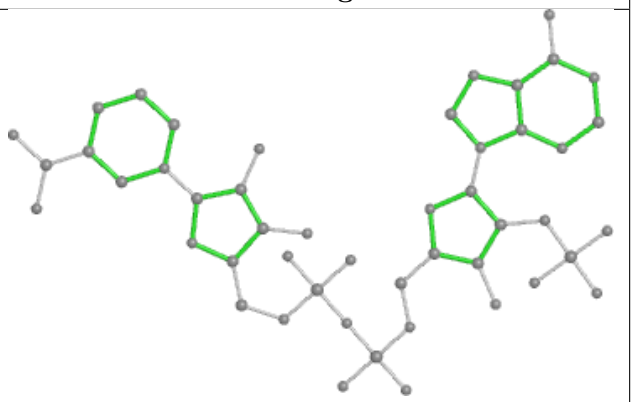
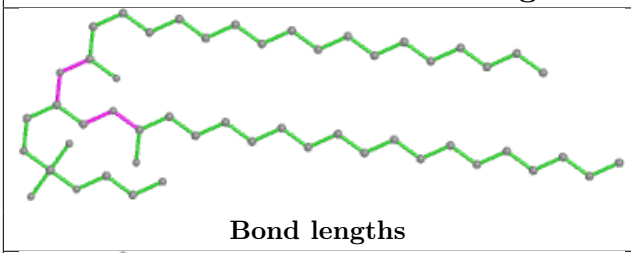


Rings

Ligand 3PE O 1201



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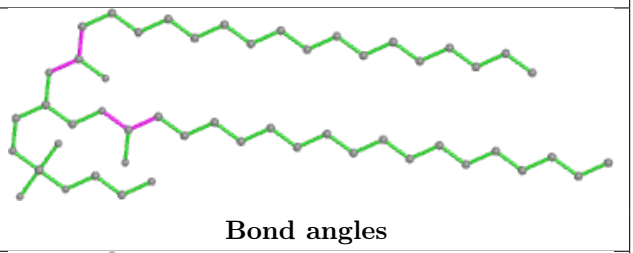
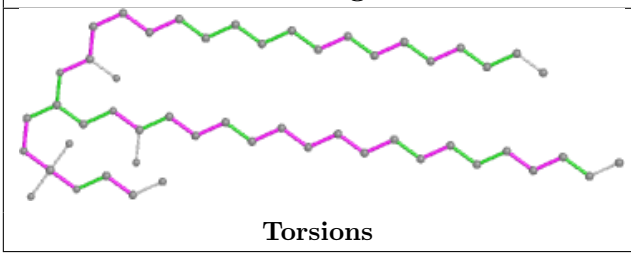


Bond angles



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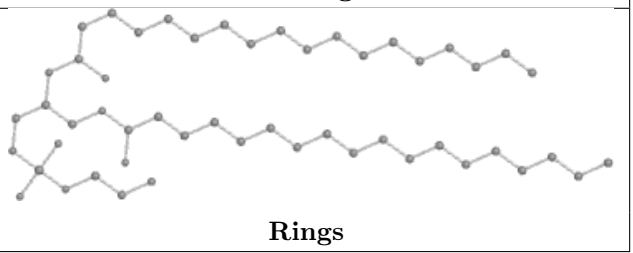
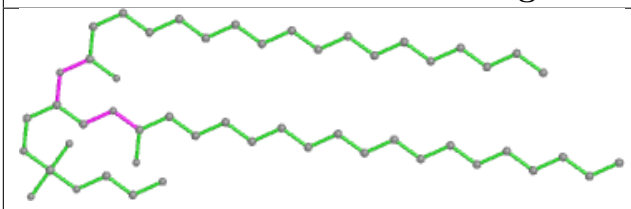


Rings

Ligand 3PE N 1301



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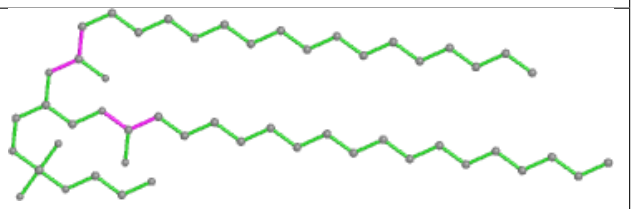
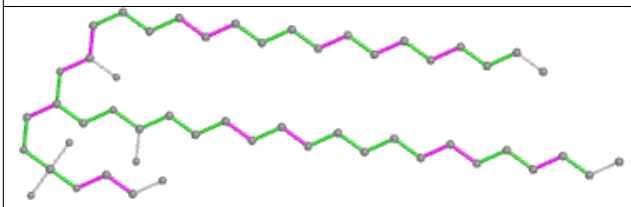


Bond angles



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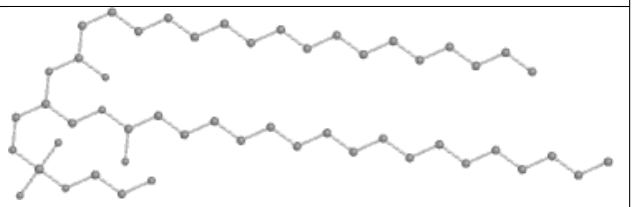
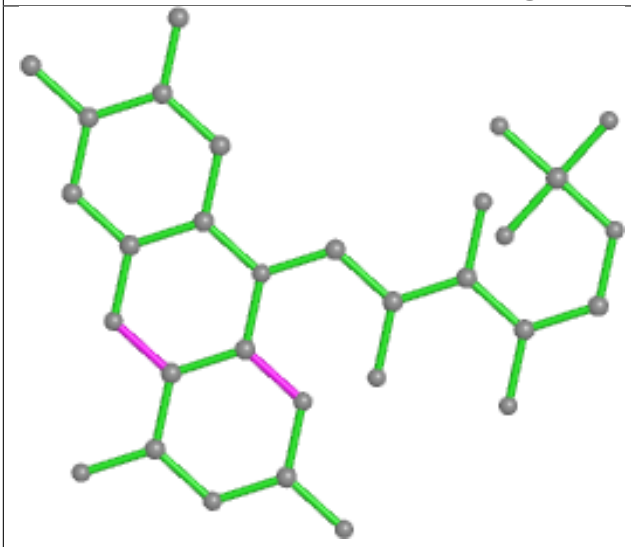


Rings

Ligand FMN F 501



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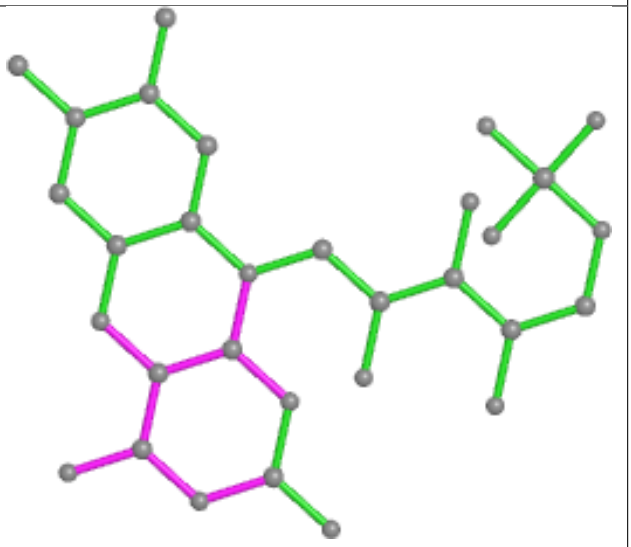
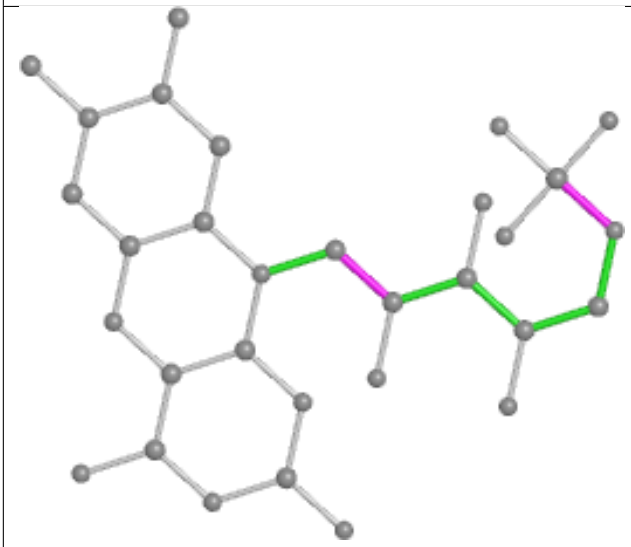
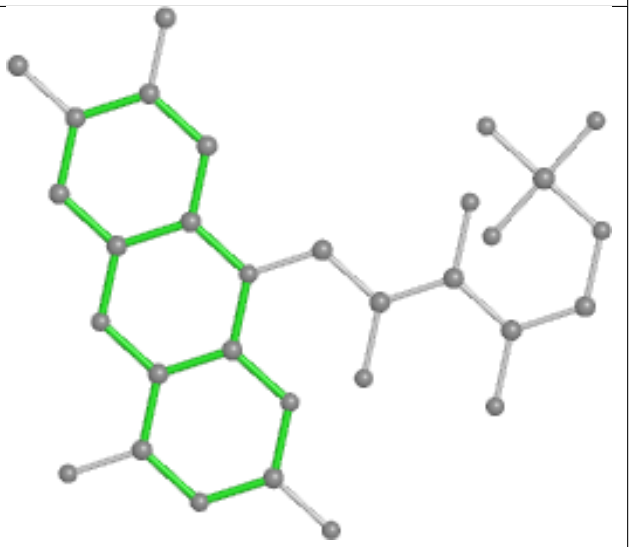


Bond angles

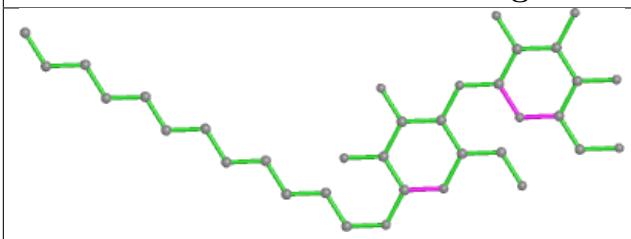


Torsions



Rings

Ligand LMT N 1303



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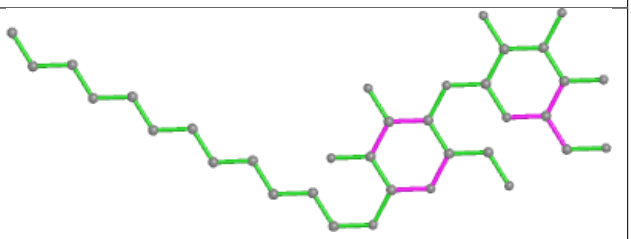
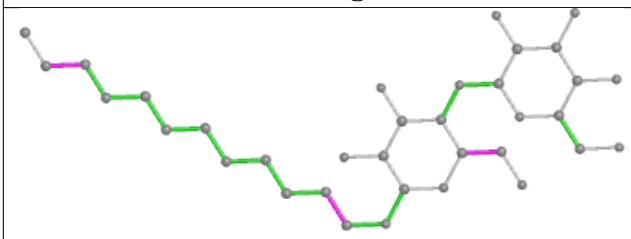


Bond angles



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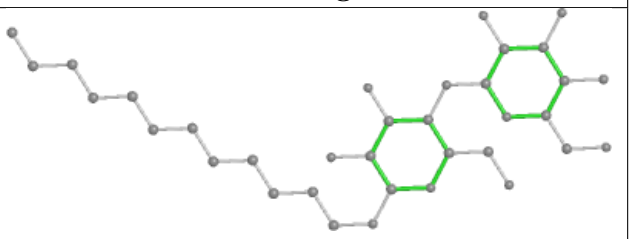
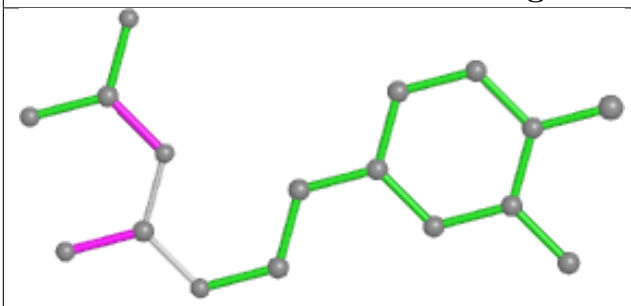
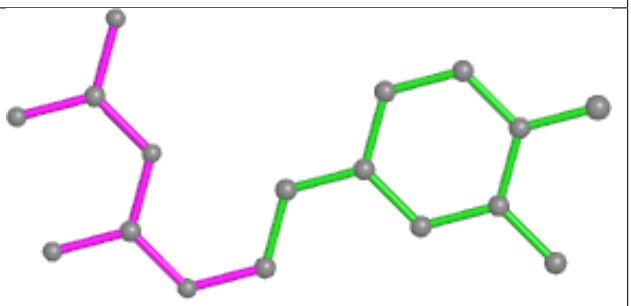


Rings

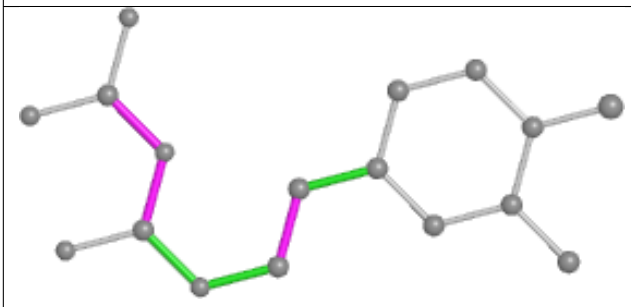
Ligand I49 N 1305



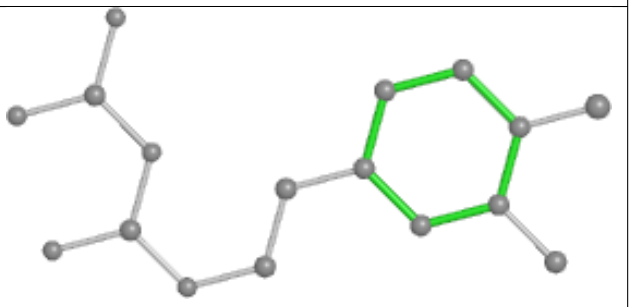
Bond lengths



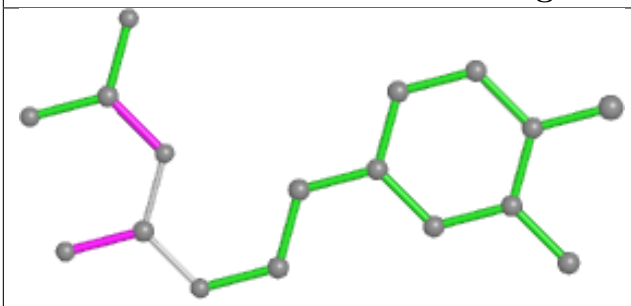
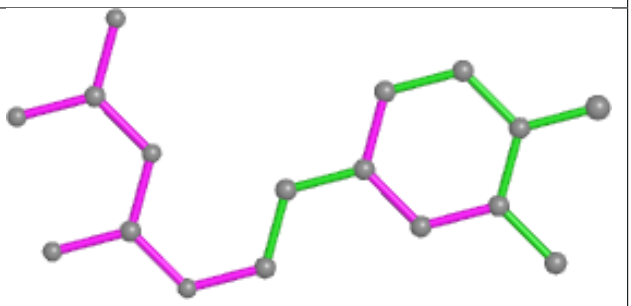
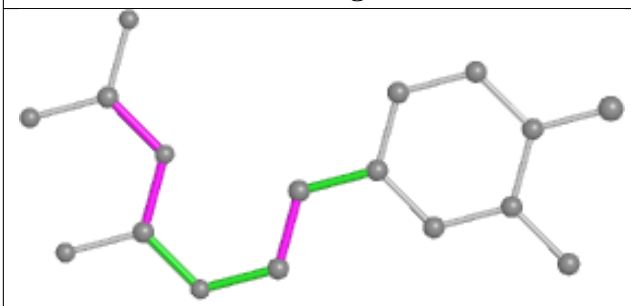
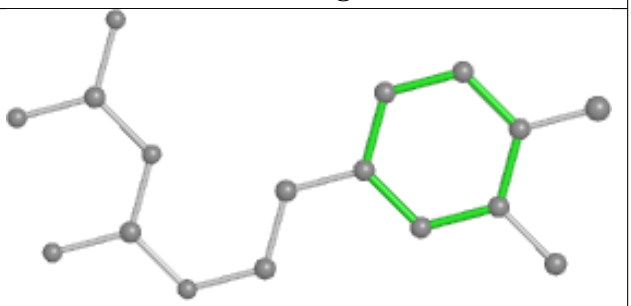
Bond angles

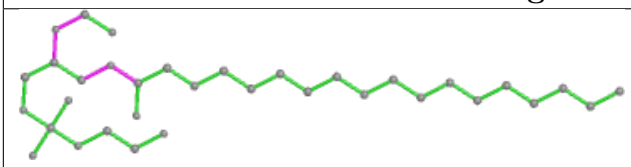
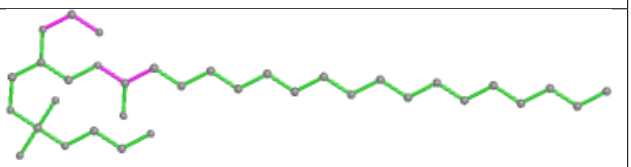
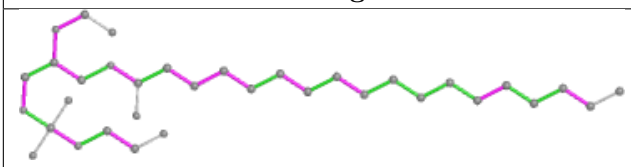
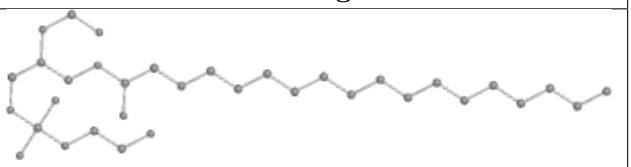


Torsions

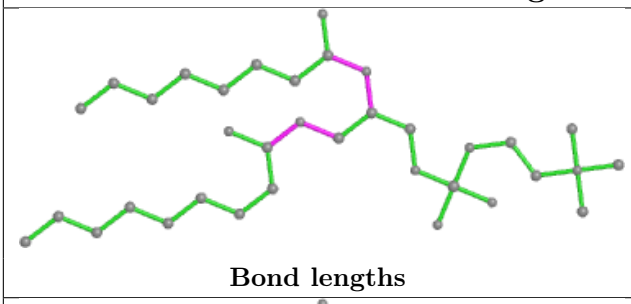


Rings

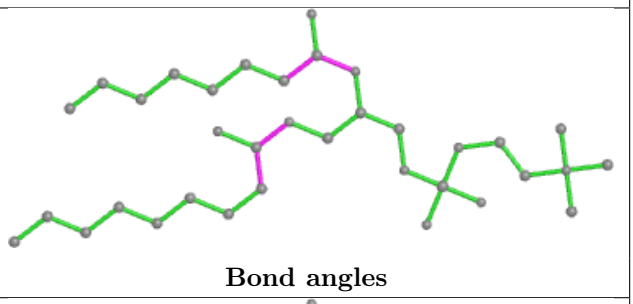
Ligand I49 H 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE H 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

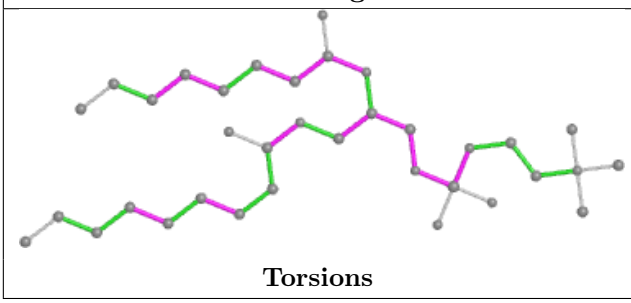
Ligand PC1 B 202



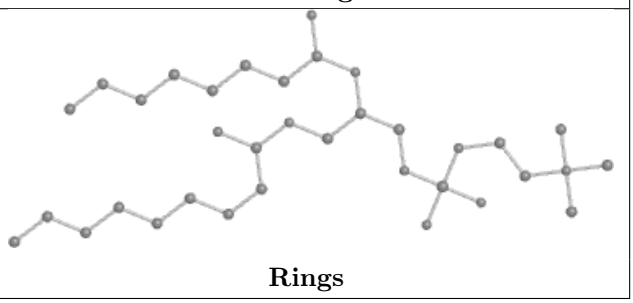
Bond lengths



Bond angles

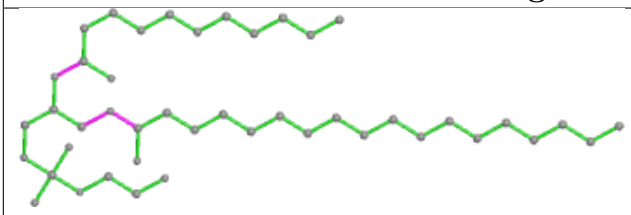


Torsions



Rings

Ligand 3PE A 902



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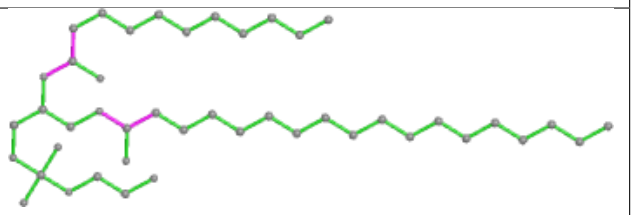
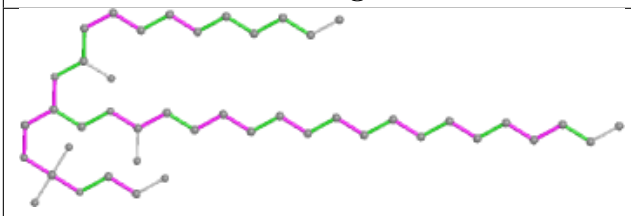
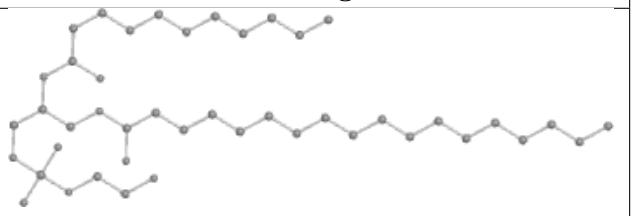


Bond angles

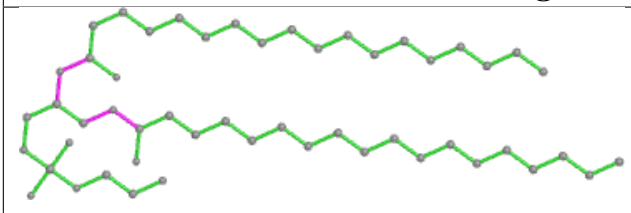


Torsions

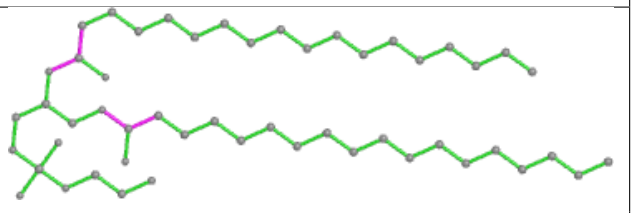


Rings

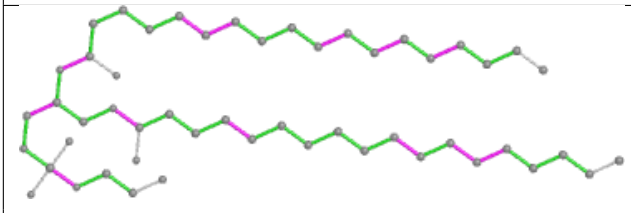
Ligand 3PE I 201



Bond lengths



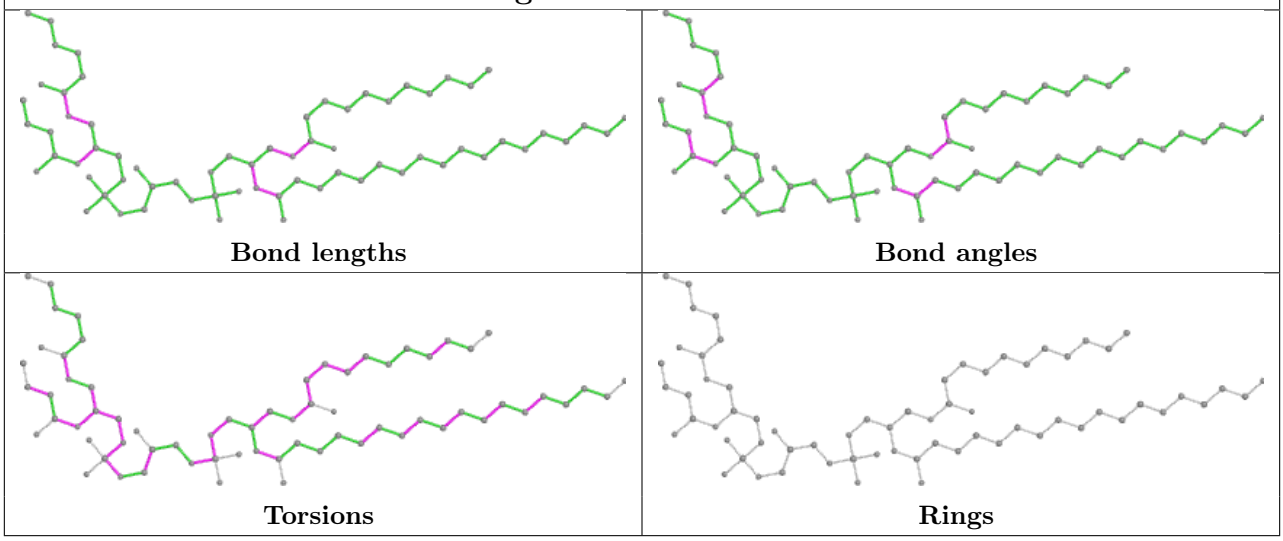
Bond angles



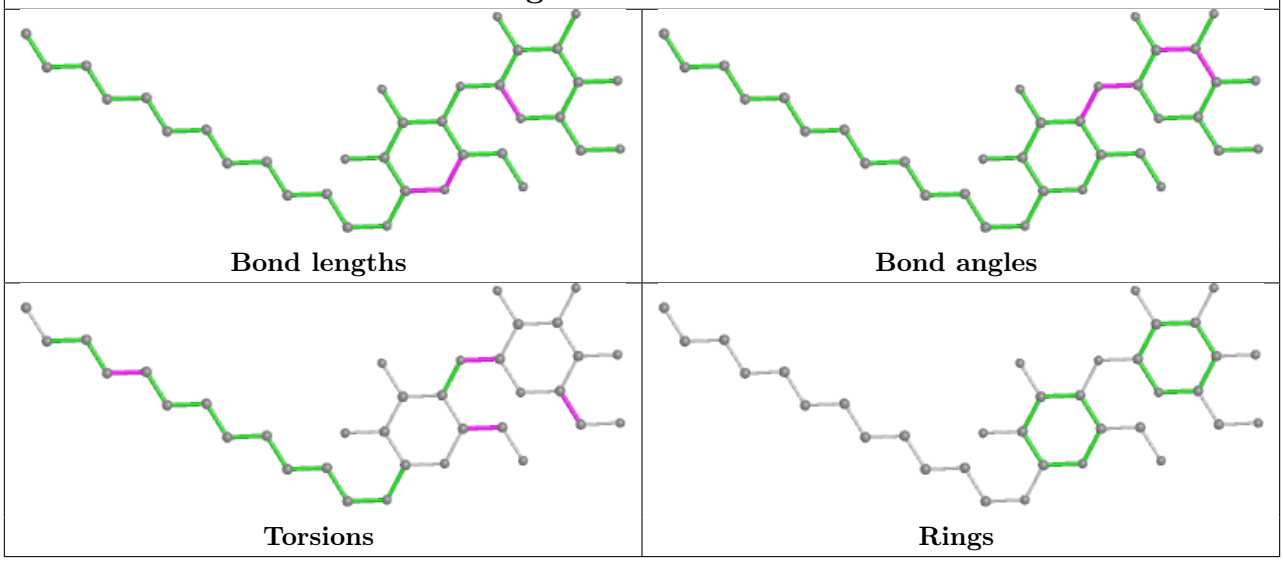
Torsions

Rings

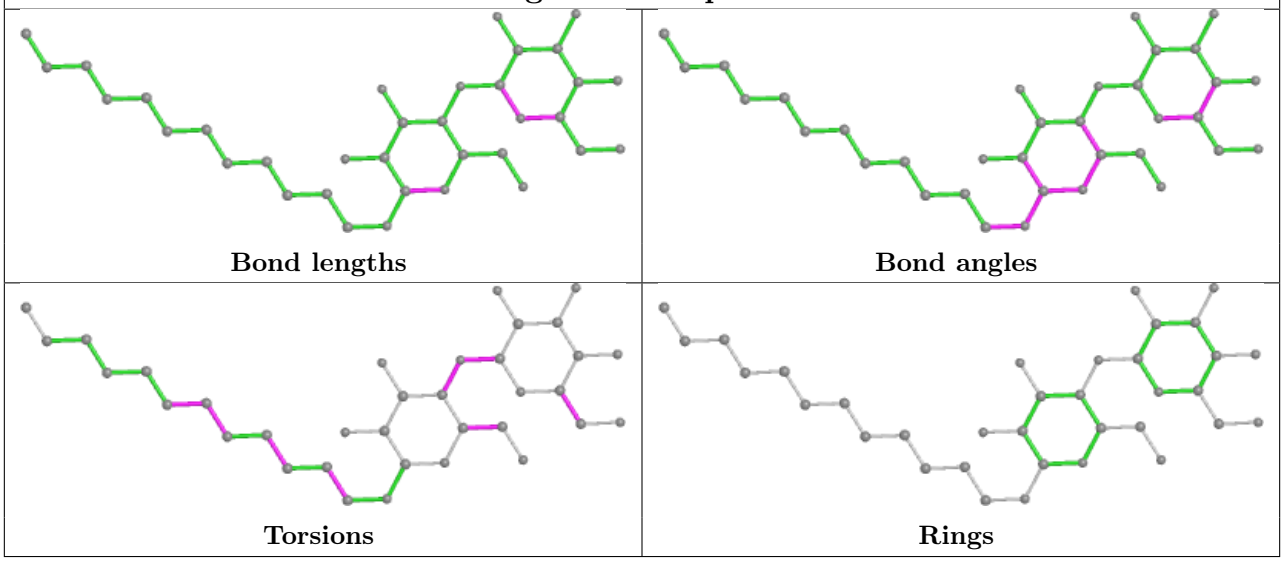
Ligand CDL N 1302



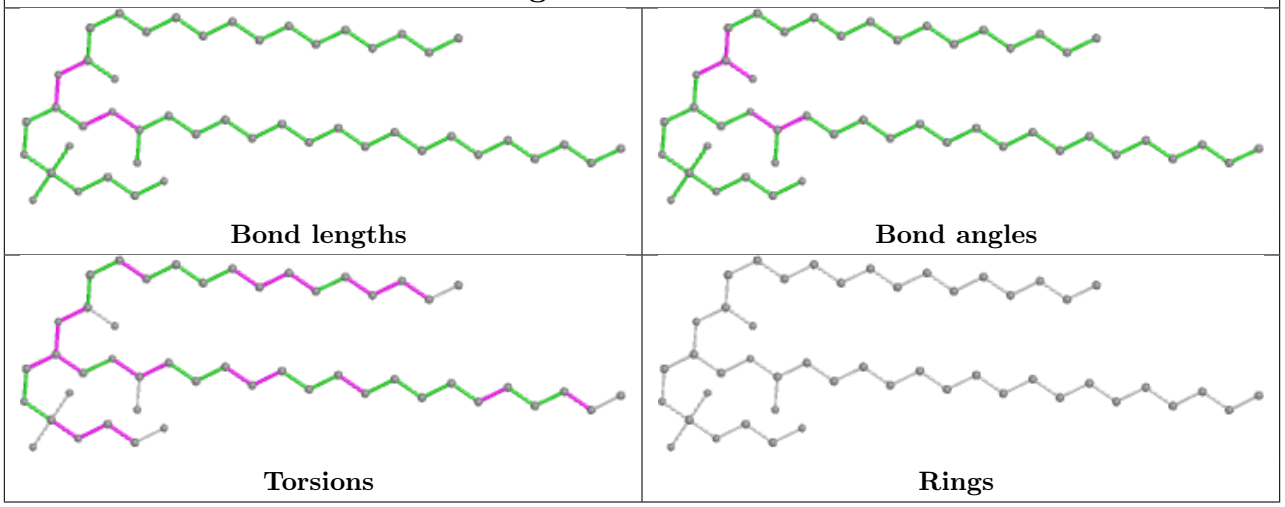
Ligand LMT J 201



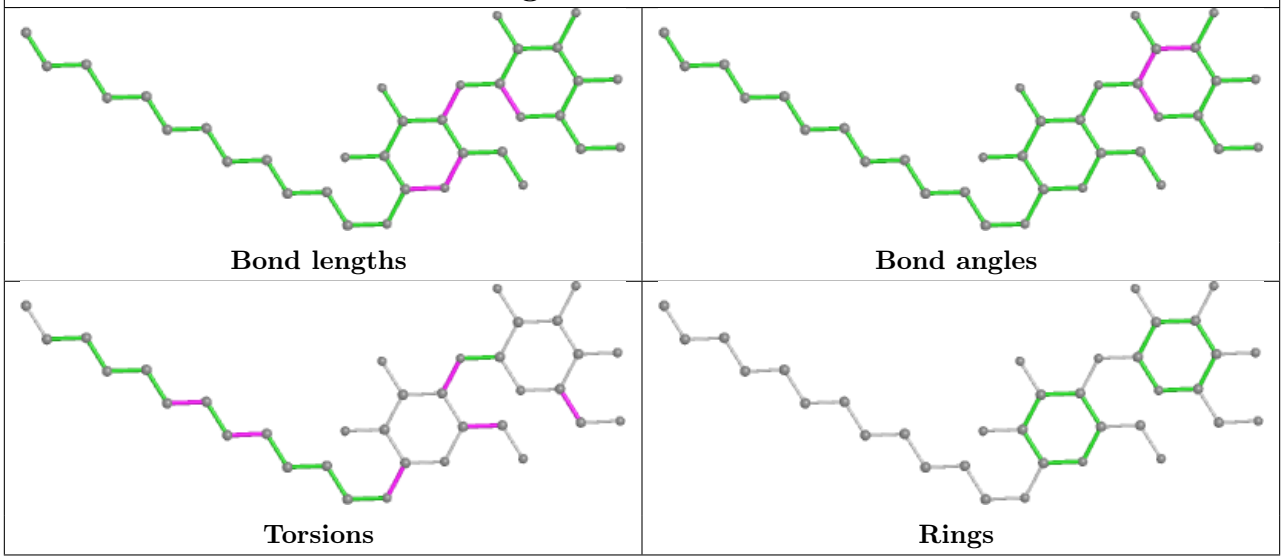
Ligand LMT p 201



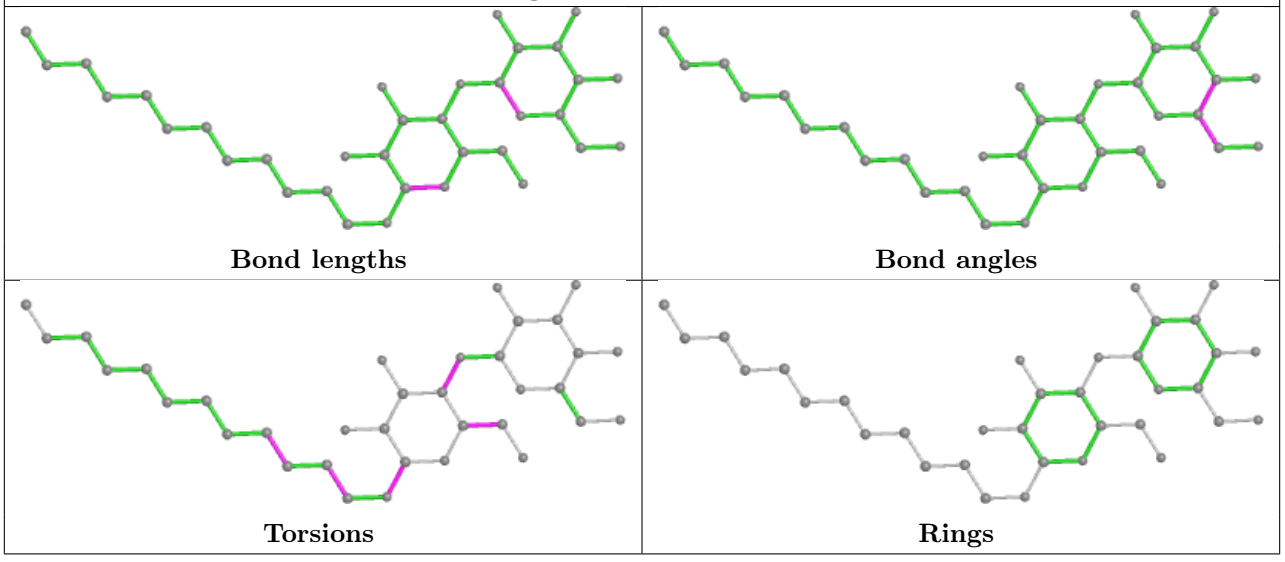
Ligand 3PE A 901



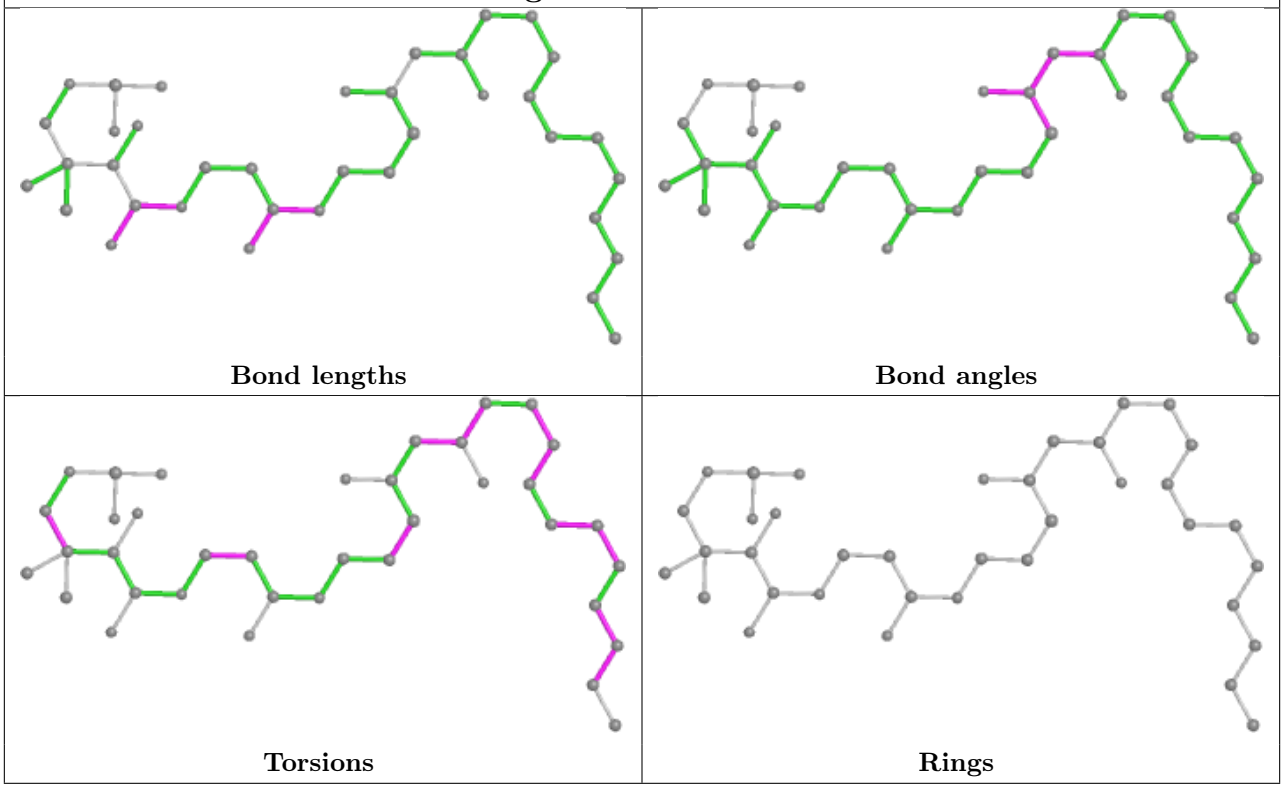
Ligand LMT H 401



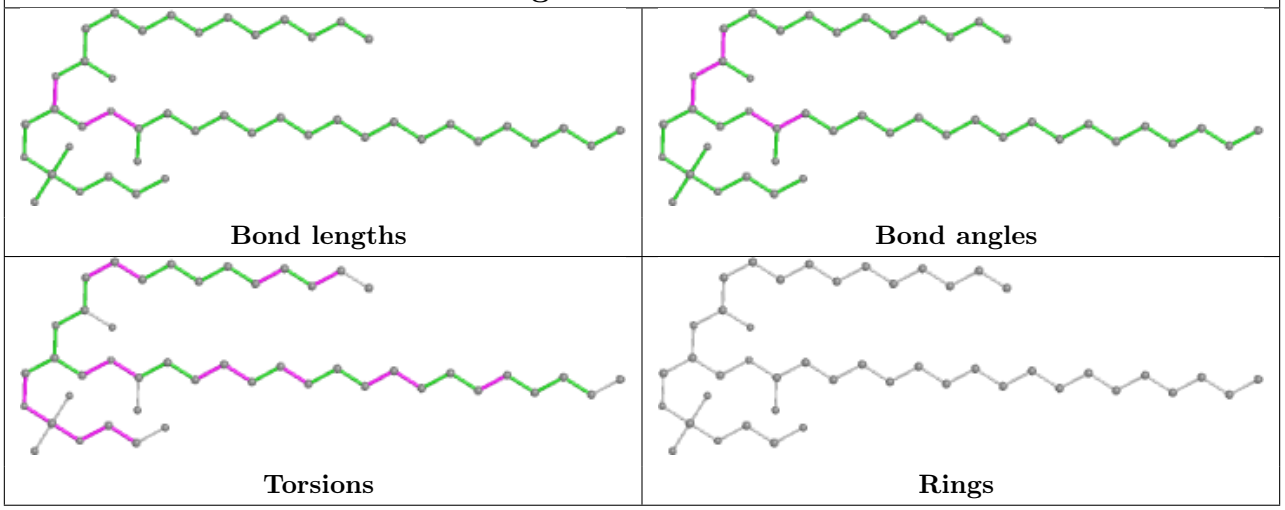
Ligand LMT b 301



Ligand EHZ U 101



Ligand 3PE L 703



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.

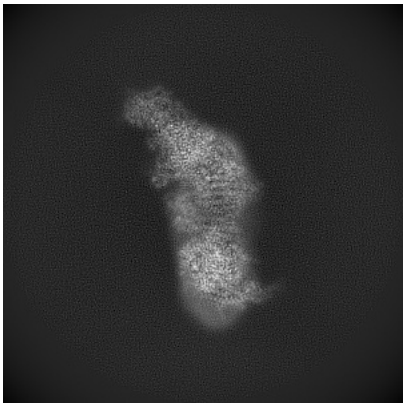
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14307. These allow visual inspection of the internal detail of the map and identification of artifacts.

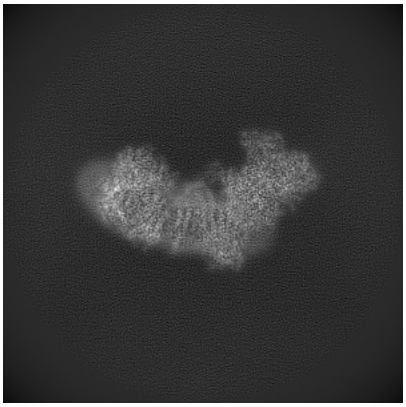
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

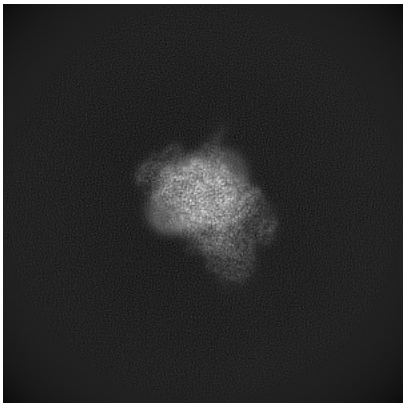
6.1.1 Primary map



X



Y

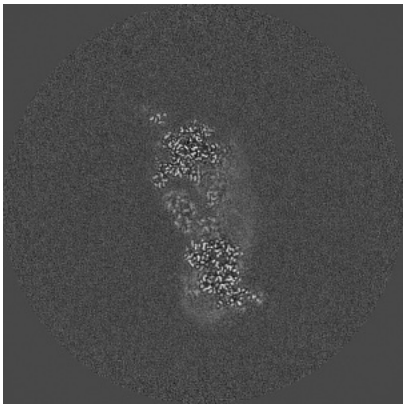


Z

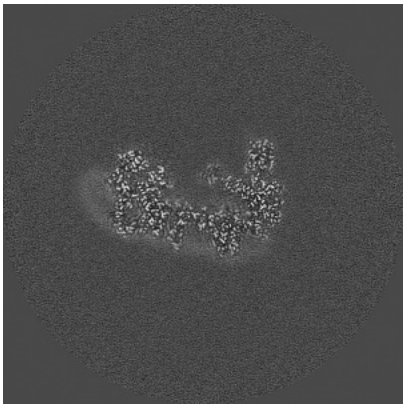
The images above show the map projected in three orthogonal directions.

6.2 Central slices

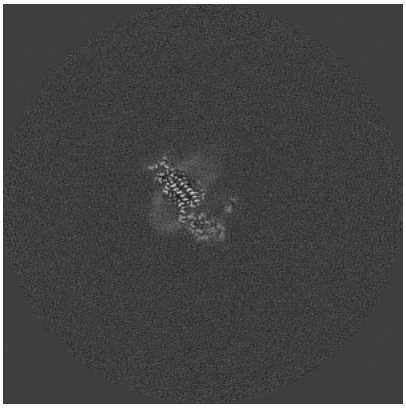
6.2.1 Primary map



X Index: 330



Y Index: 330

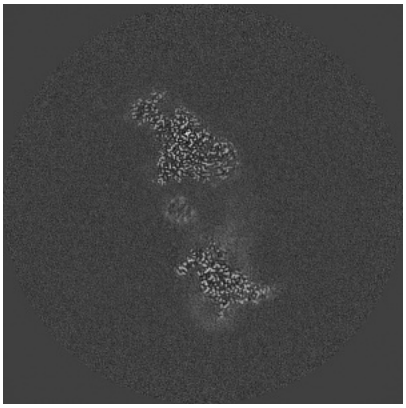


Z Index: 330

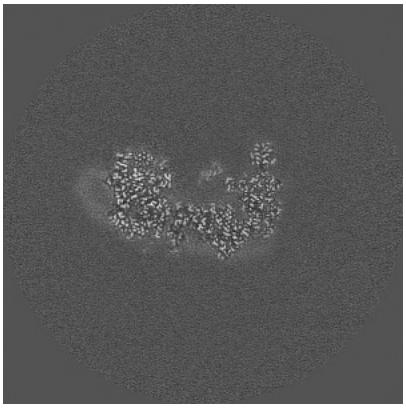
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

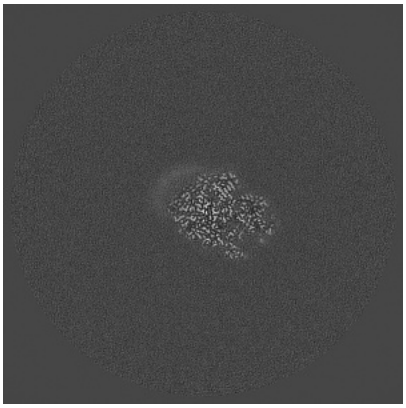
6.3.1 Primary map



X Index: 353



Y Index: 337



Z Index: 423

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.

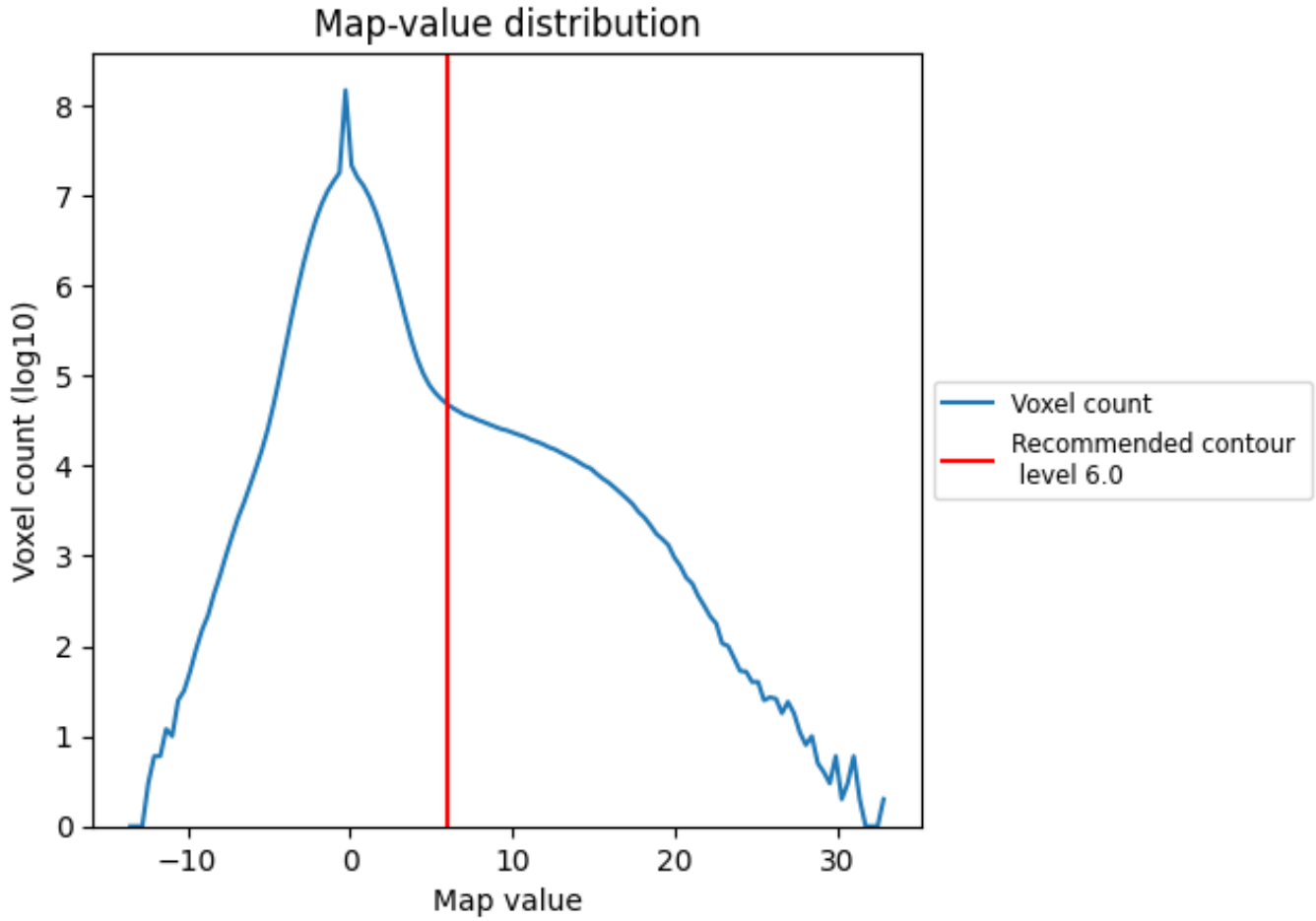
6.5 Mask visualisation (i)

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

7 Map analysis

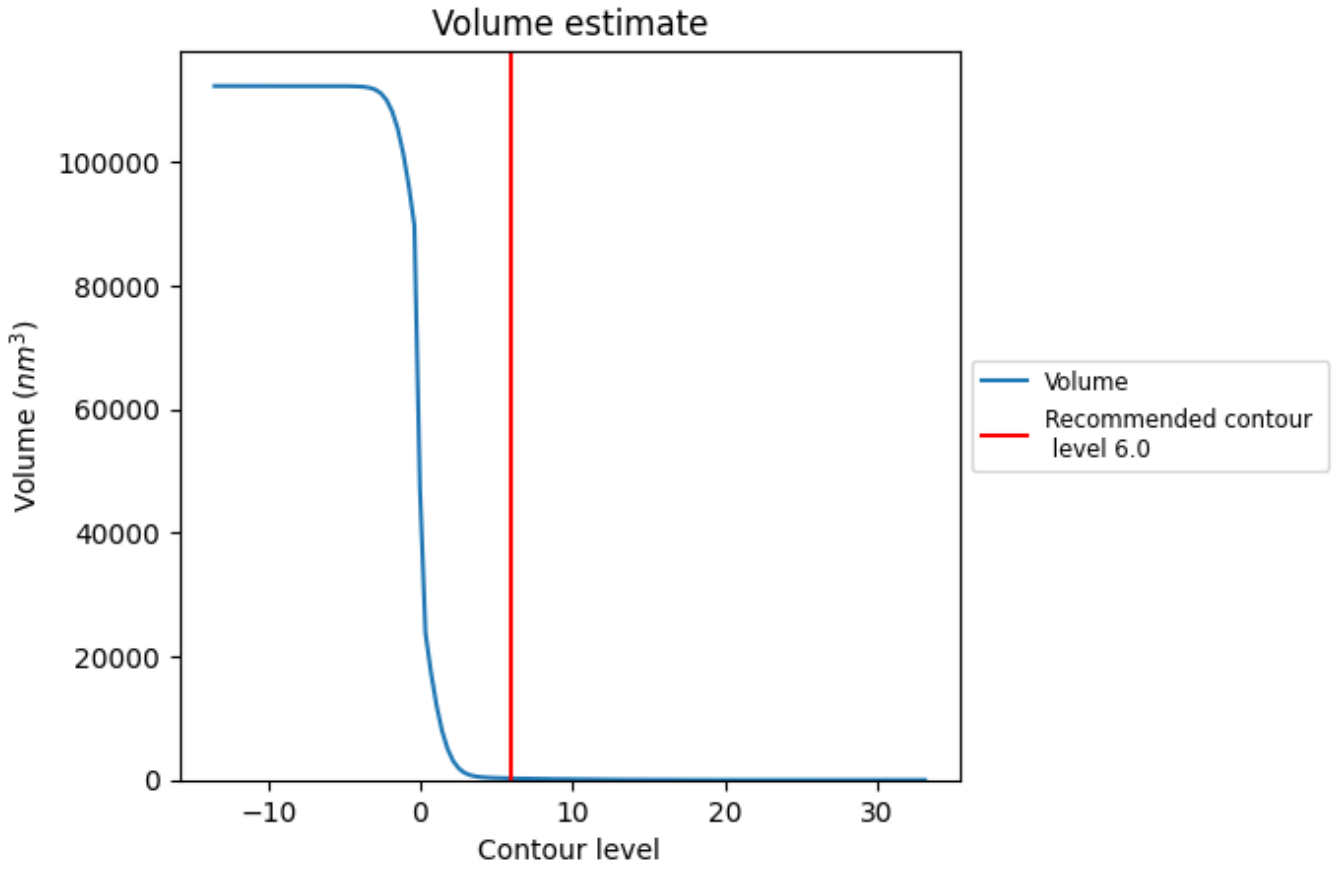
This section contains the results of statistical analysis of the map.

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.

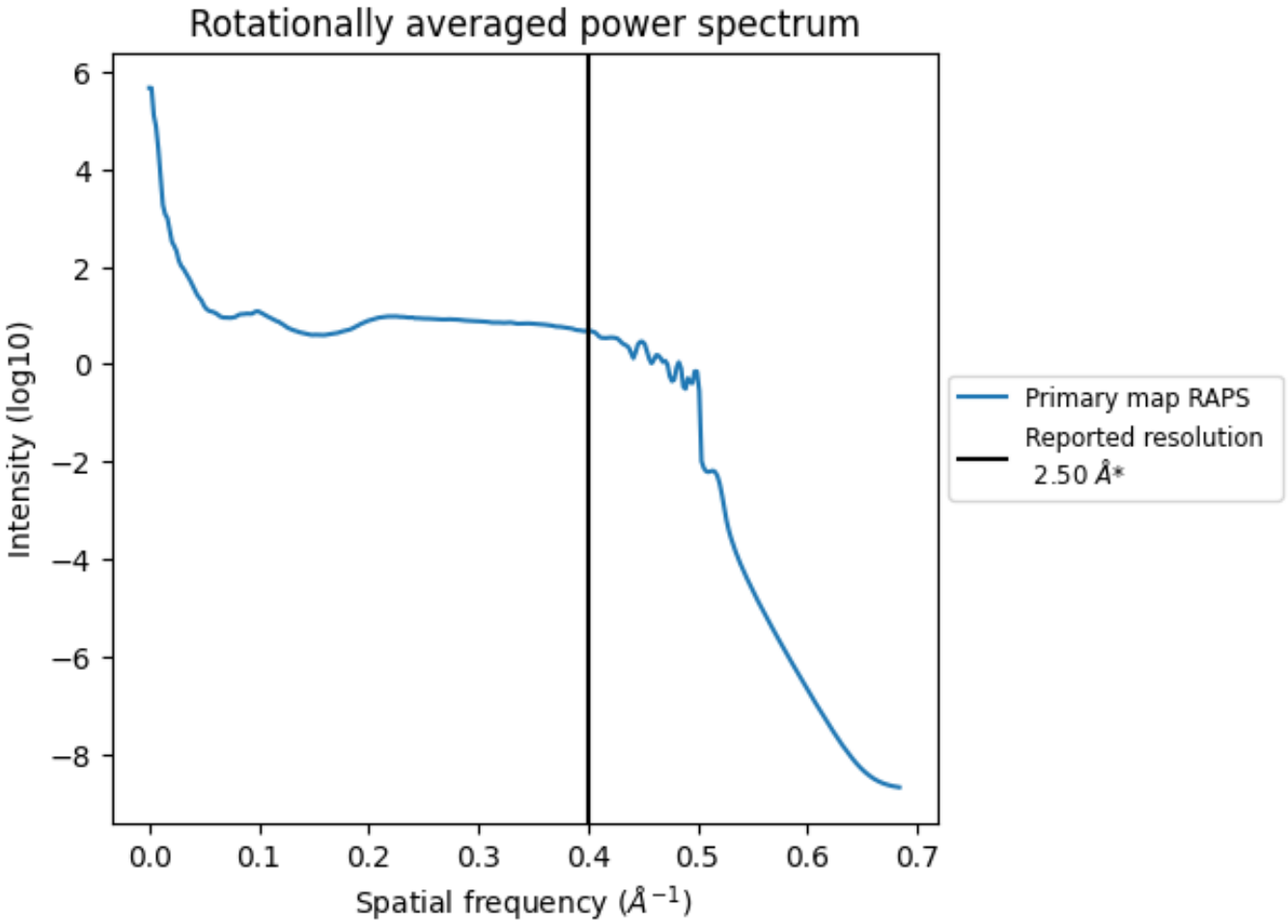
7.2 Volume estimate (i)



The volume at the recommended contour level is 253 nm^3; this corresponds to an approximate mass of 229 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 0.400 Å^{-1}

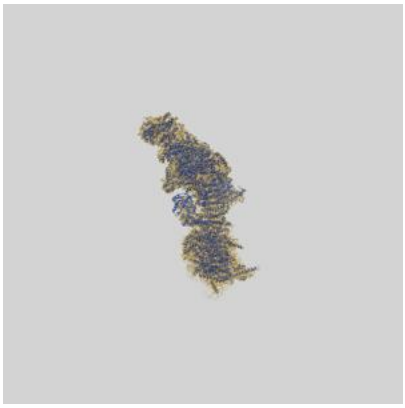
8 Fourier-Shell correlation

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

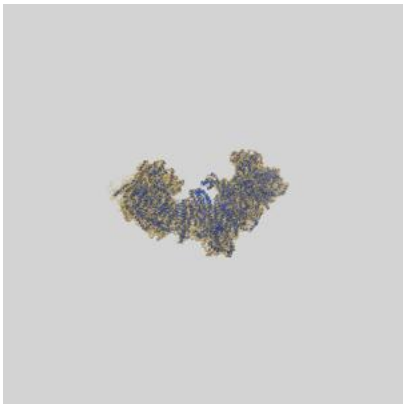
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14307 and PDB model 7R4G. Per-residue inclusion information can be found in section 3 on page 23.

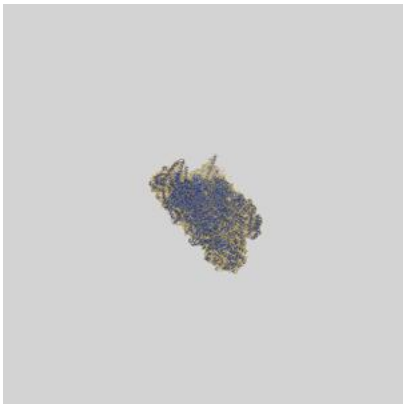
9.1 Map-model overlay



X



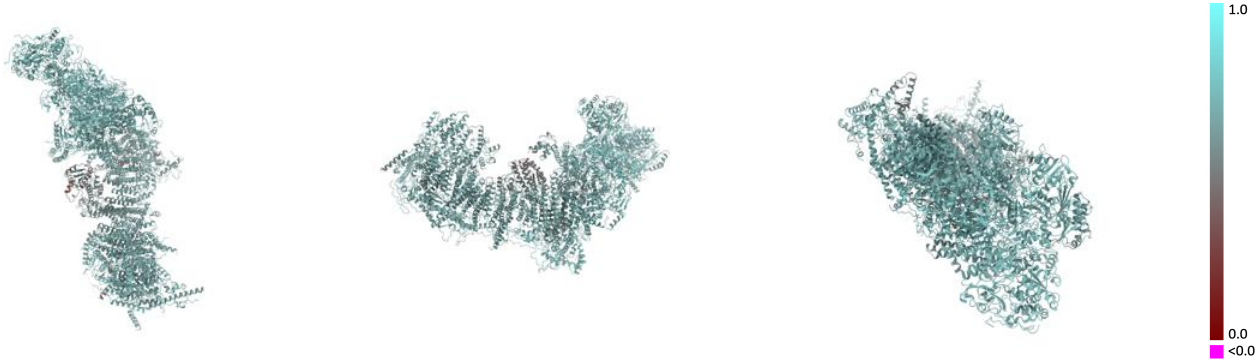
Y



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.

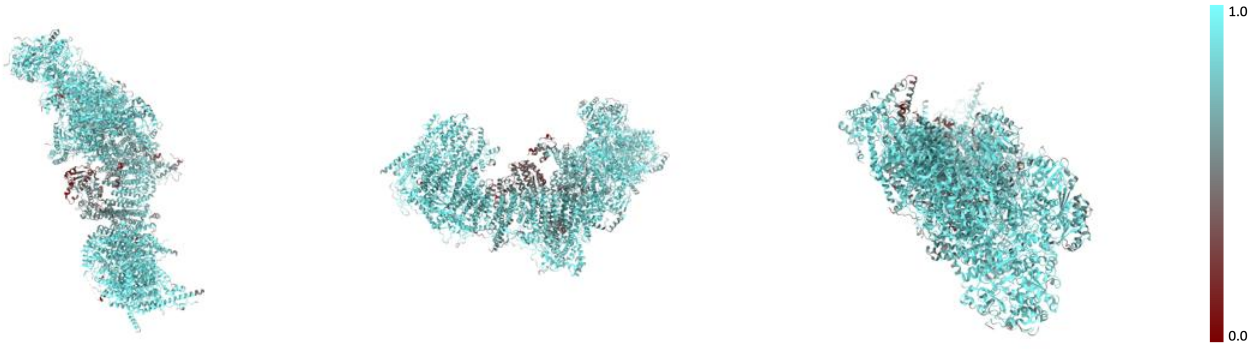
9.2 Q-score mapped to coordinate model



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.

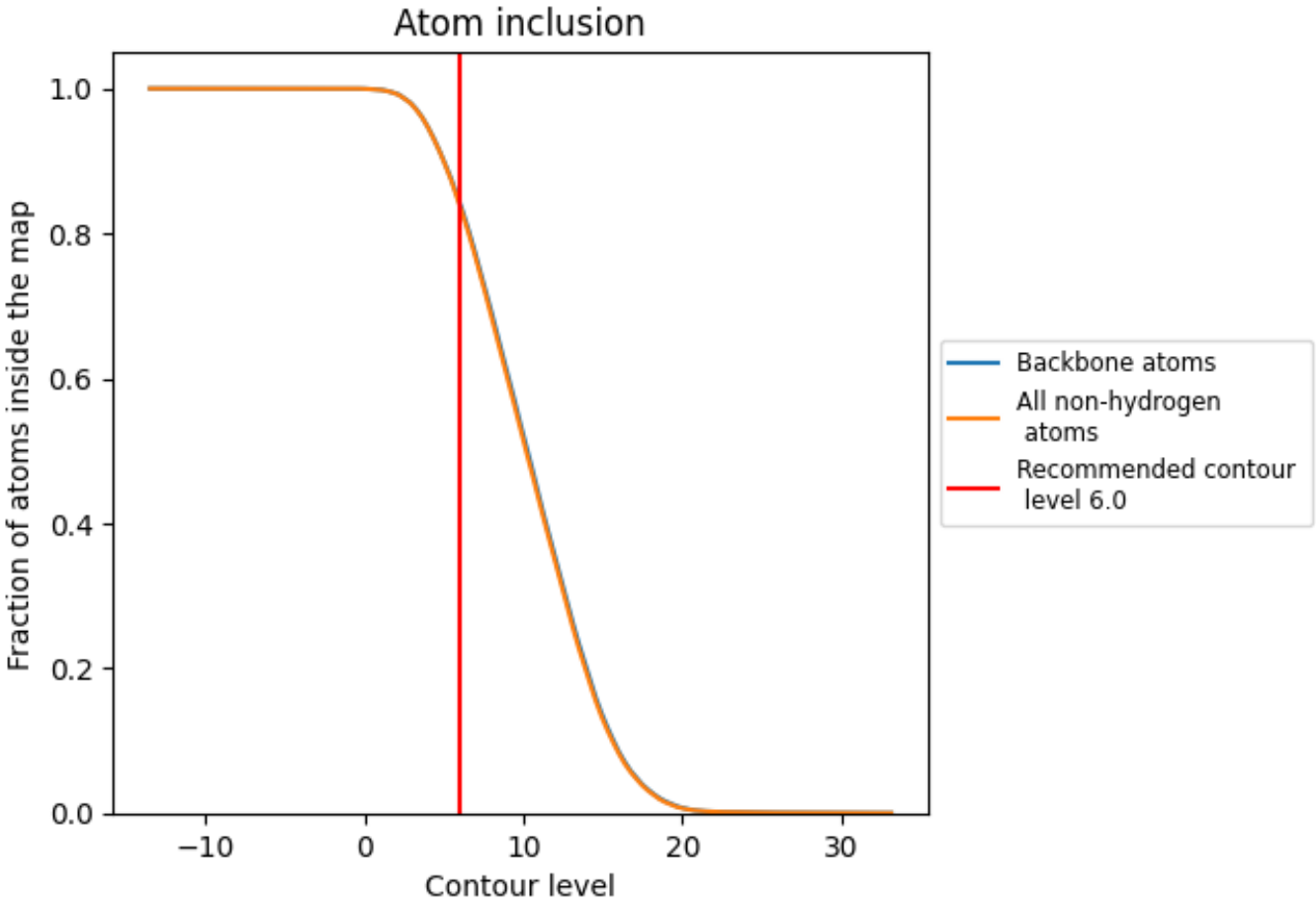
9.3 Atom inclusion mapped to coordinate model



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, 84% of all backbone atoms, 84% 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	0.8383	0.6620
A	0.7557	0.6400
B	0.8926	0.6960
C	0.9358	0.7150
D	0.9321	0.7110
E	0.8341	0.6700
F	0.8827	0.6820
G	0.8802	0.6920
H	0.8805	0.6760
I	0.9253	0.7160
J	0.7598	0.6340
K	0.8398	0.6620
L	0.9203	0.6550
M	0.9167	0.6680
N	0.8046	0.6520
O	0.4657	0.5290
P	0.8154	0.6640
Q	0.8802	0.6990
R	0.8876	0.7000
S	0.7842	0.6600
T	0.4876	0.5850
U	0.9143	0.6530
V	0.8058	0.6730
W	0.8089	0.6770
X	0.8011	0.6520
Y	0.4967	0.6310
Z	0.7471	0.6380
a	0.8854	0.6740
b	0.7693	0.6390
c	0.6162	0.5970
d	0.7830	0.6510
e	0.7668	0.6460
f	0.8151	0.6310
g	0.8945	0.6530
h	0.8751	0.6620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8616	0.6330
j	0.8850	0.6330
k	0.8794	0.6280
l	0.8603	0.6380
m	0.8542	0.6430
n	0.8988	0.6510
o	0.8731	0.6340
p	0.8806	0.6510
q	0.7998	0.6830
r	0.8531	0.6950
s	0.8197	0.6780