wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 09:06 pm BST

PDB ID	:	8OM1 / pdb_00008om1
EMDB ID	:	EMD-16965
Title	:	Mitochondrial complex I from Mus musculus in the active state
Authors	:	Grba, D.N.; Chung, I.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on	:	2023-03-31
Resolution	:	2.39 Å(reported)
Based on initial model	:	6ZR2

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:

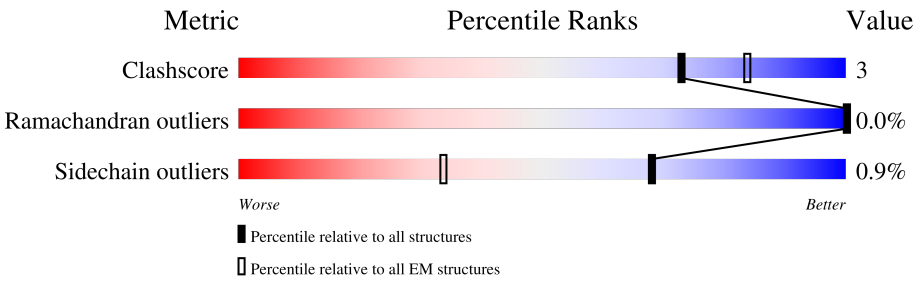
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

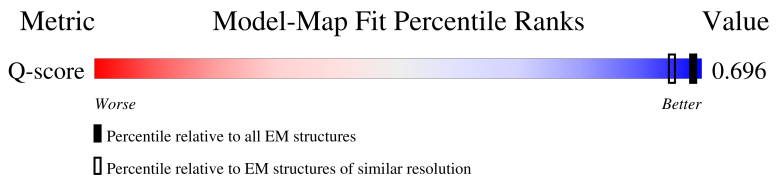
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	92% 8%
2	B	224	60% 10% 30%
3	C	263	71% 7% 21%
4	D	463	86% 7% 7%

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Mol	Chain	Length	Quality of chain
5	E	248	75% 11% 14%
6	F	464	85% 7% 7%
7	G	727	87% 8% 5%
8	H	318	88% 11%
9	I	212	79% 5% 16%
10	J	172	90% 10%
11	K	98	92% 8%
12	L	607	91% 9%
13	M	459	91% 9%
14	N	345	90% 10%
15	O	355	84% 6% 10%
16	P	377	84% 7% 9%
17	Q	175	63% 9% 28%
18	R	116	78% 18%
19	S	99	79% 8% 13%
20	T	156	39% 11% 50%
20	U	156	53% 44%
21	V	116	92% 6%
22	W	131	82% 5% 13%
23	X	172	94% 5%
24	Y	142	96%
25	Z	144	88% 9%
26	a	70	94%
27	b	84	95%
28	c	76	61% 36%

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Mol	Chain	Length	Quality of chain
29	d	120	91% 9%
30	e	106	94% 5%
31	f	57	93% 5%
32	g	151	60% 7% 33%
33	h	189	72% 26%
34	i	127	72% 9% 18%
35	j	105	58% 5% 37%
36	k	104	69% 6% 25%
37	l	186	79% 5% 16%
38	m	129	90% 8%
39	n	179	92% 8%
40	o	136	82% 5% 12%
41	p	176	91% 5%
42	q	145	94% 6%
43	r	112	85% 5% 10%
44	s	104	37% 6% 58%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 71256 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	933	633	133	160	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1259	802	227	216	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	208	1730	1116	297	314	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3464	2215	595	630	24	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	689	5301	3324	920	1016	41	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	737	477	112	137	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	607	4809	3187	747	830	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3632	2408	567	617	40	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2607	1674	431	492	10	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	126	1021	646	179	192	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	86	685	430	130	122	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	78	628	404	93	126	5	0	0
20	U	88	706	453	104	144	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	114	927	604	154	166	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	171	1396	889	250	247	10	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	648	425	105	114	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	49	407	266	70	70	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	996	651	171	165	9	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	56	482	314	85	81	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	101	850	549	136	161	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	139	1166	764	195	204	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	66	566	372	94	99	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	157	1323	855	220	237	11	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	178	1541	985	276	269	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	119	1019	642	191	178	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	145	1212	779	215	213	5	0	0

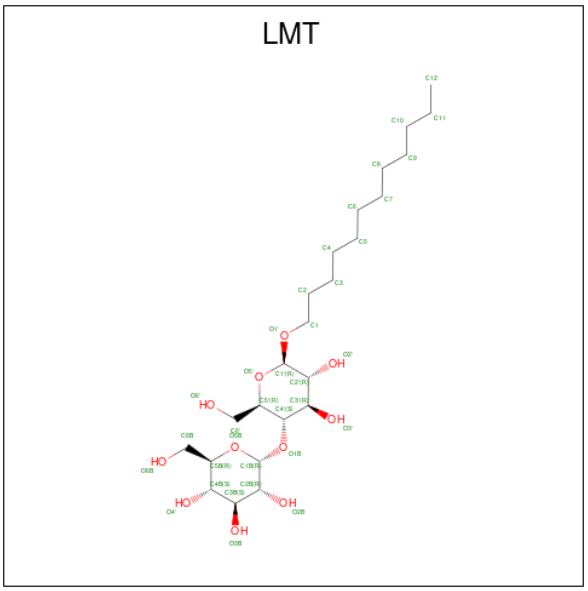
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	101	809	511	150	145	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	s	44	368	230	66	72	0	0

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



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

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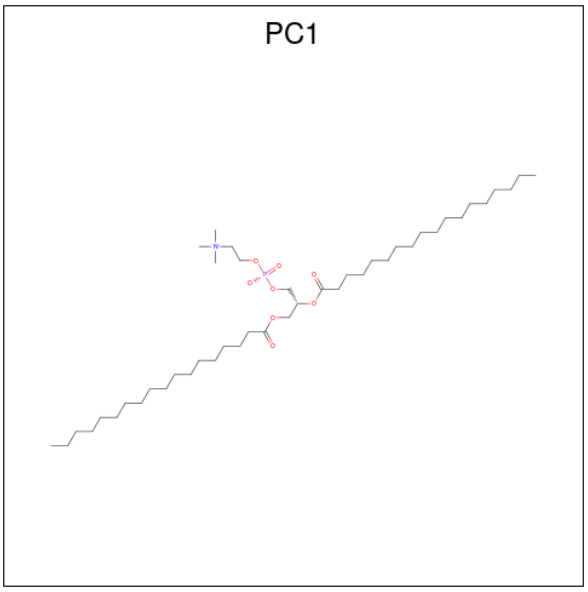
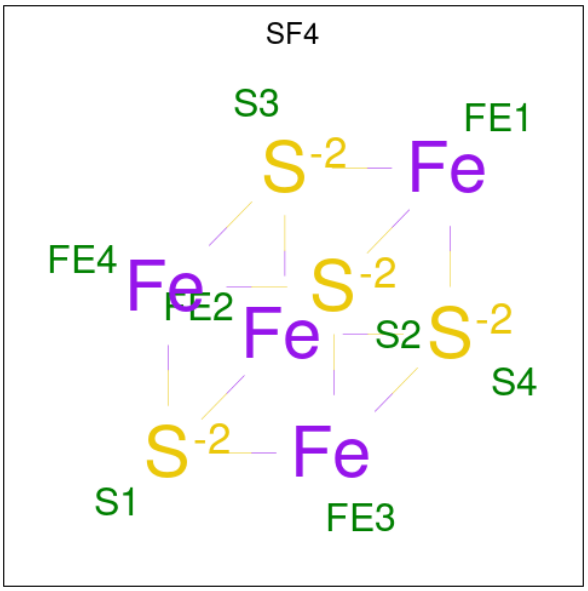
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	h	1	35	24	11	0
			Total	C	O	
45	j	1	35	24	11	0

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



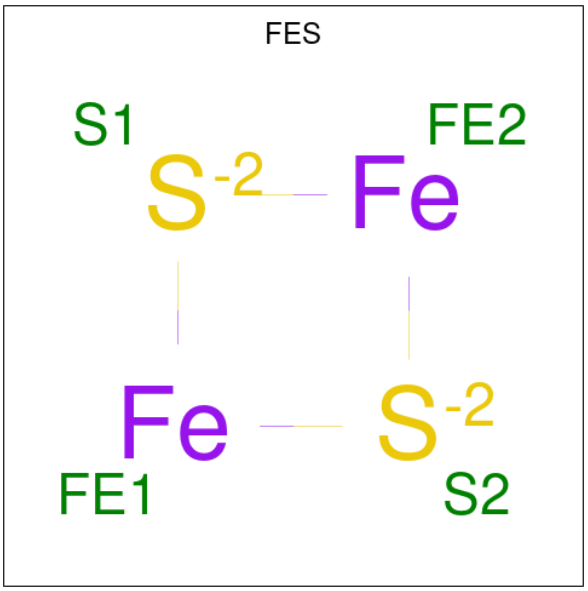
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	34	24	1	8	1	0
			Total	C	N	O	P	
46	B	1	43	33	1	8	1	0
			Total	C	N	O	P	
46	B	1	52	42	1	8	1	0
			Total	C	N	O	P	
46	L	1	27	17	1	8	1	0
			Total	C	N	O	P	
46	p	1	36	26	1	8	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



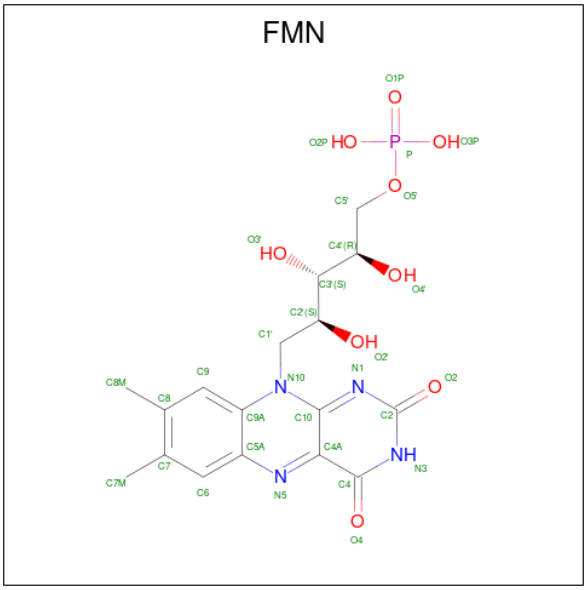
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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

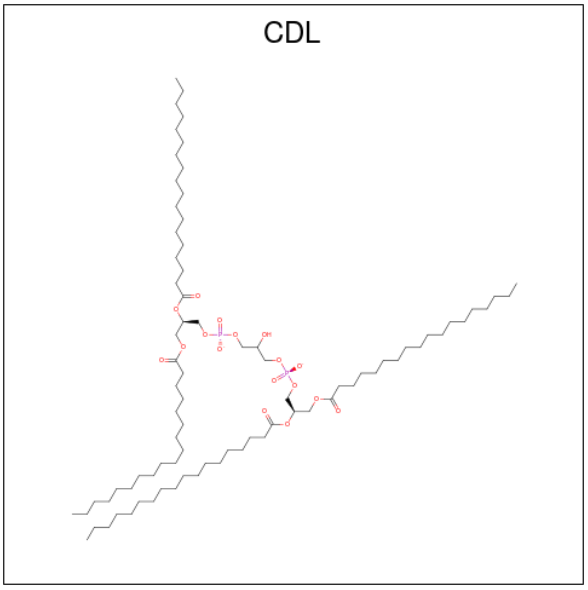


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	F	1	31	17	4	9	1	0

- Molecule 50 is SODIUM ION (CCD ID: NA) (formula: Na).

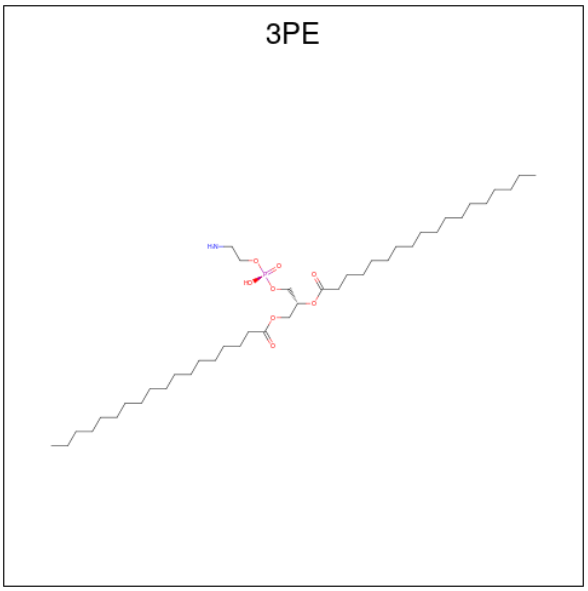
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
50	G	1	1	1	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	H	1	51	33	16	2	0
			Total	C	O	P	
51	K	1	71	52	17	2	0
			Total	C	O	P	
51	L	1	68	49	17	2	0
			Total	C	O	P	
51	h	1	58	39	17	2	0
			Total	C	O	P	
51	h	1	78	60	16	2	0
			Total	C	O	P	
51	q	1	62	43	17	2	0

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	I	1	36	26	1	8	1	0
			Total	C	N	O	P	
52	I	1	44	34	1	8	1	0
			Total	C	N	O	P	
52	L	1	43	33	1	8	1	0
			Total	C	N	O	P	
52	L	1	45	35	1	8	1	0
			Total	C	N	O	P	
52	M	1	41	31	1	8	1	0
			Total	C	N	O	P	
52	N	1	34	24	1	8	1	0
			Total	C	N	O	P	
52	N	1	38	28	1	8	1	0
			Total	C	N	O	P	
52	O	1	30	20	1	8	1	0
			Total	C	N	O	P	
52	X	1	37	27	1	8	1	0
			Total	C	N	O	P	
52	Y	1	38	28	1	8	1	0
			Total	C	N	O	P	
52	Z	1	43	33	1	8	1	0
			Total	C	N	O	P	
52	d	1	43	33	1	8	1	0
			Total	C	N	O	P	
52	d	1	32	22	1	8	1	0
			Total	C	N	O	P	
52	f	1	42	32	1	8	1	0

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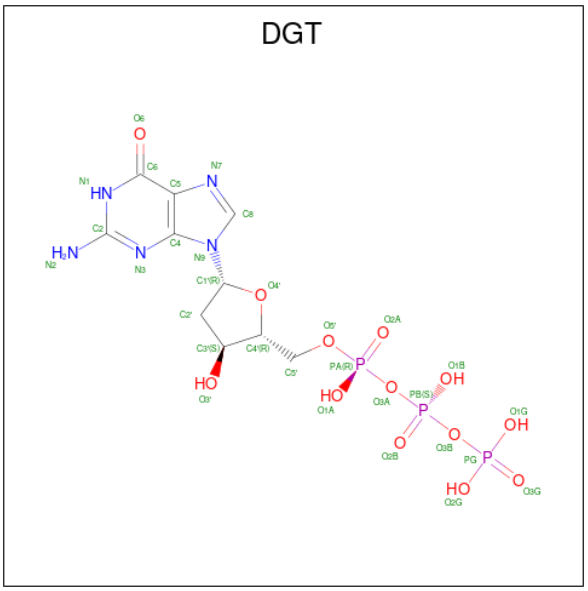
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	i	1	30	20	1	8	1	0
			Total	C	N	O	P	
52	r	1	46	36	1	8	1	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

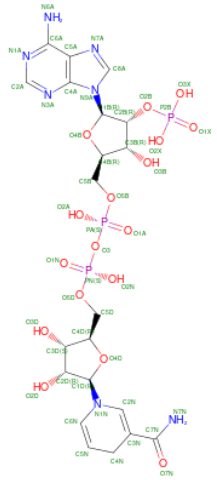
- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

NDP



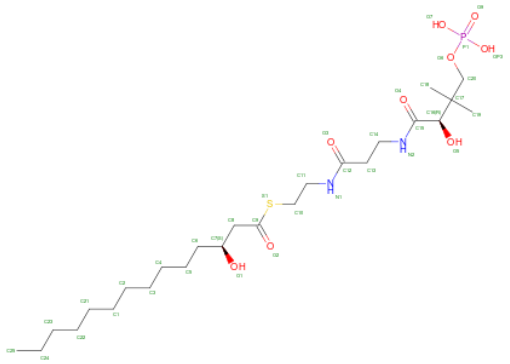
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	P	1	48	21	7	17	3	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

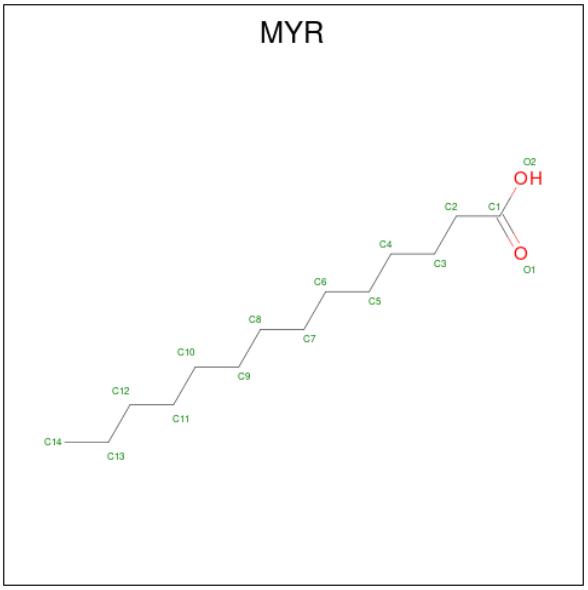
- Molecule 57 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

EHZ



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

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
59	A	59	59	59	0
59	B	96	96	96	0
59	C	160	160	160	0
59	D	257	257	257	0
59	E	43	43	43	0
59	F	85	85	85	0
59	G	300	300	300	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
59	H	120	120	120	0
			Total	O	
59	I	124	124	124	0
			Total	O	
59	J	60	60	60	0
			Total	O	
59	K	41	41	41	0
			Total	O	
59	L	105	105	105	0
			Total	O	
59	M	190	190	190	0
			Total	O	
59	N	123	123	123	0
			Total	O	
59	O	108	108	108	0
			Total	O	
59	P	149	149	149	0
			Total	O	
59	Q	120	120	120	0
			Total	O	
59	R	52	52	52	0
			Total	O	
59	S	2	2	2	0
			Total	O	
59	T	1	1	1	0
			Total	O	
59	U	3	3	3	0
			Total	O	
59	V	35	35	35	0
			Total	O	
59	W	58	58	58	0
			Total	O	
59	X	64	64	64	0
			Total	O	
59	Y	2	2	2	0
			Total	O	
59	Z	73	73	73	0
			Total	O	
59	a	37	37	37	0
			Total	O	
59	b	15	15	15	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
59	c	4	4	4	0
			Total	O	
59	d	31	31	31	0
			Total	O	
59	e	44	44	44	0
			Total	O	
59	f	11	11	11	0
			Total	O	
59	g	27	27	27	0
			Total	O	
59	h	45	45	45	0
			Total	O	
59	i	6	6	6	0
			Total	O	
59	j	2	2	2	0
			Total	O	
59	k	3	3	3	0
			Total	O	
59	l	37	37	37	0
			Total	O	
59	m	34	34	34	0
			Total	O	
59	n	31	31	31	0
			Total	O	
59	p	45	45	45	0
			Total	O	
59	q	84	84	84	0
			Total	O	
59	r	51	51	51	0
			Total	O	
59	s	8	8	8	0

3 Residue-property plots (i)

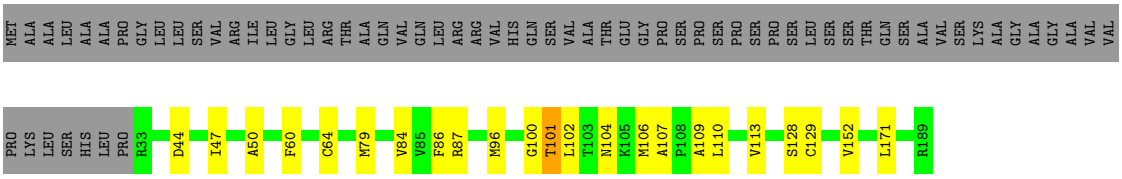
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 92% 8%

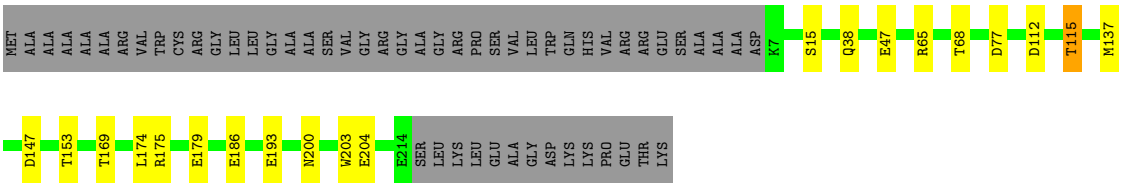
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 60% 10% 30%



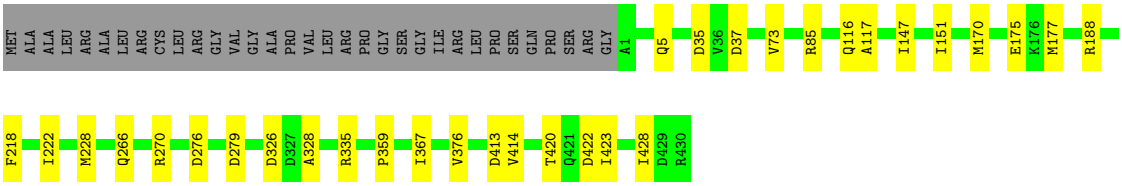
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 71% 7% 21%



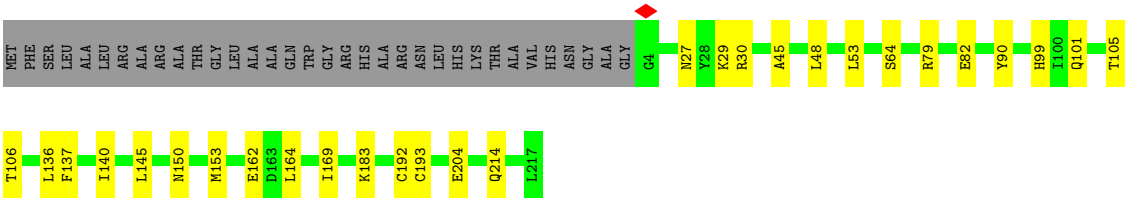
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 86% 7% 7%



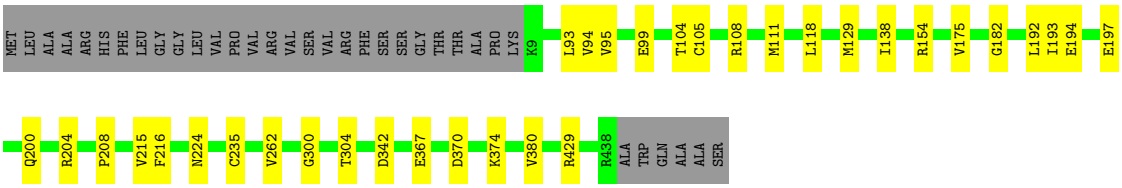
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 75% 11% 14%



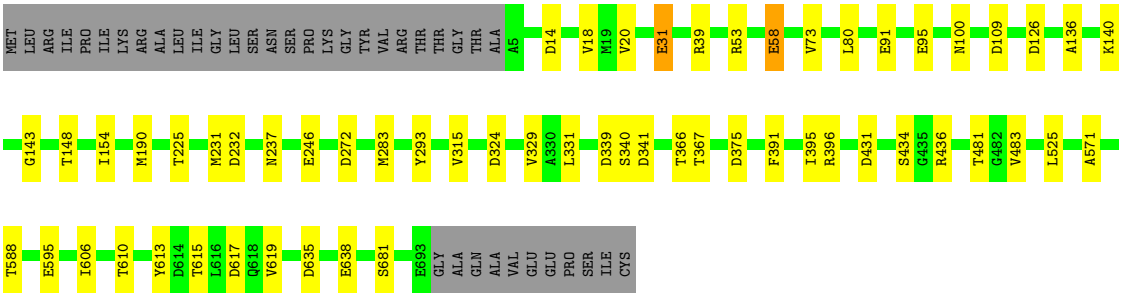
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 85% 7% 7%



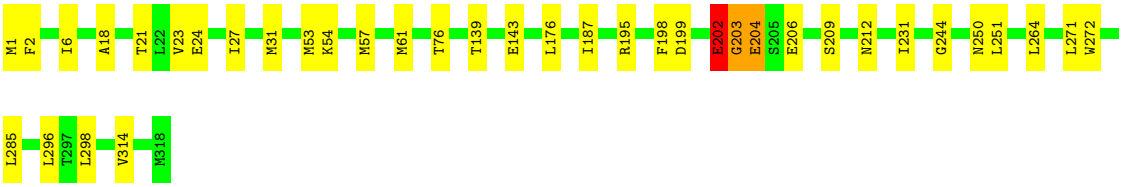
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 87% 8% 5%



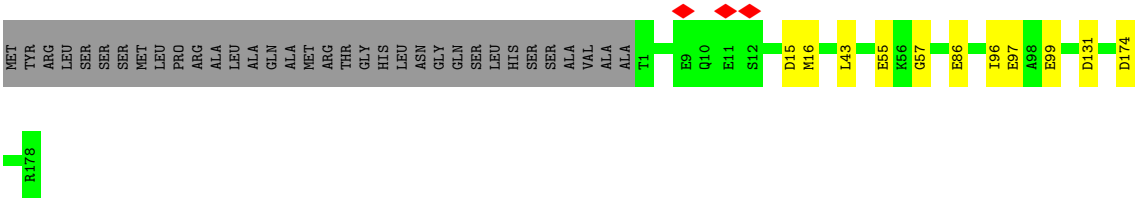
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 88% 11%



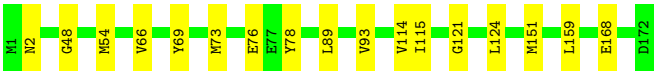
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I: 79% 5% 16%



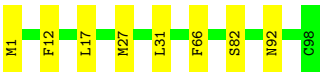
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 90% 10%



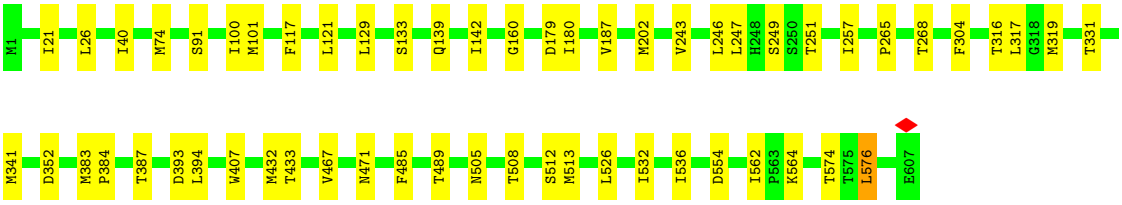
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 92% 8%



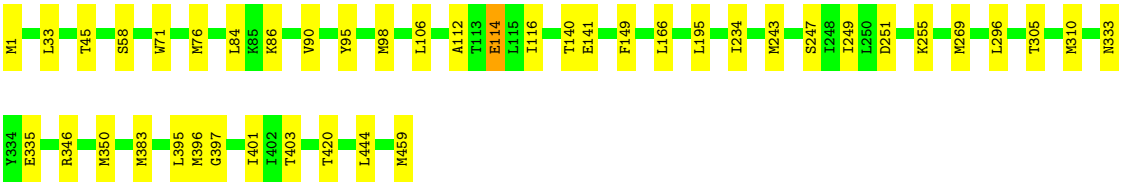
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 91% 9%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 91% 9%



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 90% 10%

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

Chain O:

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

Chain P:

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

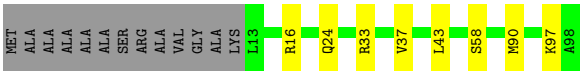
Chain Q:

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

Chain R:

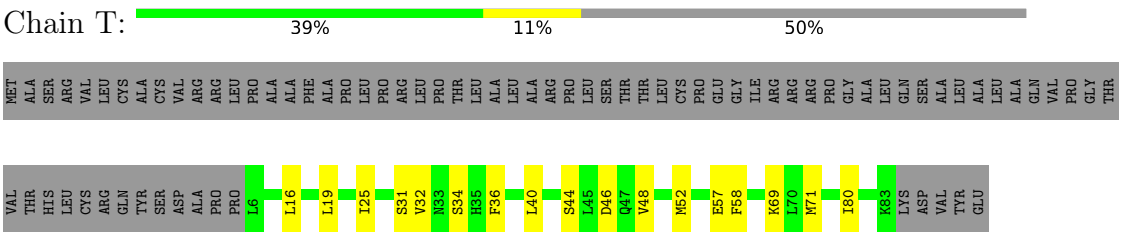
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



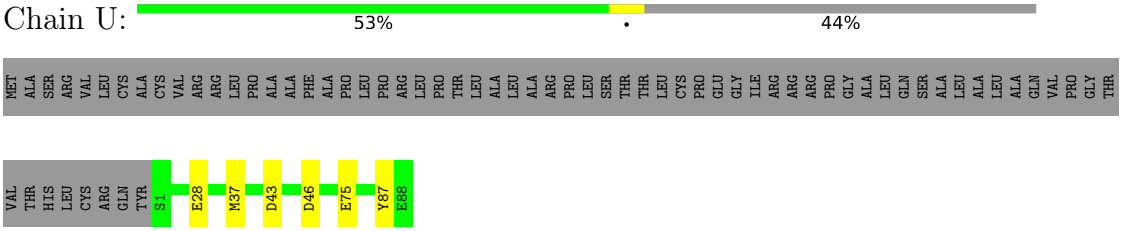
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



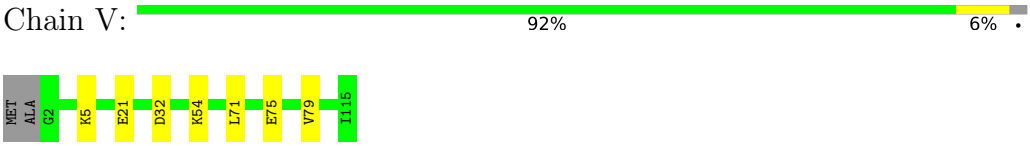
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



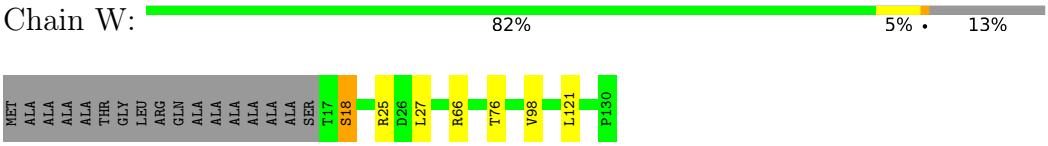
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



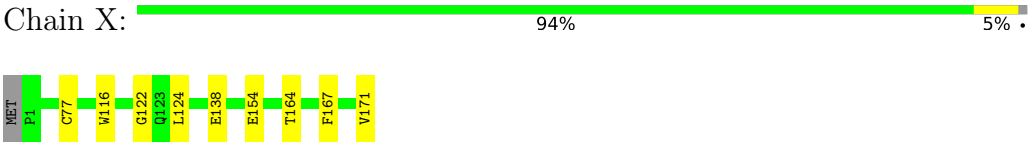
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



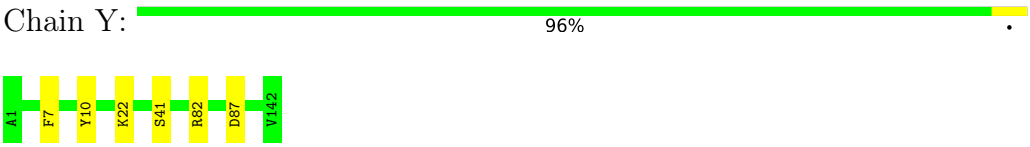
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



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

Chain Y:



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

Chain Z: 88% 9%

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

Chain a: 94%

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

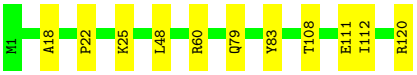
Chain b: 95%

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

Chain c: 61% 36%

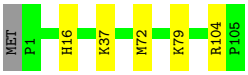
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d: 91% 9%



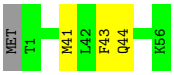
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 94% 5%



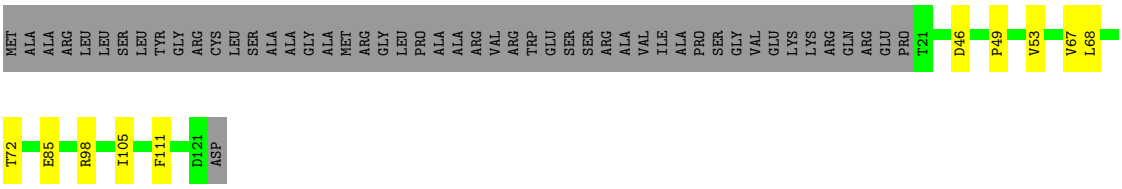
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 93% 5%



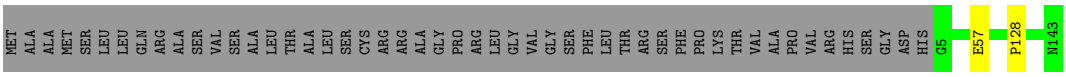
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 60% 7% 33%



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

Chain h: 72% 26%

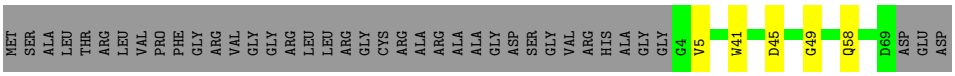


• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 72% 9% 18%

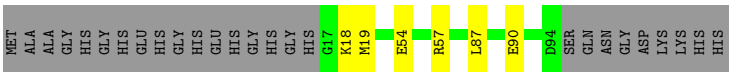
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j: 58% 5% 37%



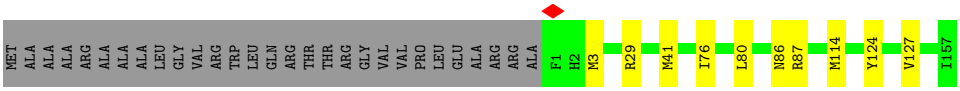
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k: 69% 6% 25%



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

Chain l: 79% 5% 16%



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

Chain m: 90% 8%

MET SER GLY S3 D23 V24 S25 T28 E34 I65 N85 W100 E117 I126 S127 Y128

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

Chain n: 92% 8%

MET A1 C30 R33 D34 K35 R44 H75 K126 E130 Q140 T143 D146 R174 E175 R176 P177 T178

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

Chain o: 82% 5% 12%

G1 R7 D11 V14 A48 Q49 L50 E82 R97 A119 ARG VAL ALA GLN GLY GLN GLY GLU GLY GLU VAL GLY PRO GLU VAL ALA LEU

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

Chain p: 91% 5%

MET PRO ASP S3 A18 P19 Y67 R68 I73 M102 E129 D144 K159 E172 ALA ALA ALA

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

Chain q: 94% 6%

M1 R34 F55 D78 G79 S80 D95 P126 R131 E136 K145

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

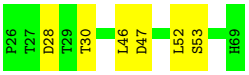
Chain r: 85% 5% 10%

A1 Q24 L25 T34 T55 L75 V76 S77 GLY LYS ALA ALA GLU SER SER ALA MET ALA ALA T89 T95 L112

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

Chain s: 37% 6% 58%

MET ALA VAL SER LEU LEU LEU ARG GLY GLY ARG ILE ARG ALA LEU LYS ALA VAL LEU LEU GLU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL VAL ARG LEU SER THR GLU SER GLU LYS SER ALA LYS GLU LYS GLU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO GLU


P26
T27
D28
T29
T30
L46
D47
L52
S53
H69

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109866	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	44.320	Depositor
Minimum map value	-20.720	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.927	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	480.62003, 480.62003, 480.62003	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6866, 0.6866, 0.6866	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, 2MR, PC1, MG, AME, NDP, EHZ, CDL, 3PE, NA, ZN, FME, LMT, WYK, SF4, FMN, MYR, FES, AYA, DGT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/949	0.40	0/1297
2	B	0.32	0/1277	0.46	0/1727
3	C	0.29	0/1780	0.45	0/2424
4	D	0.29	0/3540	0.41	0/4795
5	E	0.25	0/1700	0.41	0/2316
6	F	0.29	0/3396	0.37	0/4586
7	G	0.29	0/5388	0.39	0/7300
8	H	0.31	0/2607	0.49	1/3564 (0.0%)
9	I	0.30	0/1461	0.43	0/1974
10	J	0.25	0/1330	0.35	0/1810
11	K	0.25	0/738	0.34	0/1002
12	L	0.29	0/4922	0.36	0/6698
13	M	0.28	0/3709	0.38	0/5052
14	N	0.29	0/2755	0.41	0/3751
15	O	0.28	0/2674	0.36	0/3626
16	P	0.28	0/2823	0.39	0/3828
17	Q	0.28	0/1044	0.37	0/1409
18	R	0.28	0/762	0.36	0/1026
19	S	0.29	0/696	0.39	0/938
20	T	0.21	0/637	0.40	0/858
20	U	0.30	0/718	0.34	0/970
21	V	0.25	0/949	0.31	0/1286
22	W	0.27	0/993	0.40	0/1335
23	X	0.26	0/1434	0.38	0/1937
24	Y	0.27	0/1074	0.30	0/1456
25	Z	0.28	0/1192	0.38	0/1608
26	a	0.28	0/577	0.40	0/777
27	b	0.26	0/671	0.34	0/921
28	c	0.28	0/418	0.43	0/567
29	d	0.28	0/1028	0.40	0/1387
30	e	0.27	0/900	0.41	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.26	0/495	0.33	0/667
32	g	0.27	0/878	0.41	0/1196
33	h	0.30	0/1201	0.40	0/1626
34	i	0.29	0/889	0.42	0/1210
35	j	0.28	0/591	0.33	0/809
36	k	0.28	0/650	0.32	0/878
37	l	0.29	0/1379	0.38	0/1882
38	m	0.31	0/1079	0.42	0/1463
39	n	0.31	0/1596	0.36	0/2162
40	o	0.29	0/1044	0.40	0/1401
41	p	0.29	0/1472	0.40	0/1989
42	q	0.28	0/1243	0.39	0/1692
43	r	0.29	0/819	0.42	0/1108
44	s	0.26	0/379	0.48	0/515
All	All	0.28	0/67857	0.39	1/92022 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	202	GLU	N-CA-C	-5.01	106.01	112.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	0	969	8	0
2	B	1259	0	1255	14	0
3	C	1730	0	1686	17	0
4	D	3464	0	3416	22	0
5	E	1660	0	1653	17	0
6	F	3321	0	3278	22	0
7	G	5301	0	5327	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2540	0	2626	23	0
9	I	1431	0	1383	8	0
10	J	1308	0	1319	17	0
11	K	737	0	768	6	0
12	L	4809	0	4991	38	0
13	M	3632	0	3853	35	0
14	N	2703	0	2902	27	0
15	O	2607	0	2566	17	0
16	P	2748	0	2768	19	0
17	Q	1021	0	1022	13	0
18	R	748	0	724	4	0
19	S	685	0	706	4	0
20	T	628	0	626	9	0
20	U	706	0	698	5	0
21	V	927	0	968	5	0
22	W	970	0	991	7	0
23	X	1396	0	1385	8	0
24	Y	1050	0	1039	4	0
25	Z	1161	0	1161	9	0
26	a	564	0	579	3	0
27	b	648	0	652	3	0
28	c	407	0	407	2	0
29	d	996	0	1001	10	0
30	e	877	0	871	3	0
31	f	482	0	482	3	0
32	g	850	0	783	6	0
33	h	1166	0	1166	2	0
34	i	869	0	863	8	0
35	j	566	0	518	3	0
36	k	630	0	623	4	0
37	l	1323	0	1216	9	0
38	m	1050	0	1061	9	0
39	n	1541	0	1473	9	0
40	o	1019	0	1008	6	0
41	p	1439	0	1408	8	0
42	q	1212	0	1171	9	0
43	r	809	0	843	5	0
44	s	368	0	346	5	0
45	A	70	0	88	1	0
45	H	35	0	45	2	0
45	J	70	0	89	2	0
45	L	105	0	131	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	M	35	0	40	0	0
45	N	70	0	89	0	0
45	Y	105	0	133	1	0
45	h	35	0	46	0	0
45	j	35	0	45	0	0
46	A	34	0	42	0	0
46	B	95	0	141	1	0
46	L	27	0	28	0	0
46	p	36	0	46	0	0
47	B	8	0	0	1	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	G	1	0	0	0	0
51	H	51	0	52	0	0
51	K	71	0	86	0	0
51	L	68	0	80	0	0
51	h	136	0	174	0	0
51	q	62	0	68	0	0
52	I	80	0	108	1	0
52	L	88	0	127	2	0
52	M	41	0	59	0	0
52	N	72	0	97	1	0
52	O	30	0	34	0	0
52	X	37	0	48	1	0
52	Y	38	0	50	1	0
52	Z	43	0	60	0	0
52	d	75	0	98	2	0
52	f	42	0	58	0	0
52	i	30	0	34	1	0
52	r	46	0	66	1	0
53	O	1	0	0	0	0
54	O	31	0	12	2	0
55	P	48	0	26	2	0
56	R	1	0	0	0	0
57	T	37	0	0	0	0
57	U	37	0	0	1	0
58	o	15	0	27	0	0
59	A	59	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B	96	0	0	2	0
59	C	160	0	0	11	0
59	D	257	0	0	10	0
59	E	43	0	0	3	0
59	F	85	0	0	6	0
59	G	300	0	0	21	0
59	H	120	0	0	6	0
59	I	124	0	0	3	0
59	J	60	0	0	4	0
59	K	41	0	0	2	0
59	L	105	0	0	6	0
59	M	190	0	0	14	0
59	N	123	0	0	7	0
59	O	108	0	0	6	0
59	P	149	0	0	13	0
59	Q	120	0	0	6	0
59	R	52	0	0	3	0
59	S	2	0	0	0	0
59	T	1	0	0	0	0
59	U	3	0	0	0	0
59	V	35	0	0	2	0
59	W	58	0	0	0	0
59	X	64	0	0	3	0
59	Y	2	0	0	0	0
59	Z	73	0	0	4	0
59	a	37	0	0	0	0
59	b	15	0	0	1	0
59	c	4	0	0	0	0
59	d	31	0	0	2	0
59	e	44	0	0	2	0
59	f	11	0	0	1	0
59	g	27	0	0	1	0
59	h	45	0	0	1	0
59	i	6	0	0	0	0
59	j	2	0	0	0	0
59	k	3	0	0	0	0
59	l	37	0	0	2	0
59	m	34	0	0	2	0
59	n	31	0	0	1	0
59	p	45	0	0	1	0
59	q	84	0	0	2	0
59	r	51	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	s	8	0	0	0	0
All	All	71256	0	68897	449	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 449 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:41:MET:SD	38:m:85:ASN:ND2	2.42	0.93
14:N:47:LYS:NZ	59:N:504:HOH:O	2.07	0.85
14:N:34:GLU:OE1	59:N:501:HOH:O	1.94	0.84
45:L:701:LMT:O2B	45:L:701:LMT:O3'	1.95	0.83
3:C:112:ASP:OD2	3:C:115:THR:OG1	1.98	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	206/263 (78%)	201 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
5	E	212/248 (86%)	205 (97%)	6 (3%)	1 (0%)	24	37
6	F	428/464 (92%)	417 (97%)	11 (3%)	0	100	100
7	G	687/727 (94%)	667 (97%)	20 (3%)	0	100	100
8	H	316/318 (99%)	305 (96%)	9 (3%)	2 (1%)	21	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
10	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	605/607 (100%)	583 (96%)	21 (4%)	1 (0%)	43	58
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	343/345 (99%)	340 (99%)	3 (1%)	0	100	100
15	O	318/355 (90%)	313 (98%)	5 (2%)	0	100	100
16	P	340/377 (90%)	332 (98%)	8 (2%)	0	100	100
17	Q	124/175 (71%)	123 (99%)	1 (1%)	0	100	100
18	R	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
20	T	76/156 (49%)	71 (93%)	5 (7%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	112 (100%)	0	0	100	100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	118 (100%)	0	0	100	100
30	e	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	f	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
32	g	99/151 (66%)	98 (99%)	1 (1%)	0	100	100
33	h	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
34	i	100/127 (79%)	94 (94%)	6 (6%)	0	100	100
35	j	64/105 (61%)	62 (97%)	2 (3%)	0	100	100
36	k	76/104 (73%)	73 (96%)	3 (4%)	0	100	100
37	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
40	o	117/136 (86%)	112 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	165 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	97/112 (87%)	90 (93%)	7 (7%)	0	100	100
44	s	42/104 (40%)	39 (93%)	3 (7%)	0	100	100
All	All	8150/9210 (88%)	7934 (97%)	212 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	183	LYS
8	H	203	GLY
8	H	244	GLY
12	L	562	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	B	132/184 (72%)	128 (97%)	4 (3%)	36	58
3	C	190/227 (84%)	188 (99%)	2 (1%)	65	82
4	D	370/394 (94%)	368 (100%)	2 (0%)	81	91
5	E	184/206 (89%)	181 (98%)	3 (2%)	55	76
6	F	345/370 (93%)	342 (99%)	3 (1%)	70	85
7	G	580/610 (95%)	575 (99%)	5 (1%)	70	85
8	H	279/279 (100%)	273 (98%)	6 (2%)	45	67
9	I	152/178 (85%)	150 (99%)	2 (1%)	61	80
10	J	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	87/87 (100%)	85 (98%)	2 (2%)	44	66
12	L	549/549 (100%)	545 (99%)	4 (1%)	76	88
13	M	414/414 (100%)	406 (98%)	8 (2%)	50	71
14	N	307/307 (100%)	305 (99%)	2 (1%)	76	88
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	296 (99%)	3 (1%)	68	84
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	75/80 (94%)	73 (97%)	2 (3%)	39	62
20	T	72/135 (53%)	69 (96%)	3 (4%)	26	45
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	85
23	X	153/154 (99%)	152 (99%)	1 (1%)	76	88
24	Y	106/106 (100%)	106 (100%)	0	100	100
25	Z	121/123 (98%)	119 (98%)	2 (2%)	53	74
26	a	59/60 (98%)	59 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	43/67 (64%)	43 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	91 (98%)	2 (2%)	45	67
31	f	52/53 (98%)	52 (100%)	0	100	100
32	g	92/129 (71%)	91 (99%)	1 (1%)	65	82
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	95/118 (80%)	95 (100%)	0	100	100
35	j	61/87 (70%)	60 (98%)	1 (2%)	55	76
36	k	60/78 (77%)	59 (98%)	1 (2%)	53	74
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	89
40	o	109/120 (91%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	155/158 (98%)	154 (99%)	1 (1%)	78	89
42	q	130/130 (100%)	130 (100%)	0	100	100
43	r	90/95 (95%)	90 (100%)	0	100	100
44	s	43/95 (45%)	42 (98%)	1 (2%)	44	66
All	All	7222/7942 (91%)	7159 (99%)	63 (1%)	68	85

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	82	SER
30	e	37	LYS
13	M	86	LYS
25	Z	113	THR
36	k	90	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
40	o	83	GLN
42	q	54	GLN
13	M	374	ASN
13	M	366	ASN
42	q	112	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	AME	q	1	42	9,10,11	1.46	1 (11%)	9,11,13	1.83	3 (33%)
1	FME	A	1	1	8,9,10	0.97	1 (12%)	7,9,11	0.82	0
12	FME	L	1	12	8,9,10	0.93	0	7,9,11	1.09	0
11	FME	K	1	11	8,9,10	0.98	1 (12%)	7,9,11	1.21	1 (14%)
34	SAC	i	1	34	7,8,9	0.50	0	8,9,11	0.78	1 (12%)
8	FME	H	1	8	8,9,10	0.97	1 (12%)	7,9,11	1.14	0
43	AYA	r	1	43	6,7,8	1.16	1 (16%)	5,8,10	1.13	0
14	FME	N	1	14	8,9,10	1.02	1 (12%)	7,9,11	0.82	0
4	2MR	D	85	4	10,12,13	2.37	3 (30%)	5,13,15	1.14	0
10	FME	J	1	10	8,9,10	0.94	0	7,9,11	0.96	0
13	FME	M	1	13	8,9,10	0.91	0	7,9,11	1.40	1 (14%)
2	WYK	B	87	2	9,11,12	2.48	2 (22%)	7,13,15	1.36	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	q	1	42	-	3/9/10/12	-
1	FME	A	1	1	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
34	SAC	i	1	34	-	5/7/8/10	-
8	FME	H	1	8	-	4/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
14	FME	N	1	14	-	0/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
10	FME	J	1	10	-	4/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
2	WYK	B	87	2	-	0/10/11/13	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	WYK	CZ-NE	6.37	1.45	1.33
4	D	85	2MR	CZ-NH2	4.82	1.44	1.33
4	D	85	2MR	CZ-NE	4.75	1.44	1.34
42	q	1	AME	CT1-N	3.37	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	WYK	CZ-NH2	-2.47	1.24	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	1	FME	C-CA-N	3.17	115.45	109.73
42	q	1	AME	CE-SD-CG	3.08	110.99	100.40
2	B	87	WYK	CB-CA-N	2.93	116.84	110.32
42	q	1	AME	CT2-CT1-N	2.58	120.47	116.10
42	q	1	AME	O-C-CA	-2.47	118.31	124.78

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	C-CA-CB-CG
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	q	1	AME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	$\#\|Z\| > 2$
57	EHZ	U	201	20	29,36,37	1.65	5 (17%)	35,44,47	1.71	8 (22%)
48	FES	E	301	5	0,4,4	-	-	-		
49	FMN	F	502	-	33,33,33	2.43	7 (21%)	48,50,50	1.67	13 (27%)
45	LMT	L	705	-	36,36,36	1.20	6 (16%)	47,47,47	0.97	2 (4%)
52	3PE	I	204	-	43,43,50	0.91	4 (9%)	46,48,55	1.04	2 (4%)
52	3PE	L	702	-	42,42,50	0.98	4 (9%)	45,47,55	0.93	1 (2%)
52	3PE	L	706	-	44,44,50	0.89	4 (9%)	47,49,55	1.02	2 (4%)
52	3PE	Z	201	-	42,42,50	0.95	3 (7%)	45,47,55	1.00	2 (4%)
52	3PE	r	201	-	45,45,50	0.92	4 (8%)	48,50,55	1.09	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
47	SF4	I	201	9	0,12,12	-	-	-		
45	LMT	M	502	-	36,36,36	1.33	6 (16%)	47,47,47	1.03	1 (2%)
46	PC1	A	203	-	33,33,53	1.20	4 (12%)	39,41,61	1.00	2 (5%)
46	PC1	L	707	-	26,26,53	1.28	4 (15%)	32,34,61	1.04	2 (6%)
45	LMT	A	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.90	1 (2%)
51	CDL	h	202	-	77,77,99	0.91	6 (7%)	82,88,111	1.07	3 (3%)
52	3PE	I	203	-	35,35,50	1.03	4 (11%)	38,40,55	1.02	2 (5%)
45	LMT	N	404	-	36,36,36	1.16	5 (13%)	47,47,47	0.89	0
45	LMT	H	402	-	36,36,36	1.23	6 (16%)	47,47,47	1.07	5 (10%)
58	MYR	o	201	40	14,14,15	0.76	0	13,13,15	0.63	0
45	LMT	j	101	-	36,36,36	1.20	6 (16%)	47,47,47	0.90	0
45	LMT	Y	201	-	36,36,36	1.17	6 (16%)	47,47,47	1.11	3 (6%)
46	PC1	B	204	-	51,51,53	0.95	4 (7%)	57,59,61	0.92	2 (3%)
51	CDL	K	101	-	70,70,99	1.05	6 (8%)	76,82,111	1.09	4 (5%)
52	3PE	N	402	-	33,33,50	0.94	2 (6%)	34,37,55	0.98	1 (2%)
52	3PE	d	201	-	42,42,50	0.95	3 (7%)	45,47,55	1.09	2 (4%)
52	3PE	Y	203	-	37,37,50	0.99	4 (10%)	40,42,55	1.14	2 (5%)
45	LMT	Y	204	-	36,36,36	1.22	6 (16%)	47,47,47	0.97	1 (2%)
51	CDL	H	401	-	50,50,99	1.10	6 (12%)	55,61,111	1.04	3 (5%)
45	LMT	J	201	-	36,36,36	1.20	5 (13%)	47,47,47	0.93	1 (2%)
52	3PE	f	101	-	41,41,50	0.96	4 (9%)	44,46,55	1.11	2 (4%)
52	3PE	i	201	-	29,29,50	1.16	4 (13%)	32,34,55	1.23	3 (9%)
47	SF4	I	202	9	0,12,12	-	-	-		
46	PC1	B	203	-	42,42,53	1.07	4 (9%)	48,50,61	1.15	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	DGT	O	502	53	29,33,33	3.03	12 (41%)	44,52,52	2.06	15 (34%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	p	302	-	35,35,53	1.14	3 (8%)	41,43,61	1.11	2 (4%)
52	3PE	X	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.09	2 (5%)
45	LMT	L	704	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	1 (2%)
45	LMT	N	401	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
47	SF4	F	501	6	0,12,12	-	-	-		
52	3PE	d	202	-	31,31,50	1.11	4 (12%)	34,36,55	1.09	2 (5%)
52	3PE	O	503	-	29,29,50	1.10	4 (13%)	32,34,55	1.08	2 (6%)
45	LMT	Y	202	-	36,36,36	1.19	6 (16%)	47,47,47	0.94	0
45	LMT	A	201	-	36,36,36	1.12	5 (13%)	47,47,47	1.28	3 (6%)
51	CDL	L	703	-	67,67,99	1.07	7 (10%)	73,79,111	1.12	4 (5%)
45	LMT	J	202	-	36,36,36	1.12	5 (13%)	47,47,47	1.15	5 (10%)
45	LMT	h	203	-	36,36,36	1.17	4 (11%)	47,47,47	0.96	1 (2%)
47	SF4	G	802	7	0,12,12	-	-	-		
52	3PE	N	403	-	37,37,50	1.00	4 (10%)	40,42,55	1.09	2 (5%)
55	NDP	P	501	-	49,52,52	2.07	7 (14%)	66,80,80	1.57	14 (21%)
45	LMT	L	701	-	36,36,36	1.28	5 (13%)	47,47,47	0.96	1 (2%)
51	CDL	q	201	-	61,61,99	1.10	6 (9%)	67,73,111	1.13	4 (5%)
52	3PE	M	501	-	40,40,50	0.98	3 (7%)	43,45,55	0.97	2 (4%)
51	CDL	h	201	-	57,57,99	1.36	8 (14%)	61,68,111	1.19	4 (6%)
57	EHZ	T	201	20	29,36,37	1.73	5 (17%)	35,44,47	1.63	7 (20%)
48	FES	G	803	7	0,4,4	-	-	-		

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
57	EHZ	U	201	20	-	15/42/44/45	-
52	3PE	I	204	-	-	15/47/47/54	-
49	FMN	F	502	-	-	8/18/18/18	0/3/3/3
45	LMT	L	705	-	-	7/21/61/61	0/2/2/2
52	3PE	L	702	-	-	23/46/46/54	-
52	3PE	L	706	-	-	20/48/48/54	-
52	3PE	Z	201	-	-	16/46/46/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FES	E	301	5	-	-	0/1/1/1
52	3PE	r	201	-	-	22/49/49/54	-
47	SF4	G	801	7	-	-	0/6/5/5
47	SF4	I	201	9	-	-	0/6/5/5
45	LMT	M	502	-	-	11/21/61/61	0/2/2/2
46	PC1	A	203	-	-	10/37/37/57	-
46	PC1	L	707	-	-	16/30/30/57	-
45	LMT	A	202	-	-	8/21/61/61	0/2/2/2
52	3PE	I	203	-	-	19/39/39/54	-
45	LMT	N	404	-	-	12/21/61/61	0/2/2/2
48	FES	G	803	7	-	-	0/1/1/1
45	LMT	H	402	-	-	10/21/61/61	0/2/2/2
58	MYR	o	201	40	-	6/11/12/13	-
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
45	LMT	Y	201	-	-	12/21/61/61	0/2/2/2
46	PC1	B	204	-	-	28/55/55/57	-
51	CDL	K	101	-	-	32/81/81/110	-
52	3PE	N	402	-	-	11/36/36/54	-
52	3PE	d	201	-	-	21/46/46/54	-
52	3PE	Y	203	-	-	24/41/41/54	-
45	LMT	Y	204	-	-	11/21/61/61	0/2/2/2
51	CDL	H	401	-	-	33/59/59/110	-
45	LMT	J	201	-	-	5/21/61/61	0/2/2/2
52	3PE	f	101	-	-	14/45/45/54	-
52	3PE	i	201	-	-	14/33/33/54	-
47	SF4	I	202	9	-	-	0/6/5/5
46	PC1	B	203	-	-	19/46/46/57	-
54	DGT	O	502	53	-	10/22/34/34	0/3/3/3
47	SF4	B	201	2	-	-	0/6/5/5
46	PC1	p	302	-	-	11/39/39/57	-
52	3PE	X	201	-	-	21/40/40/54	-
45	LMT	L	704	-	-	7/21/61/61	0/2/2/2
45	LMT	N	401	-	-	8/21/61/61	0/2/2/2
47	SF4	F	501	6	-	-	0/6/5/5
52	3PE	d	202	-	-	20/35/35/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	O	503	-	-	14/33/33/54	-
45	LMT	Y	202	-	-	7/21/61/61	0/2/2/2
45	LMT	A	201	-	-	8/21/61/61	0/2/2/2
51	CDL	L	703	-	-	29/78/78/110	-
45	LMT	J	202	-	-	7/21/61/61	0/2/2/2
45	LMT	h	203	-	-	7/21/61/61	0/2/2/2
47	SF4	G	802	7	-	-	0/6/5/5
52	3PE	N	403	-	-	13/41/41/54	-
55	NDP	P	501	-	-	5/34/77/77	0/5/5/5
45	LMT	L	701	-	-	12/21/61/61	0/2/2/2
51	CDL	q	201	-	-	35/72/72/110	-
52	3PE	M	501	-	-	26/44/44/54	-
51	CDL	h	201	-	-	30/67/67/110	-
57	EHZ	T	201	20	-	20/42/44/45	-
51	CDL	h	202	-	-	42/87/87/110	-

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	11.60	1.81	1.59
54	O	502	DGT	O6-C6	8.51	1.39	1.23
49	F	502	FMN	O4-C4	8.35	1.39	1.23
49	F	502	FMN	O2-C2	7.80	1.38	1.24
54	O	502	DGT	C5-N7	6.86	1.52	1.39

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	502	DGT	C8-N9-C4	7.33	120.01	106.05
55	P	501	NDP	PN-O3-PA	-6.09	111.94	132.83
57	U	201	EHZ	C8-C9-S1	5.76	120.75	113.63
46	B	203	PC1	O21-C21-C22	5.29	122.90	111.50
57	T	201	EHZ	C8-C9-S1	5.24	120.11	113.63

There are no chirality outliers.

5 of 783 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	H	402	LMT	C2'-C1'-O1'-C1
45	H	402	LMT	O5'-C1'-O1'-C1
45	L	701	LMT	C2'-C1'-O1'-C1
45	L	701	LMT	O5'-C1'-O1'-C1
45	Y	204	LMT	C2-C1-O1'-C1'

There are no ring outliers.

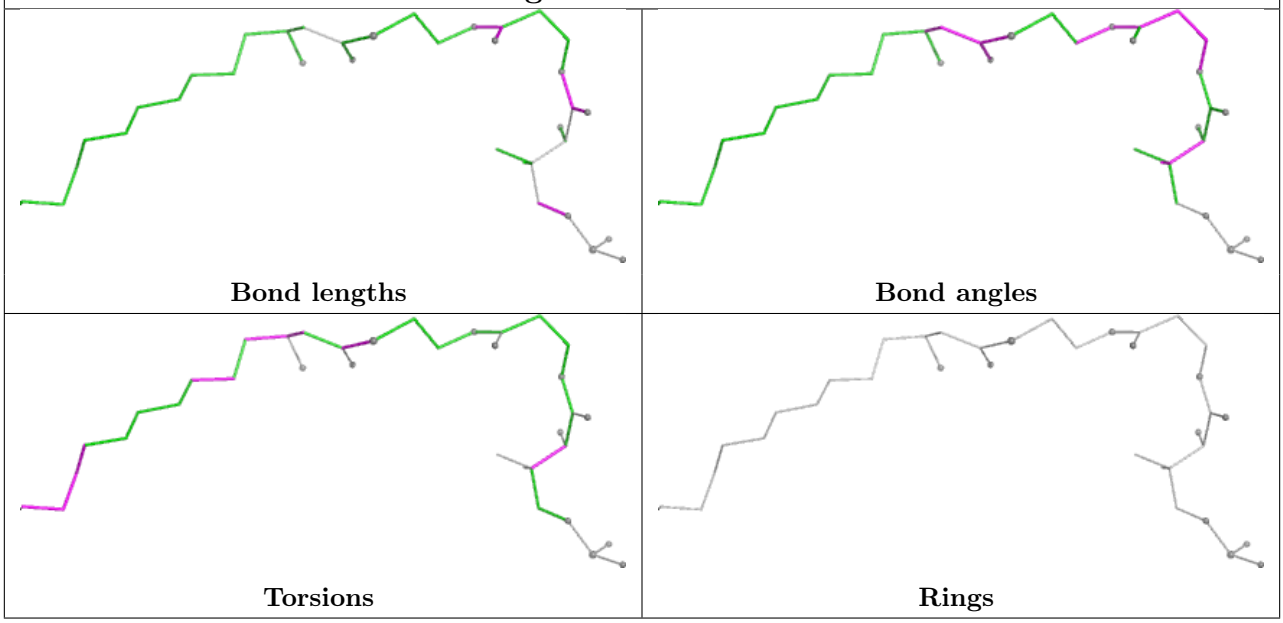
21 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	U	201	EHZ	1	0
49	F	502	FMN	2	0
45	L	705	LMT	2	0
52	I	204	3PE	1	0
52	L	702	3PE	1	0
52	L	706	3PE	1	0
52	r	201	3PE	1	0
45	H	402	LMT	2	0
45	Y	201	LMT	1	0
46	B	204	PC1	1	0
52	N	402	3PE	1	0
52	d	201	3PE	2	0
52	Y	203	3PE	1	0
52	i	201	3PE	1	0
54	O	502	DGT	2	0
47	B	201	SF4	1	0
52	X	201	3PE	1	0
45	A	201	LMT	1	0
45	J	202	LMT	2	0
55	P	501	NDP	2	0
45	L	701	LMT	3	0

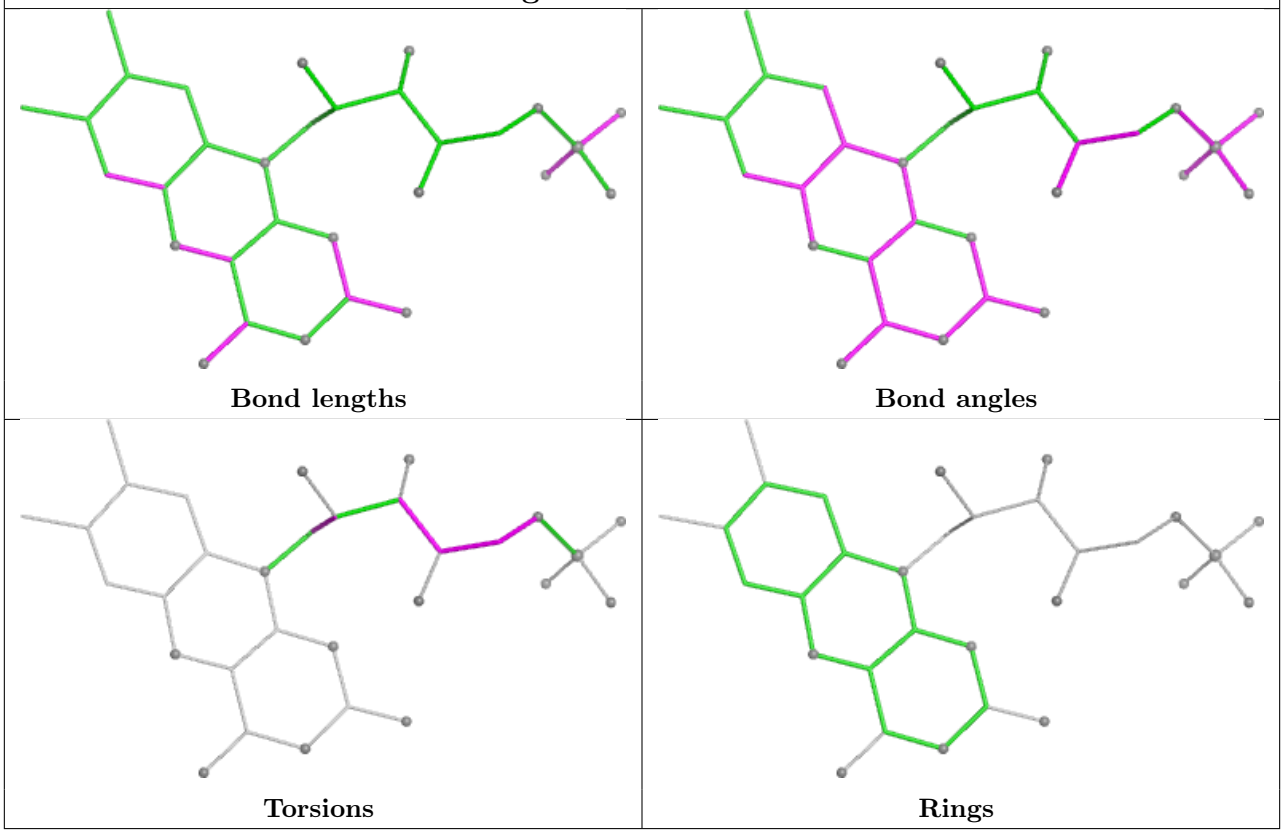
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

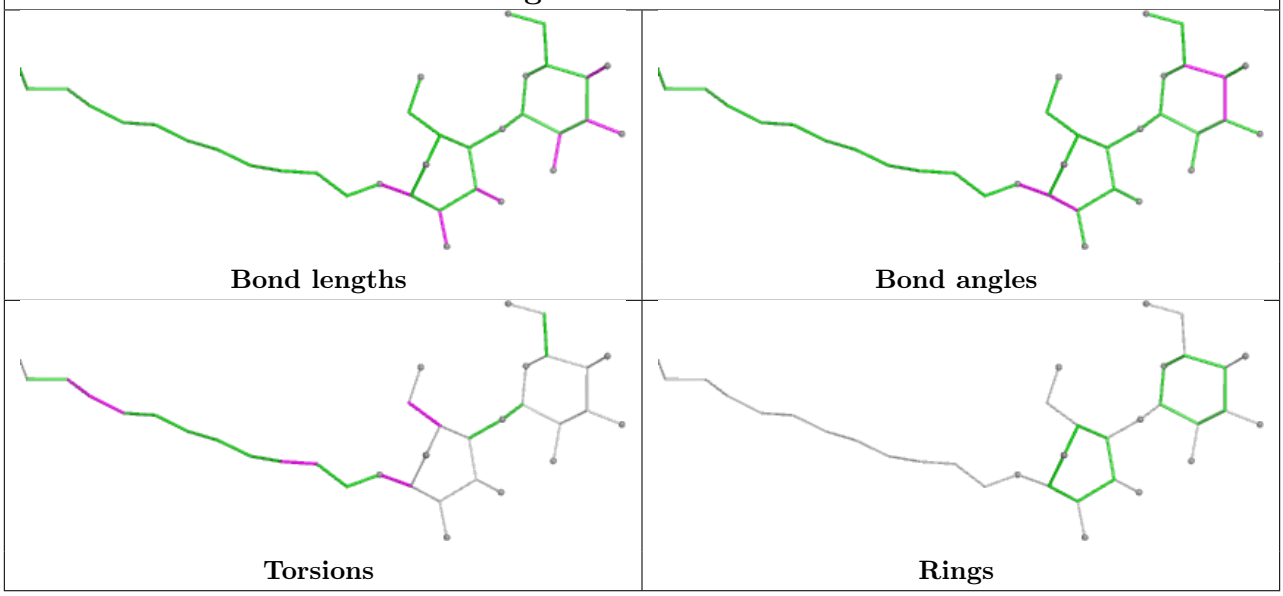
Ligand EHZ U 201



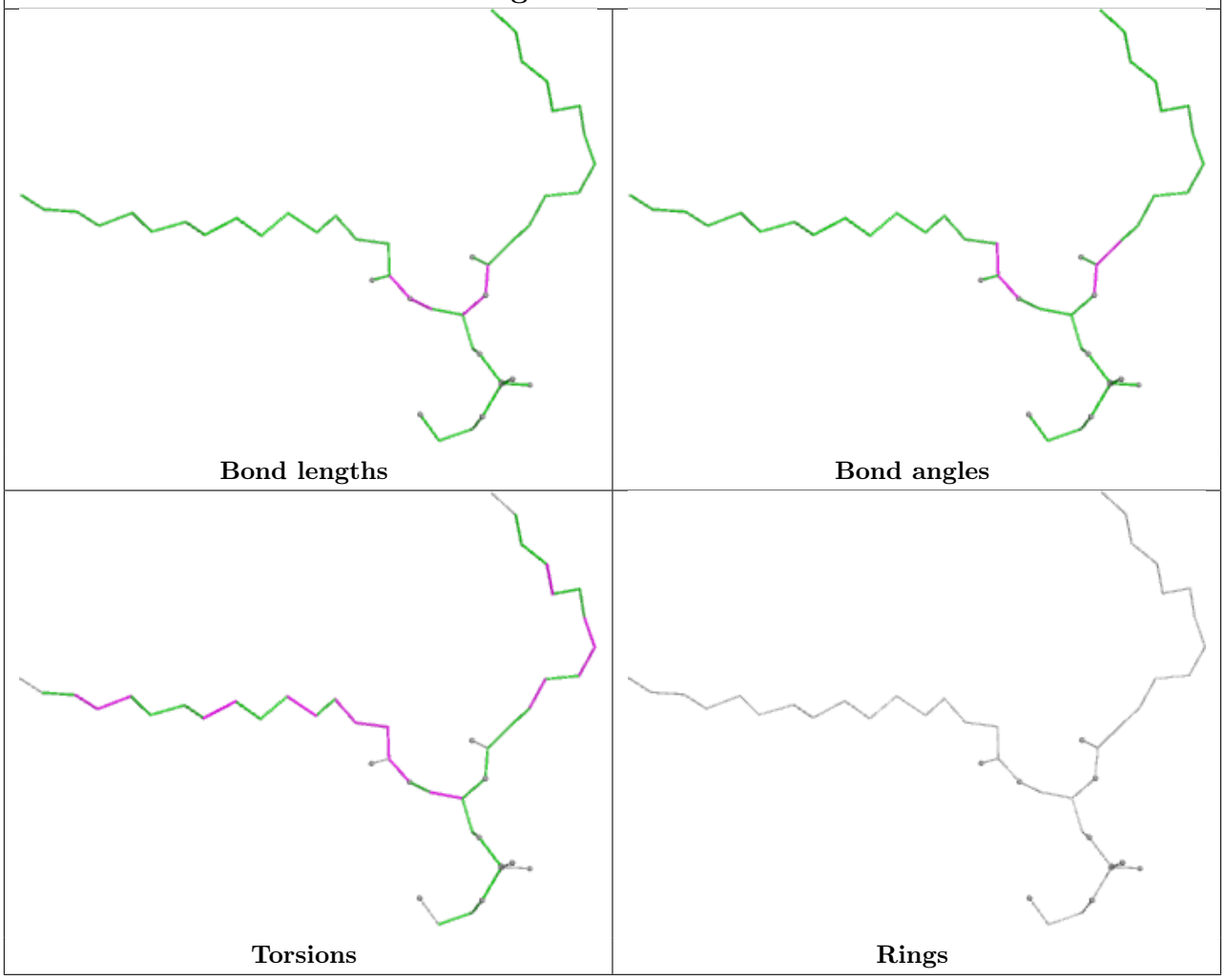
Ligand FMN F 502



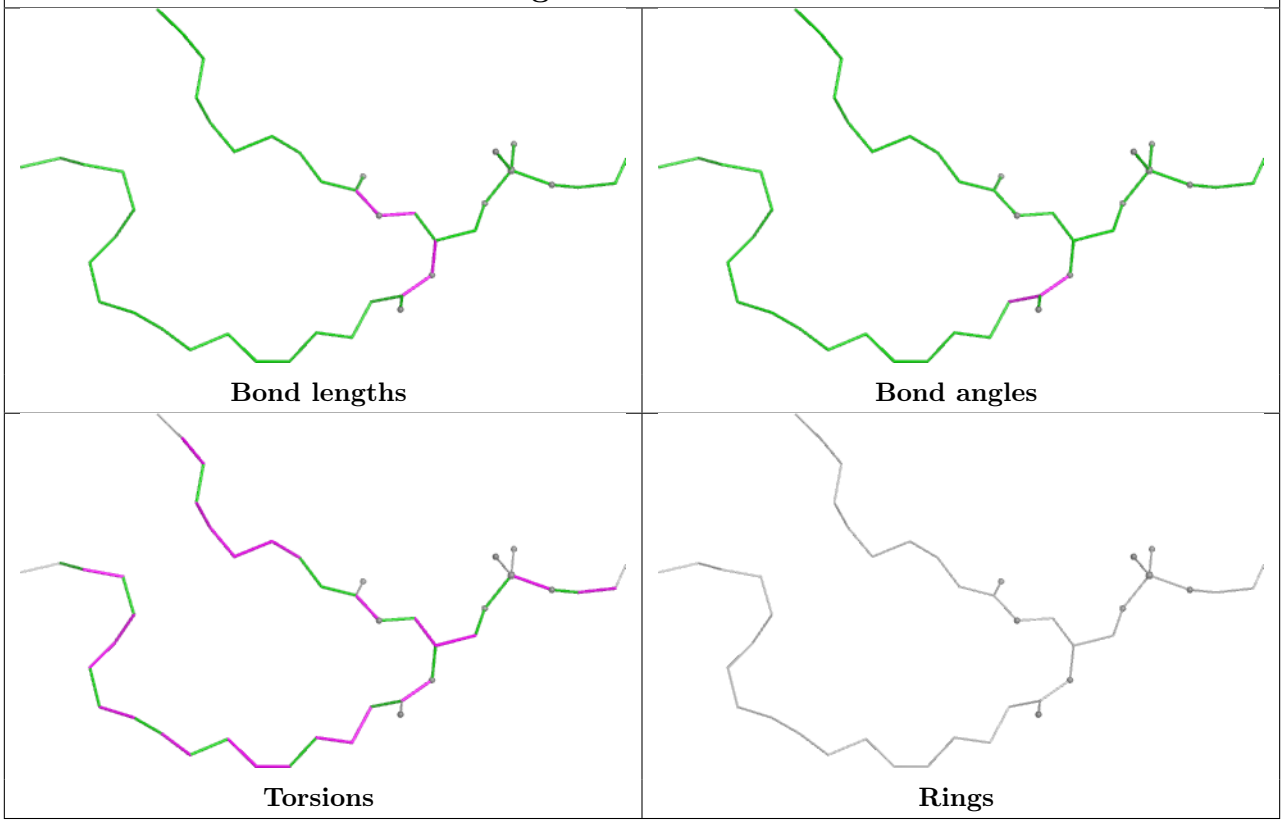
Ligand LMT L 705



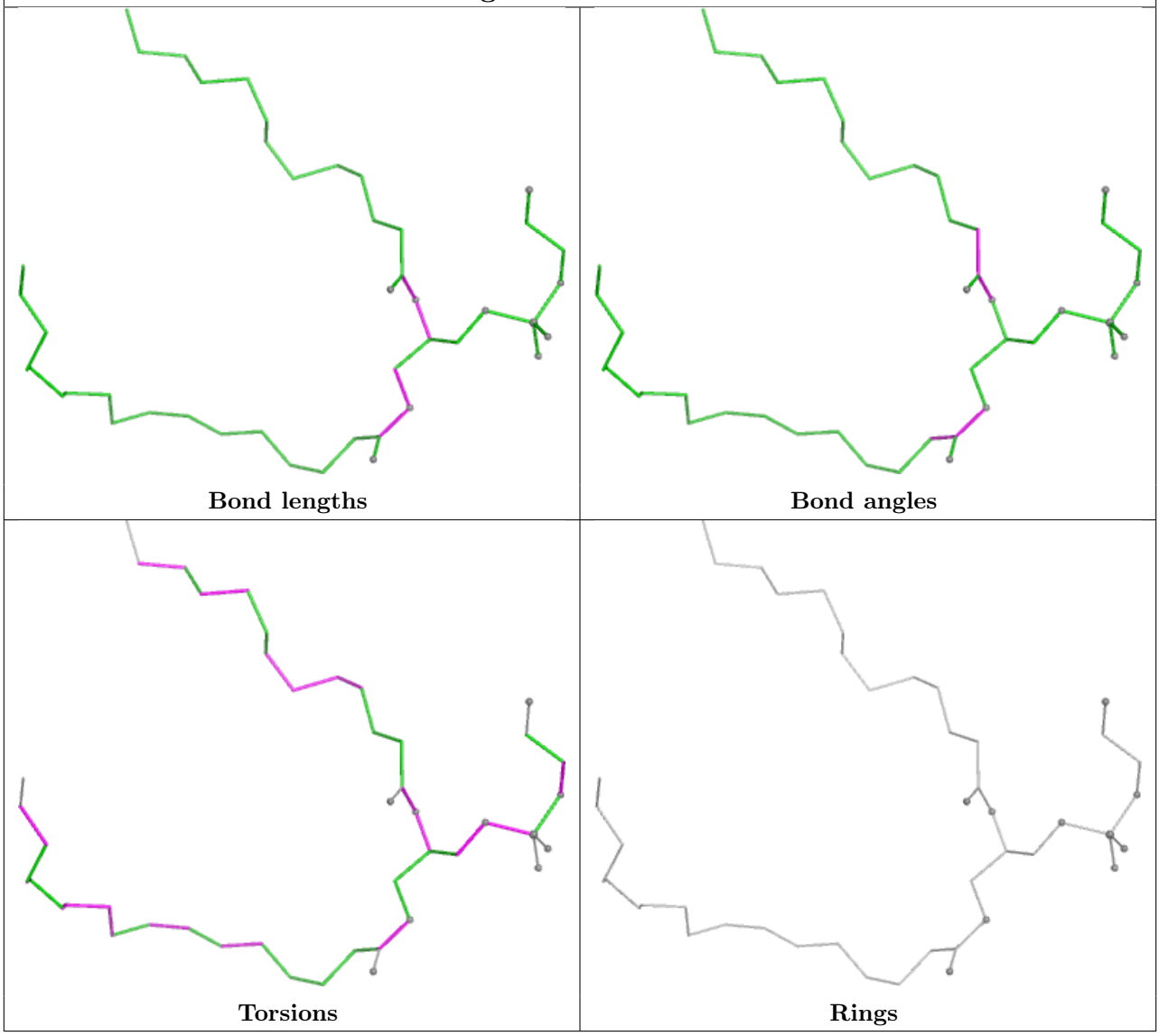
Ligand 3PE I 204



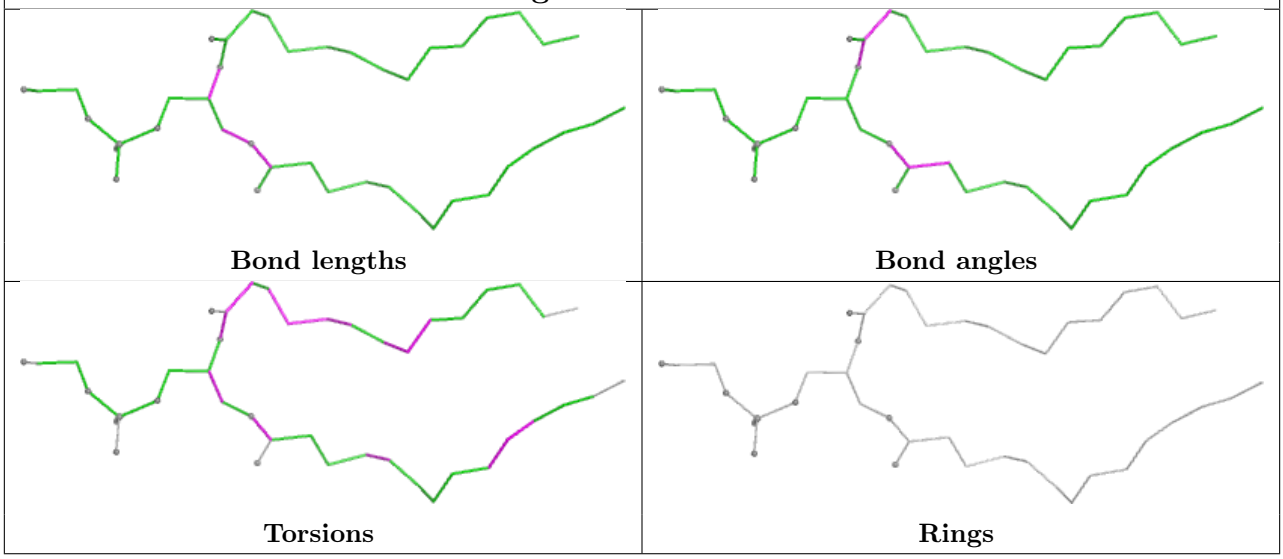
Ligand 3PE L 702

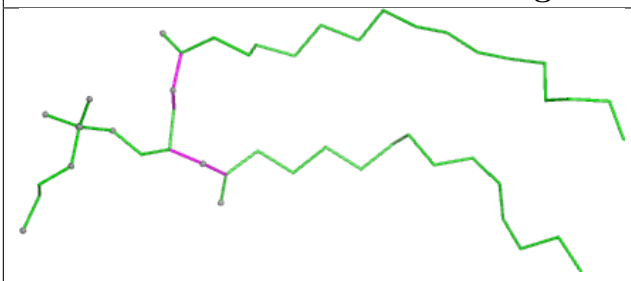
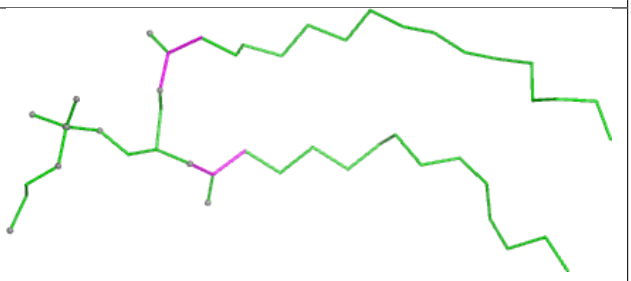
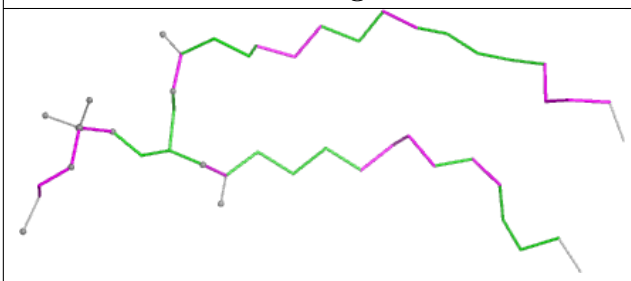
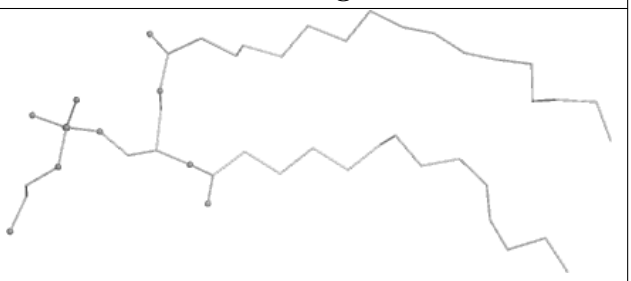


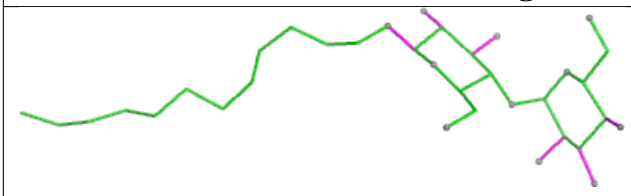
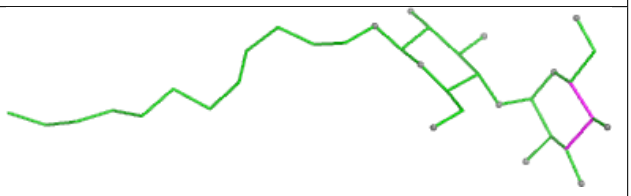
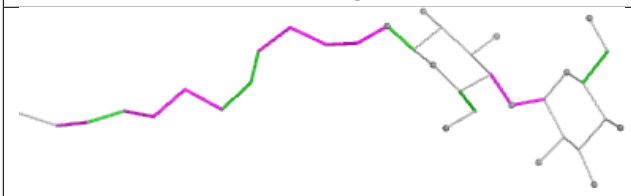
Ligand 3PE L 706



Ligand 3PE Z 201

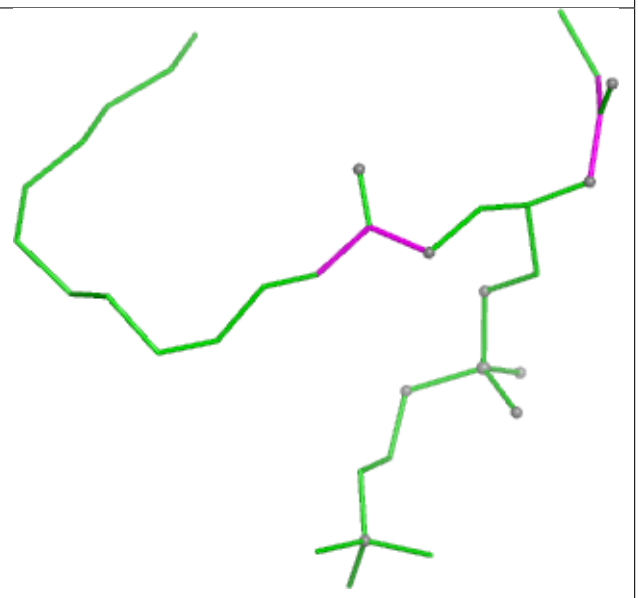


Ligand 3PE r 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT M 502	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand PC1 A 203

Bond lengths



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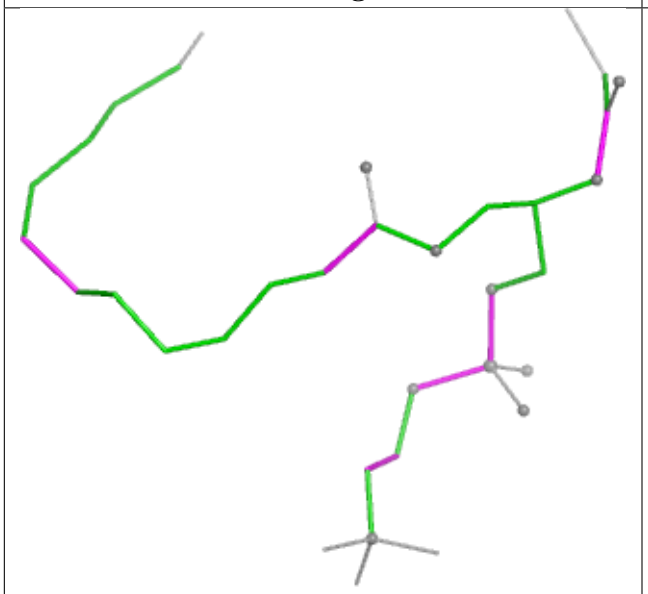

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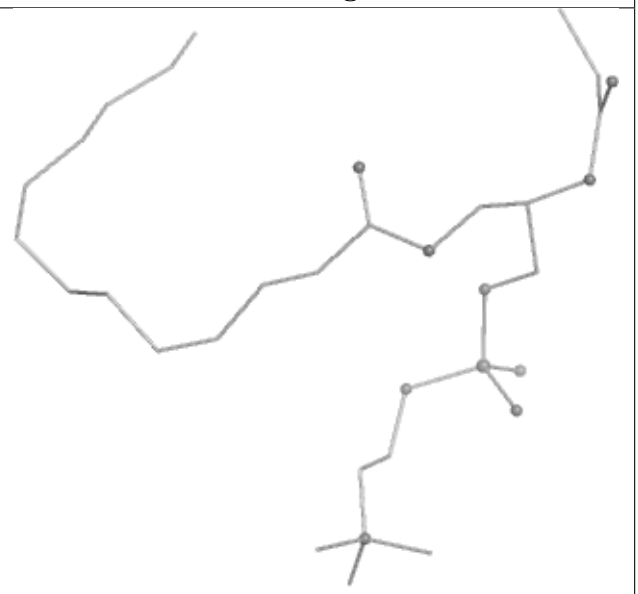

Rings

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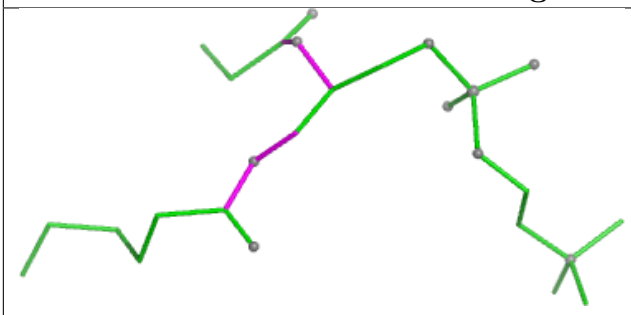
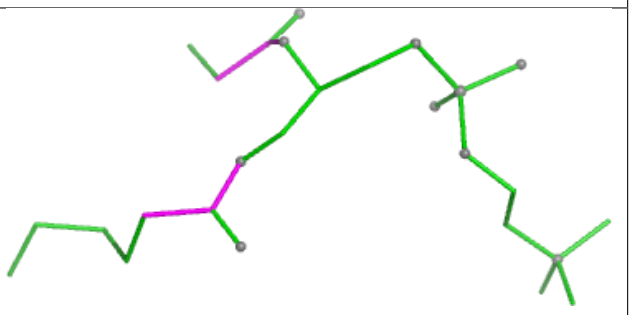
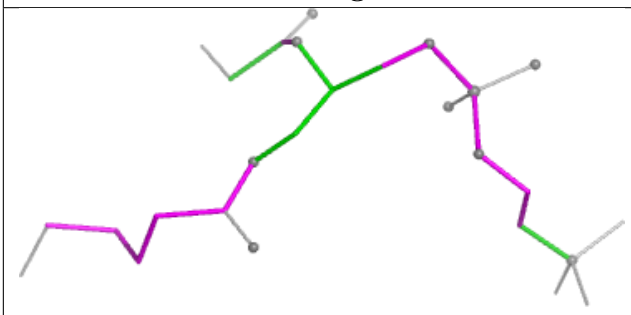
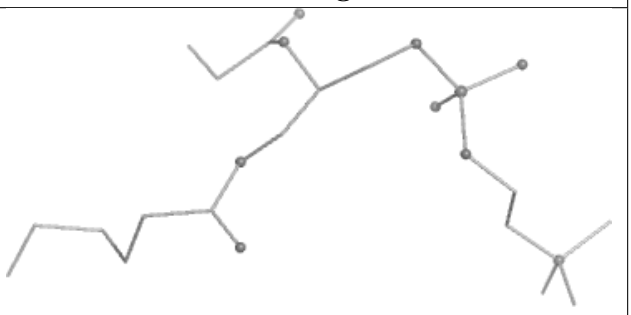
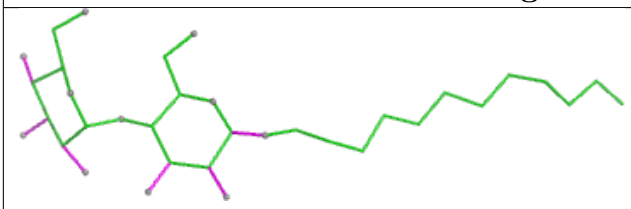
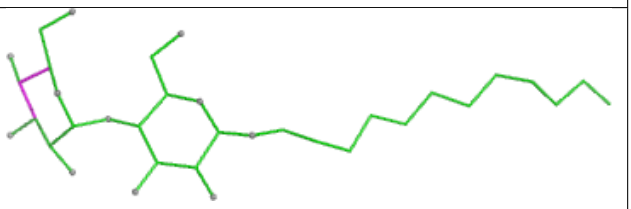
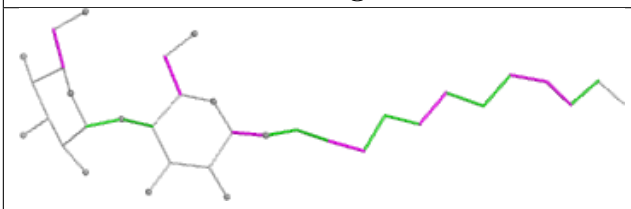
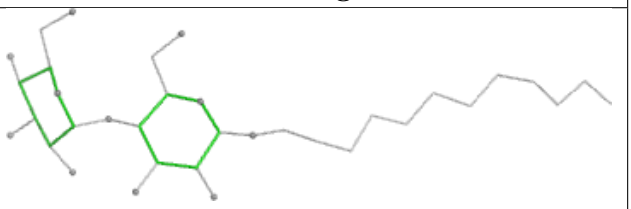
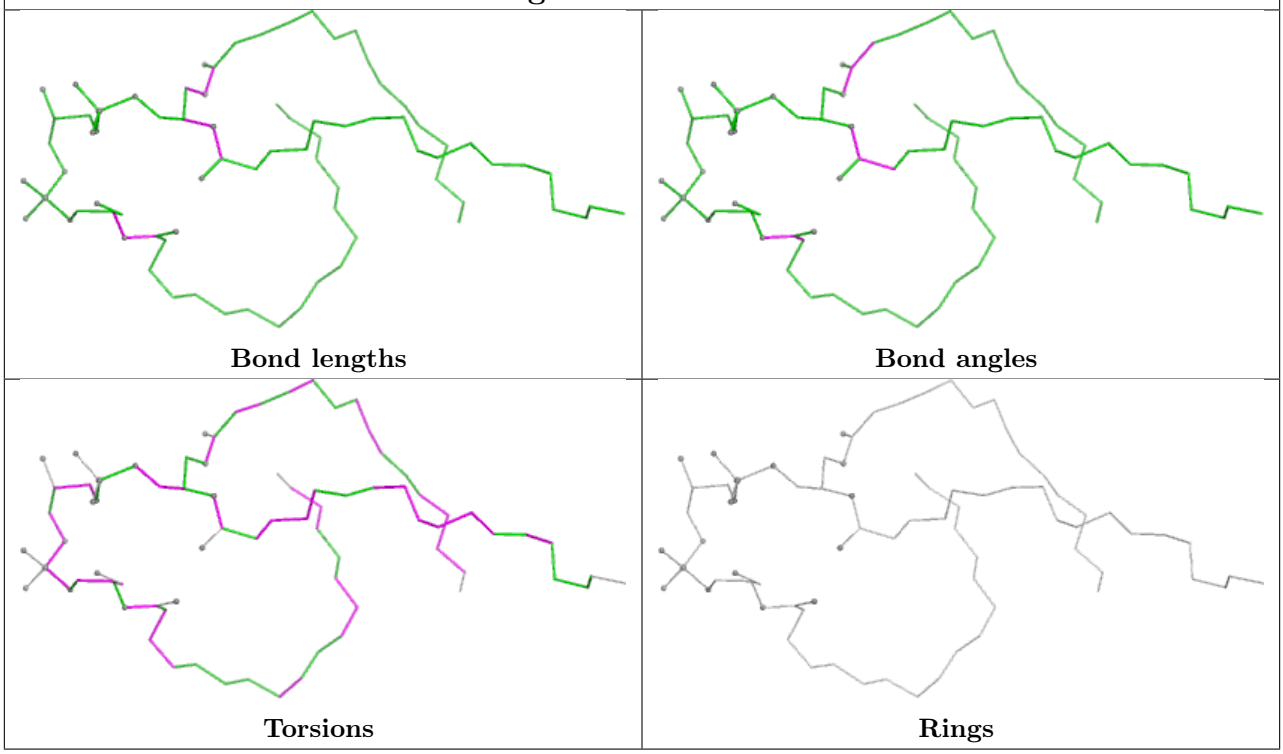
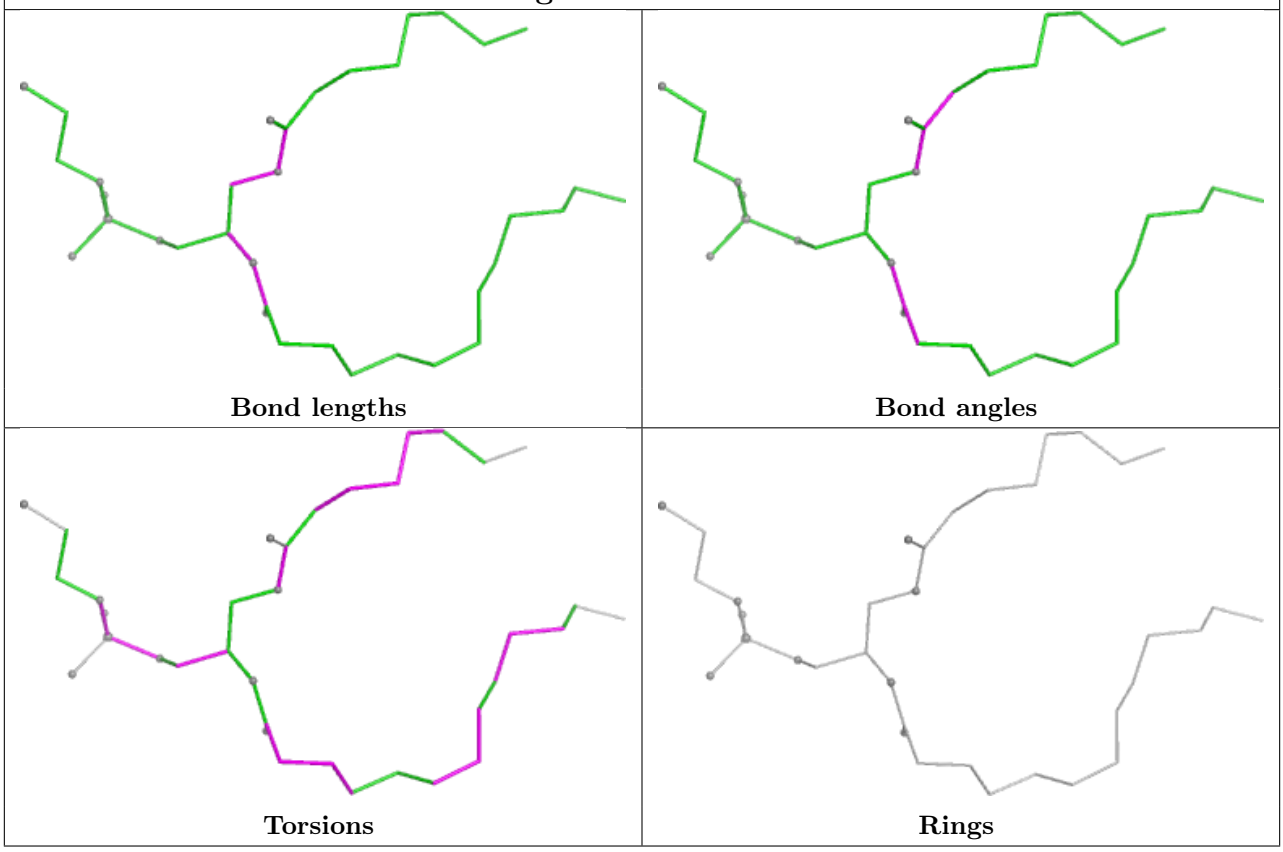
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL h 202



Ligand 3PE I 203



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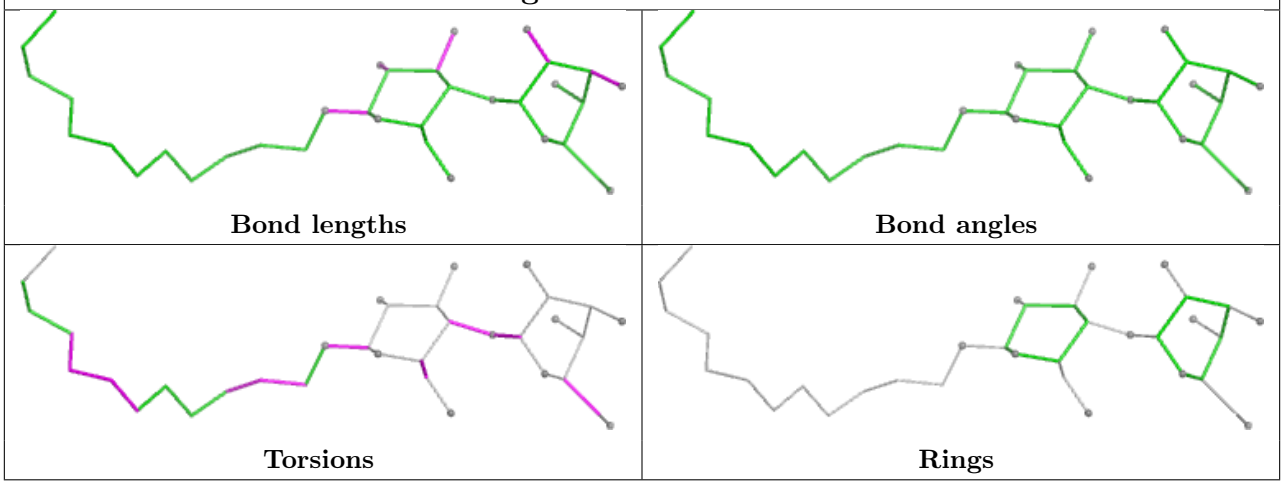

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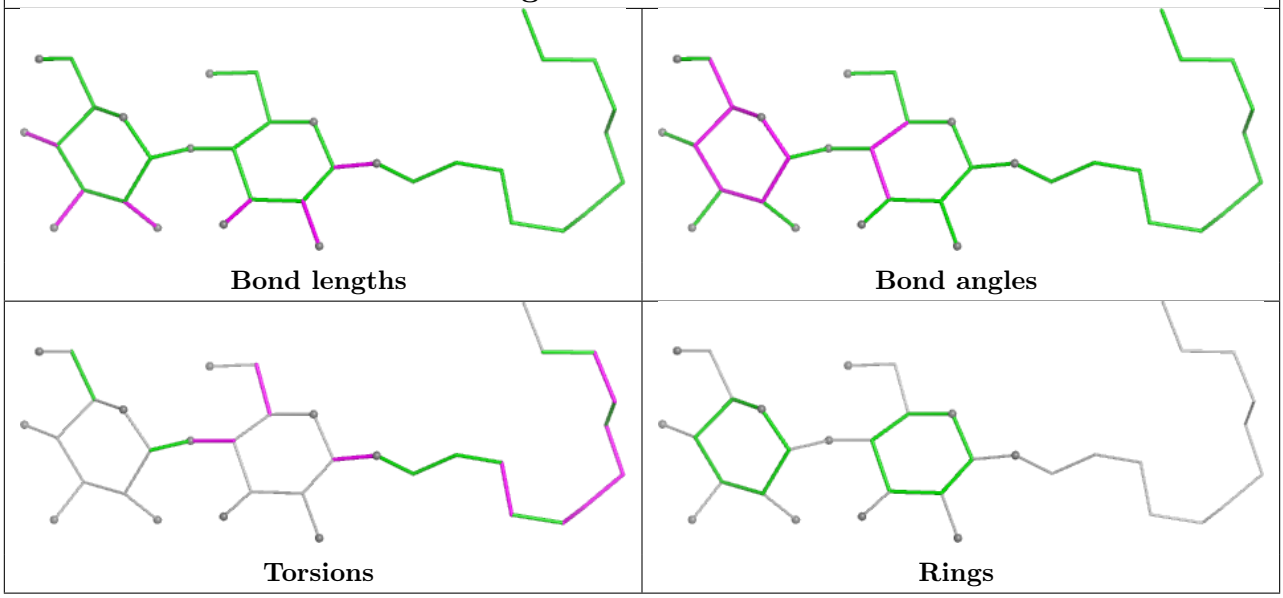
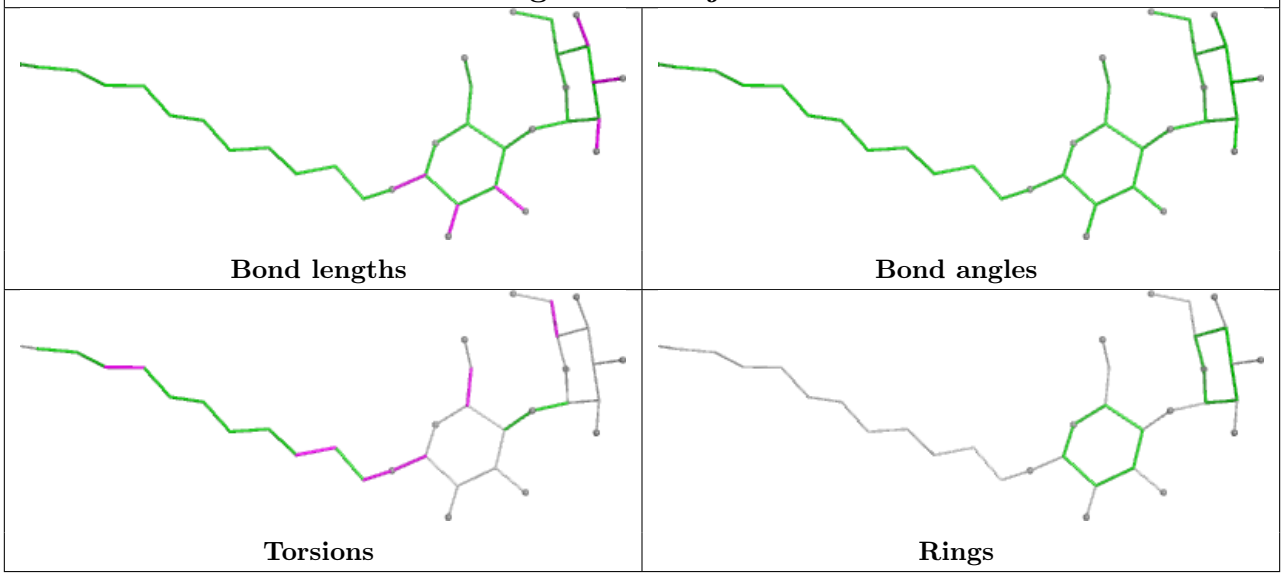


Ligand LMT j 101



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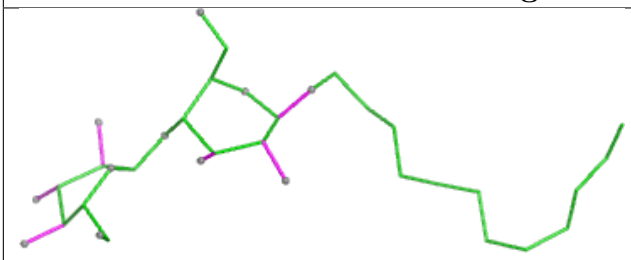
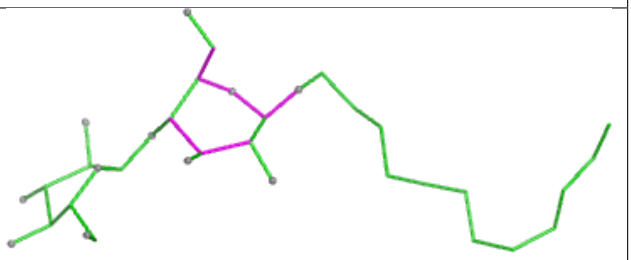
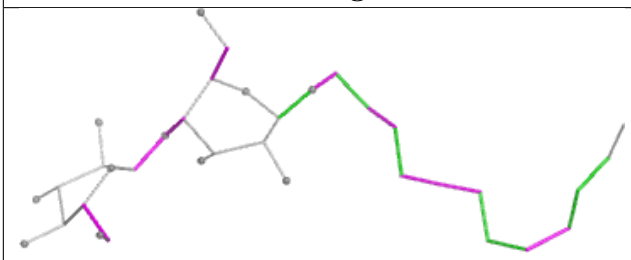
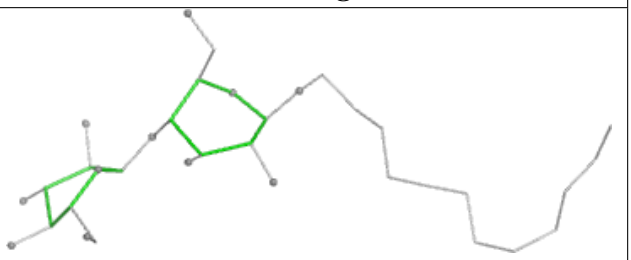
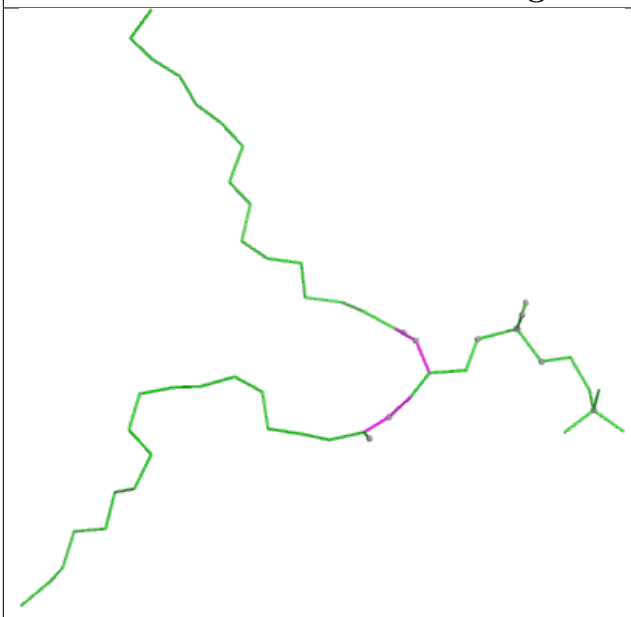
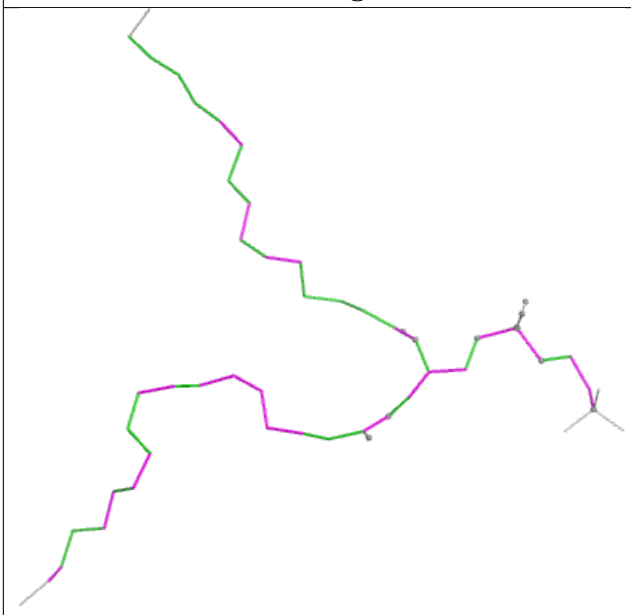
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 B 204



Bond lengths

Bond angles



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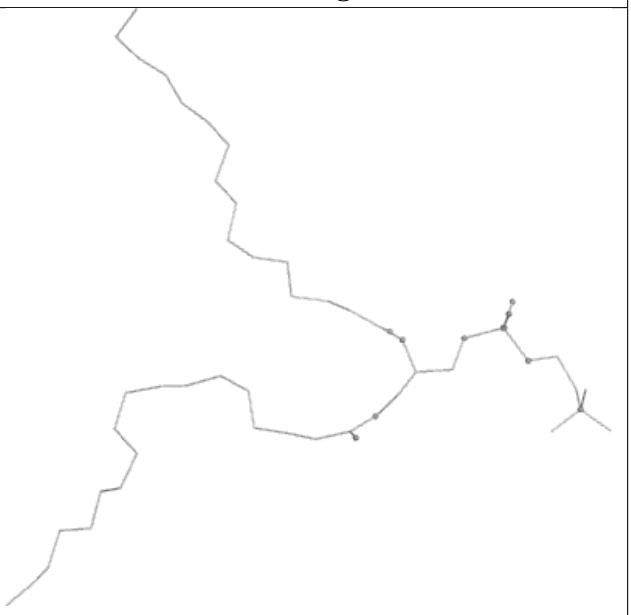
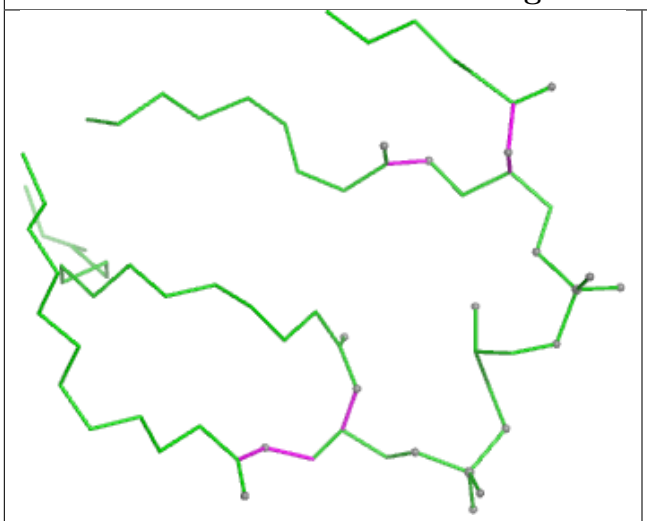


Rings

Ligand CDL K 101



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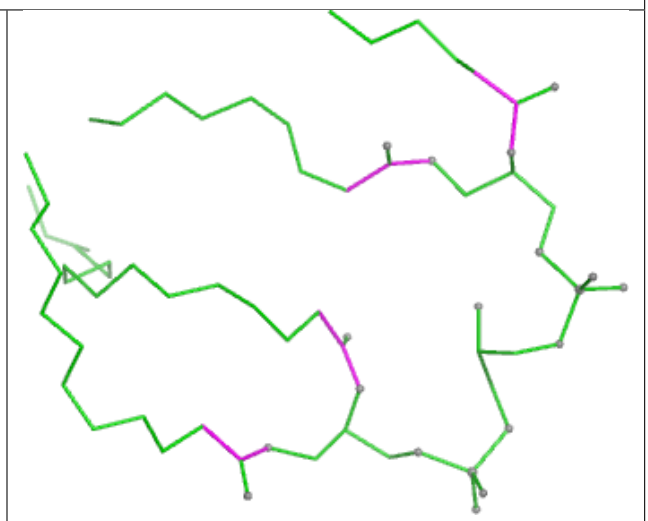

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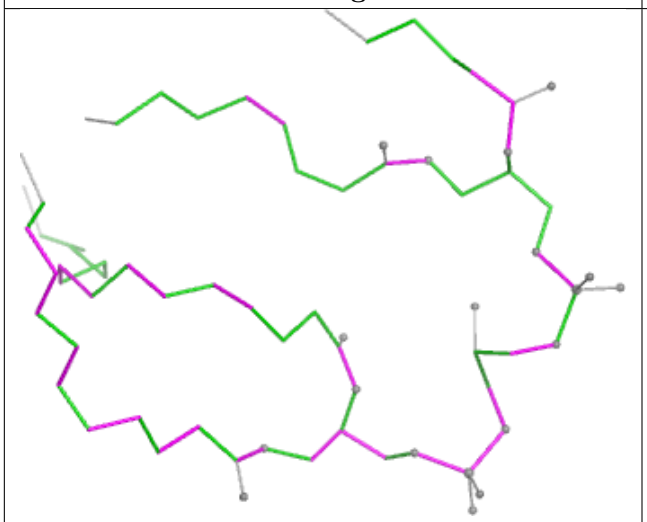

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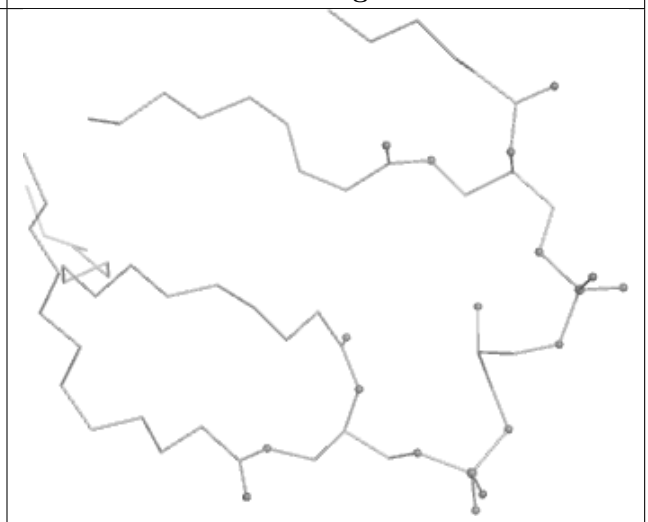
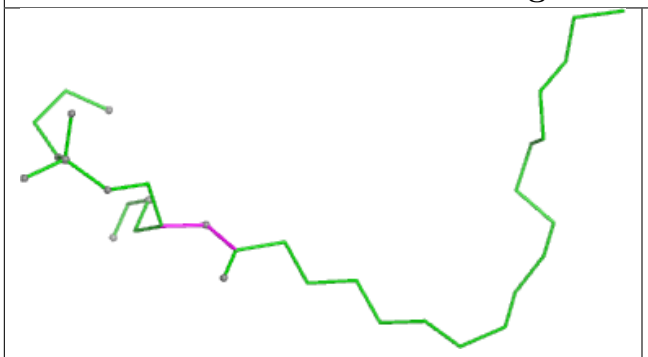


Rings

Ligand 3PE N 402



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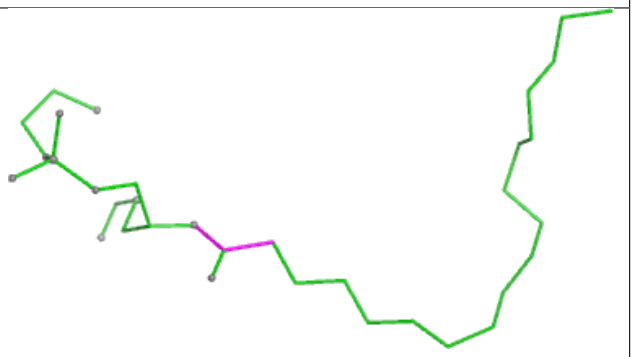

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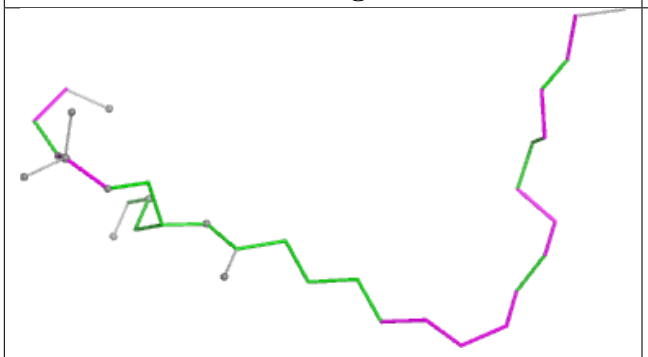

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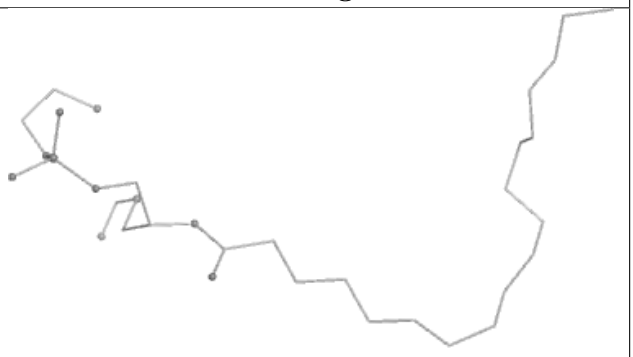
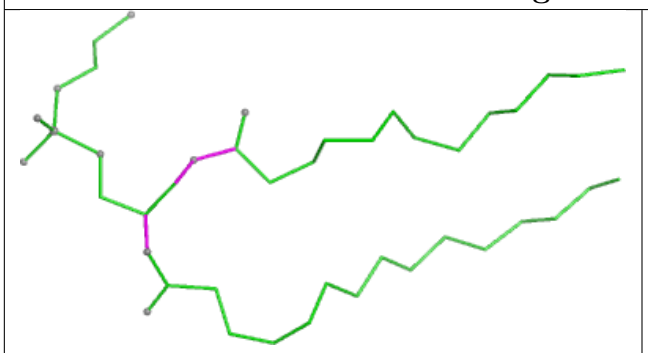


Rings

Ligand 3PE d 201



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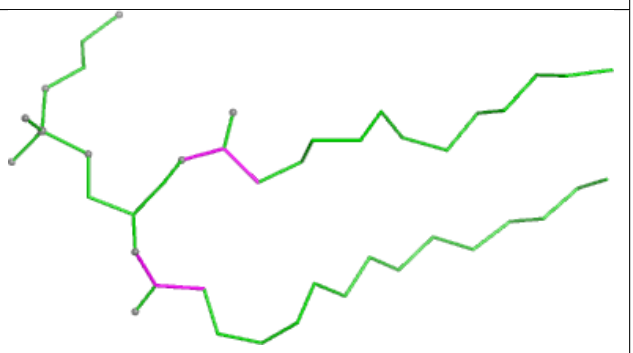

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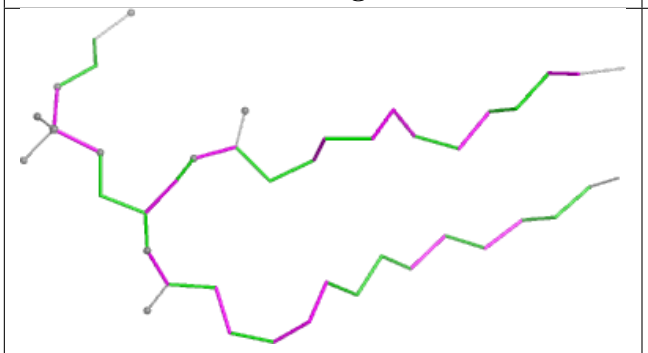

Torsions

Rings

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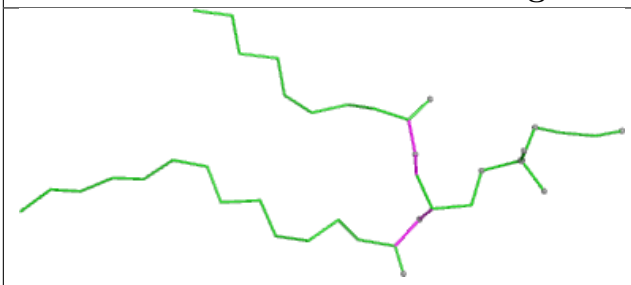
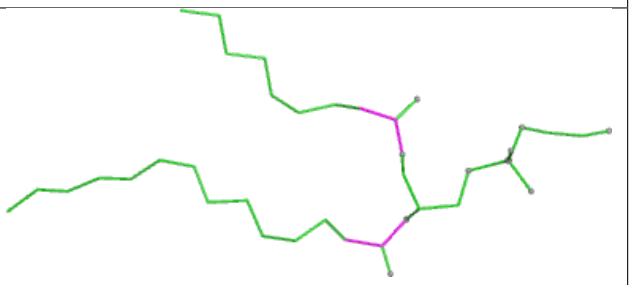
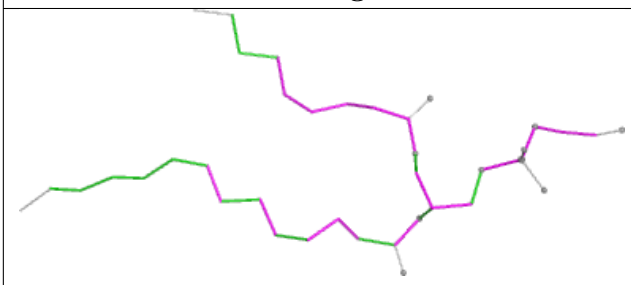
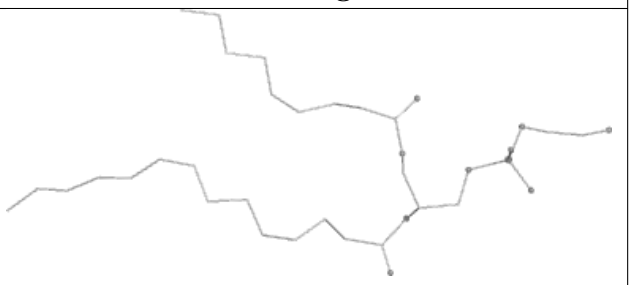
 Bond lengths	 Bond angles
 Torsions	 Rings

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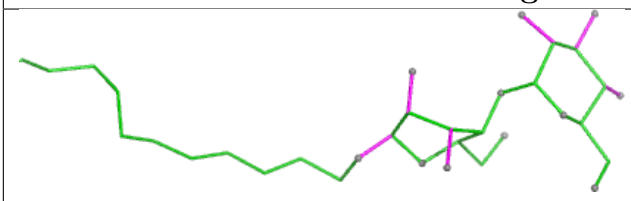
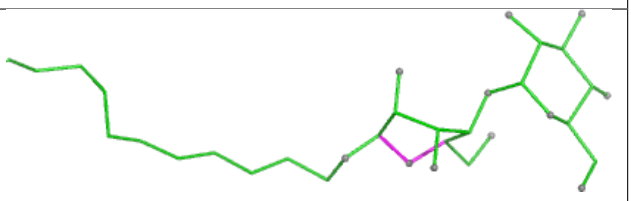
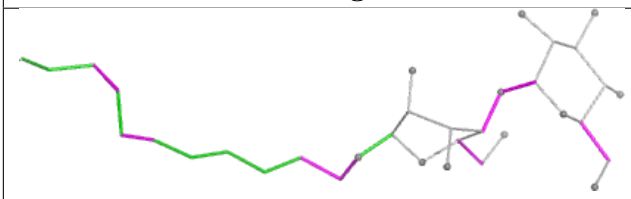
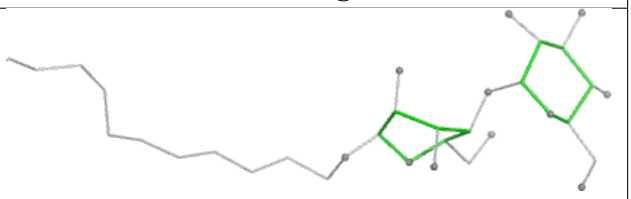
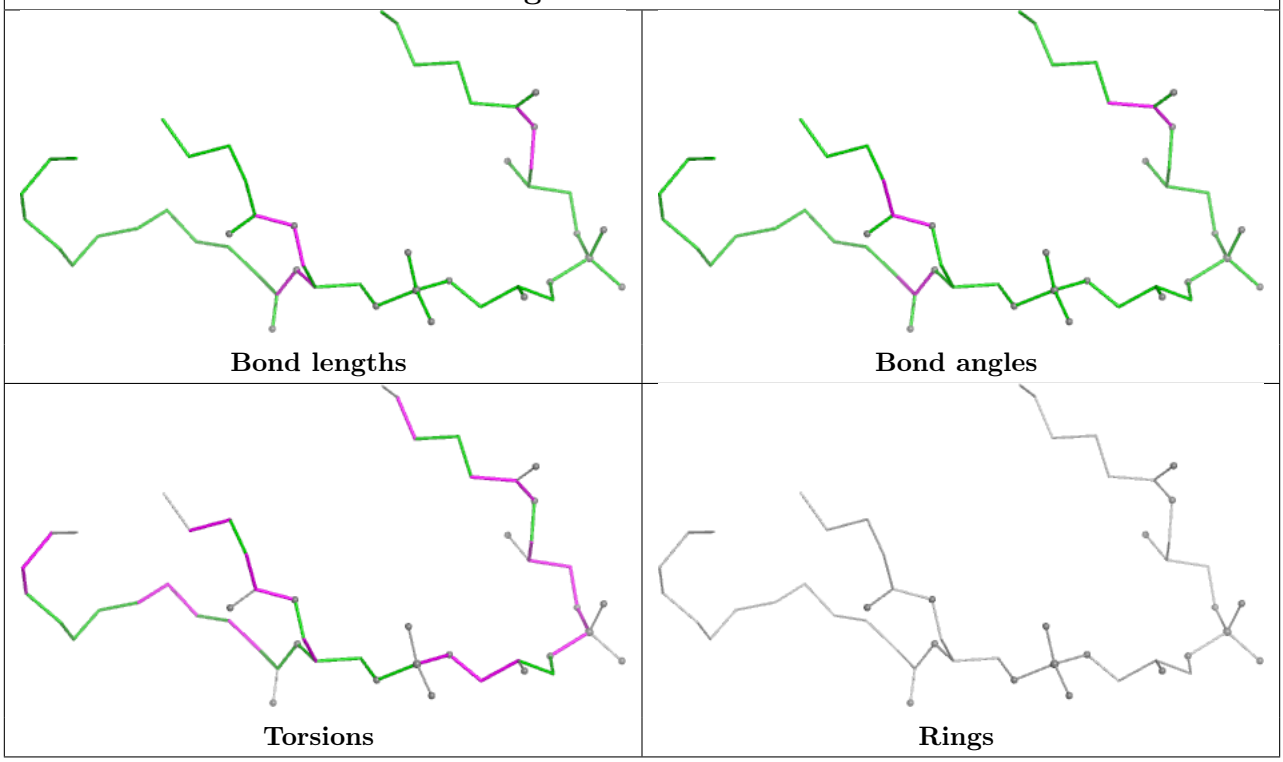
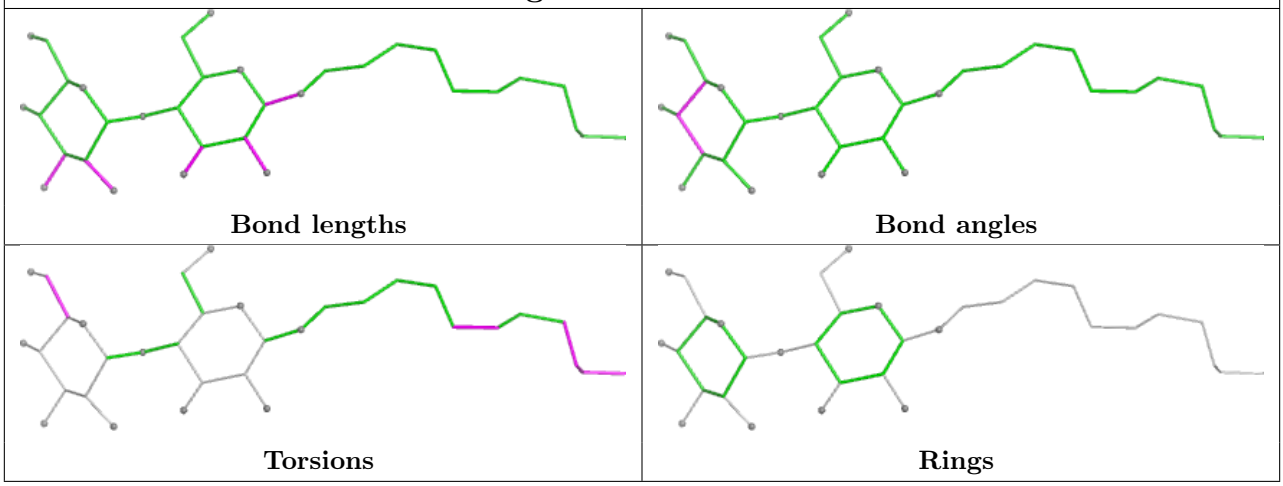
 Bond lengths	 Bond angles
 Torsions	 Rings

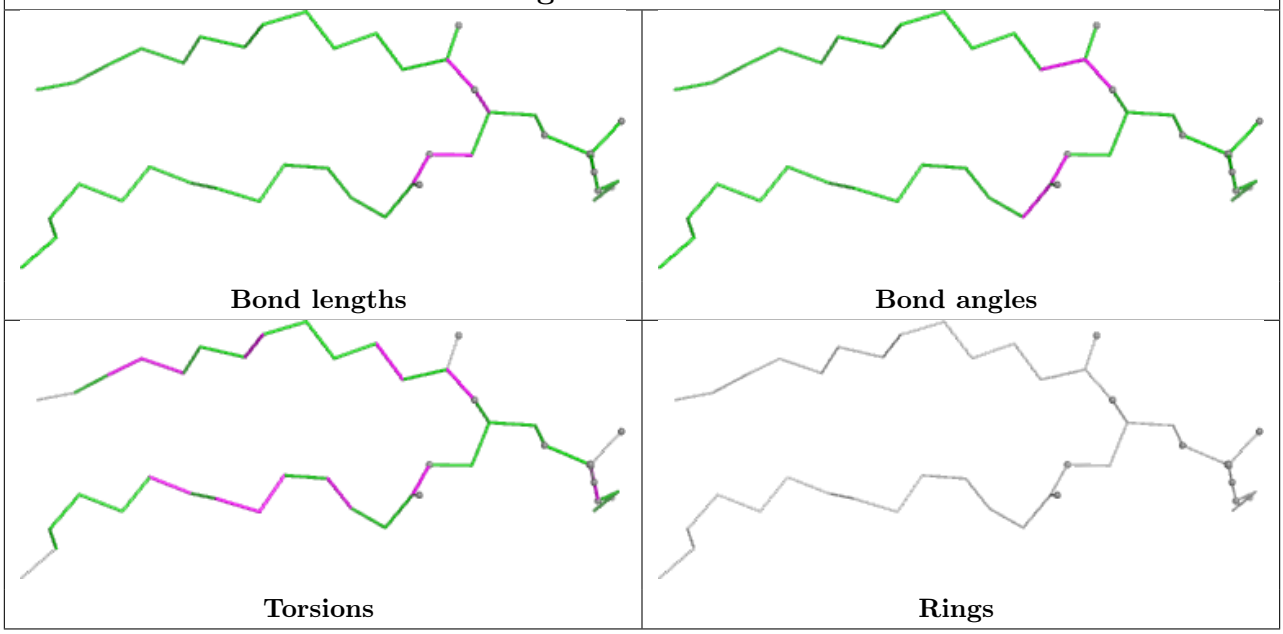
Ligand CDL H 401



Ligand LMT J 201



Ligand 3PE f 101



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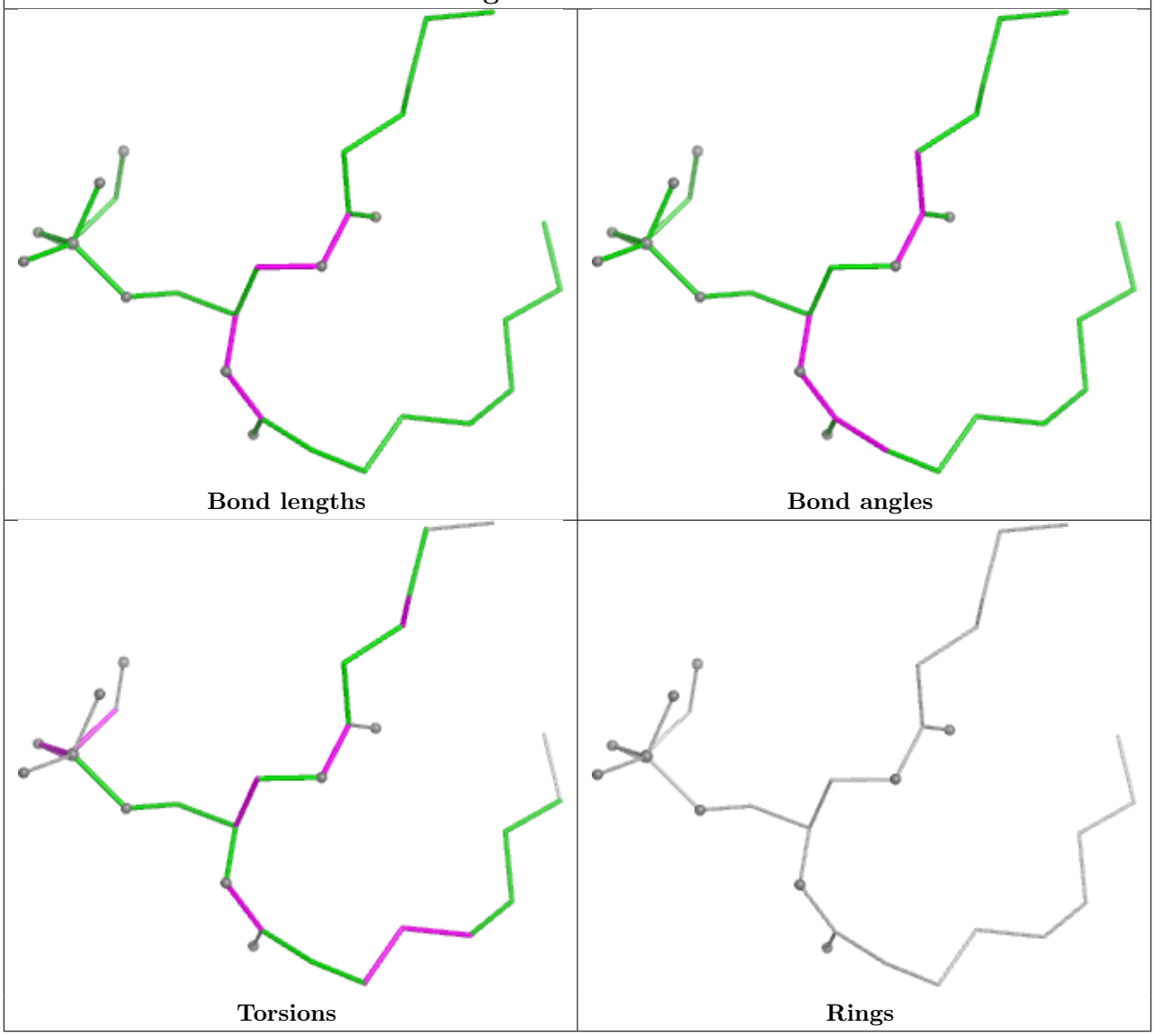
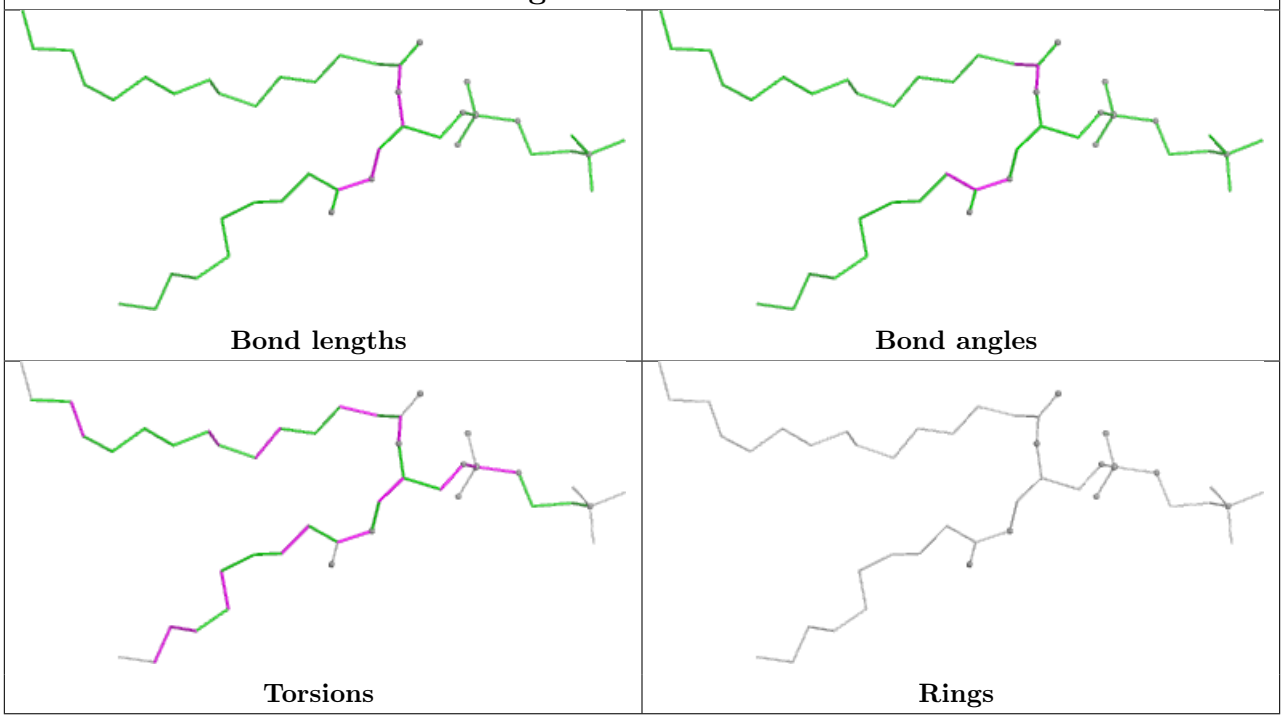
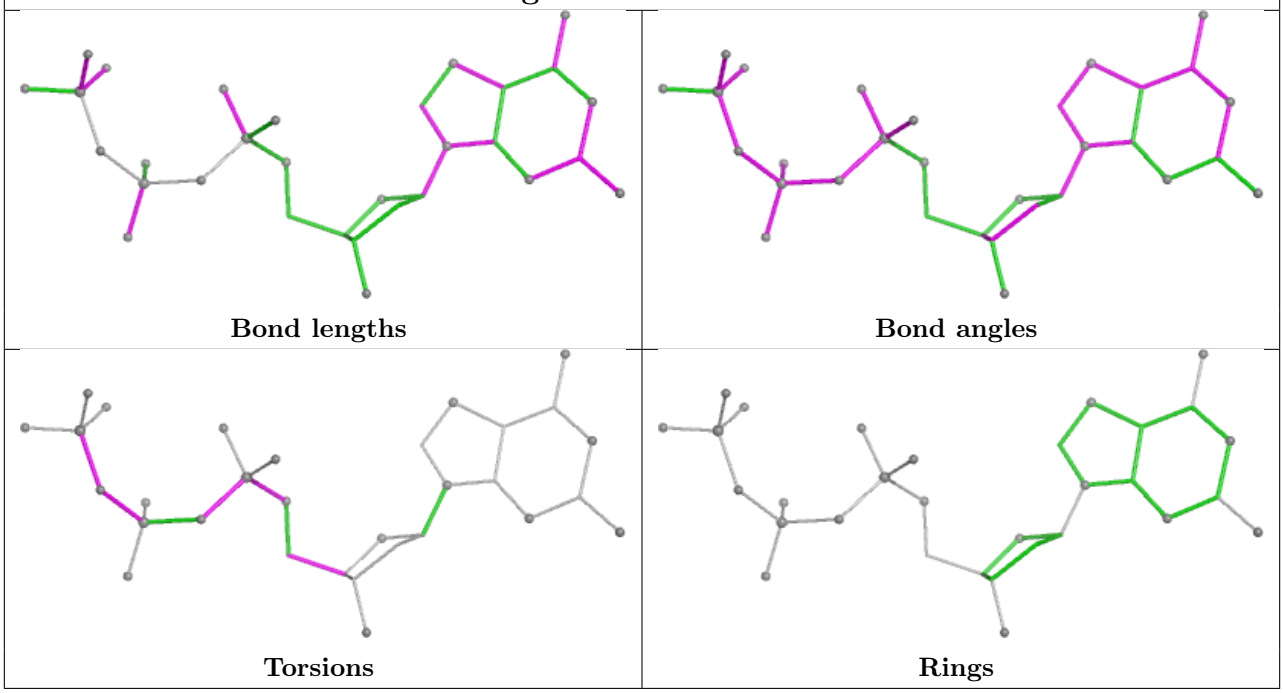


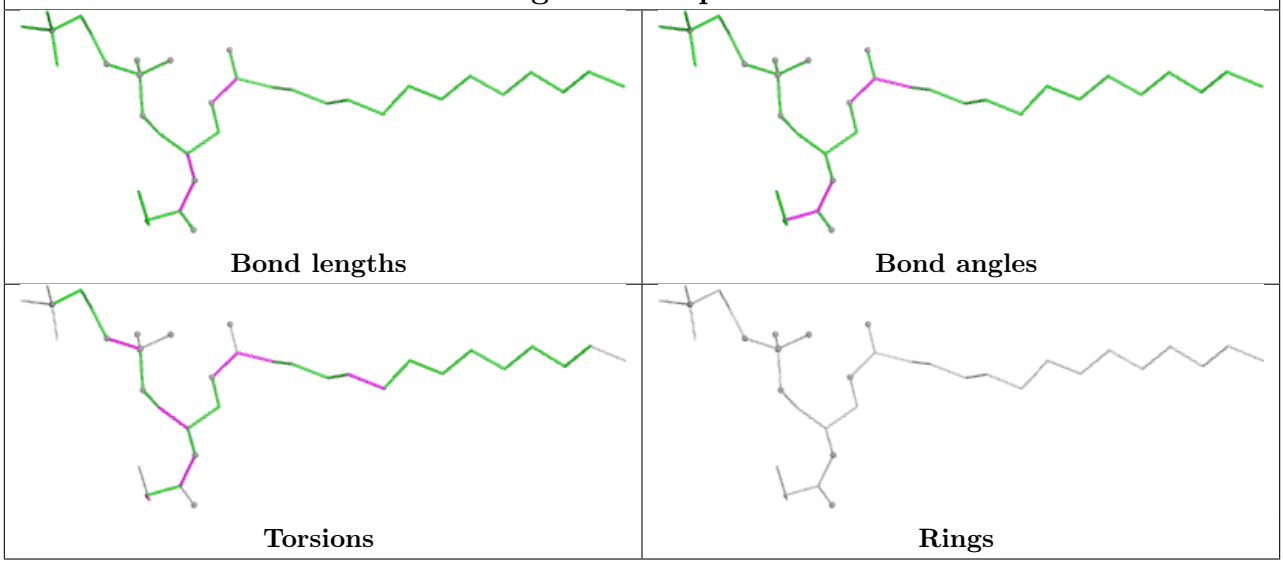
Ligand PC1 B 203



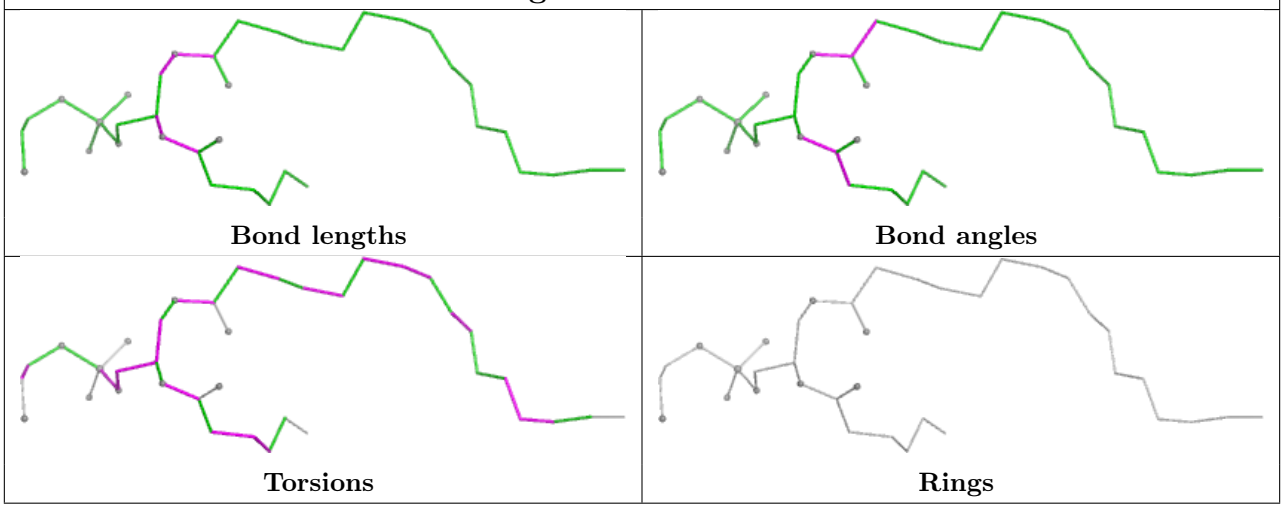
Ligand DGT O 502



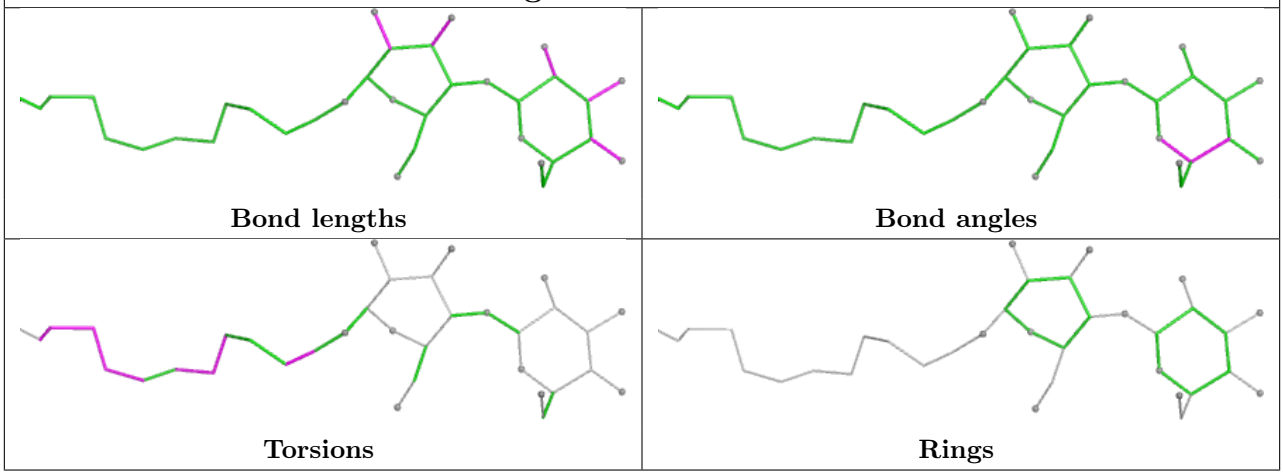
Ligand PC1 p 302

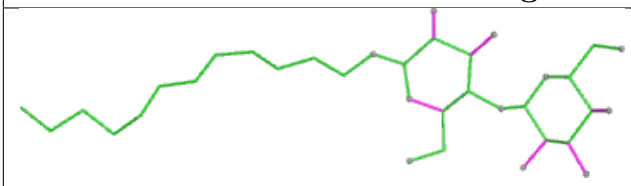
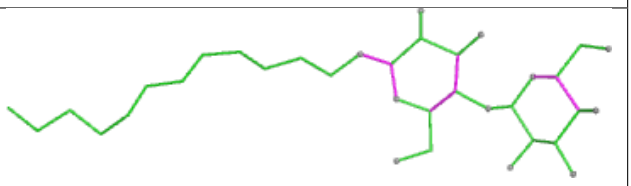
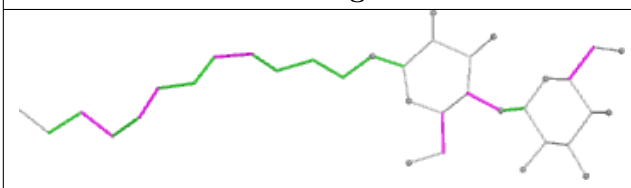
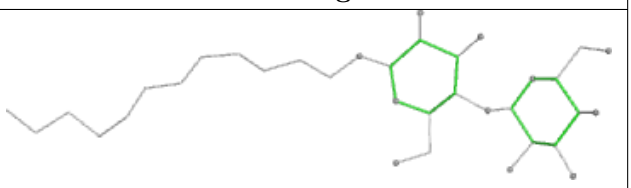


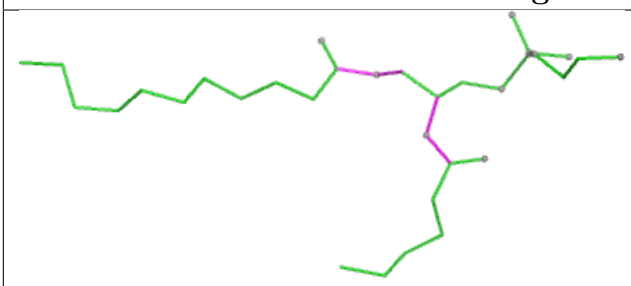
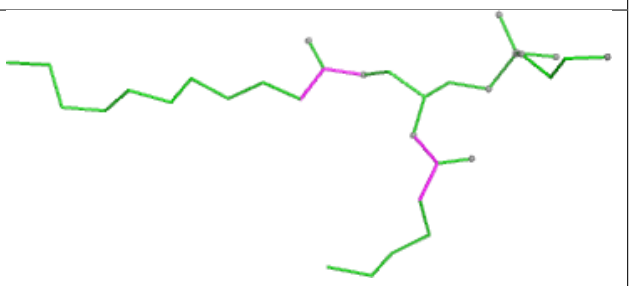
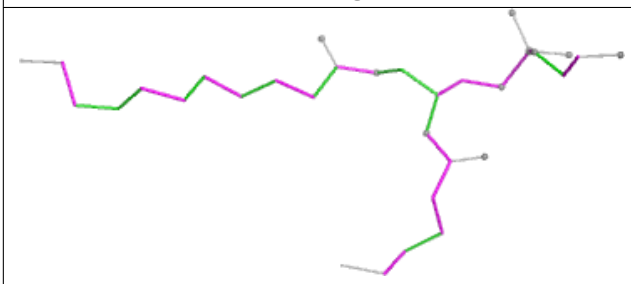
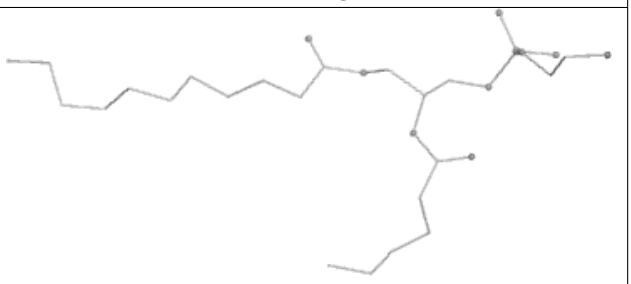
Ligand 3PE X 201



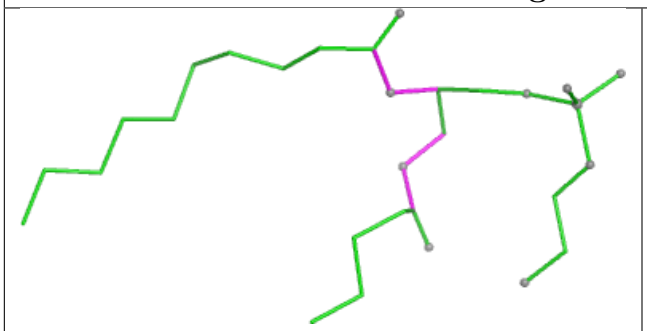
Ligand LMT L 704



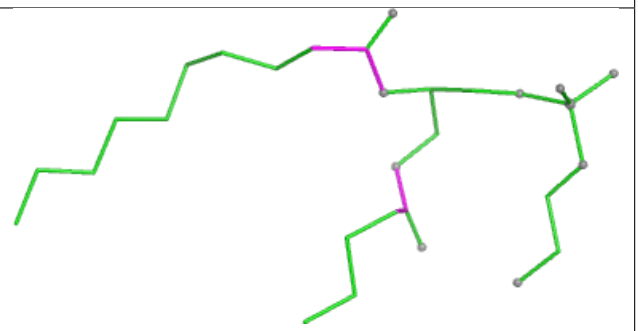
Ligand LMT N 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE d 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

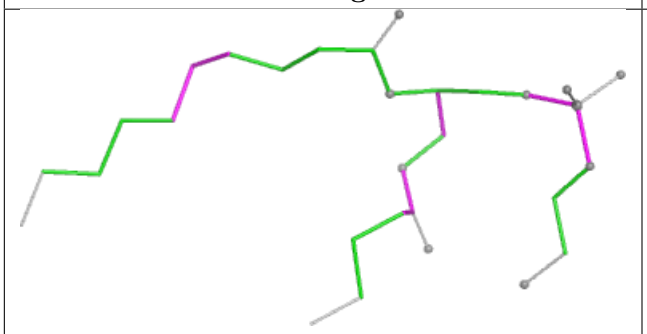
Ligand 3PE O 503



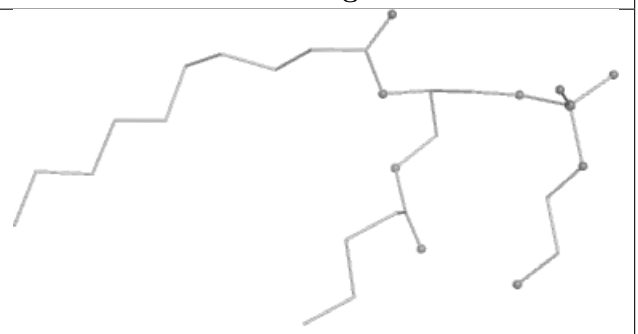
Bond lengths



Bond angles

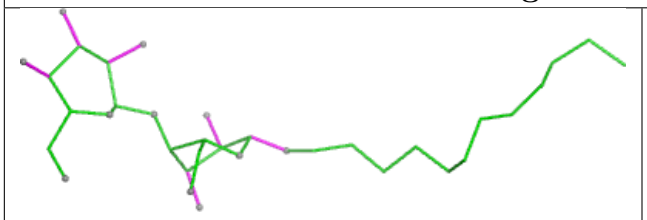


Torsions

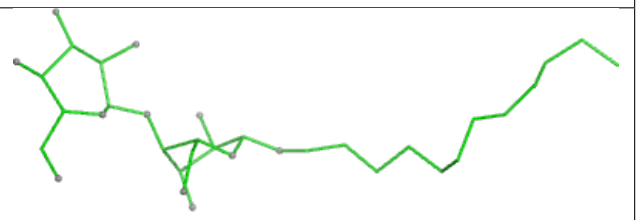


Rings

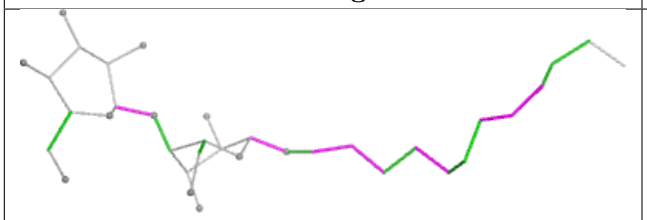
Ligand LMT Y 202



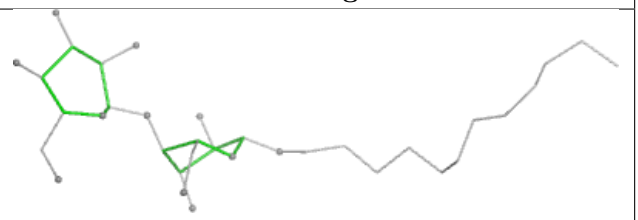
Bond lengths



Bond angles

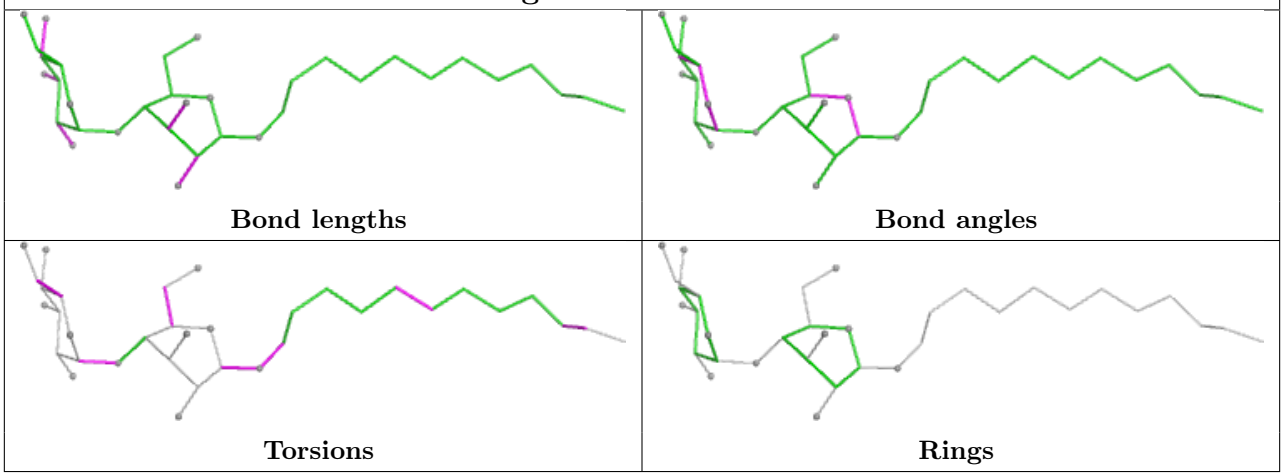


Torsions

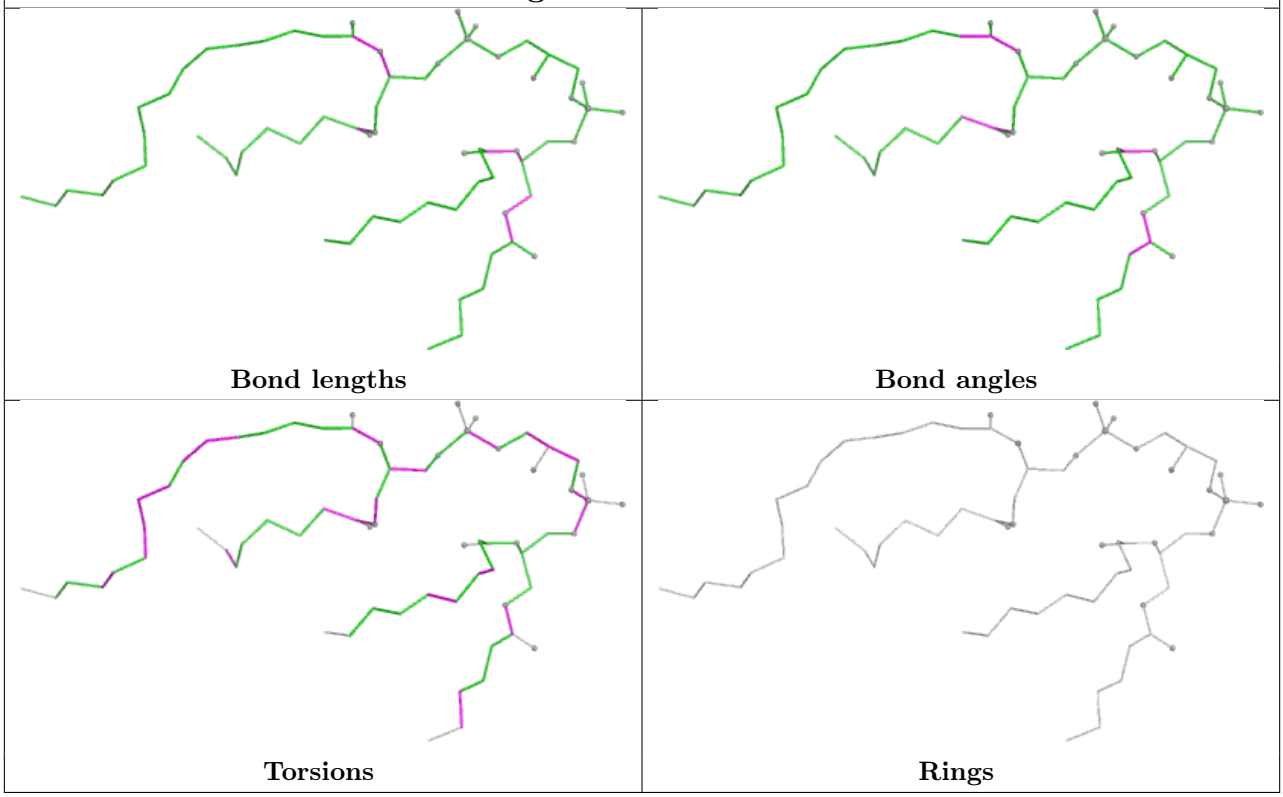


Rings

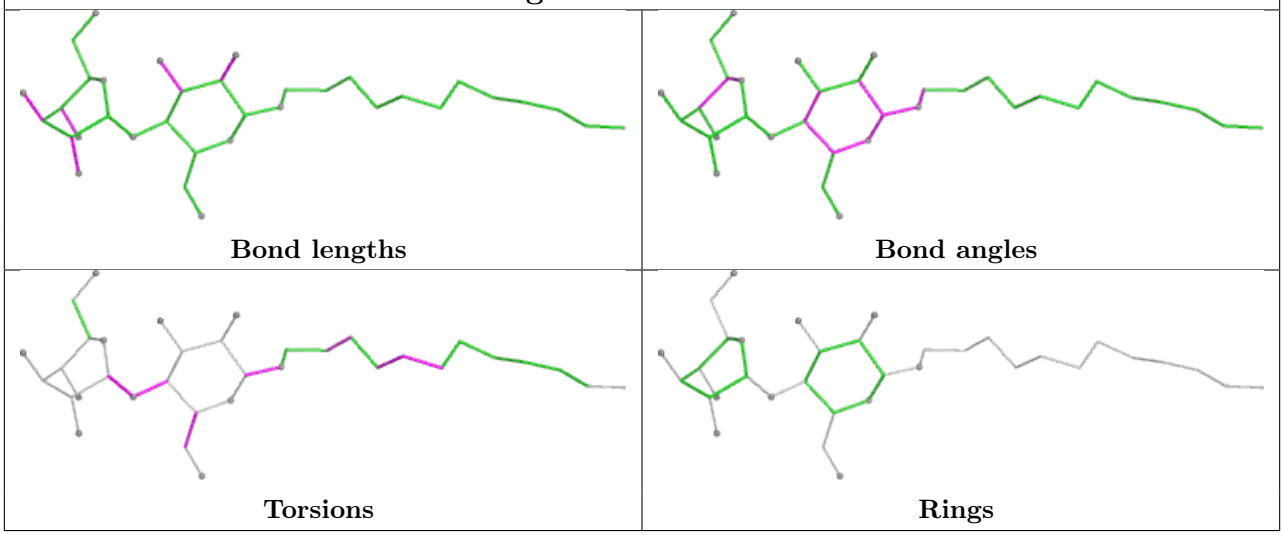
Ligand LMT A 201



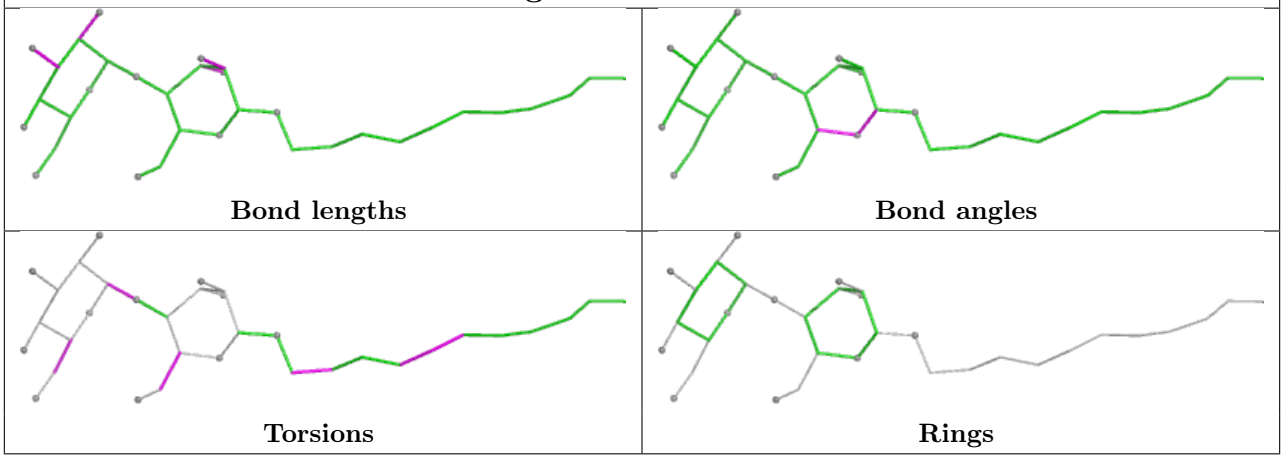
Ligand CDL L 703



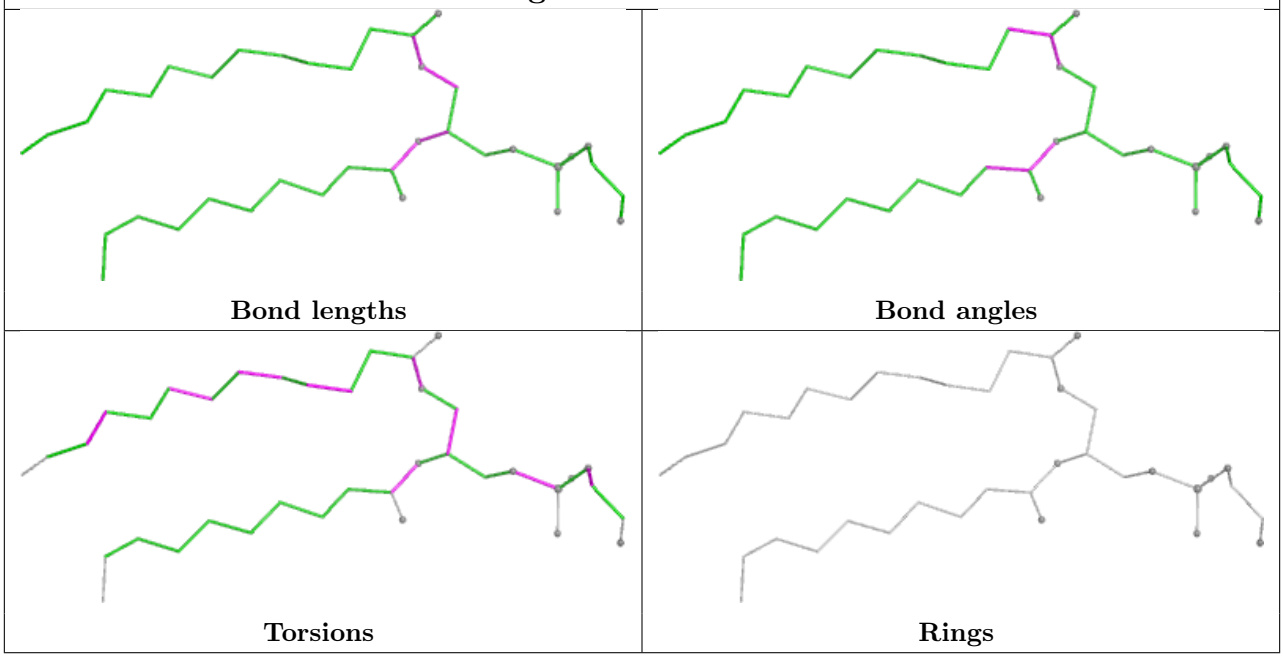
Ligand LMT J 202



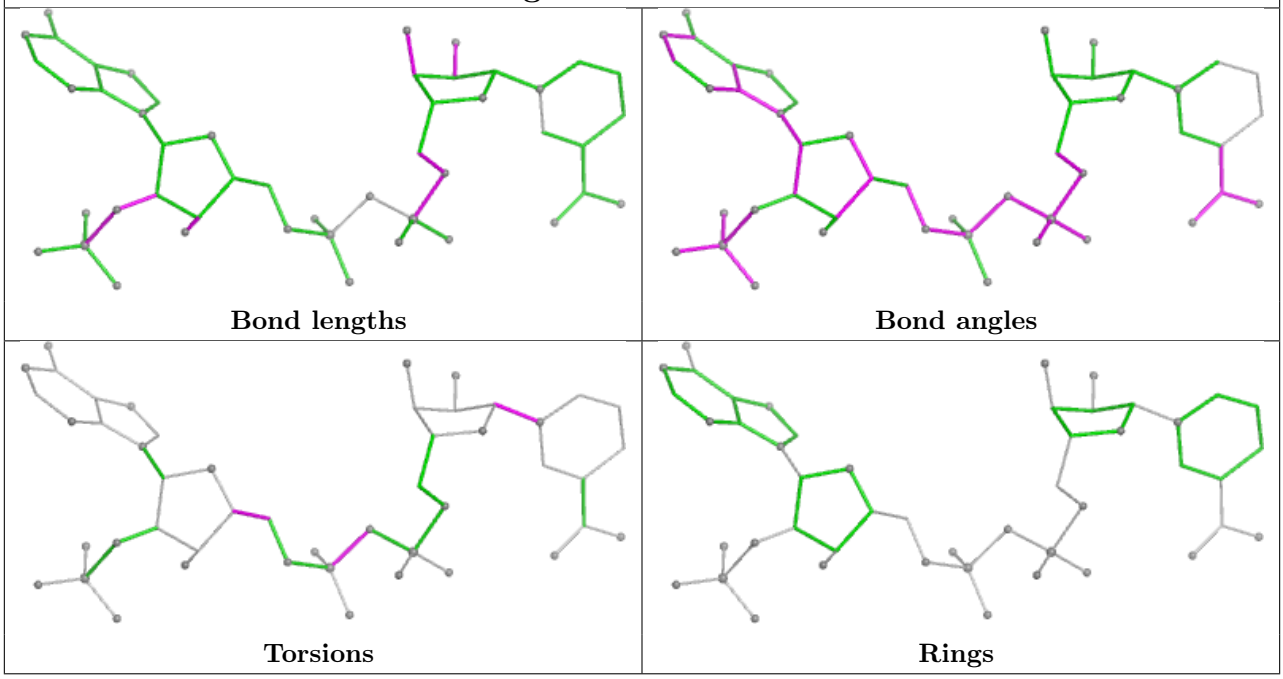
Ligand LMT h 203



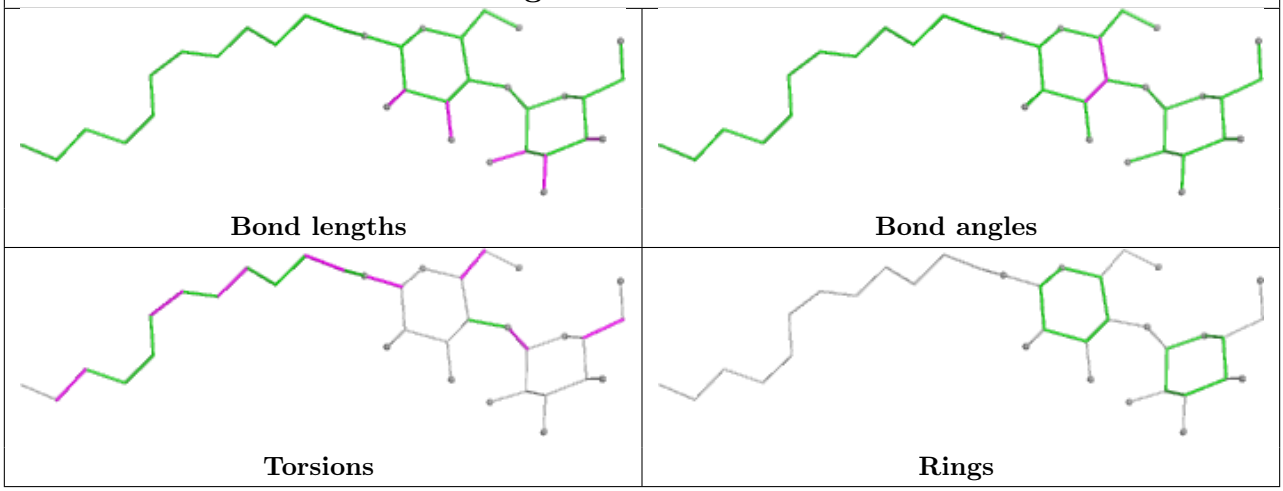
Ligand 3PE N 403



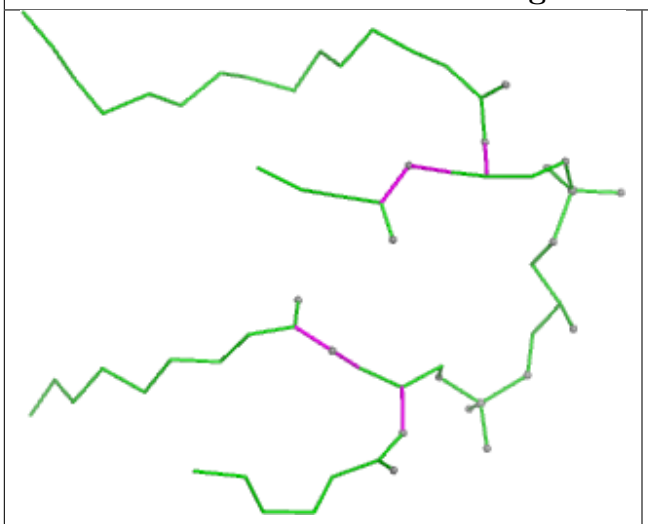
Ligand NDP P 501



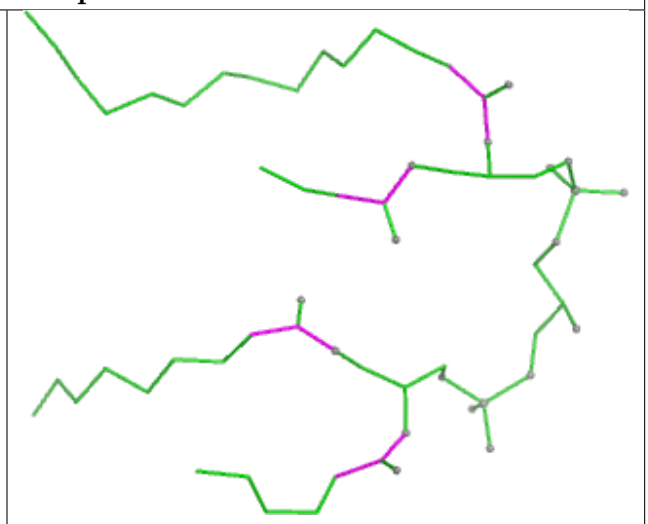
Ligand LMT L 701



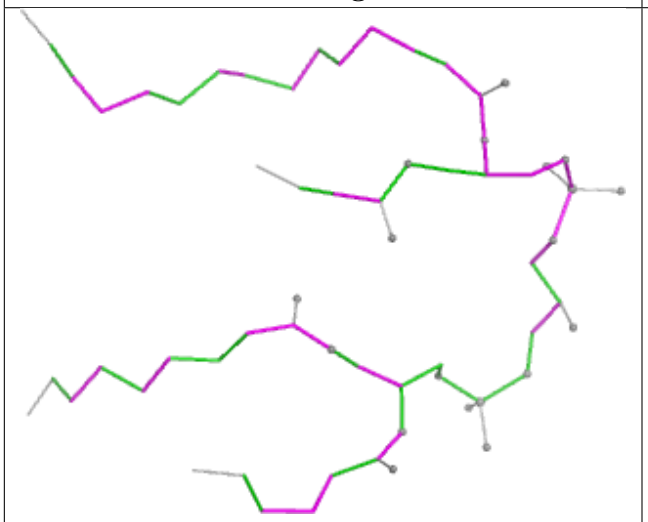
Ligand CDL q 201



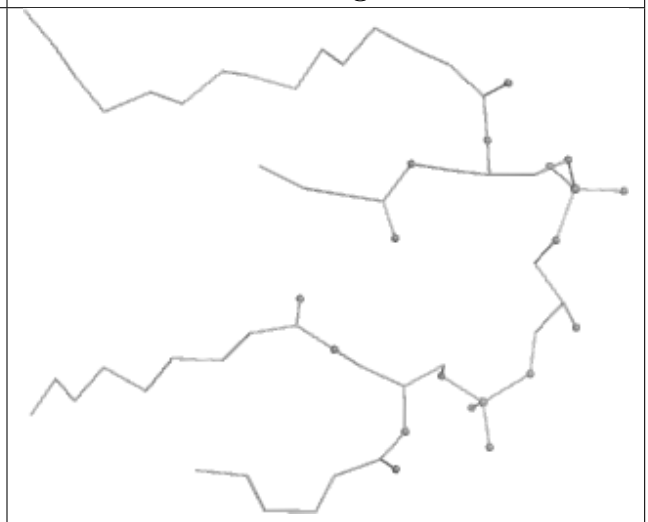
Bond lengths



Bond angles

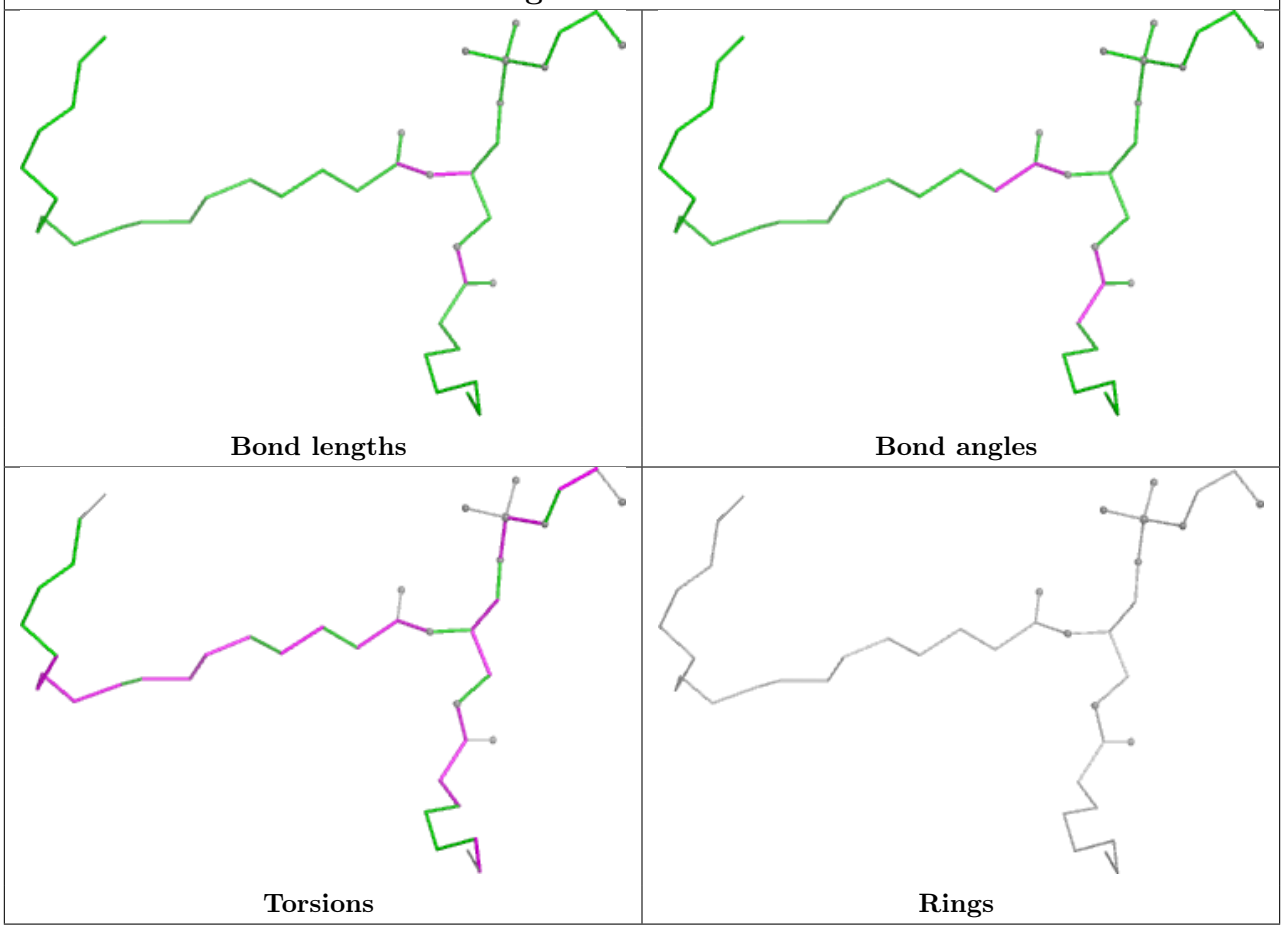


Torsions

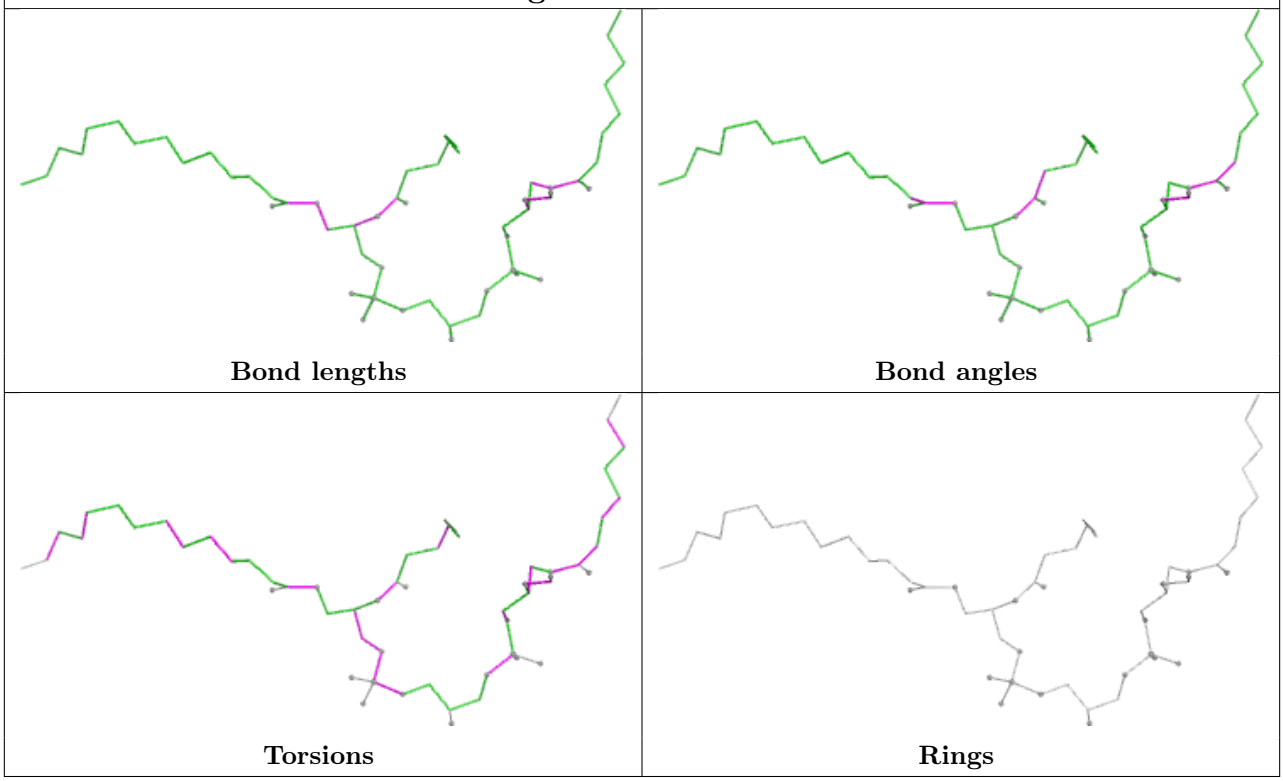


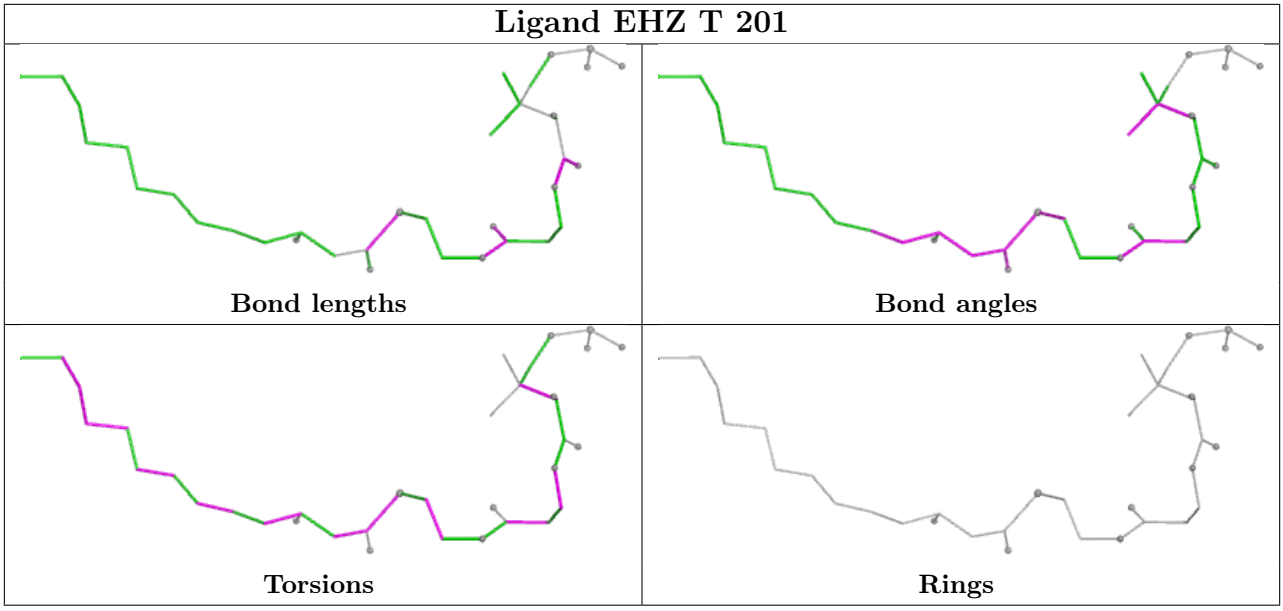
Rings

Ligand 3PE M 501



Ligand CDL h 201





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.

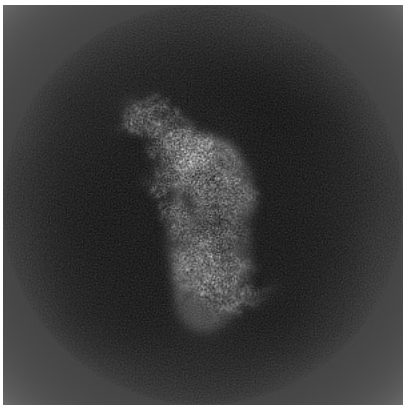
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16965. These allow visual inspection of the internal detail of the map and identification of artifacts.

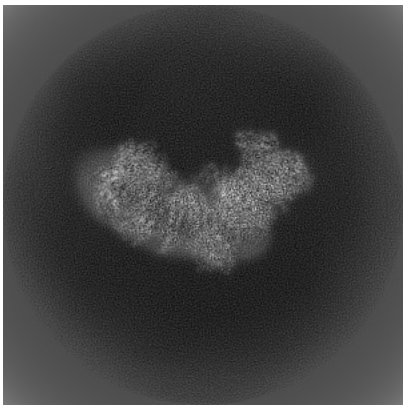
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

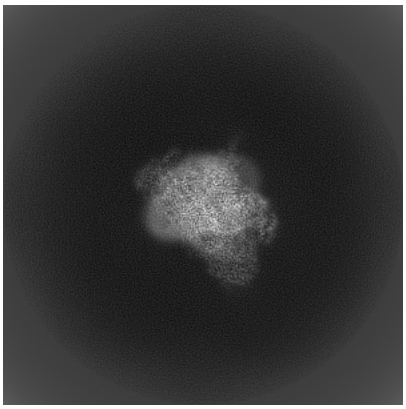
6.1.1 Primary map



X

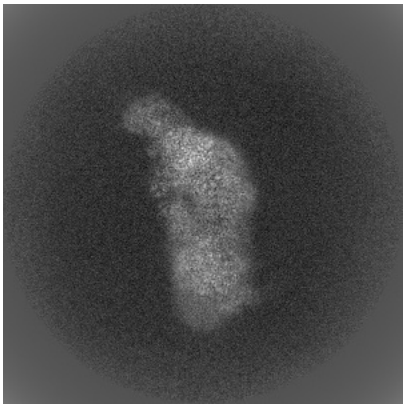


Y

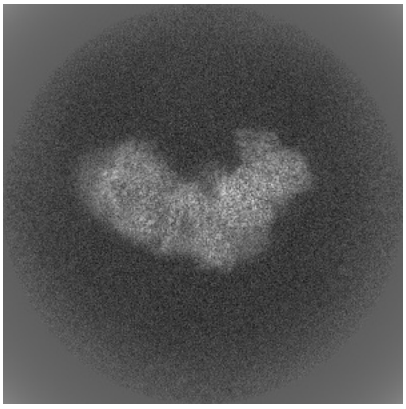


Z

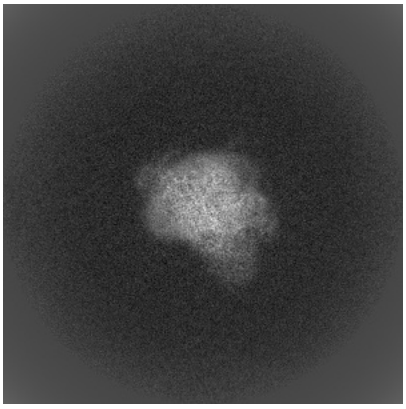
6.1.2 Raw map



X



Y

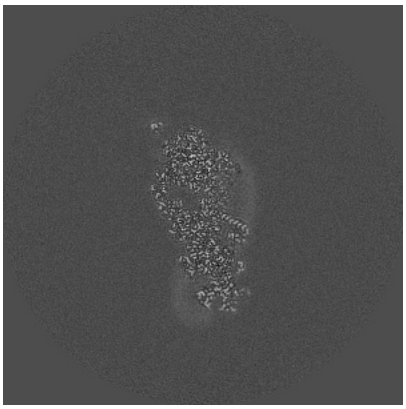


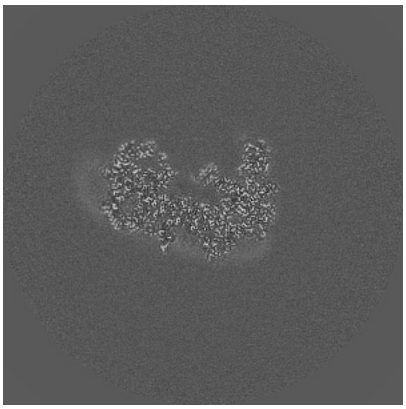
Z

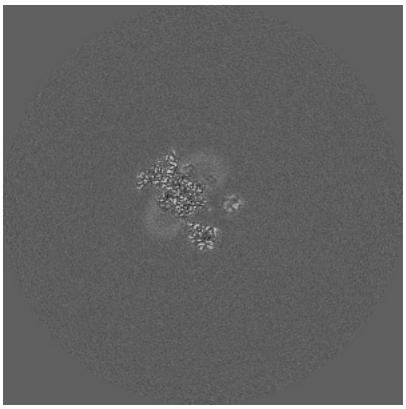
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

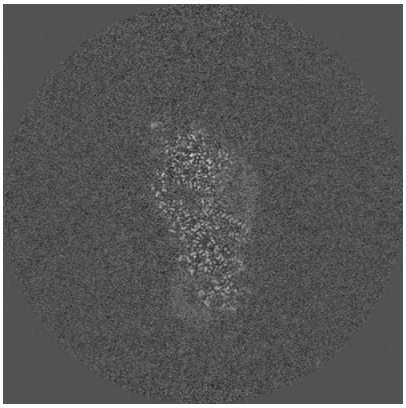
6.2.1 Primary map

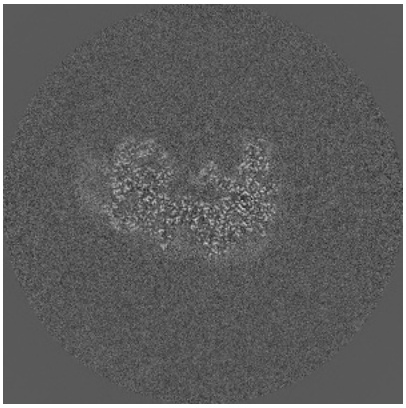

X Index: 350

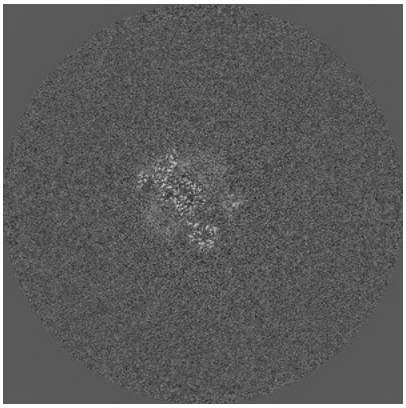

Y Index: 350


Z Index: 350

6.2.2 Raw map


X Index: 350

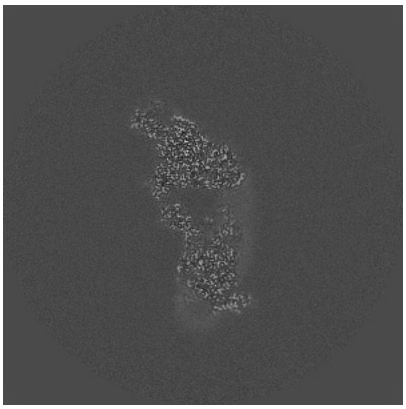

Y Index: 350

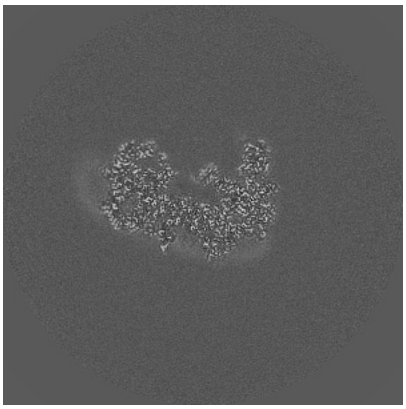

Z Index: 350

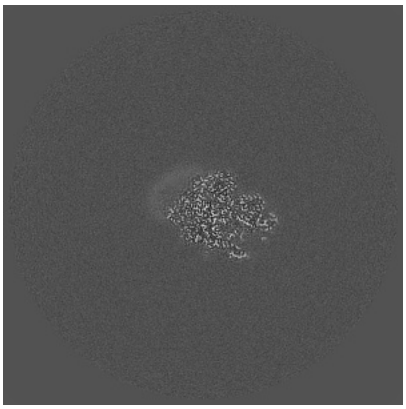
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

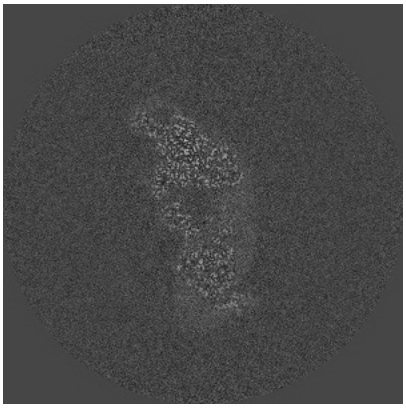
6.3.1 Primary map

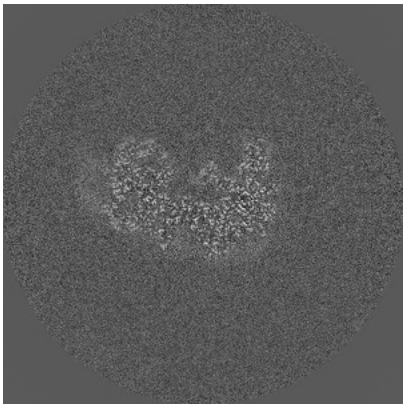

X Index: 370

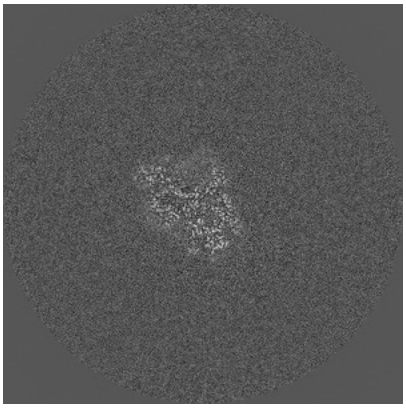

Y Index: 350


Z Index: 438

6.3.2 Raw map


X Index: 370

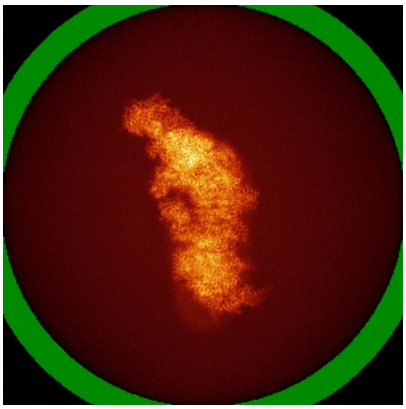

Y Index: 350

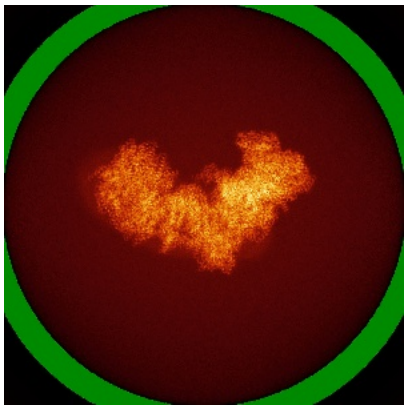

Z Index: 386

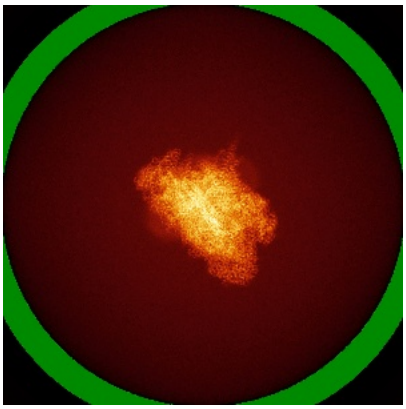
The images above show the largest variance slices of the map in three orthogonal directions.

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

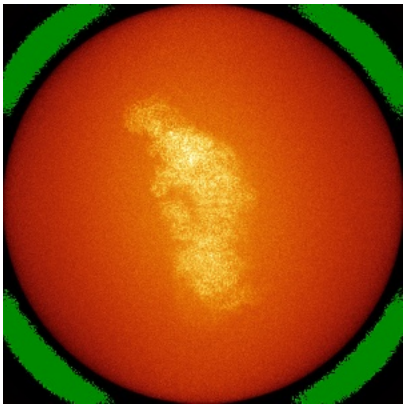
6.4.1 Primary map

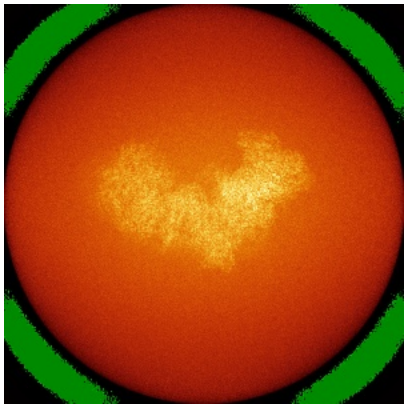

X

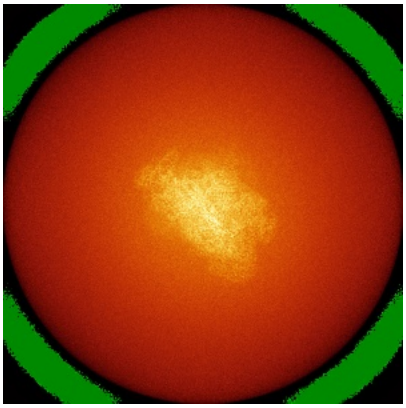

Y


Z

6.4.2 Raw map


X


Y


Z

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

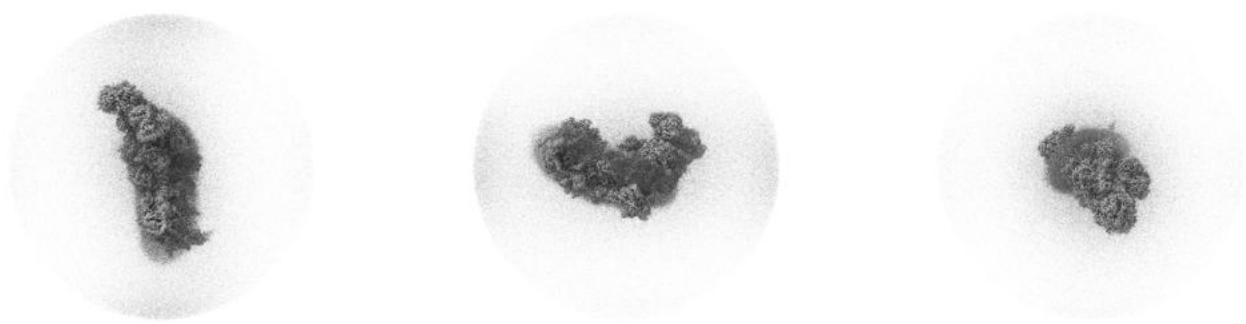
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

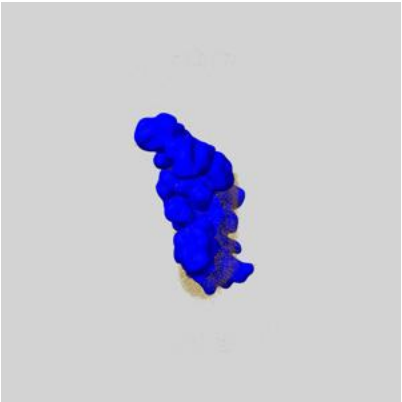
6.6 Mask visualisation (i)

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

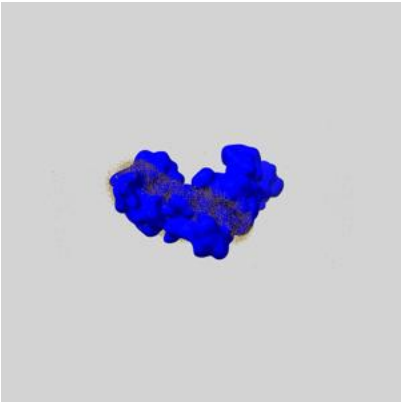
A mask typically either:

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

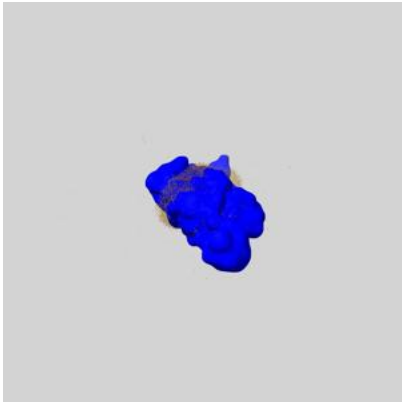
6.6.1 emd_16965_msk_1.map (i)



X



Y

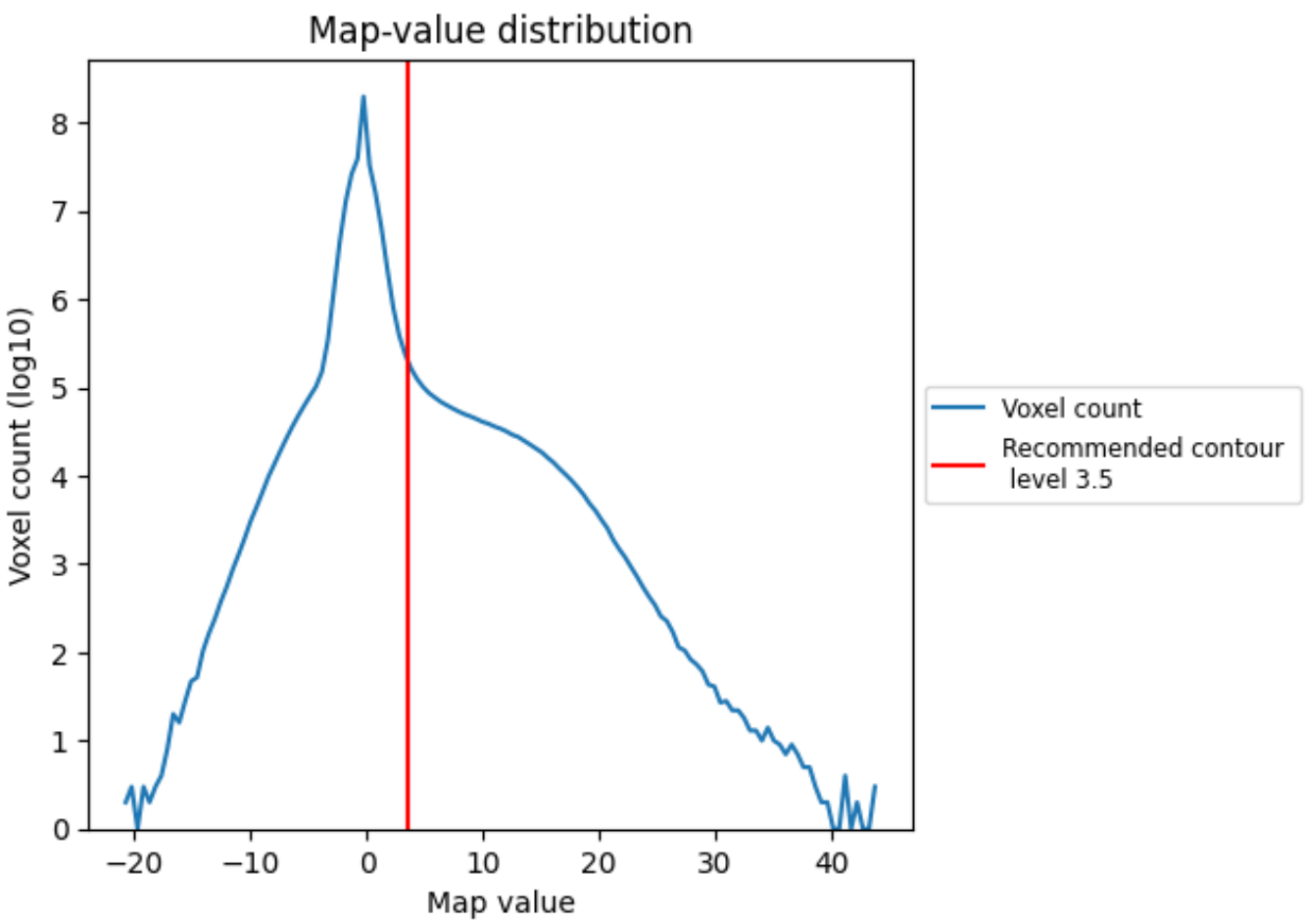


Z

7 Map analysis (i)

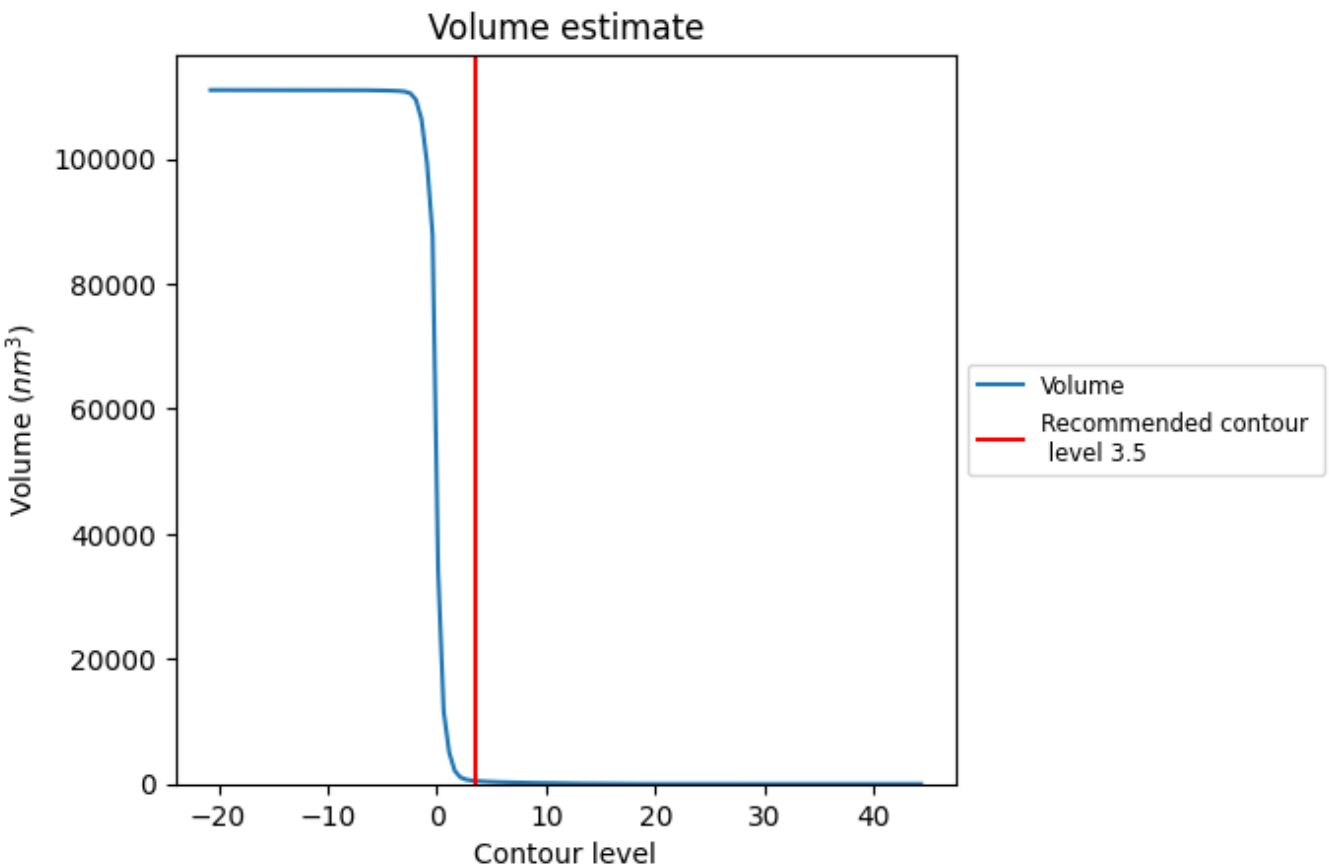
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

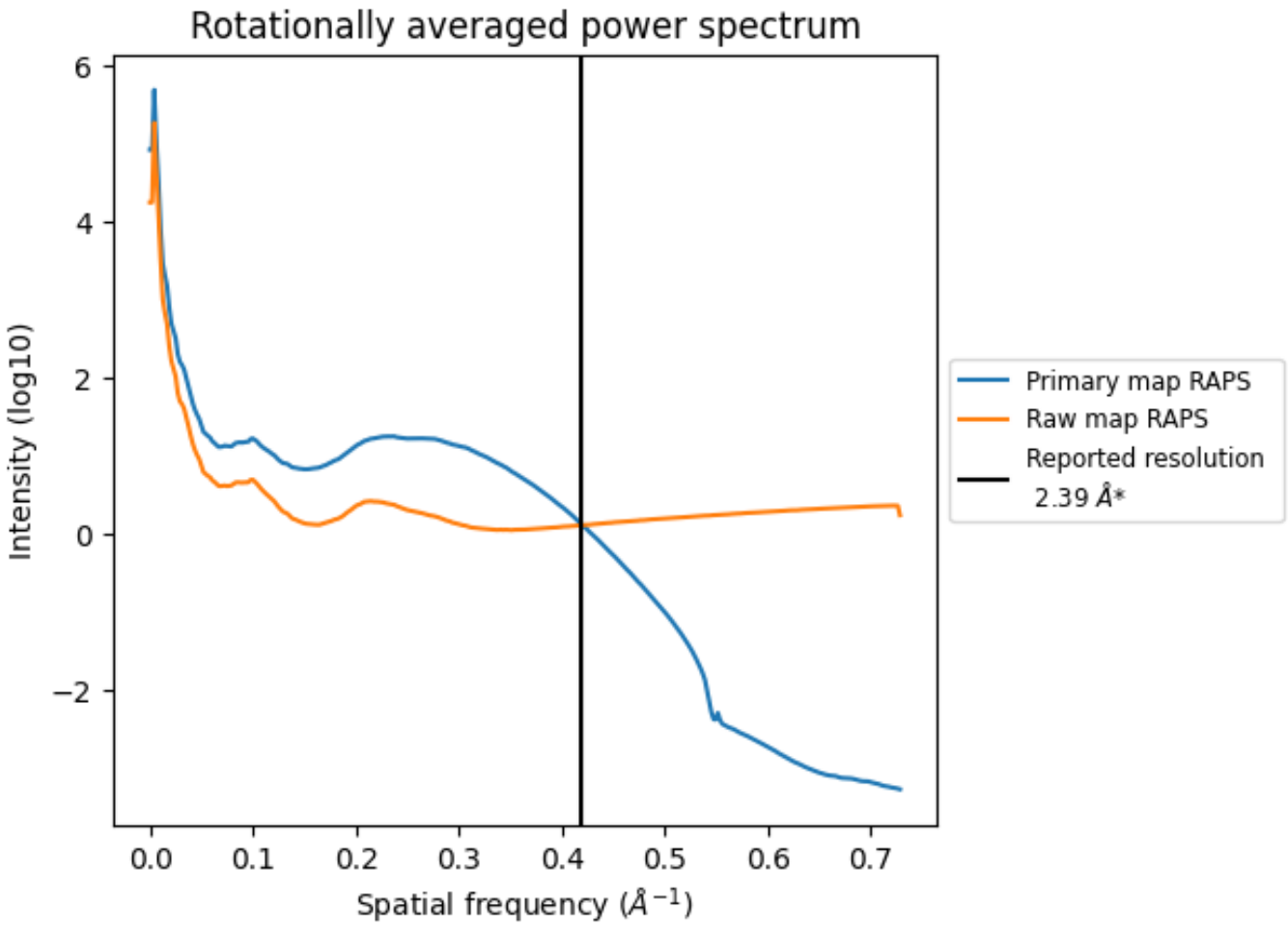
7.2 Volume estimate (i)



The volume at the recommended contour level is 496 nm^3; this corresponds to an approximate mass of 448 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)

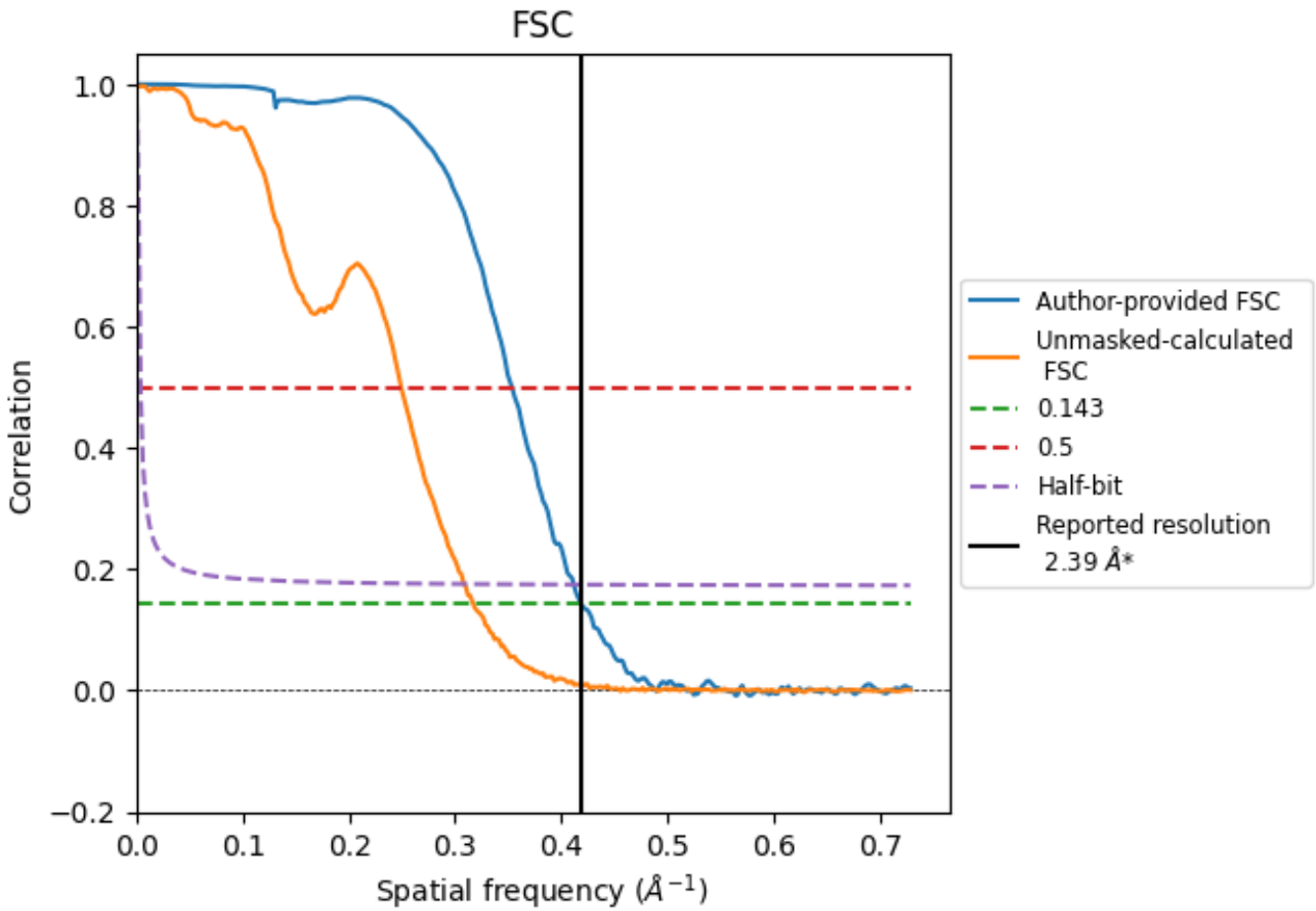


*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8.2 Resolution estimates (i)

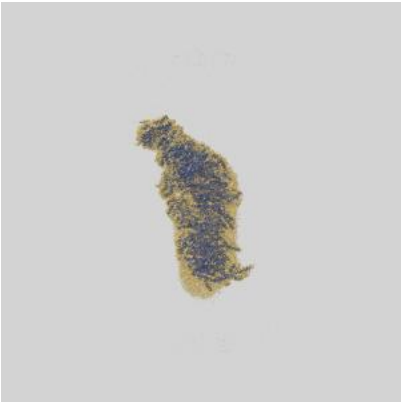
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	2.83	2.43
Unmasked-calculated*	3.15	4.01	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.39 by more than 10 %

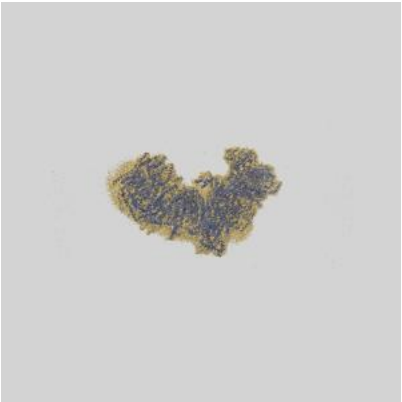
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16965 and PDB model 8OM1. Per-residue inclusion information can be found in section 3 on page 23.

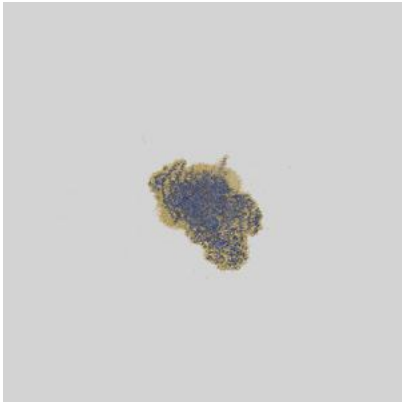
9.1 Map-model overlay (i)



X



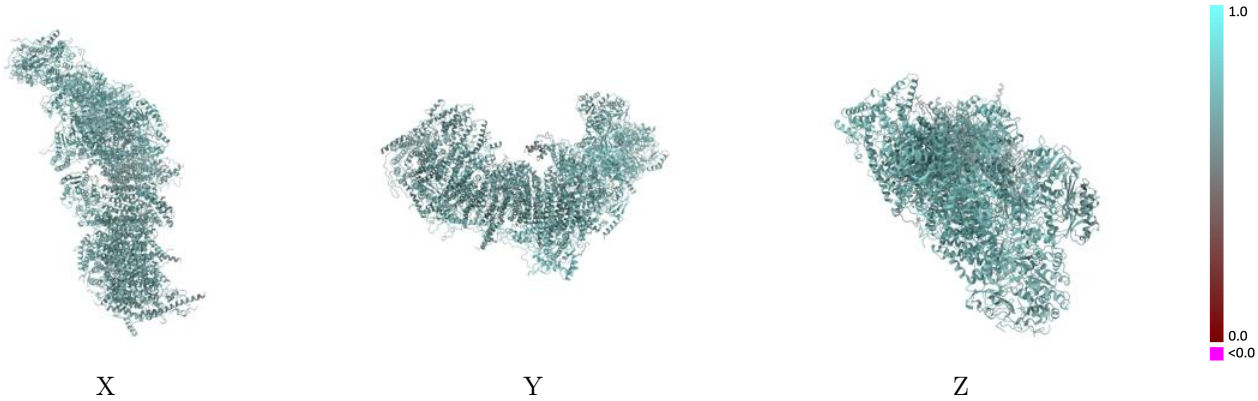
Y



Z

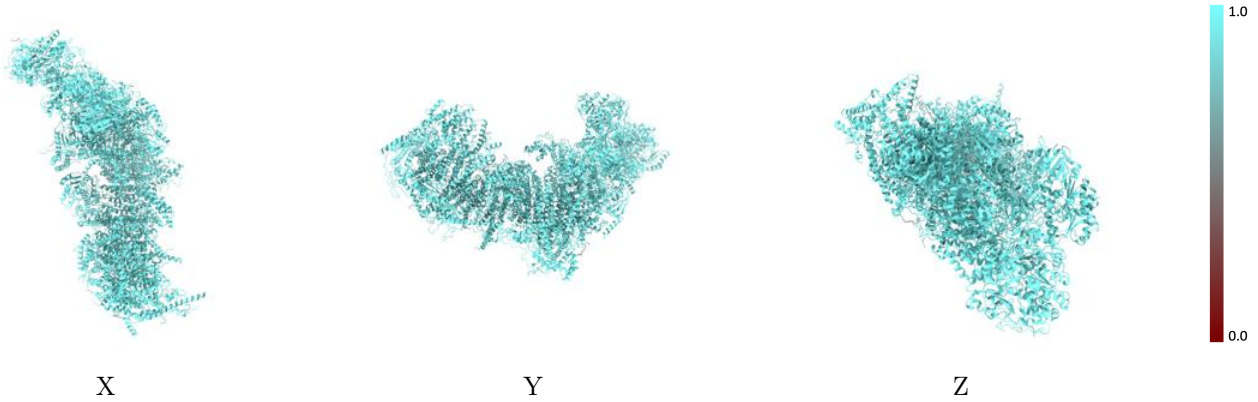
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



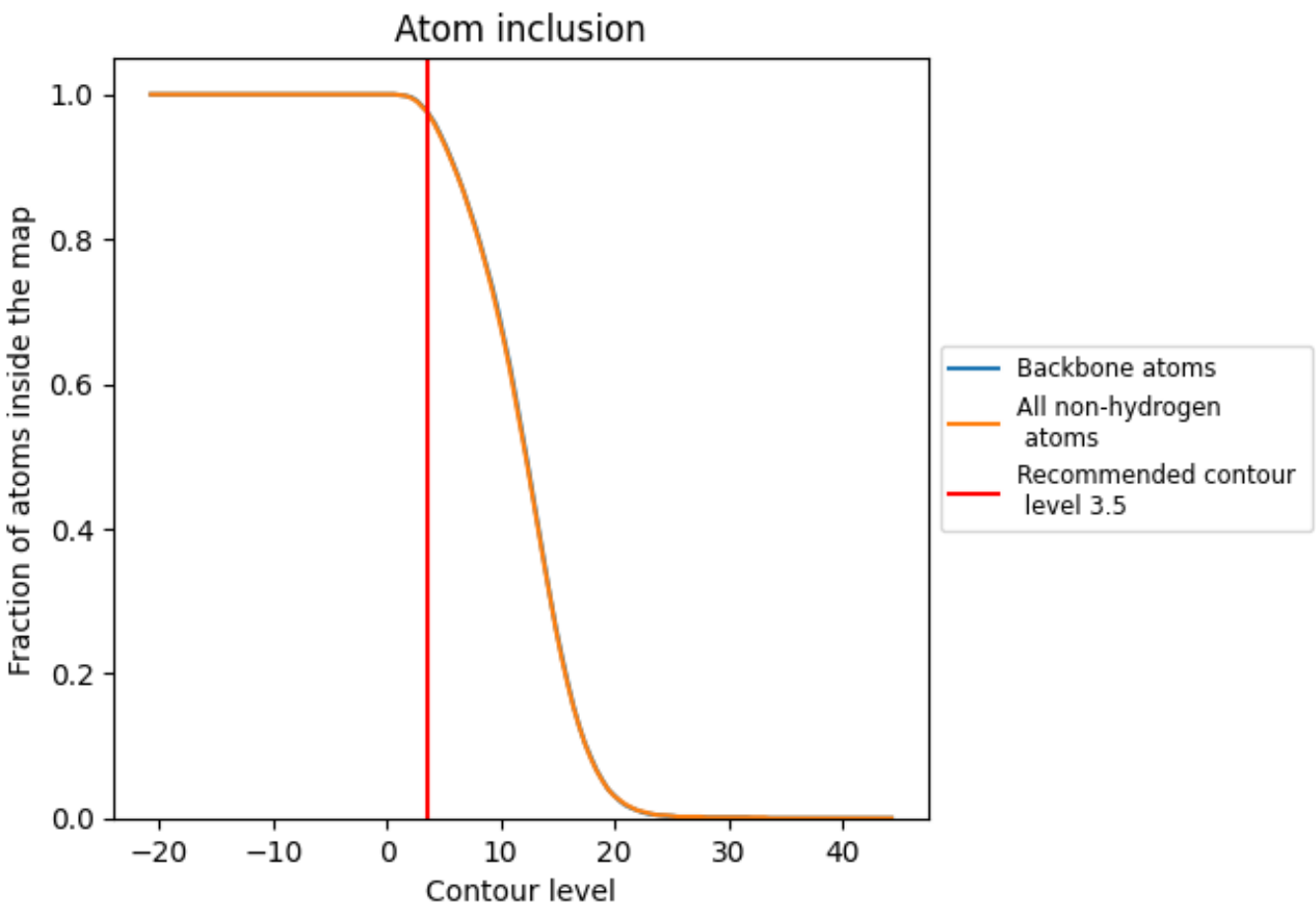
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9760	0.6960
A	0.9820	0.7130
B	0.9890	0.7390
C	0.9870	0.7410
D	0.9870	0.7410
E	0.9710	0.6690
F	0.9860	0.6800
G	0.9820	0.7010
H	0.9920	0.7310
I	0.9750	0.7350
J	0.9670	0.6970
K	0.9860	0.7290
L	0.9800	0.6810
M	0.9950	0.7290
N	0.9910	0.7270
O	0.9820	0.7090
P	0.9850	0.7150
Q	0.9750	0.7180
R	0.9840	0.7070
S	0.9700	0.6370
T	0.8920	0.5780
U	0.9610	0.6330
V	0.9710	0.7130
W	0.9790	0.7120
X	0.9740	0.6960
Y	0.9580	0.6530
Z	0.9850	0.7070
a	0.9960	0.7230
b	0.9770	0.6820
c	0.9370	0.6540
d	0.9720	0.6940
e	0.9720	0.6980
f	0.9350	0.6500
g	0.9770	0.6930
h	0.9640	0.6890

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Chain	Atom inclusion	Q-score
i	0.9520	0.6290
j	0.9420	0.6120
k	0.9580	0.6190
l	0.9620	0.6640
m	0.9640	0.6750
n	0.9600	0.6550
o	0.9410	0.6080
p	0.9700	0.6640
q	0.9790	0.7060
r	0.9600	0.6970
s	0.9440	0.6380