wwPDB EM Validation Summary Report (i)

Sep 7, 2026 – 09:40 pm BST

PDB ID	:	8Q0M / pdb_00008q0m
EMDB ID	:	EMD-18055
Title	:	Outward-facing, closed proteoliposome complex I at 3.1 A. Initially purified in DDM.
Authors	:	Grba, D.N.; Hirst, J.
Deposited on	:	2023-07-28
Resolution	:	3.10 Å(reported)
Based on initial model	:	7QSK

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:

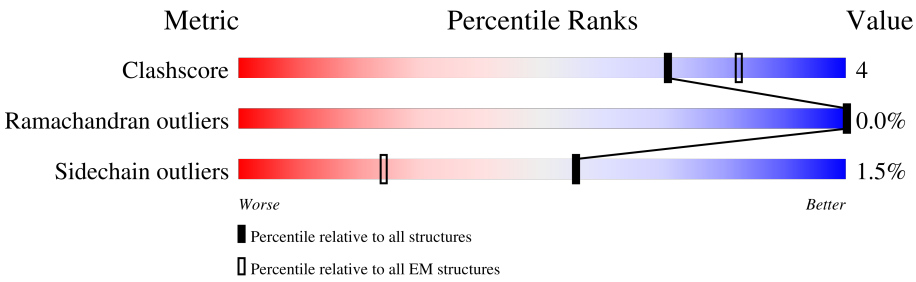
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

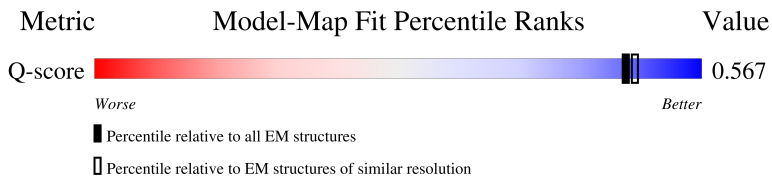
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	88% 12%
2	B	216	62% 9% 28%
3	C	266	71% 8% 21%
4	D	463	85% 7% 7%

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Mol	Chain	Length	Quality of chain
5	E	249	75% 11% 14%
6	F	464	80% 12% 7%
7	G	727	85% 9% 5%
8	H	318	86% 13%
9	I	212	73% 10% 17%
10	J	175	87% 12%
11	K	98	90% 9%
12	L	606	89% 11%
13	M	459	89% 10%
14	N	347	91% 9%
15	O	343	85% 7% 7%
16	P	380	82% 7% 10%
17	Q	175	63% 10% 26%
18	R	124	6% 74% 23%
19	S	99	74% 14% 12%
20	T	156	55% 44%
20	U	156	52% 44%
21	V	116	91% 8%
22	W	128	77% 13% 10%
23	X	172	90% 9%
24	Y	141	96%
25	Z	144	82% 16%
26	a	70	94% 6%
27	b	84	96%
28	c	76	57% 8% 36%

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Mol	Chain	Length	Quality of chain
29	d	120	91% 9%
30	e	106	85% 8% 7%
31	f	57	9% 82% 16%
32	g	154	59% 6% 34%
33	h	189	68% 5% 27%
34	i	128	8% 77% 22%
35	j	108	6% 60% 6% 34%
36	k	98	7% 78% 5% 17%
37	l	186	78% 5% 16%
38	m	129	93% 6%
39	n	179	87% 9%
40	o	137	9% 80% 9% 11%
41	p	176	91% 7%
42	q	145	91% 9%
43	r	113	79% 5% 16%
44	s	109	7% 33% 8% 59%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 70158 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	921	622	133	159	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	155	1241	792	224	211	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	209	1738	1120	298	317	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	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	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	432	3326	2096	594	616	20	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	688	5279	3307	920	1013	39	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	2509	1681	385	420	23	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	176	1414	889	243	270	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	175	1345	906	191	236	12	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	745	486	112	131	16	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	606	4802	3195	737	827	43	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	3654	2436	570	609	39	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	347	2733	1817	416	457	43	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	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	342	2754	1781	487	481	5	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	129	1049	659	188	199	3	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	96	740	454	140	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	87	700	440	131	127	2	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	88	707	454	104	144	5	0	0
20	U	88	707	454	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	115	928	600	157	168	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	115	976	625	181	166	4	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	1402	887	253	252	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	140	1030	657	176	191	6	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	141	1152	740	201	202	9	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	70	569	365	104	95	5	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	654	427	109	116	2	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		
28	c	49	414	273	70	71	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	999	650	172	172	5	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	99	829	523	158	142	6	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	57	492	322	86	82	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	846	544	140	158	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	138	1154	759	196	197	2	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	127	1097	722	191	183	1	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	71	597	390	99	107	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	81	653	427	110	114	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	156	1314	850	216	240	8	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	128	1070	686	188	196	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	171	1487	952	272	256	7	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	122	1048	653	201	185	9	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	174	1458	913	269	268	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	780	216	211	5	0	0

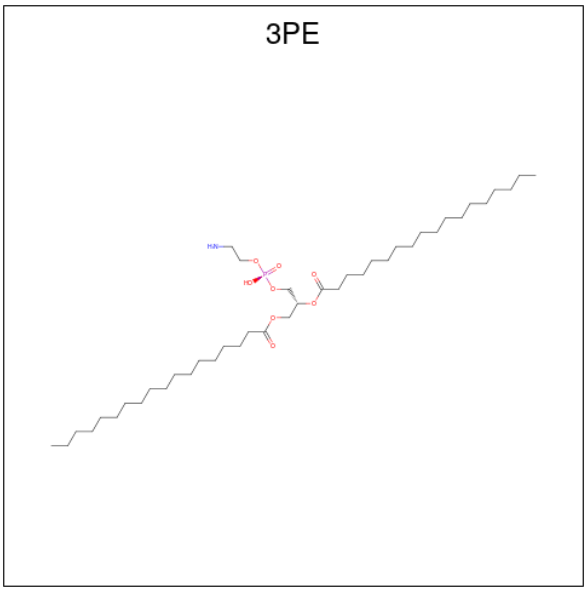
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	95	776	490	144	139	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	S		
44	s	45	380	238	67	74	1	0	0

- Molecule 45 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	
45	A	1	47	37	1	8	1	0
45	A	1	37	27	1	8	1	0
45	A	1	51	41	1	8	1	0
45	J	1	29	19	1	8	1	0
45	J	1	36	26	1	8	1	0
45	K	1	44	34	1	8	1	0
45	L	1	51	41	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	N	1	49	39	1	8	1	0
			Total	C	N	O	P	
45	N	1	45	35	1	8	1	0
			Total	C	N	O	P	
45	N	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	O	1	45	35	1	8	1	0
			Total	C	N	O	P	
45	P	1	35	25	1	8	1	0
			Total	C	N	O	P	
45	Y	1	27	17	1	8	1	0
			Total	C	N	O	P	
45	Y	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	Y	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	Y	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	Y	1	45	35	1	8	1	0
			Total	C	N	O	P	
45	Y	1	36	26	1	8	1	0
			Total	C	N	O	P	
45	Y	1	43	33	1	8	1	0
			Total	C	N	O	P	
45	Z	1	41	31	1	8	1	0
			Total	C	N	O	P	
45	Z	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	b	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	e	1	49	39	1	8	1	0
			Total	C	N	O	P	
45	f	1	34	24	1	8	1	0
			Total	C	N	O	P	
45	f	1	44	34	1	8	1	0
			Total	C	N	O	P	
45	i	1	45	35	1	8	1	0
			Total	C	N	O	P	
45	m	1	41	31	1	8	1	0
			Total	C	N	O	P	
45	m	1	32	22	1	8	1	0

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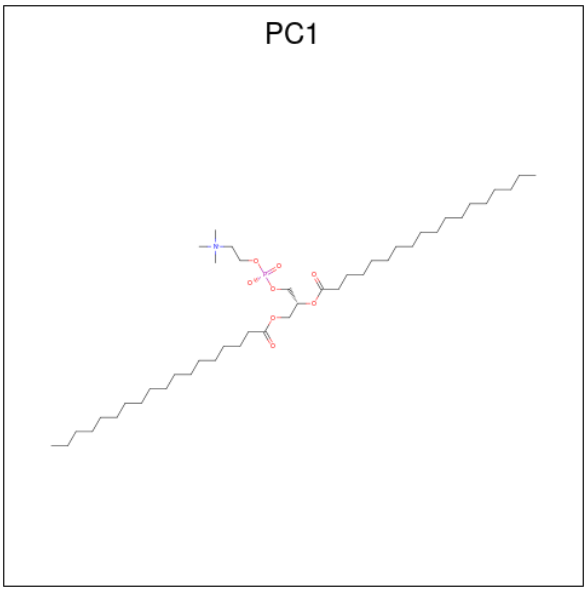
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	m	1	50	40	1	8	1	0
			Total	C	N	O	P	
45	m	1	41	31	1	8	1	0
			Total	C	N	O	P	
45	q	1	51	41	1	8	1	0
			Total	C	N	O	P	
45	r	1	34	24	1	8	1	0

- 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	35	25	1	8	1	0
			Total	C	N	O	P	
46	A	1	33	23	1	8	1	0
			Total	C	N	O	P	
46	B	1	46	36	1	8	1	0
			Total	C	N	O	P	
46	B	1	48	38	1	8	1	0
			Total	C	N	O	P	
46	H	1	48	38	1	8	1	0
			Total	C	N	O	P	
46	H	1	39	29	1	8	1	0
			Total	C	N	O	P	
46	H	1	39	29	1	8	1	0

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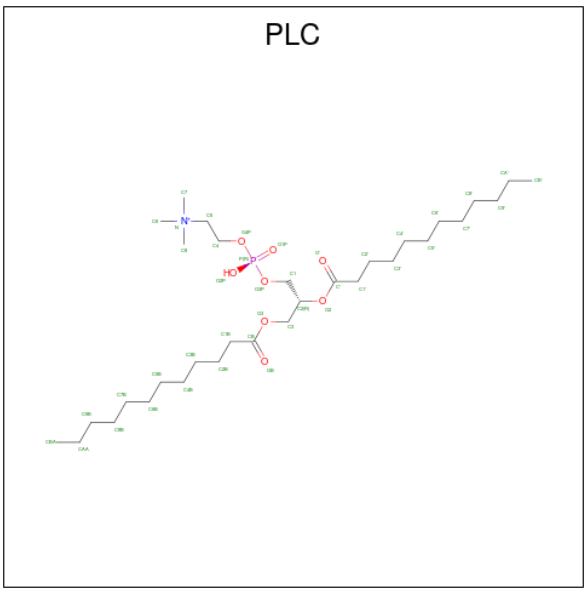
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	I	1	54	44	1	8	1	0
46	I	1	44	34	1	8	1	0
46	J	1	35	25	1	8	1	0
46	L	1	44	34	1	8	1	0
46	L	1	47	37	1	8	1	0
46	M	1	35	25	1	8	1	0
46	e	1	39	29	1	8	1	0
46	h	1	47	37	1	8	1	0
46	m	1	54	44	1	8	1	0
46	q	1	49	39	1	8	1	0

- Molecule 47 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	33	23	1	8	1	0

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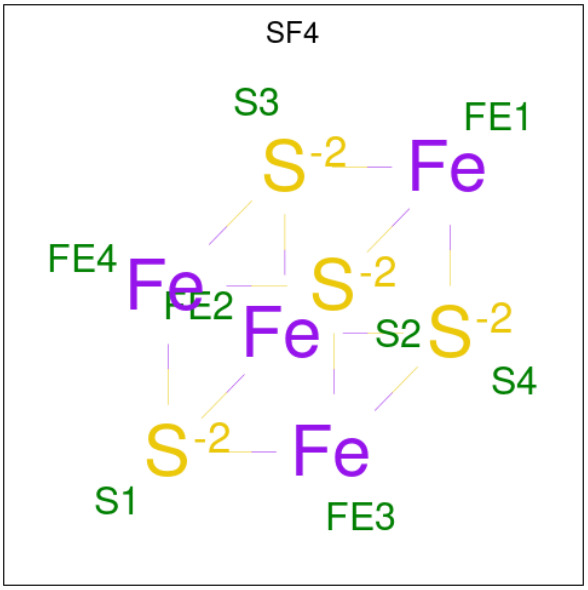
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	J	1	37	27	1	8	1	0
47	L	1	42	32	1	8	1	0
47	M	1	28	18	1	8	1	0
47	O	1	35	25	1	8	1	0
47	P	1	42	32	1	8	1	0
47	P	1	32	22	1	8	1	0
47	Y	1	42	32	1	8	1	0
47	Z	1	34	24	1	8	1	0
47	g	1	42	32	1	8	1	0

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	B	1	8	4	4	0
48	F	1	8	4	4	0

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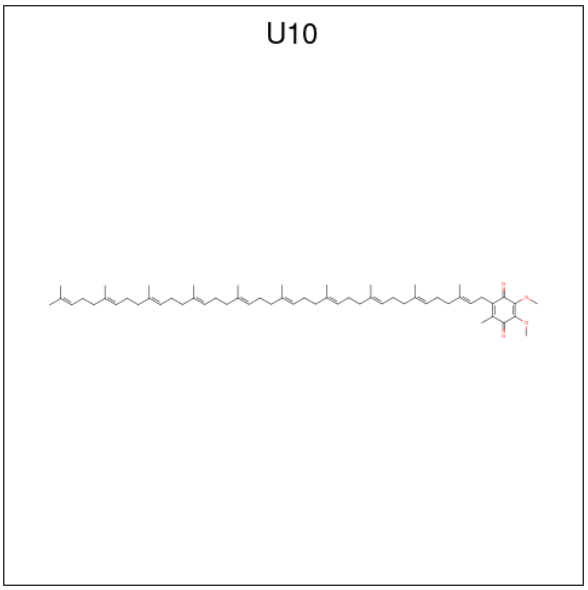
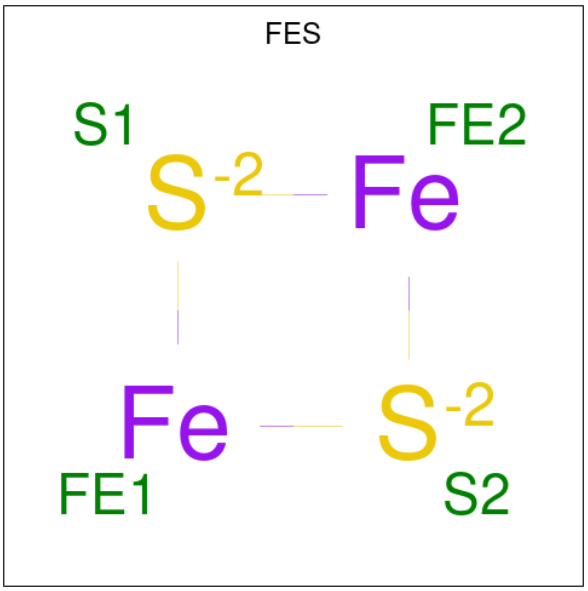
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	G	1	8	4	4	0
48	G	1	8	4	4	0
48	I	1	8	4	4	0
48	I	1	8	4	4	0

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



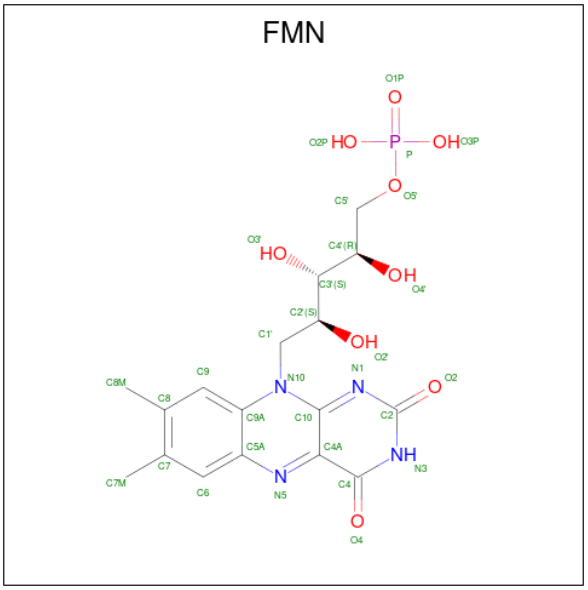
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	B	1	63	59	4	0

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

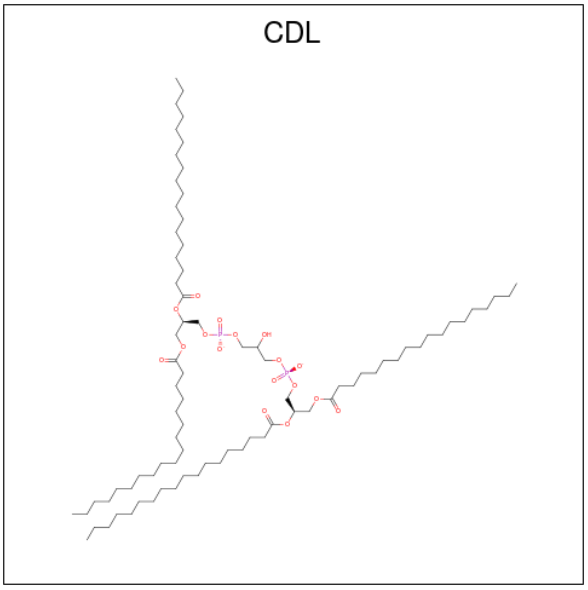


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	F	1	31	17	4	9	1	0

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

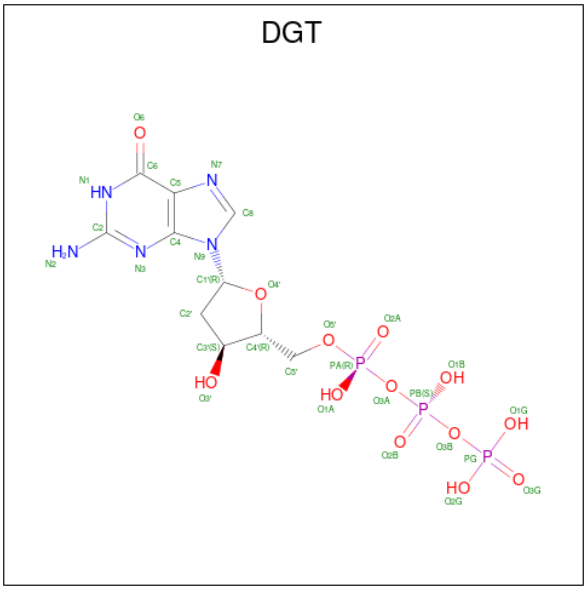


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	H	1	81	62	17	2	0
			Total	C	O	P	
53	L	1	76	57	17	2	0
			Total	C	O	P	
53	M	1	100	81	17	2	0
			Total	C	O	P	
53	N	1	100	81	17	2	0
			Total	C	O	P	
53	P	1	59	40	17	2	0
			Total	C	O	P	
53	d	1	65	46	17	2	0
			Total	C	O	P	
53	d	1	86	67	17	2	0
			Total	C	O	P	
53	h	1	80	61	17	2	0
			Total	C	O	P	
53	r	1	61	42	17	2	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	M	1	1	1	0
			Total	Zn	
54	R	1	1	1	0

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

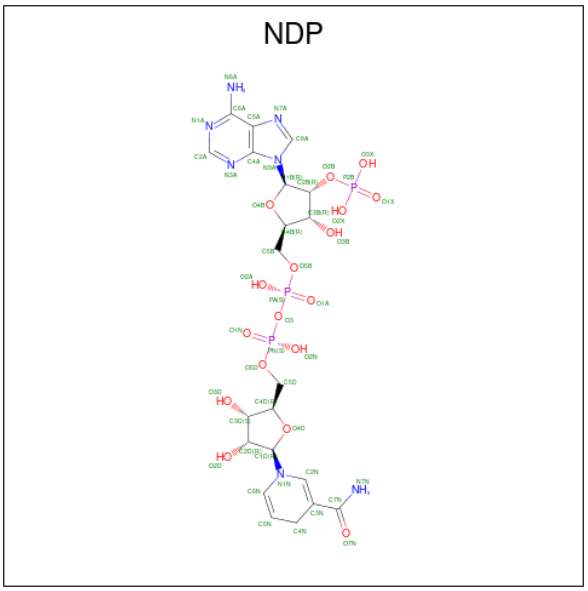


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	O	1	31	10	5	13	3	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

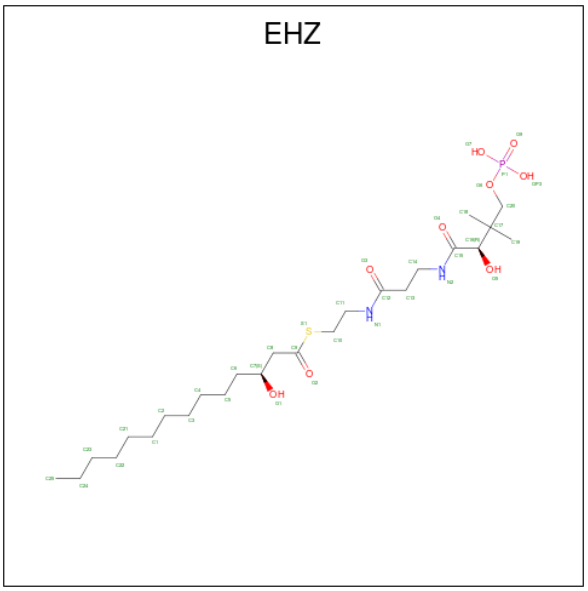
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	O	1	1	1	0

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



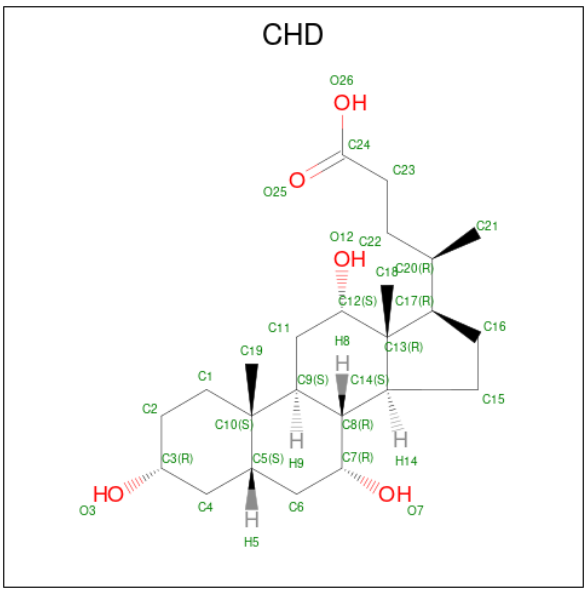
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	P	1	48	21	7	17	3	0

- Molecule 58 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: $C_{25}H_{49}N_2O_9PS$).



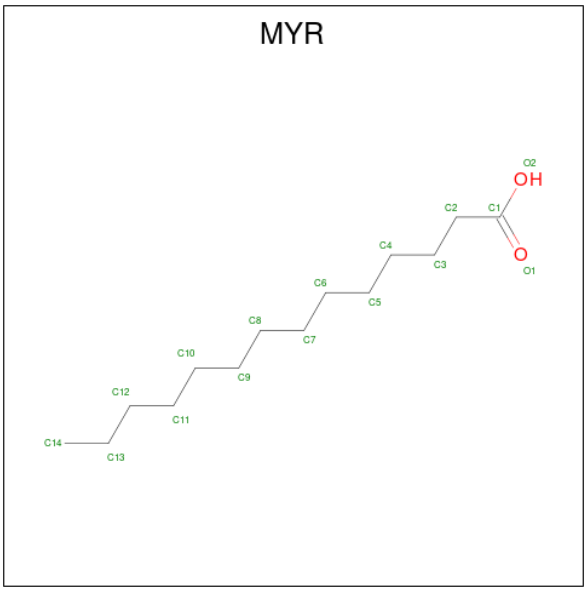
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	T	1	37	25	2	8	1	1	0
58	U	1	37	25	2	8	1	1	0

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
59	i	1	29	24	5	0

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



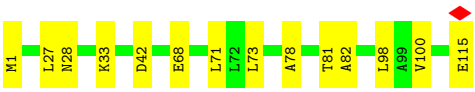
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
60	o	1	15	14	1	0

3 Residue-property plots (i)

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

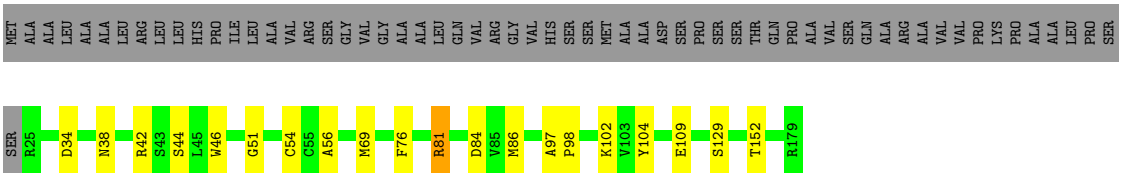
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



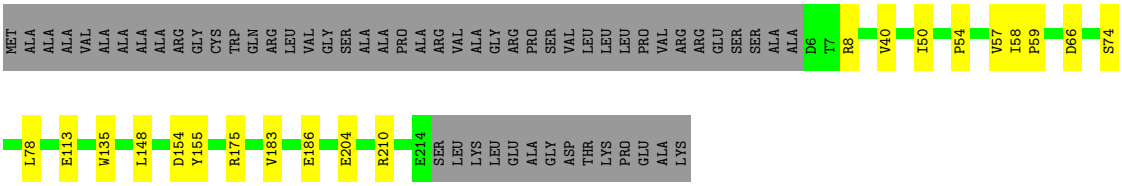
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



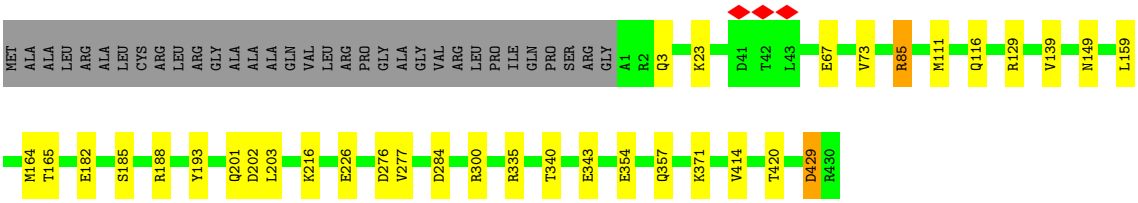
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



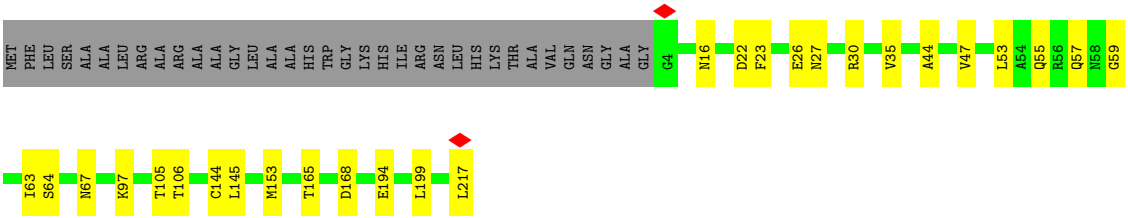
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



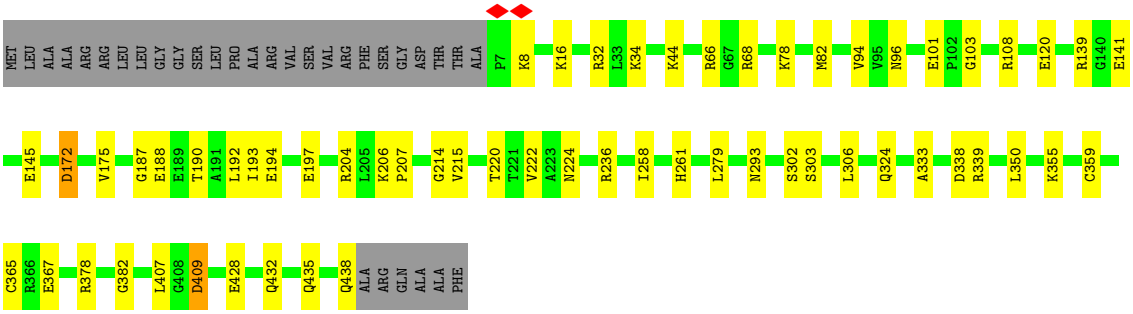
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



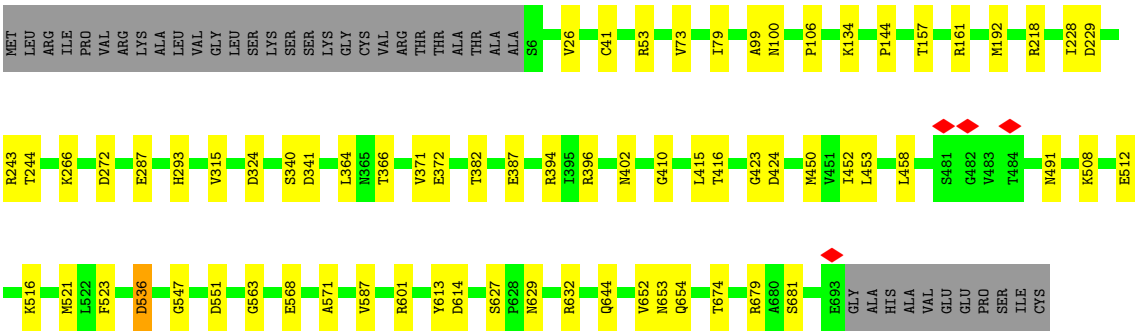
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



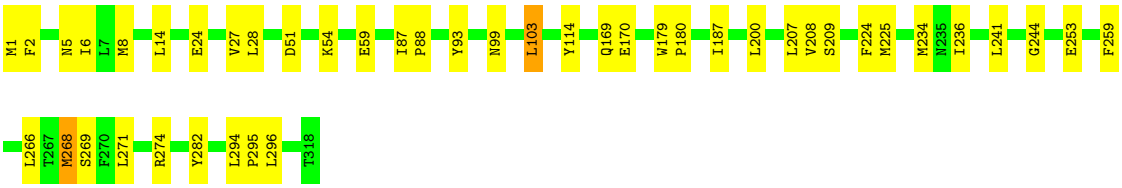
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



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

Chain I: 73% 10% 17%

MET ARG CYS LEU THR MET PRO MET LEU LEU ARG ALA LEU ALA GLN ALA GLN ALA ALA ARG ALA GLY HIS ALA SER VAL ARG GLY LEU HIS SER SER ALA VAL ALA ALA T1 E9 L26 W27 T28 R32 M36 S39 E53 S58 R62 R69 E75

I78 A79 R105 T106 D110 I111 D112 M113 T114 D129 K151 R176

• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 87% 12%

M1 M2 I5 V6 K23 L33 M64 M65 E77 E100 V104 V115 V116 F117 W125 D129 T130 F135 M141 Y147 T157 I168 T172 N175

• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 90% 9%

M1 N9 S15 G18 M37 M43 M59 I62 L73 C98

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 89% 11%

M1 N2 M3 L14 F24 K28 N31 Y35 I49 P50 F54 G58 H67 W68 L69 T70 I71 K81 M82 M87 E102 K116 F117 L121 V132 W144 A171 N175 D179 N194 T221 Q226 H230 P231 R262 F263

Y264 P265 L286 K336 D355 T356 R357 T370 M383 L394 I421 I427 L431 N446 R456 I467 M471 Q479 M480 T481 Y485 L486 K487 T488 T489 A501 L502 E503 K509 H514 Y515 H534 A537 P538 E559 A560 I561 L562

T565 Q580 Y587 S590 L601 E606

• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 89% 10%

M1 I6 M12 P13 D47 N48 L54 F57 S58 D59 L66 N88 L89 T90 R91 M98 T111 I116 L126 T134 G137 N138 T153 L158 P159 Q168 G172 M201 V205 K206 M207 L216 P217 K218 I225 R245 M271

R278 L285 L315 N331 R346 L369 I373 N390 I393 I394 V398 L444 I453 I454 P457 L458 Y459

• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 91% 9%

M1 N2 I13 I19 I22 S23 N36 M37 L38 I41 M44 Y59 M68 M71 M72 I76 M79 A137 P138 F146 P147 Y181 M220 I267 T271 N289 Y298 L302 T303 S307 M313 K321 K322 E347

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

Chain O: 85% 7% • 7%

MET ALA LEU ARG LEU LEU ARG LEU VAL PRO PRO ARG VAL GLY GLY ILE HIS THR SER VAL GLN PHE LYS L1 G11 K16 L24 K35 Y83 Q97 A102 A111 H114 T118 V122 D131 R145 K146 Q147 Y163 D173 E191 Y206

K207 Y240 L249 D250 V269 E281 V284 D290 Q294 K320

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

Chain P: 82% 7% 10%

MET ALA ALA ALA VAL HIS PRO ARG VAL VAL ARG VAL LEU PRO MET SER ARG SER SER VAL PRO ALA LEU ALA ALA SER VAL PHE HIS SER PRO PRO GLN ARG GLN L1 H2 H3 K10 R32 R97 I113 P114 Q119 K122 E127 K140 I185 K199

D209 R224 R251 F270 T279 D282 R286 G299 D302 T308 P309 L312 H321 E332 Q335 T342 SER GLY PRO

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

Chain Q: 63% 10% • 26%

MET ALA ALA VAL SER MET SER VAL ALA LEU ARG GLN ALA LEU TRP GLY ARG ARG VAL ALA THR VAL ALA ALA VAL SER VAL SER LYS VAL SER THR ARG SER LEU SER THR SER THR TRP ARG LEU ALA GLN ASP GLN T5 R6 D7 T8 D14 T20 R33 R36 R42

N43 N44 M45 Q46 D77 D91 F95 N99 E106 E107 R108 F122 R129 K133

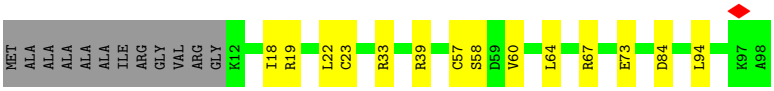
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 6% 74% • 23%

MET ALA ALA VAL LEU THR PHE LEU ARG PHE LEU GLY ARG GLY GLY GLY ALA VAL THR ARG GLY LEU PRO GLY GLY ALA ARG CYS PHE G1 V2 R3 T4 S5 P6 T7 G8 Q32 N36 Q51 R92 H95 H96

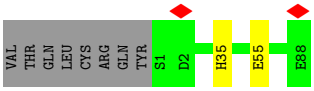
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 74% 14% 12%



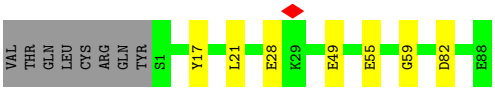
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



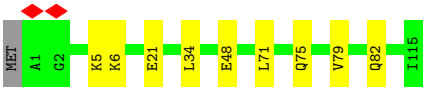
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



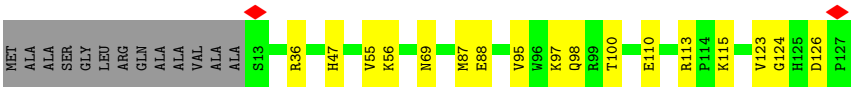
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



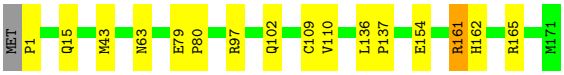
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



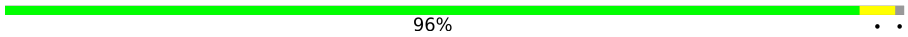
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

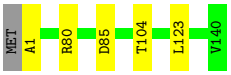
Chain X:



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

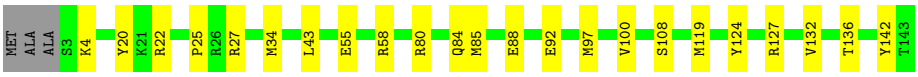
Chain Y:





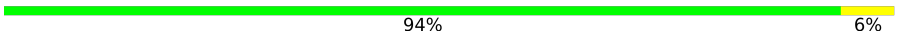
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



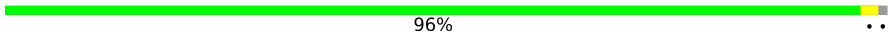
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

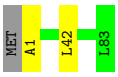
Chain a:



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

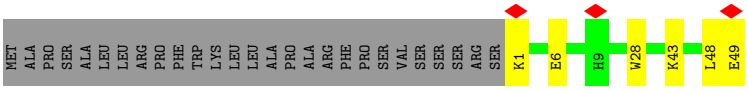
Chain b:





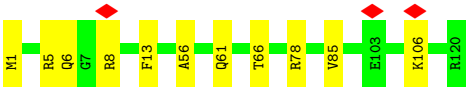
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



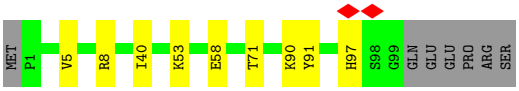
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



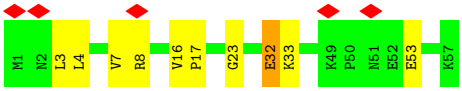
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



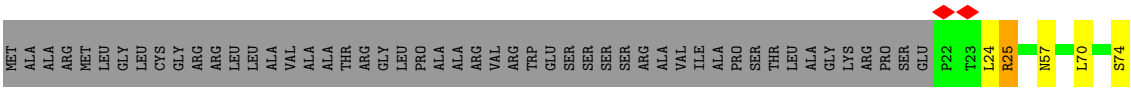
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

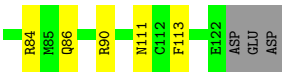
Chain f:



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

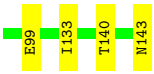
Chain g:





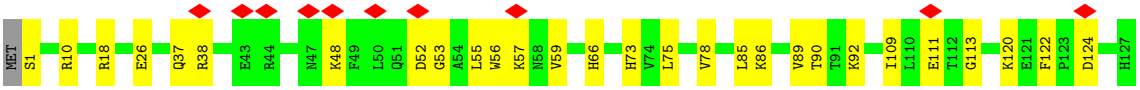
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



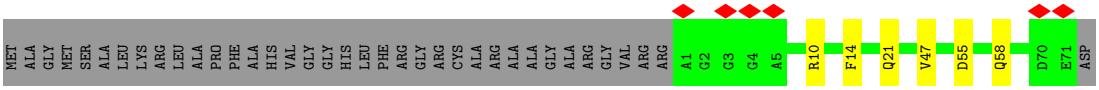
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



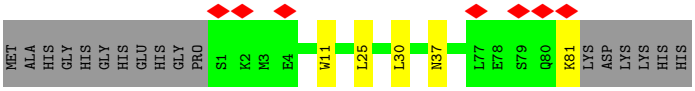
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



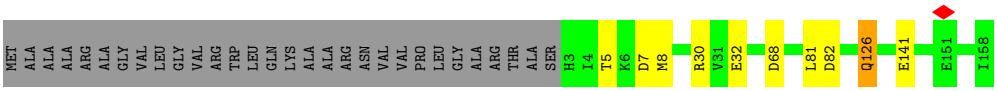
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



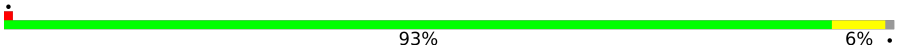
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

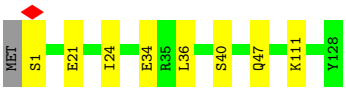
Chain l:



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

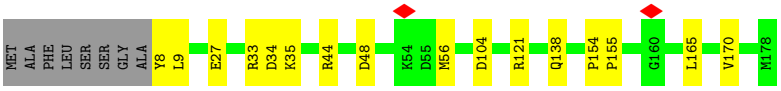
Chain m:





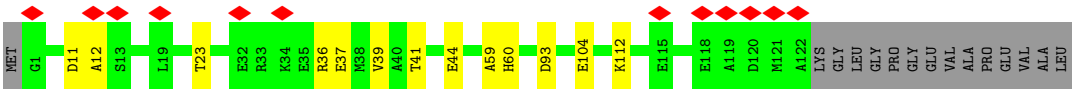
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



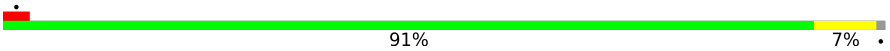
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



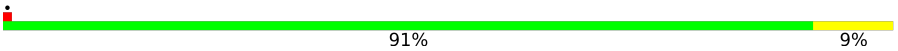
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

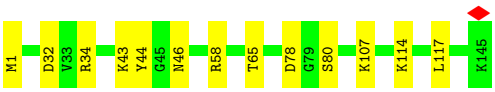
Chain p:



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

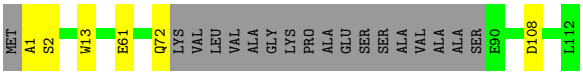
Chain q:





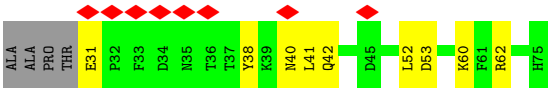
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81459	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 ($e^-/Å^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: CHD, DGT, EHZ, FES, FME, AYA, ZN, CDL, MYR, SF4, K, AME, NDP, U10, 3PE, SAC, 2MR, PC1, PLC, MG, FMN

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	0.13	0/936	0.22	0/1281
2	B	0.16	0/1272	0.27	0/1720
3	C	0.15	0/1789	0.24	0/2436
4	D	0.15	0/3537	0.24	0/4794
5	E	0.11	0/1699	0.25	0/2312
6	F	0.11	0/3401	0.25	0/4595
7	G	0.13	0/5367	0.24	0/7274
8	H	0.14	0/2571	0.25	0/3513
9	I	0.16	0/1445	0.26	0/1956
10	J	0.13	0/1370	0.21	0/1859
11	K	0.13	0/745	0.22	0/1008
12	L	0.11	0/4920	0.23	0/6694
13	M	0.13	0/3738	0.22	0/5097
14	N	0.14	0/2792	0.24	0/3800
15	O	0.11	0/2651	0.21	0/3587
16	P	0.13	0/2831	0.22	0/3841
17	Q	0.13	0/1072	0.23	0/1449
18	R	0.14	0/753	0.20	0/1014
19	S	0.10	0/711	0.22	0/956
20	T	0.11	0/719	0.21	0/971
20	U	0.11	0/719	0.21	0/971
21	V	0.13	0/948	0.21	0/1284
22	W	0.12	0/1000	0.27	0/1344
23	X	0.11	0/1439	0.22	0/1942
24	Y	0.10	0/1042	0.19	0/1414
25	Z	0.12	0/1181	0.20	0/1592
26	a	0.14	0/584	0.21	0/786
27	b	0.10	0/667	0.21	0/916
28	c	0.12	0/427	0.18	0/579
29	d	0.12	0/1018	0.20	0/1375
30	e	0.12	0/850	0.22	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.12	0/505	0.22	0/681
32	g	0.11	0/873	0.23	0/1186
33	h	0.11	0/1188	0.21	0/1607
34	i	0.09	0/1127	0.23	0/1534
35	j	0.11	0/624	0.20	0/855
36	k	0.10	0/672	0.19	0/906
37	l	0.10	0/1369	0.22	0/1873
38	m	0.10	0/1088	0.21	0/1472
39	n	0.09	0/1540	0.21	0/2085
40	o	0.12	0/1073	0.22	0/1437
41	p	0.10	0/1491	0.21	0/2011
42	q	0.12	0/1242	0.21	0/1688
43	r	0.12	0/789	0.23	0/1068
44	s	0.08	0/392	0.21	0/531
All	All	0.12	0/68167	0.23	0/92430

There are no bond length outliers.

There are no bond angle outliers.

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	921	0	952	13	0
2	B	1241	0	1251	18	0
3	C	1738	0	1685	13	0
4	D	3459	0	3404	25	0
5	E	1659	0	1664	18	0
6	F	3326	0	3282	36	0
7	G	5279	0	5301	46	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	18	0
10	J	1345	0	1352	14	0
11	K	745	0	785	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	39	0
13	M	3654	0	3852	35	0
14	N	2733	0	2912	28	0
15	O	2589	0	2566	18	0
16	P	2754	0	2773	18	0
17	Q	1049	0	1045	11	0
18	R	740	0	714	2	0
19	S	700	0	719	9	0
20	T	707	0	700	1	0
20	U	707	0	700	5	0
21	V	928	0	972	5	0
22	W	976	0	991	11	0
23	X	1402	0	1381	9	0
24	Y	1030	0	1039	3	0
25	Z	1152	0	1151	23	0
26	a	569	0	568	3	0
27	b	654	0	663	2	0
28	c	414	0	415	6	0
29	d	999	0	988	6	0
30	e	829	0	829	8	0
31	f	492	0	501	6	0
32	g	846	0	798	7	0
33	h	1154	0	1168	7	0
34	i	1097	0	1108	17	0
35	j	597	0	536	3	0
36	k	653	0	642	3	0
37	l	1314	0	1210	10	0
38	m	1070	0	1068	4	0
39	n	1487	0	1433	11	0
40	o	1048	0	1016	9	0
41	p	1458	0	1430	9	0
42	q	1212	0	1183	7	0
43	r	776	0	782	5	0
44	s	380	0	349	9	0
45	A	135	0	201	0	0
45	J	65	0	81	0	0
45	K	44	0	62	0	0
45	L	51	0	82	1	0
45	N	145	0	221	2	0
45	O	45	0	67	2	0
45	P	35	0	44	0	0
45	Y	304	0	450	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	92	0	141	1	0
45	b	51	0	82	0	0
45	e	49	0	75	2	0
45	f	78	0	107	0	0
45	i	45	0	67	2	0
45	m	164	0	233	0	0
45	q	51	0	82	0	0
45	r	34	0	42	0	0
46	A	68	0	84	2	0
46	B	94	0	136	1	0
46	H	126	0	183	4	0
46	I	98	0	150	2	0
46	J	35	0	44	0	0
46	L	91	0	136	3	0
46	M	35	0	44	0	0
46	e	39	0	52	0	0
46	h	47	0	71	0	0
46	m	54	0	88	0	0
46	q	49	0	75	0	0
47	A	33	0	43	0	0
47	J	37	0	51	0	0
47	L	42	0	64	0	0
47	M	28	0	30	0	0
47	O	35	0	47	0	0
47	P	74	0	105	1	0
47	Y	42	0	64	0	0
47	Z	34	0	45	0	0
47	g	42	0	64	1	0
48	B	8	0	0	0	0
48	F	8	0	0	0	0
48	G	16	0	0	1	0
48	I	16	0	0	0	0
49	B	63	0	90	11	0
50	E	4	0	0	0	0
50	G	4	0	0	1	0
51	F	31	0	19	1	0
52	G	1	0	0	0	0
53	H	81	0	109	0	0
53	L	76	0	99	1	0
53	M	100	0	156	2	0
53	N	100	0	156	0	0
53	P	59	0	62	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	d	151	0	202	1	0
53	h	80	0	104	0	0
53	r	61	0	66	1	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	2	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	T	37	0	0	0	0
58	U	37	0	0	0	0
59	i	29	0	38	5	0
60	o	15	0	27	1	0
All	All	70158	0	71608	498	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 4.

The worst 5 of 498 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)
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.14	0.90
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.08	0.85
40:o:59:ALA:O	40:o:60:HIS:ND1	2.10	0.84
15:O:191:GLU:OE2	55:O:401:DGT:O3'	1.95	0.84
6:F:194:GLU:OE2	6:F:204:ARG:NH1	2.11	0.83

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	153/216 (71%)	147 (96%)	6 (4%)	0	100	100
3	C	207/266 (78%)	203 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	418 (98%)	9 (2%)	0	100	100
5	E	212/249 (85%)	200 (94%)	12 (6%)	0	100	100
6	F	430/464 (93%)	417 (97%)	13 (3%)	0	100	100
7	G	686/727 (94%)	658 (96%)	28 (4%)	0	100	100
8	H	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	36	67
9	I	174/212 (82%)	168 (97%)	6 (3%)	0	100	100
10	J	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	579 (96%)	25 (4%)	0	100	100
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	314 (99%)	4 (1%)	0	100	100
16	P	340/380 (90%)	332 (98%)	8 (2%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	92 (98%)	2 (2%)	0	100	100
19	S	85/99 (86%)	83 (98%)	2 (2%)	0	100	100
20	T	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
20	U	86/156 (55%)	86 (100%)	0	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	110 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	Y	138/141 (98%)	138 (100%)	0	0	100	100
25	Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	97/106 (92%)	97 (100%)	0	0	100	100
31	f	55/57 (96%)	55 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	65 (94%)	4 (6%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	169/179 (94%)	162 (96%)	7 (4%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	172 (100%)	0	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	91/113 (80%)	86 (94%)	5 (6%)	0	100	100
44	s	43/109 (39%)	40 (93%)	3 (7%)	0	100	100
All	All	8193/9213 (89%)	7969 (97%)	223 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	208	VAL

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	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	128 (98%)	3 (2%)	44	70
3	C	190/228 (83%)	188 (99%)	2 (1%)	65	78
4	D	370/392 (94%)	366 (99%)	4 (1%)	65	78
5	E	183/205 (89%)	182 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	336 (97%)	10 (3%)	37	66
7	G	578/608 (95%)	576 (100%)	2 (0%)	86	87
8	H	274/274 (100%)	267 (97%)	7 (3%)	40	68
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	77
10	J	141/141 (100%)	139 (99%)	2 (1%)	59	76
11	K	85/85 (100%)	82 (96%)	3 (4%)	32	62
12	L	533/533 (100%)	523 (98%)	10 (2%)	50	73
13	M	412/412 (100%)	405 (98%)	7 (2%)	53	74
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	79
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	69
16	P	296/327 (90%)	289 (98%)	7 (2%)	43	69
17	Q	116/153 (76%)	114 (98%)	2 (2%)	53	74
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	77
19	S	77/82 (94%)	77 (100%)	0	100	100
20	T	81/135 (60%)	80 (99%)	1 (1%)	63	78
20	U	81/135 (60%)	80 (99%)	1 (1%)	63	78
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	79
22	W	107/114 (94%)	103 (96%)	4 (4%)	30	61
23	X	154/155 (99%)	150 (97%)	4 (3%)	40	68
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	81
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	104 (99%)	1 (1%)	68	79
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	63
31	f	54/54 (100%)	51 (94%)	3 (6%)	19	49
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	63
33	h	121/158 (77%)	120 (99%)	1 (1%)	73	81
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	69
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	75
37	l	140/159 (88%)	138 (99%)	2 (1%)	59	76
38	m	113/114 (99%)	112 (99%)	1 (1%)	70	80
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	109 (99%)	1 (1%)	70	80
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/130 (100%)	128 (98%)	2 (2%)	57	75
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	44/92 (48%)	43 (98%)	1 (2%)	44	70
All	All	7218/7891 (92%)	7110 (98%)	108 (2%)	55	75

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	16	LYS
17	Q	91	ASP
35	j	47	VAL
15	O	35	LYS
16	P	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	92	ASN
37	l	132	GLN
22	W	69	ASN
29	d	79	GLN
39	n	77	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

15 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	$\#\|Z\| > 2$
29	AME	d	1	29	9,10,11	1.46	1 (11%)	9,11,13	1.51	2 (22%)
42	AME	q	1	42	9,10,11	1.45	1 (11%)	9,11,13	1.51	2 (22%)
34	SAC	i	1	34	7,8,9	1.65	1 (14%)	8,9,11	1.43	1 (12%)
38	SAC	m	1	38	7,8,9	1.66	1 (14%)	8,9,11	1.22	1 (12%)
13	FME	M	1	13	8,9,10	1.50	1 (12%)	7,9,11	1.58	1 (14%)
10	FME	J	1	10	8,9,10	1.53	1 (12%)	7,9,11	1.64	1 (14%)
24	AYA	Y	1	24	6,7,8	1.80	1 (16%)	5,8,10	1.39	1 (20%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.70	3 (42%)
43	AYA	r	1	43	6,7,8	1.80	1 (16%)	5,8,10	1.39	1 (20%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.76	2 (28%)
4	2MR	D	85	4	10,12,13	2.41	2 (20%)	5,13,15	1.33	1 (20%)
12	FME	L	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.64	1 (14%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	7,9,11	1.60	1 (14%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.72	3 (42%)
27	AYA	b	1	27	6,7,8	1.80	1 (16%)	5,8,10	1.31	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	AME	d	1	29	-	0/9/10/12	-
42	AME	q	1	42	-	5/9/10/12	-
34	SAC	i	1	34	-	3/7/8/10	-
38	SAC	m	1	38	-	1/7/8/10	-
13	FME	M	1	13	-	1/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
1	FME	A	1	1	-	4/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	1/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	1/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
27	AYA	b	1	27	-	0/4/6/8	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.25	1.45	1.33
4	D	85	2MR	CZ-NE	5.14	1.45	1.34
10	J	1	FME	CN-N	3.72	1.45	1.33
14	N	1	FME	CN-N	3.68	1.45	1.33
13	M	1	FME	CN-N	3.65	1.45	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	C2A-C1A-N	2.84	120.91	116.10
14	N	1	FME	CE-SD-CG	2.79	109.97	100.40
10	J	1	FME	CE-SD-CG	2.77	109.92	100.40
8	H	1	FME	CE-SD-CG	2.76	109.88	100.40
1	A	1	FME	CE-SD-CG	2.62	109.38	100.40

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
10	J	1	FME	O1-CN-N-CA
11	K	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
38	m	1	SAC	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
4	D	85	2MR	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 88 ligands modelled in this entry, 4 are monoatomic - leaving 84 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	3PE	Y	201	-	26,26,50	1.17	4 (15%)	29,31,55	1.18	2 (6%)
45	3PE	N	402	-	44,44,50	0.92	4 (9%)	47,49,55	1.01	2 (4%)
51	FMN	F	501	-	33,33,33	2.75	10 (30%)	48,50,50	1.74	14 (29%)
45	3PE	Y	206	-	35,35,50	1.02	4 (11%)	38,40,55	1.12	2 (5%)
46	PC1	L	703	-	46,46,53	1.00	4 (8%)	52,54,61	0.97	2 (3%)
45	3PE	P	502	-	34,34,50	1.03	4 (11%)	37,39,55	1.09	2 (5%)
53	CDL	d	202	-	85,85,99	0.93	8 (9%)	91,97,111	1.10	4 (4%)
53	CDL	d	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.13	4 (5%)
45	3PE	Y	205	-	44,44,50	0.91	4 (9%)	47,49,55	1.10	2 (4%)
53	CDL	P	505	-	58,58,99	1.12	8 (13%)	64,70,111	1.15	4 (6%)
45	3PE	Y	204	-	50,50,50	0.86	4 (8%)	53,55,55	1.02	2 (3%)
46	PC1	m	205	-	53,53,53	0.94	4 (7%)	59,61,61	1.03	2 (3%)
58	EHZ	T	101	20	29,36,37	1.68	5 (17%)	35,44,47	1.51	6 (17%)
45	3PE	b	101	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
46	PC1	L	702	-	43,43,53	1.03	4 (9%)	49,51,61	1.02	2 (4%)
45	3PE	Y	207	-	42,42,50	0.93	4 (9%)	45,47,55	1.05	2 (4%)
45	3PE	m	203	-	49,49,50	0.87	4 (8%)	52,54,55	1.02	2 (3%)
48	SF4	F	502	6	0,12,12	-	-	-		
45	3PE	m	202	-	31,31,50	1.08	4 (12%)	34,36,55	1.17	2 (5%)
45	3PE	f	101	-	33,33,50	1.04	4 (12%)	36,38,55	1.13	2 (5%)
53	CDL	L	705	-	75,75,99	0.99	8 (10%)	81,87,111	1.09	4 (4%)
53	CDL	M	604	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	PLC	g	201	-	41,41,41	0.50	0	47,49,49	0.51	0
45	3PE	K	101	-	43,43,50	0.92	4 (9%)	46,48,55	1.06	2 (4%)
45	3PE	Y	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2 (3%)
47	PLC	O	404	-	34,34,41	0.55	0	40,42,49	0.55	0
50	FES	G	803	7	0,4,4	-	-	-		
45	3PE	r	201	-	33,33,50	1.04	4 (12%)	36,38,55	1.03	2 (5%)
45	3PE	Z	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.05	2 (3%)
48	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	H	403	-	38,38,53	1.10	4 (10%)	44,46,61	1.00	2 (4%)
46	PC1	H	402	-	38,38,53	1.09	4 (10%)	44,46,61	1.12	2 (4%)
45	3PE	q	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	L	701	-	50,50,50	0.86	4 (8%)	53,55,55	1.05	2 (3%)
45	3PE	O	403	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
59	CHD	i	201	-	32,32,32	3.21	10 (31%)	51,51,51	2.40	21 (41%)
47	PLC	A	206	-	32,32,41	0.56	0	38,40,49	0.56	0
53	CDL	h	202	-	79,79,99	0.97	8 (10%)	85,91,111	1.14	4 (4%)
47	PLC	P	503	-	41,41,41	0.51	0	47,49,49	0.52	0
45	3PE	A	202	-	36,36,50	1.00	4 (11%)	39,41,55	1.09	2 (5%)
58	EHZ	U	101	20	29,36,37	1.70	5 (17%)	35,44,47	1.57	5 (14%)
46	PC1	H	401	-	47,47,53	1.00	4 (8%)	53,55,61	1.04	2 (3%)
45	3PE	f	102	-	43,43,50	0.93	4 (9%)	46,48,55	1.08	2 (4%)
48	SF4	I	201	9	0,12,12	-	-	-		
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.14	2 (4%)
45	3PE	J	202	-	35,35,50	1.01	4 (11%)	38,40,55	1.15	2 (5%)
53	CDL	r	202	-	60,60,99	1.11	8 (13%)	66,72,111	1.12	4 (6%)
47	PLC	P	504	-	31,31,41	0.56	0	37,39,49	0.57	0
57	NDP	P	501	-	49,52,52	3.98	25 (51%)	66,80,80	2.02	14 (21%)
47	PLC	J	204	-	36,36,41	0.53	0	42,44,49	0.51	0
53	CDL	N	404	-	99,99,99	0.87	8 (8%)	105,111,111	1.03	4 (3%)
48	SF4	G	801	7	0,12,12	-	-	-		
45	3PE	m	204	-	40,40,50	0.95	4 (10%)	43,45,55	1.10	2 (4%)
46	PC1	M	602	-	34,34,53	1.16	4 (11%)	40,42,61	1.06	2 (5%)
46	PC1	A	204	-	34,34,53	1.16	4 (11%)	40,42,61	1.06	2 (5%)
47	PLC	Y	208	-	41,41,41	0.51	0	47,49,49	0.49	0
46	PC1	B	204	-	47,47,53	0.99	4 (8%)	53,55,61	1.11	2 (3%)
45	3PE	Y	202	-	50,50,50	0.85	4 (8%)	53,55,55	1.10	2 (3%)
45	3PE	A	201	-	46,46,50	0.89	4 (8%)	49,51,55	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	PC1	q	202	-	48,48,53	0.98	4 (8%)	54,56,61	0.96	2 (3%)
45	3PE	N	401	-	48,48,50	0.88	4 (8%)	51,53,55	1.08	2 (3%)
47	PLC	L	704	-	41,41,41	0.52	0	47,49,49	0.50	0
46	PC1	J	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.02	2 (5%)
46	PC1	B	203	-	45,45,53	1.01	4 (8%)	51,53,61	0.99	2 (3%)
46	PC1	I	204	-	43,43,53	1.04	4 (9%)	49,51,61	1.03	2 (4%)
48	SF4	G	802	7	0,12,12	-	-	-		
48	SF4	I	202	9	0,12,12	-	-	-		
49	U10	B	202	-	63,63,63	1.85	24 (38%)	76,79,79	1.30	12 (15%)
46	PC1	A	205	-	32,32,53	1.19	4 (12%)	38,40,61	1.08	2 (5%)
45	3PE	e	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.05	2 (3%)
55	DGT	O	401	56	29,33,33	3.07	11 (37%)	44,52,52	2.06	15 (34%)
45	3PE	J	201	-	28,28,50	1.13	4 (14%)	31,33,55	1.18	2 (6%)
46	PC1	e	202	-	38,38,53	1.10	4 (10%)	44,46,61	1.04	2 (4%)
45	3PE	A	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
47	PLC	M	603	-	27,27,41	0.61	0	33,35,49	0.57	0
60	MYR	o	201	40	14,14,15	0.46	0	13,13,15	0.87	0
46	PC1	I	203	-	53,53,53	0.93	4 (7%)	59,61,61	1.00	2 (3%)
46	PC1	h	201	-	46,46,53	1.00	4 (8%)	52,54,61	1.02	2 (3%)
45	3PE	Z	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.08	2 (4%)
47	PLC	Z	203	-	33,33,41	0.56	0	39,41,49	0.56	0
45	3PE	i	202	-	44,44,50	0.90	4 (9%)	47,49,55	1.06	2 (4%)
45	3PE	N	403	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)
53	CDL	H	404	-	80,80,99	0.97	8 (10%)	86,92,111	1.07	4 (4%)
50	FES	E	301	5	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
45	3PE	Y	201	-	-	11/30/30/54	-
45	3PE	N	402	-	-	20/48/48/54	-
51	FMN	F	501	-	-	5/18/18/18	0/3/3/3
45	3PE	Y	206	-	-	20/39/39/54	-
46	PC1	L	703	-	-	15/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	P	502	-	-	11/38/38/54	-
53	CDL	d	202	-	-	46/96/96/110	-
53	CDL	d	201	-	-	35/75/75/110	-
45	3PE	Y	205	-	-	21/48/48/54	-
53	CDL	P	505	-	-	36/69/69/110	-
45	3PE	Y	204	-	-	24/54/54/54	-
46	PC1	m	205	-	-	16/57/57/57	-
58	EHZ	T	101	20	-	14/42/44/45	-
45	3PE	b	101	-	-	20/54/54/54	-
46	PC1	L	702	-	-	20/47/47/57	-
45	3PE	Y	207	-	-	19/46/46/54	-
45	3PE	m	203	-	-	18/53/53/54	-
48	SF4	F	502	6	-	-	0/6/5/5
45	3PE	m	202	-	-	16/35/35/54	-
45	3PE	f	101	-	-	22/37/37/54	-
53	CDL	L	705	-	-	28/86/86/110	-
53	CDL	M	604	-	-	49/110/110/110	-
47	PLC	g	201	-	-	11/45/45/45	-
45	3PE	K	101	-	-	19/47/47/54	-
45	3PE	Y	203	-	-	27/54/54/54	-
47	PLC	O	404	-	-	4/38/38/45	-
50	FES	G	803	7	-	-	0/1/1/1
45	3PE	r	201	-	-	15/37/37/54	-
45	3PE	Z	202	-	-	28/54/54/54	-
48	SF4	B	201	2	-	-	0/6/5/5
46	PC1	H	403	-	-	16/42/42/57	-
46	PC1	H	402	-	-	14/42/42/57	-
45	3PE	q	201	-	-	25/54/54/54	-
45	3PE	L	701	-	-	25/54/54/54	-
45	3PE	O	403	-	-	20/48/48/54	-
59	CHD	i	201	-	-	4/9/74/74	0/4/4/4
47	PLC	A	206	-	-	7/36/36/45	-
53	CDL	h	202	-	-	39/90/90/110	-
47	PLC	P	503	-	-	15/45/45/45	-
45	3PE	A	202	-	-	16/40/40/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	U	101	20	-	17/42/44/45	-
46	PC1	H	401	-	-	20/51/51/57	-
45	3PE	f	102	-	-	25/47/47/54	-
48	SF4	I	201	9	-	-	0/6/5/5
45	3PE	m	201	-	-	18/44/44/54	-
45	3PE	J	202	-	-	21/39/39/54	-
53	CDL	r	202	-	-	30/71/71/110	-
47	PLC	P	504	-	-	14/34/34/45	-
57	NDP	P	501	-	-	11/34/77/77	0/5/5/5
47	PLC	J	204	-	-	14/40/40/45	-
53	CDL	N	404	-	-	49/110/110/110	-
48	SF4	G	801	7	-	-	0/6/5/5
45	3PE	m	204	-	-	18/44/44/54	-
46	PC1	M	602	-	-	16/38/38/57	-
46	PC1	A	204	-	-	20/38/38/57	-
47	PLC	Y	208	-	-	16/45/45/45	-
46	PC1	B	204	-	-	17/51/51/57	-
45	3PE	Y	202	-	-	27/54/54/54	-
45	3PE	A	201	-	-	22/50/50/54	-
46	PC1	q	202	-	-	24/52/52/57	-
45	3PE	N	401	-	-	30/52/52/54	-
47	PLC	L	704	-	-	11/45/45/45	-
46	PC1	J	203	-	-	14/38/38/57	-
46	PC1	B	203	-	-	13/49/49/57	-
46	PC1	I	204	-	-	20/47/47/57	-
48	SF4	G	802	7	-	-	0/6/5/5
48	SF4	I	202	9	-	-	0/6/5/5
49	U10	B	202	-	-	13/63/87/87	0/1/1/1
46	PC1	A	205	-	-	17/36/36/57	-
45	3PE	e	201	-	-	14/52/52/54	-
55	DGT	O	401	56	-	2/22/34/34	0/3/3/3
45	3PE	J	201	-	-	14/32/32/54	-
46	PC1	e	202	-	-	25/42/42/57	-
45	3PE	A	203	-	-	21/54/54/54	-
47	PLC	M	603	-	-	10/31/31/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	MYR	o	201	40	-	7/11/12/13	-
46	PC1	I	203	-	-	19/57/57/57	-
46	PC1	h	201	-	-	24/50/50/57	-
45	3PE	Z	201	-	-	21/44/44/54	-
47	PLC	Z	203	-	-	15/37/37/45	-
45	3PE	i	202	-	-	26/48/48/54	-
45	3PE	N	403	-	-	25/54/54/54	-
53	CDL	H	404	-	-	33/91/91/110	-
50	FES	E	301	5	-	-	0/1/1/1

The worst 5 of 358 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	C6N-C5N	12.08	1.54	1.33
55	O	401	DGT	O6-C6	8.82	1.40	1.23
59	i	201	CHD	C11-C12	8.71	1.68	1.53
57	P	501	NDP	C2B-C1B	-8.66	1.30	1.53
57	P	501	NDP	O4B-C1B	8.43	1.62	1.42

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	O	401	DGT	C8-N9-C4	7.44	120.21	106.05
59	i	201	CHD	C13-C17-C20	-7.16	110.95	119.50
57	P	501	NDP	N6A-C6A-N1A	-5.75	105.75	118.35
59	i	201	CHD	C14-C13-C12	5.58	112.60	107.40
57	P	501	NDP	C4A-N9A-C1B	-5.40	113.72	126.59

There are no chirality outliers.

5 of 1504 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	O13-C11-C12-N
45	A	203	3PE	C1-O11-P-O14
45	A	203	3PE	C12-C11-O13-P
45	A	203	3PE	O22-C21-O21-C2

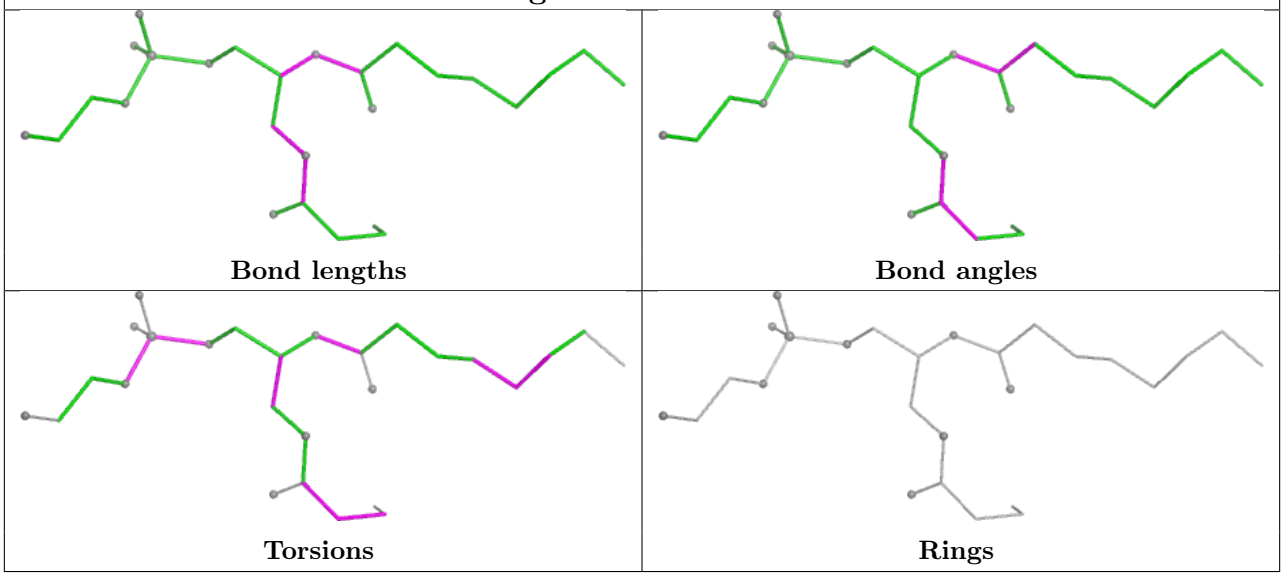
There are no ring outliers.

28 monomers are involved in 51 short contacts:

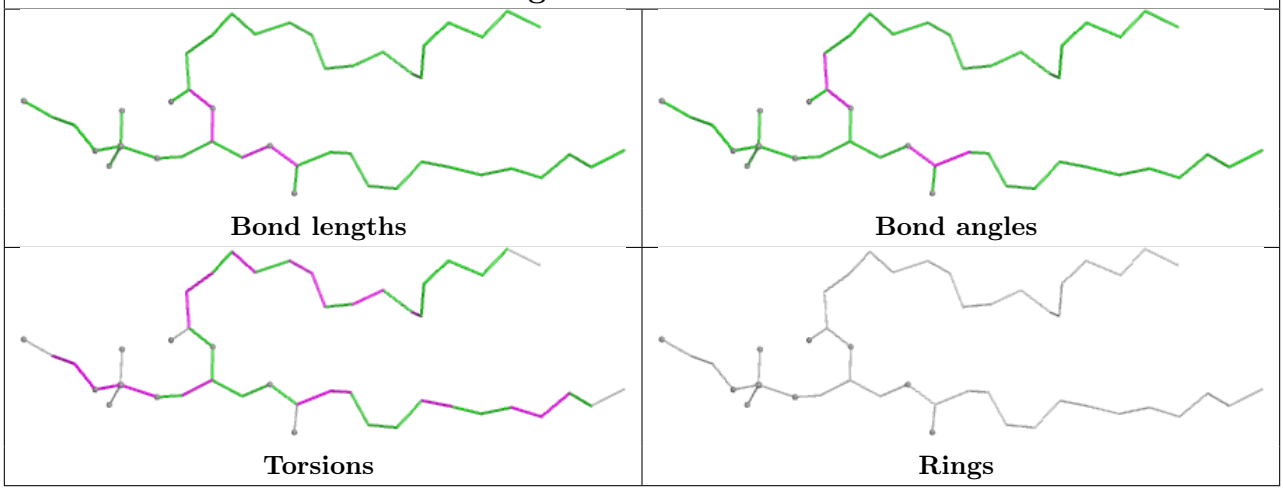
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	N	402	3PE	1	0
51	F	501	FMN	1	0
46	L	703	PC1	3	0
53	d	202	CDL	1	0
45	Y	204	3PE	1	0
53	L	705	CDL	1	0
53	M	604	CDL	2	0
47	g	201	PLC	1	0
50	G	803	FES	1	0
45	Z	202	3PE	1	0
46	H	403	PC1	2	0
45	L	701	3PE	1	0
45	O	403	3PE	2	0
59	i	201	CHD	5	0
47	P	503	PLC	1	0
46	H	401	PC1	2	0
53	r	202	CDL	1	0
46	A	204	PC1	2	0
46	B	204	PC1	1	0
45	Y	202	3PE	2	0
45	N	401	3PE	1	0
48	G	802	SF4	1	0
49	B	202	U10	11	0
45	e	201	3PE	2	0
55	O	401	DGT	2	0
60	o	201	MYR	1	0
46	I	203	PC1	2	0
45	i	202	3PE	2	0

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

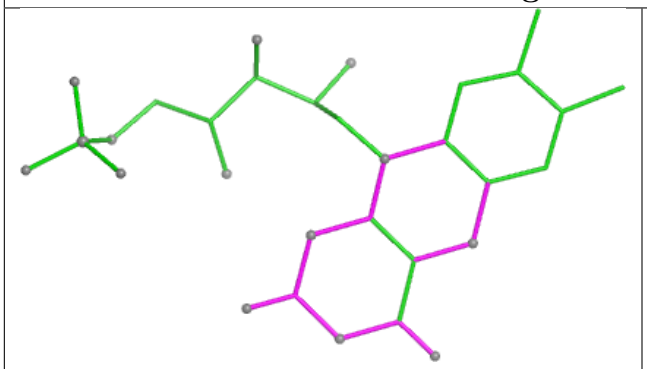
Ligand 3PE Y 201



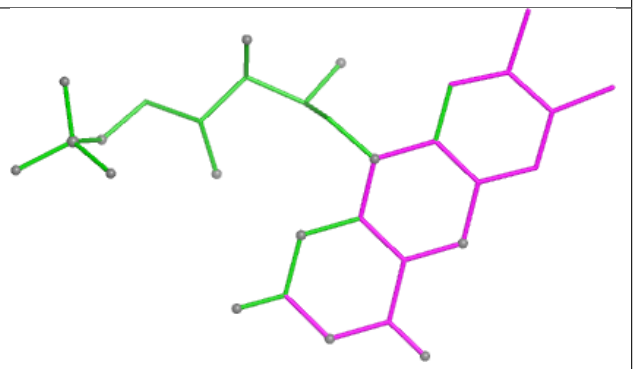
Ligand 3PE N 402



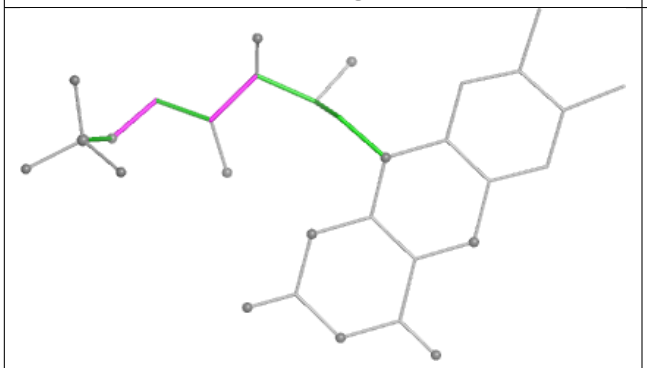
Ligand FMN F 501



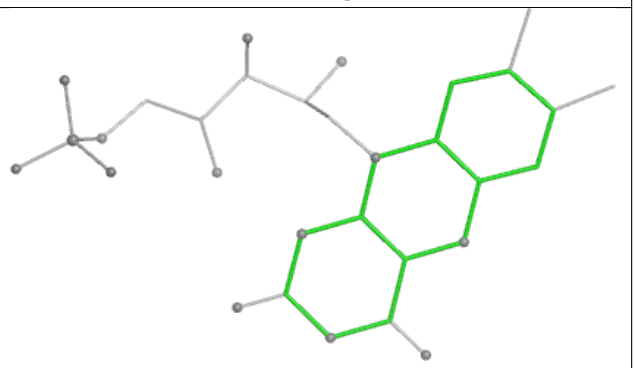
Bond lengths



Bond angles

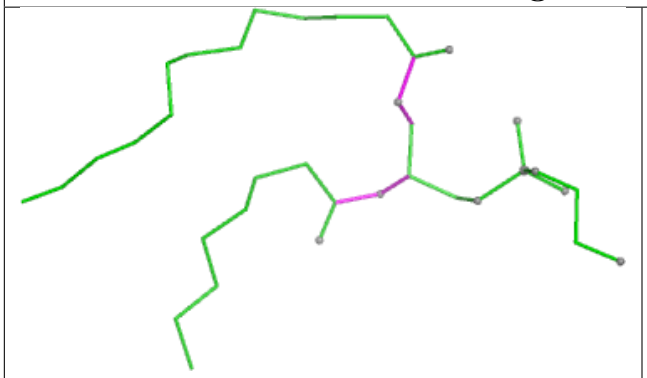


Torsions

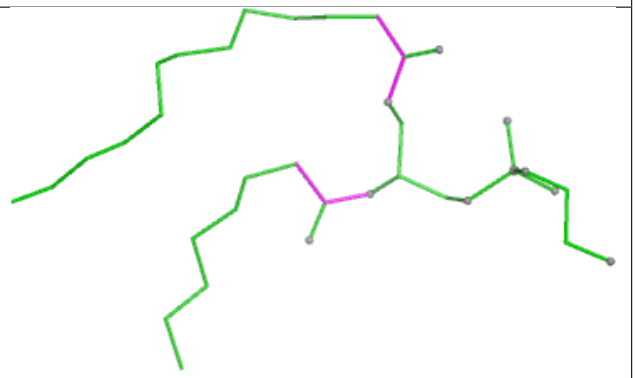


Rings

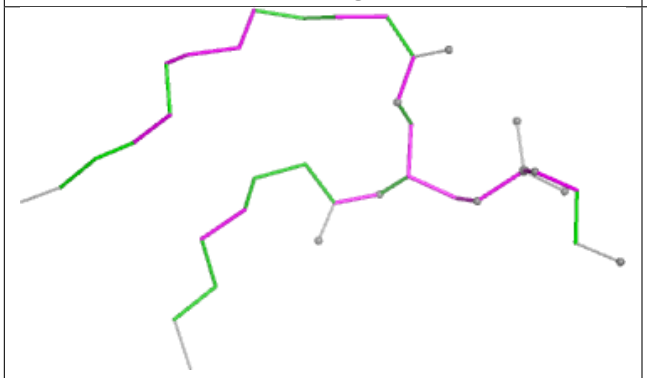
Ligand 3PE Y 206



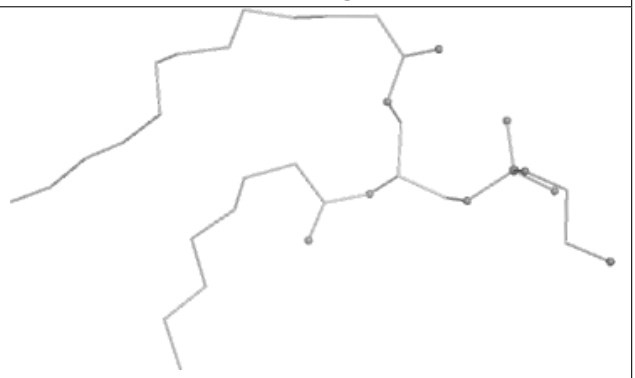
Bond lengths



Bond angles

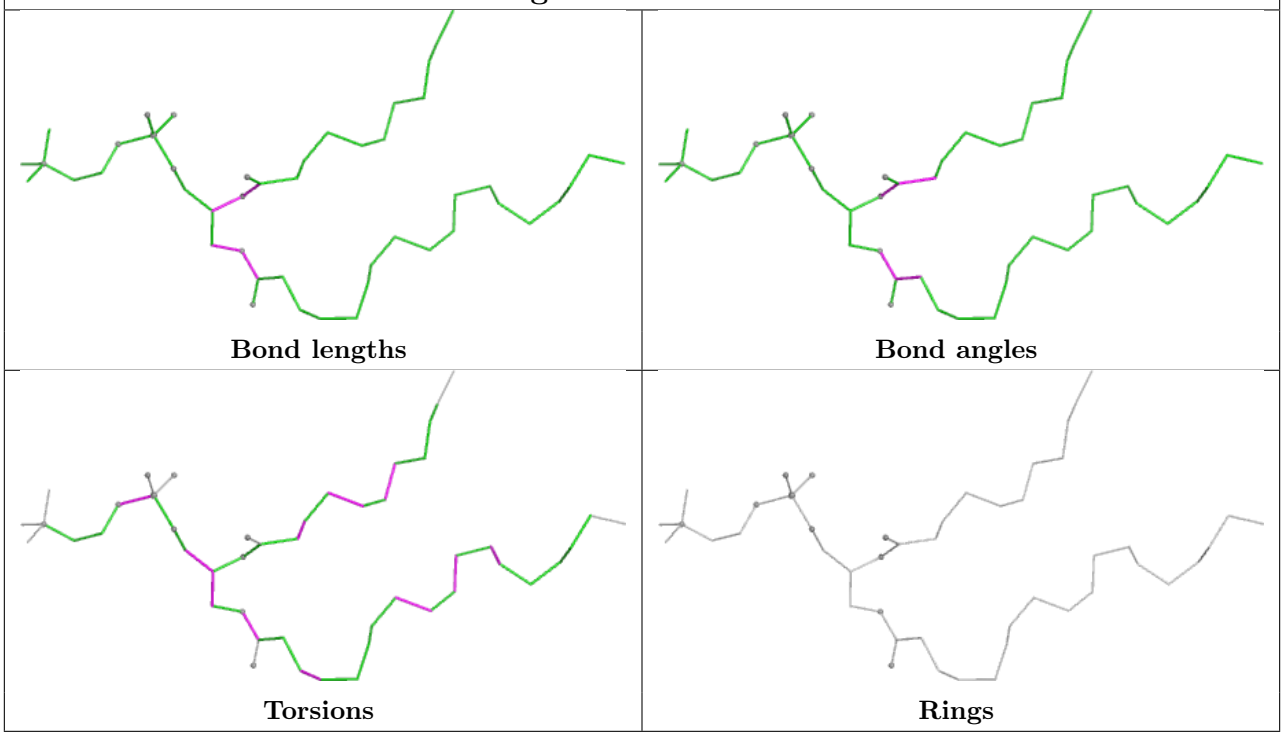


Torsions

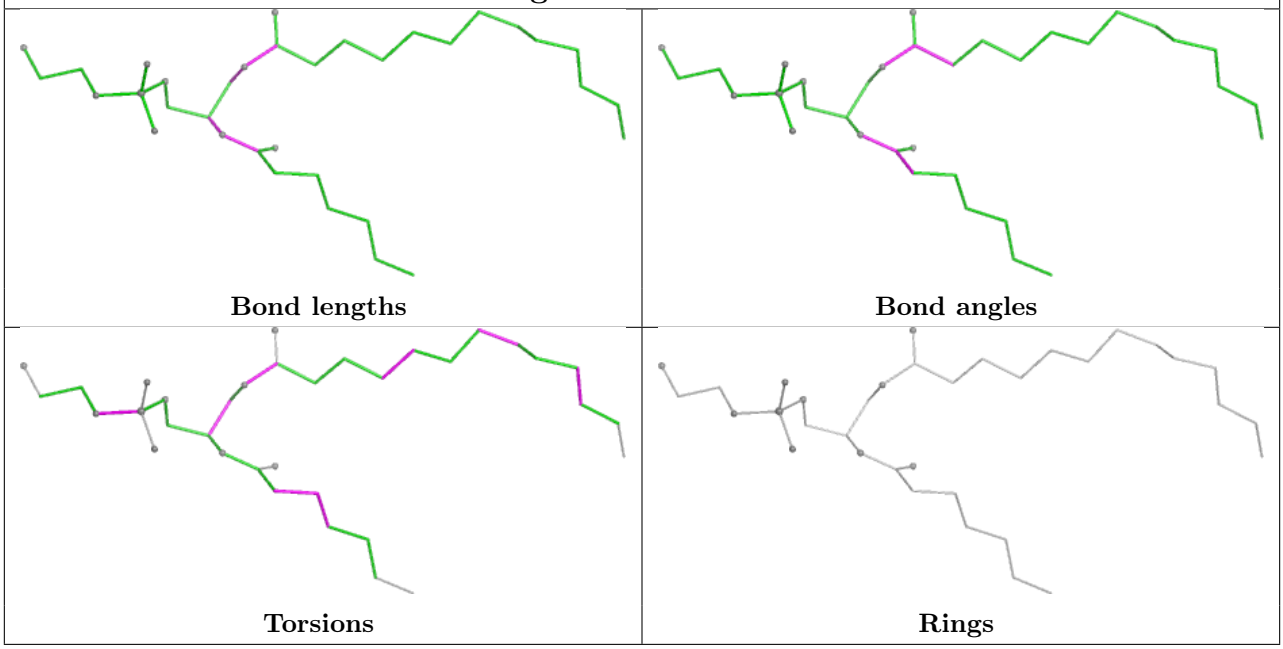


Rings

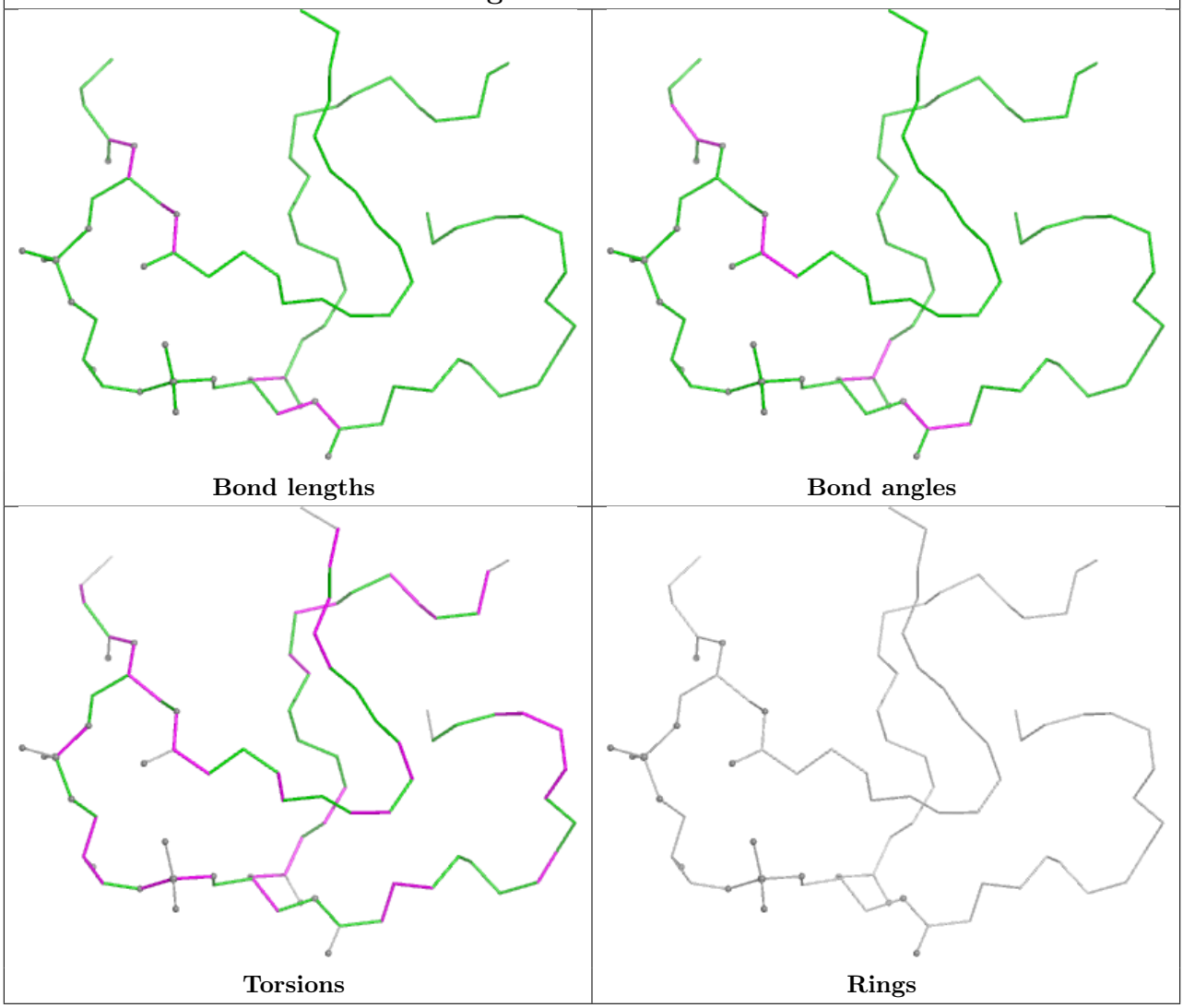
Ligand PC1 L 703



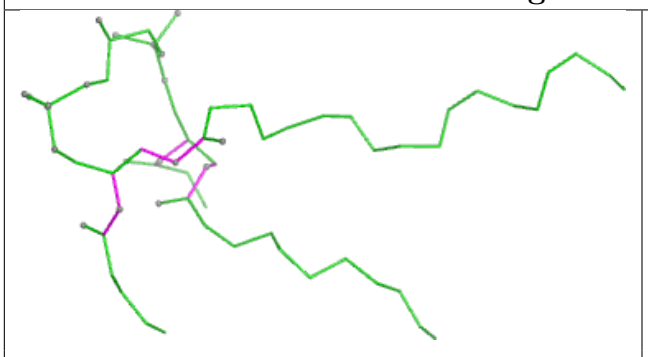
Ligand 3PE P 502



Ligand CDL d 202



Ligand CDL d 201



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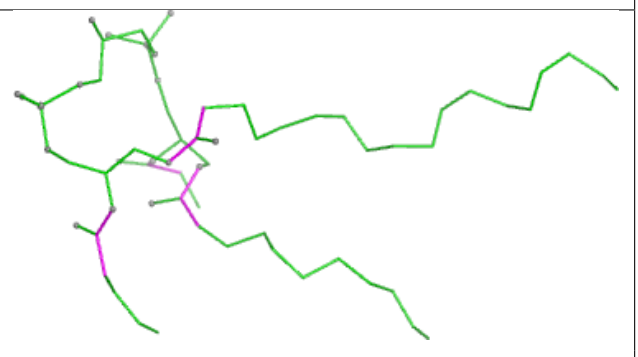
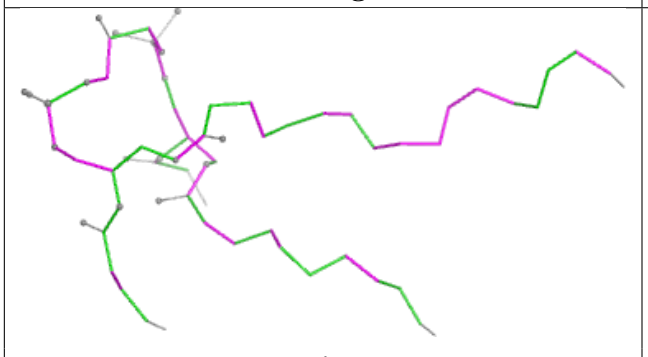
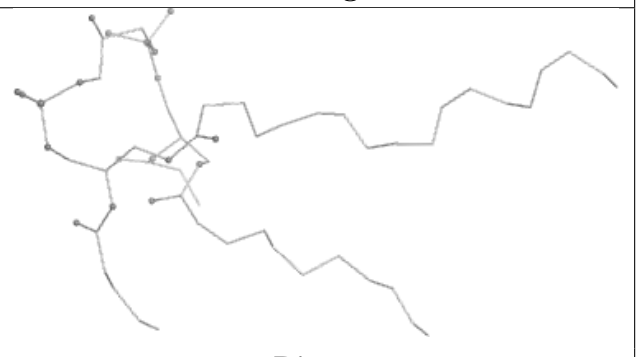


Bond angles

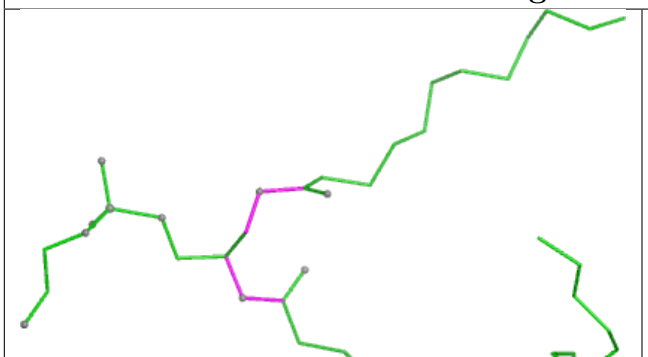


Torsions



Rings

Ligand 3PE Y 205



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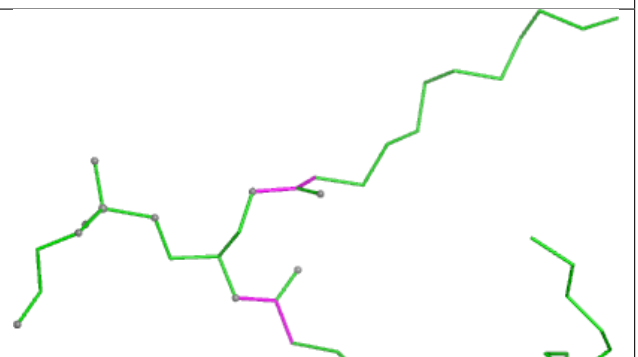
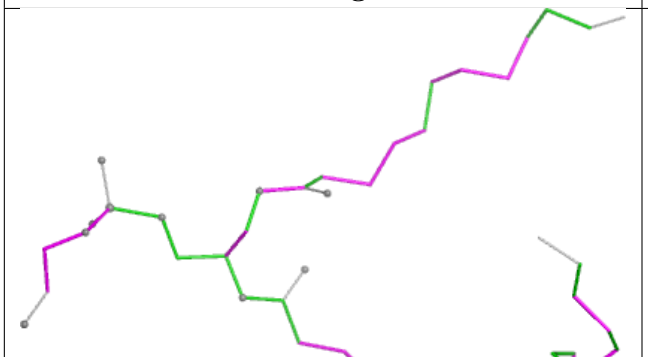


Bond angles



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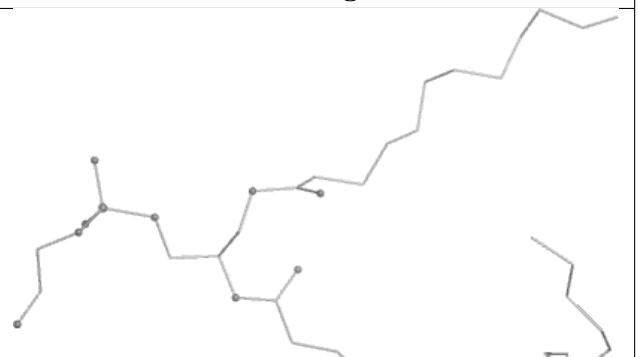

Rings

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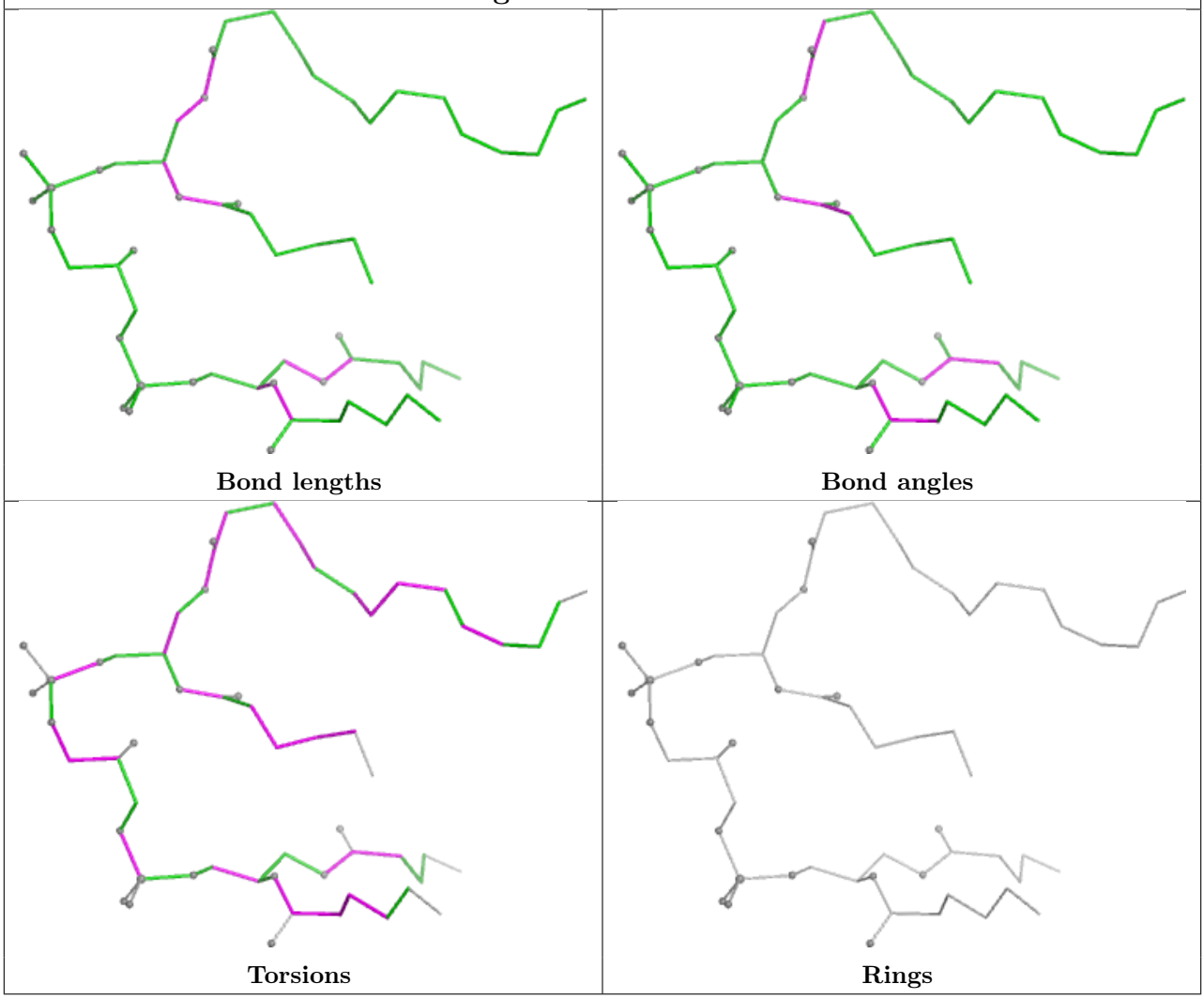

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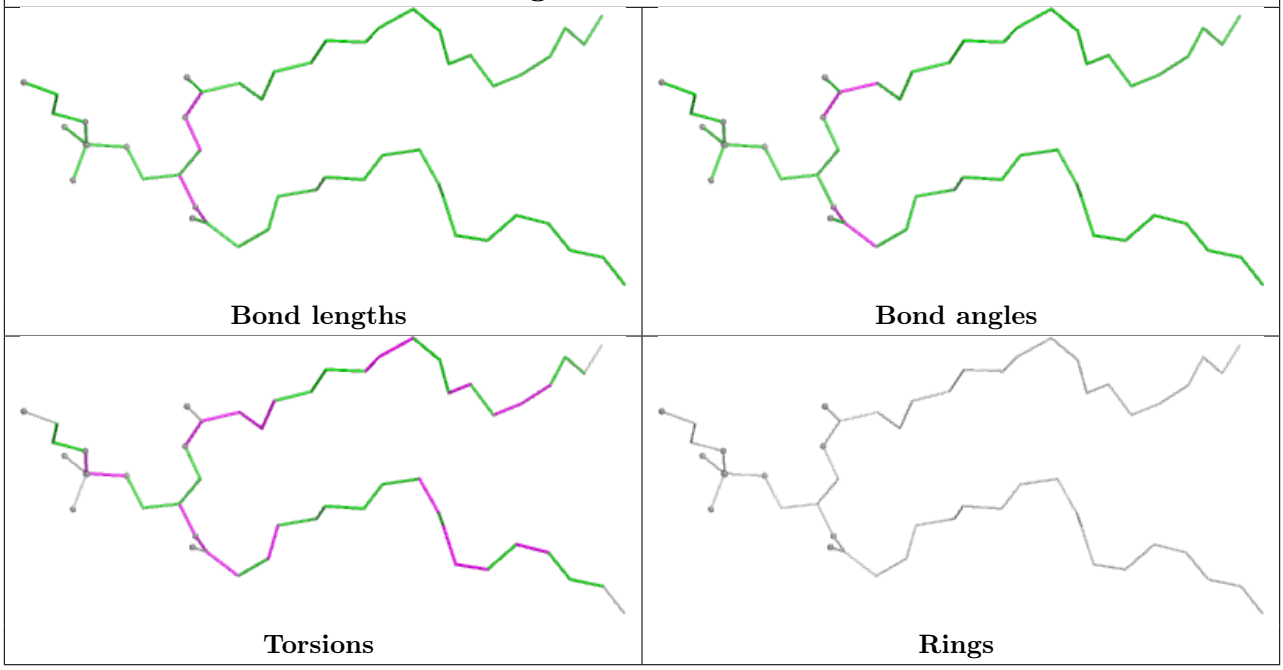
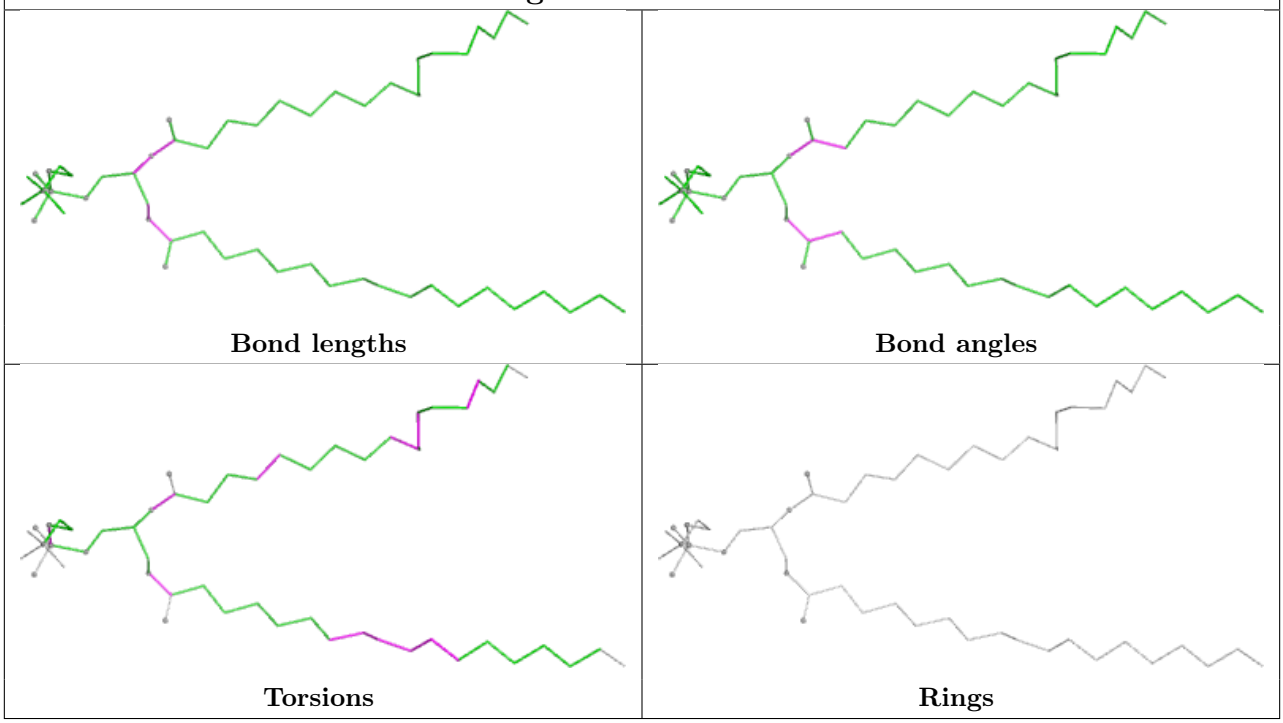
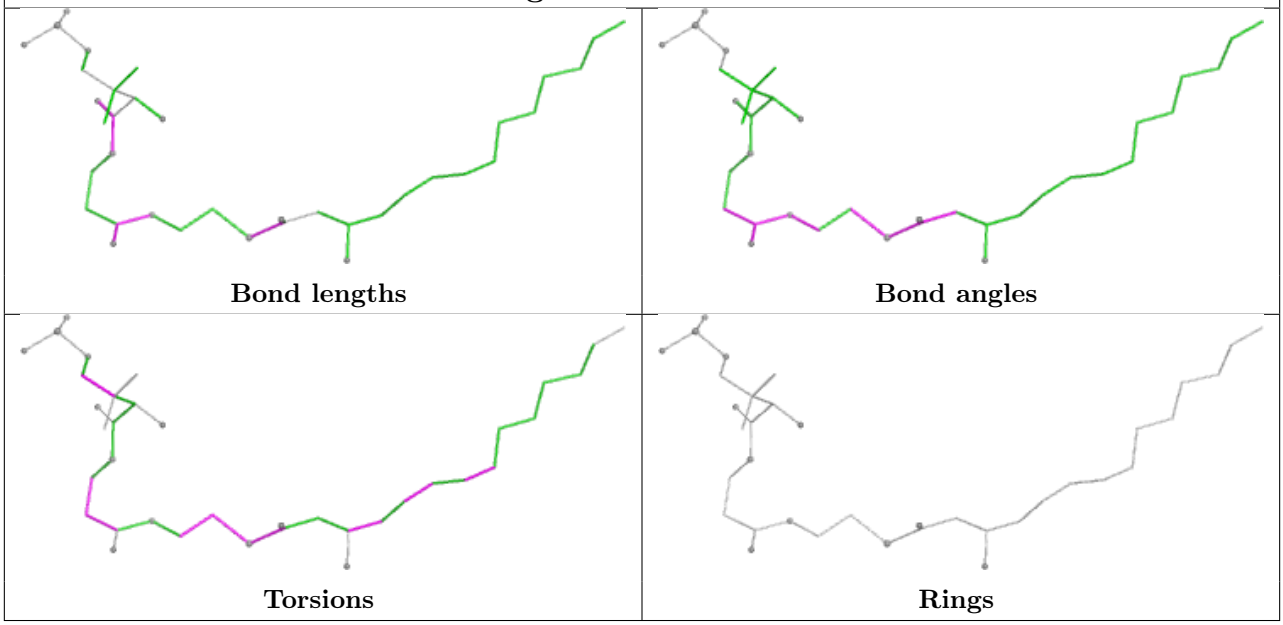


Ligand PC1 m 205



Ligand EHZ T 101



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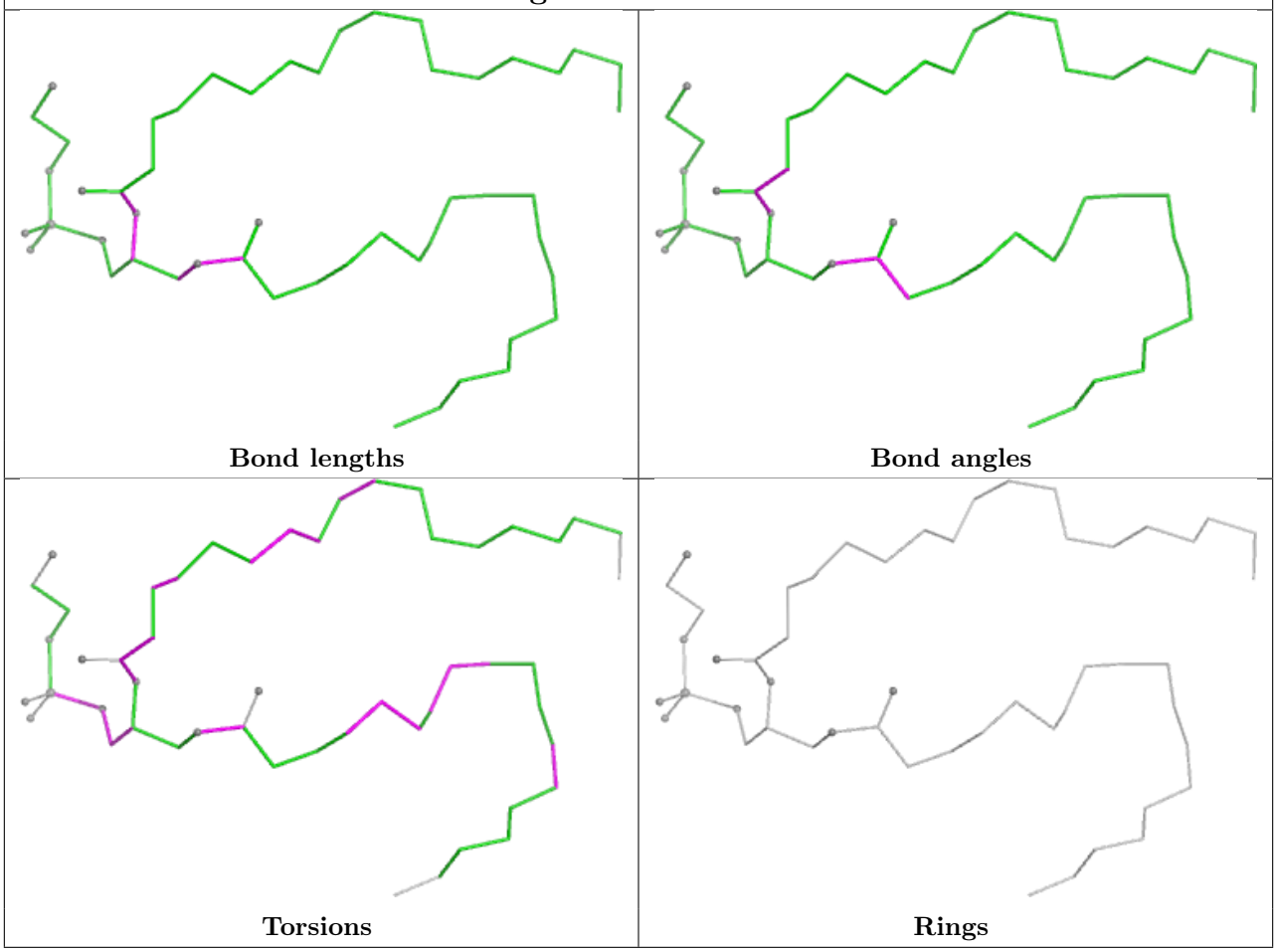
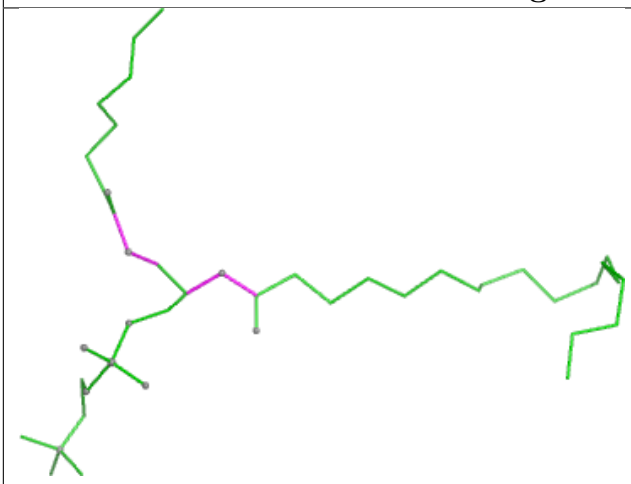
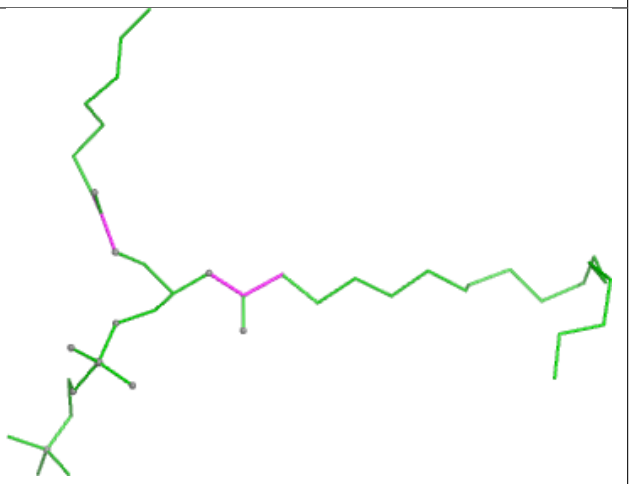
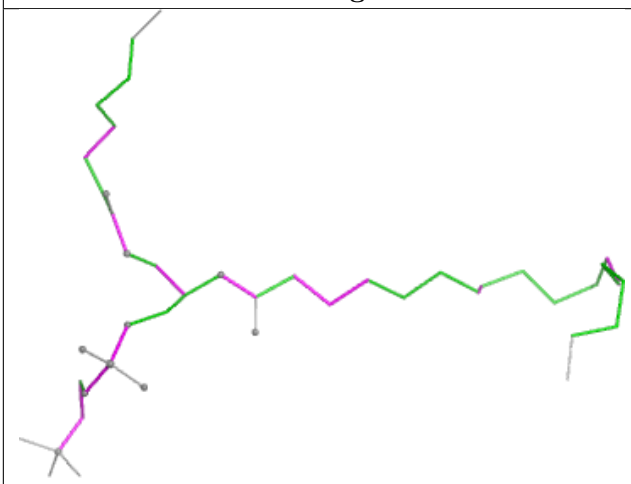
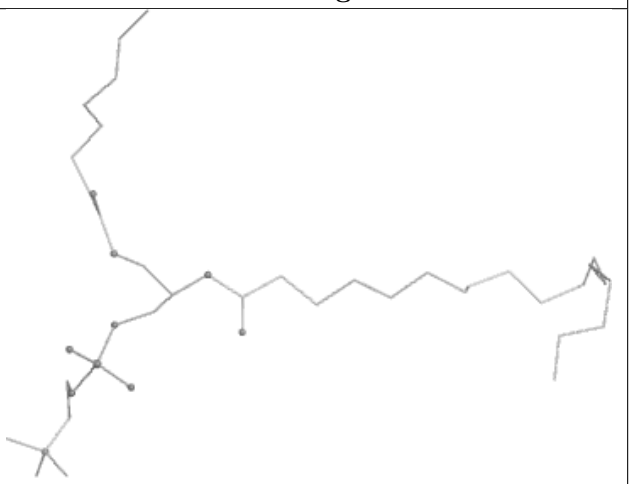
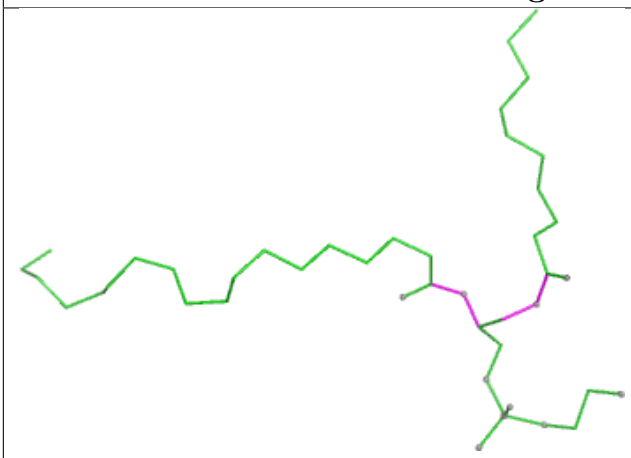


Ligand PC1 L 702	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand 3PE Y 207



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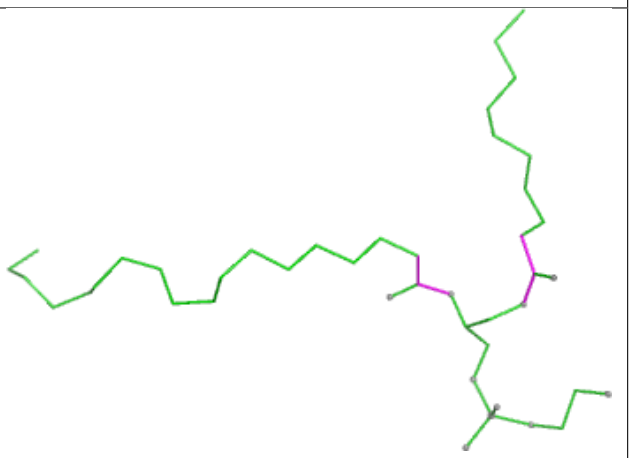
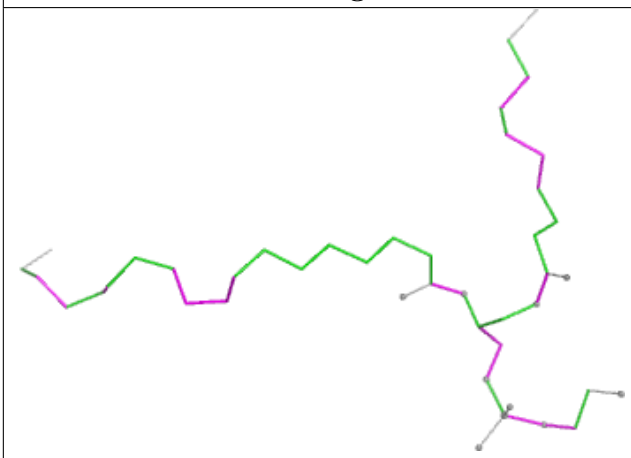


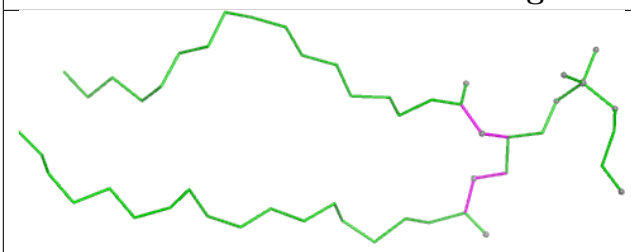
Bond angles



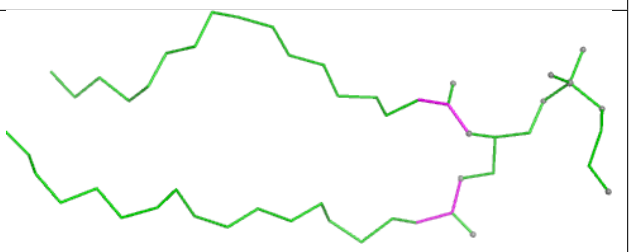
Torsions

Rings

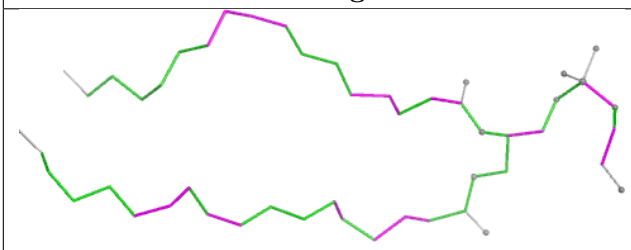
Ligand 3PE m 203



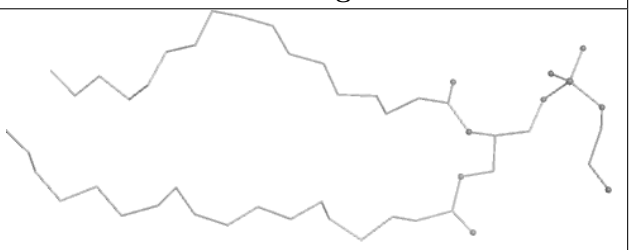
Bond lengths



Bond angles

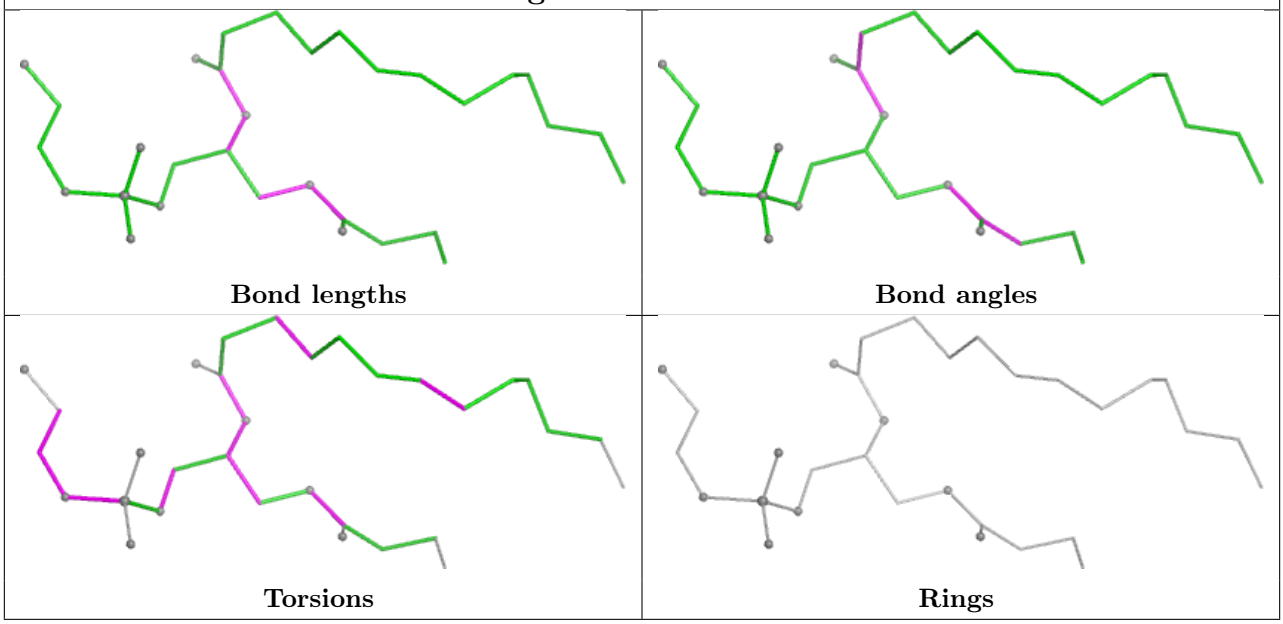


Torsions

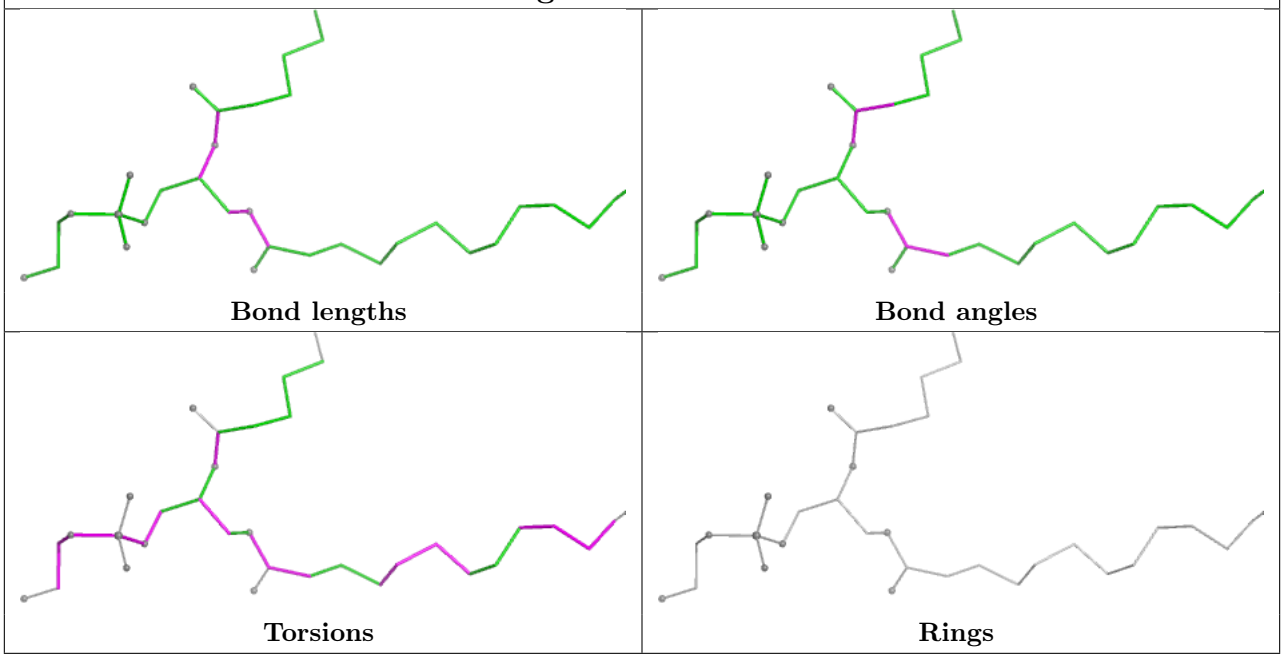


Rings

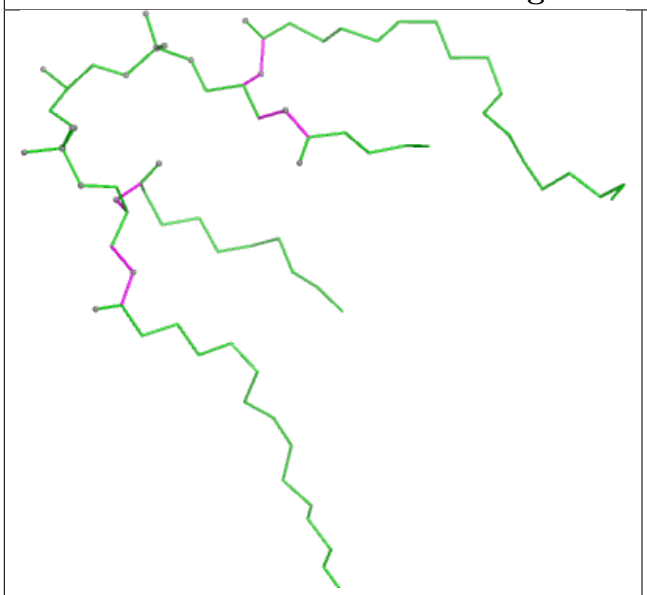
Ligand 3PE m 202



Ligand 3PE f 101

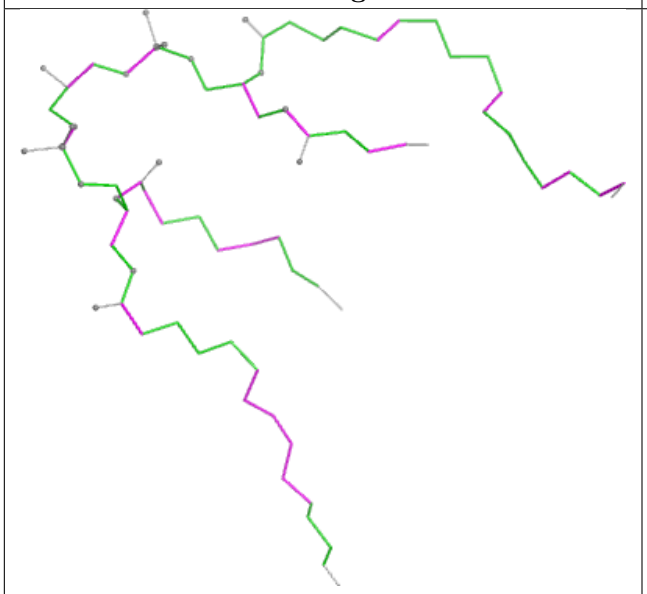


Ligand CDL L 705



Bond lengths

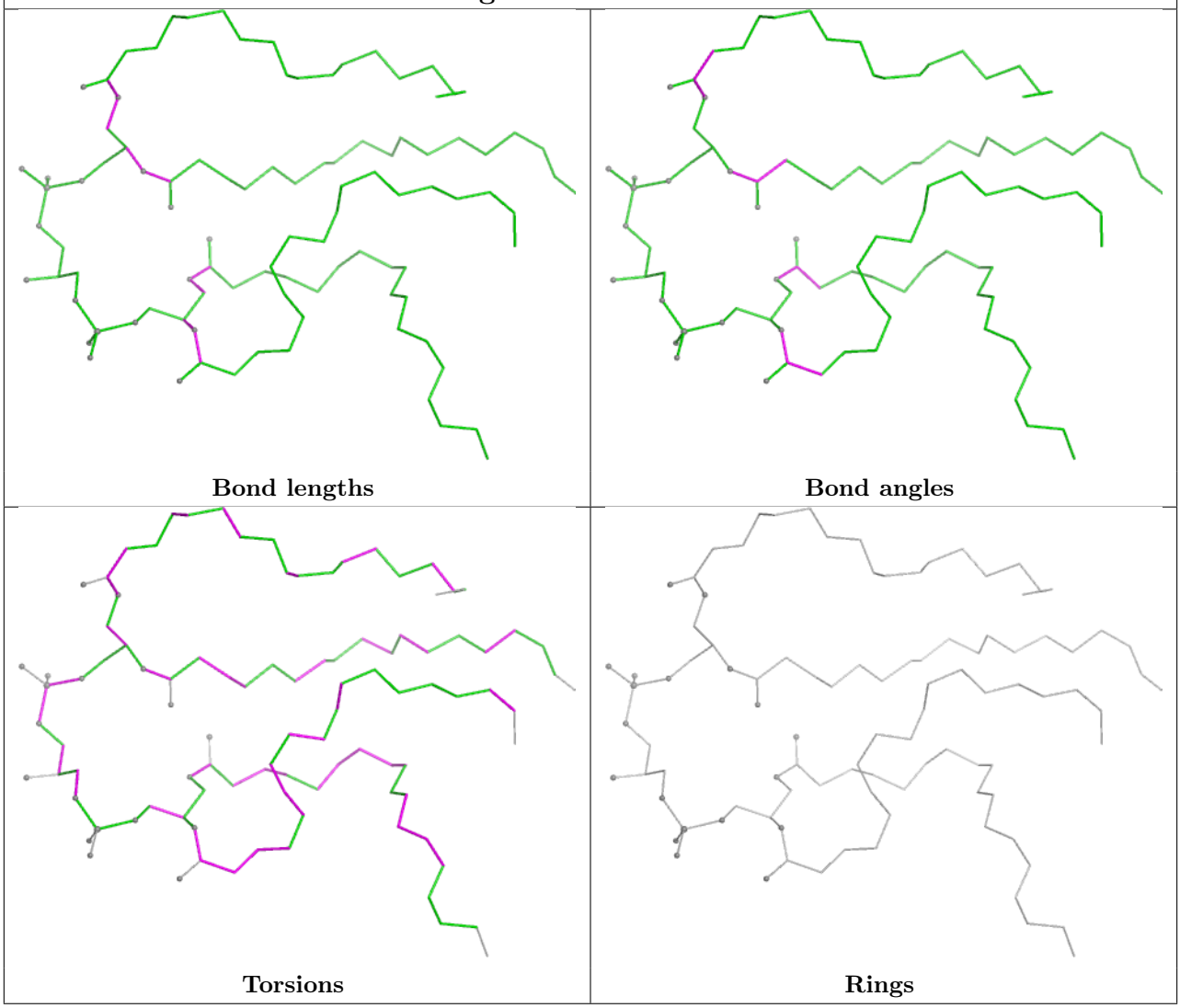
Bond angles



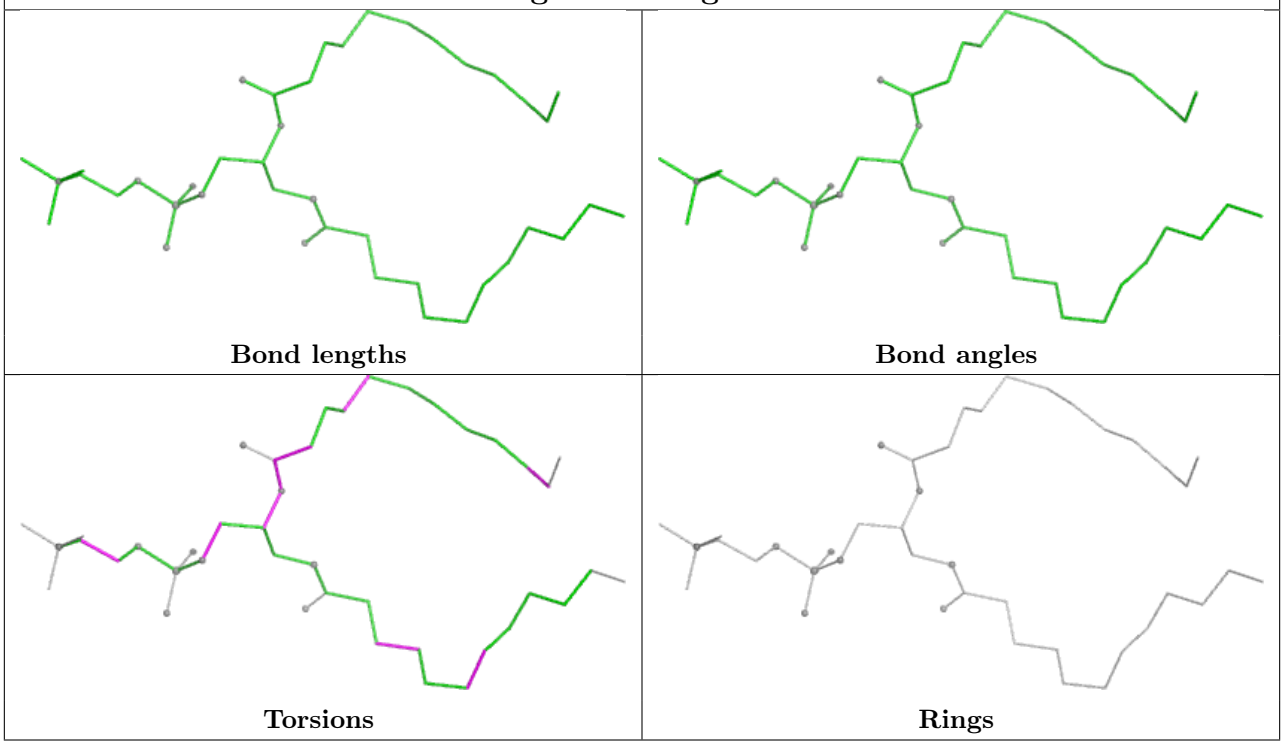
Torsions

Rings

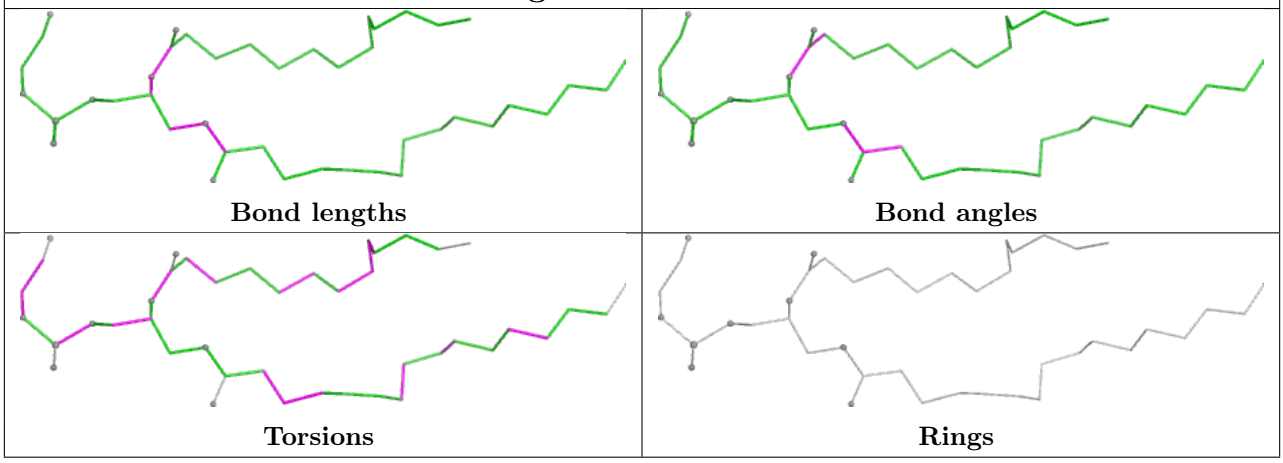
Ligand CDL M 604



Ligand PLC g 201



Ligand 3PE K 101



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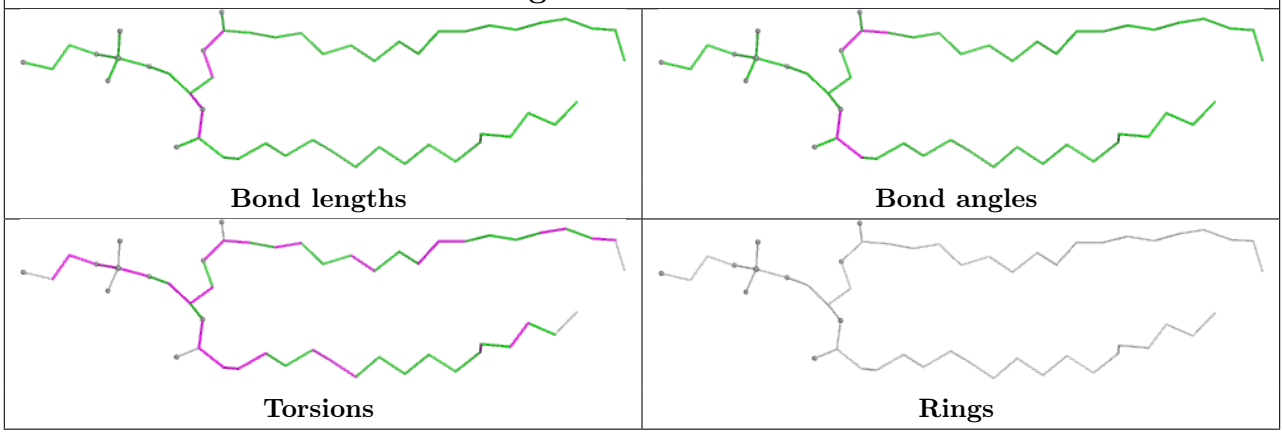
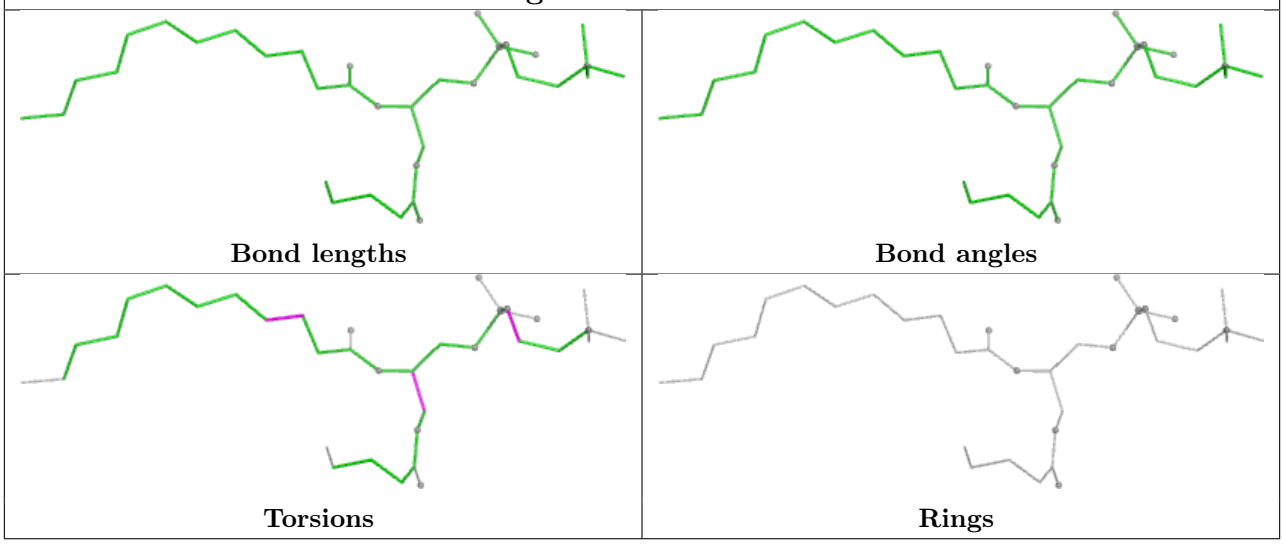


Ligand PLC O 404



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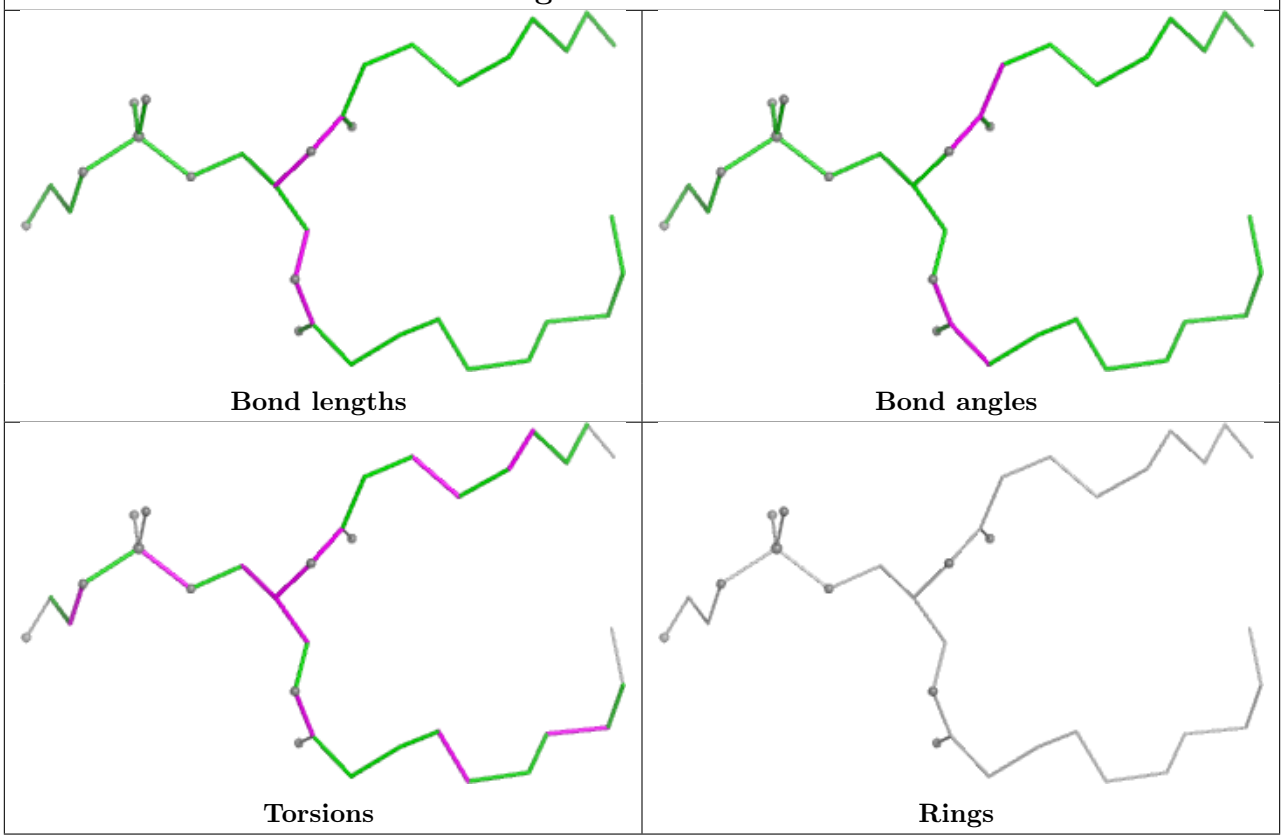
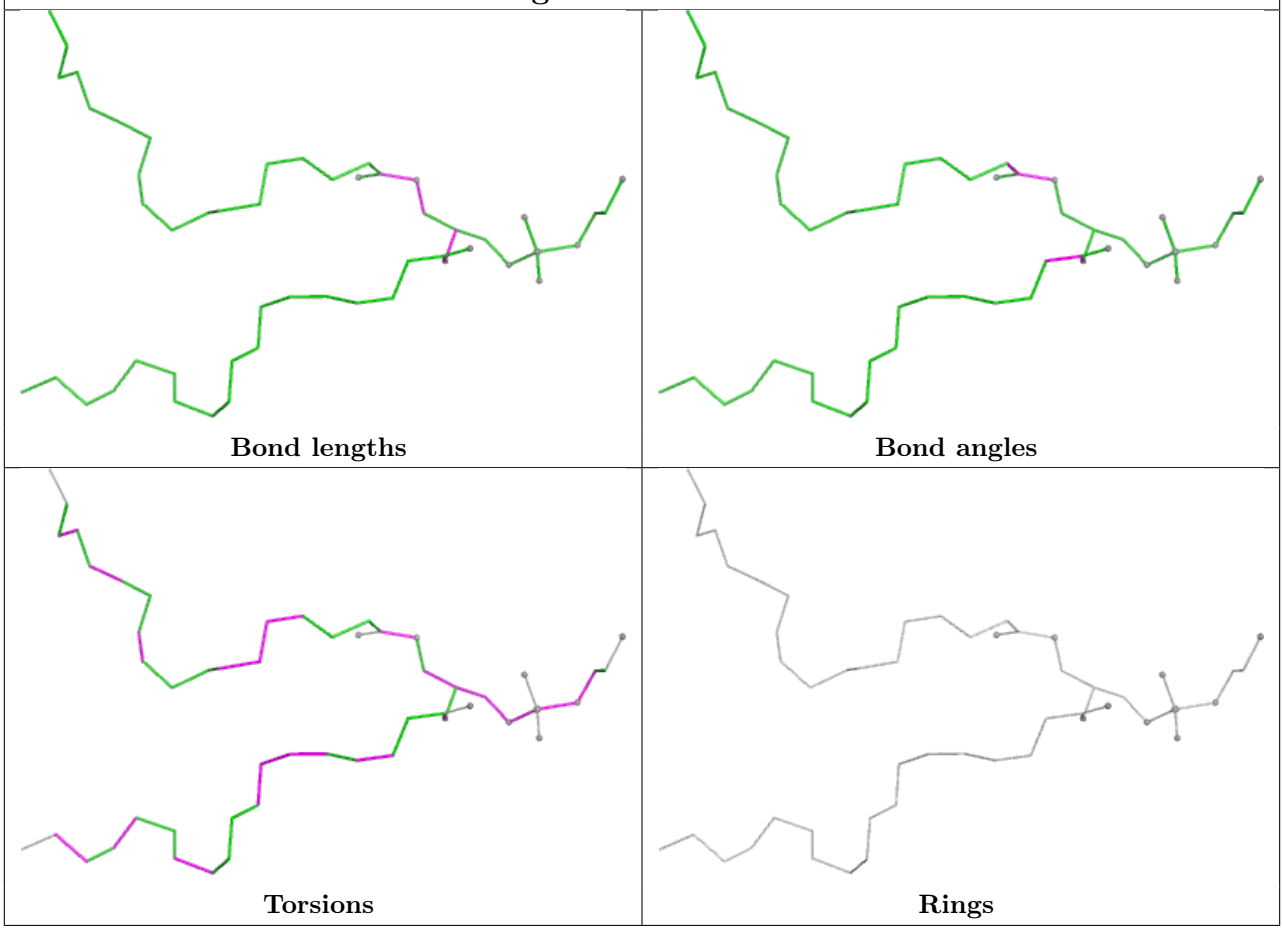
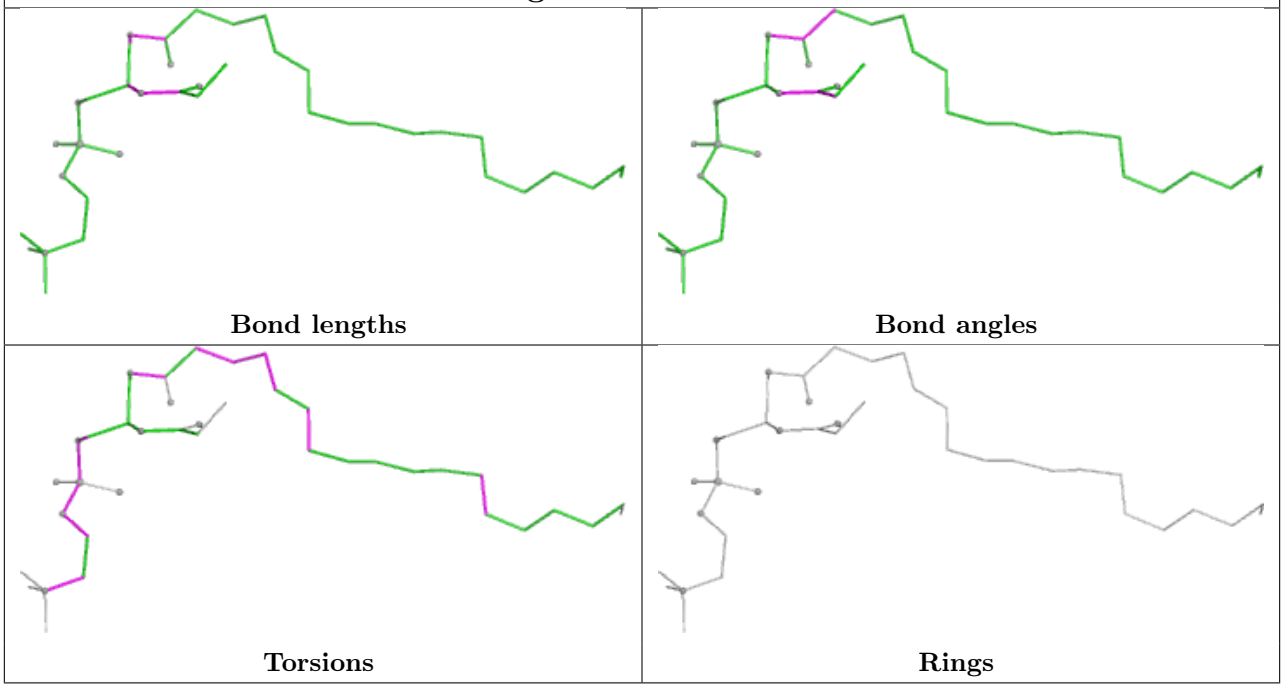


Ligand 3PE Z 202



Ligand PC1 H 403



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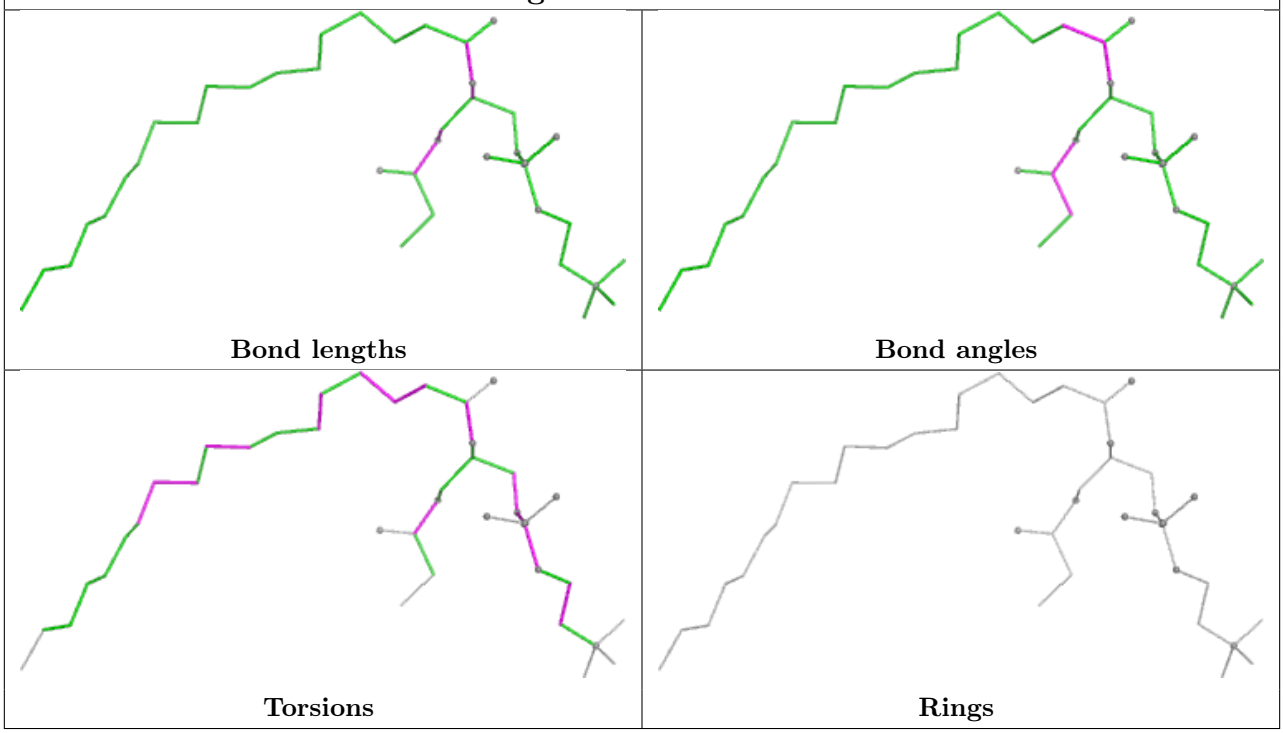
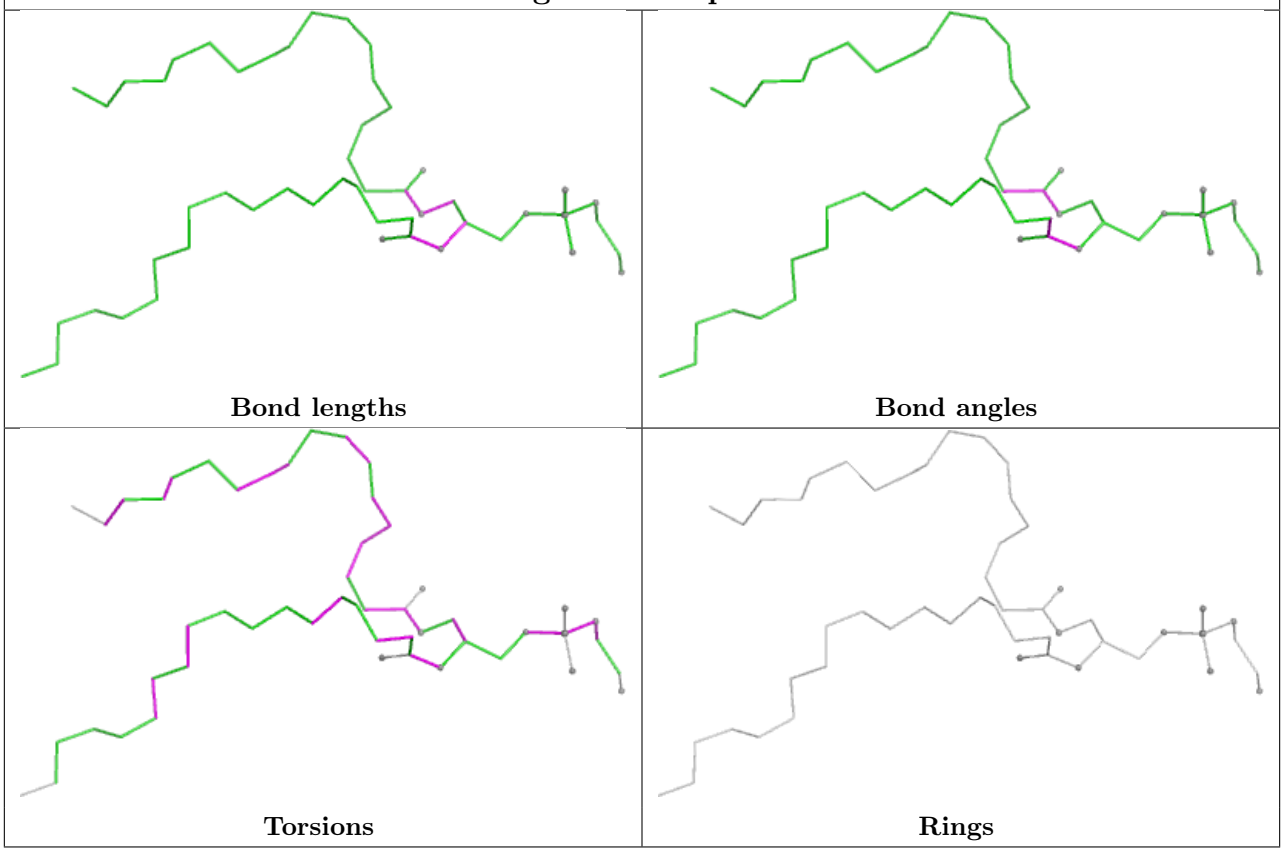
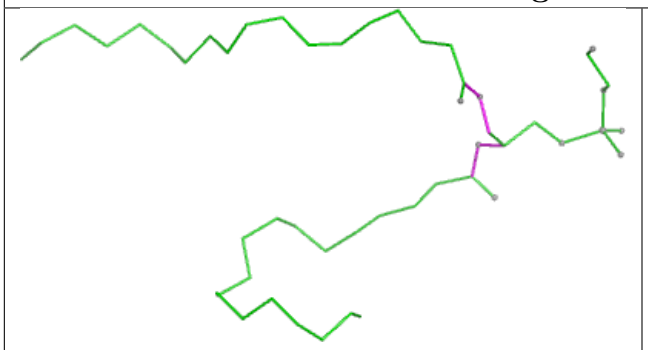


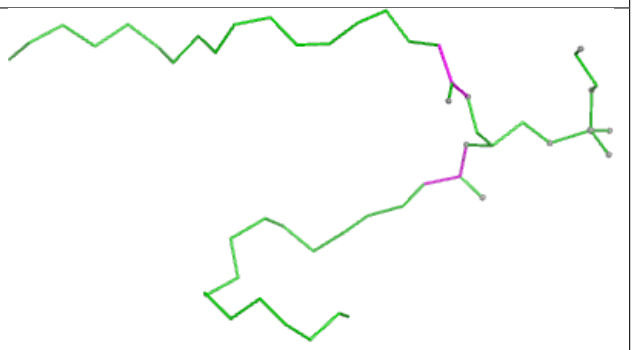
Ligand 3PE q 201



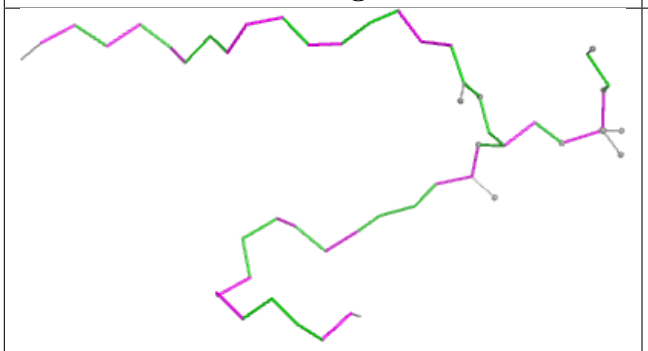
Ligand 3PE L 701



Bond lengths



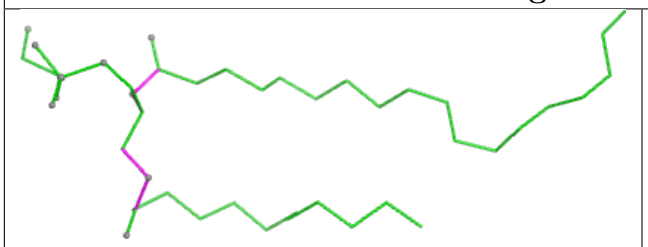
Bond angles



Torsions

Rings

Ligand 3PE O 403



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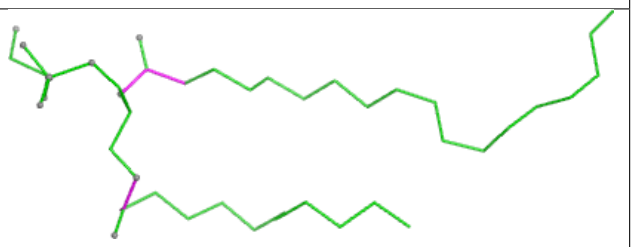
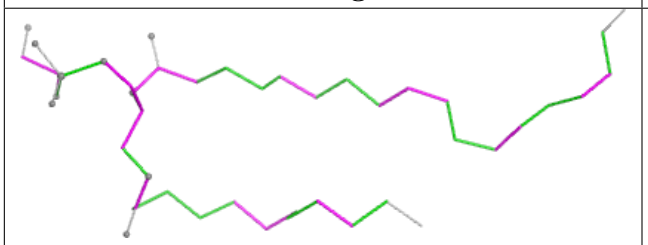
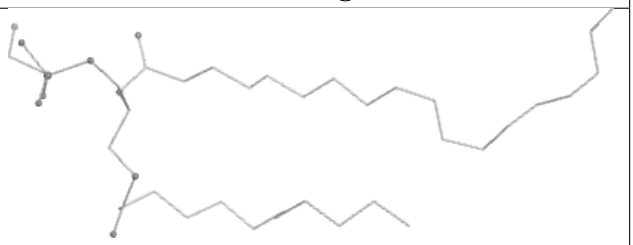


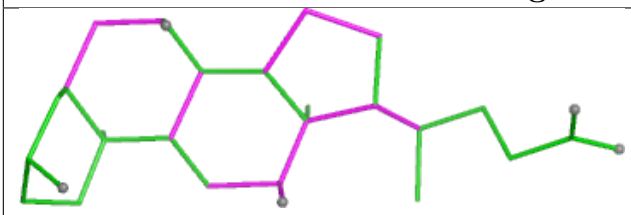
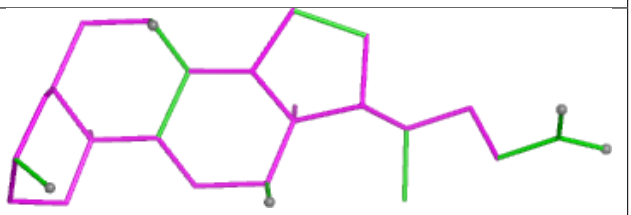
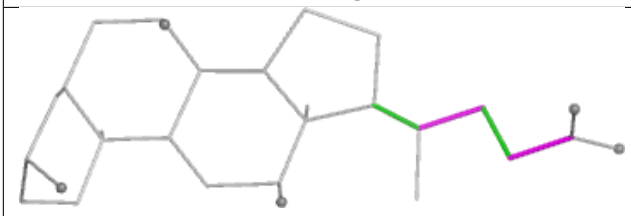
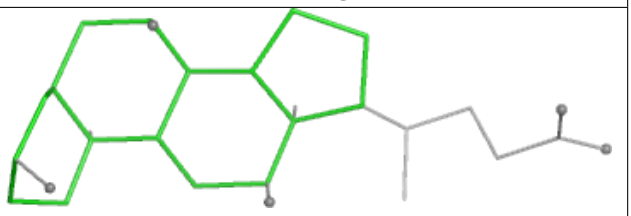
Bond angles

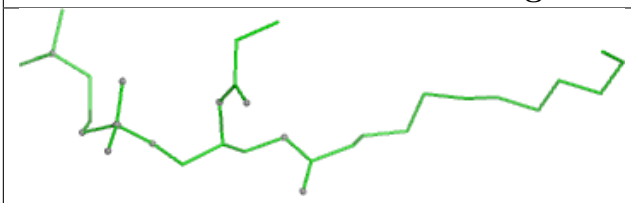
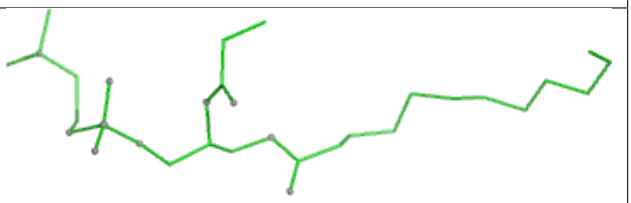
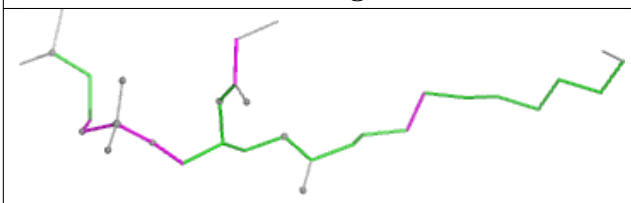
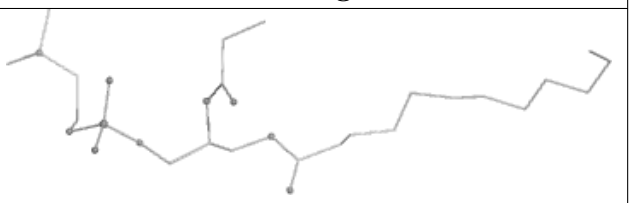


Torsions

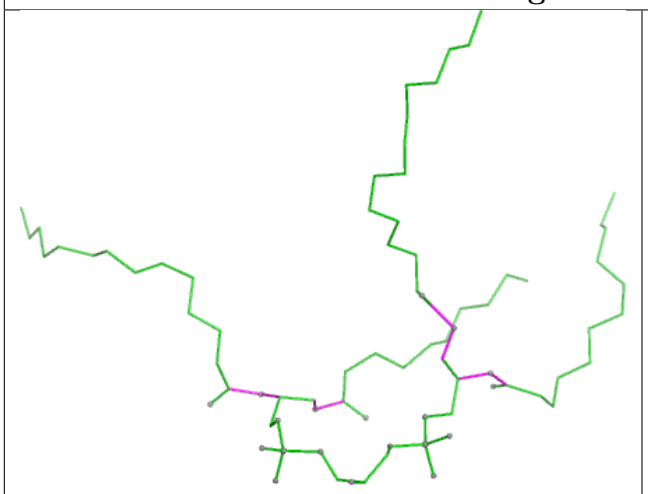


Rings

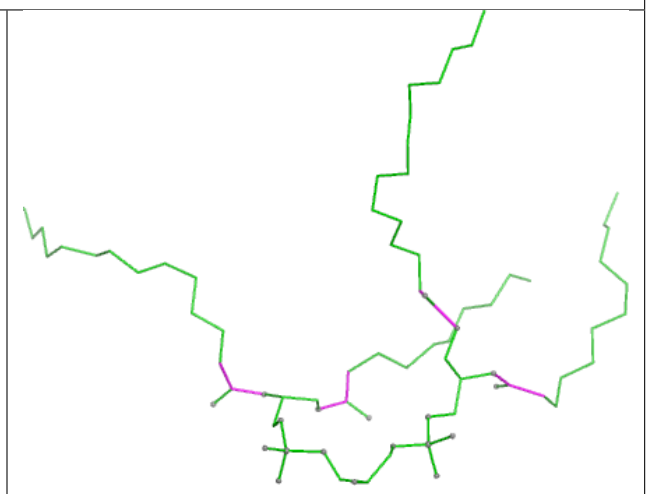
Ligand CHD i 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLC A 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

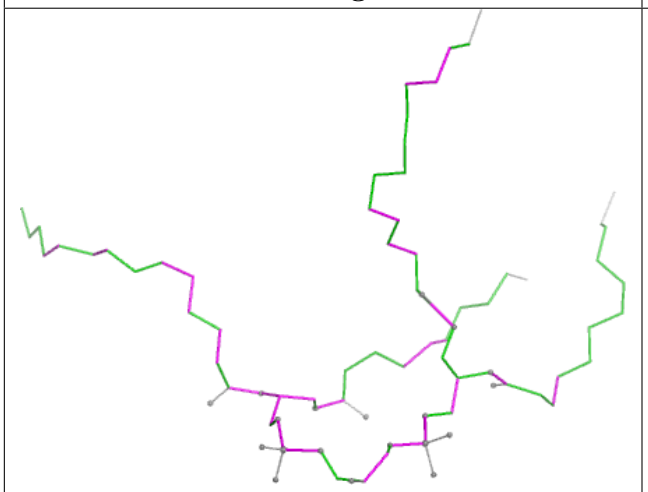
Ligand CDL h 202



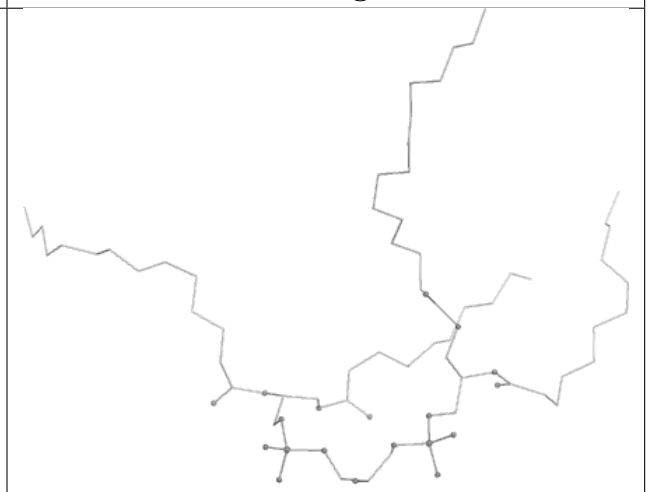
Bond lengths



Bond angles

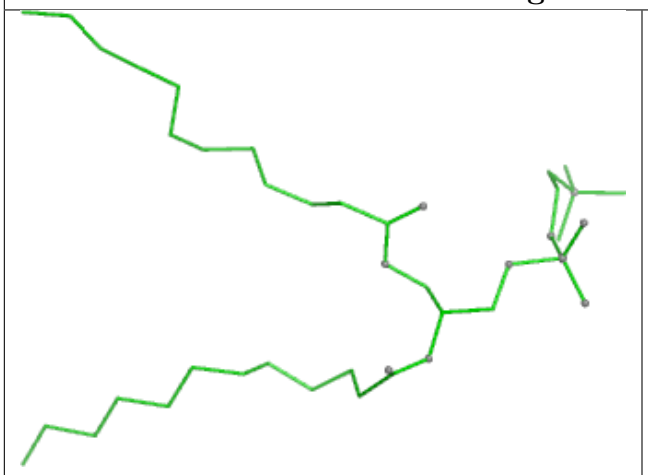


Torsions

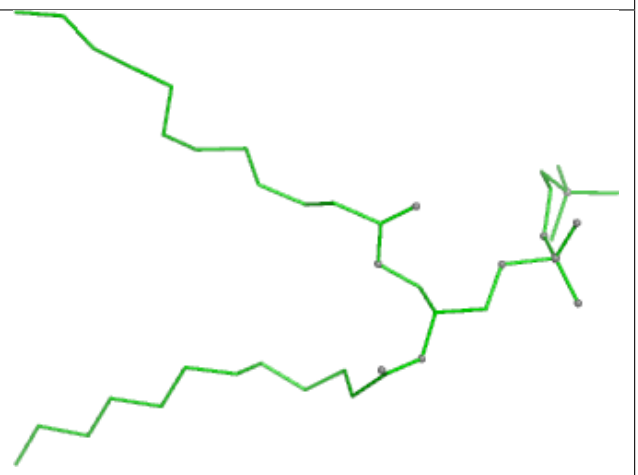


Rings

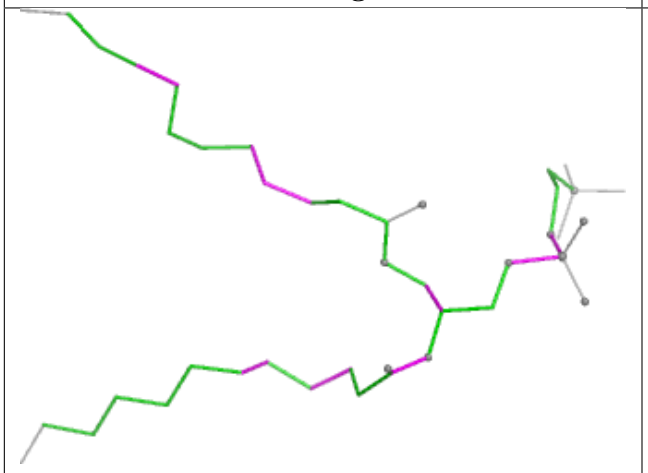
Ligand PLC P 503



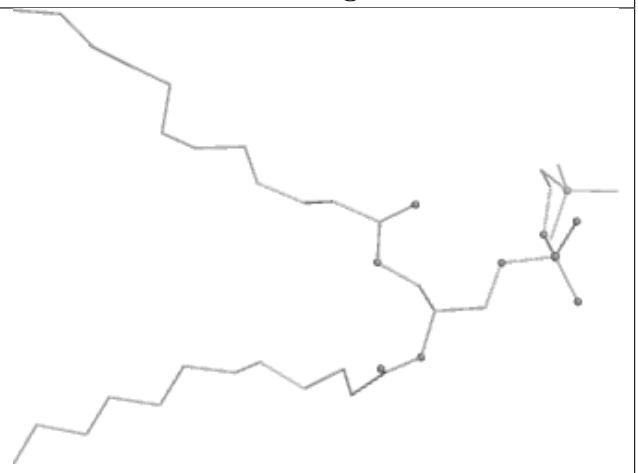
Bond lengths



Bond angles

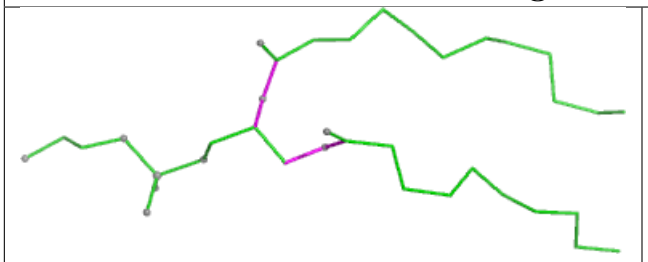


Torsions



Rings

Ligand 3PE A 202



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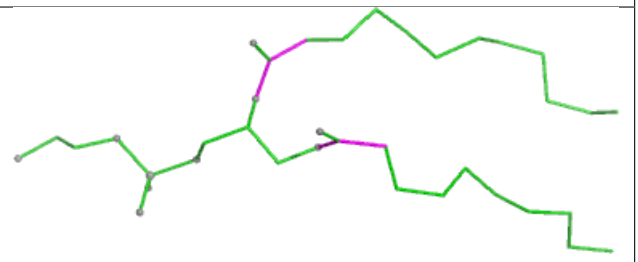
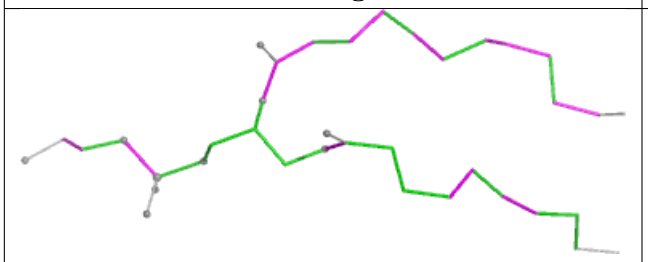


Bond angles



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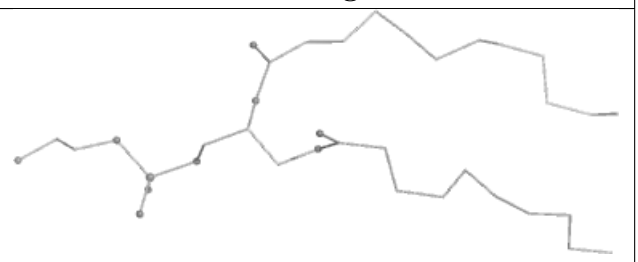
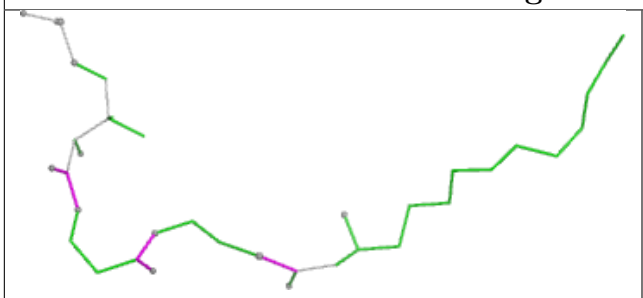
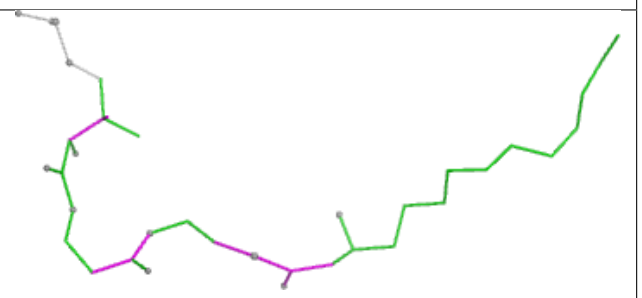
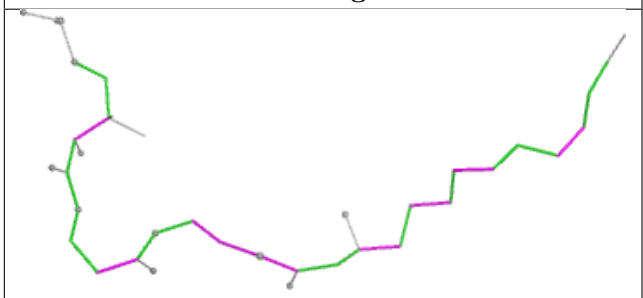
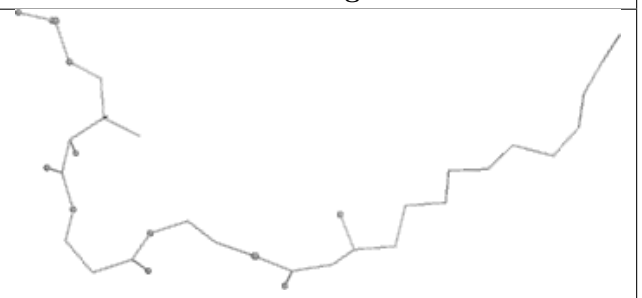
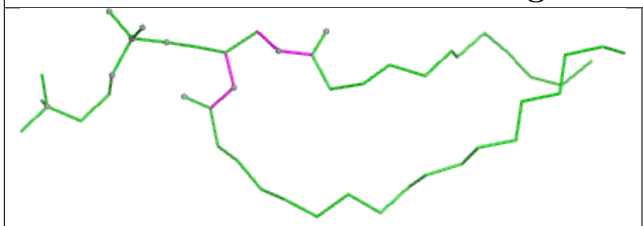
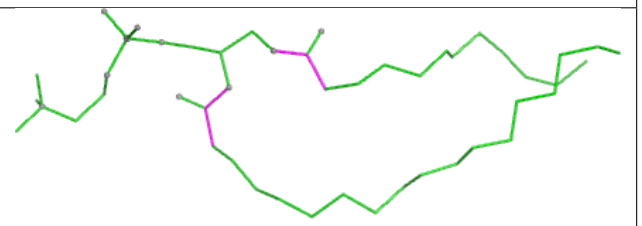
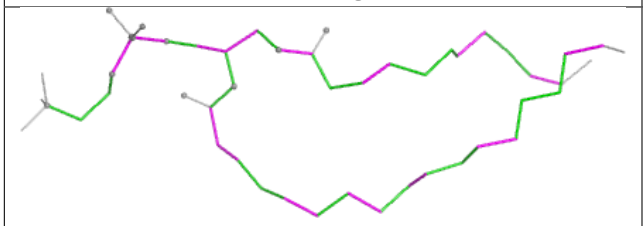
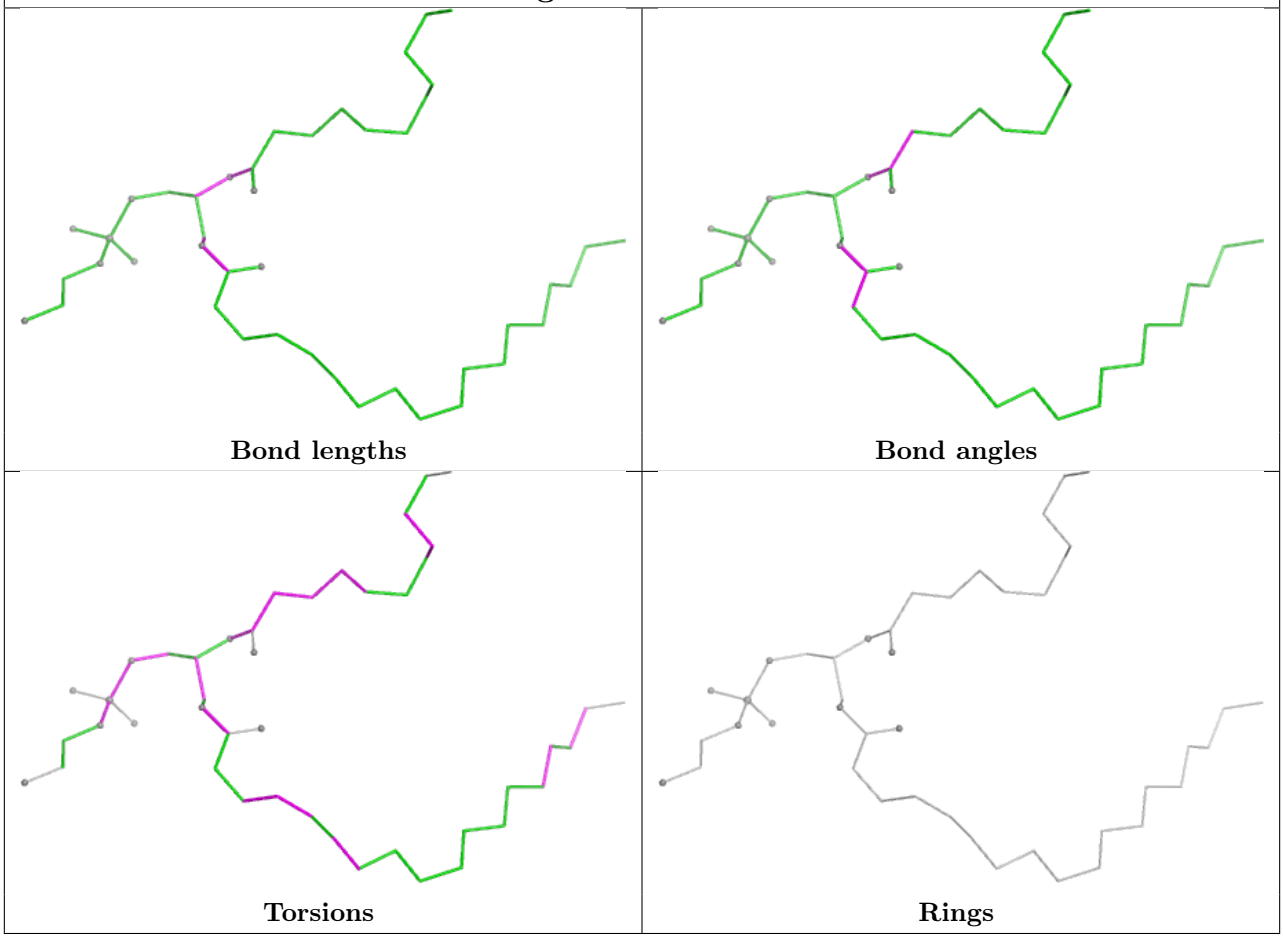


Rings

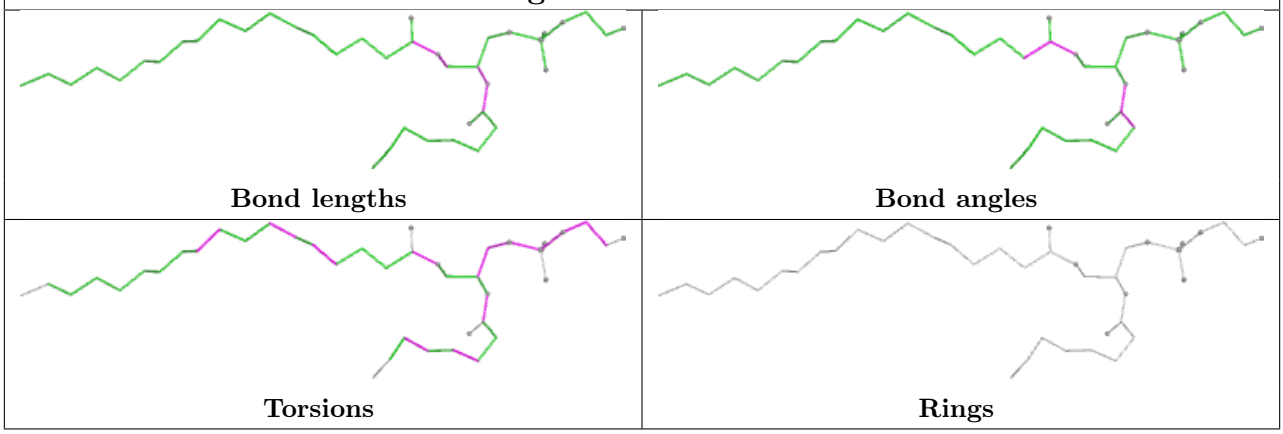
Ligand EHZ U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

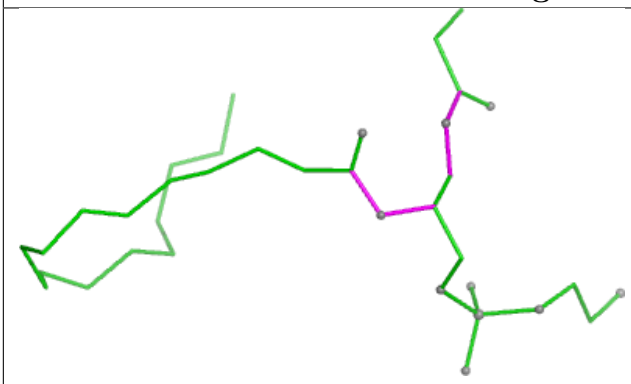
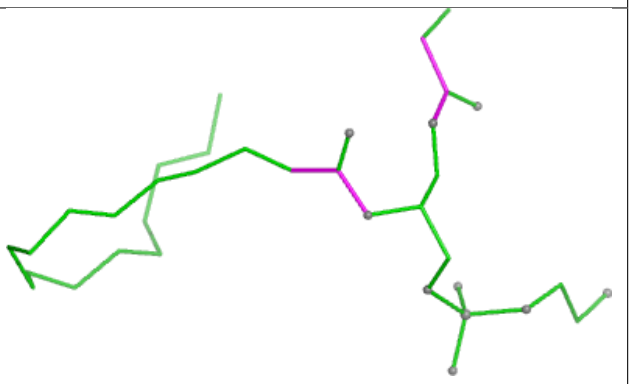
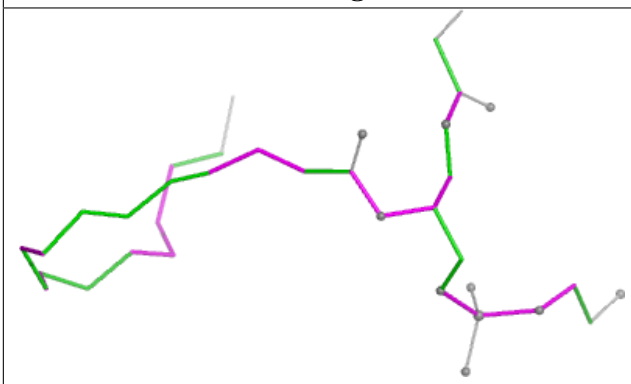
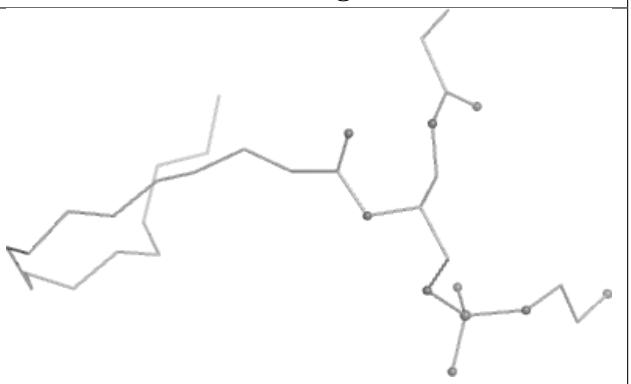
Ligand PC1 H 401	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 3PE f 102

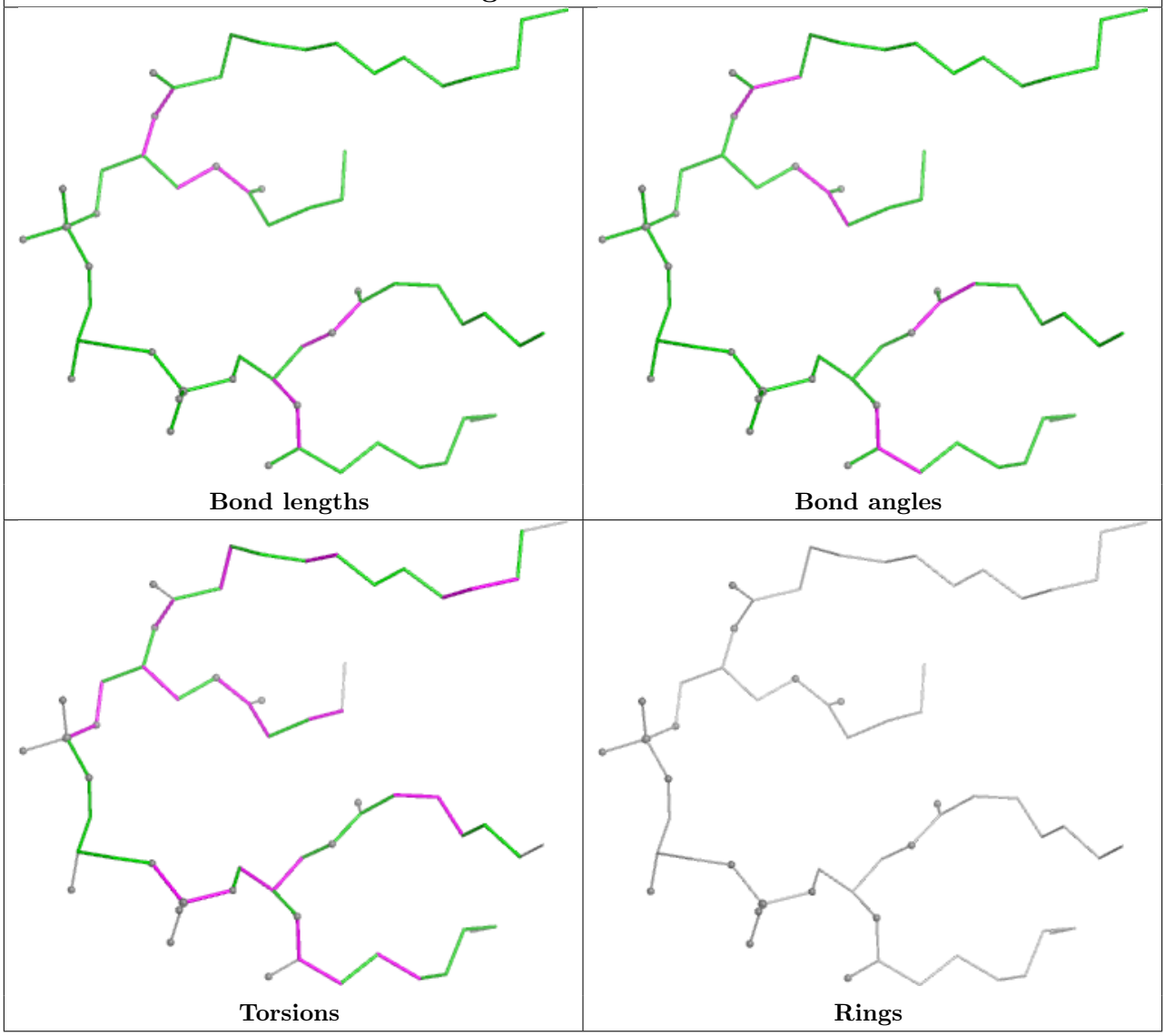


Ligand 3PE m 201

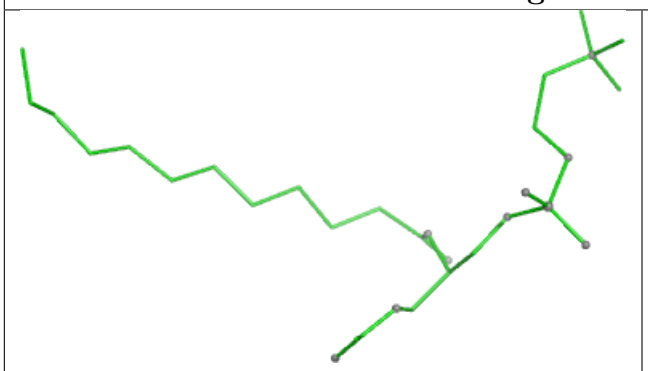


Ligand 3PE J 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

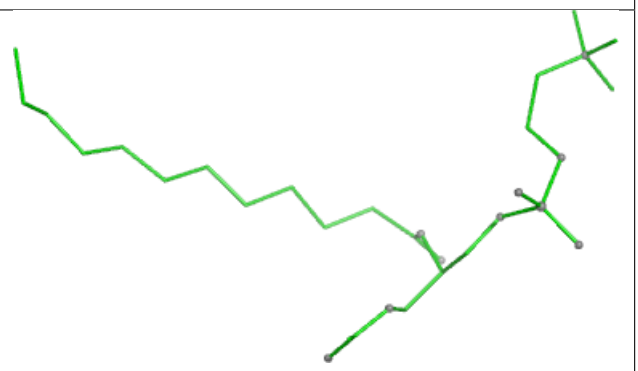
Ligand CDL r 202



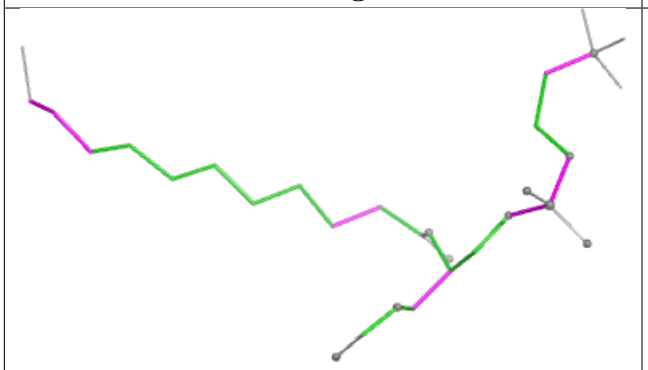
Ligand PLC P 504



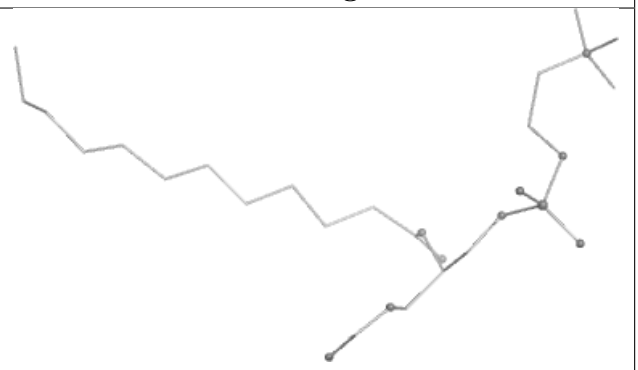
Bond lengths



Bond angles

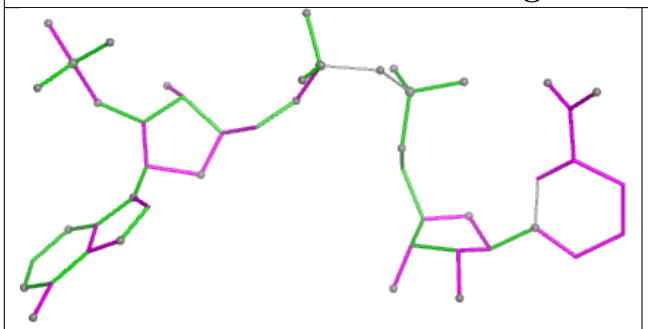


Torsions

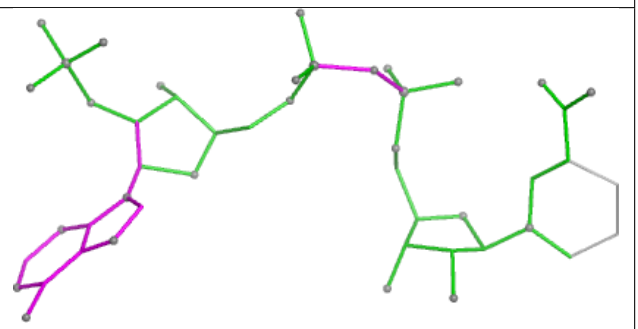


Rings

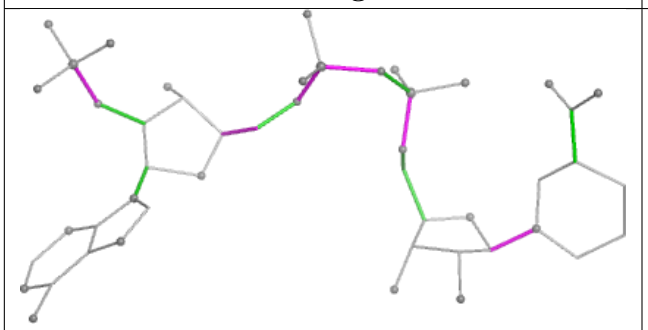
Ligand NDP P 501



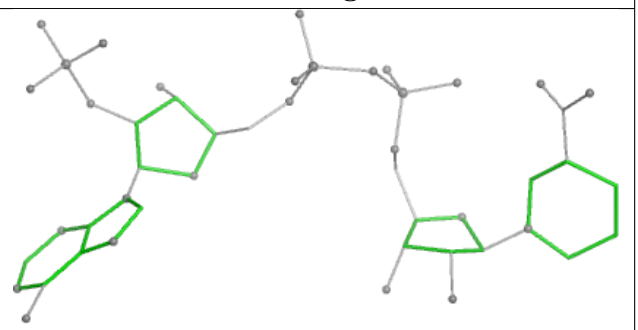
Bond lengths



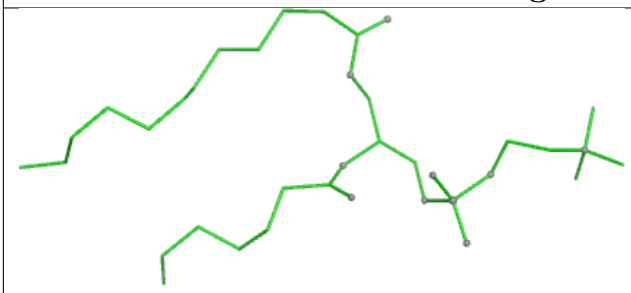
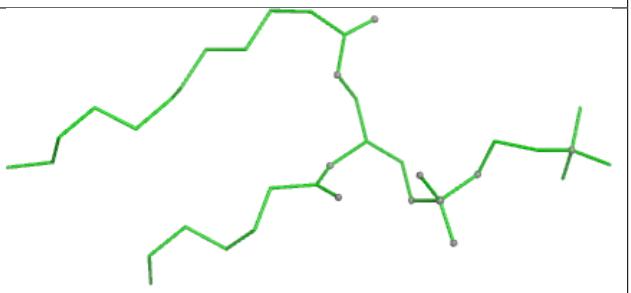
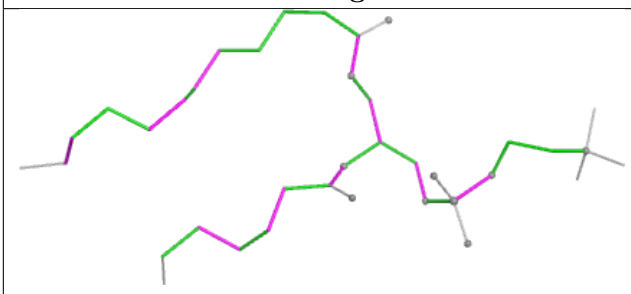
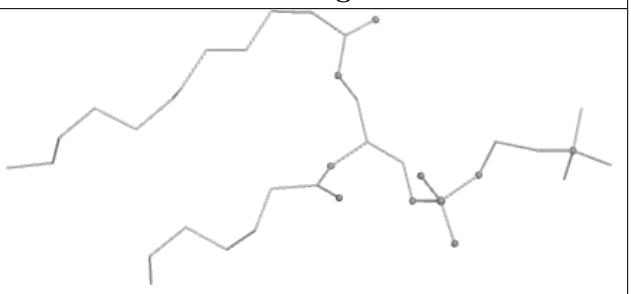
Bond angles



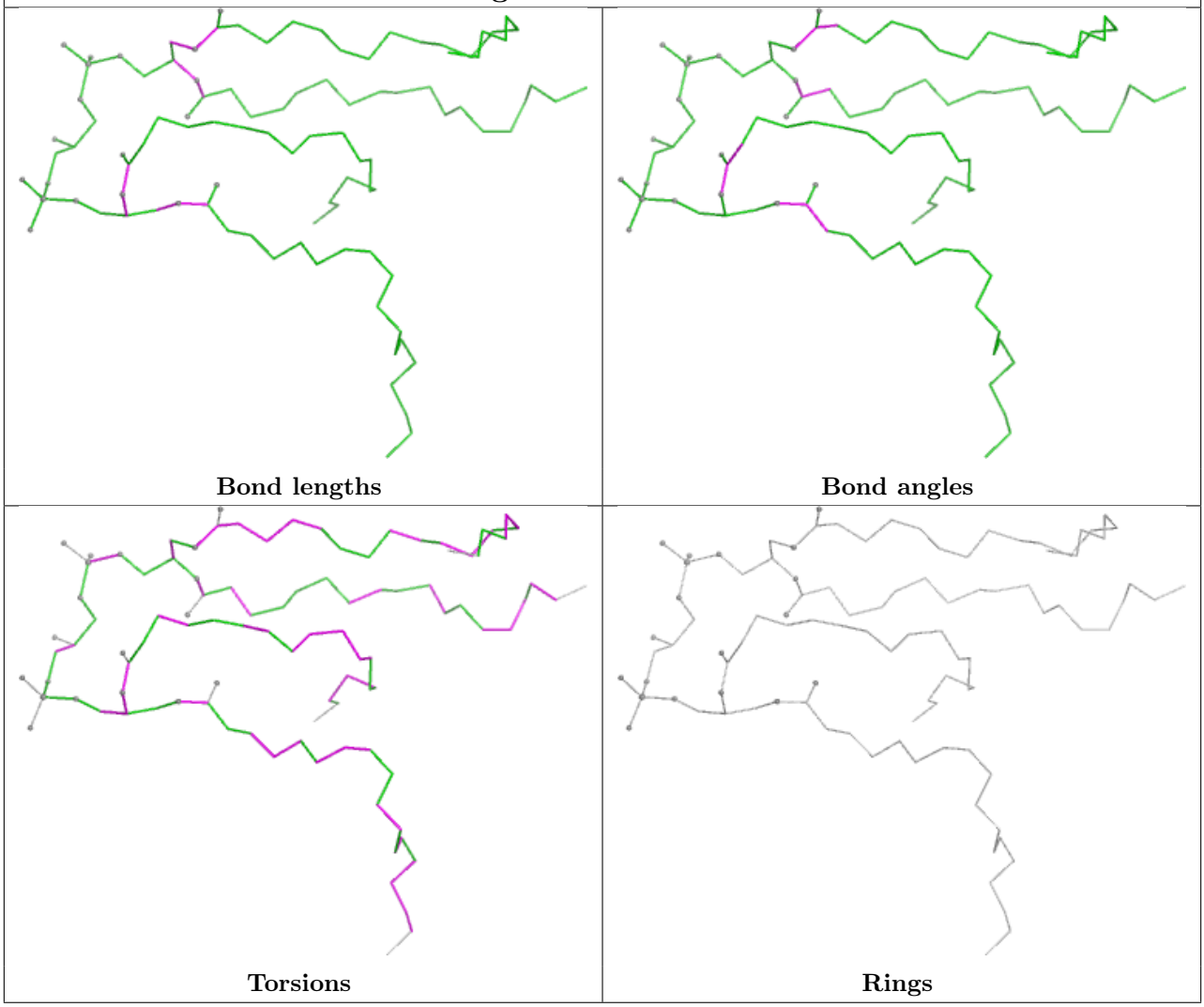
Torsions



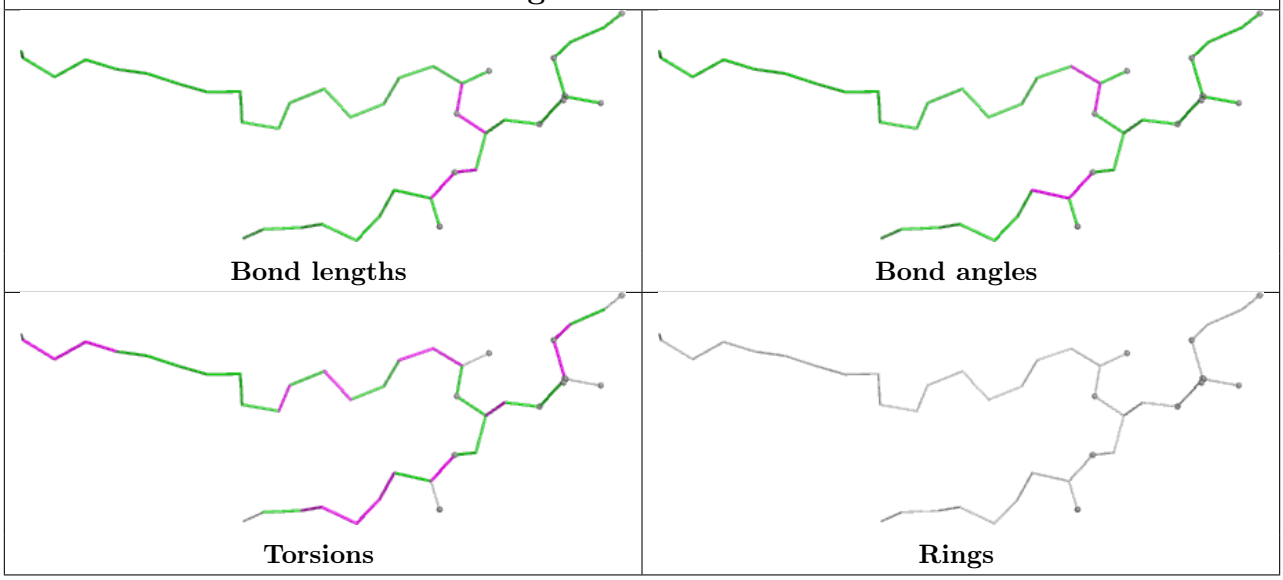
Rings

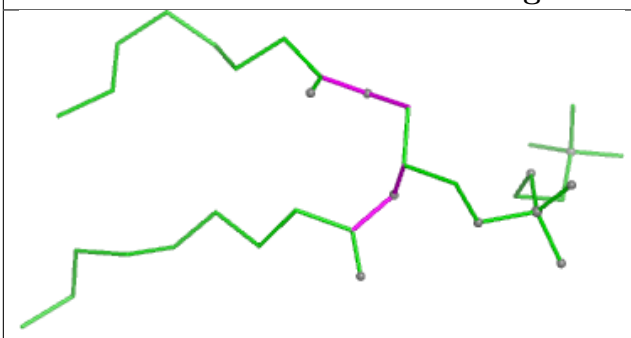
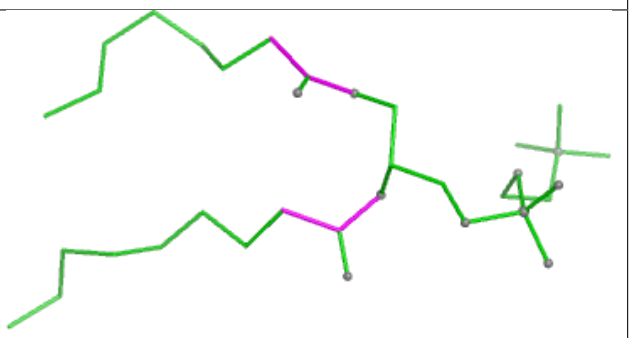
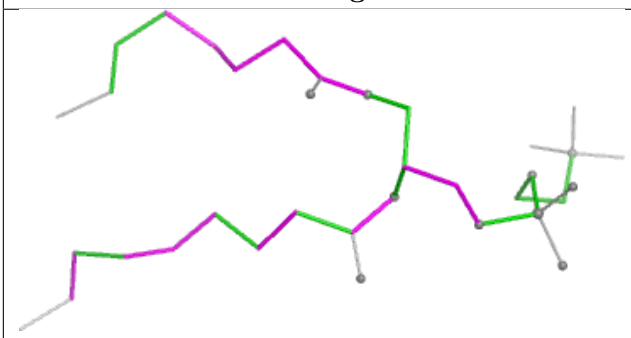
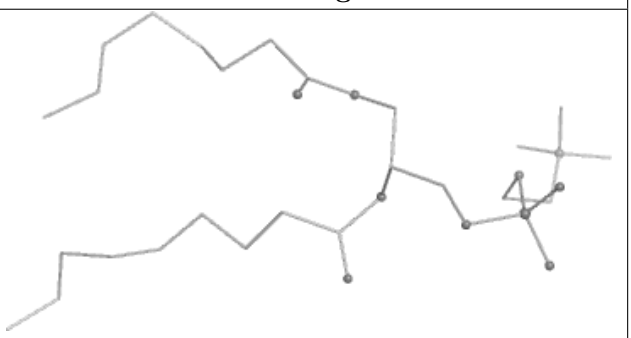
Ligand PLC J 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL N 404



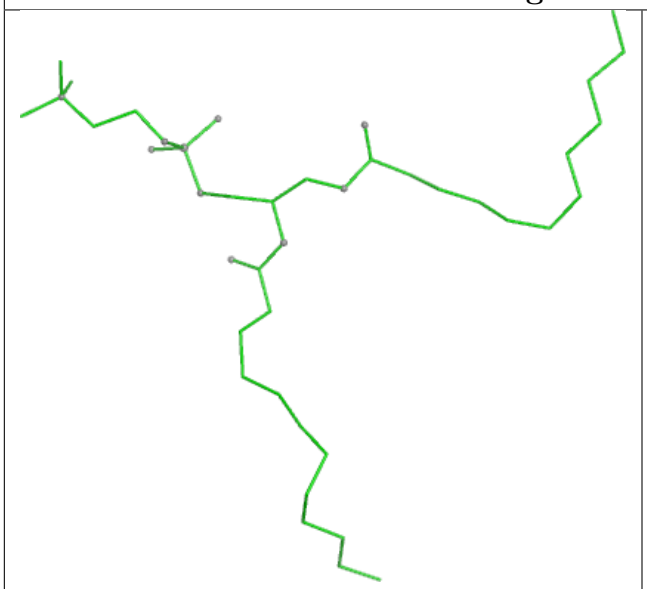
Ligand 3PE m 204



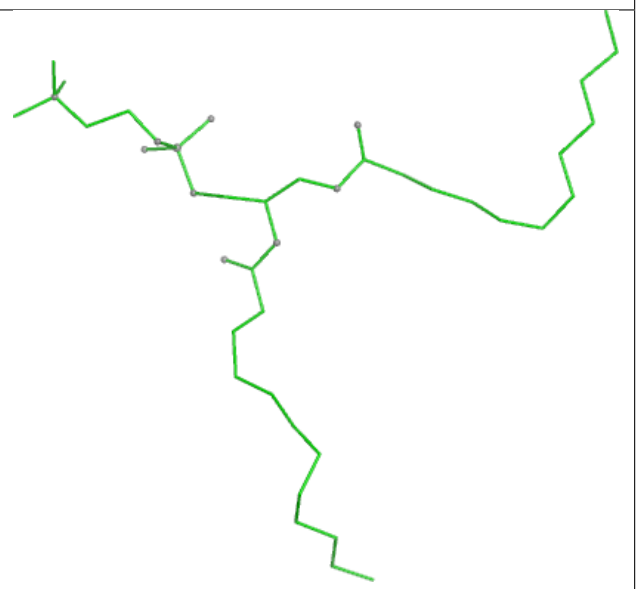
Ligand PC1 M 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 A 204

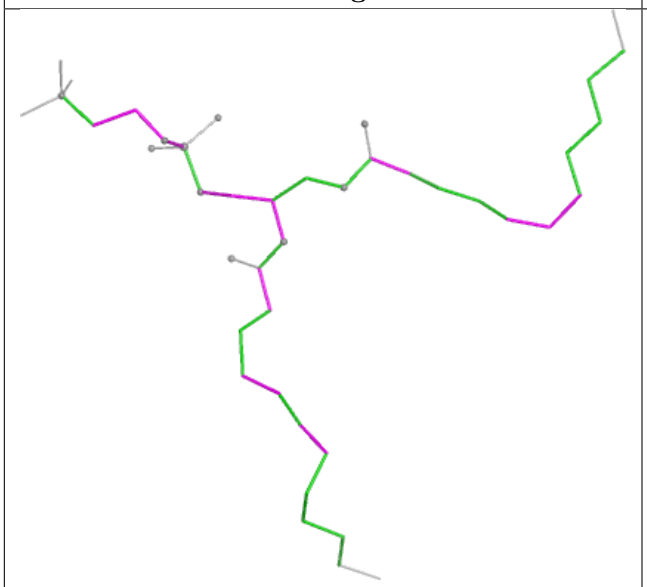
Ligand PLC Y 208



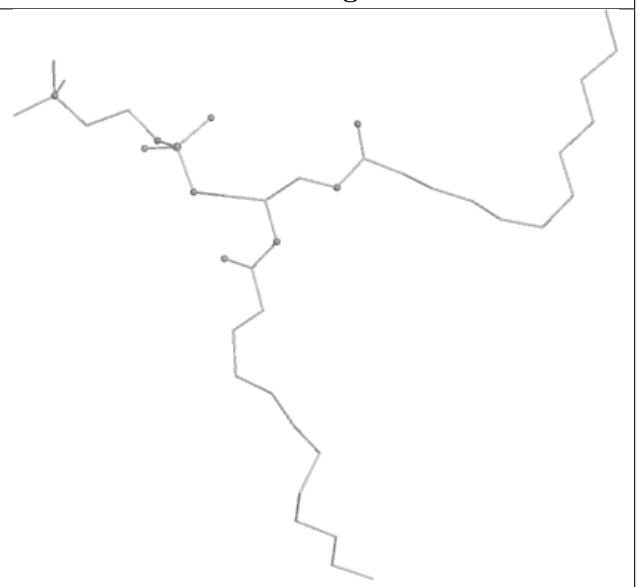
Bond lengths



Bond angles

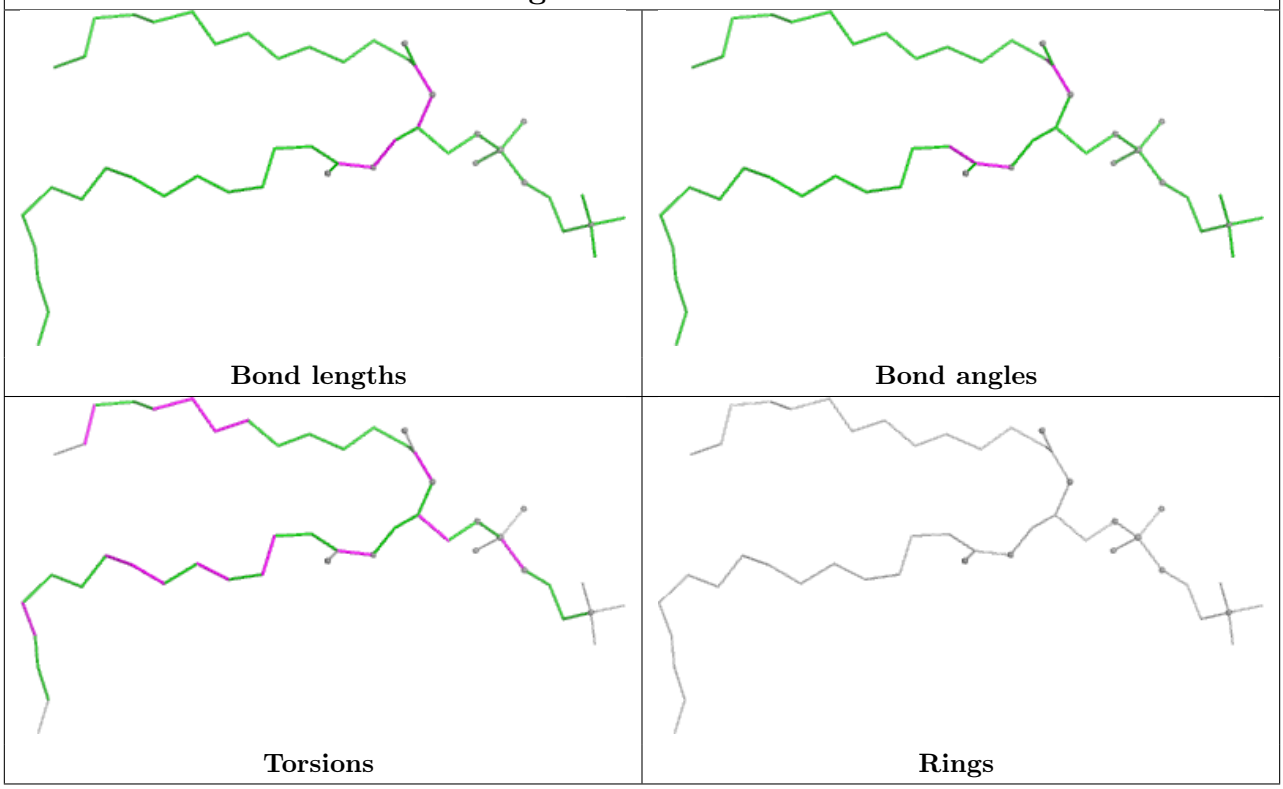


Torsions

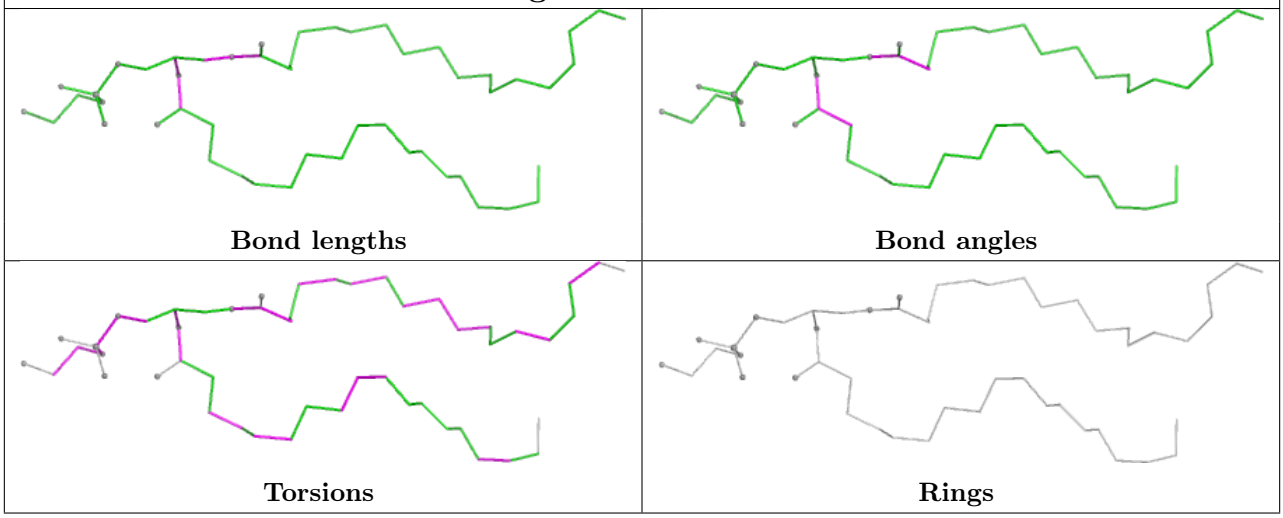


Rings

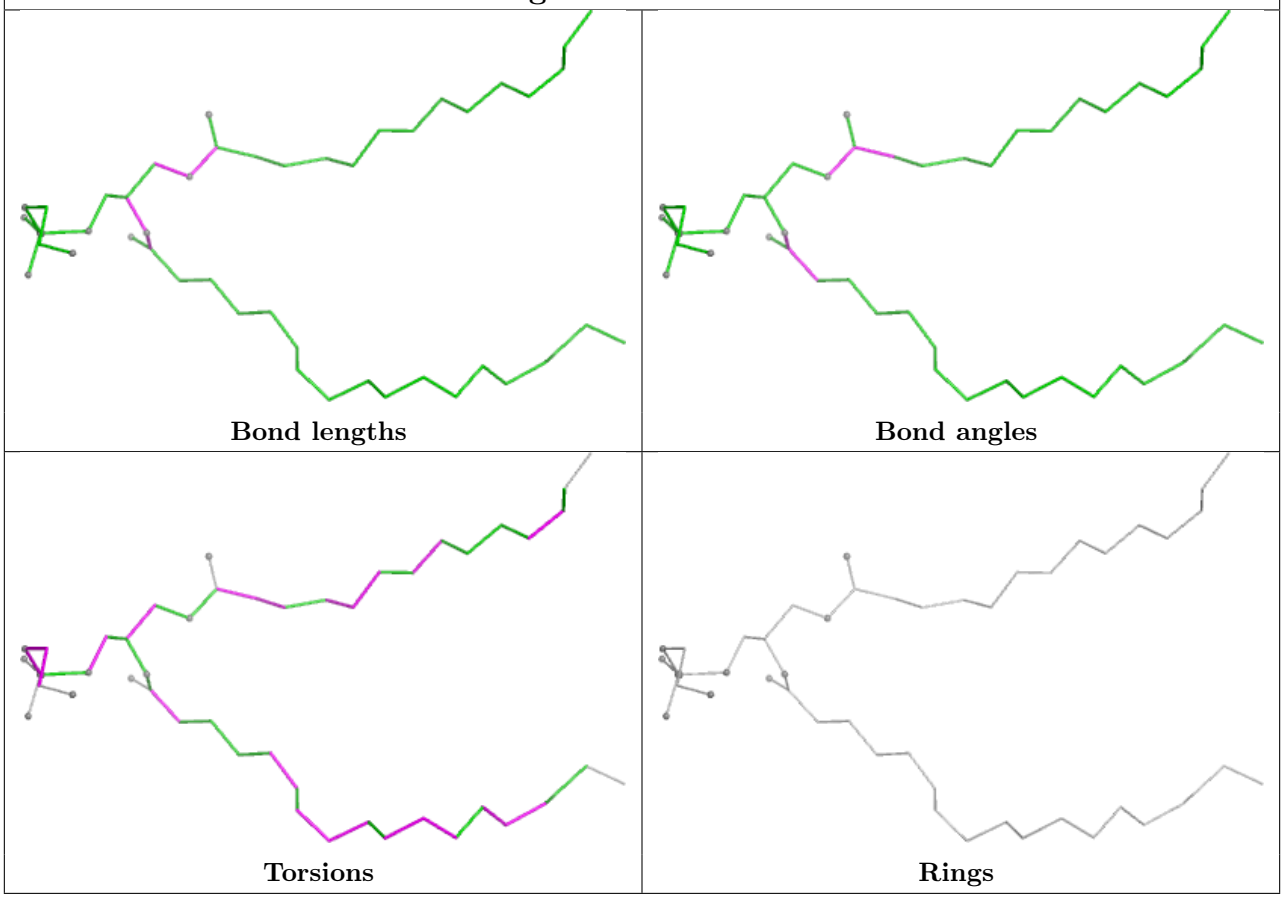
Ligand PC1 B 204



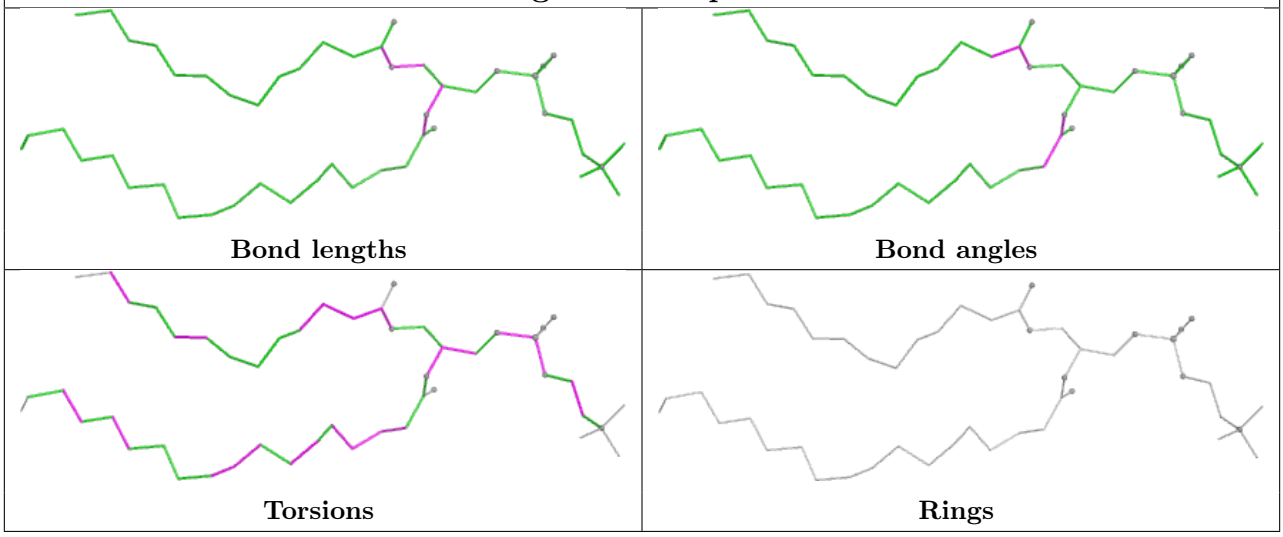
Ligand 3PE Y 202



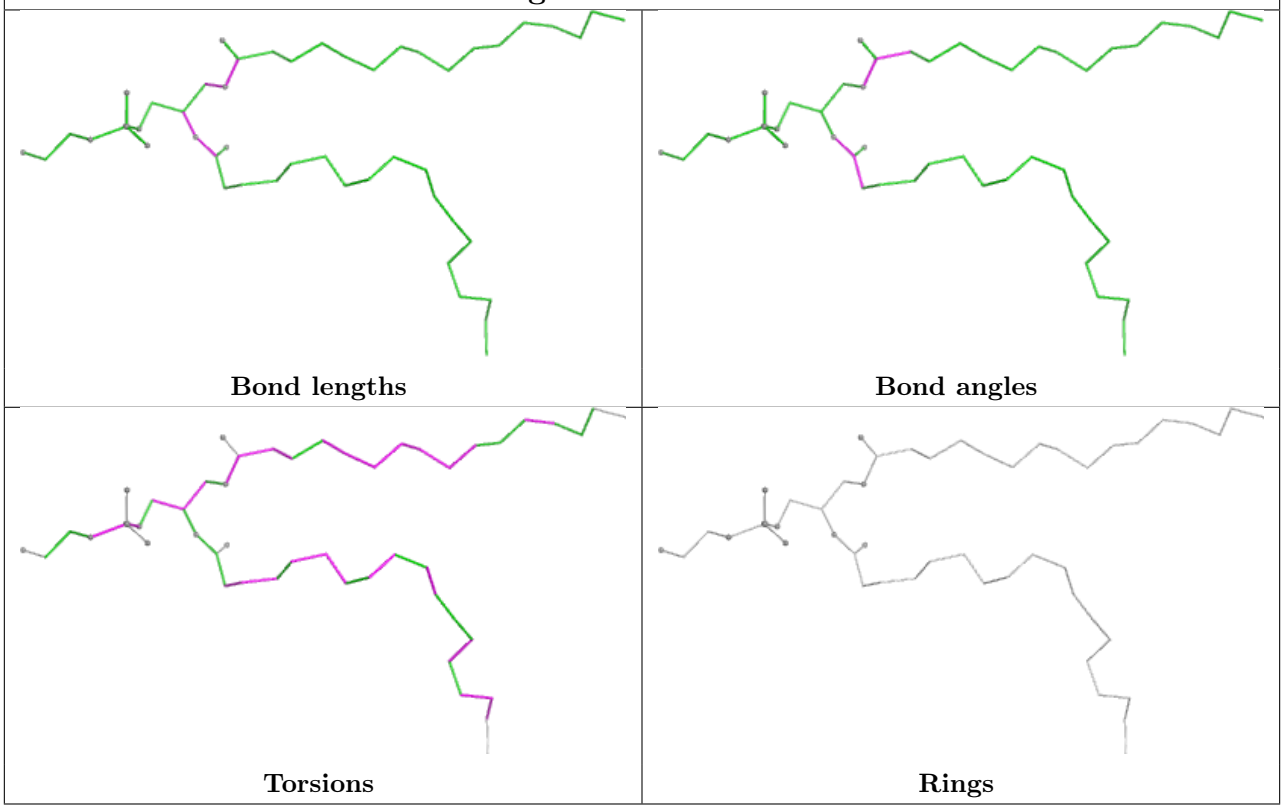
Ligand 3PE A 201



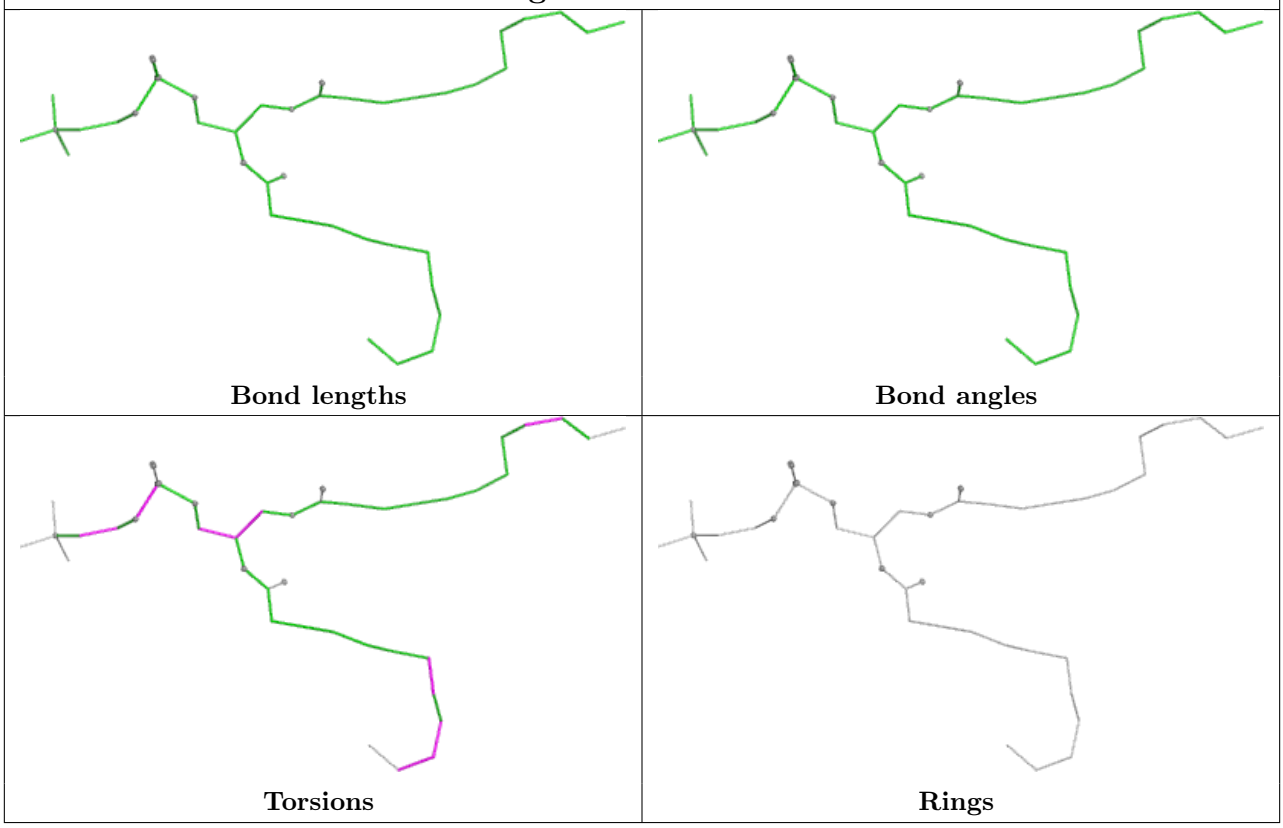
Ligand PC1 q 202



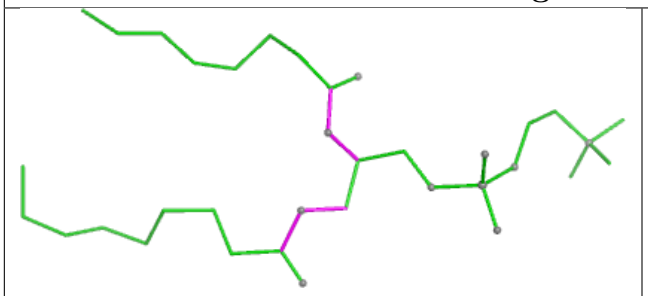
Ligand 3PE N 401



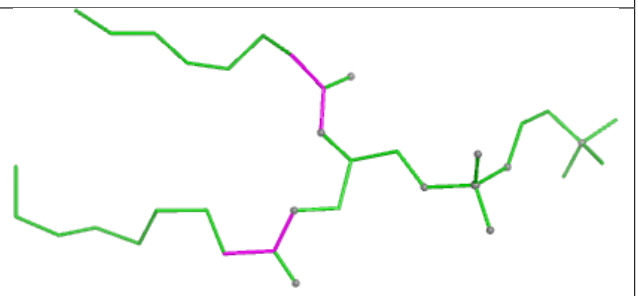
Ligand PLC L 704



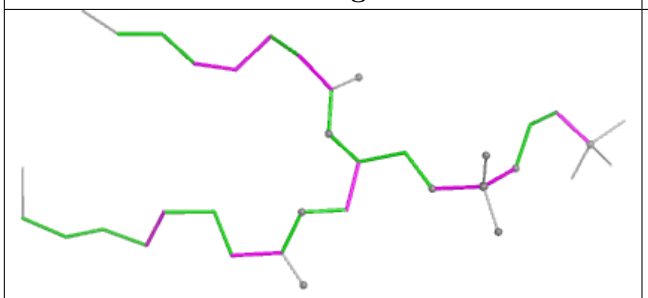
Ligand PC1 J 203



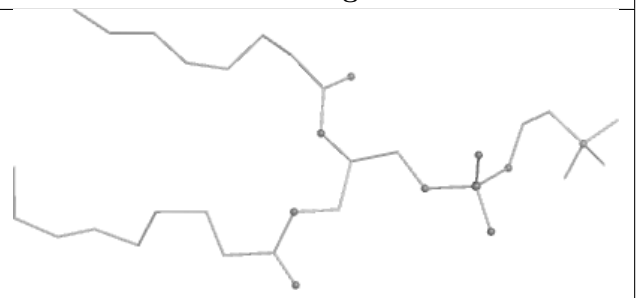
Bond lengths



Bond angles

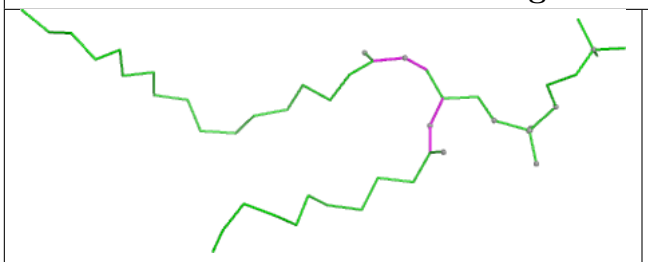


Torsions

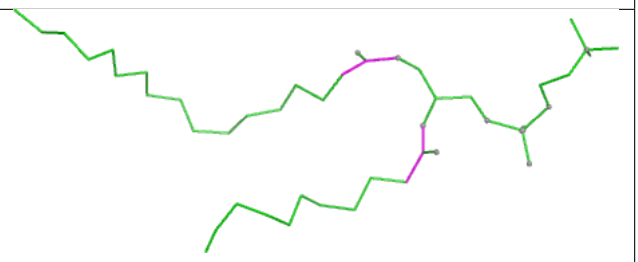


Rings

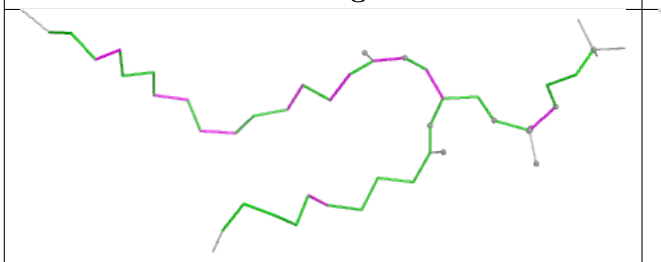
Ligand PC1 B 203



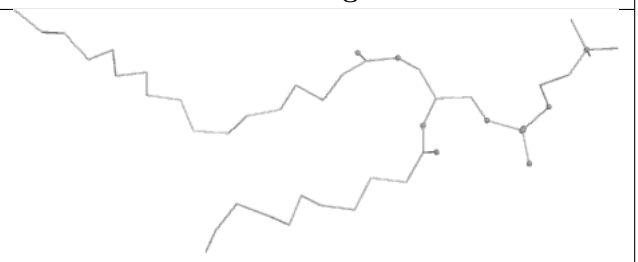
Bond lengths



Bond angles

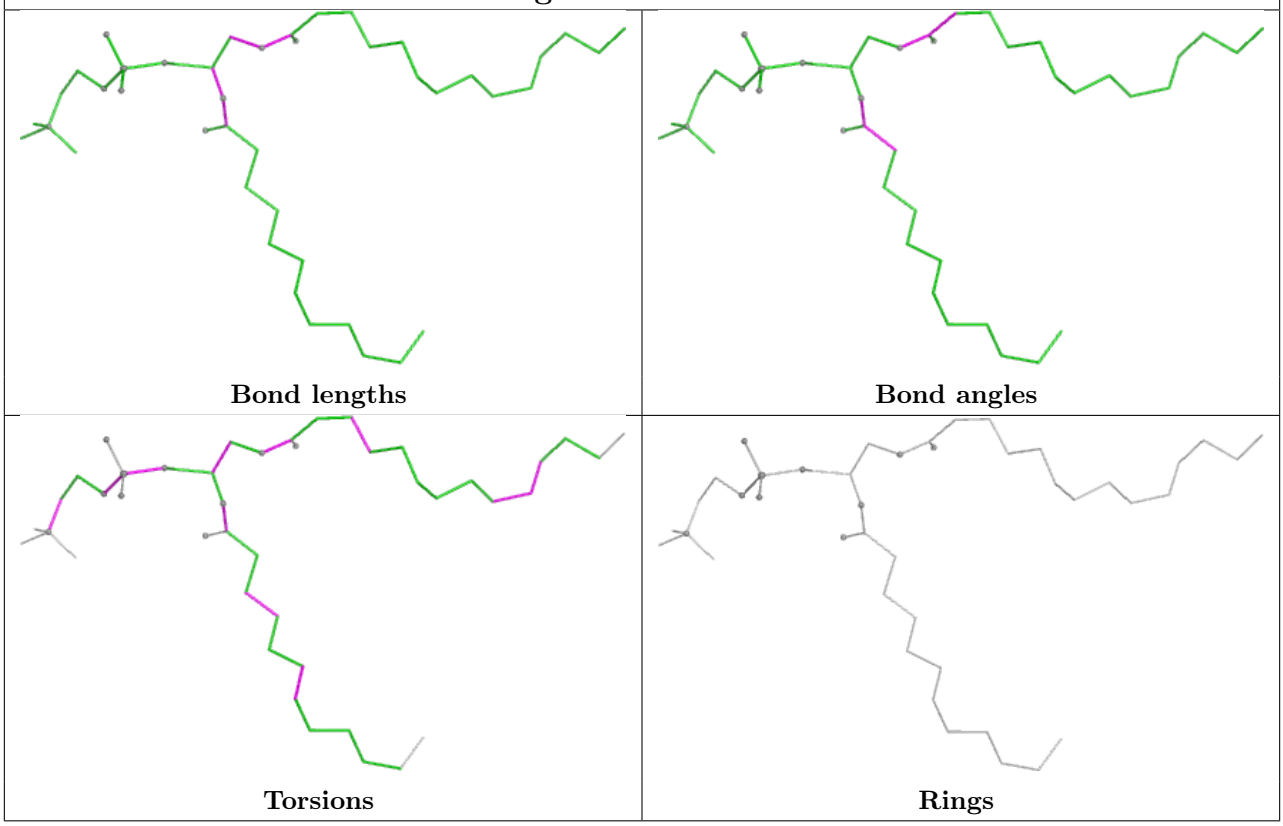


Torsions

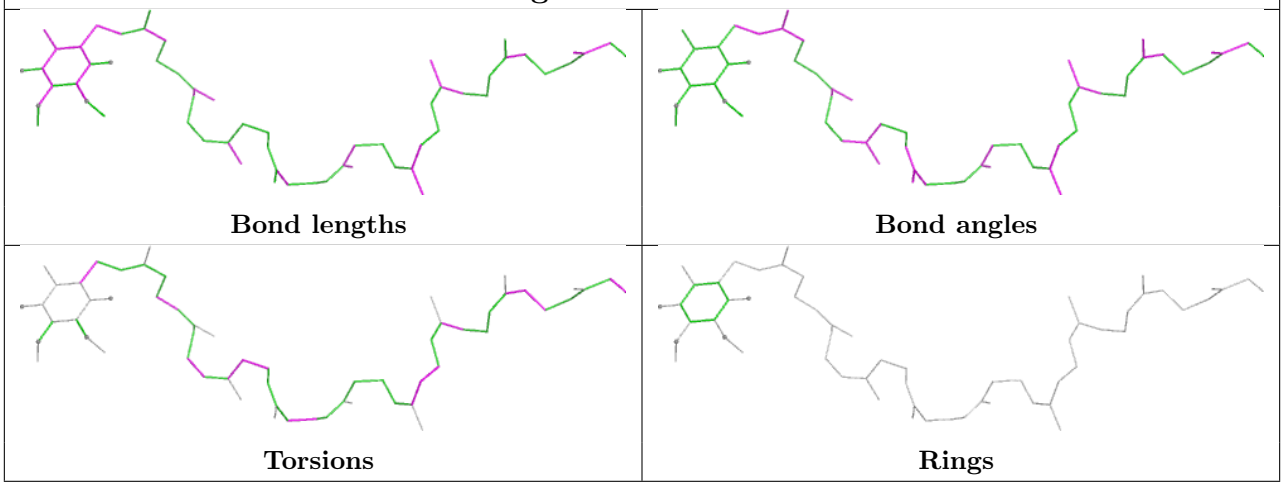


Rings

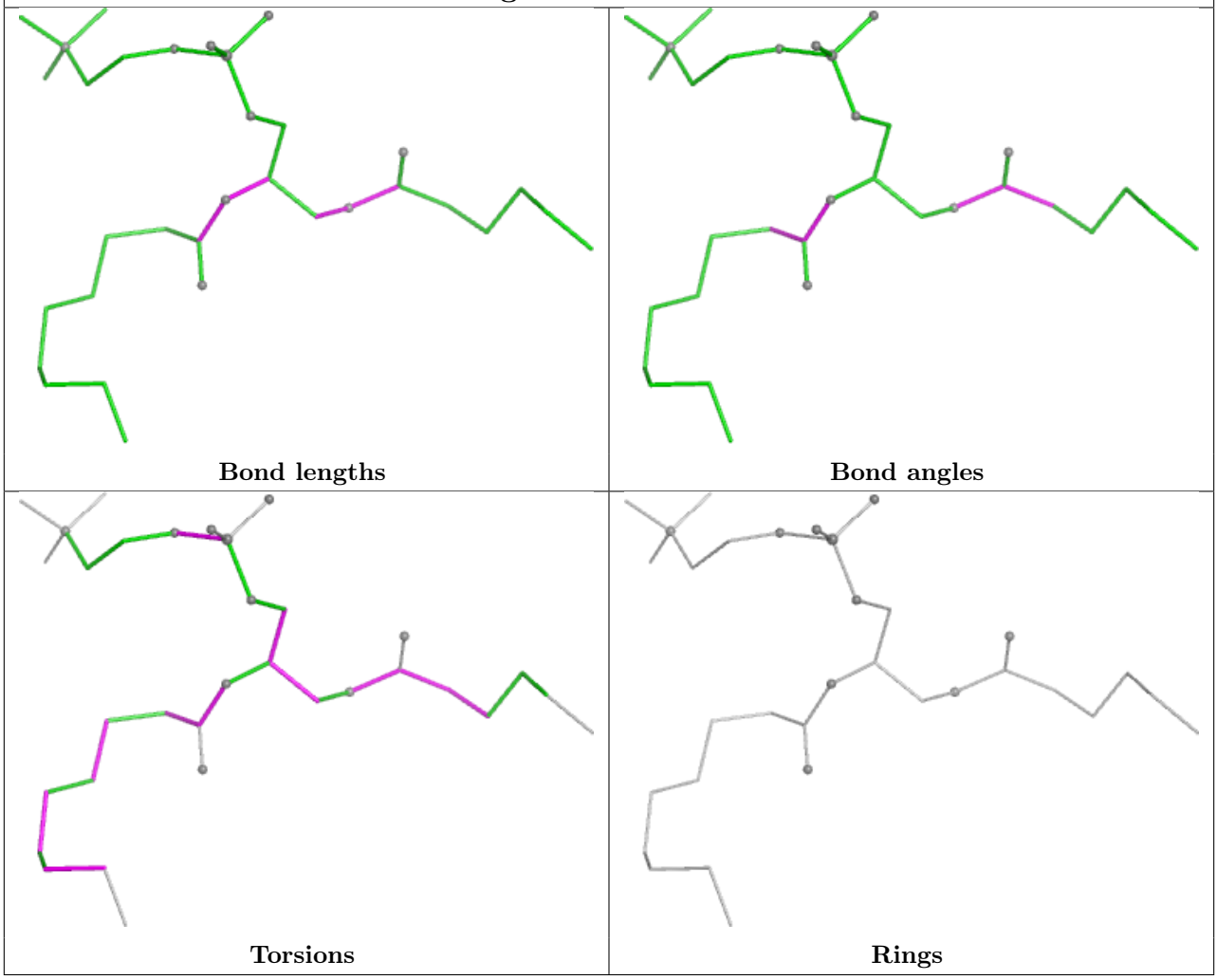
Ligand PC1 I 204



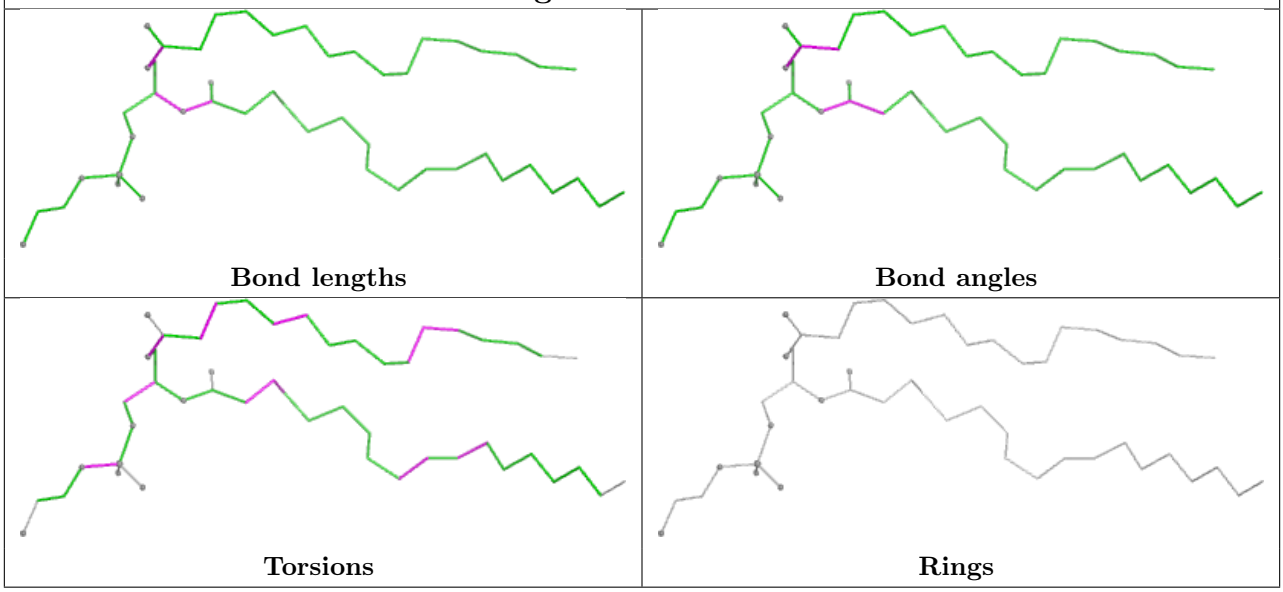
Ligand U10 B 202



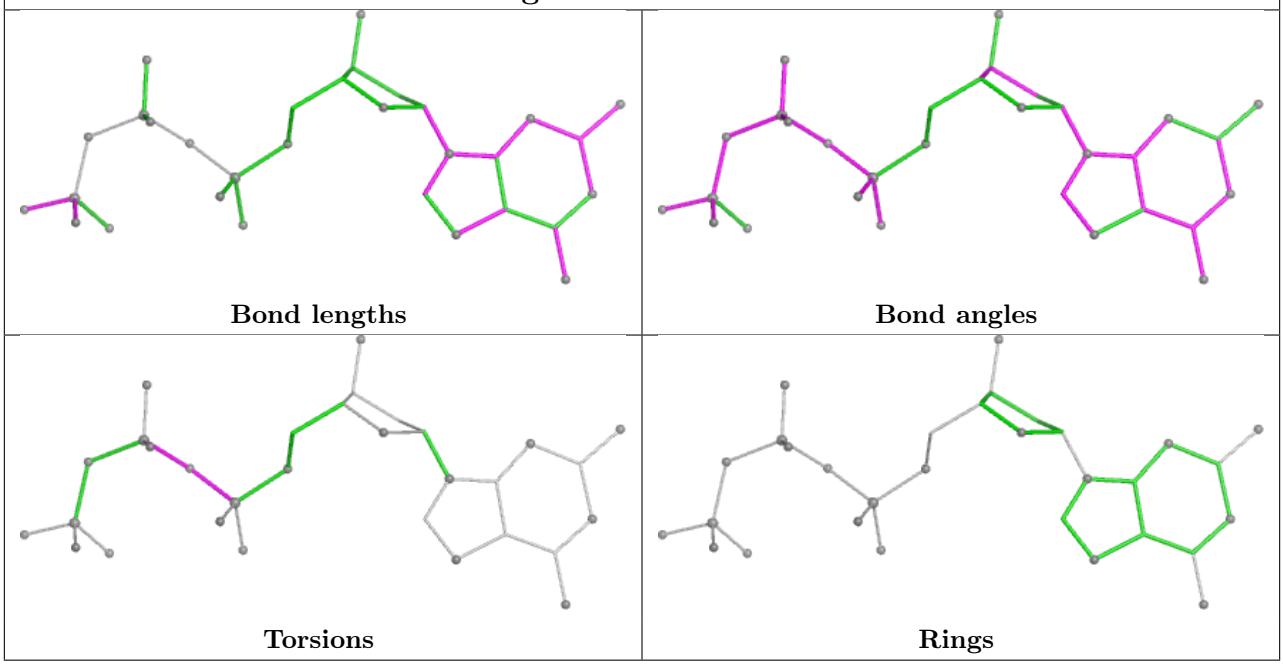
Ligand PC1 A 205



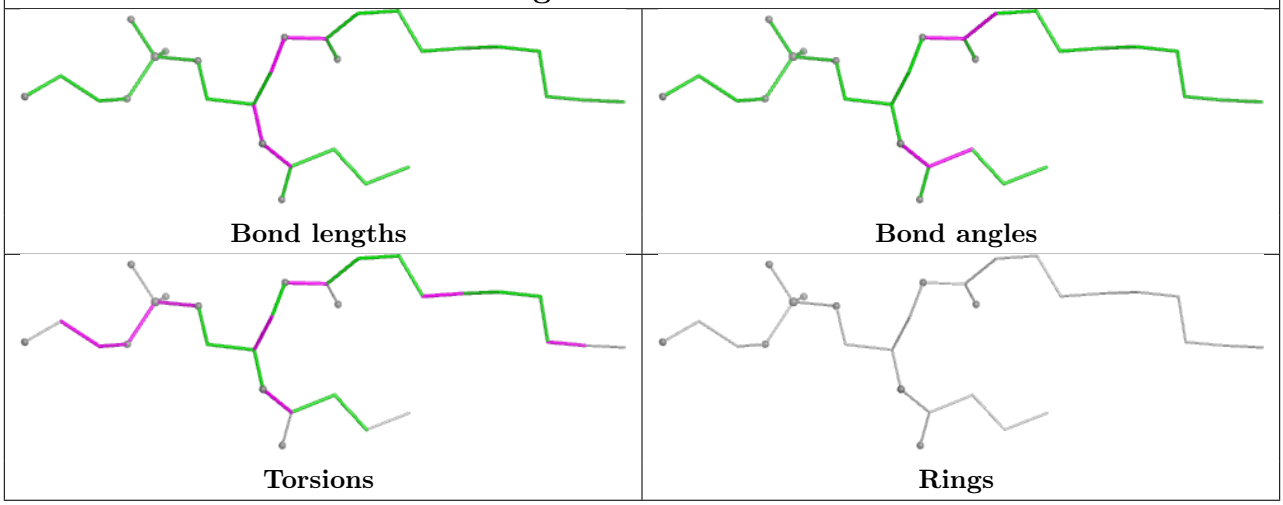
Ligand 3PE e 201



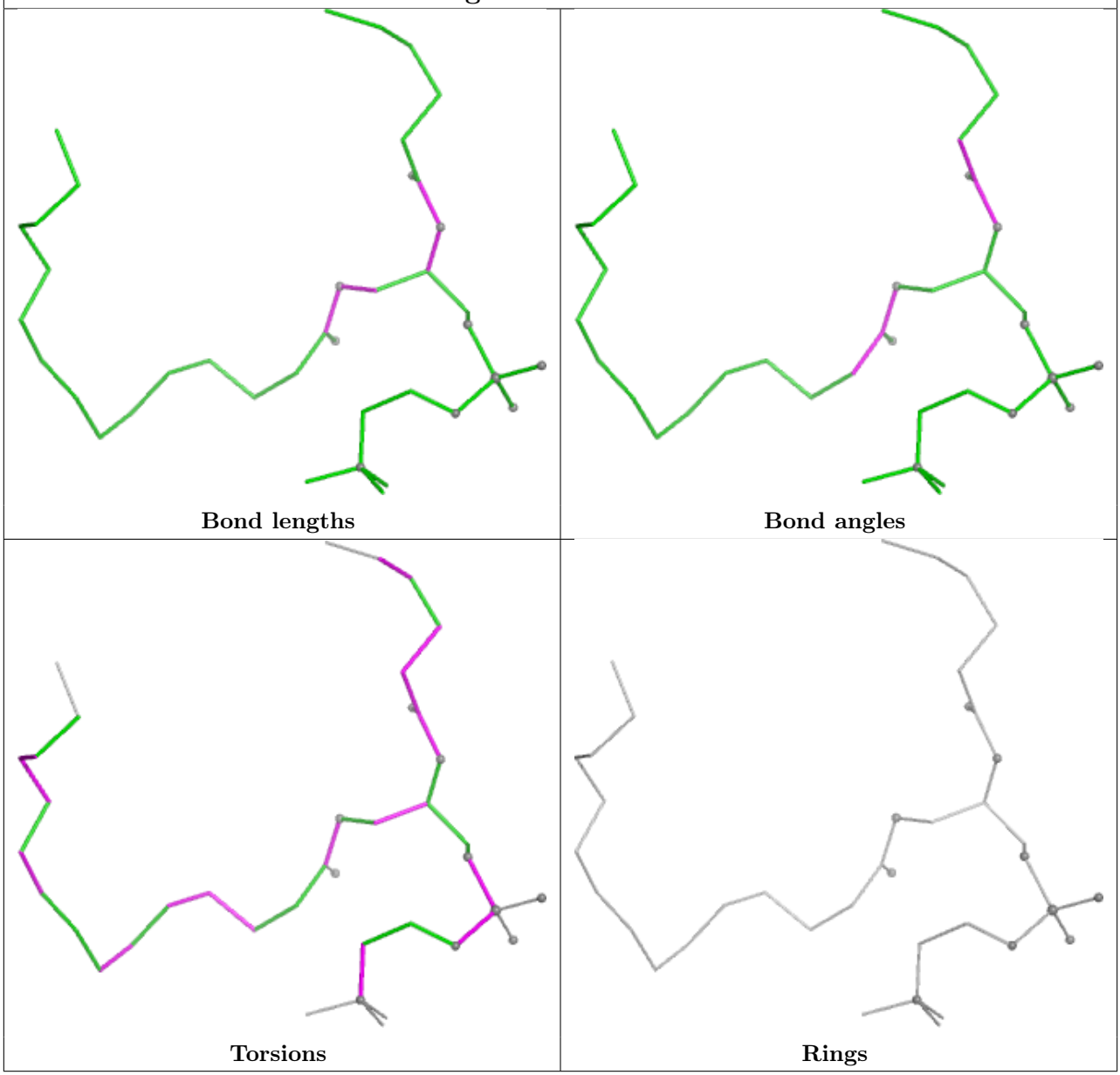
Ligand DGT O 401



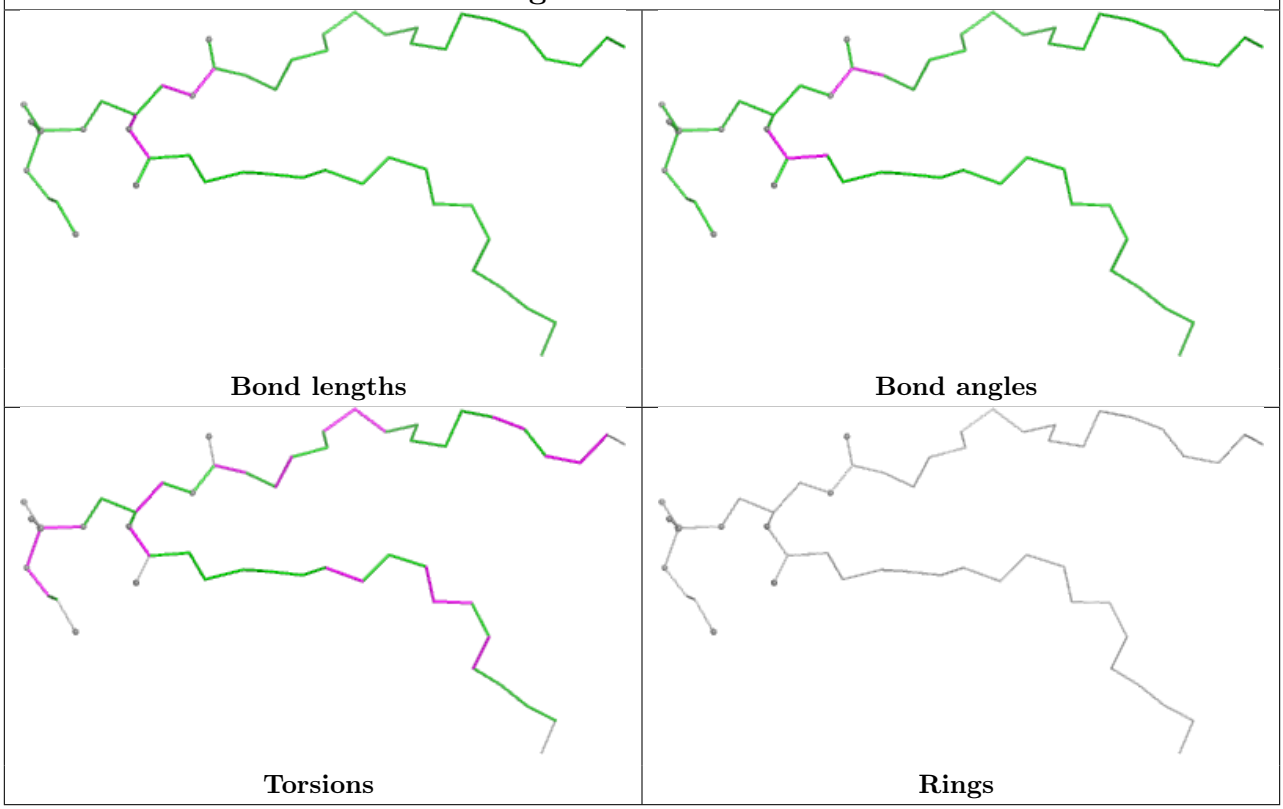
Ligand 3PE J 201



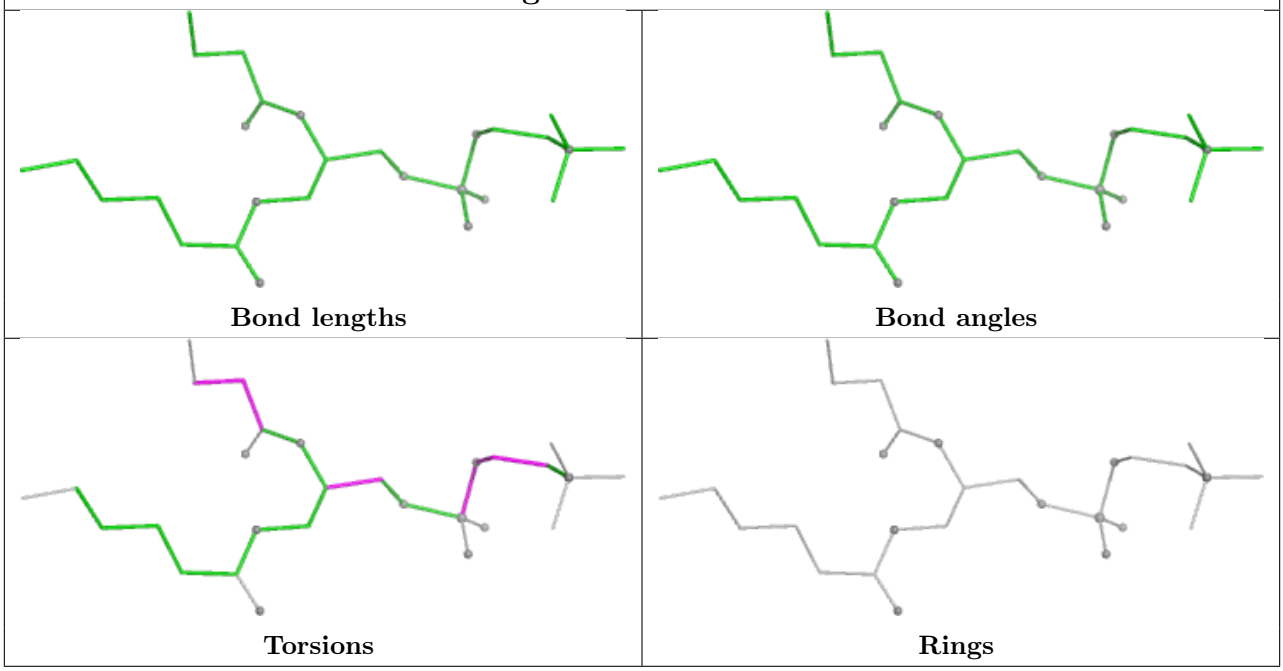
Ligand PC1 e 202



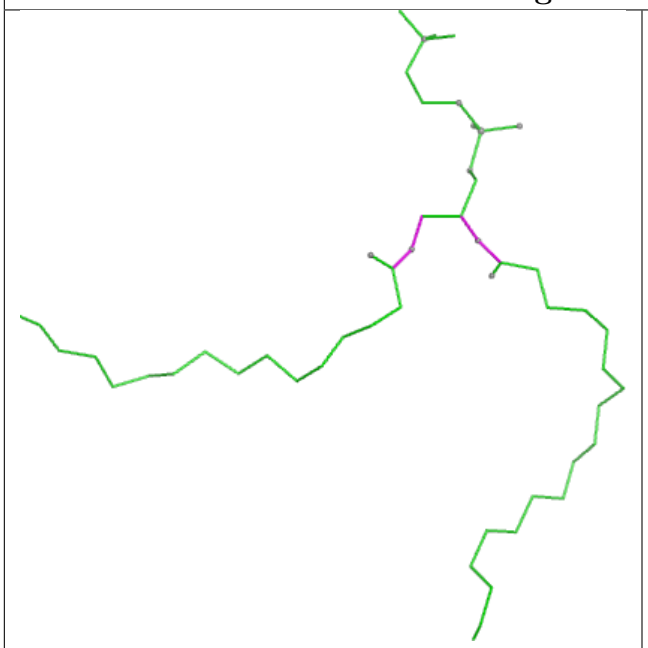
Ligand 3PE A 203



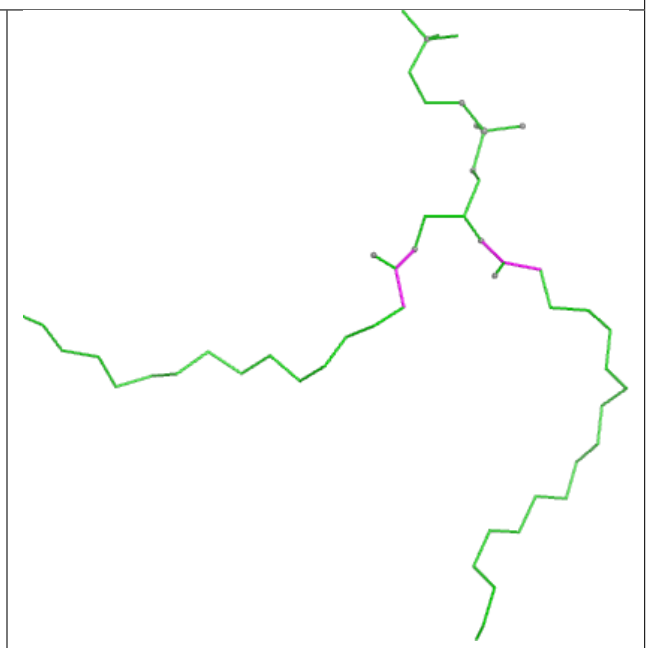
Ligand PLC M 603



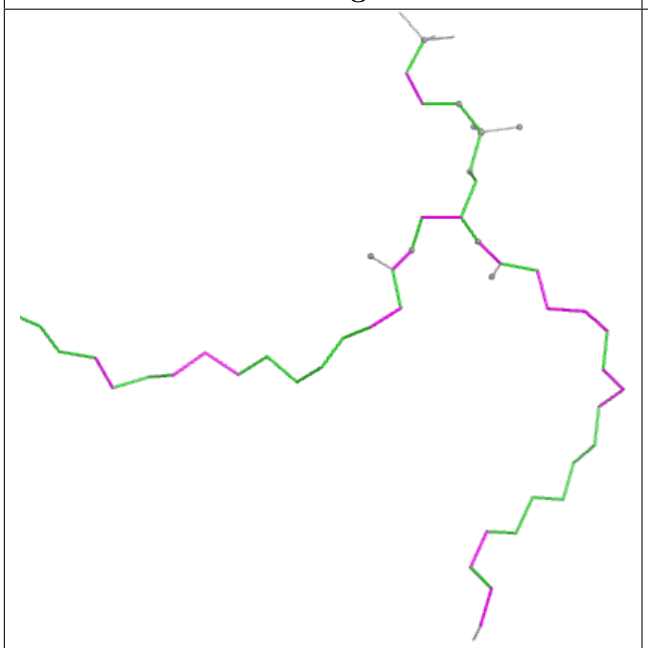
Ligand PC1 I 203



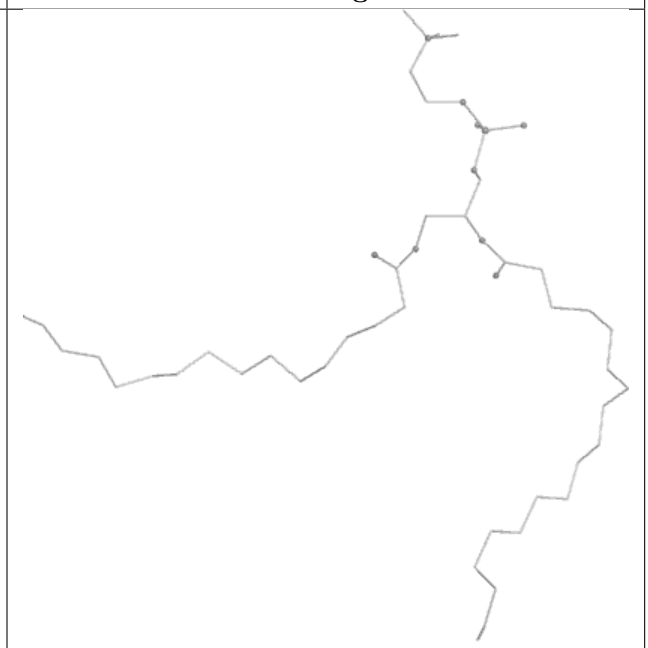
Bond lengths



Bond angles

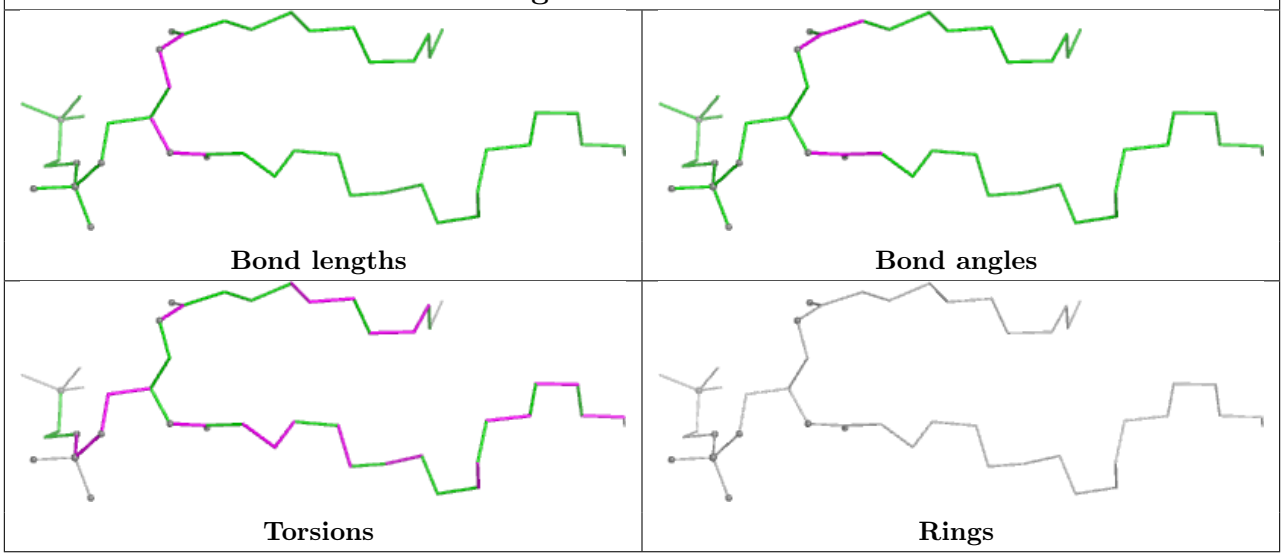


Torsions

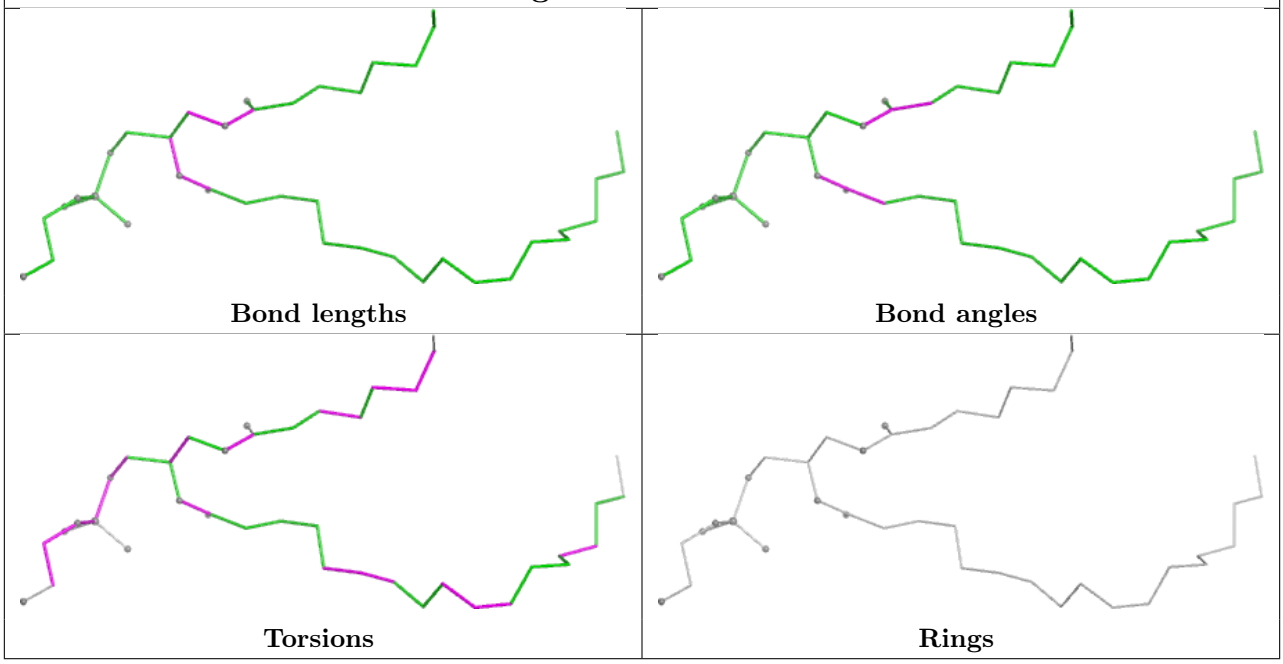


Rings

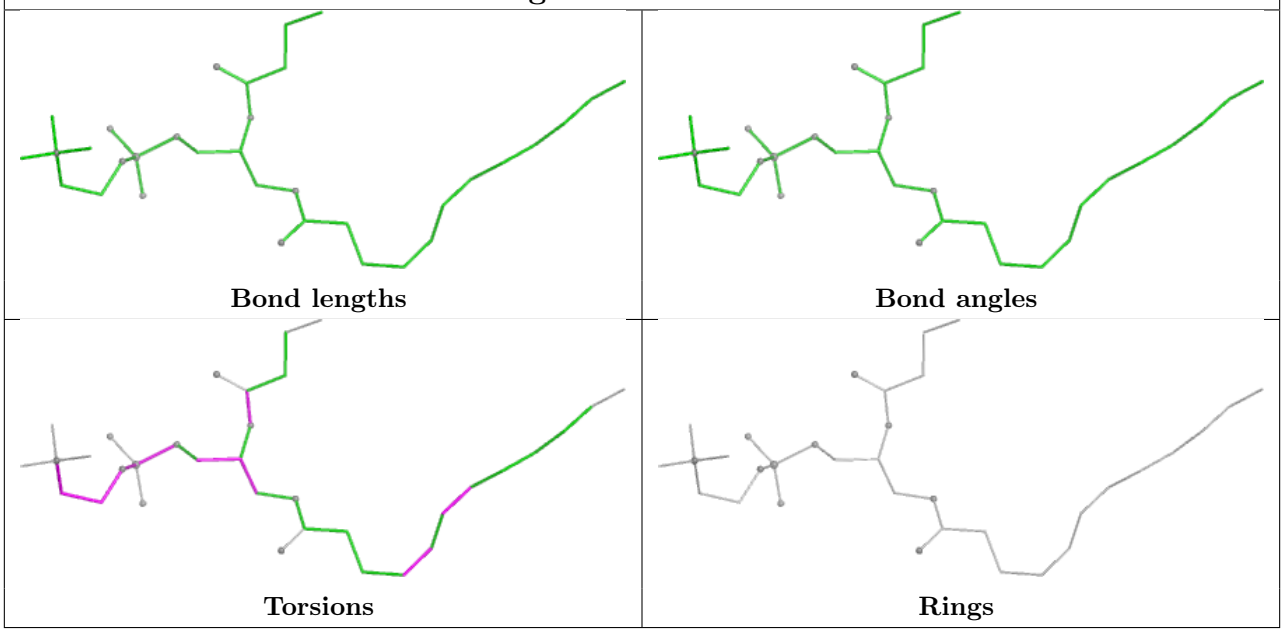
Ligand PC1 h 201



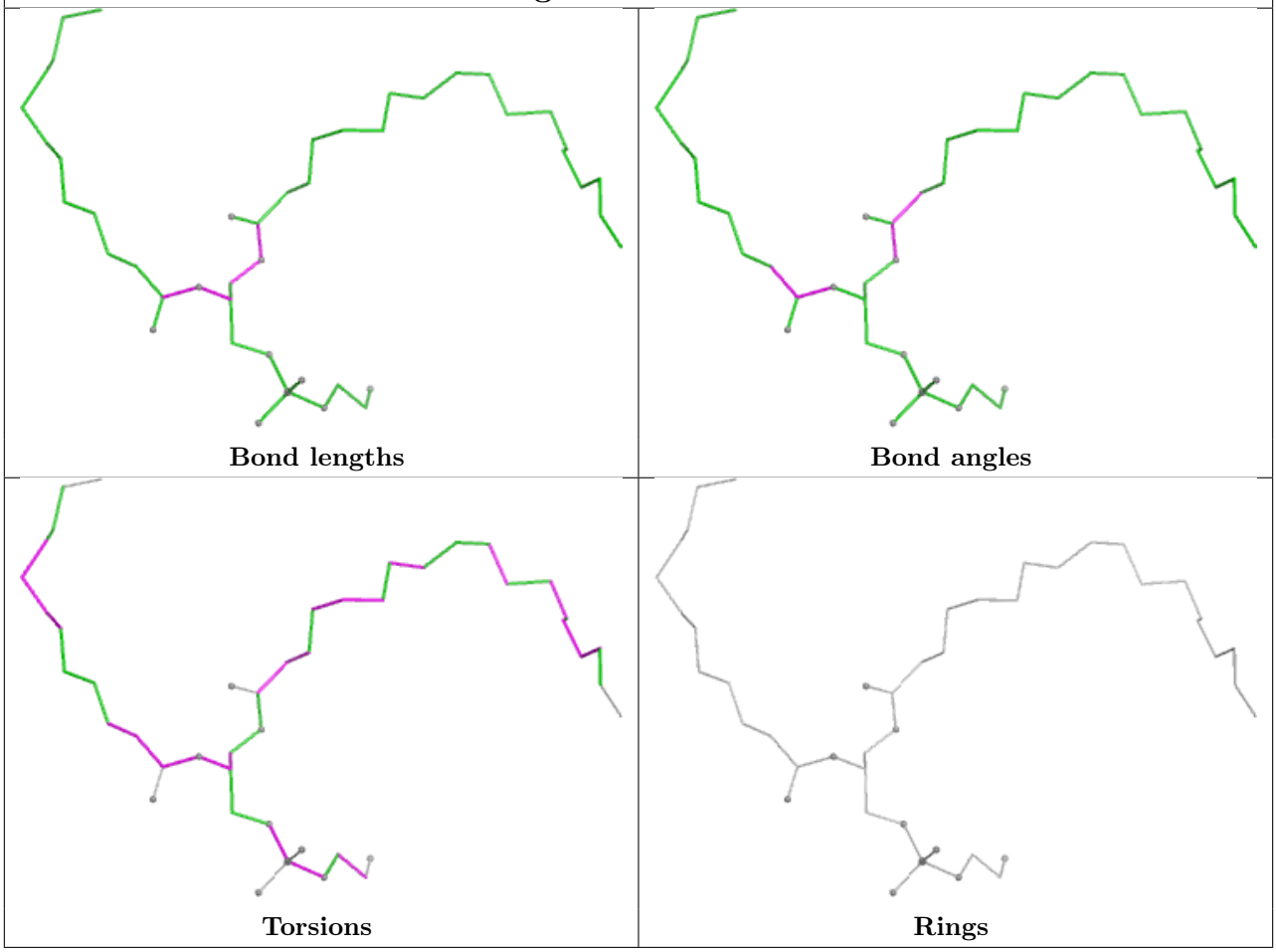
Ligand 3PE Z 201



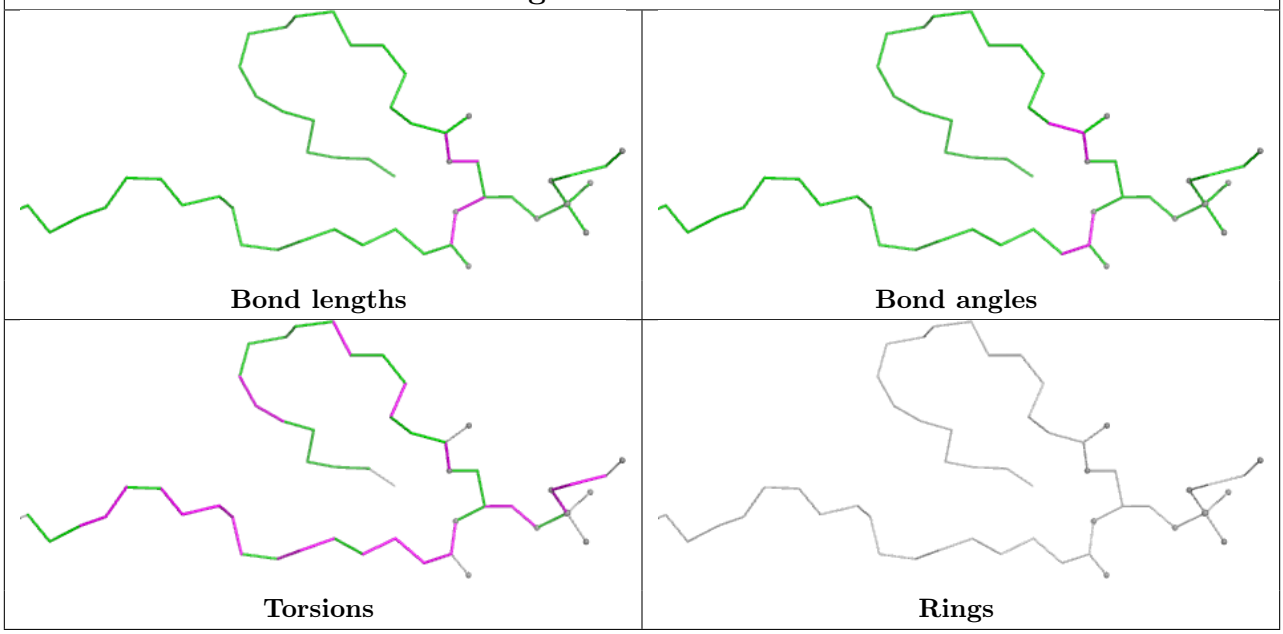
Ligand PLC Z 203



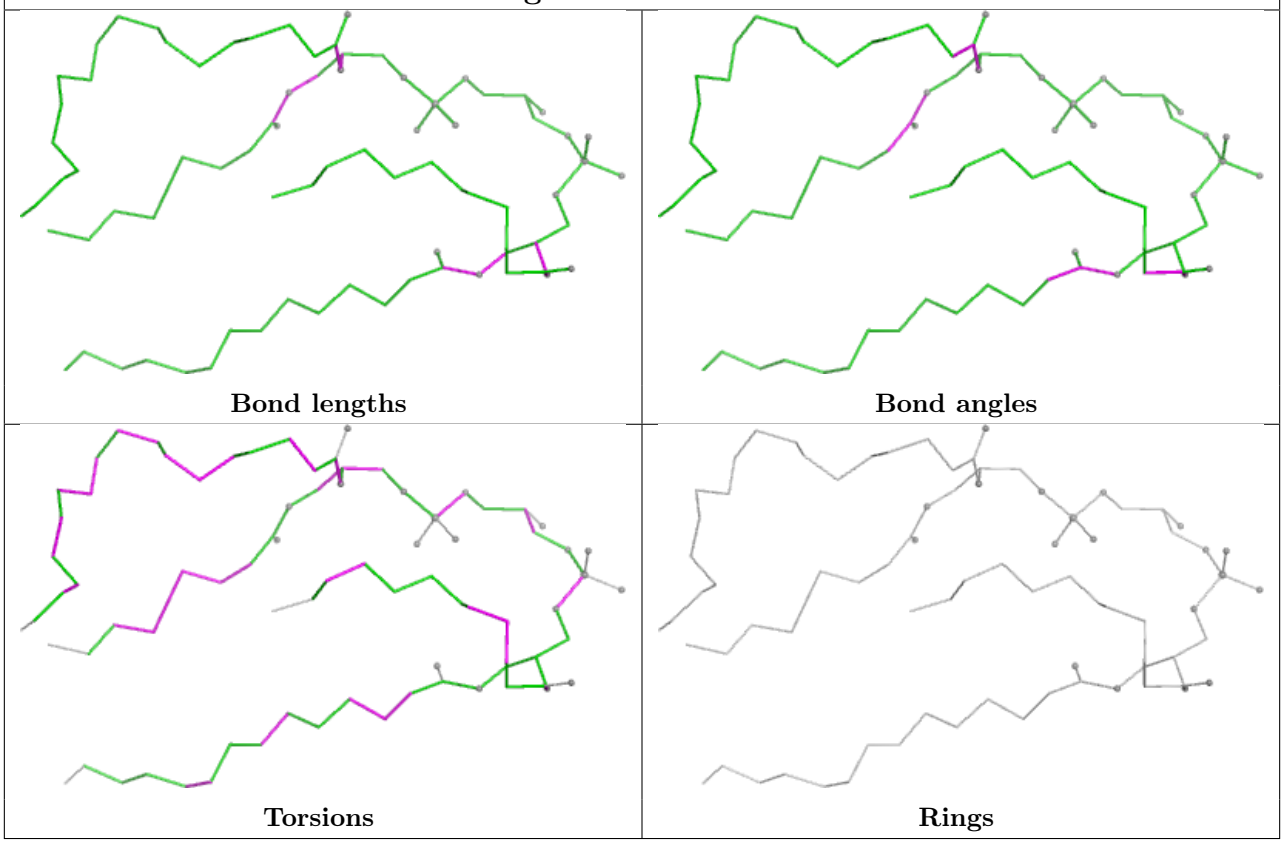
Ligand 3PE i 202



Ligand 3PE N 403



Ligand CDL H 404



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.

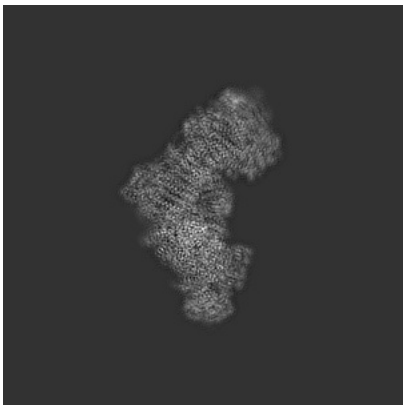
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-18055. These allow visual inspection of the internal detail of the map and identification of artifacts.

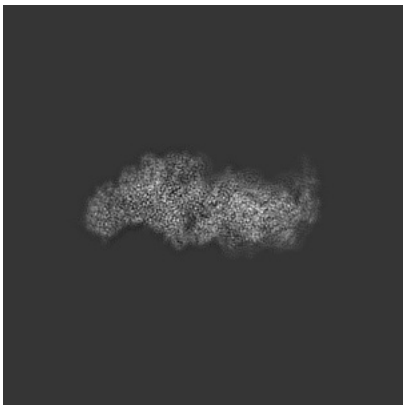
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

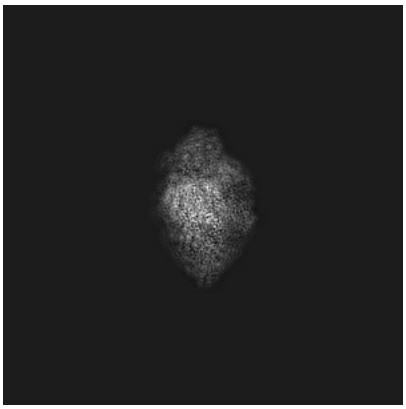
6.1.1 Primary map



X

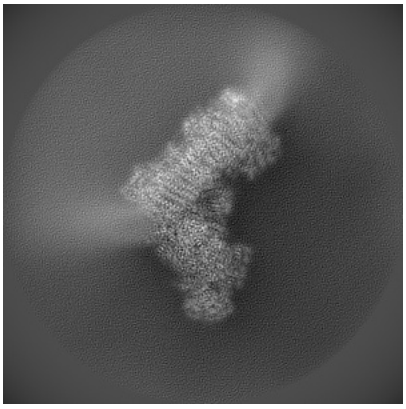


Y

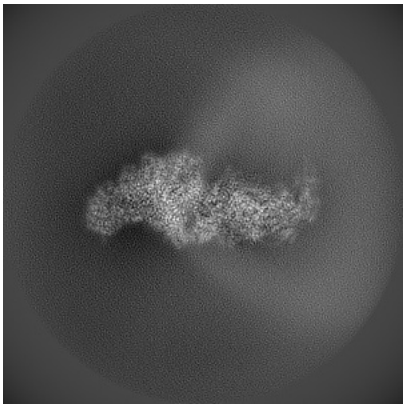


Z

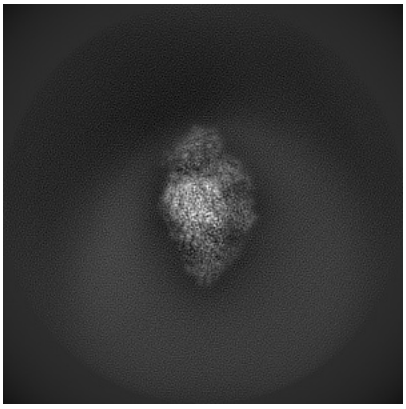
6.1.2 Raw map



X



Y

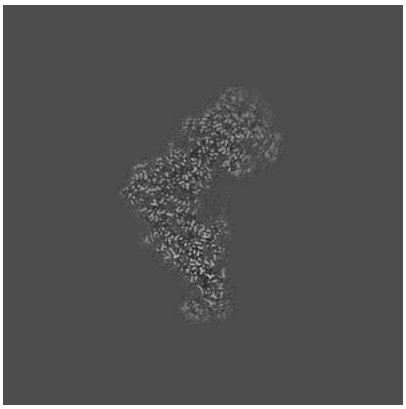


Z

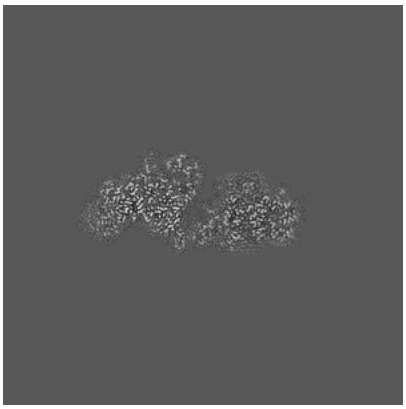
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

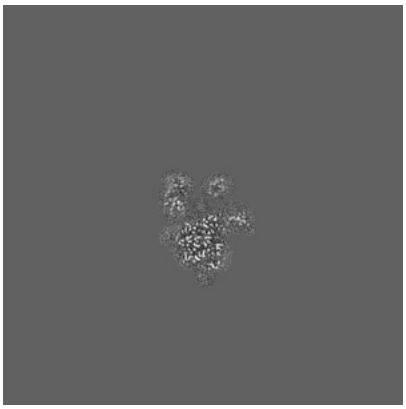
6.2.1 Primary map



X Index: 180

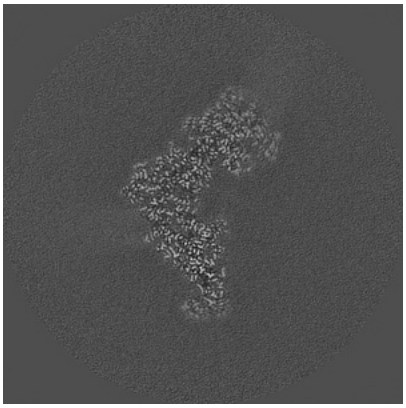


Y Index: 180

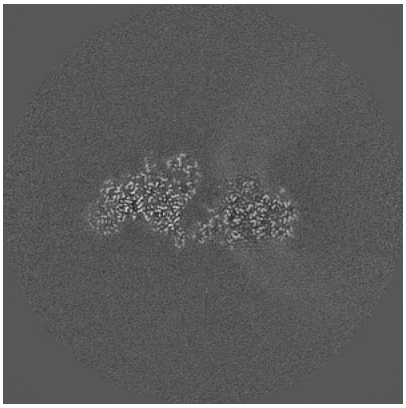


Z Index: 180

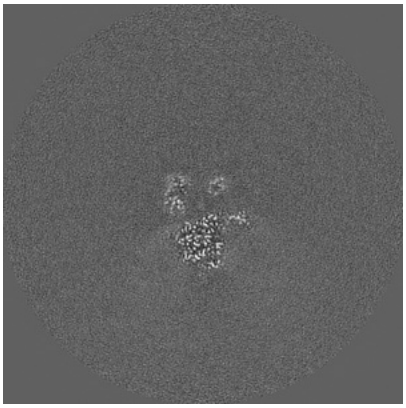
6.2.2 Raw map



X Index: 180



Y Index: 180

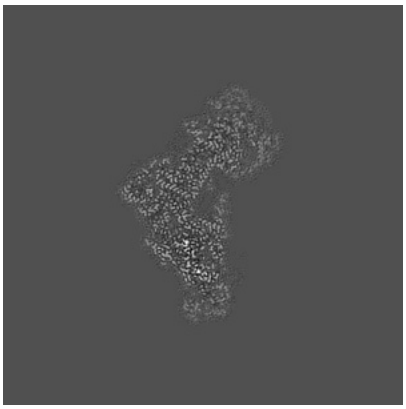


Z Index: 180

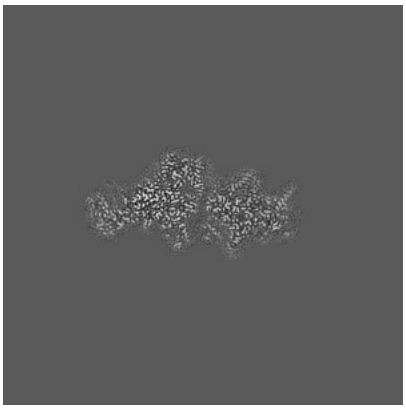
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

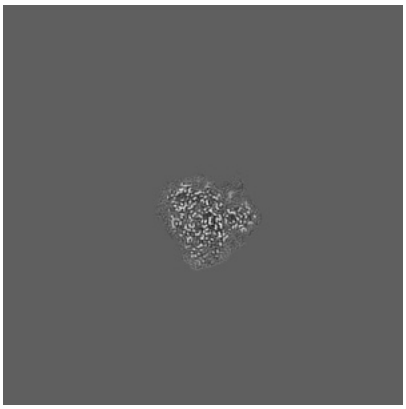
6.3.1 Primary map



X Index: 184

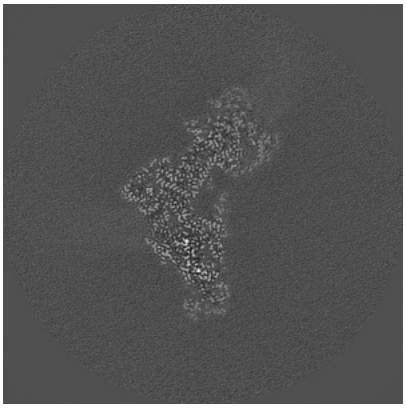


Y Index: 171

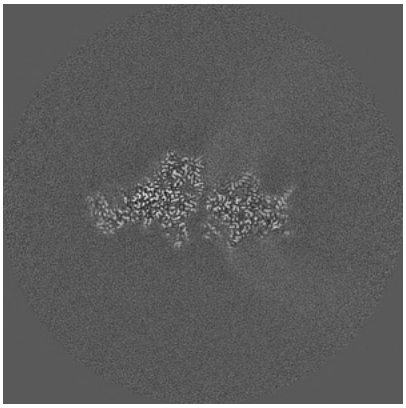


Z Index: 150

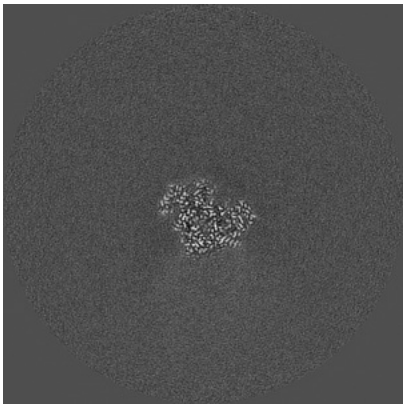
6.3.2 Raw map



X Index: 184



Y Index: 171

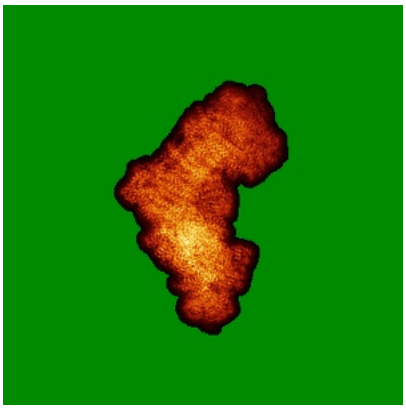


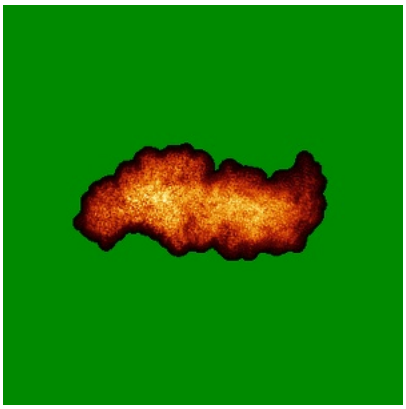
Z Index: 155

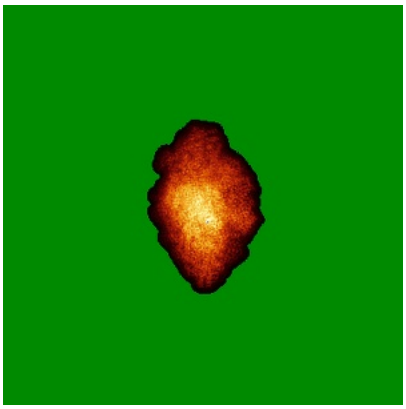
The images above show the largest variance slices of the map in three orthogonal directions.

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

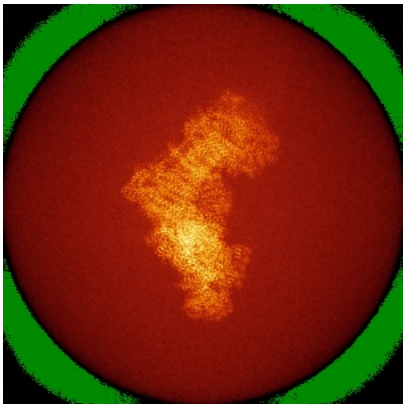
6.4.1 Primary map

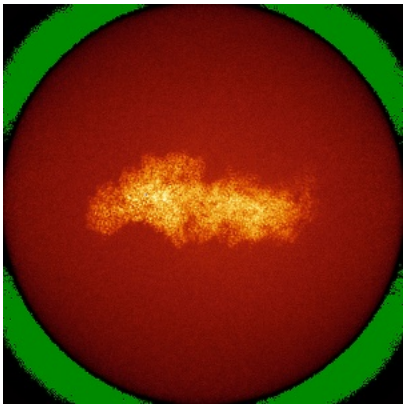

X

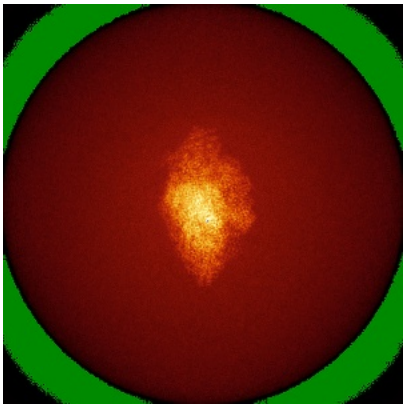

Y


Z

6.4.2 Raw map


X

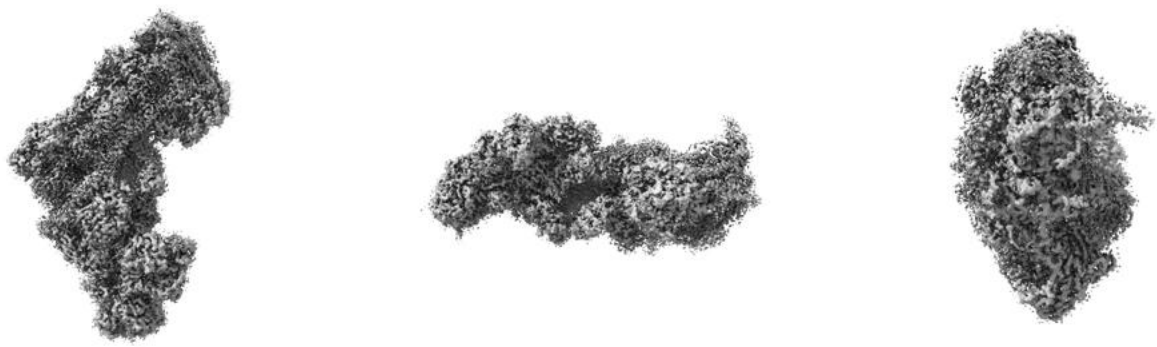

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

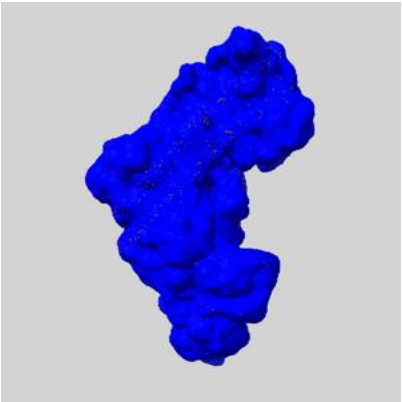
6.6 Mask visualisation (i)

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

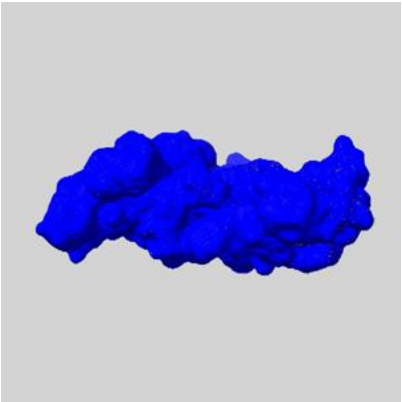
A mask typically either:

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

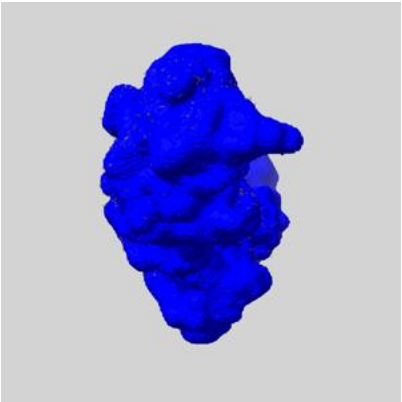
6.6.1 emd_18055_msk_1.map (i)



X



Y

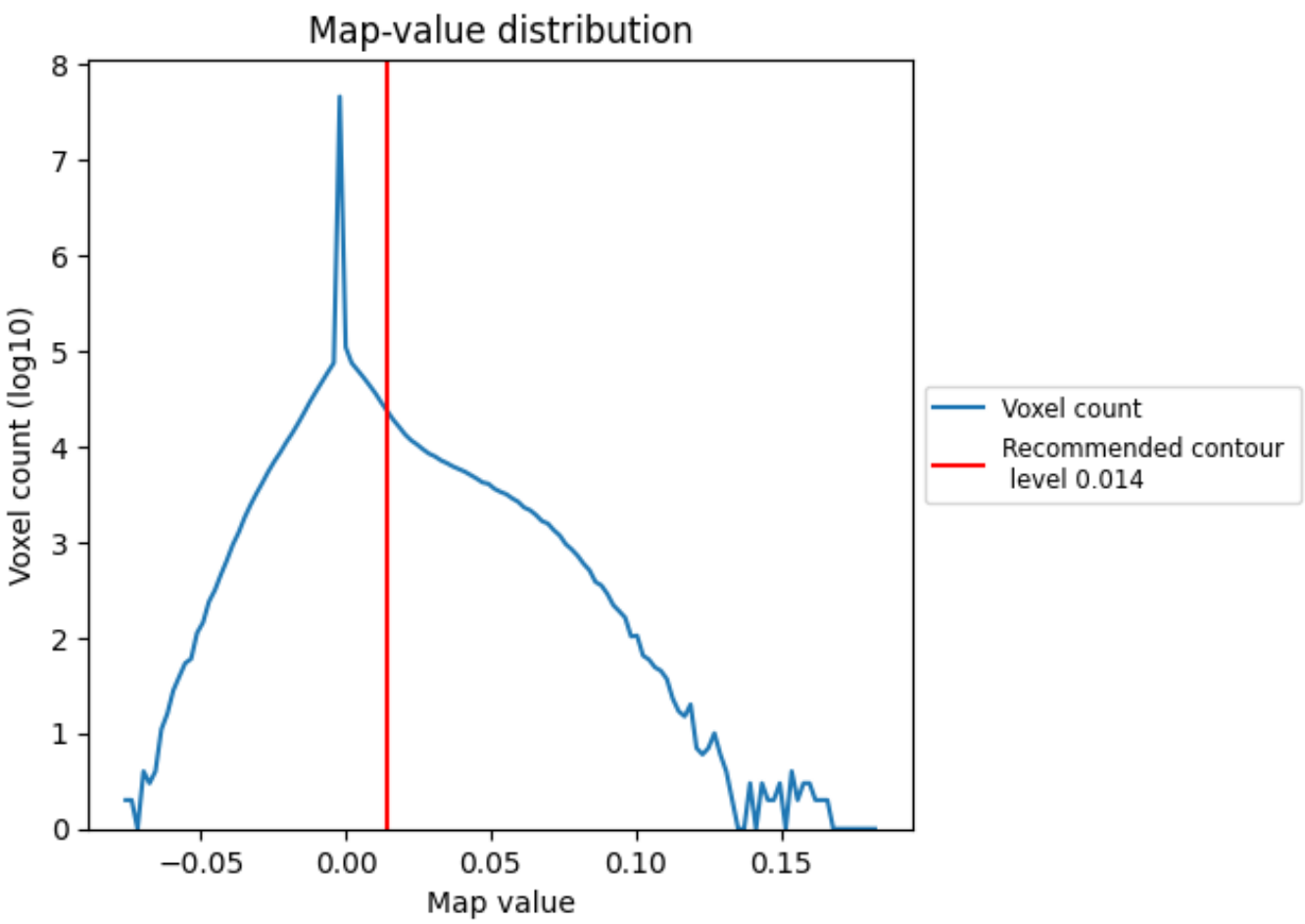


Z

7 Map analysis (i)

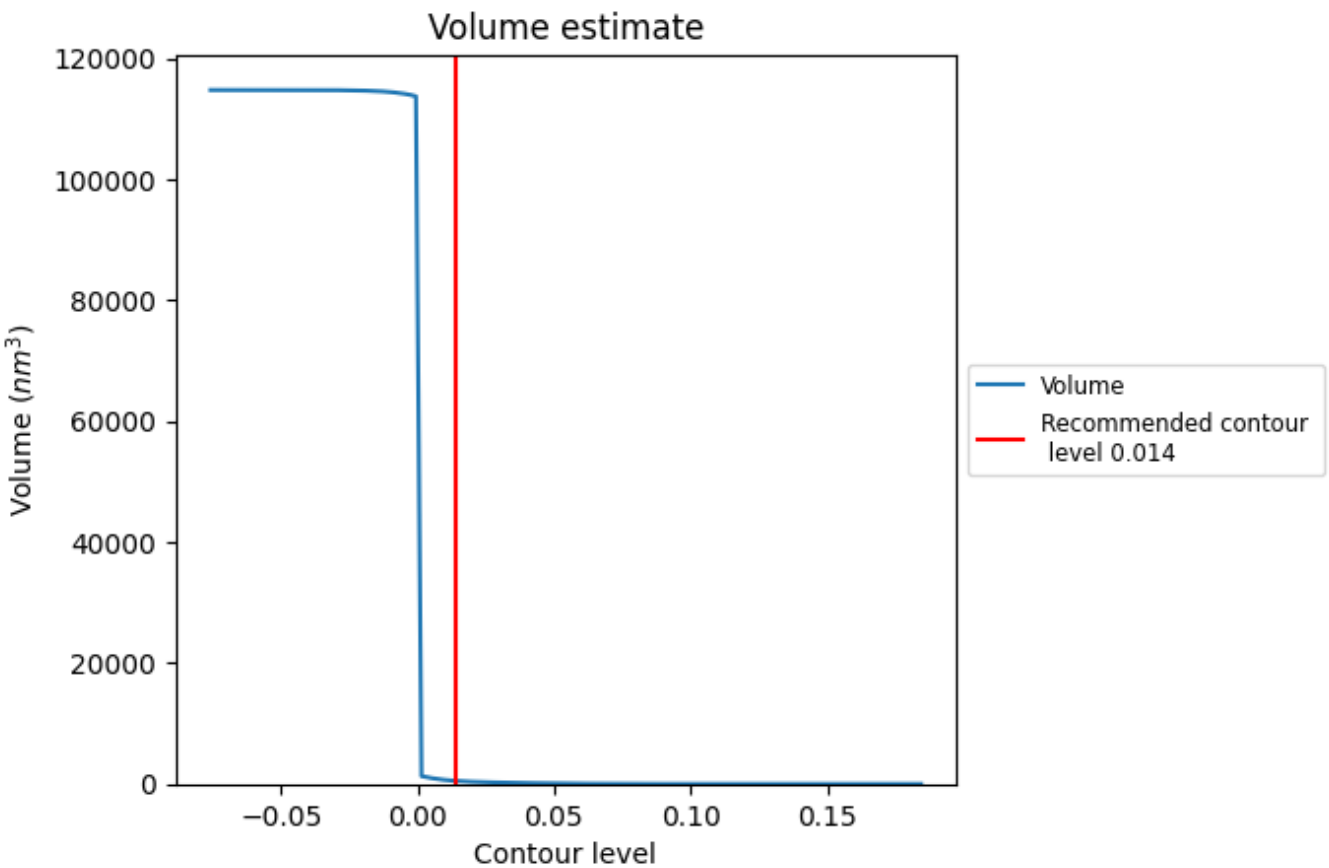
This section contains the results of statistical analysis of the map.

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.

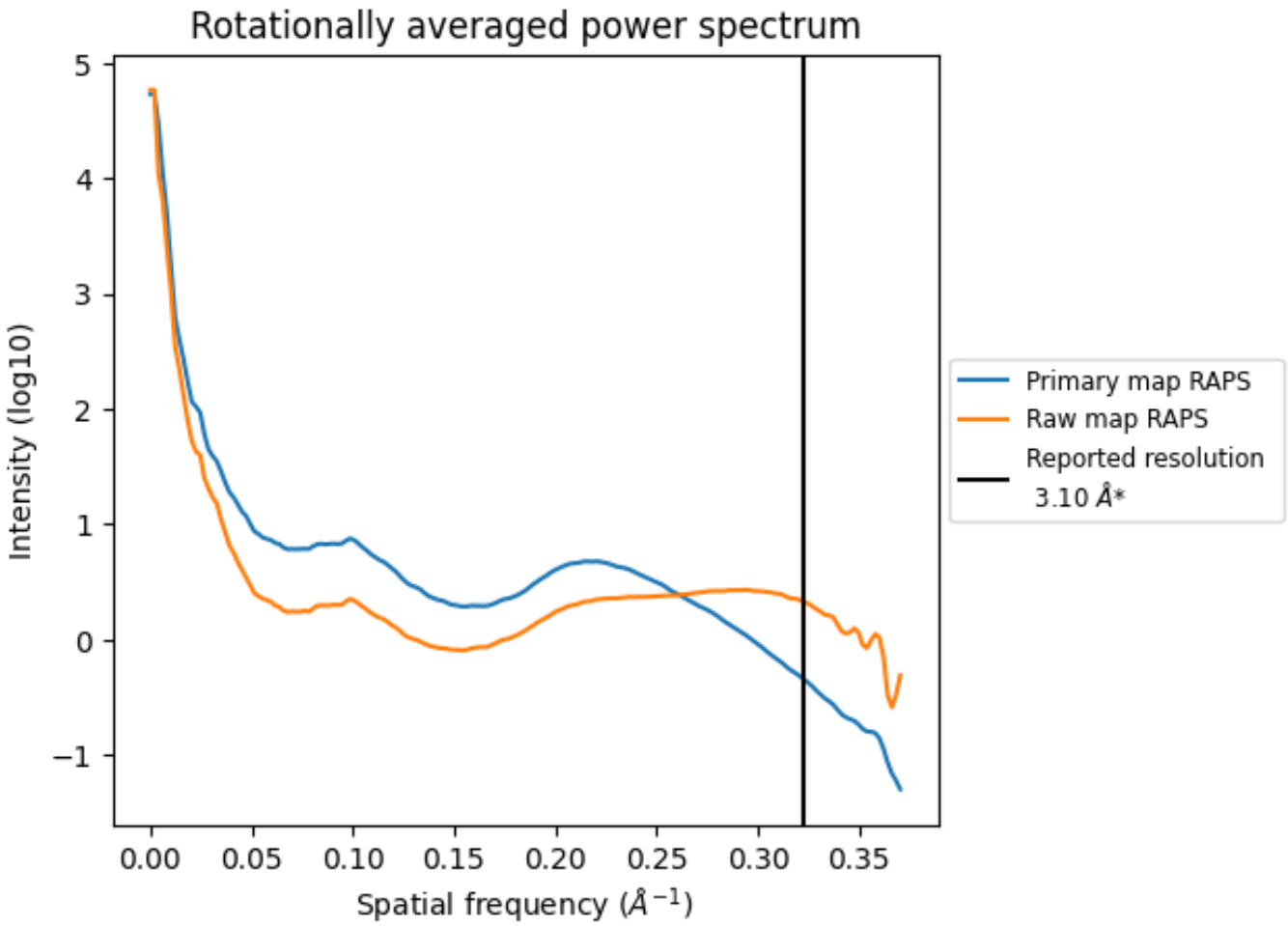
7.2 Volume estimate (i)



The volume at the recommended contour level is 511 nm^3; this corresponds to an approximate mass of 461 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)

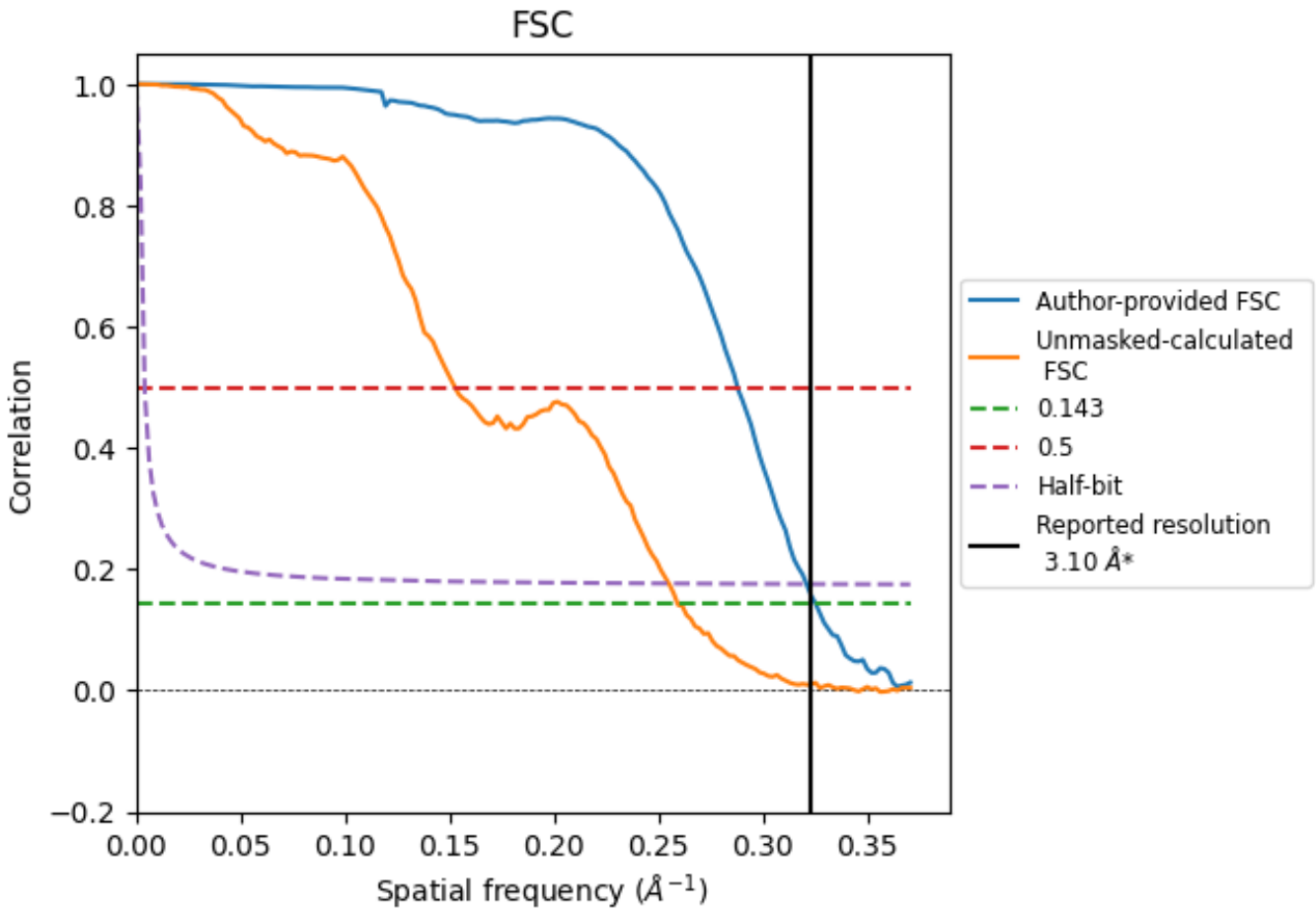


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

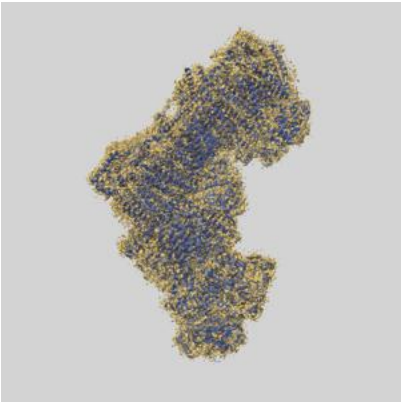
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.48	3.12
Unmasked-calculated*	3.86	6.56	3.92

*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 3.86 differs from the reported value 3.1 by more than 10 %

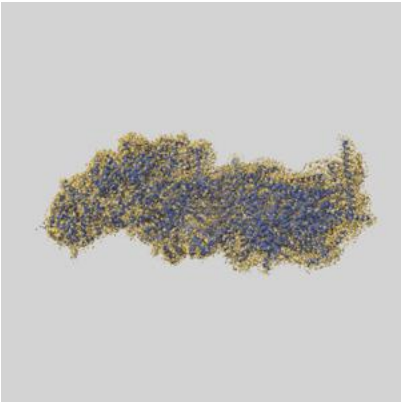
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-18055 and PDB model 8Q0M. Per-residue inclusion information can be found in section 3 on page 23.

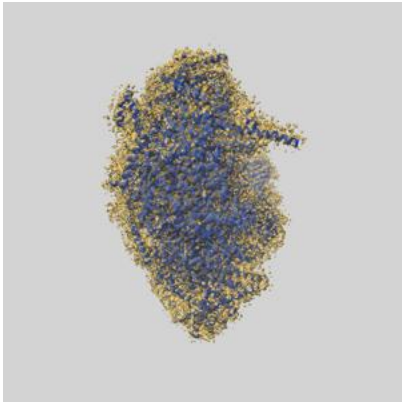
9.1 Map-model overlay (i)



X



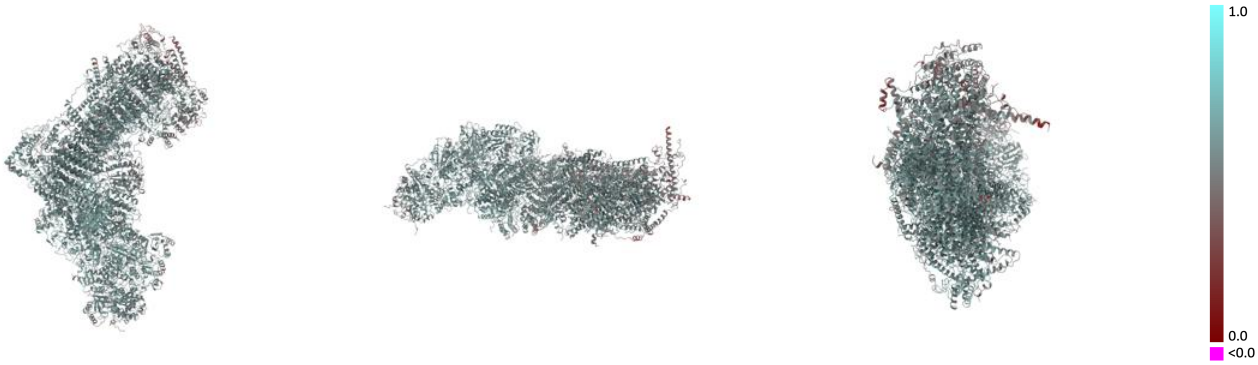
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

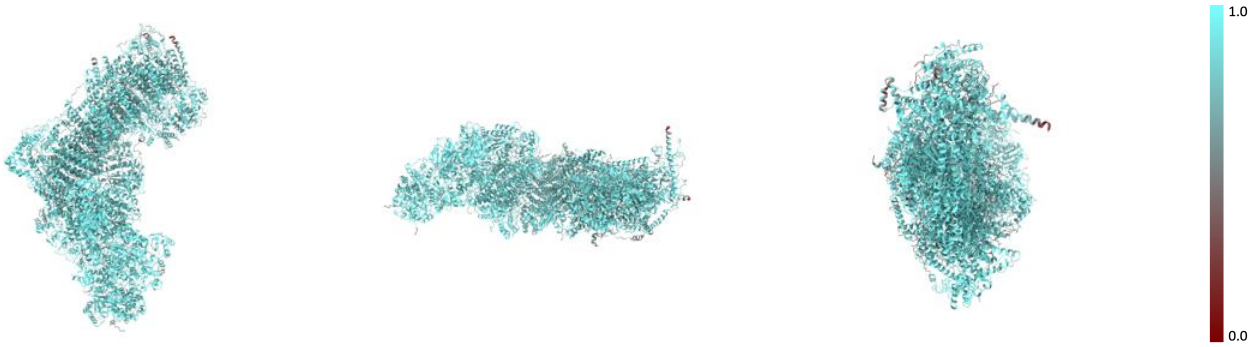
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

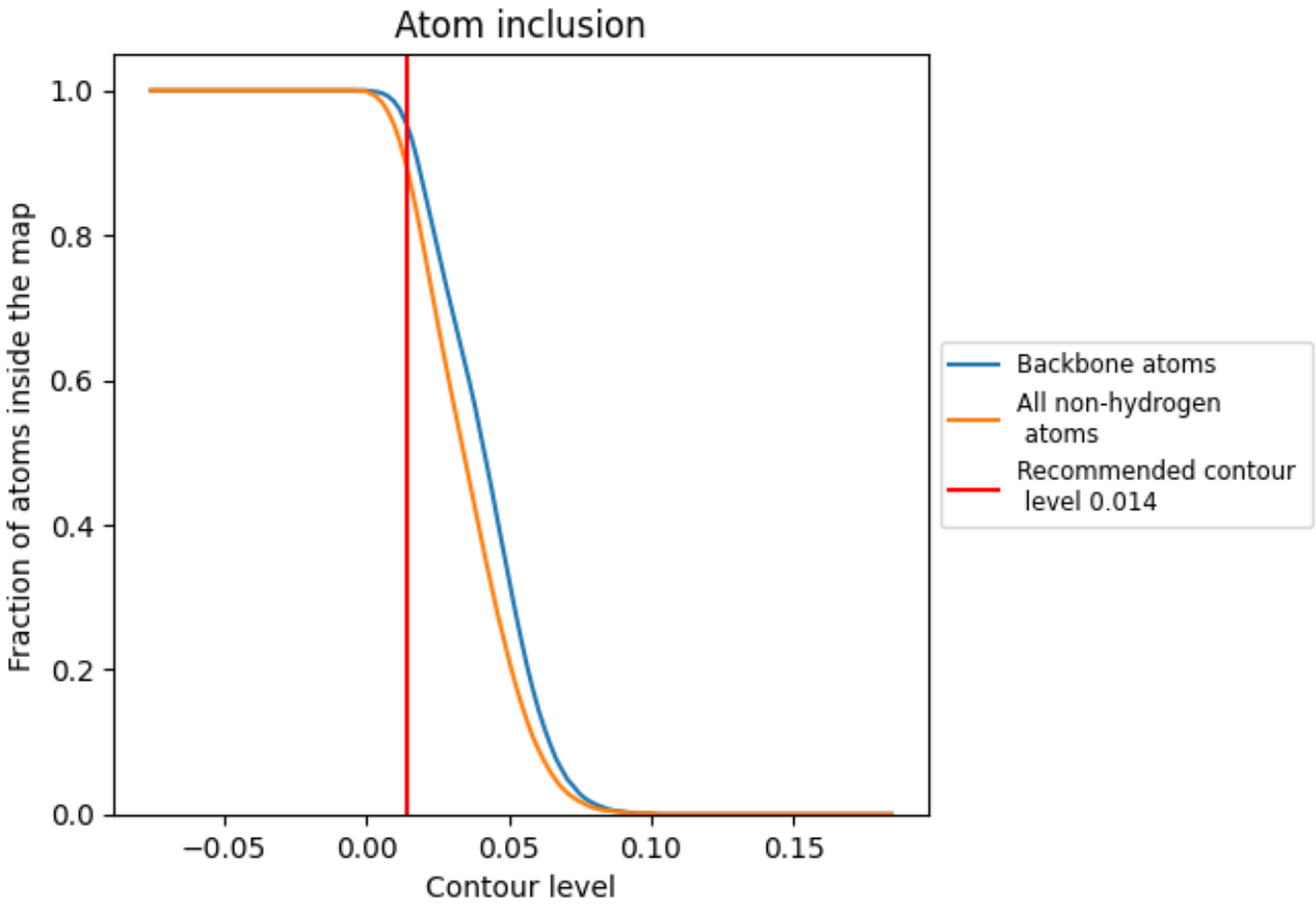
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.5670
A	0.8830	0.5900
B	0.9270	0.6060
C	0.9530	0.6130
D	0.9500	0.6060
E	0.9000	0.5430
F	0.9250	0.5630
G	0.9340	0.5810
H	0.9380	0.6030
I	0.9620	0.6140
J	0.8870	0.5780
K	0.9450	0.6030
L	0.8730	0.5580
M	0.9470	0.6020
N	0.9350	0.6010
O	0.8970	0.5510
P	0.9140	0.5840
Q	0.9030	0.5840
R	0.8400	0.5610
S	0.8650	0.5180
T	0.8460	0.5100
U	0.8050	0.4910
V	0.9050	0.5700
W	0.9220	0.5830
X	0.9160	0.5770
Y	0.8250	0.5550
Z	0.8920	0.5710
a	0.9510	0.5950
b	0.8750	0.5620
c	0.7800	0.5130
d	0.8940	0.5730
e	0.8690	0.5580
f	0.7430	0.5130
g	0.8440	0.5440
h	0.8950	0.5760

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.7690	0.4730
j	0.7770	0.4610
k	0.7350	0.4410
l	0.8780	0.5310
m	0.8440	0.5490
n	0.8730	0.5120
o	0.7620	0.4490
p	0.8550	0.5320
q	0.9100	0.5910
r	0.9050	0.5800
s	0.7220	0.4720