wwPDB EM Validation Summary Report (i)

Aug 24, 2026 – 09:15 am BST

PDB ID	:	7R42 / pdb_00007r42
EMDB ID	:	EMD-14256
Title	:	Bovine complex I in the presence of IM1761092, active class ii (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.30 Å(reported)

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

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

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

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

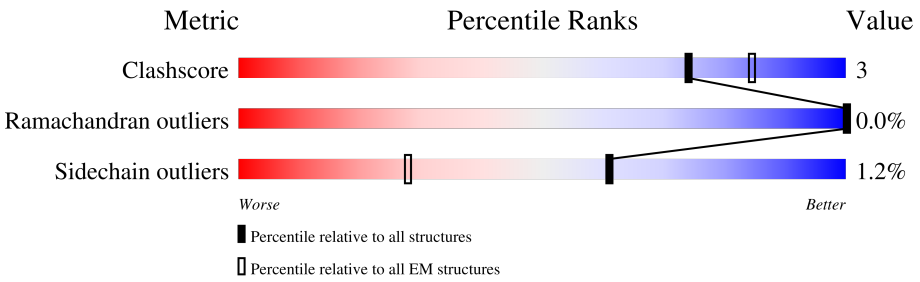
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

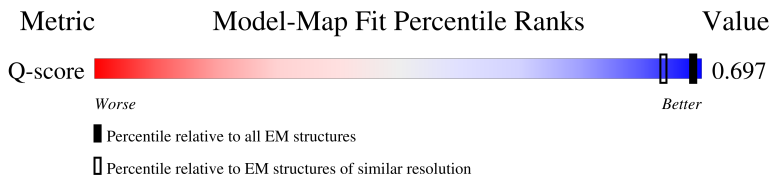
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	95% 5%
2	B	216	67% 28%
3	C	266	74% 22%
4	D	463	83% 10% 7%

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Mol	Chain	Length	Quality of chain
5	E	249	74% 12% 14%
6	F	464	84% 8% 7%
7	G	727	89% 6% 5%
8	H	318	90% 10%
9	I	212	78% 5% 17%
10	J	175	89% 10%
11	K	98	89% 11%
12	L	606	88% 12%
13	M	459	91% 9%
14	N	347	92% 8%
15	O	343	82% 11% 7%
16	P	380	82% 7% 10%
17	Q	175	69% 29%
18	R	124	72% 23%
19	S	99	5% 76% 11% 13%
20	T	156	11% 37% 12% 51%
20	U	156	51% 45%
21	V	116	91% 6%
22	W	128	84% 5% 11%
23	X	172	87% 12%
24	Y	141	7% 96%
25	Z	144	85% 13%
26	a	70	91% 9%
27	b	84	6% 86% 13%
28	c	76	54% 8% 37%

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Mol	Chain	Length	Quality of chain
29	d	120	88% 6% 6%
30	e	106	84% 7% 8%
31	f	57	11% 84% 7% 9%
32	g	154	59% 5% 36%
33	h	189	71% 27%
34	i	127	9% 74% 7% 18%
35	j	108	56% 6% 38%
36	k	98	78% 18%
37	l	186	80% 17%
38	m	129	87% 12%
39	n	179	93%
40	o	137	81% 7% 12%
41	p	176	93%
42	q	145	95% 5%
43	r	113	77% 6% 17%
44	s	109	35% 5% 60%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 69480 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	207	1721	1111	296	311	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	213	1655	1057	277	311	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	431	3319	2091	593	615	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	174	1337	902	189	234	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	4780	3178	735	824	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	341	2747	1777	486	479	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	125	1016	641	181	191	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	95	730	448	137	142	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	86	691	434	129	126	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	76	612	393	90	124	5	0	0
20	U	86	693	447	102	139	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	114	923	597	156	167	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	114	971	622	180	165	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	651	425	109	115	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	48	405	268	69	68	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	113	945	619	161	162	3	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	97	819	518	156	139	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	52	451	296	79	75	1	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	98	824	529	137	154	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	104	898	590	155	152	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	67	580	381	95	103	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	80	644	421	108	113	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	155	1304	844	213	239	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	127	1061	681	187	193	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	172	1492	955	273	257	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	120	1035	645	199	183	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	171	1443	904	266	265	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	1209	778	216	210	5	0	0

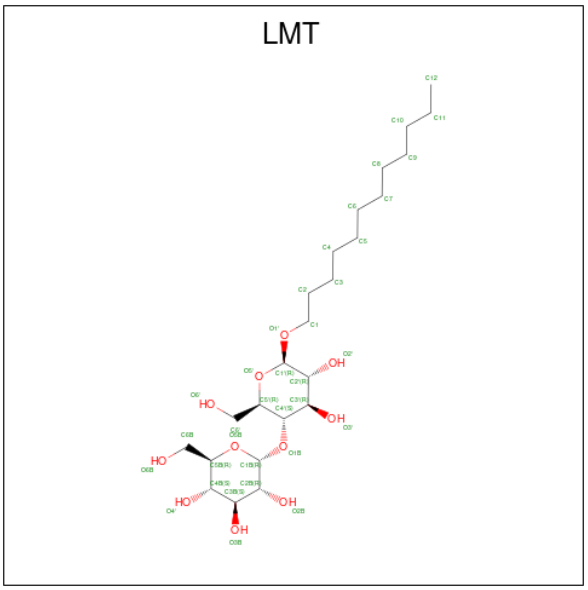
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	94	767	485	143	136	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	44	371	233	66	71	1	0	0

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



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

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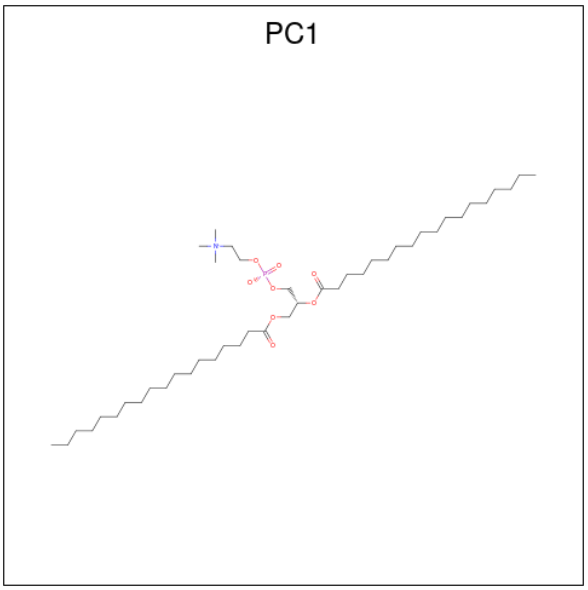
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	M	1	35	24	11	0
45	M	1	35	24	11	0
45	M	1	35	24	11	0
45	Y	1	35	24	11	0
45	Y	1	35	24	11	0
45	Y	1	35	24	11	0
45	b	1	35	24	11	0
45	h	1	35	24	11	0
45	j	1	35	24	11	0
45	l	1	35	24	11	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	21	11	1	8	1	0

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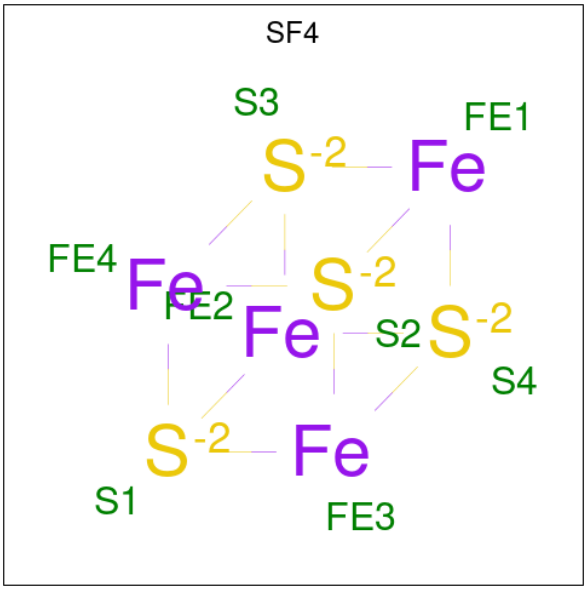
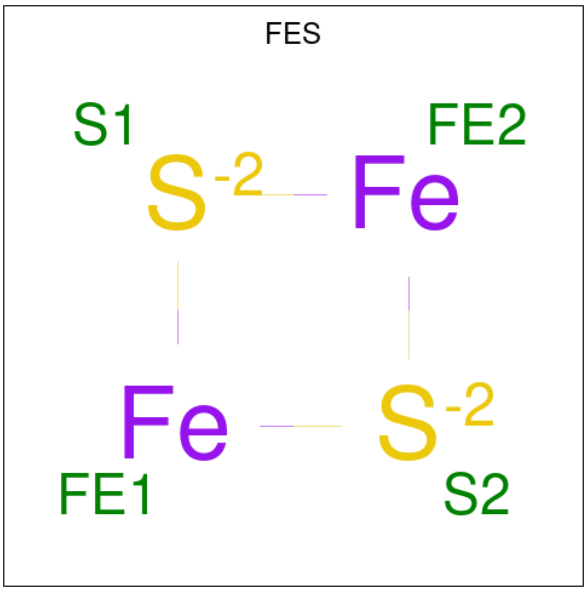
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	B	1	54	44	1	8	1	0
46	B	1	35	25	1	8	1	0
46	L	1	49	39	1	8	1	0

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



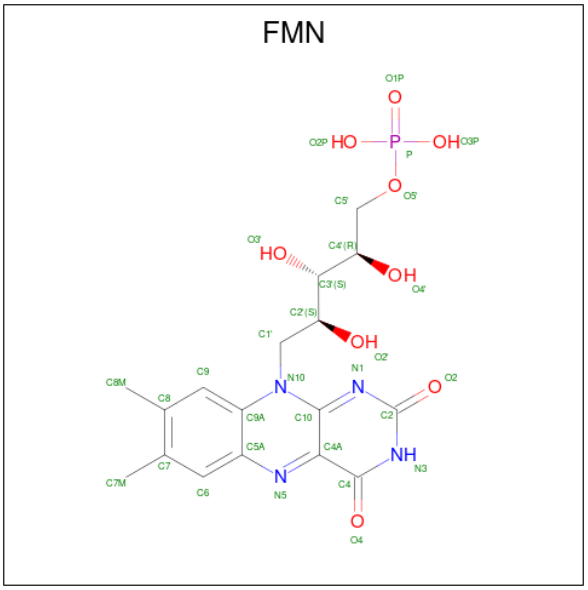
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0
47	I	1	8	4	4	0
47	I	1	8	4	4	0

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



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

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

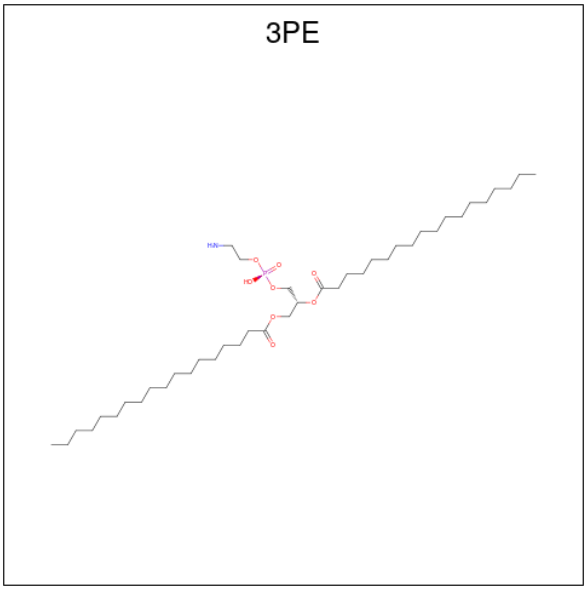


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	F	1	31	17	4	9	1	0

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 51 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	
51	H	1	44	34	1	8	1	0
			Total	C	N	O	P	
51	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
51	H	1	34	24	1	8	1	0
			Total	C	N	O	P	
51	L	1	49	39	1	8	1	0
			Total	C	N	O	P	
51	L	1	45	35	1	8	1	0
			Total	C	N	O	P	
51	M	1	46	36	1	8	1	0
			Total	C	N	O	P	
51	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
51	N	1	41	31	1	8	1	0
			Total	C	N	O	P	
51	N	1	29	19	1	8	1	0
			Total	C	N	O	P	
51	P	1	37	27	1	8	1	0

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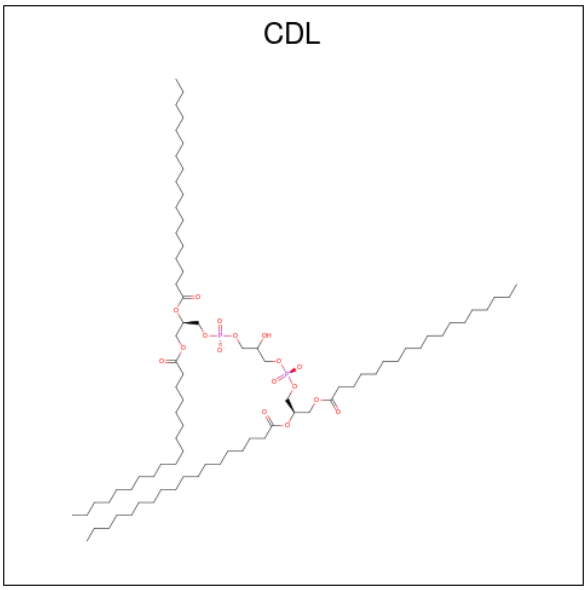
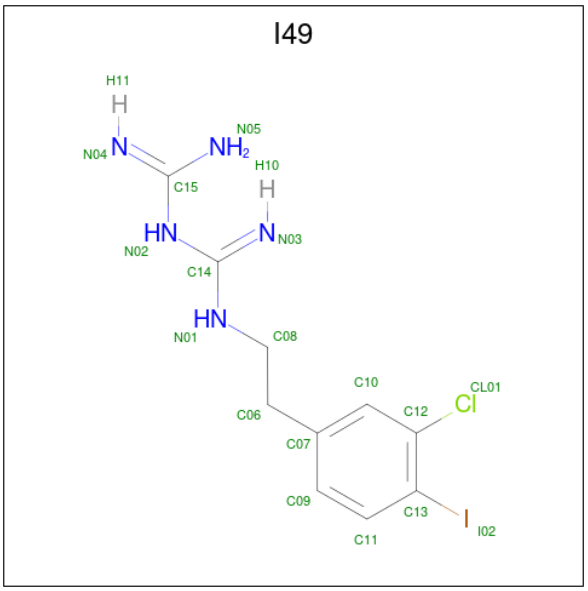
Mol	Chain	Residues	Atoms					AltConf
51	X	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



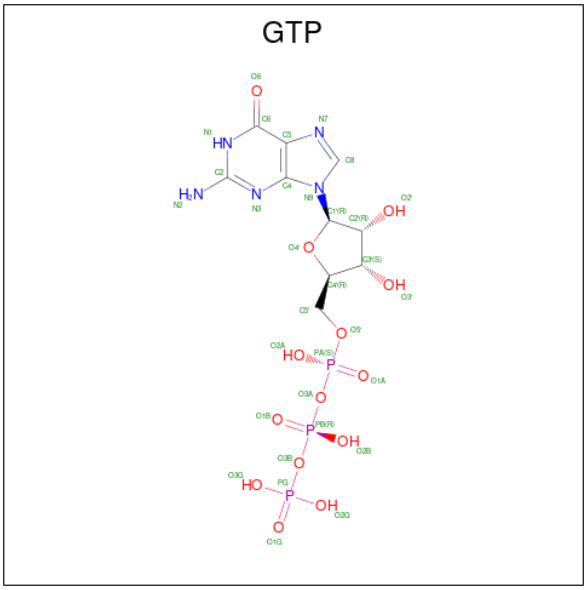
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			62	43	17	2	
52	K	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	r	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (CCD ID: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



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

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

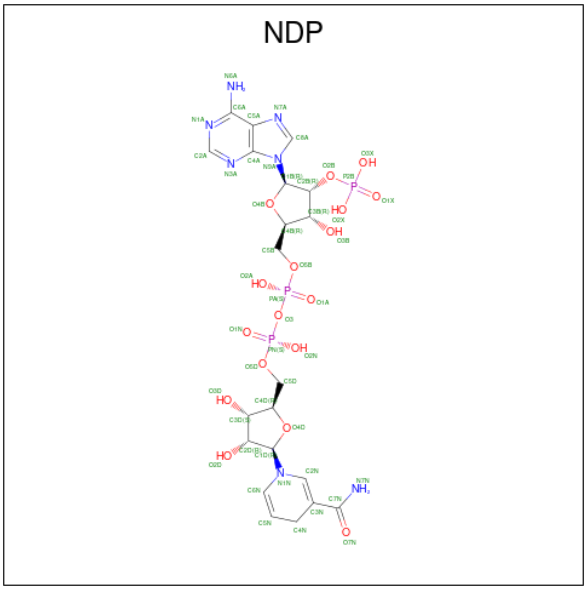


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	O	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

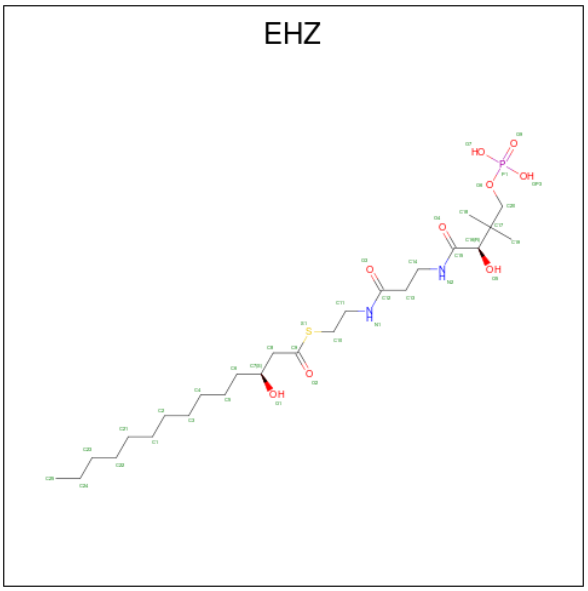


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	P	1	48	21	7	17	3	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

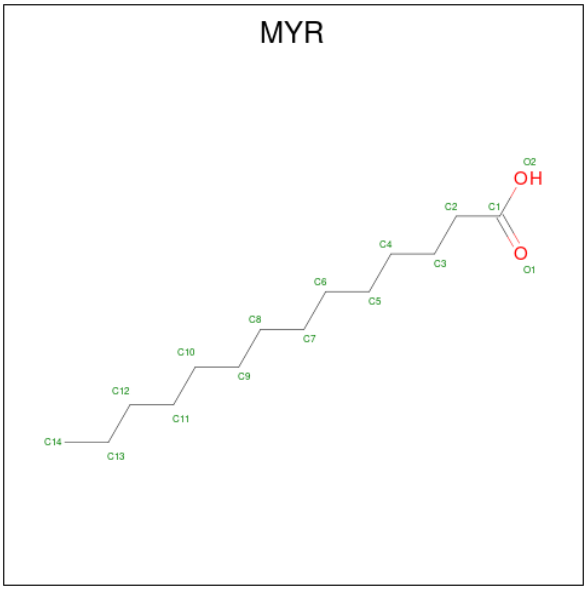
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	R	1	1	1	0

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



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	A	30	30	30	0
60	B	65	65	65	0
60	C	92	92	92	0
60	D	168	168	168	0
60	E	15	15	15	0
60	F	63	63	63	0
60	G	203	203	203	0
60	H	70	70	70	0
60	I	92	92	92	0
60	J	27	27	27	0
60	K	18	18	18	0
60	L	52	52	52	0
60	M	65	65	65	0
60	N	52	52	52	0
60	O	27	27	27	0
60	P	80	80	80	0
60	Q	64	64	64	0
60	R	44	44	44	0
60	S	4	4	4	0
60	U	1	1	1	0
60	V	17	17	17	0
60	W	13	13	13	0

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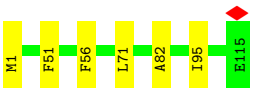
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	X	28	28	28	0
			Total	O	
60	Y	2	2	2	0
			Total	O	
60	Z	22	22	22	0
			Total	O	
60	a	16	16	16	0
			Total	O	
60	b	8	8	8	0
			Total	O	
60	d	17	17	17	0
			Total	O	
60	e	18	18	18	0
			Total	O	
60	f	3	3	3	0
			Total	O	
60	g	5	5	5	0
			Total	O	
60	h	23	23	23	0
			Total	O	
60	i	3	3	3	0
			Total	O	
60	j	2	2	2	0
			Total	O	
60	k	1	1	1	0
			Total	O	
60	l	13	13	13	0
			Total	O	
60	m	11	11	11	0
			Total	O	
60	n	7	7	7	0
			Total	O	
60	o	2	2	2	0
			Total	O	
60	p	16	16	16	0
			Total	O	
60	q	47	47	47	0
			Total	O	
60	r	33	33	33	0
			Total	O	
60	s	6	6	6	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.

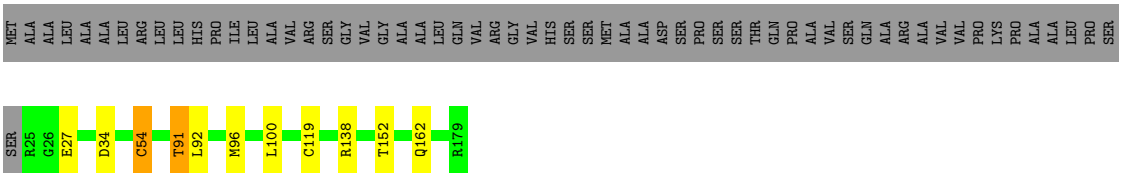
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 95% 5%



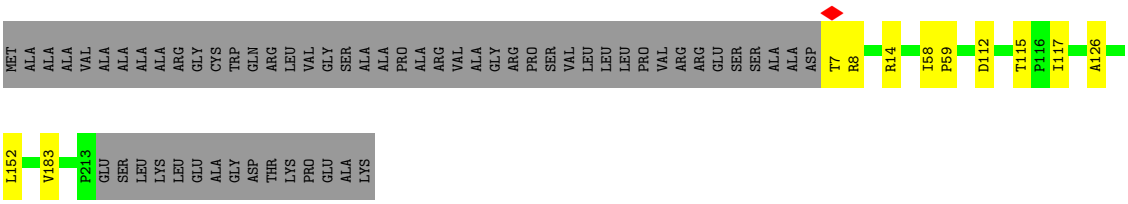
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 67% 28%



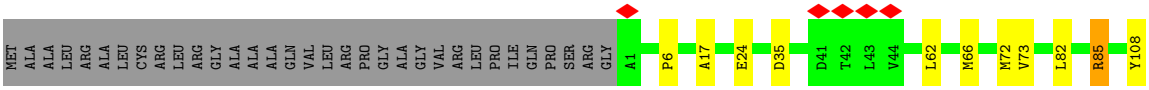
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

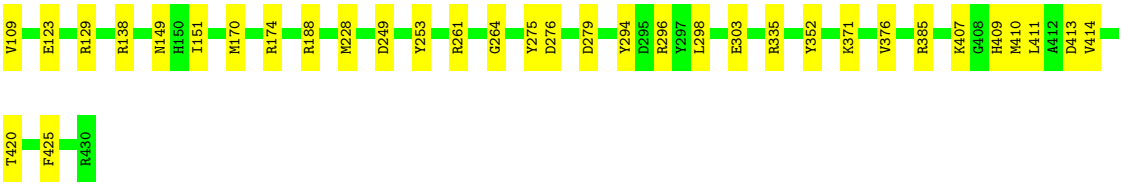
Chain C: 74% 22%



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

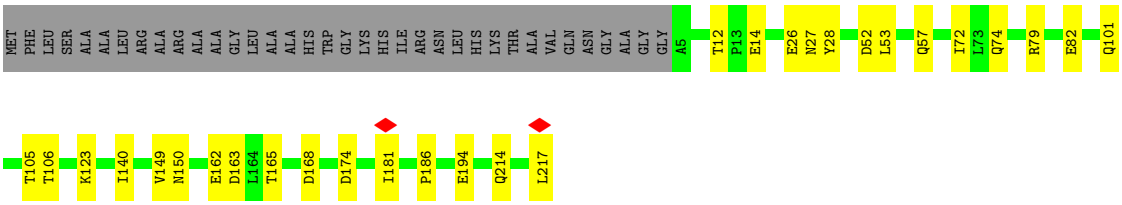
Chain D: 83% 10% 7%





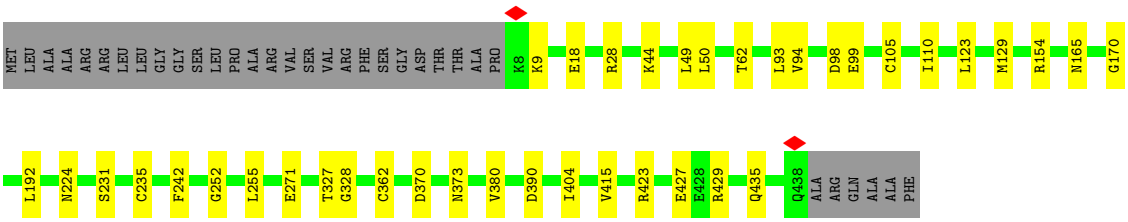
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



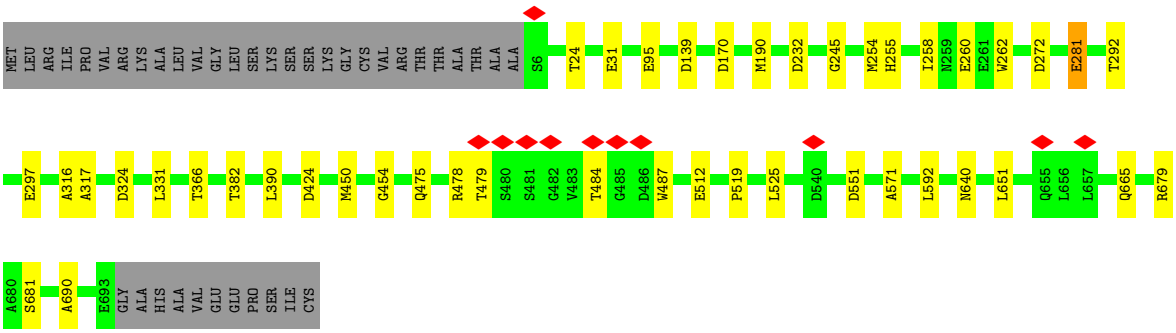
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

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: 78% 5% 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 P10 S11 M14 T28 R32 T37 V86 S103 E124 D129 S140

R176

• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 89% 10%

M1 S10 V11 F17 F20 M55 Y70 E77 F101 F102 M103 V115 D124 W125 G131 F135 F136 Y147 L153 T157 V167 G174 ASN

• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 89% 11%

M1 V4 N7 L16 L19 M27 M36 M37 L46 I62 A67 C98

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 88% 12%

M1 N2 M3 F4 S5 S6 V10 L13 L14 S23 Y27 S30 V36 I49 H67 T70 F80 K81 M82 M101 E102 L140 F141 W144 I149 D179 I183 D197 M203 H230 P231 W232 L233 P234 S235 A236 M237 H248 S249 S250

T251 M252 V253 V254 Y264 P265 L286 F287 T288 F304 S307 L310 T331 L373 T387 D393 A398 S402 N405 A406 W407 M411 L431 N442 E445 I451 R456 Q479 M480 T481 M482 P483 L486 S505 T508 H514

L526 P530 A537 P538 D554 E559 L562 P563 K564 T565 T594 I595 E606

• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

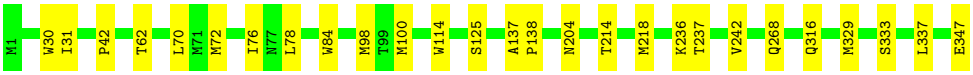
Chain M: 91% 9%

M1 N20 S27 S31 L66 W71 L72 M76 S80 K86 F105 T109 F110 T111 A112 M113 I116 L126 N144 T153 I165 N175 M207 P208 L214 W215 L216 P217 A226 V230 A233 G240 M243 M271 I301

P306 G320 E335 L369 Y406 H422 S427 S438 I441 L458 Y459

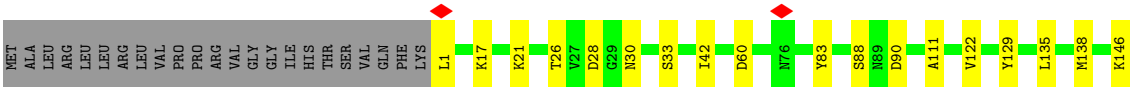
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

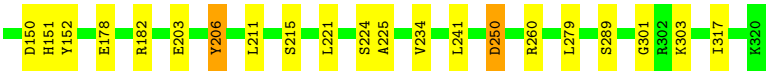
Chain N:



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

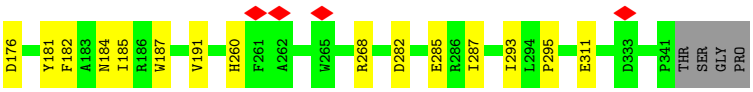
Chain O:





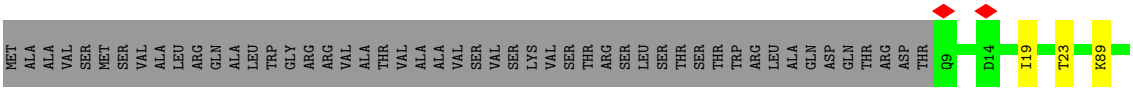
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



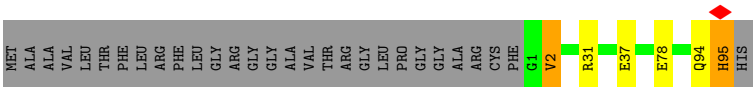
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



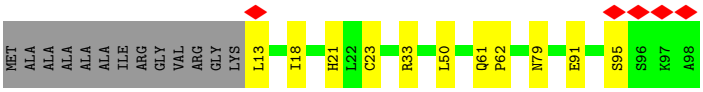
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



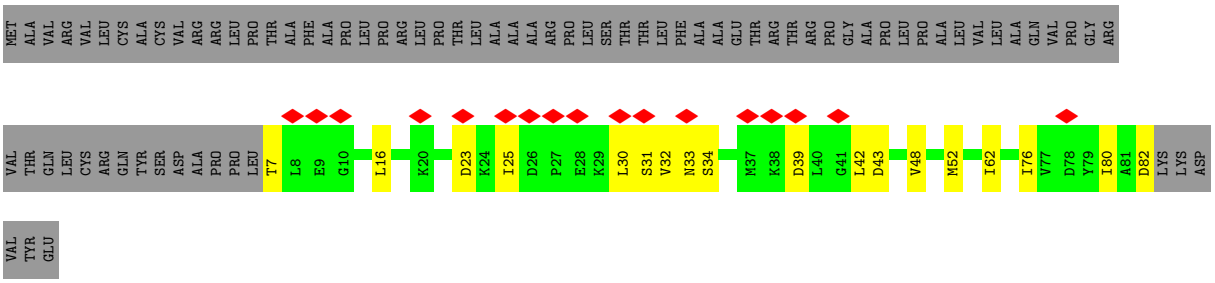
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



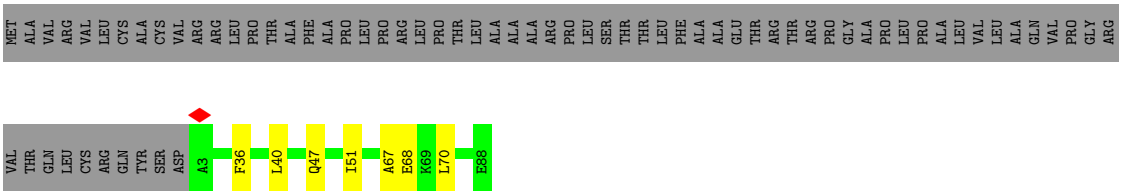
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



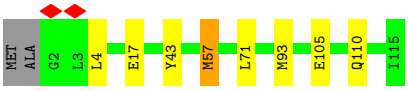
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



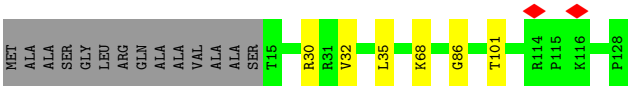
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



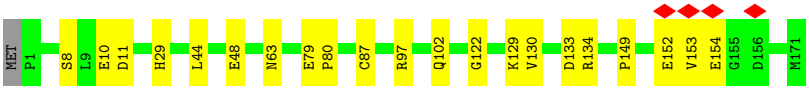
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



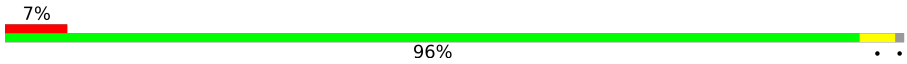
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

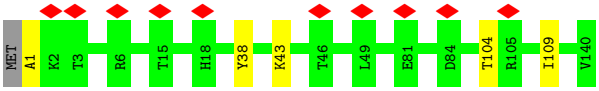
Chain X:



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

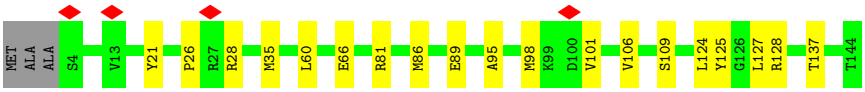
Chain Y:





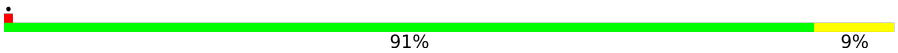
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

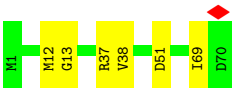
Chain Z:



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

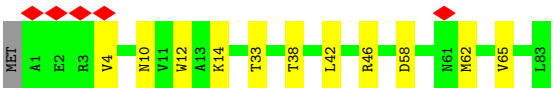
Chain a:





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

Chain b:



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

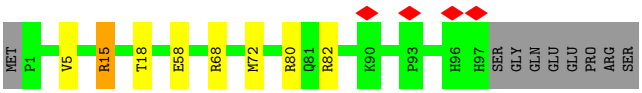
Chain c:

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

Chain d:

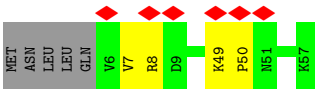
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



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

Chain f:

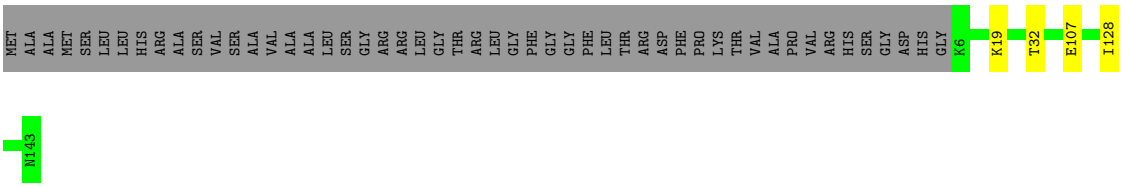


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:

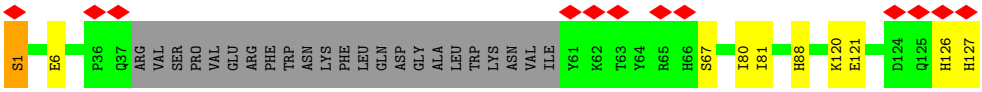
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



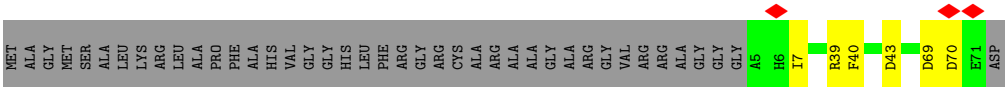
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



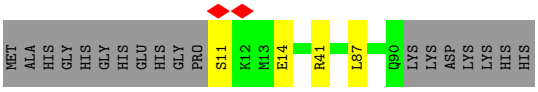
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



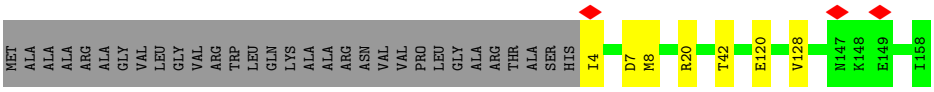
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



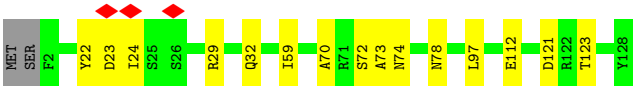
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



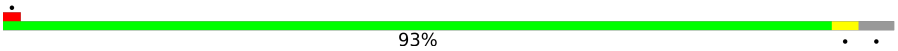
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

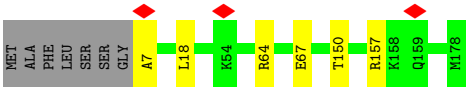
Chain m:



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

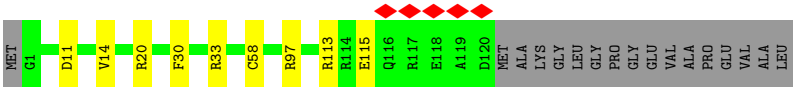
Chain n:





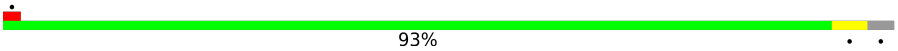
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

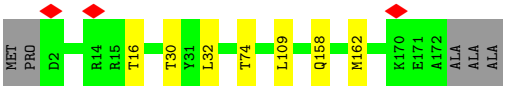
Chain o:



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

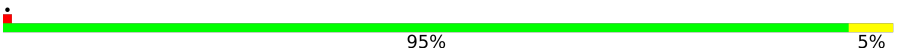
Chain p:

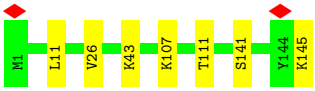




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



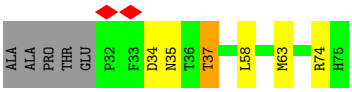


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:

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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53763	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	32.833	Depositor
Minimum map value	-14.121	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.032	Depositor
Recommended contour level	5	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.23	0/936	0.28	0/1281
2	B	0.27	0/1272	0.37	0/1720
3	C	0.25	0/1772	0.32	0/2413
4	D	0.26	0/3537	0.33	0/4794
5	E	0.22	0/1695	0.31	0/2307
6	F	0.23	0/3393	0.30	0/4584
7	G	0.24	0/5367	0.32	0/7274
8	H	0.27	0/2571	0.35	0/3513
9	I	0.27	0/1445	0.35	0/1956
10	J	0.24	0/1362	0.31	0/1848
11	K	0.24	0/745	0.28	0/1008
12	L	0.26	0/4896	0.30	0/6663
13	M	0.27	0/3738	0.31	0/5097
14	N	0.26	0/2792	0.30	0/3800
15	O	0.24	0/2651	0.29	0/3587
16	P	0.23	0/2824	0.32	0/3831
17	Q	0.24	0/1039	0.32	0/1404
18	R	0.26	0/742	0.33	0/999
19	S	0.22	0/702	0.31	0/945
20	T	0.18	0/621	0.31	0/837
20	U	0.28	0/705	0.30	0/952
21	V	0.21	0/943	0.27	0/1277
22	W	0.24	0/995	0.31	0/1337
23	X	0.24	0/1439	0.33	0/1942
24	Y	0.19	0/1042	0.29	0/1414
25	Z	0.23	0/1181	0.29	0/1592
26	a	0.25	0/584	0.32	0/786
27	b	0.22	0/672	0.31	0/923
28	c	0.22	0/418	0.28	0/567
29	d	0.24	0/975	0.31	0/1319
30	e	0.23	0/840	0.36	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.22	0/464	0.33	0/626
32	g	0.23	0/850	0.29	0/1154
33	h	0.25	0/1188	0.31	0/1607
34	i	0.25	0/920	0.34	0/1251
35	j	0.25	0/607	0.29	0/833
36	k	0.24	0/663	0.30	0/895
37	l	0.25	0/1358	0.30	0/1858
38	m	0.26	0/1088	0.31	0/1472
39	n	0.25	0/1545	0.29	0/2092
40	o	0.26	0/1060	0.34	0/1420
41	p	0.27	0/1476	0.28	0/1990
42	q	0.23	0/1250	0.32	0/1698
43	r	0.22	0/780	0.31	0/1056
44	s	0.20	0/383	0.28	0/518
All	All	0.25	0/67526	0.31	0/91563

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	275	TYR	Peptide
4	D	85	2MR	Mainchain

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	5	0
2	B	1241	0	1251	8	0
3	C	1721	0	1675	8	0
4	D	3459	0	3404	32	0
5	E	1655	0	1661	18	0
6	F	3319	0	3274	24	0
7	G	5279	0	5301	28	0
8	H	2509	0	2621	18	0
9	I	1414	0	1370	8	0
10	J	1337	0	1346	17	0
11	K	745	0	785	10	0
12	L	4780	0	4926	46	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	20	0
15	O	2589	0	2565	22	0
16	P	2747	0	2766	18	0
17	Q	1016	0	1014	3	0
18	R	730	0	707	4	0
19	S	691	0	706	4	0
20	T	612	0	604	9	0
20	U	693	0	688	4	0
21	V	923	0	964	5	0
22	W	971	0	989	4	0
23	X	1402	0	1385	14	0
24	Y	1030	0	1039	5	0
25	Z	1152	0	1151	18	0
26	a	569	0	568	5	0
27	b	651	0	662	8	0
28	c	405	0	409	6	0
29	d	945	0	932	9	0
30	e	819	0	821	6	0
31	f	451	0	453	2	0
32	g	824	0	772	6	0
33	h	1154	0	1168	3	0
34	i	898	0	907	7	0
35	j	580	0	519	3	0
36	k	644	0	626	1	0
37	l	1304	0	1203	9	0
38	m	1061	0	1059	14	0
39	n	1492	0	1438	6	0
40	o	1035	0	1004	7	0
41	p	1443	0	1415	6	0
42	q	1209	0	1182	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	767	0	776	6	0
44	s	371	0	344	5	0
45	A	70	0	92	2	0
45	J	35	0	46	2	0
45	K	35	0	46	0	0
45	L	105	0	138	0	0
45	M	105	0	138	6	0
45	Y	105	0	138	1	0
45	b	35	0	46	0	0
45	h	35	0	46	1	0
45	j	35	0	46	0	0
45	l	35	0	46	0	0
46	A	21	0	18	1	0
46	B	89	0	132	4	0
46	L	49	0	75	3	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	H	129	0	194	0	0
51	L	94	0	142	2	0
51	M	97	0	151	4	0
51	N	70	0	88	0	0
51	P	37	0	48	0	0
51	X	51	0	82	2	0
51	Y	35	0	44	1	0
51	d	102	0	164	0	0
52	J	62	0	68	1	0
52	K	71	0	86	0	0
52	L	69	0	82	0	0
52	h	67	0	81	2	0
52	r	76	0	96	1	0
53	N	17	0	0	4	0
54	O	32	0	12	3	0
55	O	1	0	0	0	0
56	P	48	0	26	1	0
57	R	1	0	0	0	0
58	T	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	U	37	0	0	0	0
59	o	15	0	27	0	0
60	A	30	0	0	0	0
60	B	65	0	0	3	0
60	C	92	0	0	2	0
60	D	168	0	0	7	0
60	E	15	0	0	1	0
60	F	63	0	0	4	0
60	G	203	0	0	8	0
60	H	70	0	0	0	0
60	I	92	0	0	1	0
60	J	27	0	0	1	0
60	K	18	0	0	0	0
60	L	52	0	0	1	0
60	M	65	0	0	3	0
60	N	52	0	0	2	0
60	O	27	0	0	5	0
60	P	80	0	0	4	0
60	Q	64	0	0	1	0
60	R	44	0	0	1	0
60	S	4	0	0	0	0
60	U	1	0	0	0	0
60	V	17	0	0	2	0
60	W	13	0	0	0	0
60	X	28	0	0	2	0
60	Y	2	0	0	0	0
60	Z	22	0	0	1	0
60	a	16	0	0	1	0
60	b	8	0	0	0	0
60	d	17	0	0	0	0
60	e	18	0	0	0	0
60	f	3	0	0	0	0
60	g	5	0	0	0	0
60	h	23	0	0	2	0
60	i	3	0	0	0	0
60	j	2	0	0	0	0
60	k	1	0	0	0	0
60	l	13	0	0	1	0
60	m	11	0	0	2	0
60	n	7	0	0	0	0
60	o	2	0	0	0	0
60	p	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	q	47	0	0	0	0
60	r	33	0	0	2	0
60	s	6	0	0	0	0
All	All	69480	0	68583	434	0

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

The worst 5 of 434 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)
53:N:703:I49:I02	29:d:82:MET:HB3	2.31	1.01
53:N:703:I49:I02	29:d:82:MET:O	2.57	0.92
16:P:51:CYS:O	60:P:601:HOH:O	1.93	0.85
16:P:98:GLU:OE1	60:P:602:HOH:O	1.97	0.81
52:J:701:CDL:OB4	60:J:801:HOH:O	1.97	0.81

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	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	409 (96%)	18 (4%)	0	100	100
5	E	211/249 (85%)	204 (97%)	7 (3%)	0	100	100
6	F	429/464 (92%)	419 (98%)	10 (2%)	0	100	100
7	G	686/727 (94%)	673 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	582 (96%)	21 (4%)	1 (0%)	43	55
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	339/380 (89%)	330 (97%)	9 (3%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	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%)	77 (95%)	4 (5%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	111/120 (92%)	111 (100%)	0	0	100	100
30	e	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	96/154 (62%)	91 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	63 (97%)	2 (3%)	0	100	100
36	k	78/98 (80%)	77 (99%)	1 (1%)	0	100	100
37	l	153/186 (82%)	150 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
39	n	170/179 (95%)	167 (98%)	3 (2%)	0	100	100
40	o	118/137 (86%)	113 (96%)	5 (4%)	0	100	100
41	p	169/176 (96%)	168 (99%)	1 (1%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
All	All	8109/9212 (88%)	7899 (97%)	209 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

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	63
3	C	188/228 (82%)	187 (100%)	1 (0%)	81	90
4	D	370/392 (94%)	368 (100%)	2 (0%)	81	90
5	E	183/205 (89%)	181 (99%)	2 (1%)	65	81
6	F	345/368 (94%)	339 (98%)	6 (2%)	53	72
7	G	578/608 (95%)	573 (99%)	5 (1%)	70	84
8	H	274/274 (100%)	273 (100%)	1 (0%)	84	92
9	I	151/175 (86%)	148 (98%)	3 (2%)	48	67
10	J	140/141 (99%)	139 (99%)	1 (1%)	76	87
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	528/533 (99%)	520 (98%)	8 (2%)	57	75
13	M	412/412 (100%)	407 (99%)	5 (1%)	63	79
14	N	315/315 (100%)	314 (100%)	1 (0%)	86	93
15	O	283/303 (93%)	275 (97%)	8 (3%)	38	56
16	P	295/327 (90%)	293 (99%)	2 (1%)	76	87
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	76 (97%)	2 (3%)	40	59
19	S	76/82 (93%)	73 (96%)	3 (4%)	28	43
20	T	70/135 (52%)	67 (96%)	3 (4%)	26	39
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	82
22	W	107/114 (94%)	106 (99%)	1 (1%)	70	84
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	89
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	86
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	56
28	c	44/68 (65%)	43 (98%)	1 (2%)	44	63
29	d	101/105 (96%)	101 (100%)	0	100	100
30	e	88/96 (92%)	86 (98%)	2 (2%)	44	63
31	f	49/54 (91%)	49 (100%)	0	100	100
32	g	89/131 (68%)	88 (99%)	1 (1%)	65	81
33	h	121/158 (77%)	120 (99%)	1 (1%)	73	86
34	i	99/120 (82%)	97 (98%)	2 (2%)	48	67
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	50
36	k	62/76 (82%)	59 (95%)	3 (5%)	23	35
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	155 (99%)	1 (1%)	78	89
40	o	109/120 (91%)	107 (98%)	2 (2%)	51	70
41	p	155/157 (99%)	153 (99%)	2 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	q	131/131 (100%)	126 (96%)	5 (4%)	29	44
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	43/92 (47%)	42 (98%)	1 (2%)	44	63
All	All	7150/7892 (91%)	7064 (99%)	86 (1%)	61	79

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	V	57	MET
35	j	40	PHE
23	X	154	GLU
30	e	15	ARG
39	n	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	268	GLN
40	o	42	GLN
16	P	8	HIS
39	n	77	GLN
44	s	43	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.91	0	7,9,11	1.09	1 (14%)
11	FME	K	1	11	8,9,10	0.91	0	7,9,11	0.81	0
12	FME	L	1	12	8,9,10	1.00	1 (12%)	7,9,11	0.72	0
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	0.97	0
8	FME	H	1	8	8,9,10	1.03	1 (12%)	7,9,11	0.86	0
34	SAC	i	1	34	7,8,9	0.98	0	8,9,11	1.71	2 (25%)
43	AYA	r	1	43	6,7,8	1.81	2 (33%)	5,8,10	1.26	1 (20%)
13	FME	M	1	13	8,9,10	0.98	1 (12%)	7,9,11	0.88	0
24	AYA	Y	1	24	6,7,8	1.76	1 (16%)	5,8,10	1.42	1 (20%)
14	FME	N	1	14	8,9,10	0.97	0	7,9,11	0.91	0
4	2MR	D	85	4	10,12,13	2.62	4 (40%)	5,13,15	1.18	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
1	FME	A	1	1	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
34	SAC	i	1	34	-	6/7/8/10	-
43	AYA	r	1	43	-	0/4/6/8	-
13	FME	M	1	13	-	0/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
14	FME	N	1	14	-	5/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.92	1.44	1.33
4	D	85	2MR	CZ-NE	4.55	1.44	1.34
4	D	85	2MR	O-C	3.94	1.35	1.19
43	r	1	AYA	CT-N	3.26	1.45	1.34
24	Y	1	AYA	CT-N	3.13	1.45	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	C-CA-N	3.26	115.61	109.73
4	D	85	2MR	NE-CZ-NH2	-2.41	117.27	119.48
24	Y	1	AYA	CM-CT-N	2.36	120.10	116.10
43	r	1	AYA	CM-CT-N	2.30	120.00	116.10
1	A	1	FME	C-CA-N	2.23	113.75	109.73

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	2	0
34	i	1	SAC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 58 ligands modelled in this entry, 3 are monoatomic - leaving 55 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	PC1	A	303	-	20,20,53	1.89	3 (15%)	24,27,61	1.17	1 (4%)
47	SF4	I	202	9	0,12,12	-	-	-		
45	LMT	Y	804	-	36,36,36	1.19	3 (8%)	47,47,47	1.07	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
51	3PE	d	1202	-	50,50,50	0.82	3 (6%)	53,55,55	1.19	4 (7%)
45	LMT	j	101	-	36,36,36	1.21	3 (8%)	47,47,47	0.96	2 (4%)
56	NDP	P	501	-	49,52,52	2.10	4 (8%)	66,80,80	1.60	14 (21%)
46	PC1	B	202	-	53,53,53	0.92	3 (5%)	59,61,61	1.05	2 (3%)
47	SF4	I	201	9	0,12,12	-	-	-		
46	PC1	L	707	-	48,48,53	0.98	4 (8%)	54,56,61	1.07	2 (3%)
52	CDL	J	701	-	61,61,99	1.06	7 (11%)	67,73,111	1.25	5 (7%)
51	3PE	N	701	-	40,40,50	0.97	3 (7%)	43,45,55	1.09	2 (4%)
45	LMT	M	604	-	36,36,36	1.22	3 (8%)	47,47,47	0.96	0
45	LMT	L	704	-	36,36,36	1.23	4 (11%)	47,47,47	0.91	0
45	LMT	Y	803	-	36,36,36	1.17	3 (8%)	47,47,47	1.00	1 (2%)
45	LMT	M	603	-	36,36,36	1.15	2 (5%)	47,47,47	0.98	1 (2%)
46	PC1	B	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.12	2 (5%)
51	3PE	H	403	-	33,33,50	1.38	3 (9%)	34,37,55	1.23	2 (5%)
45	LMT	b	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.17	3 (6%)
49	FMN	F	501	-	33,33,33	1.11	2 (6%)	48,50,50	1.29	6 (12%)
45	LMT	Y	801	-	36,36,36	1.15	3 (8%)	47,47,47	1.15	4 (8%)
45	LMT	L	706	-	36,36,36	1.18	2 (5%)	47,47,47	1.12	3 (6%)
48	FES	E	301	5	0,4,4	-	-	-		
51	3PE	X	401	-	50,50,50	0.85	4 (8%)	53,55,55	1.14	2 (3%)
47	SF4	G	802	7	0,12,12	-	-	-		
45	LMT	M	602	-	36,36,36	1.13	2 (5%)	47,47,47	1.01	2 (4%)
54	GTP	O	401	55	30,34,34	3.05	11 (36%)	46,54,54	1.92	15 (32%)
51	3PE	M	601	-	45,45,50	0.91	4 (8%)	48,50,55	0.99	2 (4%)
51	3PE	P	502	-	36,36,50	1.03	4 (11%)	39,41,55	1.16	2 (5%)
51	3PE	L	701	-	48,48,50	0.90	4 (8%)	51,53,55	1.14	2 (3%)
53	I49	N	703	-	15,17,17	1.45	2 (13%)	21,22,22	1.90	6 (28%)
47	SF4	B	201	2	0,12,12	-	-	-		
59	MYR	o	201	40	14,14,15	0.87	0	13,13,15	0.68	0
51	3PE	M	605	-	50,50,50	0.87	3 (6%)	53,55,55	1.12	2 (3%)
51	3PE	H	402	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	3 (5%)
52	CDL	K	502	-	70,70,99	1.03	6 (8%)	76,82,111	1.08	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	LMT	l	201	-	36,36,36	1.23	3 (8%)	47,47,47	1.15	3 (6%)
51	3PE	d	1201	-	50,50,50	0.86	3 (6%)	53,55,55	1.10	2 (3%)
51	3PE	L	705	-	44,44,50	0.91	3 (6%)	47,49,55	1.08	2 (4%)
45	LMT	L	702	-	36,36,36	1.17	3 (8%)	47,47,47	0.92	0
45	LMT	A	302	-	36,36,36	1.23	2 (5%)	47,47,47	1.09	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
52	CDL	L	703	-	68,68,99	1.03	6 (8%)	74,80,111	1.10	4 (5%)
48	FES	G	803	7	0,4,4	-	-	-		
45	LMT	h	1002	-	36,36,36	1.16	2 (5%)	47,47,47	0.92	2 (4%)
45	LMT	K	501	-	36,36,36	1.19	3 (8%)	47,47,47	1.01	0
58	EHZ	U	101	20	29,36,37	1.68	6 (20%)	35,44,47	1.50	4 (11%)
51	3PE	N	702	-	28,28,50	1.13	3 (10%)	31,33,55	1.16	2 (6%)
51	3PE	Y	802	-	34,34,50	1.05	4 (11%)	37,39,55	1.19	2 (5%)
52	CDL	r	201	-	75,75,99	0.99	6 (8%)	81,87,111	1.11	4 (4%)
52	CDL	h	1001	-	66,66,99	1.06	8 (12%)	72,78,111	1.23	4 (5%)
58	EHZ	T	101	20	29,36,37	1.67	6 (20%)	35,44,47	1.67	5 (14%)
45	LMT	J	702	-	36,36,36	1.21	3 (8%)	47,47,47	1.11	2 (4%)
45	LMT	A	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.13	3 (6%)
51	3PE	H	401	-	43,43,50	0.93	3 (6%)	46,48,55	1.10	2 (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
46	PC1	A	303	-	-	8/22/22/57	-
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	Y	804	-	-	8/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
51	3PE	d	1202	-	-	19/54/54/54	-
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
56	NDP	P	501	-	-	5/34/77/77	0/5/5/5
46	PC1	B	202	-	-	23/57/57/57	-
47	SF4	I	201	9	-	-	0/6/5/5
46	PC1	L	707	-	-	25/52/52/57	-
52	CDL	J	701	-	-	31/71/71/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	N	701	-	-	19/44/44/54	-
45	LMT	M	604	-	-	11/21/61/61	0/2/2/2
45	LMT	L	704	-	-	8/21/61/61	0/2/2/2
45	LMT	Y	803	-	-	11/21/61/61	0/2/2/2
45	LMT	M	603	-	-	10/21/61/61	0/2/2/2
46	PC1	B	203	-	-	14/38/38/57	-
51	3PE	H	403	-	-	19/36/36/54	-
45	LMT	b	101	-	-	3/21/61/61	0/2/2/2
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
45	LMT	Y	801	-	-	8/21/61/61	0/2/2/2
45	LMT	L	706	-	-	8/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
51	3PE	X	401	-	-	24/54/54/54	-
54	GTP	O	401	55	-	3/22/38/38	0/3/3/3
45	LMT	M	602	-	-	7/21/61/61	0/2/2/2
47	SF4	G	802	7	-	-	0/6/5/5
51	3PE	M	601	-	-	17/49/49/54	-
51	3PE	P	502	-	-	23/40/40/54	-
51	3PE	L	701	-	-	24/52/52/54	-
53	I49	N	703	-	-	5/10/10/10	0/1/1/1
47	SF4	B	201	2	-	-	0/6/5/5
59	MYR	o	201	40	-	8/11/12/13	-
51	3PE	M	605	-	-	22/54/54/54	-
51	3PE	H	402	-	-	17/54/54/54	-
52	CDL	K	502	-	-	33/81/81/110	-
45	LMT	l	201	-	-	6/21/61/61	0/2/2/2
51	3PE	d	1201	-	-	27/54/54/54	-
51	3PE	L	705	-	-	15/48/48/54	-
45	LMT	L	702	-	-	9/21/61/61	0/2/2/2
45	LMT	A	302	-	-	14/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5
52	CDL	L	703	-	-	32/79/79/110	-
48	FES	G	803	7	-	-	0/1/1/1
45	LMT	h	1002	-	-	6/21/61/61	0/2/2/2
45	LMT	K	501	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	U	101	20	-	6/42/44/45	-
51	3PE	N	702	-	-	18/32/32/54	-
51	3PE	Y	802	-	-	17/38/38/54	-
52	CDL	r	201	-	-	32/86/86/110	-
52	CDL	h	1001	-	-	35/77/77/110	-
58	EHZ	T	101	20	-	10/42/44/45	-
45	LMT	J	702	-	-	9/21/61/61	0/2/2/2
45	LMT	A	301	-	-	1/21/61/61	0/2/2/2
51	3PE	H	401	-	-	23/47/47/54	-

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.00	1.82	1.59
54	O	401	GTP	O6-C6	8.62	1.40	1.23
54	O	401	GTP	C5-N7	6.89	1.52	1.39
46	A	303	PC1	O21-C2	-5.95	1.40	1.46
51	H	403	3PE	O21-C2	-5.41	1.40	1.46

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	401	GTP	C8-N9-C4	7.39	120.12	106.05
56	P	501	NDP	PN-O3-PA	-6.69	109.86	132.83
58	T	101	EHZ	C8-C9-S1	6.50	121.68	113.63
58	U	101	EHZ	C8-C9-S1	6.02	121.08	113.63
51	H	403	3PE	O21-C21-O22	-5.21	118.94	125.57

There are no chirality outliers.

5 of 694 torsion outliers are listed below:

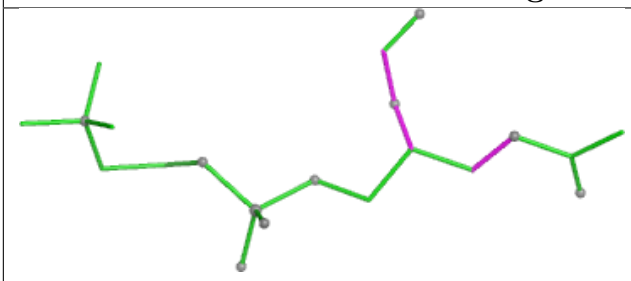
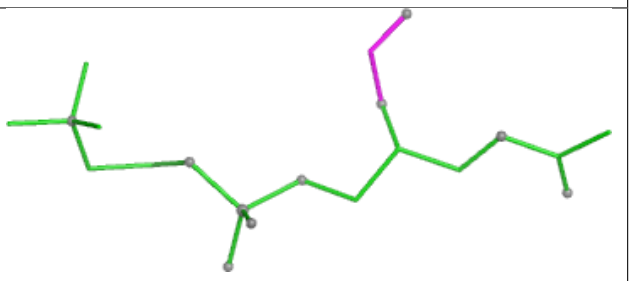
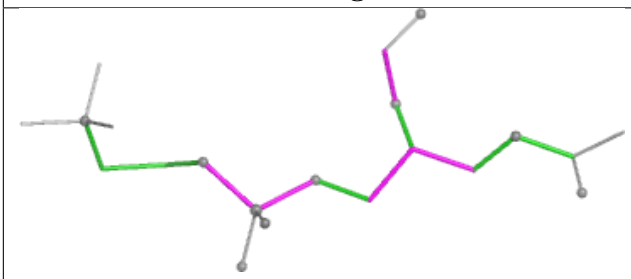
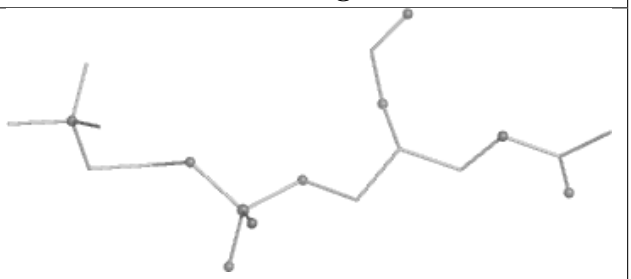
Mol	Chain	Res	Type	Atoms
45	A	302	LMT	O5'-C1'-O1'-C1
45	L	702	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	O5'-C1'-O1'-C1
45	L	702	LMT	C2-C1-O1'-C1'
45	L	706	LMT	C2'-C1'-O1'-C1

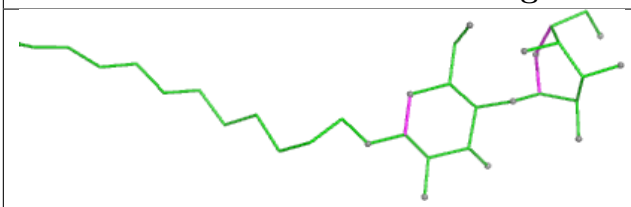
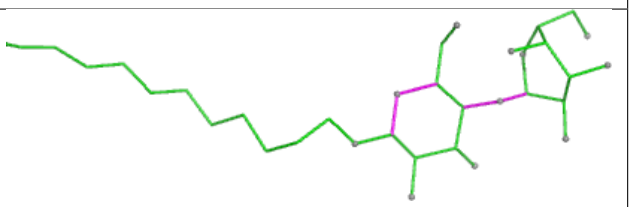
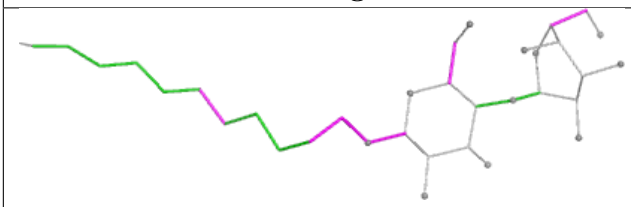
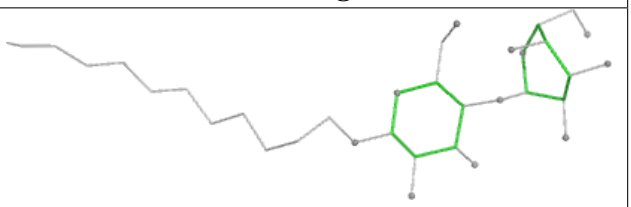
There are no ring outliers.

23 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	303	PC1	1	0
45	Y	804	LMT	1	0
56	P	501	NDP	1	0
46	B	202	PC1	2	0
46	L	707	PC1	3	0
52	J	701	CDL	1	0
45	M	603	LMT	1	0
46	B	203	PC1	2	0
49	F	501	FMN	1	0
51	X	401	3PE	2	0
45	M	602	LMT	5	0
54	O	401	GTP	3	0
51	M	601	3PE	2	0
53	N	703	I49	4	0
51	M	605	3PE	2	0
51	L	705	3PE	2	0
45	h	1002	LMT	1	0
51	Y	802	3PE	1	0
52	r	201	CDL	1	0
52	h	1001	CDL	2	0
58	T	101	EHZ	1	0
45	J	702	LMT	2	0
45	A	301	LMT	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 PC1 A 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT Y 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

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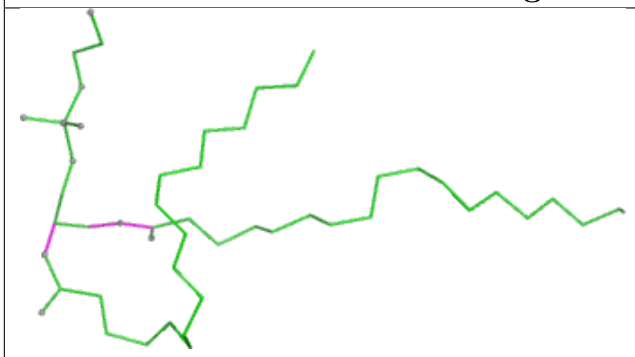
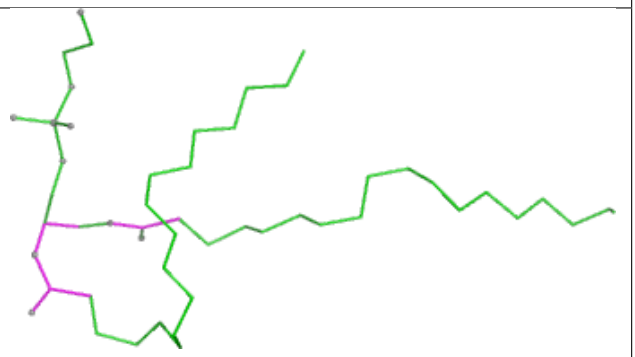
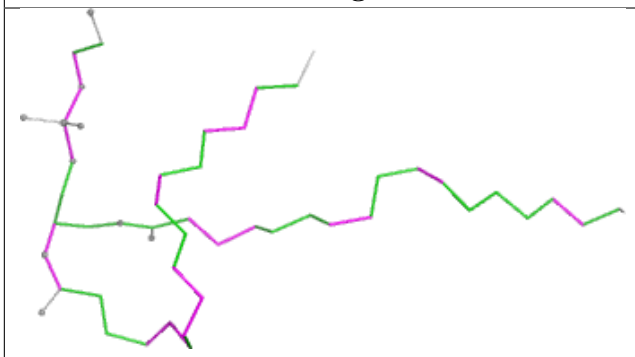
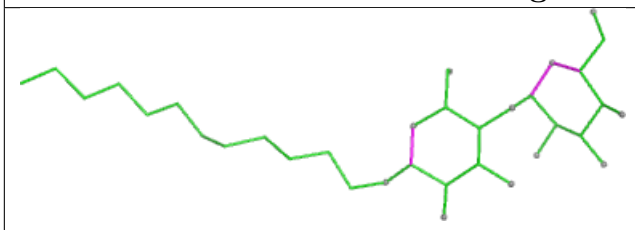
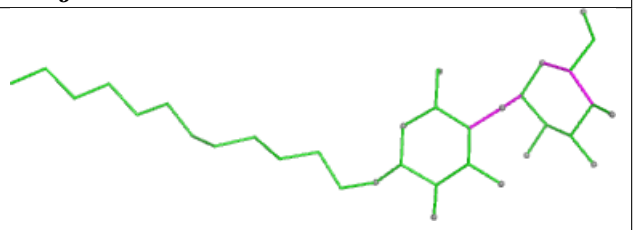
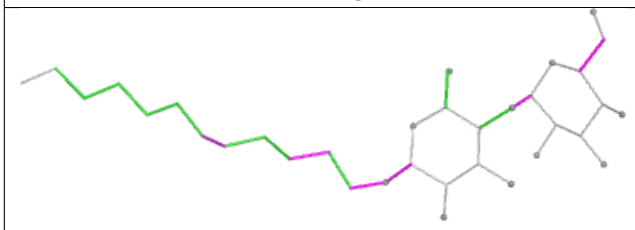
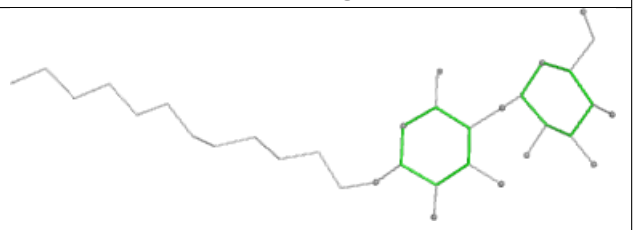
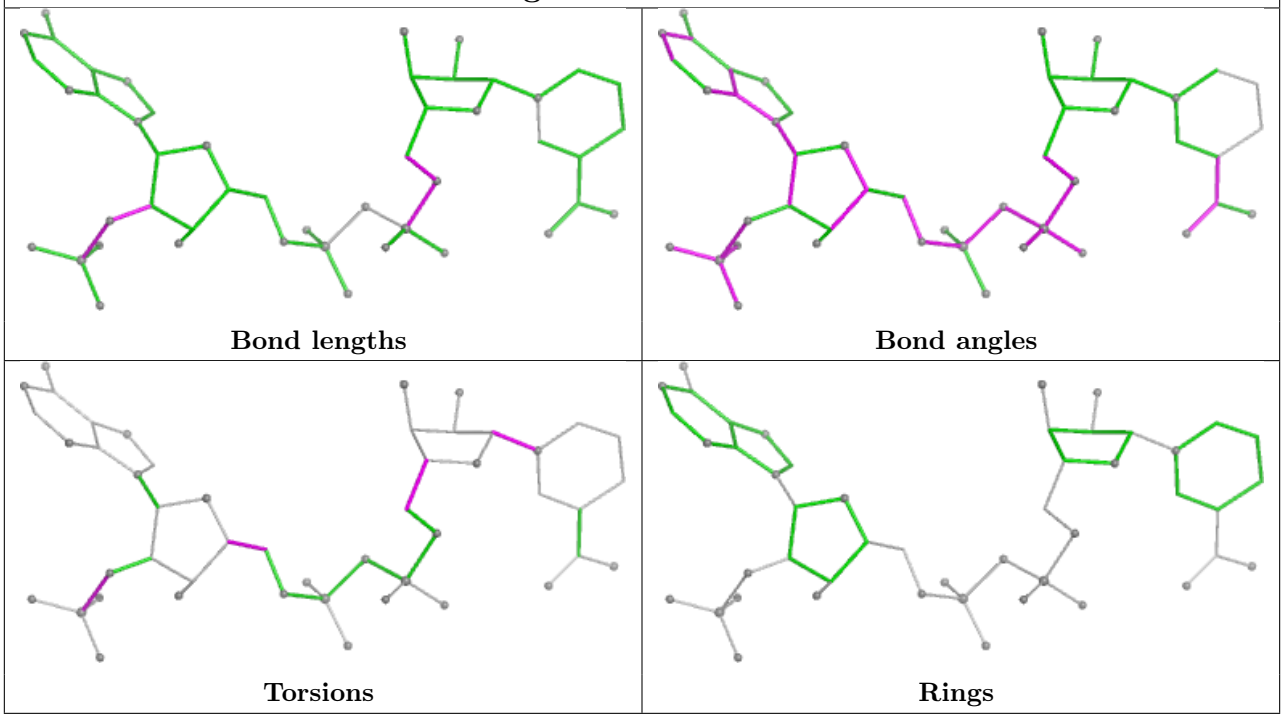
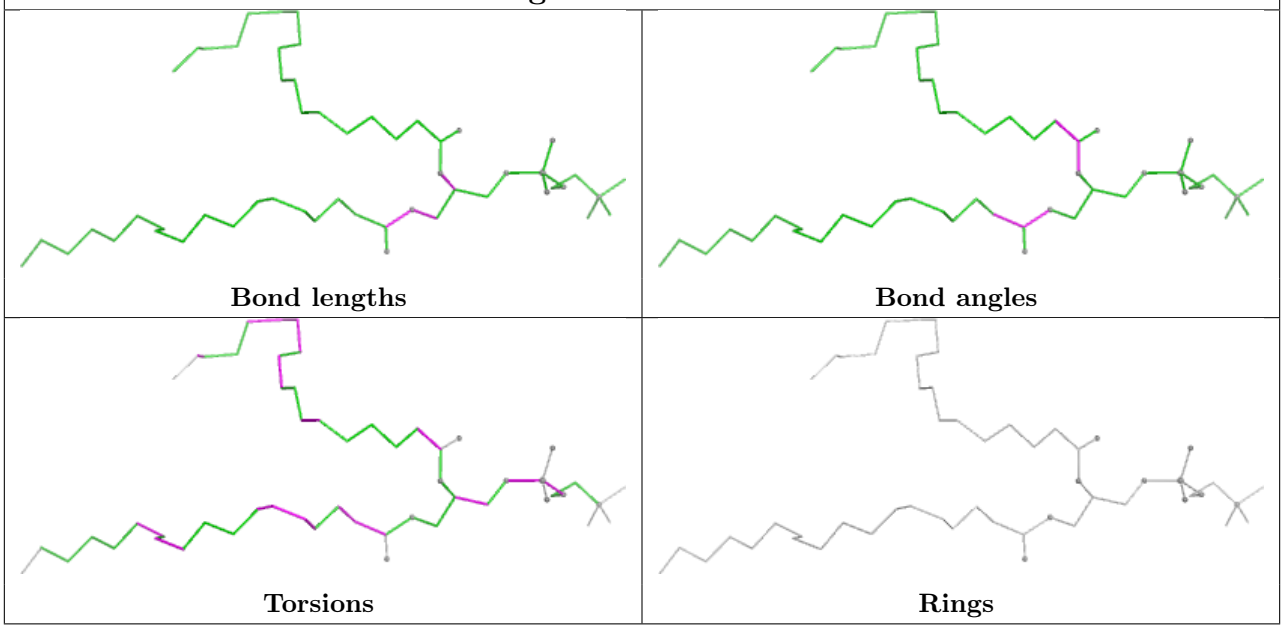
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LMT j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NDP P 501



Ligand PC1 B 202



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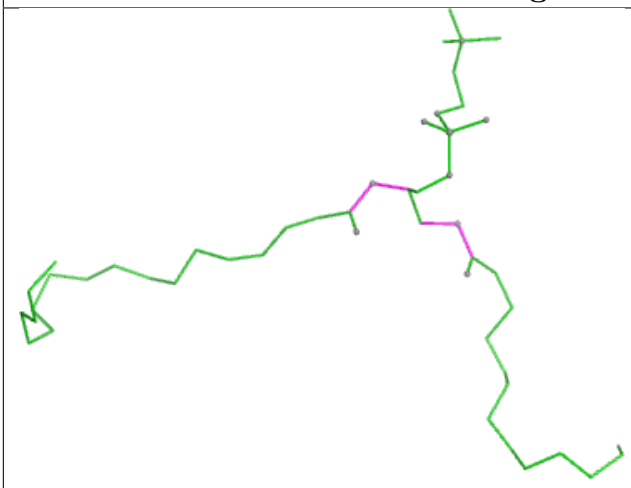
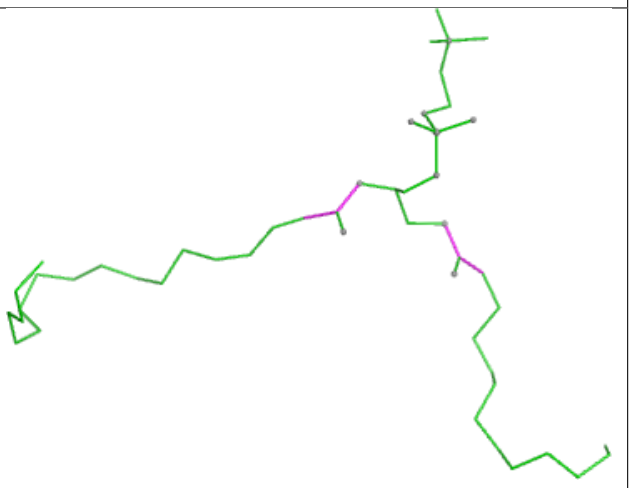
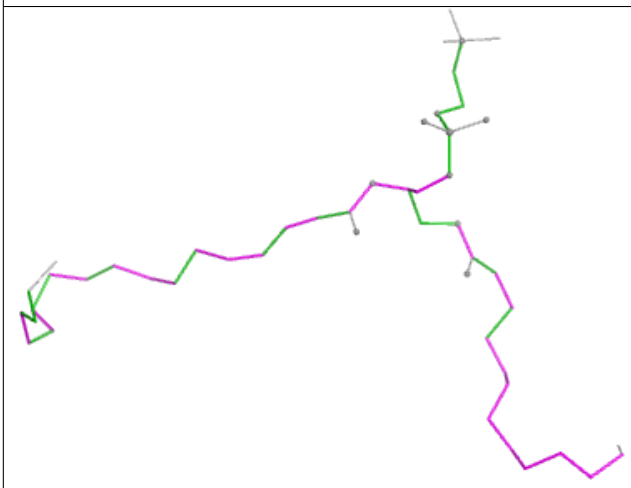
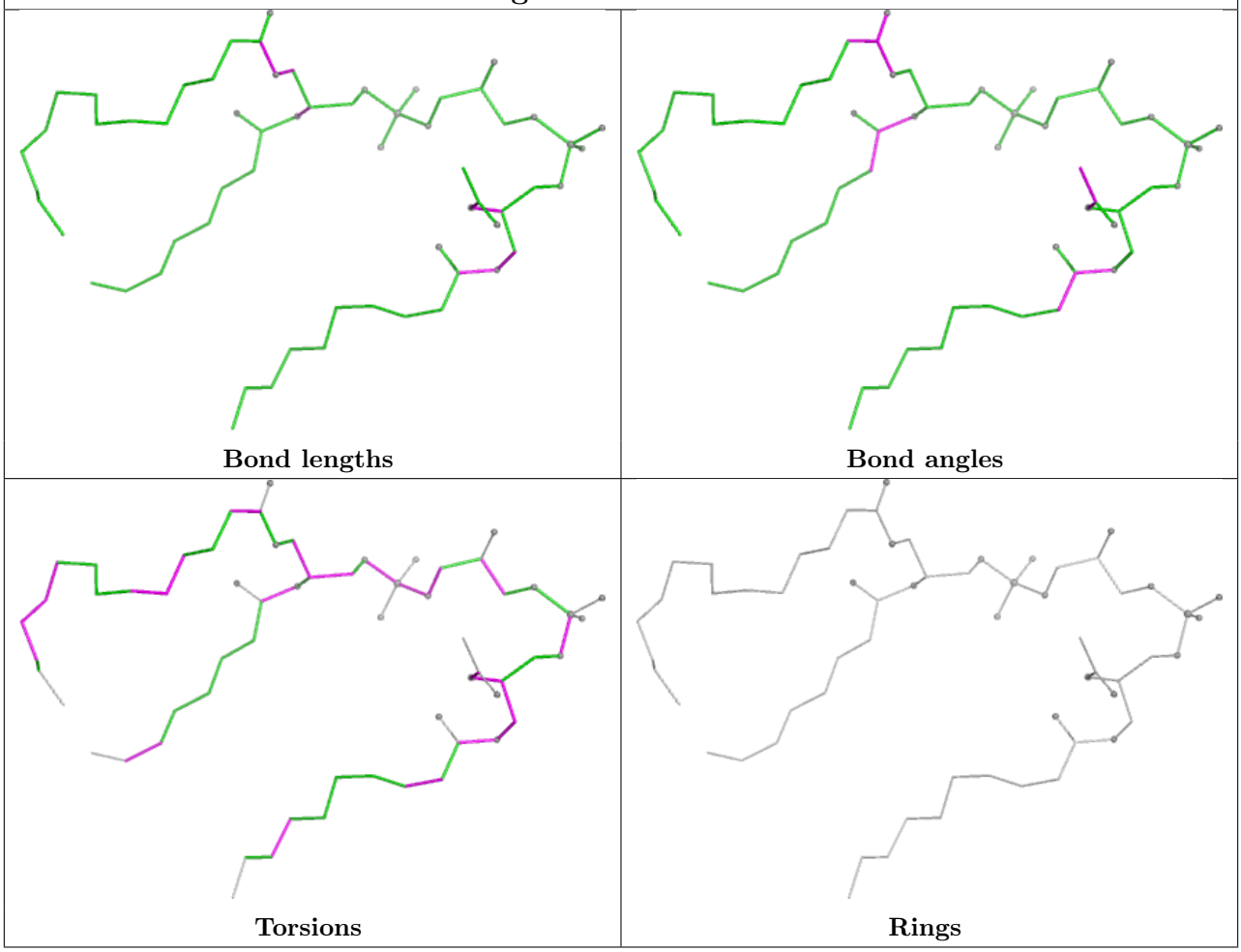
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL J 701



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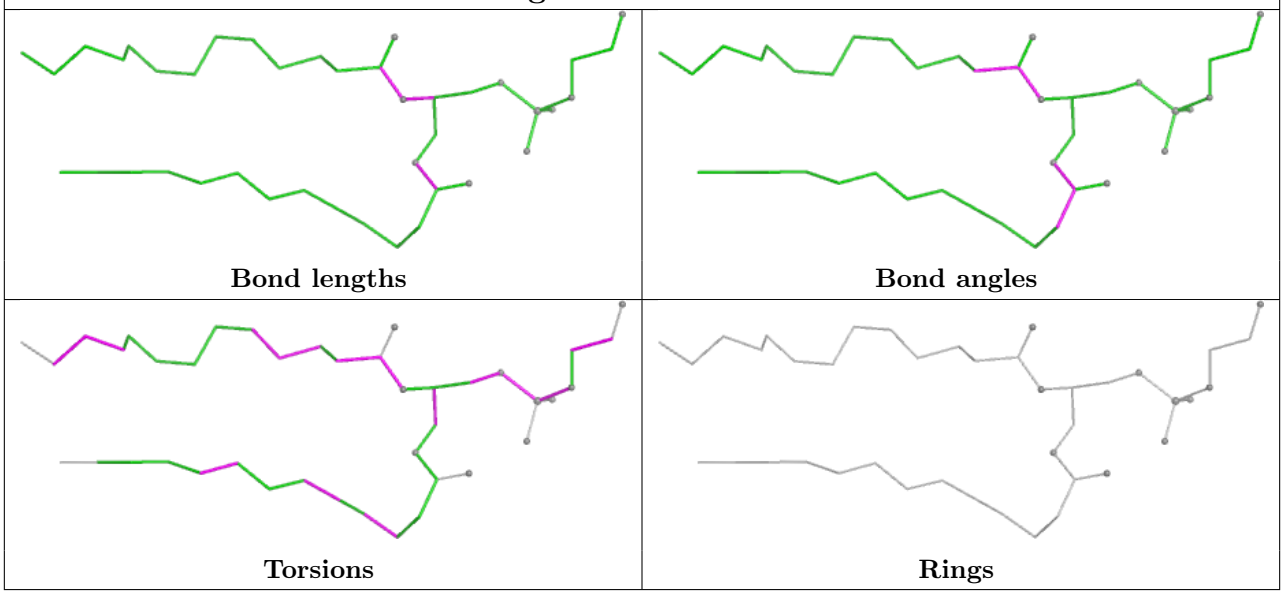
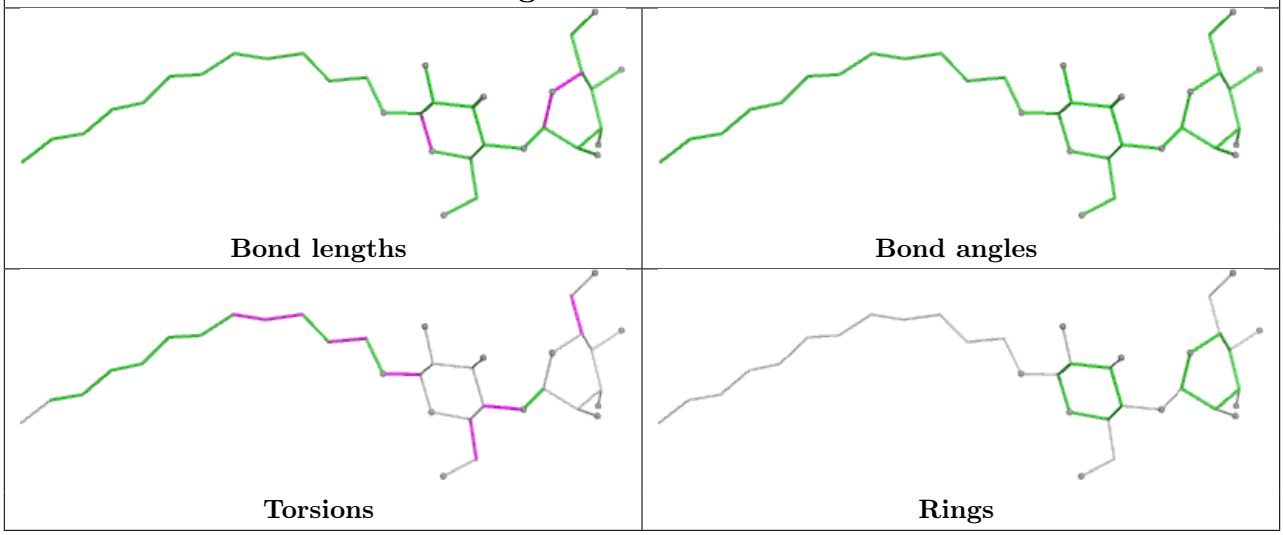


Ligand LMT M 604



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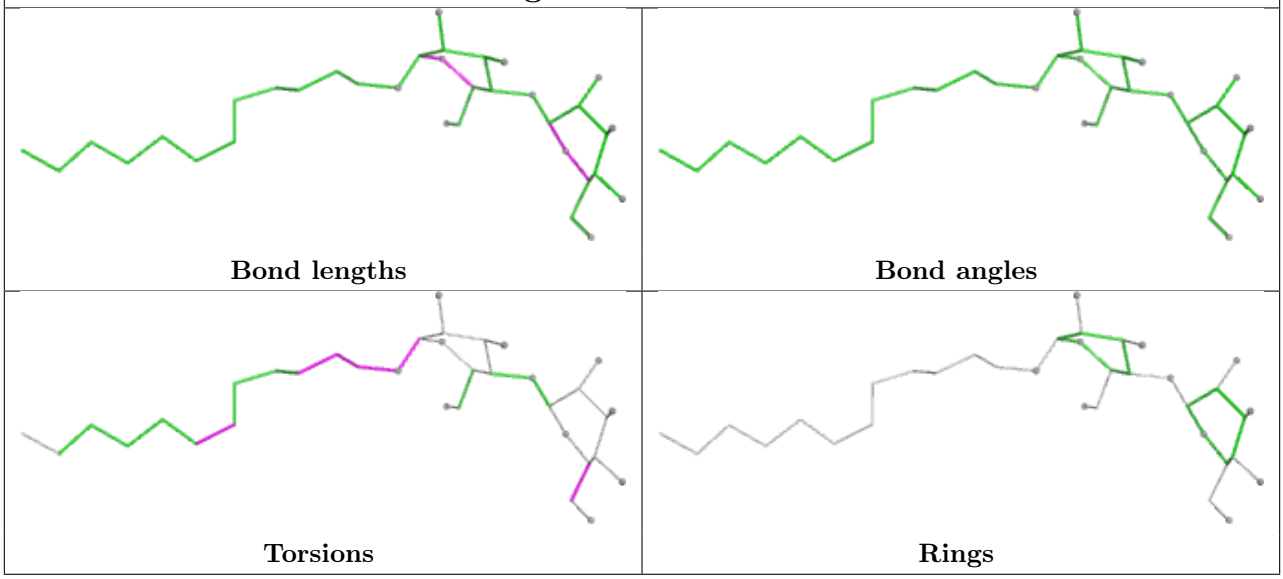

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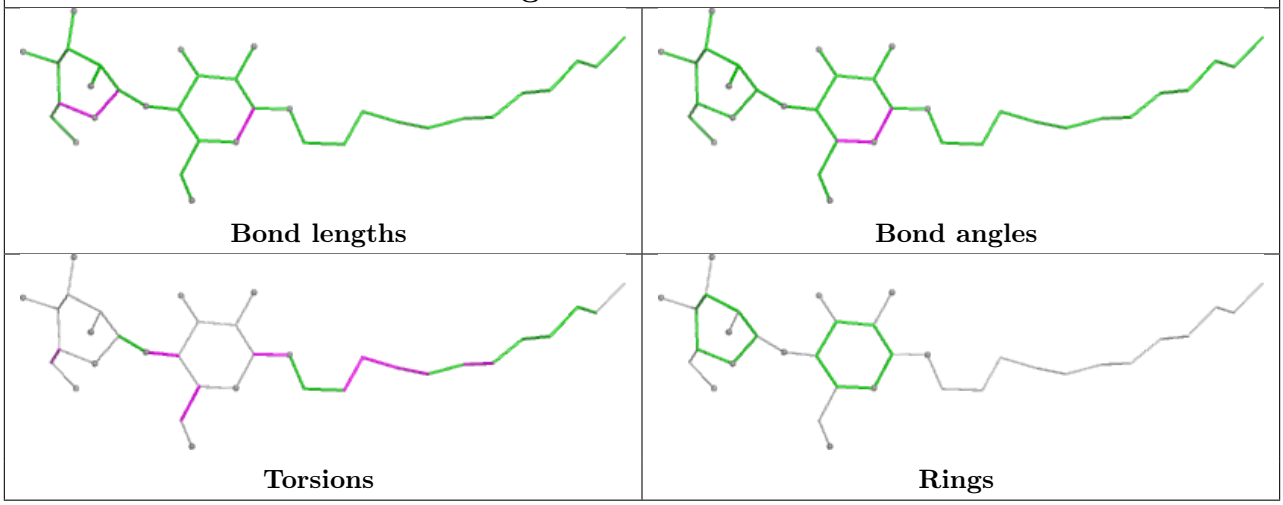

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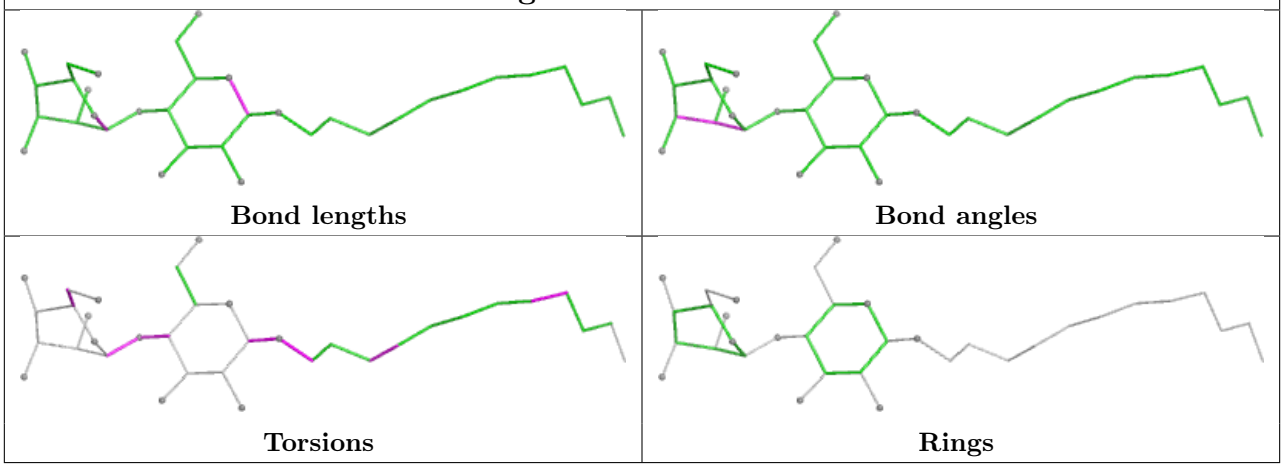
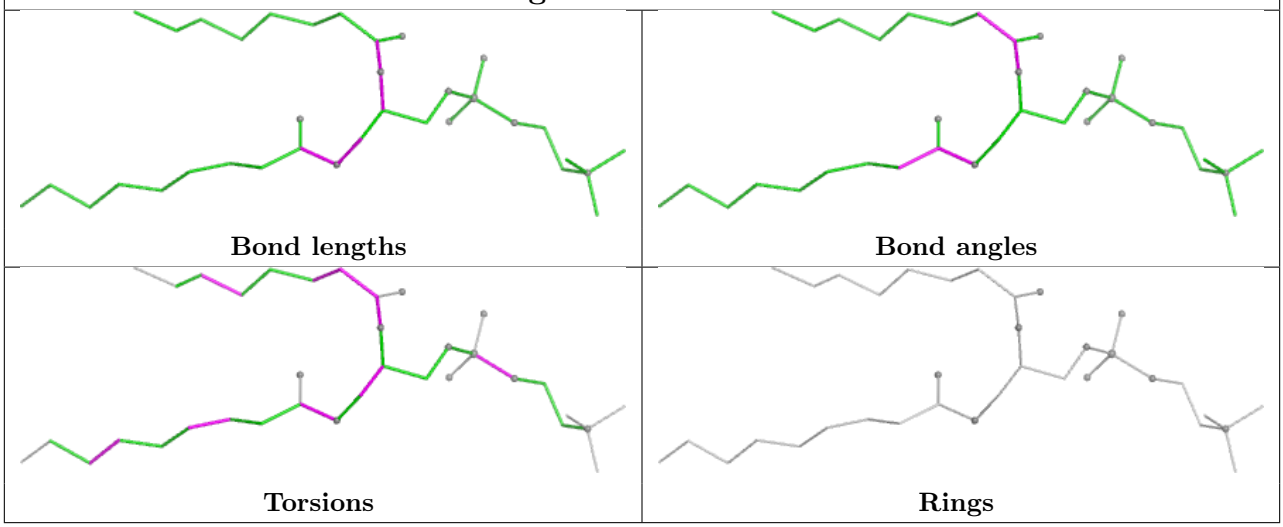


Ligand PC1 B 203



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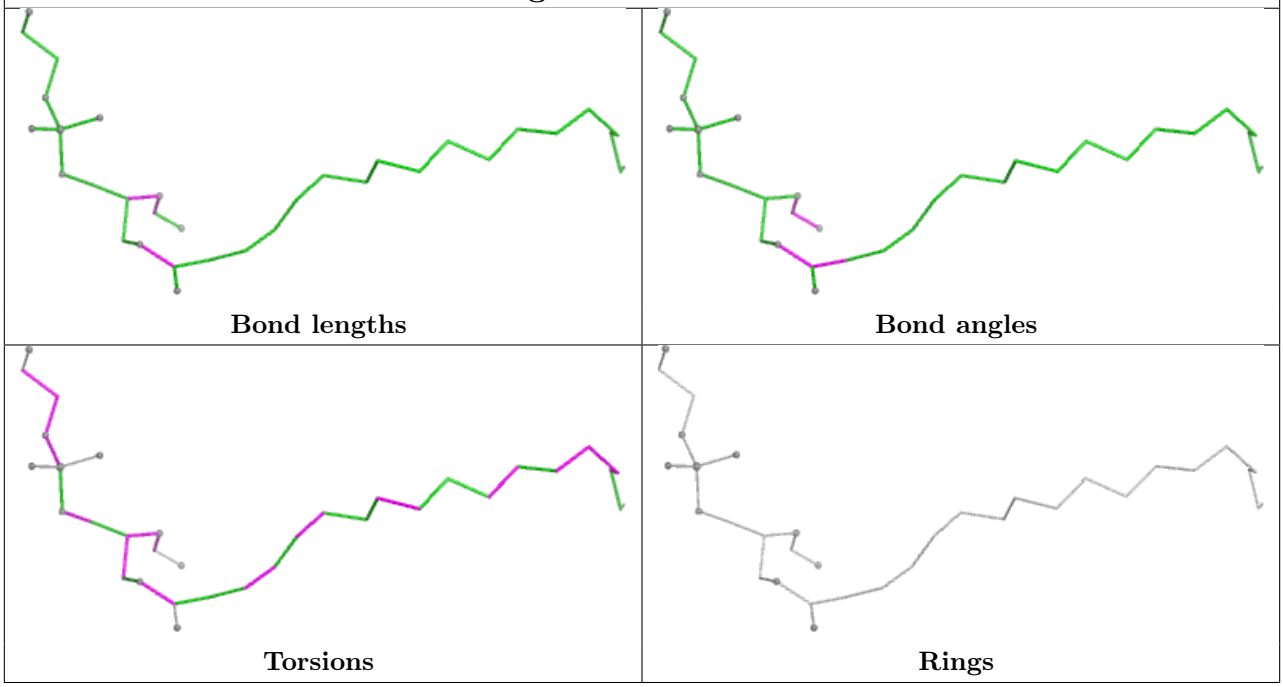

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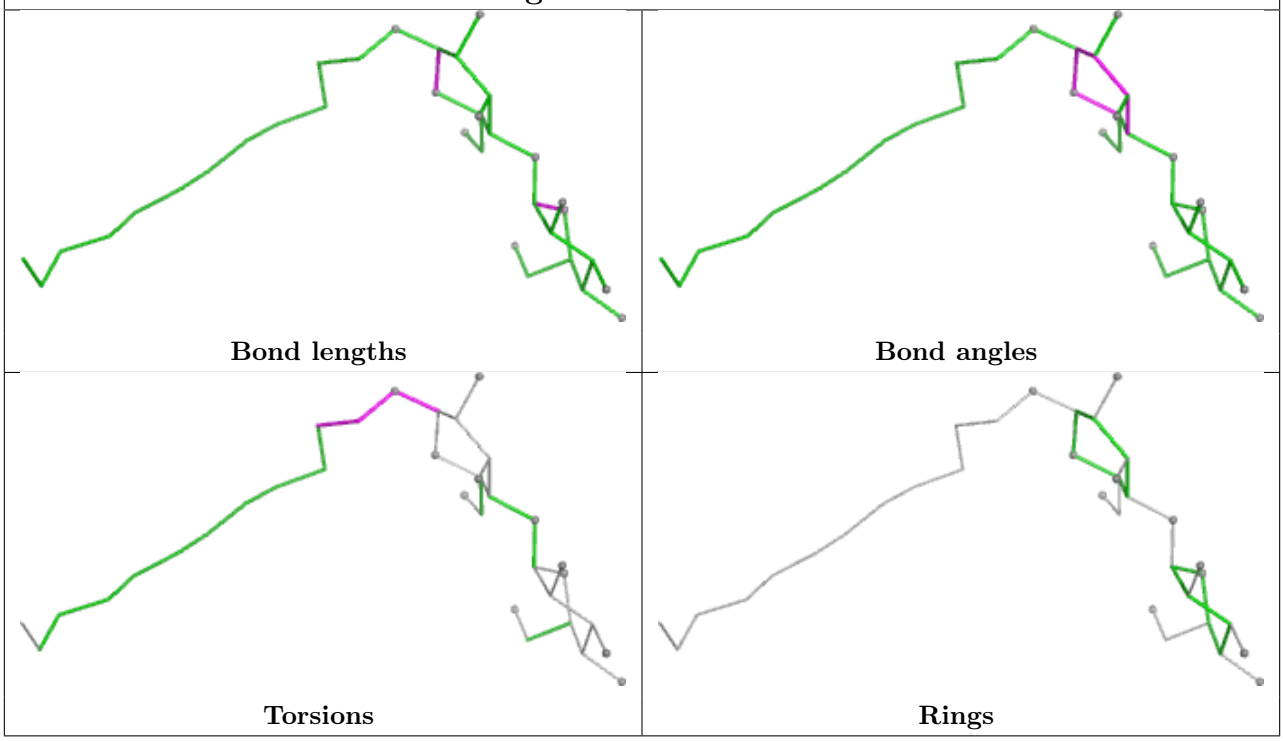
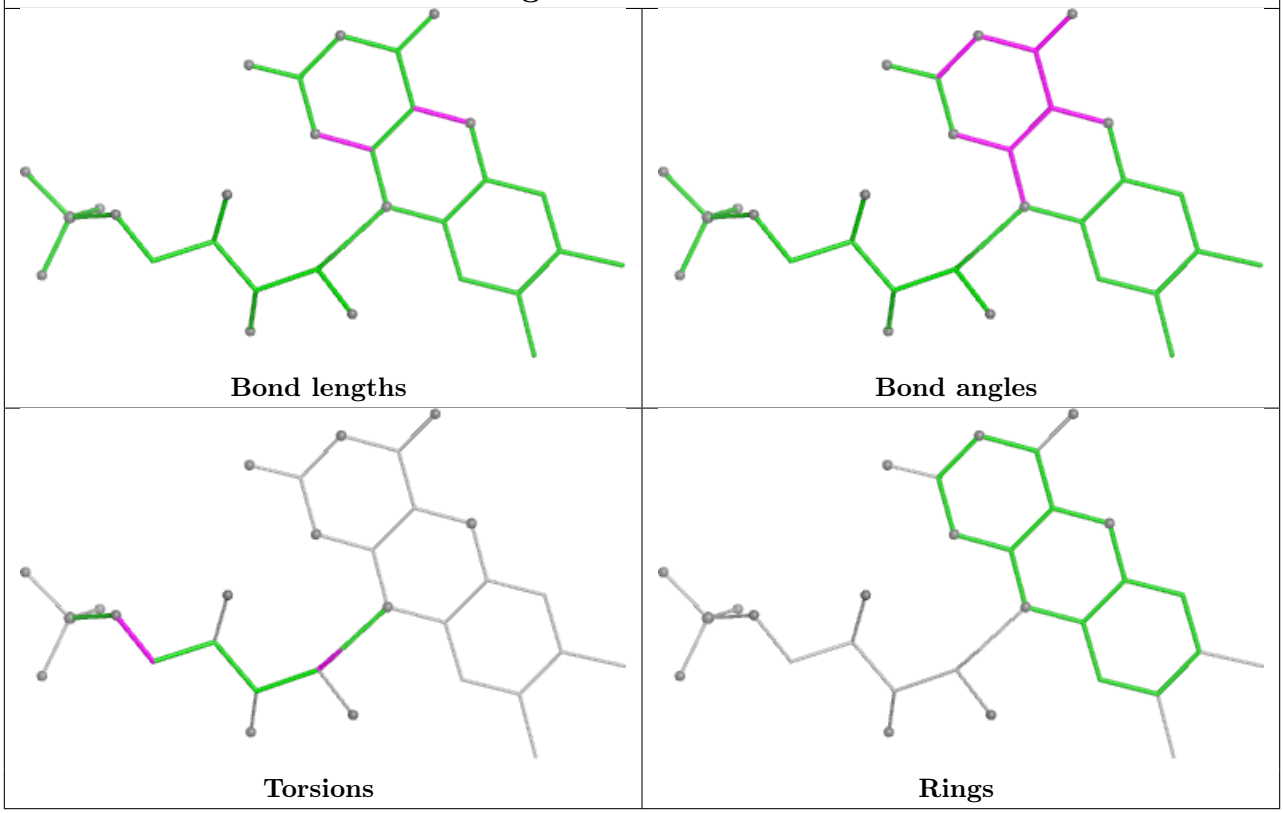
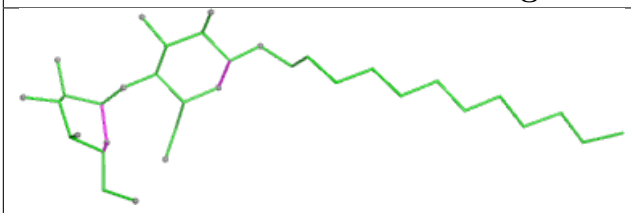
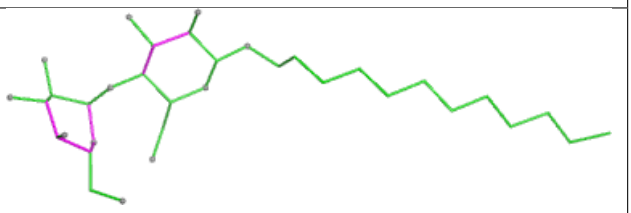
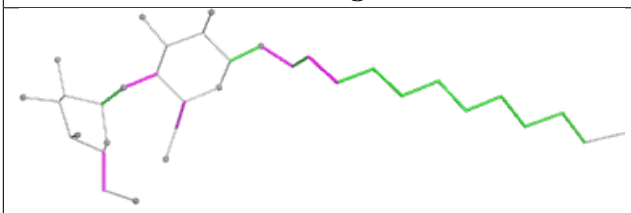
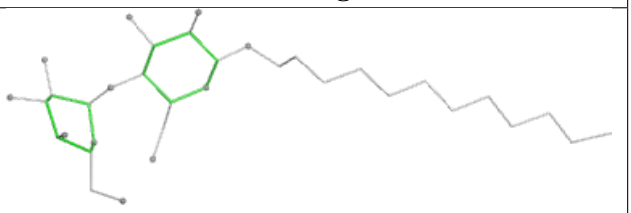


Ligand FMN F 501



Ligand LMT Y 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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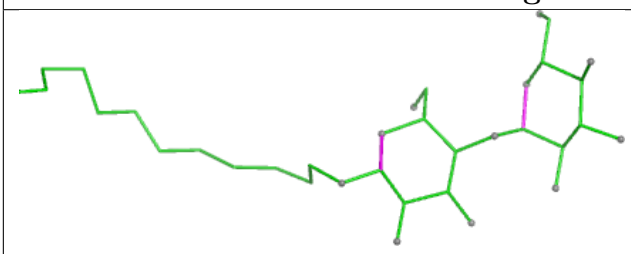
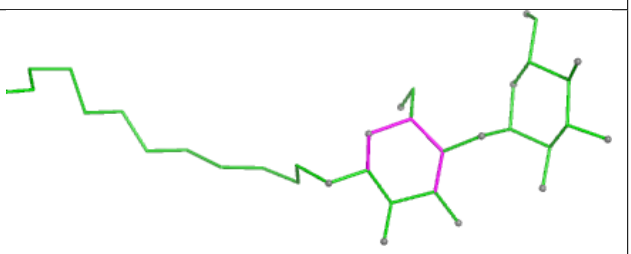
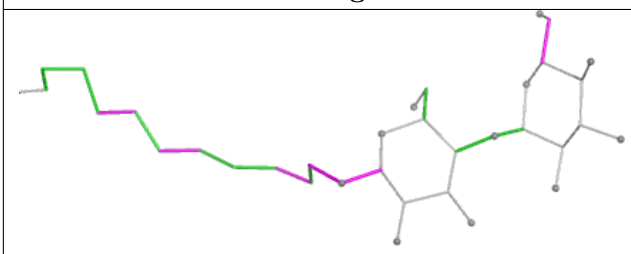
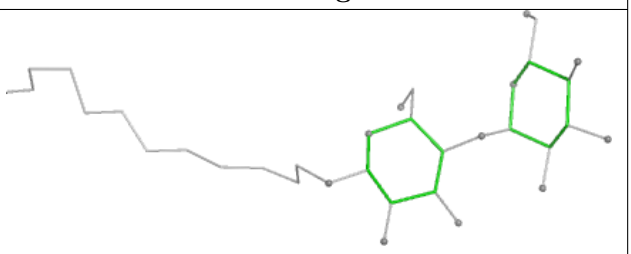
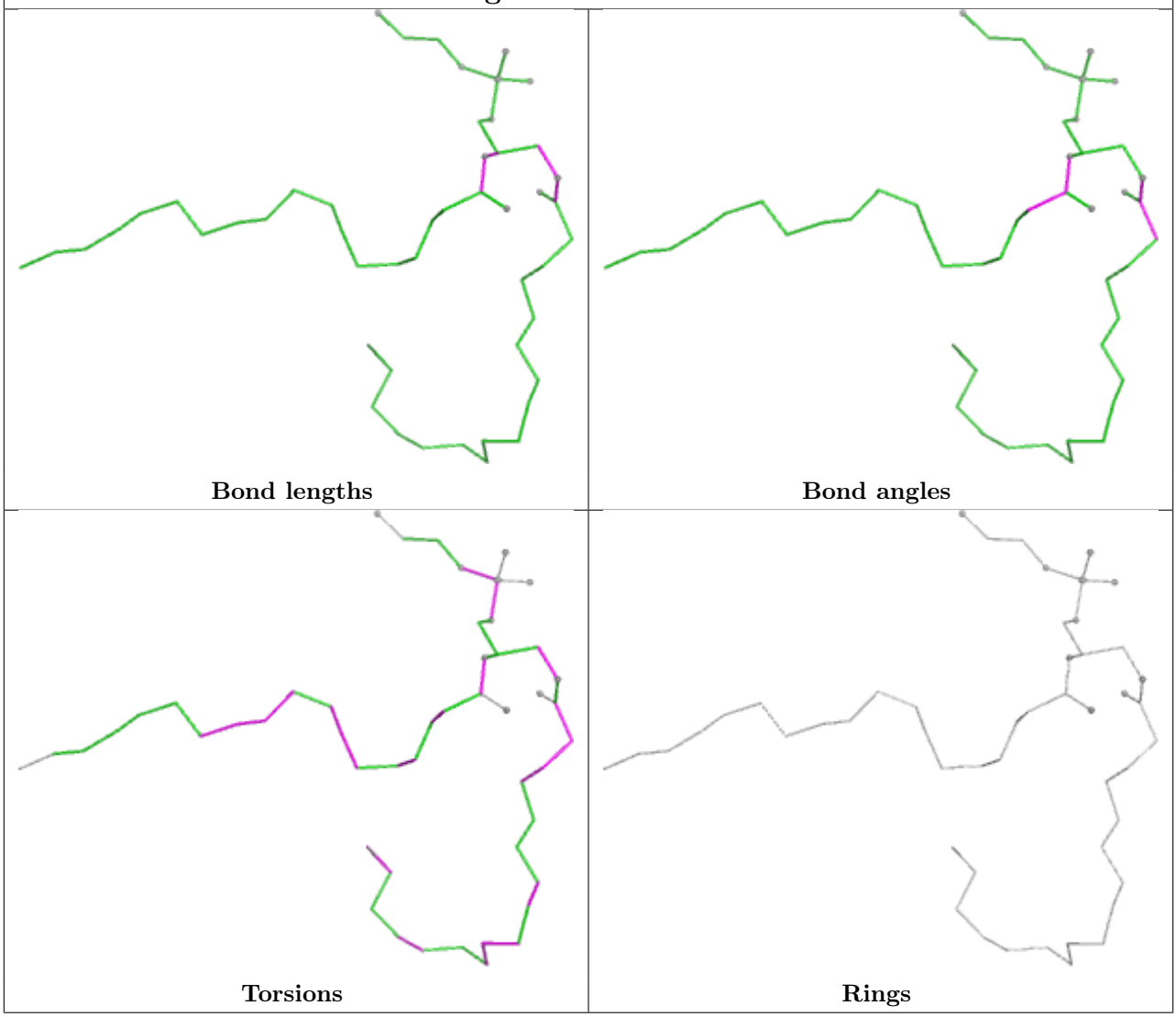
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE X 401



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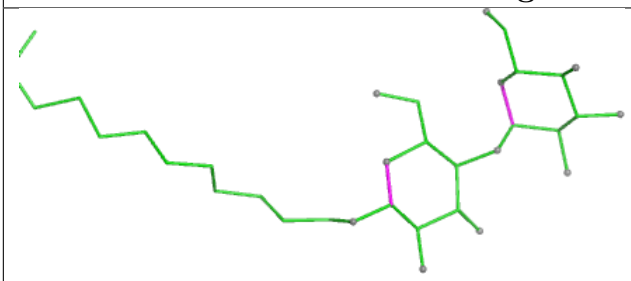
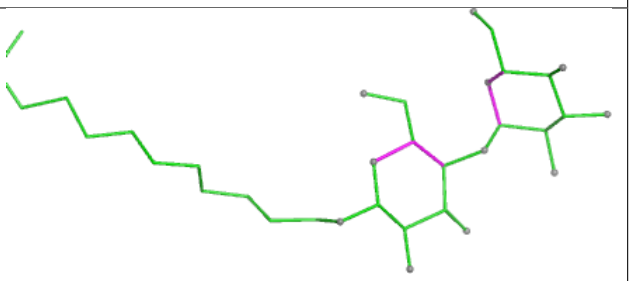
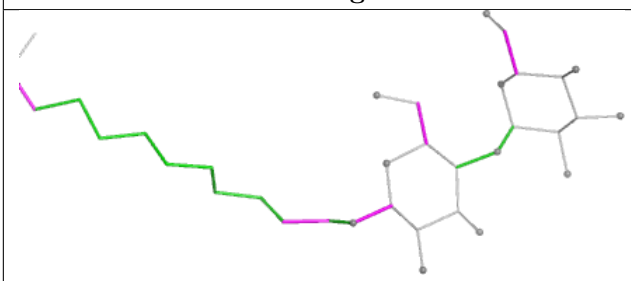
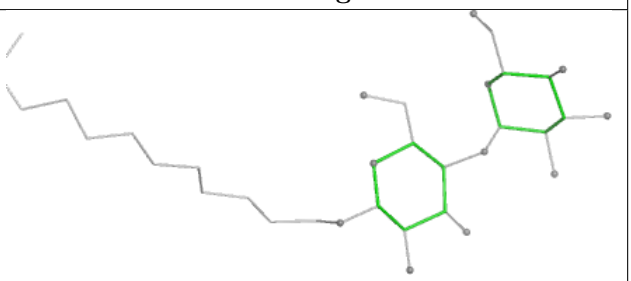
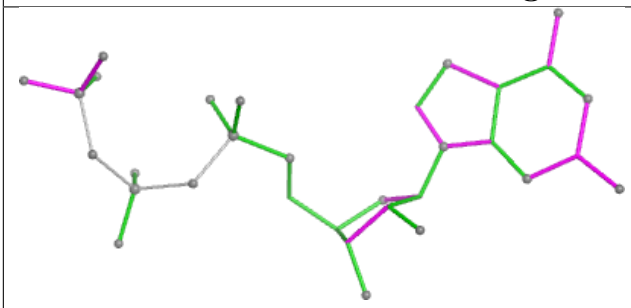
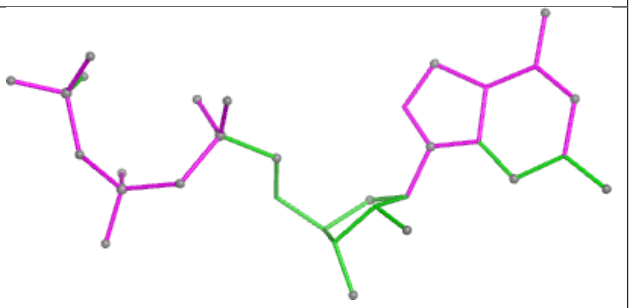
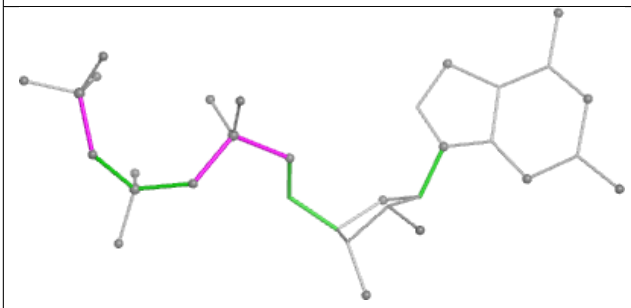
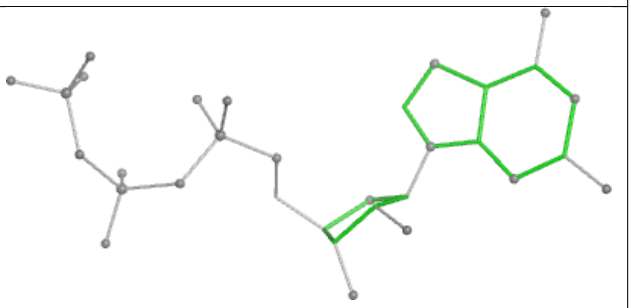
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP O 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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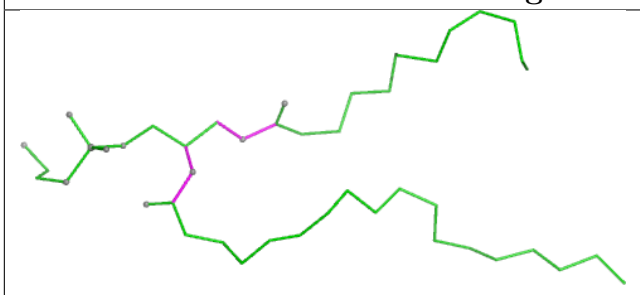
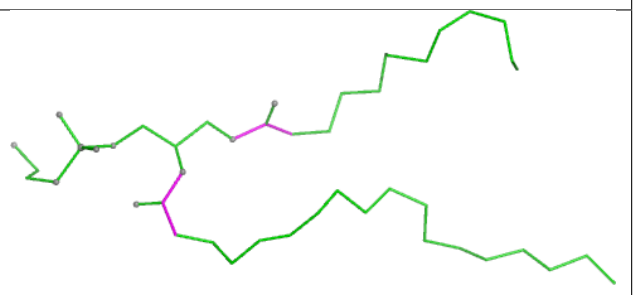
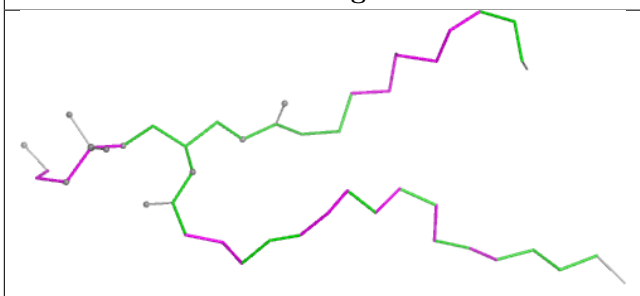
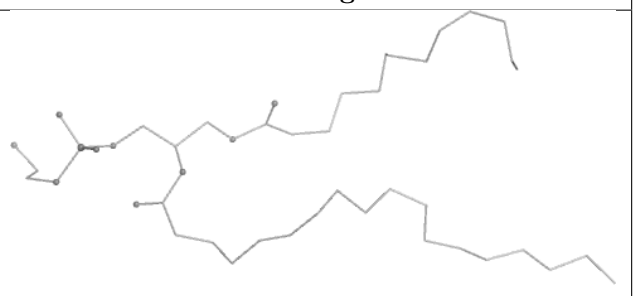
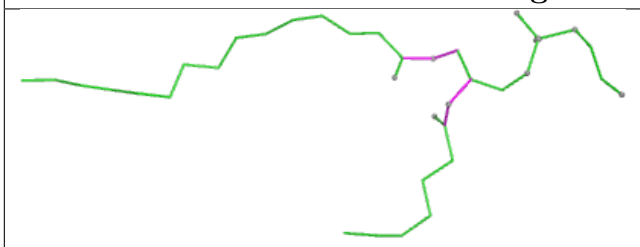
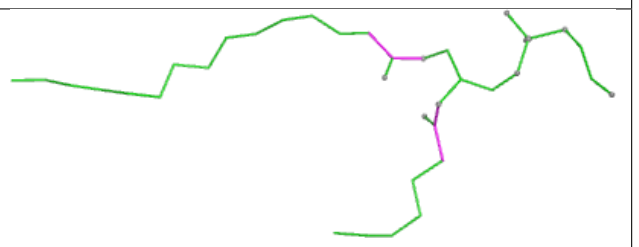
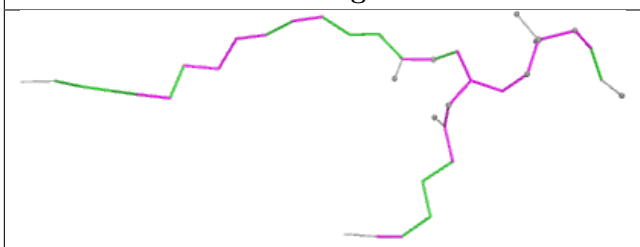
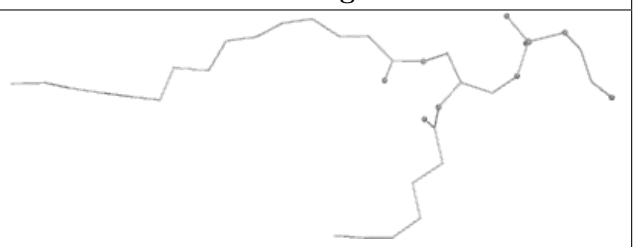
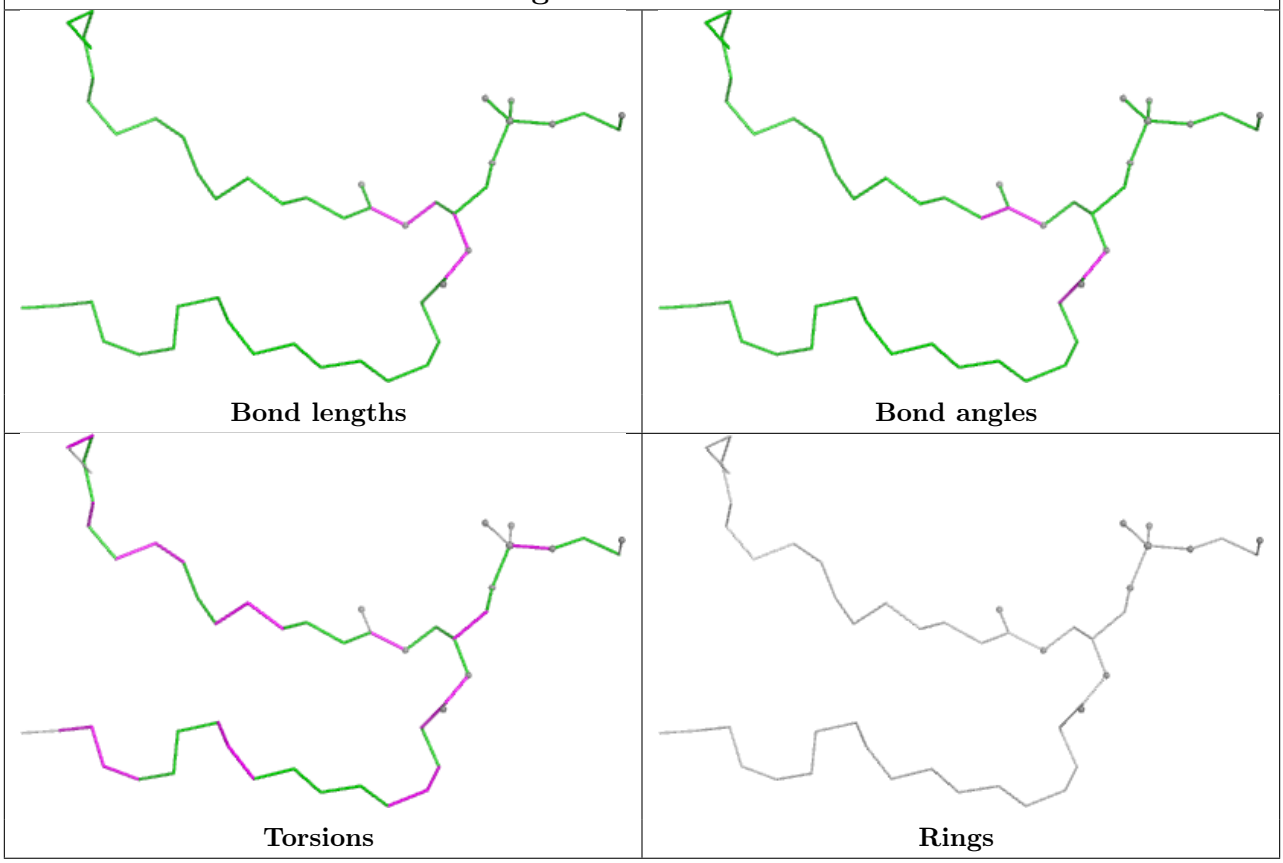
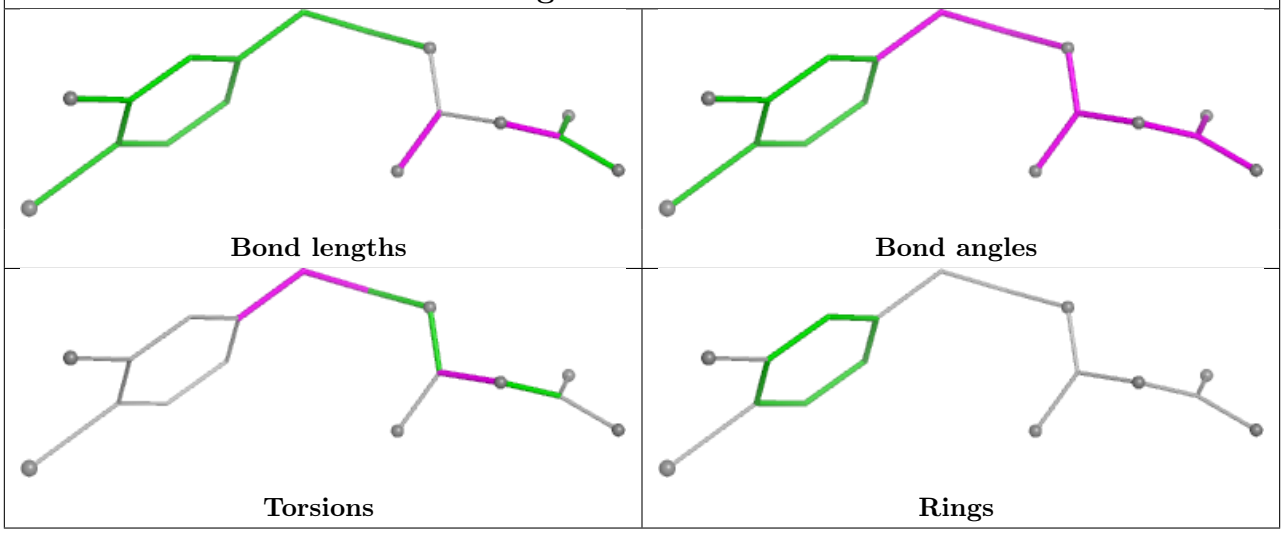
 Bond lengths	 Bond angles
 Torsions	 Rings

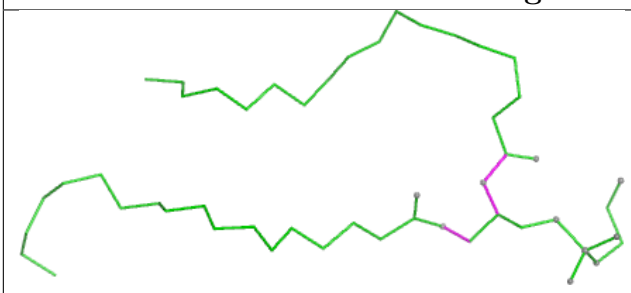
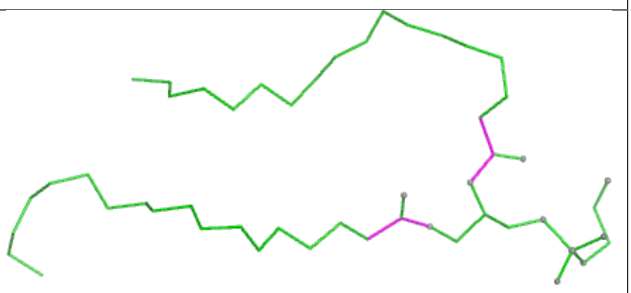
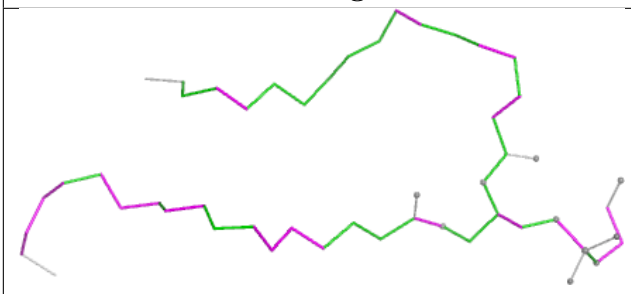
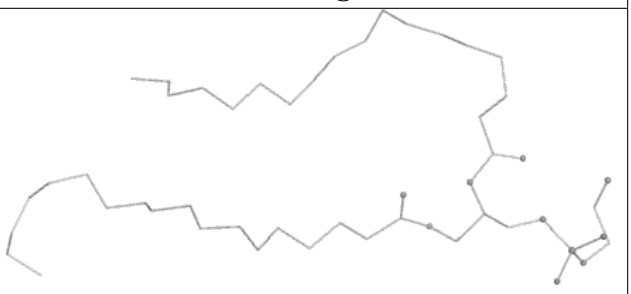
Ligand 3PE P 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 701

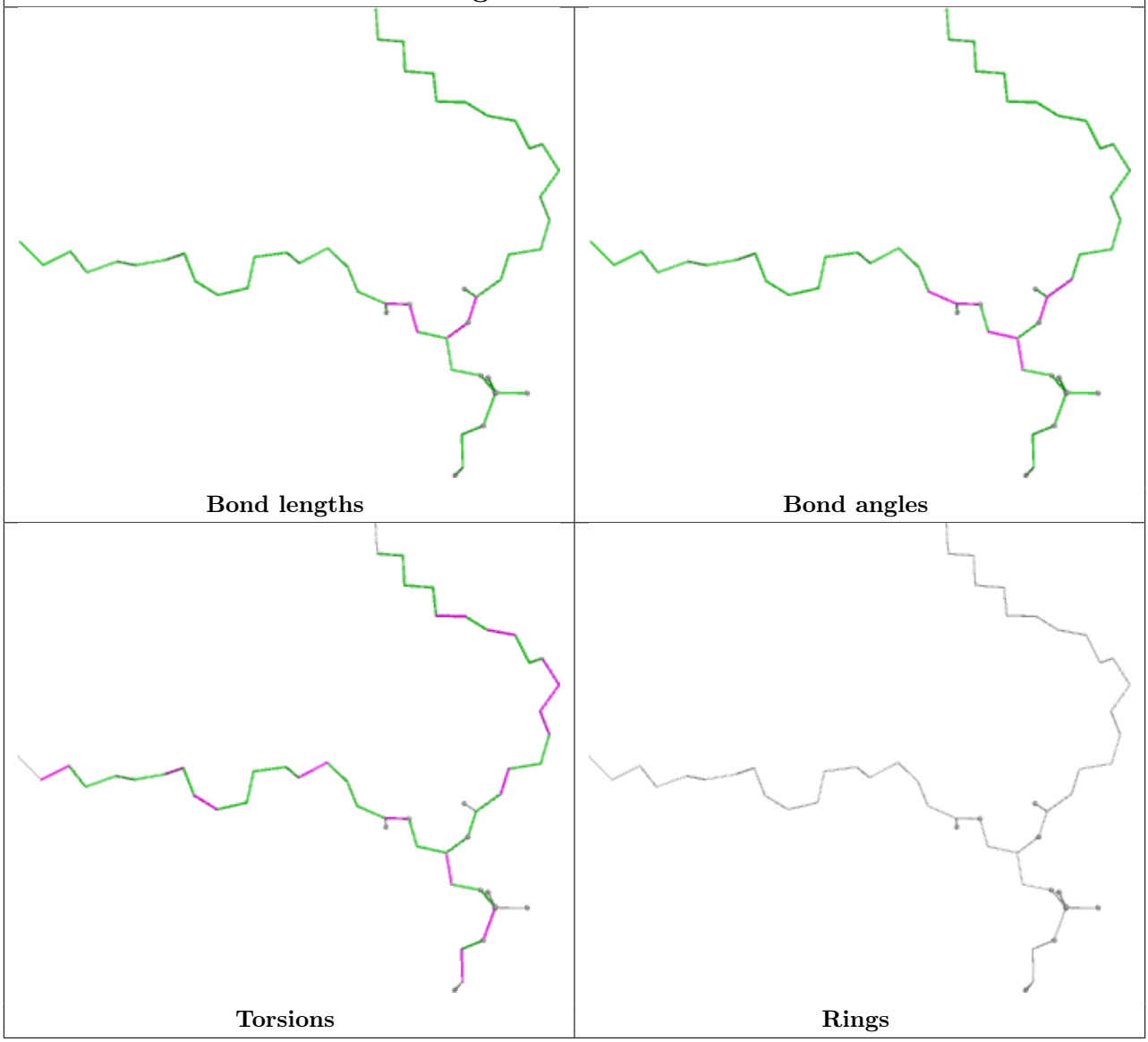


Ligand I49 N 703

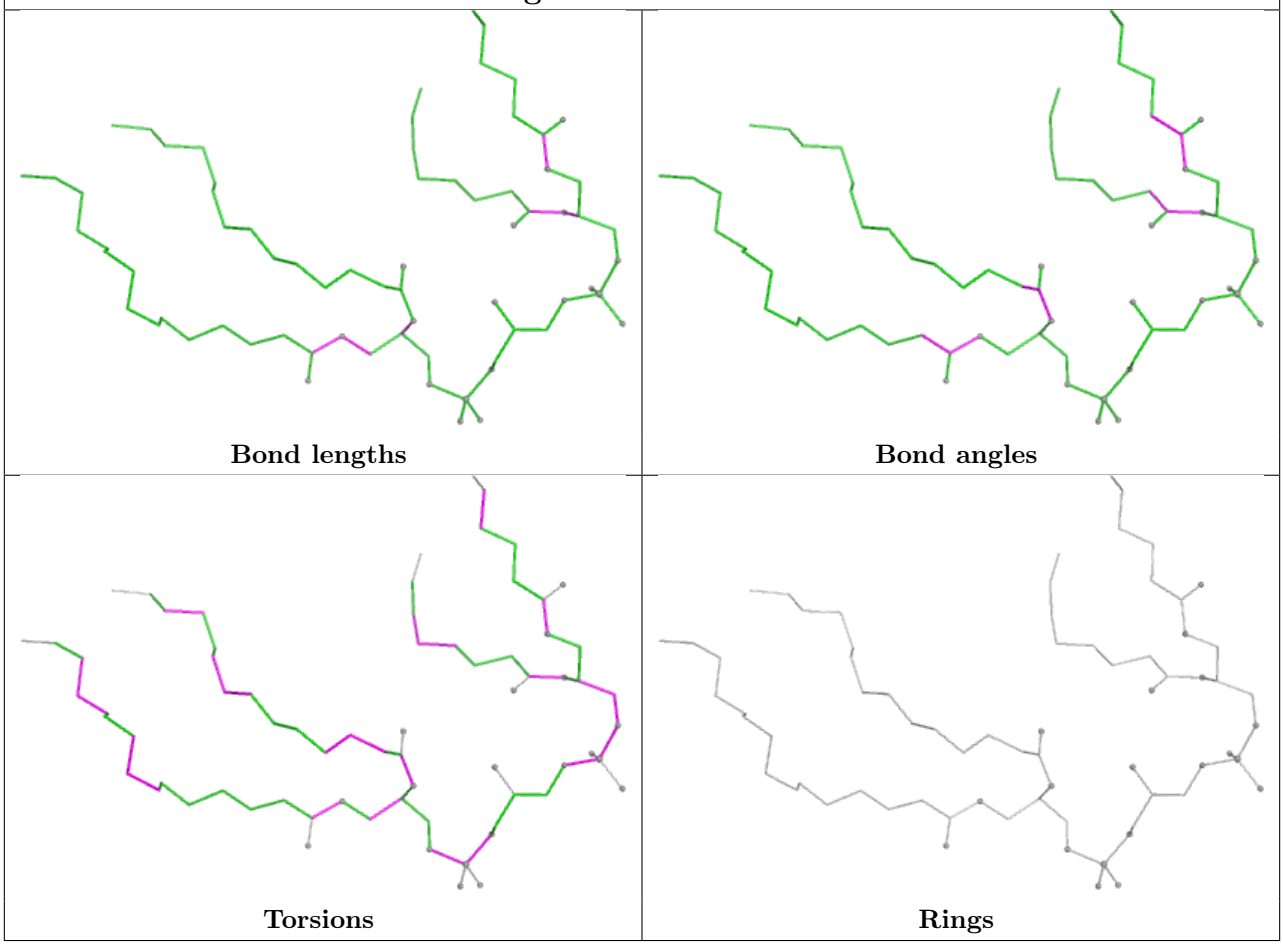


Ligand 3PE M 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

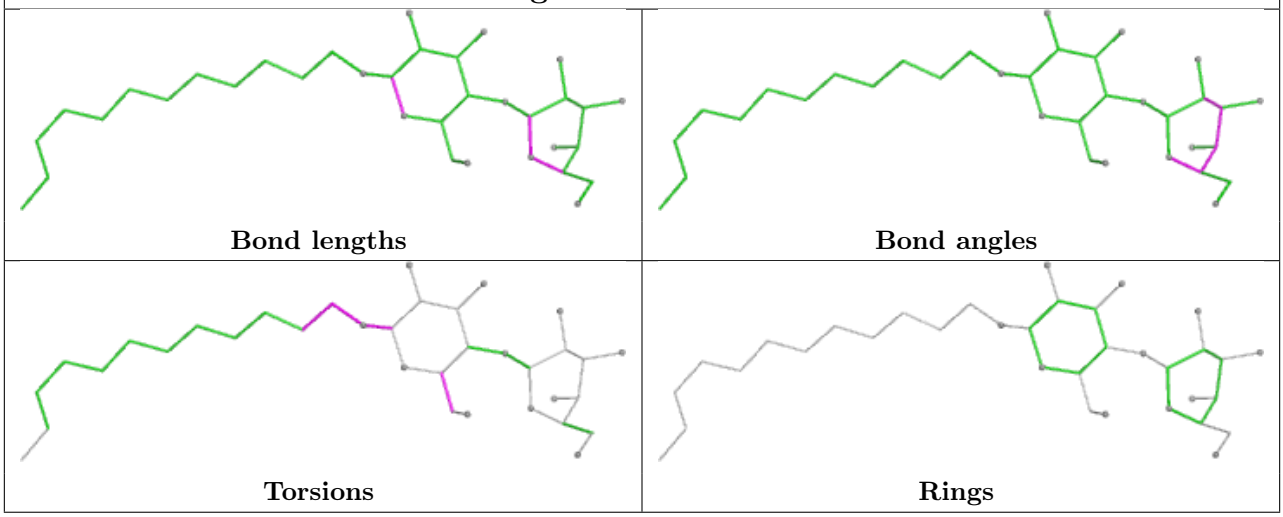
Ligand 3PE H 402



Ligand CDL K 502

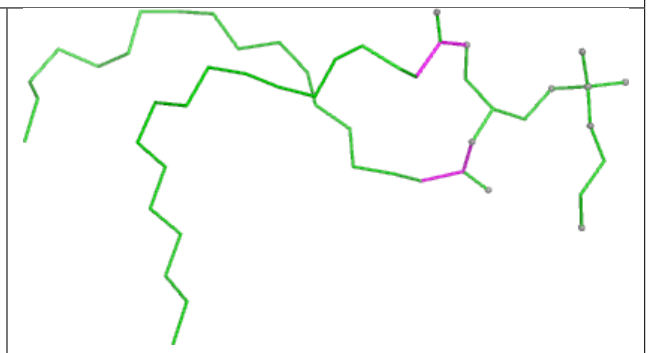


Ligand LMT l 201



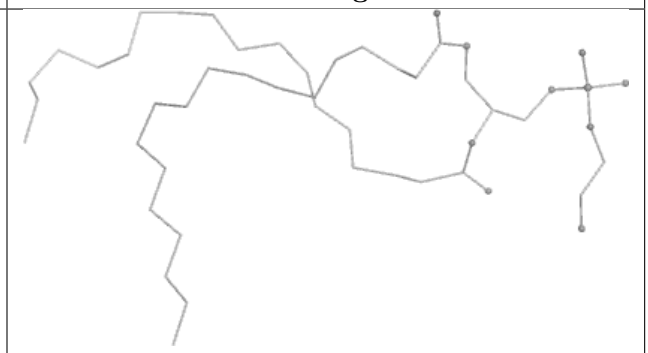
Ligand 3PE d 1201

Bond lengths



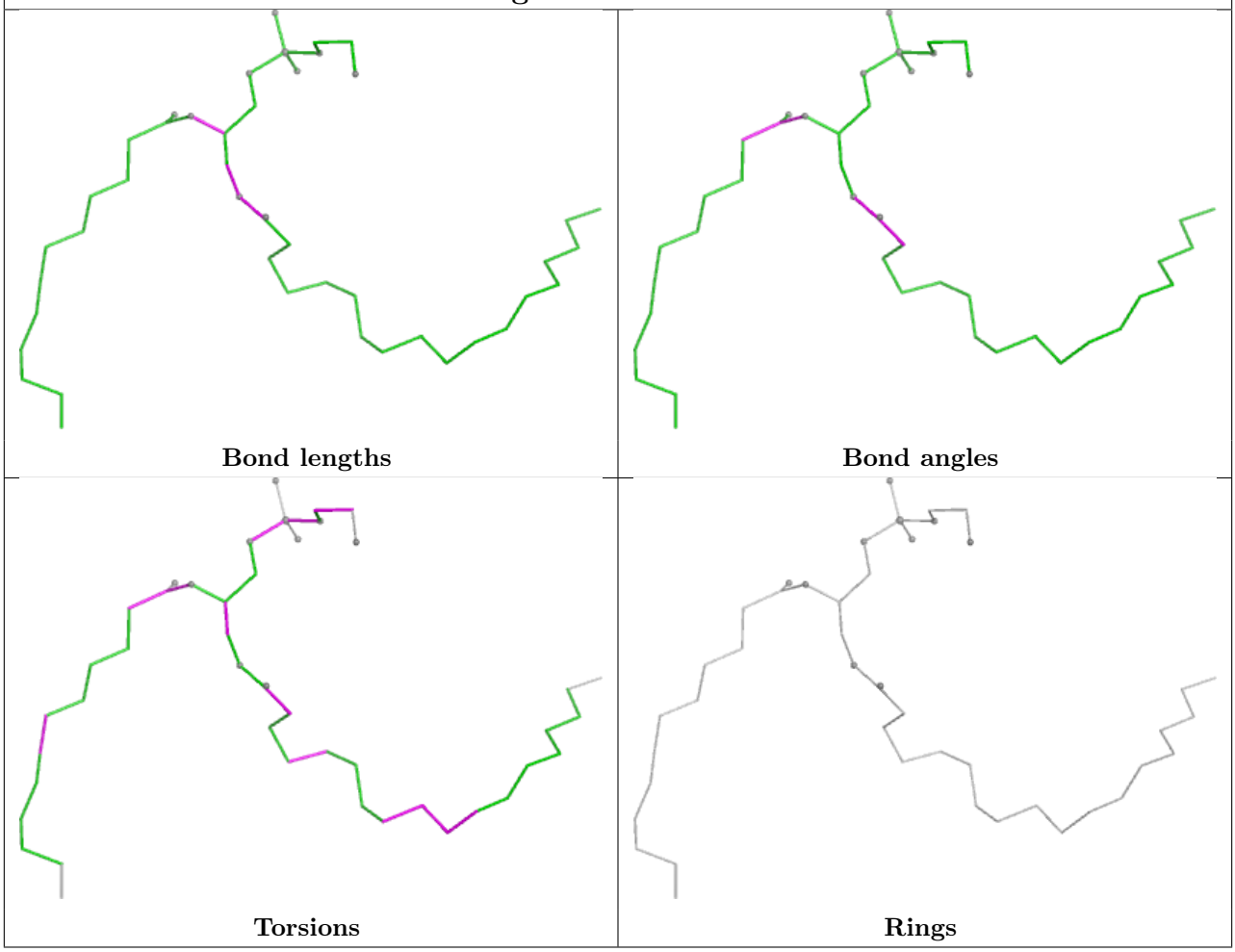
Bond angles

Torsions

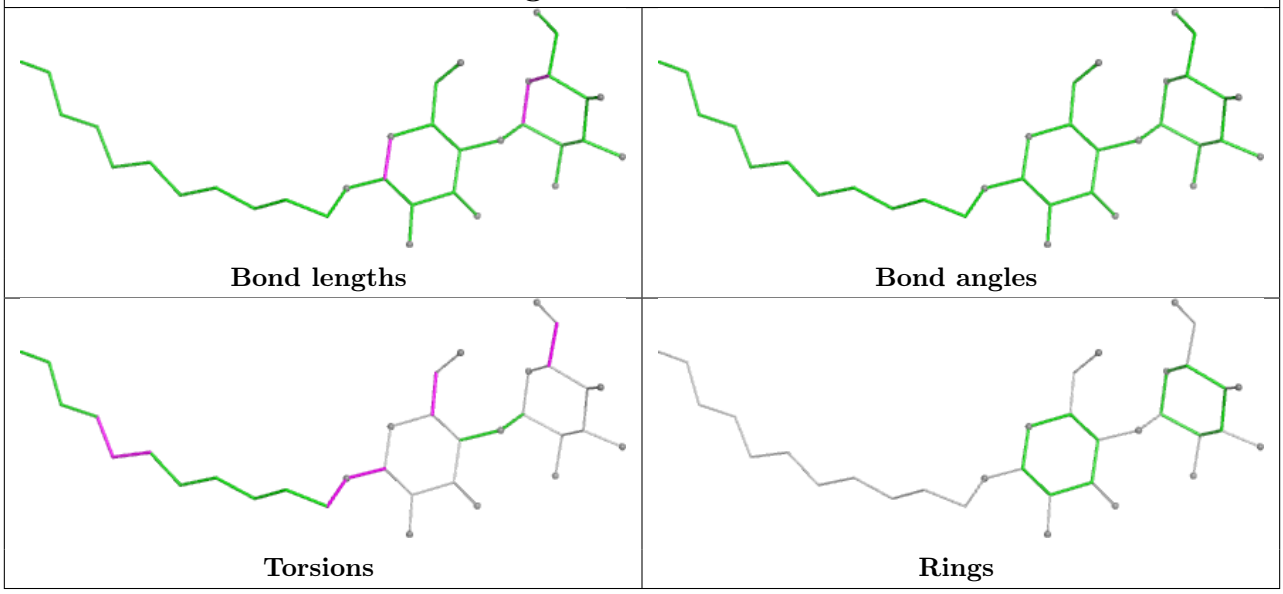


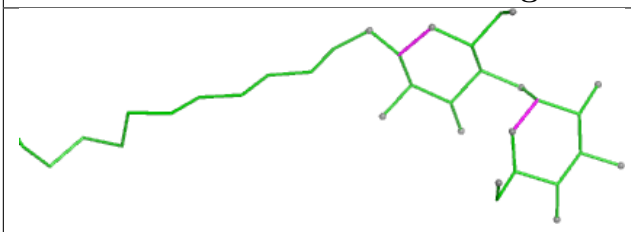
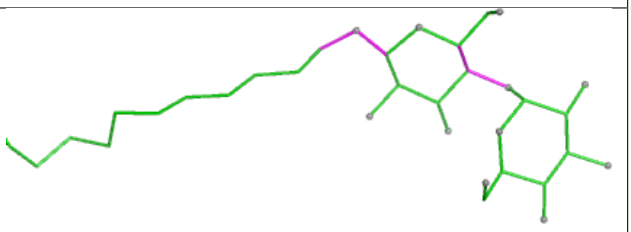
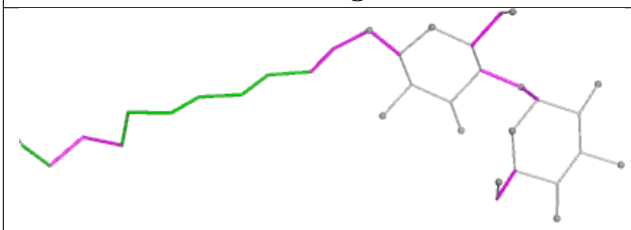
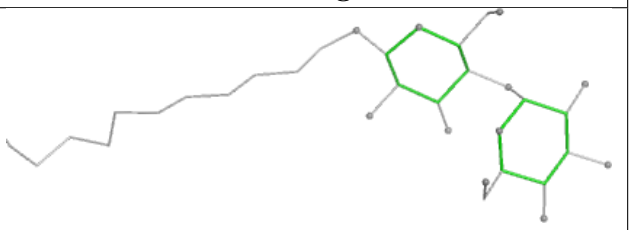
Rings

Ligand 3PE L 705

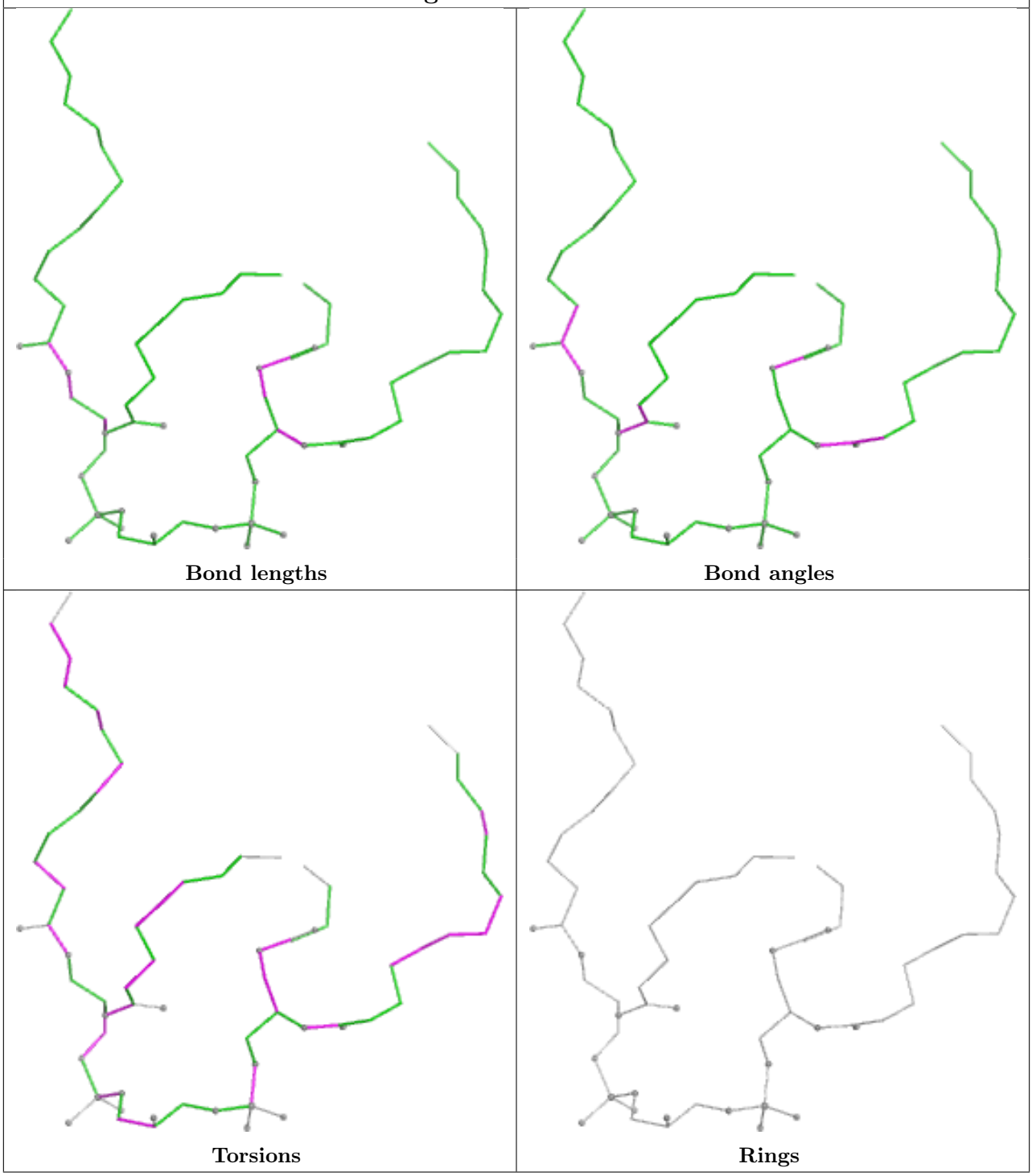


Ligand LMT L 702

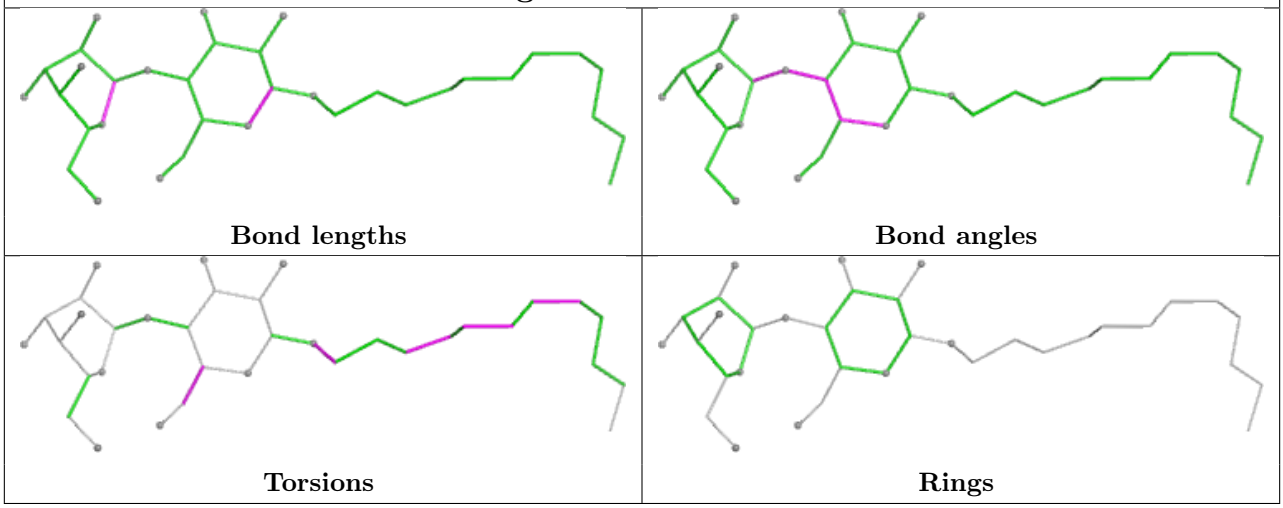


Ligand LMT A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

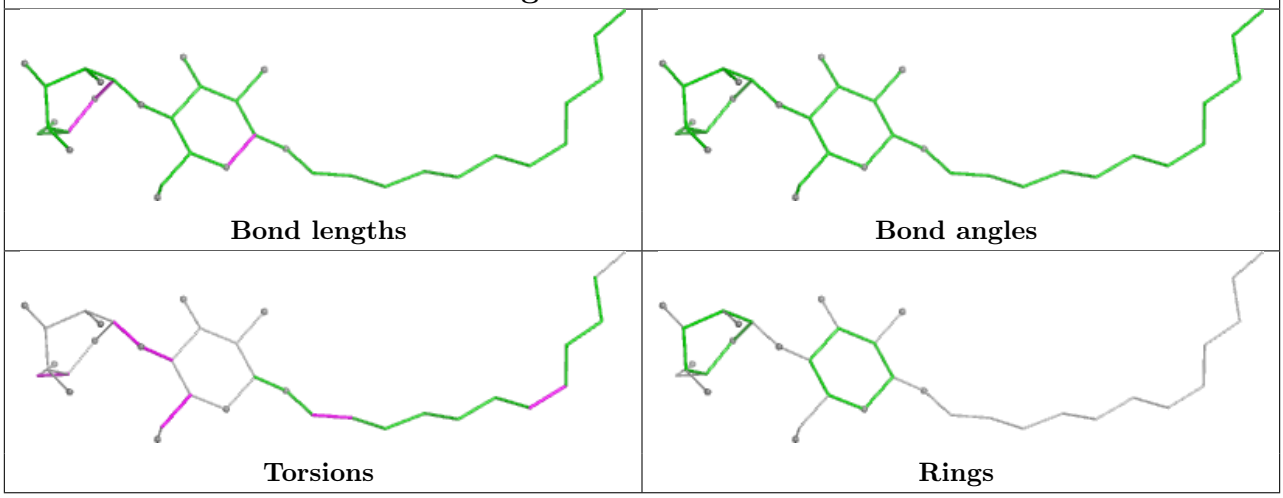
Ligand CDL L 703



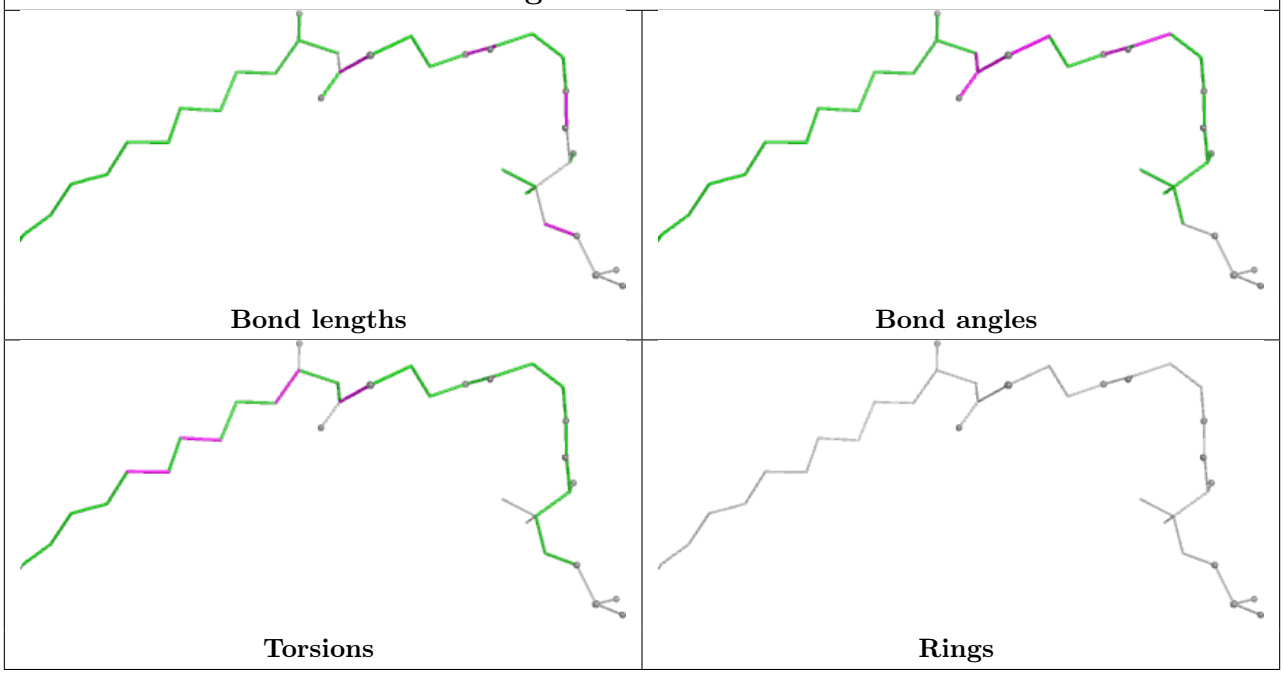
Ligand LMT h 1002

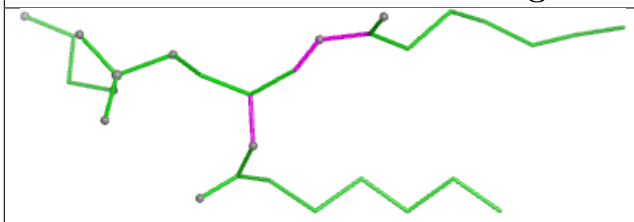
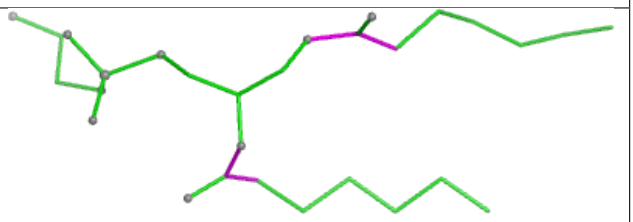
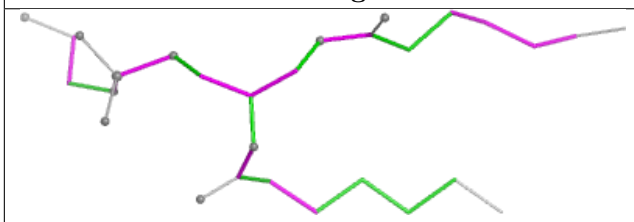
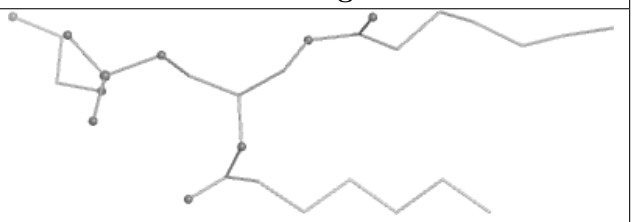


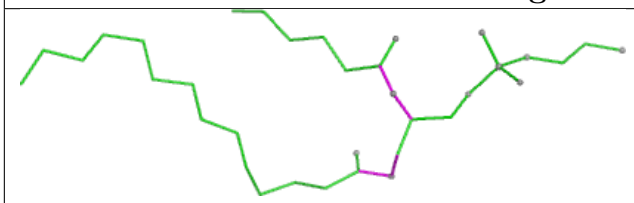
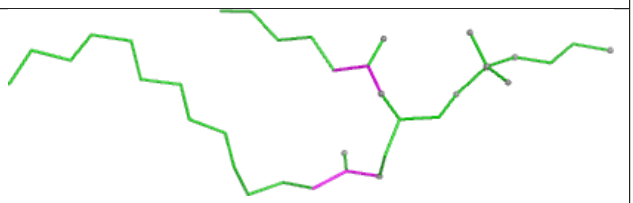
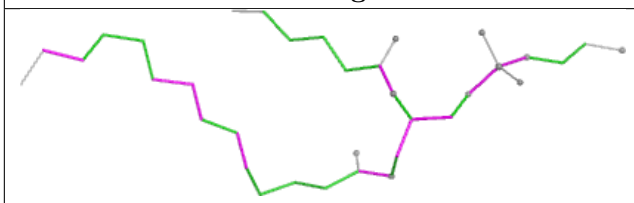
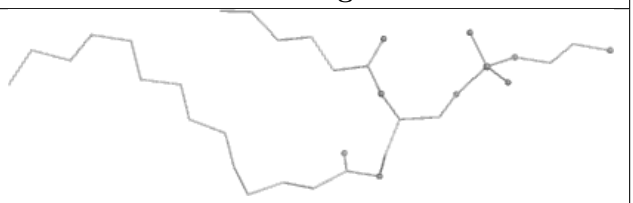
Ligand LMT K 501



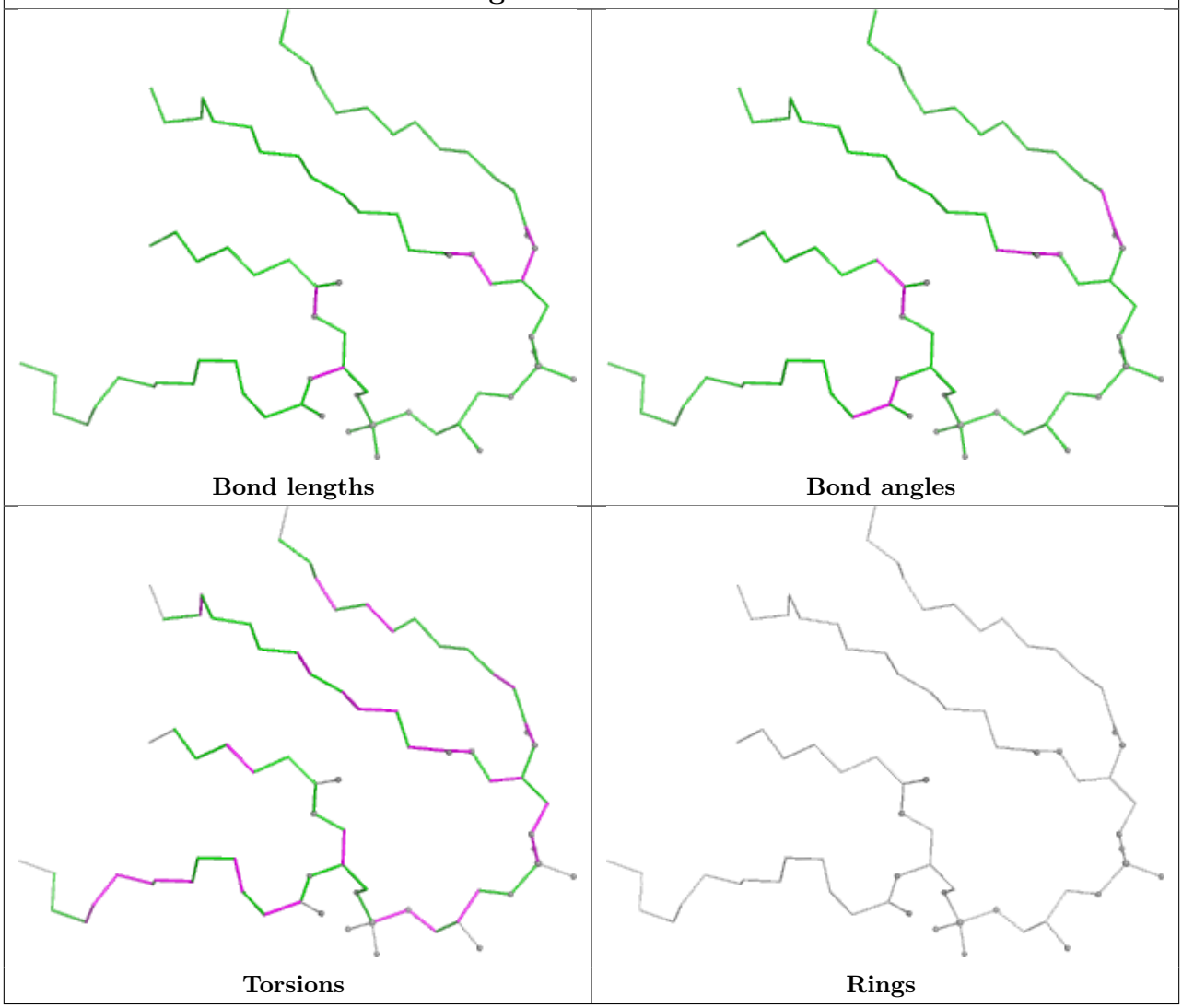
Ligand EHZ U 101



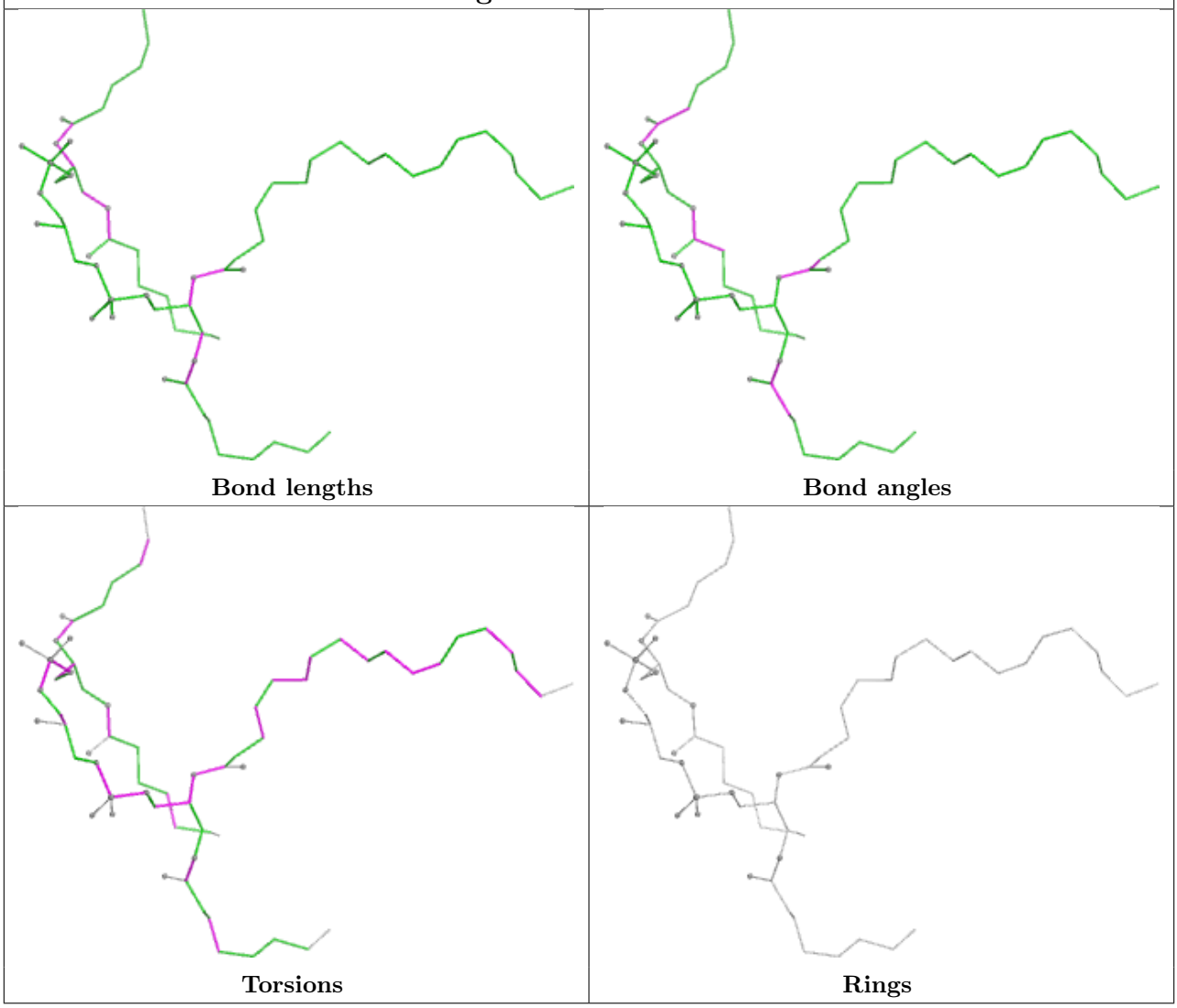
Ligand 3PE N 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE Y 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

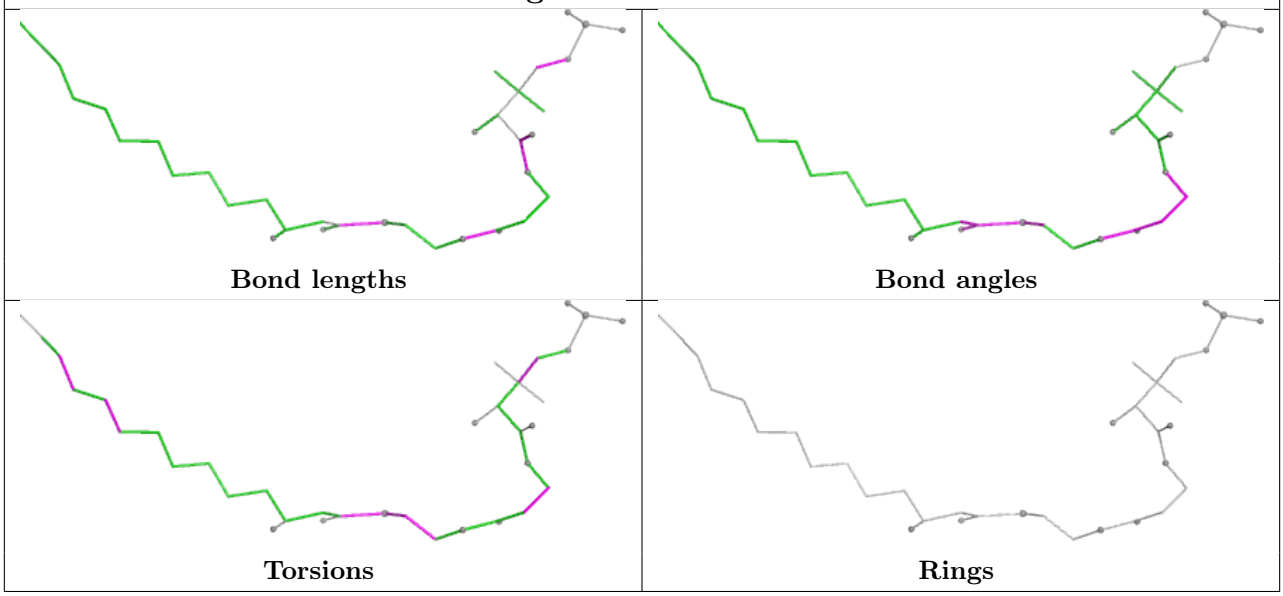
Ligand CDL r 201



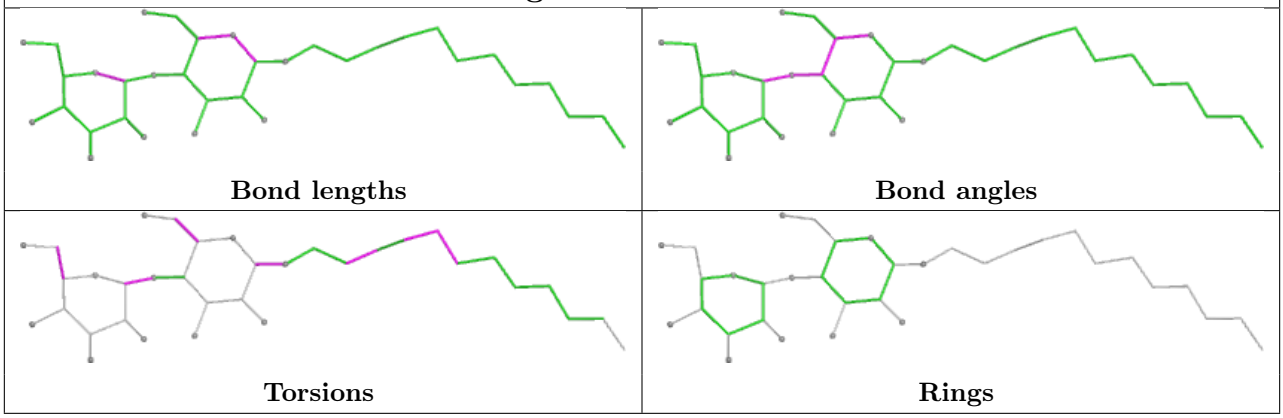
Ligand CDL h 1001



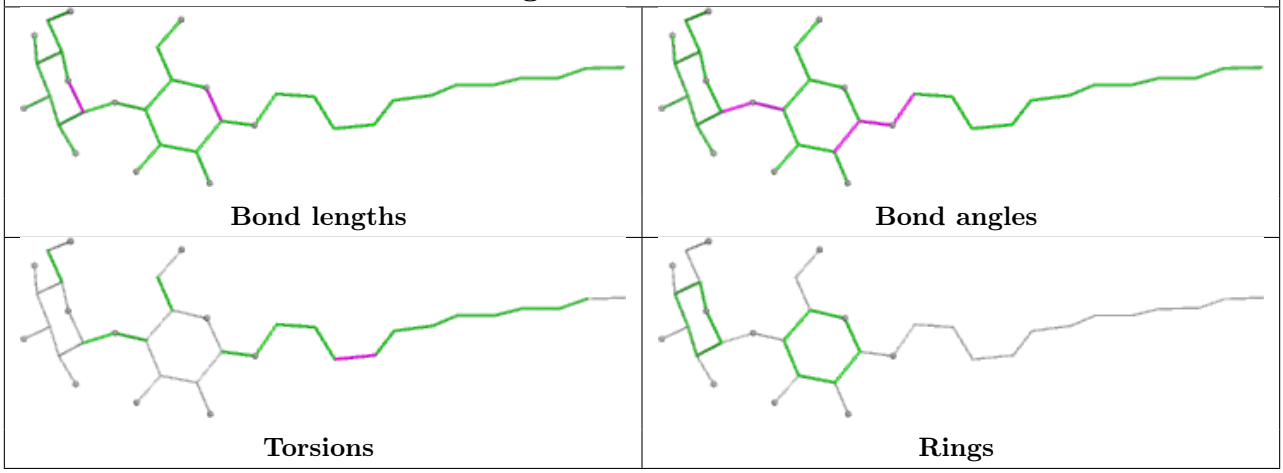
Ligand EHZ T 101



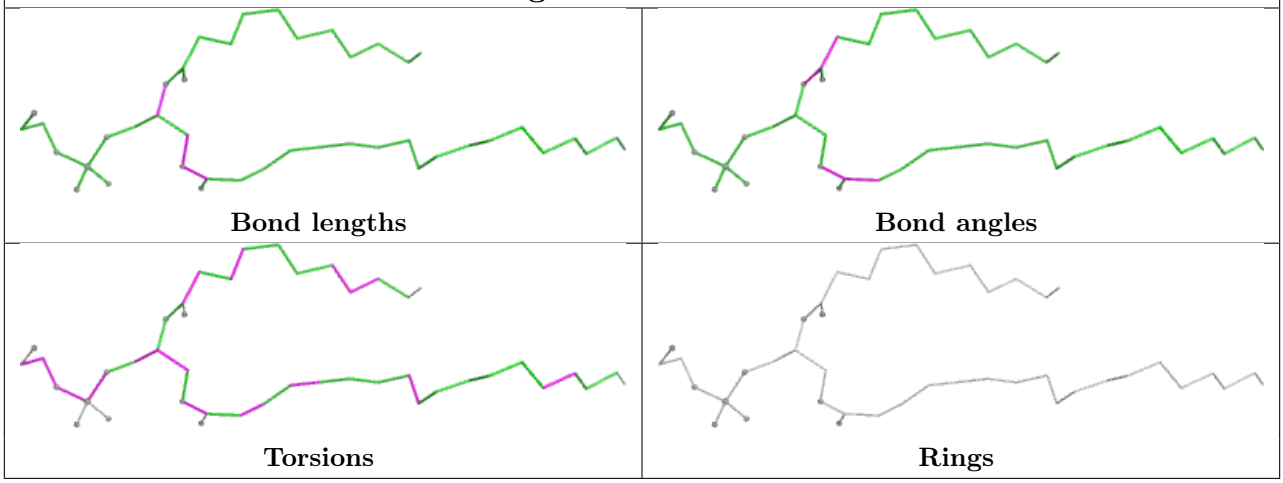
Ligand LMT J 702



Ligand LMT A 301



Ligand 3PE H 401



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.

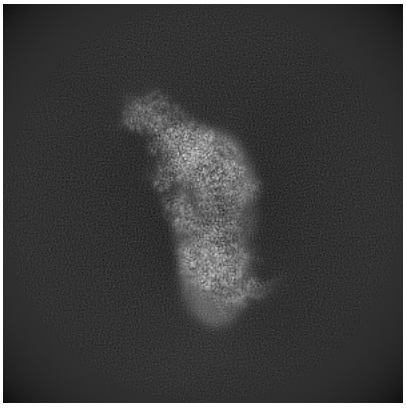
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14256. These allow visual inspection of the internal detail of the map and identification of artifacts.

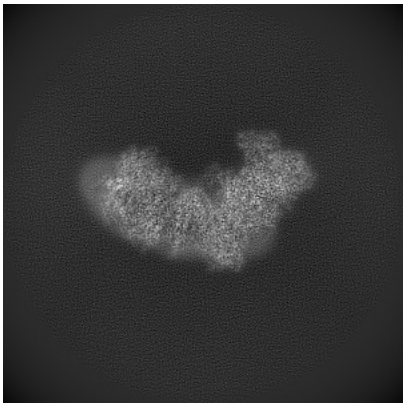
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

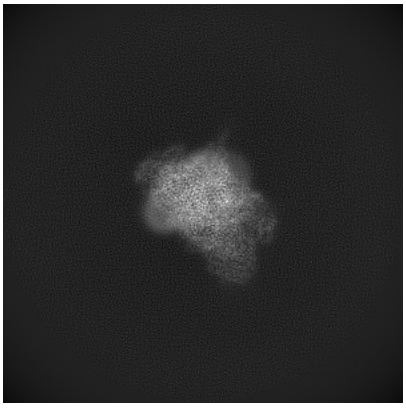
6.1.1 Primary map



X



Y

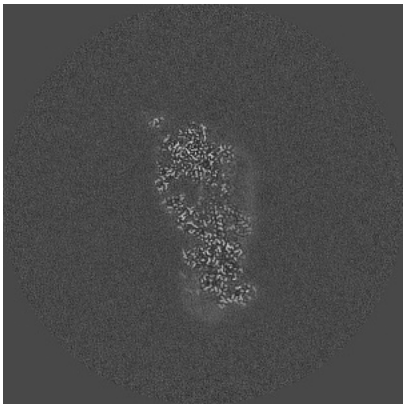


Z

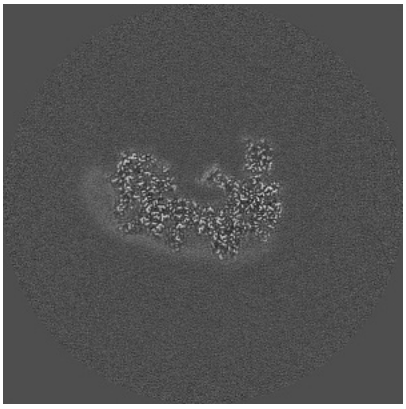
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

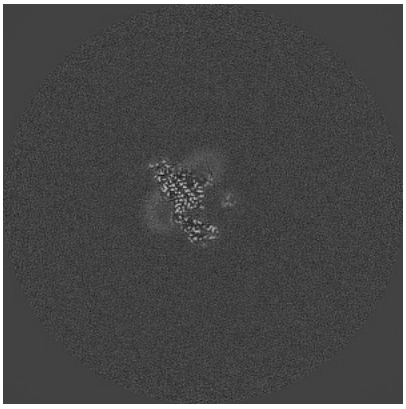
6.2.1 Primary map



X Index: 330



Y Index: 330

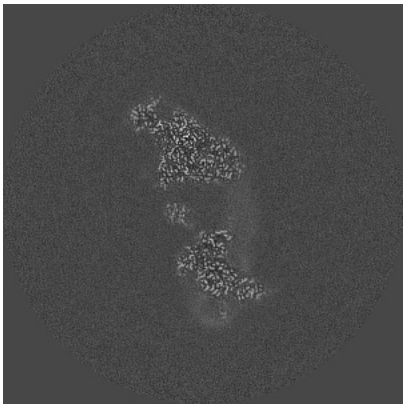


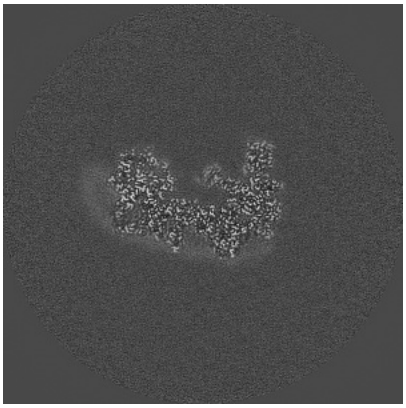
Z Index: 330

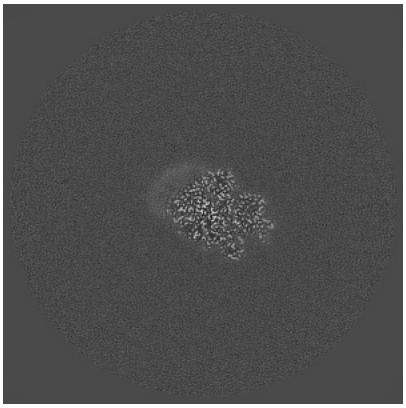
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 353

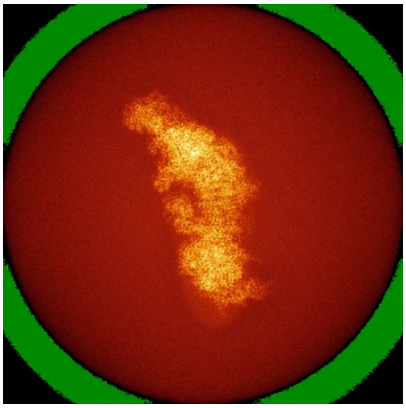

Y Index: 333

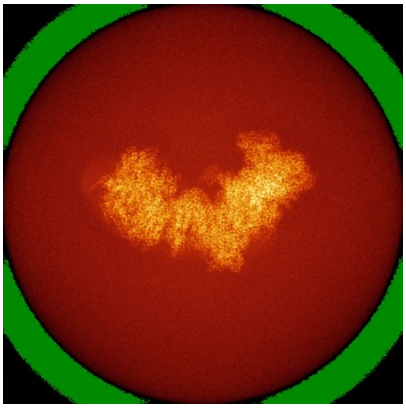

Z Index: 421

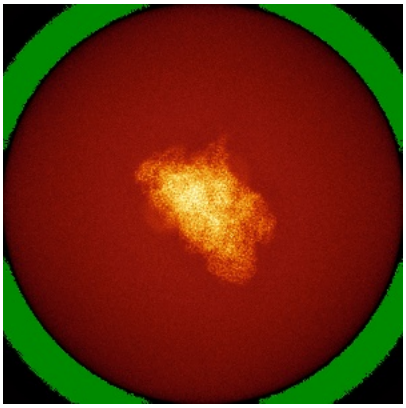
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

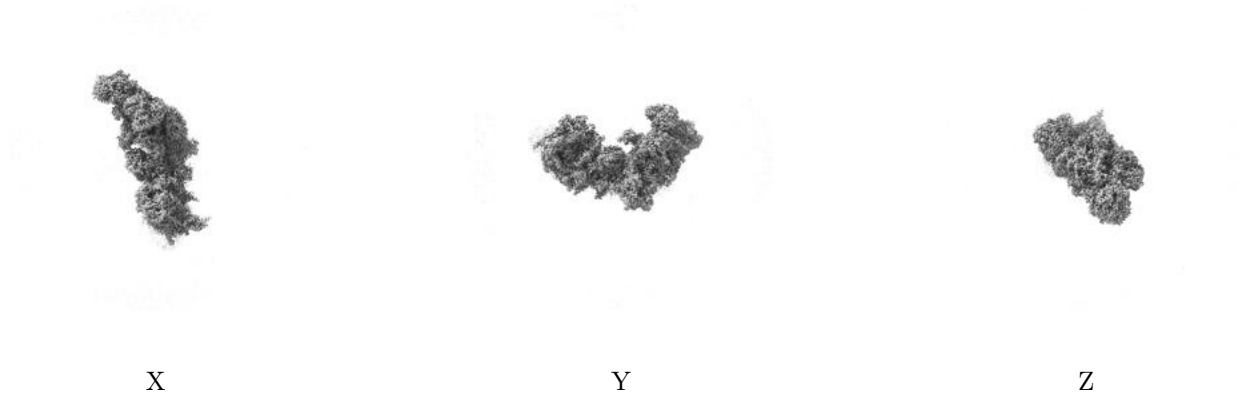

Y


Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

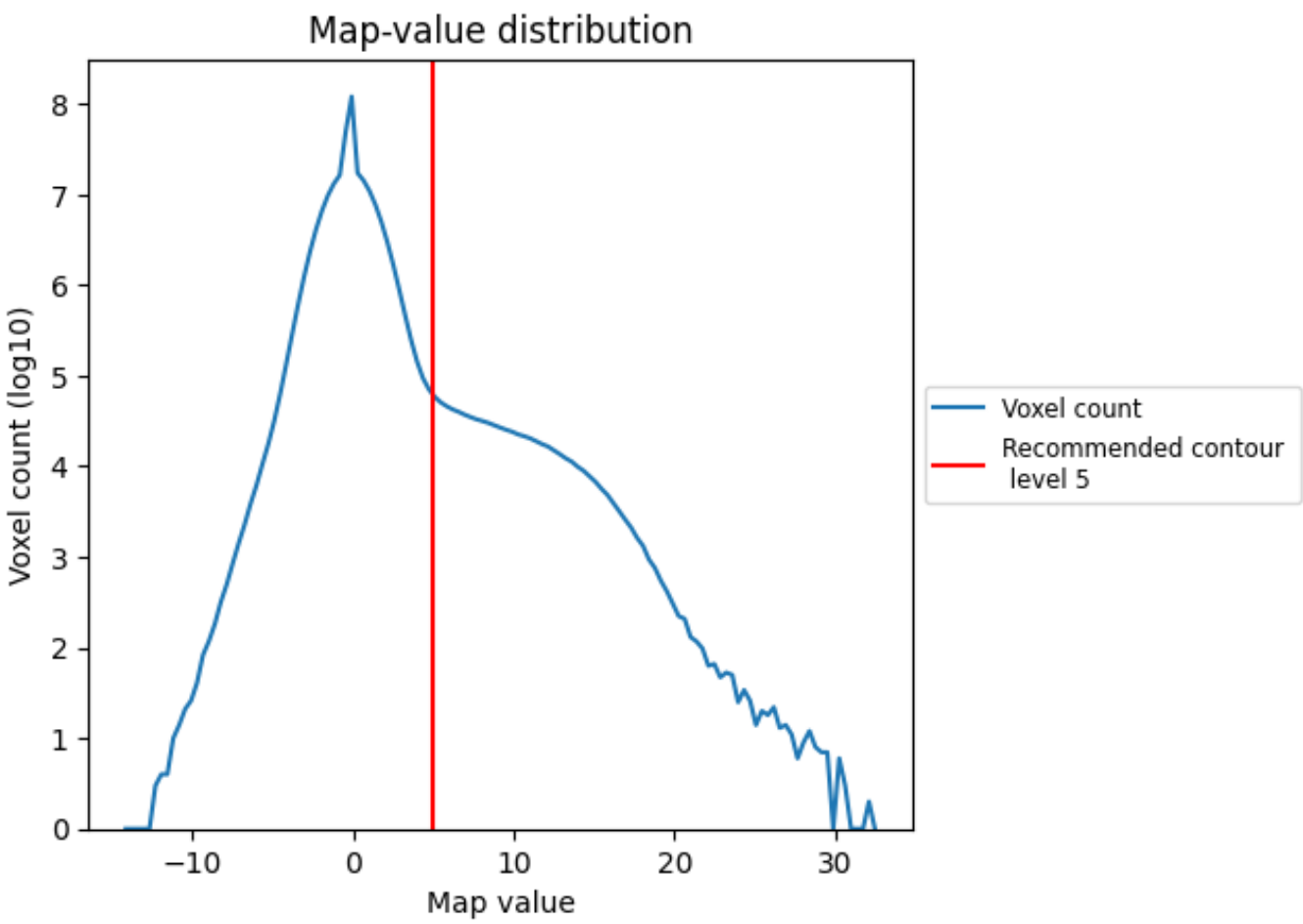
6.6 Mask visualisation (i)

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

7 Map analysis (i)

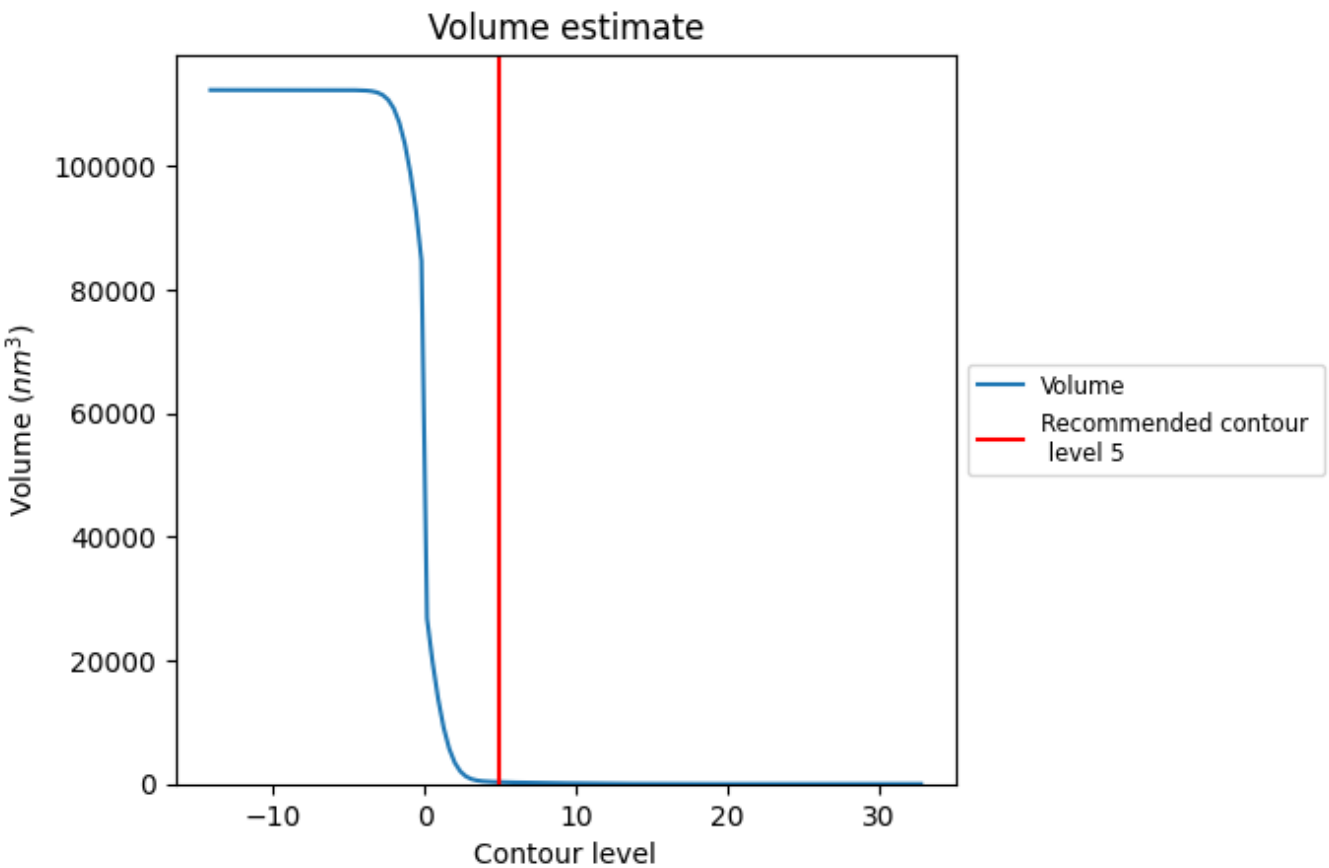
This section contains the results of statistical analysis of the map.

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.

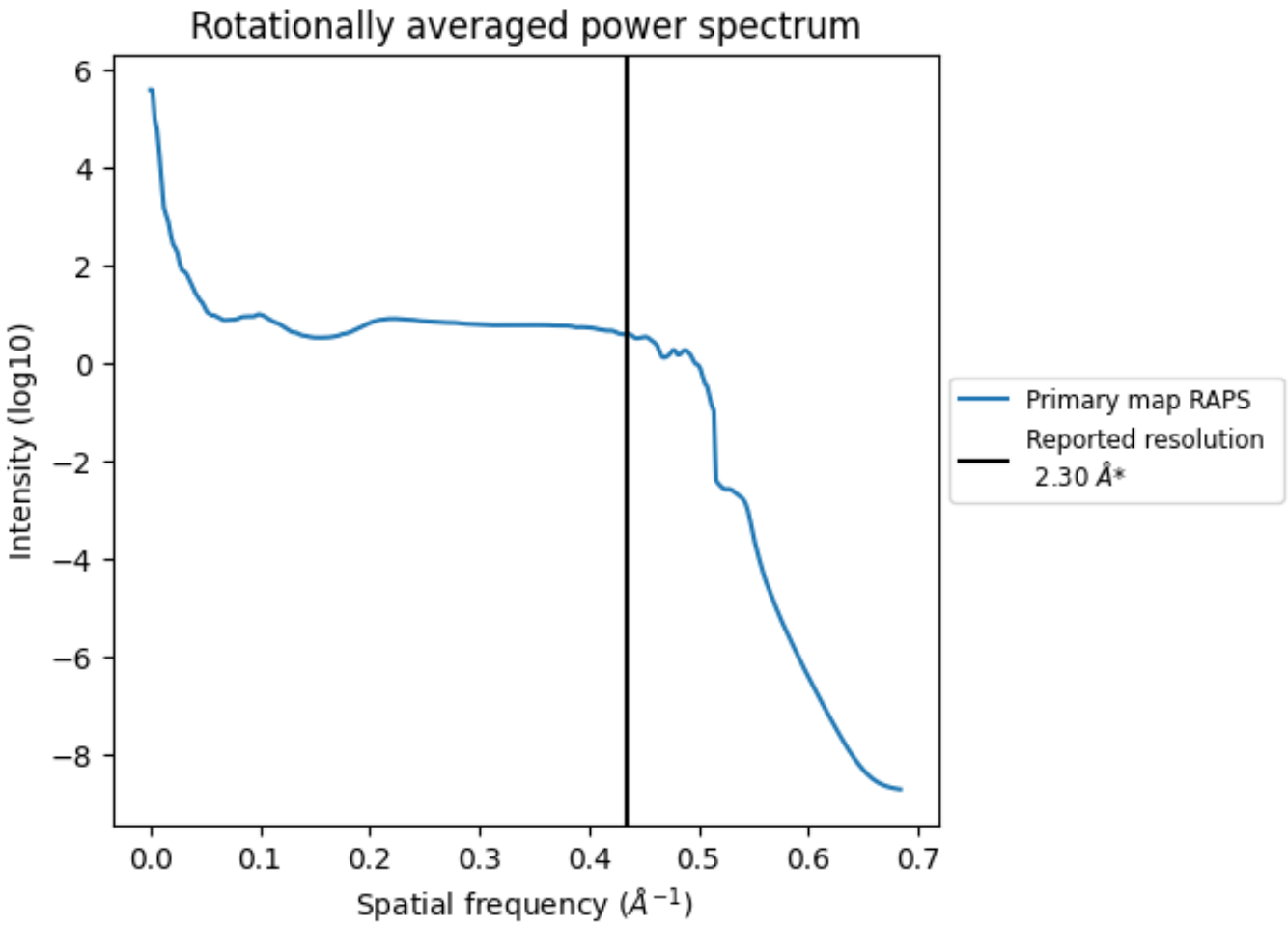
7.2 Volume estimate (i)



The volume at the recommended contour level is 297 nm^3; this corresponds to an approximate mass of 269 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

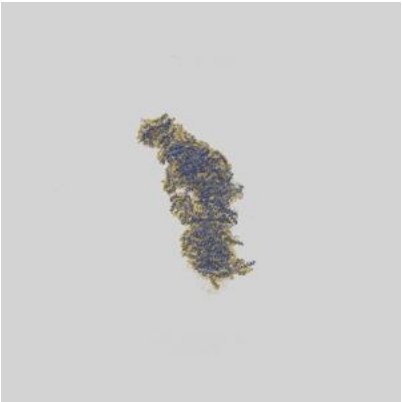
8 Fourier-Shell correlation (i)

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

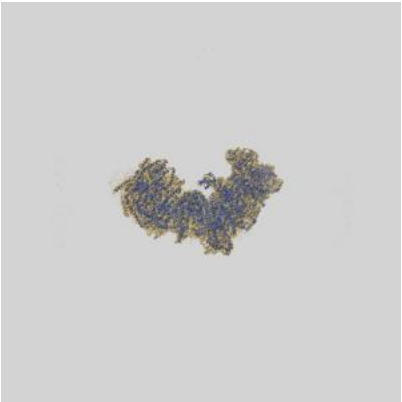
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14256 and PDB model 7R42. Per-residue inclusion information can be found in section 3 on page 23.

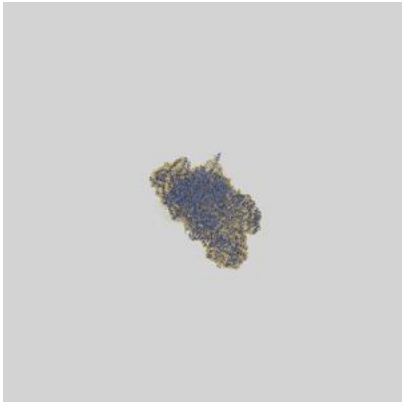
9.1 Map-model overlay (i)



X



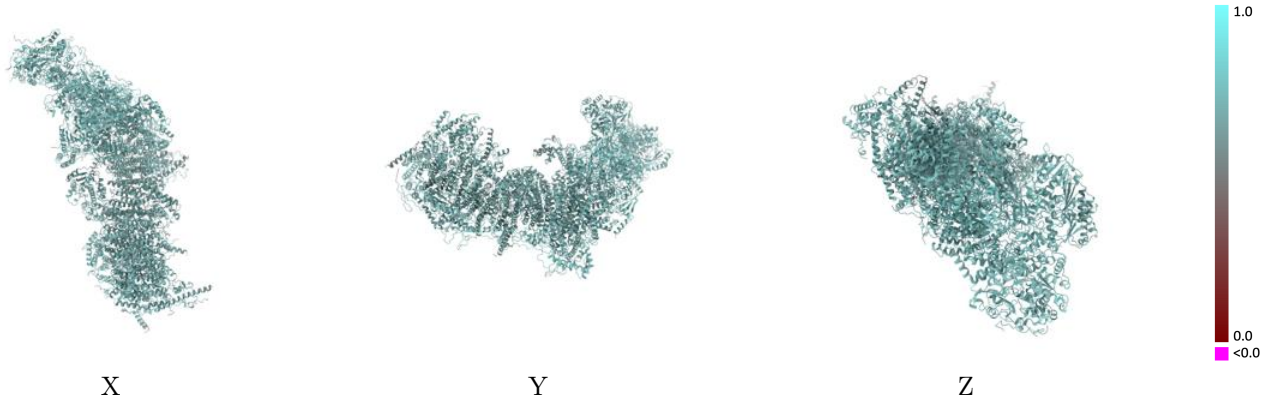
Y



Z

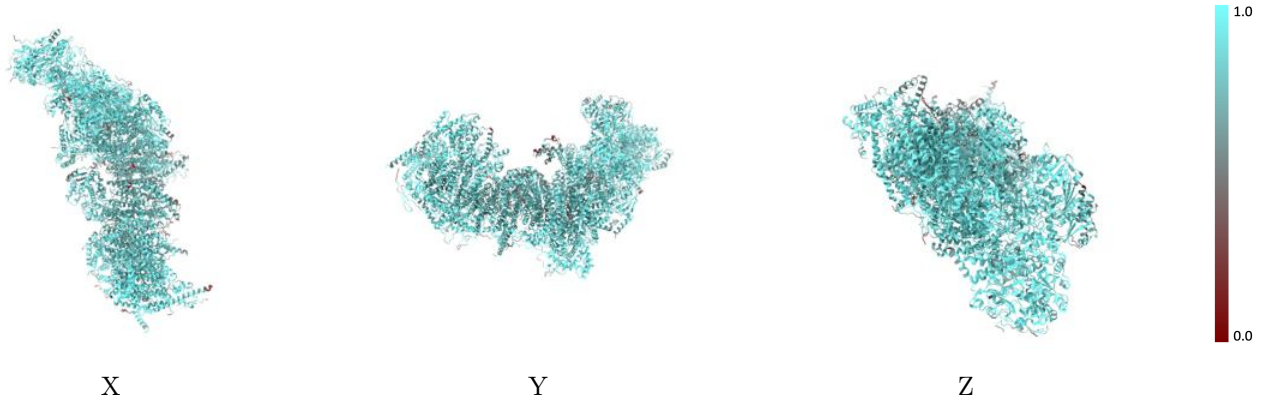
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



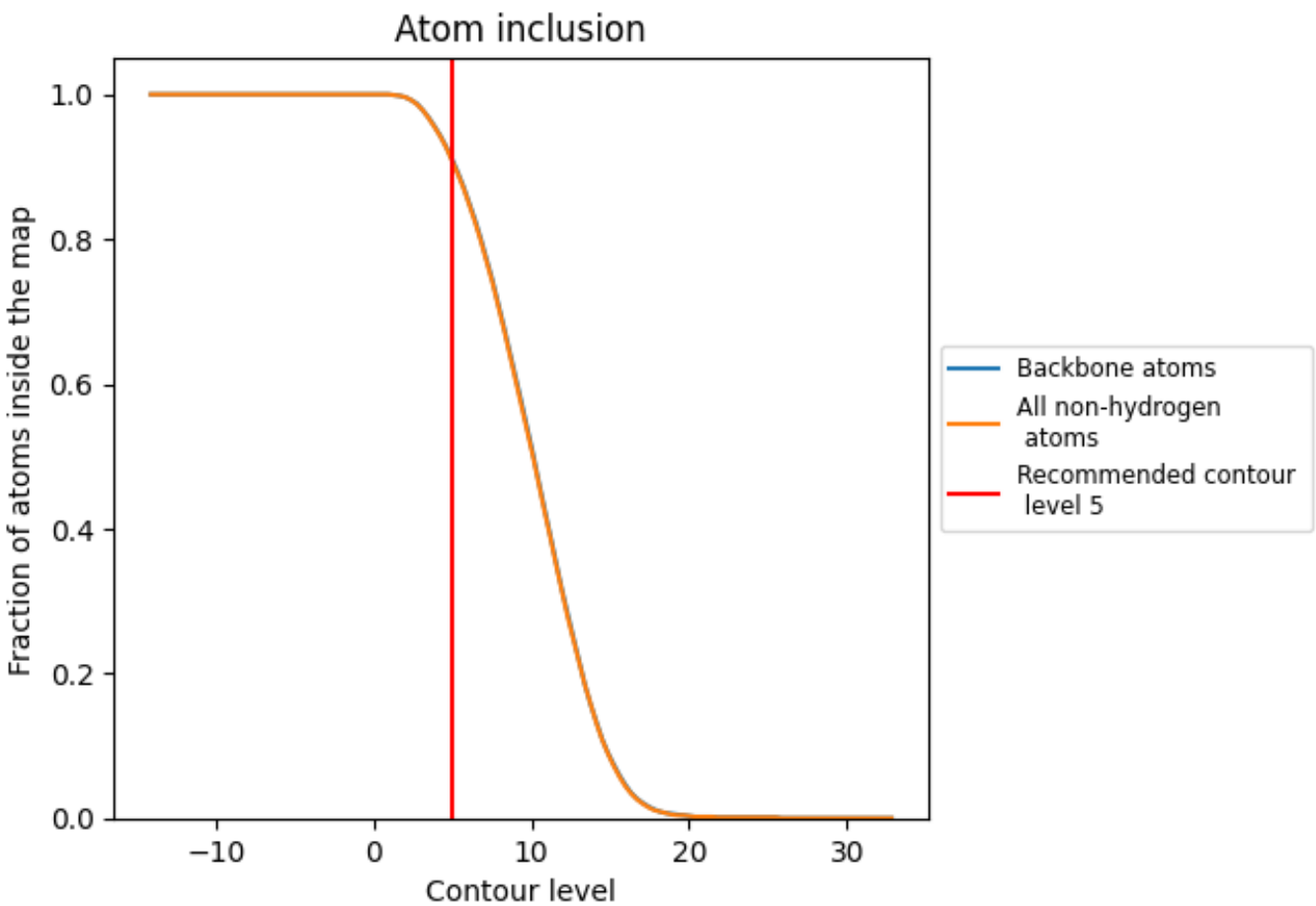
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.6970
A	0.9030	0.7040
B	0.9640	0.7340
C	0.9610	0.7350
D	0.9550	0.7320
E	0.8870	0.6830
F	0.9340	0.7000
G	0.9170	0.7090
H	0.9710	0.7220
I	0.9740	0.7400
J	0.8920	0.6930
K	0.9050	0.7070
L	0.9380	0.6860
M	0.9570	0.7060
N	0.9700	0.7160
O	0.8990	0.6840
P	0.8950	0.7030
Q	0.9220	0.7200
R	0.9170	0.7140
S	0.8270	0.6730
T	0.6150	0.6110
U	0.9100	0.6740
V	0.8780	0.7050
W	0.8850	0.7030
X	0.8910	0.6780
Y	0.7100	0.6520
Z	0.8880	0.6850
a	0.9400	0.7020
b	0.8200	0.6560
c	0.8430	0.6530
d	0.8880	0.6870
e	0.8580	0.6780
f	0.8130	0.6630
g	0.8880	0.6830
h	0.9220	0.6910

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Chain	Atom inclusion	Q-score
i	0.8210	0.6530
j	0.8570	0.6470
k	0.8900	0.6460
l	0.8960	0.6760
m	0.8730	0.6750
n	0.9010	0.6810
o	0.8610	0.6520
p	0.9030	0.6810
q	0.9060	0.7090
r	0.8870	0.7070
s	0.8540	0.6780