wwPDB EM Validation Summary Report (i)

Aug 25, 2026 – 03:47 am BST

PDB ID	:	7ZM7 / pdb_00007zm7
EMDB ID	:	EMD-14791
Title	:	CryoEM structure of mitochondrial complex I from Chaetomium thermophilum (inhibited by DDM)
Authors	:	Laube, E.; Kuehlbrandt, W.
Deposited on	:	2022-04-19
Resolution	:	2.77 Å(reported)
Based on initial models	:	6RFR, 6RFQ

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:

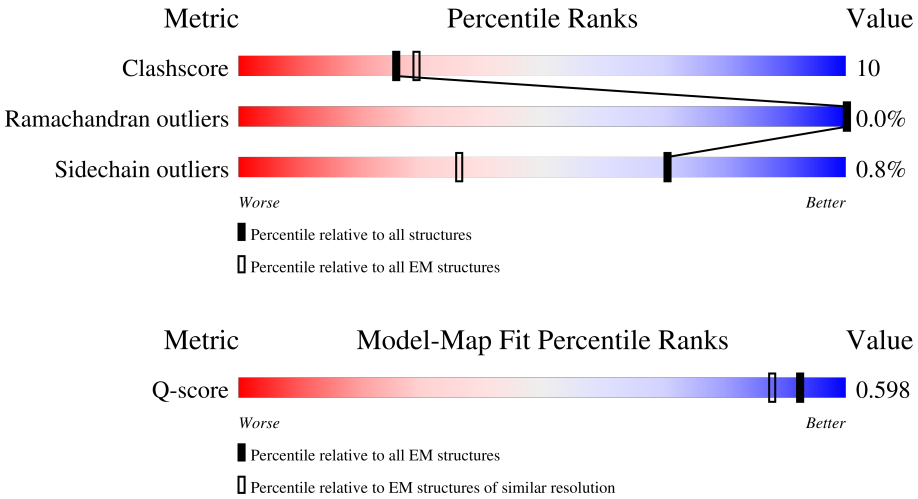
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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	1	378	11% 78% 21%
2	2	571	72% 25%
3	3	146	53% 26% 21%
4	4	542	66% 24% 9%

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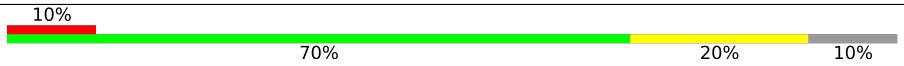
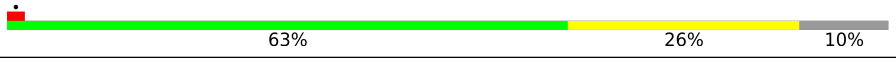
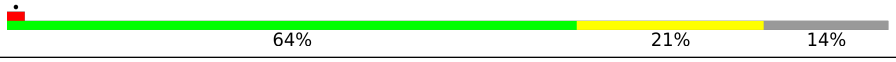
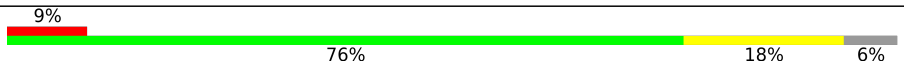
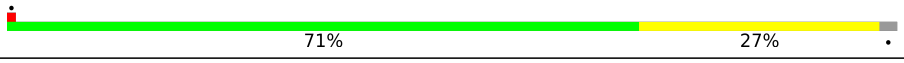
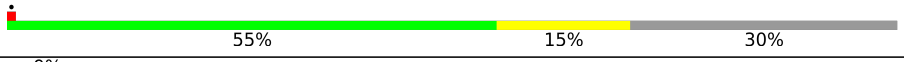
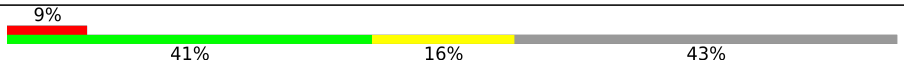
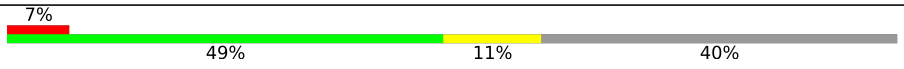
Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	A	749	
10	B	507	
11	C	499	
12	D	86	
13	E	378	
14	F	261	
15	G	293	
16	H	318	
17	I	223	
18	J	199	
19	K	230	
20	L	89	
21	M	168	
22	O	141	
22	Q	141	
23	P	124	
24	R	99	
25	S	143	
26	U	186	
27	W	121	
28	X	191	

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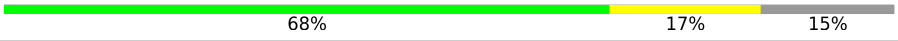
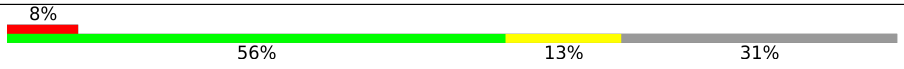
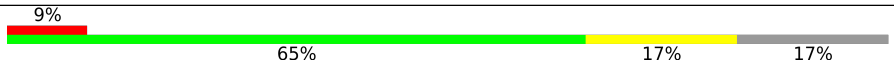
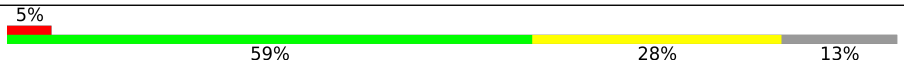
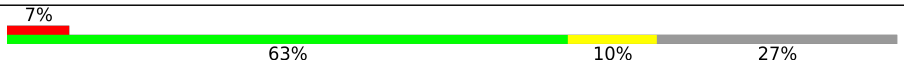
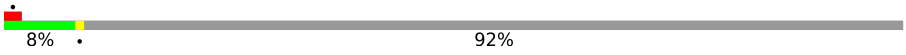
Mol	Chain	Length	Quality of chain
29	Y	210	
30	Z	196	
31	a	203	
32	b	94	
33	c	93	
34	d	105	
35	e	46	
36	f	95	
37	g	82	
38	h	134	
39	i	93	
40	j	75	
41	n	184	
42	o	380	

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 69157 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	378	2852	1916	430	496	10	0	0

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4456	2993	672	780	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	116	897	608	134	153	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	494	3904	2650	572	670	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	670	5276	3552	793	906	25	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	189	Total	C	N	O	S	0	0
			1460	985	219	250	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			654	405	125	118	6		

- Molecule 8 is a protein called Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	102	Total	C	N	O	S	0	0
			802	497	146	153	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	711	Total	C	N	O	S	0	0
			5476	3444	966	1035	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0RYA1
A	72	TYR	VAL	conflict	UNP G0RYA1
A	73	CYS	SER	conflict	UNP G0RYA1
A	74	TYR	MET	conflict	UNP G0RYA1
A	75	HIS	ARG	conflict	UNP G0RYA1
A	76	GLU	ARG	conflict	UNP G0RYA1

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	456	3538	2225	638	648	27	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	427	3376	2152	585	620	19	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP G0SCG0
C	?	-	LEU	deletion	UNP G0SCG0
C	?	-	THR	deletion	UNP G0SCG0
C	?	-	ILE	deletion	UNP G0SCG0
C	?	-	ALA	deletion	UNP G0SCG0
C	?	-	PRO	deletion	UNP G0SCG0
C	?	-	LYS	deletion	UNP G0SCG0

- Molecule 12 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	85	678	432	127	115	4	0	0

- Molecule 13 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	353	Total	C	N	O	S	0	0
			2866	1816	510	530	10		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	GLU	-	insertion	UNP G0SB35
E	104	PHE	-	insertion	UNP G0SB35
E	105	ASP	-	insertion	UNP G0SB35
E	106	LEU	-	insertion	UNP G0SB35
E	107	ARG	-	insertion	UNP G0SB35
E	108	ASN	-	insertion	UNP G0SB35
E	109	THR	-	insertion	UNP G0SB35
E	110	GLN	-	insertion	UNP G0SB35
E	233	HIS	-	insertion	UNP G0SB35
E	234	VAL	-	insertion	UNP G0SB35

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	237	Total	C	N	O	S	0	0
			1877	1185	328	363	1		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	242	Total	C	N	O	S	0	0
			1968	1271	329	361	7		

- Molecule 16 is a protein called Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	220	Total	C	N	O	S	0	0
			1695	1069	288	324	14		

- Molecule 17 is a protein called Oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	185	Total	C	N	O	S	0	0
			1487	941	252	282	12		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	188	Total	C	N	O	S	0	0
			1408	892	263	251	2		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	182	Total	C	N	O	S	0	0
			1439	916	253	255	15		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	118	Total	C	N	O	S	0	0
			937	585	178	169	5		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	149	ALA	SER	conflict	UNP G0S6J1
M	150	ASN	-	insertion	UNP G0S6J1
M	151	GLU	-	insertion	UNP G0S6J1
M	152	HIS	-	insertion	UNP G0S6J1
M	153	HIS	-	insertion	UNP G0S6J1
M	154	ARG	-	insertion	UNP G0S6J1
M	155	LYS	-	insertion	UNP G0S6J1
M	156	TYR	-	insertion	UNP G0S6J1
M	157	LEU	-	insertion	UNP G0S6J1
M	158	GLU	-	insertion	UNP G0S6J1
M	159	SER	-	insertion	UNP G0S6J1
M	160	LEU	-	insertion	UNP G0S6J1
M	161	PRO	-	insertion	UNP G0S6J1
M	162	GLN	-	insertion	UNP G0S6J1
M	163	THR	-	insertion	UNP G0S6J1
M	164	SER	-	insertion	UNP G0S6J1
M	165	TYR	-	insertion	UNP G0S6J1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	166	PRO	-	insertion	UNP G0S6J1
M	167	LEU	-	insertion	UNP G0S6J1
M	168	ASN	-	insertion	UNP G0S6J1

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	80	Total	C	N	O	S	0	0
			617	389	100	127	1		
22	Q	85	Total	C	N	O	S	0	0
			670	421	109	139	1		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase B14 subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	122	Total	C	N	O	S	0	0
			1035	658	197	177	3		

- Molecule 24 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 25 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	72	Total	C	N	O	0	0
			598	393	96	109		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	167	Total	C	N	O	S	0	0
			1353	852	252	240	9		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	120	Total	C	N	O	S	0	0
			976	623	182	168	3		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	186	Total	C	N	O	S	0	0
			1467	934	266	259	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	154	Total	C	N	O	S	0	0
			1240	788	219	229	4		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	186	Total	C	N	O	S	0	0
			1432	898	254	278	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	189	SER	-	insertion	UNP G0SEF0
Z	190	TYR	-	insertion	UNP G0SEF0
Z	191	PRO	-	insertion	UNP G0SEF0
Z	192	CYS	-	insertion	UNP G0SEF0
Z	193	ARG	-	insertion	UNP G0SEF0
Z	194	SER	-	insertion	UNP G0SEF0
Z	195	PHE	-	insertion	UNP G0SEF0
Z	196	VAL	-	insertion	UNP G0SEF0

- Molecule 31 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 32 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	80	Total	C	N	O	S	0	0
			675	440	124	109	2		

- Molecule 33 is a protein called Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	64	Total	C	N	O	S	0	0
			510	332	90	86	2		

- Molecule 34 is a protein called Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	100	Total	C	N	O	S	0	0
			827	526	146	151	4		

- Molecule 35 is a protein called Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	38	Total	C	N	O	S	0	0
			320	217	58	44	1		

- Molecule 36 is a protein called NADH dehydrogenase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	88	Total	C	N	O	S	0	0
			717	459	127	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	ALA	deletion	UNP G0S1P3

- Molecule 37 is a protein called Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	77	Total	C	N	O	S	0	0
			604	395	104	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	133	Total	C	N	O	S	0	0
			1124	726	197	200	1		

- Molecule 39 is a protein called Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	81	Total	C	N	O	S	0	0
			686	453	119	112	2		

- Molecule 40 is a protein called Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

- Molecule 41 is a protein called Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	135	Total	C	N	O	S	0	0
			1068	683	189	195	1		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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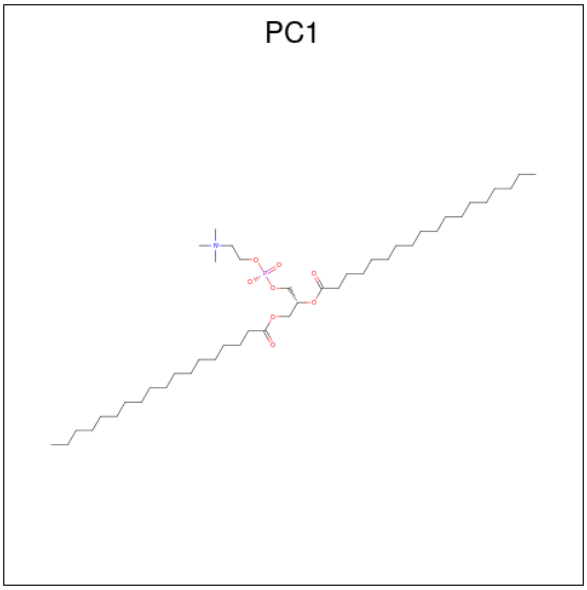
Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 42 is a protein called Oxidoreductase-like domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	o	32	Total	C	N	O	0	0
			252	165	43	44		

- Molecule 43 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
43	5	1	Total	C	N	O	P	0
			40	30	1	8	1	

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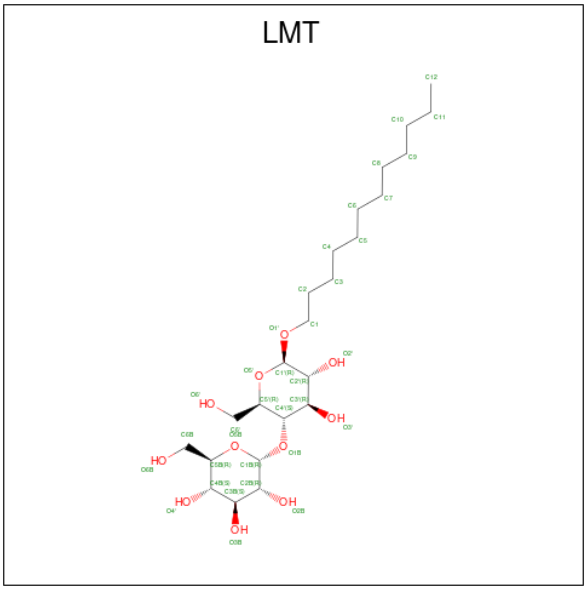
Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 44 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
44	1	1	Total	C	O	0
			35	24	11	
44	1	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			35	24	11	
44	2	1	Total	C	O	0
			33	22	11	
44	2	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	3	1	Total	C	O	0
			35	24	11	
44	4	1	Total	C	O	0
			35	24	11	
44	5	1	Total	C	O	0
			35	24	11	
44	J	1	Total	C	O	0
			31	20	11	

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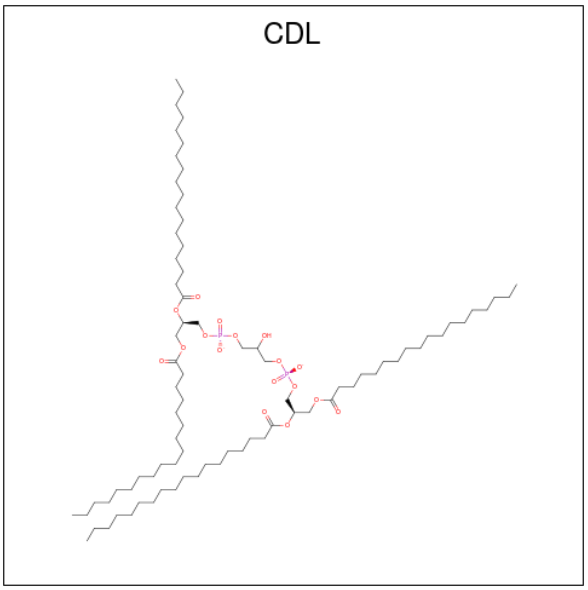
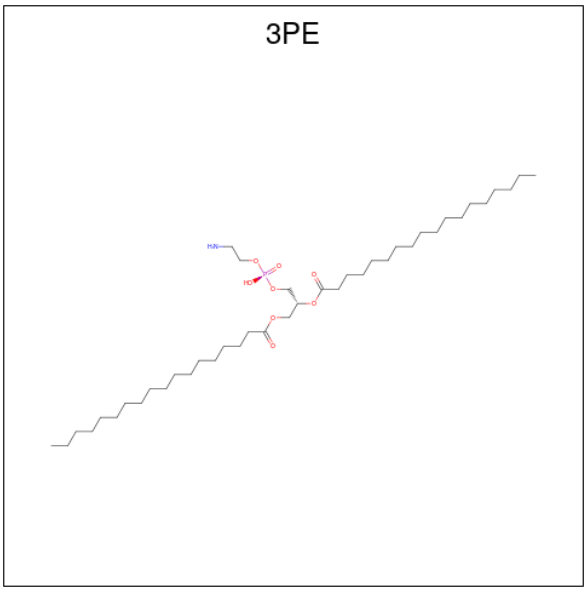
Mol	Chain	Residues	Atoms	AltConf
44	X	1	Total C O 35 24 11	0
44	a	1	Total C O 35 24 11	0
44	g	1	Total C O 34 23 11	0
44	j	1	Total C O 35 24 11	0

- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



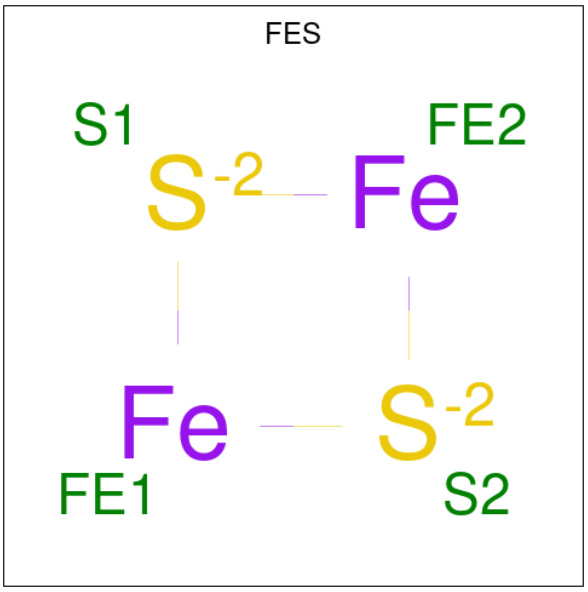
Mol	Chain	Residues	Atoms	AltConf
45	2	1	Total C O P 68 49 17 2	0
45	D	1	Total C O P 59 40 17 2	0
45	S	1	Total C O P 61 42 17 2	0
45	X	1	Total C O P 52 33 17 2	0
45	X	1	Total C O P 76 57 17 2	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



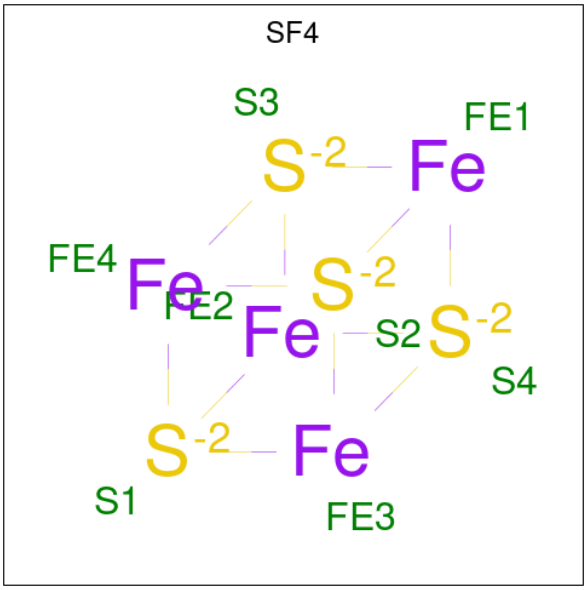
Mol	Chain	Residues	Atoms					AltConf
46	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	E	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	W	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	Fe	S	0
			4	2	2	
47	H	1	Total	Fe	S	0
			4	2	2	

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



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

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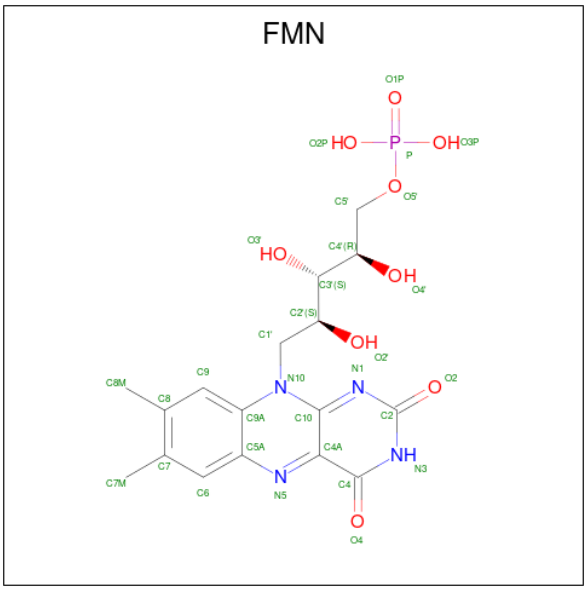
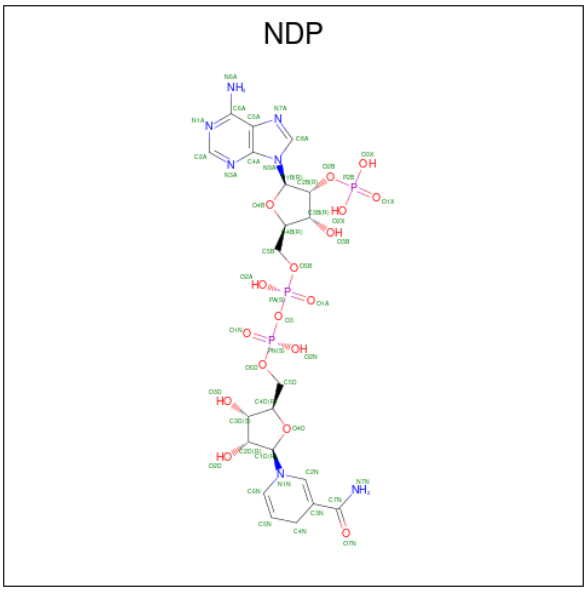
Mol	Chain	Residues	Atoms	AltConf
48	B	1	Total Fe S 8 4 4	0
48	I	1	Total Fe S 8 4 4	0
48	I	1	Total Fe S 8 4 4	0
48	K	1	Total Fe S 8 4 4	0

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



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

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

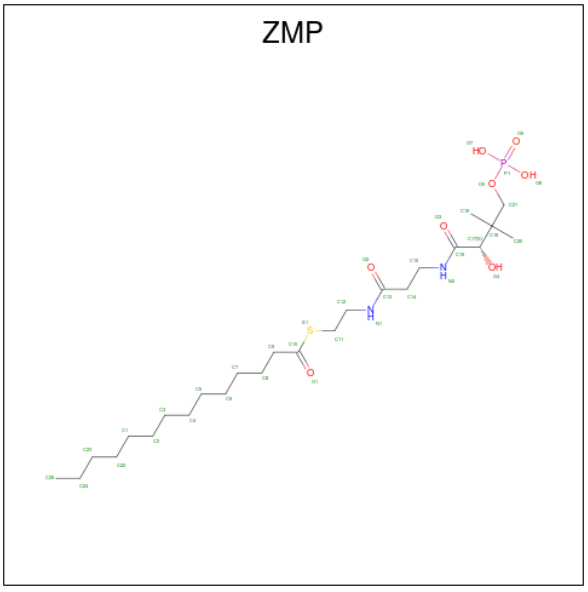


Mol	Chain	Residues	Atoms					AltConf
50	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	M	1	Total	Zn	0
			1	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	1	45	Total	O	0
			45	45	
53	2	115	Total	O	0
			115	115	
53	3	9	Total	O	0
			9	9	
53	4	79	Total	O	0
			79	79	
53	5	34	Total	O	0
			34	34	
53	6	21	Total	O	0
			21	21	
53	9	24	Total	O	0
			24	24	
53	A	123	Total	O	0
			123	123	
53	B	25	Total	O	0
			25	25	
53	C	114	Total	O	0
			114	114	
53	D	24	Total	O	0
			24	24	
53	E	31	Total	O	0
			31	31	
53	F	37	Total	O	0
			37	37	
53	G	76	Total	O	0
			76	76	
53	H	11	Total	O	0
			11	11	
53	I	68	Total	O	0
			68	68	
53	J	2	Total	O	0
			2	2	
53	K	38	Total	O	0
			38	38	

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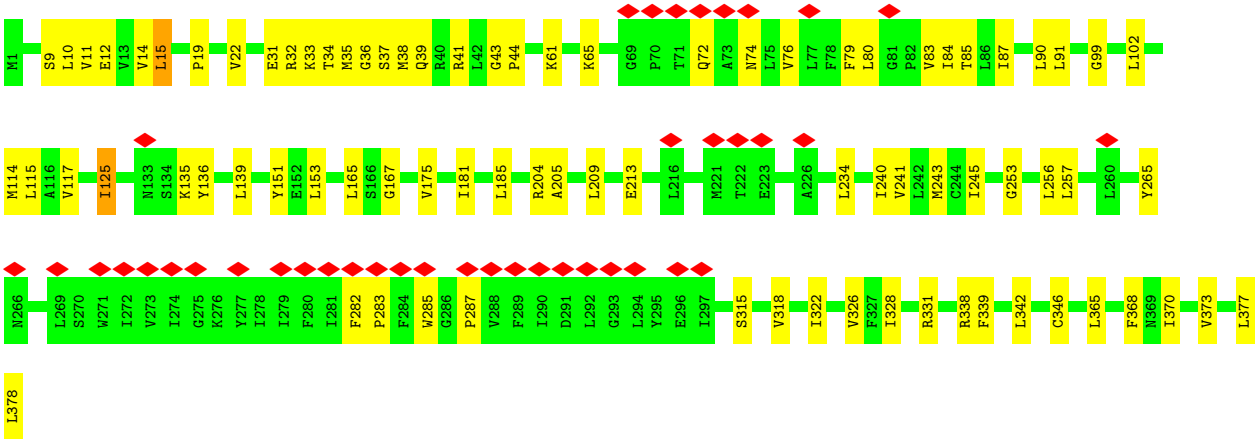
Mol	Chain	Residues	Atoms	AltConf
53	L	5	Total O 5 5	0
53	M	26	Total O 26 26	0
53	P	20	Total O 20 20	0
53	R	2	Total O 2 2	0
53	U	23	Total O 23 23	0
53	W	41	Total O 41 41	0
53	X	41	Total O 41 41	0
53	Y	60	Total O 60 60	0
53	Z	35	Total O 35 35	0
53	a	5	Total O 5 5	0
53	b	6	Total O 6 6	0
53	d	14	Total O 14 14	0
53	f	2	Total O 2 2	0
53	g	2	Total O 2 2	0
53	h	26	Total O 26 26	0
53	i	1	Total O 1 1	0
53	j	7	Total O 7 7	0
53	n	27	Total O 27 27	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.

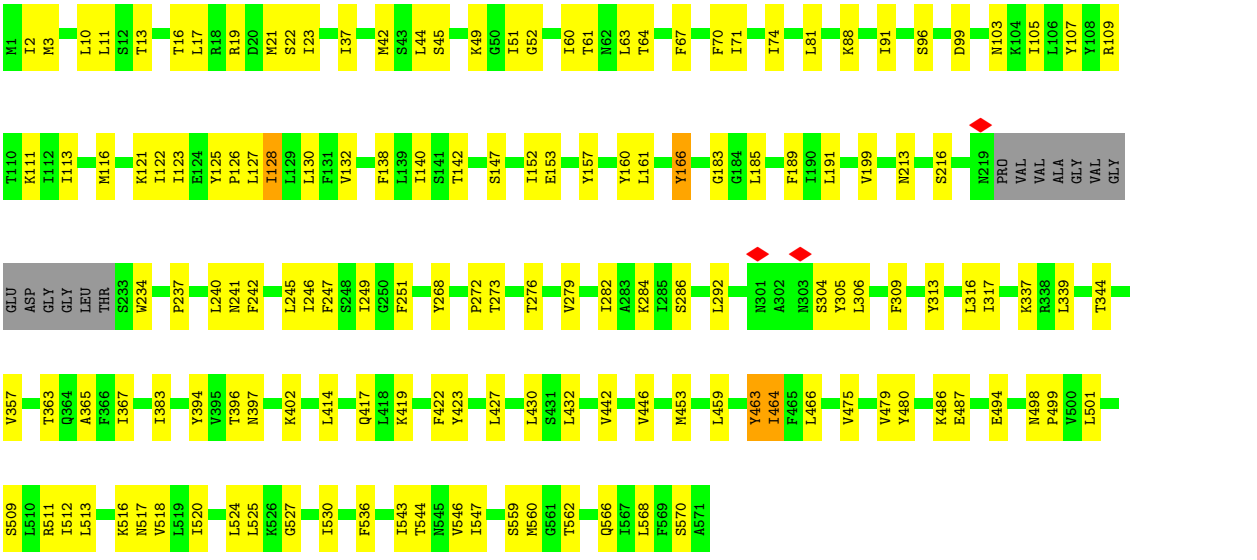
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



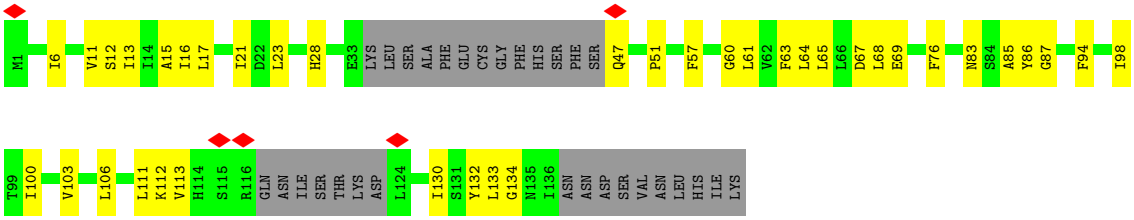
• Molecule 2: NADH dehydrogenase subunit 2

Chain 2:



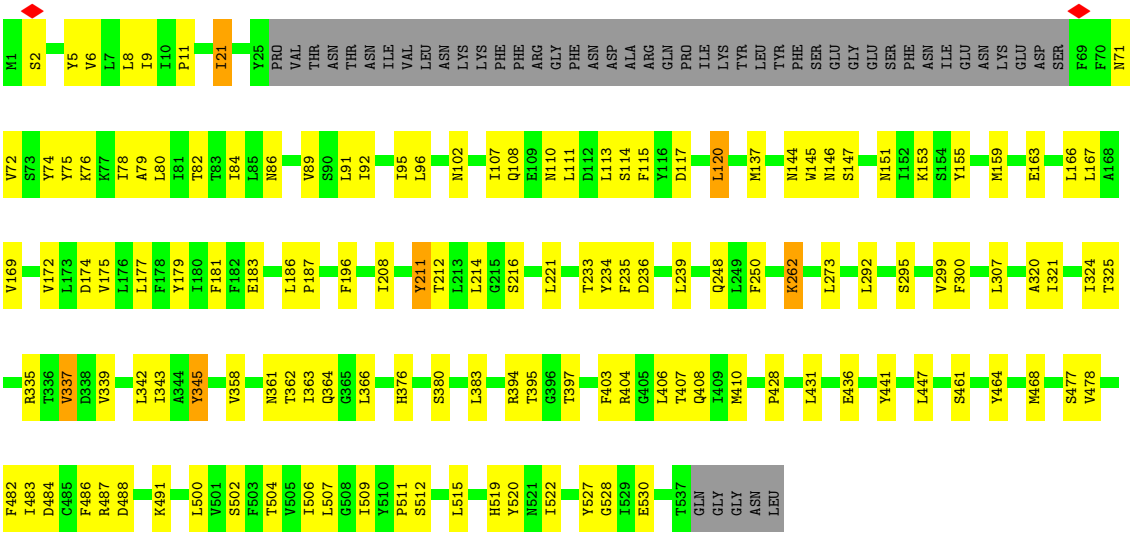
• Molecule 3: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



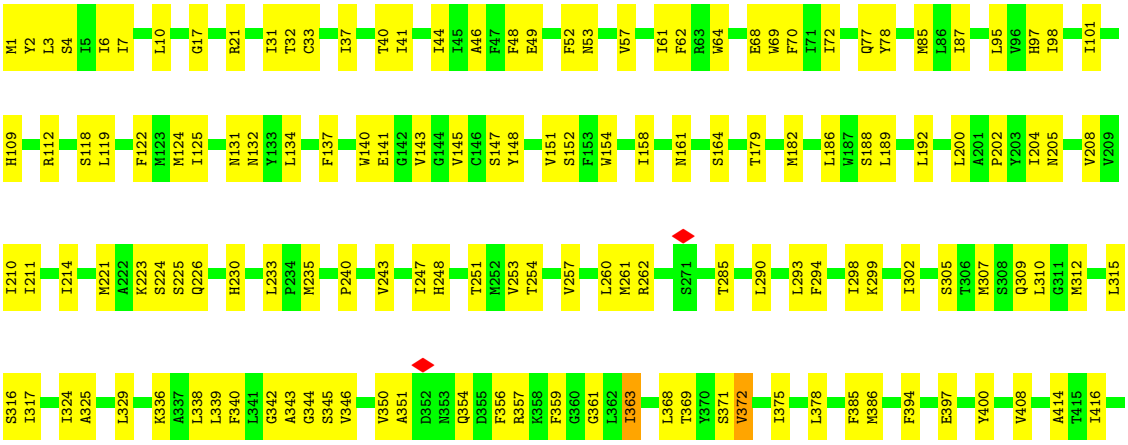
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4

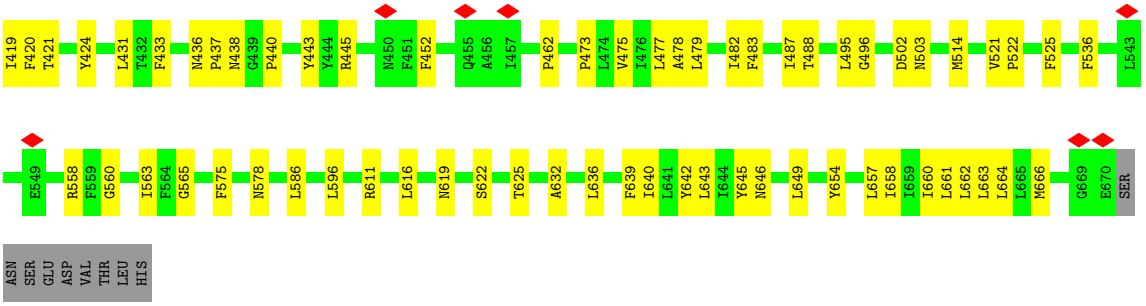
Chain 4:



• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

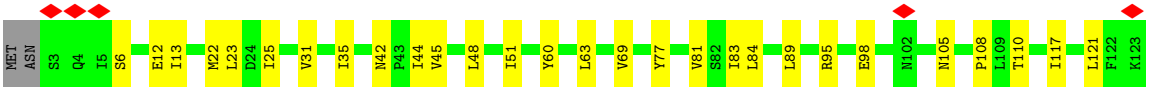
Chain 5:

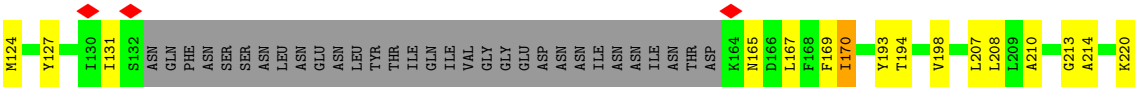




• Molecule 6: NADH-ubiquinone oxidoreductase chain 6

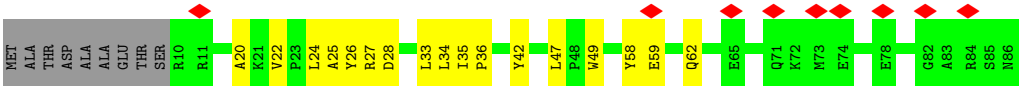
Chain 6:





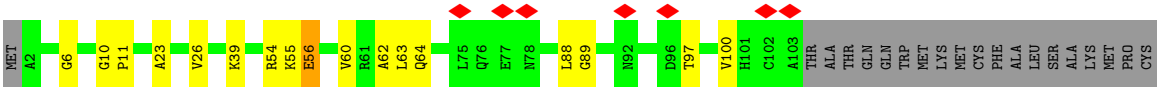
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

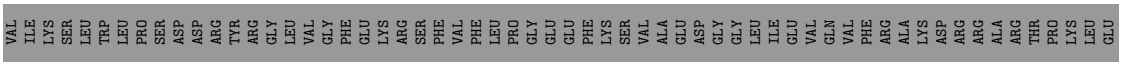
Chain 8:

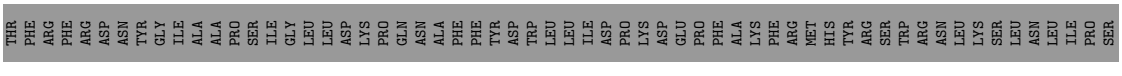


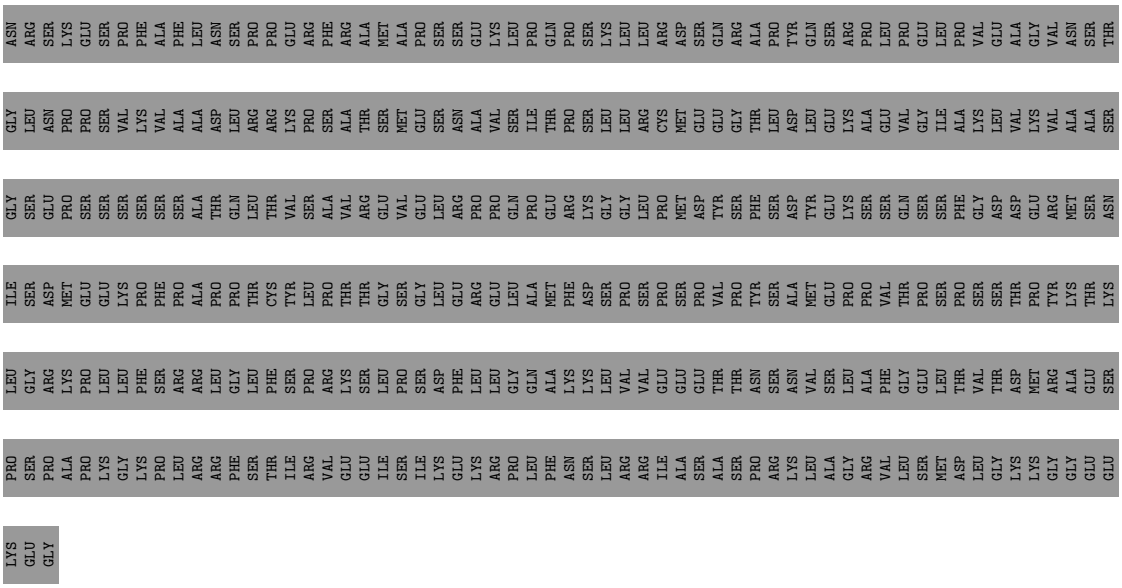
• Molecule 8: Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain 9:



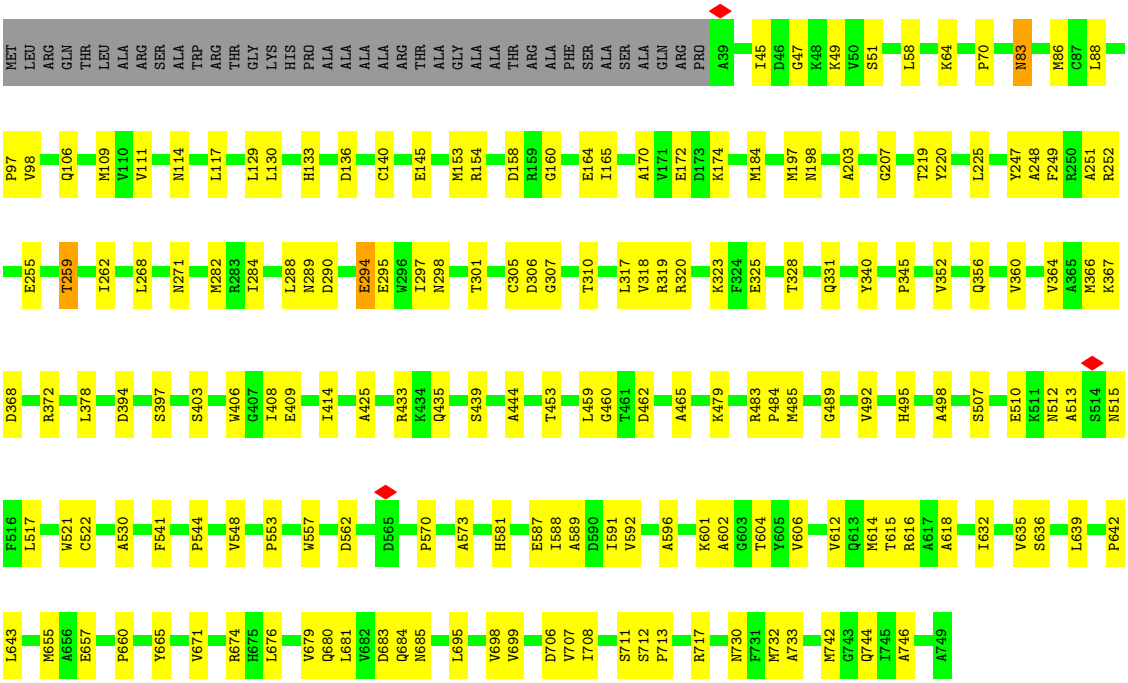






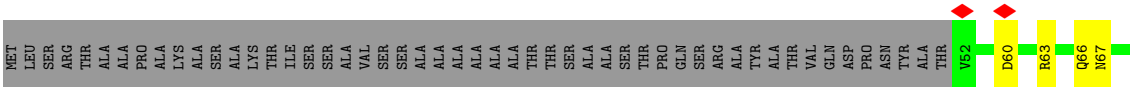
• Molecule 9: NADH-ubiquinone oxidoreductase-like protein

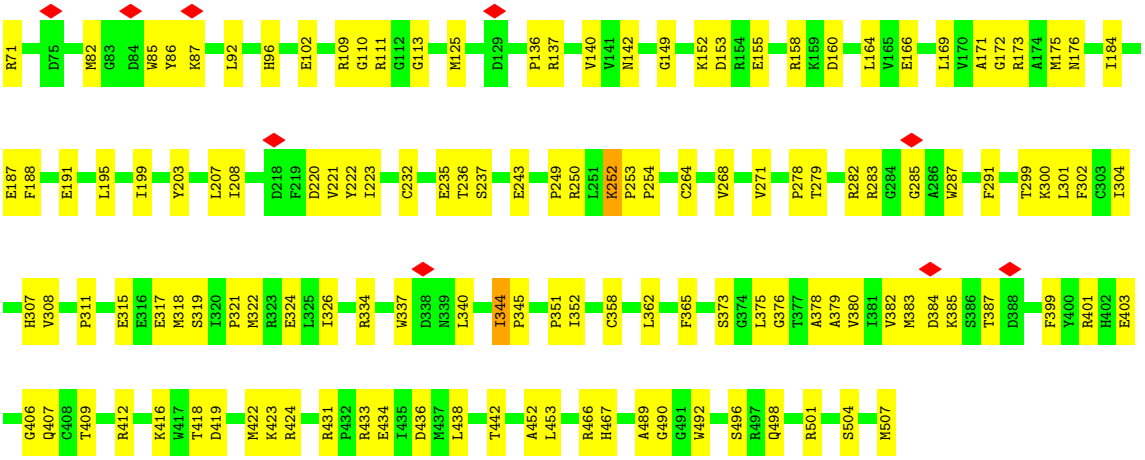
Chain A:



• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

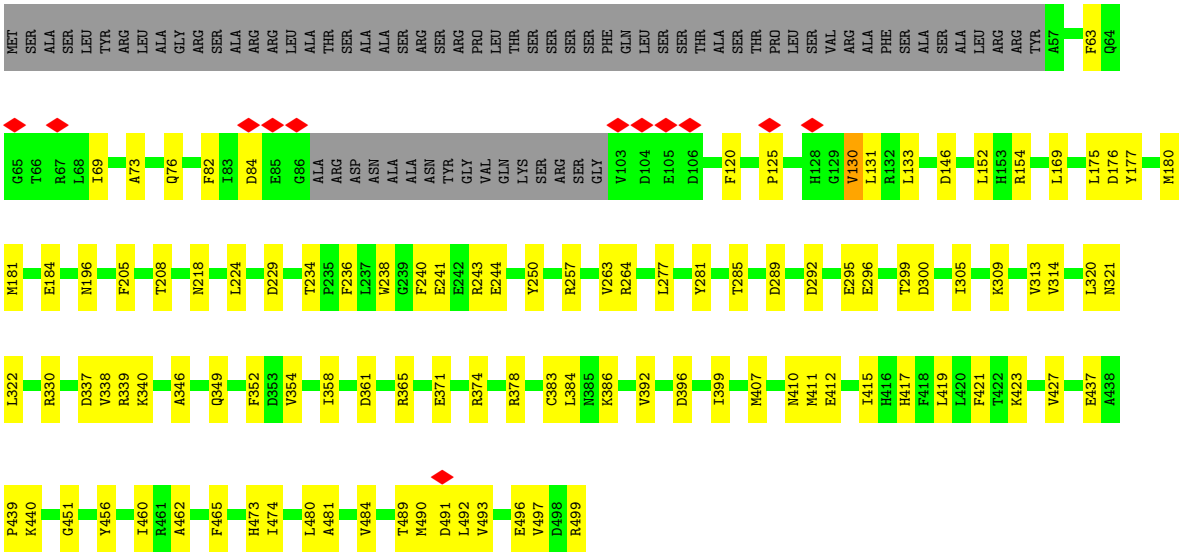
Chain B:





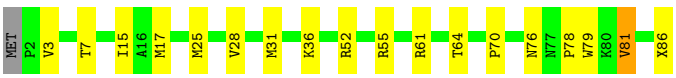
• Molecule 11: NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein

Chain C:



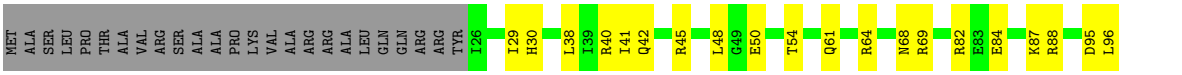
• Molecule 12: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

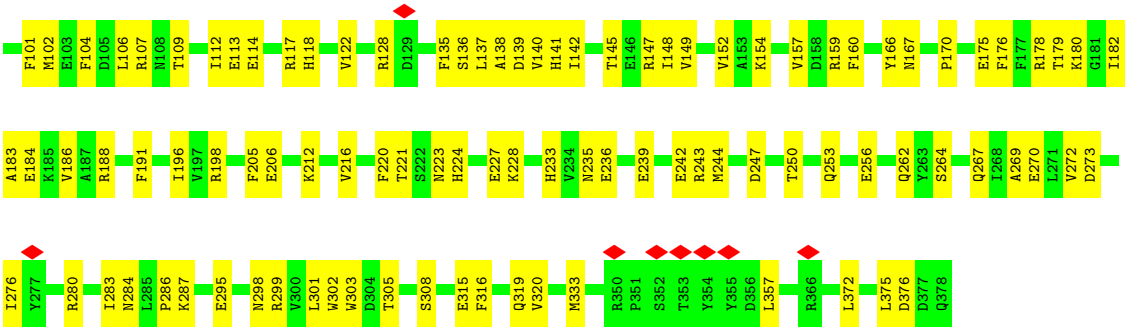
Chain D:



• Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein

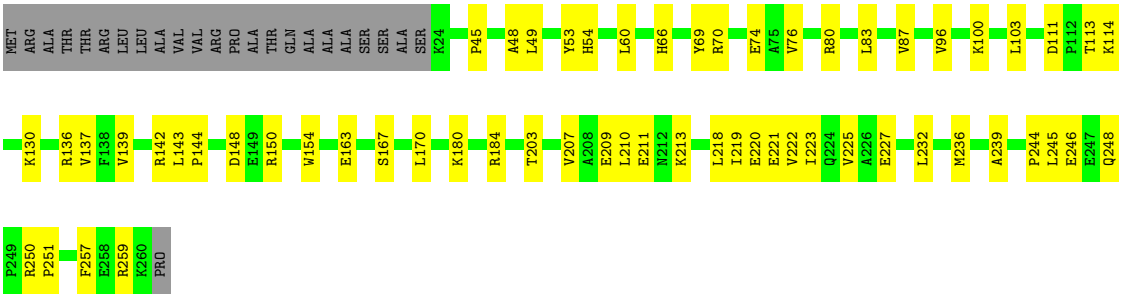
Chain E:





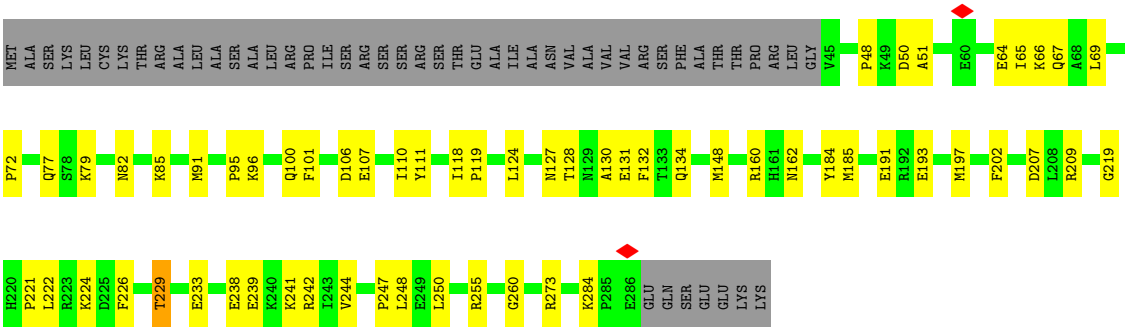
• Molecule 14: NADH-ubiquinone oxidoreductase-like protein

Chain F:



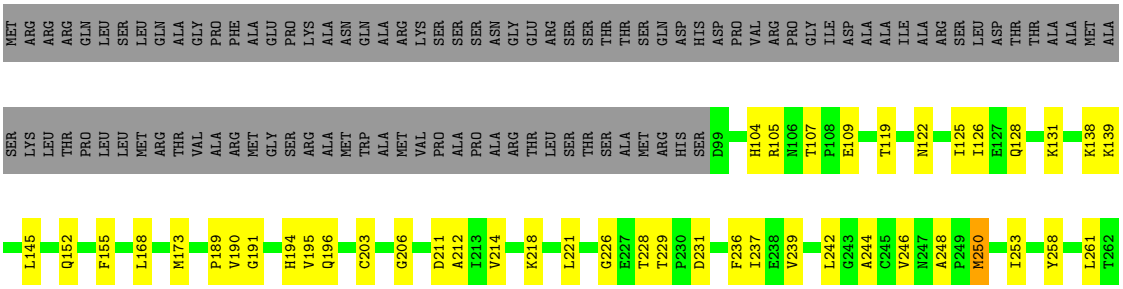
• Molecule 15: NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein

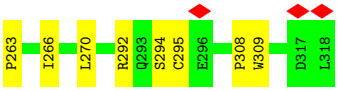
Chain G:



• Molecule 16: Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I)

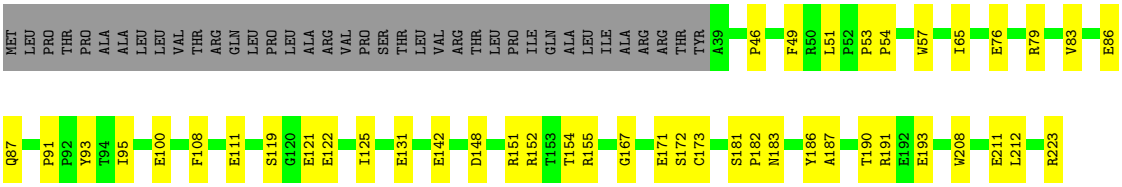
Chain H:





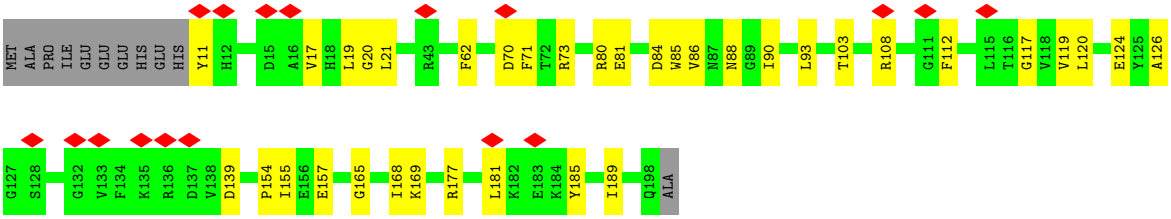
• Molecule 17: Oxidoreductase-like protein

Chain I:



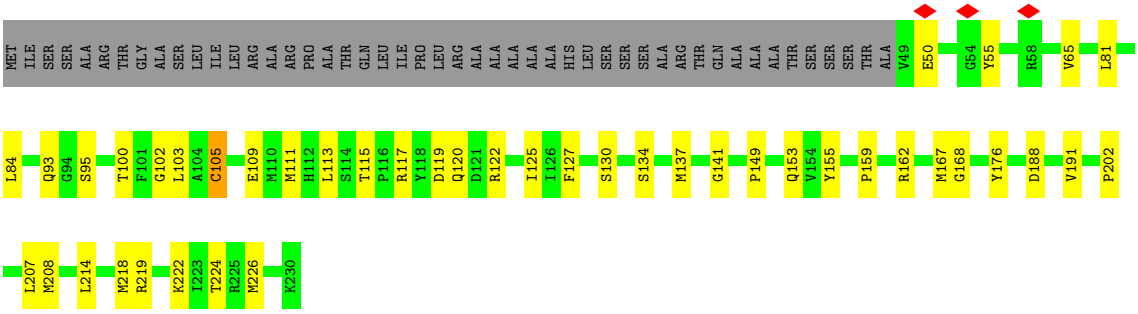
• Molecule 18: NADH-ubiquinone oxidoreductase-like protein

Chain J:



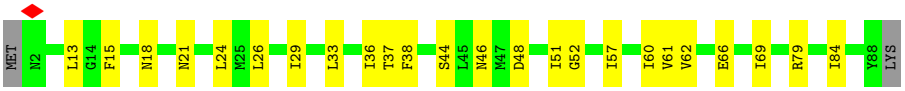
• Molecule 19: NADH-ubiquinone oxidoreductase-like protein

Chain K:



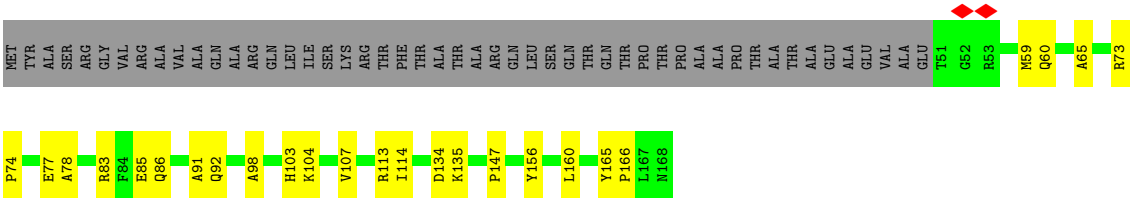
• Molecule 20: NADH-ubiquinone oxidoreductase chain 4L

Chain L:



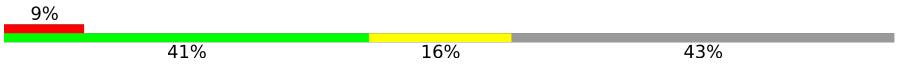
• Molecule 21: NADH-ubiquinone oxidoreductase-like protein

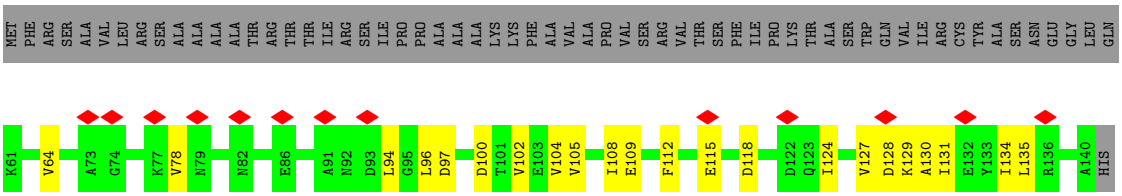
Chain M:



• Molecule 22: Acyl carrier protein

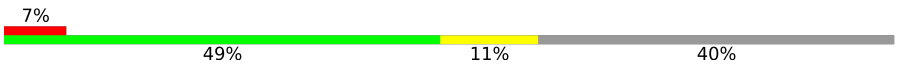
Chain O:

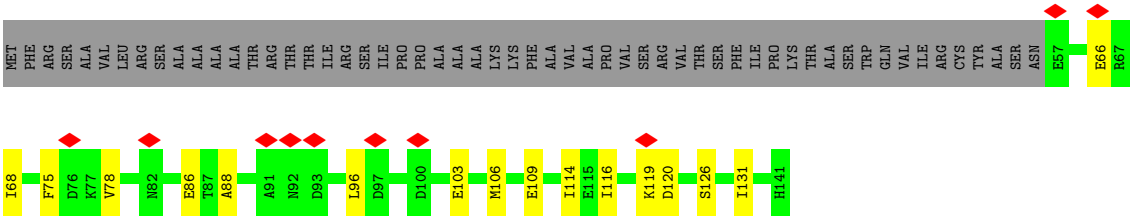




• Molecule 22: Acyl carrier protein

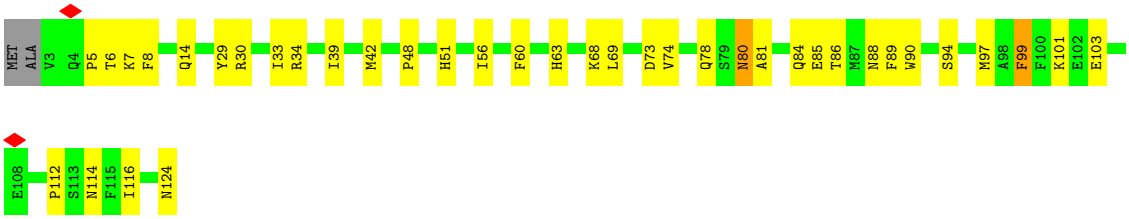
Chain Q:





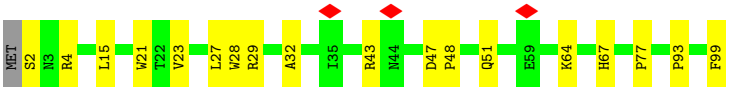
• Molecule 23: NADH-ubiquinone oxidoreductase B14 subunit-like protein

Chain P:



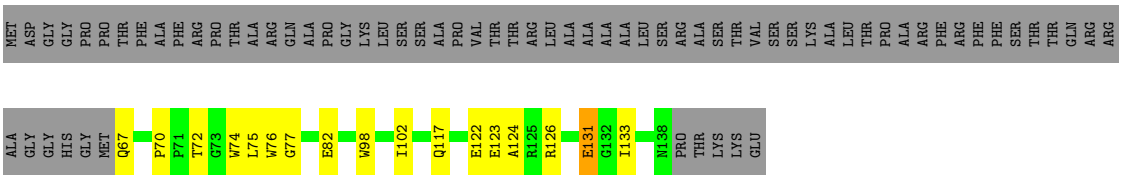
• Molecule 24: Complex I-B22

Chain R:



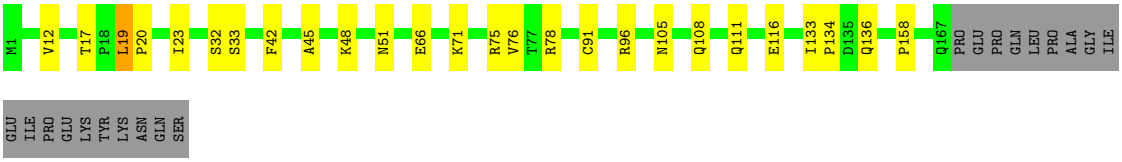
• Molecule 25: Complex I-ESSS

Chain S:



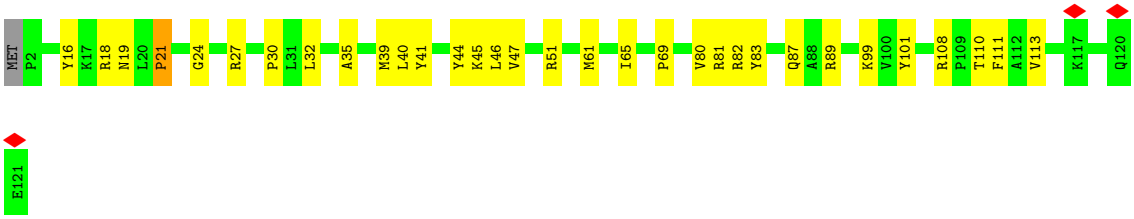
• Molecule 26: NADH-ubiquinone oxidoreductase

Chain U:



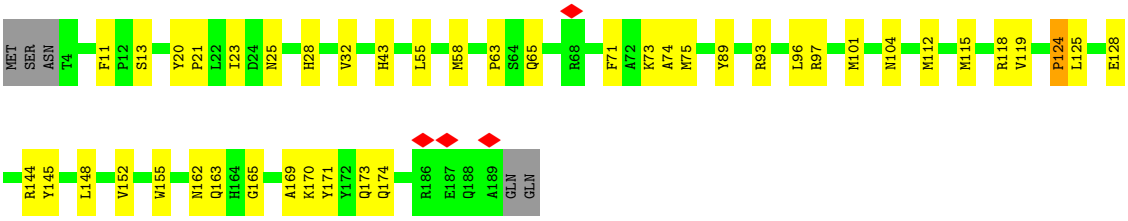
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



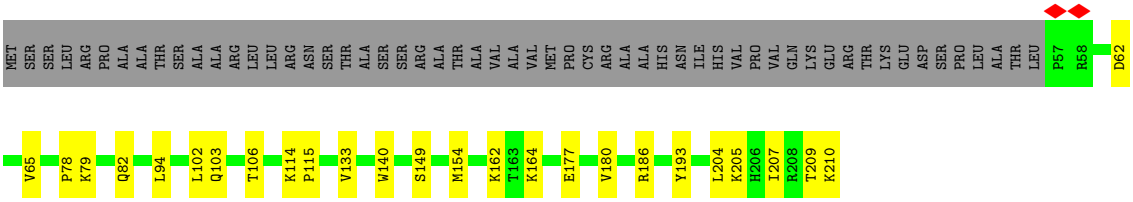
• Molecule 28: NADH-ubiquinone oxidoreductase-like protein

Chain X:



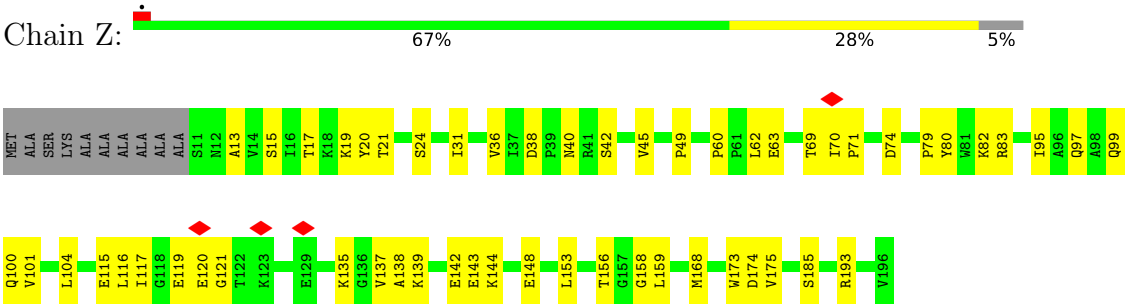
• Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Y:



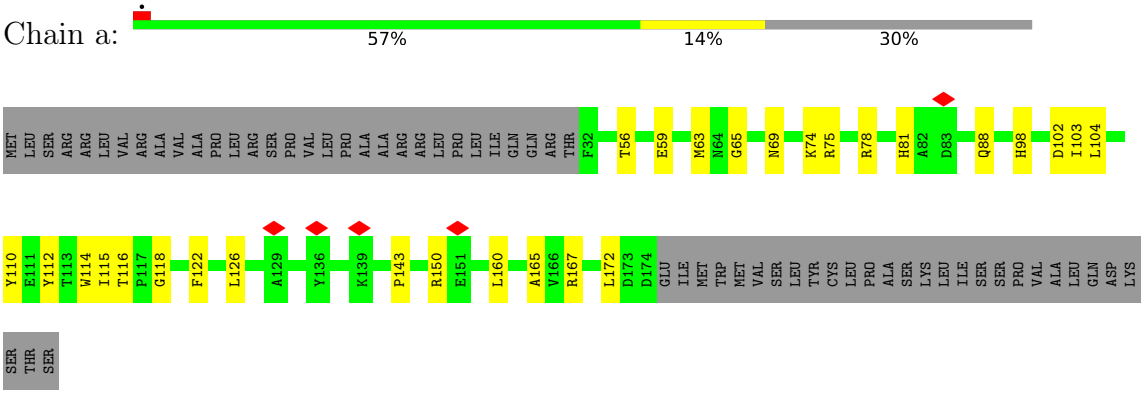
• Molecule 30: NADH-ubiquinone oxidoreductase-like protein

Chain Z:



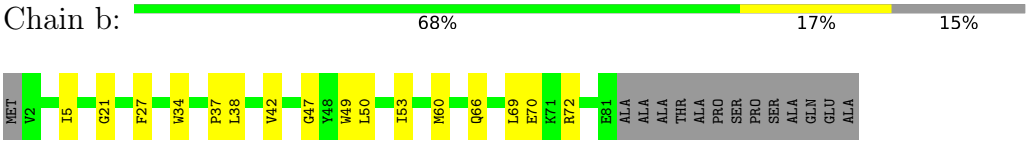
• Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein

Chain a:



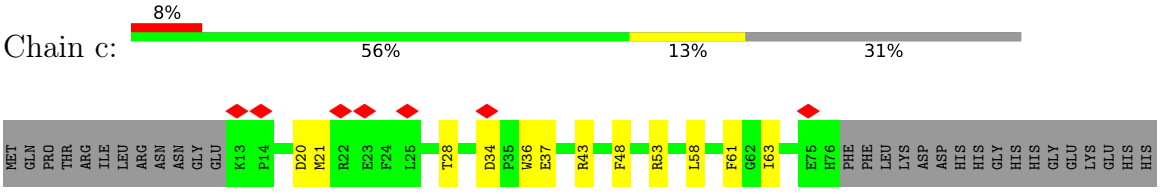
• Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain b:



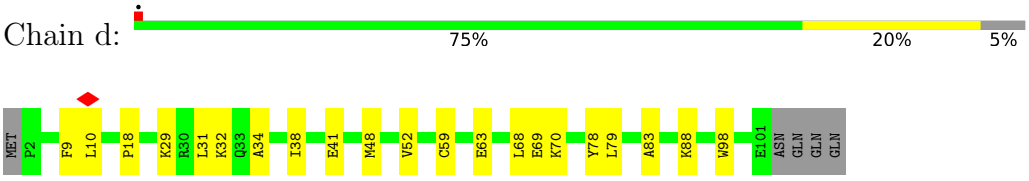
• Molecule 33: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain c:



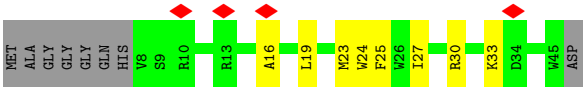
• Molecule 34: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)

Chain d:



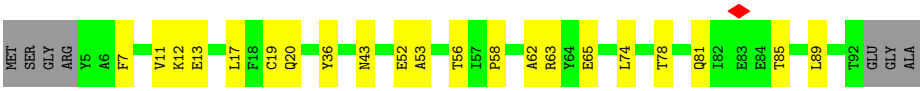
• Molecule 35: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain e:



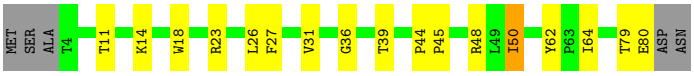
• Molecule 36: NADH dehydrogenase-like protein

Chain f:



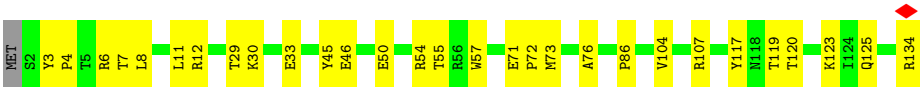
• Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain g:



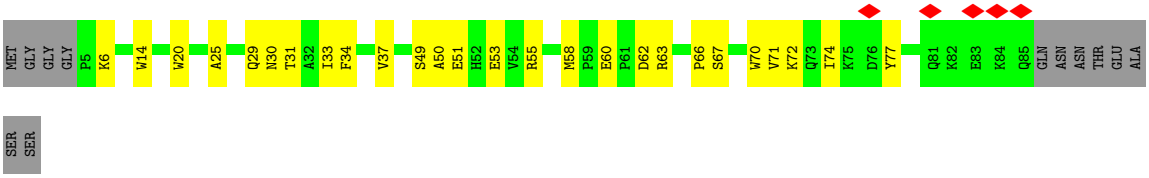
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

Chain h:



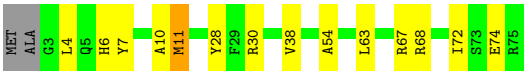
• Molecule 39: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)

Chain i:



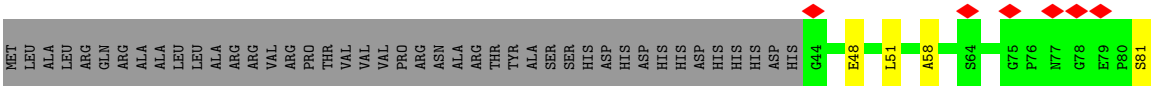
• Molecule 40: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)

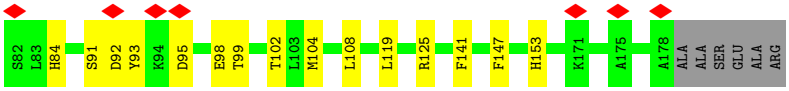
Chain j:



• Molecule 41: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)

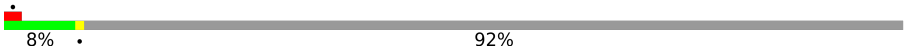
Chain n:

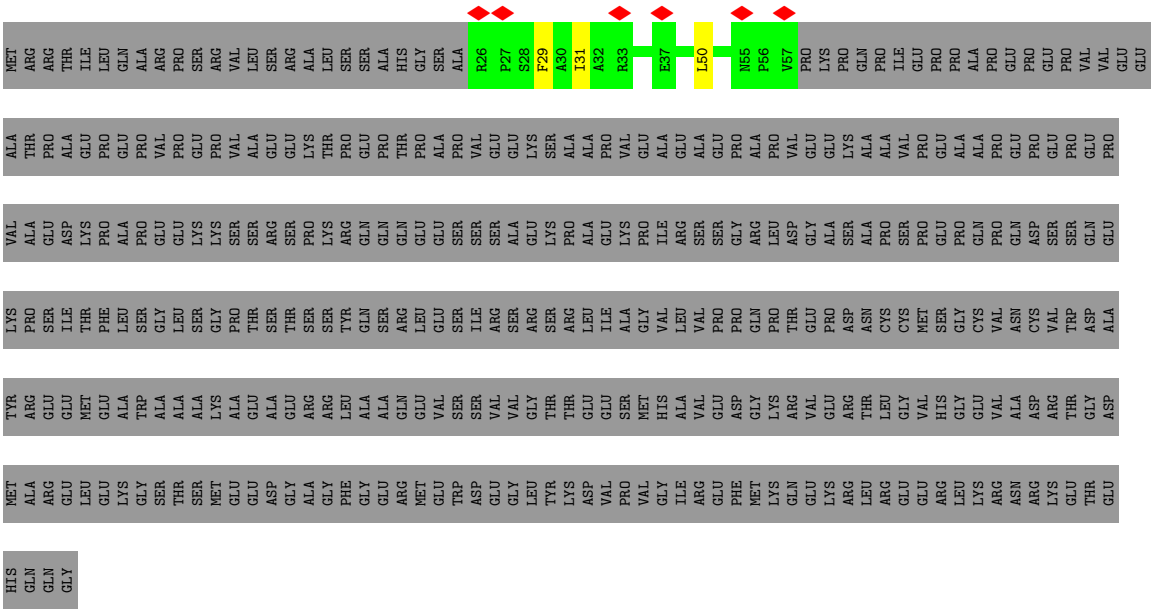




• Molecule 42: Oxidoreductase-like domain-containing protein

Chain o:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.497	Depositor
Minimum map value	-1.728	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	154.48529, 228.63824, 305.8809	wwPDB
Map dimensions	297, 222, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029902, 1.029902, 1.029902	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: FMN, LMT, FES, CDL, ZMP, NDP, ZN, 3PE, SF4, 2MR, PC1

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	1	0.68	1/2921 (0.0%)	0.96	7/3996 (0.2%)
2	2	0.77	2/4562 (0.0%)	1.06	8/6205 (0.1%)
3	3	0.56	0/918	0.75	0/1249
4	4	0.68	2/4002 (0.0%)	0.85	3/5454 (0.1%)
5	5	0.54	0/5418	0.72	3/7376 (0.0%)
6	6	0.66	0/1487	0.80	1/2026 (0.0%)
7	8	0.40	0/667	0.61	0/892
8	9	0.68	0/819	0.99	1/1105 (0.1%)
9	A	0.57	0/5589	0.76	3/7579 (0.0%)
10	B	0.49	0/3621	0.69	6/4878 (0.1%)
11	C	0.60	0/3447	0.74	1/4675 (0.0%)
12	D	0.73	0/674	1.09	1/911 (0.1%)
13	E	0.53	0/2932	0.69	0/3973
14	F	0.46	0/1916	0.57	0/2596
15	G	0.57	0/2026	0.73	2/2759 (0.1%)
16	H	0.49	0/1734	0.66	2/2358 (0.1%)
17	I	0.65	0/1527	0.81	1/2070 (0.0%)
18	J	0.49	0/1435	0.74	2/1940 (0.1%)
19	K	0.64	0/1478	0.90	2/2009 (0.1%)
20	L	0.72	0/680	1.03	1/921 (0.1%)
21	M	0.64	0/968	0.79	2/1319 (0.2%)
22	O	0.27	0/626	0.40	0/852
22	Q	0.23	0/680	0.37	0/922
23	P	0.59	0/1062	0.84	1/1432 (0.1%)
24	R	0.55	0/832	0.68	0/1133
25	S	0.66	0/622	0.97	2/850 (0.2%)
26	U	0.85	0/1390	1.23	4/1885 (0.2%)
27	W	0.76	0/1001	1.14	5/1354 (0.4%)
28	X	0.75	0/1506	1.08	2/2036 (0.1%)
29	Y	0.64	0/1277	0.78	0/1731
30	Z	0.49	0/1466	0.62	0/1997
31	a	0.46	0/1204	0.58	0/1632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.67	0/693	1.09	2/929 (0.2%)
33	c	0.37	0/529	0.57	0/720
34	d	0.56	0/845	0.89	1/1137 (0.1%)
35	e	0.54	0/335	0.73	0/454
36	f	0.42	0/731	0.60	0/981
37	g	0.67	0/624	0.87	0/857
38	h	0.53	0/1164	0.66	0/1584
39	i	0.53	0/715	0.76	0/971
40	j	0.61	0/617	0.83	0/830
41	n	0.67	0/1100	0.97	1/1491 (0.1%)
42	o	0.41	0/262	0.39	0/360
All	All	0.60	5/68102 (0.0%)	0.82	64/92429 (0.1%)

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
10	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	113	LEU	C-N	-11.55	1.23	1.33
4	4	436	GLU	C-N	-7.01	1.25	1.33
2	2	394	TYR	C-N	-6.48	1.25	1.33
2	2	122	ILE	C-N	5.81	1.41	1.33
1	1	167	GLY	C-N	5.25	1.40	1.33

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	253	PRO	N-CA-C	8.45	121.00	110.70
10	B	453	LEU	N-CA-C	-8.11	103.39	113.28
1	1	125	ILE	N-CA-C	-7.17	105.79	112.96
26	U	45	ALA	N-CA-C	-7.13	103.55	112.90
4	4	113	LEU	CA-C-N	7.06	131.48	122.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	252	LYS	Peptide

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	1	2852	0	2895	62	0
2	2	4456	0	4650	113	0
3	3	897	0	912	35	0
4	4	3904	0	4056	98	0
5	5	5276	0	5403	166	0
6	6	1460	0	1567	38	0
7	8	654	0	637	12	0
8	9	802	0	773	19	0
9	A	5476	0	5419	123	0
10	B	3538	0	3477	93	0
11	C	3376	0	3286	88	0
12	D	678	0	643	17	0
13	E	2866	0	2825	90	0
14	F	1877	0	1851	51	0
15	G	1968	0	1935	54	0
16	H	1695	0	1673	40	0
17	I	1487	0	1434	40	0
18	J	1408	0	1411	28	0
19	K	1439	0	1413	34	0
20	L	673	0	742	25	0
21	M	937	0	890	21	0
22	O	617	0	588	15	0
22	Q	670	0	644	12	0
23	P	1035	0	1018	27	0
24	R	807	0	823	15	0
25	S	598	0	548	15	0
26	U	1353	0	1324	12	0
27	W	976	0	990	31	0
28	X	1467	0	1420	37	0
29	Y	1240	0	1204	19	0
30	Z	1432	0	1411	52	0
31	a	1167	0	1104	25	0
32	b	675	0	678	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	510	0	458	10	0
34	d	827	0	814	18	0
35	e	320	0	313	12	0
36	f	717	0	735	17	0
37	g	604	0	614	13	0
38	h	1124	0	1093	27	0
39	i	686	0	666	25	0
40	j	603	0	623	17	0
41	n	1068	0	1026	14	0
42	o	252	0	235	3	0
43	1	33	0	40	1	0
43	2	45	0	67	13	0
43	5	85	0	118	11	0
44	1	70	0	92	3	0
44	2	103	0	131	6	0
44	3	70	0	92	3	0
44	4	35	0	46	4	0
44	5	35	0	46	3	0
44	J	31	0	35	0	0
44	X	35	0	46	3	0
44	a	35	0	46	2	0
44	g	34	0	41	1	0
44	j	35	0	46	4	0
45	2	68	0	80	2	0
45	D	59	0	62	3	0
45	S	61	0	66	3	0
45	X	128	0	144	3	0
46	5	125	0	175	3	0
46	E	29	0	32	1	0
46	I	37	0	48	2	0
46	W	72	0	95	4	0
46	i	38	0	50	1	0
47	A	4	0	0	0	0
47	H	4	0	0	0	0
48	A	16	0	0	0	0
48	B	8	0	0	0	0
48	I	16	0	0	0	0
48	K	8	0	0	1	0
49	B	31	0	19	2	0
50	E	48	0	26	2	0
51	M	1	0	0	0	0
52	O	36	0	47	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	Q	36	0	47	3	0
53	1	45	0	0	0	0
53	2	115	0	0	0	0
53	3	9	0	0	0	0
53	4	79	0	0	1	0
53	5	34	0	0	3	0
53	6	21	0	0	0	0
53	9	24	0	0	1	0
53	A	123	0	0	1	0
53	B	25	0	0	0	0
53	C	114	0	0	1	0
53	D	24	0	0	1	0
53	E	31	0	0	2	0
53	F	37	0	0	4	0
53	G	76	0	0	0	0
53	H	11	0	0	0	0
53	I	68	0	0	6	0
53	J	2	0	0	0	0
53	K	38	0	0	0	0
53	L	5	0	0	0	0
53	M	26	0	0	3	0
53	P	20	0	0	1	0
53	R	2	0	0	0	0
53	U	23	0	0	0	0
53	W	41	0	0	0	0
53	X	41	0	0	2	0
53	Y	60	0	0	1	0
53	Z	35	0	0	3	0
53	a	5	0	0	1	0
53	b	6	0	0	0	0
53	d	14	0	0	0	0
53	f	2	0	0	0	0
53	g	2	0	0	0	0
53	h	26	0	0	1	0
53	i	1	0	0	0	0
53	j	7	0	0	0	0
53	n	27	0	0	0	0
All	All	69157	0	67958	1384	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 10.

The worst 5 of 1384 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)
2:2:19:ARG:HA	2:2:123:ILE:HD11	1.28	1.09
2:2:546:VAL:HG21	43:2:605:PC1:C3I	1.99	0.92
8:9:63:LEU:HD22	27:W:113:VAL:HG21	1.55	0.88
9:A:366:MET:HE2	9:A:632:ILE:HG12	1.54	0.87
4:4:408:GLN:HA	43:5:702:PC1:H131	1.57	0.84

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	1	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
2	2	554/571 (97%)	541 (98%)	13 (2%)	0	100	100
3	3	110/146 (75%)	107 (97%)	3 (3%)	0	100	100
4	4	490/542 (90%)	472 (96%)	18 (4%)	0	100	100
5	5	668/679 (98%)	632 (95%)	36 (5%)	0	100	100
6	6	185/224 (83%)	175 (95%)	10 (5%)	0	100	100
7	8	75/86 (87%)	72 (96%)	3 (4%)	0	100	100
8	9	100/785 (13%)	98 (98%)	2 (2%)	0	100	100
9	A	709/749 (95%)	680 (96%)	29 (4%)	0	100	100
10	B	454/507 (90%)	434 (96%)	20 (4%)	0	100	100
11	C	422/499 (85%)	404 (96%)	18 (4%)	0	100	100
12	D	79/86 (92%)	76 (96%)	3 (4%)	0	100	100
13	E	351/378 (93%)	337 (96%)	13 (4%)	1 (0%)	36	63
14	F	235/261 (90%)	232 (99%)	3 (1%)	0	100	100
15	G	240/293 (82%)	233 (97%)	7 (3%)	0	100	100
16	H	218/318 (69%)	205 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	I	183/223 (82%)	179 (98%)	4 (2%)	0	100	100
18	J	186/199 (94%)	182 (98%)	4 (2%)	0	100	100
19	K	180/230 (78%)	172 (96%)	7 (4%)	1 (1%)	21	47
20	L	85/89 (96%)	85 (100%)	0	0	100	100
21	M	116/168 (69%)	114 (98%)	2 (2%)	0	100	100
22	O	78/141 (55%)	76 (97%)	2 (3%)	0	100	100
22	Q	83/141 (59%)	81 (98%)	2 (2%)	0	100	100
23	P	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
24	R	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
25	S	70/143 (49%)	66 (94%)	4 (6%)	0	100	100
26	U	165/186 (89%)	161 (98%)	4 (2%)	0	100	100
27	W	118/121 (98%)	117 (99%)	1 (1%)	0	100	100
28	X	184/191 (96%)	179 (97%)	5 (3%)	0	100	100
29	Y	152/210 (72%)	144 (95%)	8 (5%)	0	100	100
30	Z	184/196 (94%)	174 (95%)	10 (5%)	0	100	100
31	a	141/203 (70%)	133 (94%)	8 (6%)	0	100	100
32	b	78/94 (83%)	77 (99%)	1 (1%)	0	100	100
33	c	62/93 (67%)	59 (95%)	3 (5%)	0	100	100
34	d	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
35	e	36/46 (78%)	34 (94%)	2 (6%)	0	100	100
36	f	86/95 (90%)	83 (96%)	3 (4%)	0	100	100
37	g	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
38	h	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
39	i	79/93 (85%)	75 (95%)	4 (5%)	0	100	100
40	j	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
41	n	133/184 (72%)	127 (96%)	6 (4%)	0	100	100
42	o	30/380 (8%)	29 (97%)	1 (3%)	0	100	100
All	All	8286/10547 (79%)	7971 (96%)	313 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	286	PRO

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Mol	Chain	Res	Type
19	K	102	GLY

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	1	298/326 (91%)	295 (99%)	3 (1%)	68 86
2	2	509/518 (98%)	498 (98%)	11 (2%)	45 75
3	3	95/128 (74%)	95 (100%)	0	100 100
4	4	431/477 (90%)	422 (98%)	9 (2%)	47 76
5	5	581/596 (98%)	578 (100%)	3 (0%)	81 92
6	6	167/203 (82%)	165 (99%)	2 (1%)	63 84
7	8	68/75 (91%)	68 (100%)	0	100 100
8	9	84/687 (12%)	82 (98%)	2 (2%)	43 74
9	A	577/602 (96%)	576 (100%)	1 (0%)	87 96
10	B	366/401 (91%)	365 (100%)	1 (0%)	86 94
11	C	354/416 (85%)	353 (100%)	1 (0%)	86 94
12	D	68/69 (99%)	67 (98%)	1 (2%)	57 81
13	E	311/335 (93%)	310 (100%)	1 (0%)	86 94
14	F	198/219 (90%)	198 (100%)	0	100 100
15	G	215/257 (84%)	213 (99%)	2 (1%)	70 87
16	H	190/272 (70%)	189 (100%)	1 (0%)	81 92
17	I	158/191 (83%)	156 (99%)	2 (1%)	61 83
18	J	131/146 (90%)	131 (100%)	0	100 100
19	K	154/191 (81%)	152 (99%)	2 (1%)	61 83
20	L	74/76 (97%)	73 (99%)	1 (1%)	59 82
21	M	98/135 (73%)	98 (100%)	0	100 100
22	O	67/119 (56%)	67 (100%)	0	100 100
22	Q	74/119 (62%)	74 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	P	109/110 (99%)	106 (97%)	3 (3%)	38 70
24	R	87/89 (98%)	87 (100%)	0	100 100
25	S	58/111 (52%)	57 (98%)	1 (2%)	53 80
26	U	148/167 (89%)	141 (95%)	7 (5%)	23 54
27	W	100/102 (98%)	99 (99%)	1 (1%)	68 86
28	X	143/152 (94%)	143 (100%)	0	100 100
29	Y	131/176 (74%)	130 (99%)	1 (1%)	73 89
30	Z	152/155 (98%)	152 (100%)	0	100 100
31	a	123/177 (70%)	123 (100%)	0	100 100
32	b	66/74 (89%)	66 (100%)	0	100 100
33	c	47/80 (59%)	47 (100%)	0	100 100
34	d	87/94 (93%)	86 (99%)	1 (1%)	65 85
35	e	30/35 (86%)	30 (100%)	0	100 100
36	f	76/80 (95%)	76 (100%)	0	100 100
37	g	65/69 (94%)	64 (98%)	1 (2%)	57 81
38	h	118/119 (99%)	118 (100%)	0	100 100
39	i	69/78 (88%)	69 (100%)	0	100 100
40	j	63/64 (98%)	62 (98%)	1 (2%)	55 81
41	n	108/150 (72%)	107 (99%)	1 (1%)	70 87
42	o	26/318 (8%)	26 (100%)	0	100 100
All	All	7074/8958 (79%)	7014 (99%)	60 (1%)	70 89

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	9	26	VAL
29	Y	133	VAL
15	G	107	GLU
27	W	40	LEU
41	n	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
13	E	291	GLN
17	I	87	GLN
38	h	121	GLN
14	F	42	HIS
15	G	220	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
11	2MR	C	154	11	10,12,13	0.42	0	5,13,15	1.04	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
11	2MR	C	154	11	-	0/10/13/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	154	2MR	NE-CZ-NH2	-2.20	117.46	119.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	$\#\|Z\| > 2$
44	LMT	g	101	-	35,35,36	1.10	2 (5%)	46,46,47	1.06	1 (2%)
44	LMT	X	203	-	36,36,36	0.38	0	47,47,47	0.70	0
47	FES	A	801	9	0,4,4	-	-	-		
43	PC1	5	702	-	39,39,53	0.35	0	45,47,61	0.51	0
46	3PE	W	201	-	39,39,50	0.30	0	42,44,55	0.35	0
43	PC1	1	401	-	32,32,53	0.33	0	38,40,61	0.35	0
44	LMT	5	705	-	36,36,36	0.33	0	47,47,47	1.15	4 (8%)
44	LMT	a	301	-	36,36,36	0.39	0	47,47,47	0.77	1 (2%)
46	3PE	i	101	-	37,37,50	0.32	0	40,42,55	0.36	0
48	SF4	B	601	10	0,12,12	-	-	-		
49	FMN	B	602	-	33,33,33	0.66	0	48,50,50	0.72	1 (2%)
46	3PE	5	704	-	41,41,50	0.30	0	44,46,55	0.37	0
44	LMT	J	201	-	32,32,36	0.39	0	43,43,47	0.70	1 (2%)
44	LMT	4	601	-	36,36,36	1.09	2 (5%)	47,47,47	1.09	3 (6%)
44	LMT	1	403	-	36,36,36	0.35	0	47,47,47	0.61	0
44	LMT	1	402	-	36,36,36	0.35	0	47,47,47	0.82	2 (4%)
45	CDL	2	601	-	67,67,99	0.33	0	73,79,111	0.42	0
44	LMT	2	603	-	34,34,36	0.37	0	45,45,47	0.84	1 (2%)
44	LMT	2	604	-	36,36,36	0.41	0	47,47,47	0.70	0
46	3PE	I	303	-	36,36,50	0.34	0	39,41,55	0.55	0
43	PC1	5	703	-	44,44,53	0.30	0	50,52,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	NDP	E	402	-	49,52,52	0.48	0	66,80,80	0.52	0
46	3PE	E	401	-	28,28,50	0.37	0	31,33,55	0.48	0
46	3PE	5	701	-	40,40,50	0.29	0	43,45,55	0.32	0
44	LMT	3	201	-	36,36,36	0.33	0	47,47,47	0.84	0
48	SF4	K	301	19	0,12,12	-	-	-		
44	LMT	2	602	-	36,36,36	0.48	0	47,47,47	0.97	3 (6%)
45	CDL	S	201	-	60,60,99	0.33	0	66,72,111	0.43	0
48	SF4	A	802	9	0,12,12	-	-	-		
48	SF4	A	803	9	0,12,12	-	-	-		
47	FES	H	401	16	0,4,4	-	-	-		
48	SF4	I	302	17	0,12,12	-	-	-		
45	CDL	X	202	-	75,75,99	0.33	0	81,87,111	0.38	0
45	CDL	D	101	-	58,58,99	0.35	0	64,70,111	0.42	0
46	3PE	W	202	-	31,31,50	0.36	0	34,36,55	0.39	0
45	CDL	X	201	-	51,51,99	0.38	0	57,63,111	0.51	0
48	SF4	I	301	17	0,12,12	-	-	-		
52	ZMP	O	201	22	29,35,36	0.23	0	34,42,45	0.45	0
44	LMT	j	101	-	36,36,36	0.38	0	47,47,47	0.94	3 (6%)
52	ZMP	Q	201	22	29,35,36	0.18	0	34,42,45	0.41	0
44	LMT	3	202	-	36,36,36	0.40	0	47,47,47	0.93	4 (8%)
46	3PE	5	706	-	41,41,50	0.94	4 (9%)	44,46,55	1.10	2 (4%)
43	PC1	2	605	-	44,44,53	0.28	0	50,52,61	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	LMT	g	101	-	-	10/20/60/61	0/2/2/2
44	LMT	X	203	-	-	4/21/61/61	0/2/2/2
47	FES	A	801	9	-	-	0/1/1/1
43	PC1	5	702	-	-	18/43/43/57	-
46	3PE	W	201	-	-	14/43/43/54	-
43	PC1	1	401	-	-	10/36/36/57	-
44	LMT	5	705	-	-	6/21/61/61	0/2/2/2
44	LMT	a	301	-	-	6/21/61/61	0/2/2/2
46	3PE	i	101	-	-	11/41/41/54	-
49	FMN	B	602	-	-	3/18/18/18	0/3/3/3
48	SF4	B	601	10	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	5	704	-	-	17/45/45/54	-
44	LMT	J	201	-	-	6/17/57/61	0/2/2/2
44	LMT	4	601	-	-	8/21/61/61	0/2/2/2
44	LMT	1	403	-	-	3/21/61/61	0/2/2/2
44	LMT	1	402	-	-	3/21/61/61	0/2/2/2
45	CDL	2	601	-	-	19/78/78/110	-
44	LMT	2	603	-	-	7/19/59/61	0/2/2/2
44	LMT	2	604	-	-	9/21/61/61	0/2/2/2
46	3PE	I	303	-	-	15/40/40/54	-
43	PC1	5	703	-	-	8/48/48/57	-
50	NDP	E	402	-	-	7/34/77/77	0/5/5/5
46	3PE	E	401	-	-	8/32/32/54	-
46	3PE	5	701	-	-	8/44/44/54	-
44	LMT	3	201	-	-	3/21/61/61	0/2/2/2
48	SF4	K	301	19	-	-	0/6/5/5
44	LMT	2	602	-	-	7/21/61/61	0/2/2/2
45	CDL	S	201	-	-	20/70/70/110	-
48	SF4	A	802	9	-	-	0/6/5/5
48	SF4	A	803	9	-	-	0/6/5/5
47	FES	H	401	16	-	-	0/1/1/1
48	SF4	I	302	17	-	-	0/6/5/5
45	CDL	X	202	-	-	36/86/86/110	-
45	CDL	D	101	-	-	25/69/69/110	-
46	3PE	W	202	-	-	7/35/35/54	-
45	CDL	X	201	-	-	25/62/62/110	-
48	SF4	I	301	17	-	-	0/6/5/5
52	ZMP	O	201	22	-	10/40/42/43	-
44	LMT	j	101	-	-	5/21/61/61	0/2/2/2
52	ZMP	Q	201	22	-	17/40/42/43	-
44	LMT	3	202	-	-	10/21/61/61	0/2/2/2
46	3PE	5	706	-	-	14/45/45/54	-
43	PC1	2	605	-	-	7/48/48/57	-

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	4	601	LMT	O5B-C1B	3.28	1.50	1.41
44	g	101	LMT	O5B-C1B	3.18	1.49	1.41
44	g	101	LMT	O5'-C1'	3.13	1.49	1.41
44	4	601	LMT	O5'-C1'	2.79	1.48	1.41
46	5	706	3PE	O21-C2	-2.46	1.40	1.46

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	5	706	3PE	O21-C21-C22	3.86	119.82	111.50
44	4	601	LMT	C1B-O1B-C4'	-3.46	109.40	117.96
44	5	705	LMT	C1-O1'-C1'	-3.39	108.22	113.84
44	5	705	LMT	O1'-C1'-C2'	3.35	113.53	108.30
44	j	101	LMT	C1-O1'-C1'	-2.94	108.97	113.84

There are no chirality outliers.

5 of 386 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	PC1	C11-O13-P-O14
43	1	401	PC1	C11-O13-P-O11
43	1	401	PC1	C1-O11-P-O12
43	1	401	PC1	C1-O11-P-O14
43	1	401	PC1	C22-C21-O21-C2

There are no ring outliers.

34 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	g	101	LMT	1	0
44	X	203	LMT	3	0
43	5	702	PC1	7	0
46	W	201	3PE	1	0
43	1	401	PC1	1	0
44	5	705	LMT	3	0
44	a	301	LMT	2	0
46	i	101	3PE	1	0
49	B	602	FMN	2	0
46	5	704	3PE	1	0

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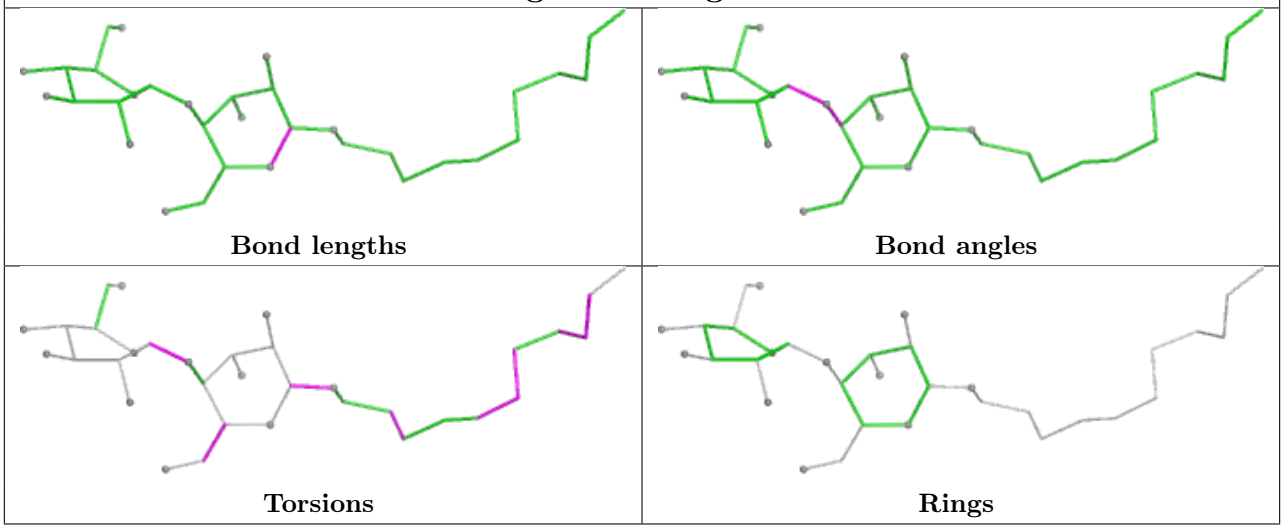
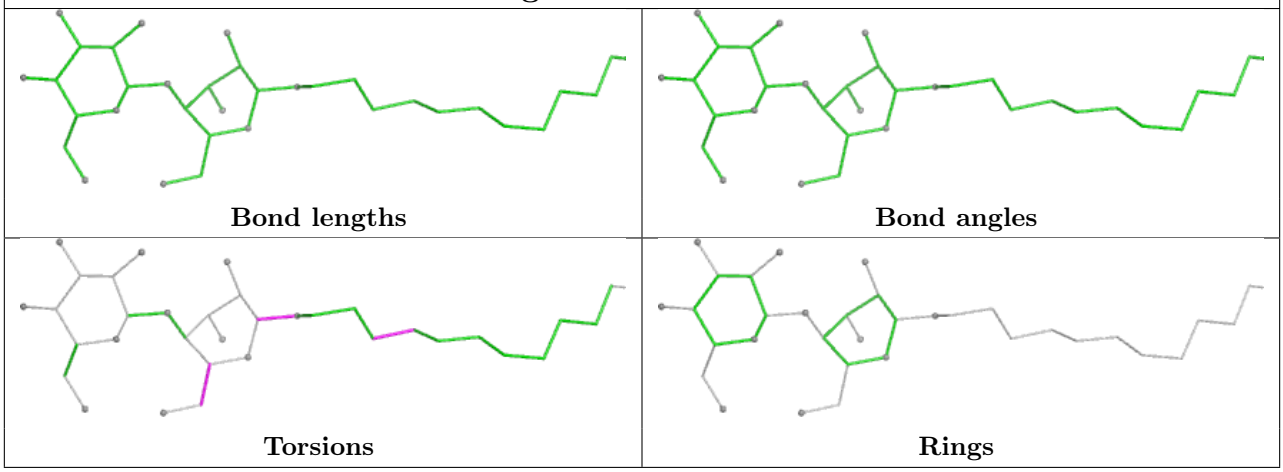
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	4	601	LMT	4	0
44	1	403	LMT	1	0
44	1	402	LMT	2	0
45	2	601	CDL	2	0
44	2	603	LMT	1	0
44	2	604	LMT	2	0
46	I	303	3PE	2	0
43	5	703	PC1	4	0
50	E	402	NDP	2	0
46	E	401	3PE	1	0
46	5	701	3PE	1	0
44	3	201	LMT	2	0
48	K	301	SF4	1	0
44	2	602	LMT	3	0
45	S	201	CDL	3	0
45	X	202	CDL	3	0
45	D	101	CDL	3	0
46	W	202	3PE	3	0
52	O	201	ZMP	1	0
44	j	101	LMT	4	0
52	Q	201	ZMP	3	0
44	3	202	LMT	1	0
46	5	706	3PE	1	0
43	2	605	PC1	13	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.

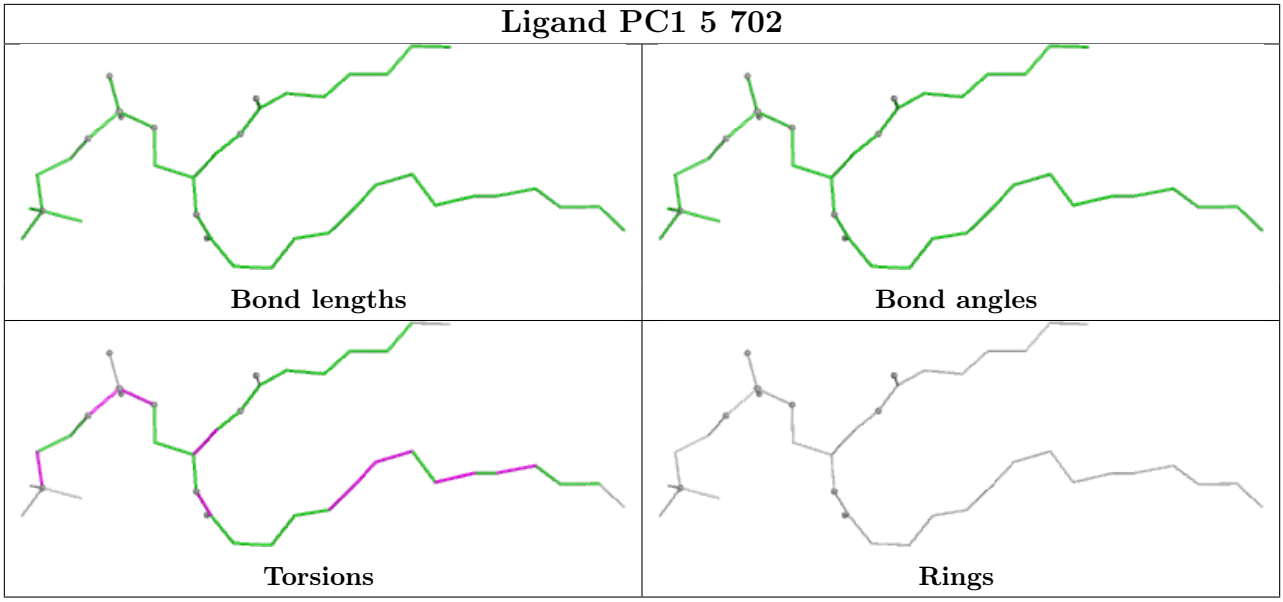
Ligand LMT g 101



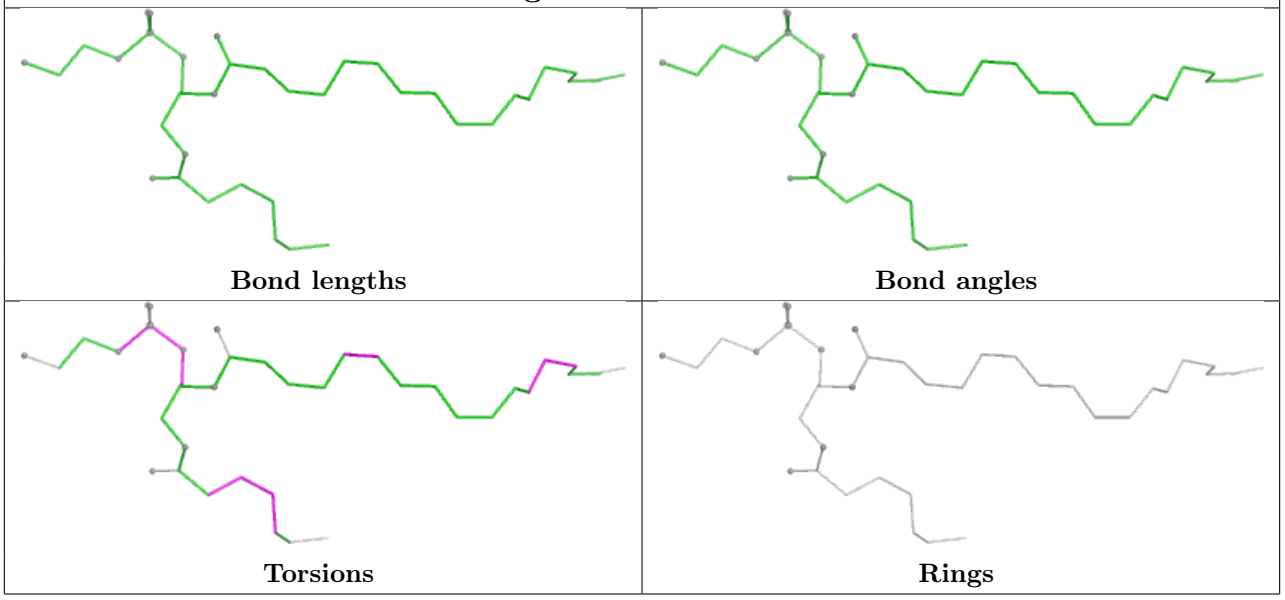
Ligand LMT X 203



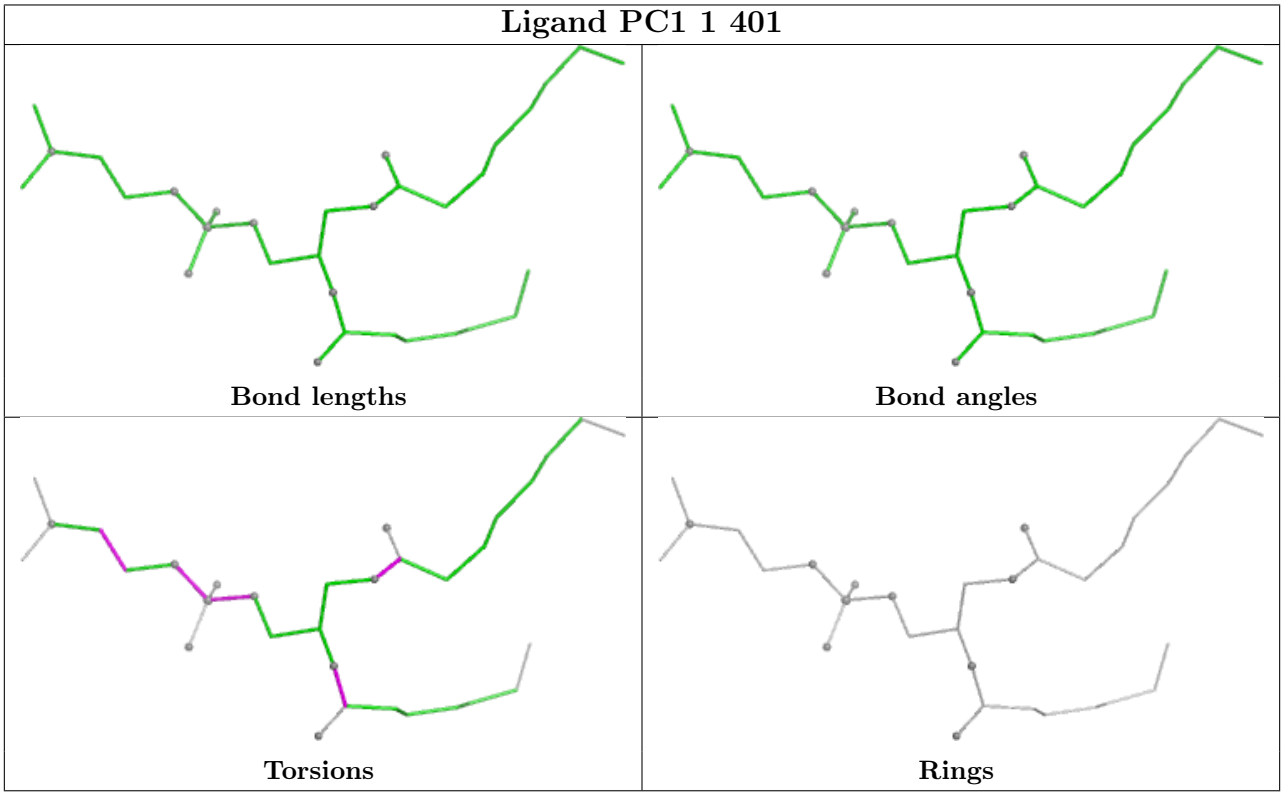
Ligand PC1 5 702



Ligand 3PE W 201



Ligand PC1 1 401



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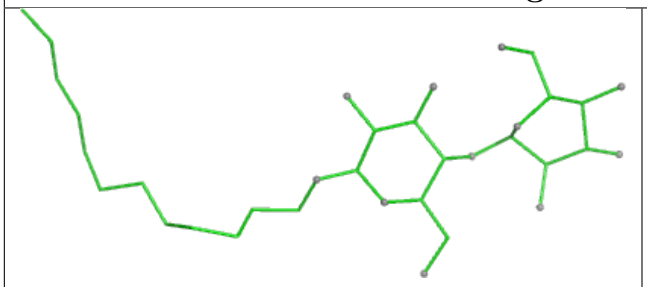
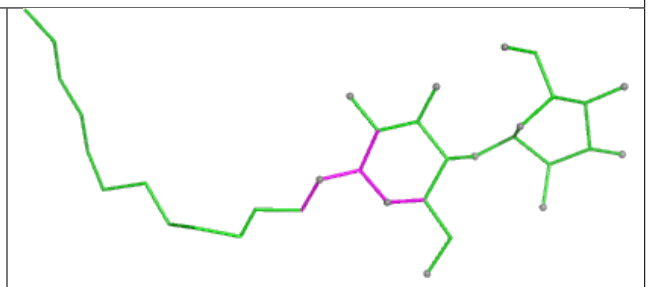
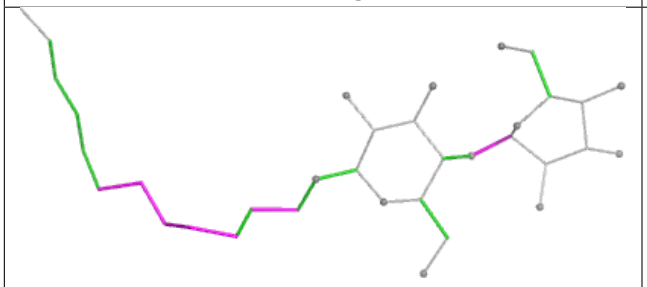


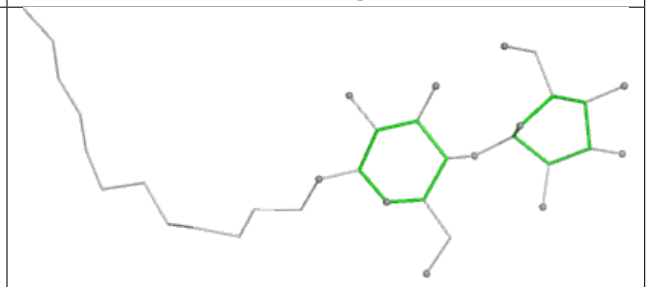
Bond lengths



Bond angles

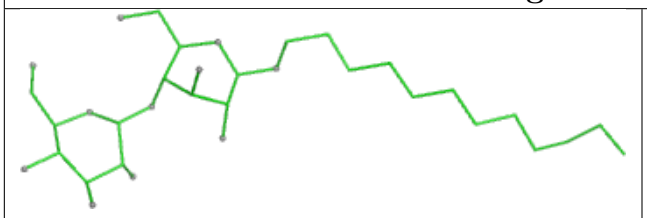


Torsions

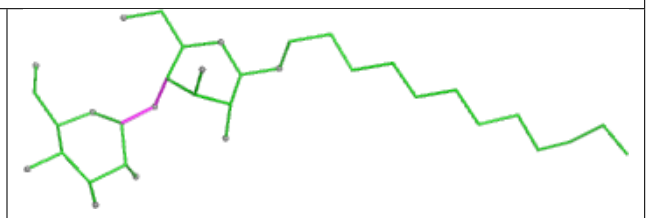


Rings

Ligand LMT a 301



Bond lengths



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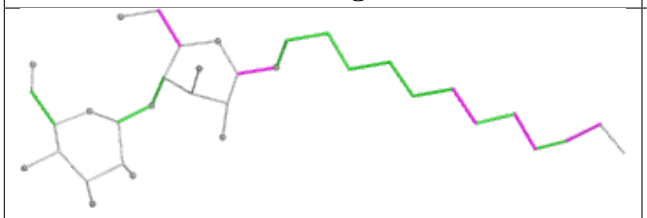

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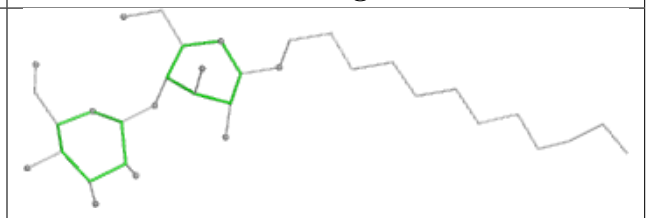
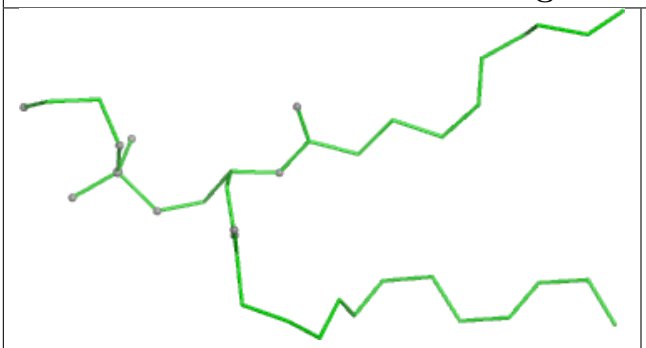


Rings

Ligand 3PE i 101



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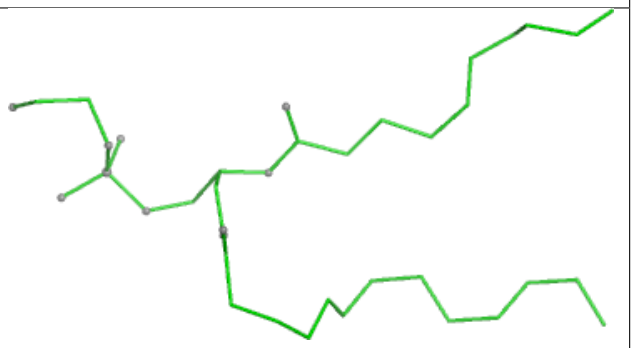

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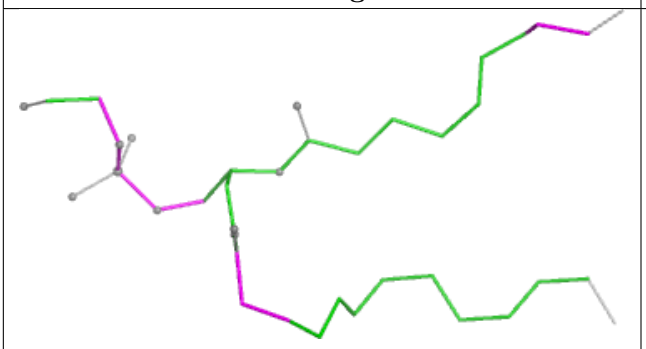

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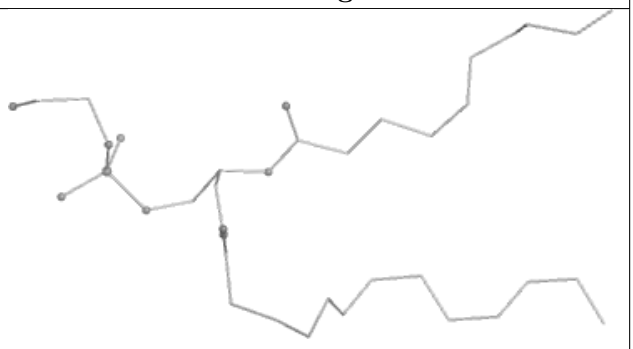
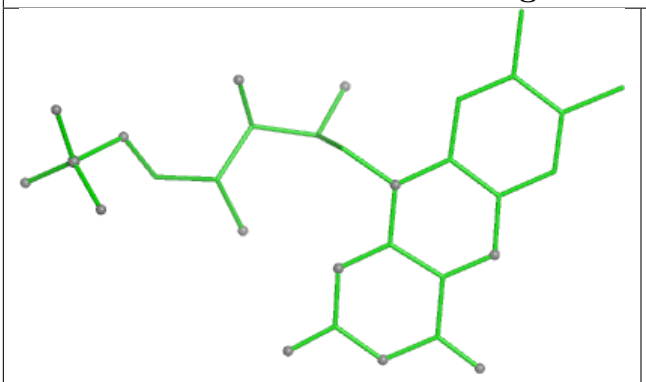


Rings

Ligand FMN B 602



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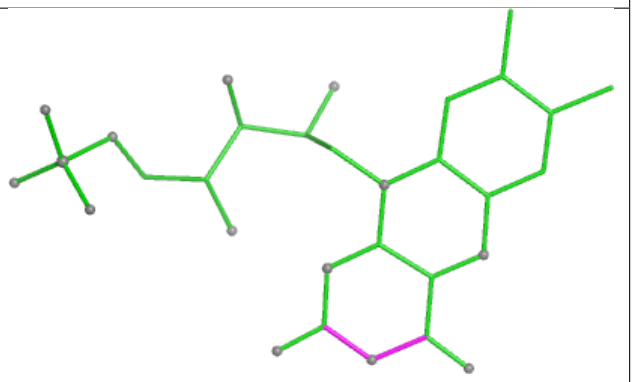

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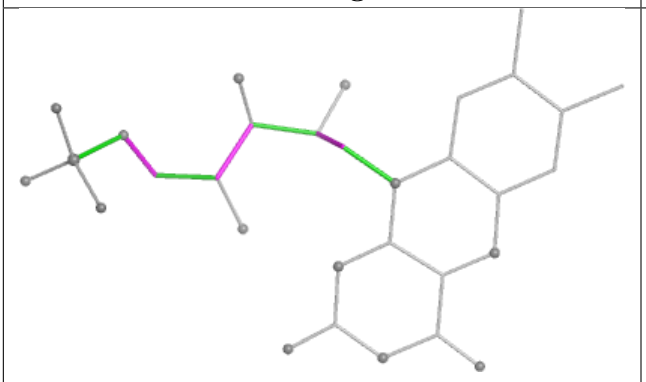

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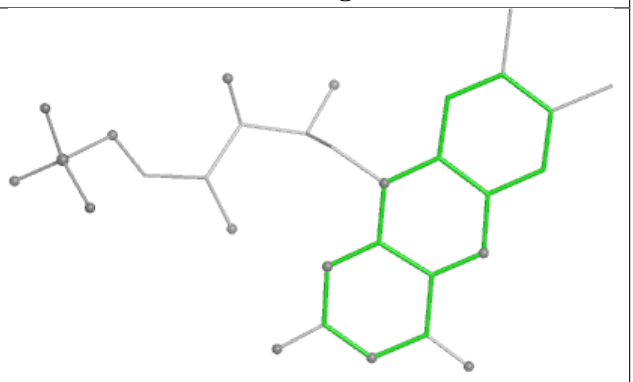
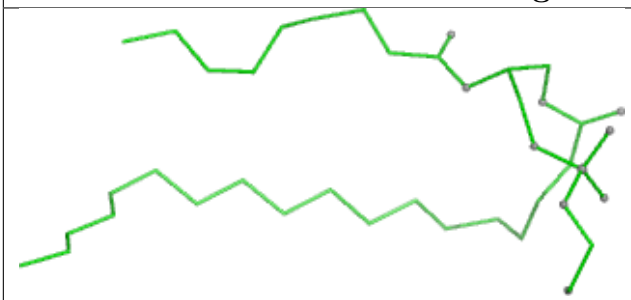


Rings

Ligand 3PE 5 704



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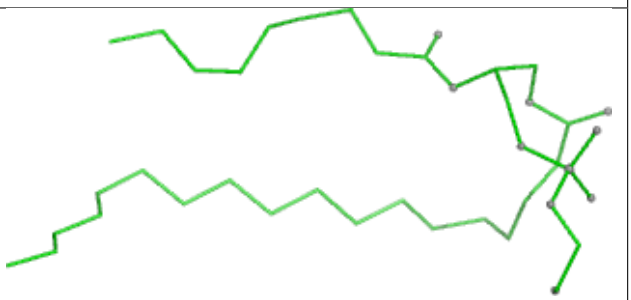

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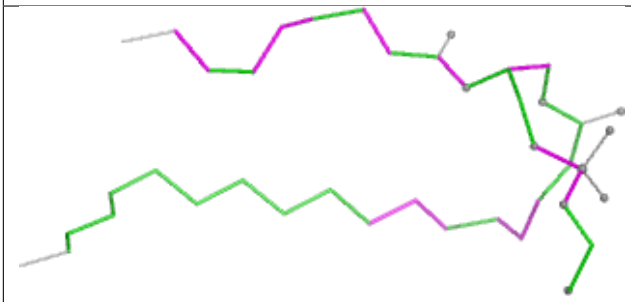
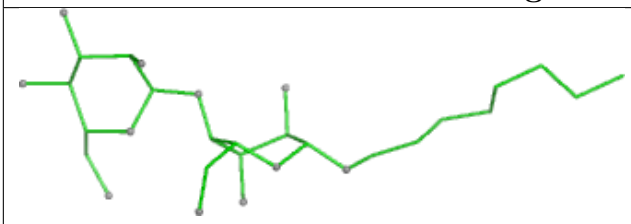


Torsions

Rings

Ligand LMT J 201



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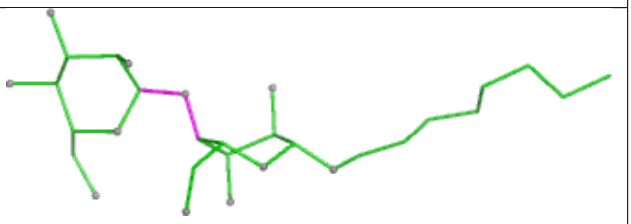

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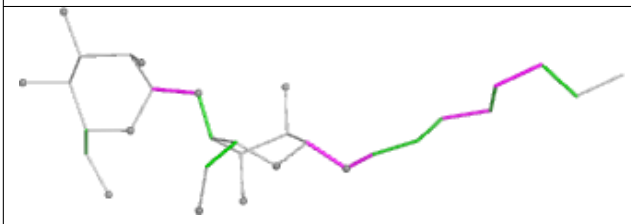

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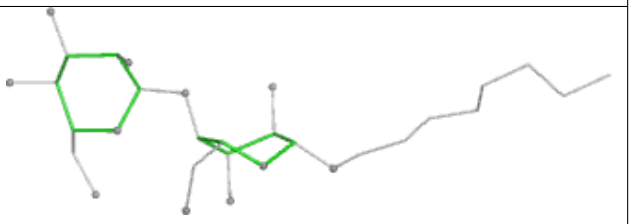
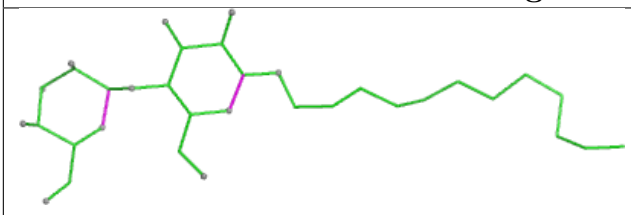


Rings

Ligand LMT 4 601



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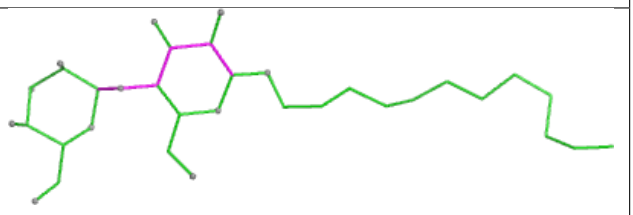

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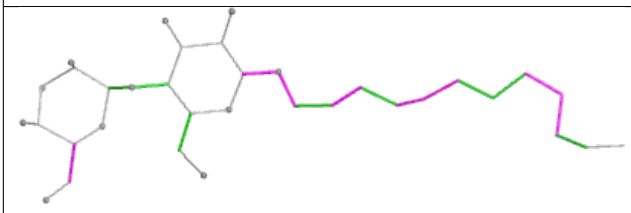

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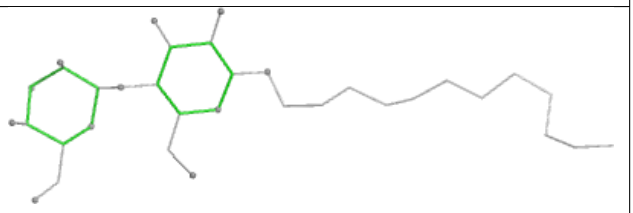
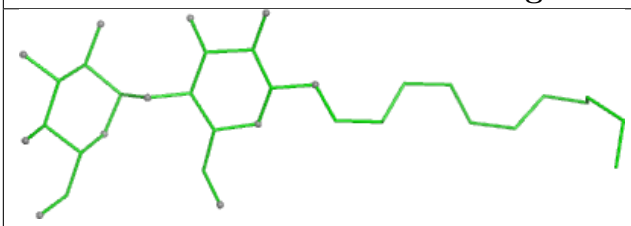
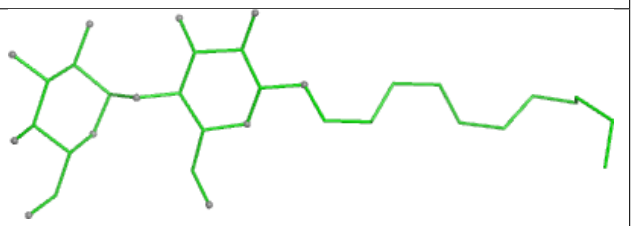


Rings

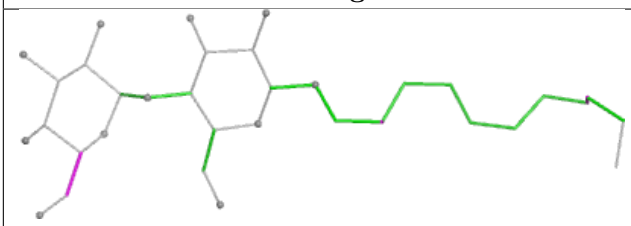
Ligand LMT 1 403



Bond lengths



Bond angles



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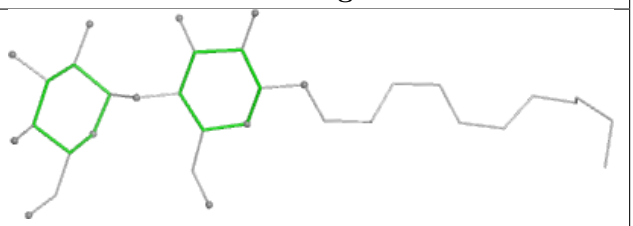
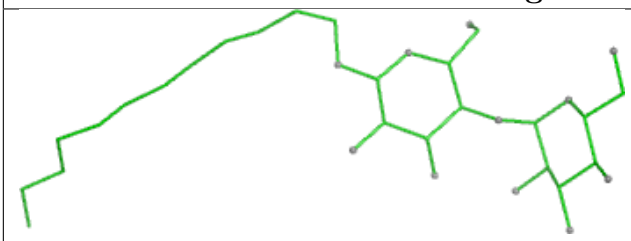
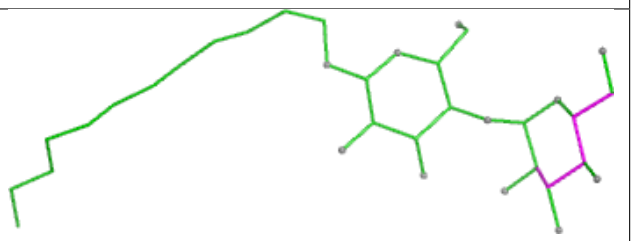


Rings

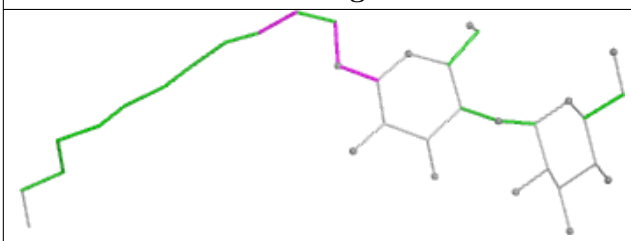
Ligand LMT 1 402



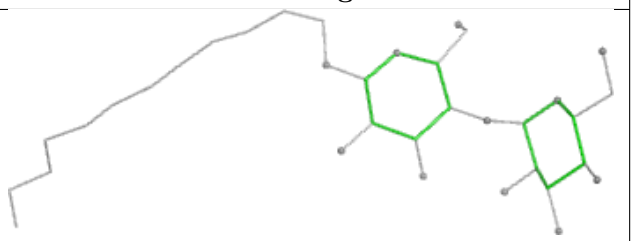
Bond lengths



Bond angles

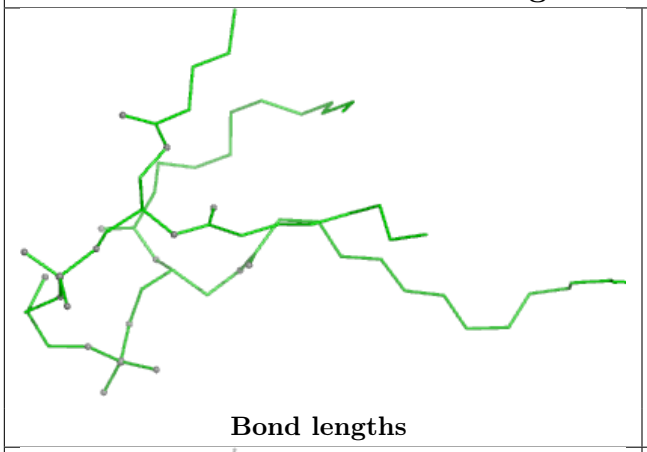


Torsions



Rings

Ligand CDL 2 601



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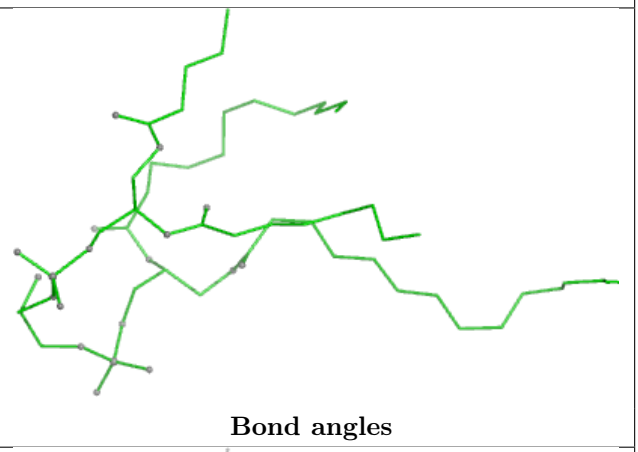

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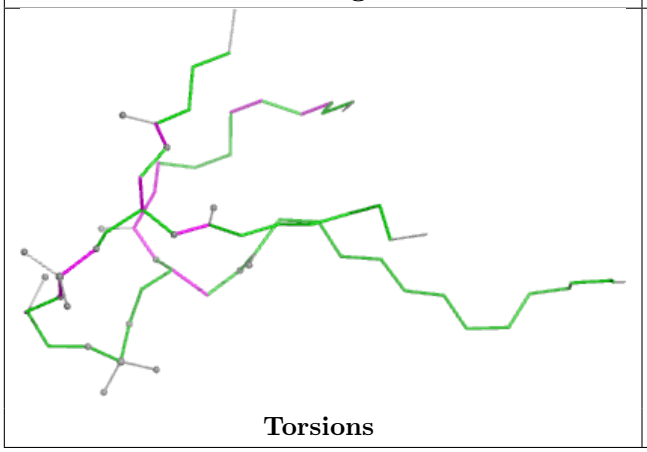

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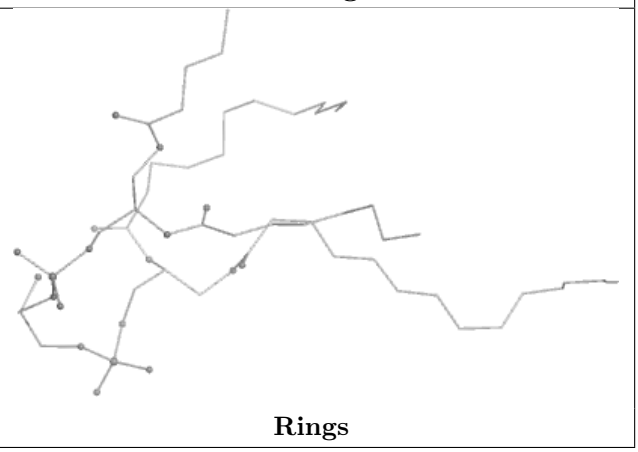

Rings

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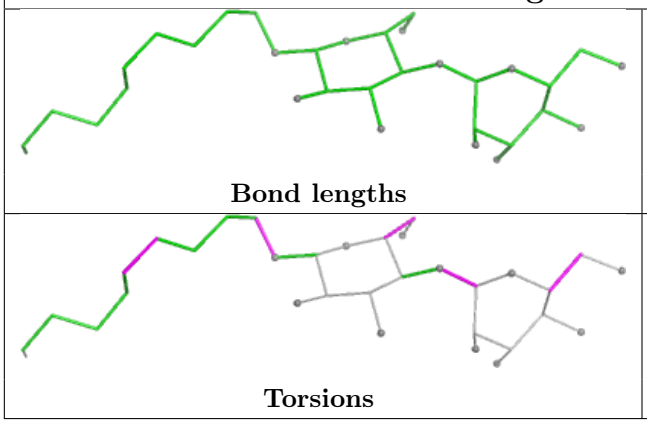

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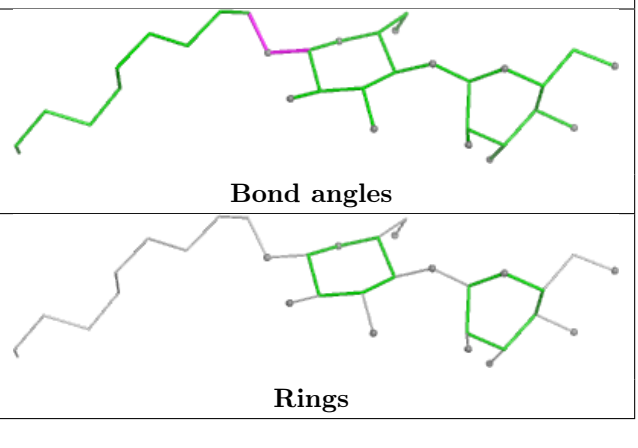
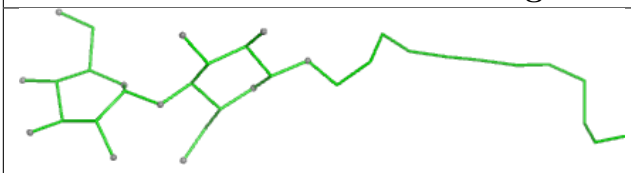


Bond angles

Torsions

Rings

Ligand LMT 2 604



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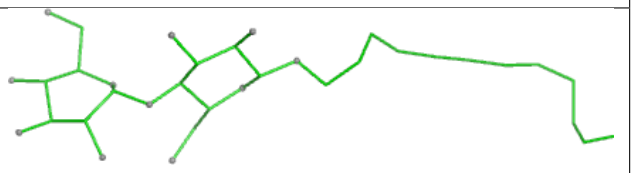

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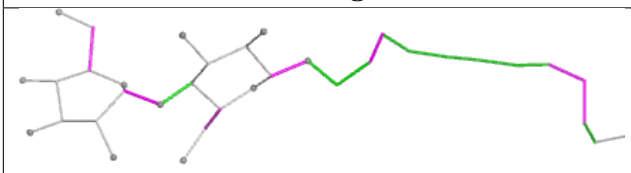

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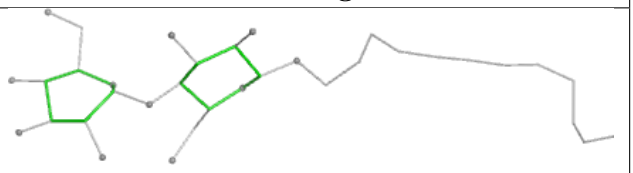

Rings

Ligand 3PE I 303

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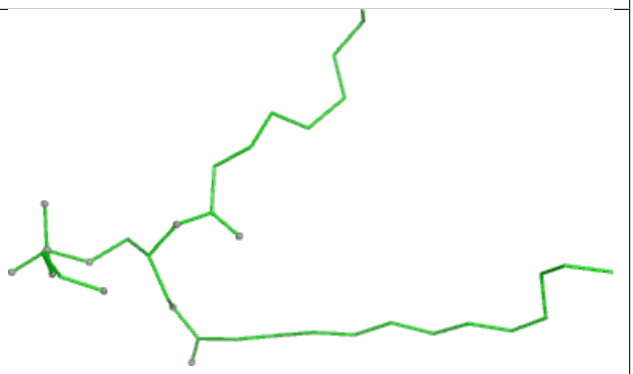

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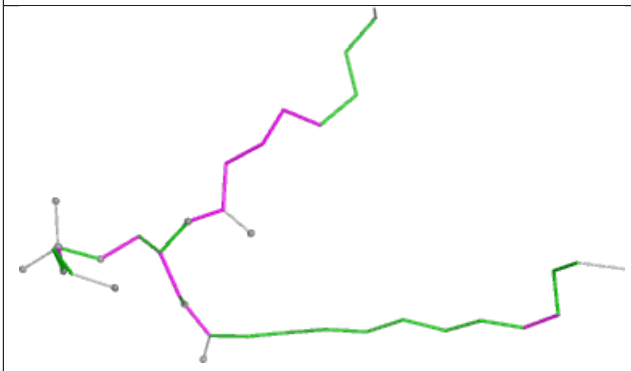

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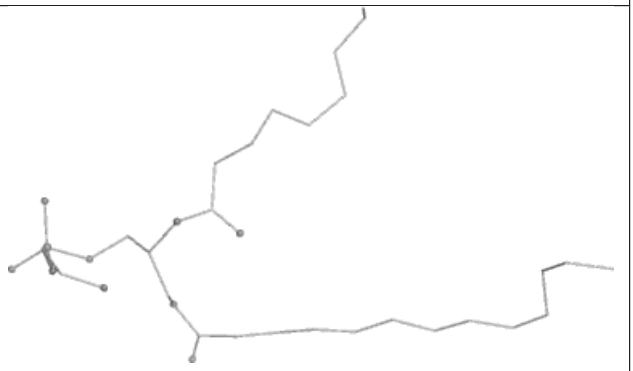
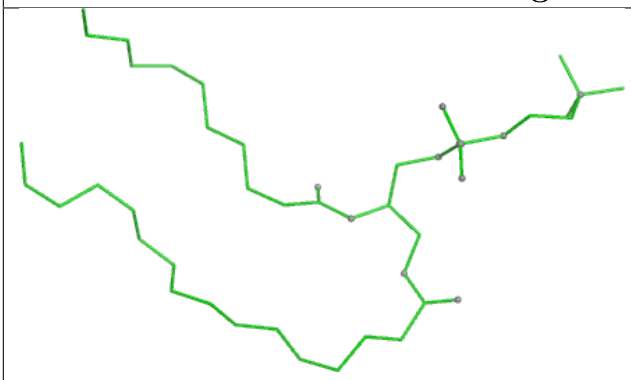


Rings

Ligand PC1 5 703



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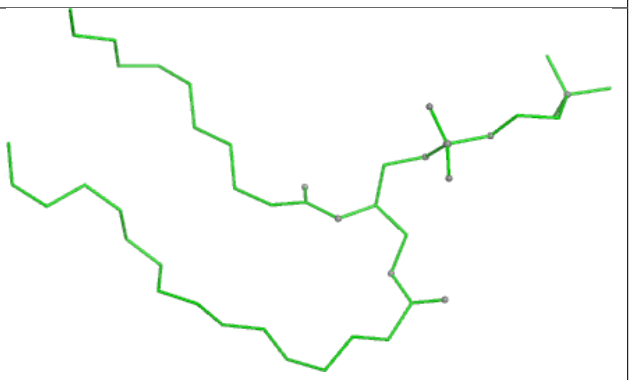

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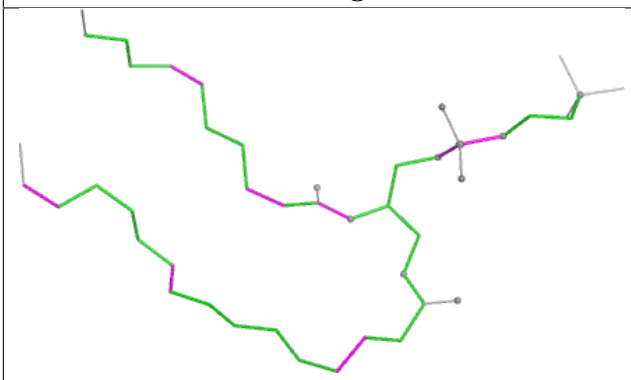

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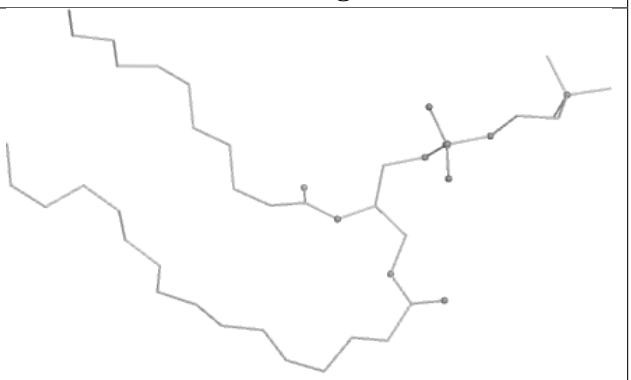
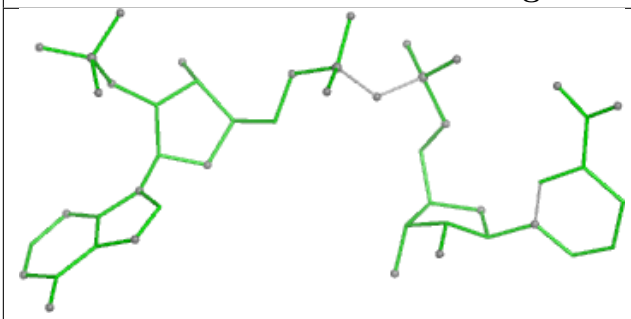


Rings

Ligand NDP E 402



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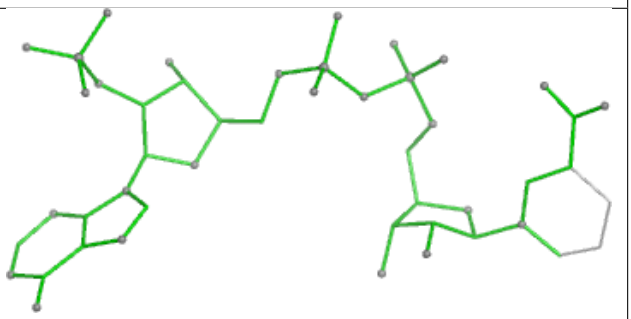

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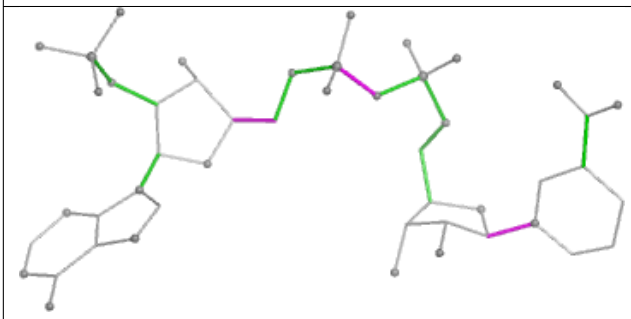

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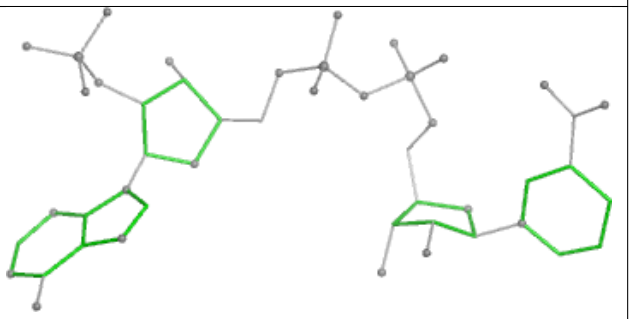

Rings

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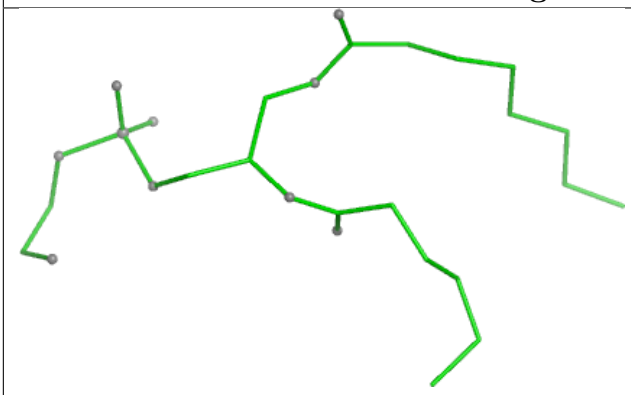

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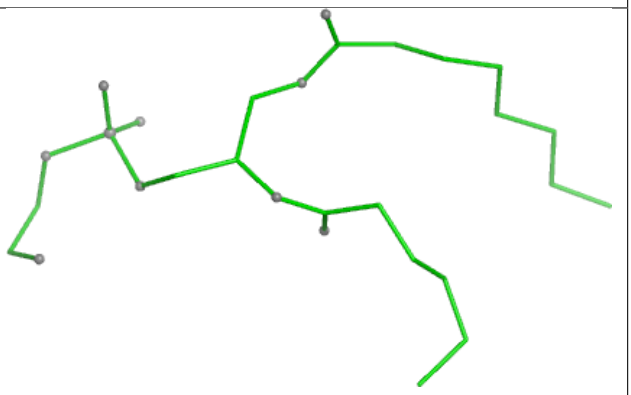

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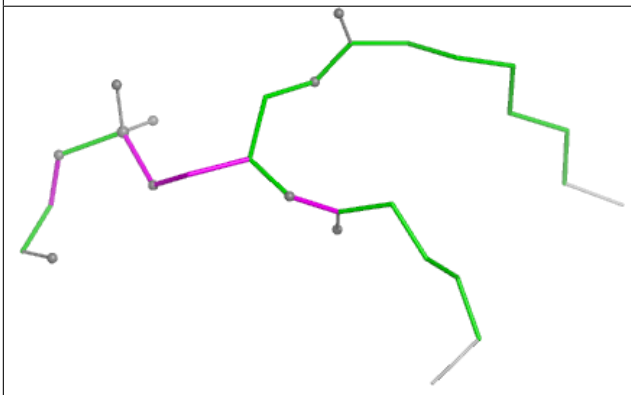

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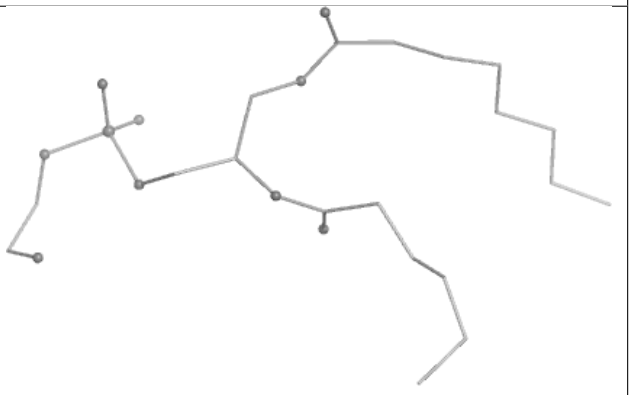

Rings

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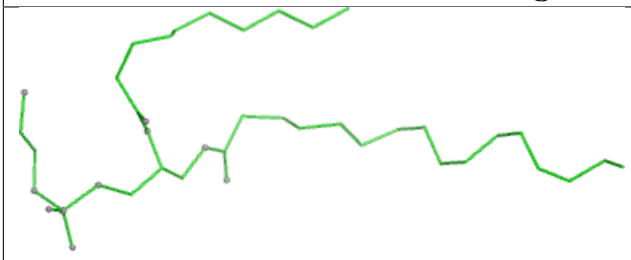

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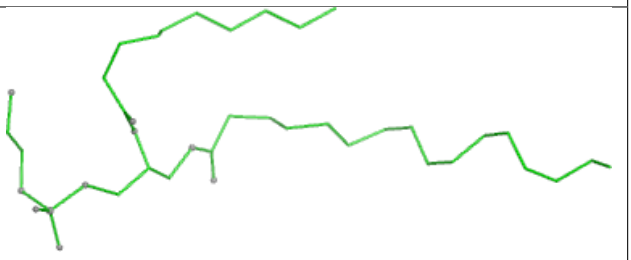
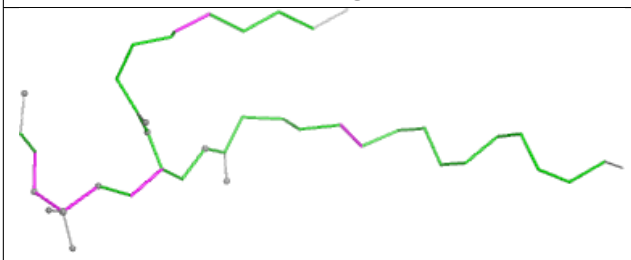


Bond angles



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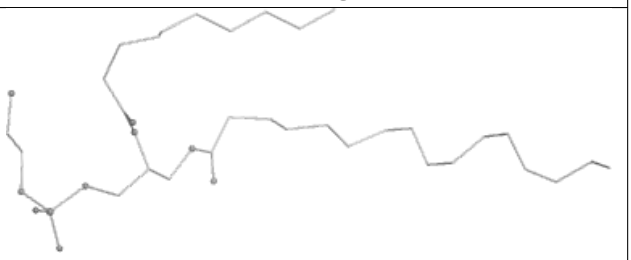

Rings

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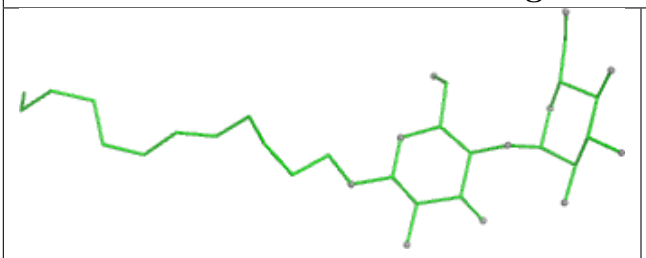

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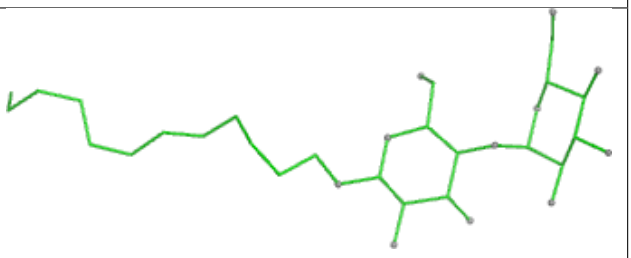

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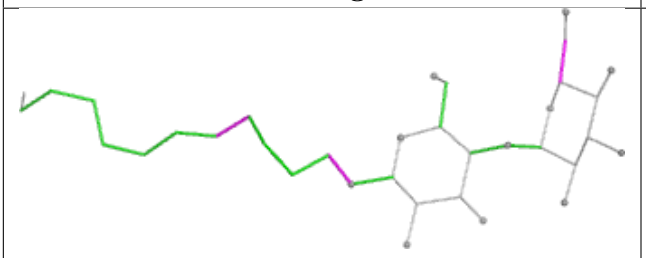

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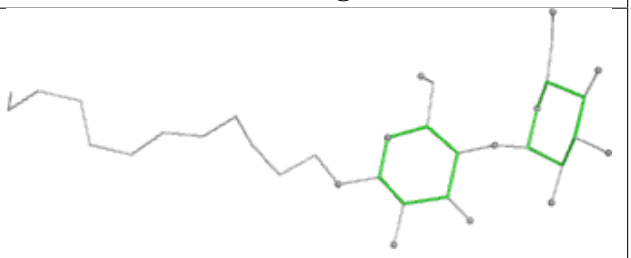

Rings

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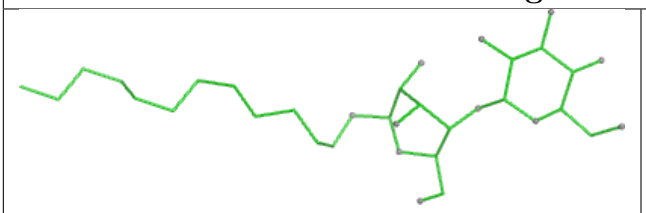

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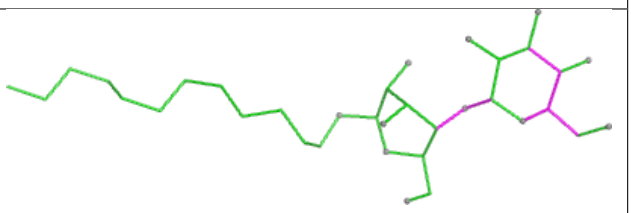
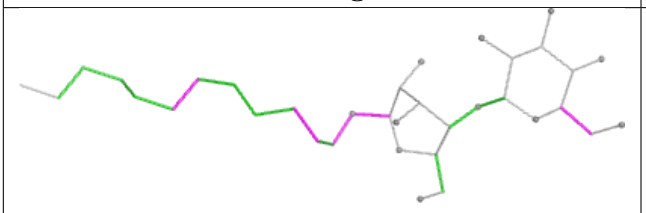


Bond angles



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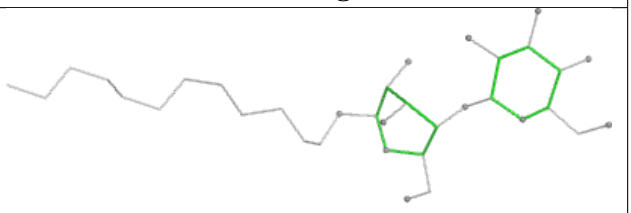
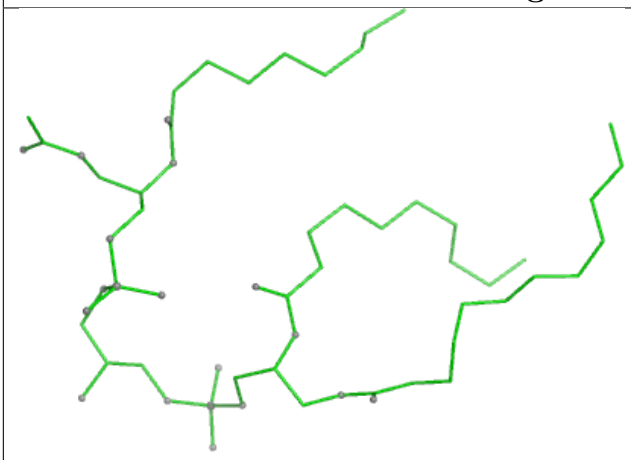


Rings

Ligand CDL S 201



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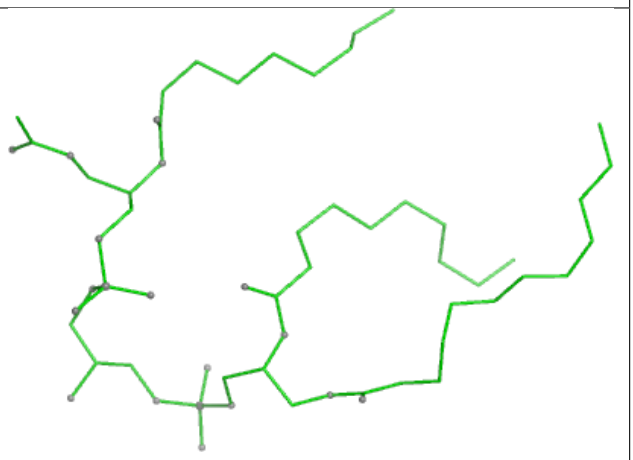
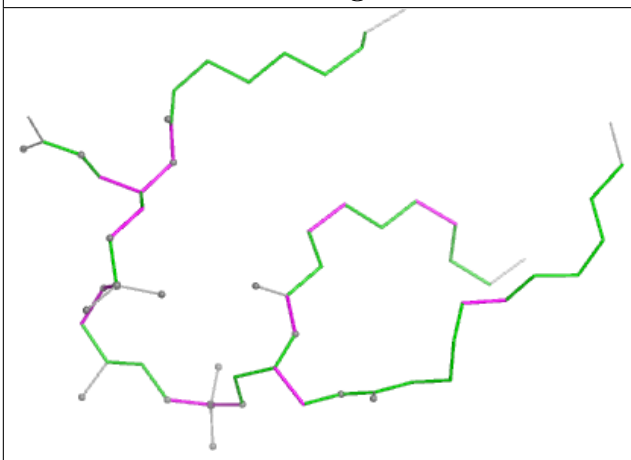


Bond angles



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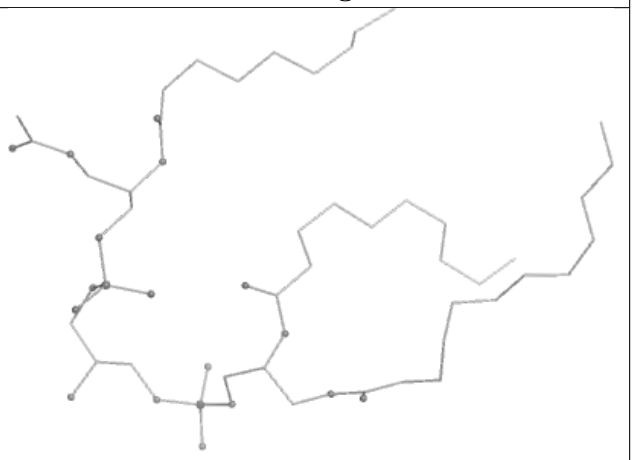
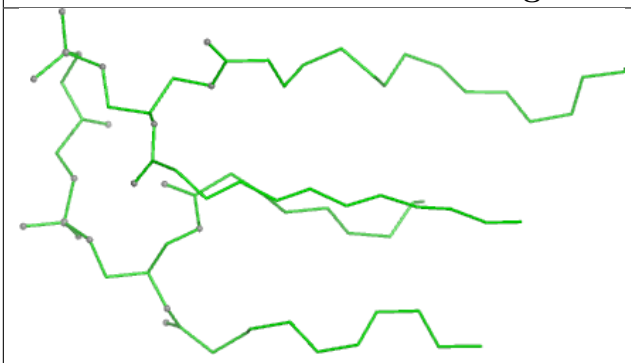


Rings

Ligand CDL X 202



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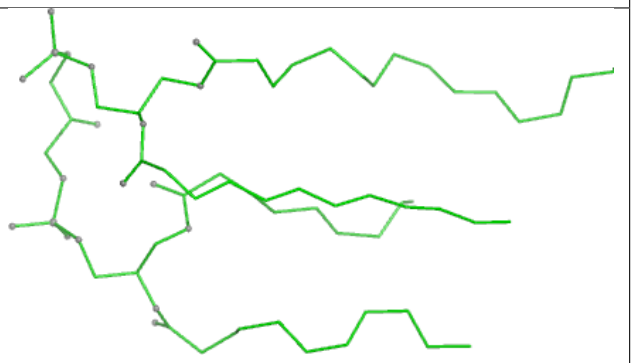
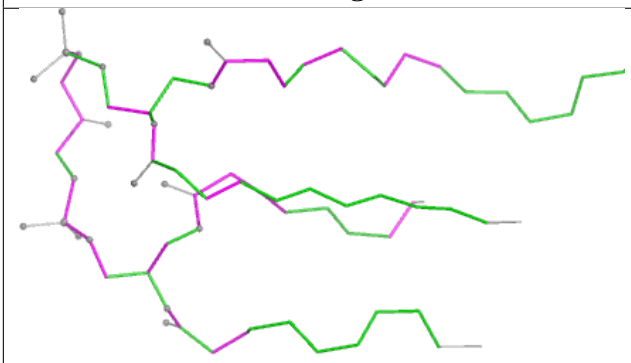


Bond angles



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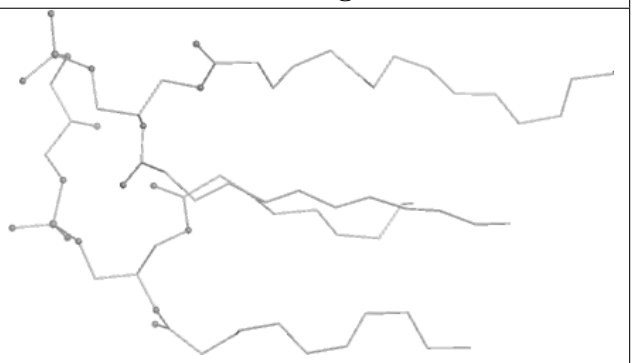
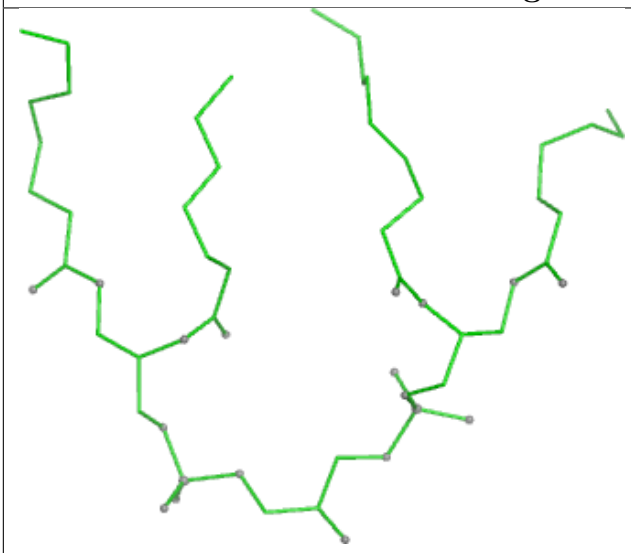


Rings

Ligand CDL D 101



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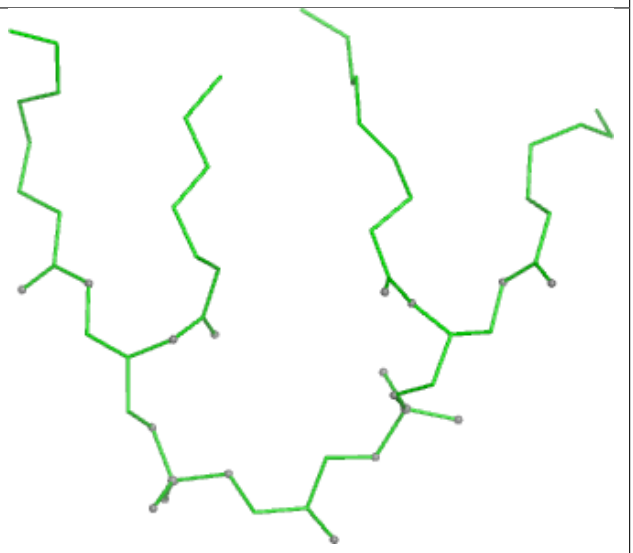
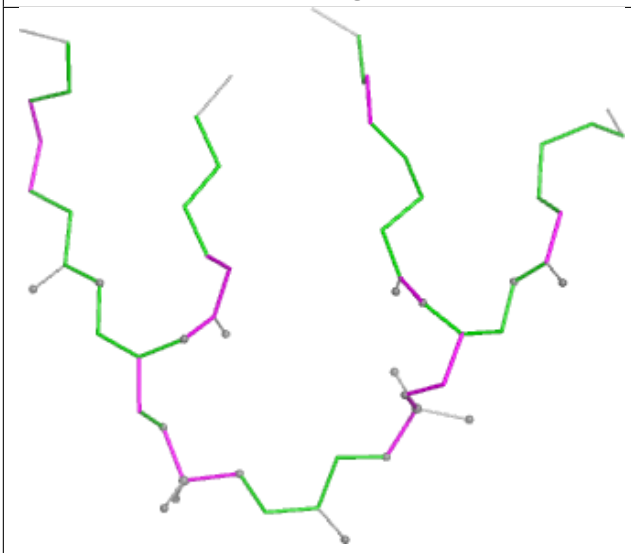


Bond angles



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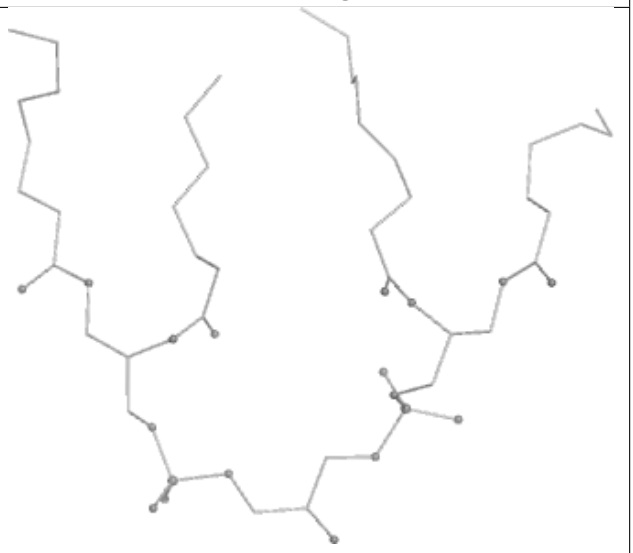
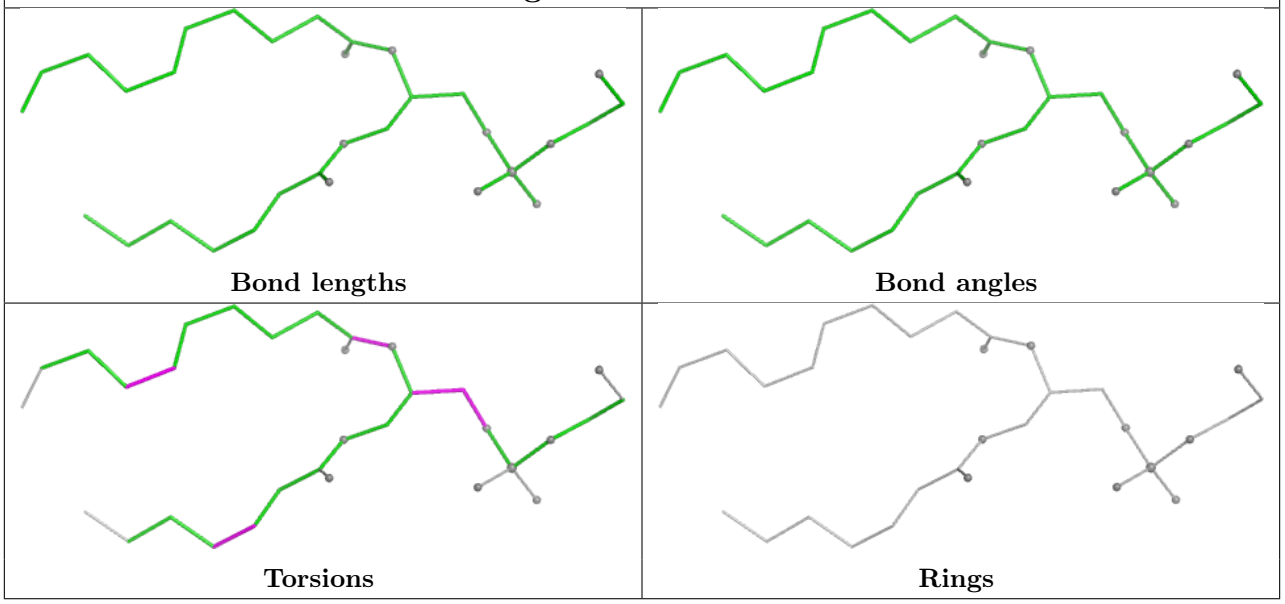
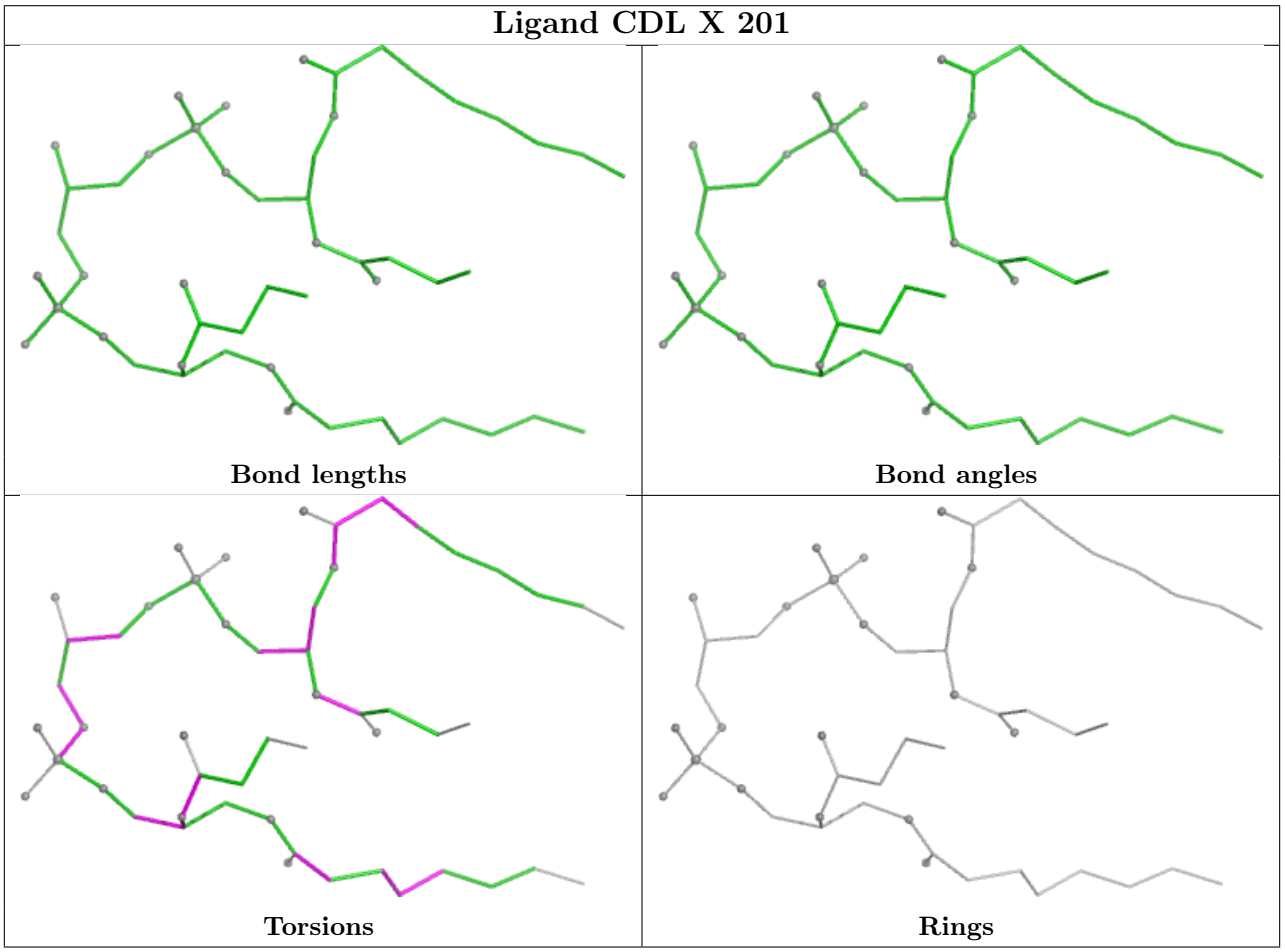


Rings

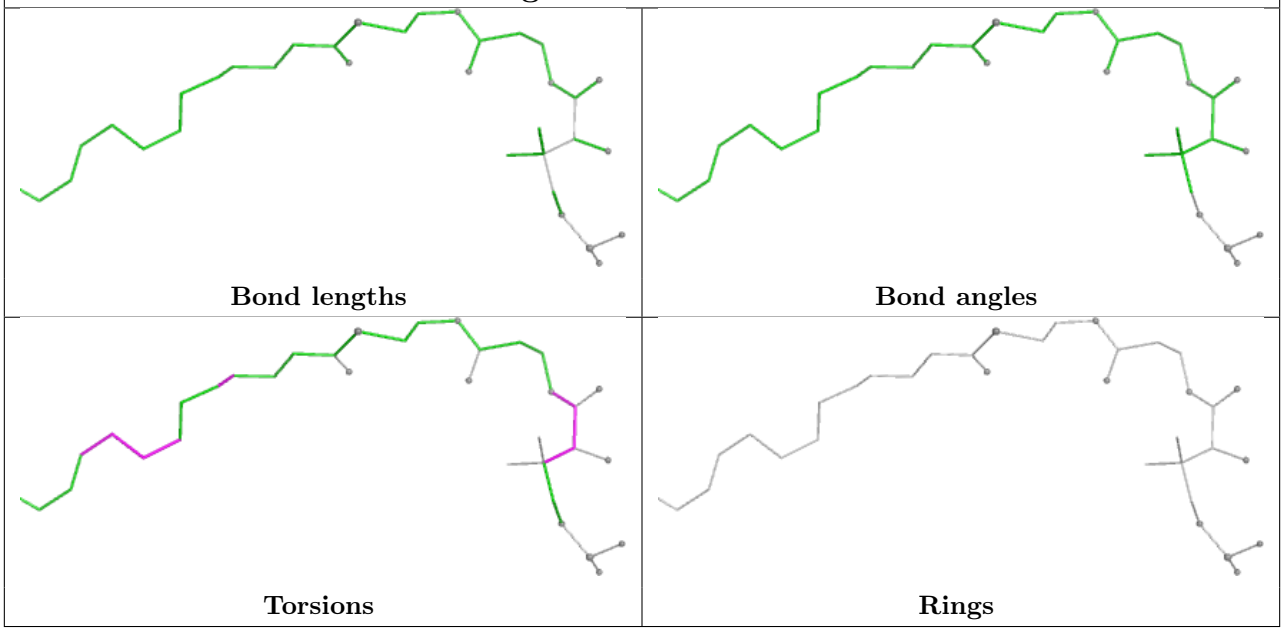
Ligand 3PE W 202



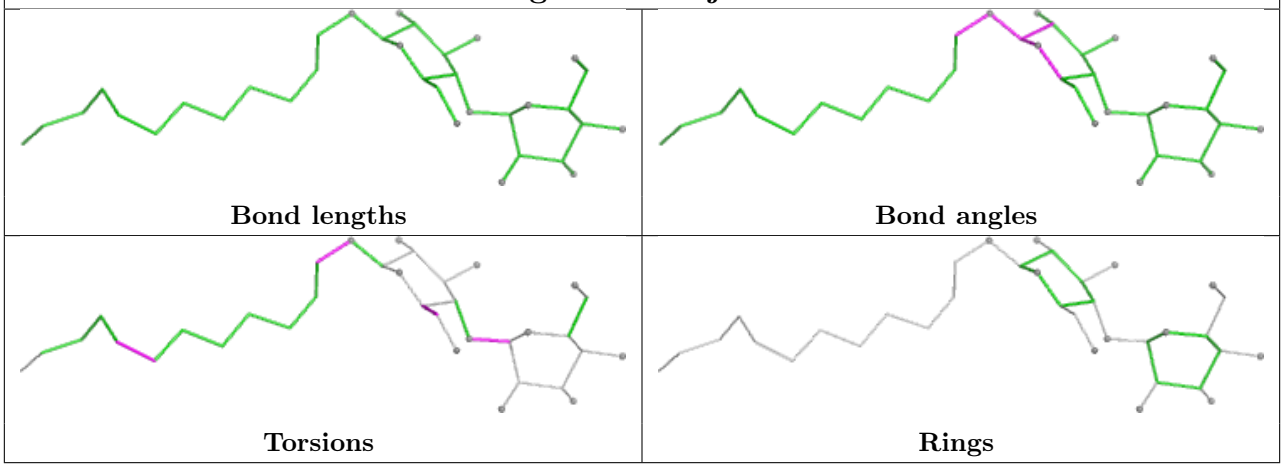
Ligand CDL X 201



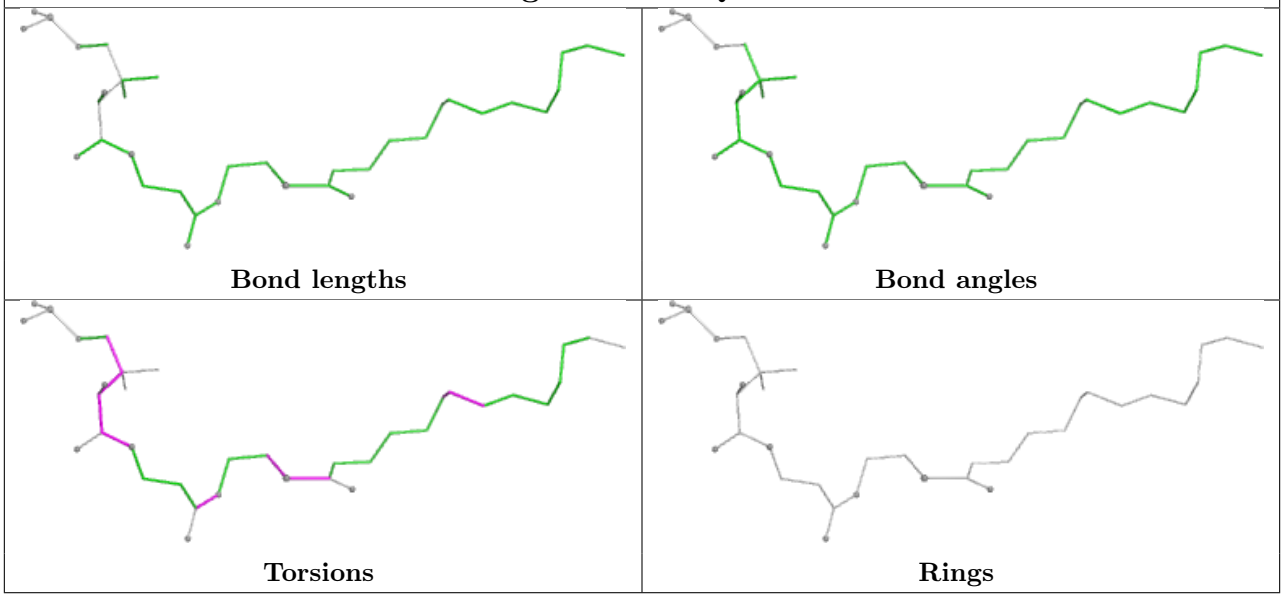
Ligand ZMP O 201



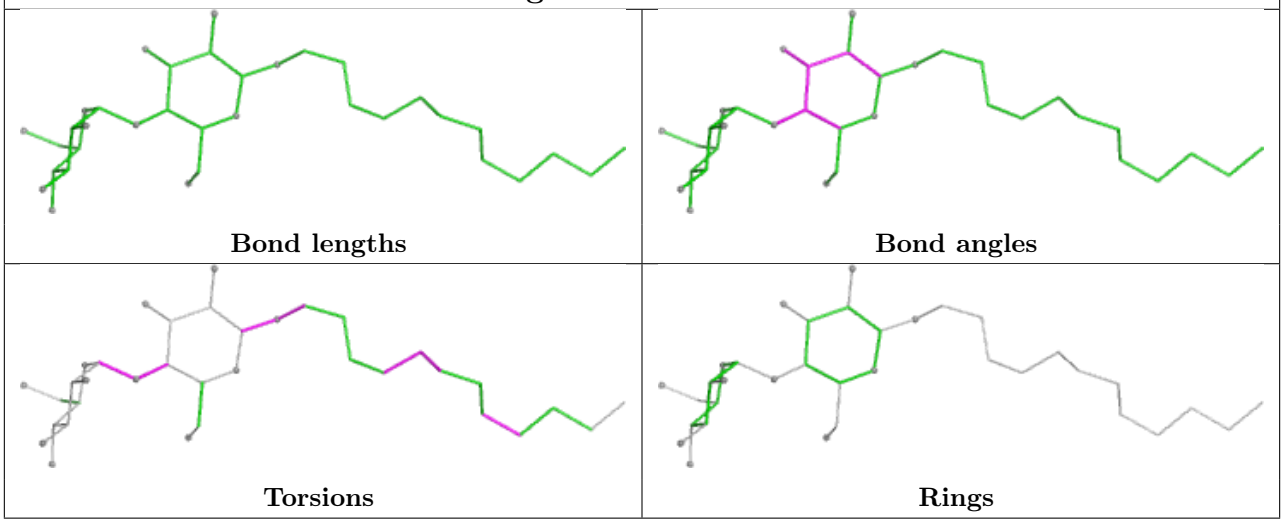
Ligand LMT j 101



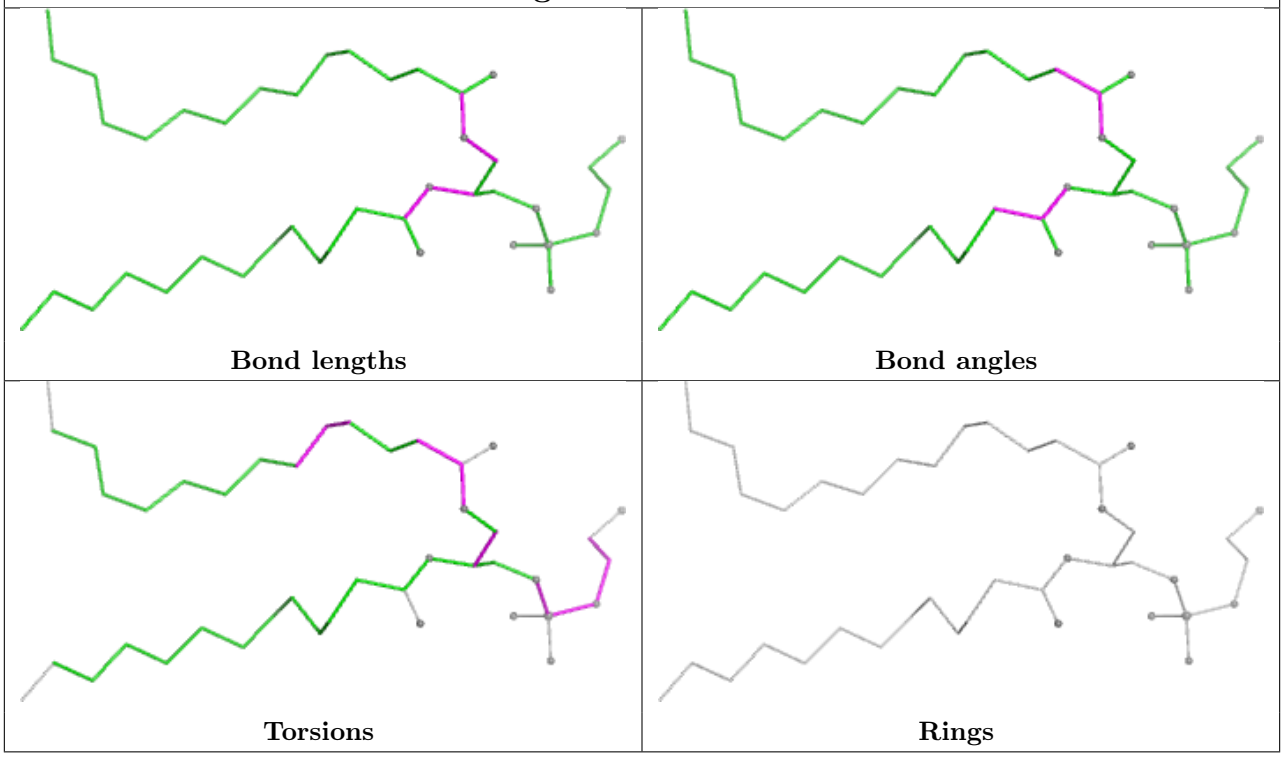
Ligand ZMP Q 201



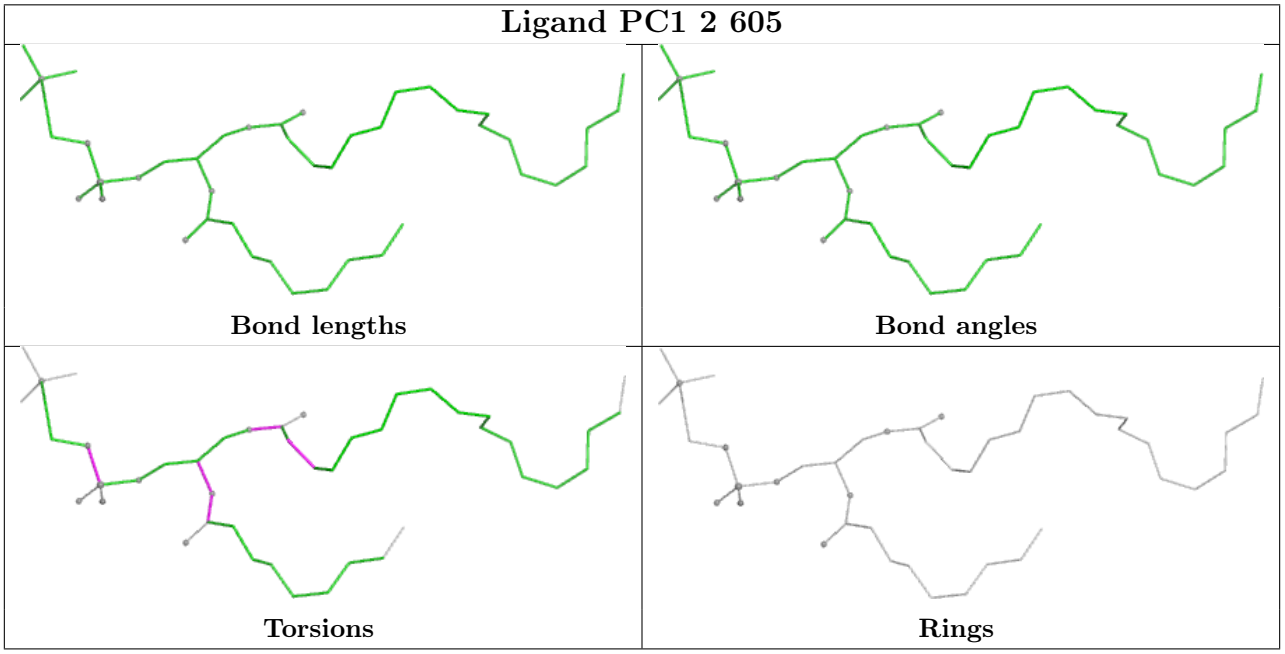
Ligand LMT 3 202



Ligand 3PE 5 706



Ligand PC1 2 605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

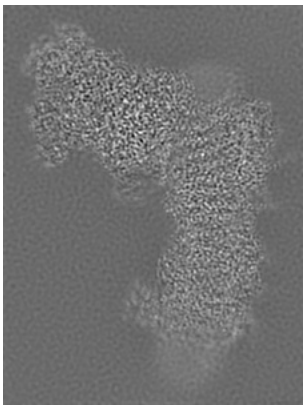
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14791. These allow visual inspection of the internal detail of the map and identification of artifacts.

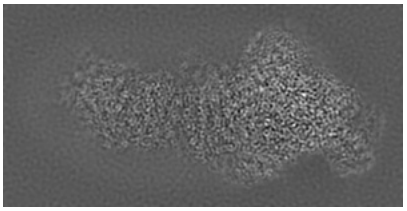
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

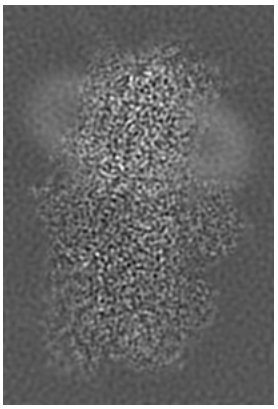
6.1.1 Primary map



X

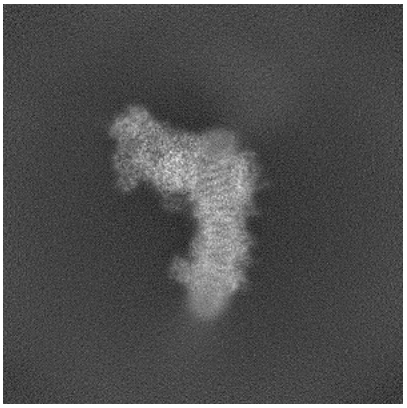


Y

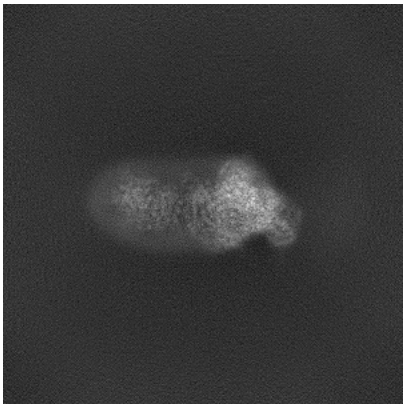


Z

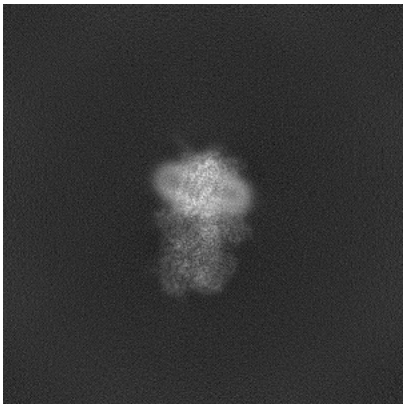
6.1.2 Raw map



X



Y

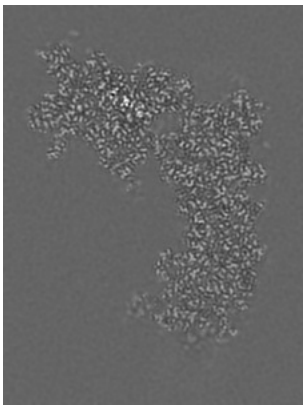


Z

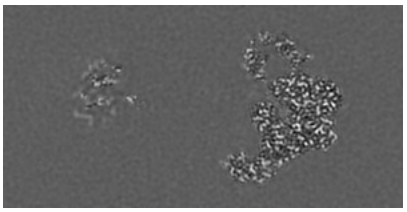
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

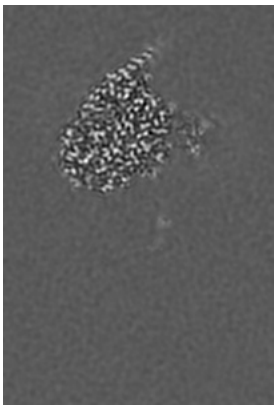
6.2.1 Primary map



X Index: 75

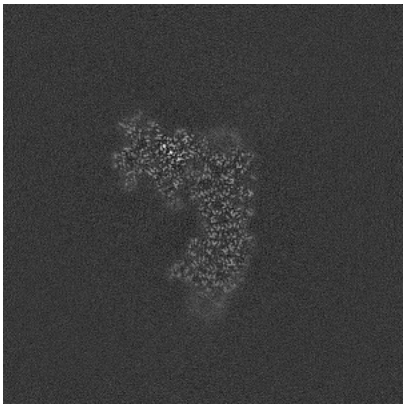


Y Index: 111

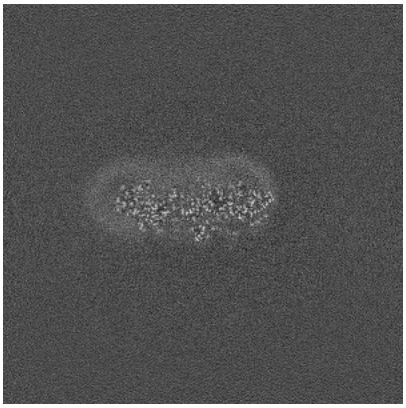


Z Index: 148

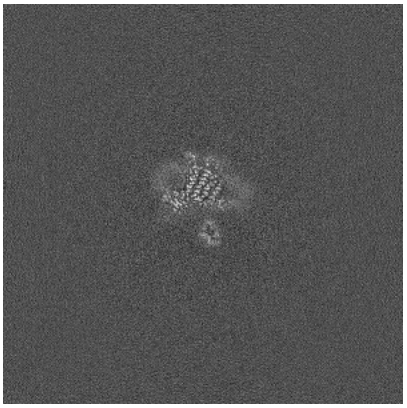
6.2.2 Raw map



X Index: 256



Y Index: 256

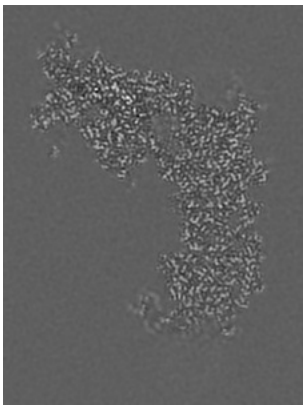


Z Index: 256

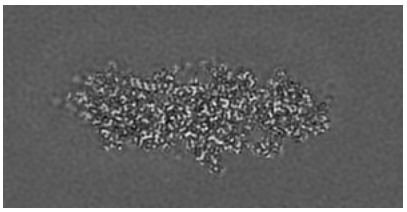
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

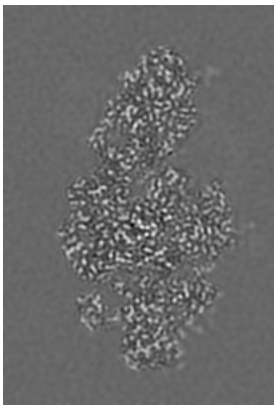
6.3.1 Primary map



X Index: 71

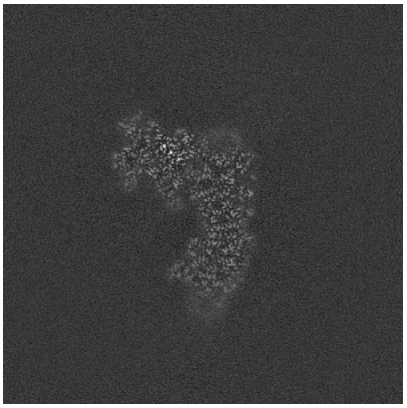


Y Index: 139

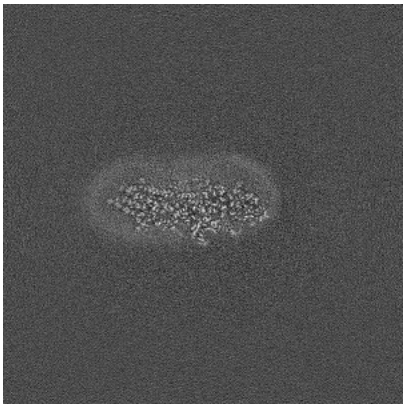


Z Index: 214

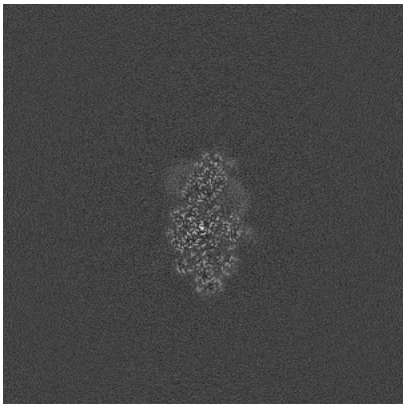
6.3.2 Raw map



X Index: 256



Y Index: 262

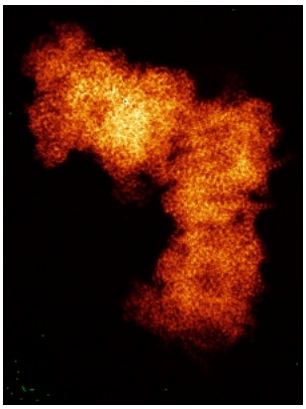


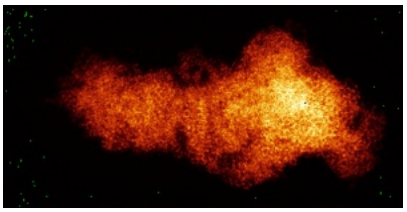
Z Index: 312

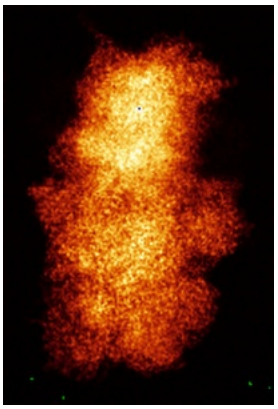
The images above show the largest variance slices of the map in three orthogonal directions.

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

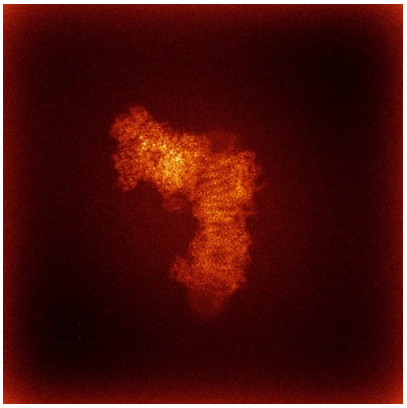
6.4.1 Primary map

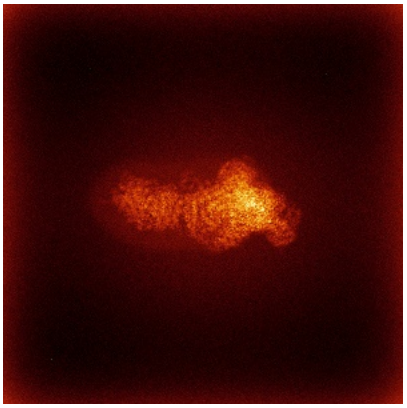

X

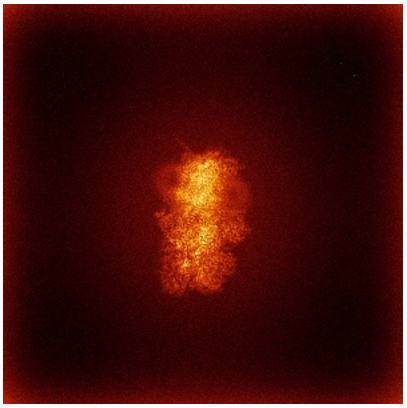

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

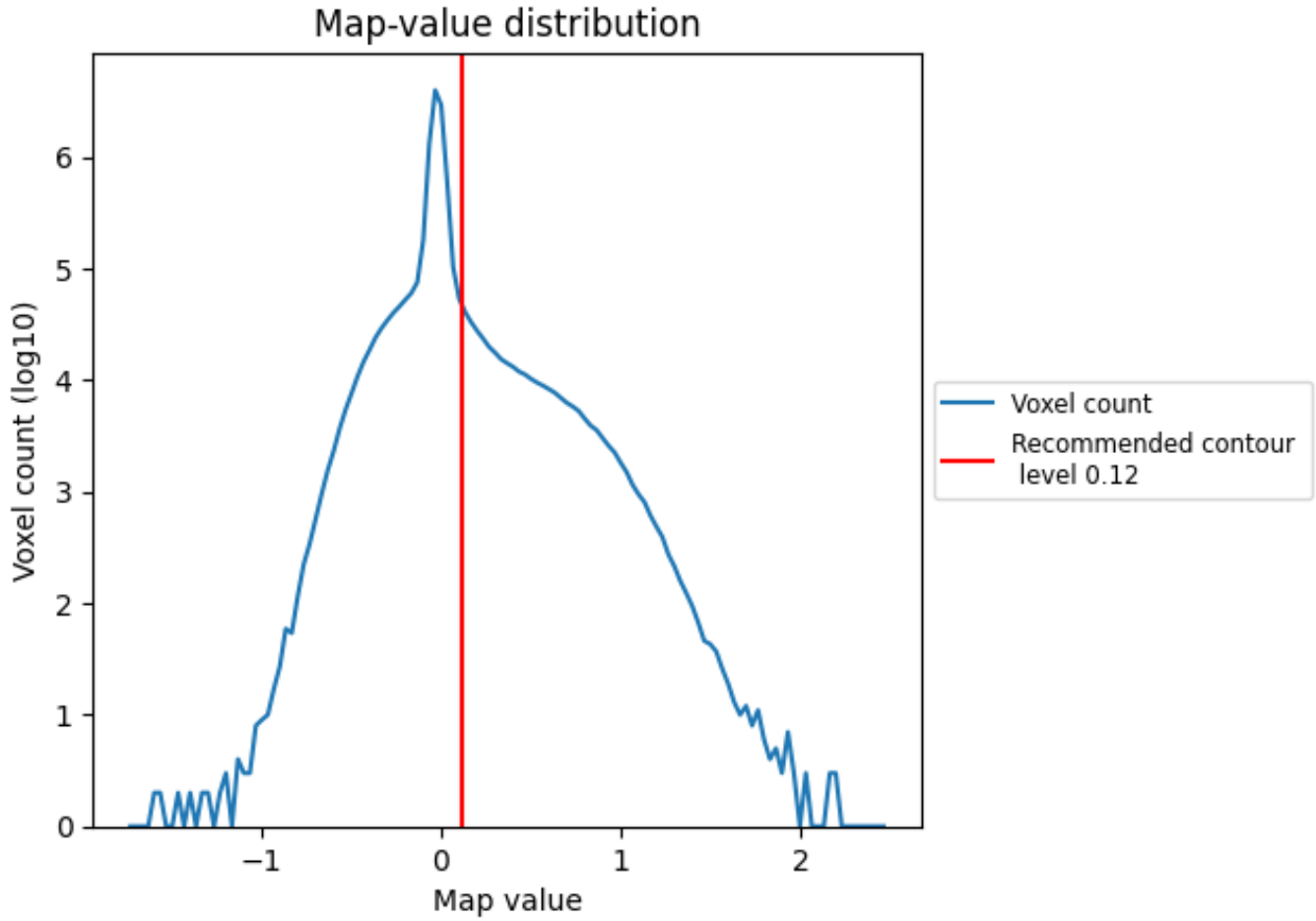
6.6 Mask visualisation (i)

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

7 Map analysis

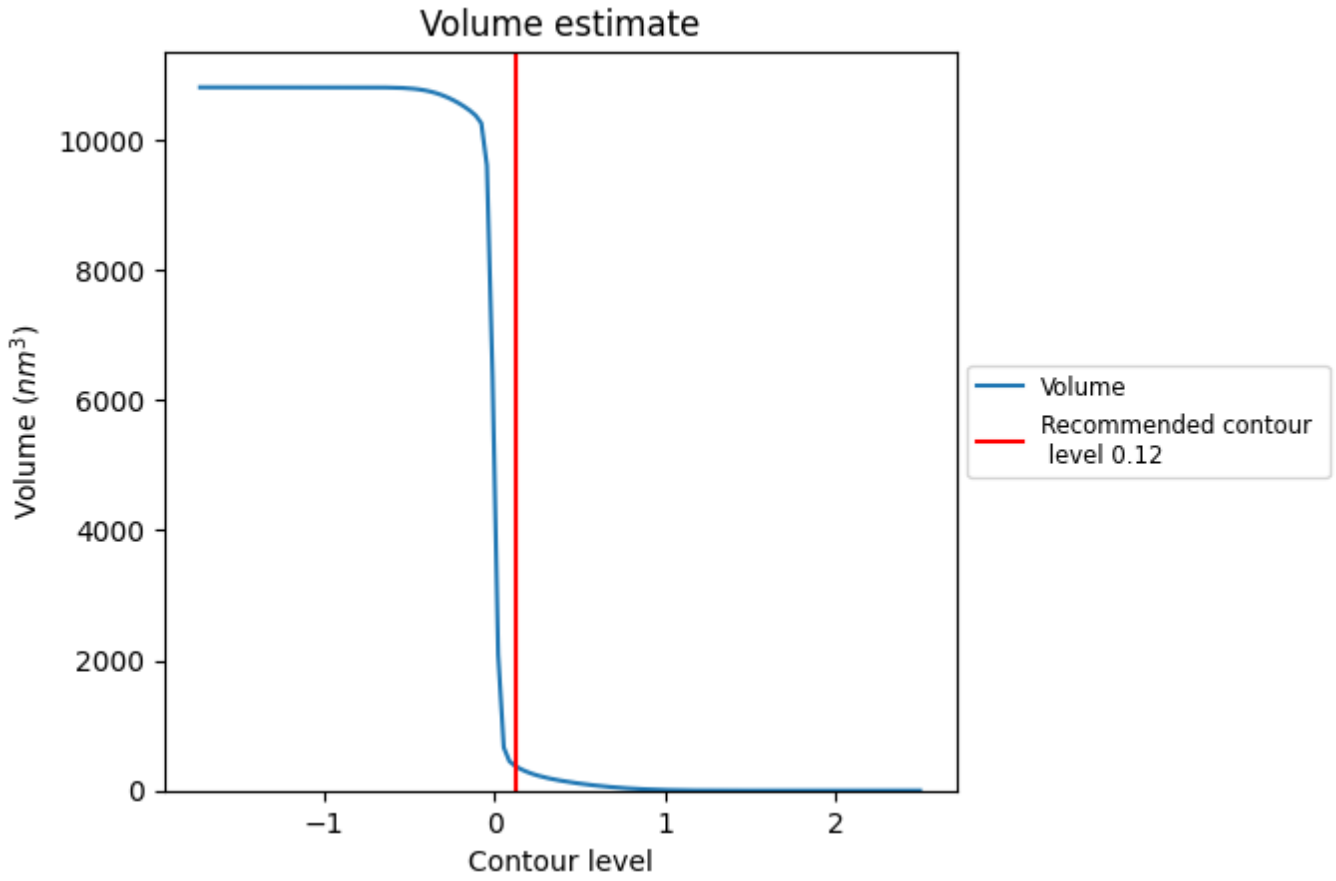
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 382 nm^3; this corresponds to an approximate mass of 345 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.

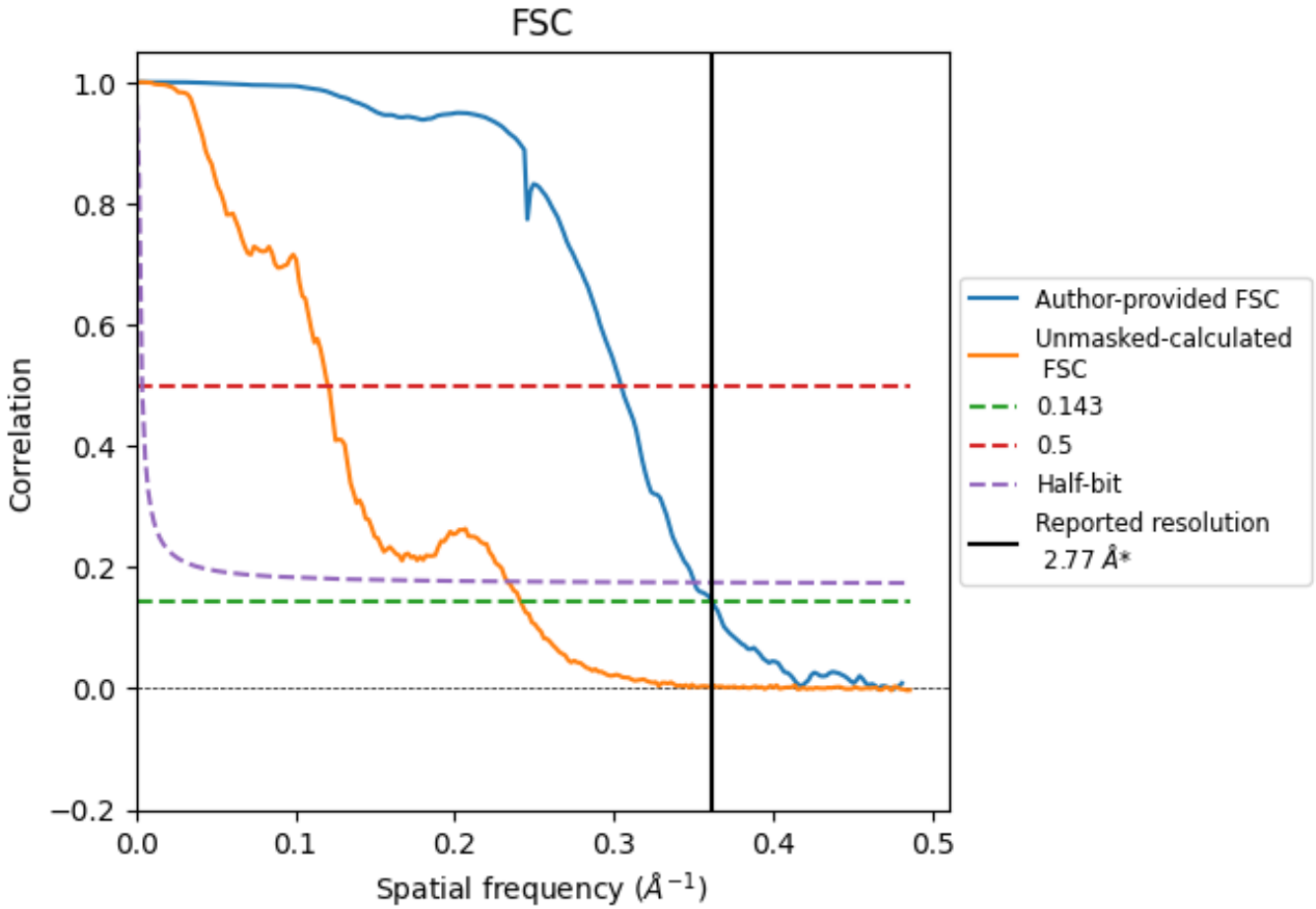
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.361 Å^{-1}

8.2 Resolution estimates (i)

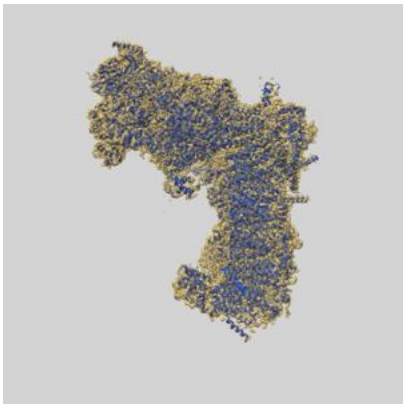
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.29	2.85
Unmasked-calculated*	4.14	8.30	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.77 by more than 10 %

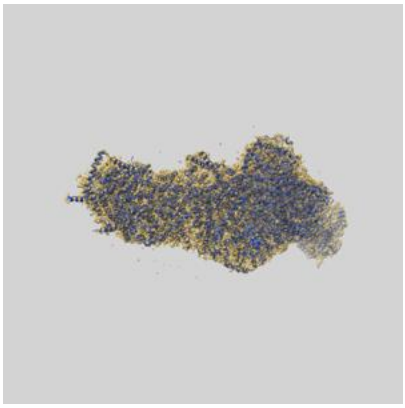
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14791 and PDB model 7ZM7. Per-residue inclusion information can be found in section 3 on page 24.

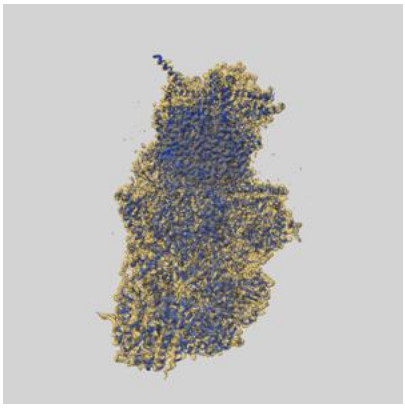
9.1 Map-model overlay



X



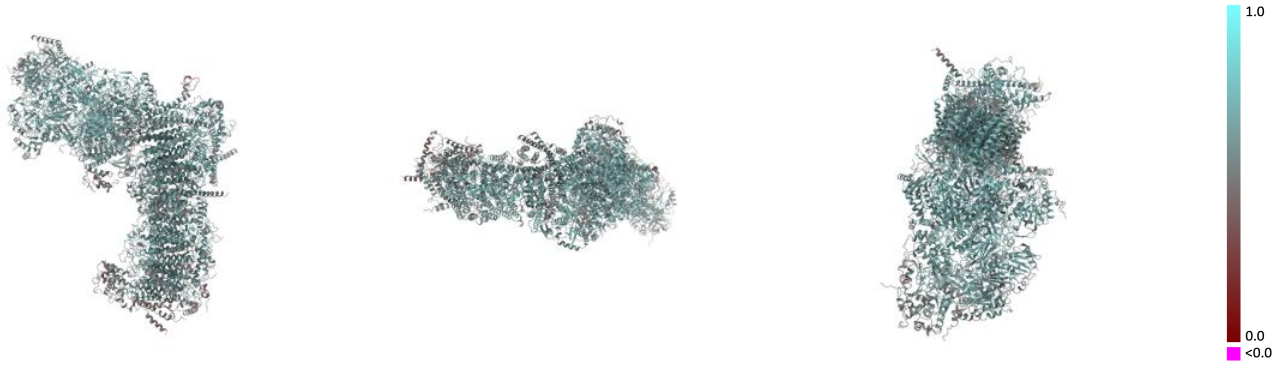
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

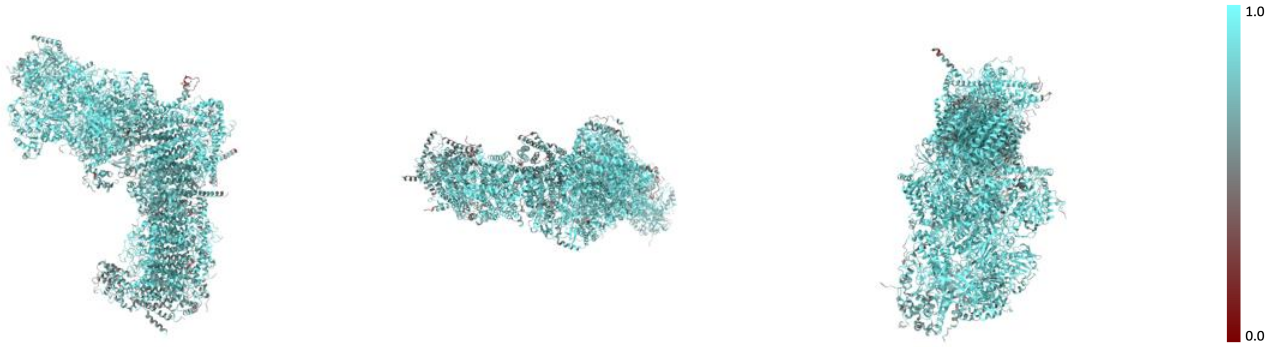
9.2 Q-score mapped to coordinate model



X Y Z

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

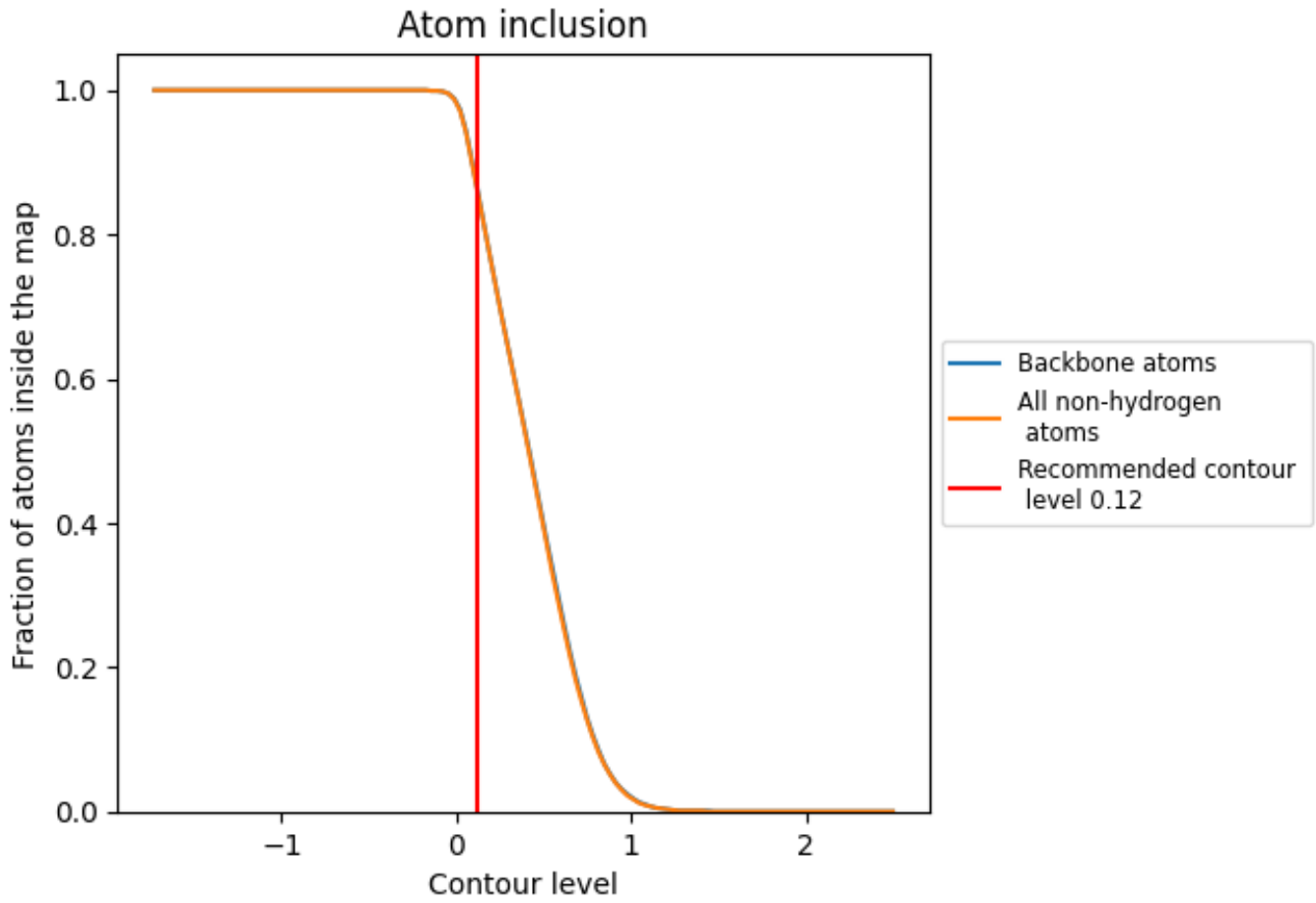
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.5980
1	0.8390	0.5950
2	0.9270	0.6390
3	0.8270	0.5880
4	0.9500	0.6400
5	0.8450	0.5820
6	0.8710	0.6040
8	0.6820	0.4830
9	0.8110	0.5780
A	0.9100	0.6200
B	0.8300	0.5650
C	0.9330	0.6490
D	0.9230	0.6350
E	0.8580	0.5840
F	0.8550	0.5930
G	0.9410	0.6580
H	0.8300	0.5630
I	0.9450	0.6540
J	0.7010	0.5290
K	0.9260	0.6300
L	0.9200	0.6260
M	0.9120	0.6240
O	0.6440	0.4590
P	0.8830	0.5880
Q	0.6160	0.4750
R	0.7400	0.5230
S	0.8520	0.5770
U	0.9030	0.6110
W	0.8530	0.6070
X	0.8960	0.6180
Y	0.9230	0.6330
Z	0.8610	0.5970
a	0.7730	0.5380
b	0.8510	0.5980
c	0.6430	0.4690

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8680	0.5980
e	0.6410	0.4690
f	0.8140	0.5510
g	0.8450	0.5910
h	0.9100	0.6340
i	0.7690	0.5560
j	0.8400	0.5850
n	0.7880	0.5660
o	0.5890	0.5030