wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 08:16 am BST

PDB ID	:	7ZMG / pdb_00007zmg
EMDB ID	:	EMD-14797
Title	:	CryoEM structure of mitochondrial complex I from Chaetomium thermophilum (state 1)
Authors	:	Laube, E.; Kuehlbrandt, W.
Deposited on	:	2022-04-19
Resolution	:	2.44 Å(reported)
Based on initial models	:	6RFQ, 6RFR

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

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

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

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

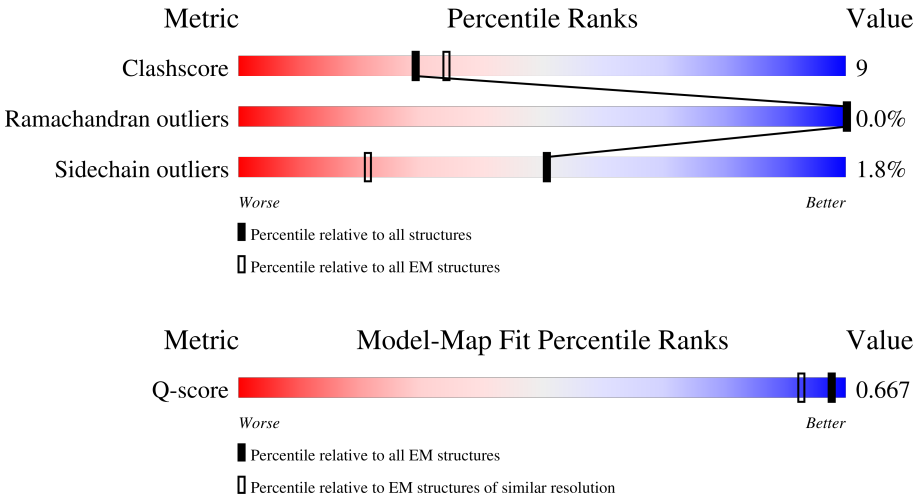
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.44 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	5856 (1.94 - 2.94)

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	70% 18% • 12%
2	2	571	74% 23% ••
3	3	146	65% 14% • 20%
4	4	542	69% 22% • 9%

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Mol	Chain	Length	Quality of chain
5	5	679	68% 29%
6	6	224	62% 21% 15%
7	8	86	9% 79% 10% 10%
8	9	785	11% 87%
9	A	749	77% 17% 5%
10	B	507	68% 20% 10%
11	C	499	72% 14% 15%
12	D	86	79% 17%
13	E	378	67% 26% 7%
14	F	261	67% 24% 9%
15	G	293	64% 18% 17%
16	H	318	53% 17% 31%
17	I	223	63% 18% 17%
18	J	199	73% 19% 7%
19	K	230	54% 23% 21%
20	L	89	61% 34%
21	M	168	61% 10% 30%
22	O	141	6% 46% 11% 43%
22	Q	141	9% 52% 8% 40%
23	P	124	72% 27%
24	R	99	7% 75% 23%
25	S	143	38% 14% 48%
26	U	186	67% 22% 10%
27	W	121	79% 20%
28	X	191	74% 22%

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Mol	Chain	Length	Quality of chain
29	Y	210	58% 15% 27%
30	Z	196	73% 21% 5%
31	a	203	56% 15% 29%
32	b	94	77% 10% 14%
33	c	93	9% 55% 11% 34%
34	d	105	77% 18%
35	e	46	65% 17% 17%
36	f	95	65% 27% 6%
37	g	82	74% 20% 5%
38	h	134	75% 25%
39	i	93	9% 72% 14% 13%
40	j	75	77% 23%
41	n	184	7% 60% 14% 26%
42	o	380	7% 92%

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 70825 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	334	2573	1728	388	446	11	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	4459	2994	672	782	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	117	894	608	130	154	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	5273	3551	792	905	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	190	Total	C	N	O	S	0	0
			1465	985	221	253	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
			658	408	126	118	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	103	Total	C	N	O	S	0	0
			807	500	147	154	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
10	B	456	Total	C	N	O	S	0	0
			3538	2225	638	648	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	425	Total	C	N	O	S	0	0
			3376	2152	587	618	19		

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
12	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- 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
			2886	1832	511	533	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	238	Total	C	N	O	S	0	0
			1899	1198	330	370	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	221	Total	C	N	O	S	0	0
			1702	1071	288	329	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	186	Total	C	N	O	S	0	0
			1388	877	259	250	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
			1446	922	254	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
			935	584	178	168	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
			633	398	101	133	1		
22	Q	85	Total	C	N	O	S	0	0
			673	422	109	141	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
			1033	656	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	74	Total	C	N	O	0	0
			612	402	98	112		

- 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
			1357	854	253	241	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
			980	625	182	170	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	187	Total	C	N	O	S	0	0
			1484	943	268	265	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
			1428	895	253	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	144	Total	C	N	O	S	0	0
			1172	753	196	218	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	81	Total	C	N	O	S	0	0
			683	445	125	110	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	61	Total	C	N	O	S	0	0
			505	329	91	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	101	Total	C	N	O	S	0	0
			843	535	149	155	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
			317	215	55	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	89	Total	C	N	O	S	0	0
			722	462	128	129	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	78	Total	C	N	O	S	0	0
			610	399	105	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	134	Total	C	N	O	S	0	0
			1132	731	198	201	2		

- 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
			682	450	118	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	75	Total	C	N	O	S	0	0
			616	399	110	103	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	136	Total	C	N	O	S	0	0
			1067	683	187	196	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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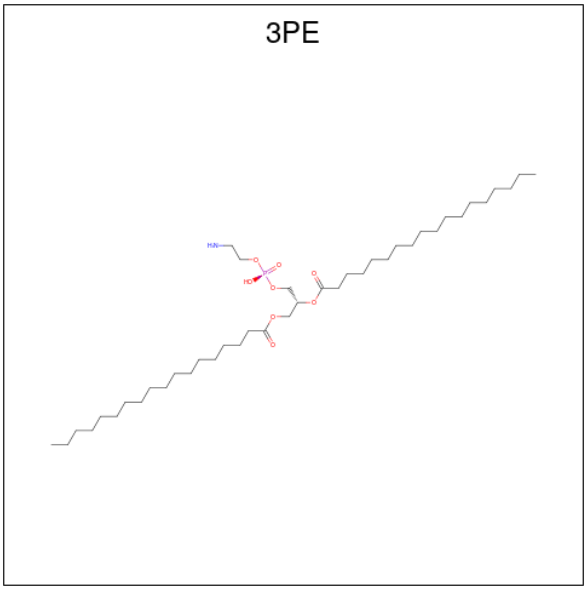
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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



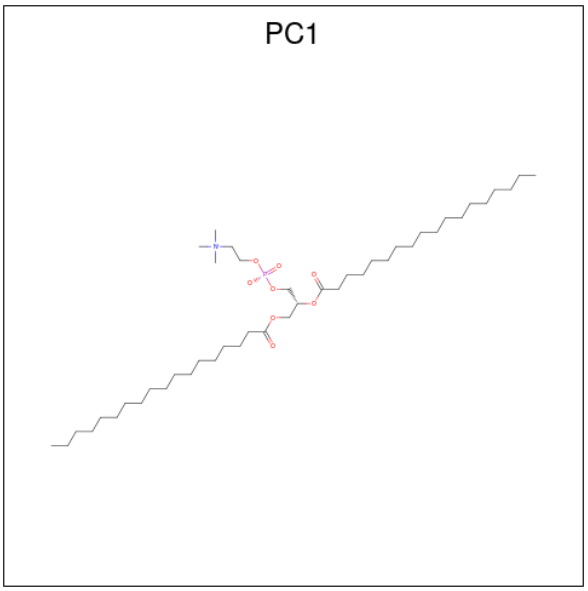
Mol	Chain	Residues	Atoms					AltConf
43	1	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	4	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	4	1	Total	C	N	O	P	0
			33	23	1	8	1	

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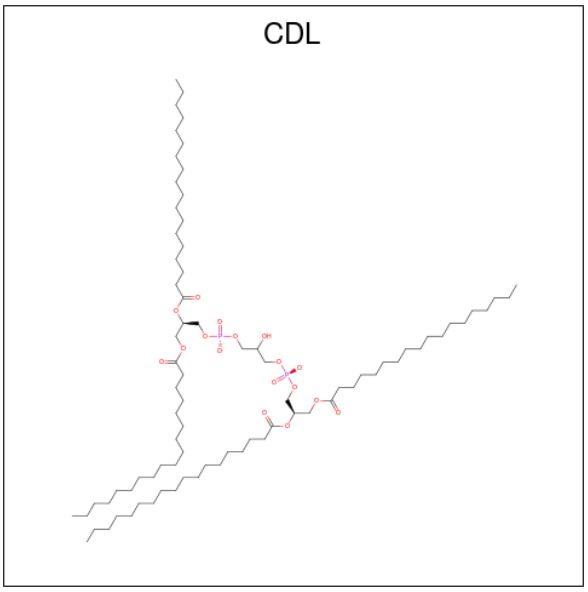
Mol	Chain	Residues	Atoms					AltConf
43	4	1	Total	C	N	O	P	0
			34	24	1	8	1	
43	5	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
43	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	E	1	Total	C	N	O	P	0
			31	21	1	8	1	
43	I	1	Total	C	N	O	P	0
			42	32	1	8	1	
43	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
43	J	1	Total	C	N	O	P	0
			30	20	1	8	1	
43	W	1	Total	C	N	O	P	0
			35	25	1	8	1	
43	W	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	g	1	Total	C	N	O	P	0
			36	26	1	8	1	
43	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	i	1	Total	C	N	O	P	0
			41	31	1	8	1	
43	n	1	Total	C	N	O	P	0
			39	29	1	8	1	

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



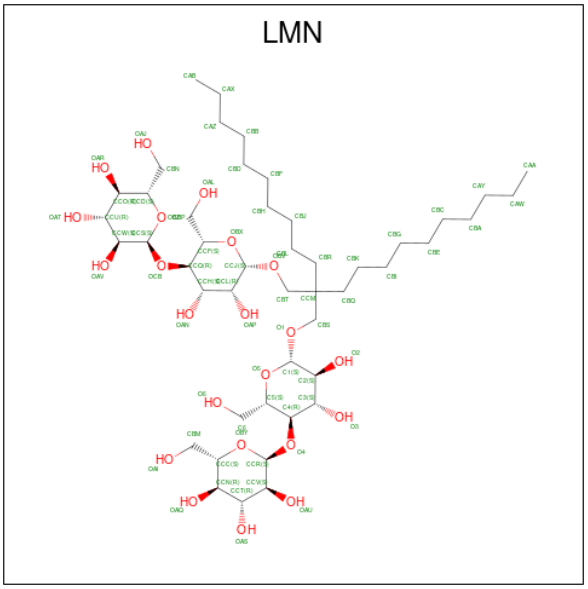
Mol	Chain	Residues	Atoms					AltConf
44	1	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	3	1	Total	C	N	O	P	0
			48	38	1	8	1	
44	4	1	Total	C	N	O	P	0
			50	40	1	8	1	
44	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
44	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
44	K	1	Total	C	N	O	P	0
			47	37	1	8	1	
44	S	1	Total	C	N	O	P	0
			51	41	1	8	1	
44	X	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	X	1	Total	C	N	O	P	0
			32	22	1	8	1	

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



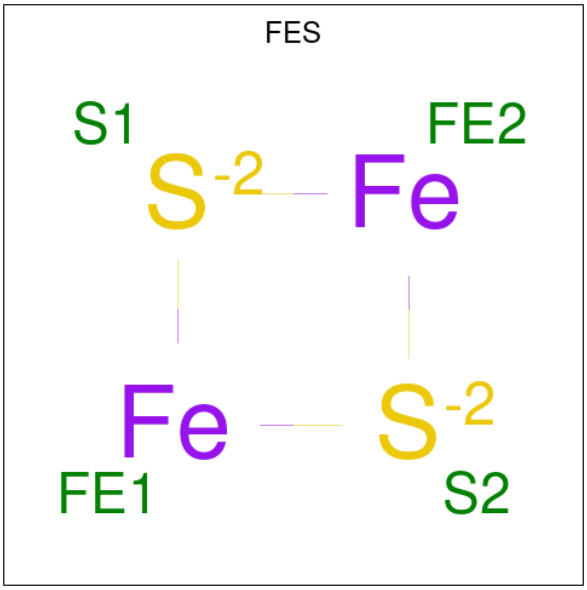
Mol	Chain	Residues	Atoms				AltConf
45	2	1	Total	C	O	P	0
			74	55	17	2	
45	D	1	Total	C	O	P	0
			74	55	17	2	
45	S	1	Total	C	O	P	0
			79	60	17	2	
45	X	1	Total	C	O	P	0
			77	58	17	2	
45	g	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 46 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



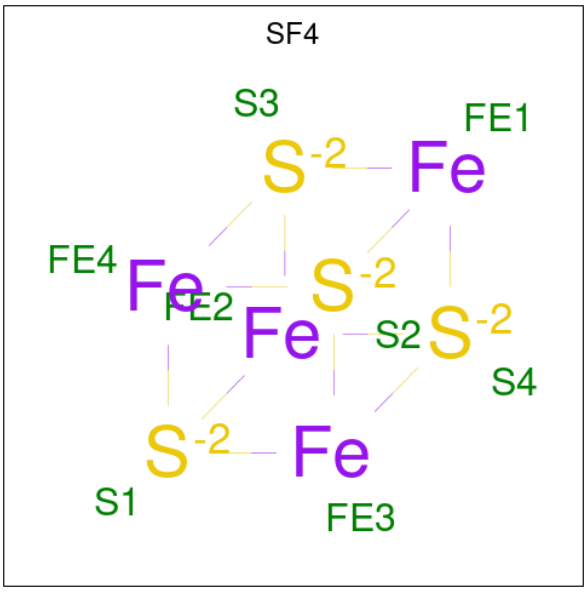
Mol	Chain	Residues	Atoms	AltConf
46	2	1	Total C O 58 41 17	0
46	4	1	Total C O 47 35 12	0
46	5	1	Total C O 69 47 22	0

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



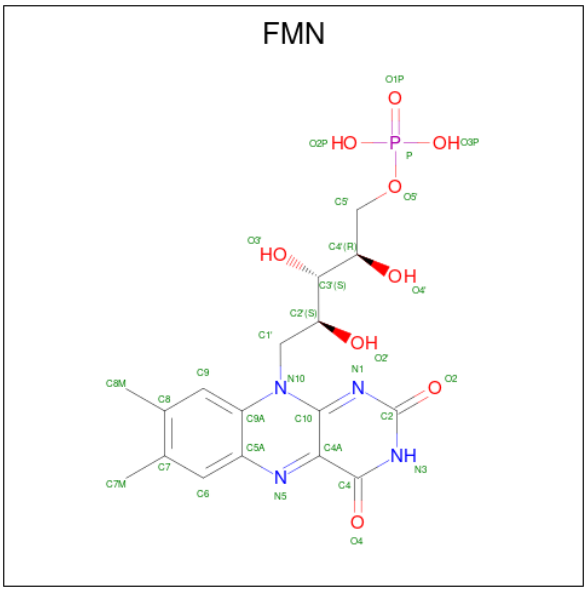
Mol	Chain	Residues	Atoms	AltConf
47	A	1	Total Fe S 4 2 2	0
47	H	1	Total Fe S 4 2 2	0

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



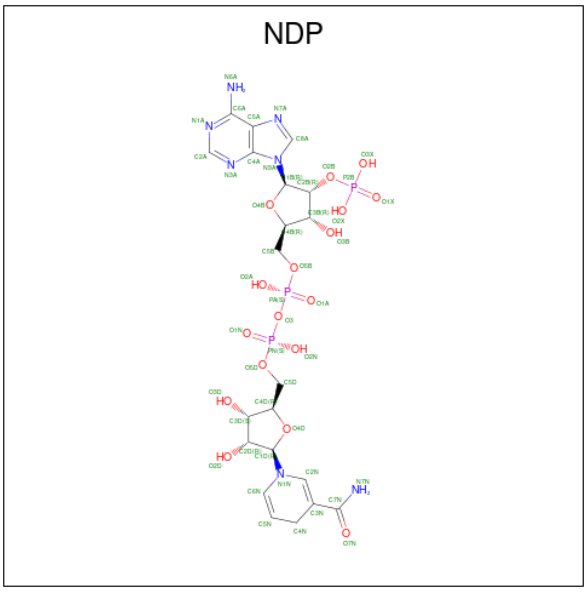
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	
48	B	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	K	1	Total	Fe	S	0
			8	4	4	

- 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	0
			31	17	4	9	1	

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

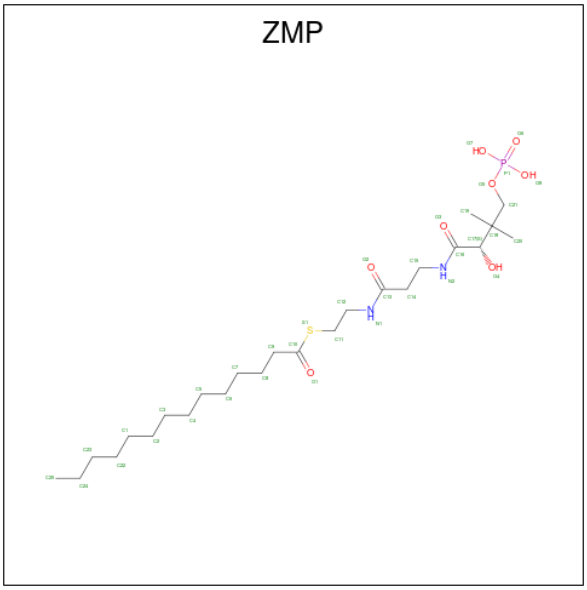


Mol	Chain	Residues	Atoms					AltConf
50	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

- 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 36 25 2 7 1 1	0
52	Q	1	Total C N O P S 36 25 2 7 1 1	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms	AltConf
53	1	134	Total O 134 134	0
53	2	214	Total O 214 214	0
53	3	31	Total O 31 31	0
53	4	115	Total O 115 115	0
53	5	28	Total O 28 28	0
53	6	56	Total O 56 56	0

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Mol	Chain	Residues	Atoms	AltConf
53	9	19	Total O 19 19	0
53	A	319	Total O 319 319	0
53	B	73	Total O 73 73	0
53	C	257	Total O 257 257	0
53	D	41	Total O 41 41	0
53	E	88	Total O 88 88	0
53	F	65	Total O 65 65	0
53	G	172	Total O 172 172	0
53	H	34	Total O 34 34	0
53	I	124	Total O 124 124	0
53	J	1	Total O 1 1	0
53	K	107	Total O 107 107	0
53	L	25	Total O 25 25	0
53	M	81	Total O 81 81	0
53	P	42	Total O 42 42	0
53	R	3	Total O 3 3	0
53	S	3	Total O 3 3	0
53	U	67	Total O 67 67	0
53	W	64	Total O 64 64	0
53	X	81	Total O 81 81	0
53	Y	163	Total O 163 163	0

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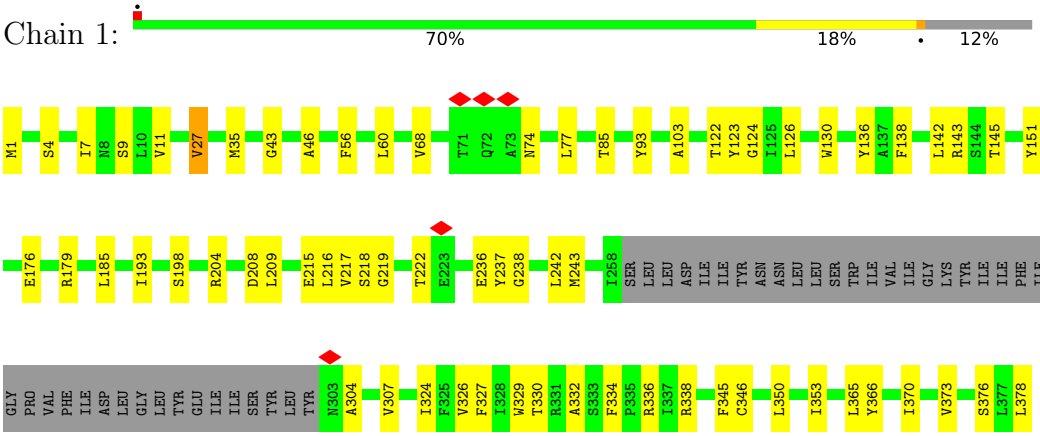
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Mol	Chain	Residues	Atoms	AltConf
53	Z	84	Total O 84 84	0
53	a	8	Total O 8 8	0
53	b	11	Total O 11 11	0
53	d	8	Total O 8 8	0
53	f	6	Total O 6 6	0
53	g	20	Total O 20 20	0
53	h	58	Total O 58 58	0
53	j	9	Total O 9 9	0
53	n	37	Total O 37 37	0
53	o	1	Total O 1 1	0

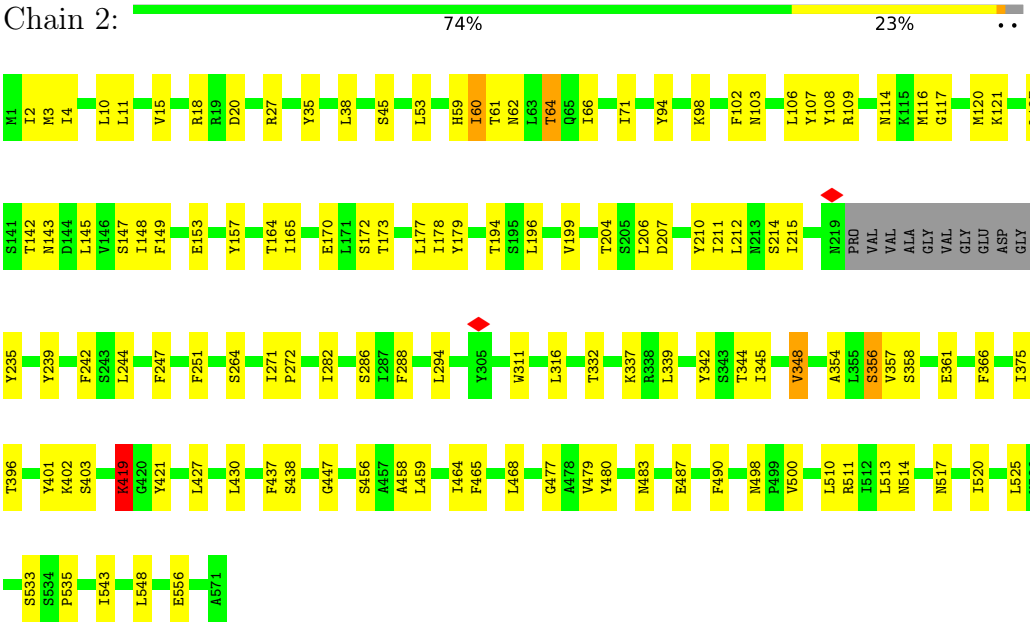
3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 1



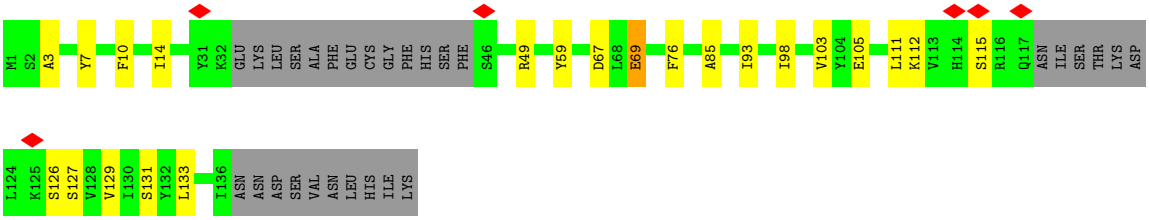
• Molecule 2: NADH dehydrogenase subunit 2



• Molecule 3: NADH-ubiquinone oxidoreductase chain 3

Chain 3:

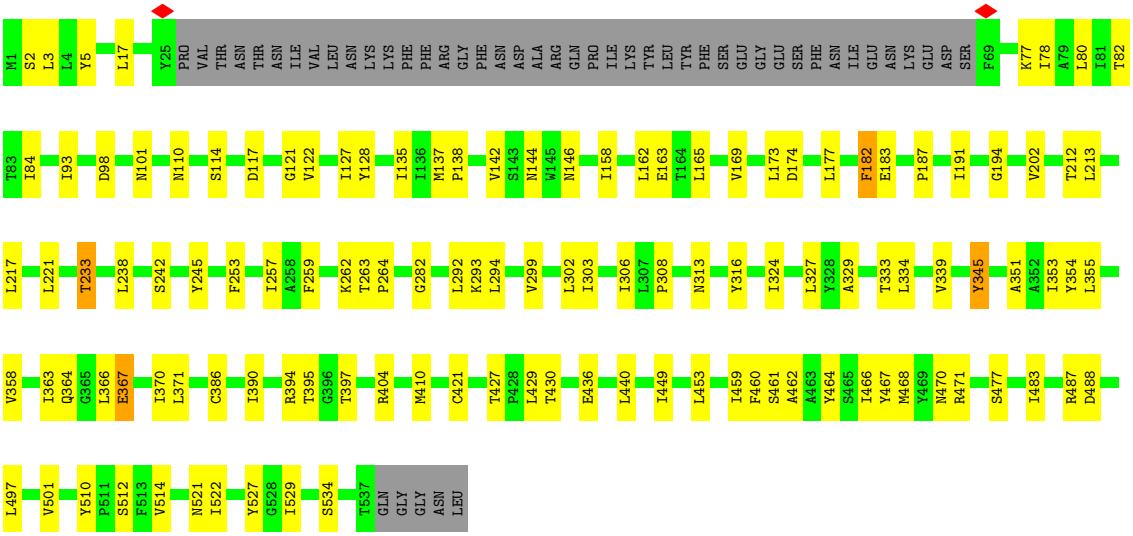




• Molecule 4: NADH-ubiquinone oxidoreductase chain 4

Chain 4:

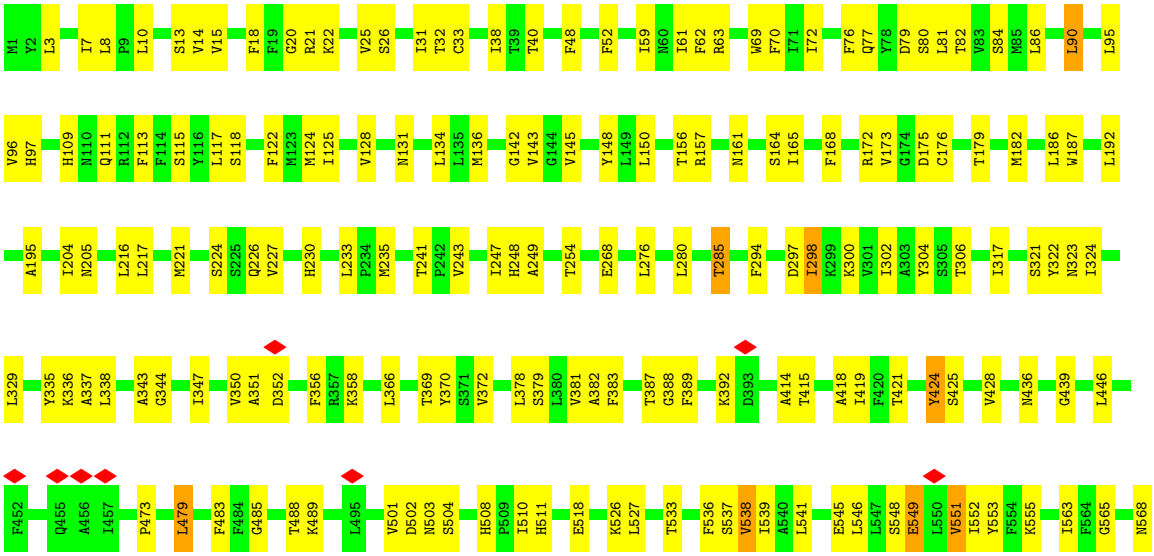


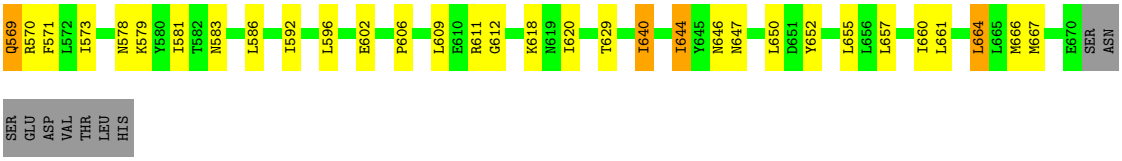


• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

Chain 5:



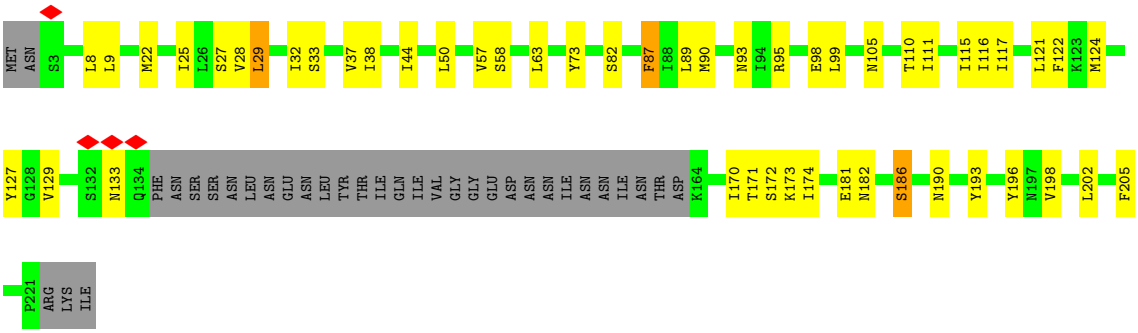




• Molecule 6: NADH-ubiquinone oxidoreductase chain 6

Chain 6:

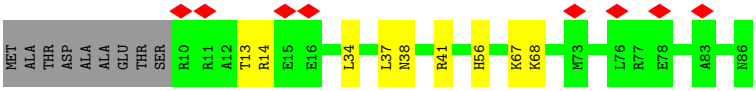




• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 8:

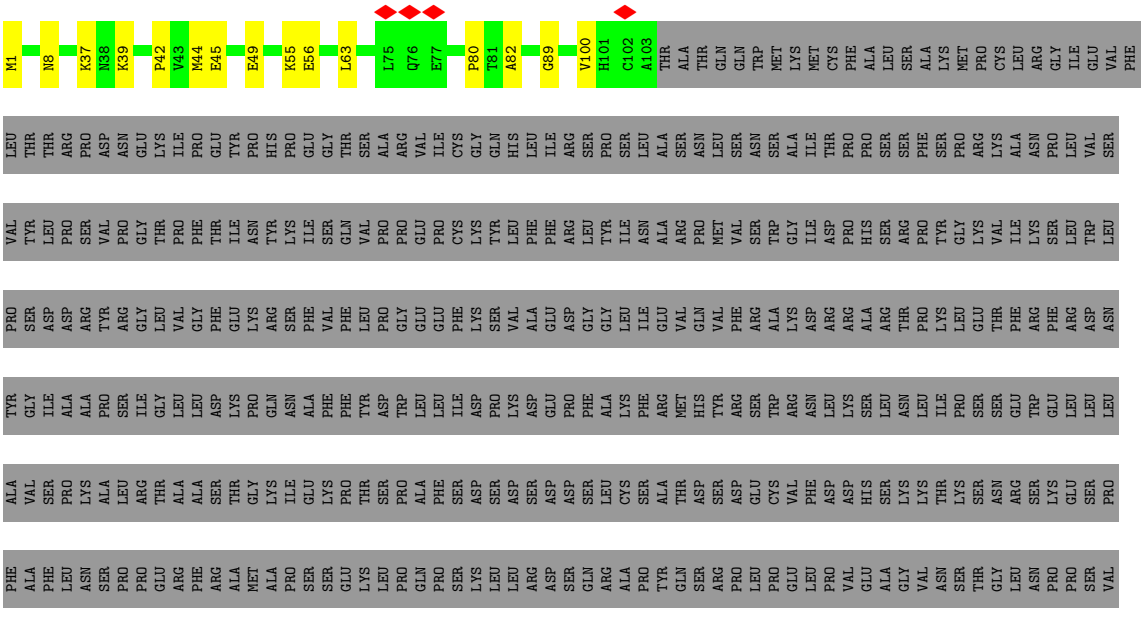


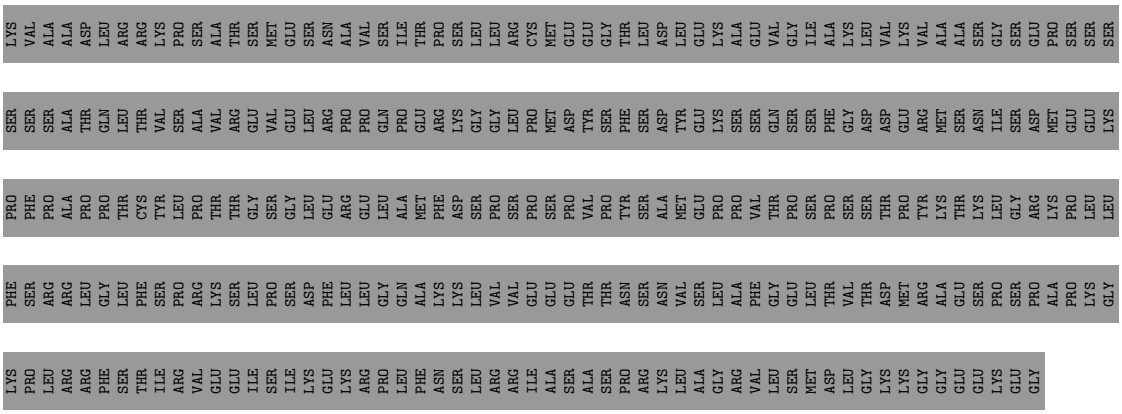


• Molecule 8: Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain 9:



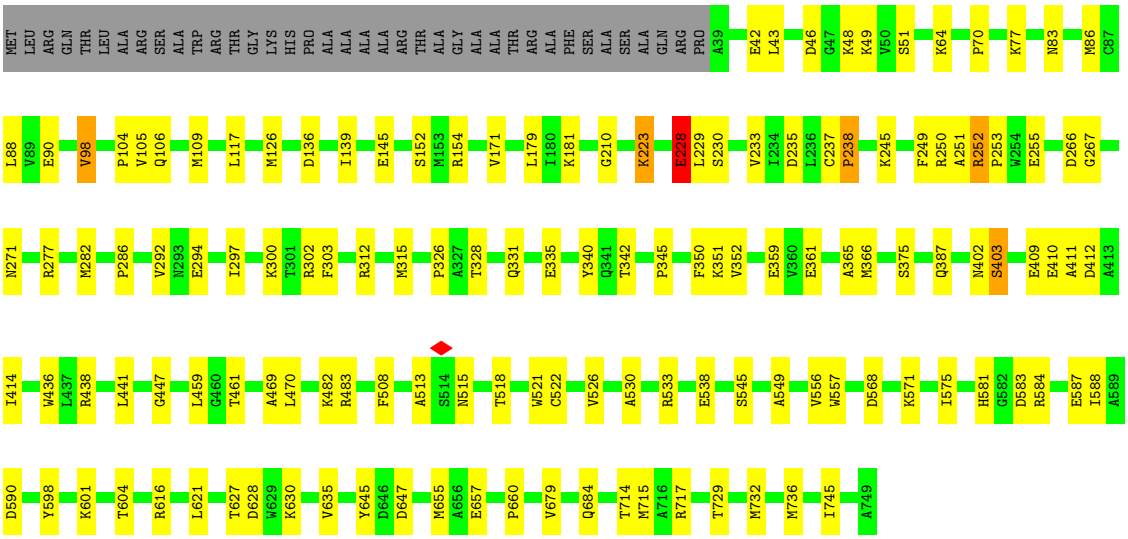




• Molecule 9: NADH-ubiquinone oxidoreductase-like protein

Chain A:

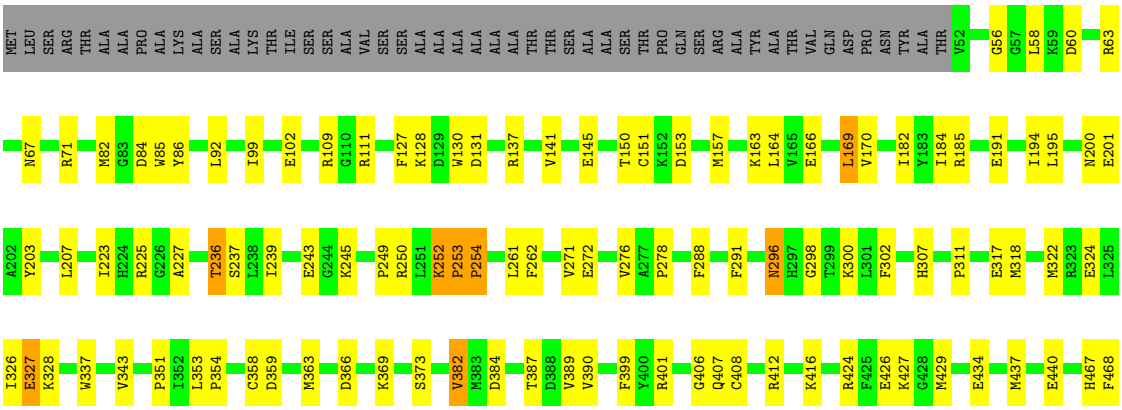




• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:



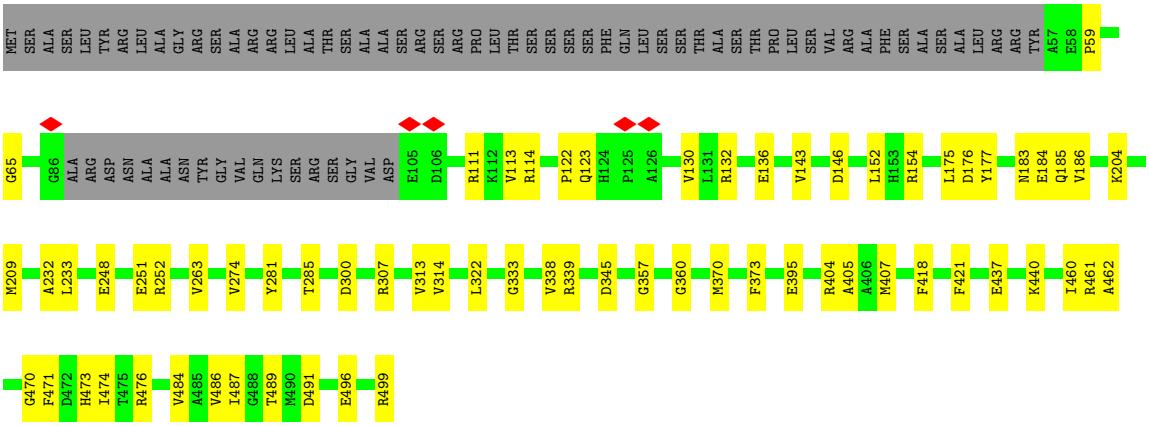




• Molecule 11: NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein

Chain C:





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

Chain D:

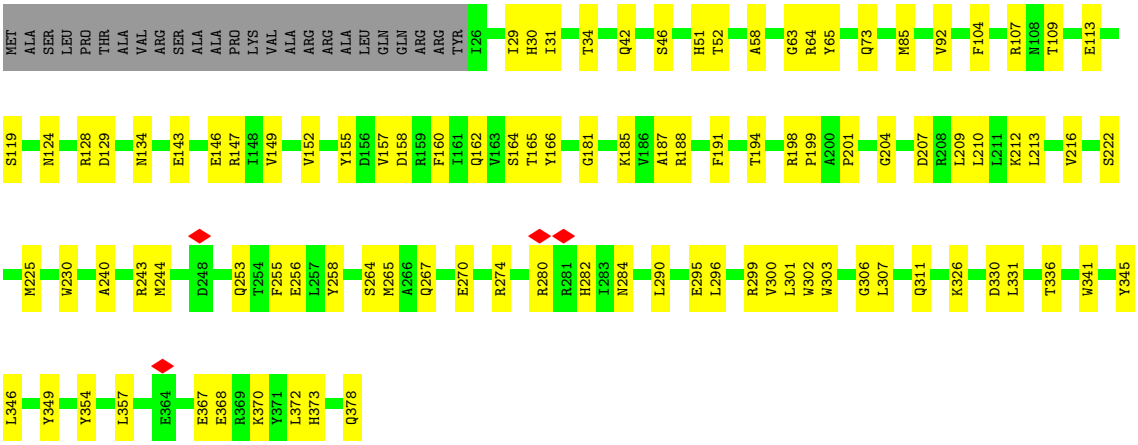




• Molecule 13: NADH dehydrogenase (Ubiquinone)-like protein

Chain E:

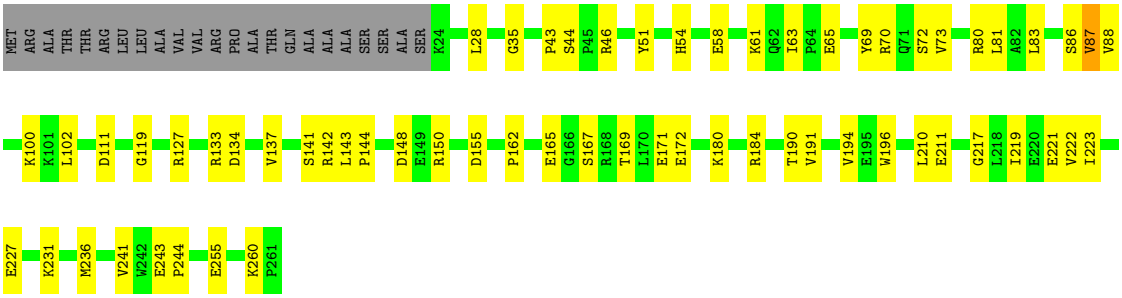




• Molecule 14: NADH-ubiquinone oxidoreductase-like protein

Chain F:

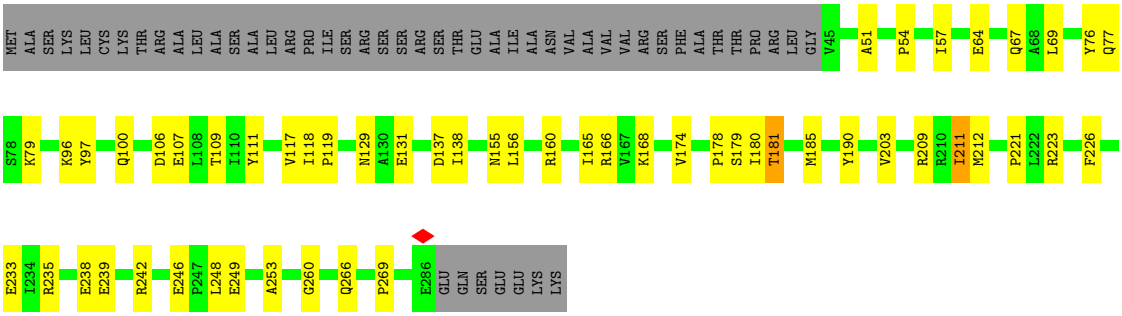




• Molecule 15: NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein

Chain G:

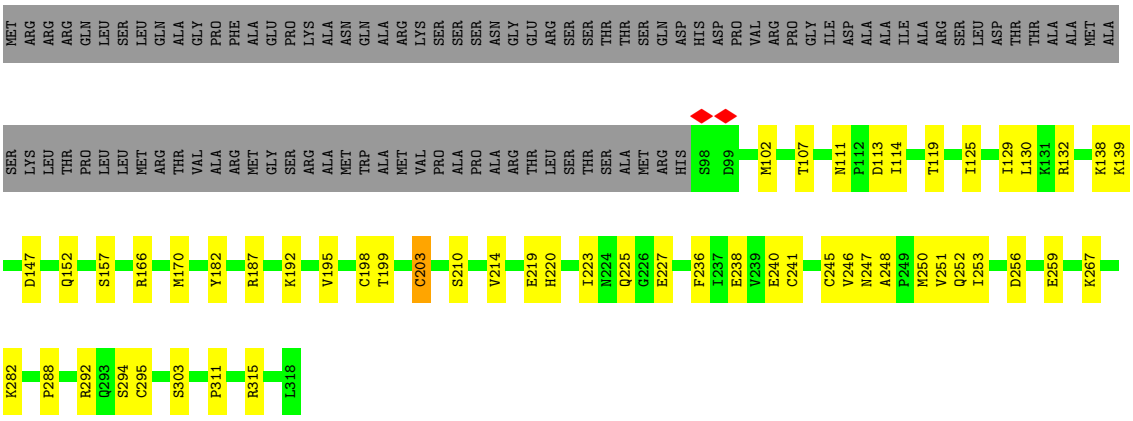




• Molecule 16: Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain H:

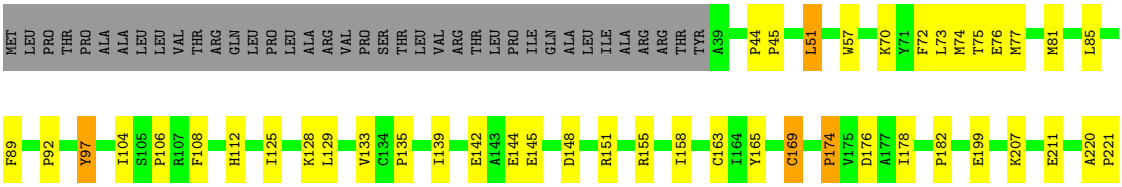




• Molecule 17: Oxidoreductase-like protein

Chain I:



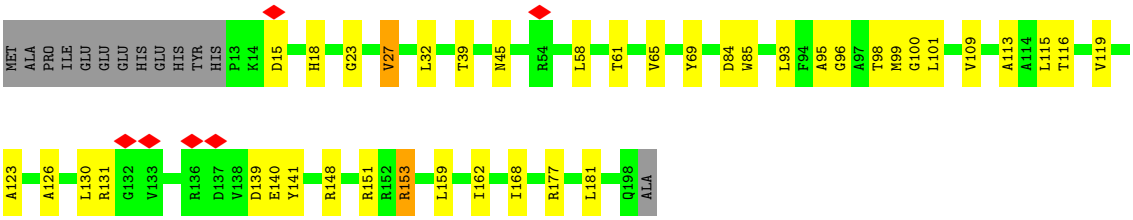




• Molecule 18: NADH-ubiquinone oxidoreductase-like protein

Chain J:

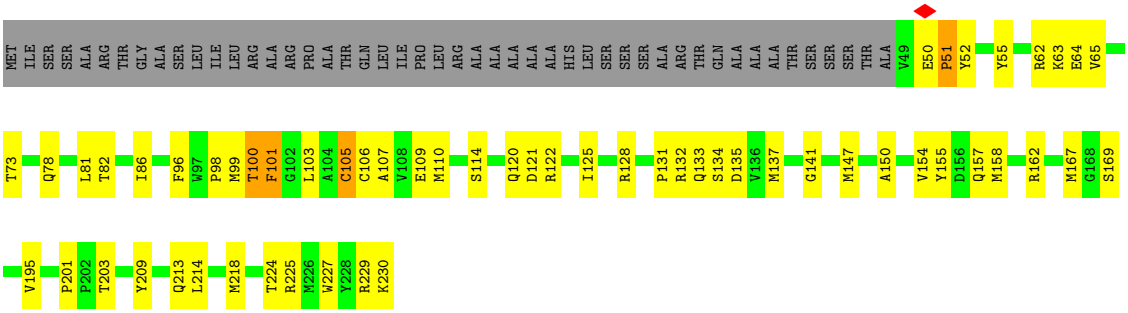




• Molecule 19: NADH-ubiquinone oxidoreductase-like protein

Chain K:

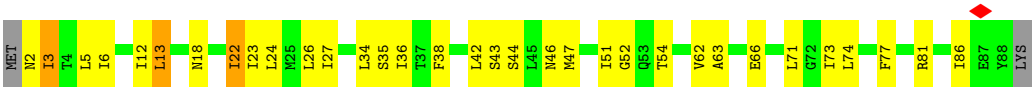




• Molecule 20: NADH-ubiquinone oxidoreductase chain 4L

Chain L:

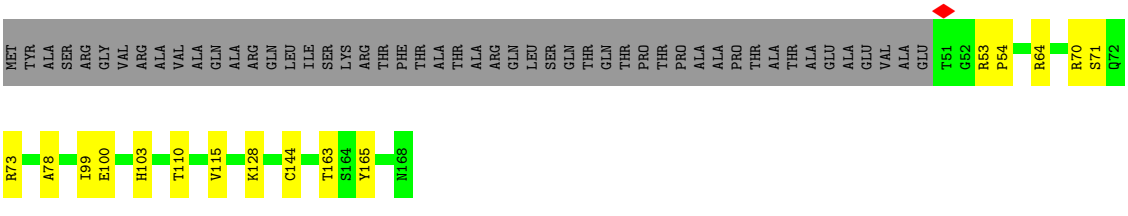




• Molecule 21: NADH-ubiquinone oxidoreductase-like protein

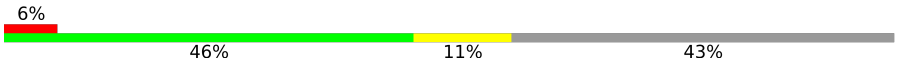
Chain M:

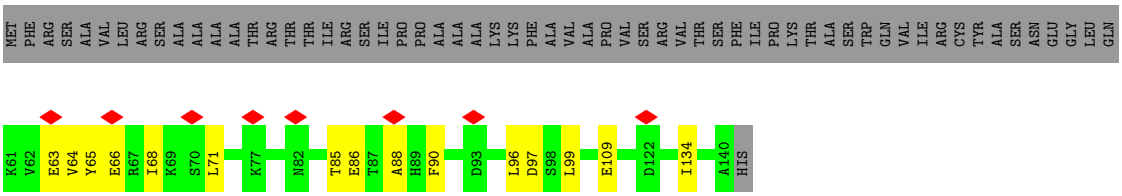




• Molecule 22: Acyl carrier protein

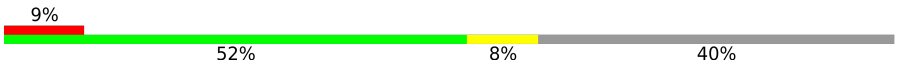
Chain O:

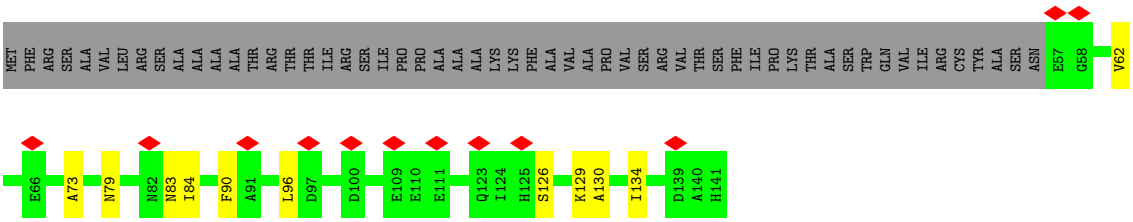




• Molecule 22: Acyl carrier protein

Chain Q:





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

Chain P:

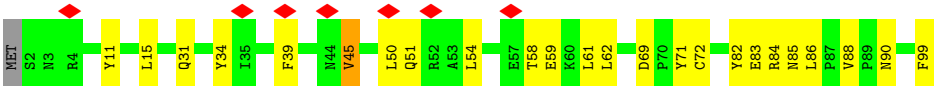




• Molecule 24: Complex I-B22

Chain R:

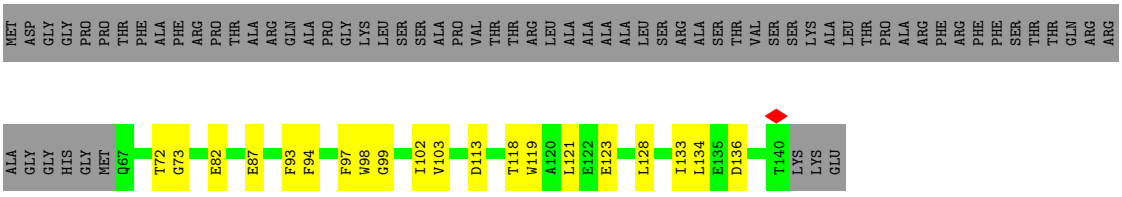




• Molecule 25: Complex I-ESSS

Chain S:

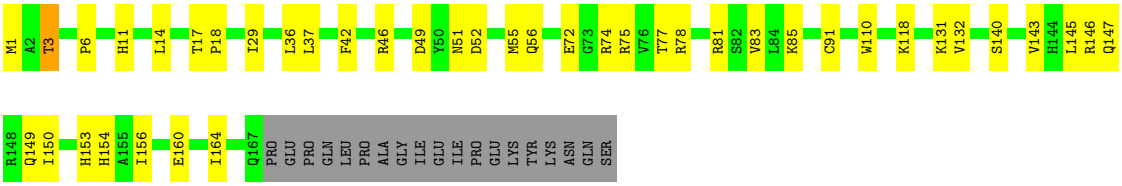




• Molecule 26: NADH-ubiquinone oxidoreductase

Chain U:

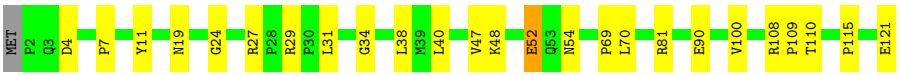




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:

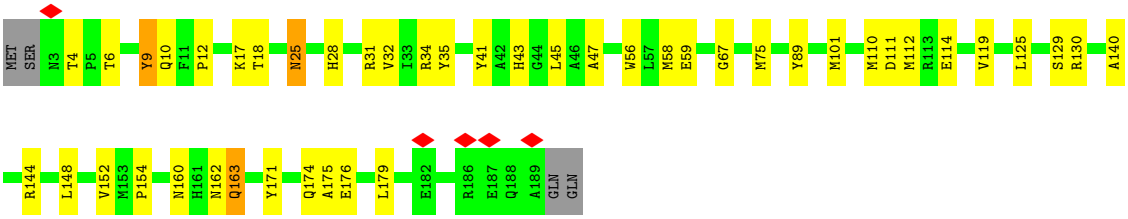




• Molecule 28: NADH-ubiquinone oxidoreductase-like protein

Chain X:

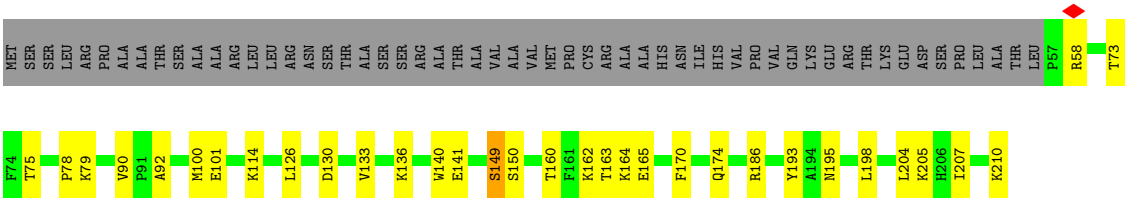




• Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Y:

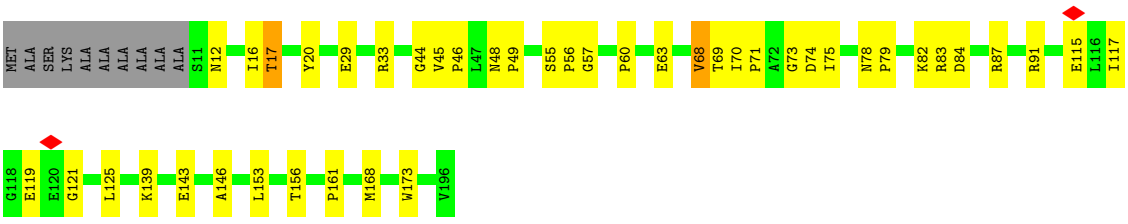




• Molecule 30: NADH-ubiquinone oxidoreductase-like protein

Chain Z:

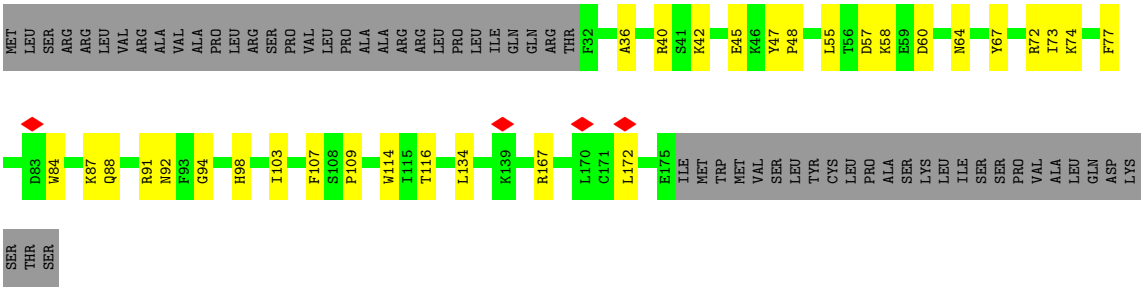




• Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein

Chain a:

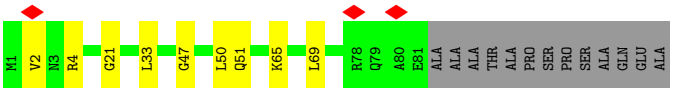




• Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain b:

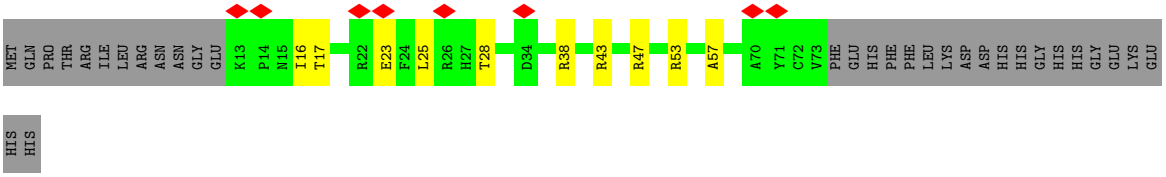




• Molecule 33: Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain c:

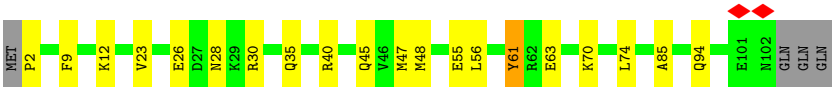




• Molecule 34: Subunit NDUFB10 of NADH-ubiquinone oxidoreductase (Complex I)

Chain d:





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

Chain e:

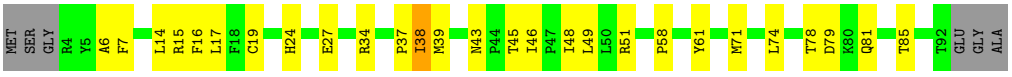




• Molecule 36: NADH dehydrogenase-like protein

Chain f:

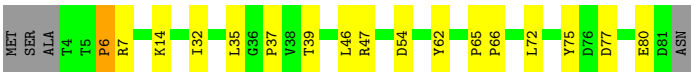




• Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain g:

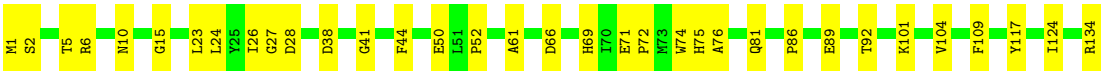




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

Chain h:

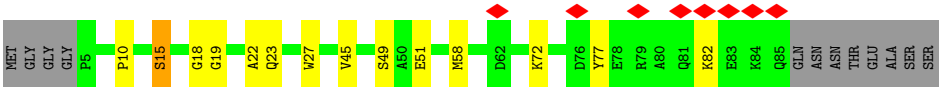




• Molecule 39: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)

Chain i:

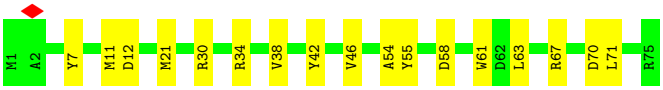




• Molecule 40: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)

Chain j:

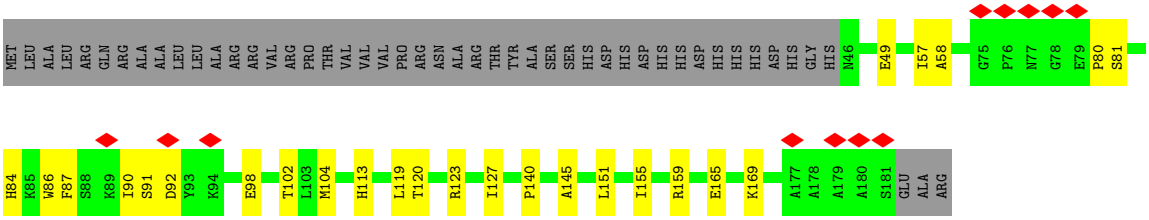




• Molecule 41: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)

Chain n:

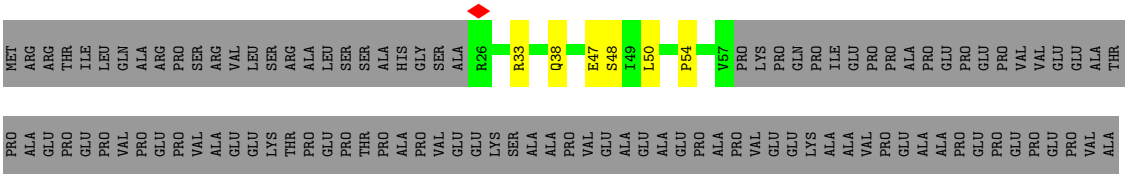




• Molecule 42: Oxidoreductase-like domain-containing protein

Chain o:





GLU ASP LYS PRO ALA PRO GLU GLU LYS LYS SER SER ARG SER PRO LYS ARG GLN GLN GLN GLU GLU SER SER SER ALA GLU LYS PRO ALA GLU LYS PRO ILE ARG SER SER GLY ARG LEU ASP GLY ALA SER ALA PRO SER PRO GLU PRO GLN PRO GLN ASP SER SER GLN GLU LYS PRO

SER ILE THR PHE LEU SER GLY LEU SER GLY PRO THR SER THR SER SER TYR GLN SER ARG LEU GLU SER ILE ARG SER ARG SER ARG LEU ILE ALA GLY VAL LEU VAL PRO PRO GLN PRO THR GLU PRO ASP ASN CYS CYS MET SER GLY CYS VAL ASN CYS VAL TRP ASP ALA TYR ARG

GLU GLU MET GLU ALA TRP ALA ALA ALA LYS ALA GLU ALA GLU ARG ARG LEU ALA ALA GLN GLU VAL SER SER VAL VAL GLY THR THR GLU GLU SER MET HIS ALA VAL GLU ASP GLY LYS ARG VAL GLU ARG THR LEU GLY VAL HIS GLY GLU VAL ALA ASP ARG THR GLY ASP MET ALA

ARG GLU LEU GLU LYS GLY SER THR SER MET GLU GLU ASP GLY ALA GLY PHE GLY GLU ARG MET GLU TRP ASP GLU GLY LEU TYR LYS ASP VAL PRO VAL GLY ILE ARG GLU PHE MET LYS GLN GLU LYS ARG LEU ARG GLU GLU ARG LEU LYS ARG ASN ARG LYS GLU THR GLU HIS GLN

GLN GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153568	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)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.669	Depositor
Minimum map value	-3.480	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	159.03, 221.80501, 319.734	wwPDB
Map dimensions	382, 265, 190	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, LMN, FES, 3PE, ZMP, PC1, CDL, 2MR, ZN, SF4, NDP

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	0.47	0/2633	0.78	2/3593 (0.1%)
2	2	0.48	6/4565 (0.1%)	0.67	5/6209 (0.1%)
3	3	0.44	0/915	0.66	0/1246
4	4	0.56	3/4002 (0.1%)	0.78	8/5454 (0.1%)
5	5	0.50	10/5415 (0.2%)	0.71	8/7372 (0.1%)
6	6	0.51	0/1492	0.81	1/2034 (0.0%)
7	8	0.40	0/671	0.62	0/896
8	9	0.40	0/824	0.63	0/1112
9	A	0.50	3/5589 (0.1%)	0.77	6/7579 (0.1%)
10	B	0.46	4/3621 (0.1%)	0.69	8/4878 (0.2%)
11	C	0.51	1/3449 (0.0%)	0.72	1/4677 (0.0%)
12	D	0.69	1/674 (0.1%)	0.96	2/911 (0.2%)
13	E	0.54	4/2954 (0.1%)	0.73	2/4002 (0.0%)
14	F	0.42	3/1939 (0.2%)	0.59	3/2626 (0.1%)
15	G	0.40	1/2026 (0.0%)	0.54	0/2759
16	H	0.42	1/1741 (0.1%)	0.69	1/2367 (0.0%)
17	I	0.71	3/1527 (0.2%)	0.91	5/2070 (0.2%)
18	J	0.41	1/1413 (0.1%)	0.57	1/1908 (0.1%)
19	K	0.41	1/1485 (0.1%)	0.67	1/2017 (0.0%)
20	L	0.60	0/680	0.86	2/921 (0.2%)
21	M	0.44	0/966	0.64	0/1316
22	O	0.79	0/642	1.05	0/871
22	Q	0.80	1/683 (0.1%)	1.00	0/926
23	P	0.48	2/1060 (0.2%)	0.56	0/1429
24	R	0.47	2/832 (0.2%)	0.60	0/1133
25	S	0.39	1/637 (0.2%)	0.42	0/872
26	U	0.58	0/1394	0.88	2/1890 (0.1%)
27	W	0.49	2/1005 (0.2%)	0.65	0/1359
28	X	0.70	6/1523 (0.4%)	0.89	4/2058 (0.2%)
29	Y	0.42	2/1277 (0.2%)	0.55	0/1731
30	Z	0.48	1/1462 (0.1%)	0.71	3/1993 (0.2%)
31	a	0.59	2/1209 (0.2%)	0.73	3/1639 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.23	0/701	0.40	0/939
33	c	0.43	0/524	0.63	0/710
34	d	0.25	0/861	0.49	1/1157 (0.1%)
35	e	0.19	0/332	0.33	0/451
36	f	0.52	2/736 (0.3%)	0.63	3/988 (0.3%)
37	g	0.49	2/631 (0.3%)	0.57	1/868 (0.1%)
38	h	0.47	0/1172	0.75	3/1594 (0.2%)
39	i	0.39	0/711	0.61	2/967 (0.2%)
40	j	0.48	1/630 (0.2%)	0.59	0/847
41	n	0.45	2/1098 (0.2%)	0.51	1/1489 (0.1%)
42	o	0.38	0/262	0.68	1/360 (0.3%)
All	All	0.50	68/67963 (0.1%)	0.71	80/92218 (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

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	232	ALA	C-N	10.45	1.47	1.33
13	E	306	GLY	C-N	10.08	1.46	1.33
31	a	77	PHE	C-N	10.05	1.46	1.33
41	n	80	PRO	C-N	9.87	1.46	1.33
36	f	38	ILE	C-N	-9.80	1.20	1.33

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	253	PRO	N-CA-C	12.96	126.52	110.70
36	f	38	ILE	O-C-N	-9.14	112.42	121.83
9	A	403	SER	N-CA-C	-8.88	97.13	110.28
2	2	527	GLY	O-C-N	-8.62	113.10	122.24
10	B	254	PRO	N-CA-C	-7.88	98.19	110.95

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	2573	0	2696	65	0
2	2	4459	0	4652	106	0
3	3	894	0	899	19	0
4	4	3904	0	4056	85	0
5	5	5273	0	5399	153	0
6	6	1465	0	1559	49	0
7	8	658	0	648	7	0
8	9	807	0	778	19	0
9	A	5476	0	5419	84	0
10	B	3538	0	3477	84	0
11	C	3376	0	3292	56	0
12	D	678	0	642	12	0
13	E	2886	0	2855	62	0
14	F	1899	0	1879	45	0
15	G	1968	0	1935	45	0
16	H	1702	0	1671	43	0
17	I	1487	0	1434	40	0
18	J	1388	0	1393	33	0
19	K	1446	0	1433	50	0
20	L	673	0	742	28	0
21	M	935	0	885	11	0
22	O	633	0	611	8	0
22	Q	673	0	646	6	0
23	P	1033	0	1011	27	0
24	R	807	0	823	21	0
25	S	612	0	562	17	0
26	U	1357	0	1330	41	0
27	W	980	0	994	24	0
28	X	1484	0	1436	35	0
29	Y	1240	0	1204	28	0
30	Z	1428	0	1400	35	0
31	a	1172	0	1106	23	0
32	b	683	0	690	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	505	0	474	9	0
34	d	843	0	835	20	0
35	e	317	0	304	6	0
36	f	722	0	737	24	0
37	g	610	0	620	15	0
38	h	1132	0	1105	25	0
39	i	682	0	655	12	0
40	j	616	0	640	18	0
41	n	1067	0	1027	24	0
42	o	252	0	235	5	0
43	1	32	0	38	0	0
43	4	118	0	164	12	0
43	5	142	0	183	4	0
43	E	31	0	36	0	0
43	I	86	0	120	7	0
43	J	30	0	34	1	0
43	W	74	0	96	2	0
43	g	36	0	46	1	0
43	i	92	0	138	5	0
43	n	39	0	52	3	0
44	1	43	0	60	4	0
44	3	48	0	70	4	0
44	4	50	0	77	3	0
44	5	97	0	148	16	0
44	K	47	0	68	3	0
44	S	51	0	79	3	0
44	X	71	0	90	2	0
45	2	74	0	92	1	0
45	D	74	0	92	4	0
45	S	79	0	105	6	0
45	X	77	0	101	3	0
45	g	70	0	84	3	0
46	2	58	0	77	1	0
46	4	47	0	66	4	0
46	5	69	0	88	3	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	0	0
49	B	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	E	48	0	26	1	0
51	M	1	0	0	0	0
52	O	36	0	47	3	0
52	Q	36	0	47	6	0
53	1	134	0	0	10	0
53	2	214	0	0	9	0
53	3	31	0	0	2	0
53	4	115	0	0	6	0
53	5	28	0	0	1	0
53	6	56	0	0	2	0
53	9	19	0	0	2	0
53	A	319	0	0	4	0
53	B	73	0	0	3	0
53	C	257	0	0	10	0
53	D	41	0	0	1	0
53	E	88	0	0	7	0
53	F	65	0	0	3	0
53	G	172	0	0	7	0
53	H	34	0	0	1	0
53	I	124	0	0	0	0
53	J	1	0	0	0	0
53	K	107	0	0	7	0
53	L	25	0	0	6	0
53	M	81	0	0	3	0
53	P	42	0	0	3	0
53	R	3	0	0	0	0
53	S	3	0	0	0	0
53	U	67	0	0	4	0
53	W	64	0	0	1	0
53	X	81	0	0	1	0
53	Y	163	0	0	6	0
53	Z	84	0	0	1	0
53	a	8	0	0	0	0
53	b	11	0	0	0	0
53	d	8	0	0	0	0
53	f	6	0	0	0	0
53	g	20	0	0	0	0
53	h	58	0	0	2	0
53	j	9	0	0	1	0
53	n	37	0	0	1	0
53	o	1	0	0	0	0
All	All	70825	0	68532	1271	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 9.

The worst 5 of 1271 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)
26:U:153:HIS:CE1	26:U:154:HIS:CD2	2.54	0.95
11:C:184:GLU:HG3	11:C:263:VAL:HB	1.52	0.91
10:B:440:GLU:HG2	53:B:767:HOH:O	1.72	0.90
26:U:153:HIS:CE1	26:U:154:HIS:HD2	1.89	0.90
9:A:77:LYS:HE2	9:A:294:GLU:HG3	1.55	0.87

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	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	548 (99%)	6 (1%)	0	100	100
3	3	111/146 (76%)	107 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	476 (97%)	14 (3%)	0	100	100
5	5	668/679 (98%)	635 (95%)	33 (5%)	0	100	100
6	6	186/224 (83%)	181 (97%)	5 (3%)	0	100	100
7	8	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	A	709/749 (95%)	683 (96%)	26 (4%)	0	100	100
10	B	454/507 (90%)	437 (96%)	17 (4%)	0	100	100
11	C	420/499 (84%)	406 (97%)	14 (3%)	0	100	100
12	D	79/86 (92%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	E	351/378 (93%)	342 (97%)	9 (3%)	0	100	100
14	F	236/261 (90%)	233 (99%)	3 (1%)	0	100	100
15	G	240/293 (82%)	233 (97%)	7 (3%)	0	100	100
16	H	219/318 (69%)	207 (94%)	12 (6%)	0	100	100
17	I	183/223 (82%)	180 (98%)	3 (2%)	0	100	100
18	J	184/199 (92%)	180 (98%)	4 (2%)	0	100	100
19	K	180/230 (78%)	174 (97%)	5 (3%)	1 (1%)	21	25
20	L	85/89 (96%)	85 (100%)	0	0	100	100
21	M	116/168 (69%)	111 (96%)	5 (4%)	0	100	100
22	O	78/141 (55%)	76 (97%)	2 (3%)	0	100	100
22	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100
23	P	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
24	R	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
25	S	72/143 (50%)	71 (99%)	1 (1%)	0	100	100
26	U	165/186 (89%)	162 (98%)	3 (2%)	0	100	100
27	W	118/121 (98%)	117 (99%)	1 (1%)	0	100	100
28	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
29	Y	152/210 (72%)	148 (97%)	4 (3%)	0	100	100
30	Z	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
31	a	142/203 (70%)	138 (97%)	4 (3%)	0	100	100
32	b	79/94 (84%)	78 (99%)	1 (1%)	0	100	100
33	c	59/93 (63%)	55 (93%)	4 (7%)	0	100	100
34	d	99/105 (94%)	95 (96%)	4 (4%)	0	100	100
35	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
36	f	87/95 (92%)	84 (97%)	3 (3%)	0	100	100
37	g	76/82 (93%)	74 (97%)	2 (3%)	0	100	100
38	h	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
39	i	79/93 (85%)	77 (98%)	2 (2%)	0	100	100
40	j	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
41	n	134/184 (73%)	129 (96%)	5 (4%)	0	100	100
42	o	30/380 (8%)	28 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8250/10547 (78%)	8005 (97%)	244 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	K	51	PRO

5.3.2 Protein sidechains

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	284/326 (87%)	281 (99%)	3 (1%)	65 75
2	2	510/518 (98%)	501 (98%)	9 (2%)	51 64
3	3	93/128 (73%)	90 (97%)	3 (3%)	34 46
4	4	431/477 (90%)	425 (99%)	6 (1%)	59 70
5	5	580/596 (97%)	562 (97%)	18 (3%)	35 47
6	6	167/203 (82%)	157 (94%)	10 (6%)	17 23
7	8	69/75 (92%)	69 (100%)	0	100 100
8	9	84/687 (12%)	84 (100%)	0	100 100
9	A	577/602 (96%)	564 (98%)	13 (2%)	44 57
10	B	366/401 (91%)	358 (98%)	8 (2%)	45 59
11	C	356/416 (86%)	353 (99%)	3 (1%)	73 81
12	D	68/69 (99%)	67 (98%)	1 (2%)	57 69
13	E	315/335 (94%)	314 (100%)	1 (0%)	86 91
14	F	203/219 (93%)	200 (98%)	3 (2%)	57 69
15	G	215/257 (84%)	212 (99%)	3 (1%)	59 70
16	H	191/272 (70%)	189 (99%)	2 (1%)	68 77
17	I	158/191 (83%)	155 (98%)	3 (2%)	50 63
18	J	129/146 (88%)	126 (98%)	3 (2%)	44 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	K	156/191 (82%)	152 (97%)	4 (3%)	40 53
20	L	74/76 (97%)	67 (90%)	7 (10%)	8 8
21	M	97/135 (72%)	97 (100%)	0	100 100
22	O	71/119 (60%)	68 (96%)	3 (4%)	26 37
22	Q	75/119 (63%)	74 (99%)	1 (1%)	61 72
23	P	108/110 (98%)	106 (98%)	2 (2%)	50 63
24	R	87/89 (98%)	84 (97%)	3 (3%)	32 45
25	S	60/111 (54%)	60 (100%)	0	100 100
26	U	149/167 (89%)	143 (96%)	6 (4%)	28 39
27	W	101/102 (99%)	99 (98%)	2 (2%)	48 62
28	X	146/152 (96%)	145 (99%)	1 (1%)	76 83
29	Y	131/176 (74%)	128 (98%)	3 (2%)	44 57
30	Z	151/155 (97%)	148 (98%)	3 (2%)	48 62
31	a	123/177 (70%)	122 (99%)	1 (1%)	73 81
32	b	67/74 (90%)	67 (100%)	0	100 100
33	c	49/80 (61%)	47 (96%)	2 (4%)	27 38
34	d	90/94 (96%)	90 (100%)	0	100 100
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%)	65 (100%)	0	100 100
38	h	119/119 (100%)	119 (100%)	0	100 100
39	i	68/78 (87%)	67 (98%)	1 (2%)	57 69
40	j	64/64 (100%)	64 (100%)	0	100 100
41	n	107/150 (71%)	107 (100%)	0	100 100
42	o	26/318 (8%)	26 (100%)	0	100 100
All	All	7086/8958 (79%)	6958 (98%)	128 (2%)	51 64

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	W	40	LEU
29	Y	133	VAL
6	6	198	VAL

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Mol	Chain	Res	Type
6	6	186	SER
30	Z	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
24	R	90	ASN
34	d	15	GLN
26	U	107	GLN
27	W	97	ASN
38	h	81	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.39	0	5,13,15	1.31	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.33	117.34	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 48 ligands modelled in this entry, 1 is monoatomic - leaving 47 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	$\#\|Z\| > 2$
47	FES	A	801	9	0,4,4	-	-	-		
45	CDL	g	101	-	69,69,99	1.03	8 (11%)	75,81,111	1.15	6 (8%)
43	3PE	5	707	-	32,32,50	1.05	4 (12%)	35,37,55	1.11	2 (5%)
52	ZMP	Q	201	22	29,35,36	0.18	0	34,42,45	0.40	0
43	3PE	I	304	-	43,43,50	0.94	4 (9%)	46,48,55	1.10	2 (4%)
48	SF4	I	301	17	0,12,12	-	-	-		
44	PC1	5	706	-	42,42,53	1.06	4 (9%)	48,50,61	1.14	3 (6%)
45	CDL	2	601	-	73,73,99	1.00	8 (10%)	79,85,111	1.23	4 (5%)
48	SF4	A	802	9	0,12,12	-	-	-		
48	SF4	I	302	17	0,12,12	-	-	-		
43	3PE	W	202	-	38,38,50	0.97	4 (10%)	41,43,55	1.30	4 (9%)
43	3PE	J	201	-	29,29,50	1.10	4 (13%)	32,34,55	1.17	2 (6%)
43	3PE	5	703	-	34,34,50	1.03	4 (11%)	37,39,55	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	3PE	4	605	-	33,33,50	1.04	4 (12%)	36,38,55	1.12	2 (5%)
44	PC1	S	202	-	50,50,53	0.96	4 (8%)	56,58,61	1.07	2 (3%)
46	LMN	2	602	-	60,60,72	1.70	12 (20%)	78,80,98	1.05	3 (3%)
46	LMN	4	603	-	48,48,72	1.85	13 (27%)	60,62,98	0.99	2 (3%)
44	PC1	4	604	-	49,49,53	0.99	4 (8%)	55,57,61	1.19	3 (5%)
45	CDL	D	101	-	73,73,99	1.00	8 (10%)	79,85,111	1.16	4 (5%)
43	3PE	I	303	-	41,41,50	0.92	2 (4%)	44,46,55	1.13	3 (6%)
44	PC1	K	302	-	46,46,53	1.01	4 (8%)	52,54,61	1.15	2 (3%)
43	3PE	i	102	-	40,40,50	0.94	4 (10%)	43,45,55	1.11	2 (4%)
43	3PE	5	704	-	42,42,50	0.94	4 (9%)	45,47,55	1.14	2 (4%)
44	PC1	3	201	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	3 (5%)
43	3PE	1	401	-	31,31,50	1.09	4 (12%)	34,36,55	1.34	3 (8%)
45	CDL	X	201	-	76,76,99	0.98	6 (7%)	82,88,111	1.26	6 (7%)
46	LMN	5	705	-	72,72,72	1.62	12 (16%)	96,98,98	1.08	5 (5%)
47	FES	H	401	16	0,4,4	-	-	-		
48	SF4	K	301	19	0,12,12	-	-	-		
43	3PE	W	201	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
43	3PE	g	102	-	35,35,50	1.00	4 (11%)	38,40,55	1.13	3 (7%)
50	NDP	E	402	-	49,52,52	0.54	0	66,80,80	0.51	1 (1%)
44	PC1	X	203	-	31,31,53	1.21	4 (12%)	37,39,61	1.17	3 (8%)
52	ZMP	O	201	22	29,35,36	0.24	0	34,42,45	0.43	0
49	FMN	B	602	-	33,33,33	0.70	0	48,50,50	0.80	1 (2%)
43	3PE	E	401	-	30,30,50	1.10	4 (13%)	33,35,55	1.21	2 (6%)
44	PC1	5	701	-	53,53,53	0.95	5 (9%)	59,61,61	1.21	3 (5%)
48	SF4	B	601	10	0,12,12	-	-	-		
43	3PE	i	101	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
43	3PE	4	602	-	32,32,50	1.05	4 (12%)	35,37,55	1.18	2 (5%)
43	3PE	4	601	-	50,50,50	0.87	4 (8%)	53,55,55	1.19	2 (3%)
48	SF4	A	803	9	0,12,12	-	-	-		
45	CDL	S	201	-	78,78,99	0.97	8 (10%)	84,90,111	1.10	4 (4%)
44	PC1	1	402	-	42,42,53	1.09	4 (9%)	48,50,61	1.23	4 (8%)
44	PC1	X	202	-	38,38,53	1.10	4 (10%)	44,46,61	1.18	3 (6%)
43	3PE	5	702	-	30,30,50	1.11	4 (13%)	33,35,55	1.20	2 (6%)
43	3PE	n	201	-	38,38,50	0.98	4 (10%)	41,43,55	1.14	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	FES	A	801	9	-	-	0/1/1/1
45	CDL	g	101	-	-	36/80/80/110	-
43	3PE	5	707	-	-	5/36/36/54	-
52	ZMP	Q	201	22	-	17/40/42/43	-
43	3PE	I	304	-	-	20/47/47/54	-
48	SF4	I	301	17	-	-	0/6/5/5
44	PC1	5	706	-	-	11/46/46/57	-
45	CDL	2	601	-	-	36/84/84/110	-
48	SF4	A	802	9	-	-	0/6/5/5
48	SF4	I	302	17	-	-	0/6/5/5
43	3PE	W	202	-	-	18/42/42/54	-
43	3PE	J	201	-	-	6/33/33/54	-
43	3PE	5	703	-	-	15/38/38/54	-
43	3PE	4	605	-	-	18/37/37/54	-
44	PC1	S	202	-	-	19/54/54/57	-
46	LMN	2	602	-	-	25/44/104/130	0/3/3/4
46	LMN	4	603	-	-	25/38/78/130	0/2/2/4
44	PC1	4	604	-	-	18/53/53/57	-
45	CDL	D	101	-	-	31/84/84/110	-
43	3PE	I	303	-	-	20/45/45/54	-
44	PC1	K	302	-	-	11/50/50/57	-
43	3PE	i	102	-	-	17/44/44/54	-
43	3PE	5	704	-	-	10/46/46/54	-
44	PC1	3	201	-	-	17/51/51/57	-
43	3PE	1	401	-	-	15/35/35/54	-
45	CDL	X	201	-	-	44/87/87/110	-
46	LMN	5	705	-	-	29/50/130/130	0/4/4/4
47	FES	H	401	16	-	-	0/1/1/1
48	SF4	K	301	19	-	-	0/6/5/5
43	3PE	W	201	-	-	14/38/38/54	-
43	3PE	g	102	-	-	18/39/39/54	-
50	NDP	E	402	-	-	6/34/77/77	0/5/5/5
44	PC1	X	203	-	-	15/35/35/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	ZMP	O	201	22	-	16/40/42/43	-
49	FMN	B	602	-	-	9/18/18/18	0/3/3/3
43	3PE	E	401	-	-	18/34/34/54	-
44	PC1	5	701	-	-	20/57/57/57	-
48	SF4	B	601	10	-	-	0/6/5/5
43	3PE	i	101	-	-	16/54/54/54	-
43	3PE	4	602	-	-	17/36/36/54	-
43	3PE	4	601	-	-	19/54/54/54	-
48	SF4	A	803	9	-	-	0/6/5/5
45	CDL	S	201	-	-	30/89/89/110	-
44	PC1	1	402	-	-	16/46/46/57	-
44	PC1	X	202	-	-	14/42/42/57	-
43	3PE	5	702	-	-	14/34/34/54	-
43	3PE	n	201	-	-	19/42/42/54	-

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	5	705	LMN	O5-C1	4.68	1.53	1.41
46	4	603	LMN	O5-C1	4.64	1.53	1.41
46	2	602	LMN	O5-C1	4.59	1.53	1.41
46	5	705	LMN	CBS-CCM	4.32	1.63	1.53
46	4	603	LMN	CBT-CCM	4.03	1.62	1.53

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	4	604	PC1	O21-C21-C22	5.28	122.89	111.50
43	1	401	3PE	O21-C21-C22	4.93	122.12	111.50
44	K	302	PC1	O21-C21-C22	4.67	121.57	111.50
45	2	601	CDL	OB6-CB5-C51	4.63	121.47	111.50
43	4	601	3PE	O21-C21-C22	4.62	121.47	111.50

There are no chirality outliers.

5 of 724 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	3PE	C1-O11-P-O12
43	1	401	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
43	4	601	3PE	C1-O11-P-O12
43	4	601	3PE	C1-O11-P-O14
43	4	601	3PE	C11-O13-P-O12

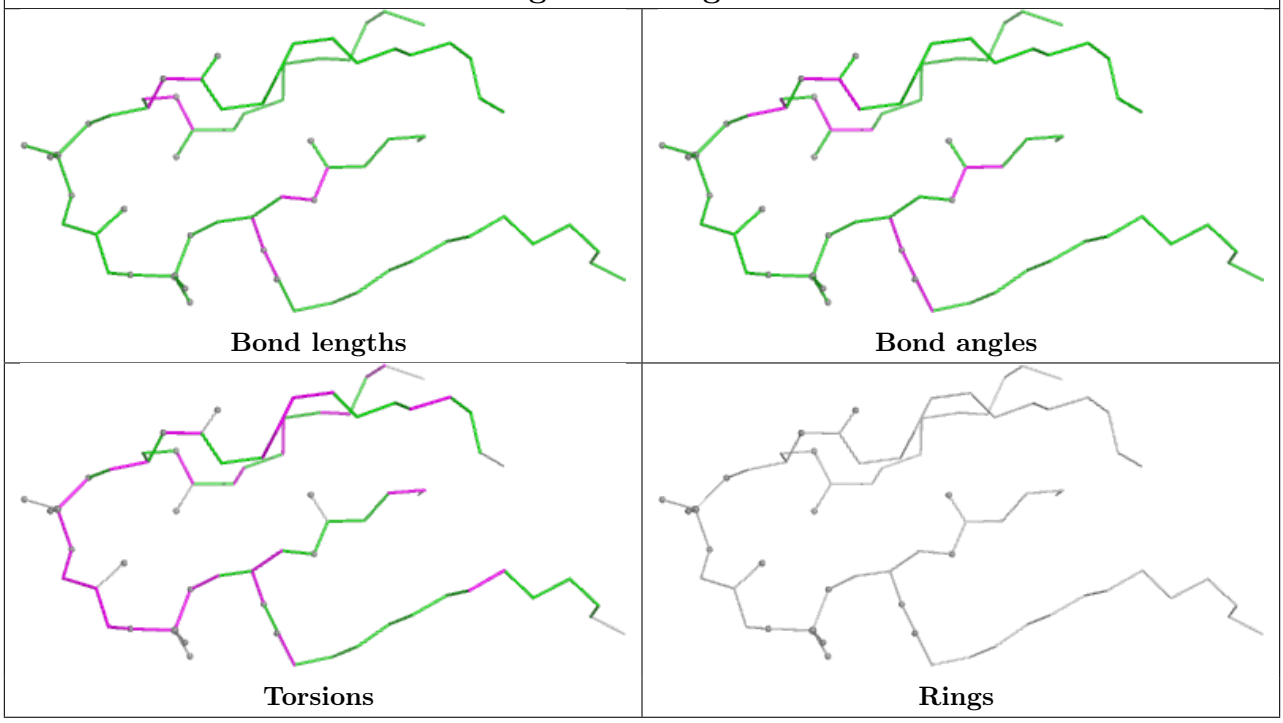
There are no ring outliers.

34 monomers are involved in 105 short contacts:

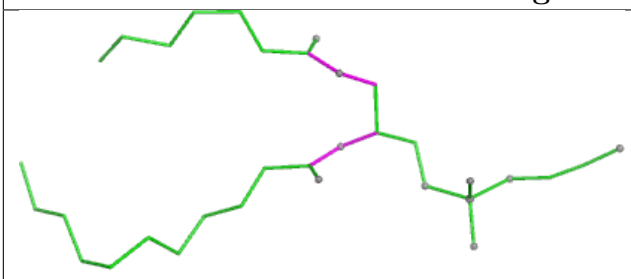
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	g	101	CDL	3	0
52	Q	201	ZMP	6	0
43	I	304	3PE	3	0
44	5	706	PC1	6	0
45	2	601	CDL	1	0
43	W	202	3PE	1	0
43	J	201	3PE	1	0
43	5	703	3PE	2	0
43	4	605	3PE	2	0
44	S	202	PC1	3	0
46	2	602	LMN	1	0
46	4	603	LMN	4	0
44	4	604	PC1	3	0
45	D	101	CDL	4	0
43	I	303	3PE	4	0
44	K	302	PC1	3	0
43	i	102	3PE	2	0
43	5	704	3PE	2	0
44	3	201	PC1	4	0
45	X	201	CDL	3	0
46	5	705	LMN	3	0
43	W	201	3PE	1	0
43	g	102	3PE	1	0
50	E	402	NDP	1	0
44	X	203	PC1	1	0
52	O	201	ZMP	3	0
44	5	701	PC1	10	0
43	i	101	3PE	3	0
43	4	602	3PE	3	0
43	4	601	3PE	7	0
45	S	201	CDL	6	0
44	1	402	PC1	4	0
44	X	202	PC1	1	0
43	n	201	3PE	3	0

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

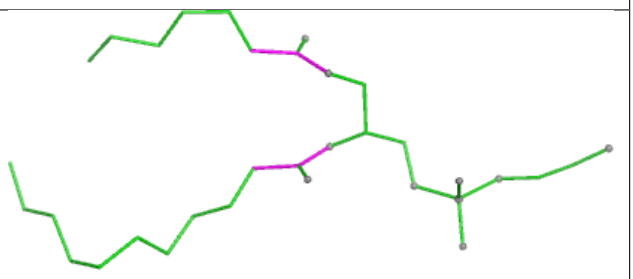
Ligand CDL g 101



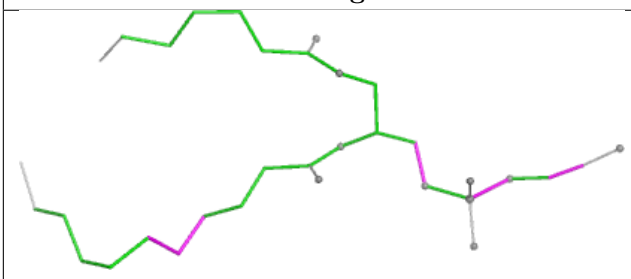
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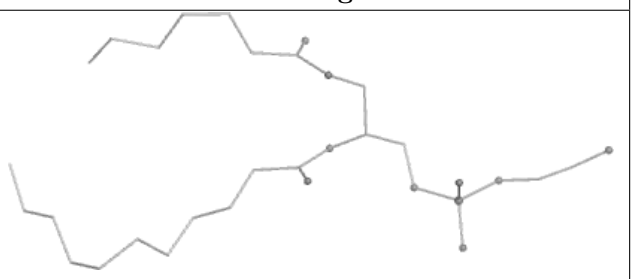
Bond lengths



Bond angles

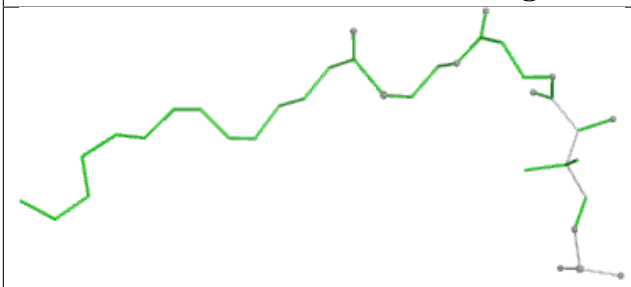


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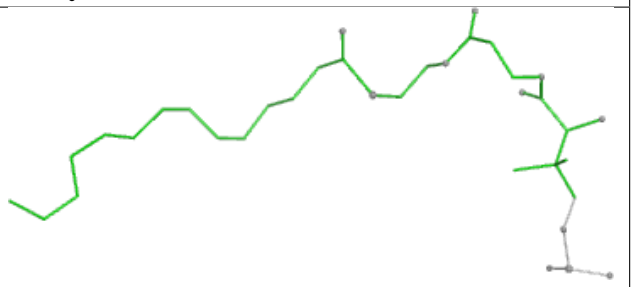


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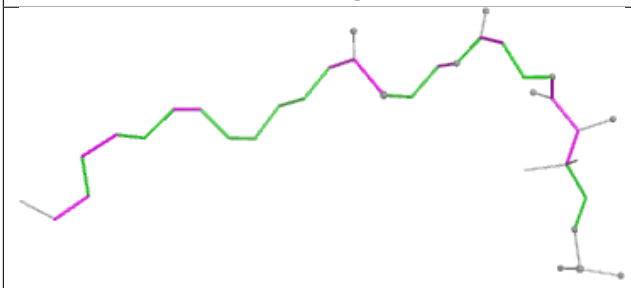
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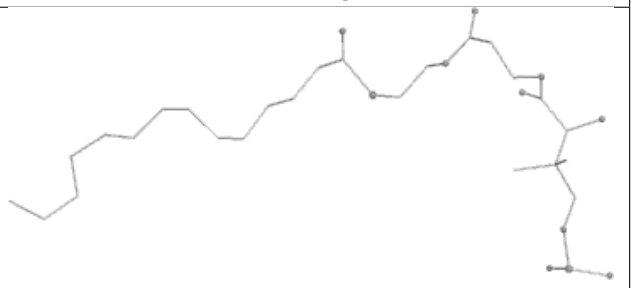
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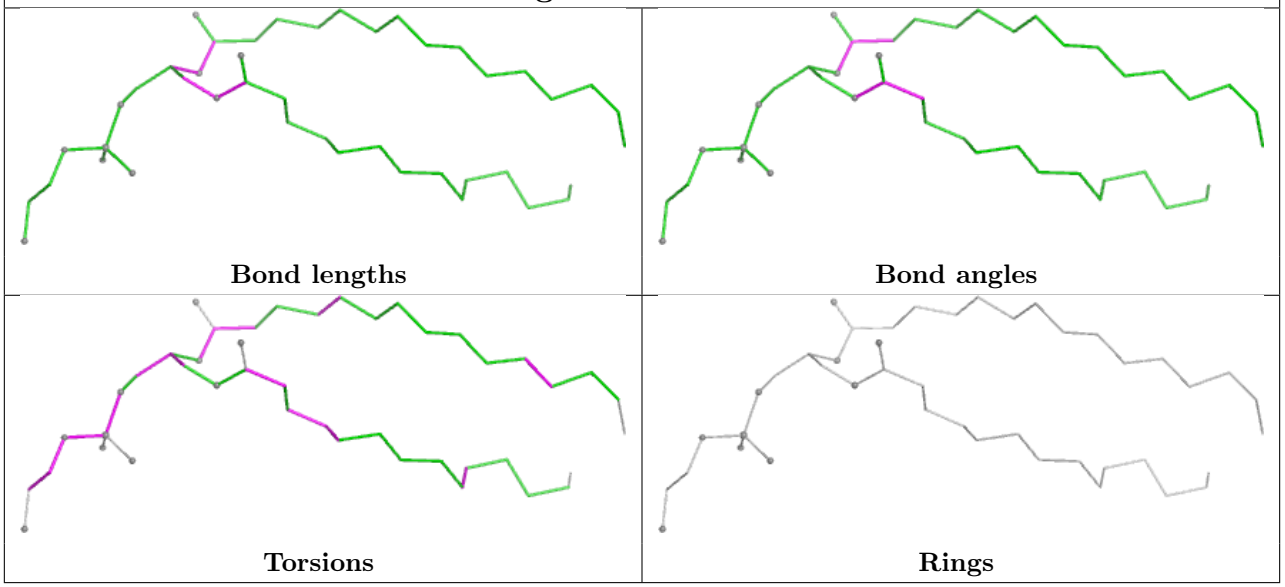


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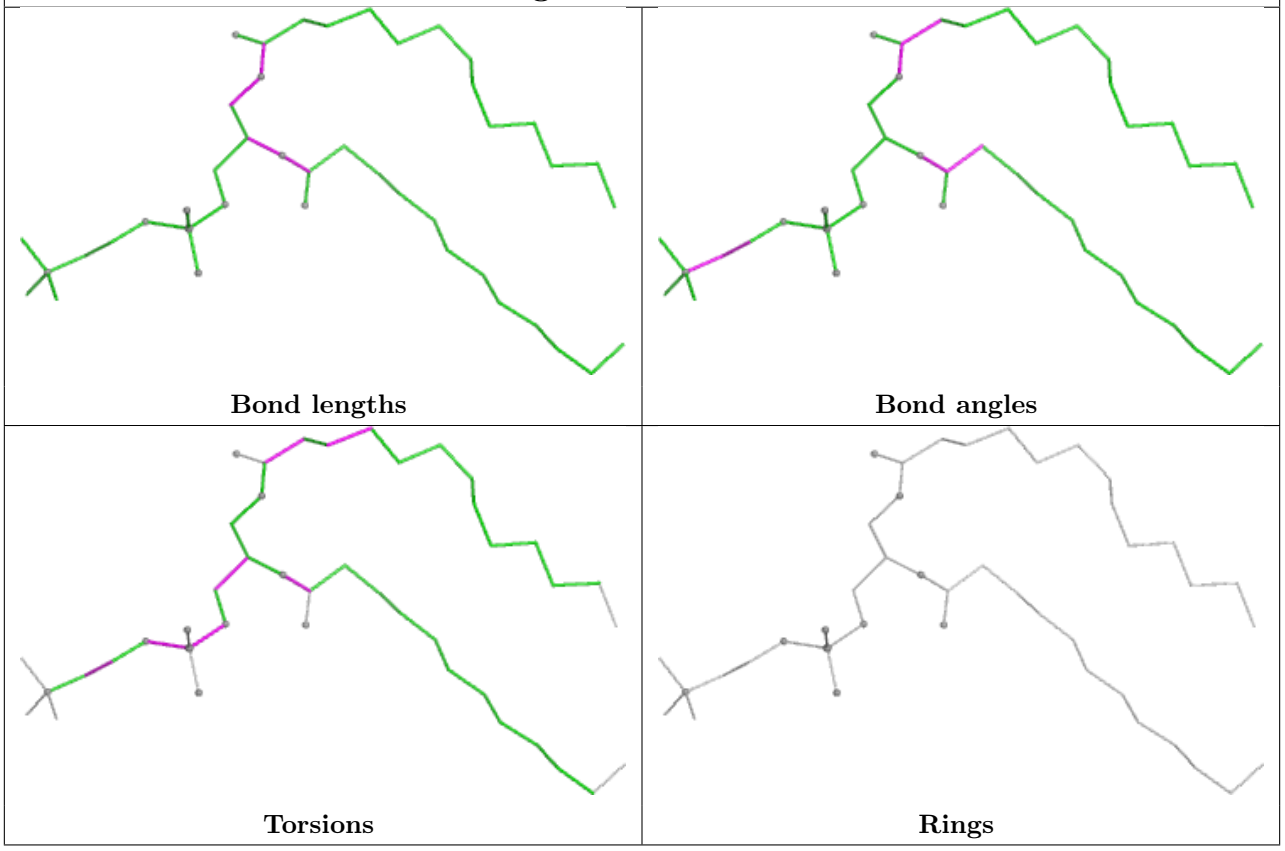


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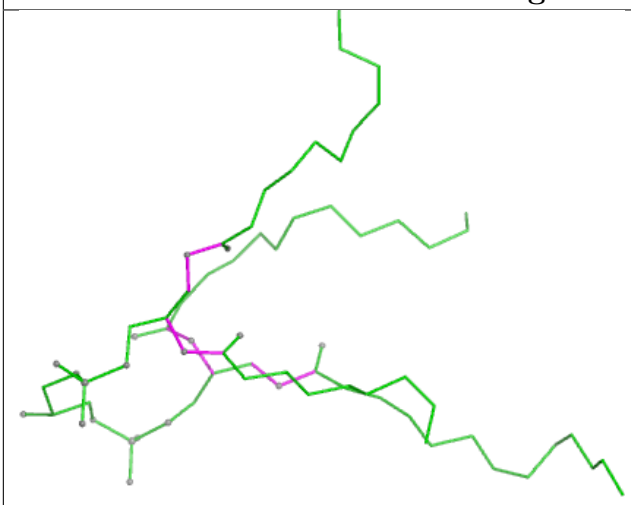
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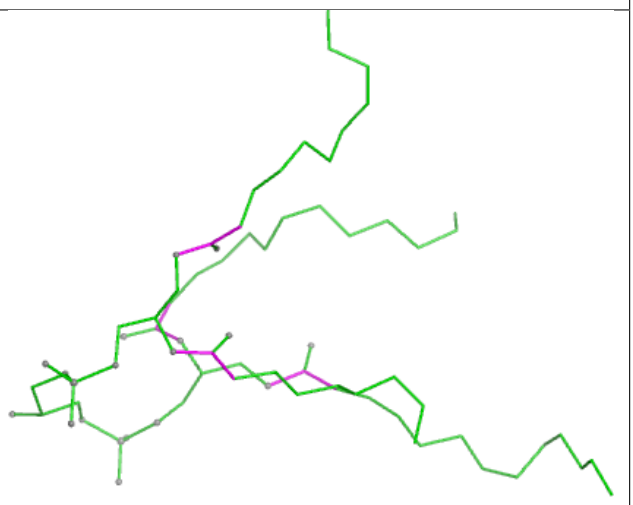
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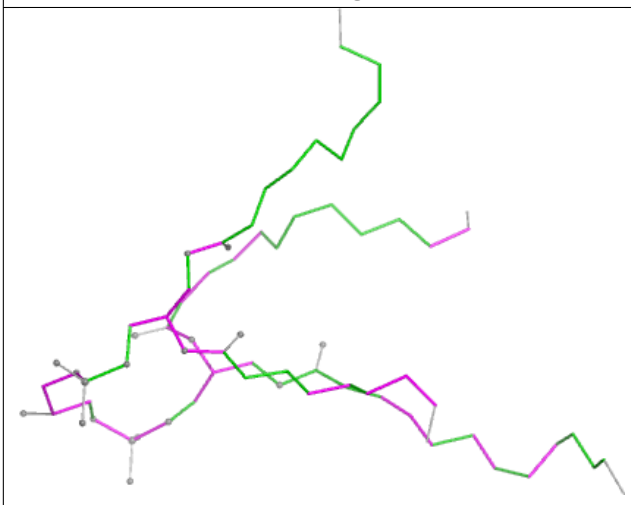
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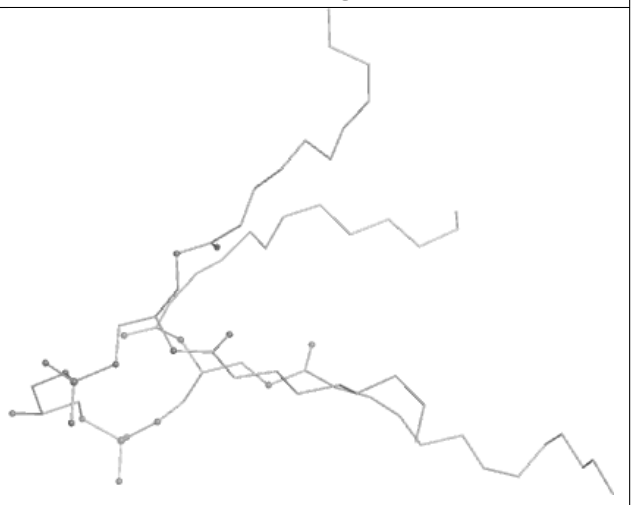
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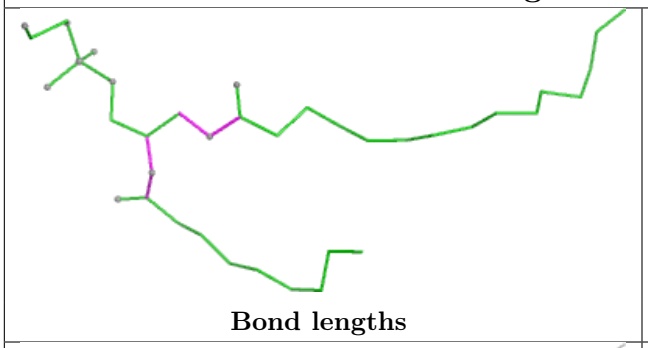


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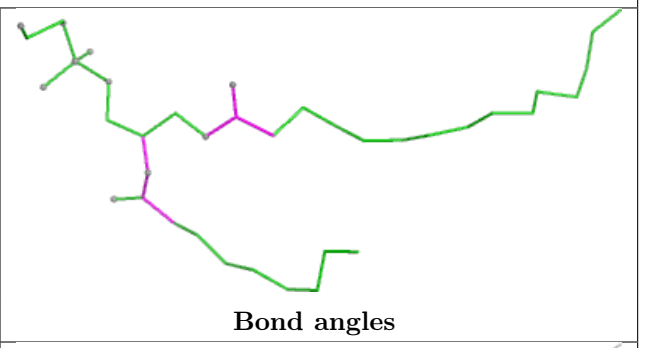


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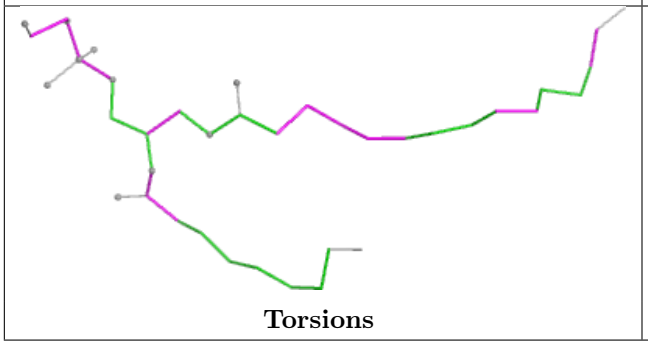
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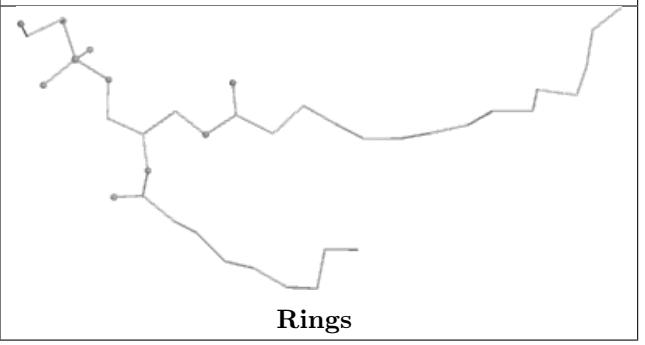
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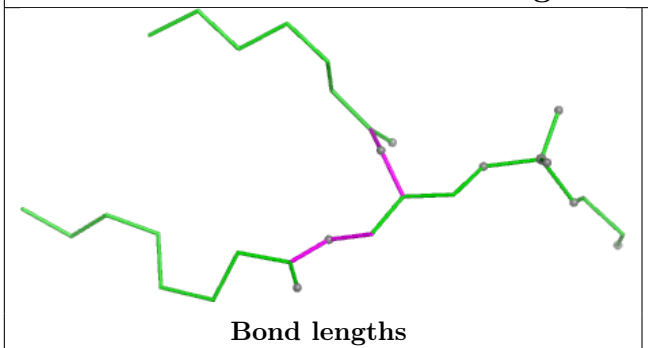


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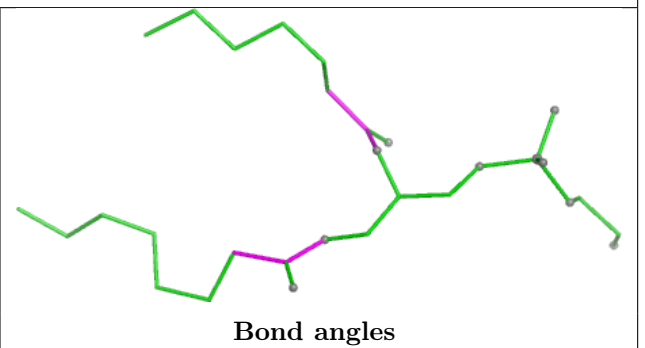


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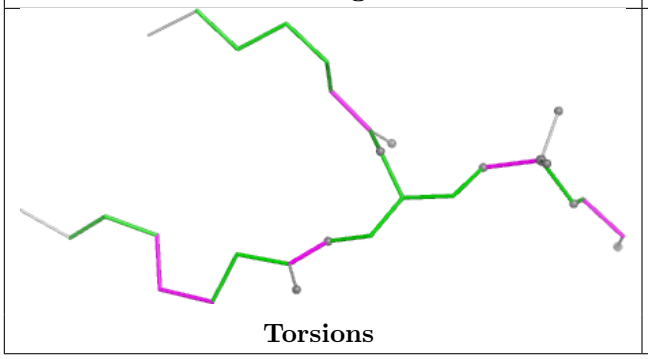
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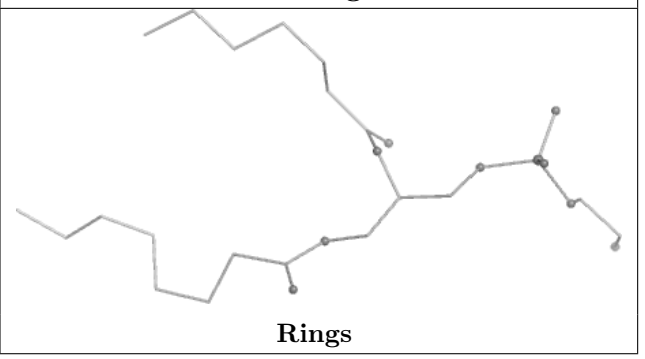
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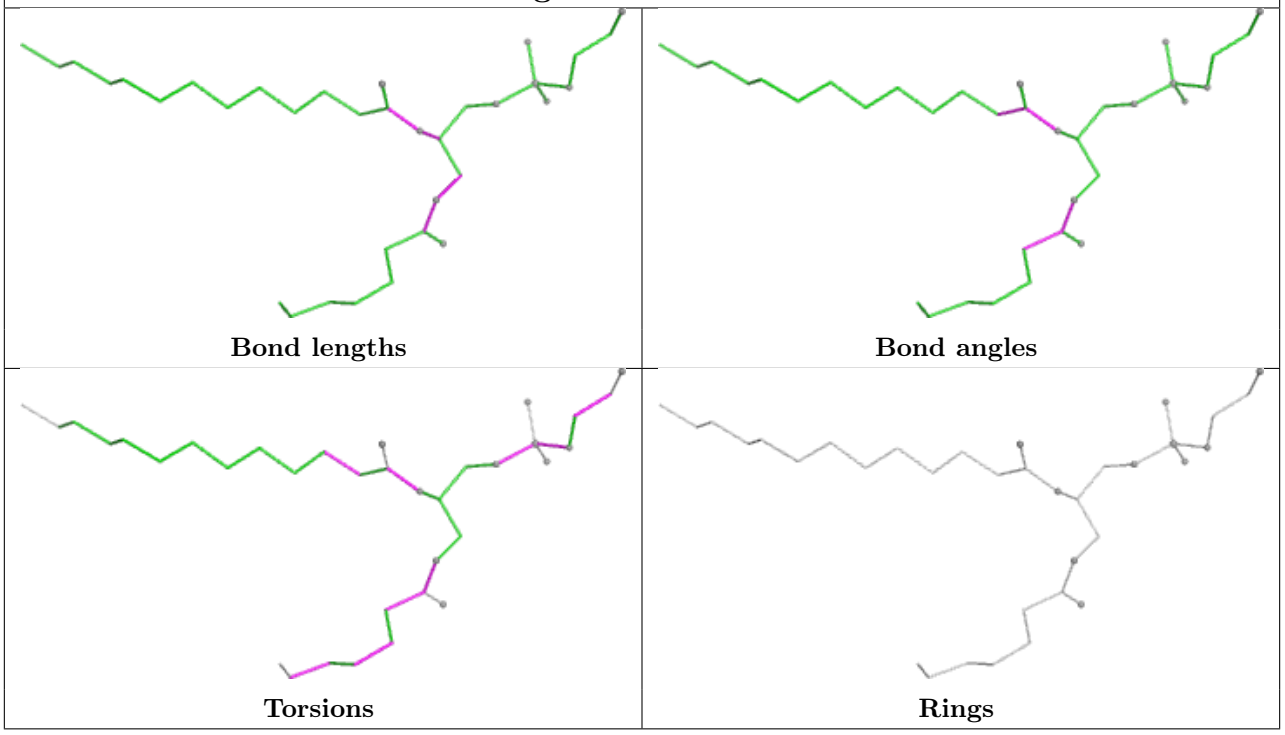


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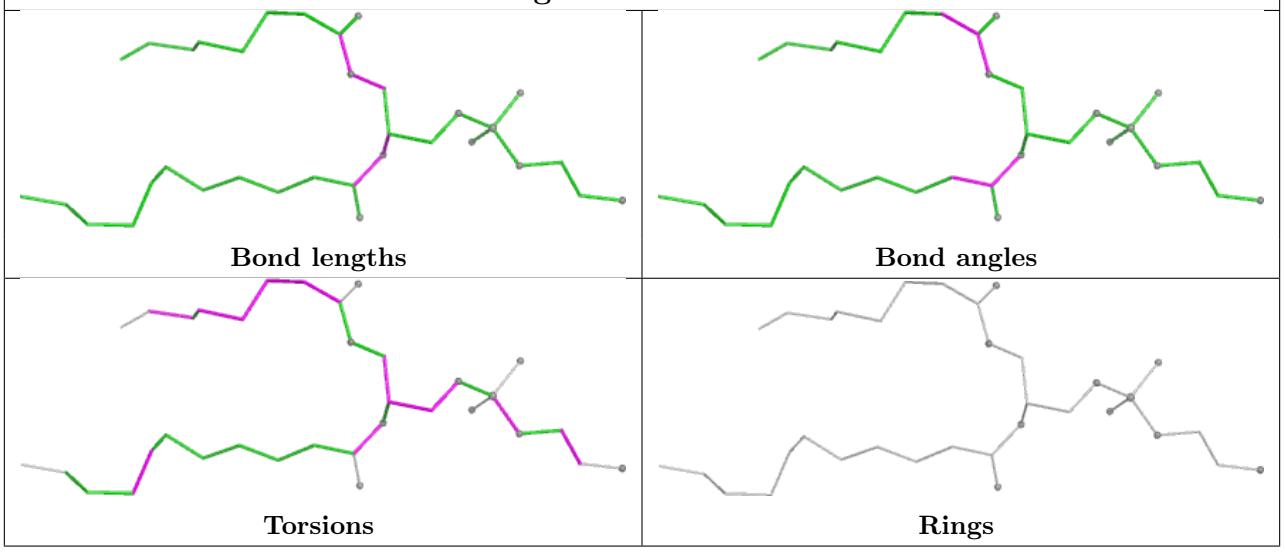


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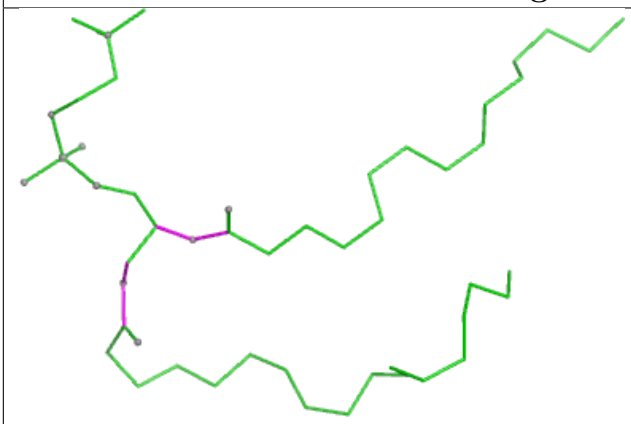
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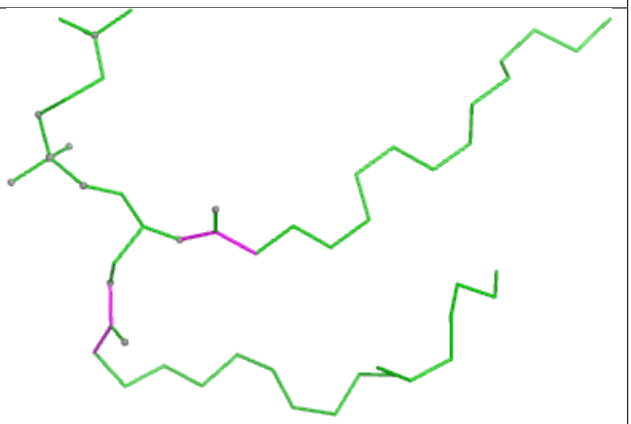
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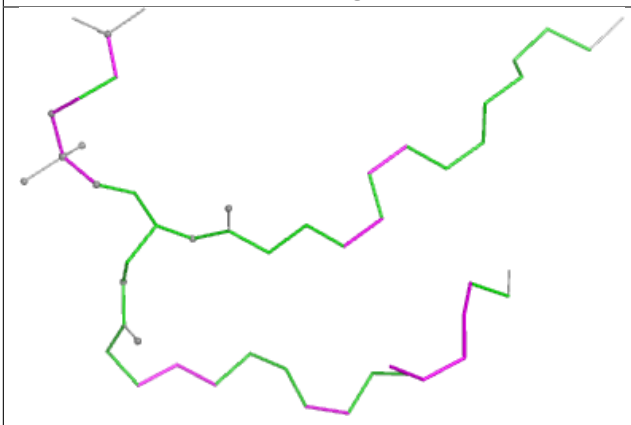
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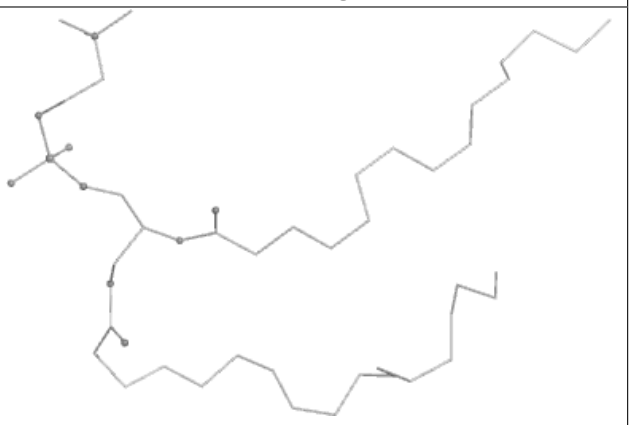
Bond lengths



Bond angles

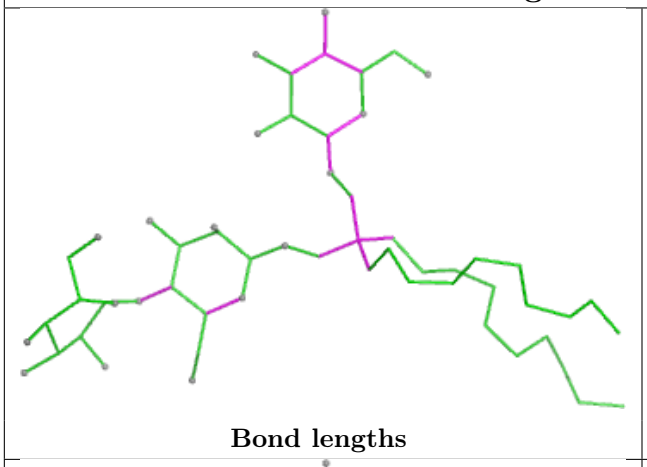


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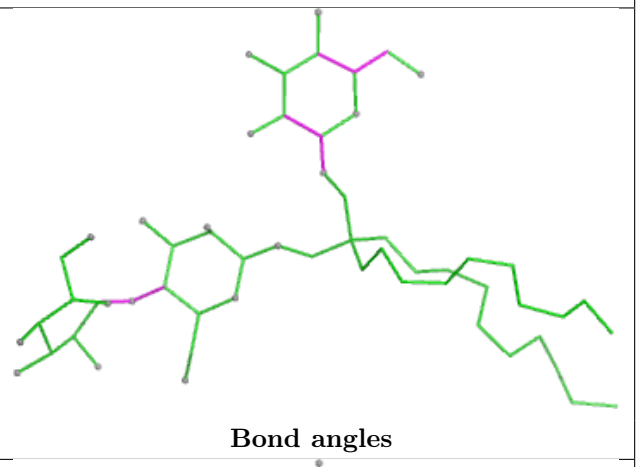


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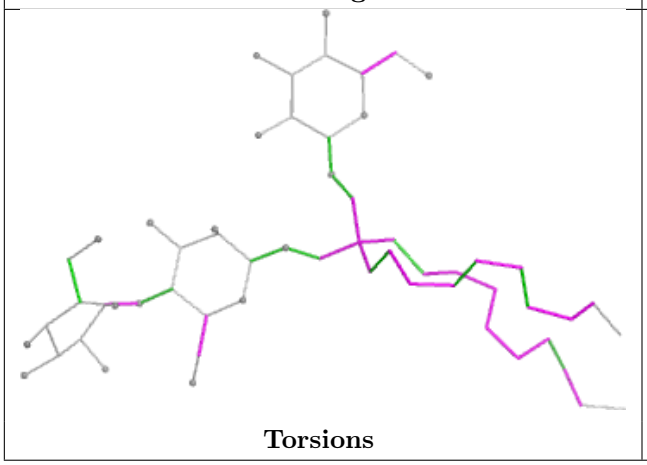
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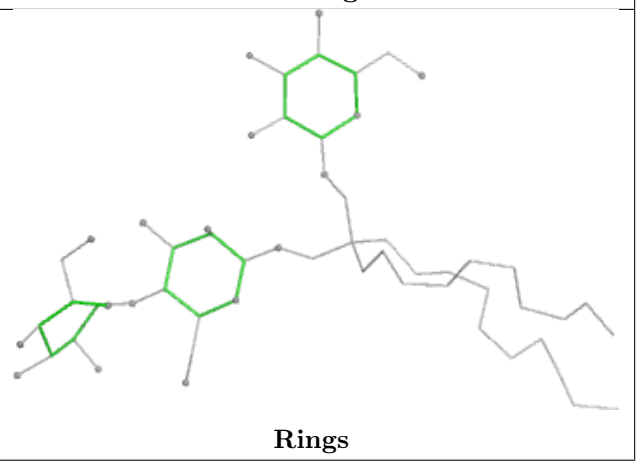
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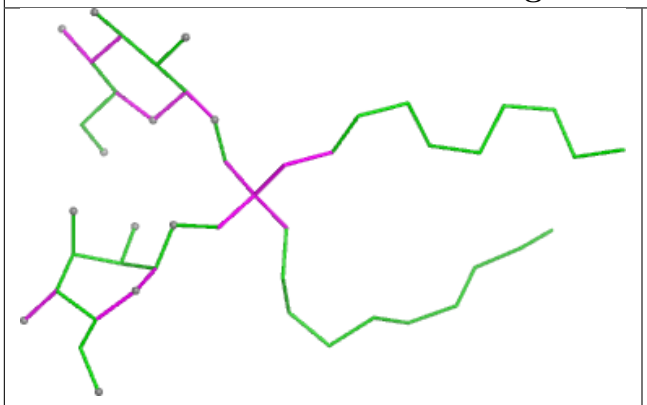


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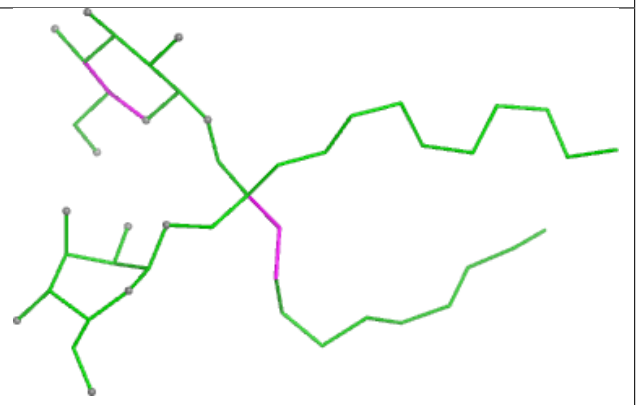


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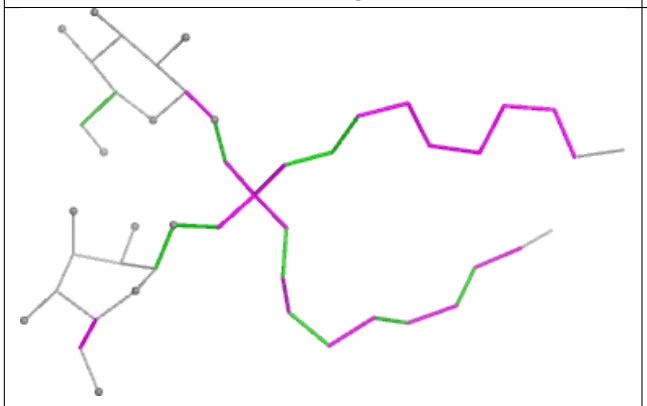
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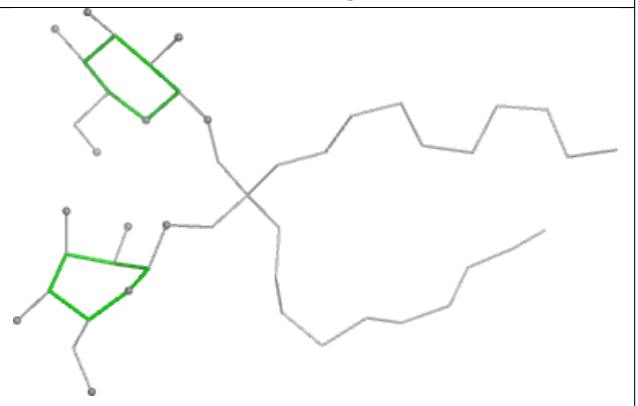
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Bond angles

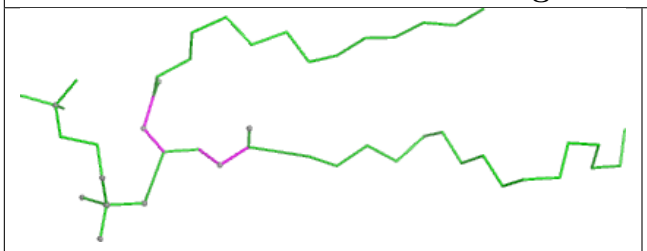


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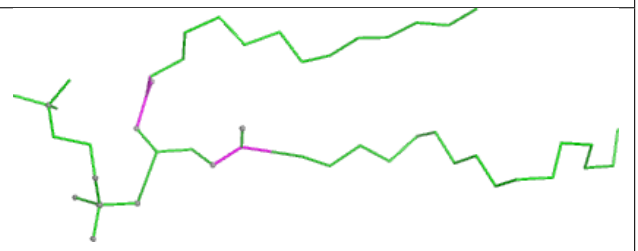


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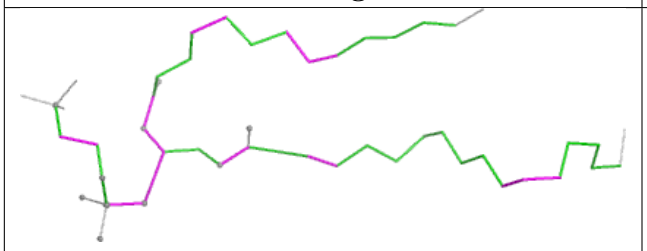
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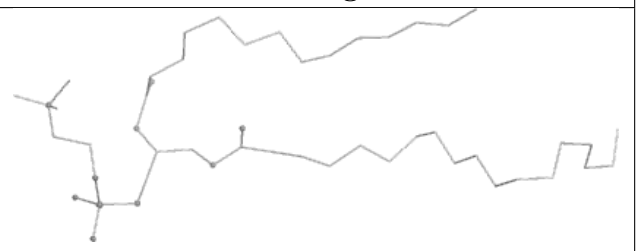
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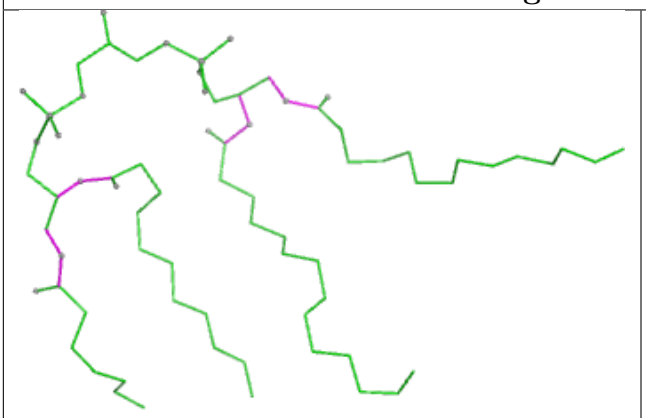


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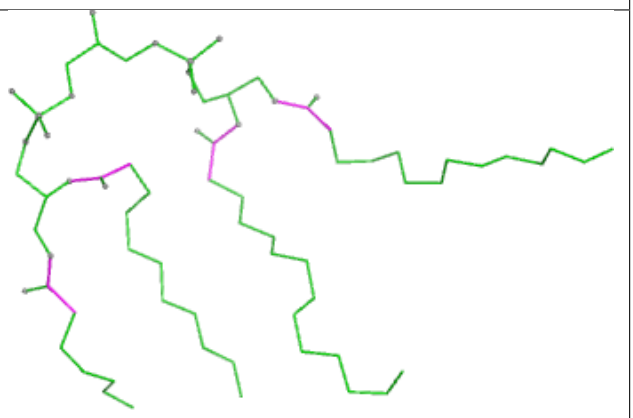


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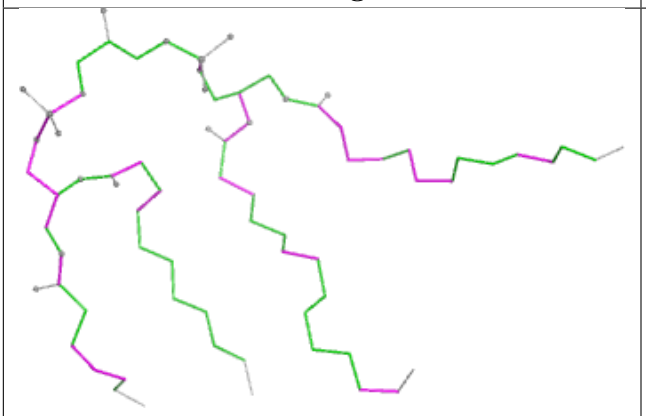
Ligand CDL D 101



Bond lengths



Bond angles

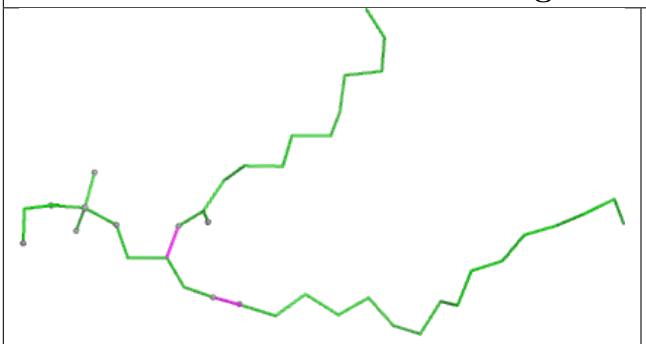


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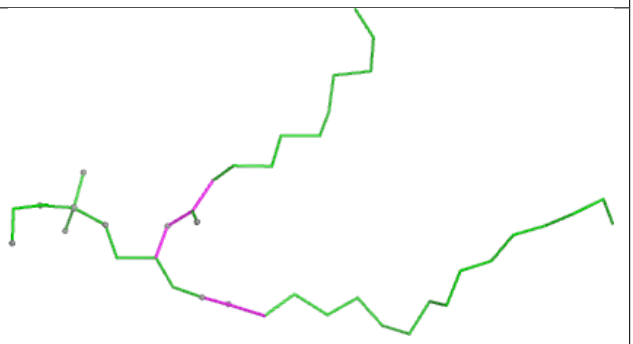


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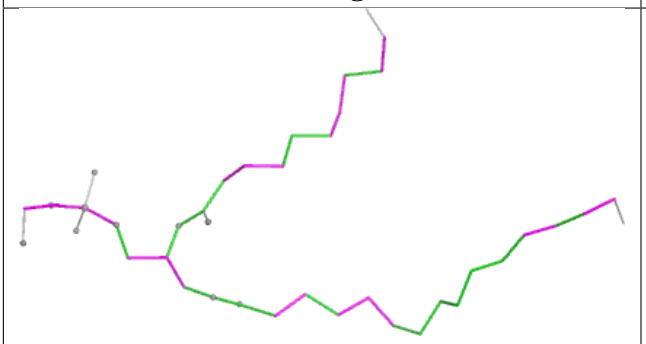
Ligand 3PE I 303



Bond lengths



Bond angles

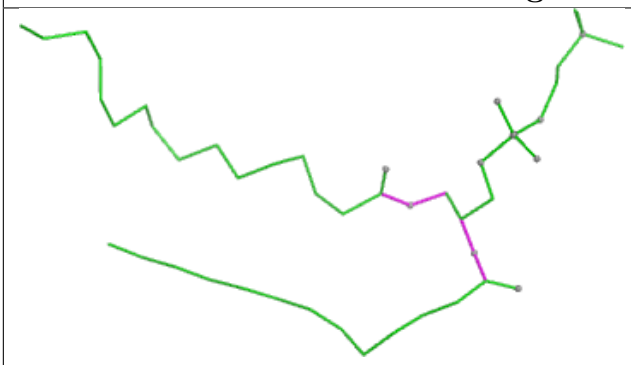


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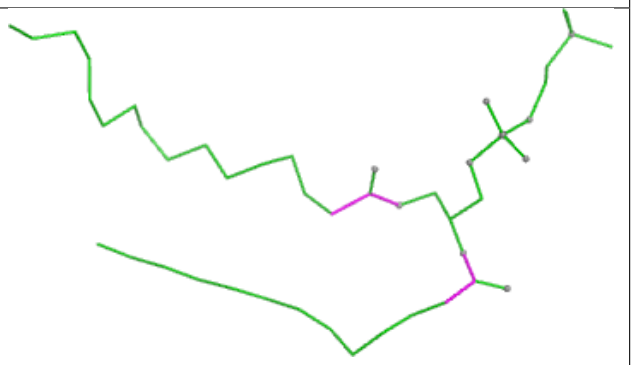


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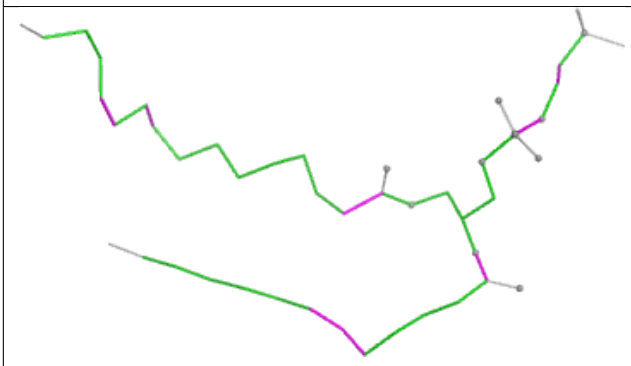
Ligand PC1 K 302



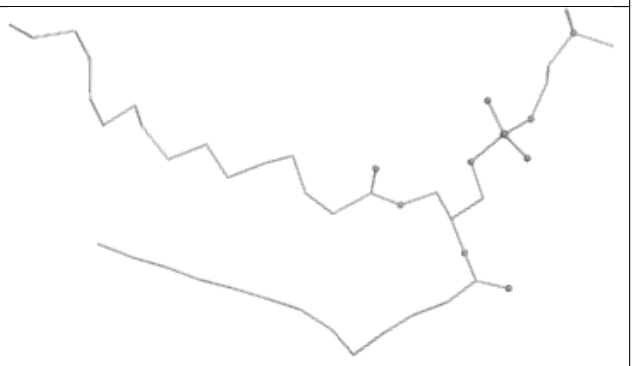
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Bond angles

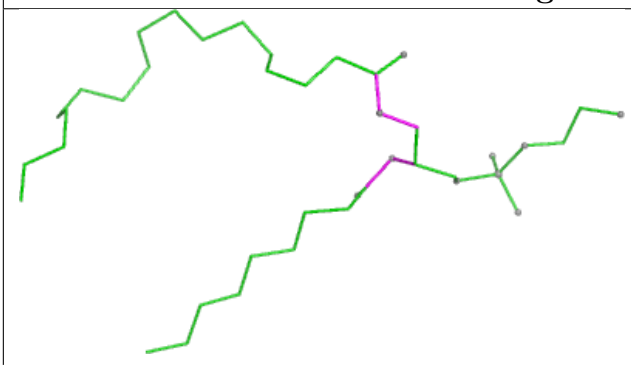


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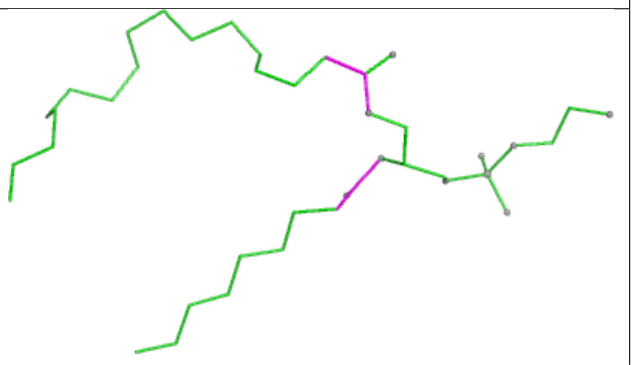


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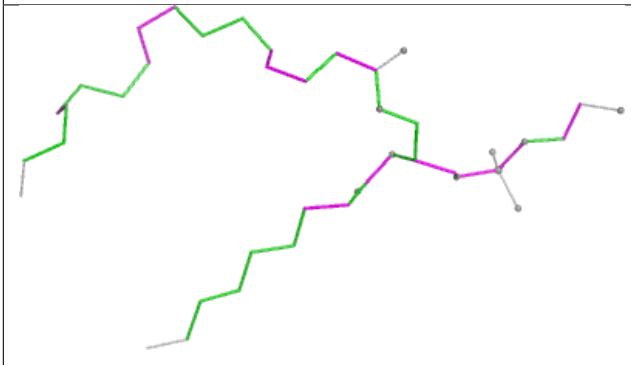
Ligand 3PE i 102



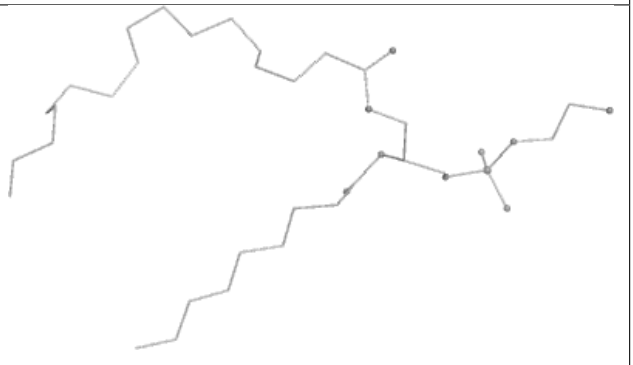
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Bond angles

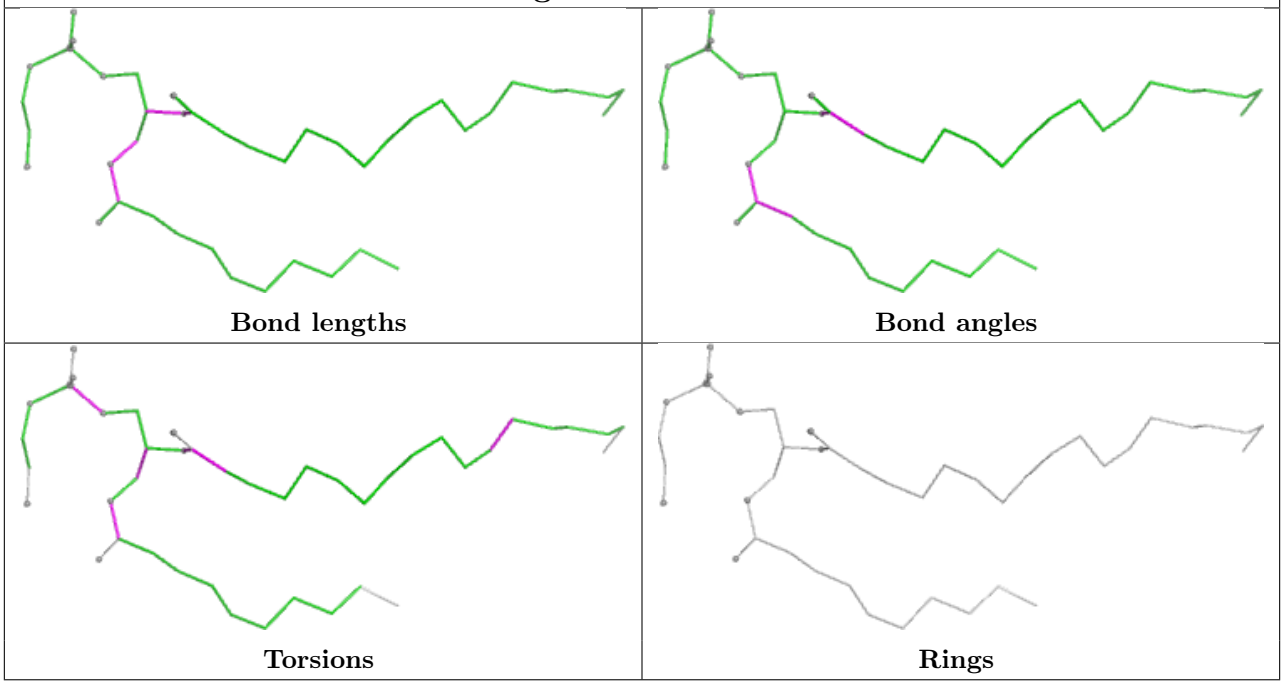


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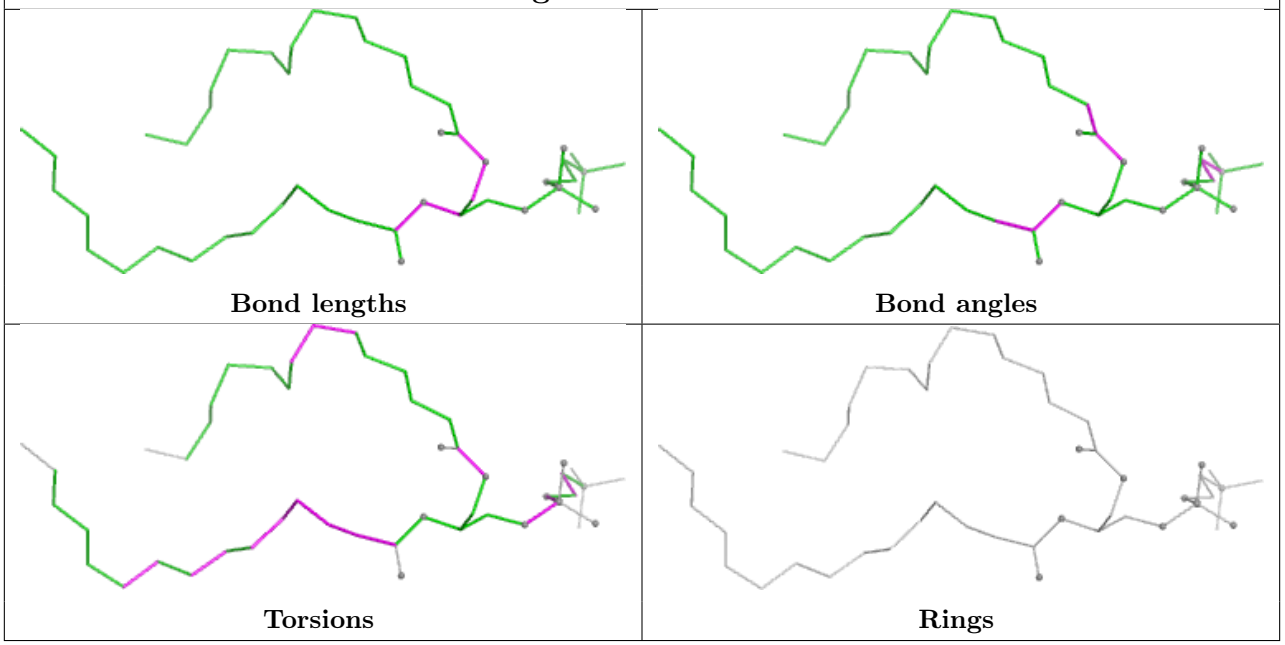


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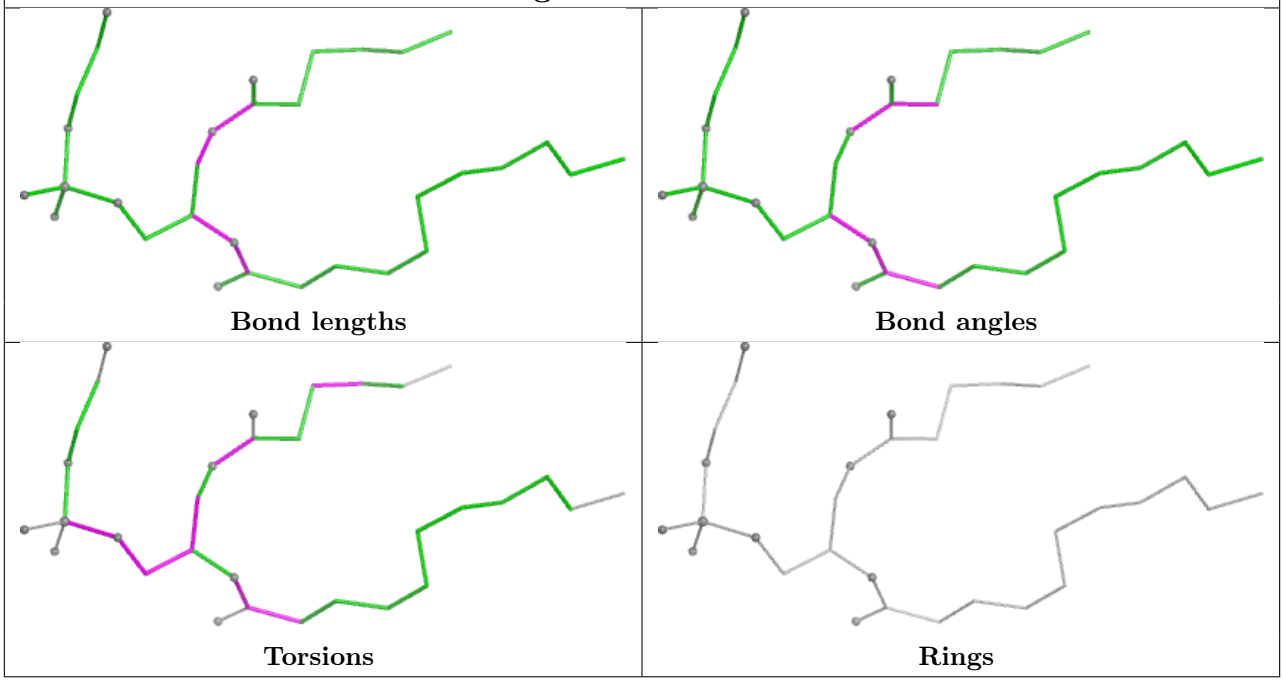
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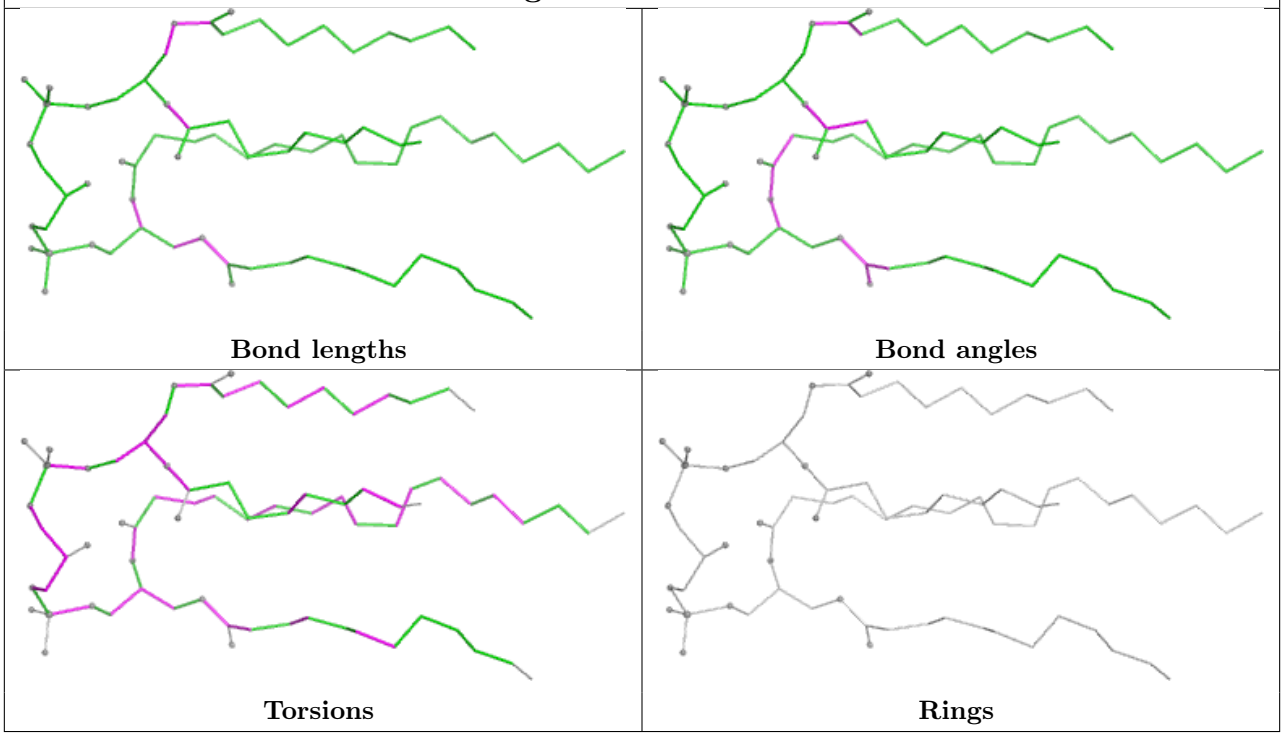
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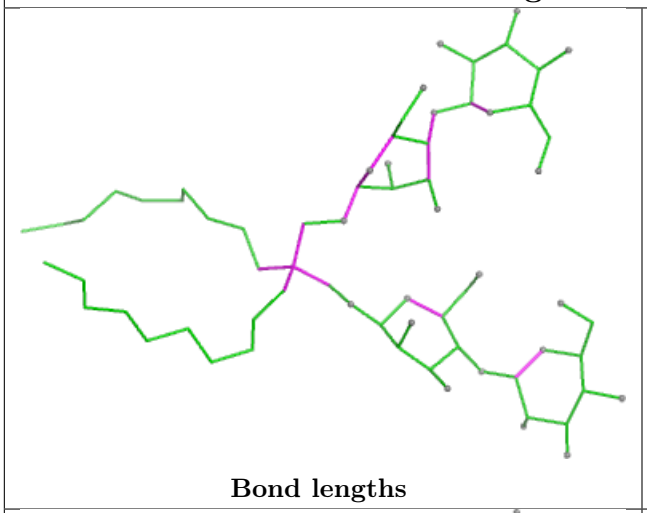
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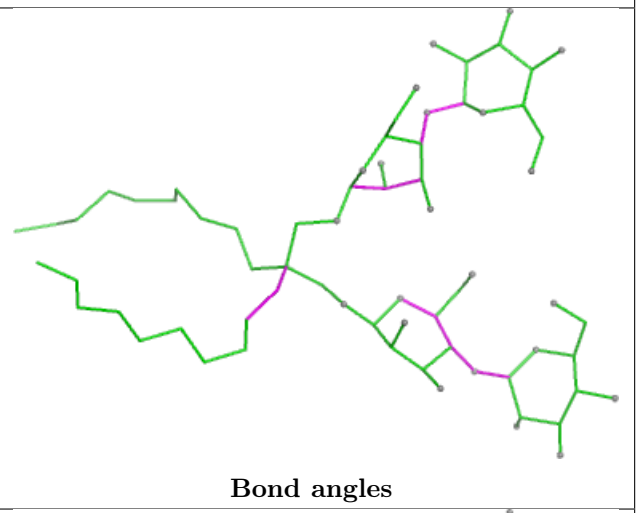
Ligand CDL X 201



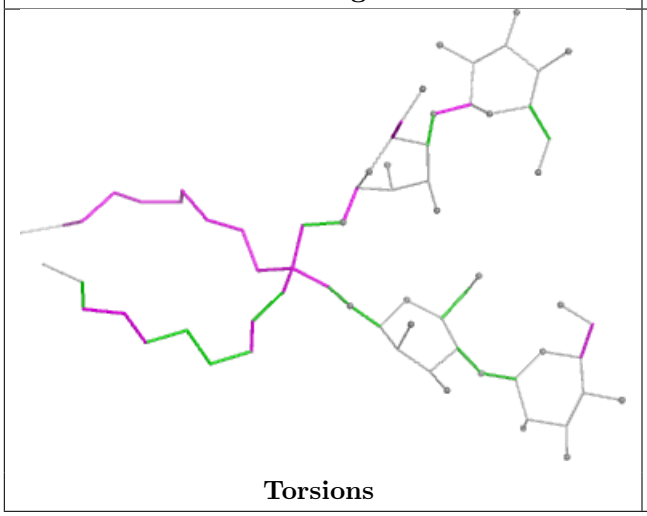
Ligand LMN 5 705



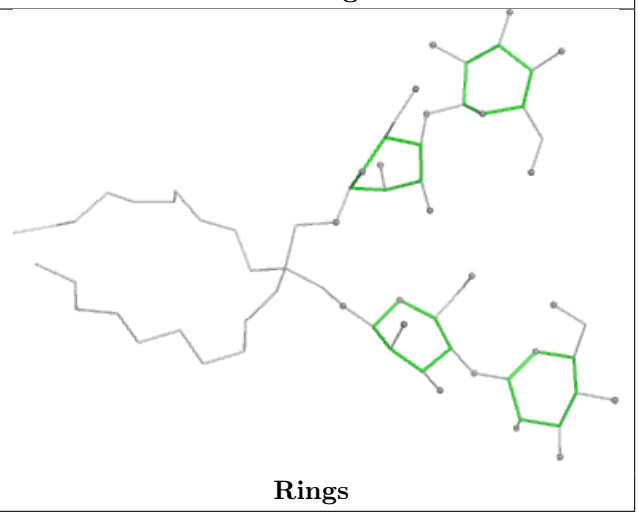
Bond lengths



Bond angles

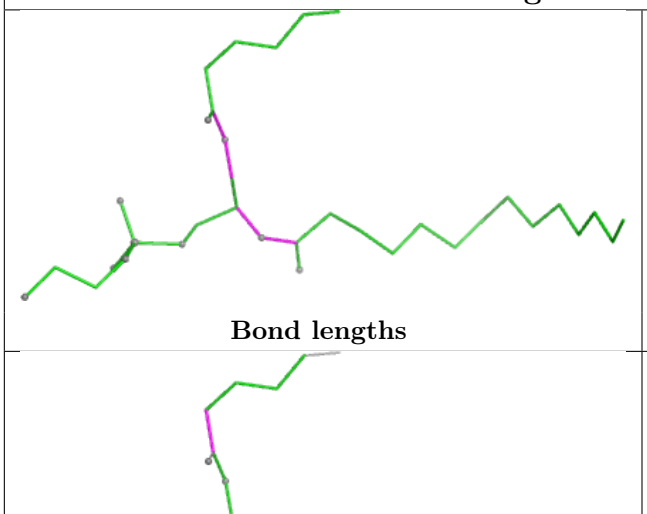


Torsions

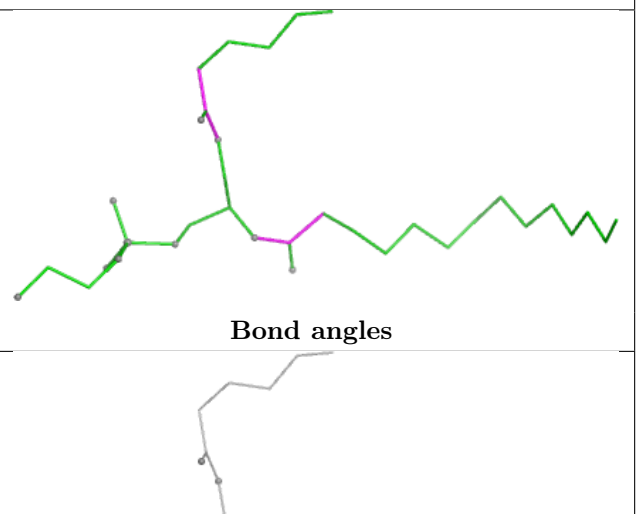


Rings

Ligand 3PE W 201



Bond lengths

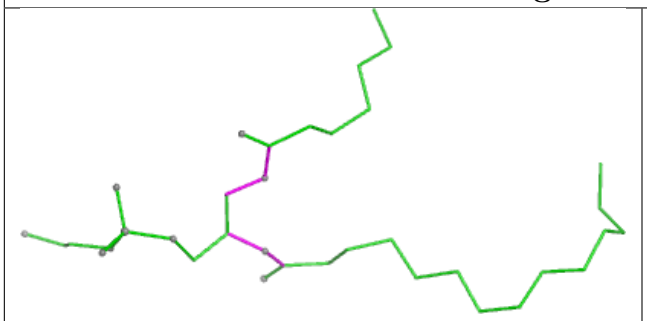


Bond angles

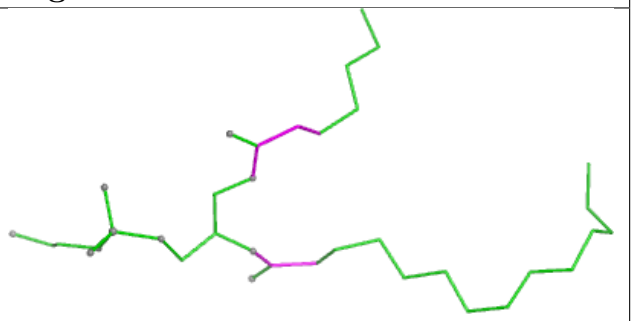
Torsions

Rings

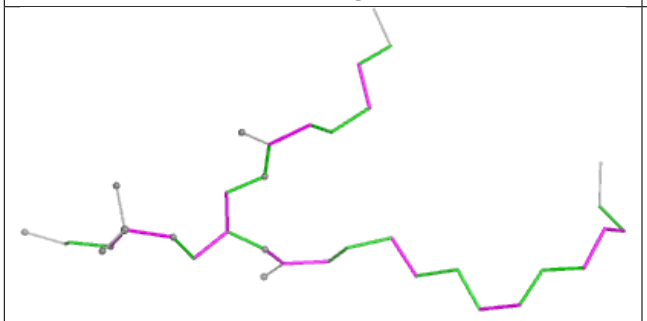
Ligand 3PE g 102



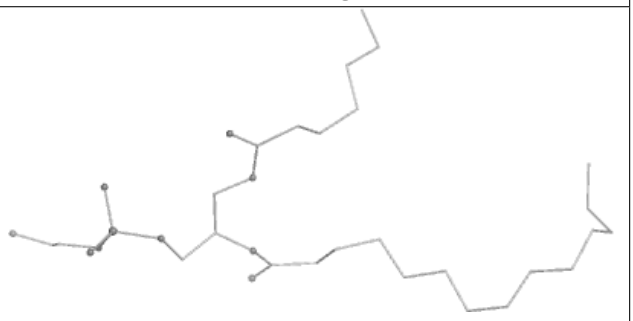
Bond lengths



Bond angles

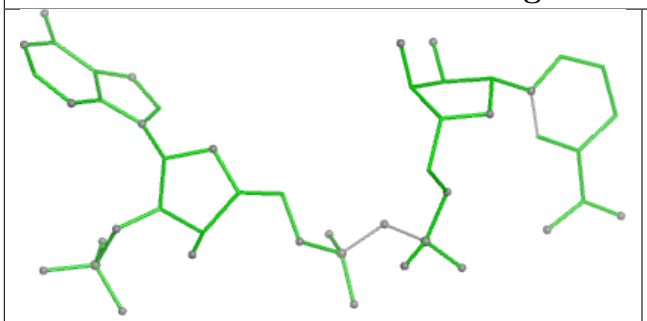


Torsions

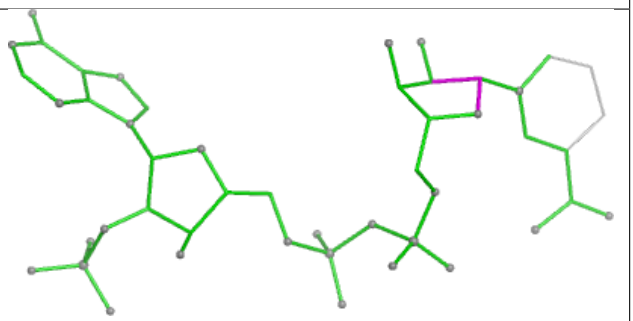


Rings

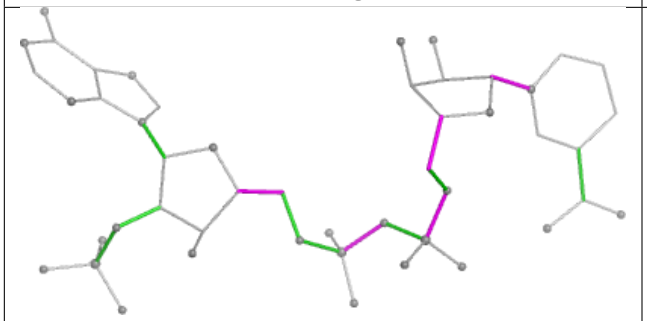
Ligand NDP E 402



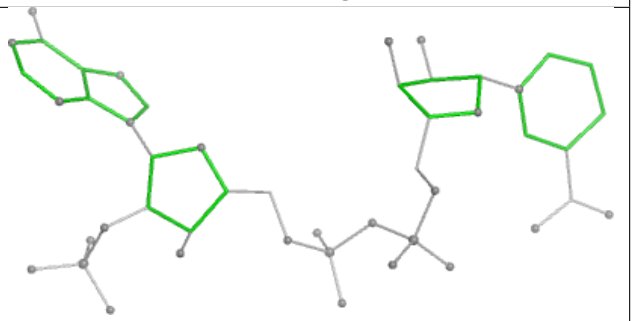
Bond lengths



Bond angles

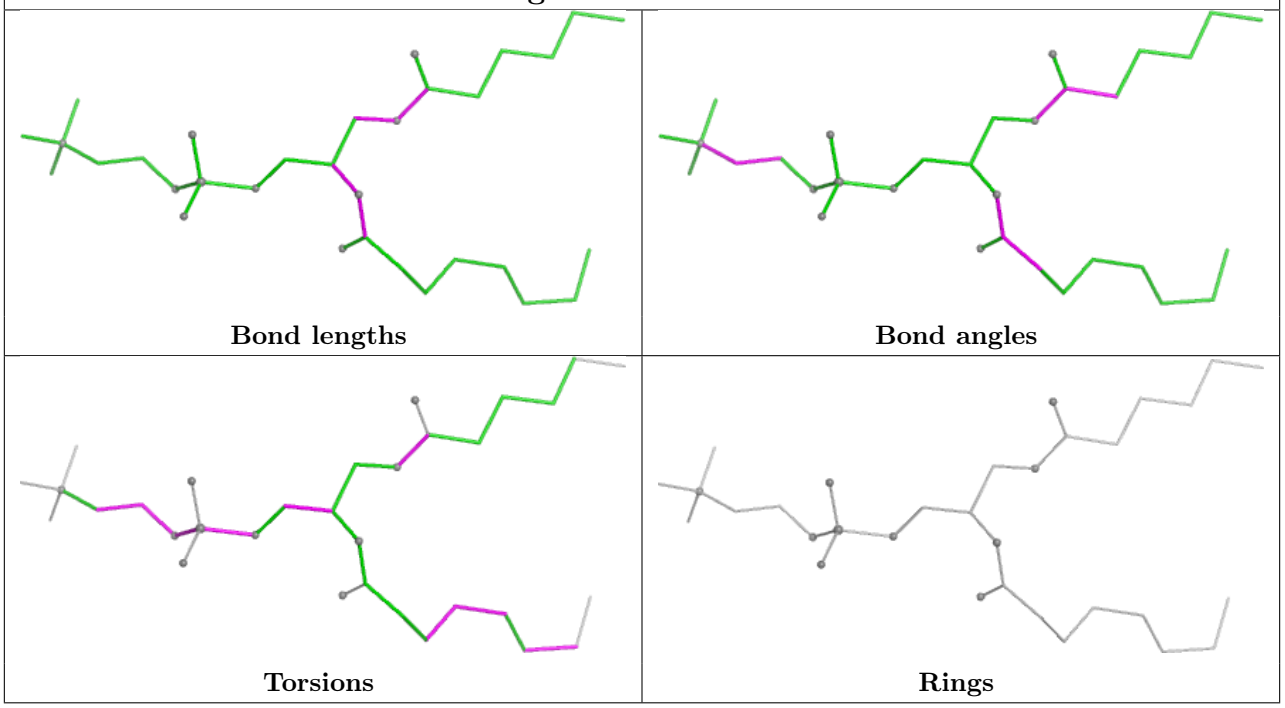


Torsions

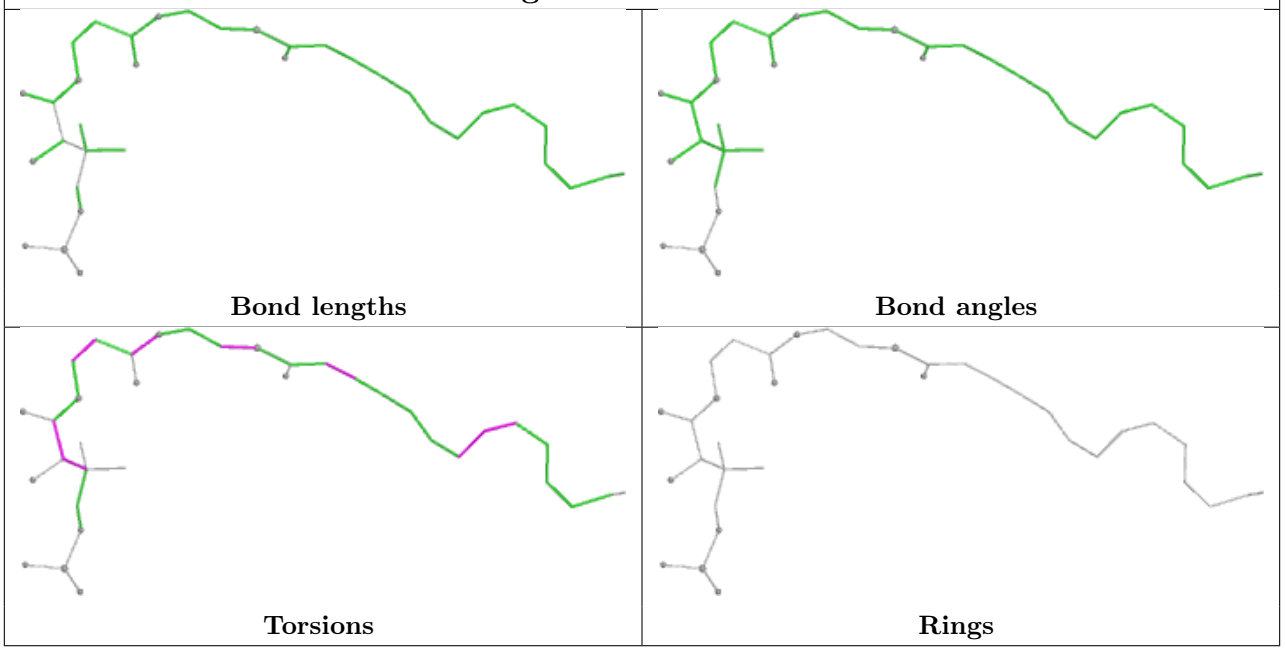


Rings

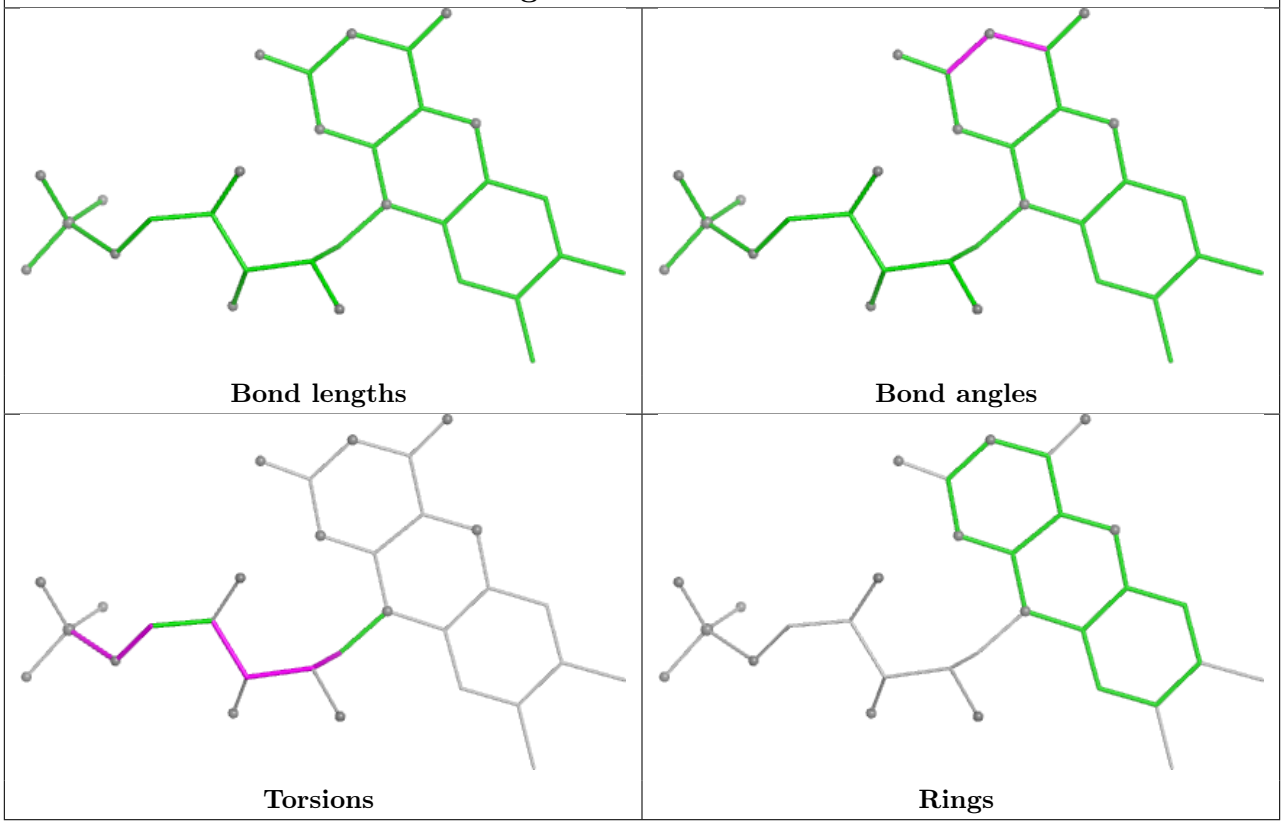
Ligand PC1 X 203



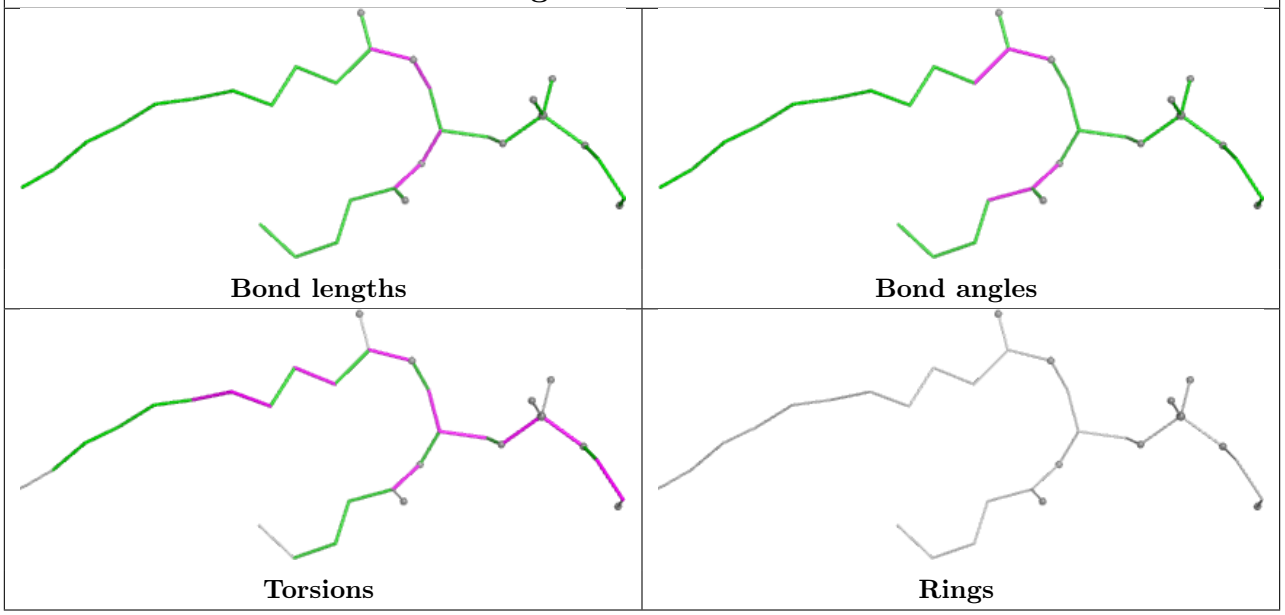
Ligand ZMP O 201



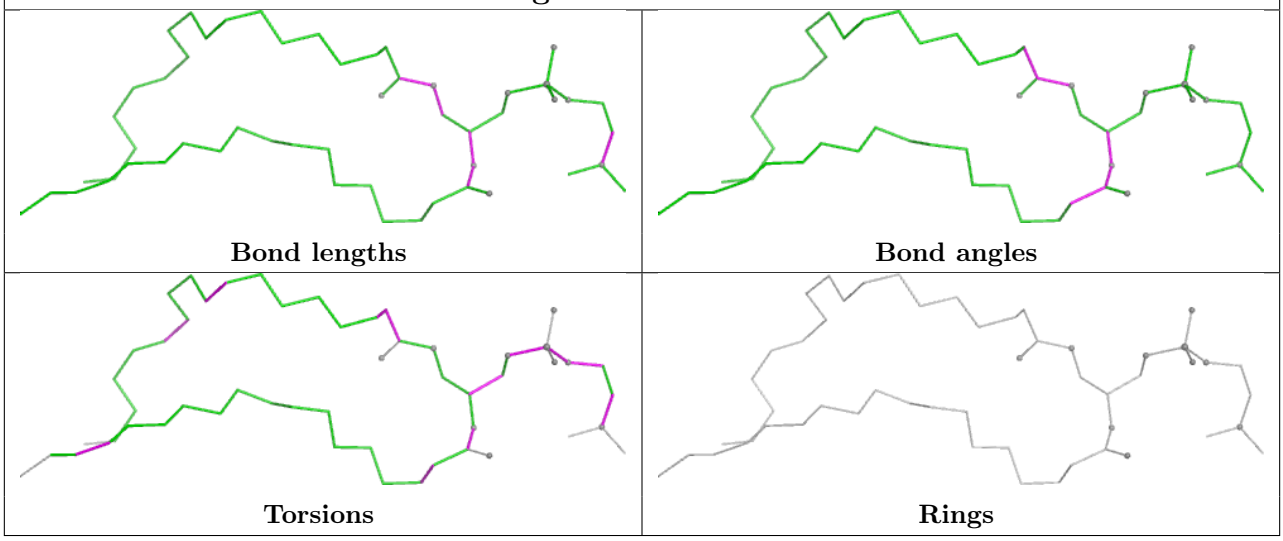
Ligand FMN B 602



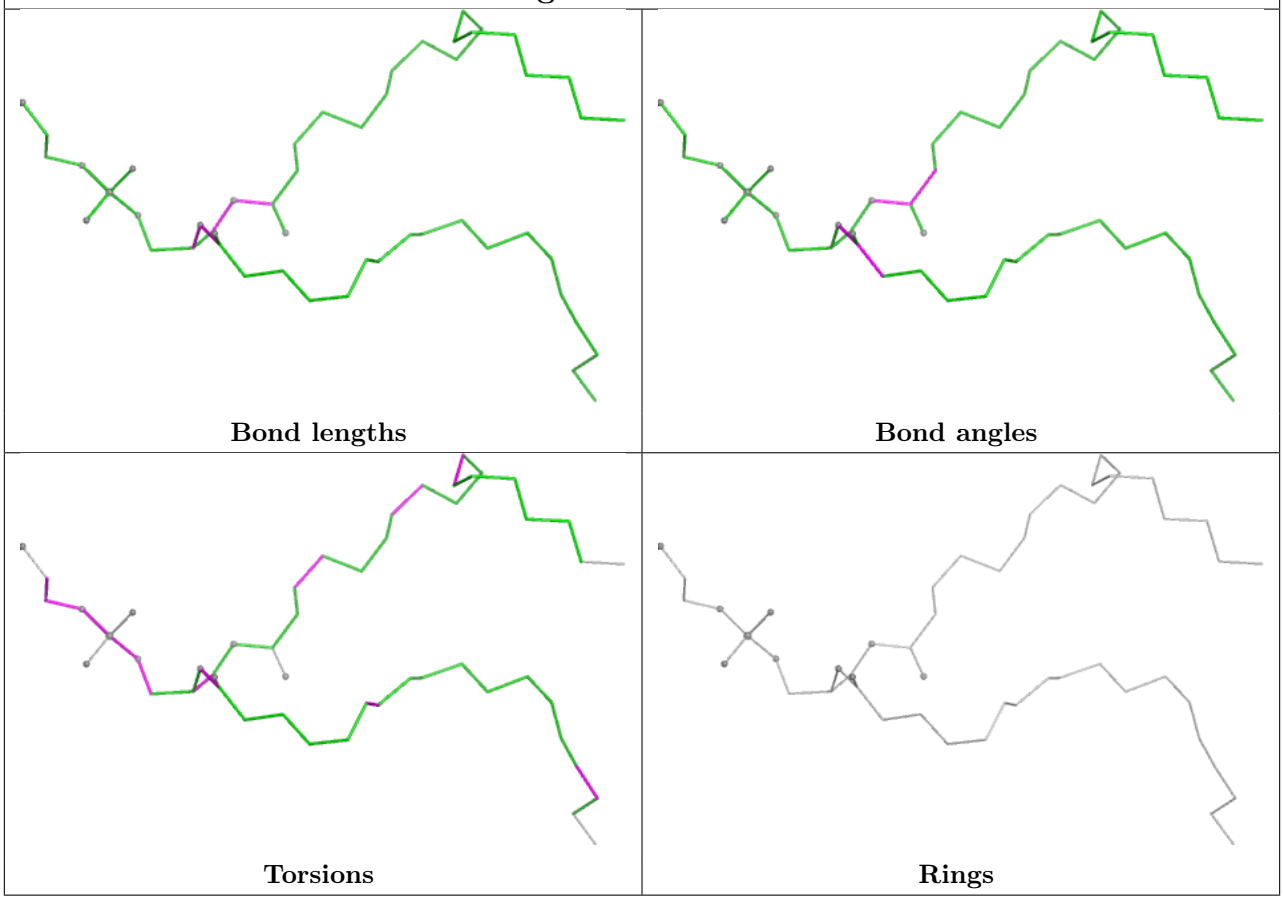
Ligand 3PE E 401



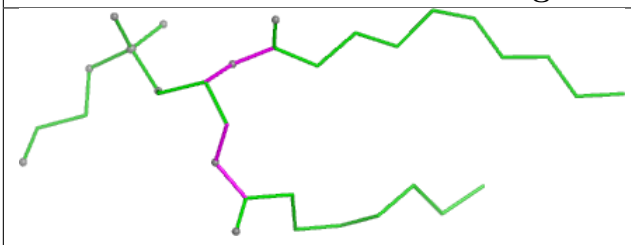
Ligand PC1 5 701



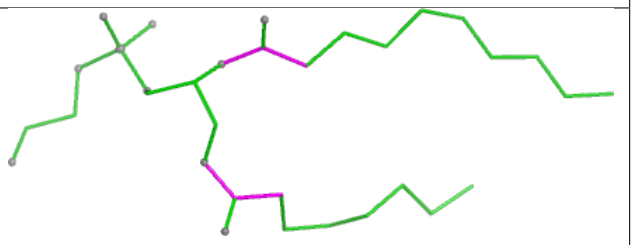
Ligand 3PE i 101



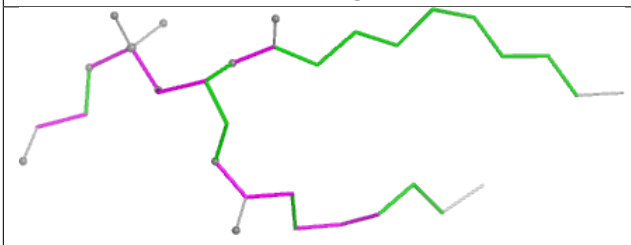
Ligand 3PE 4 602



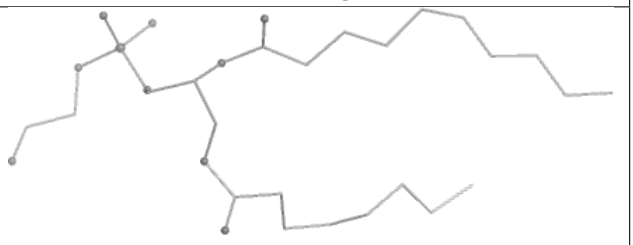
Bond lengths



Bond angles

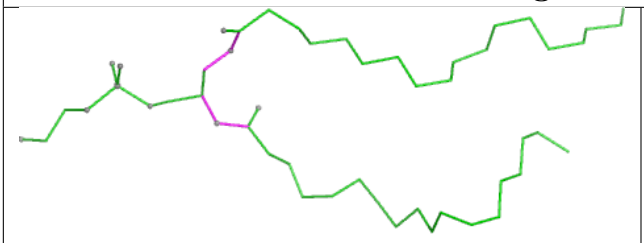


Torsions

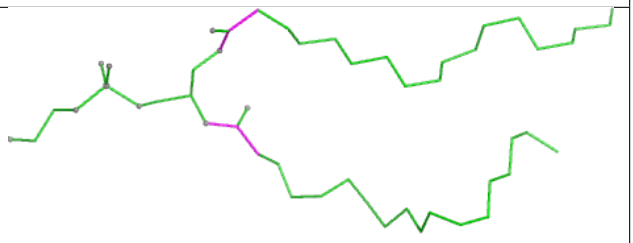


Rings

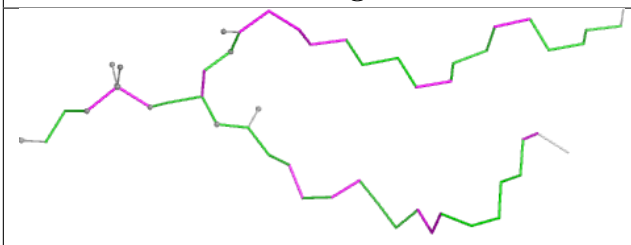
Ligand 3PE 4 601



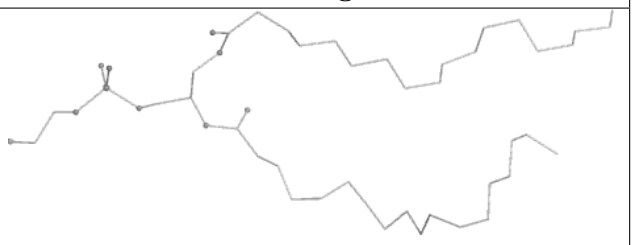
Bond lengths



Bond angles

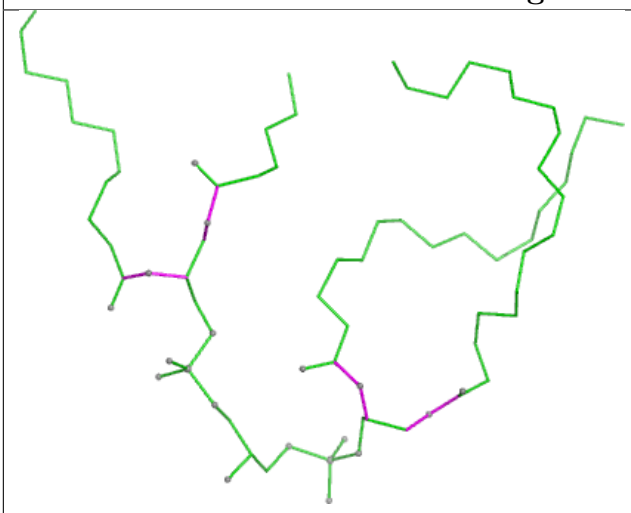


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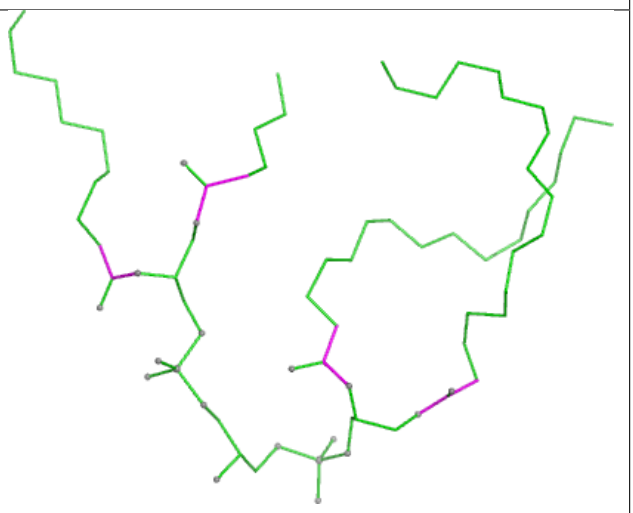


Rings

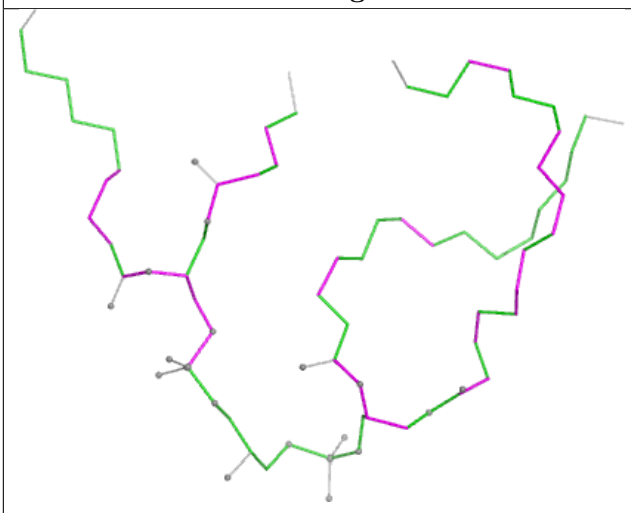
Ligand CDL S 201



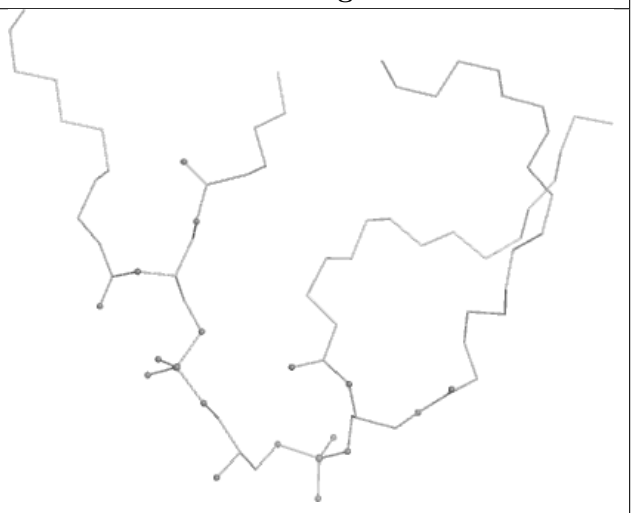
Bond lengths



Bond angles

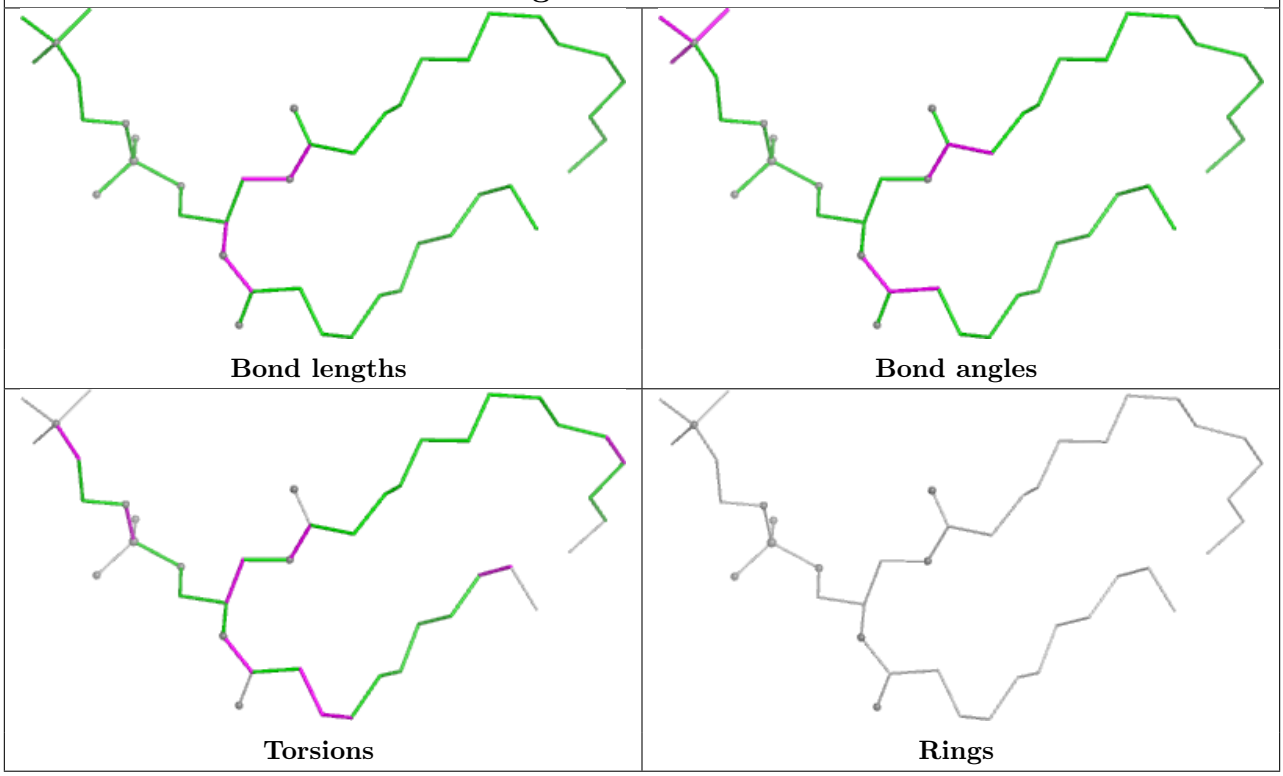


Torsions

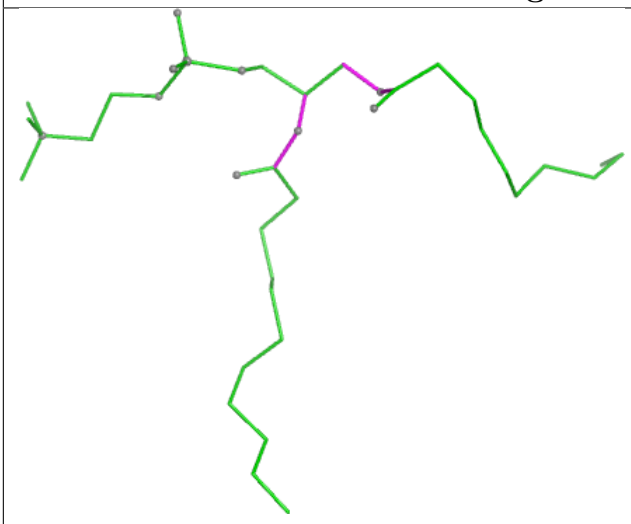


Rings

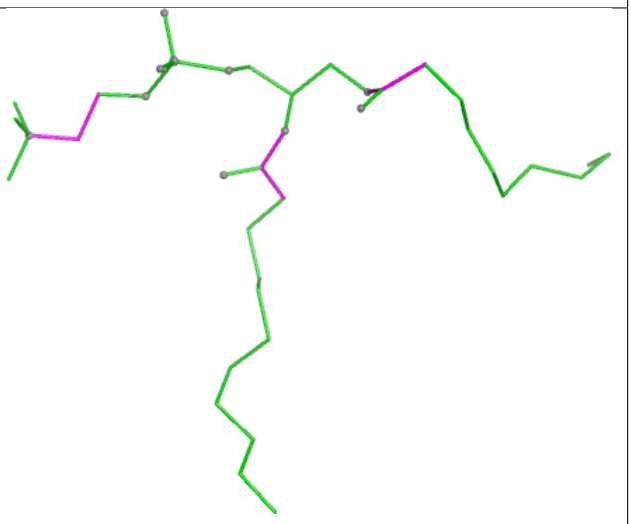
Ligand PC1 1 402



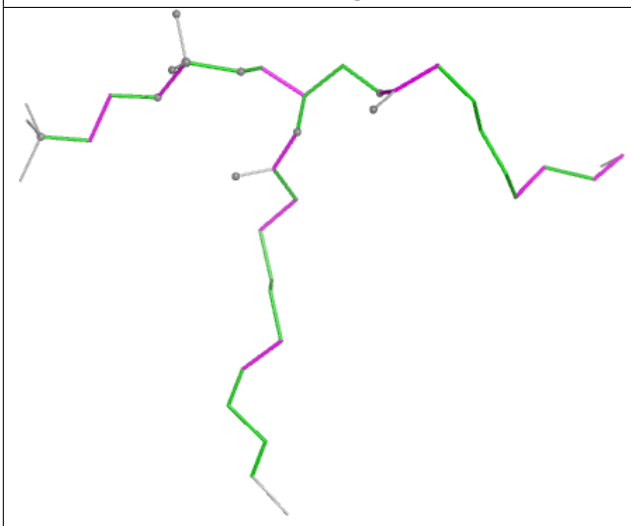
Ligand PC1 X 202



Bond lengths



Bond angles

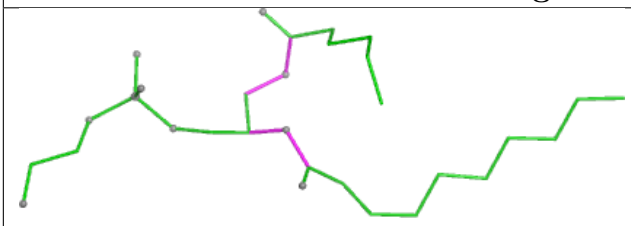


Torsions

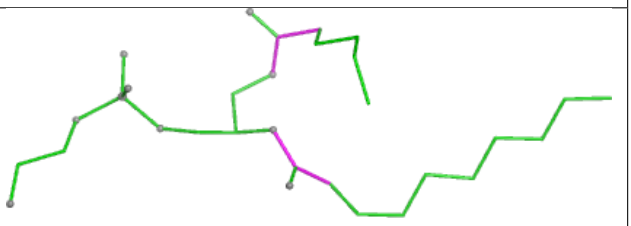


Rings

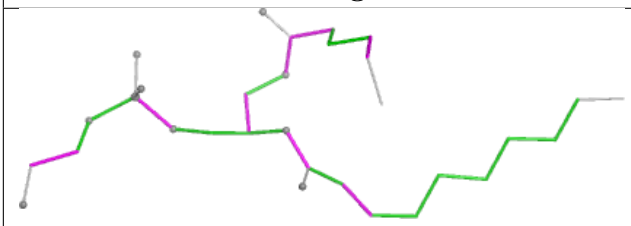
Ligand 3PE 5 702



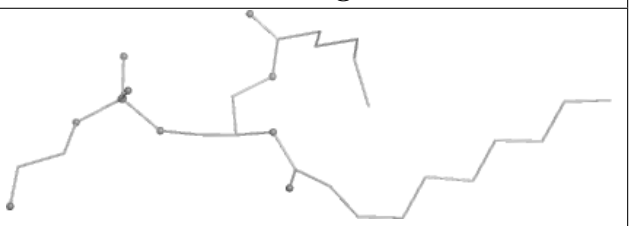
Bond lengths



Bond angles

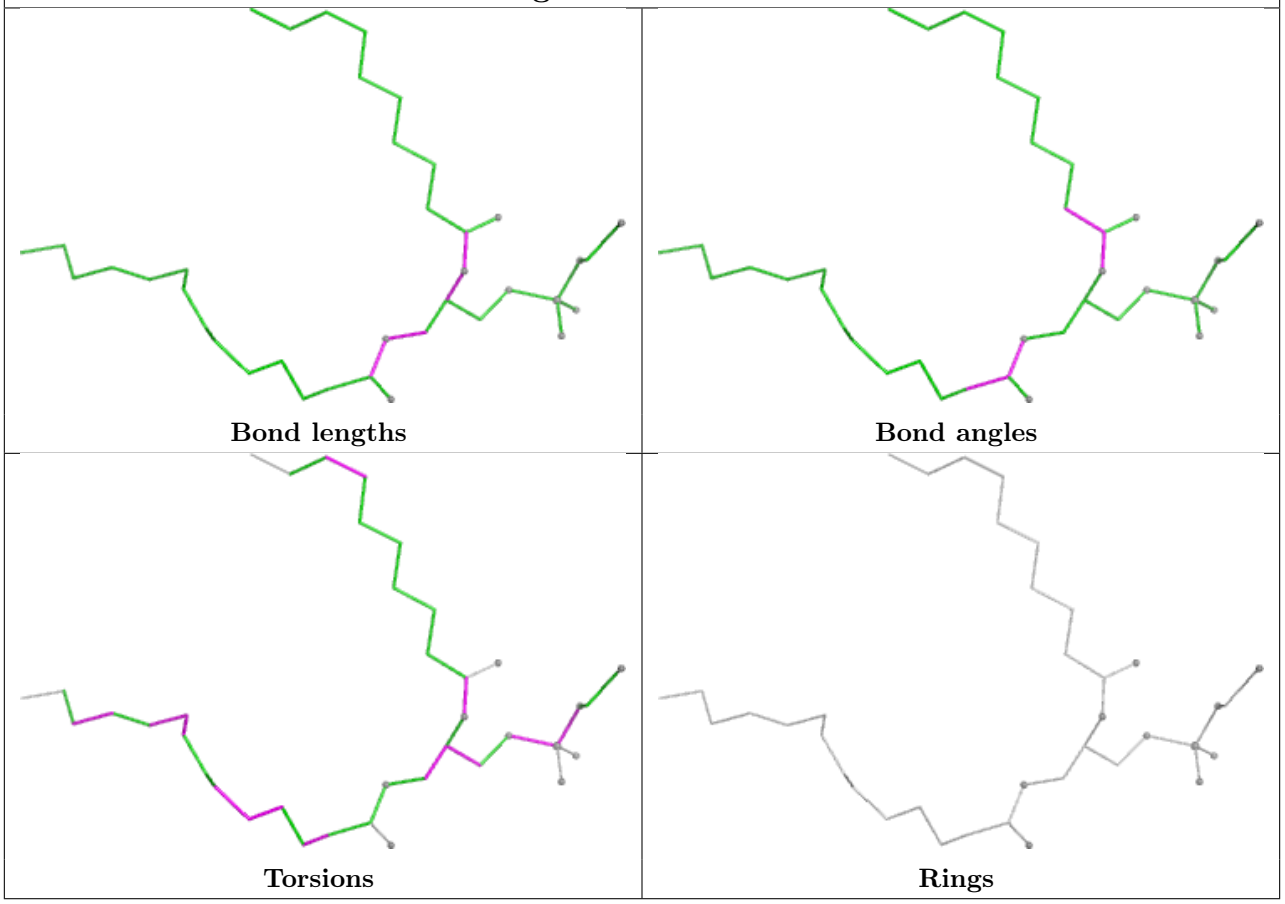


Torsions



Rings

Ligand 3PE n 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

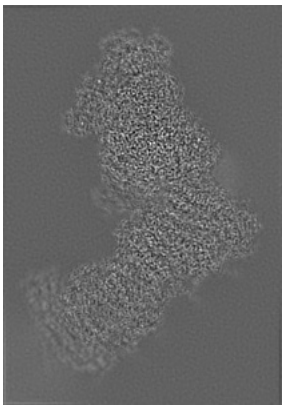
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14797. These allow visual inspection of the internal detail of the map and identification of artifacts.

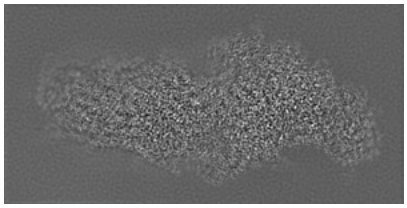
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

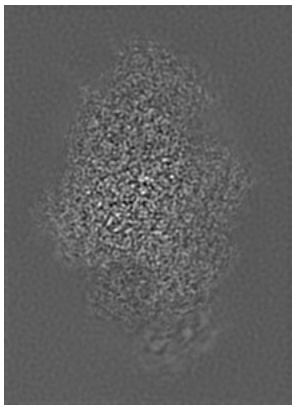
6.1.1 Primary map



X

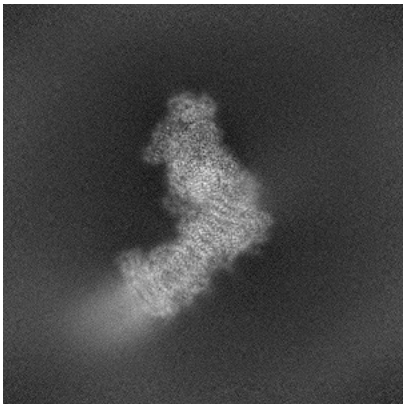


Y

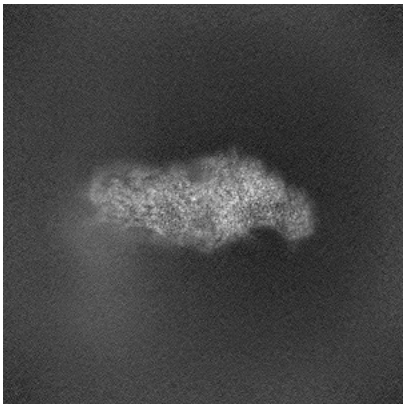


Z

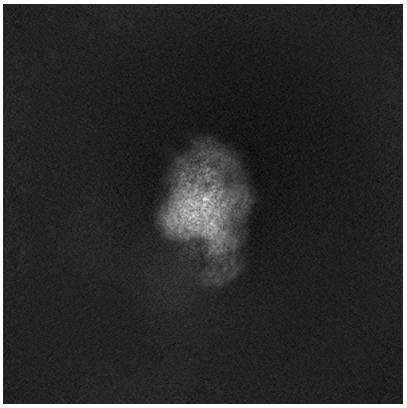
6.1.2 Raw map



X



Y

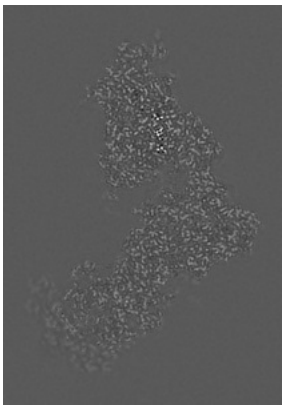


Z

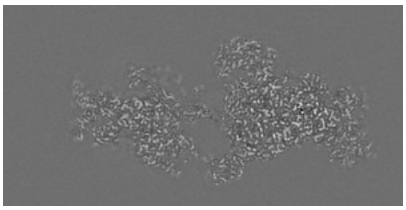
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

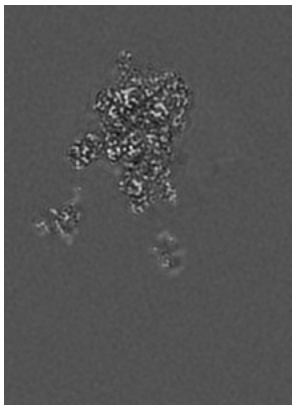
6.2.1 Primary map



X Index: 95

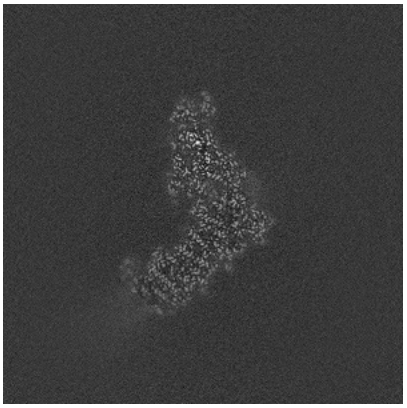


Y Index: 132

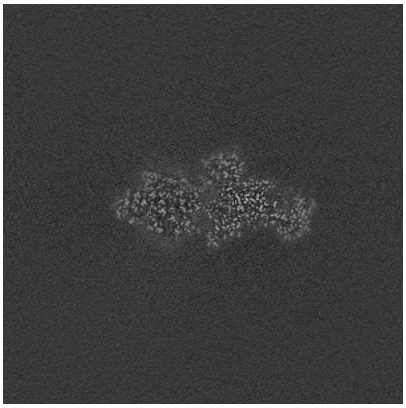


Z Index: 191

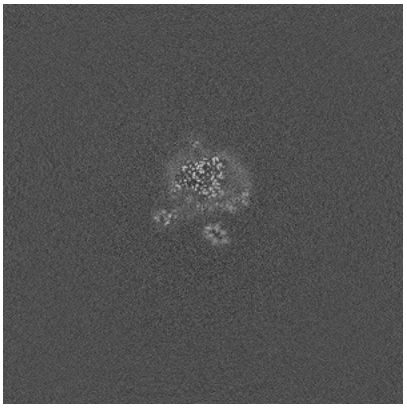
6.2.2 Raw map



X Index: 294



Y Index: 294



Z Index: 294

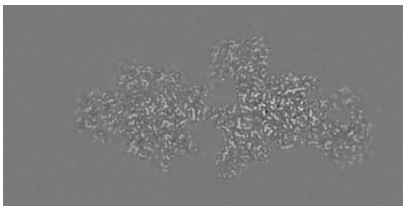
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

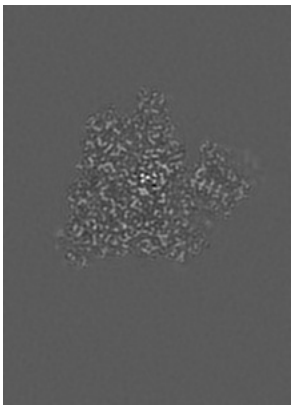
6.3.1 Primary map



X Index: 90

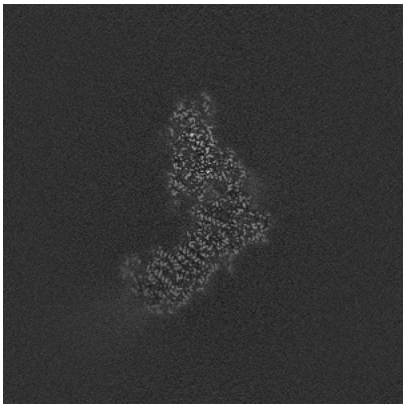


Y Index: 140

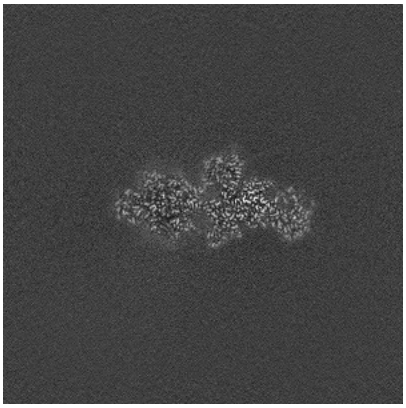


Z Index: 245

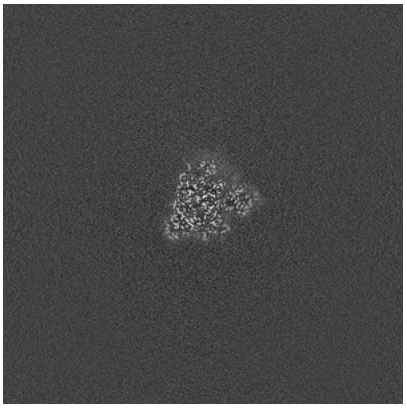
6.3.2 Raw map



X Index: 296



Y Index: 292

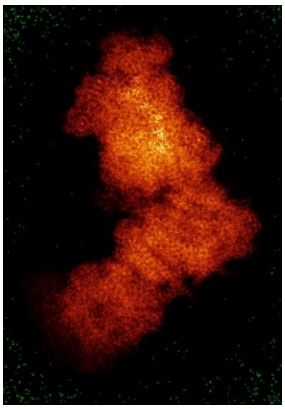


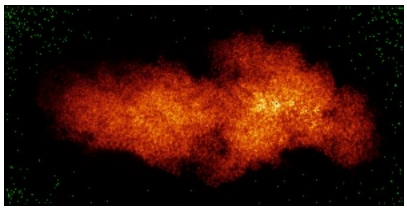
Z Index: 337

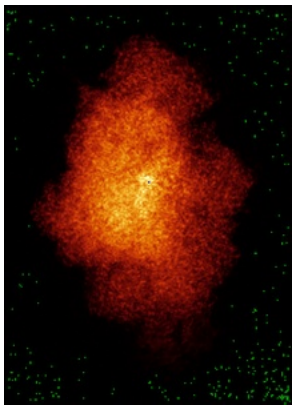
The images above show the largest variance slices of the map in three orthogonal directions.

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

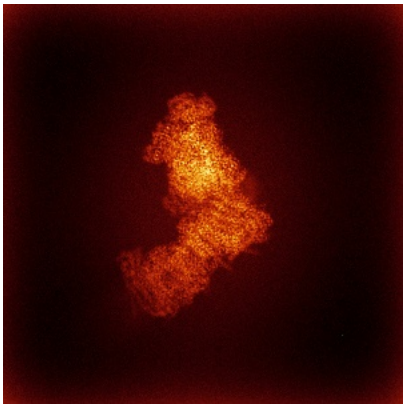
6.4.1 Primary map

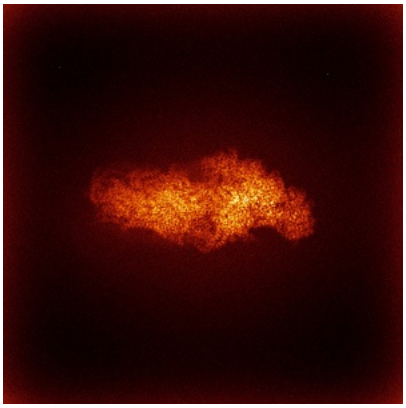

X

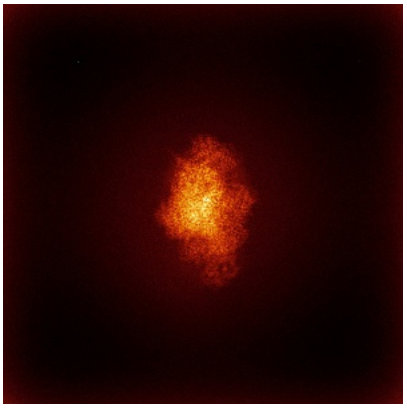

Y


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.

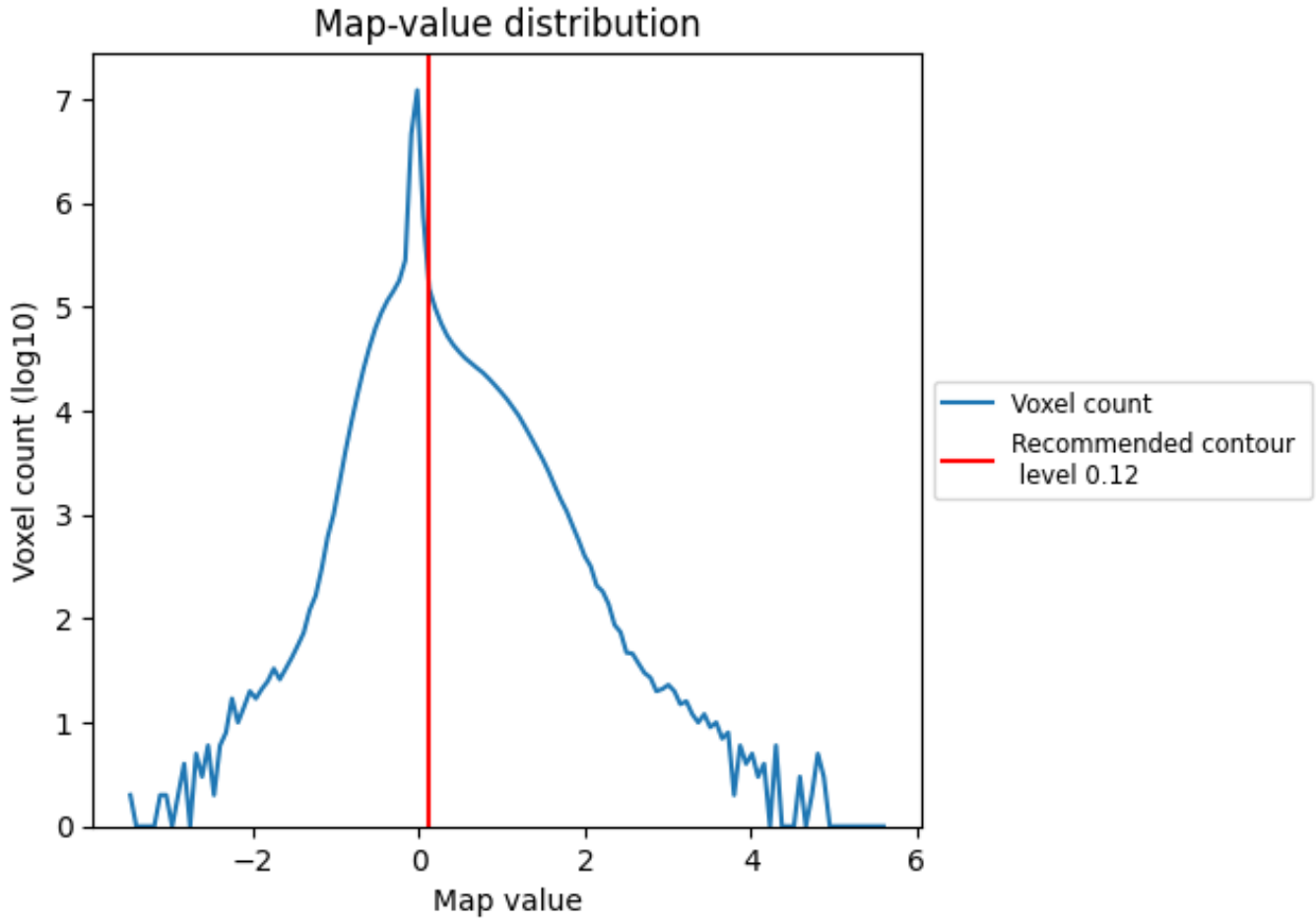
6.6 Mask visualisation (i)

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

7 Map analysis

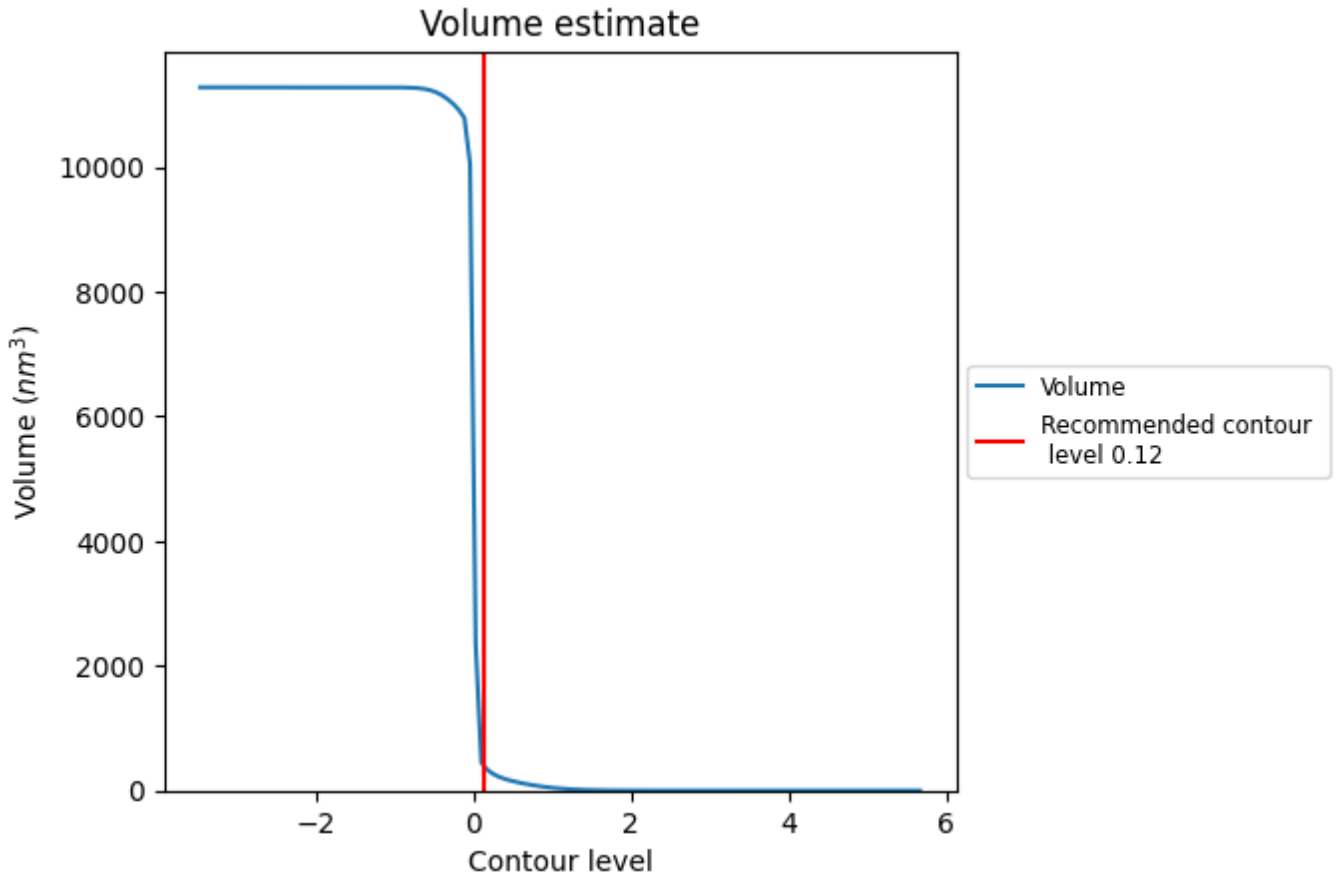
This section contains the results of statistical analysis of the map.

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 410 nm^3; this corresponds to an approximate mass of 370 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.

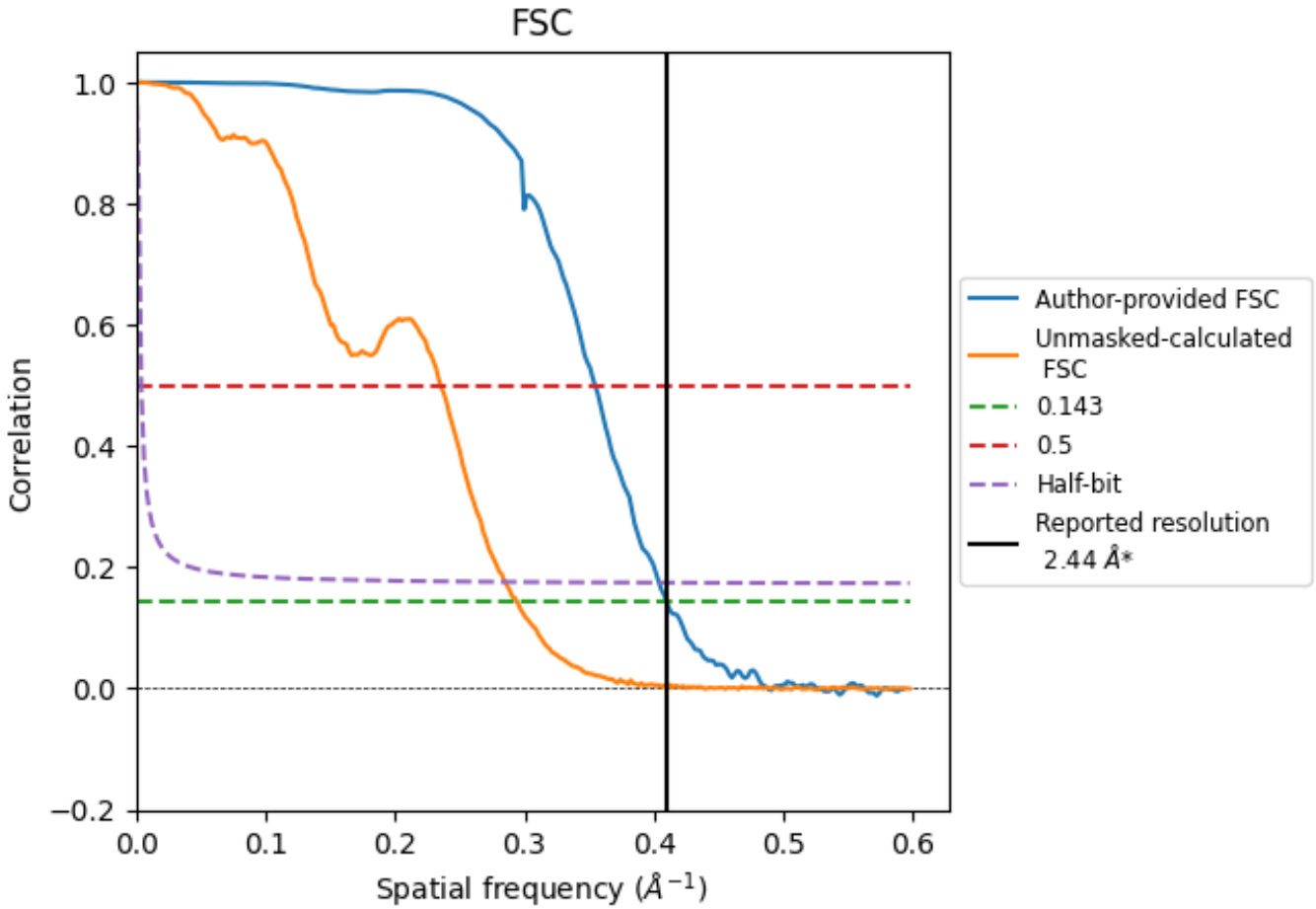
7.3 Rotationally averaged power spectrum (i)

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 0.410 Å^{-1}

8.2 Resolution estimates (i)

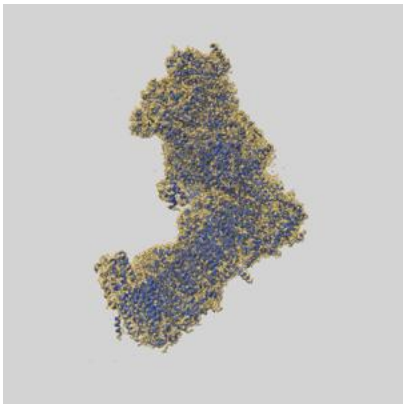
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.82	2.48
Unmasked-calculated*	3.40	4.25	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.44 by more than 10 %

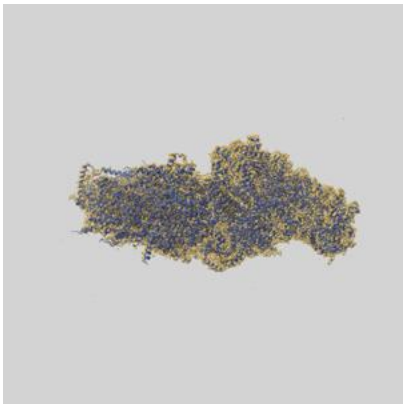
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14797 and PDB model 7ZMG. Per-residue inclusion information can be found in section 3 on page 25.

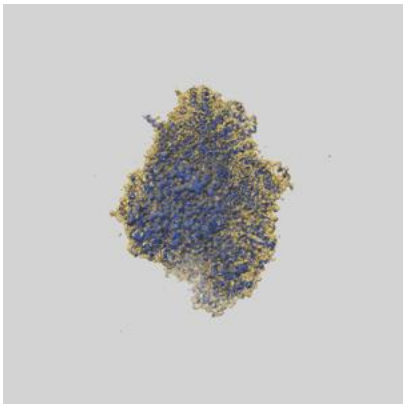
9.1 Map-model overlay



X



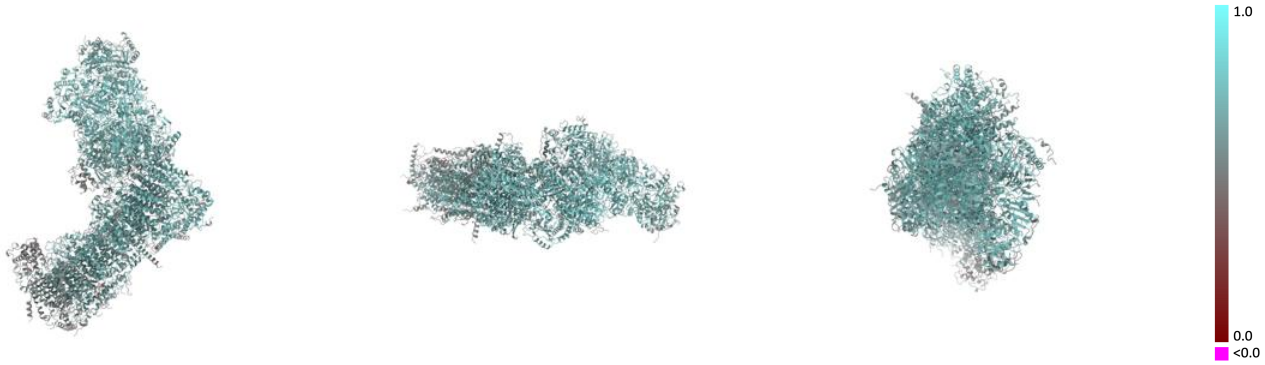
Y



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.

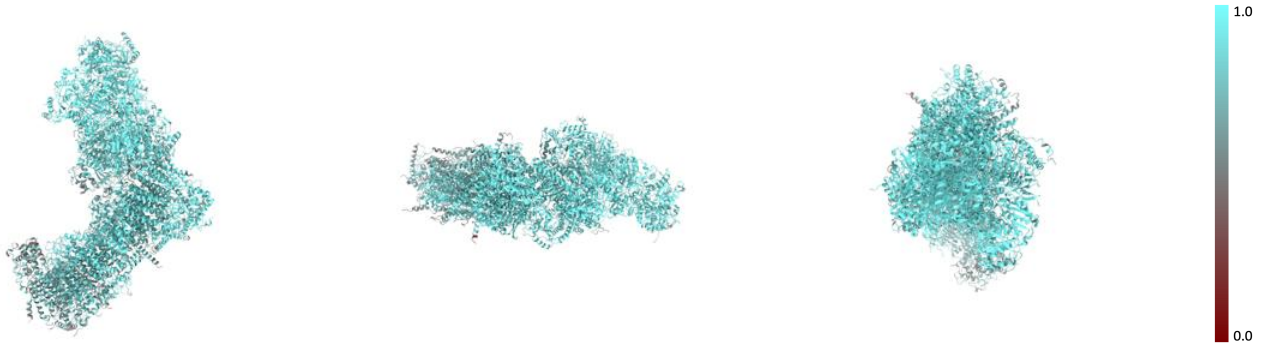
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

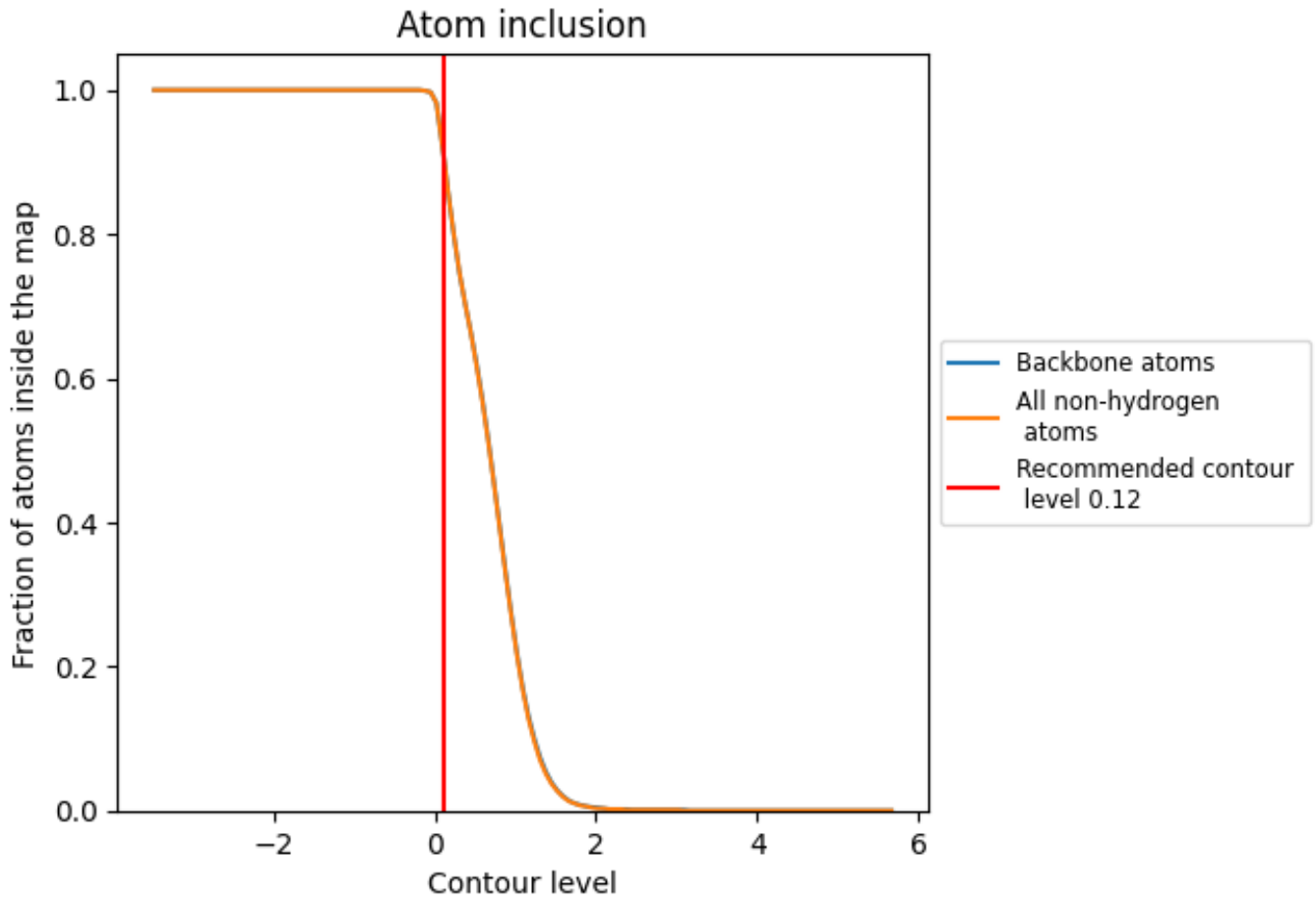
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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	0.9020	0.6670
1	0.9500	0.7140
2	0.9650	0.7240
3	0.8970	0.6640
4	0.9530	0.6980
5	0.8450	0.6060
6	0.9260	0.6900
8	0.6790	0.5170
9	0.8470	0.6410
A	0.9610	0.7110
B	0.9350	0.6570
C	0.9670	0.7340
D	0.9710	0.7020
E	0.9110	0.6510
F	0.9130	0.6660
G	0.9700	0.7350
H	0.9050	0.6400
I	0.9700	0.7340
J	0.8120	0.5910
K	0.9370	0.7070
L	0.9730	0.7200
M	0.9560	0.7060
O	0.6740	0.4750
P	0.9060	0.6630
Q	0.5660	0.4730
R	0.7140	0.5290
S	0.8150	0.5980
U	0.9430	0.6880
W	0.9240	0.6870
X	0.9200	0.6840
Y	0.9560	0.7180
Z	0.9250	0.6810
a	0.7970	0.5770
b	0.8860	0.6620
c	0.6500	0.5040



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8580	0.6290
e	0.6660	0.5240
f	0.8830	0.6270
g	0.9280	0.6630
h	0.9480	0.7030
i	0.7410	0.5790
j	0.9120	0.6570
n	0.7910	0.6120
o	0.8050	0.5670