wwPDB EM Validation Summary Report

Aug 27, 2026 – 10:32 am BST

PDB ID	:	9SMG / pdb_00009smg
EMDB ID	:	EMD-55031
Title	:	Reduced bovine complex I in lipid nanodisc, NADH-active-altQ10
Authors	:	Chung, I.; Hirst, J.
Deposited on	:	2025-09-08
Resolution	:	2.42 Å(reported)
Based on initial model	:	7QSK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

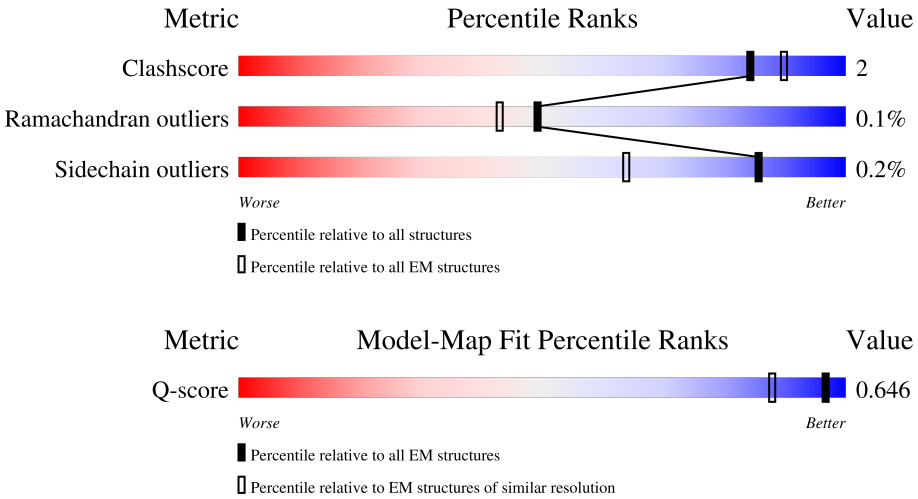
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.42 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	5729 (1.92 - 2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	86% 14%
2	B	216	66% 6% 27%
3	C	266	77% 21%
4	D	463	89% 7%

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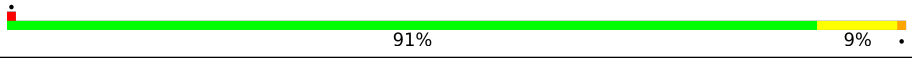
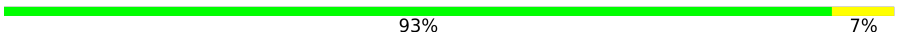
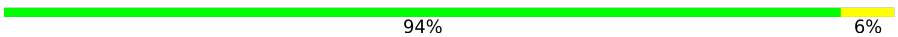
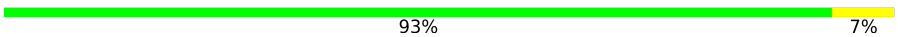
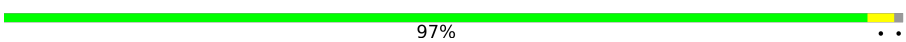
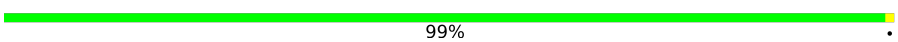
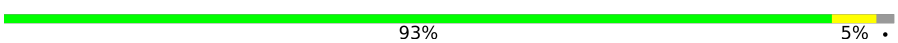
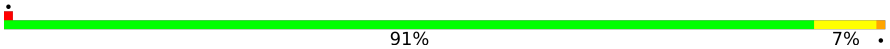
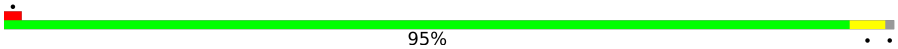
Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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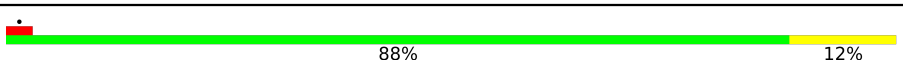
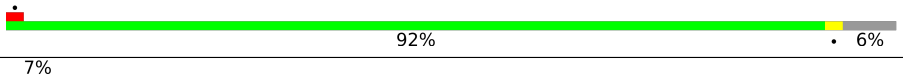
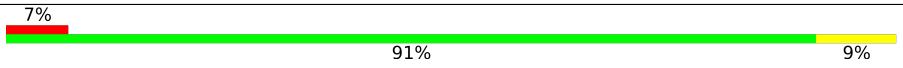
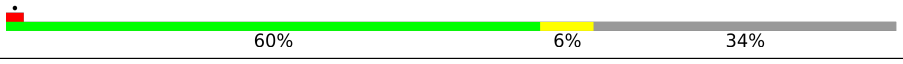
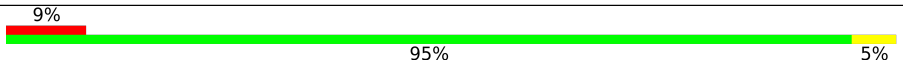
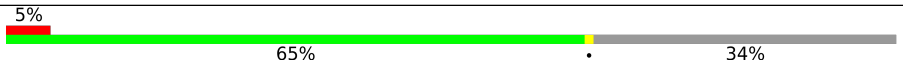
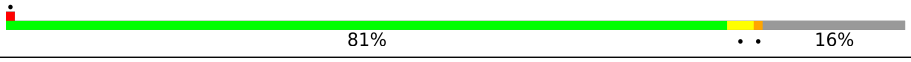
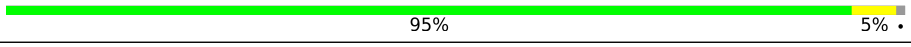
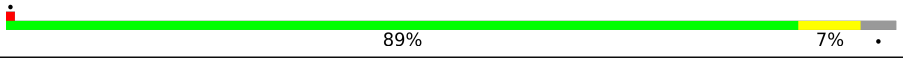
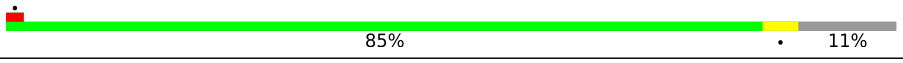
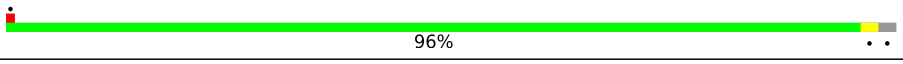
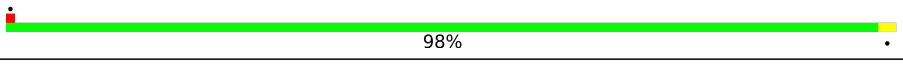
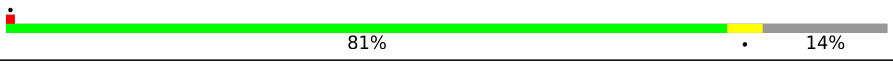
Mol	Chain	Length	Quality of chain
29	d	121	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 70726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	921	622	133	159	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	158	1261	803	227	217	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	209	1738	1120	298	317	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1668	1064	280	314	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	433	Total	C	N	O	S	0	0
			3331	2099	595	617	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	690	Total	C	N	O	S	0	0
			5288	3312	922	1015	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total 740	C 454	N 140	O 143	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total 700	C 440	N 131	O 127	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total 707	C 454	N 104	O 144	S 5	0	0
20	U	88	Total 707	C 454	N 104	O 144	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total 928	C 600	N 157	O 168	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total 976	C 625	N 181	O 166	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total 1402	C 887	N 253	O 252	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	ACE	-	acetylation	UNP Q8HXG6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	121	Total	C	N	O	S	0	0
			999	650	172	172	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	ACE	-	acetylation	UNP Q02827

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	100	Total	C	N	O	S	0	0
			838	528	160	144	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			854	548	141	161	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	143	Total	C	N	O	S	0	0
			1186	776	203	205	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	ACE	-	acetylation	UNP Q02367

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	128	Total	C	N	O	0	0
			1067	684	188	195		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1453	910	268	267	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	97	Total	C	N	O	S	0	0
			785	496	146	140	3		

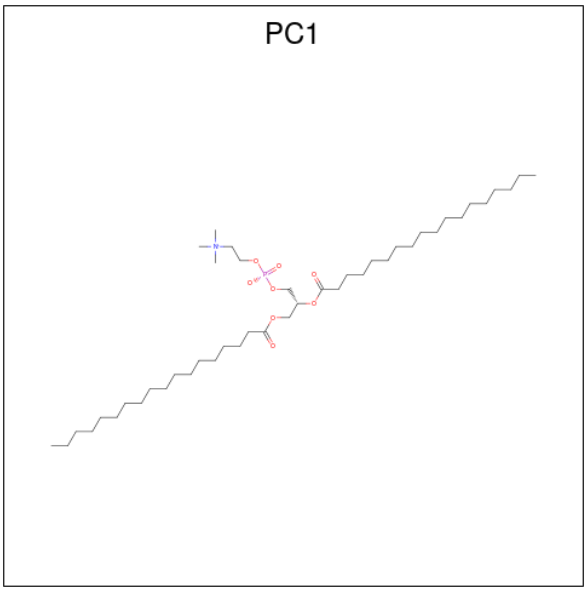
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	1	ACE	-	acetylation	UNP Q05752

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

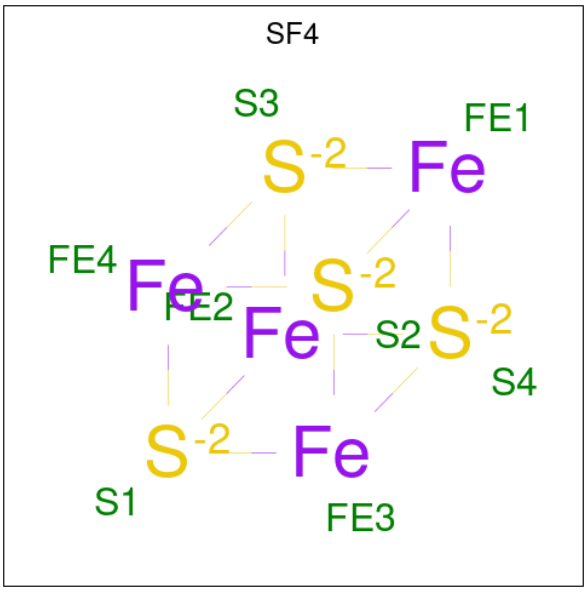
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



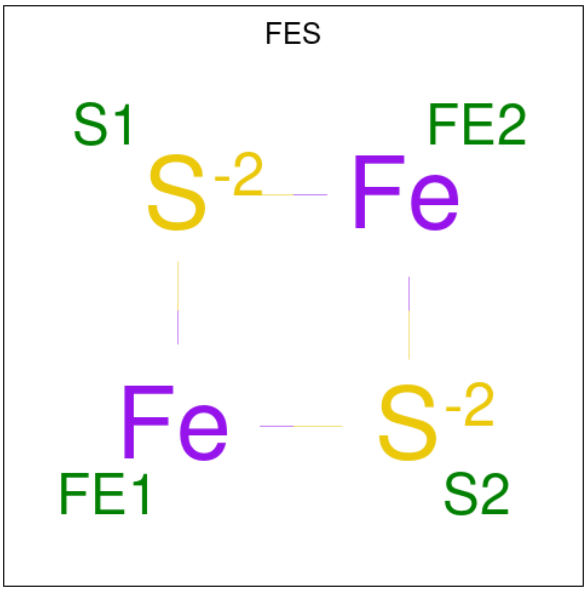
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	I	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	P	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	h	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



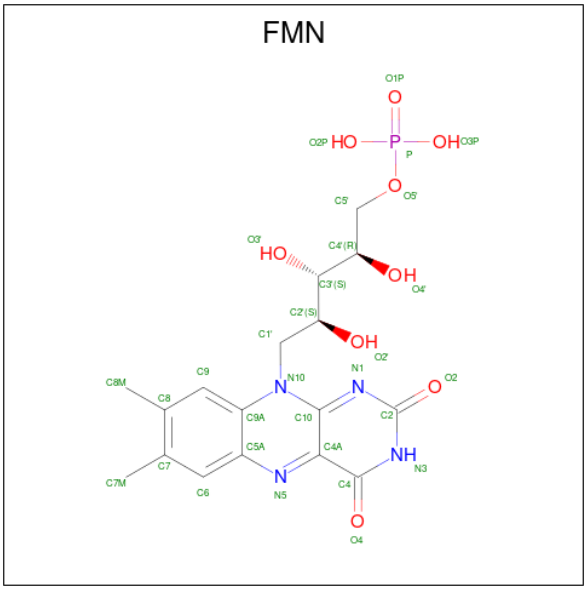
Mol	Chain	Residues	Atoms	AltConf
46	B	1	Total Fe S 8 4 4	0
46	F	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0

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



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

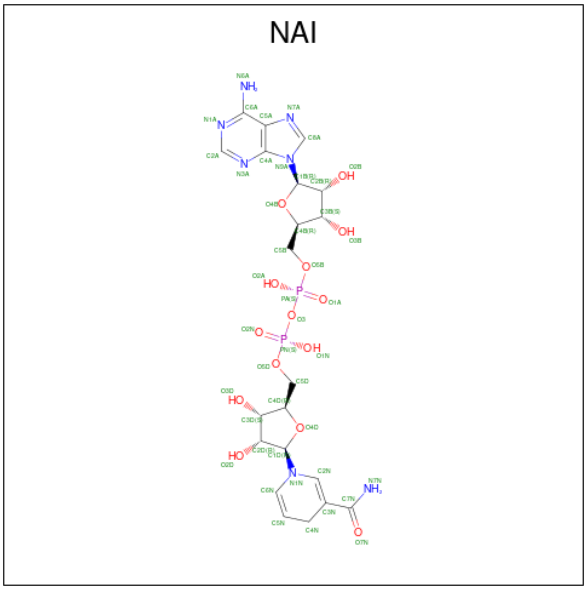
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 49 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID:

NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

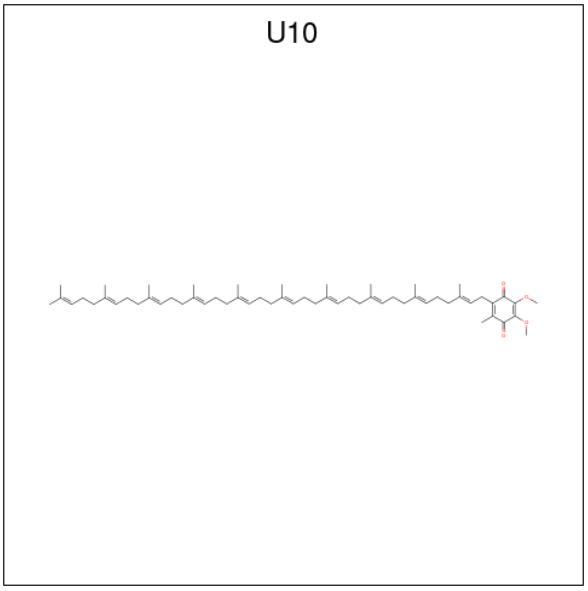


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

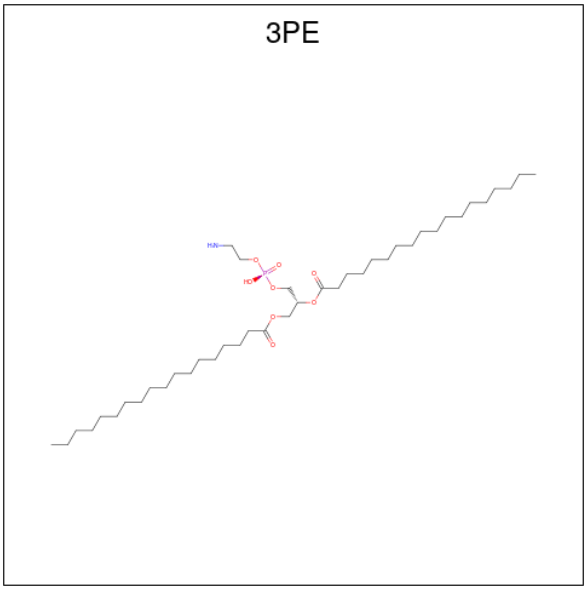
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			63	59	4	

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



Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
52	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	K	1	Total	C	N	O	P	0
			42	32	1	8	1	
52	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
52	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
52	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	N	1	Total	C	N	O	P	0
			49	39	1	8	1	

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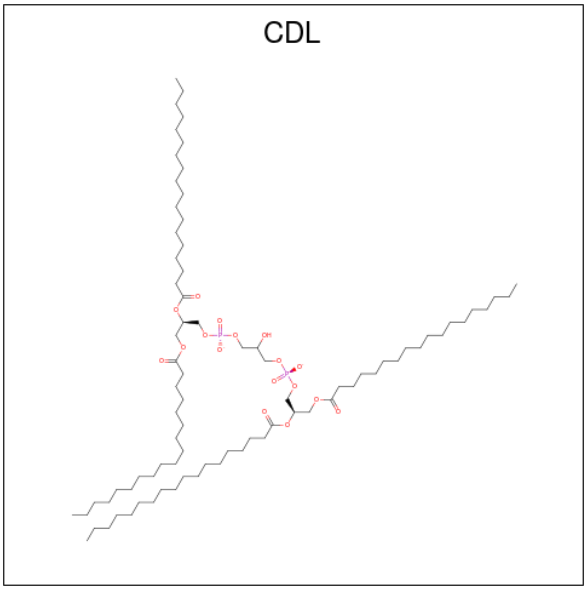
Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
52	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	Y	1	Total	C	N	O	P	0
			34	24	1	8	1	
52	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
52	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
52	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
52	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			69	50	17	2	
53	M	1	Total	C	O	P	0
			81	62	17	2	
53	P	1	Total	C	O	P	0
			69	50	17	2	

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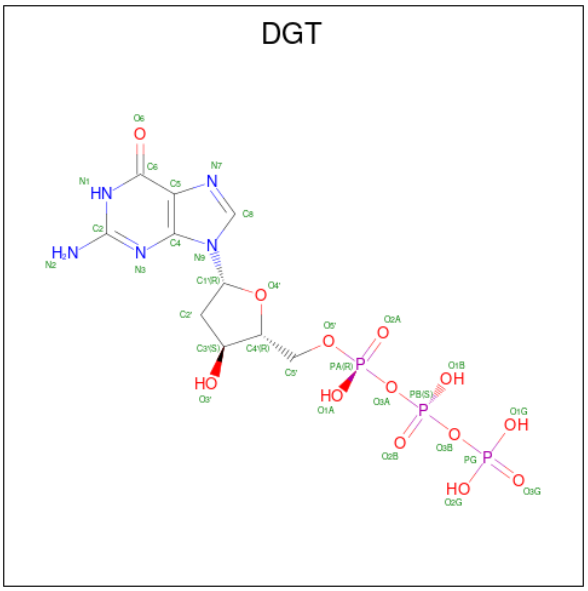
Mol	Chain	Residues	Atoms				AltConf
53	X	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			78	59	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

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

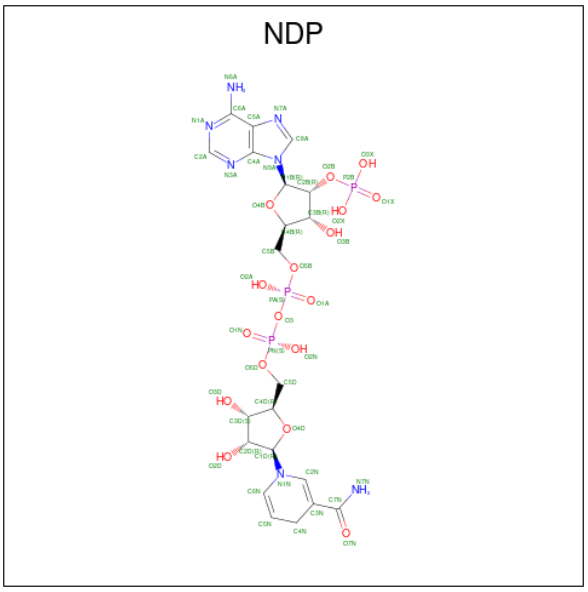


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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

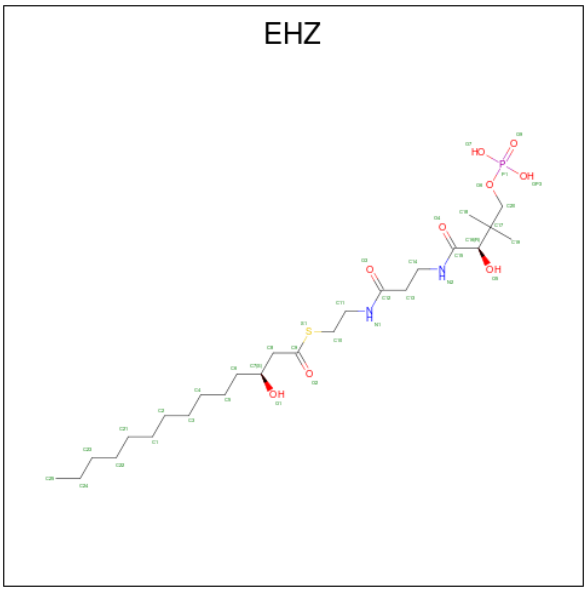


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

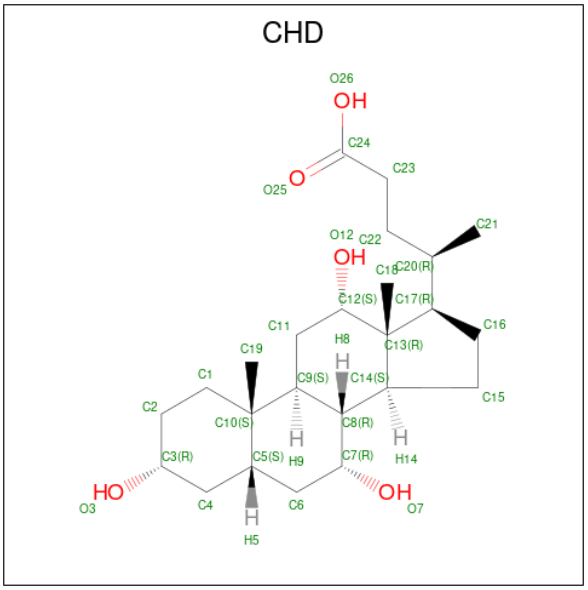
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



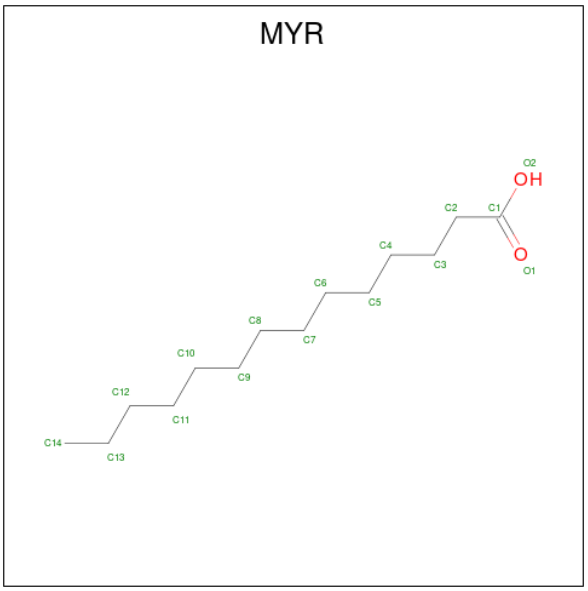
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	A	32	Total O 32 32	0
61	B	76	Total O 76 76	0
61	C	111	Total O 111 111	0
61	D	200	Total O 200 200	0
61	E	31	Total O 31 31	0
61	F	81	Total O 81 81	0
61	G	223	Total O 223 223	0
61	H	107	Total O 107 107	0
61	I	100	Total O 100 100	0
61	J	41	Total O 41 41	0
61	K	24	Total O 24 24	0

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Mol	Chain	Residues	Atoms	AltConf
61	L	61	Total O 61 61	0
61	M	131	Total O 131 131	0
61	N	77	Total O 77 77	0
61	O	25	Total O 25 25	0
61	P	87	Total O 87 87	0
61	Q	101	Total O 101 101	0
61	R	35	Total O 35 35	0
61	S	1	Total O 1 1	0
61	T	1	Total O 1 1	0
61	V	14	Total O 14 14	0
61	W	24	Total O 24 24	0
61	X	33	Total O 33 33	0
61	Y	2	Total O 2 2	0
61	Z	52	Total O 52 52	0
61	a	32	Total O 32 32	0
61	b	6	Total O 6 6	0
61	d	23	Total O 23 23	0
61	e	31	Total O 31 31	0
61	f	3	Total O 3 3	0
61	g	14	Total O 14 14	0
61	h	33	Total O 33 33	0

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Mol	Chain	Residues	Atoms	AltConf
61	i	2	Total O 2 2	0
61	l	22	Total O 22 22	0
61	m	14	Total O 14 14	0
61	n	13	Total O 13 13	0
61	o	1	Total O 1 1	0
61	p	36	Total O 36 36	0
61	q	35	Total O 35 35	0
61	r	25	Total O 25 25	0
61	s	11	Total O 11 11	0

3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:

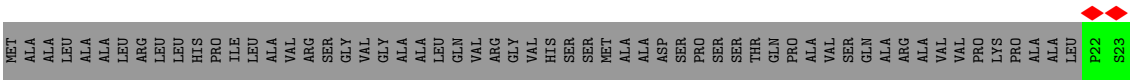


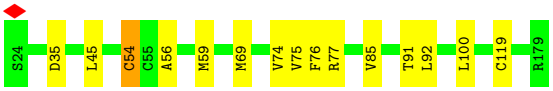


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



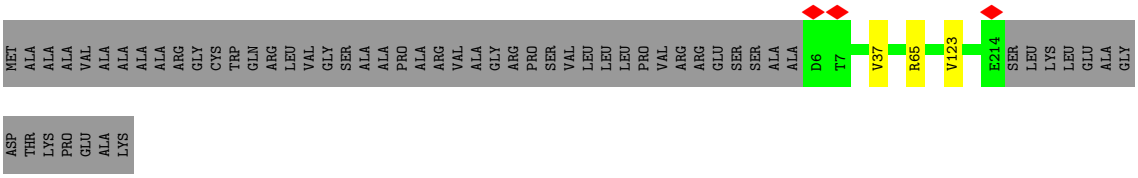




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

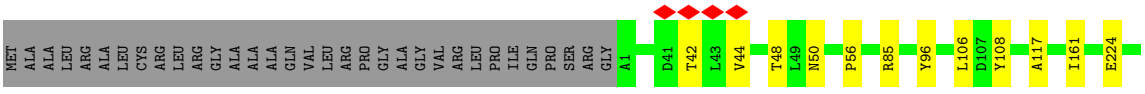




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



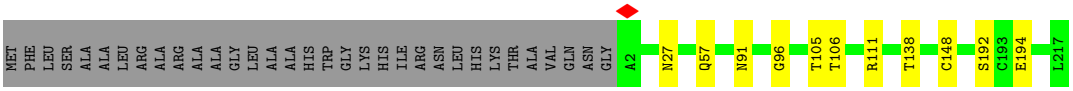




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

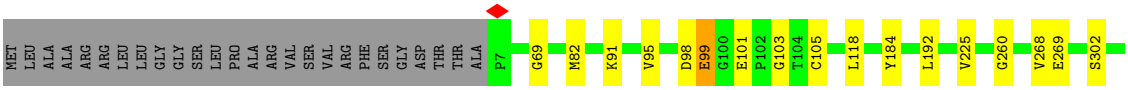


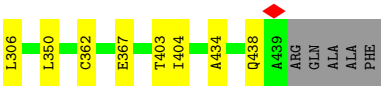


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:







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

Chain G:







• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

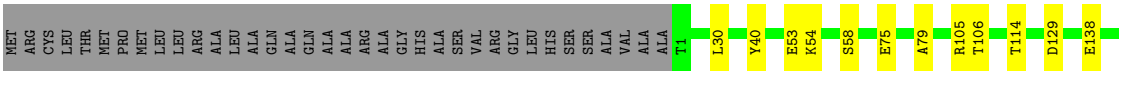




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:

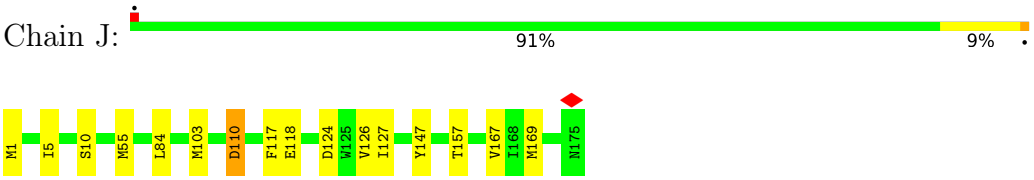






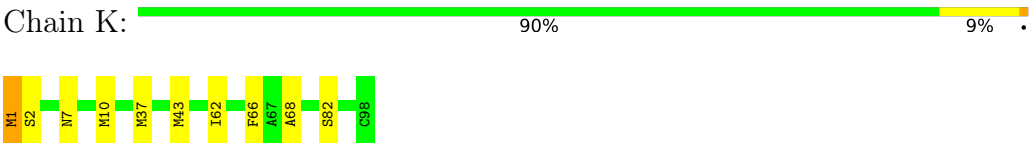
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



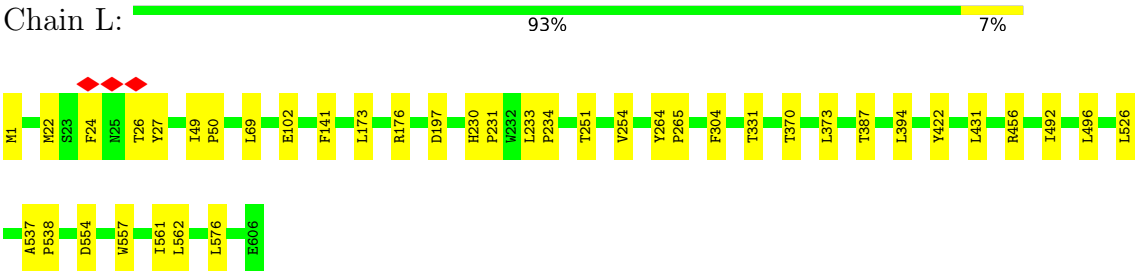
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



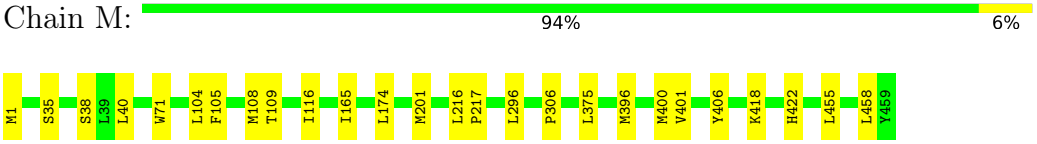
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



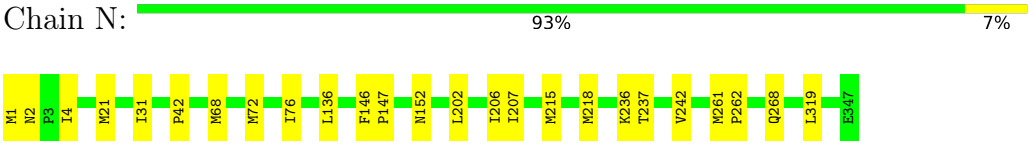
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



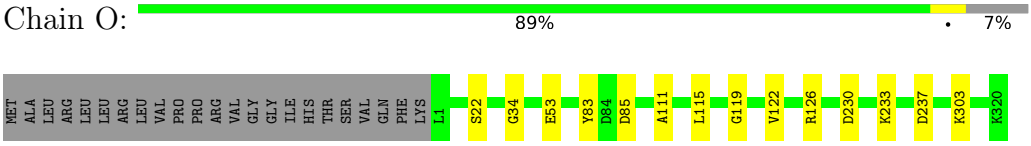
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



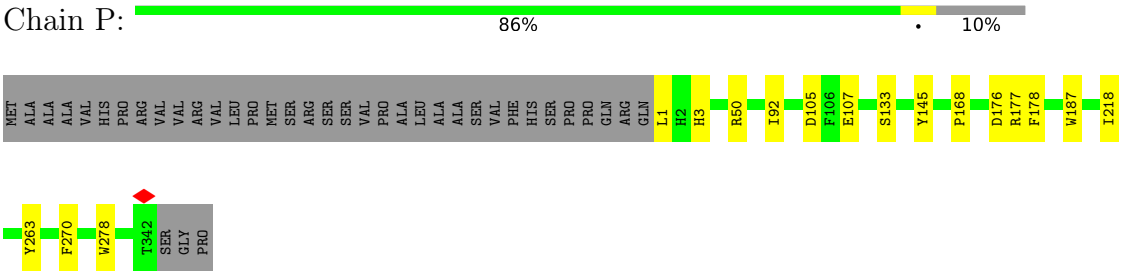
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



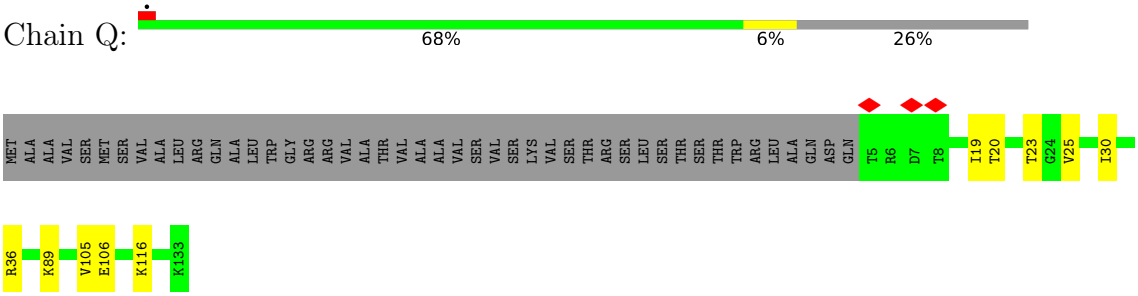
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



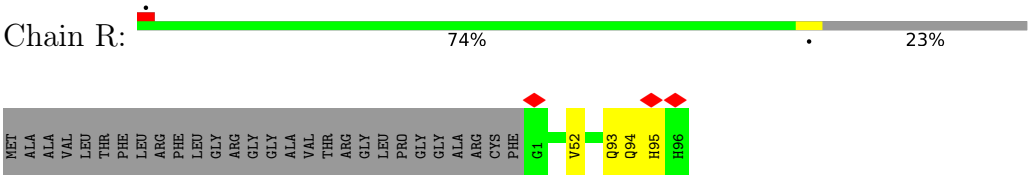
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



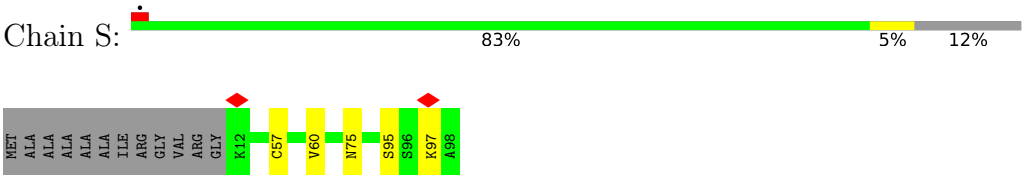
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



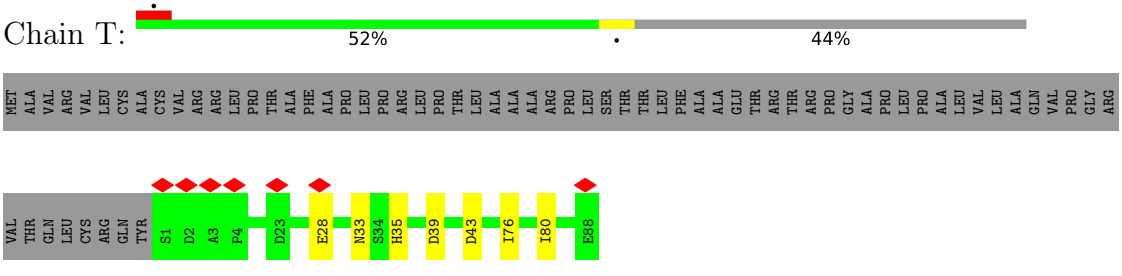
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



• Molecule 20: Acyl carrier protein, mitochondrial

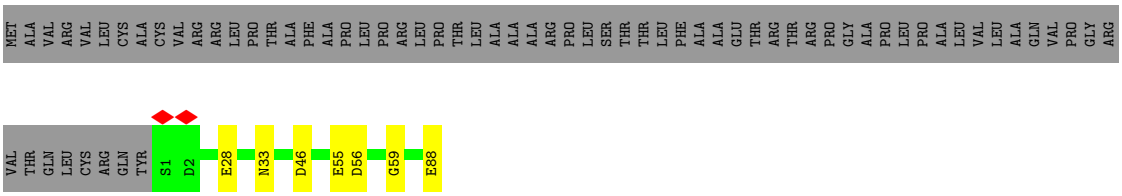
Chain T:



• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:

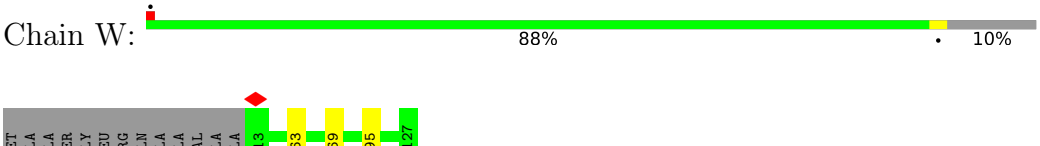




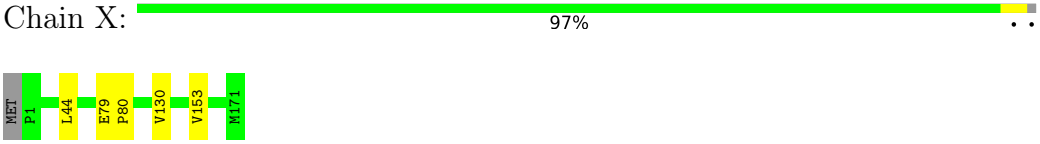
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



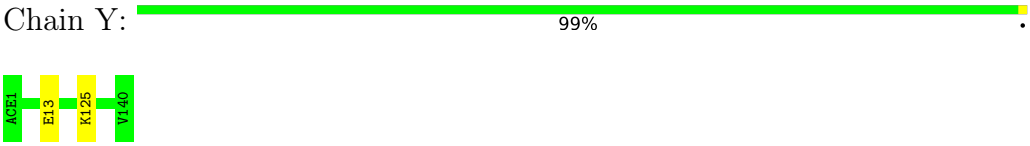
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



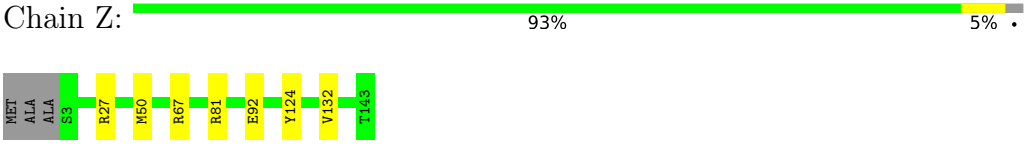
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



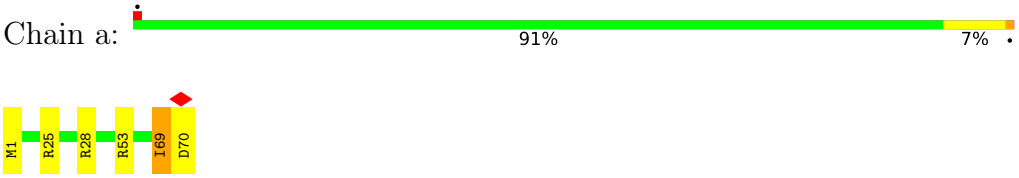
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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

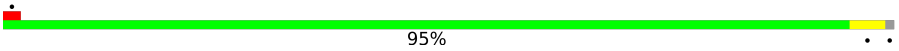


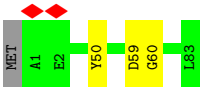
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

Chain b:

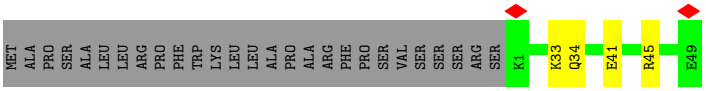




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:

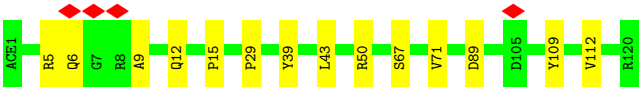




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

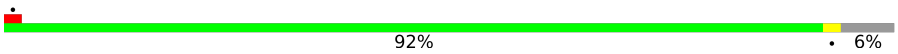
Chain d:

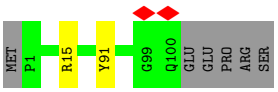




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

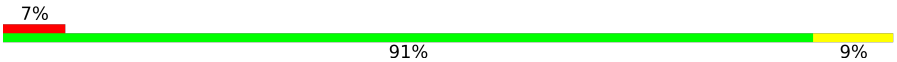
Chain e:

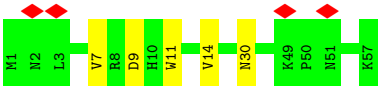




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

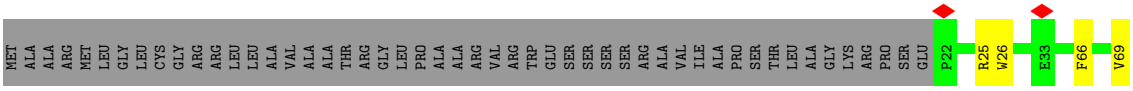


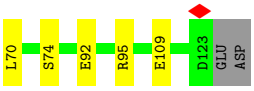


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:

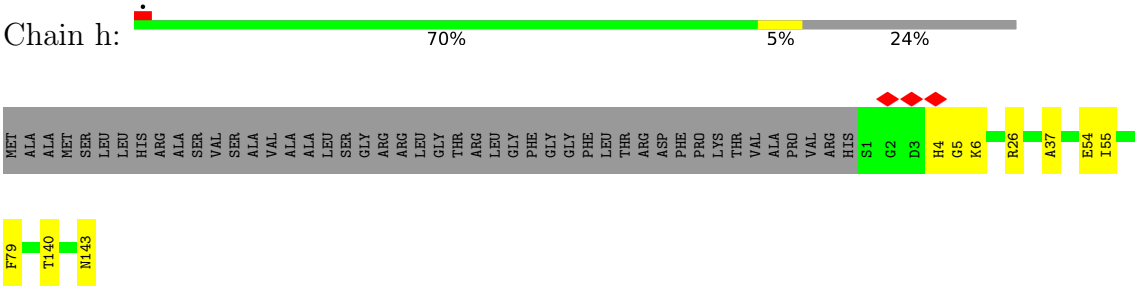






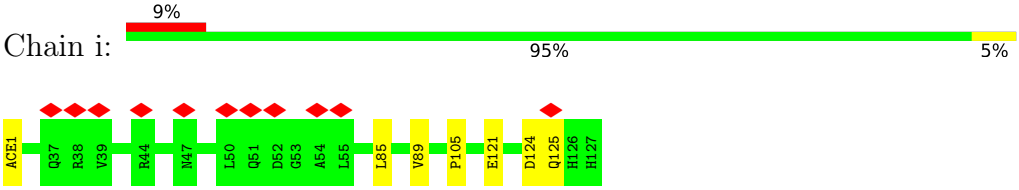
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



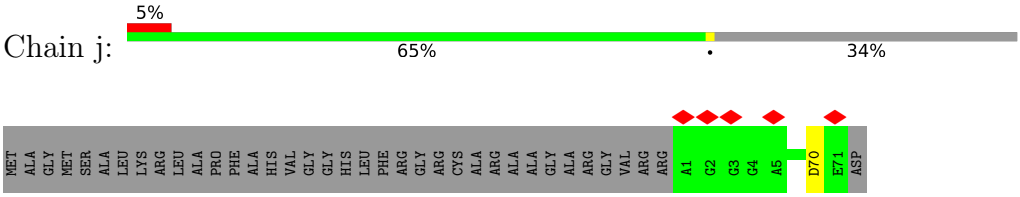
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



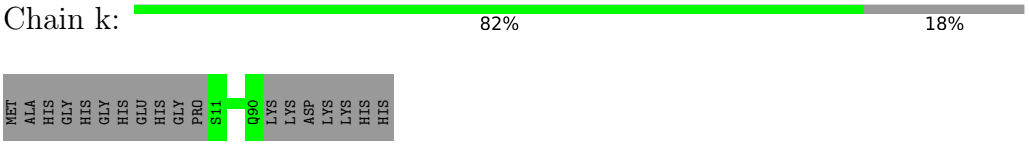
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



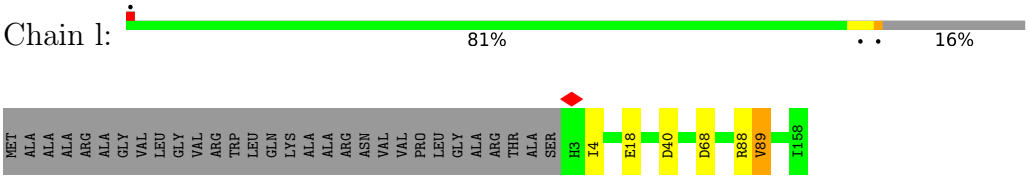
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



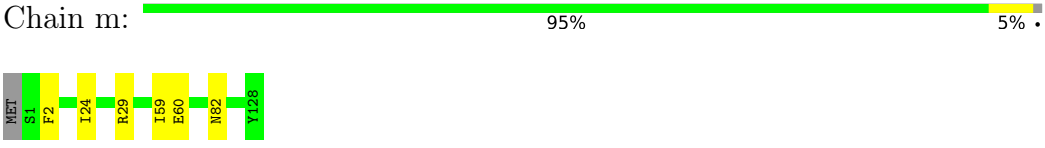
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



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

Chain m:



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

Chain n:

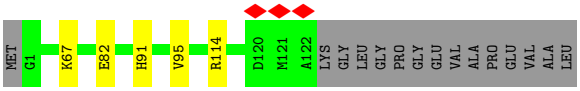




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

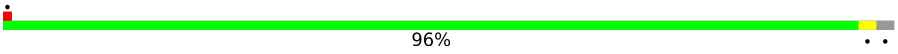
Chain o:

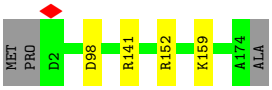




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

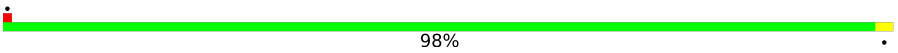
Chain p:

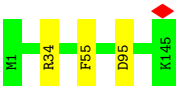




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

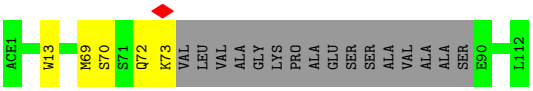




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



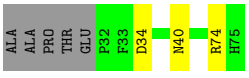


• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.29	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	33.956	Depositor
Minimum map value	-14.378	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.906	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75375, 0.75375, 0.75375	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: PC1, NDP, SF4, FME, WYK, U10, NAI, MYR, DGT, 3PE, ACE, CHD, K, MG, ZN, EHZ, FES, 2MR, FMN, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.10	0/936	0.24	0/1281
2	B	0.12	0/1280	0.29	0/1730
3	C	0.10	0/1789	0.26	0/2436
4	D	0.12	0/3537	0.26	0/4794
5	E	0.10	0/1708	0.27	0/2324
6	F	0.11	0/3406	0.25	0/4602
7	G	0.09	0/5376	0.25	0/7286
8	H	0.11	0/2571	0.30	0/3513
9	I	0.10	0/1445	0.26	0/1956
10	J	0.09	0/1370	0.23	0/1859
11	K	0.10	0/745	0.25	0/1008
12	L	0.09	0/4920	0.25	0/6694
13	M	0.09	0/3738	0.24	0/5097
14	N	0.10	0/2792	0.26	0/3800
15	O	0.09	0/2651	0.22	0/3587
16	P	0.17	0/2831	0.31	0/3841
17	Q	0.10	0/1072	0.28	0/1449
18	R	0.13	0/753	0.24	0/1014
19	S	0.08	0/711	0.22	0/956
20	T	0.11	0/719	0.30	0/971
20	U	0.10	0/719	0.19	0/971
21	V	0.10	0/948	0.20	0/1284
22	W	0.10	0/1000	0.26	0/1344
23	X	0.10	0/1439	0.25	0/1942
24	Y	0.18	0/1048	0.21	0/1423
25	Z	0.09	0/1181	0.22	0/1592
26	a	0.15	0/584	0.34	0/786
27	b	0.12	0/672	0.23	0/923
28	c	0.11	0/427	0.18	0/579
29	d	0.19	0/1027	0.26	0/1387
30	e	0.10	0/859	0.24	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.11	0/505	0.25	0/681
32	g	0.10	0/881	0.27	0/1197
33	h	0.09	0/1221	0.23	0/1651
34	i	0.18	1/1134 (0.1%)	0.24	0/1544
35	j	0.11	0/624	0.20	0/855
36	k	0.07	0/663	0.17	0/895
37	l	0.09	0/1369	0.23	0/1873
38	m	0.10	0/1094	0.21	0/1480
39	n	0.08	0/1545	0.21	0/2092
40	o	0.08	0/1073	0.22	0/1437
41	p	0.09	0/1486	0.24	0/2004
42	q	0.10	0/1250	0.22	0/1698
43	r	0.21	0/804	0.26	0/1088
44	s	0.09	0/383	0.24	0/518
All	All	0.11	1/68286 (0.0%)	0.25	0/92590

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
26	a	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1	ACE	C-N	5.04	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	a	25	ARG	Sidechain
26	a	28	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	16	0
2	B	1261	0	1256	13	0
3	C	1738	0	1685	2	0
4	D	3459	0	3404	15	0
5	E	1668	0	1672	8	0
6	F	3331	0	3287	17	0
7	G	5288	0	5309	21	0
8	H	2509	0	2621	20	0
9	I	1414	0	1370	8	0
10	J	1345	0	1352	15	0
11	K	745	0	785	12	0
12	L	4802	0	4960	25	0
13	M	3654	0	3852	19	0
14	N	2733	0	2912	20	0
15	O	2589	0	2565	10	0
16	P	2754	0	2773	14	0
17	Q	1049	0	1045	7	0
18	R	740	0	714	2	0
19	S	700	0	719	3	0
20	T	707	0	700	5	0
20	U	707	0	700	6	0
21	V	928	0	972	1	0
22	W	976	0	991	2	0
23	X	1402	0	1379	3	0
24	Y	1030	0	1039	1	0
25	Z	1152	0	1151	6	0
26	a	569	0	568	3	0
27	b	651	0	662	2	0
28	c	414	0	415	2	0
29	d	999	0	988	12	0
30	e	838	0	837	2	0
31	f	492	0	501	4	0
32	g	854	0	802	7	0
33	h	1186	0	1193	7	0
34	i	1097	0	1108	4	0
35	j	597	0	536	1	0
36	k	644	0	626	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1314	0	1210	5	0
38	m	1067	0	1067	5	0
39	n	1492	0	1438	8	0
40	o	1048	0	1016	4	0
41	p	1453	0	1425	4	0
42	q	1209	0	1182	2	0
43	r	785	0	795	4	0
44	s	371	0	344	3	0
45	A	70	0	88	5	0
45	B	90	0	128	2	0
45	I	40	0	54	1	0
45	M	42	0	61	1	0
45	N	39	0	52	5	0
45	P	33	0	40	2	0
45	Z	44	0	62	2	0
45	h	44	0	62	0	0
45	q	49	0	75	1	0
46	B	8	0	0	0	0
46	F	8	0	0	1	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	F	44	0	25	3	0
50	G	1	0	0	0	0
51	H	63	0	90	15	0
52	H	79	0	109	3	0
52	K	42	0	58	0	0
52	L	138	0	207	2	0
52	M	43	0	60	1	0
52	N	121	0	167	2	0
52	P	35	0	44	5	0
52	Y	173	0	219	2	0
52	b	47	0	71	2	0
52	m	41	0	59	1	0
53	L	69	0	82	0	0
53	M	81	0	112	2	0
53	P	69	0	85	1	0
53	X	86	0	125	1	0
53	d	65	0	77	2	0
53	h	78	0	100	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	q	61	0	66	2	0
54	O	31	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	0	0
57	R	1	0	0	0	0
58	T	37	0	0	3	0
58	U	37	0	0	1	0
59	i	29	0	38	1	0
60	o	15	0	27	0	0
61	A	32	0	0	0	0
61	B	76	0	0	0	0
61	C	111	0	0	0	0
61	D	200	0	0	0	0
61	E	31	0	0	1	0
61	F	81	0	0	0	0
61	G	223	0	0	1	0
61	H	107	0	0	2	0
61	I	100	0	0	0	0
61	J	41	0	0	0	0
61	K	24	0	0	0	0
61	L	61	0	0	1	0
61	M	131	0	0	0	0
61	N	77	0	0	0	0
61	O	25	0	0	0	0
61	P	87	0	0	0	0
61	Q	101	0	0	0	0
61	R	35	0	0	0	0
61	S	1	0	0	0	0
61	T	1	0	0	0	0
61	V	14	0	0	0	0
61	W	24	0	0	0	0
61	X	33	0	0	0	0
61	Y	2	0	0	0	0
61	Z	52	0	0	1	0
61	a	32	0	0	1	0
61	b	6	0	0	0	0
61	d	23	0	0	0	0
61	e	31	0	0	1	0
61	f	3	0	0	0	0
61	g	14	0	0	0	0
61	h	33	0	0	0	0
61	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	l	22	0	0	0	0
61	m	14	0	0	0	0
61	n	13	0	0	0	0
61	o	1	0	0	0	0
61	p	36	0	0	0	0
61	q	35	0	0	0	0
61	r	25	0	0	0	0
61	s	11	0	0	1	0
All	All	70726	0	69378	321	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 2.

The worst 5 of 321 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)
25:Z:92:GLU:OE1	30:e:91:TYR:OH	2.02	0.78
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.67	0.75
7:G:675:ASP:OD1	7:G:678:SER:OG	2.03	0.75
51:H:701:U10:H38	51:H:701:U10:H351	1.69	0.75
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	155/216 (72%)	150 (97%)	5 (3%)	0	100	100
3	C	207/266 (78%)	203 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	427/463 (92%)	417 (98%)	9 (2%)	1 (0%)	43	57
5	E	214/249 (86%)	207 (97%)	7 (3%)	0	100	100
6	F	431/464 (93%)	425 (99%)	5 (1%)	1 (0%)	43	57
7	G	688/727 (95%)	674 (98%)	14 (2%)	0	100	100
8	H	316/318 (99%)	311 (98%)	4 (1%)	1 (0%)	36	49
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	585 (97%)	19 (3%)	0	100	100
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	340/380 (90%)	335 (98%)	4 (1%)	1 (0%)	36	49
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	85/99 (86%)	83 (98%)	2 (2%)	0	100	100
20	T	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	110 (97%)	2 (2%)	1 (1%)	14	20
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
25	Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	119/121 (98%)	119 (100%)	0	0	100	100
30	e	98/106 (92%)	98 (100%)	0	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	100/154 (65%)	94 (94%)	6 (6%)	0	100	100
33	h	141/189 (75%)	137 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	78/98 (80%)	76 (97%)	2 (3%)	0	100	100
37	l	154/186 (83%)	150 (97%)	3 (2%)	1 (1%)	21	30
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	o	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
41	p	171/176 (97%)	171 (100%)	0	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	93/113 (82%)	90 (97%)	3 (3%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8210/9214 (89%)	8056 (98%)	148 (2%)	6 (0%)	49	63

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	99	GLU
16	P	3	HIS
4	D	359	PRO
8	H	208	VAL
37	l	89	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	133/174 (76%)	132 (99%)	1 (1%)	73	85
3	C	190/228 (83%)	190 (100%)	0	100	100
4	D	370/392 (94%)	369 (100%)	1 (0%)	86	93
5	E	183/205 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	346/368 (94%)	345 (100%)	1 (0%)	86 93
7	G	578/608 (95%)	578 (100%)	0	100 100
8	H	274/274 (100%)	273 (100%)	1 (0%)	84 92
9	I	151/175 (86%)	150 (99%)	1 (1%)	76 87
10	J	141/141 (100%)	139 (99%)	2 (1%)	59 77
11	K	85/85 (100%)	84 (99%)	1 (1%)	63 79
12	L	533/533 (100%)	531 (100%)	2 (0%)	84 92
13	M	412/412 (100%)	412 (100%)	0	100 100
14	N	315/315 (100%)	315 (100%)	0	100 100
15	O	283/303 (93%)	283 (100%)	0	100 100
16	P	296/327 (90%)	295 (100%)	1 (0%)	86 93
17	Q	116/153 (76%)	116 (100%)	0	100 100
18	R	79/97 (81%)	79 (100%)	0	100 100
19	S	77/82 (94%)	77 (100%)	0	100 100
20	T	81/135 (60%)	81 (100%)	0	100 100
20	U	81/135 (60%)	81 (100%)	0	100 100
21	V	101/102 (99%)	101 (100%)	0	100 100
22	W	107/114 (94%)	107 (100%)	0	100 100
23	X	154/155 (99%)	154 (100%)	0	100 100
24	Y	101/101 (100%)	101 (100%)	0	100 100
25	Z	120/121 (99%)	120 (100%)	0	100 100
26	a	59/59 (100%)	58 (98%)	1 (2%)	53 73
27	b	71/72 (99%)	71 (100%)	0	100 100
28	c	45/68 (66%)	45 (100%)	0	100 100
29	d	106/106 (100%)	106 (100%)	0	100 100
30	e	90/96 (94%)	90 (100%)	0	100 100
31	f	54/54 (100%)	54 (100%)	0	100 100
32	g	93/131 (71%)	93 (100%)	0	100 100
33	h	124/158 (78%)	124 (100%)	0	100 100
34	i	121/121 (100%)	121 (100%)	0	100 100
35	j	61/84 (73%)	61 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	k	62/76 (82%)	62 (100%)	0	100 100
37	l	140/159 (88%)	140 (100%)	0	100 100
38	m	114/115 (99%)	113 (99%)	1 (1%)	70 84
39	n	156/161 (97%)	156 (100%)	0	100 100
40	o	110/120 (92%)	110 (100%)	0	100 100
41	p	155/157 (99%)	155 (100%)	0	100 100
42	q	131/131 (100%)	130 (99%)	1 (1%)	73 85
43	r	86/96 (90%)	86 (100%)	0	100 100
44	s	43/92 (47%)	43 (100%)	0	100 100
All	All	7228/7891 (92%)	7214 (100%)	14 (0%)	85 94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	82	SER
12	L	554	ASP
42	q	95	ASP
26	a	69	ILE
38	m	2	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	172	GLN
42	q	5	GLN
16	P	131	HIS
41	p	143	HIS
39	n	11	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	FME	K	1	11	8,9,10	1.52	1 (12%)	7,9,11	1.70	2 (28%)
2	WYK	B	77	2	9,11,12	2.53	2 (22%)	7,13,15	0.58	0
14	FME	N	1	14	8,9,10	1.52	1 (12%)	7,9,11	1.73	2 (28%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	7,9,11	1.62	2 (28%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	7,9,11	1.77	1 (14%)
12	FME	L	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.61	1 (14%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.71	2 (28%)
13	FME	M	1	13	8,9,10	1.53	1 (12%)	7,9,11	1.79	1 (14%)
4	2MR	D	85	4	10,12,13	2.45	2 (20%)	5,13,15	1.26	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	FME	K	1	11	-	2/7/9/11	-
2	WYK	B	77	2	-	1/10/11/13	-
14	FME	N	1	14	-	1/7/9/11	-
10	FME	J	1	10	-	5/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
12	FME	L	1	12	-	4/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	WYK	CZ-NE	6.69	1.46	1.33
4	D	85	2MR	CZ-NH2	5.37	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.22	1.45	1.34
13	M	1	FME	CN-N	3.73	1.45	1.33
14	N	1	FME	CN-N	3.71	1.45	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	1	FME	CE-SD-CG	3.46	112.27	100.40
14	N	1	FME	CE-SD-CG	3.15	111.23	100.40
8	H	1	FME	CE-SD-CG	2.94	110.51	100.40
11	K	1	FME	CE-SD-CG	2.94	110.51	100.40
1	A	1	FME	CE-SD-CG	2.73	109.78	100.40

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 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	$\#\|Z\| > 2$
52	3PE	N	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.15	2 (4%)
52	3PE	Y	802	-	39,39,50	0.96	4 (10%)	42,44,55	1.14	2 (4%)
52	3PE	N	403	-	48,48,50	0.89	4 (8%)	51,53,55	1.01	2 (3%)
52	3PE	M	501	-	42,42,50	0.94	4 (9%)	45,47,55	1.07	2 (4%)
51	U10	H	701	-	63,63,63	0.62	2 (3%)	76,79,79	0.60	0
46	SF4	G	801	7	0,12,12	-	-	-		
45	PC1	A	202	-	34,34,53	1.53	6 (17%)	40,42,61	1.13	3 (7%)
53	CDL	M	502	-	80,80,99	1.02	7 (8%)	86,92,111	1.20	5 (5%)
46	SF4	F	502	6	0,12,12	-	-	-		
52	3PE	Y	804	-	26,26,50	1.20	4 (15%)	29,31,55	1.23	2 (6%)
47	FES	G	803	7	0,4,4	-	-	-		
45	PC1	I	203	-	39,39,53	1.46	6 (15%)	45,47,61	1.03	2 (4%)
52	3PE	H	702	-	33,33,50	1.09	4 (12%)	36,38,55	1.37	3 (8%)
52	3PE	Y	805	-	40,40,50	0.96	3 (7%)	43,45,55	1.11	2 (4%)
45	PC1	B	202	-	45,45,53	1.41	6 (13%)	51,53,61	0.94	2 (3%)
46	SF4	B	201	2	0,12,12	-	-	-		
45	PC1	M	503	-	41,41,53	1.41	6 (14%)	47,49,61	1.18	2 (4%)
46	SF4	I	201	9	0,12,12	-	-	-		
45	PC1	P	401	-	32,32,53	1.58	6 (18%)	38,40,61	0.94	2 (5%)
59	CHD	i	201	-	32,32,32	3.28	10 (31%)	51,51,51	1.85	13 (25%)
53	CDL	L	702	-	68,68,99	1.08	7 (10%)	74,80,111	0.99	4 (5%)
45	PC1	B	203	-	43,43,53	1.40	6 (13%)	49,51,61	0.95	2 (4%)
52	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.08	2 (4%)
52	3PE	P	404	-	34,34,50	1.04	4 (11%)	37,39,55	1.21	2 (5%)
45	PC1	N	404	-	38,38,53	1.45	6 (15%)	44,46,61	1.04	2 (4%)
52	3PE	Y	801	-	30,30,50	1.07	4 (13%)	33,35,55	1.15	3 (9%)
53	CDL	h	201	-	77,77,99	1.02	7 (9%)	83,89,111	1.14	5 (6%)
53	CDL	X	201	-	85,85,99	0.99	7 (8%)	91,97,111	1.08	6 (6%)
52	3PE	b	201	-	46,46,50	0.97	4 (8%)	49,51,55	1.12	2 (4%)
58	EHZ	T	101	20	29,36,37	1.71	5 (17%)	35,44,47	1.26	2 (5%)
53	CDL	d	201	-	64,64,99	1.10	6 (9%)	70,76,111	1.09	4 (5%)
60	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	3PE	m	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.12	2 (4%)
47	FES	E	301	5	0,4,4	-	-	-		
52	3PE	L	704	-	48,48,50	0.90	4 (8%)	51,53,55	1.01	2 (3%)
54	DGT	O	401	55	29,33,33	3.19	14 (48%)	44,52,52	2.10	12 (27%)
45	PC1	A	201	-	34,34,53	1.51	6 (17%)	40,42,61	1.00	2 (5%)
52	3PE	N	402	-	30,30,50	1.10	4 (13%)	33,35,55	1.06	2 (6%)
52	3PE	H	703	-	44,44,50	0.91	4 (9%)	47,49,55	1.13	3 (6%)
53	CDL	P	402	-	68,68,99	1.07	7 (10%)	74,80,111	1.05	3 (4%)
45	PC1	Z	200	-	43,43,53	1.44	6 (13%)	49,51,61	0.97	2 (4%)
46	SF4	G	802	7	0,12,12	-	-	-		
56	NDP	P	403	-	49,52,52	3.97	24 (48%)	66,80,80	2.08	14 (21%)
45	PC1	h	202	-	43,43,53	1.41	6 (13%)	49,51,61	1.02	2 (4%)
53	CDL	q	202	-	60,60,99	1.14	7 (11%)	66,72,111	1.15	5 (7%)
52	3PE	Y	803	-	33,33,50	1.09	4 (12%)	36,38,55	1.09	2 (5%)
48	FMN	F	501	-	33,33,33	2.81	10 (30%)	48,50,50	1.70	12 (25%)
45	PC1	q	201	-	48,48,53	1.35	6 (12%)	54,56,61	1.06	2 (3%)
52	3PE	K	101	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)
49	NAI	F	503	-	45,48,48	3.75	19 (42%)	60,73,73	1.85	15 (25%)
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.51	5 (14%)
46	SF4	I	202	9	0,12,12	-	-	-		
52	3PE	L	701	-	43,43,50	0.94	4 (9%)	46,48,55	1.02	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
52	3PE	N	401	-	-	19/44/44/54	-
52	3PE	Y	802	-	-	18/43/43/54	-
52	3PE	N	403	-	-	18/52/52/54	-
52	3PE	M	501	-	-	17/46/46/54	-
51	U10	H	701	-	-	24/63/87/87	0/1/1/1
46	SF4	G	801	7	-	-	0/6/5/5
45	PC1	A	202	-	-	11/38/38/57	-
53	CDL	M	502	-	-	39/91/91/110	-
52	3PE	Y	804	-	-	17/30/30/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SF4	F	502	6	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
45	PC1	I	203	-	-	11/43/43/57	-
52	3PE	H	702	-	-	17/37/37/54	-
52	3PE	Y	805	-	-	13/44/44/54	-
45	PC1	B	202	-	-	14/49/49/57	-
59	CHD	i	201	-	-	0/9/74/74	0/4/4/4
45	PC1	M	503	-	-	6/45/45/57	-
46	SF4	B	201	2	-	-	0/6/5/5
45	PC1	P	401	-	-	10/36/36/57	-
46	SF4	I	201	9	-	-	0/6/5/5
53	CDL	L	702	-	-	24/79/79/110	-
45	PC1	B	203	-	-	13/47/47/57	-
52	3PE	L	703	-	-	19/48/48/54	-
52	3PE	P	404	-	-	15/38/38/54	-
45	PC1	N	404	-	-	11/42/42/57	-
52	3PE	Y	801	-	-	23/34/34/54	-
53	CDL	h	201	-	-	34/88/88/110	-
53	CDL	X	201	-	-	38/96/96/110	-
52	3PE	b	201	-	-	18/50/50/54	-
58	EHZ	T	101	20	-	17/42/44/45	-
53	CDL	d	201	-	-	33/75/75/110	-
60	MYR	o	201	40	-	2/11/12/13	-
52	3PE	m	201	-	-	18/44/44/54	-
47	FES	E	301	5	-	-	0/1/1/1
52	3PE	L	704	-	-	19/52/52/54	-
54	DGT	O	401	55	-	3/22/34/34	0/3/3/3
45	PC1	A	201	-	-	9/38/38/57	-
52	3PE	N	402	-	-	15/34/34/54	-
52	3PE	H	703	-	-	13/48/48/54	-
53	CDL	P	402	-	-	33/79/79/110	-
45	PC1	Z	200	-	-	21/47/47/57	-
46	SF4	G	802	7	-	-	0/6/5/5
56	NDP	P	403	-	-	3/34/77/77	0/5/5/5
45	PC1	h	202	-	-	14/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	q	202	-	-	28/71/71/110	-
52	3PE	Y	803	-	-	12/37/37/54	-
48	FMN	F	501	-	-	1/18/18/18	0/3/3/3
45	PC1	q	201	-	-	18/52/52/57	-
52	3PE	K	101	-	-	18/45/45/54	-
49	NAI	F	503	-	-	6/29/72/72	0/5/5/5
58	EHZ	U	101	20	-	9/42/44/45	-
46	SF4	I	202	9	-	-	0/6/5/5
52	3PE	L	701	-	-	21/47/47/54	-

The worst 5 of 273 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	403	NDP	C6N-C5N	12.12	1.55	1.33
49	F	503	NAI	C6N-C5N	11.32	1.53	1.33
59	i	201	CHD	C11-C12	9.01	1.68	1.53
49	F	503	NAI	O4B-C1B	8.64	1.62	1.42
49	F	503	NAI	O4D-C1D	8.56	1.62	1.42

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	P	403	NDP	N6A-C6A-N1A	-6.40	104.33	118.35
54	O	401	DGT	C5-C4-N3	-5.55	119.46	128.46
56	P	403	NDP	C5A-C6A-N6A	5.45	135.30	123.43
56	P	403	NDP	C5A-C4A-N3A	-5.42	119.68	126.75
54	O	401	DGT	C1'-N9-C8	5.38	139.91	127.85

There are no chirality outliers.

5 of 742 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PC1	O13-C11-C12-N
45	A	201	PC1	C22-C21-O21-C2
45	B	203	PC1	C22-C21-O21-C2
45	I	203	PC1	C1-O11-P-O12
45	I	203	PC1	C1-O11-P-O14

There are no ring outliers.

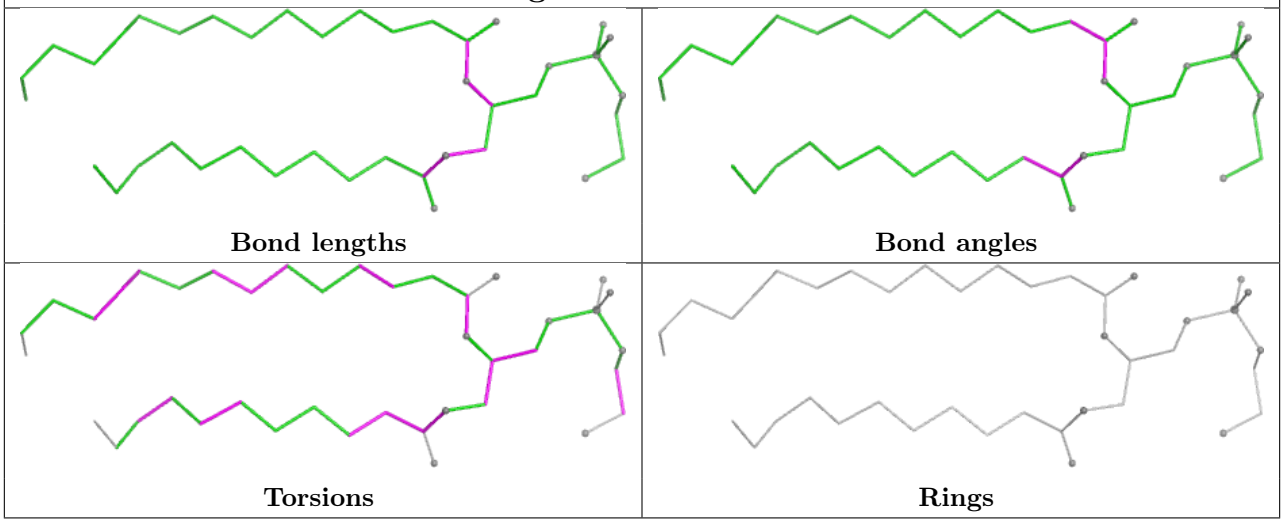
34 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	Y	802	3PE	2	0
52	N	403	3PE	1	0
52	M	501	3PE	1	0
51	H	701	U10	15	0
45	A	202	PC1	2	0
53	M	502	CDL	2	0
46	F	502	SF4	1	0
45	I	203	PC1	1	0
52	H	702	3PE	2	0
45	B	202	PC1	1	0
45	M	503	PC1	1	0
45	P	401	PC1	2	0
59	i	201	CHD	1	0
45	B	203	PC1	1	0
52	P	404	3PE	5	0
45	N	404	PC1	5	0
53	h	201	CDL	1	0
53	X	201	CDL	1	0
52	b	201	3PE	2	0
58	T	101	EHZ	3	0
53	d	201	CDL	2	0
52	m	201	3PE	1	0
54	O	401	DGT	2	0
45	A	201	PC1	3	0
52	N	402	3PE	1	0
52	H	703	3PE	1	0
53	P	402	CDL	1	0
45	Z	200	PC1	2	0
53	q	202	CDL	2	0
52	Y	803	3PE	2	0
45	q	201	PC1	1	0
49	F	503	NAI	3	0
58	U	101	EHZ	1	0
52	L	701	3PE	2	0

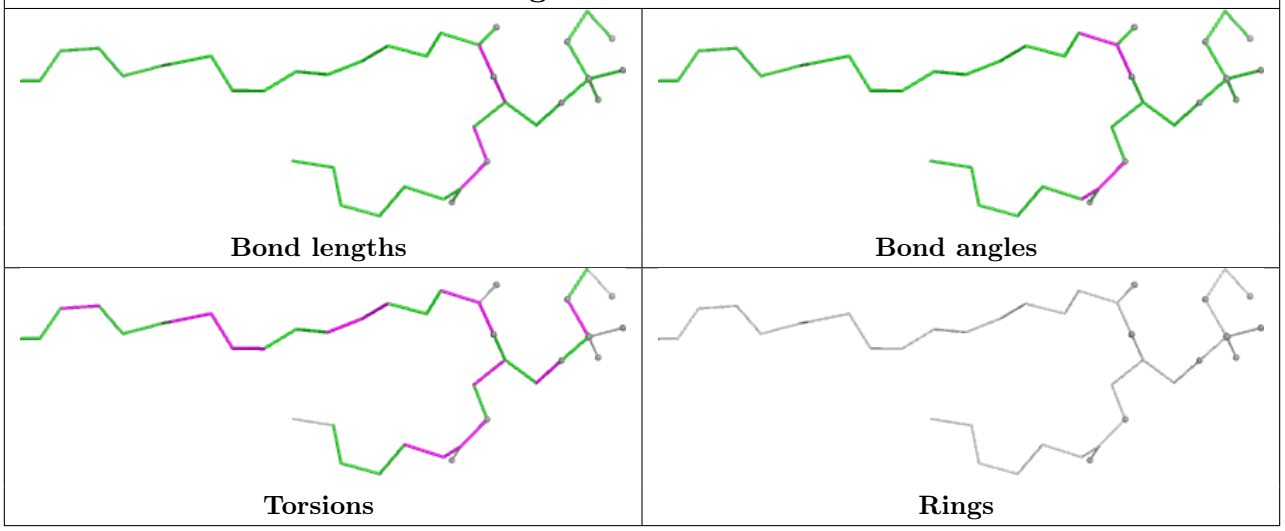
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

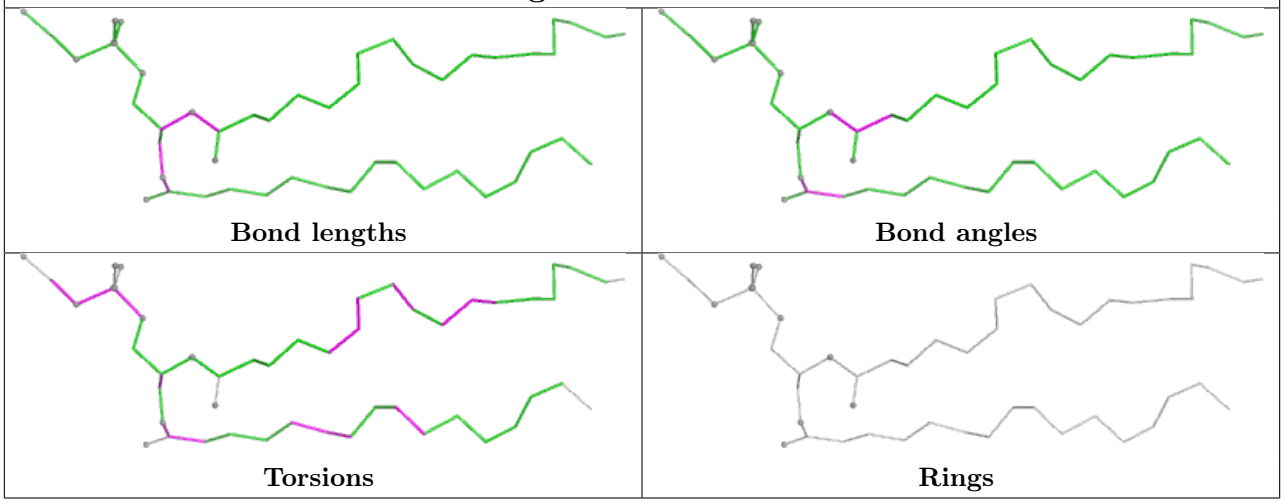
Ligand 3PE N 401



Ligand 3PE Y 802



Ligand 3PE N 403



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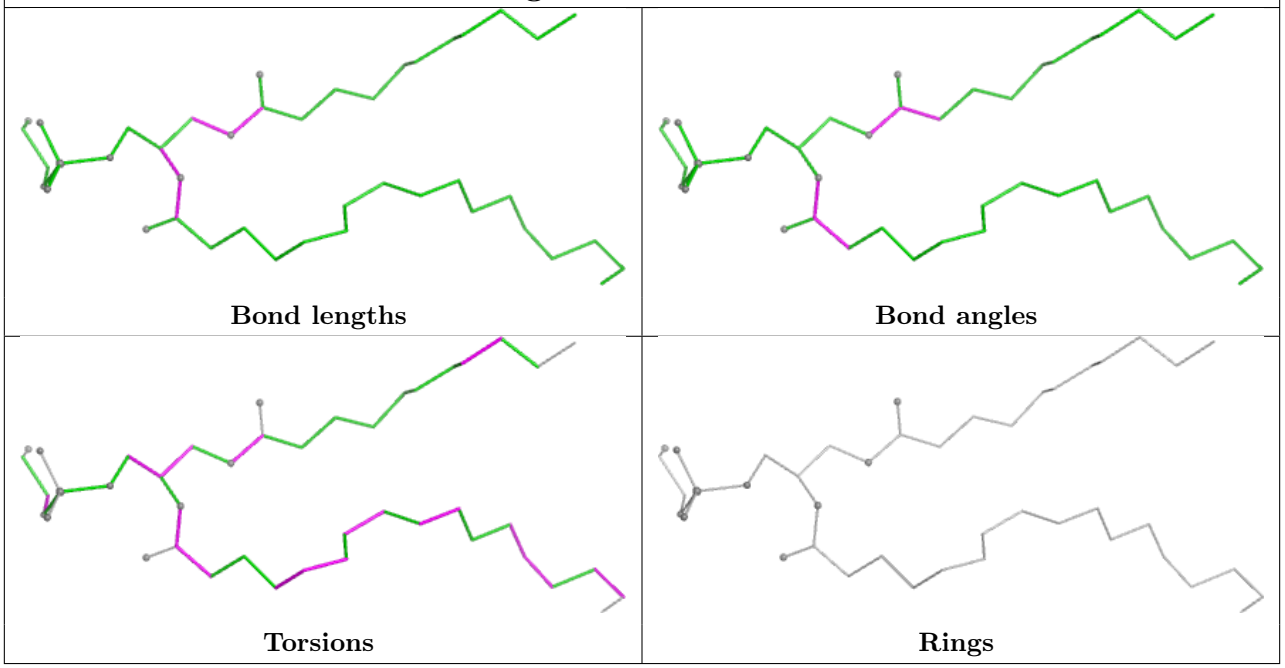

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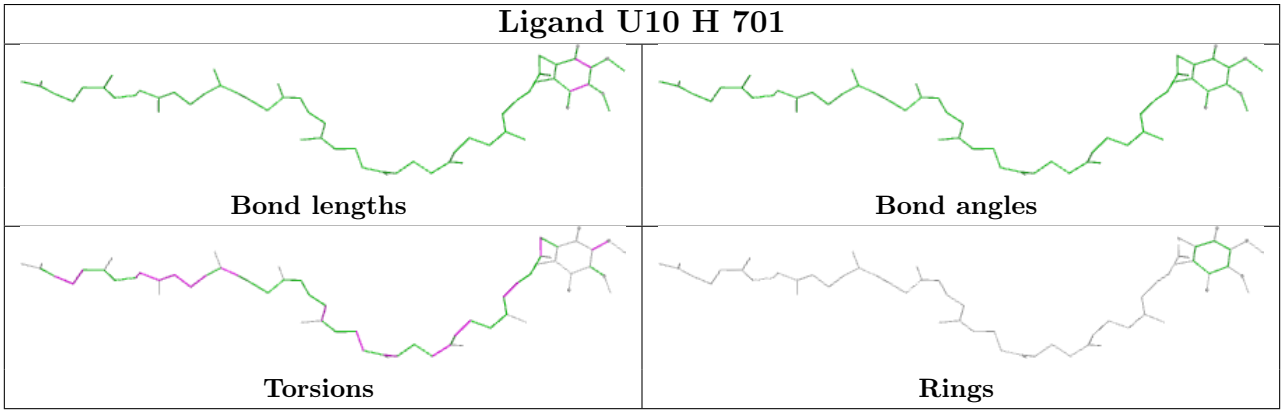
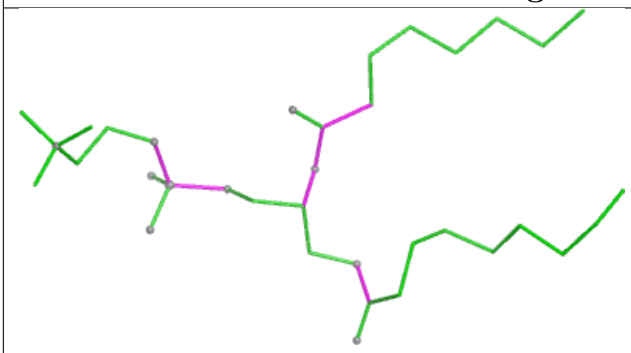


Ligand PC1 A 202



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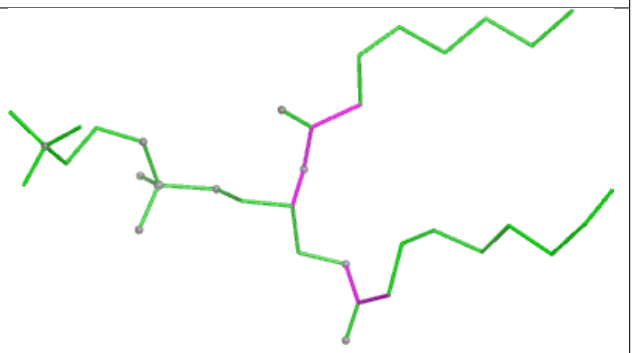
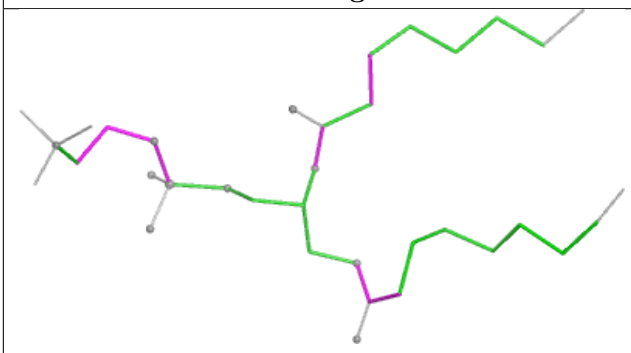
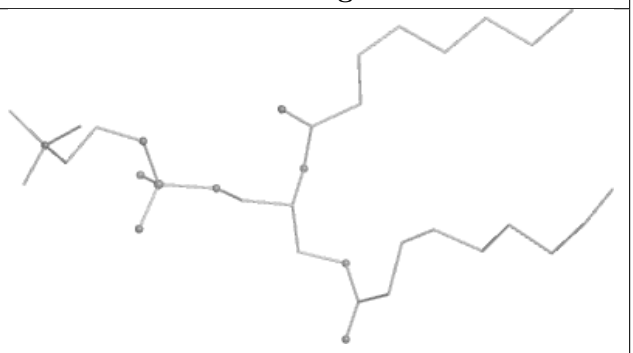


Bond angles

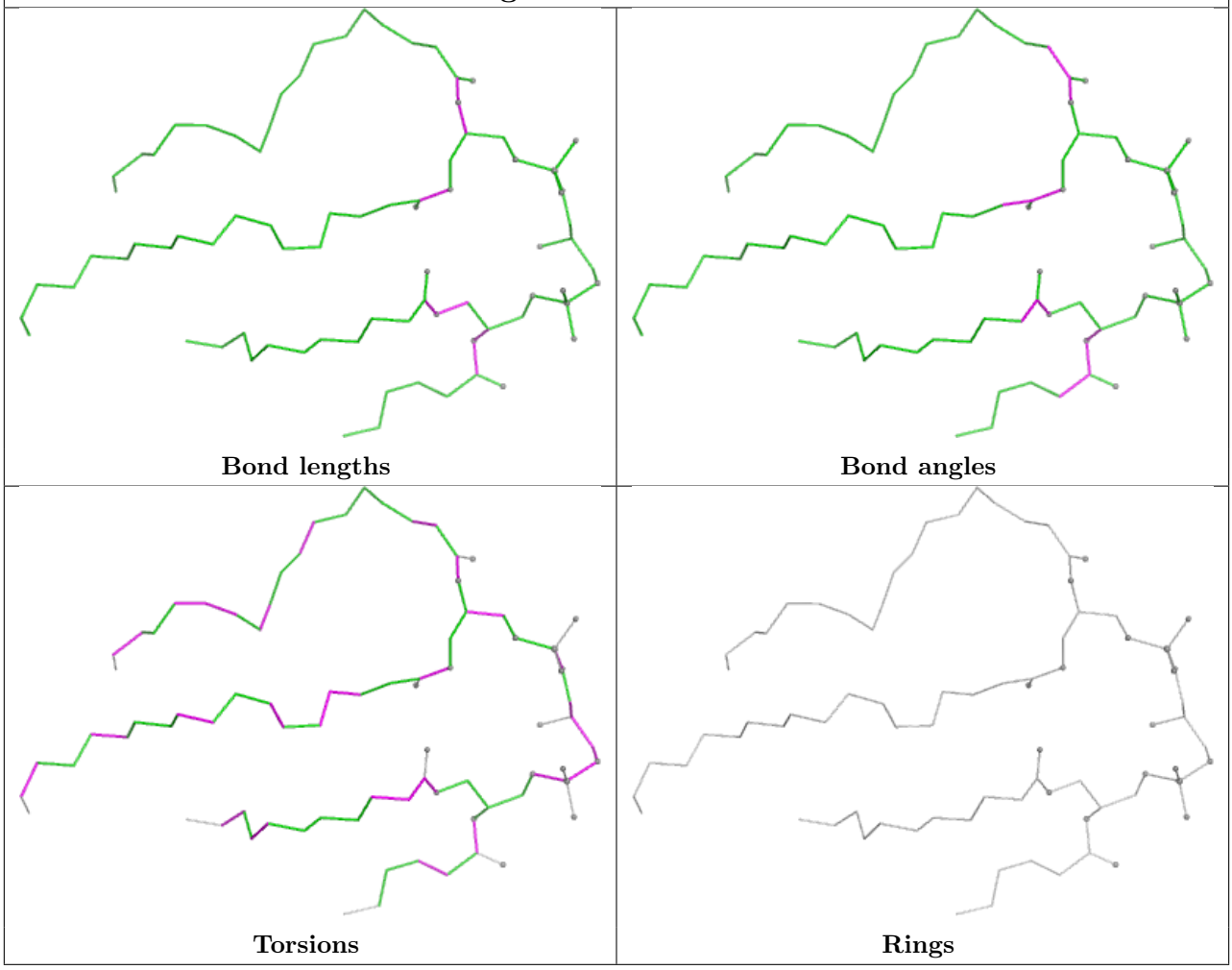


Torsions



Rings

Ligand CDL M 502



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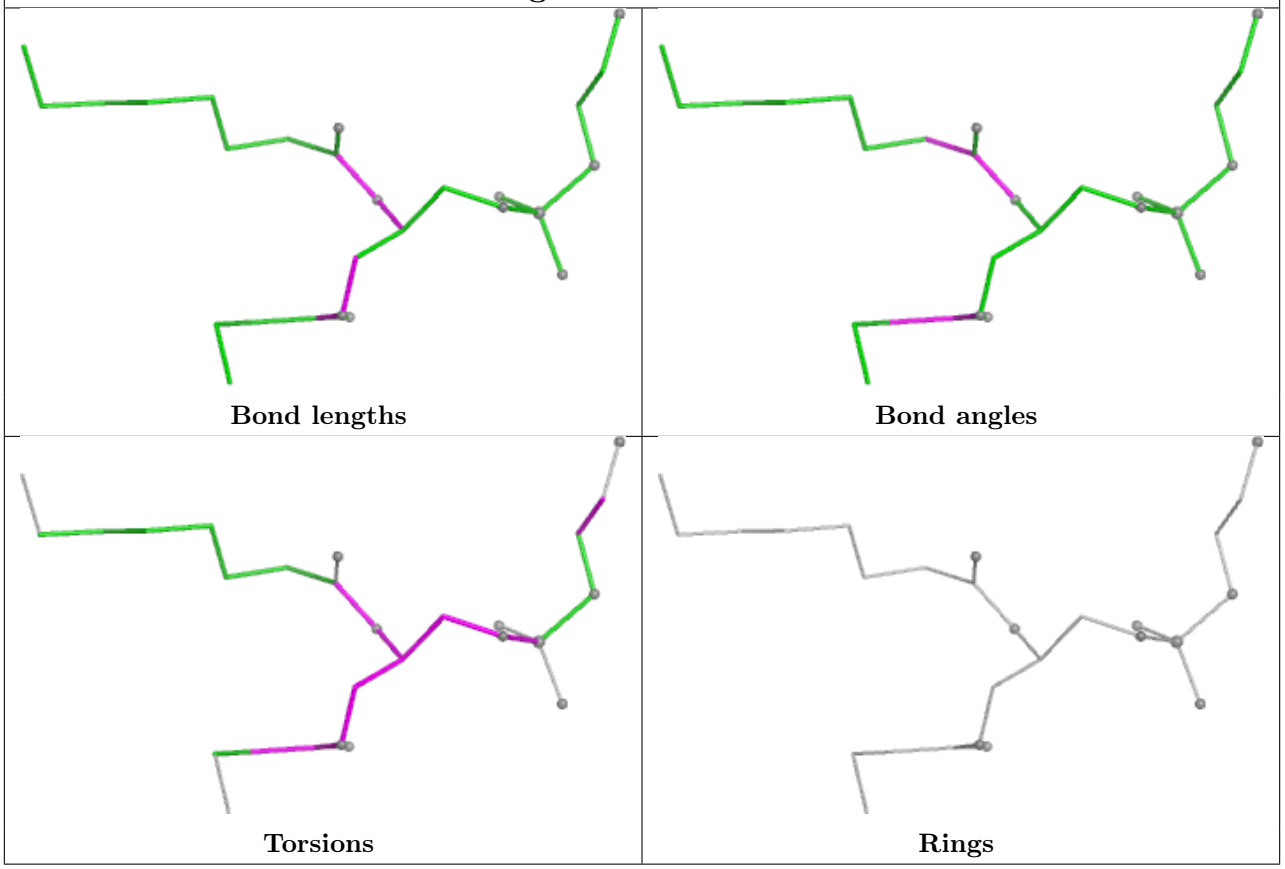

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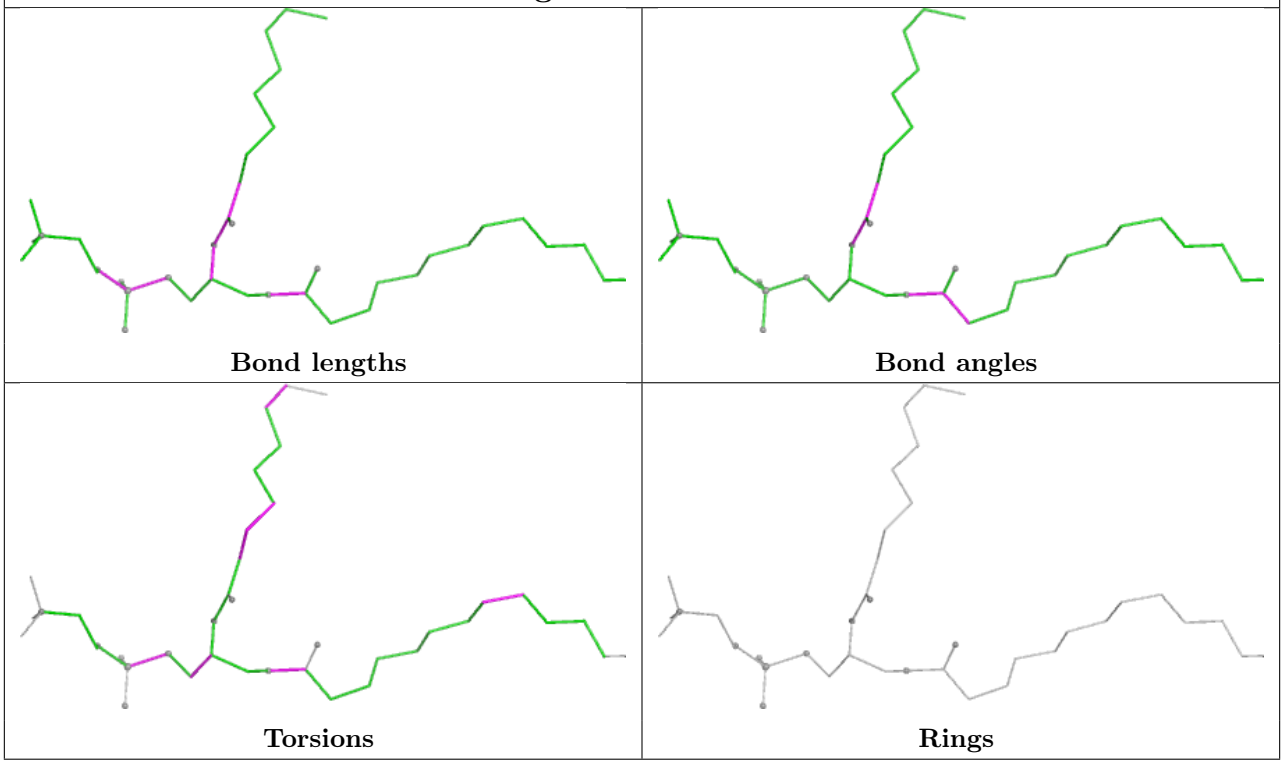

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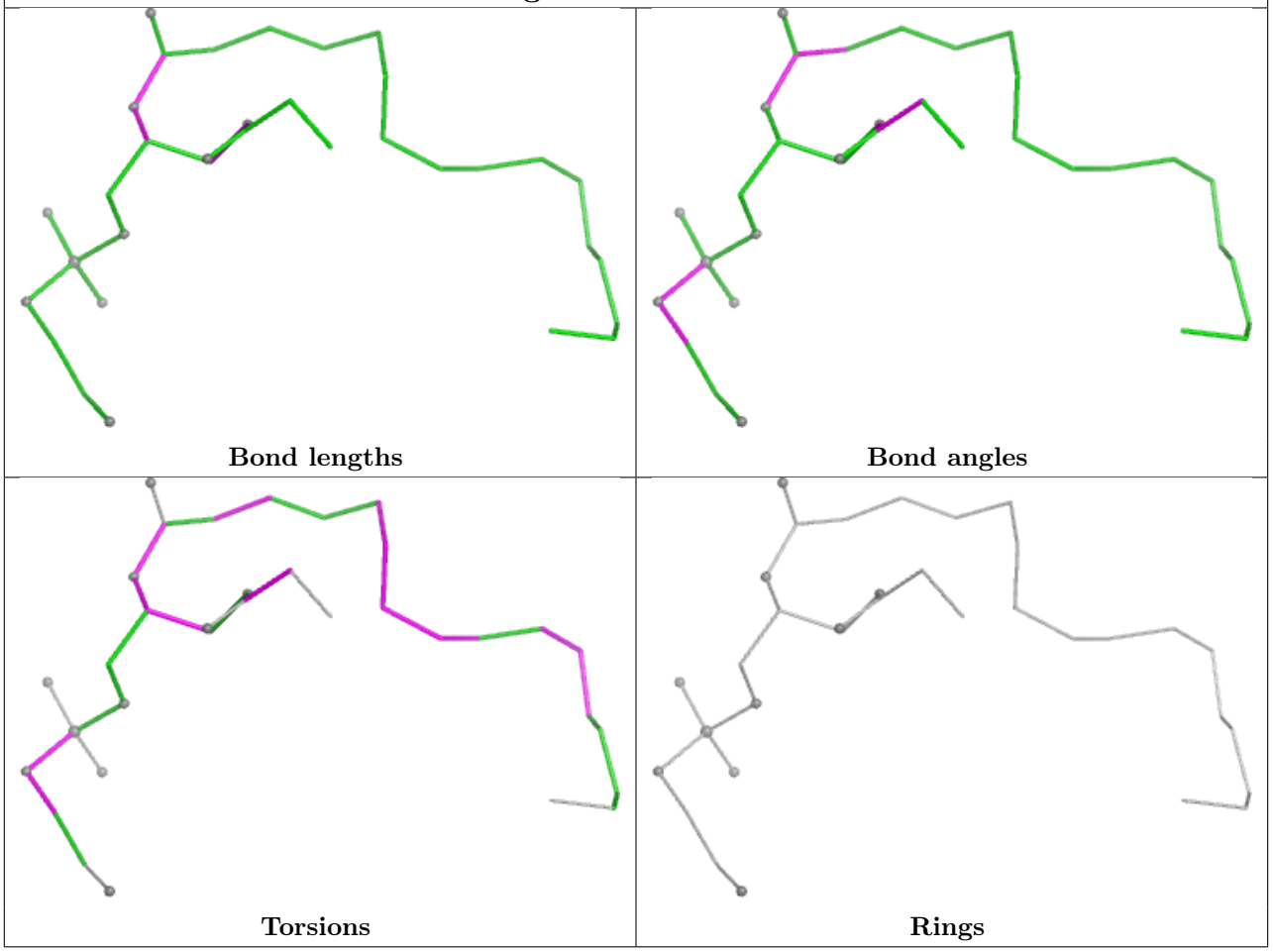

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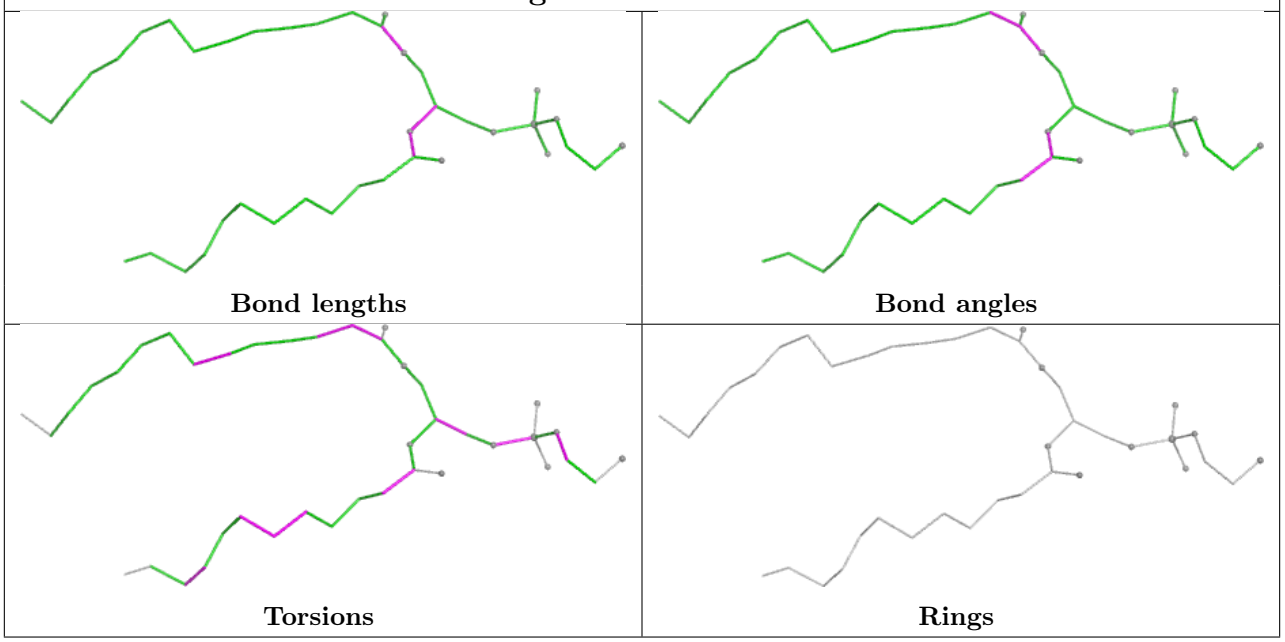

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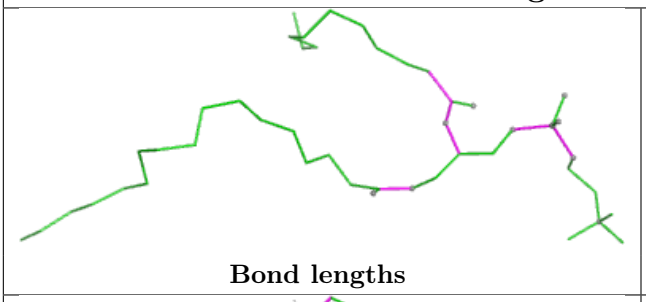
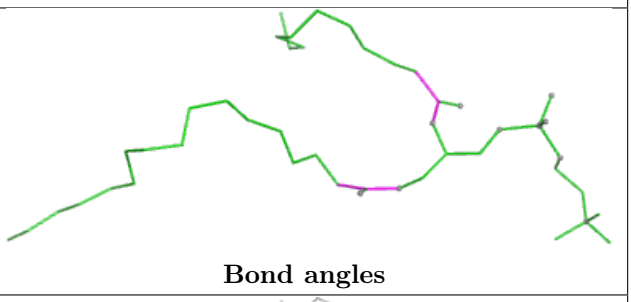
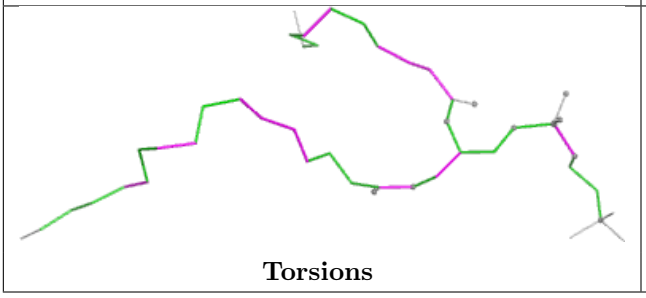


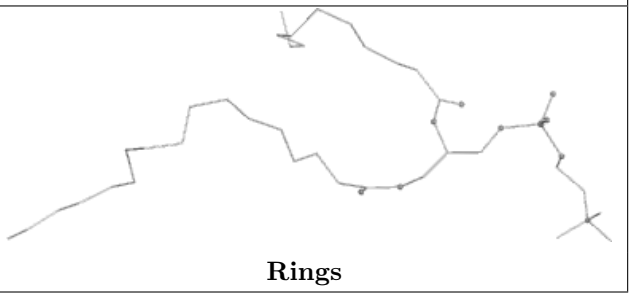
Bond lengths



Bond angles



Torsions



Rings

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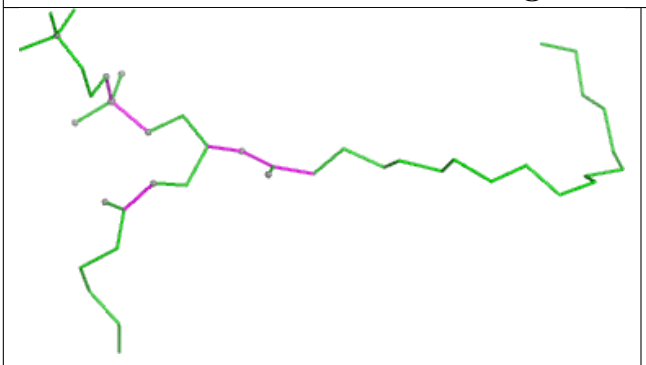

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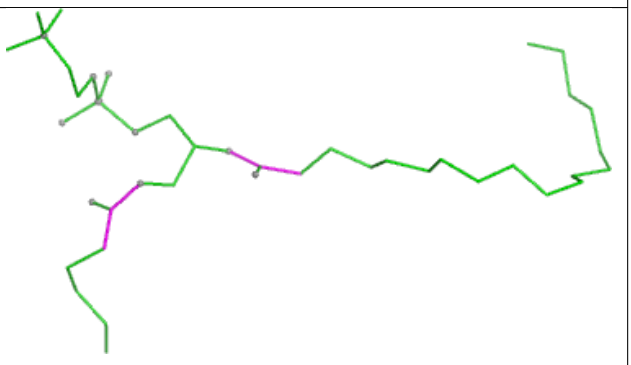

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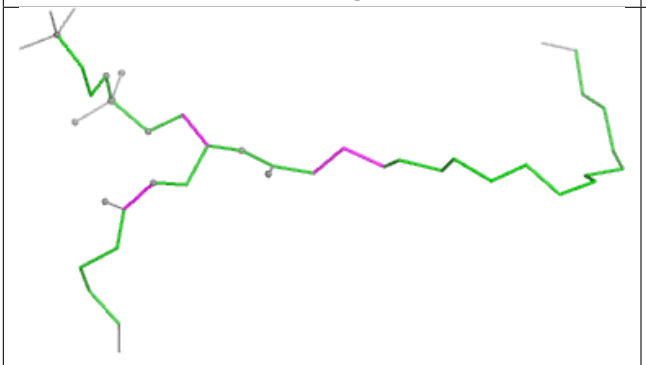

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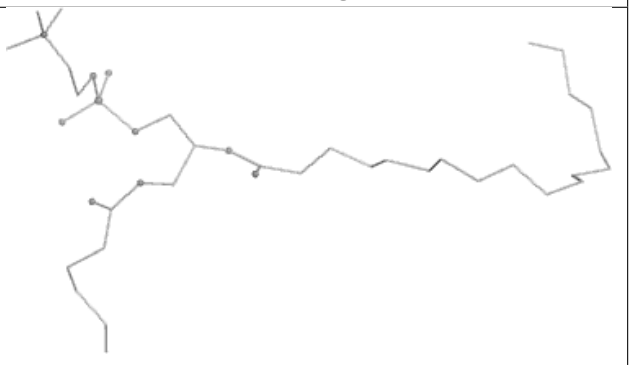
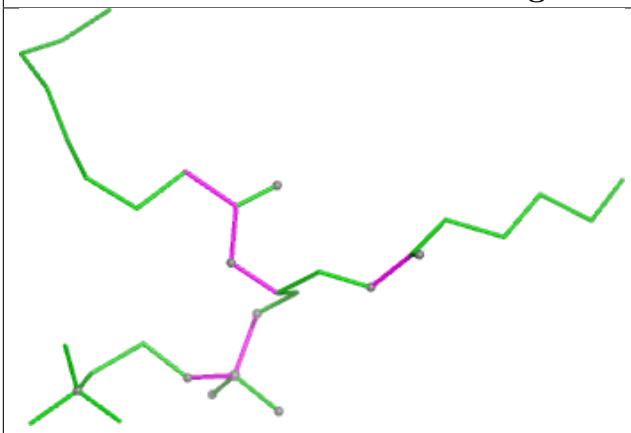


Rings

Ligand PC1 P 401



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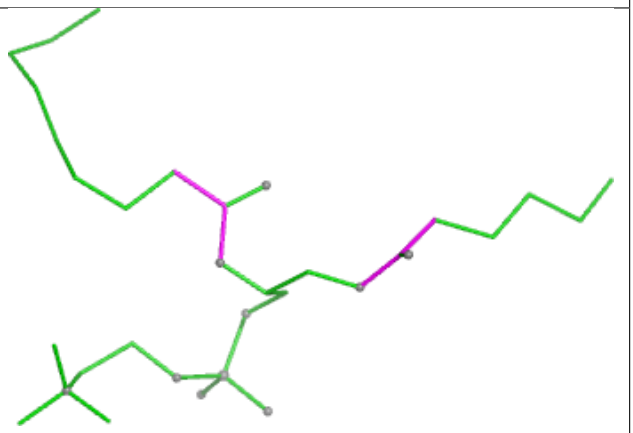

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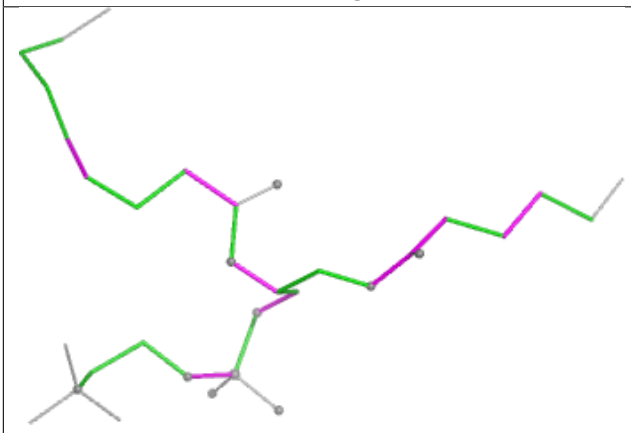

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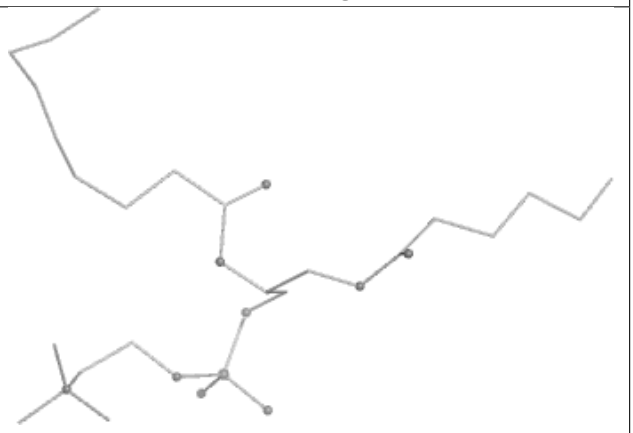
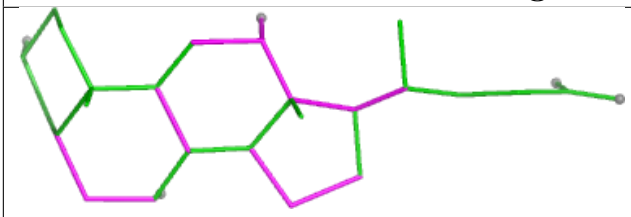


Rings

Ligand CHD i 201



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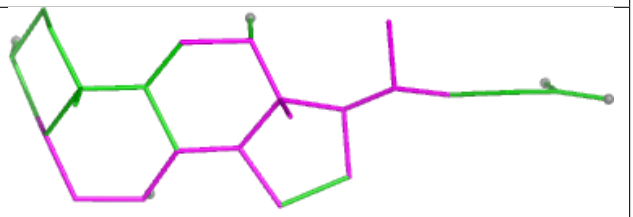

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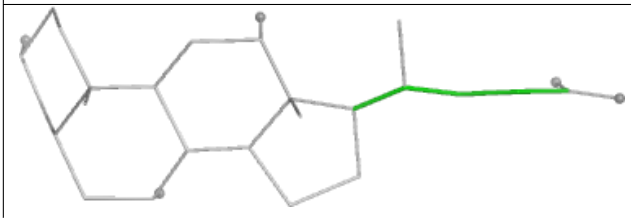

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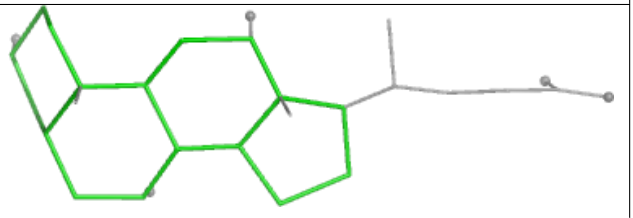
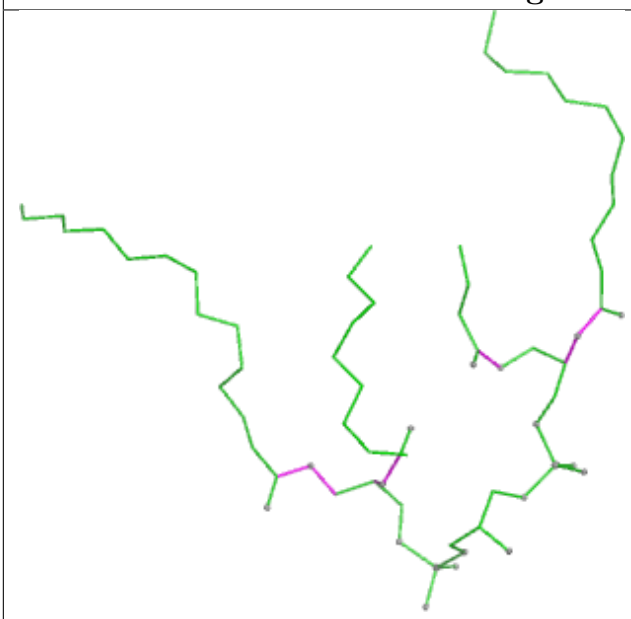


Rings

Ligand CDL L 702



Bond lengths



Bond angles

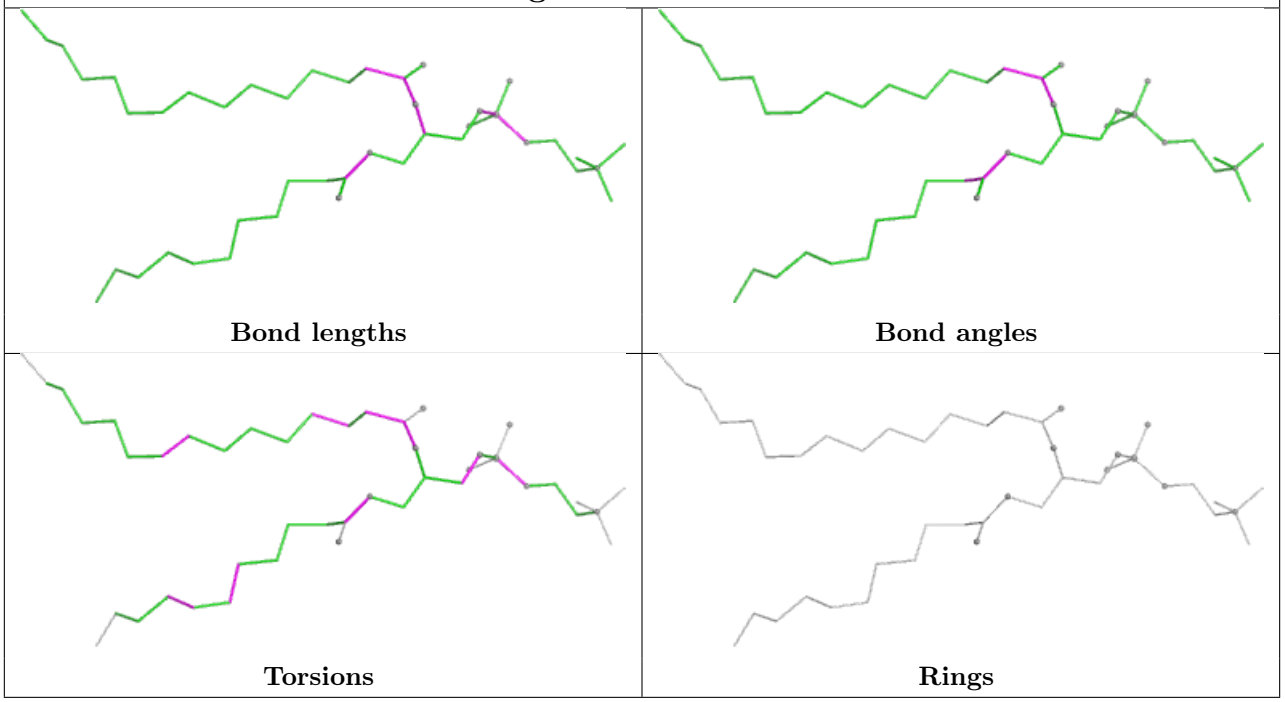


Torsions

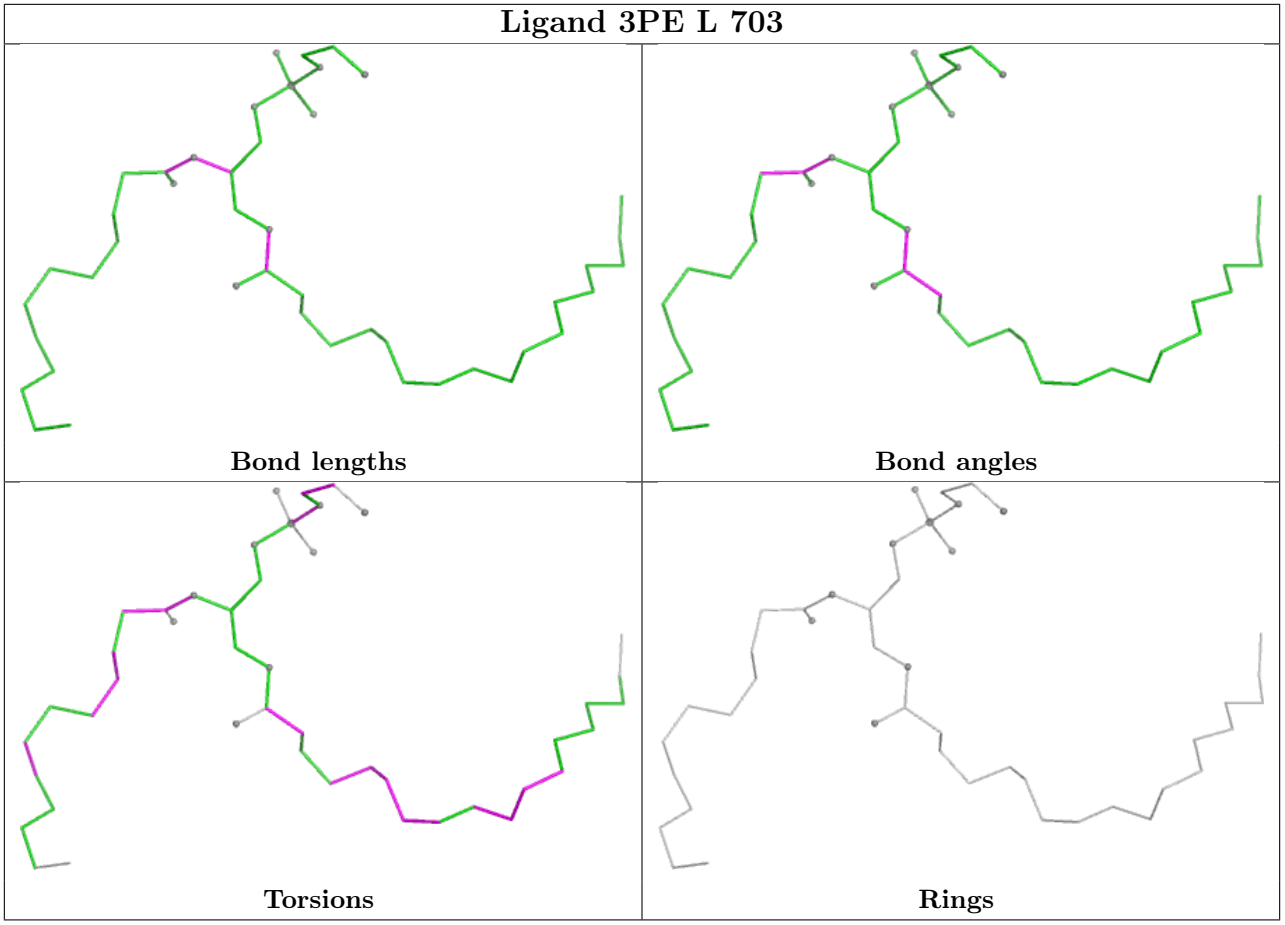


Rings

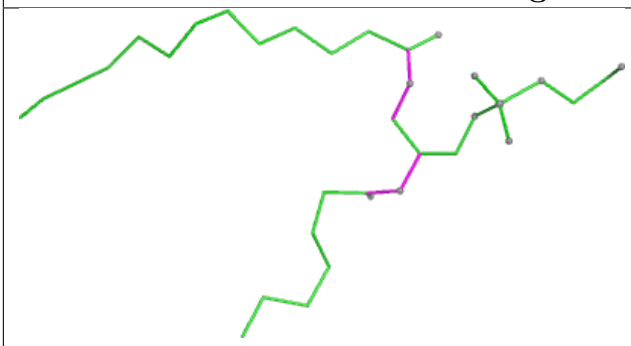
Ligand PC1 B 203



Ligand 3PE L 703



Ligand 3PE P 404



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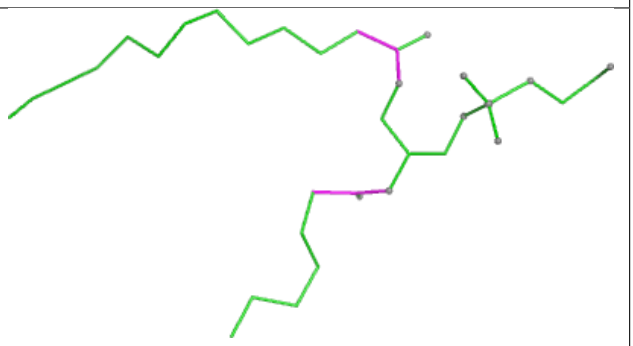

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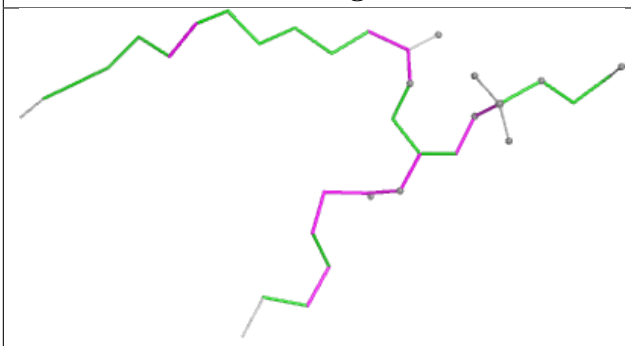
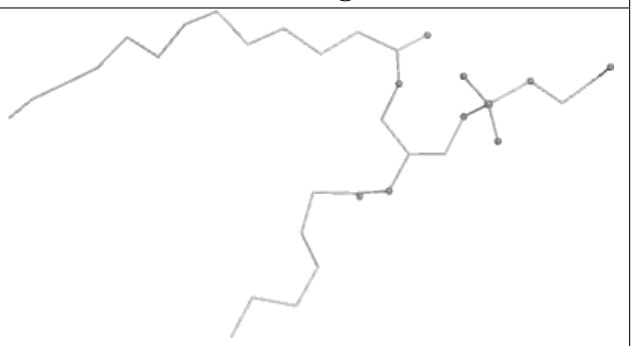
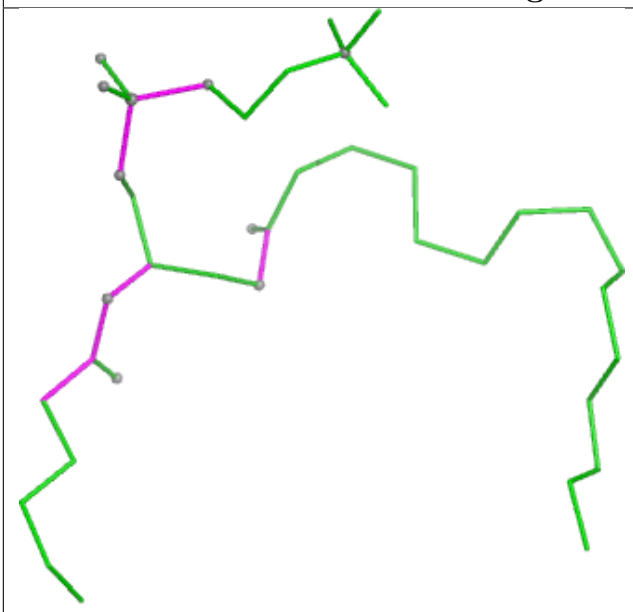


Torsions



Rings

Ligand PC1 N 404



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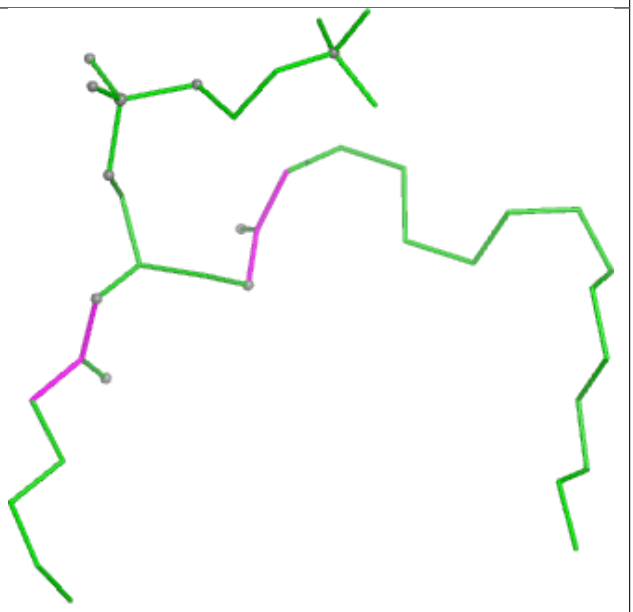
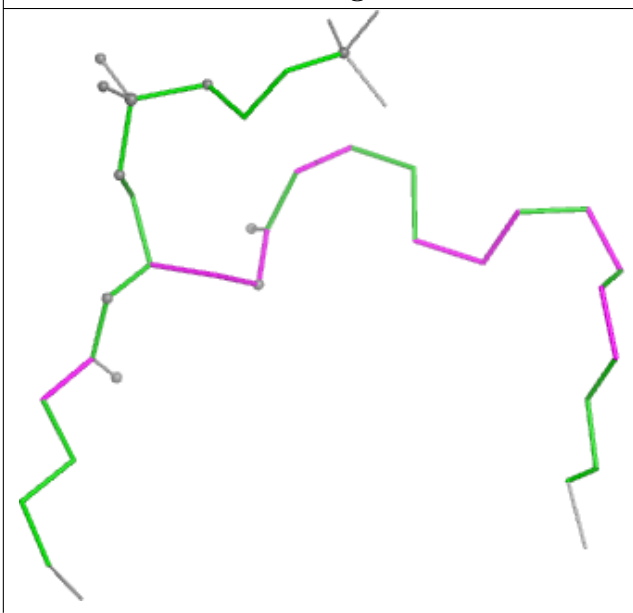


Bond angles

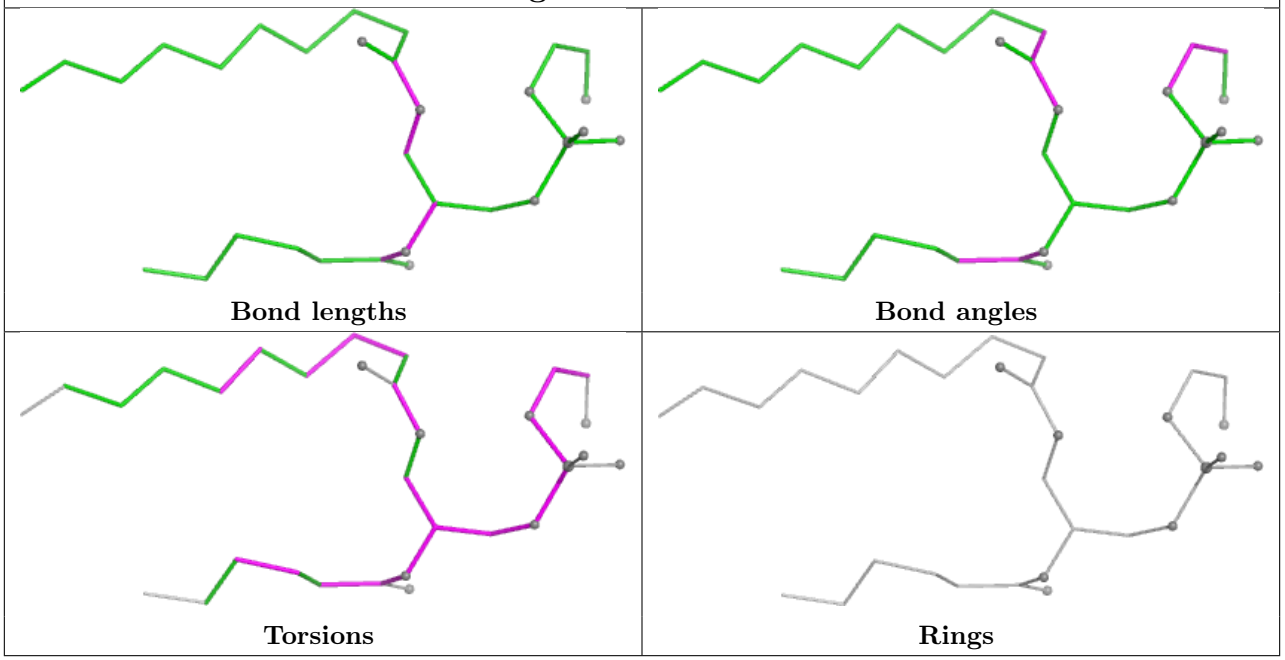


Torsions

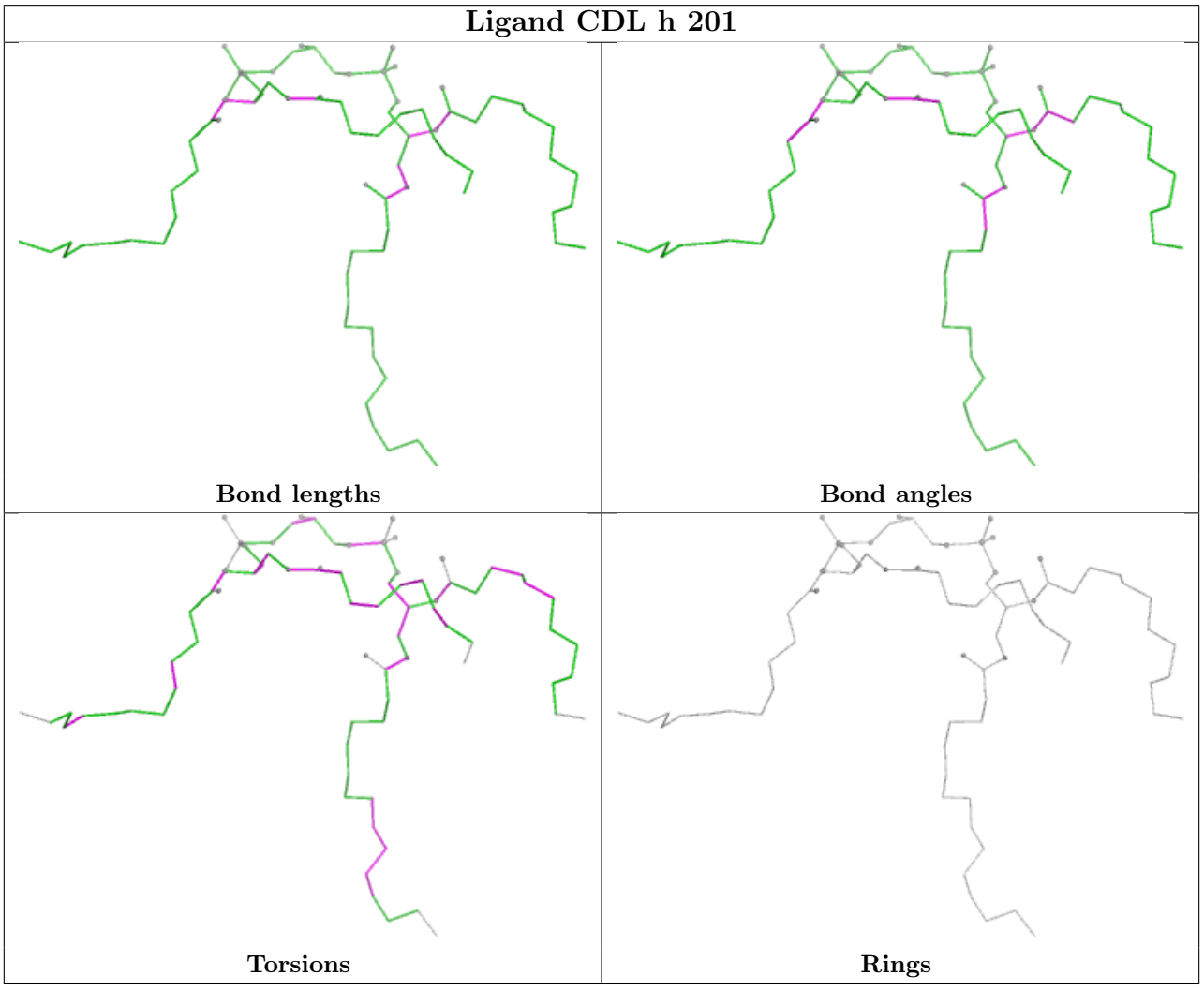


Rings

Ligand 3PE Y 801



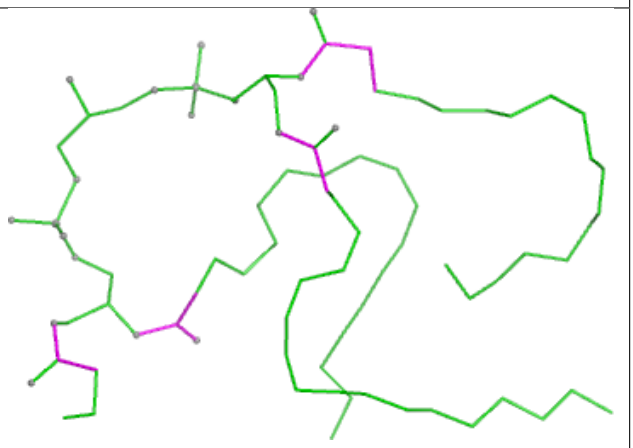
Ligand CDL h 201



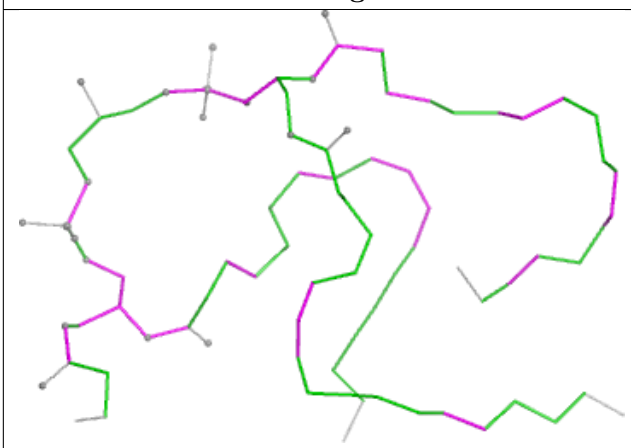
Ligand CDL X 201



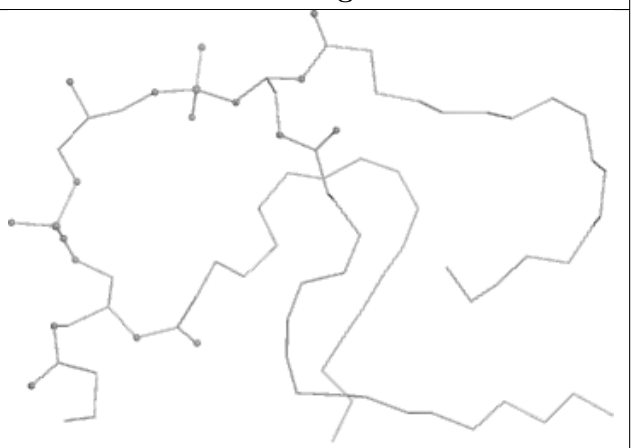
Bond lengths



Bond angles

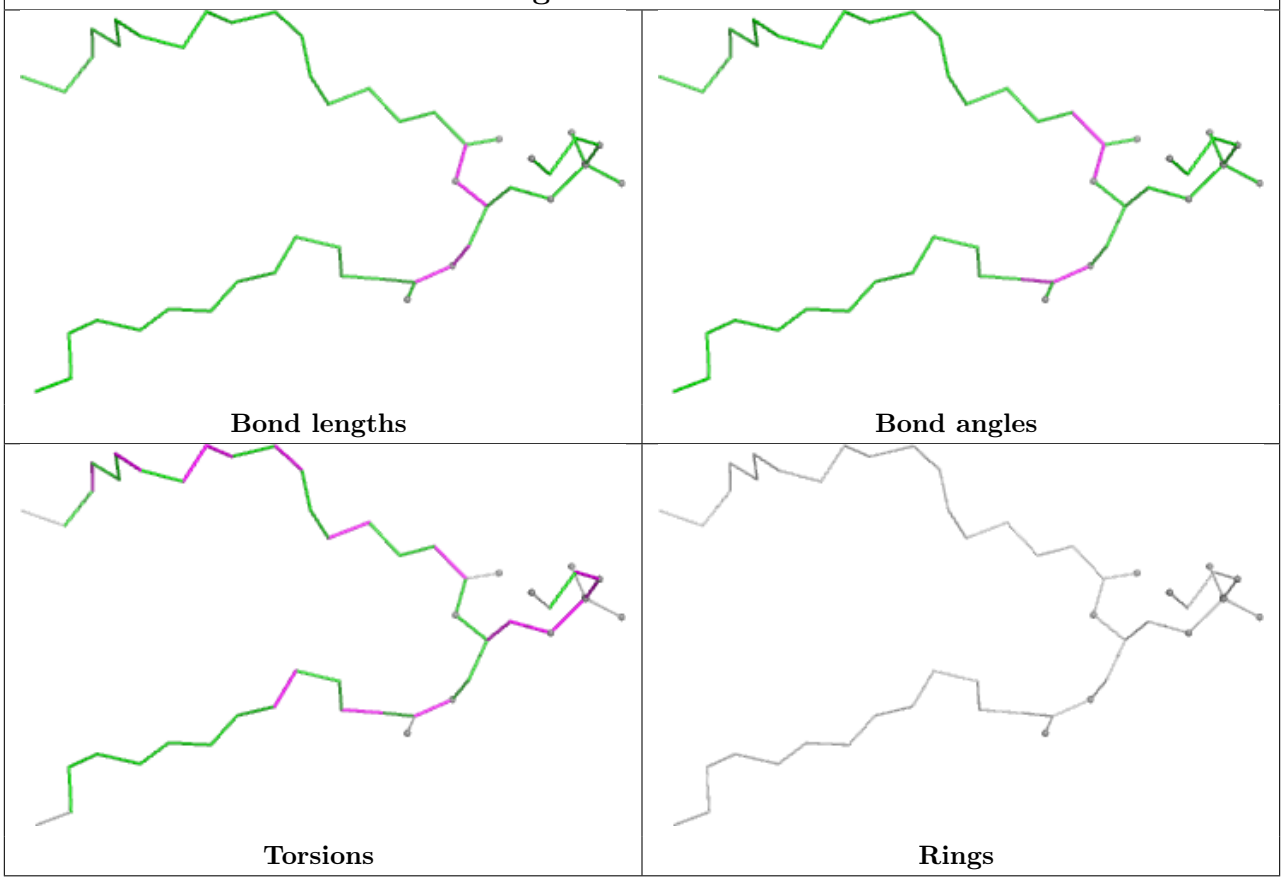


Torsions

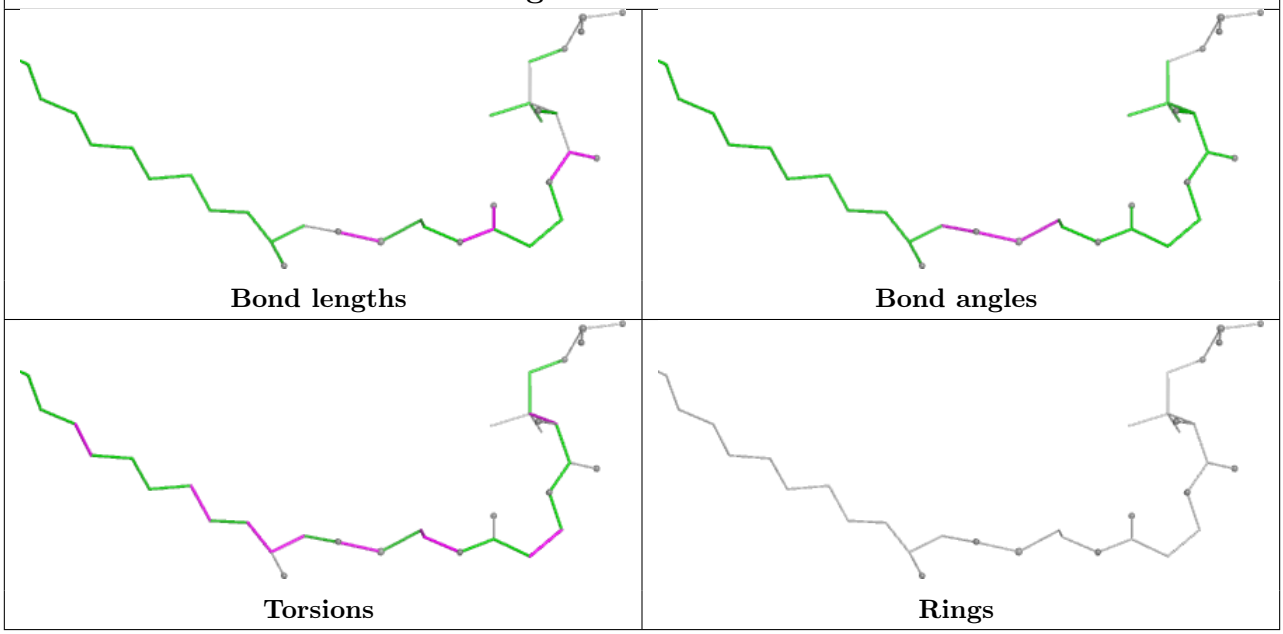


Rings

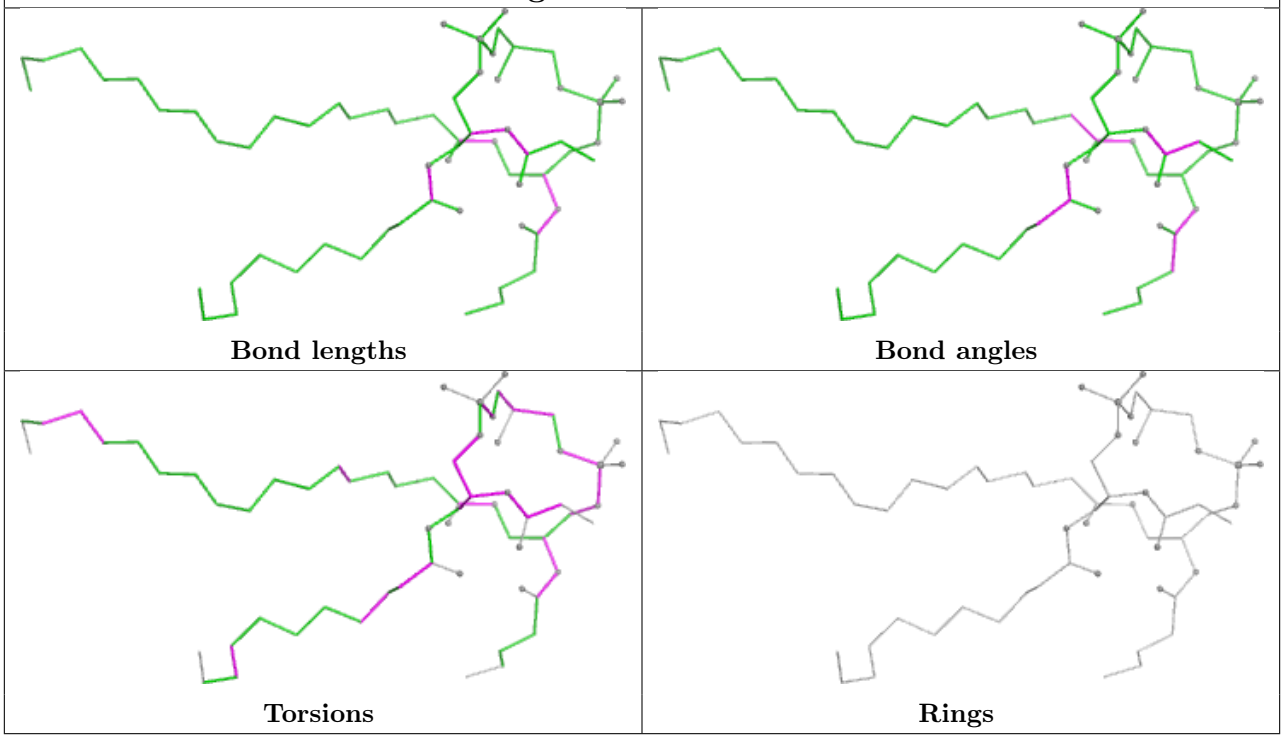
Ligand 3PE b 201



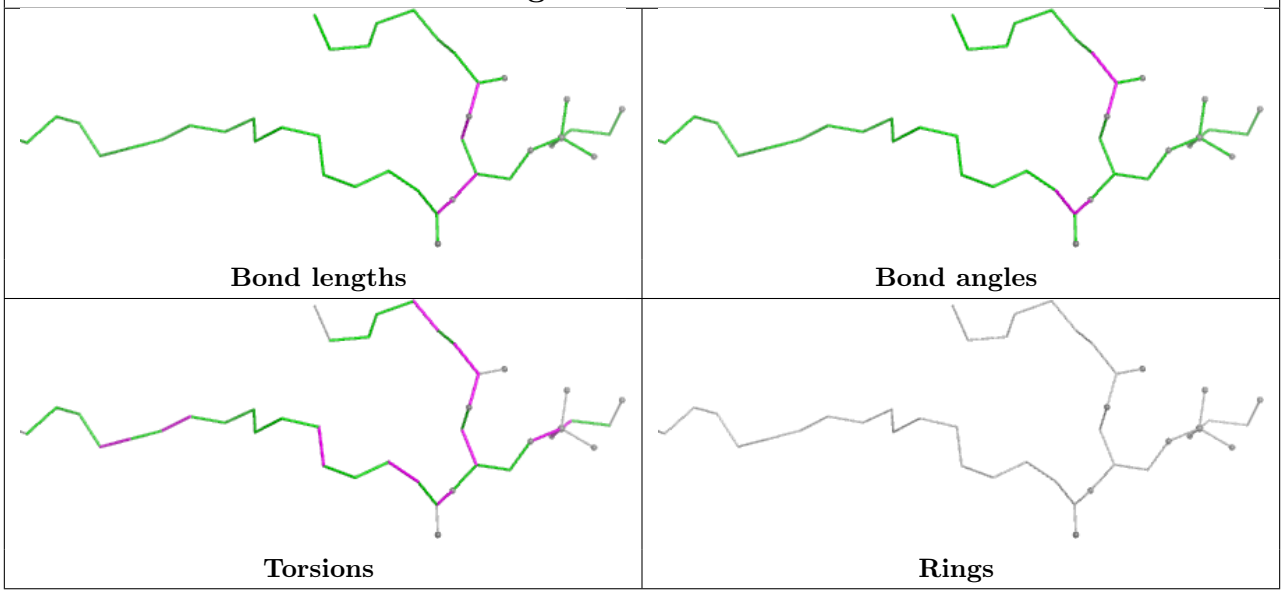
Ligand EHZ T 101



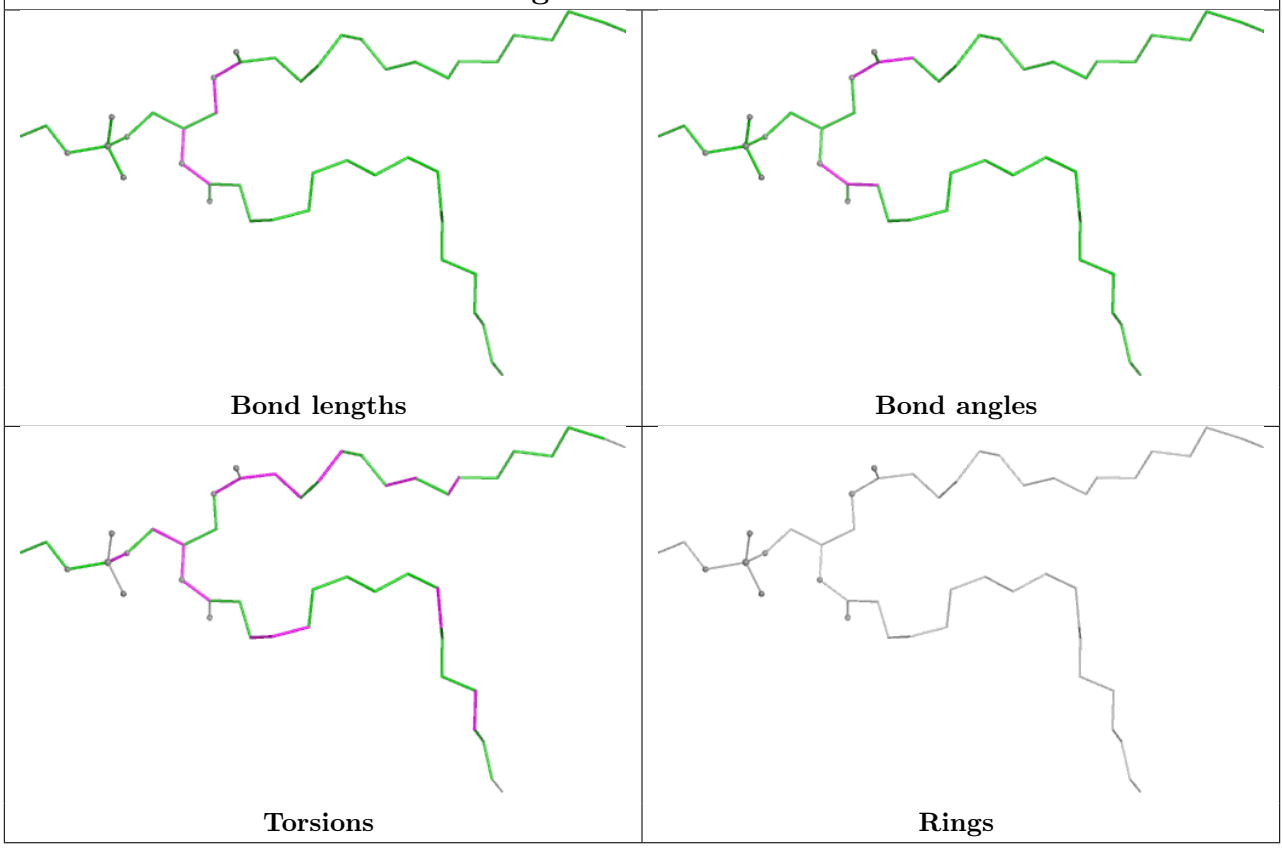
Ligand CDL d 201



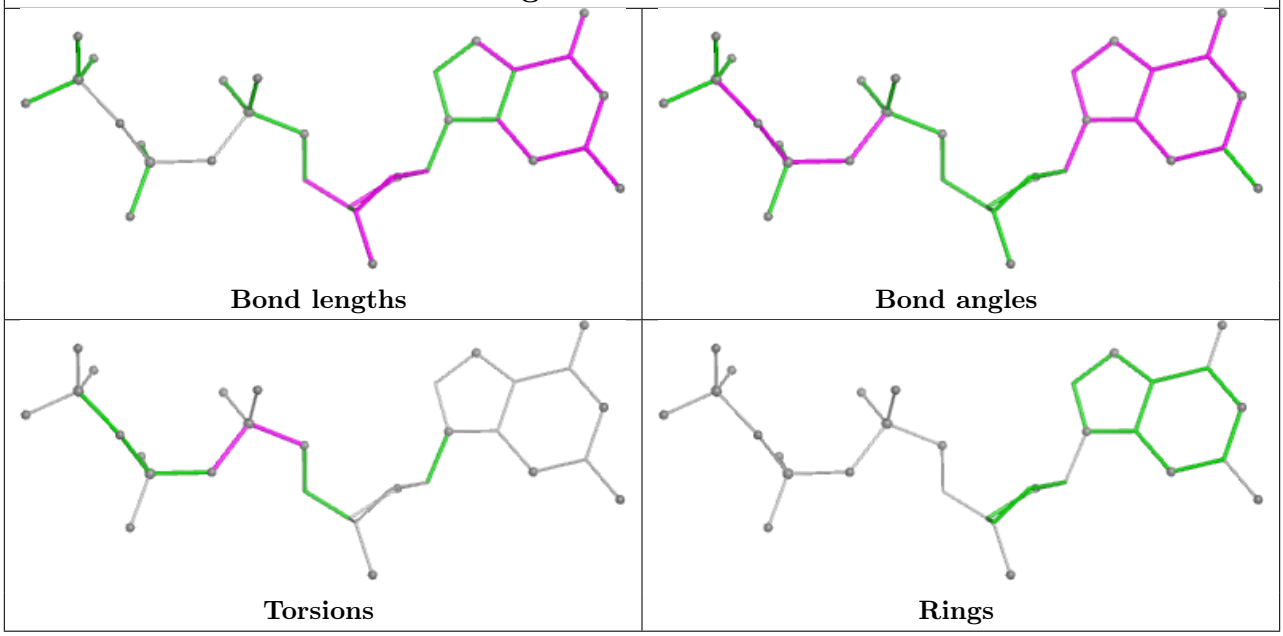
Ligand 3PE m 201



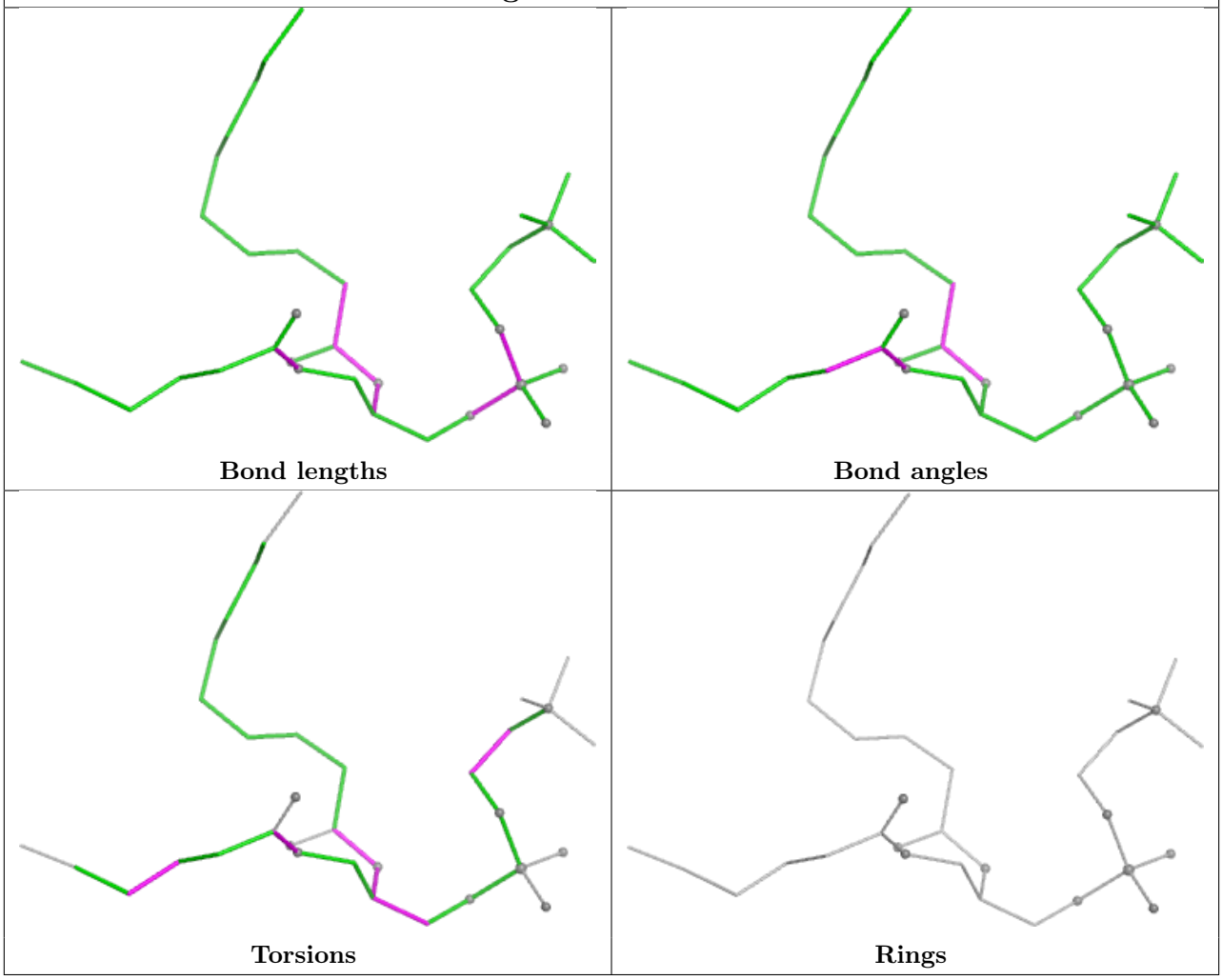
Ligand 3PE L 704



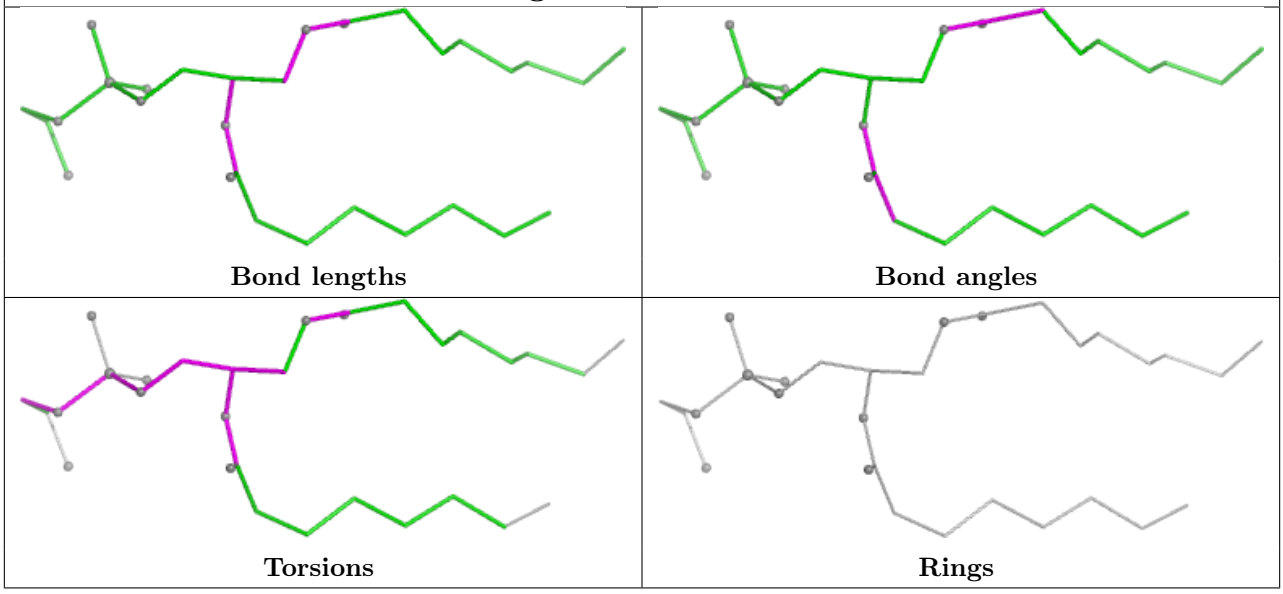
Ligand DGT O 401



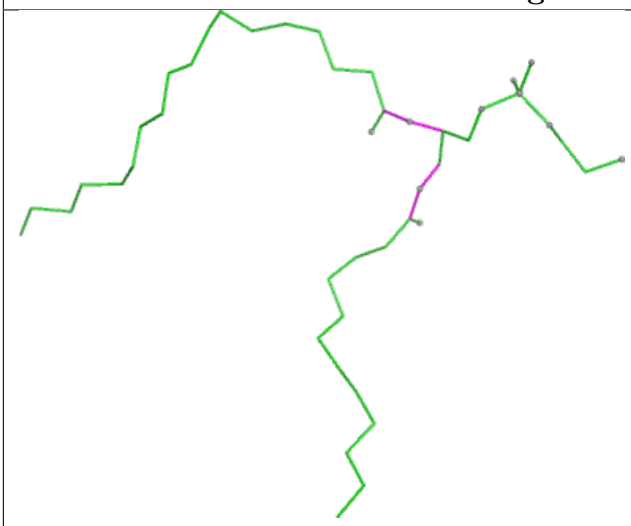
Ligand PC1 A 201



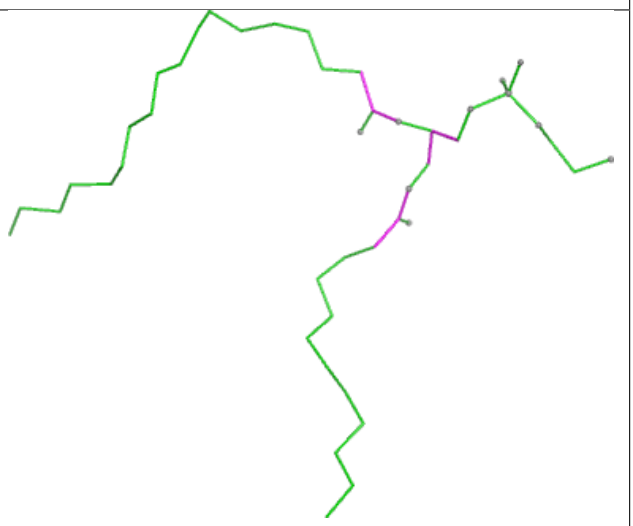
Ligand 3PE N 402



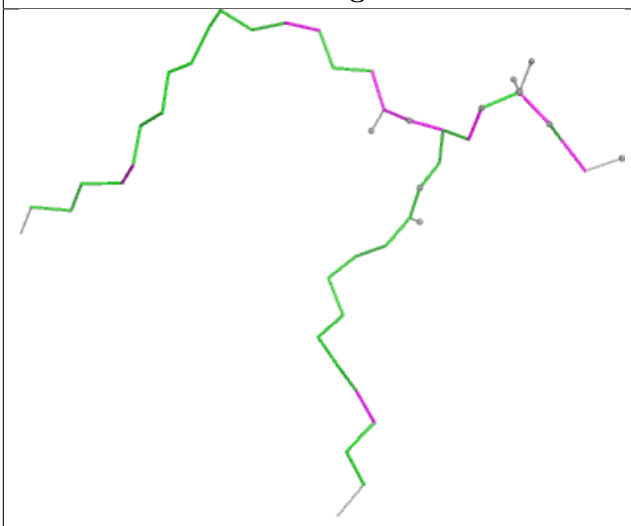
Ligand 3PE H 703



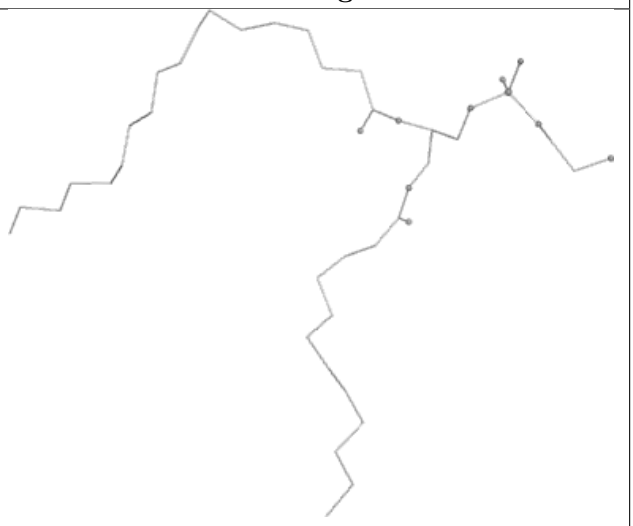
Bond lengths



Bond angles

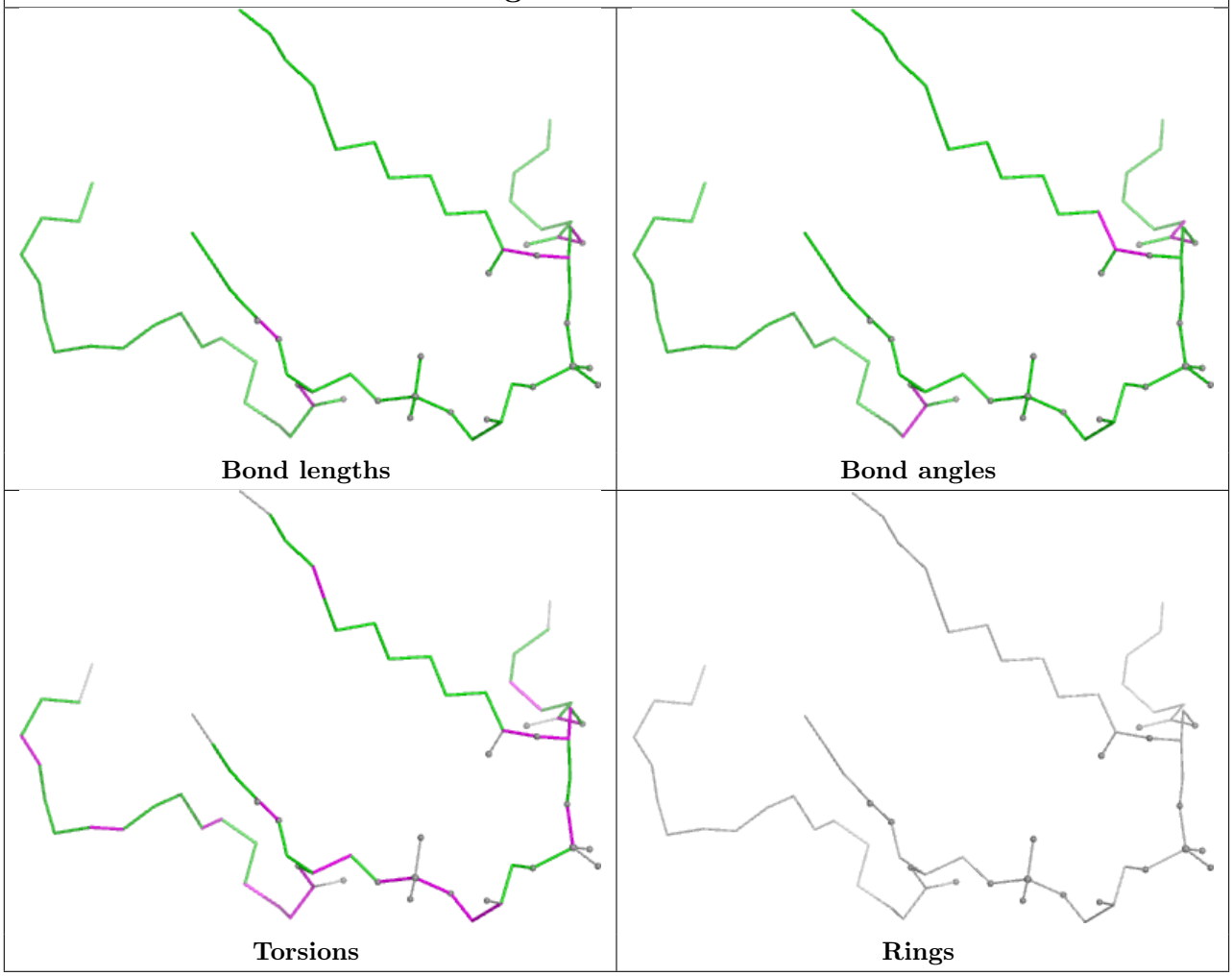


Torsions

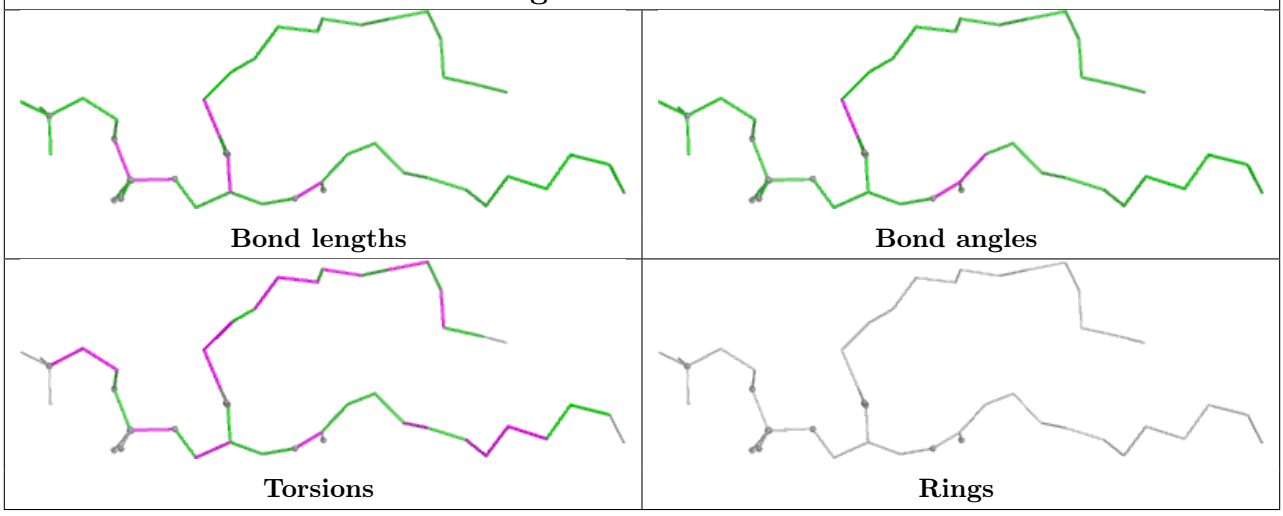


Rings

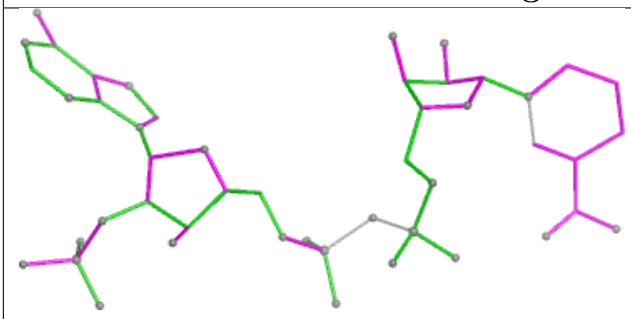
Ligand CDL P 402



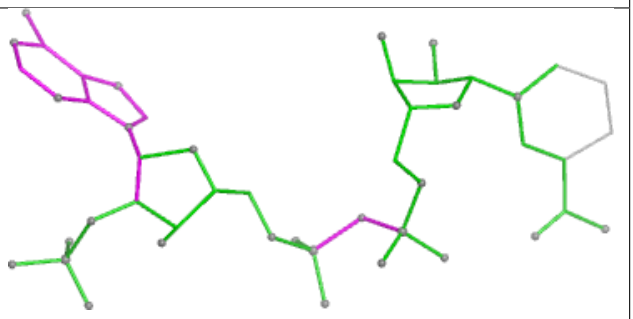
Ligand PC1 Z 200



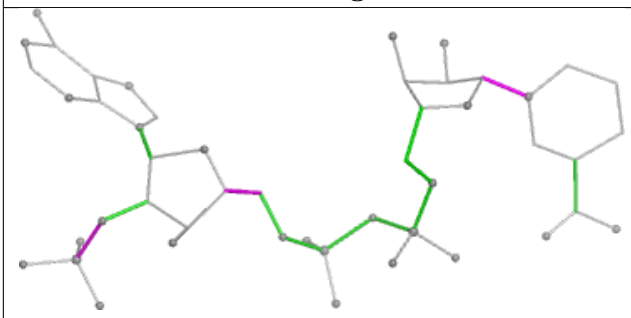
Ligand NDP P 403



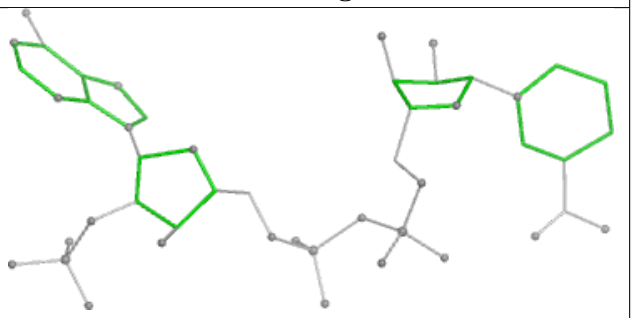
Bond lengths



Bond angles

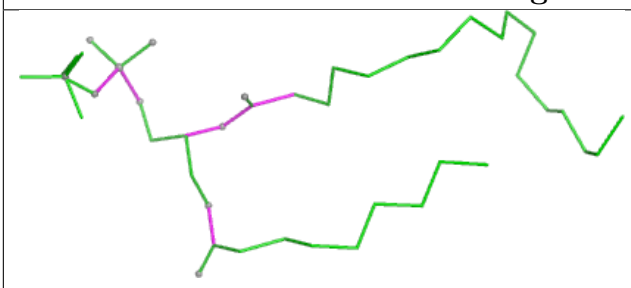


Torsions

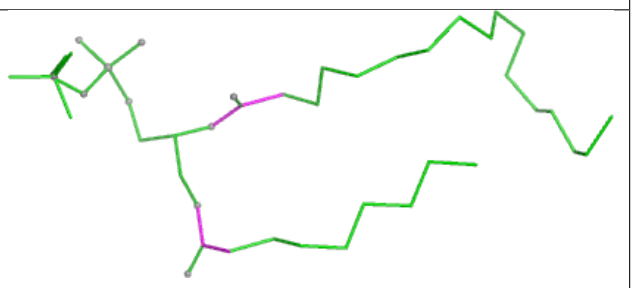


Rings

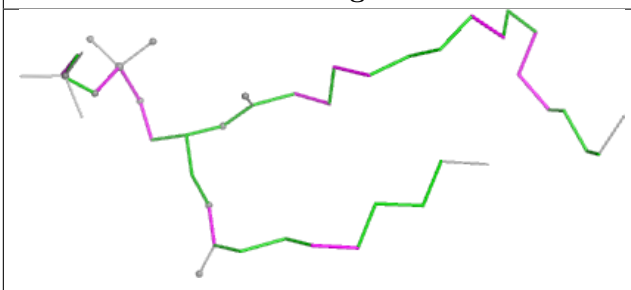
Ligand PC1 h 202



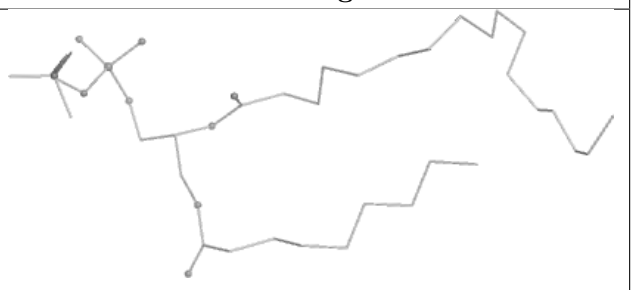
Bond lengths



Bond angles

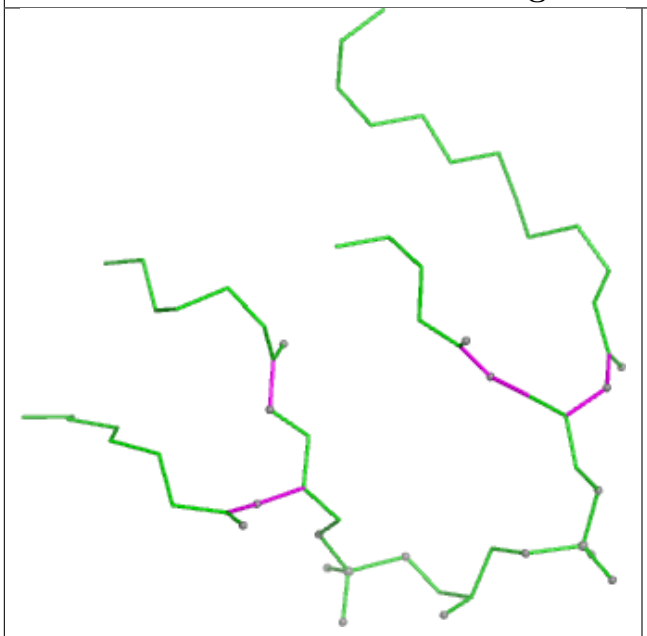


Torsions

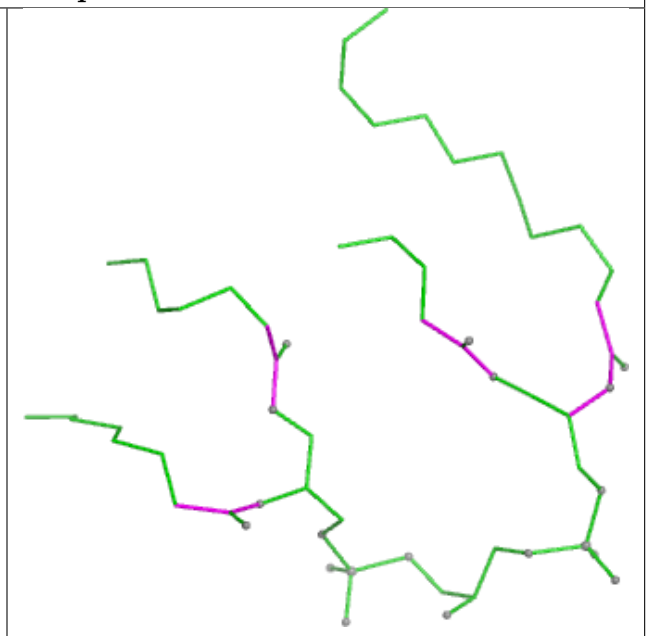


Rings

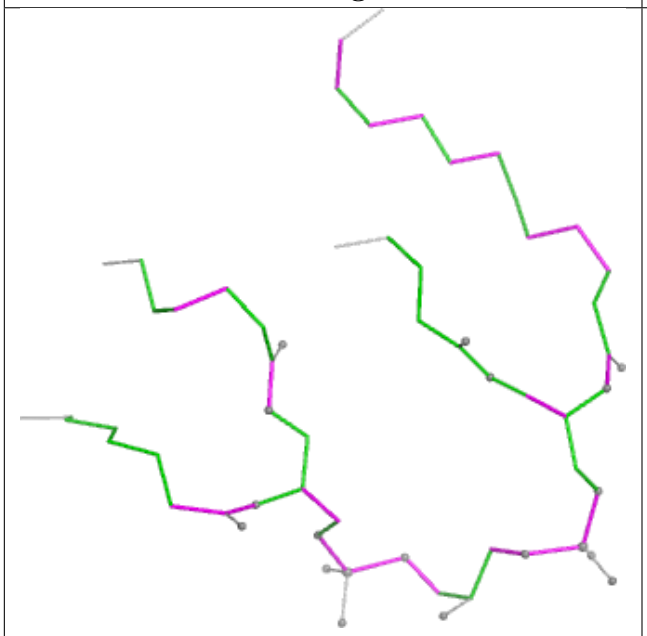
Ligand CDL q 202



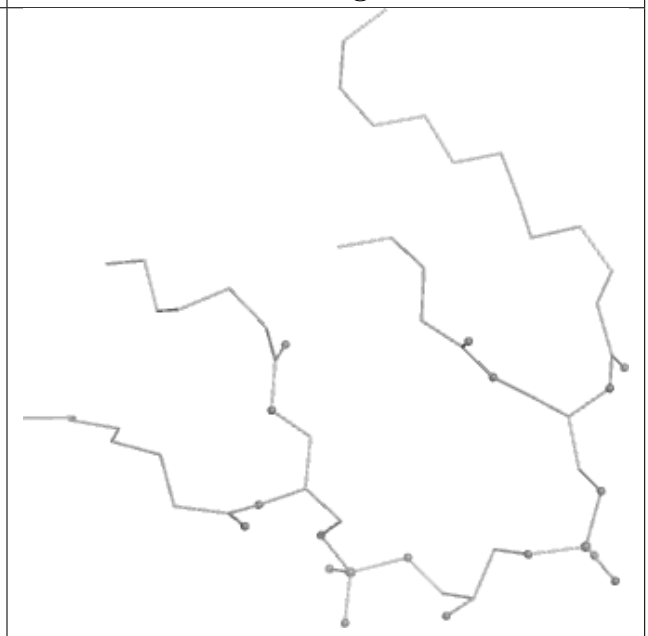
Bond lengths



Bond angles

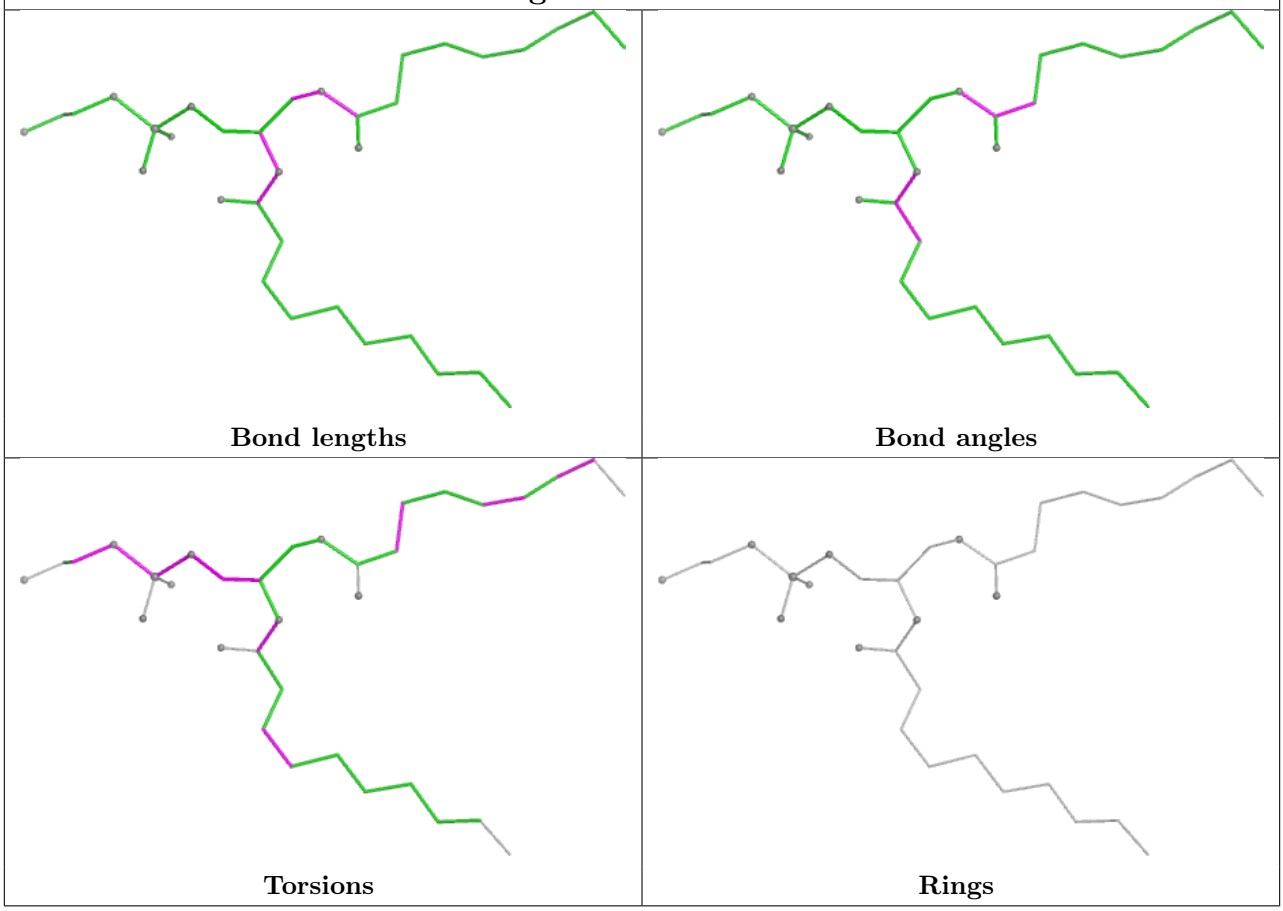


Torsions

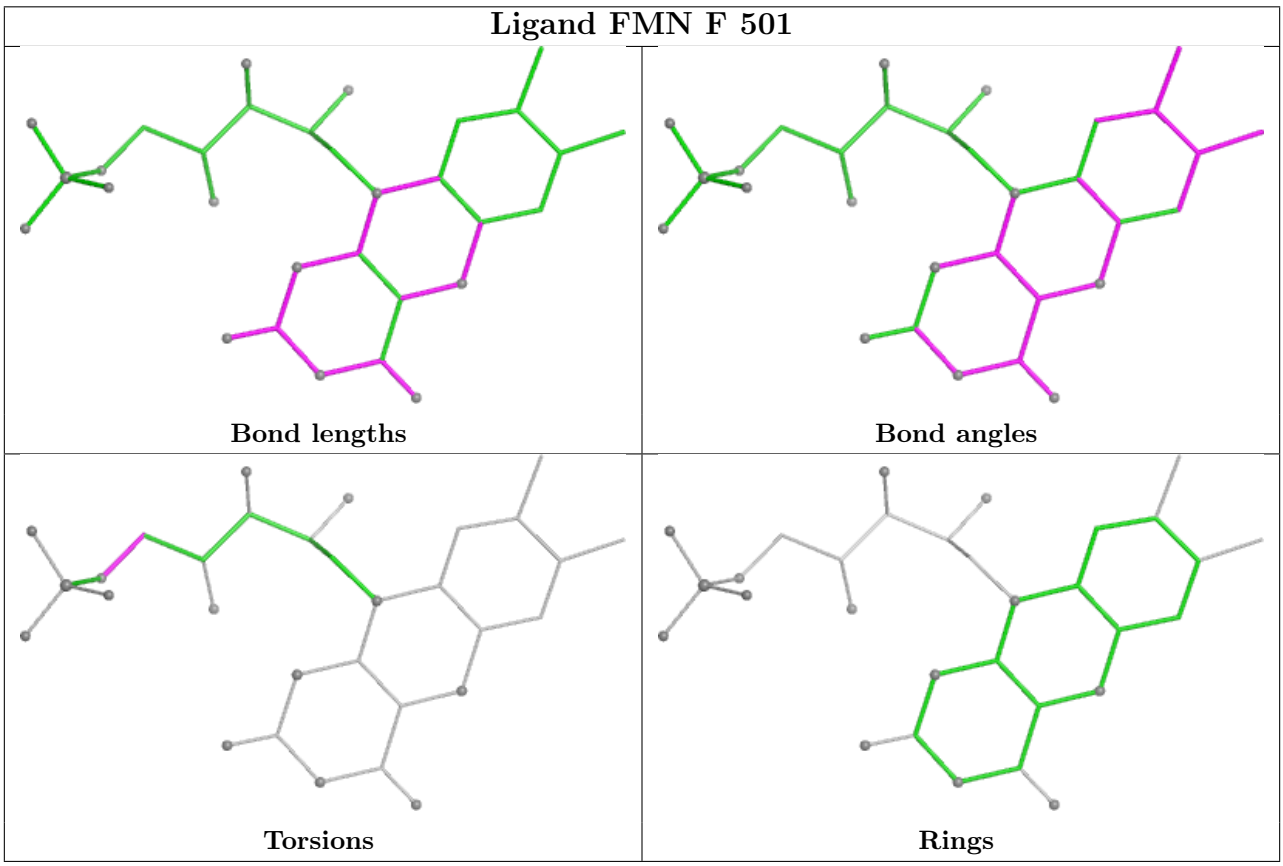


Rings

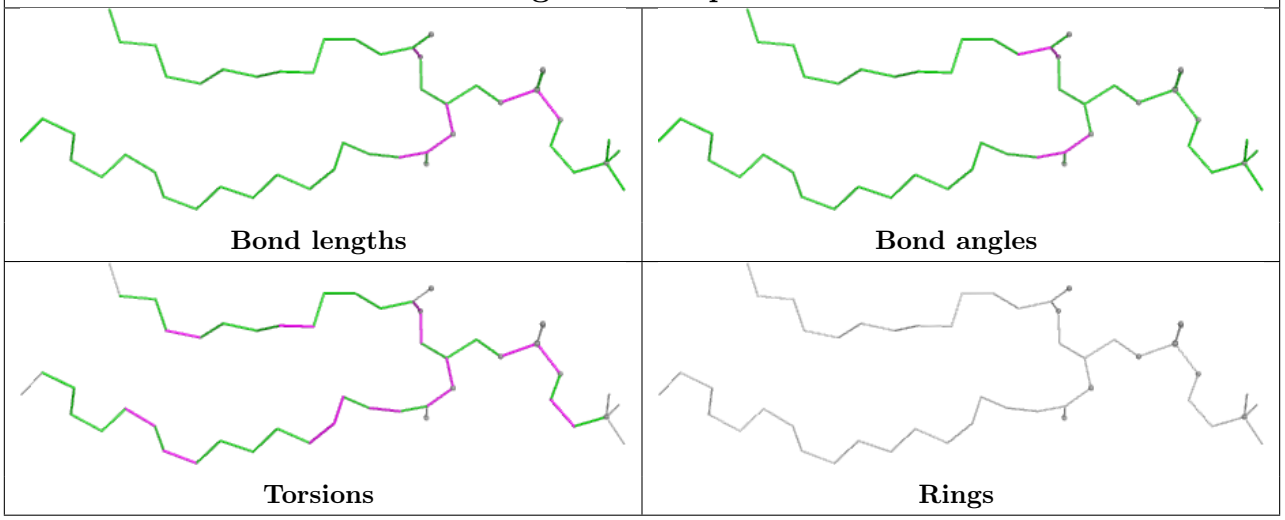
Ligand 3PE Y 803



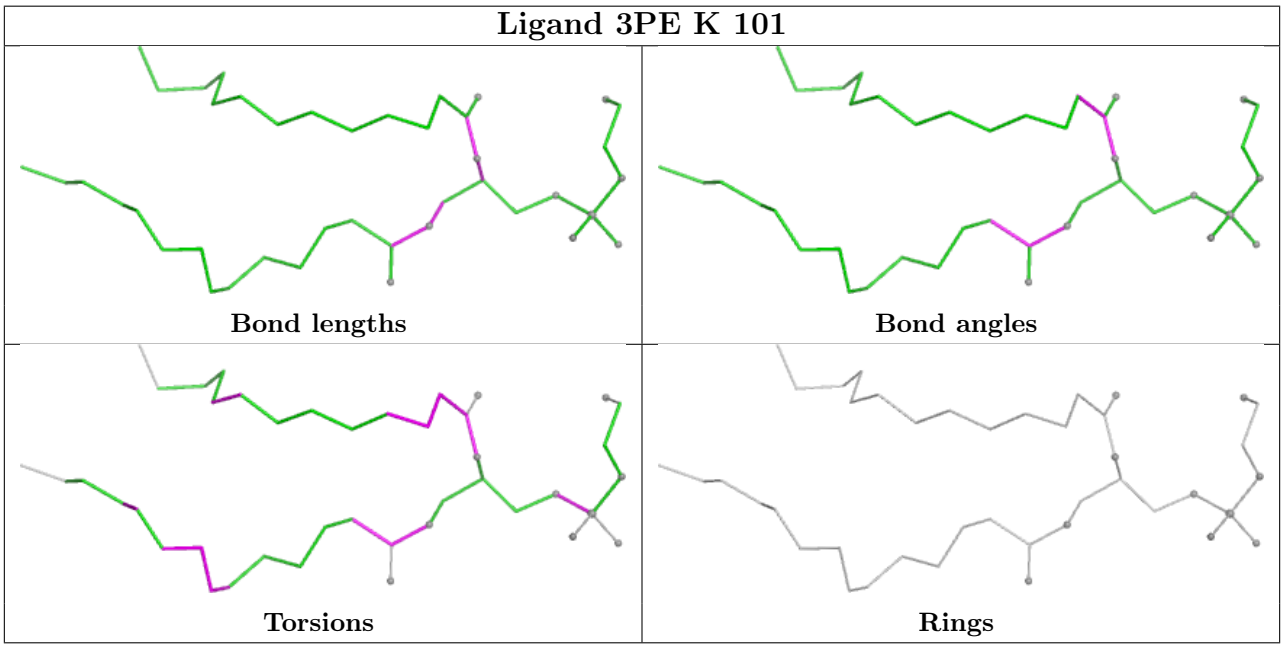
Ligand FMN F 501



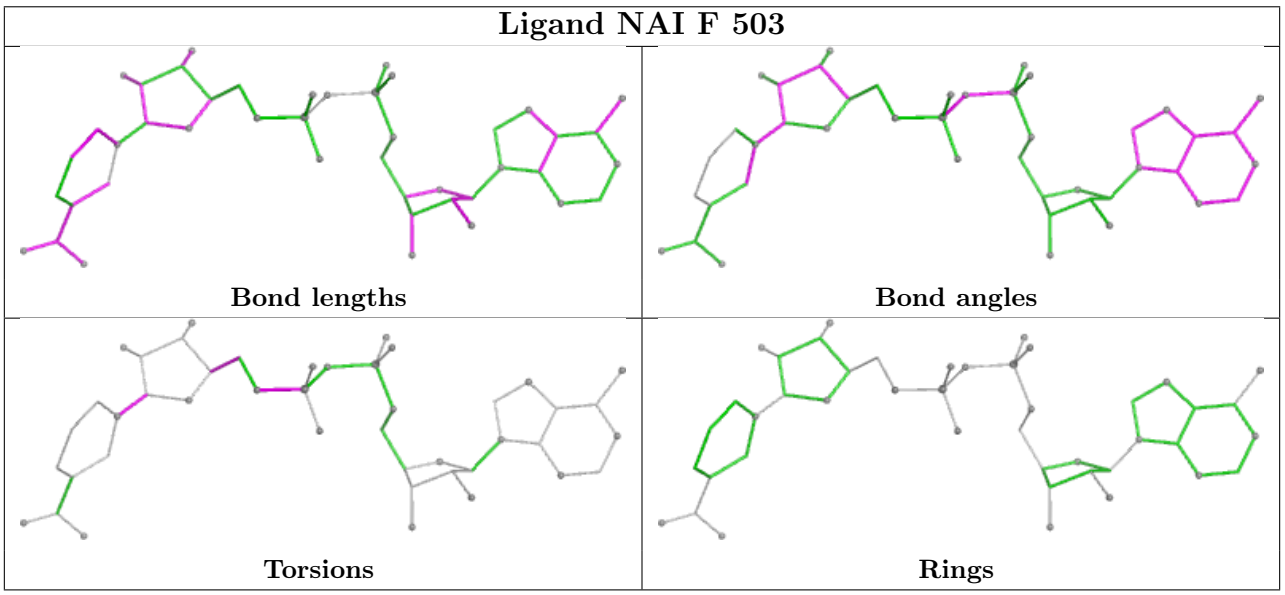
Ligand PC1 q 201

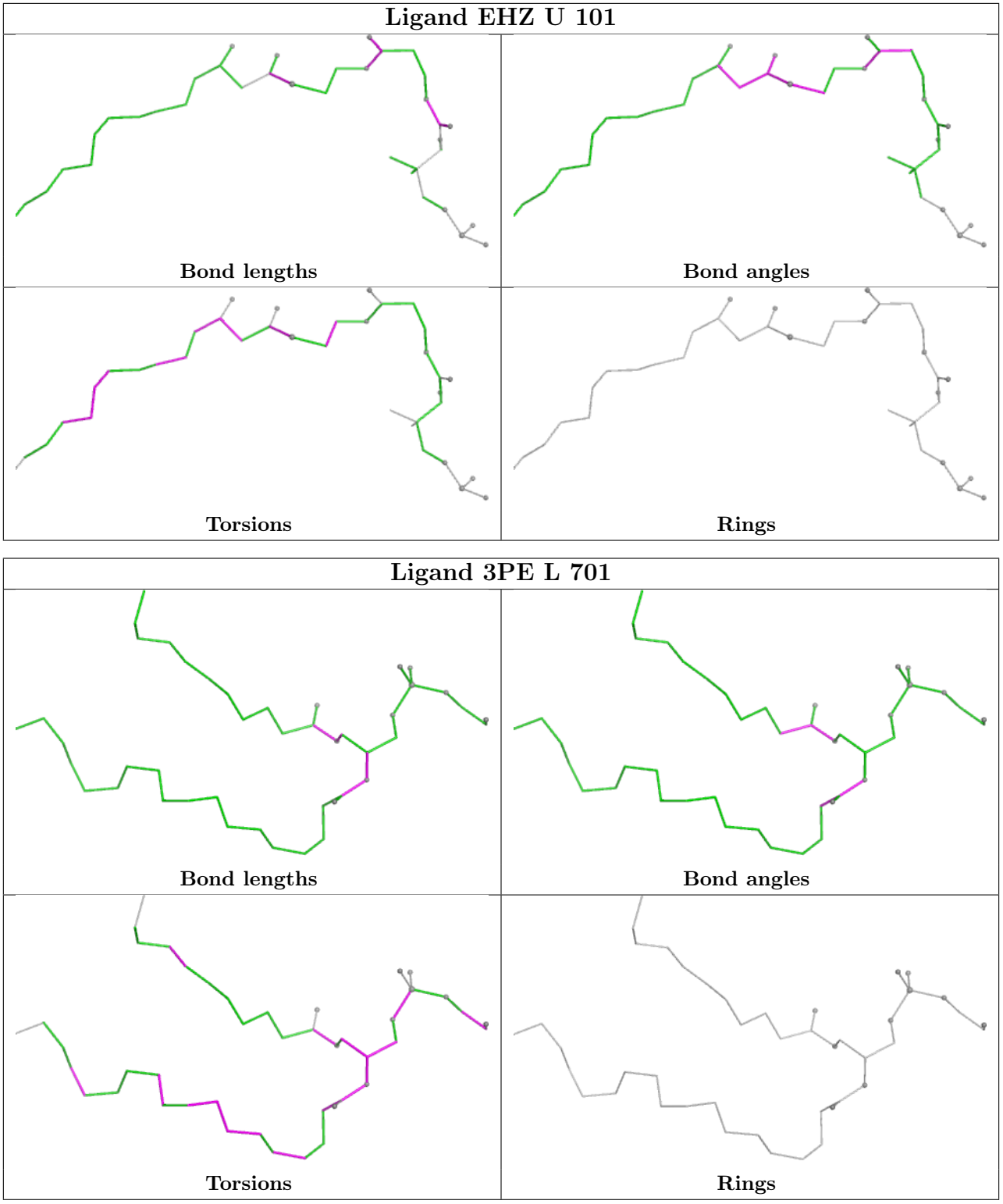


Ligand 3PE K 101



Ligand NAI F 503





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.

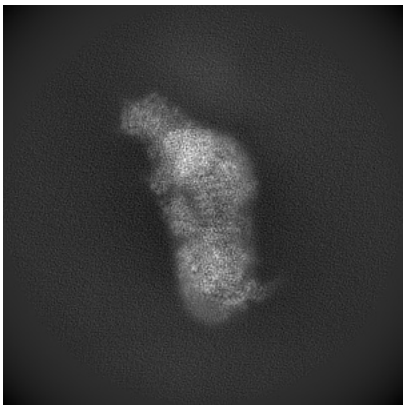
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55031. These allow visual inspection of the internal detail of the map and identification of artifacts.

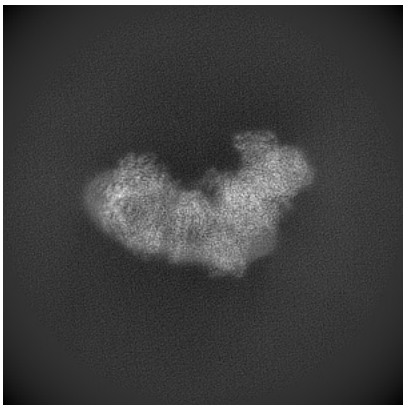
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

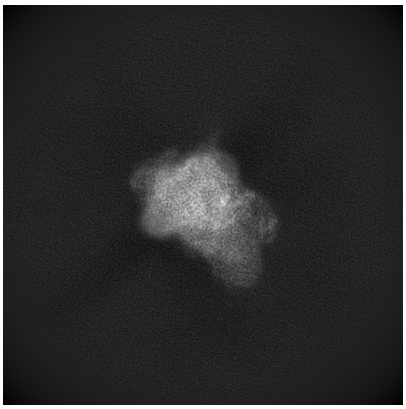
6.1.1 Primary map



X

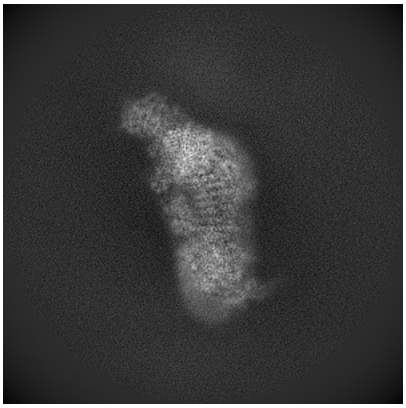


Y

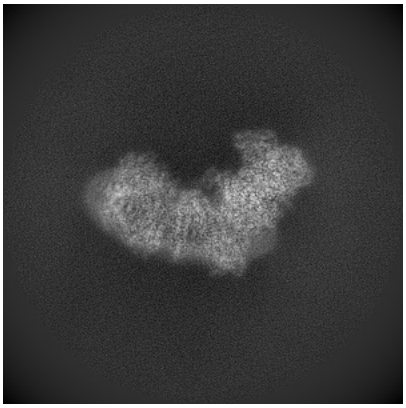


Z

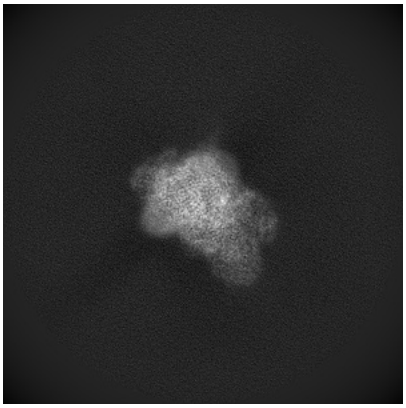
6.1.2 Raw map



X



Y

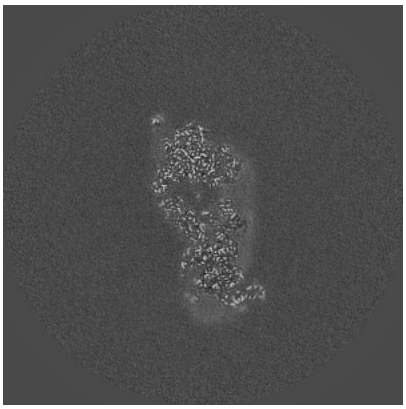


Z

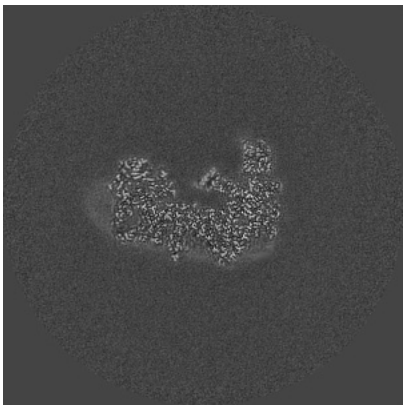
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

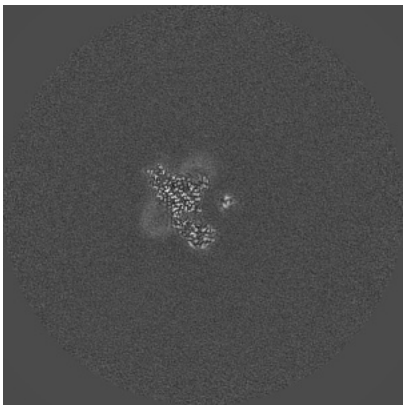
6.2.1 Primary map



X Index: 320

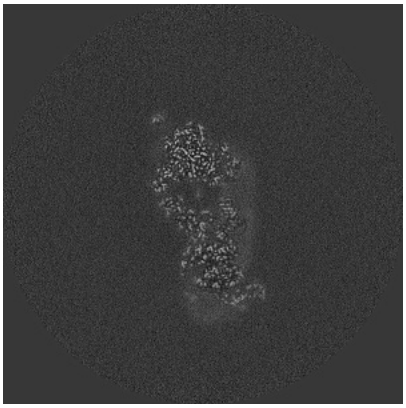


Y Index: 320

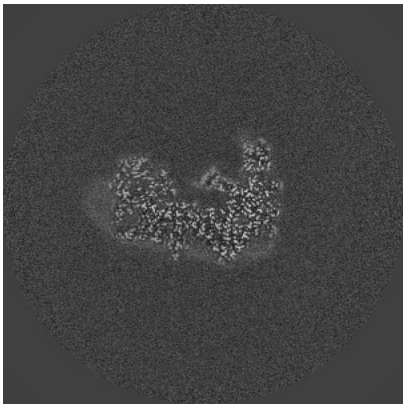


Z Index: 320

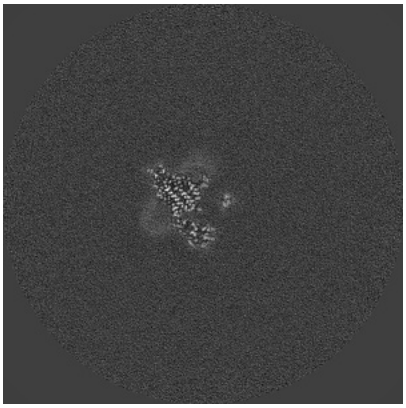
6.2.2 Raw map



X Index: 320



Y Index: 320

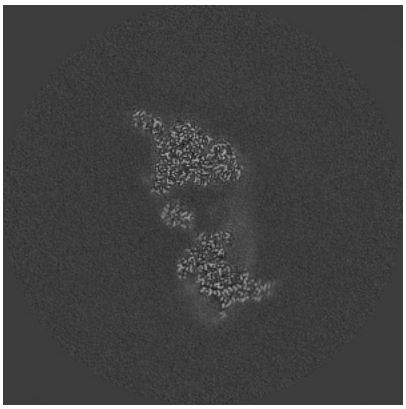


Z Index: 320

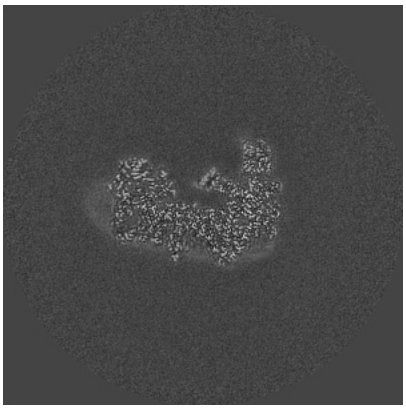
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

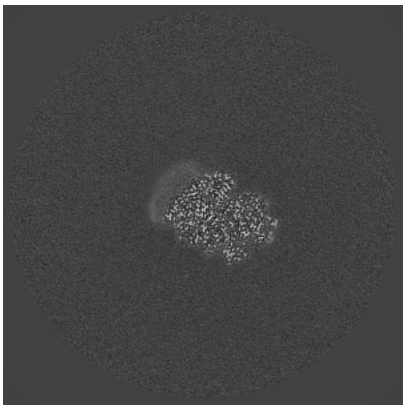
6.3.1 Primary map



X Index: 336

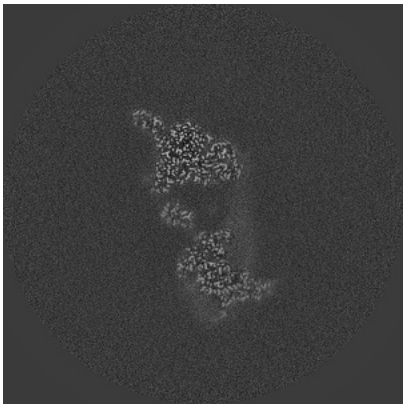


Y Index: 320

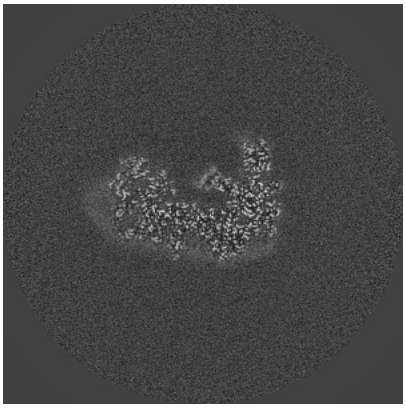


Z Index: 408

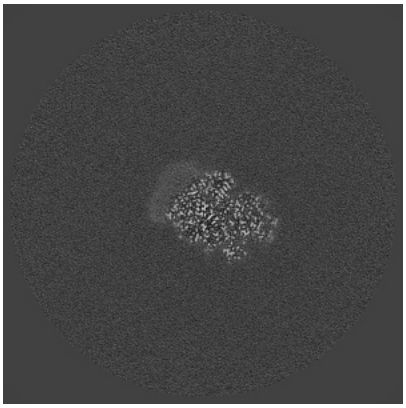
6.3.2 Raw map



X Index: 336



Y Index: 319

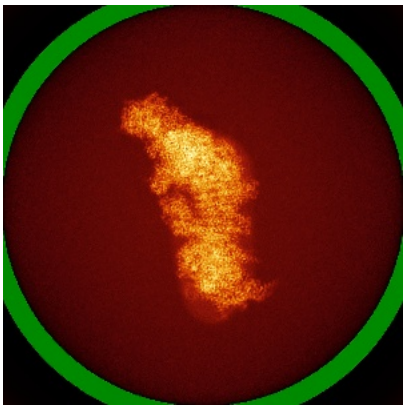


Z Index: 408

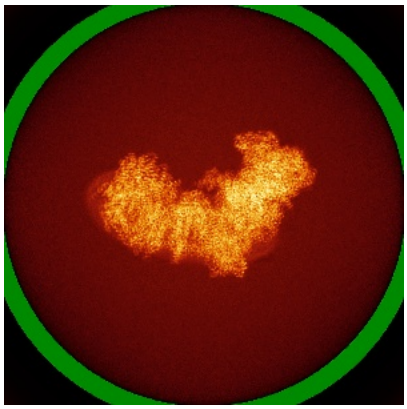
The images above show the largest variance slices of the map in three orthogonal directions.

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

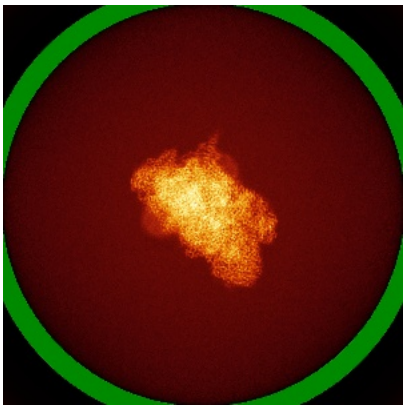
6.4.1 Primary map



X

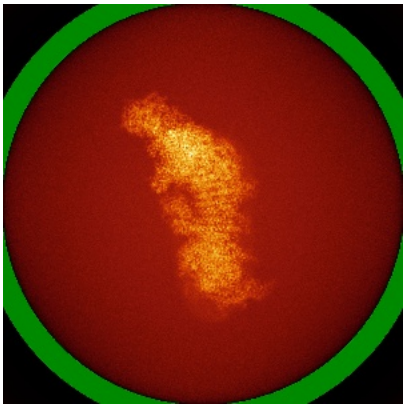


Y

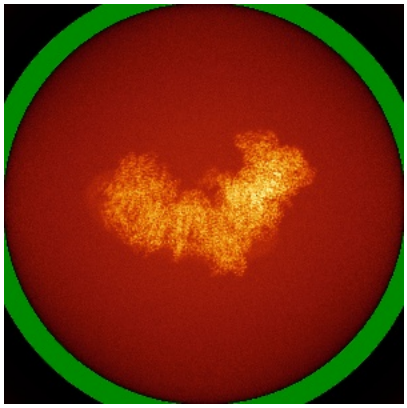


Z

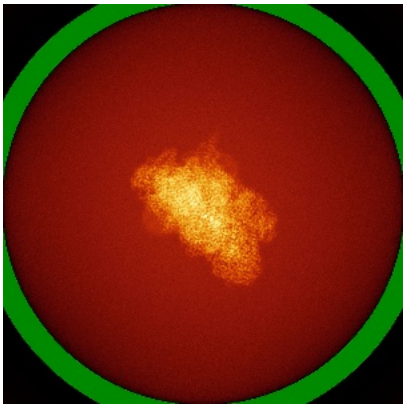
6.4.2 Raw map



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)

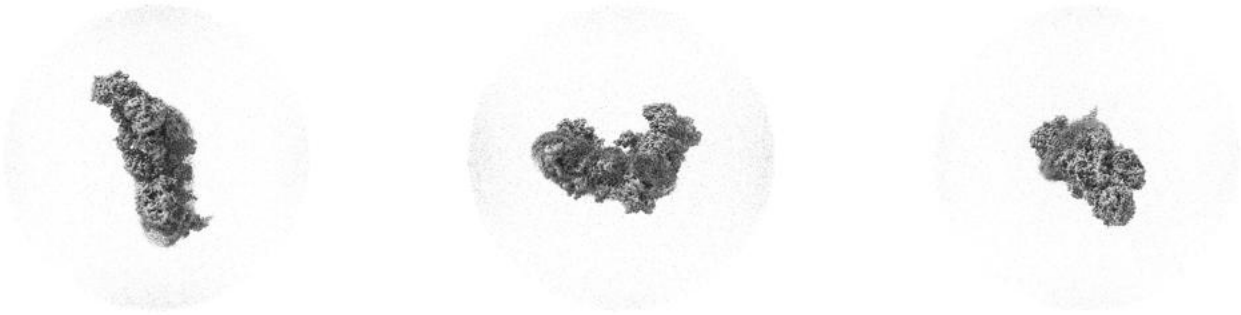
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

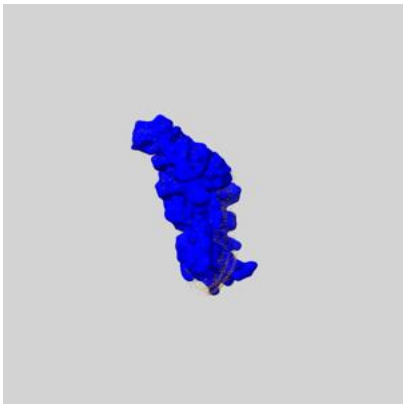
6.6 Mask visualisation (i)

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

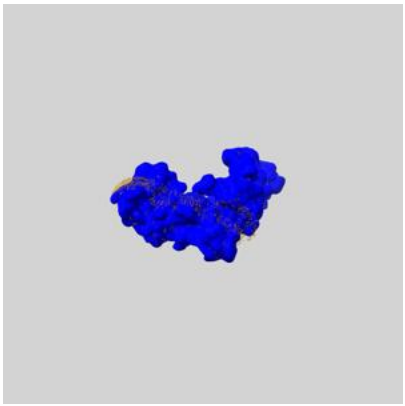
A mask typically either:

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

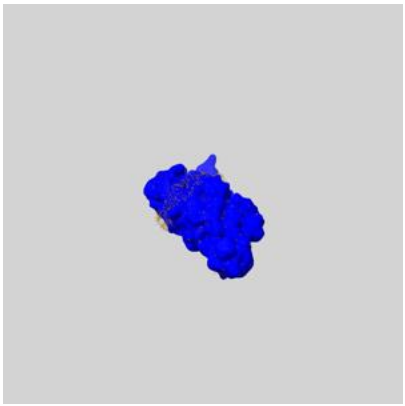
6.6.1 emd_55031_msk_1.map (i)



X



Y

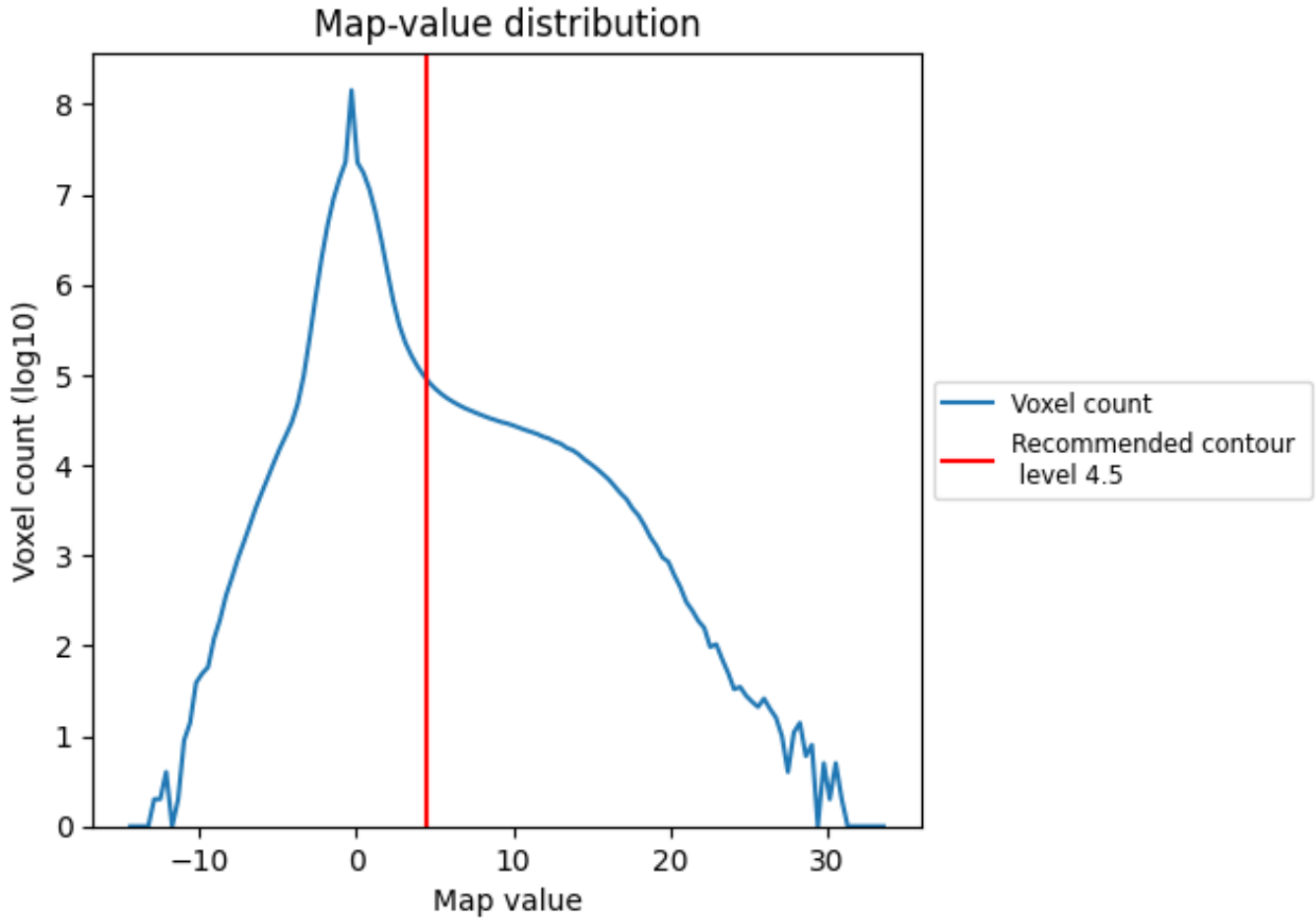


Z

7 Map analysis

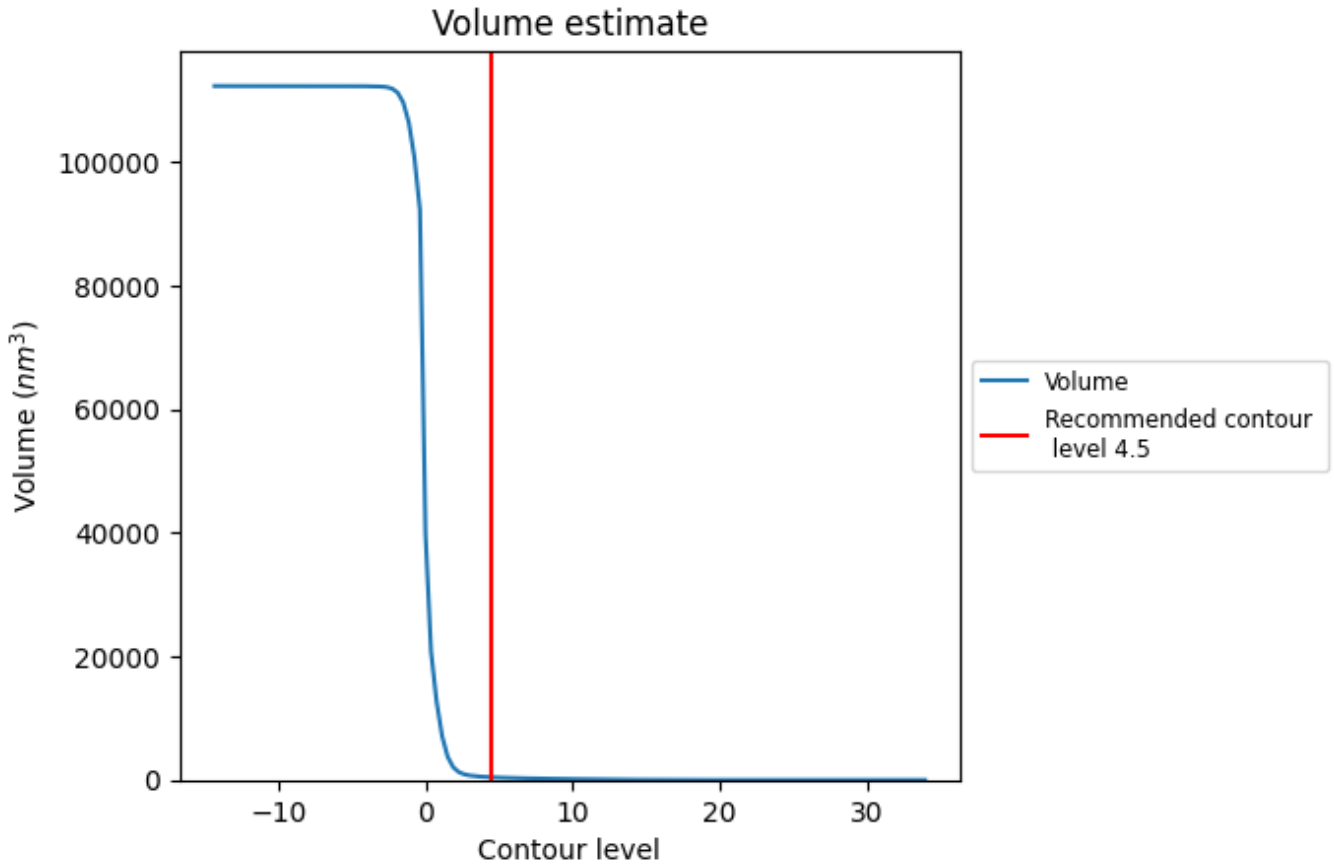
This section contains the results of statistical analysis of the map.

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.

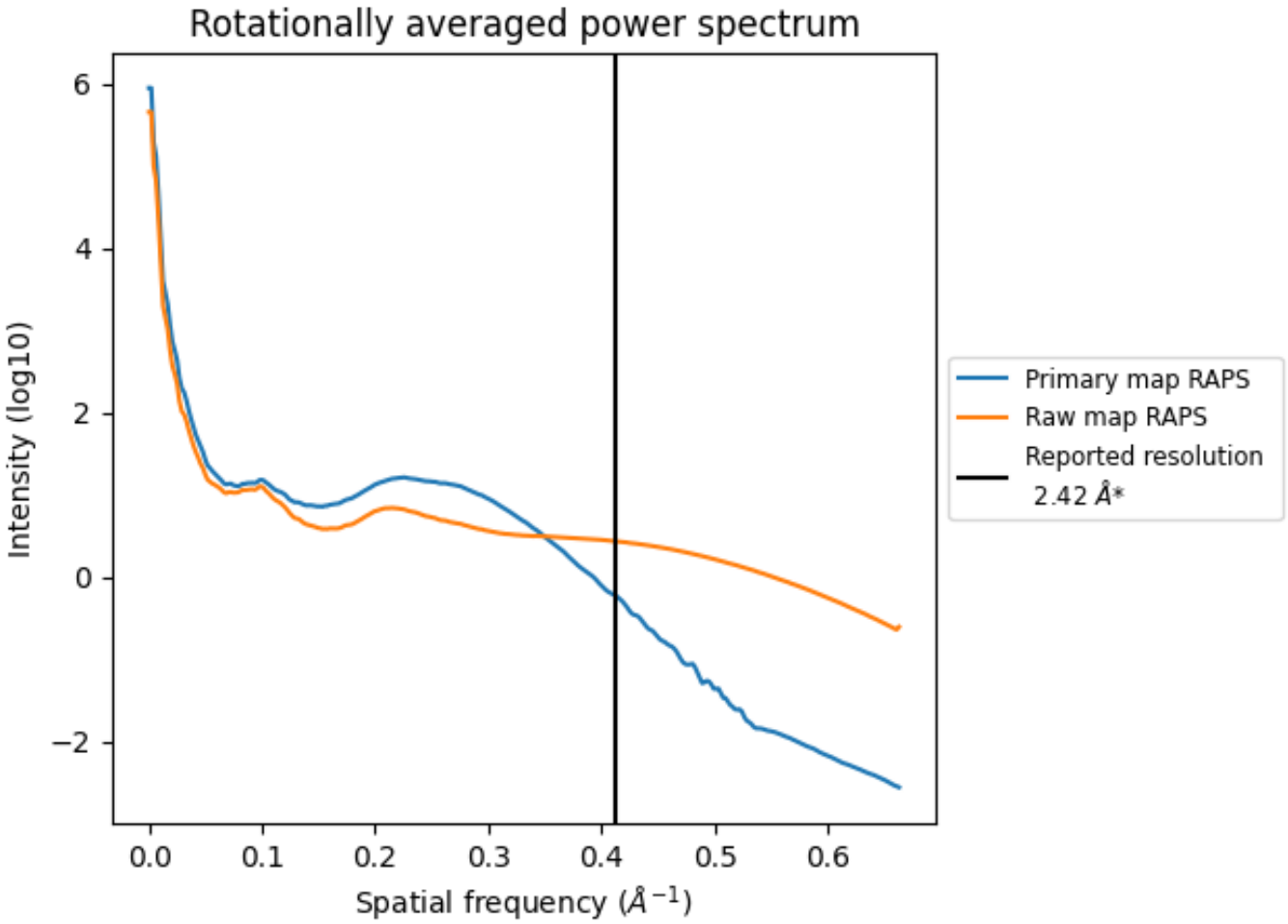
7.2 Volume estimate (i)



The volume at the recommended contour level is 430 nm^3; this corresponds to an approximate mass of 389 kDa.

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

7.3 Rotationally averaged power spectrum (i)

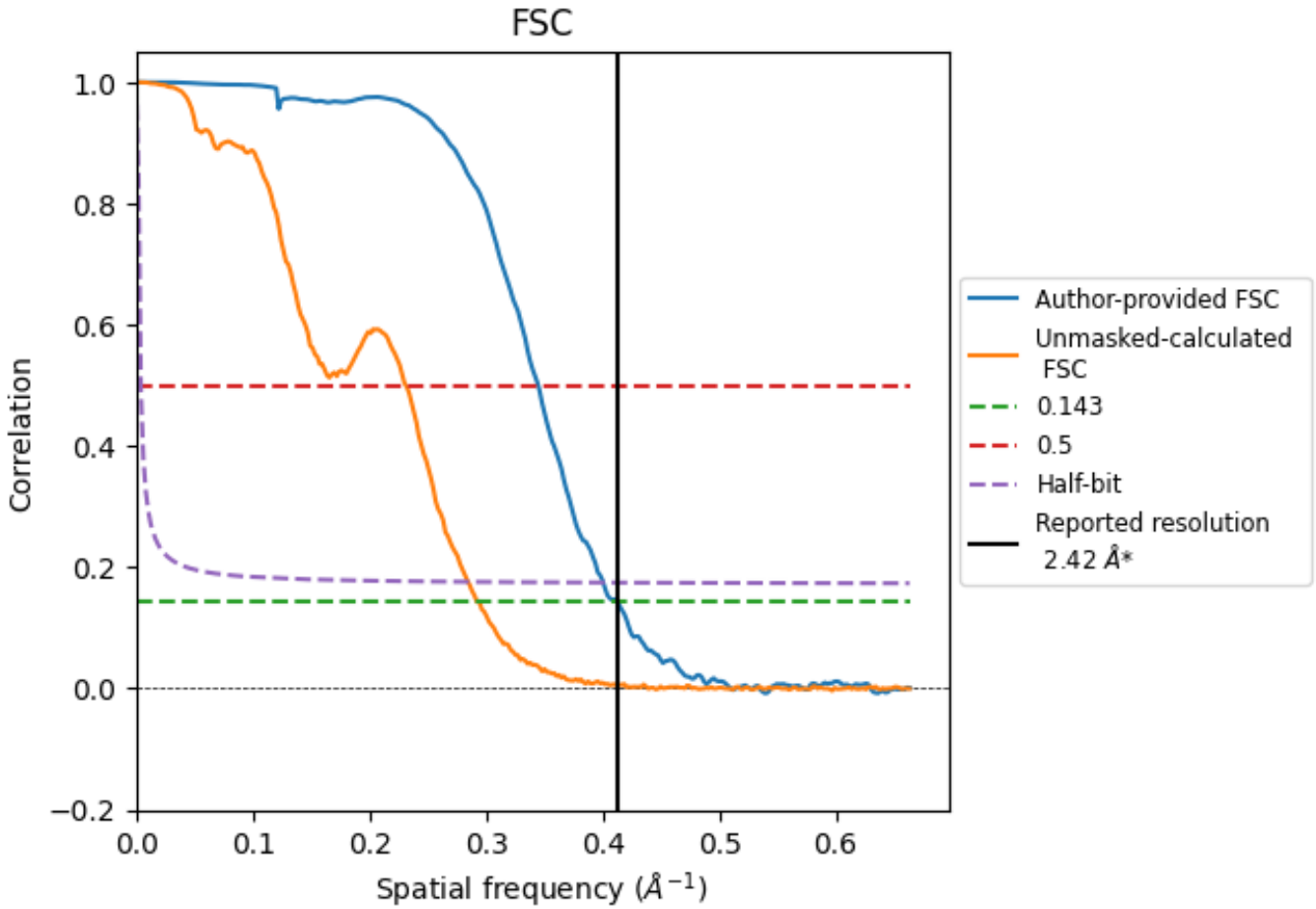


*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

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 0.413 Å^{-1}

8.2 Resolution estimates (i)

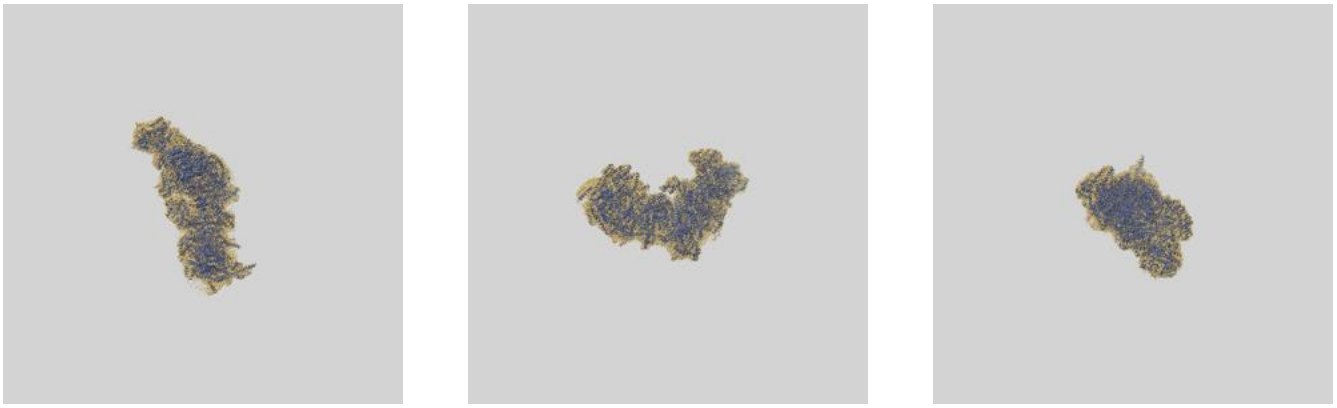
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.90	2.50
Unmasked-calculated*	3.42	4.32	3.51

*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 3.42 differs from the reported value 2.42 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55031 and PDB model 9SMG. Per-residue inclusion information can be found in section 3 on page 25.

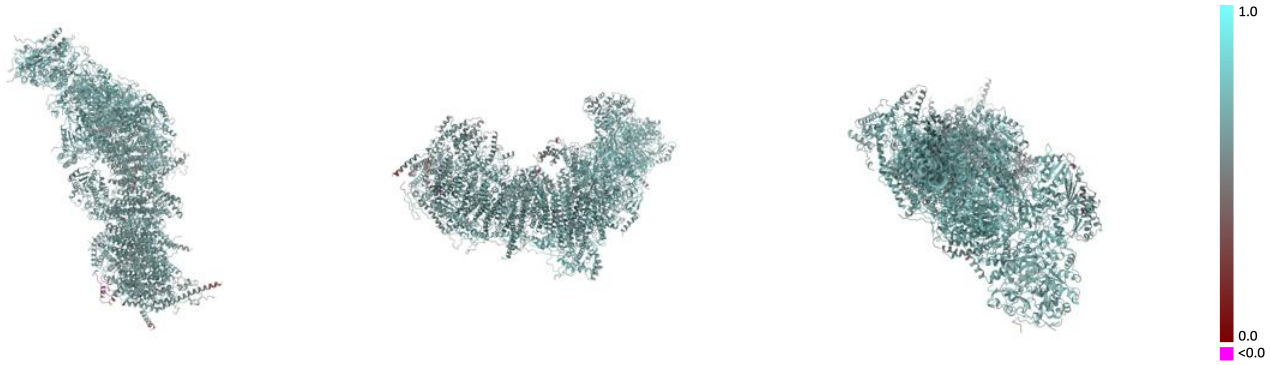
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

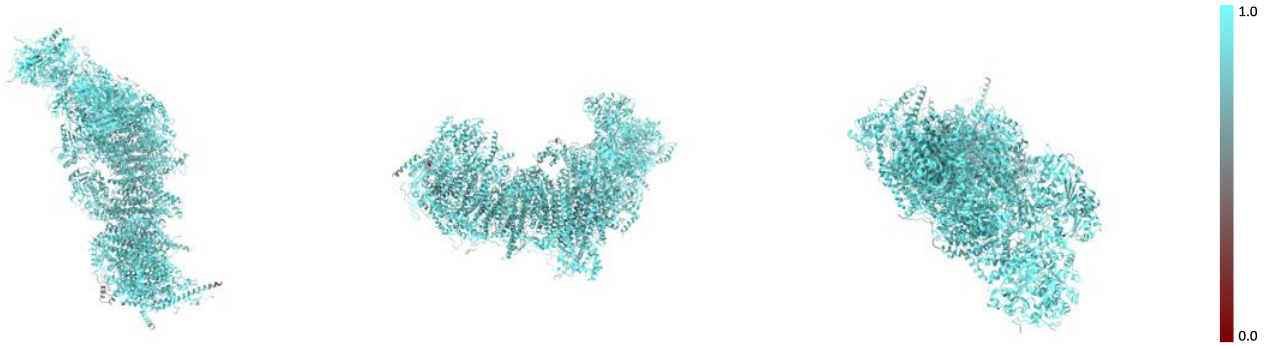
9.2 Q-score mapped to coordinate model (i)



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.

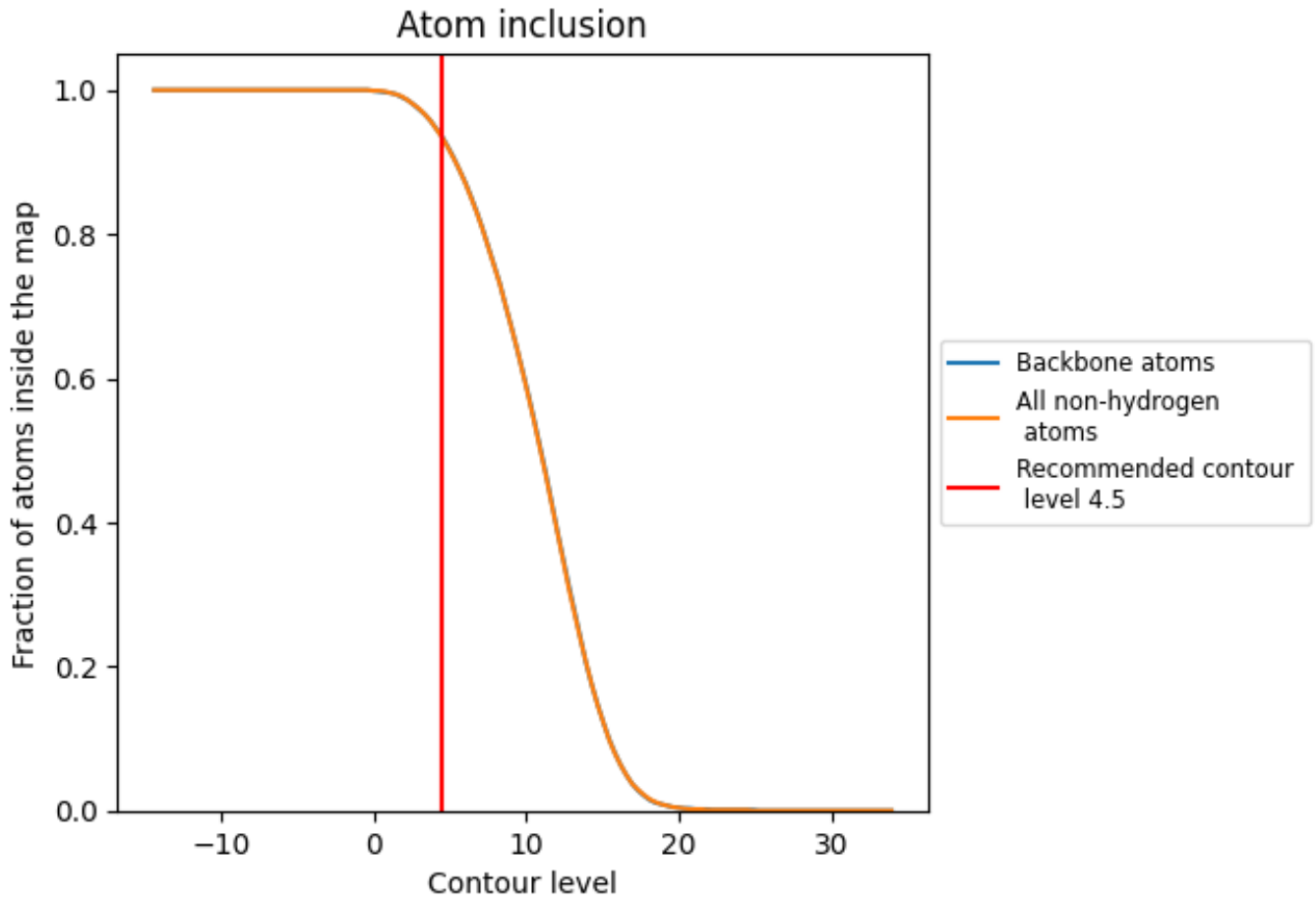
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.6460
A	0.9520	0.6810
B	0.9680	0.6940
C	0.9650	0.6990
D	0.9710	0.7020
E	0.9400	0.6300
F	0.9590	0.6510
G	0.9510	0.6640
H	0.9690	0.6930
I	0.9820	0.7060
J	0.9590	0.6720
K	0.9760	0.6930
L	0.9490	0.6370
M	0.9800	0.6890
N	0.9750	0.6930
O	0.9250	0.6190
P	0.9340	0.6540
Q	0.9270	0.6750
R	0.9250	0.6630
S	0.8910	0.5650
T	0.7600	0.5040
U	0.8750	0.5630
V	0.9100	0.6440
W	0.9220	0.6530
X	0.9160	0.6290
Y	0.8900	0.6030
Z	0.9370	0.6540
a	0.9730	0.6710
b	0.8920	0.6210
c	0.8910	0.5950
d	0.9230	0.6400
e	0.9140	0.6370
f	0.8100	0.5640
g	0.8890	0.6120
h	0.9190	0.6330



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Chain	Atom inclusion	Q-score
i	0.8220	0.5230
j	0.8640	0.5360
k	0.8540	0.5410
l	0.9260	0.6080
m	0.9110	0.6080
n	0.9160	0.5970
o	0.8660	0.5460
p	0.9190	0.6180
q	0.9200	0.6560
r	0.9340	0.6540
s	0.9360	0.6200