



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 09:49 PM UTC

PDB ID : 9W2U / pdb_00009w2u
EMDB ID : EMD-65580
Title : Cryo-EM structure of complex I on the bovine heart submitochondrial particles, open
Authors : Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.
Deposited on : 2025-07-28
Resolution : 2.60 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

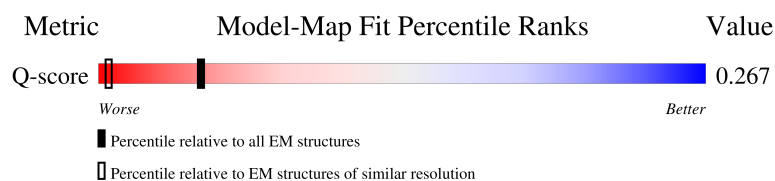
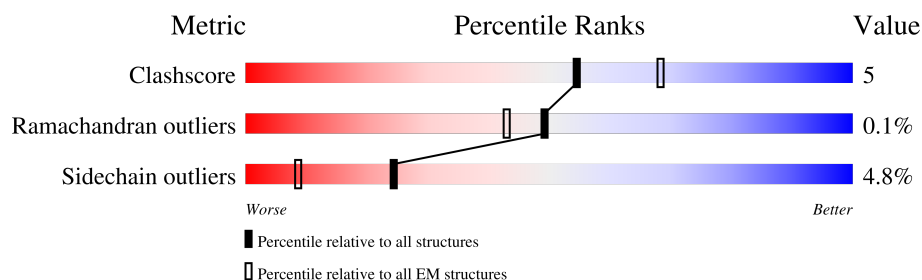
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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 $\leq 5\%$. 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	J	175	<div> <div>25%</div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>
2	A	114	<div> <div>35%</div> <div>66%</div> <div>11%</div> <div>• 21%</div> </div>
3	B	155	<div> <div>17%</div> <div>85%</div> <div>14%</div> <div>••</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	209	
5	D	430	
6	E	214	
7	F	432	
8	G	699	
9	H	317	
10	I	176	
11	K	97	
12	L	605	
13	M	458	
14	N	346	
15	O	320	
16	P	342	
17	Q	129	
18	R	96	
19	S	87	
20	T	85	
21	U	86	
22	V	115	
23	W	115	
24	X	171	
25	t	141	
26	Z	141	
27	a	70	
28	b	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	c	49	<div> <div>51%</div> <div>80%</div> <div>20%</div> </div>
30	d	119	<div> <div>35%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>
31	e	99	<div> <div>27%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
32	f	57	<div> <div>35%</div> <div>74%</div> <div>26%</div> </div>
33	g	100	<div> <div>25%</div> <div>85%</div> <div>15%</div> </div>
34	h	138	<div> <div>22%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
35	u	128	<div> <div>28%</div> <div>77%</div> <div>23%</div> </div>
36	j	71	<div> <div>18%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
37	k	81	<div> <div>22%</div> <div>78%</div> <div>22%</div> </div>
38	l	156	<div> <div>10%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
39	m	128	<div> <div>11%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
40	n	172	<div> <div>17%</div> <div>87%</div> <div>13%</div> </div>
41	o	122	<div> <div>9%</div> <div>77%</div> <div>23%</div> </div>
42	p	173	<div> <div>12%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
43	q	145	<div> <div>15%</div> <div>90%</div> <div>10%</div> <div>.</div> </div>
44	v	113	<div> <div>26%</div> <div>72%</div> <div>13%</div> <div>15%</div> </div>
45	s	45	<div> <div>16%</div> <div>84%</div> <div>16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	SF4	F	502	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68035 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 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	167	Total	C	N	O	S	0	0
			1269	854	181	222	12		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	90	Total	C	N	O	S	0	0
			724	499	102	119	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	THR	conflict	UNP Q8WAB4

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	416	Total	C	N	O	S	0	0
			3362	2150	577	610	25		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	432	Total	C	N	O	S	1	0
			3336	2102	597	617	20		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	699	Total	C	N	O	S	1	0
			5366	3362	934	1030	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	294	Total	C	N	O	S	0	0
			2338	1577	360	379	22		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			735	480	111	129	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	605	Total	C	N	O	S	0	0
			4792	3189	736	825	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3644	2430	569	607	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	346	Total	C	N	O	S	0	0
			2723	1811	415	455	42		

- 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	conflict	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	1	0
			2768	1792	489	482	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	C	N	O	S	0	0
			740	454	140	143	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	9	GLU	ASP	conflict	UNP Q9CR21

- Molecule 21 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	t	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
t	0	ACE	-	acetylation	UNP Q8HXG6

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 13.

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

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

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	119	Total	C	N	O	S	0	0
			988	643	171	170	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

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

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	100	Total	C	N	O	S	0	0
			839	539	139	157	4		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	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
u	0	ACE	-	acetylation	UNP Q02367

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	96	Total	C	N	O	S	0	0
			776	490	144	139	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	0	ACE	-	acetylation	UNP Q05752

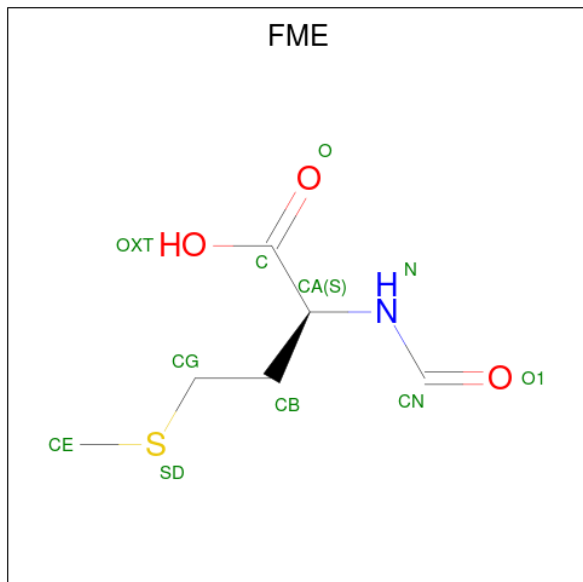
- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	45	Total	C	N	O	S	1	0
			391	244	71	75	1		

There is a discrepancy between the modelled and reference sequences:

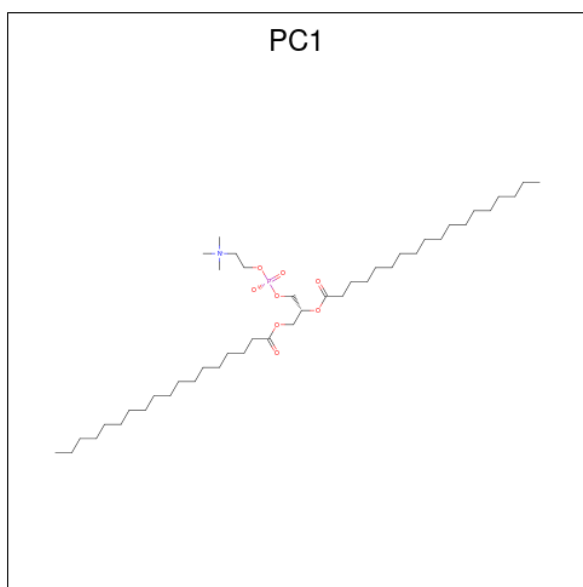
Chain	Residue	Modelled	Actual	Comment	Reference
s	57	ASP	GLU	conflict	UNP P56181

- Molecule 46 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	H	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	K	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	L	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	M	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	N	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
47	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



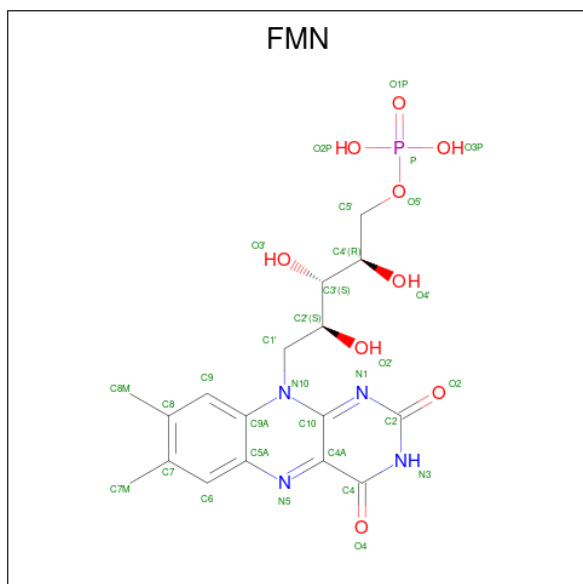
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

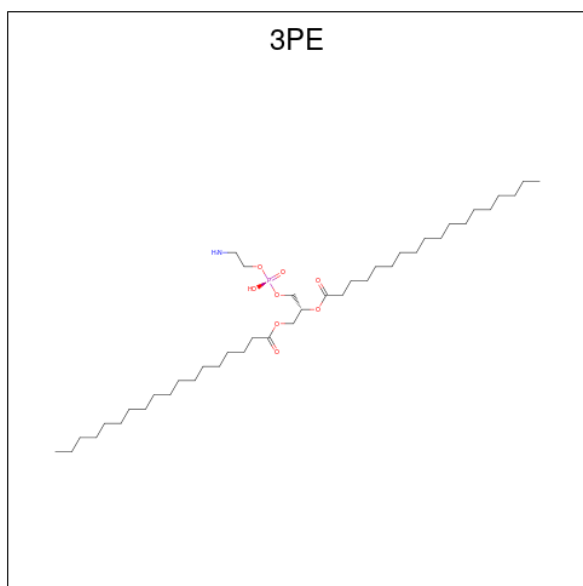


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



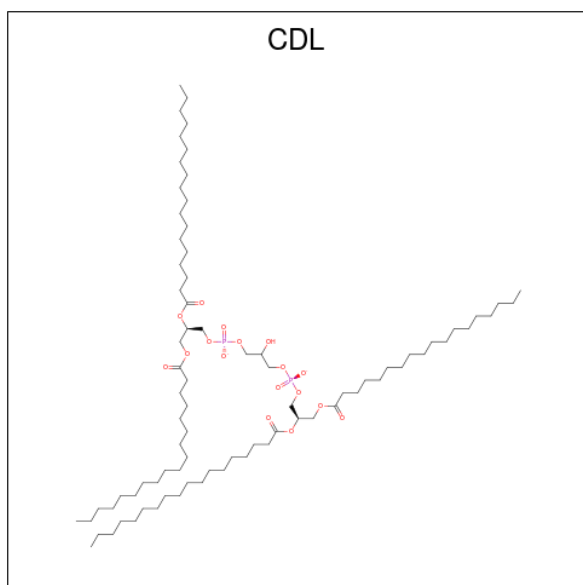
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
52	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
52	O	1	Total	C	N	O	P	0
			48	38	1	8	1	
52	t	1	Total	C	N	O	P	0
			31	21	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
52	t	1	Total	C	N	O	P	0
			40	30	1	8	1	
52	t	1	Total	C	N	O	P	0
			30	20	1	8	1	
52	t	1	Total	C	N	O	P	0
			33	23	1	8	1	
52	t	1	Total	C	N	O	P	0
			27	17	1	8	1	
52	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
52	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	u	1	Total	C	N	O	P	0
			45	35	1	8	1	
52	j	1	Total	C	N	O	P	0
			44	34	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: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



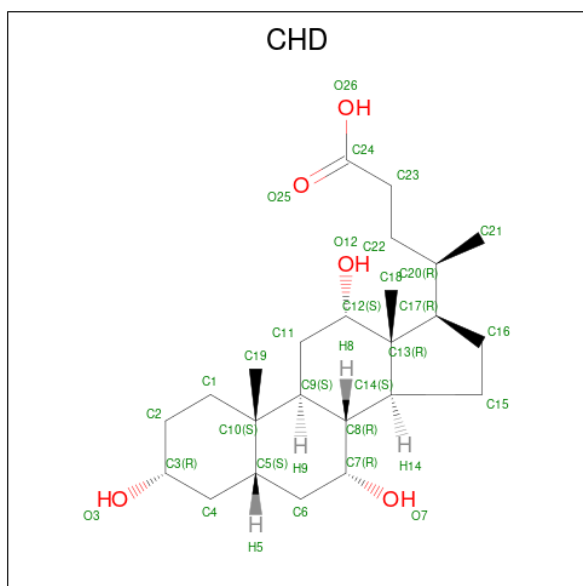
Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	O	1	Total	C	O	P	0
			62	43	17	2	

Continued on next page...

Continued from previous page...

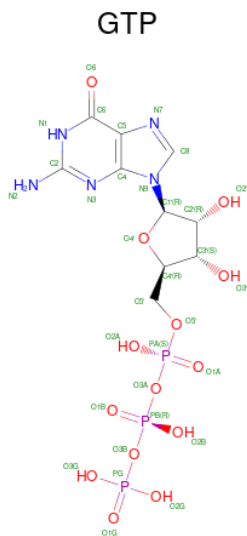
Mol	Chain	Residues	Atoms				AltConf
53	d	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			80	61	17	2	
53	v	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
54	L	1	Total	C	O		0
			29	24	5		

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

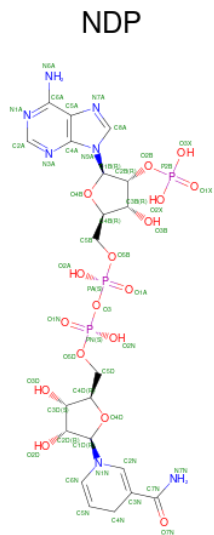


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total 32	C 10	N 5	O 14	P 3	0

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

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

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

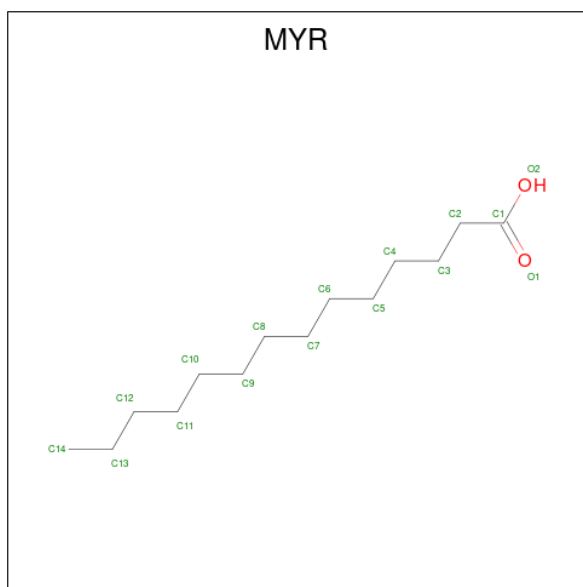


Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

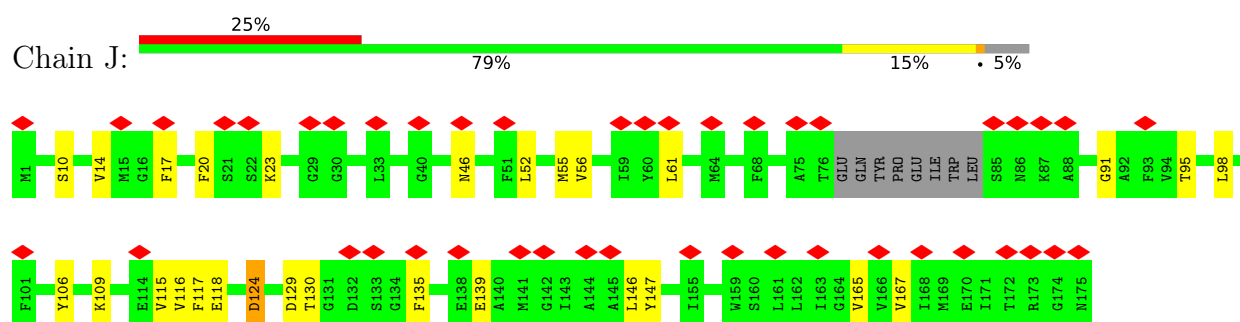


Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

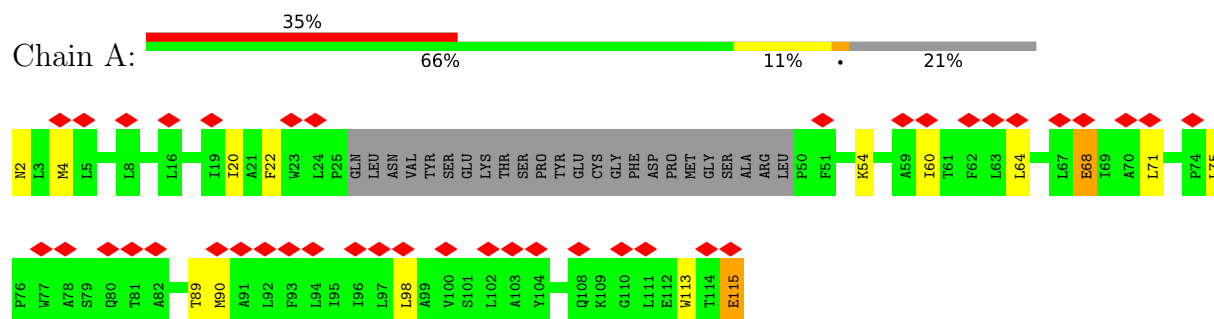
3 Residue-property plots [i](#)

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.

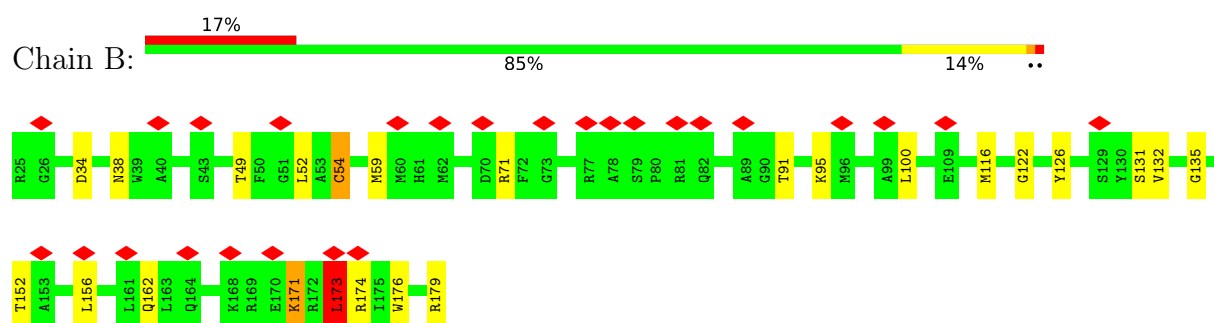
- Molecule 1: NADH-ubiquinone oxidoreductase chain 6



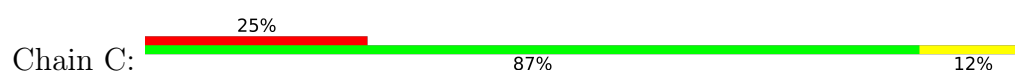
- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

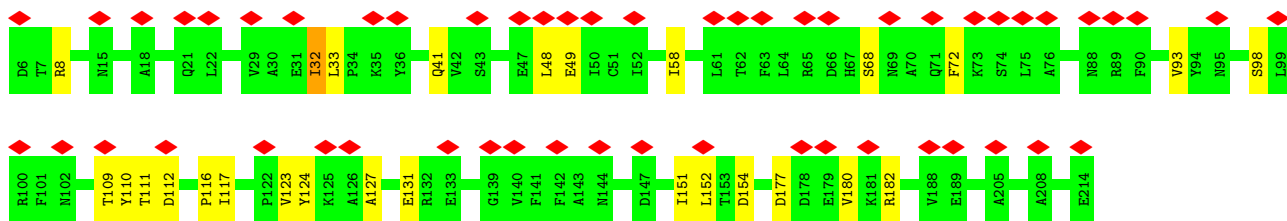


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

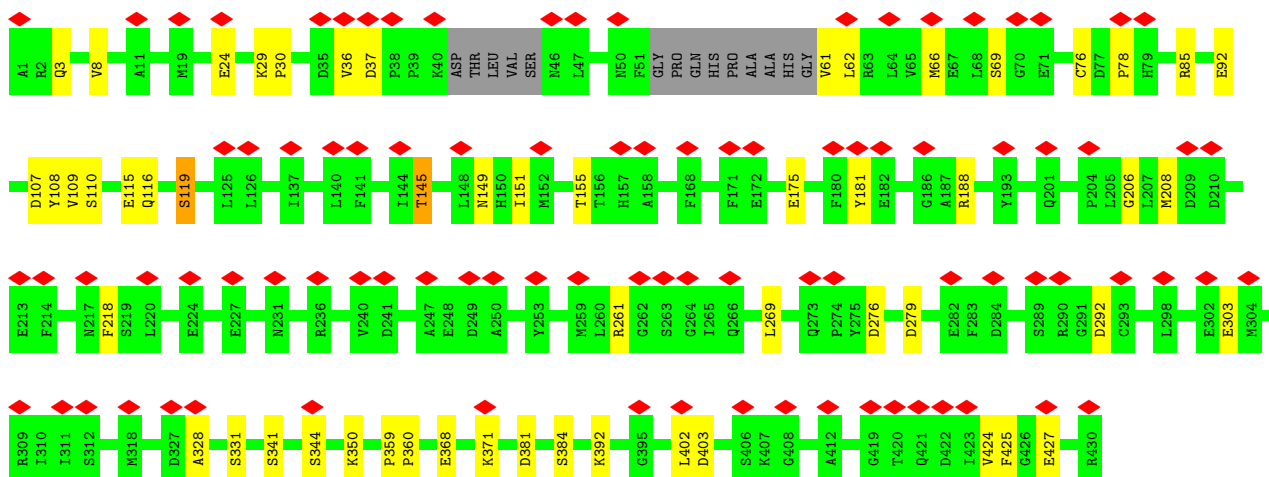
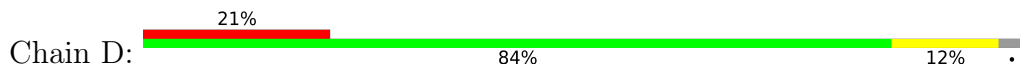


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

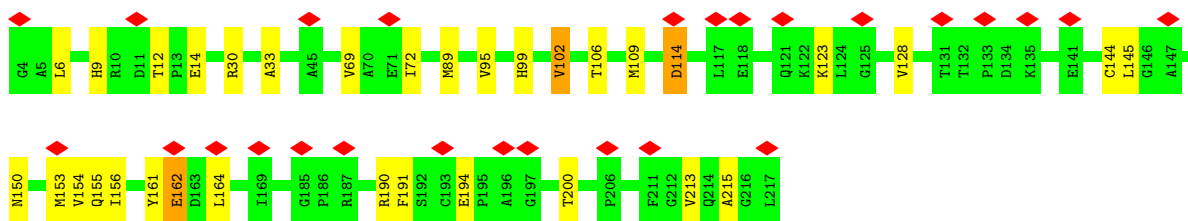
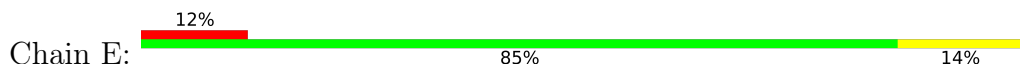




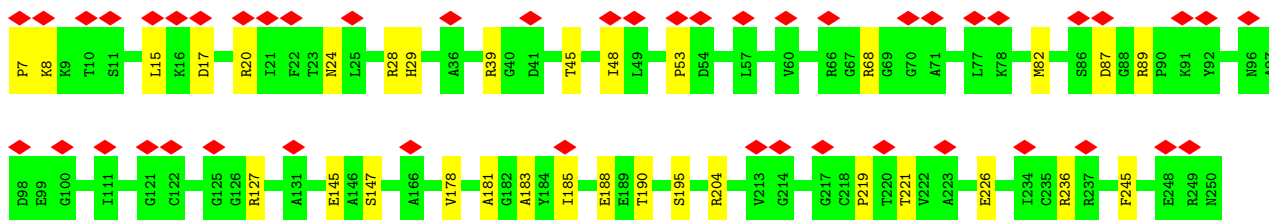
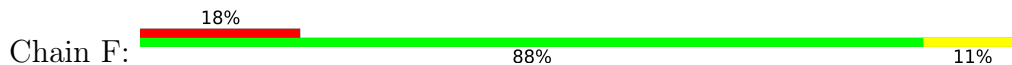
- Molecule 5: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

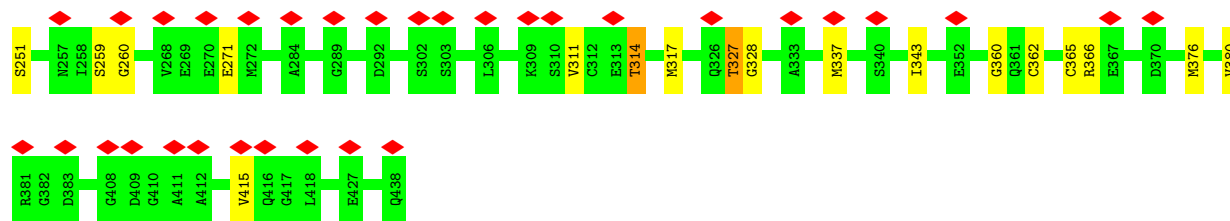


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

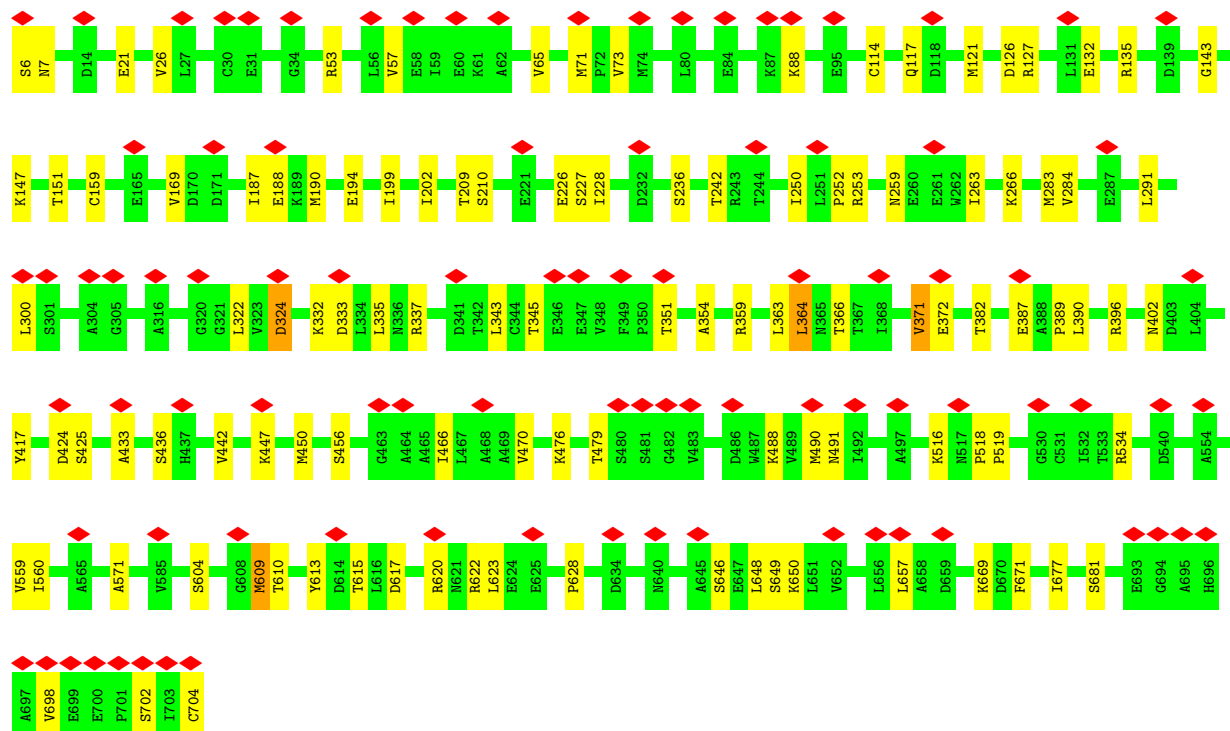
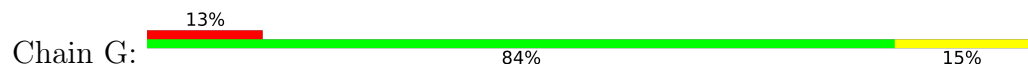


- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

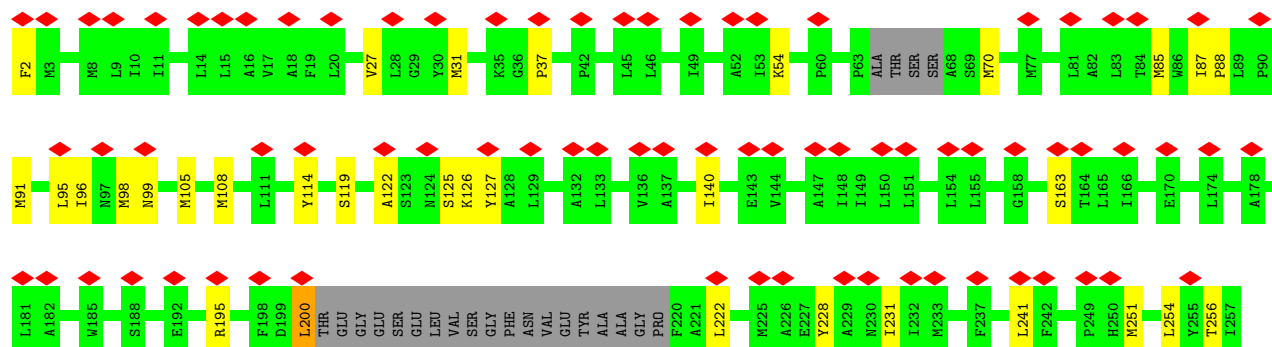
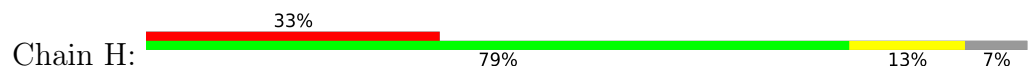


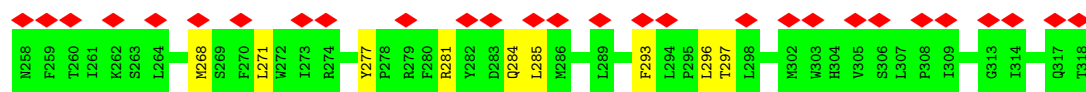


- Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

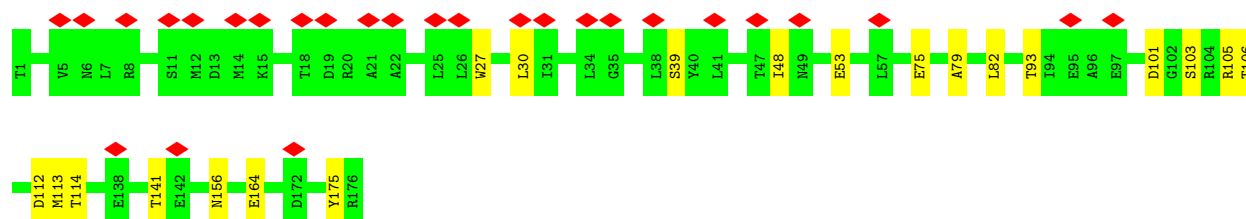
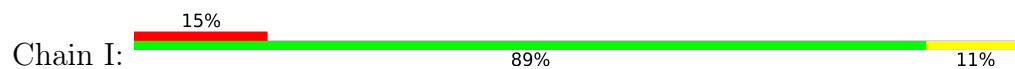


- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

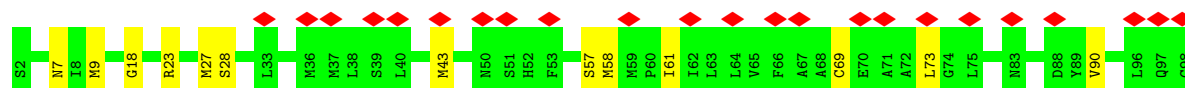
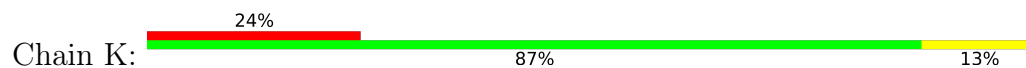




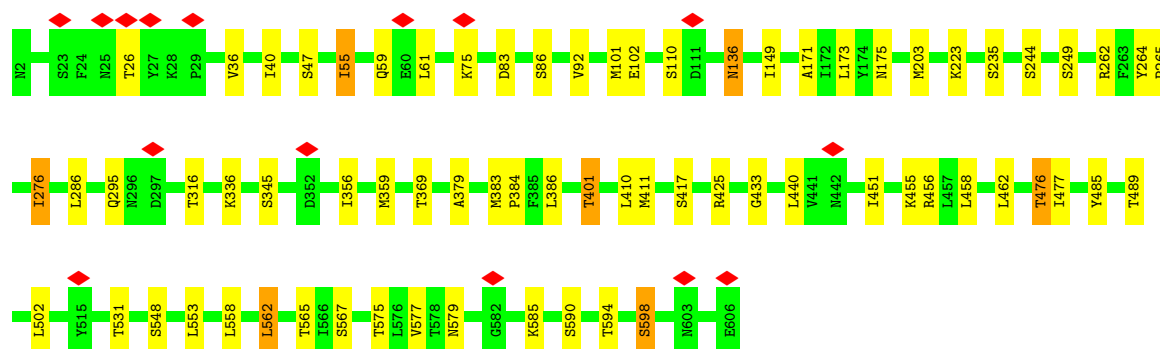
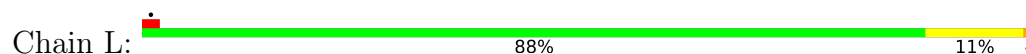
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



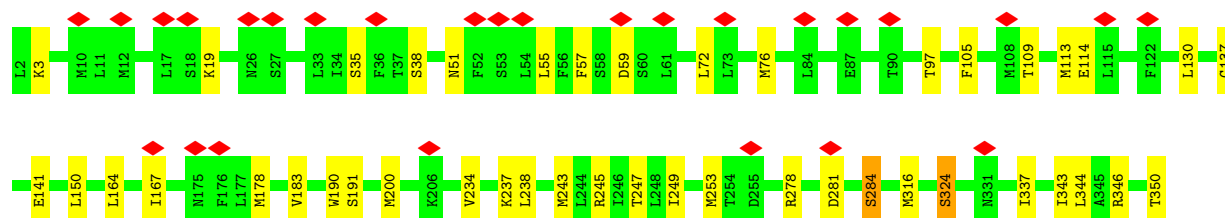
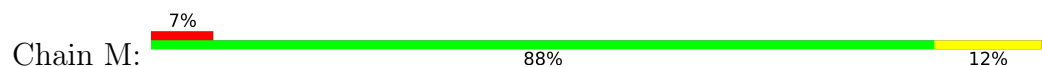
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

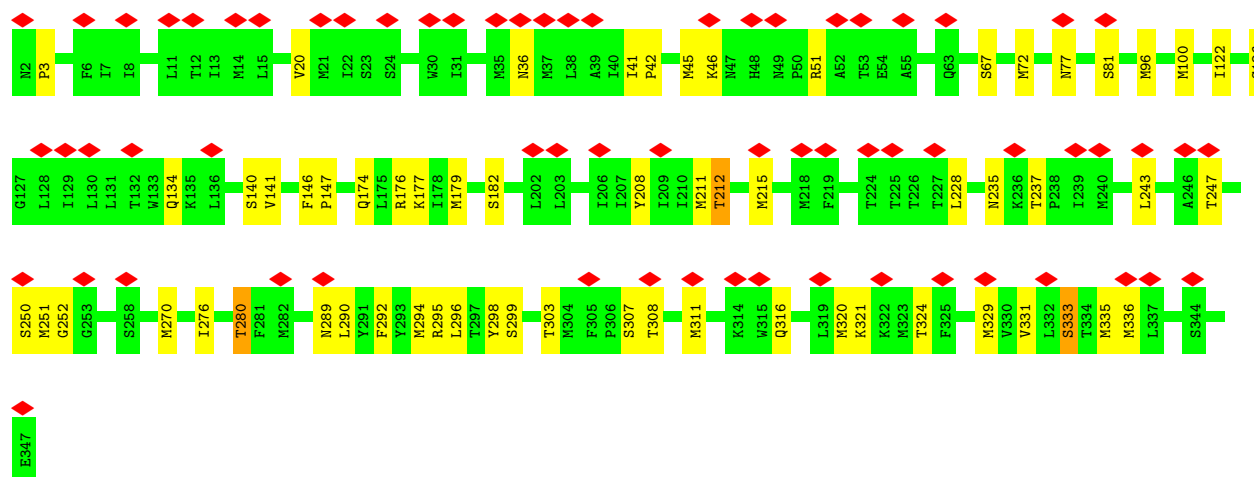
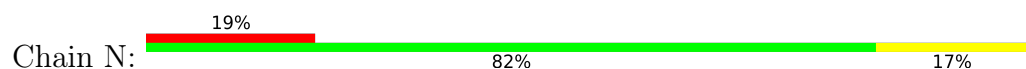


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

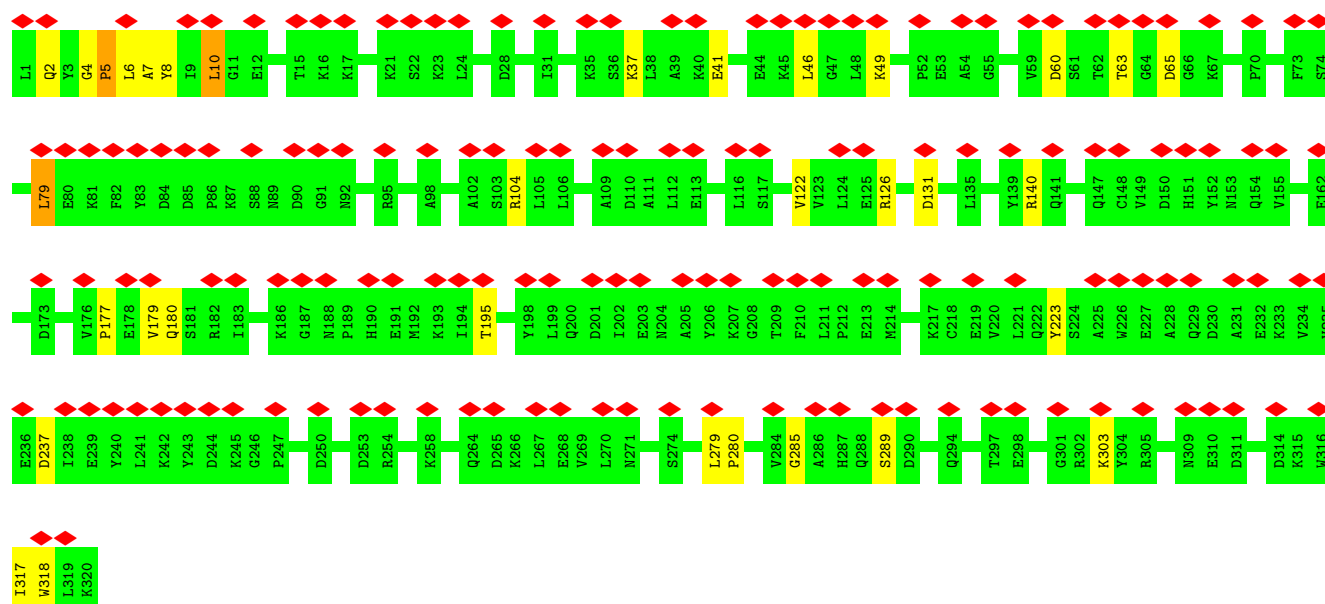
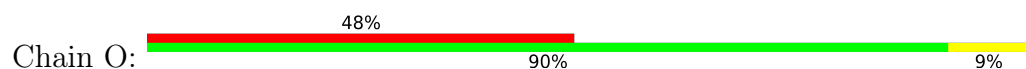




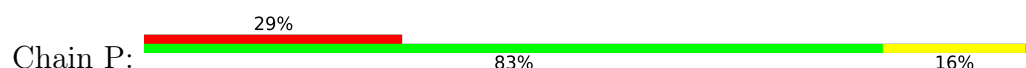
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

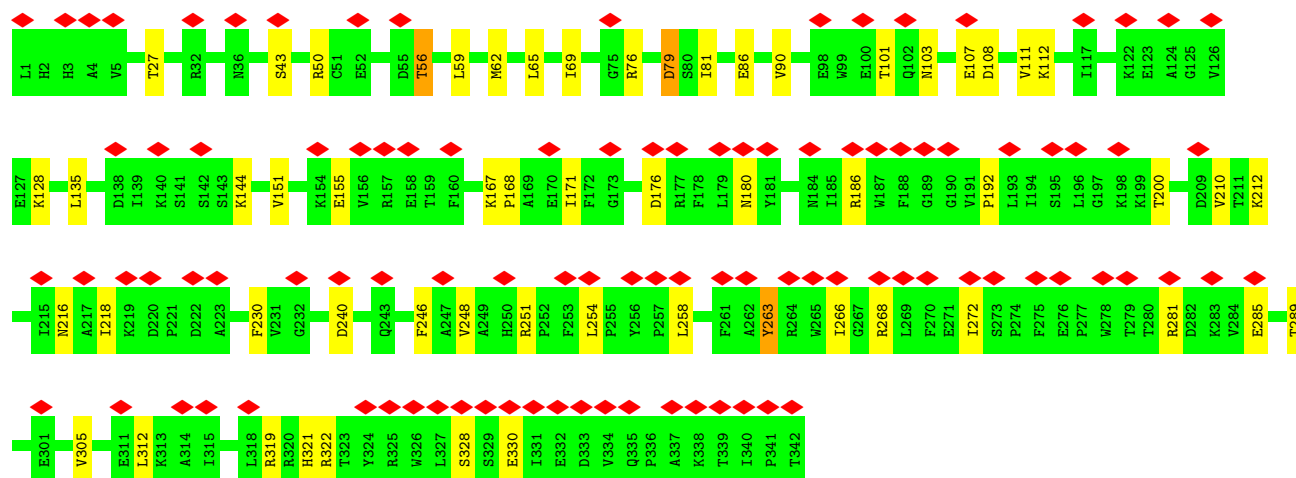


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

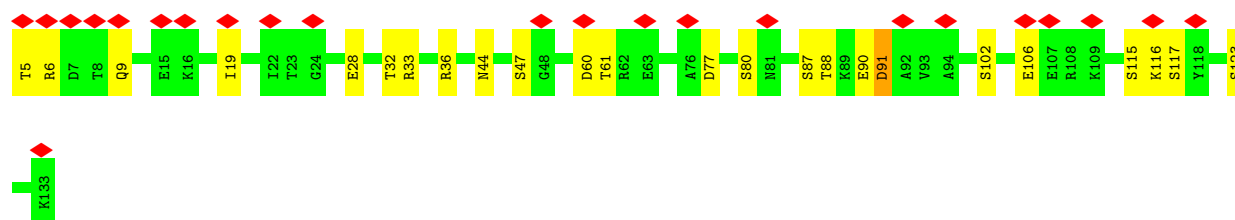
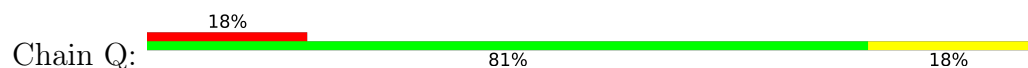


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

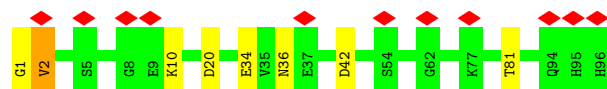




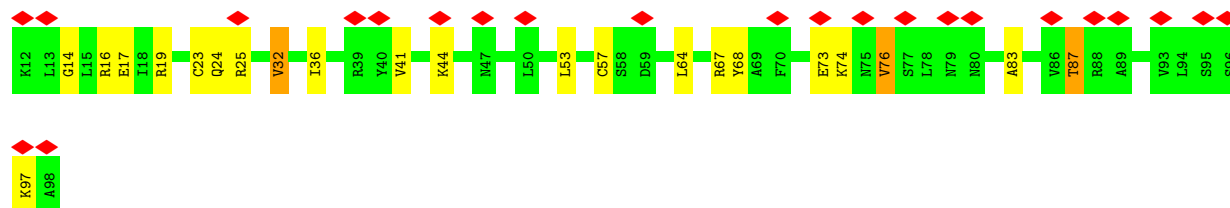
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

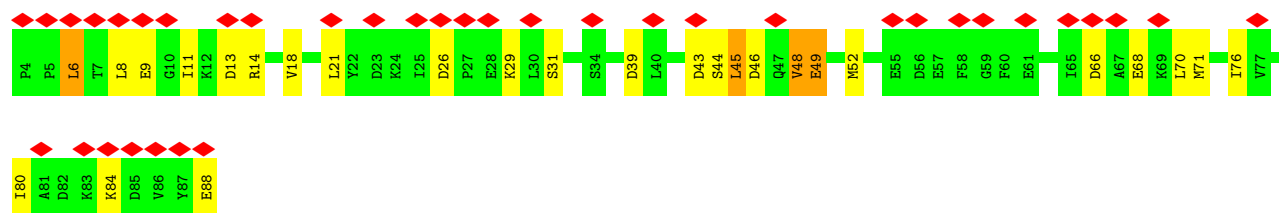


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

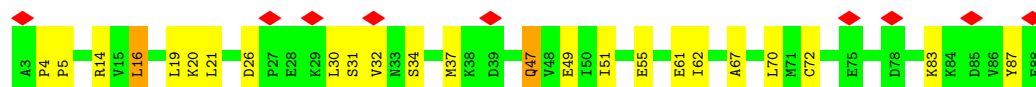
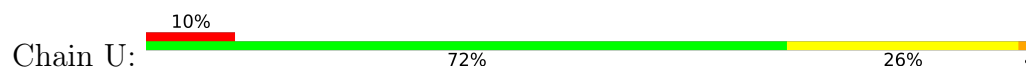


- Molecule 20: Acyl carrier protein, mitochondrial

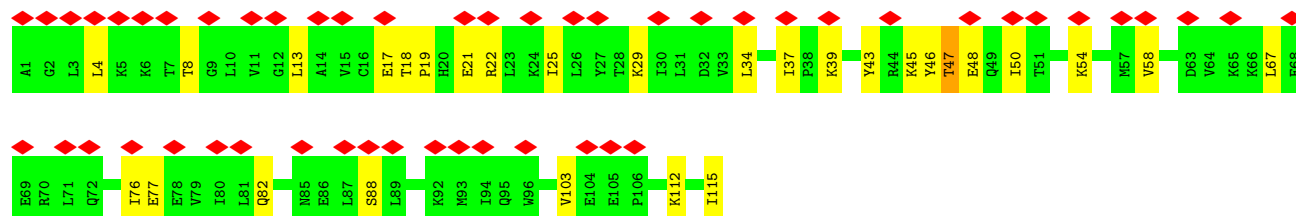
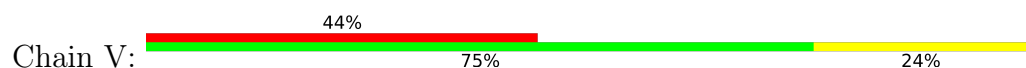




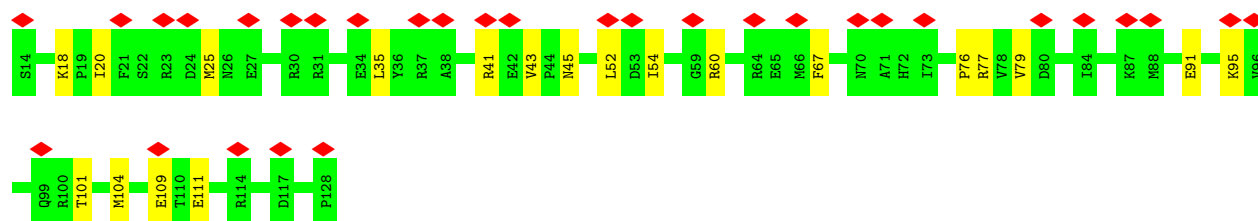
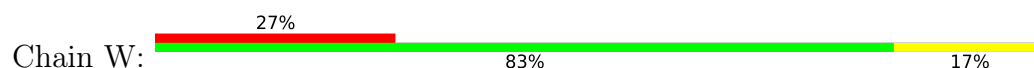
- Molecule 21: Acyl carrier protein, mitochondrial



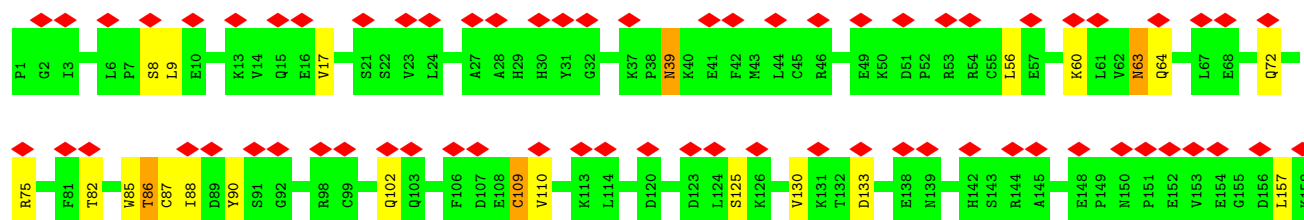
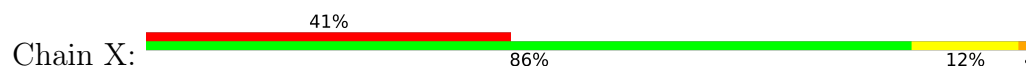
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

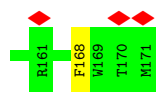


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

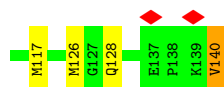
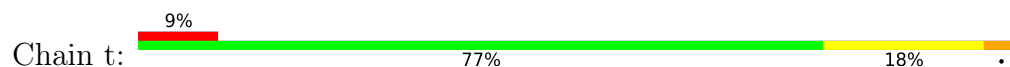


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

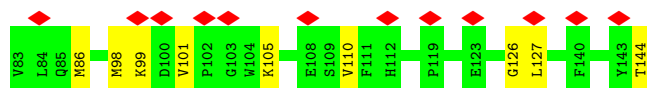
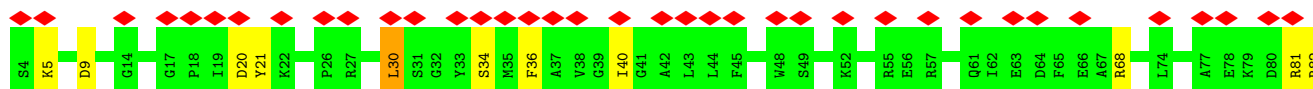
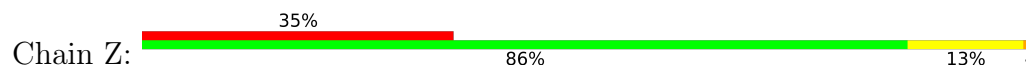




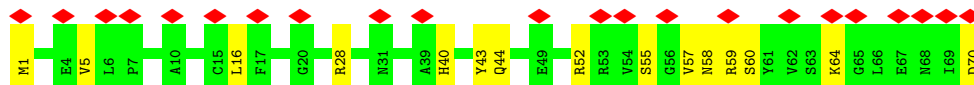
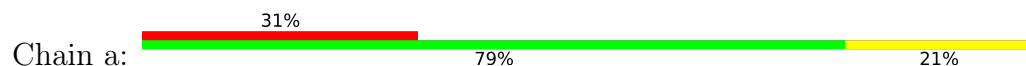
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



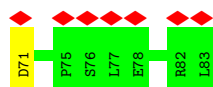
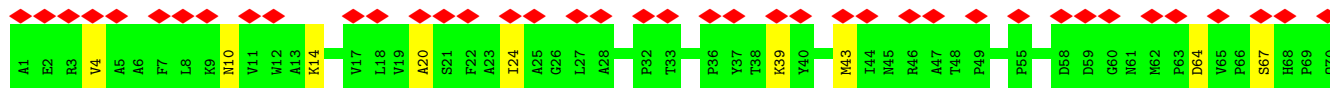
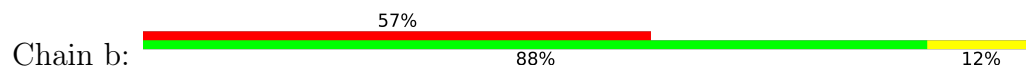
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

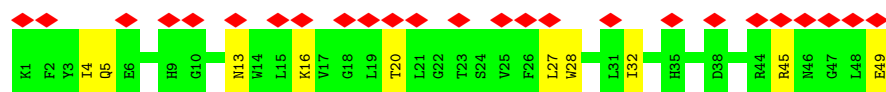


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

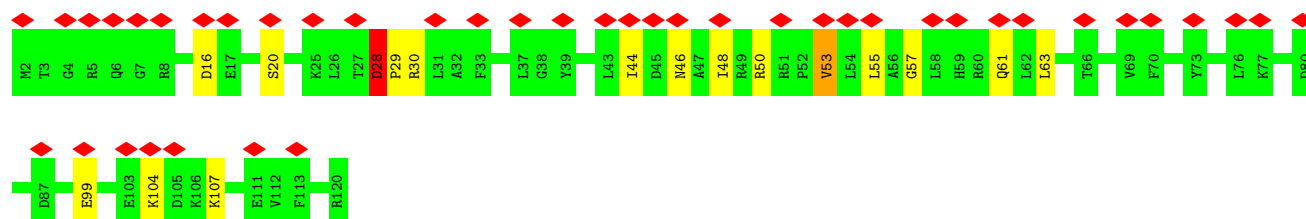
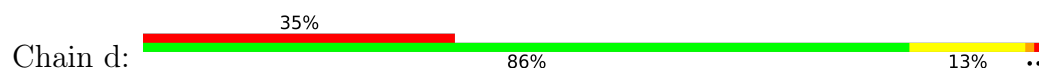


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

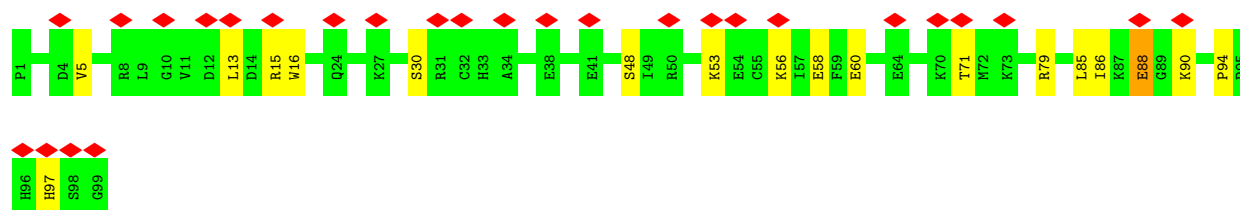
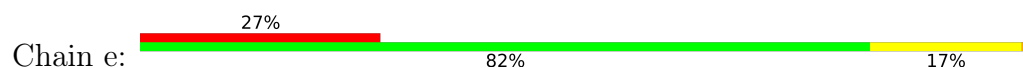




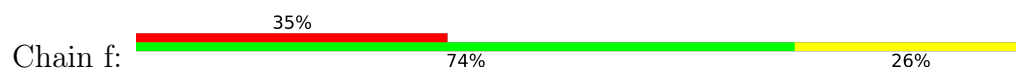
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



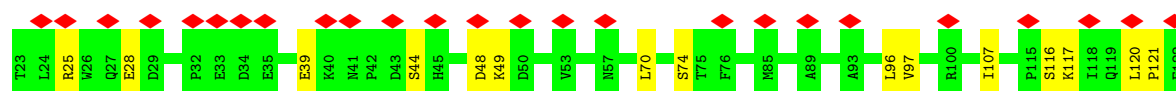
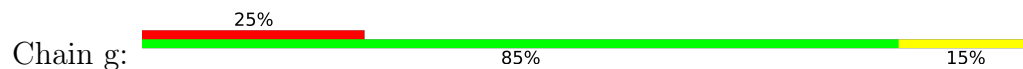
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



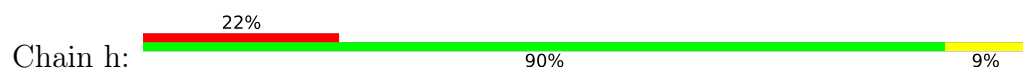
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

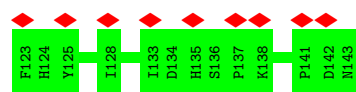


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

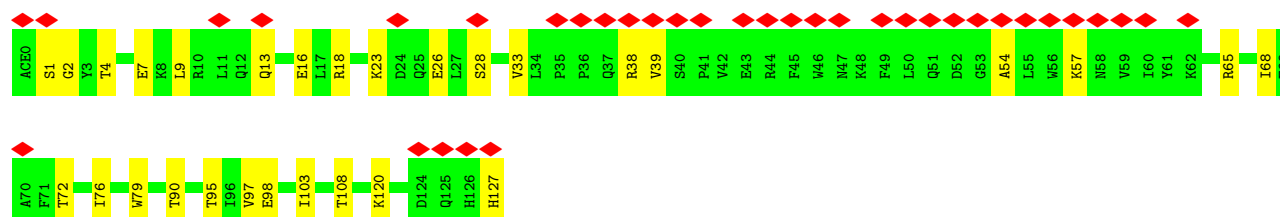
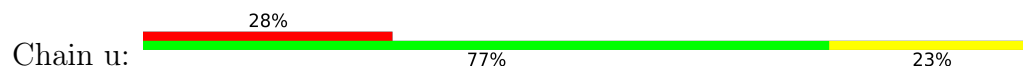


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

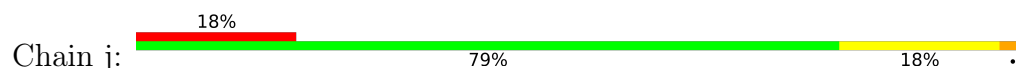




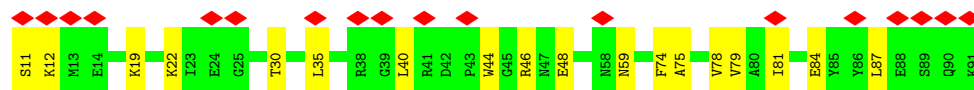
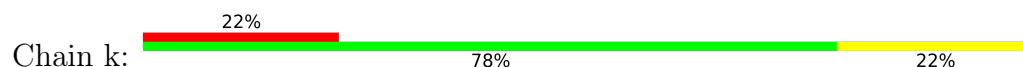
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



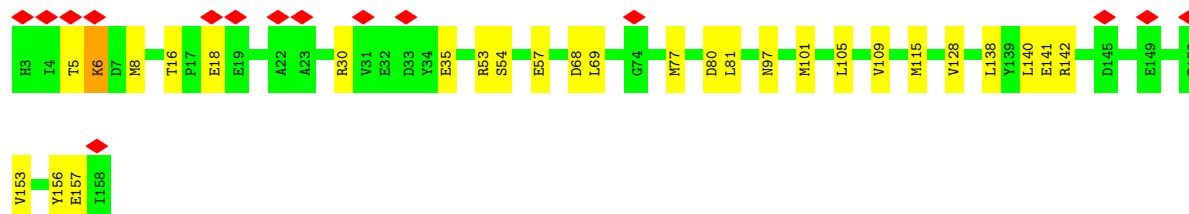
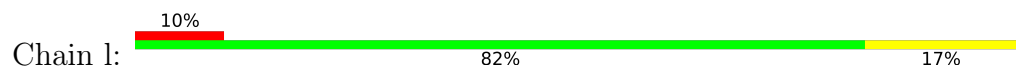
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



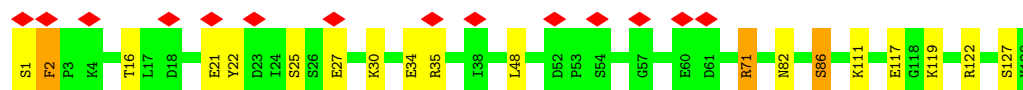
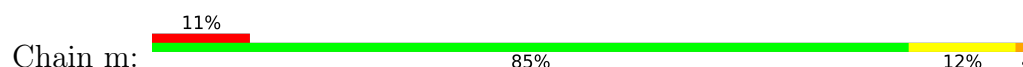
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



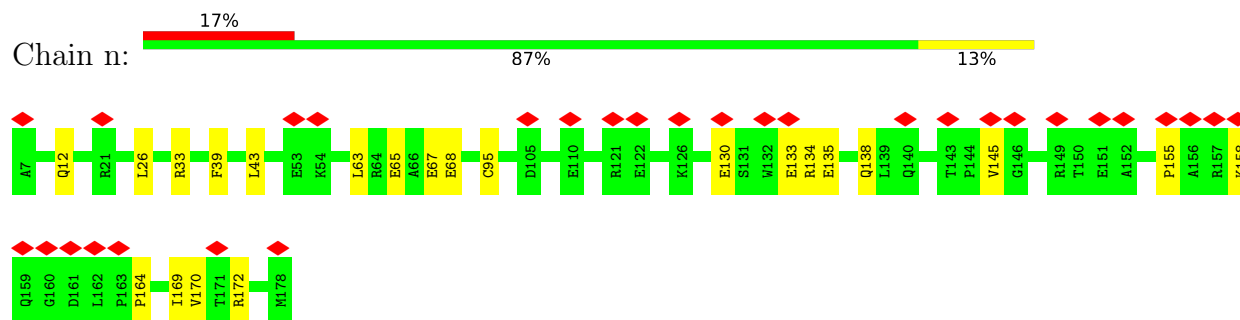
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



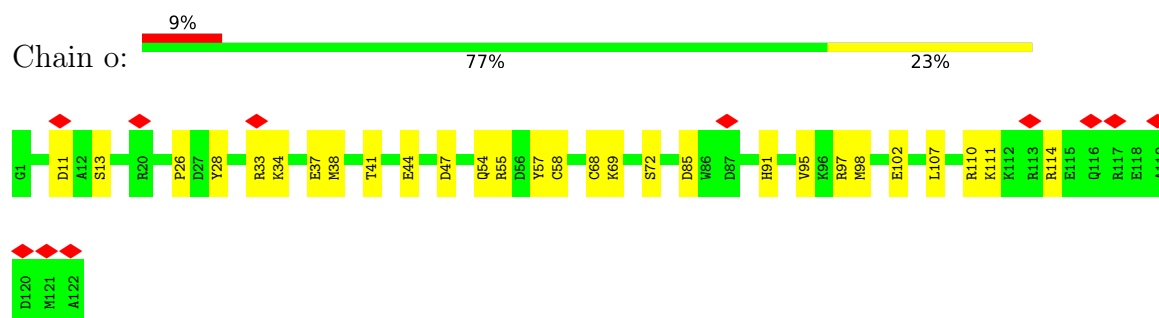
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



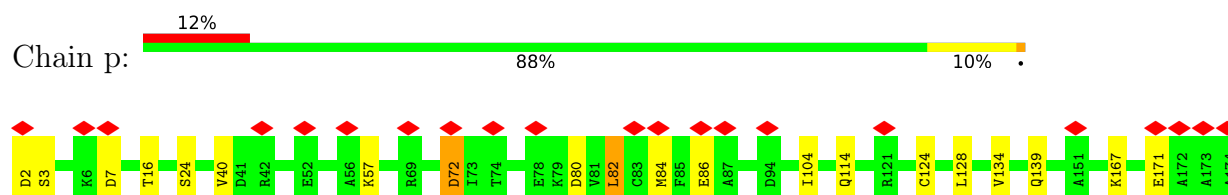
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



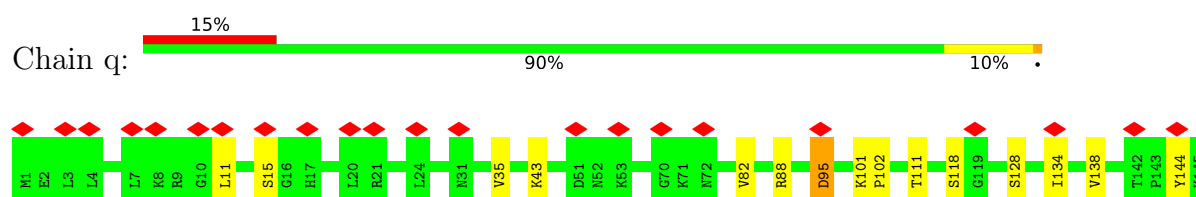
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



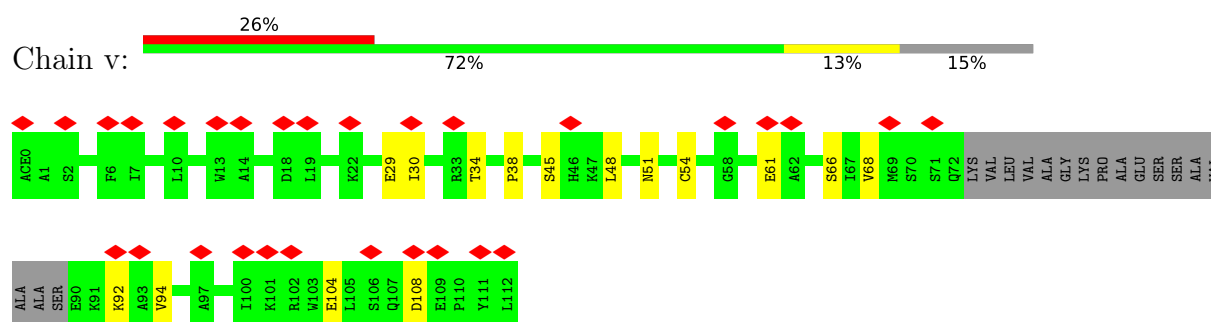
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



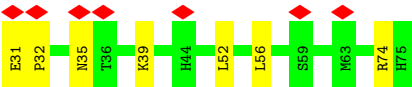
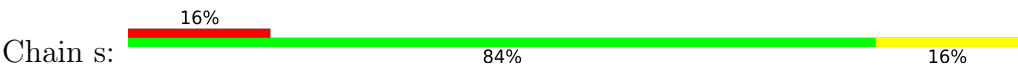
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 45: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252601	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.020	Depositor
Minimum map value	-0.612	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	654.0, 654.0, 654.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	J	0.18	0/1289	0.42	0/1745
2	A	0.16	0/743	0.37	0/1017
3	B	0.19	0/1272	0.42	1/1720 (0.1%)
4	C	0.14	0/1789	0.29	0/2436
5	D	0.16	0/3434	0.34	0/4648
6	E	0.13	0/1699	0.35	0/2312
7	F	0.13	0/3412	0.32	0/4610
8	G	0.14	0/5457	0.33	0/7397
9	H	0.17	0/2405	0.38	0/3283
10	I	0.16	0/1445	0.30	0/1956
11	K	0.15	0/745	0.36	0/1008
12	L	0.14	0/4920	0.34	0/6694
13	M	0.16	0/3738	0.31	0/5097
14	N	0.17	0/2792	0.34	0/3800
15	O	0.16	0/2651	0.35	0/3587
16	P	0.16	0/2847	0.36	0/3864
17	Q	0.15	0/1072	0.37	0/1449
18	R	0.14	0/753	0.30	0/1014
19	S	0.22	0/711	0.56	0/956
20	T	0.26	0/700	0.75	3/944 (0.3%)
21	U	0.18	0/705	0.48	0/952
22	V	0.19	0/948	0.45	0/1284
23	W	0.21	0/1000	0.45	0/1344
24	X	0.14	0/1439	0.33	0/1942
25	t	0.24	0/1048	0.50	0/1423
26	Z	0.21	0/1181	0.39	0/1592
27	a	0.14	0/584	0.29	0/786
28	b	0.18	0/672	0.44	0/923
29	c	0.20	0/427	0.52	0/579
30	d	0.20	0/1018	0.38	0/1375
31	e	0.18	0/850	0.47	0/1136
32	f	0.20	0/505	0.57	0/681

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.22	0/865	0.52	0/1175
34	h	0.14	0/1188	0.28	0/1607
35	u	0.23	0/1134	0.54	0/1544
36	j	0.20	0/624	0.47	0/855
37	k	0.21	0/672	0.56	0/906
38	l	0.18	0/1369	0.46	0/1873
39	m	0.21	0/1094	0.51	0/1480
40	n	0.16	0/1545	0.40	0/2092
41	o	0.18	0/1073	0.46	0/1437
42	p	0.13	0/1486	0.31	0/2004
43	q	0.15	0/1250	0.32	0/1698
44	v	0.22	0/795	0.50	0/1077
45	s	0.16	0/403	0.35	0/545
All	All	0.17	0/67749	0.39	4/91847 (0.0%)

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
7	F	0	1
30	d	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	48	VAL	CA-C-N	-6.22	109.44	121.58
20	T	48	VAL	C-N-CA	-6.22	109.44	121.58
20	T	49	GLU	CA-CB-CG	5.77	125.64	114.10
3	B	173	LEU	CA-CB-CG	5.48	135.48	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	236	ARG	Peptide
30	d	28	ASP	Mainchain

5.2 Too-close contacts ⓘ

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	J	1269	0	1283	19	0
2	A	724	0	766	12	0
3	B	1241	0	1251	13	0
4	C	1738	0	1685	12	0
5	D	3362	0	3314	35	0
6	E	1659	0	1664	14	0
7	F	3336	0	3286	28	0
8	G	5366	0	5378	51	0
9	H	2338	0	2466	22	0
10	I	1414	0	1370	11	0
11	K	735	0	774	8	0
12	L	4792	0	4949	31	0
13	M	3644	0	3841	33	0
14	N	2723	0	2901	34	0
15	O	2589	0	2566	24	0
16	P	2768	0	2782	32	0
17	Q	1049	0	1045	11	0
18	R	740	0	714	4	0
19	S	700	0	719	15	0
20	T	688	0	685	20	0
21	U	693	0	689	17	0
22	V	928	0	972	17	0
23	W	976	0	991	16	0
24	X	1402	0	1381	16	0
25	t	1030	0	1039	20	0
26	Z	1152	0	1151	19	0
27	a	569	0	568	8	0
28	b	651	0	662	7	0
29	c	414	0	415	7	0
30	d	988	0	975	14	0
31	e	829	0	829	10	0
32	f	492	0	501	9	0
33	g	839	0	790	11	0
34	h	1154	0	1168	11	0
35	u	1097	0	1108	18	0
36	j	597	0	536	10	0
37	k	653	0	639	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	1314	0	1210	20	0
39	m	1067	0	1067	17	0
40	n	1492	0	1438	12	0
41	o	1048	0	1020	22	0
42	p	1453	0	1425	12	0
43	q	1209	0	1182	4	0
44	v	776	0	782	7	0
45	s	391	0	361	5	0
46	A	10	0	10	2	0
46	H	10	0	10	1	0
46	K	10	0	10	0	0
46	L	10	0	10	1	0
46	M	10	0	10	0	0
46	N	10	0	10	1	0
47	A	35	0	44	0	0
47	B	94	0	132	4	0
47	H	48	0	73	3	0
47	I	54	0	88	2	0
47	L	44	0	65	0	0
47	M	35	0	44	1	0
47	Z	44	0	62	0	0
47	d	39	0	52	2	0
47	h	47	0	71	1	0
47	m	46	0	66	0	0
48	B	8	0	0	0	0
48	F	8	0	0	2	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	2	0
51	G	1	0	0	0	0
52	H	36	0	46	0	0
52	K	44	0	62	0	0
52	L	95	0	144	1	0
52	M	146	0	223	6	0
52	O	48	0	73	1	0
52	b	47	0	71	2	0
52	d	49	0	75	1	0
52	j	44	0	65	1	0
52	m	41	0	59	1	0
52	t	161	0	195	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	u	45	0	67	1	0
53	L	76	0	99	4	0
53	O	62	0	67	5	0
53	d	151	0	202	10	0
53	h	80	0	104	2	0
53	v	61	0	66	2	0
54	L	29	0	39	2	0
55	O	32	0	12	1	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	R	1	0	0	0	0
59	o	15	0	27	0	0
All	All	68035	0	68836	691	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 5.

The worst 5 of 691 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:383:MET:HE3	12:L:384:PRO:HD2	1.55	0.89
30:d:28:ASP:N	53:d:201:CDL:OB9	1.98	0.89
25:t:68:ILE:HD11	25:t:99:ILE:HG12	1.70	0.72
33:g:97:VAL:HG23	33:g:107:ILE:HD11	1.71	0.71
11:K:43:MET:HE1	14:N:72:MET:HE1	1.72	0.70

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	J	163/175 (93%)	157 (96%)	5 (3%)	1 (1%)	21	42
2	A	86/114 (75%)	84 (98%)	2 (2%)	0	100	100
3	B	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
4	C	207/209 (99%)	204 (99%)	3 (1%)	0	100	100
5	D	409/430 (95%)	397 (97%)	12 (3%)	0	100	100
6	E	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	14	30
7	F	431/432 (100%)	423 (98%)	8 (2%)	0	100	100
8	G	698/699 (100%)	679 (97%)	18 (3%)	1 (0%)	48	70
9	H	288/317 (91%)	279 (97%)	9 (3%)	0	100	100
10	I	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
11	K	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
12	L	603/605 (100%)	576 (96%)	26 (4%)	1 (0%)	43	66
13	M	456/458 (100%)	448 (98%)	8 (2%)	0	100	100
14	N	344/346 (99%)	334 (97%)	10 (3%)	0	100	100
15	O	318/320 (99%)	314 (99%)	2 (1%)	2 (1%)	21	42
16	P	341/342 (100%)	329 (96%)	12 (4%)	0	100	100
17	Q	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
18	R	94/96 (98%)	94 (100%)	0	0	100	100
19	S	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
20	T	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
21	U	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
22	V	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
23	W	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
24	X	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
25	t	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
26	Z	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
27	a	68/70 (97%)	68 (100%)	0	0	100	100
28	b	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
29	c	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	d	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
31	e	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
32	f	55/57 (96%)	51 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	g	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
34	h	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
35	u	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
36	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
37	k	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
38	l	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
39	m	126/128 (98%)	126 (100%)	0	0	100	100
40	n	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	21	42
41	o	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
42	p	171/173 (99%)	171 (100%)	0	0	100	100
43	q	143/145 (99%)	143 (100%)	0	0	100	100
44	v	92/113 (81%)	91 (99%)	1 (1%)	0	100	100
45	s	44/45 (98%)	44 (100%)	0	0	100	100
All	All	8117/8304 (98%)	7903 (97%)	206 (2%)	8 (0%)	49	70

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	5	PRO
8	G	188	GLU
6	E	215	ALA
12	L	562	LEU
15	O	126	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	133/141 (94%)	127 (96%)	6 (4%)	24	50
2	A	79/100 (79%)	75 (95%)	4 (5%)	21	45
3	B	131/131 (100%)	123 (94%)	8 (6%)	17	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	190/190 (100%)	181 (95%)	9 (5%)	23	48
5	D	360/370 (97%)	351 (98%)	9 (2%)	42	69
6	E	183/183 (100%)	171 (93%)	12 (7%)	15	34
7	F	347/346 (100%)	336 (97%)	11 (3%)	34	62
8	G	587/586 (100%)	548 (93%)	39 (7%)	15	34
9	H	257/274 (94%)	246 (96%)	11 (4%)	26	51
10	I	151/151 (100%)	146 (97%)	5 (3%)	33	61
11	K	85/85 (100%)	80 (94%)	5 (6%)	18	38
12	L	533/533 (100%)	499 (94%)	34 (6%)	16	35
13	M	412/412 (100%)	399 (97%)	13 (3%)	34	62
14	N	315/315 (100%)	298 (95%)	17 (5%)	20	42
15	O	283/283 (100%)	277 (98%)	6 (2%)	47	73
16	P	297/296 (100%)	282 (95%)	15 (5%)	21	45
17	Q	116/116 (100%)	105 (90%)	11 (10%)	8	18
18	R	79/79 (100%)	76 (96%)	3 (4%)	29	56
19	S	77/77 (100%)	73 (95%)	4 (5%)	21	44
20	T	79/79 (100%)	75 (95%)	4 (5%)	21	45
21	U	79/79 (100%)	74 (94%)	5 (6%)	16	36
22	V	101/101 (100%)	94 (93%)	7 (7%)	14	32
23	W	107/108 (99%)	105 (98%)	2 (2%)	50	75
24	X	154/154 (100%)	146 (95%)	8 (5%)	21	44
25	t	101/101 (100%)	95 (94%)	6 (6%)	18	38
26	Z	120/120 (100%)	116 (97%)	4 (3%)	33	61
27	a	59/59 (100%)	55 (93%)	4 (7%)	14	32
28	b	71/71 (100%)	69 (97%)	2 (3%)	38	66
29	c	45/45 (100%)	44 (98%)	1 (2%)	45	72
30	d	105/105 (100%)	102 (97%)	3 (3%)	37	65
31	e	89/89 (100%)	82 (92%)	7 (8%)	11	26
32	f	54/54 (100%)	49 (91%)	5 (9%)	8	18
33	g	91/91 (100%)	89 (98%)	2 (2%)	45	72
34	h	121/121 (100%)	119 (98%)	2 (2%)	53	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	u	121/121 (100%)	114 (94%)	7 (6%)	18	39
36	j	61/61 (100%)	57 (93%)	4 (7%)	15	34
37	k	63/63 (100%)	61 (97%)	2 (3%)	34	62
38	l	140/140 (100%)	134 (96%)	6 (4%)	26	51
39	m	114/114 (100%)	108 (95%)	6 (5%)	20	43
40	n	156/156 (100%)	152 (97%)	4 (3%)	40	68
41	o	110/110 (100%)	108 (98%)	2 (2%)	51	76
42	p	155/155 (100%)	148 (96%)	7 (4%)	24	50
43	q	131/131 (100%)	120 (92%)	11 (8%)	10	23
44	v	85/96 (88%)	78 (92%)	7 (8%)	10	24
45	s	45/44 (102%)	43 (96%)	2 (4%)	25	50
All	All	7172/7236 (99%)	6830 (95%)	342 (5%)	24	47

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	4	LEU
35	u	39	VAL
23	W	45	ASN
27	a	55	SER
38	l	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
29	c	35	HIS
40	n	13	GLN
30	d	117	HIS
34	h	143	ASN
42	p	106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
5	2MR	D	85	5	10,12,13	2.49	2 (20%)	5,13,15	0.92	0
1	FME	J	1	1	8,9,10	0.97	0	8,9,11	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2MR	D	85	5	-	0/10/13/15	-
1	FME	J	1	1	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	85	2MR	CZ-NH2	5.36	1.44	1.33
5	D	85	2MR	CZ-NE	5.13	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	1	FME	N-CA-CB-CG
1	J	1	FME	C-CA-CB-CG
1	J	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 3 are monoatomic - leaving 54 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	$\# Z > 2$
53	CDL	L	703	-	75,75,99	0.35	0	81,87,111	0.23	0
46	FME	A	201	-	8,9,10	0.99	0	8,9,11	0.87	0
47	PC1	Z	201	-	43,43,53	0.54	0	49,51,61	0.53	1 (2%)
52	3PE	t	803	-	29,29,50	0.64	0	32,34,55	0.82	2 (6%)
52	3PE	M	502	-	44,44,50	0.54	0	47,49,55	0.59	1 (2%)
47	PC1	M	503	-	34,34,53	0.60	0	40,42,61	0.57	1 (2%)
48	SF4	I	203	10	0,12,12	-	-	-	-	-
53	CDL	h	201	-	79,79,99	0.35	0	85,91,111	0.22	0
52	3PE	t	804	-	32,32,50	0.62	0	35,37,55	0.76	2 (5%)
47	PC1	I	201	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
52	3PE	L	702	-	45,45,50	0.55	0	48,50,55	0.57	1 (2%)
53	CDL	O	402	-	61,61,99	0.46	0	67,73,111	0.47	0
46	FME	H	401	-	8,9,10	0.97	0	8,9,11	0.96	0
48	SF4	F	502	7	0,12,12	-	-	-	-	-
55	GTP	O	403	56	33,34,34	1.01	4 (12%)	50,54,54	1.57	9 (18%)
53	CDL	d	201	-	85,85,99	0.42	1 (1%)	91,97,111	0.28	0
52	3PE	L	704	-	48,48,50	0.53	0	51,53,55	0.53	1 (1%)
46	FME	L	701	-	8,9,10	1.00	0	8,9,11	0.91	0
46	FME	K	101	-	8,9,10	0.97	0	8,9,11	0.92	0
47	PC1	H	403	-	47,47,53	0.53	0	53,55,61	0.52	1 (1%)
48	SF4	B	201	3	0,12,12	-	-	-	-	-
47	PC1	L	705	-	43,43,53	0.54	0	49,51,61	0.51	1 (2%)
49	FES	E	301	6	0,4,4	-	-	-	-	-
46	FME	M	501	-	8,9,10	0.99	0	8,9,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	FME	N	401	-	8,9,10	1.00	0	8,9,11	0.92	0
52	3PE	K	102	-	43,43,50	0.56	0	46,48,55	0.56	1 (2%)
52	3PE	t	802	-	39,39,50	0.58	0	42,44,55	0.58	1 (2%)
54	CHD	L	706	-	32,32,32	0.62	0	51,51,51	1.12	5 (9%)
47	PC1	B	202	-	45,45,53	0.54	0	51,53,61	0.65	2 (3%)
48	SF4	G	802	8	0,12,12	-	-	-		
47	PC1	B	203	-	47,47,53	0.52	0	53,55,61	0.54	1 (1%)
52	3PE	d	202	-	48,48,50	0.53	0	51,53,55	0.54	1 (1%)
47	PC1	A	202	-	34,34,53	0.60	0	40,42,61	0.57	1 (2%)
47	PC1	d	203	-	38,38,53	0.58	0	44,46,61	0.54	1 (2%)
47	PC1	h	202	-	46,46,53	0.52	0	52,54,61	0.50	1 (1%)
50	FMN	F	501	-	33,33,33	1.07	2 (6%)	48,50,50	1.23	9 (18%)
52	3PE	t	801	-	30,30,50	0.62	0	33,35,55	0.82	2 (6%)
52	3PE	u	201	-	44,44,50	0.55	0	47,49,55	0.57	1 (2%)
48	SF4	G	801	8	0,12,12	-	-	-		
53	CDL	v	201	-	60,60,99	0.39	0	66,72,111	0.25	0
52	3PE	b	201	-	46,46,50	0.53	0	49,51,55	0.54	1 (2%)
59	MYR	o	201	-	13,14,15	0.33	0	12,13,15	0.64	0
48	SF4	I	202	10	0,12,12	-	-	-		
52	3PE	M	505	-	49,49,50	0.51	0	52,54,55	0.53	1 (1%)
57	NDP	P	501	-	51,52,52	2.40	6 (11%)	71,80,80	1.52	15 (21%)
52	3PE	j	101	-	43,43,50	0.55	0	46,48,55	0.59	1 (2%)
52	3PE	M	504	-	50,50,50	0.50	0	53,55,55	0.66	2 (3%)
52	3PE	t	805	-	26,26,50	0.69	0	29,31,55	0.68	1 (3%)
52	3PE	m	202	-	40,40,50	0.57	0	43,45,55	0.58	1 (2%)
47	PC1	m	201	-	45,45,53	0.53	0	51,53,61	0.51	1 (1%)
53	CDL	d	204	-	64,64,99	0.38	0	70,76,111	0.27	0
52	3PE	O	401	-	47,47,50	0.54	0	50,52,55	0.55	1 (2%)
49	FES	G	803	8	0,4,4	-	-	-		
52	3PE	H	402	-	35,35,50	0.60	0	38,40,55	0.62	1 (2%)

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
53	CDL	L	703	-	-	48/86/86/110	-
46	FME	A	201	-	-	2/7/9/11	-
47	PC1	Z	201	-	-	17/47/47/57	-
52	3PE	t	803	-	-	21/33/33/54	-
52	3PE	M	502	-	-	12/48/48/54	-
47	PC1	M	503	-	-	20/38/38/57	-
48	SF4	I	203	10	-	-	0/6/5/5
53	CDL	h	201	-	-	53/90/90/110	-
52	3PE	t	804	-	-	19/36/36/54	-
47	PC1	I	201	-	-	17/57/57/57	-
52	3PE	L	702	-	-	21/49/49/54	-
53	CDL	O	402	-	-	46/71/71/110	-
46	FME	H	401	-	-	4/7/9/11	-
55	GTP	O	403	56	-	4/22/38/38	0/3/3/3
48	SF4	F	502	7	-	-	0/6/5/5
53	CDL	d	201	-	-	54/96/96/110	-
52	3PE	L	704	-	-	20/52/52/54	-
46	FME	L	701	-	-	4/7/9/11	-
46	FME	K	101	-	-	2/7/9/11	-
47	PC1	H	403	-	-	16/51/51/57	-
48	SF4	B	201	3	-	-	0/6/5/5
47	PC1	L	705	-	-	15/47/47/57	-
52	3PE	t	802	-	-	16/43/43/54	-
46	FME	M	501	-	-	1/7/9/11	-
46	FME	N	401	-	-	2/7/9/11	-
52	3PE	K	102	-	-	14/47/47/54	-
54	CHD	L	706	-	-	3/9/74/74	0/4/4/4
49	FES	E	301	6	-	-	0/1/1/1
47	PC1	B	202	-	-	24/49/49/57	-
48	SF4	G	802	8	-	-	0/6/5/5
47	PC1	B	203	-	-	16/51/51/57	-
52	3PE	d	202	-	-	17/52/52/54	-
47	PC1	A	202	-	-	17/38/38/57	-
47	PC1	d	203	-	-	11/42/42/57	-
47	PC1	h	202	-	-	22/50/50/57	-
50	FMN	F	501	-	-	1/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	t	801	-	-	15/34/34/54	-
52	3PE	u	201	-	-	21/48/48/54	-
53	CDL	v	201	-	-	33/71/71/110	-
48	SF4	G	801	8	-	-	0/6/5/5
52	3PE	b	201	-	-	25/50/50/54	-
59	MYR	o	201	-	-	1/12/12/13	-
48	SF4	I	202	10	-	-	0/6/5/5
52	3PE	M	505	-	-	25/53/53/54	-
57	NDP	P	501	-	-	12/34/77/77	0/5/5/5
52	3PE	j	101	-	-	11/47/47/54	-
52	3PE	M	504	-	-	17/54/54/54	-
52	3PE	t	805	-	-	14/30/30/54	-
52	3PE	m	202	-	-	15/44/44/54	-
47	PC1	m	201	-	-	23/49/49/57	-
53	CDL	d	204	-	-	42/75/75/110	-
52	3PE	O	401	-	-	18/51/51/54	-
49	FES	G	803	8	-	-	0/1/1/1
52	3PE	H	402	-	-	12/39/39/54	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	P2B-O2B	13.50	1.83	1.59
57	P	501	NDP	PA-O3	5.21	1.65	1.59
57	P	501	NDP	PN-O5D	4.27	1.76	1.59
50	F	501	FMN	C4A-N5	3.43	1.38	1.30
57	P	501	NDP	O2B-C2B	-3.20	1.33	1.44

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	403	GTP	C5-C4-N3	-5.00	120.43	128.39
55	O	403	GTP	C2-N3-C4	4.55	120.13	112.30
57	P	501	NDP	P2B-O2B-C2B	-4.54	111.30	123.43
57	P	501	NDP	O2B-P2B-O1X	-3.66	96.29	109.33
57	P	501	NDP	O3-PA-O1A	-3.54	100.07	110.70

There are no chirality outliers.

5 of 823 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	201	FME	O1-CN-N-CA
46	H	401	FME	N-CA-CB-CG
46	H	401	FME	O-C-CA-CB
46	K	101	FME	O1-CN-N-CA
46	K	101	FME	O-C-CA-CB

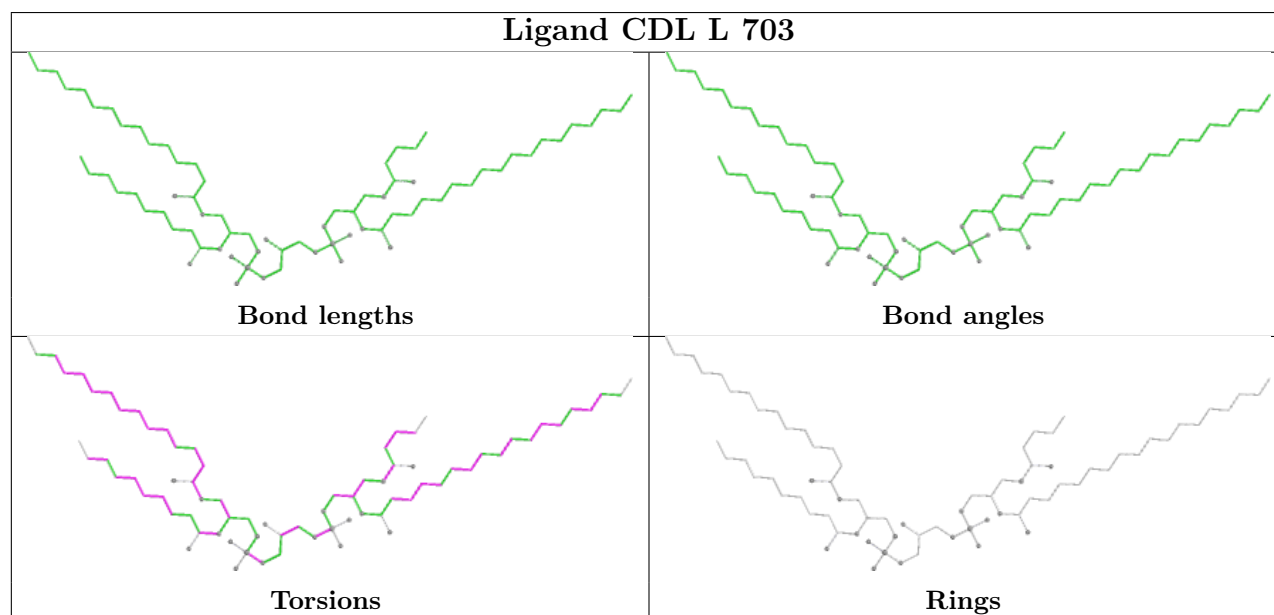
There are no ring outliers.

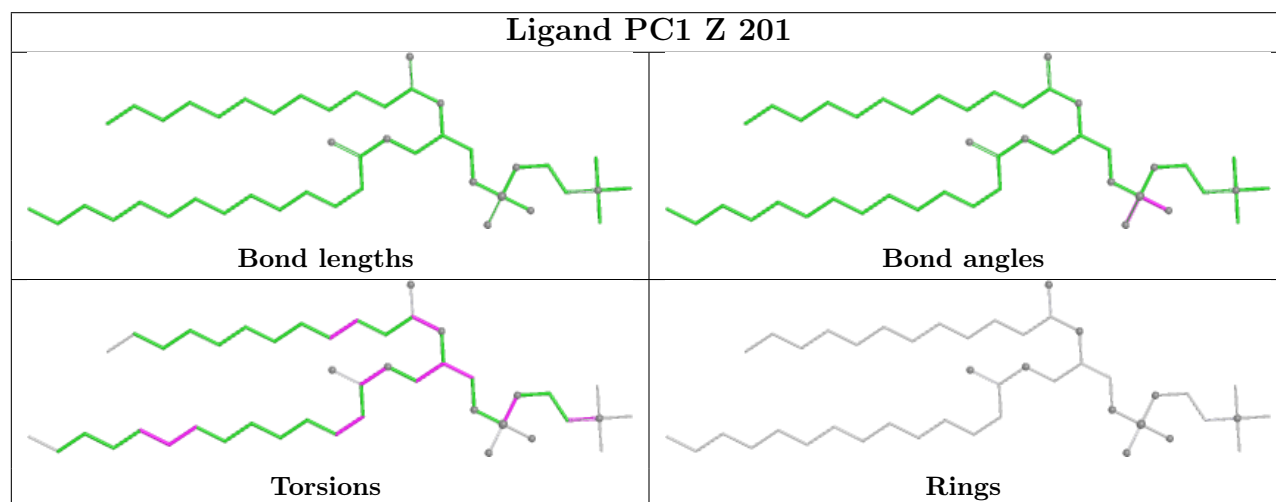
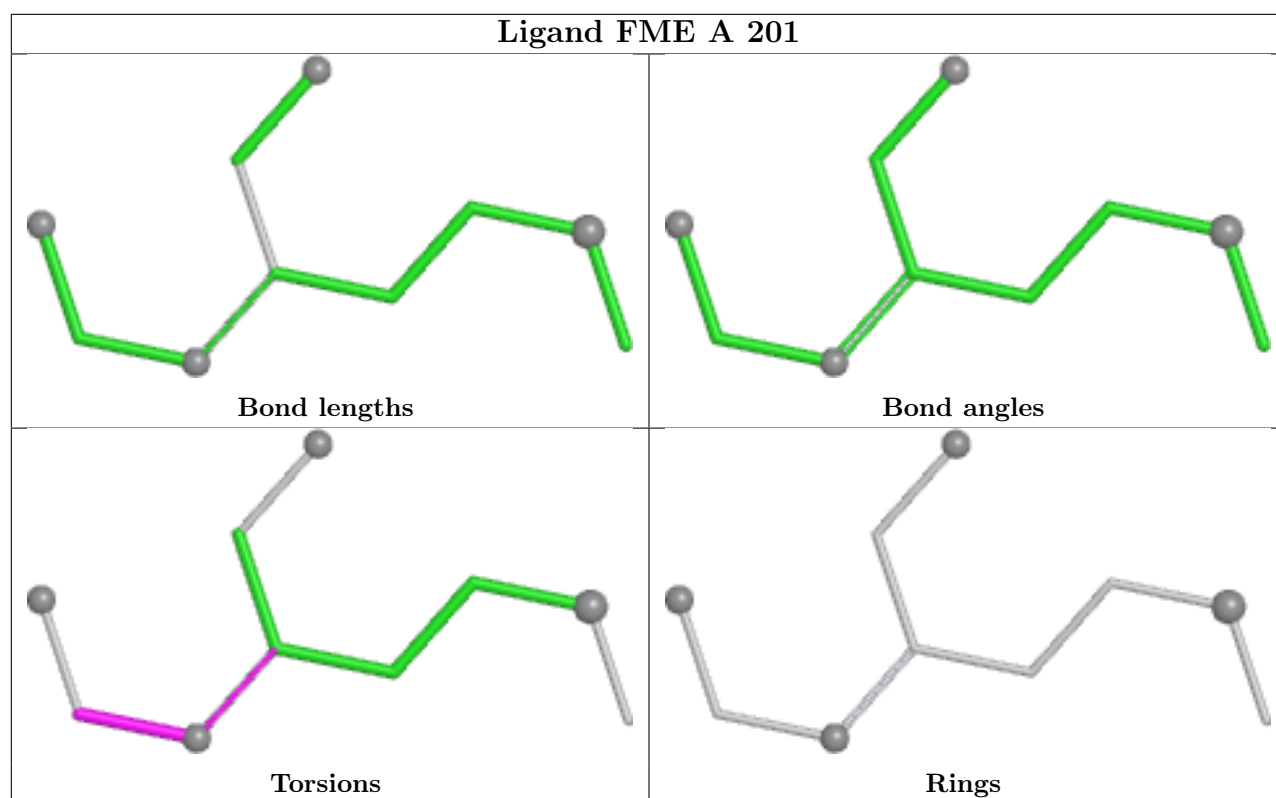
31 monomers are involved in 60 short contacts:

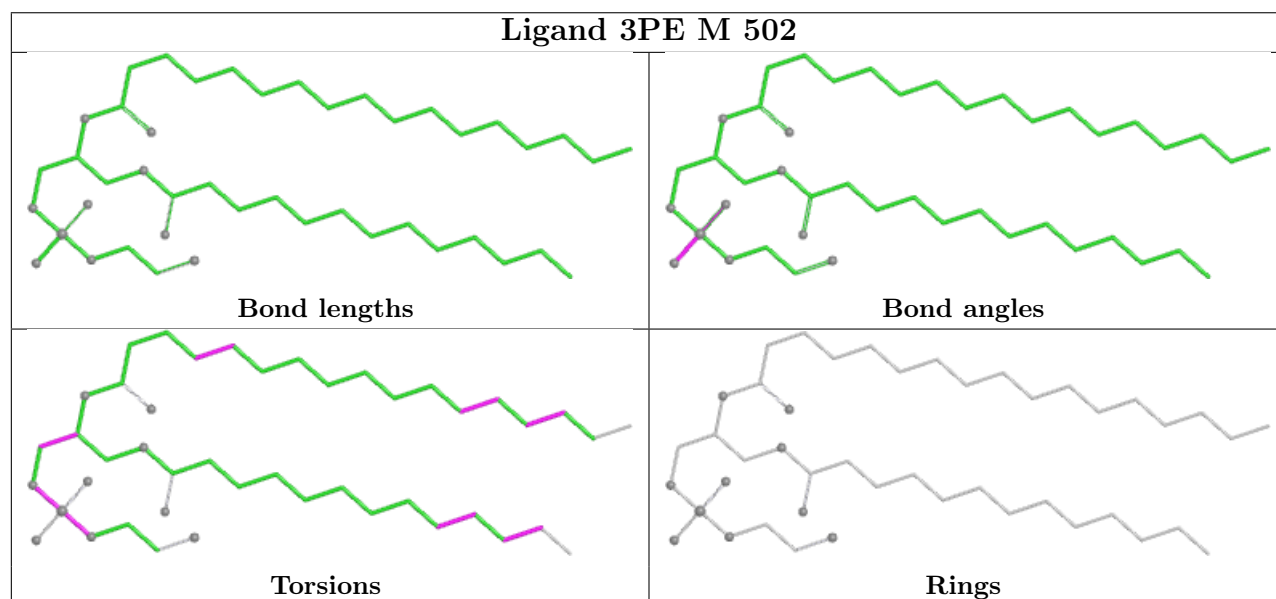
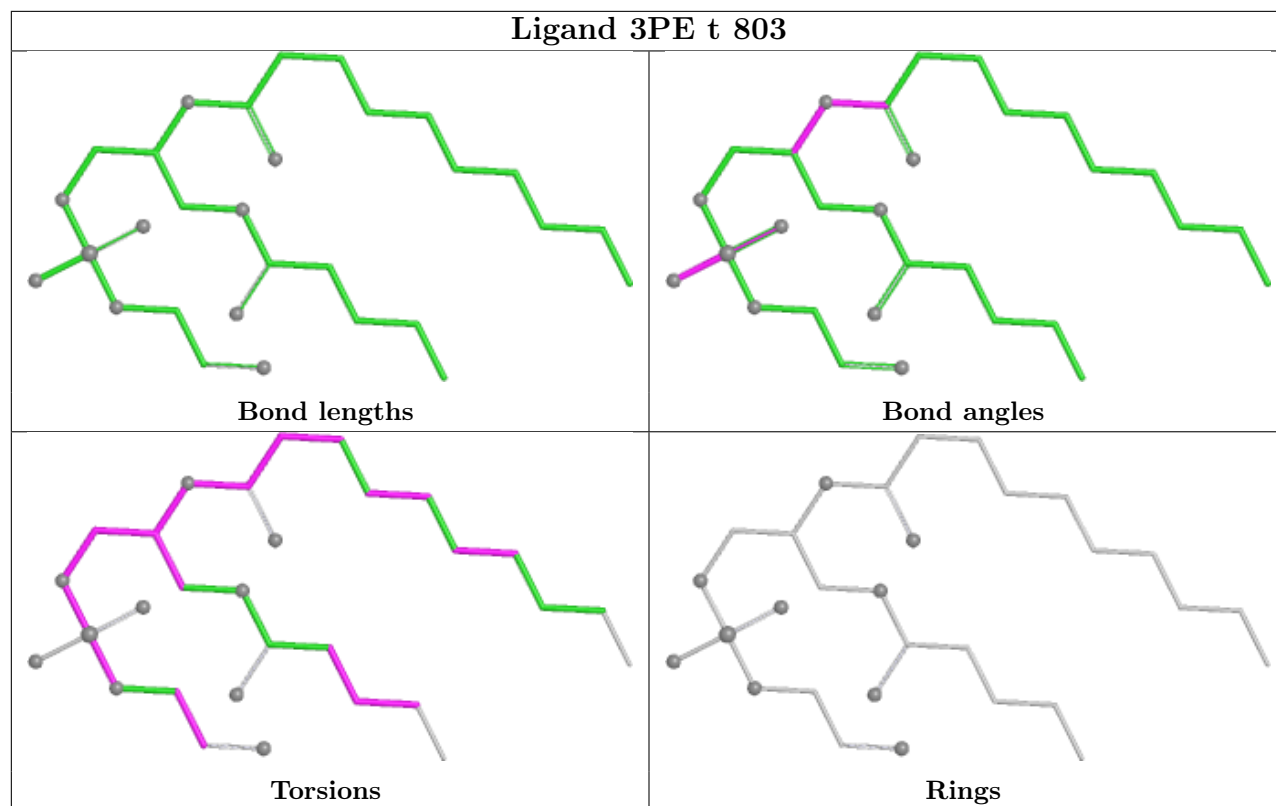
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	L	703	CDL	4	0
46	A	201	FME	2	0
52	M	502	3PE	1	0
47	M	503	PC1	1	0
53	h	201	CDL	2	0
52	t	804	3PE	1	0
47	I	201	PC1	2	0
53	O	402	CDL	5	0
46	H	401	FME	1	0
48	F	502	SF4	2	0
55	O	403	GTP	1	0
53	d	201	CDL	8	0
52	L	704	3PE	1	0
46	L	701	FME	1	0
47	H	403	PC1	3	0
46	N	401	FME	1	0
54	L	706	CHD	2	0
47	B	202	PC1	4	0
52	d	202	3PE	1	0
47	d	203	PC1	2	0
47	h	202	PC1	1	0
50	F	501	FMN	2	0
52	u	201	3PE	1	0
53	v	201	CDL	2	0
52	b	201	3PE	2	0
52	M	505	3PE	1	0
52	j	101	3PE	1	0
52	M	504	3PE	4	0
52	m	202	3PE	1	0
53	d	204	CDL	2	0
52	O	401	3PE	1	0

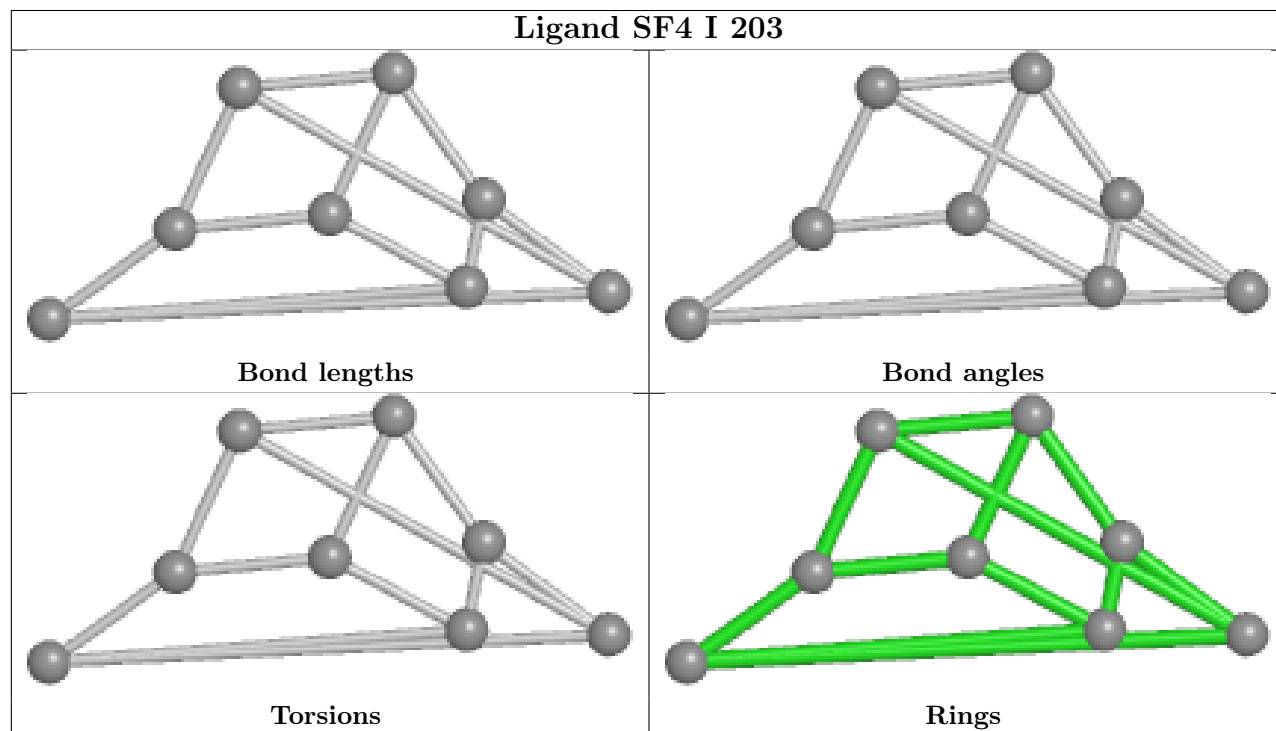
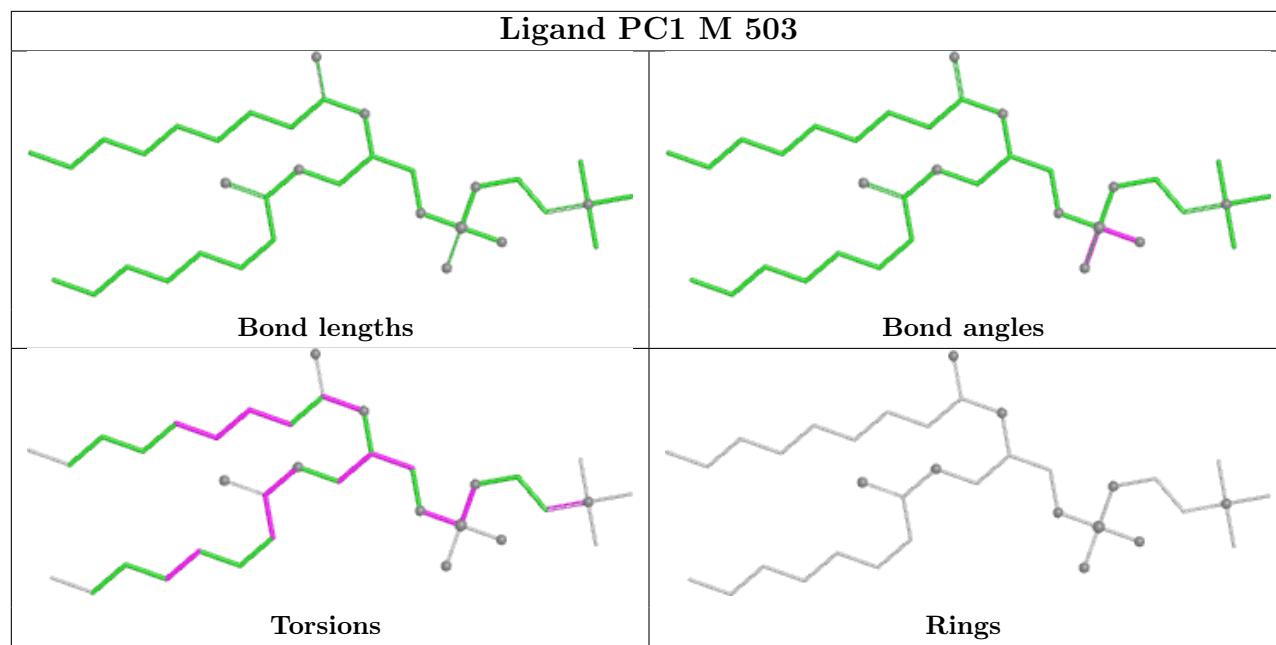
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

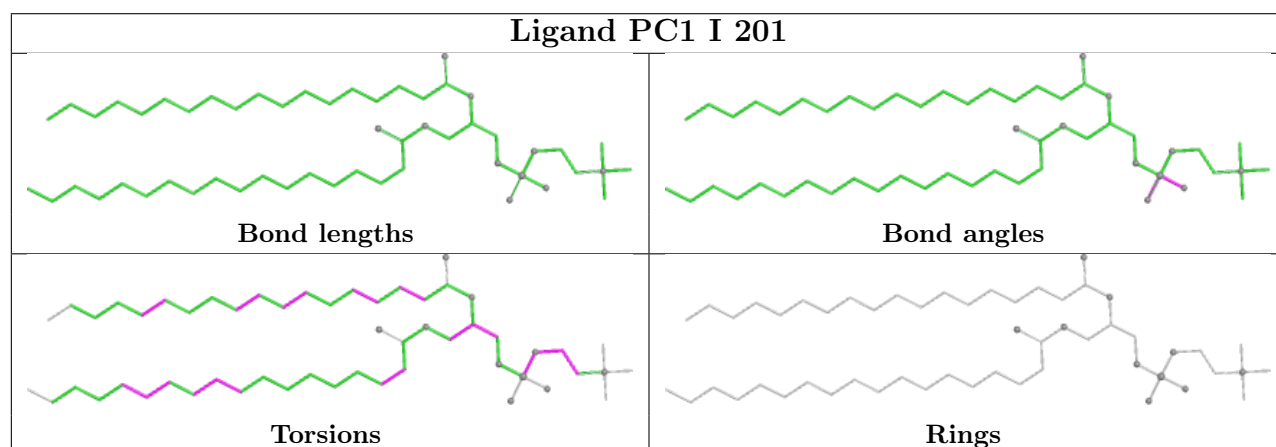
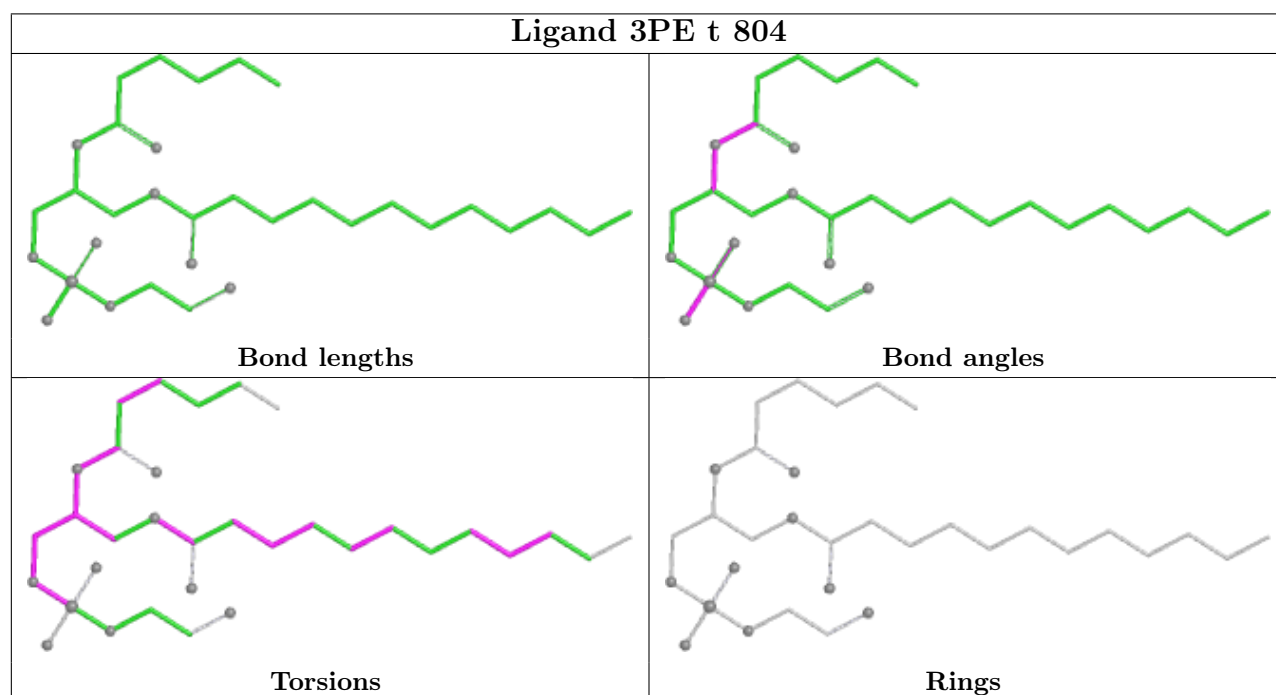
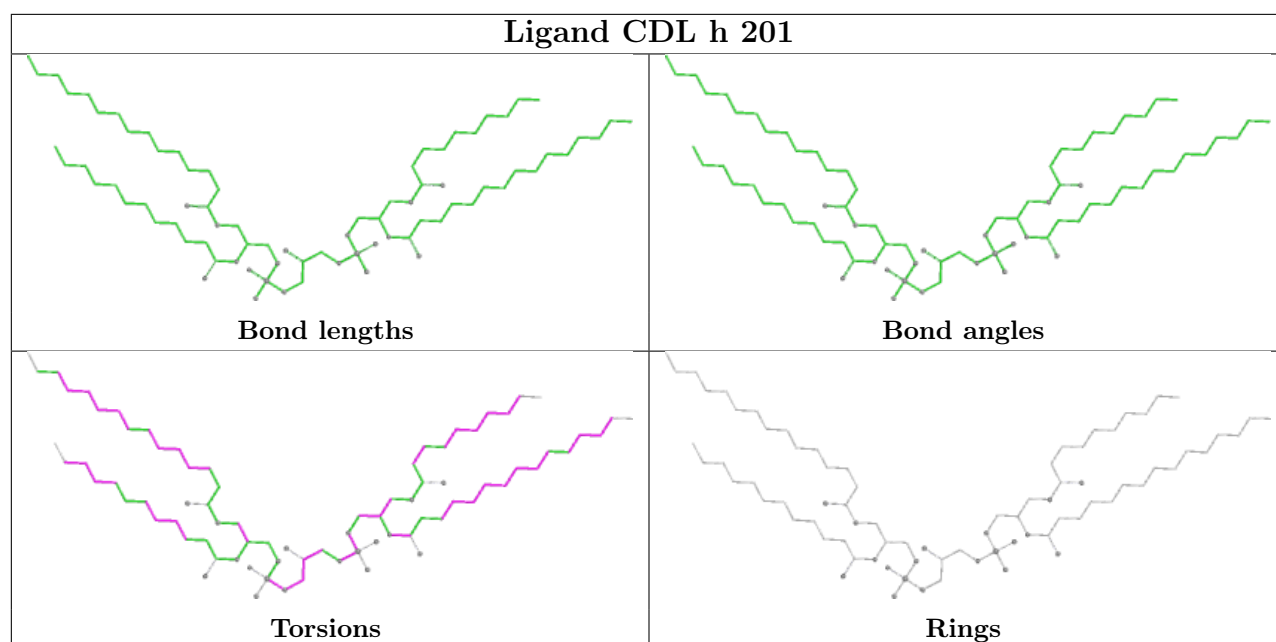
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

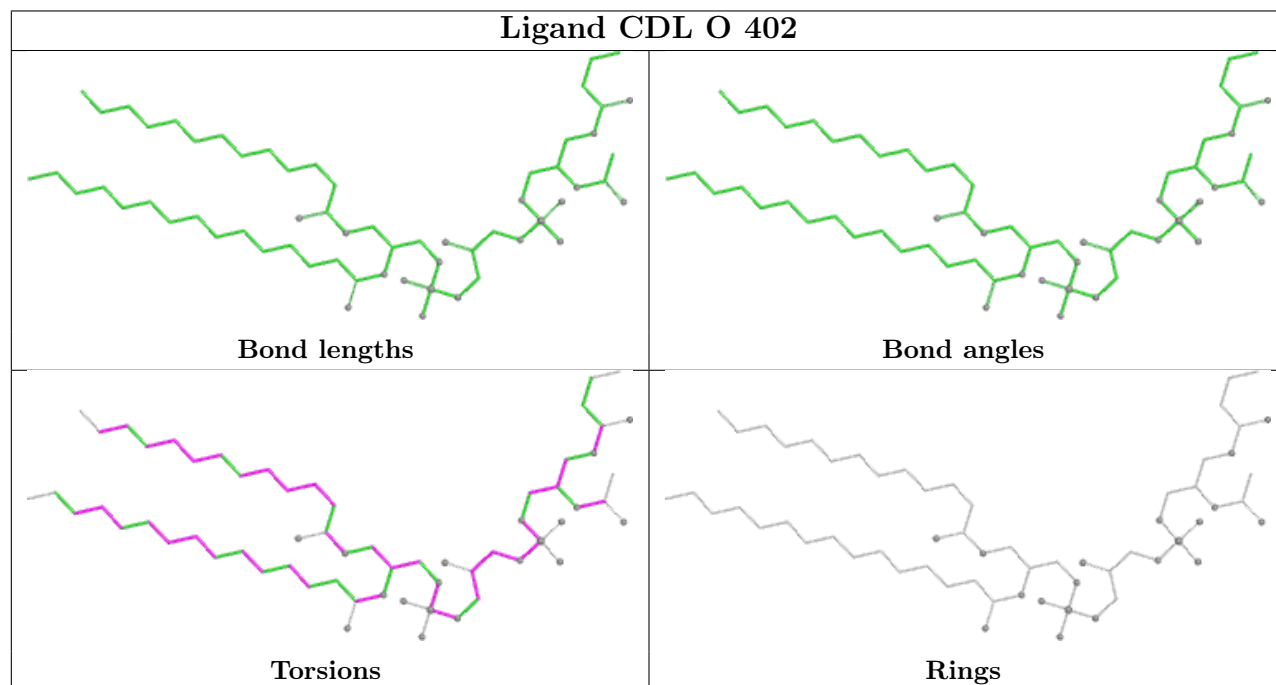
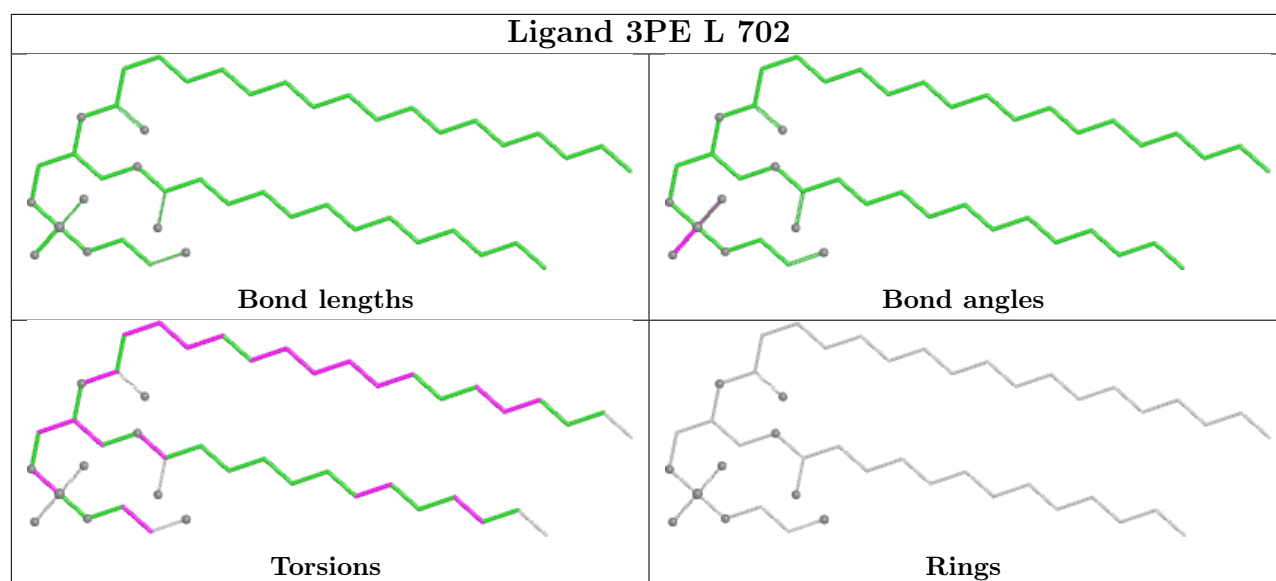


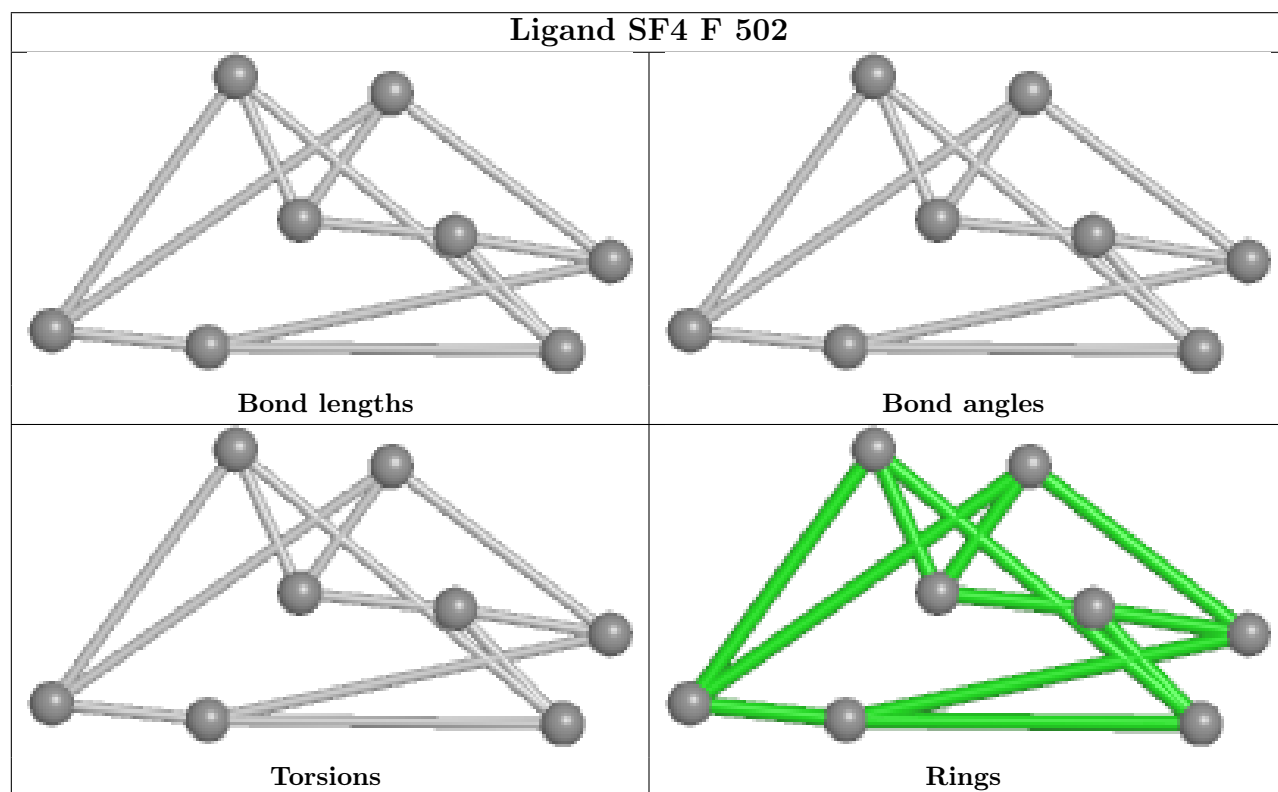
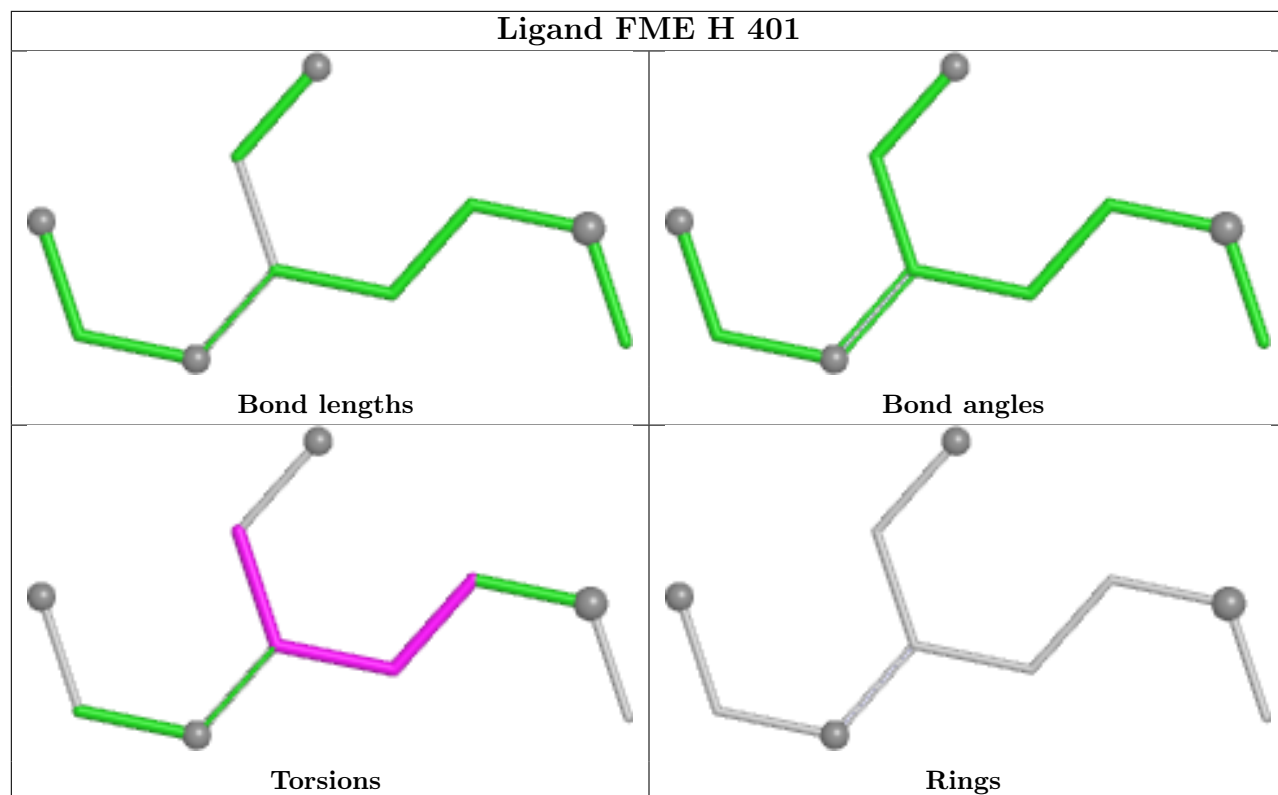


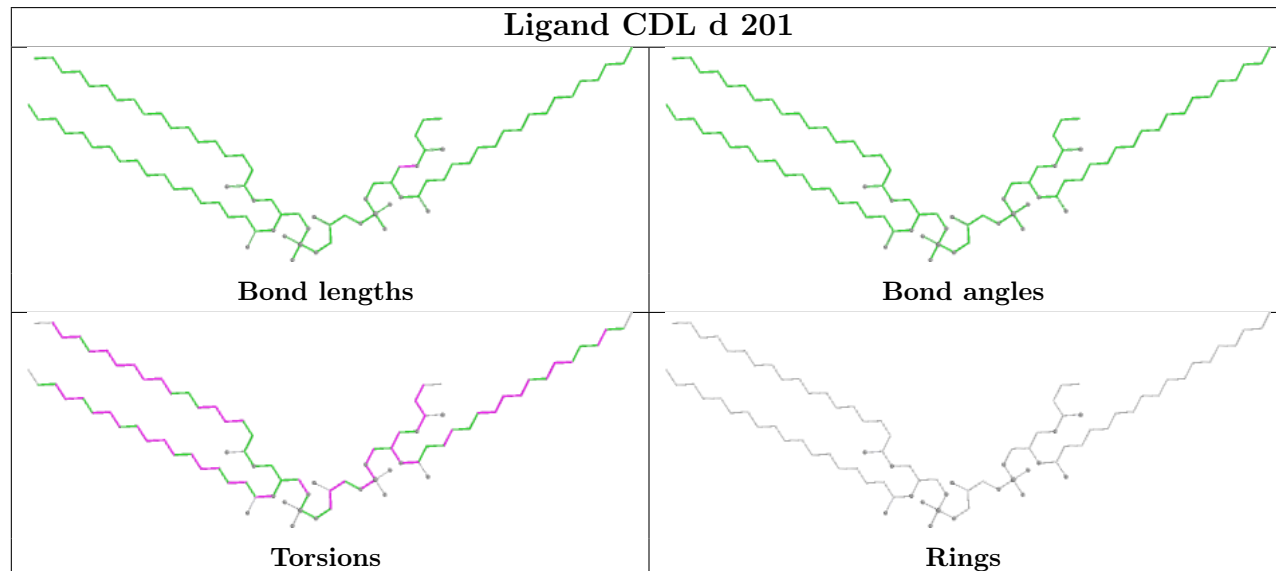
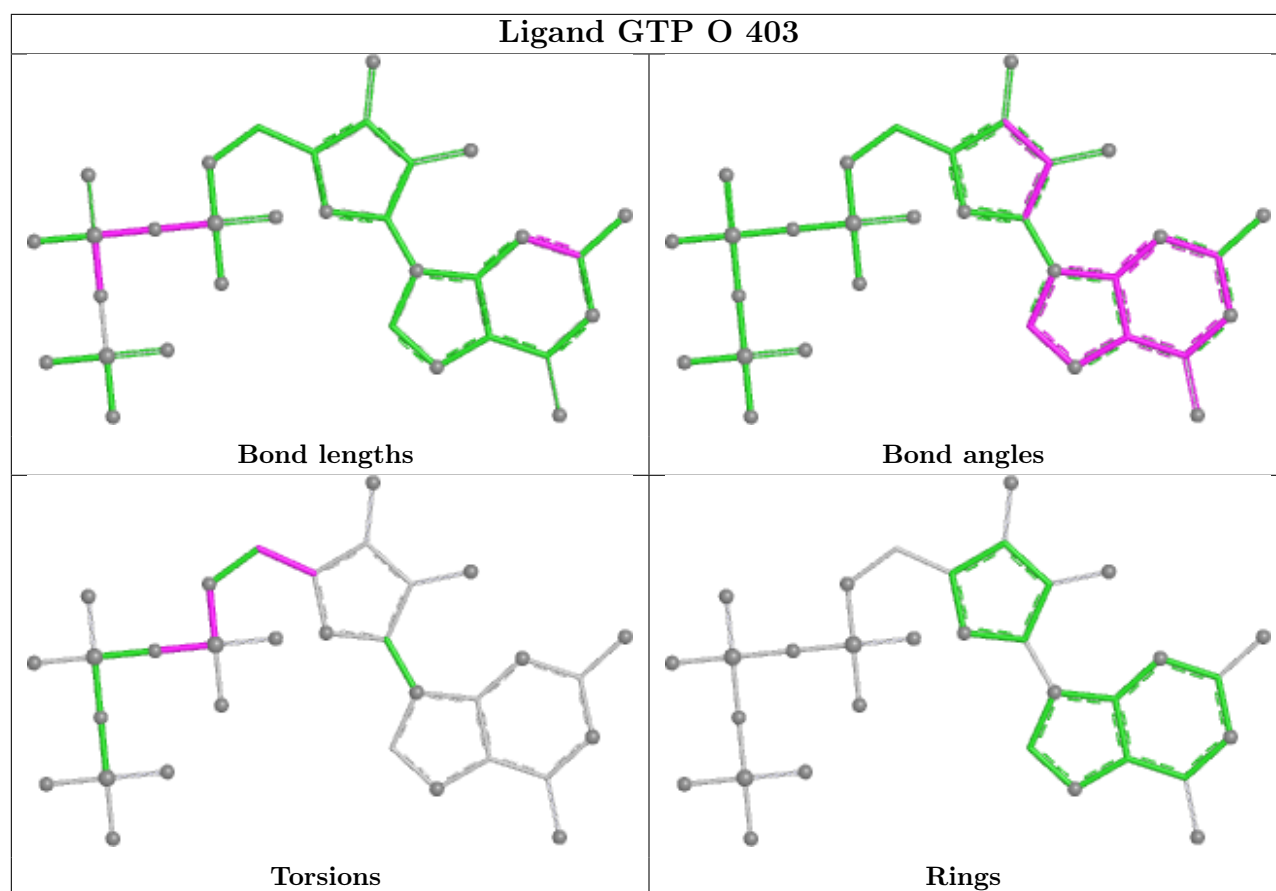


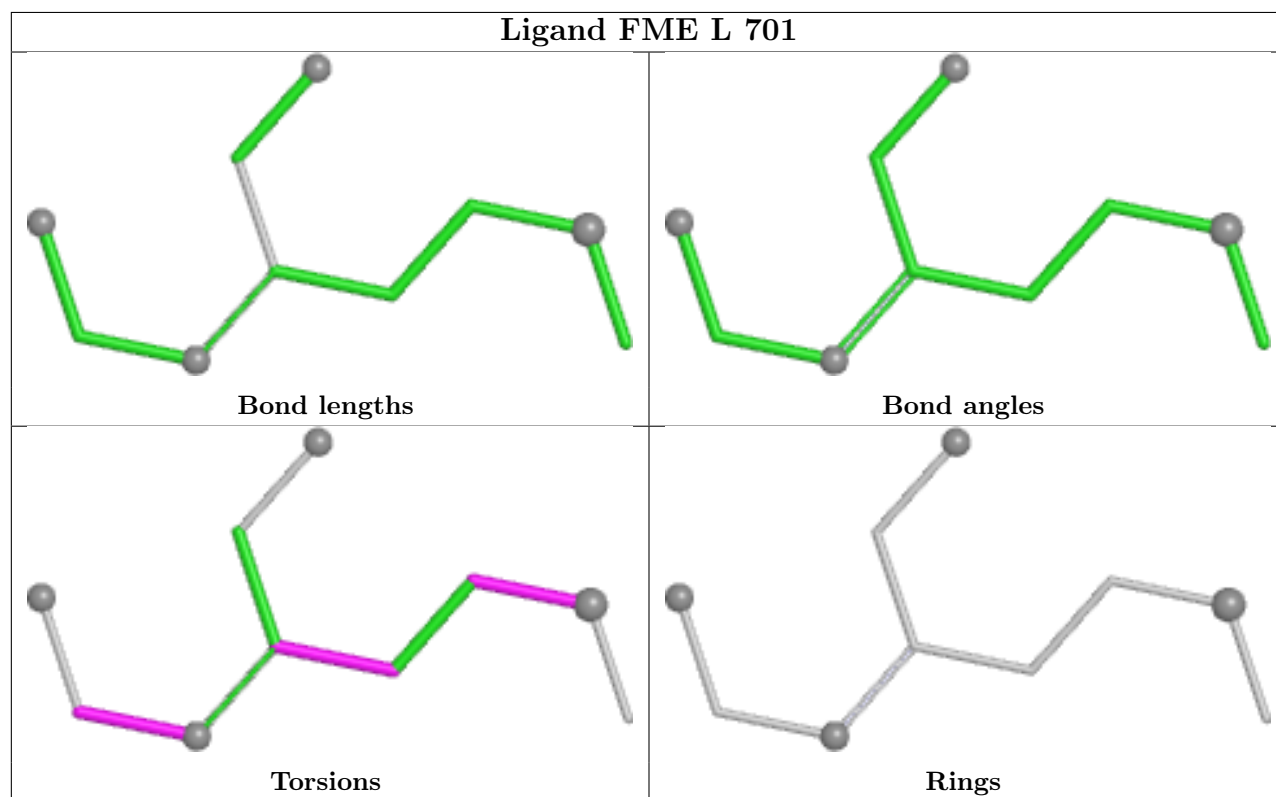
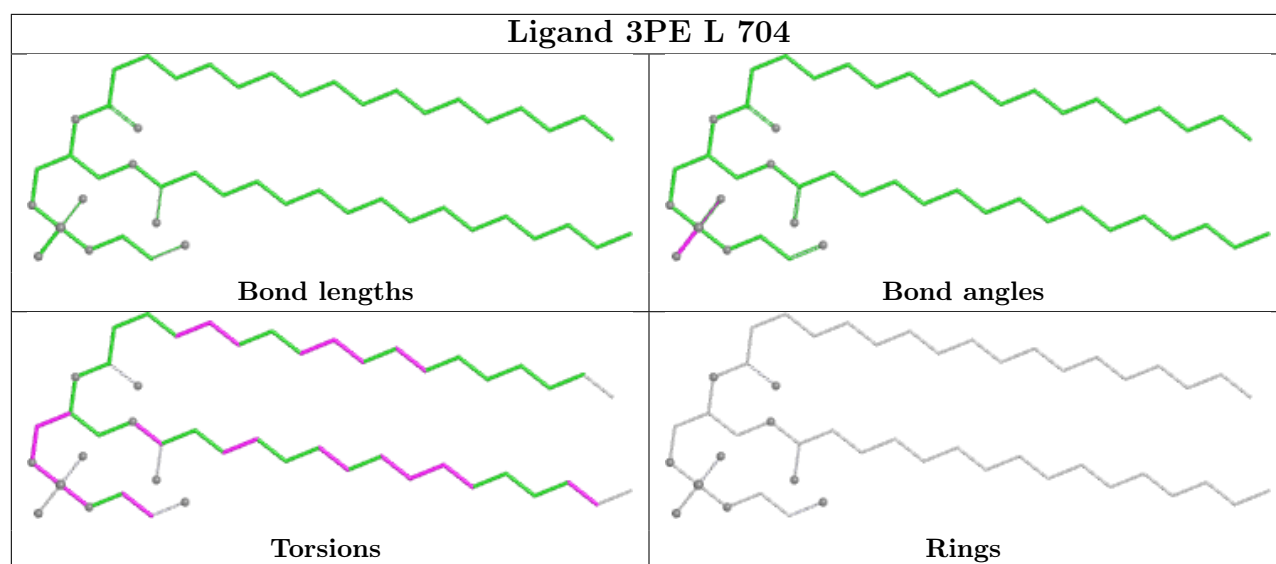


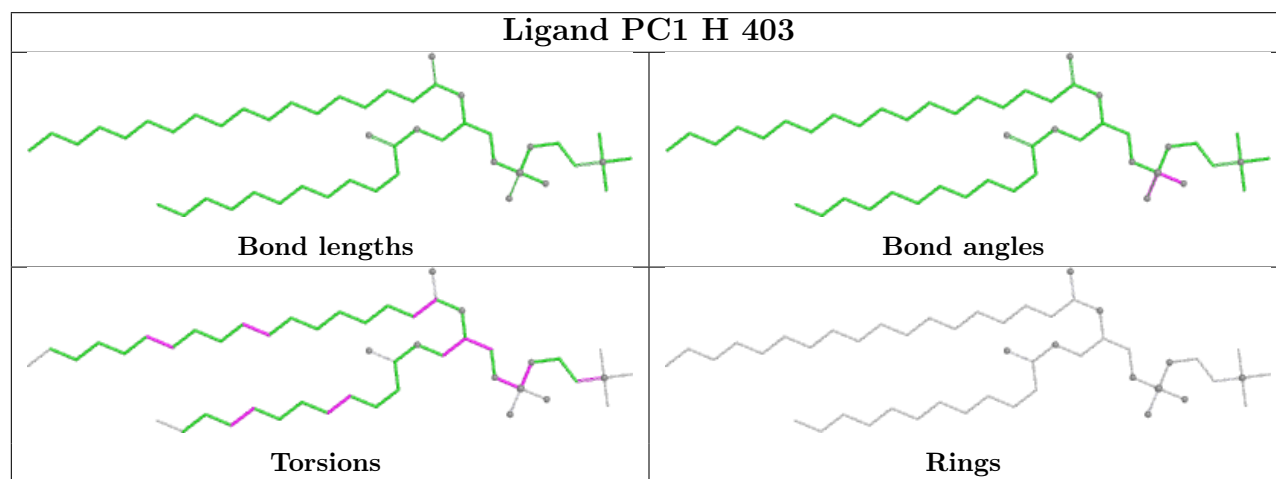
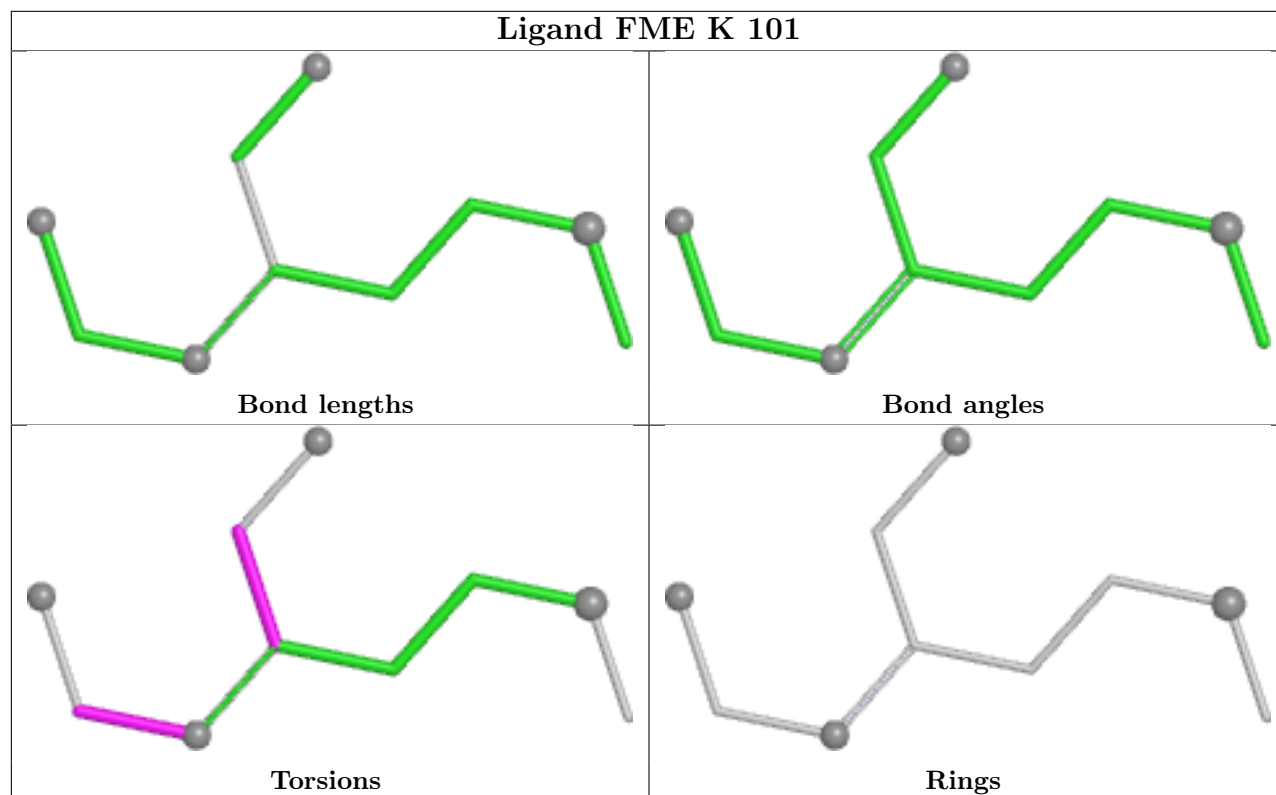


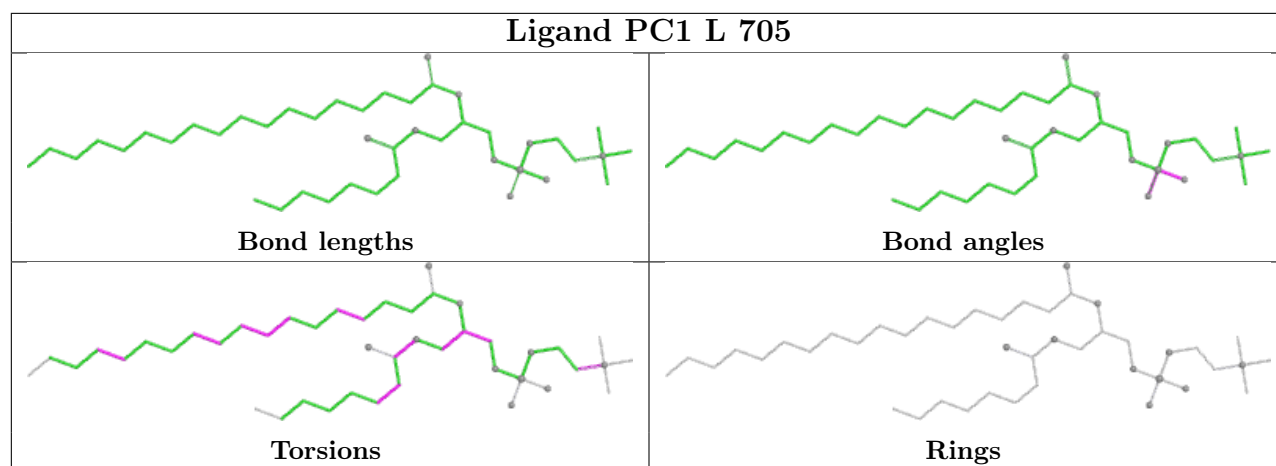
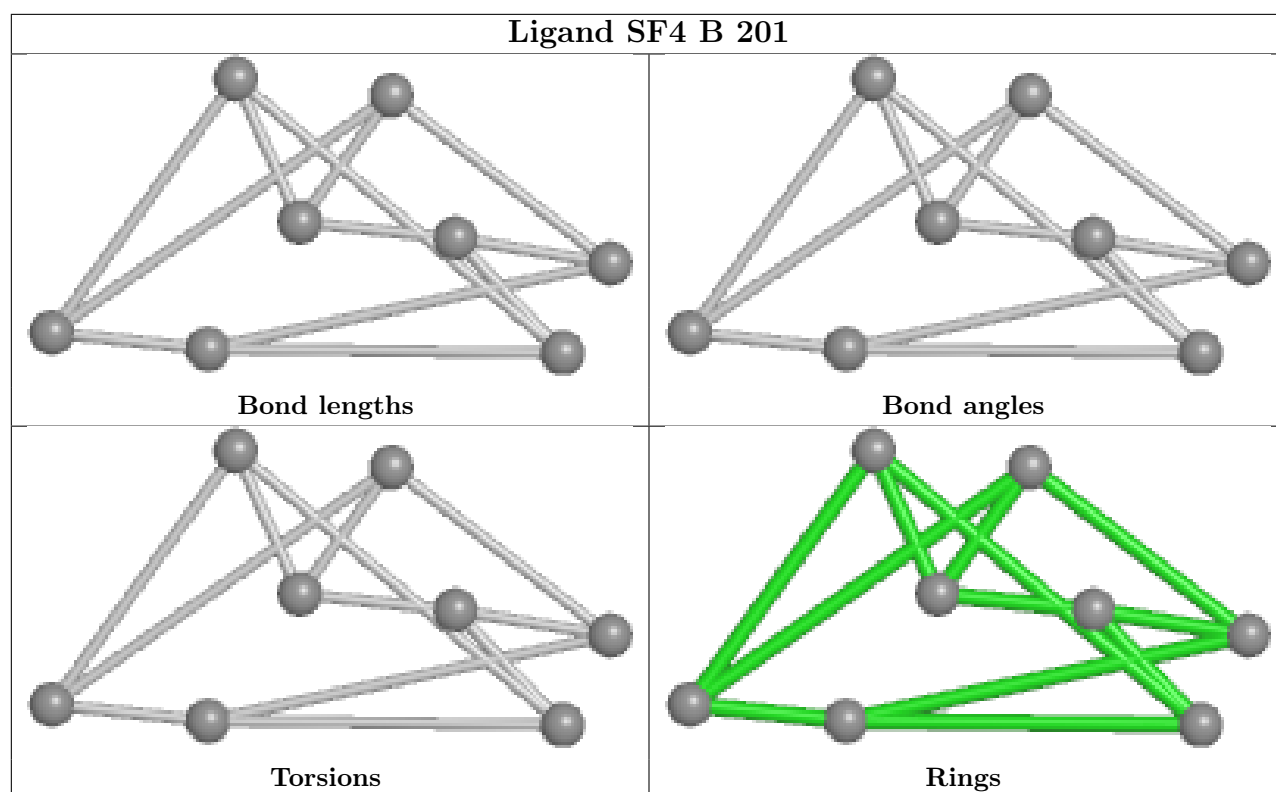


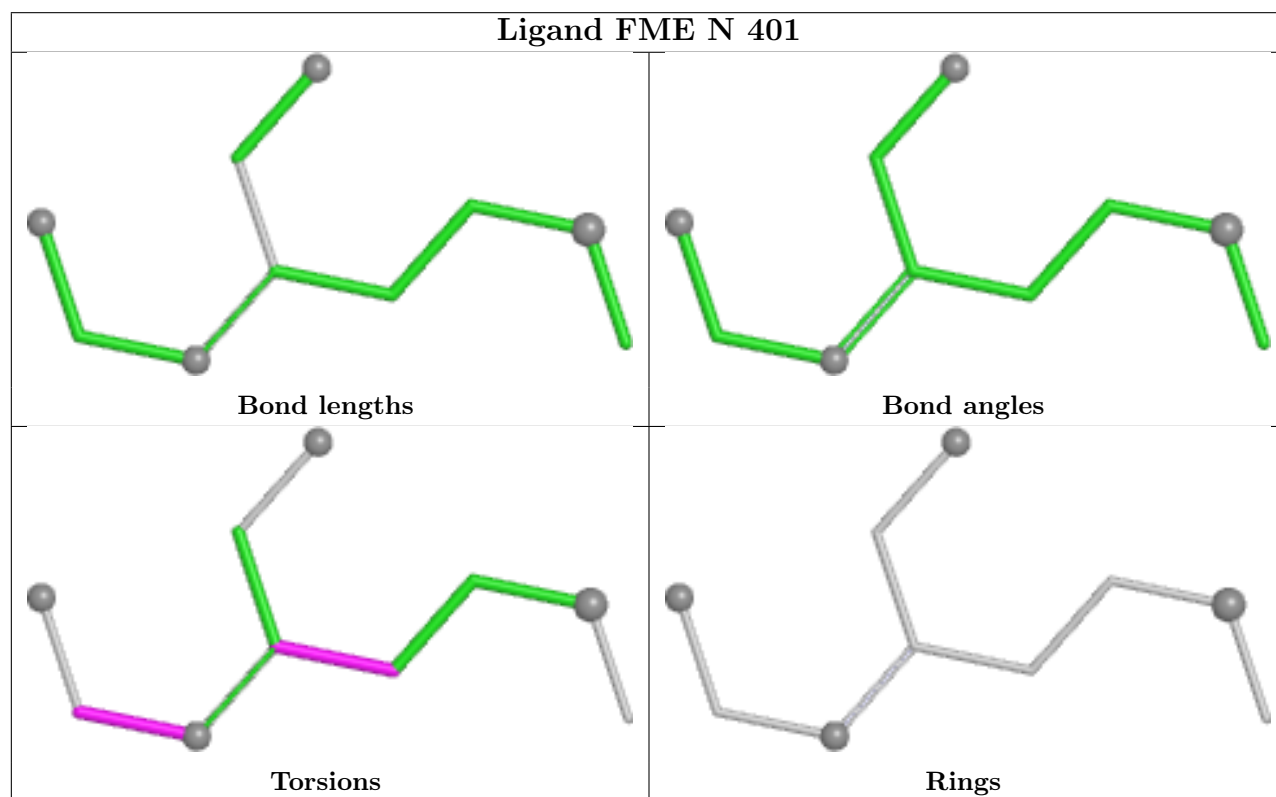
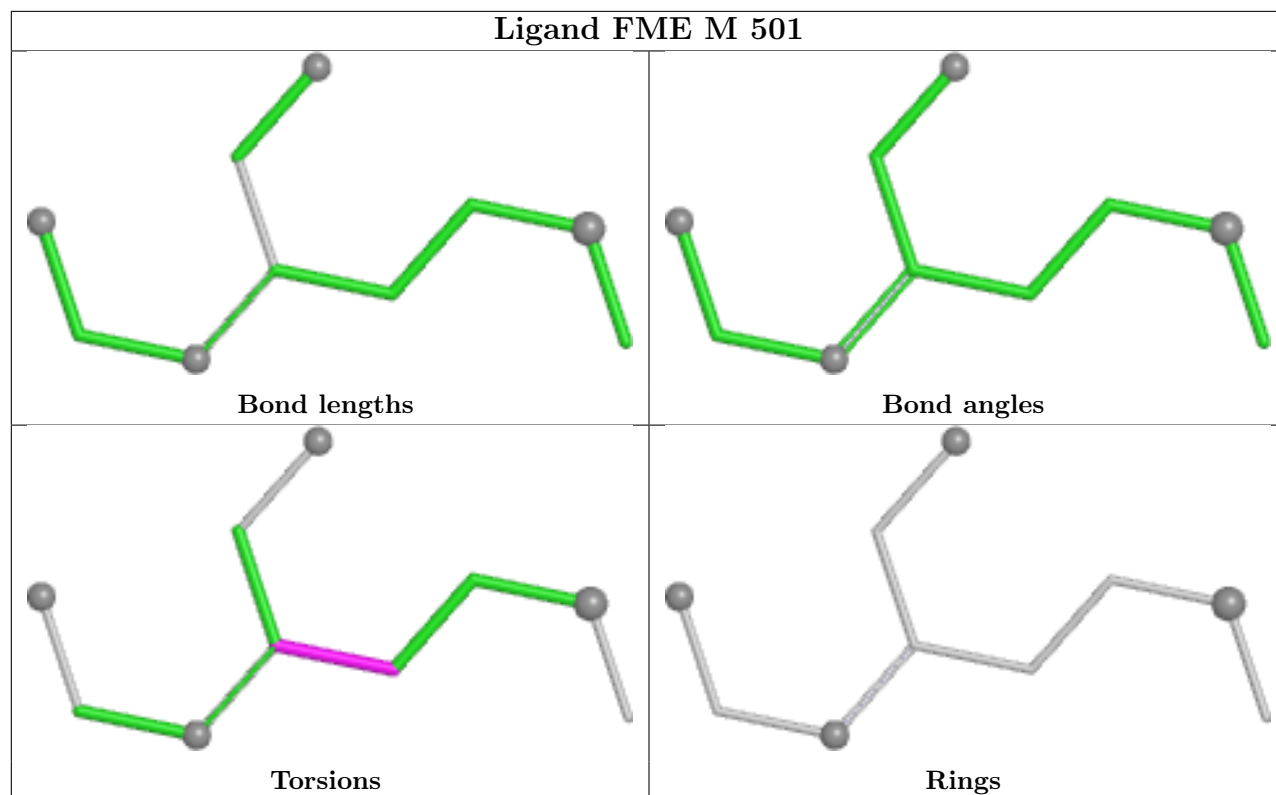


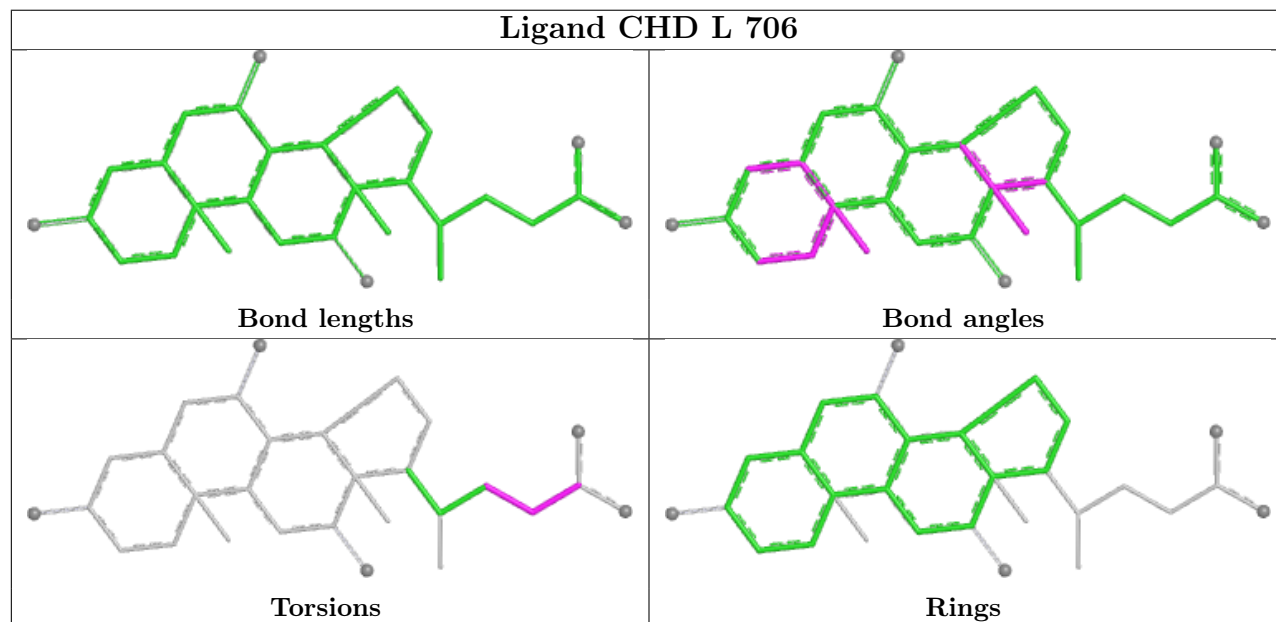
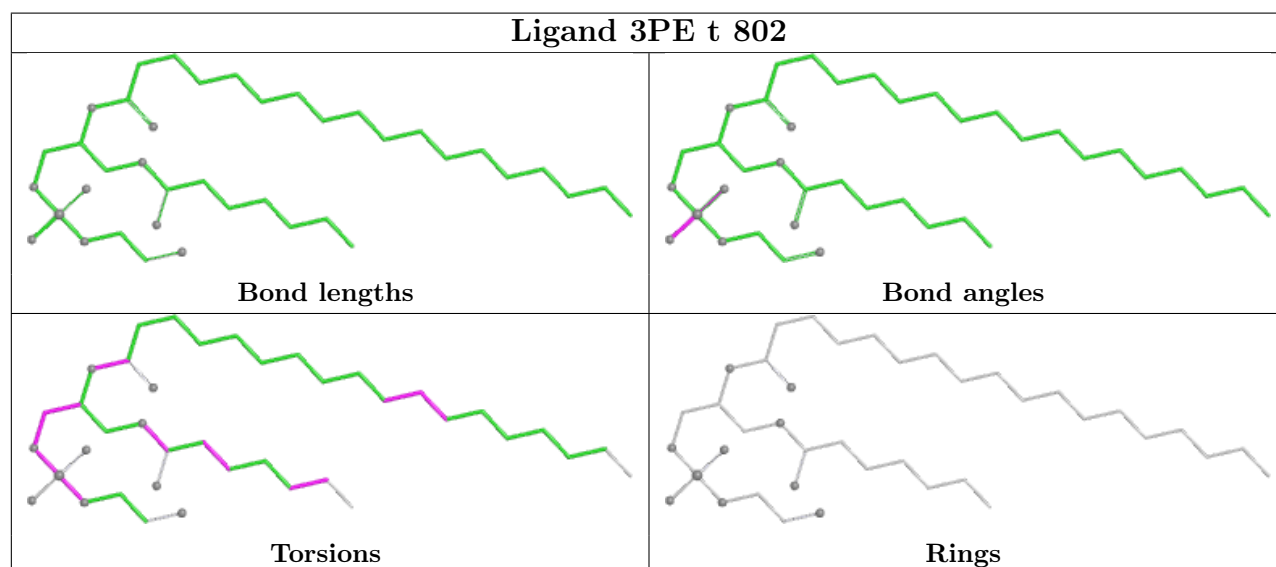
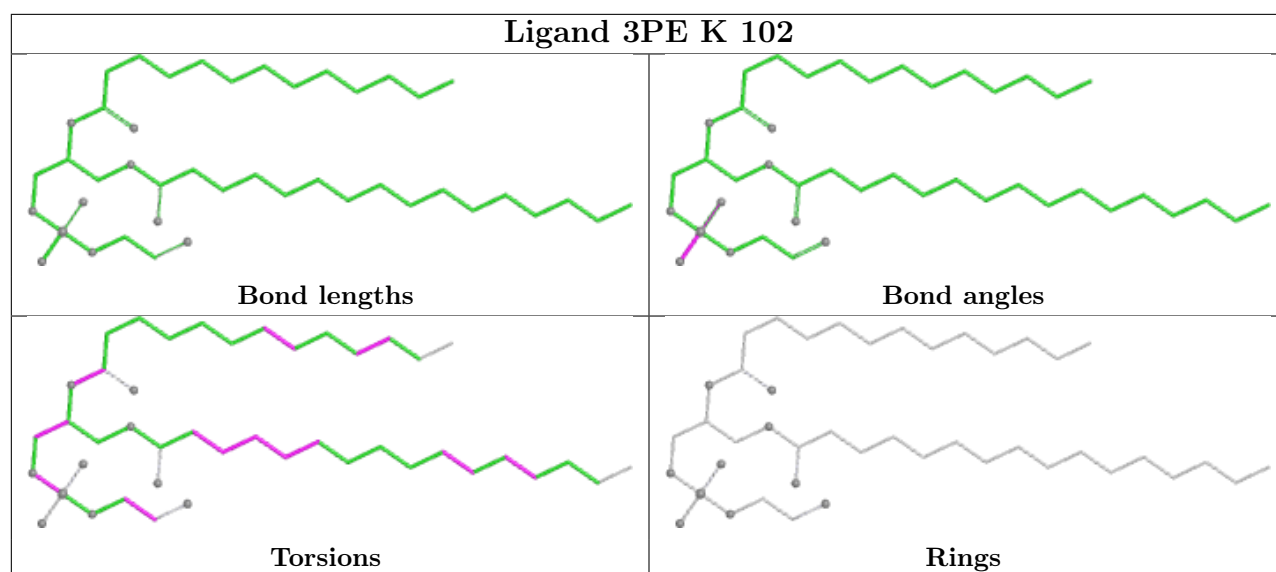


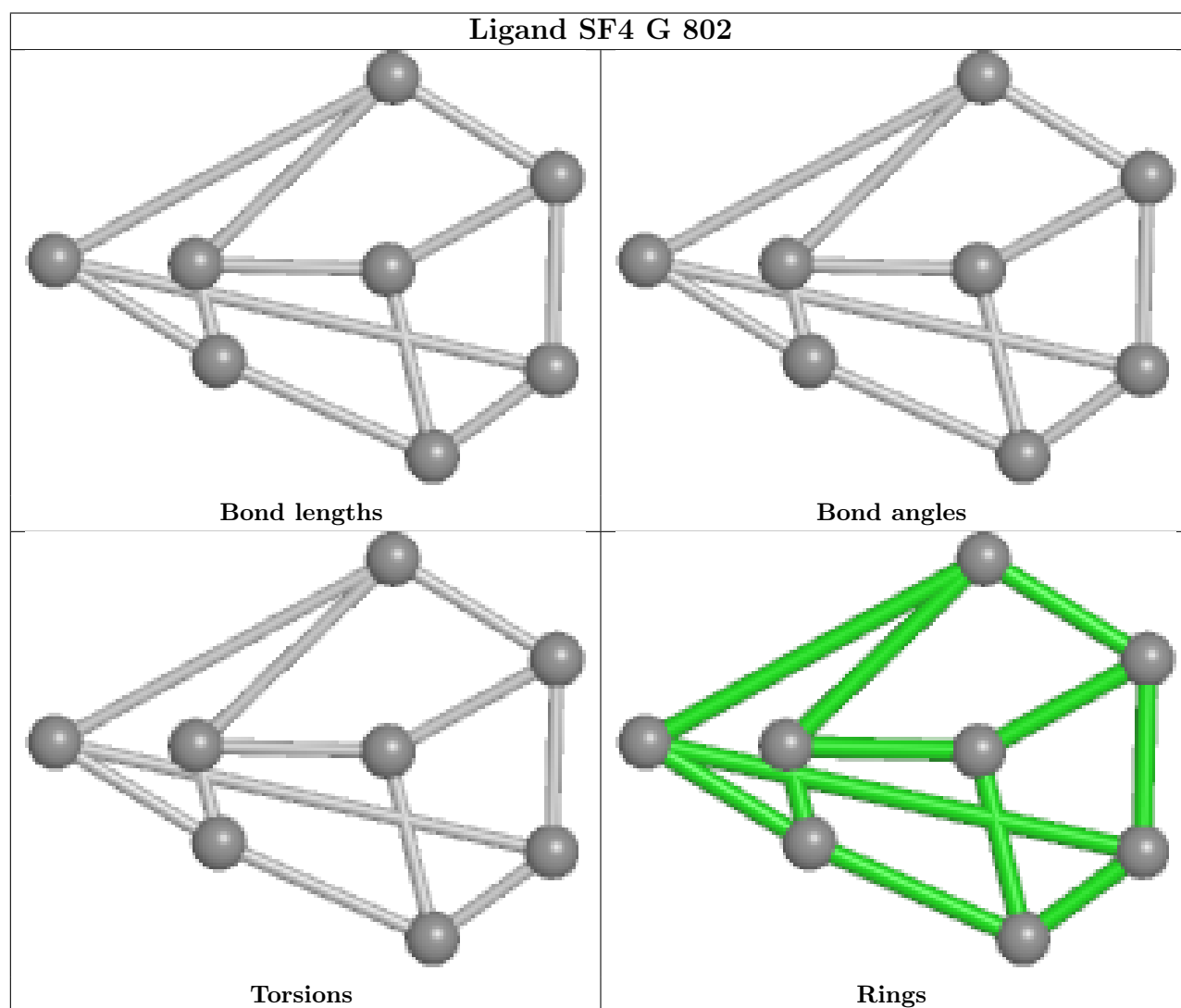
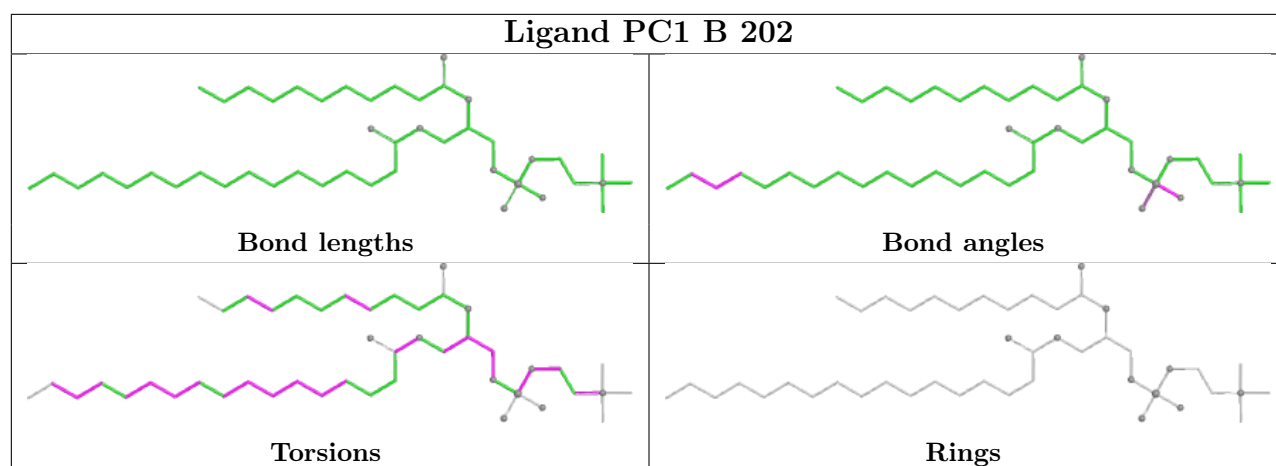


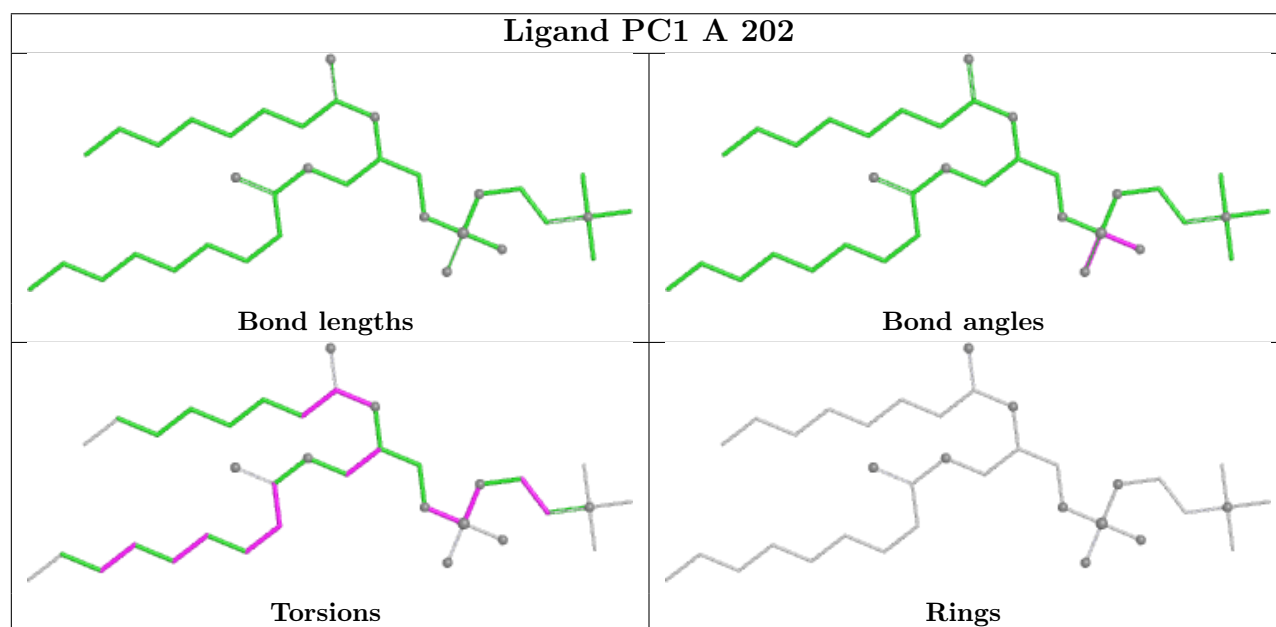
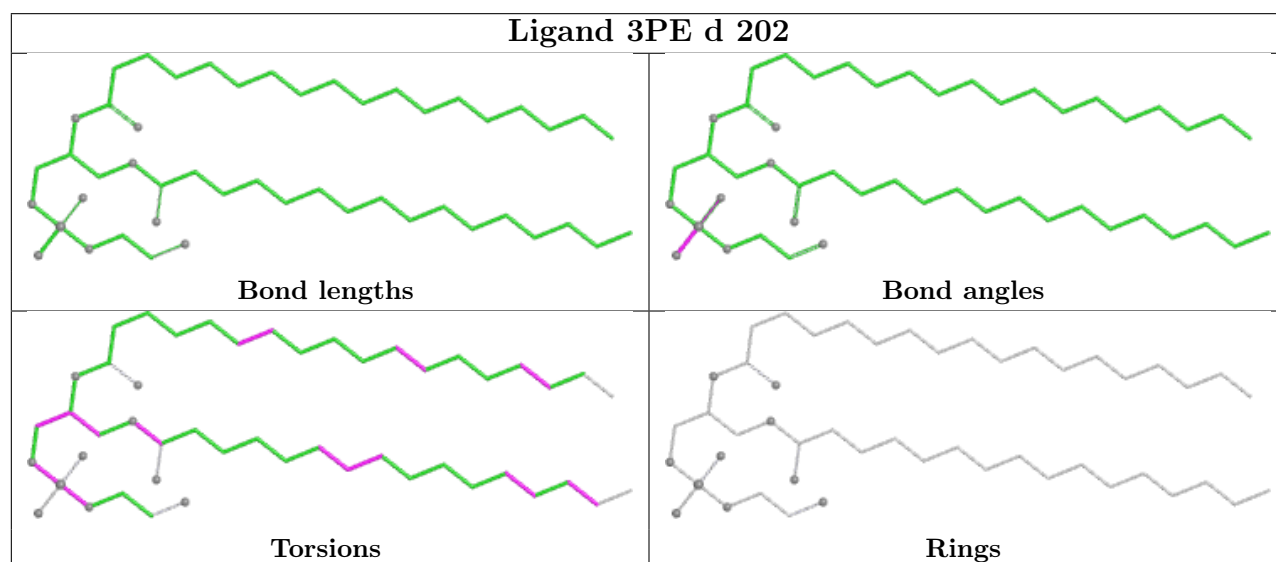
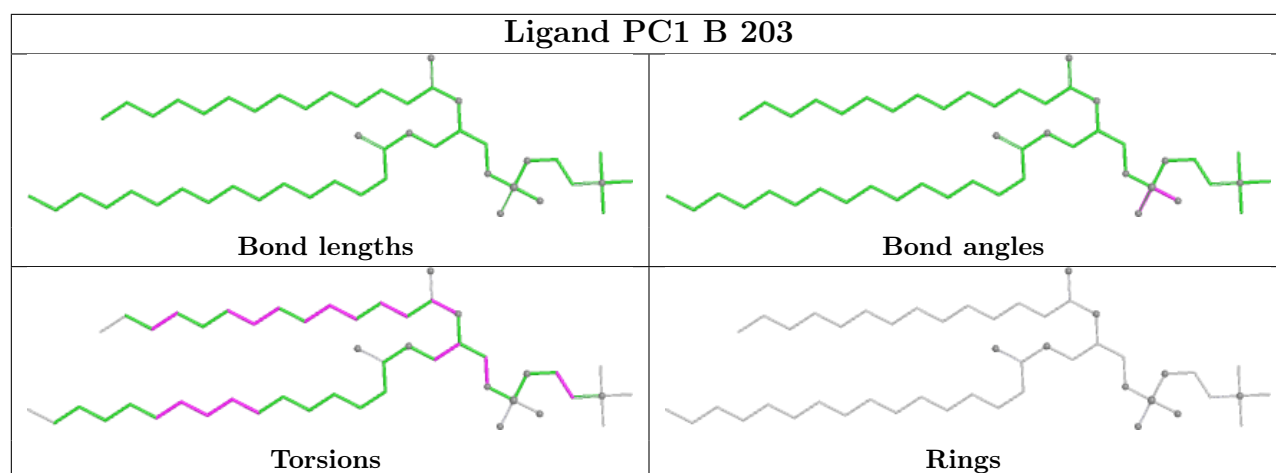


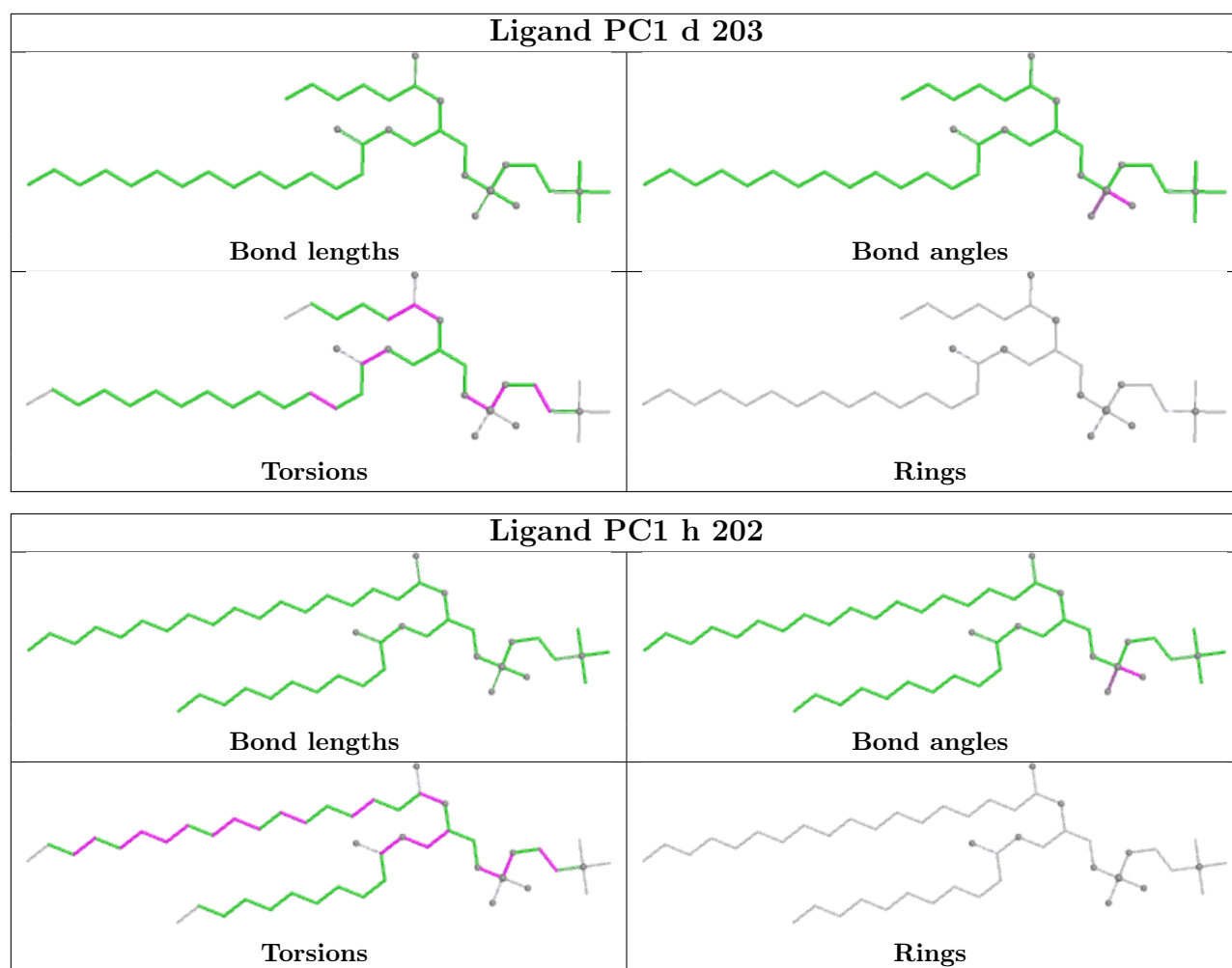


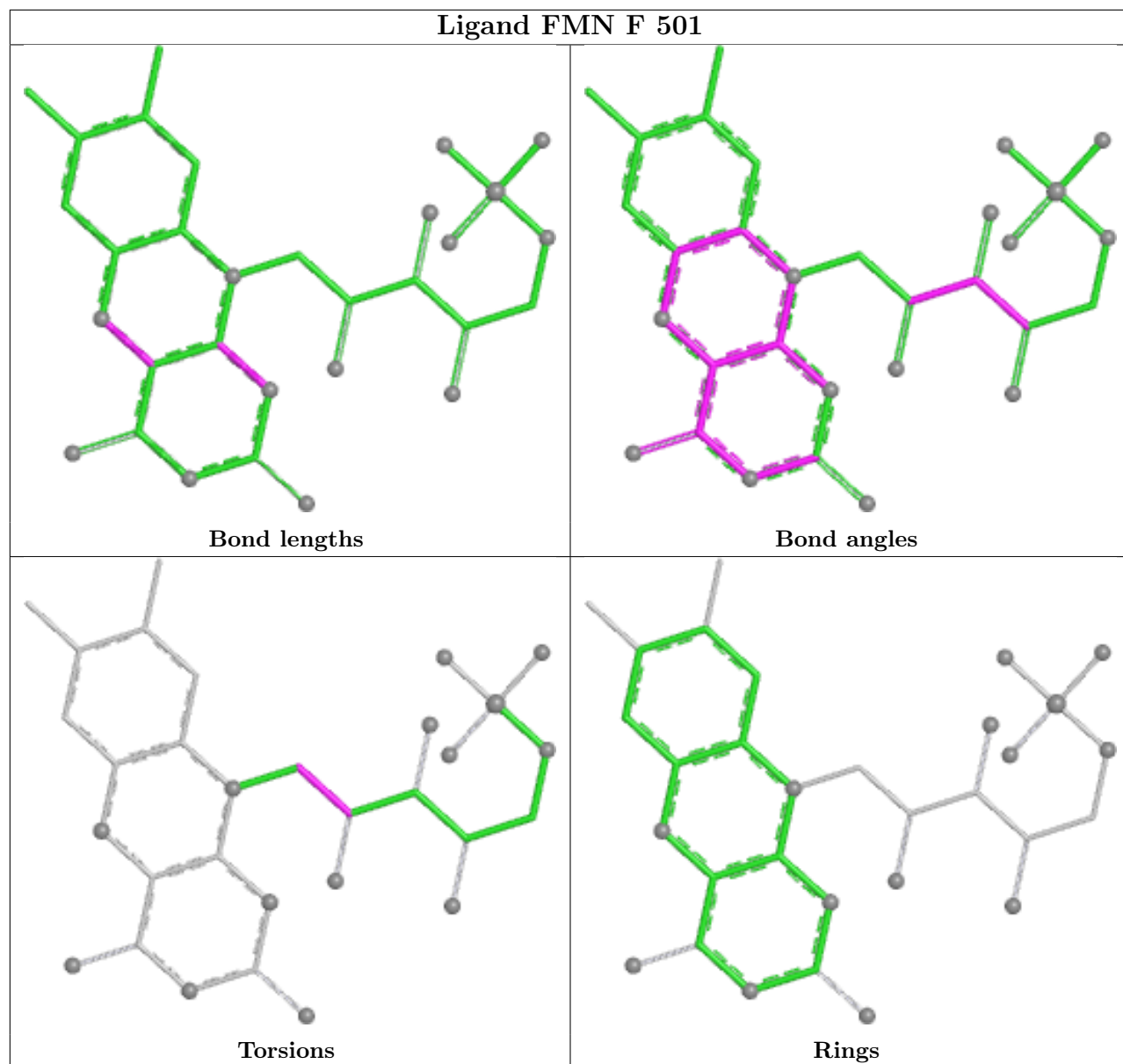


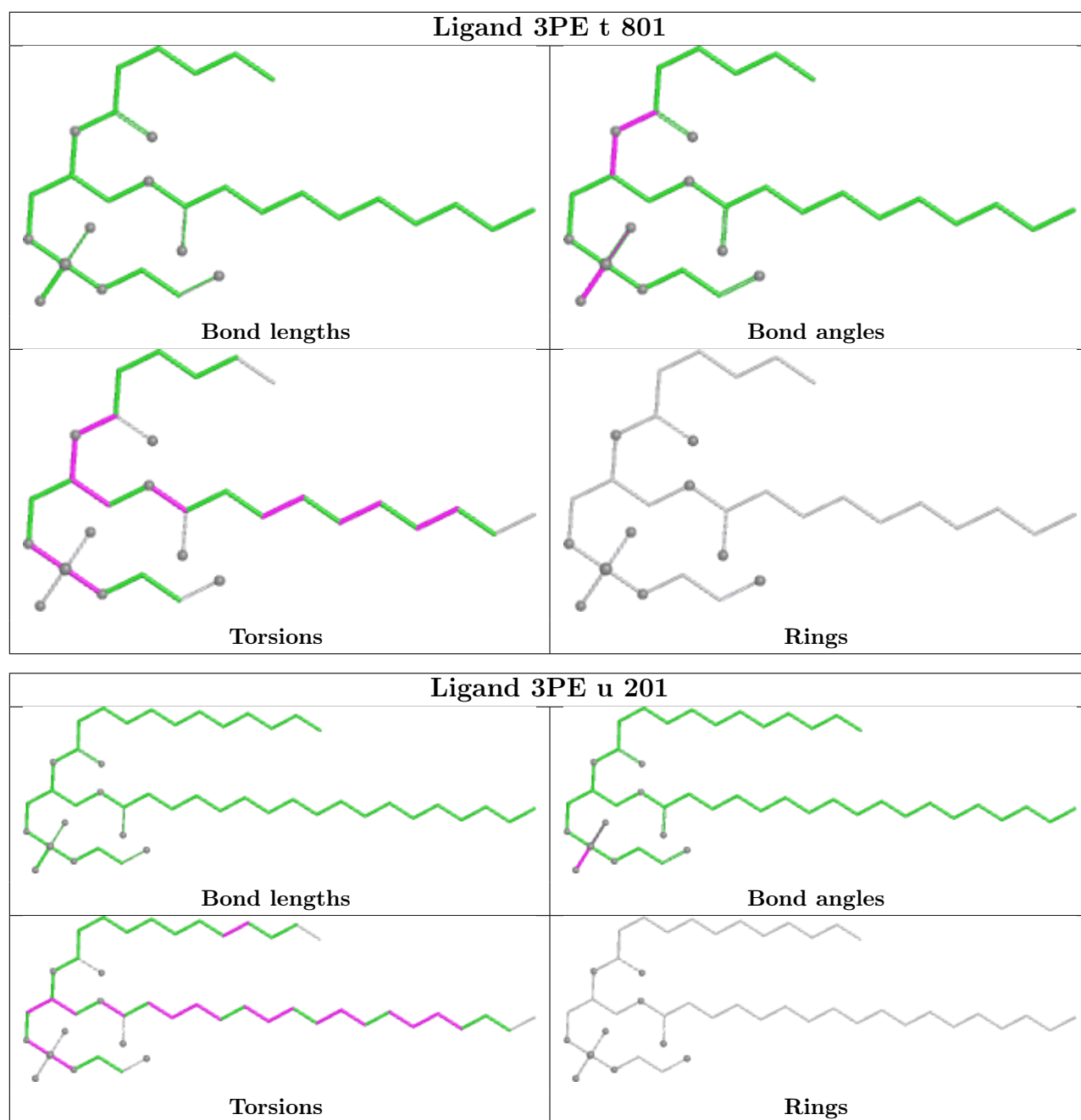


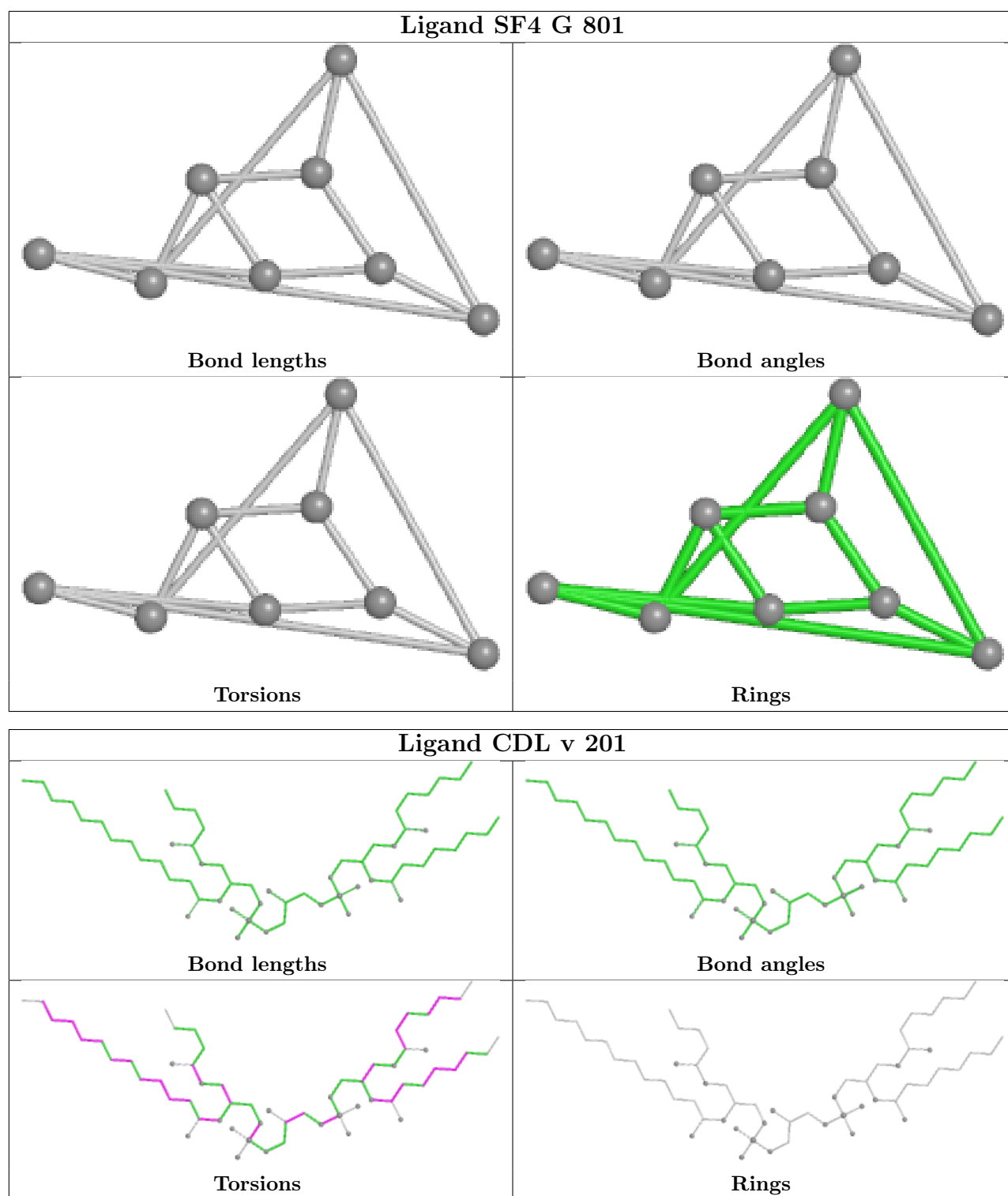


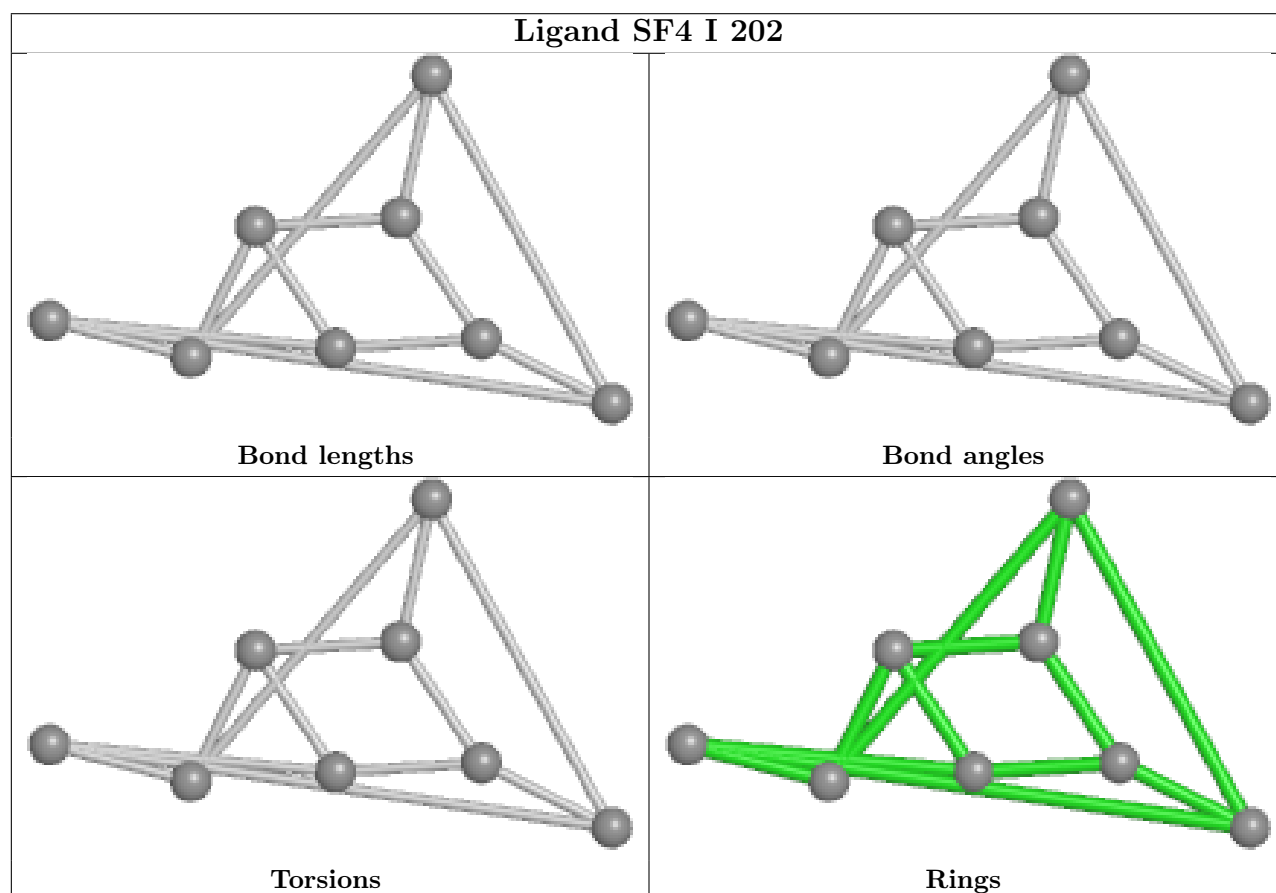
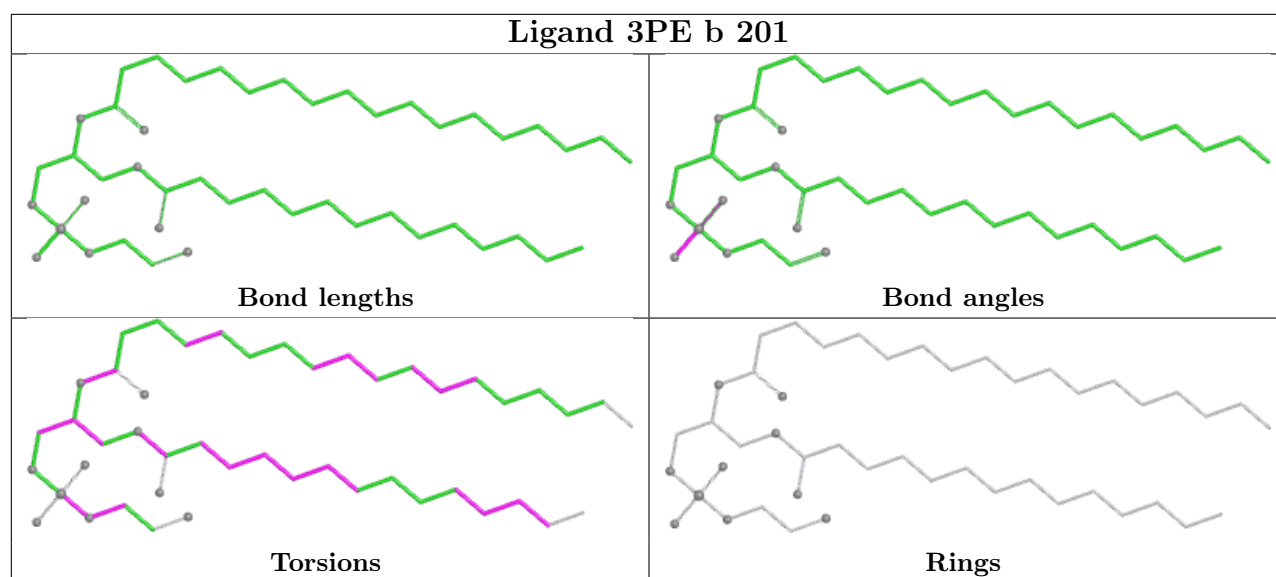


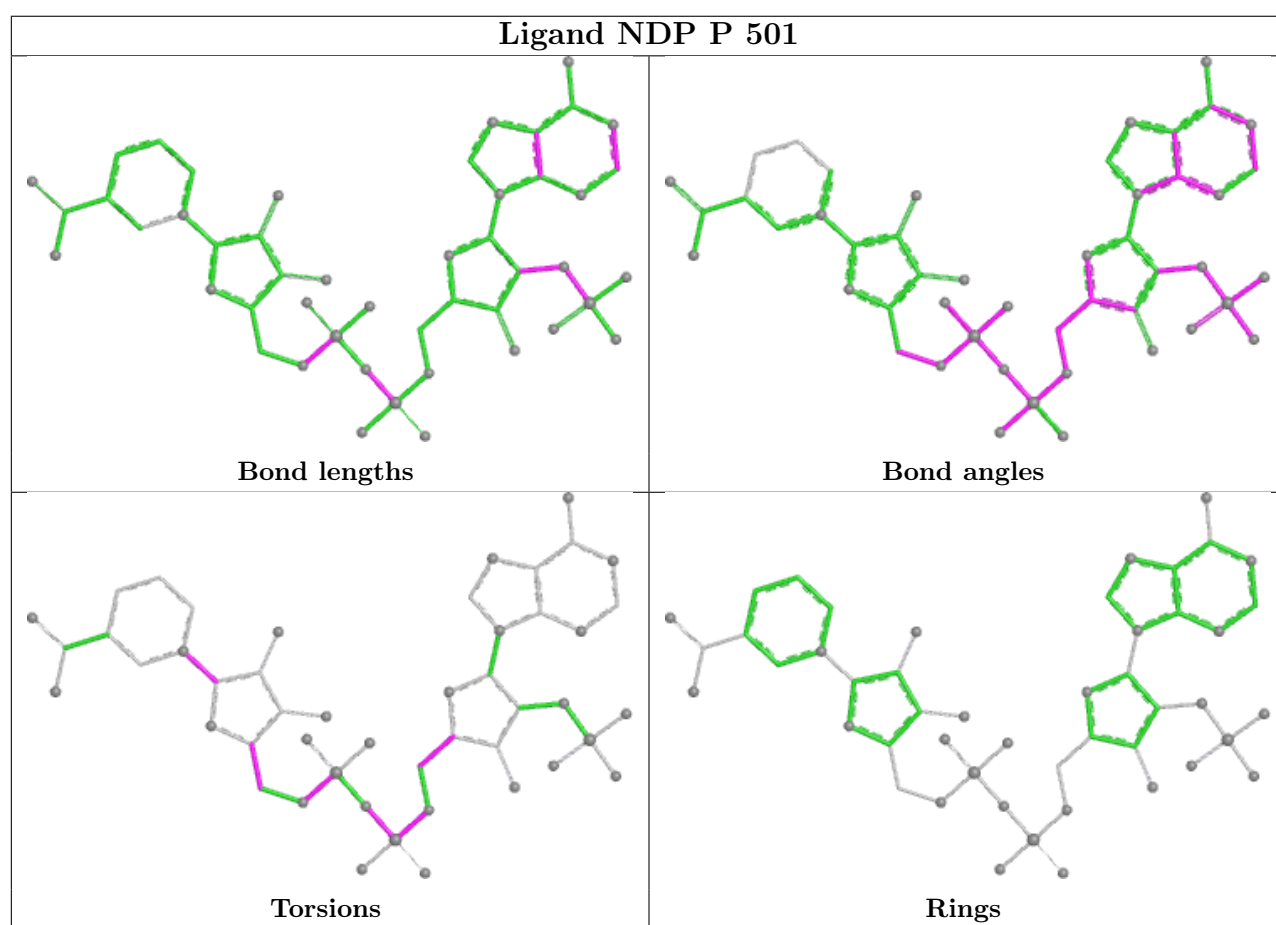
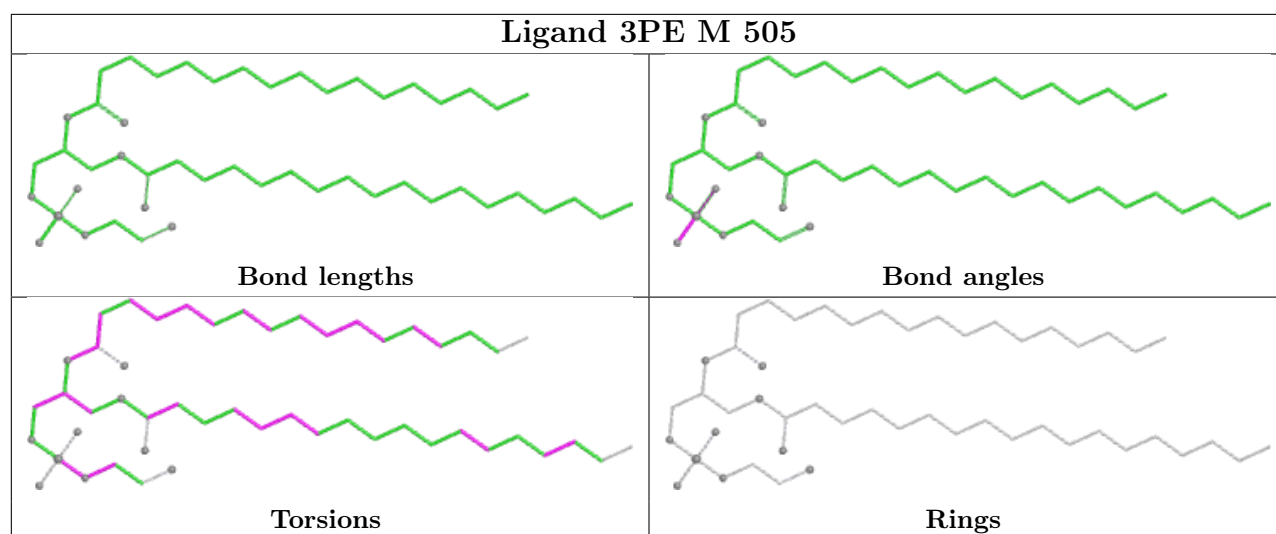


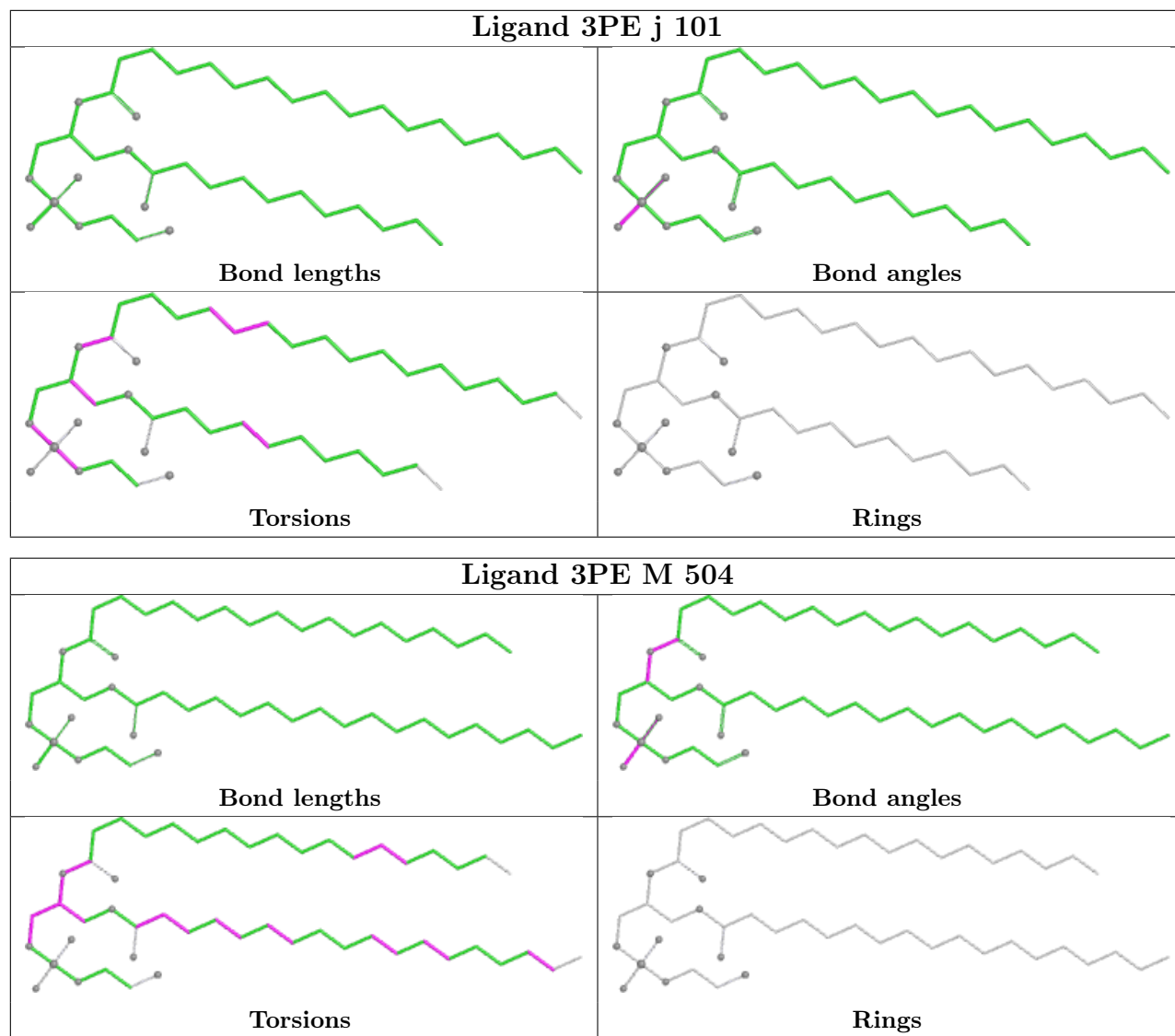


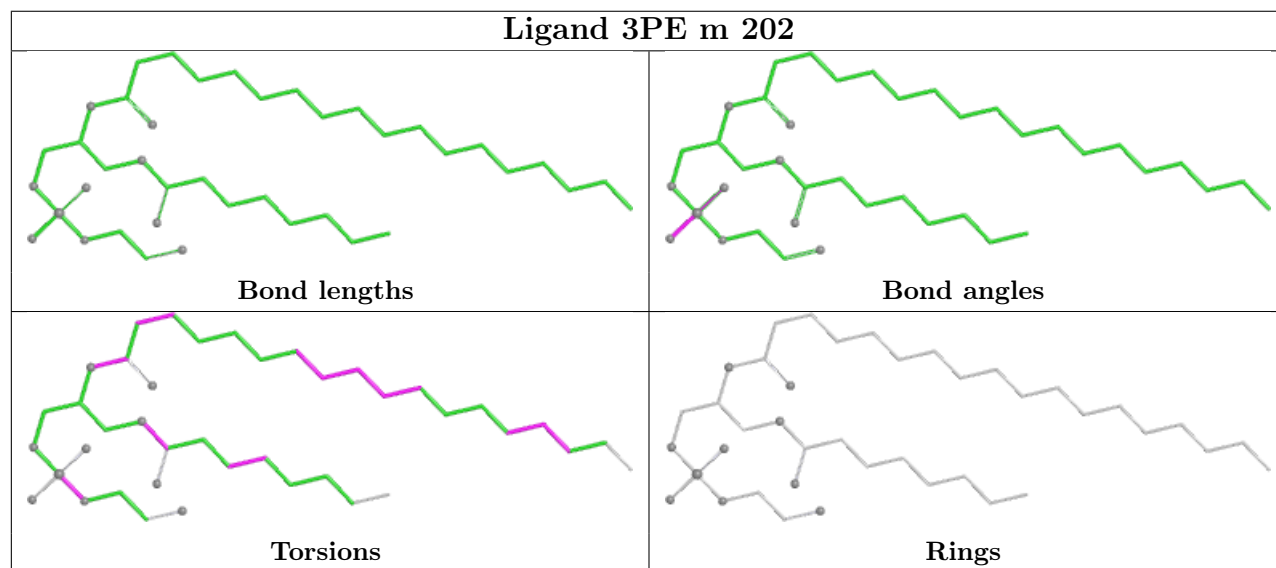
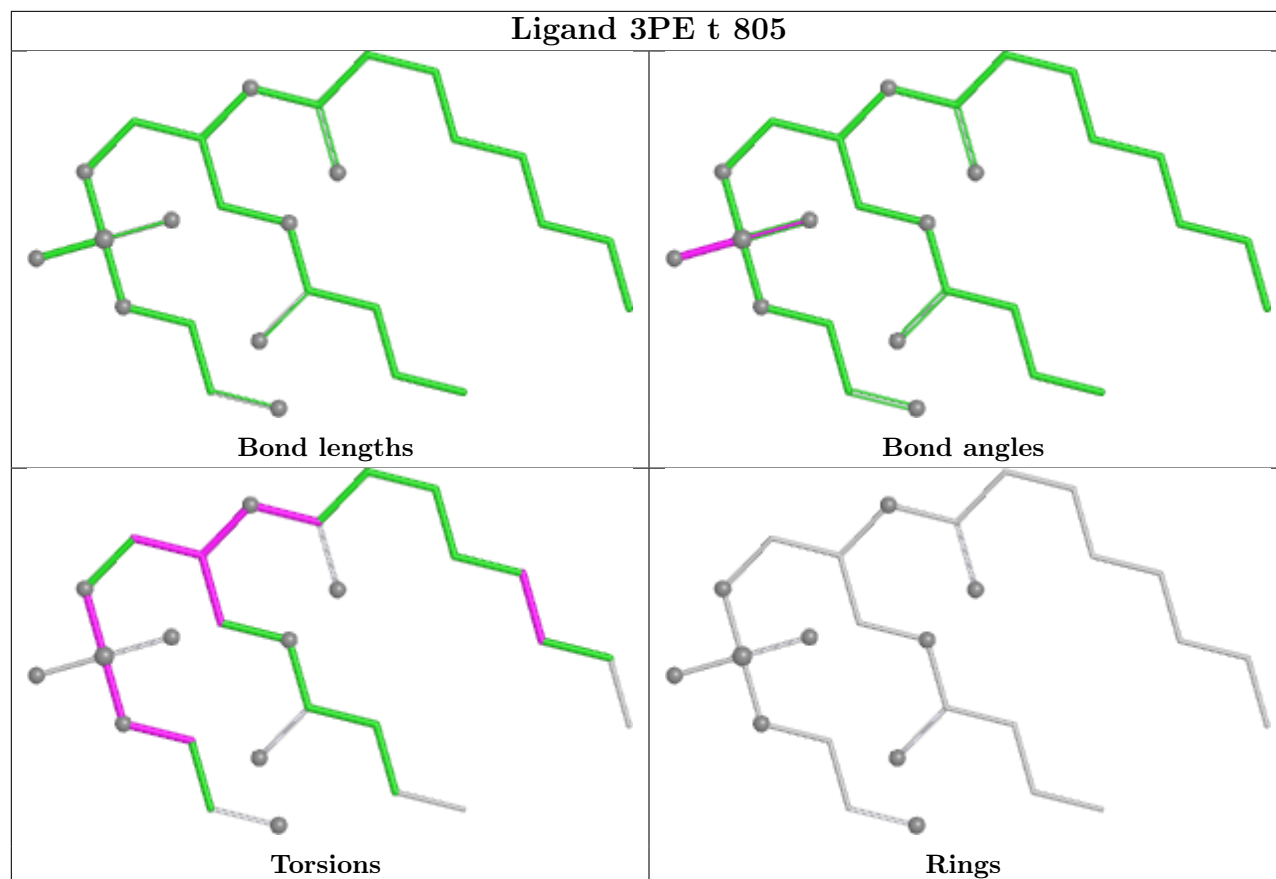


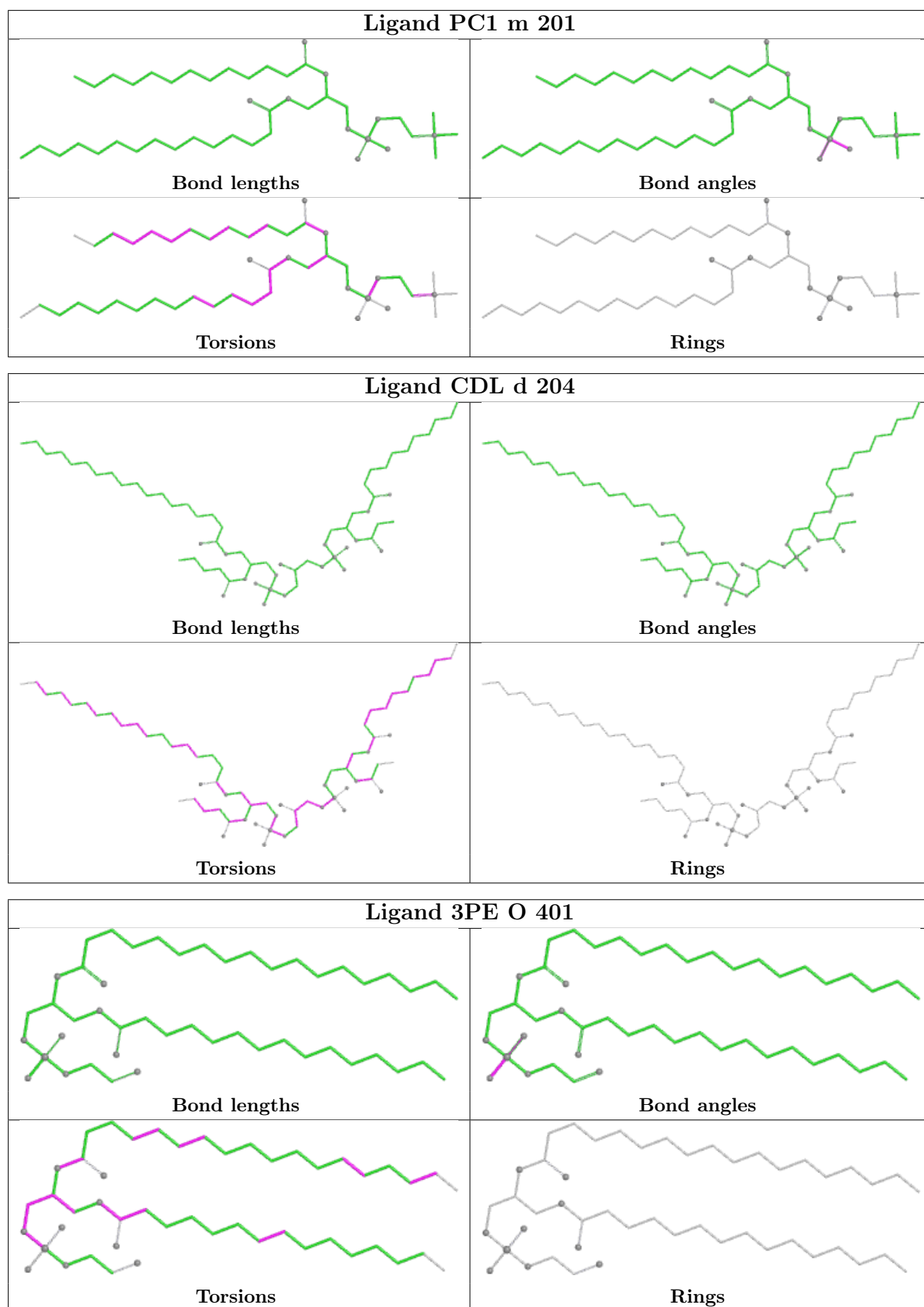


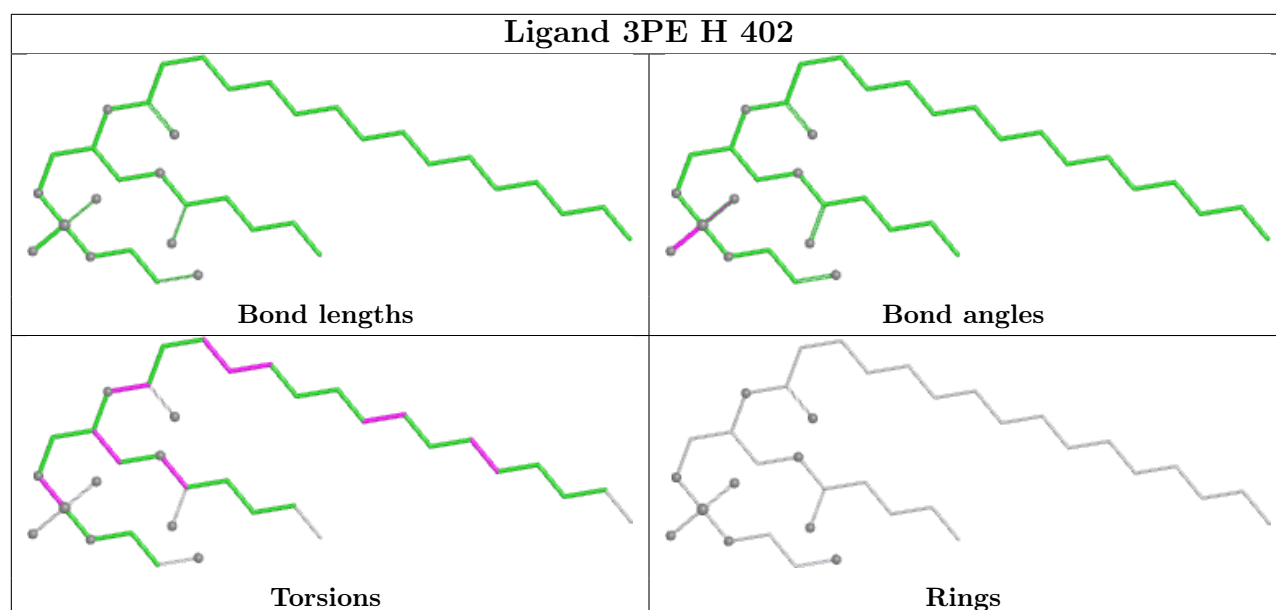












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

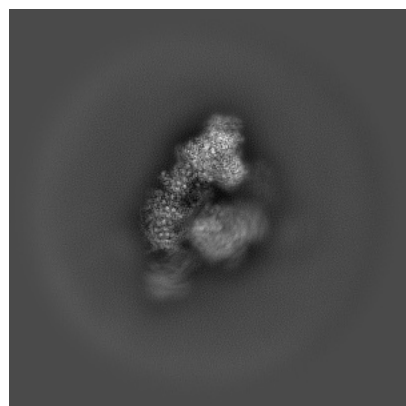
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65580. These allow visual inspection of the internal detail of the map and identification of artifacts.

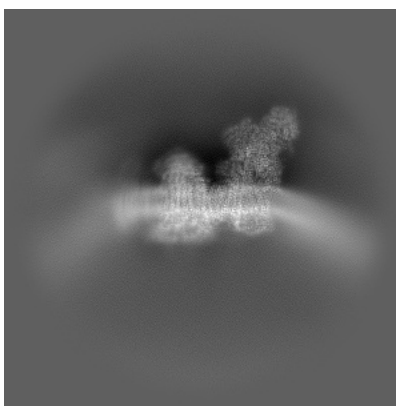
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

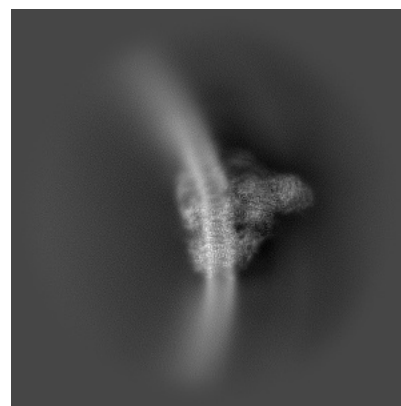
6.1.1 Primary map



X

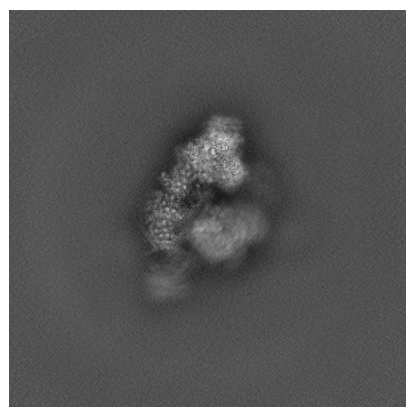


Y

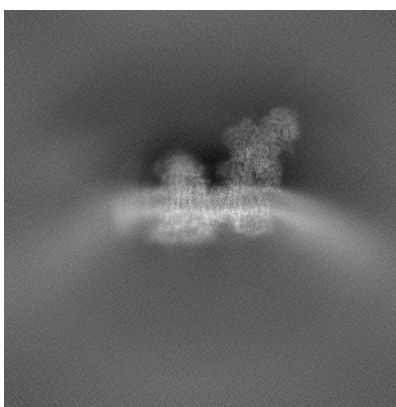


Z

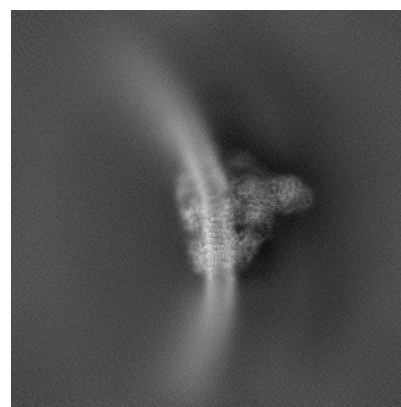
6.1.2 Raw map



X



Y

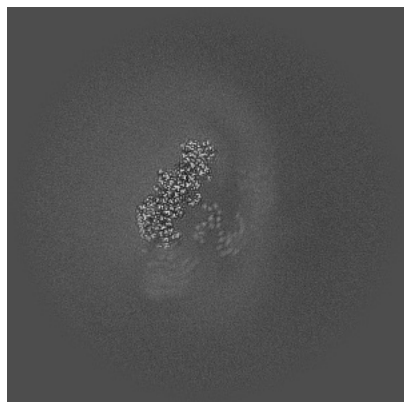


Z

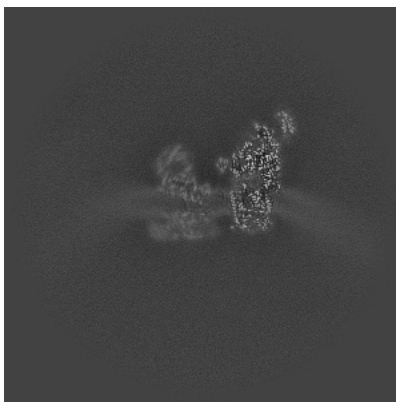
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

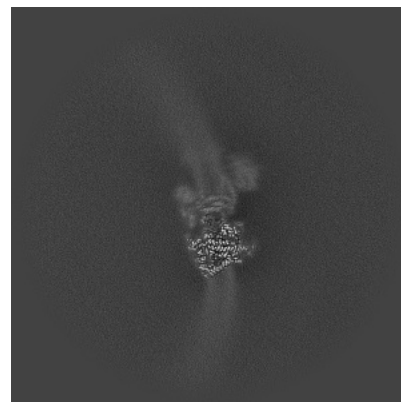
6.2.1 Primary map



X Index: 300

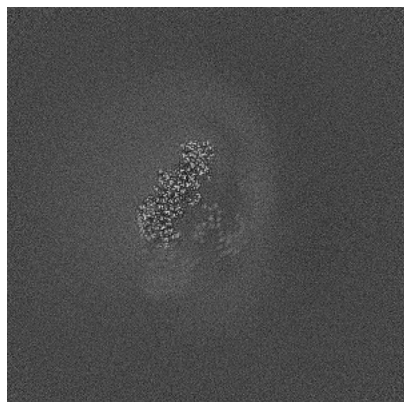


Y Index: 300

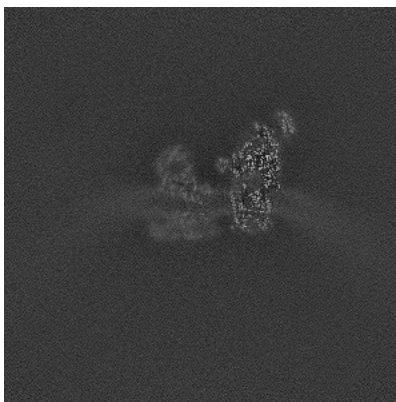


Z Index: 300

6.2.2 Raw map



X Index: 300



Y Index: 300

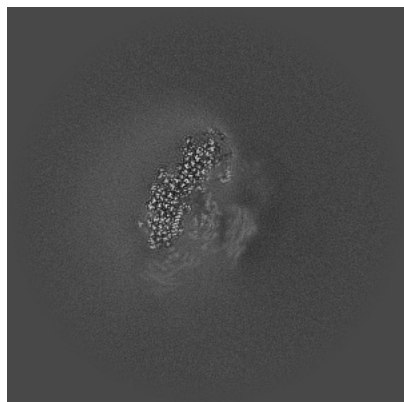


Z Index: 300

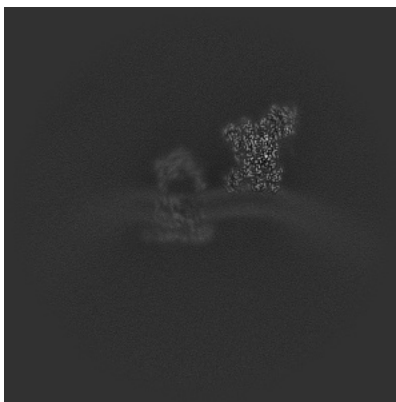
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

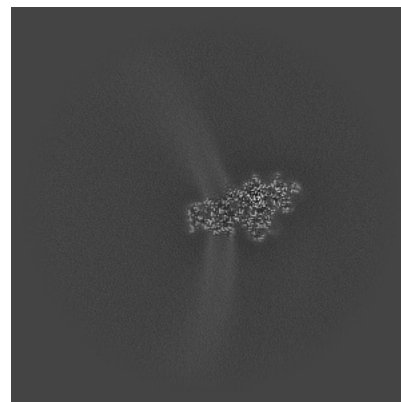
6.3.1 Primary map



X Index: 322

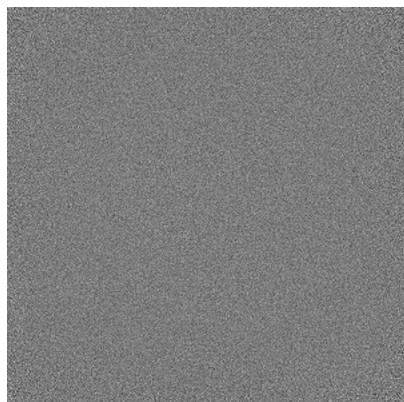


Y Index: 323

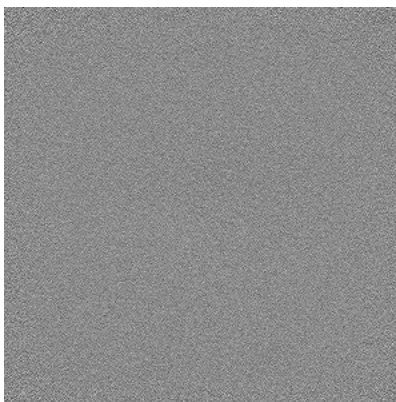


Z Index: 386

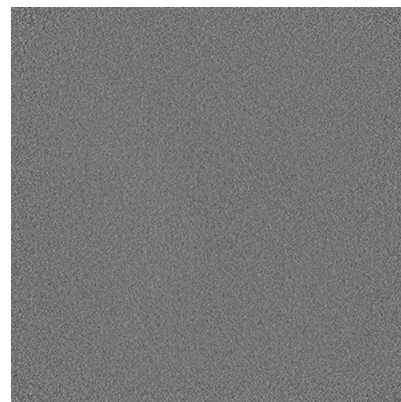
6.3.2 Raw map



X Index: 0



Y Index: 0

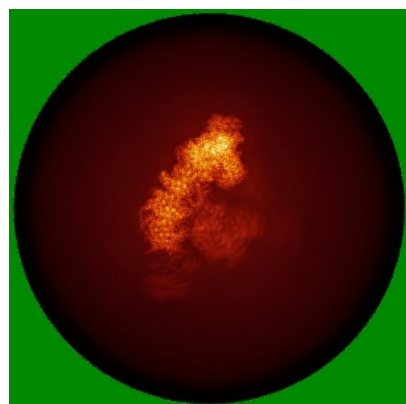


Z Index: 0

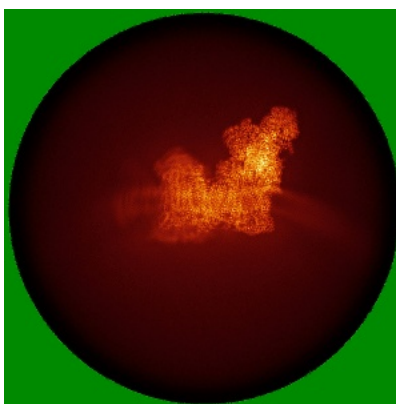
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

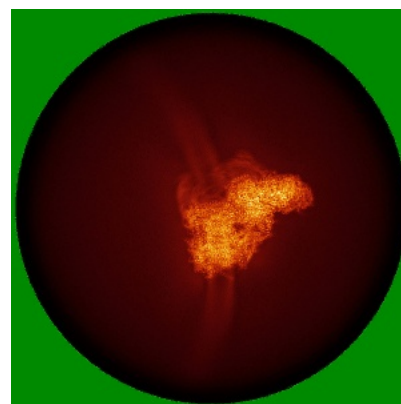
6.4.1 Primary map



X

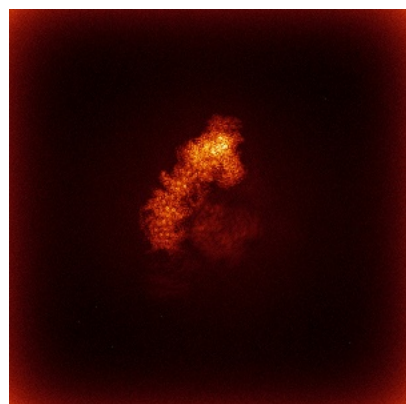


Y

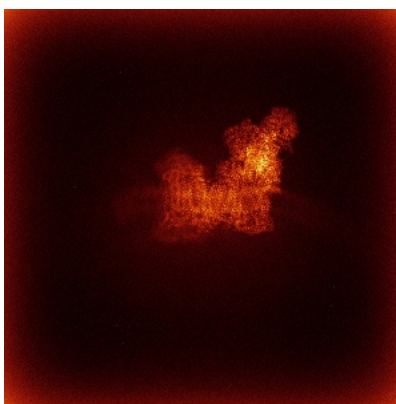


Z

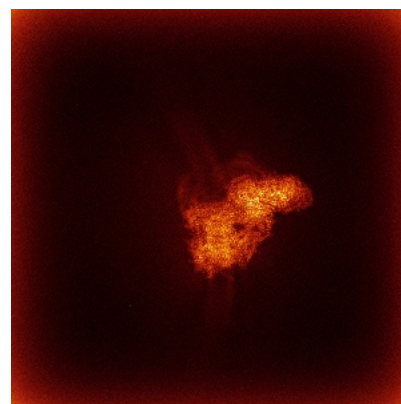
6.4.2 Raw map



X



Y



Z

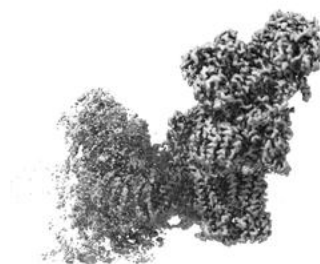
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

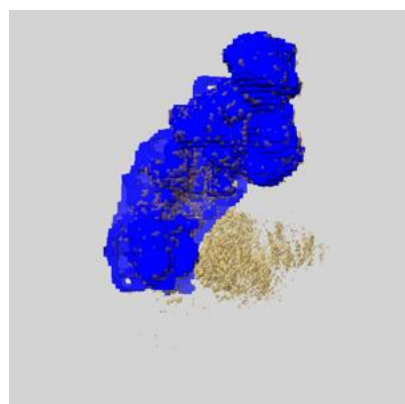
6.6 Mask visualisation [i](#)

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

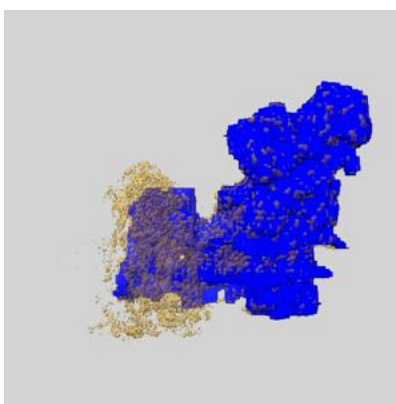
A mask typically either:

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

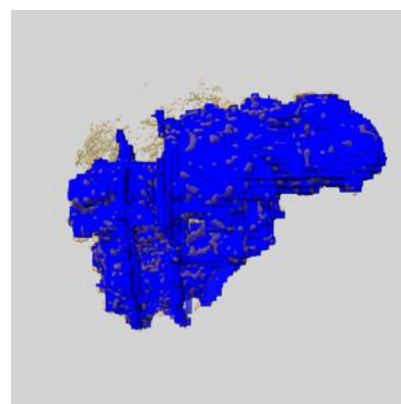
6.6.1 emd_65580_msk_1.map [i](#)



X



Y

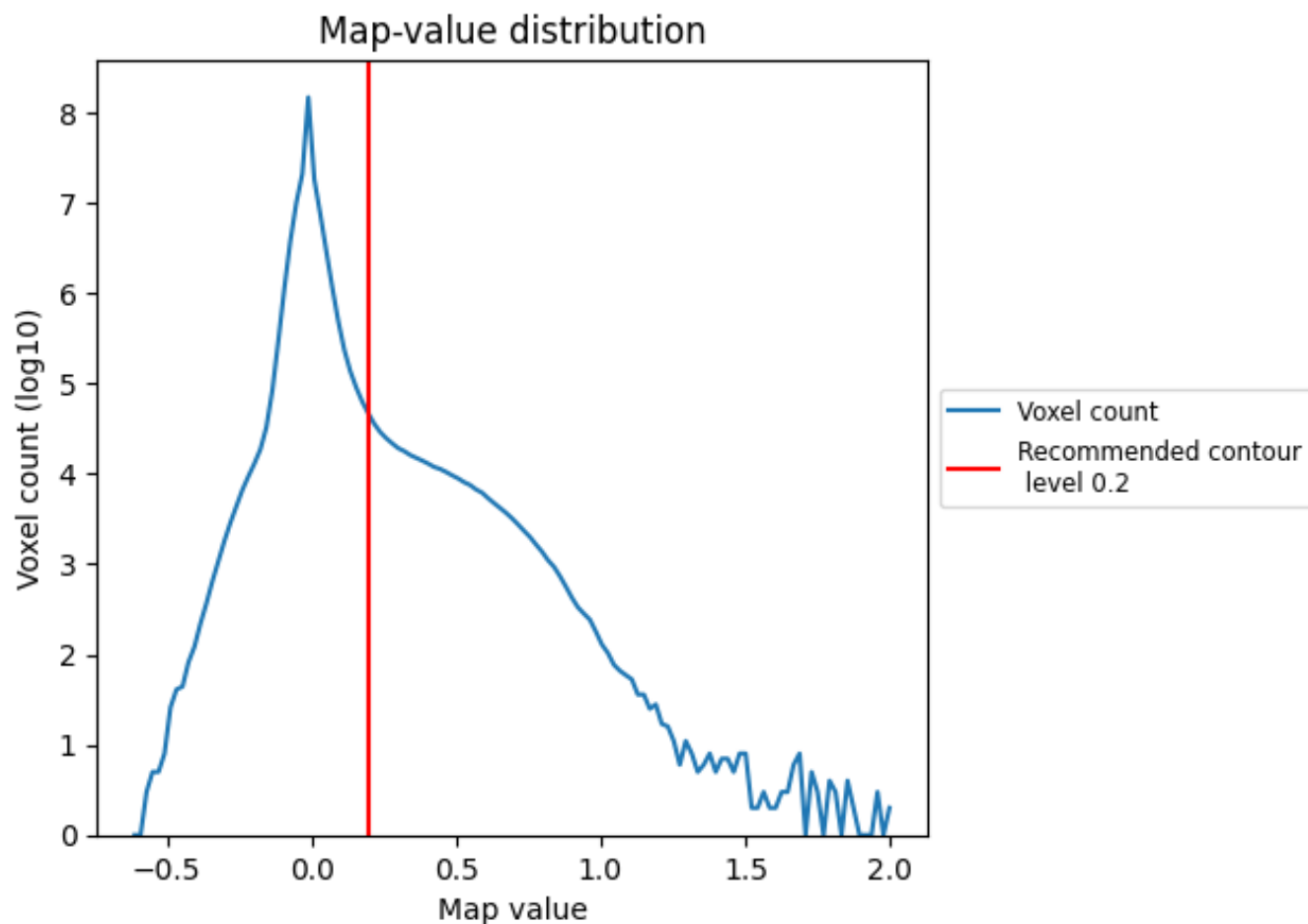


Z

7 Map analysis [i](#)

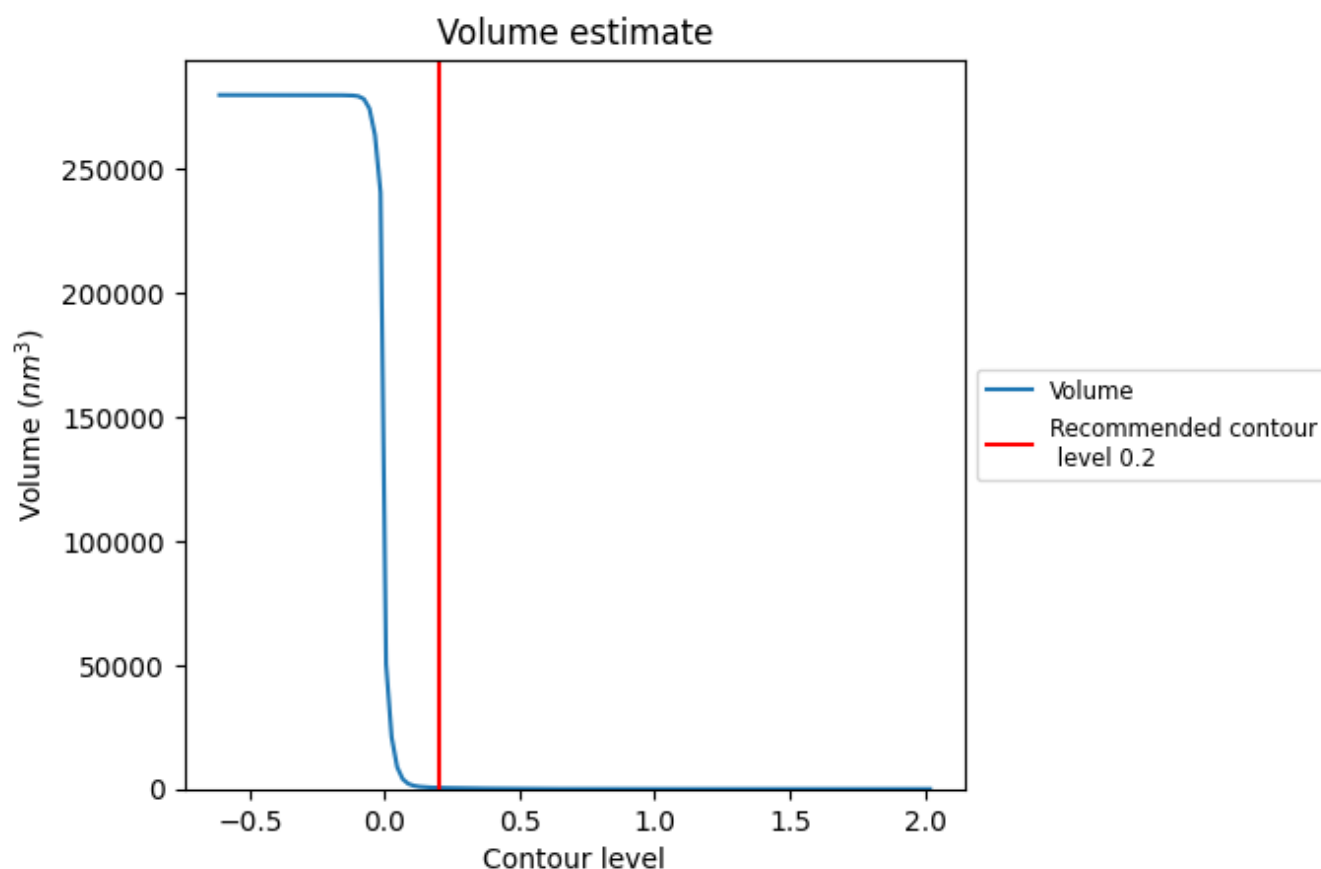
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

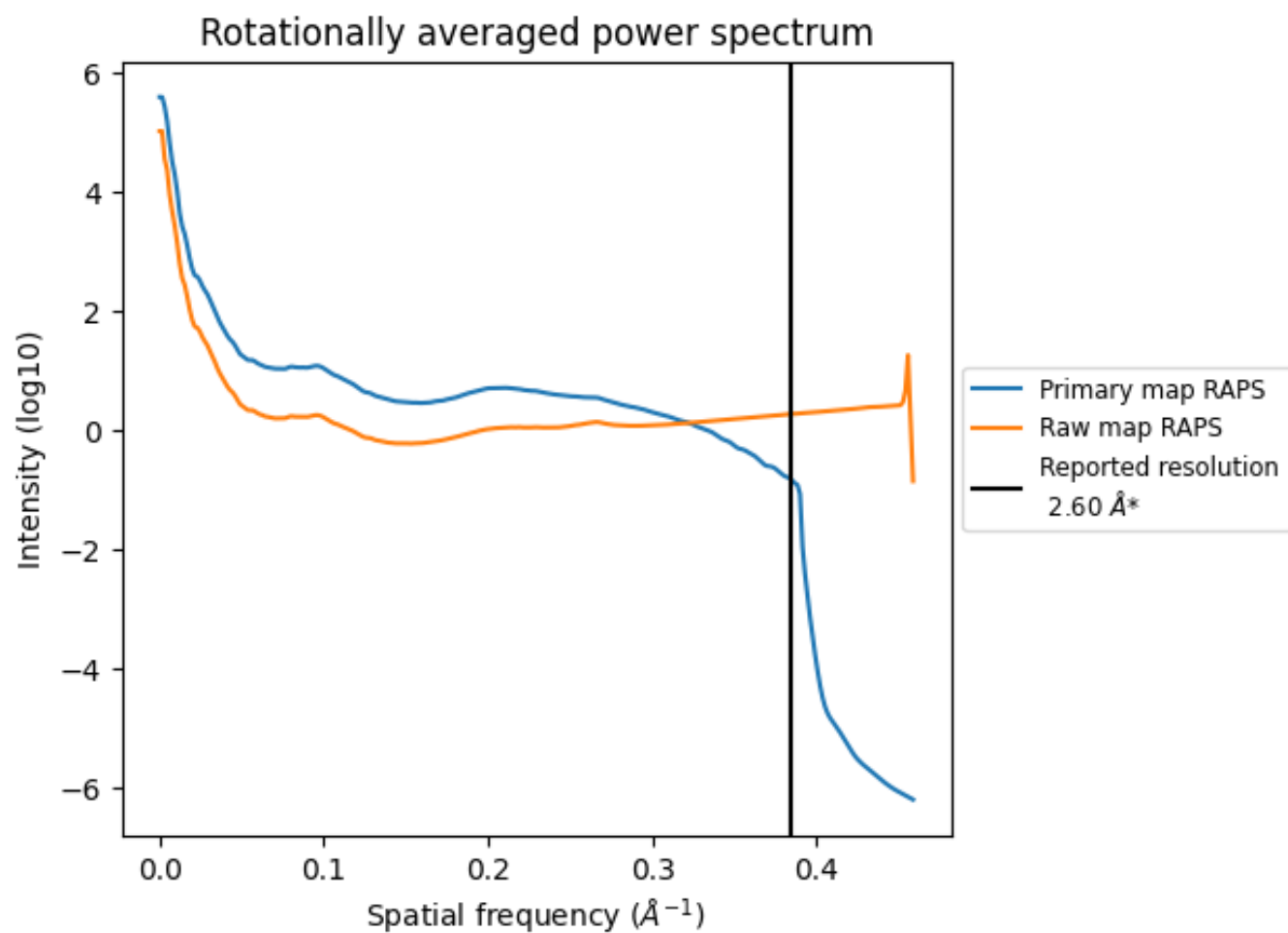
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 472 nm^3 ; this corresponds to an approximate mass of 426 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 ⓘ

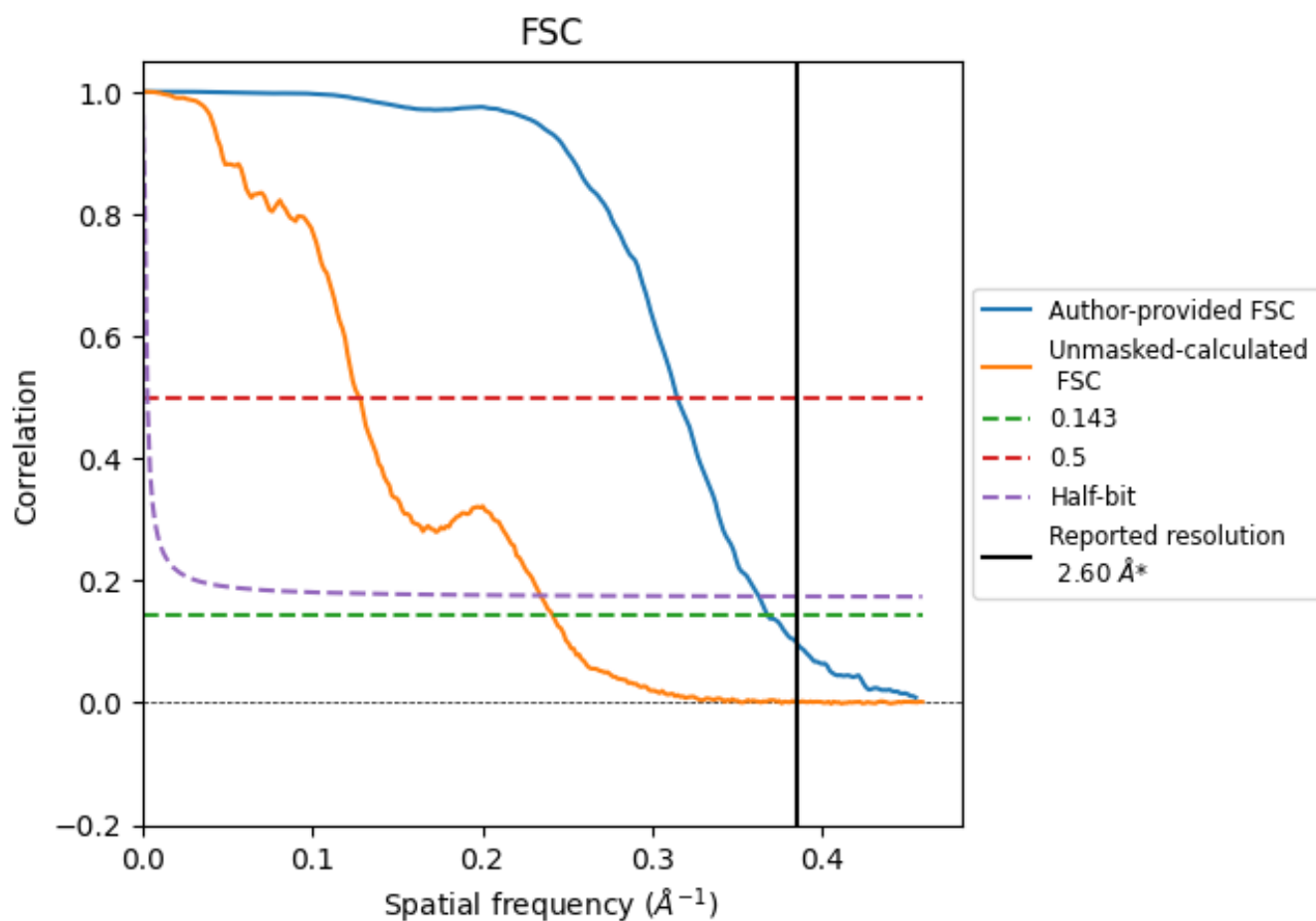


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

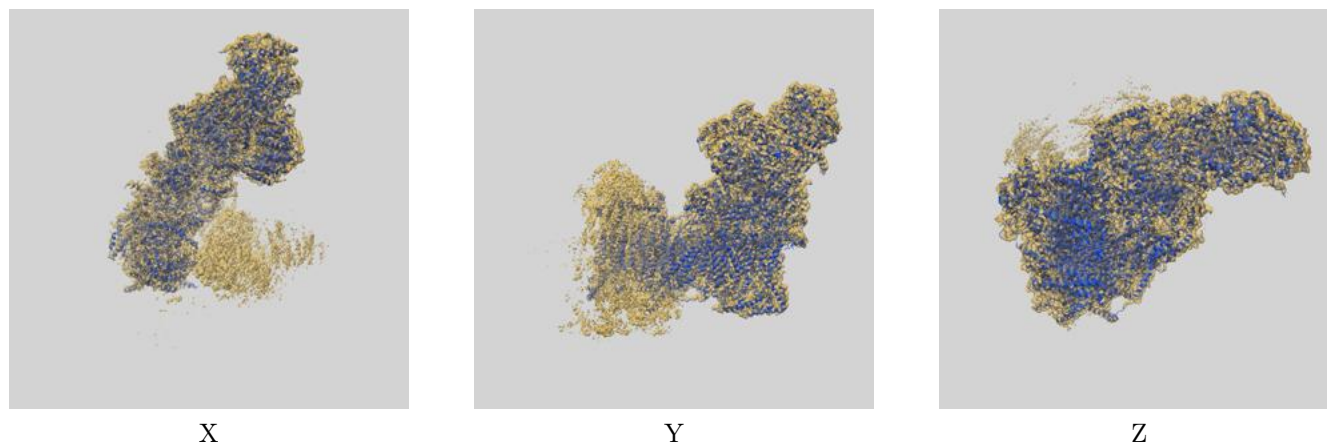
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.72	3.18	2.76
Unmasked-calculated*	4.14	7.83	4.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

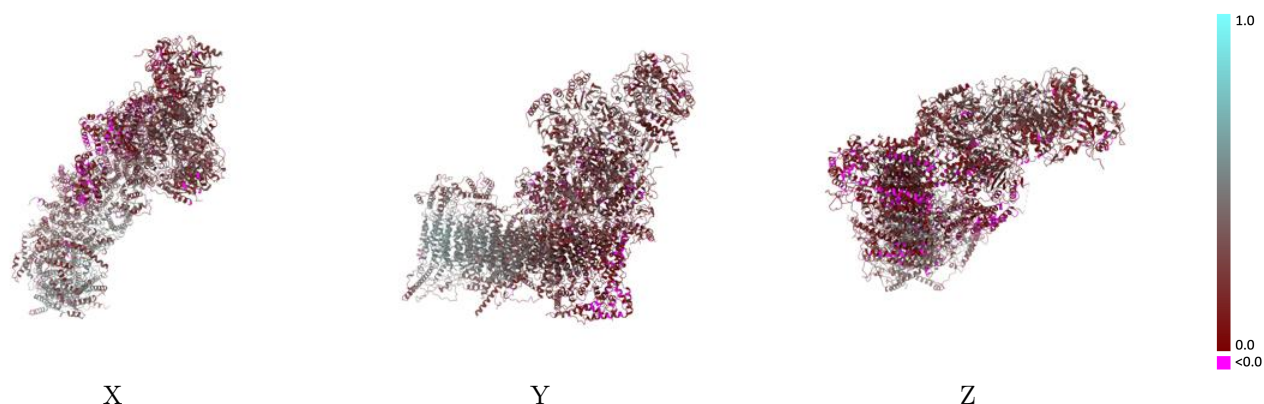
This section contains information regarding the fit between EMDB map EMD-65580 and PDB model 9W2U. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



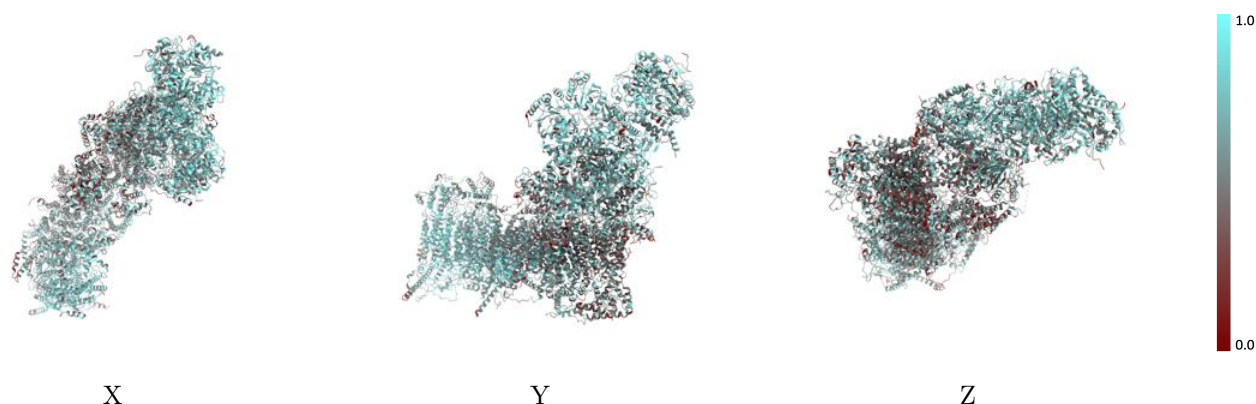
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



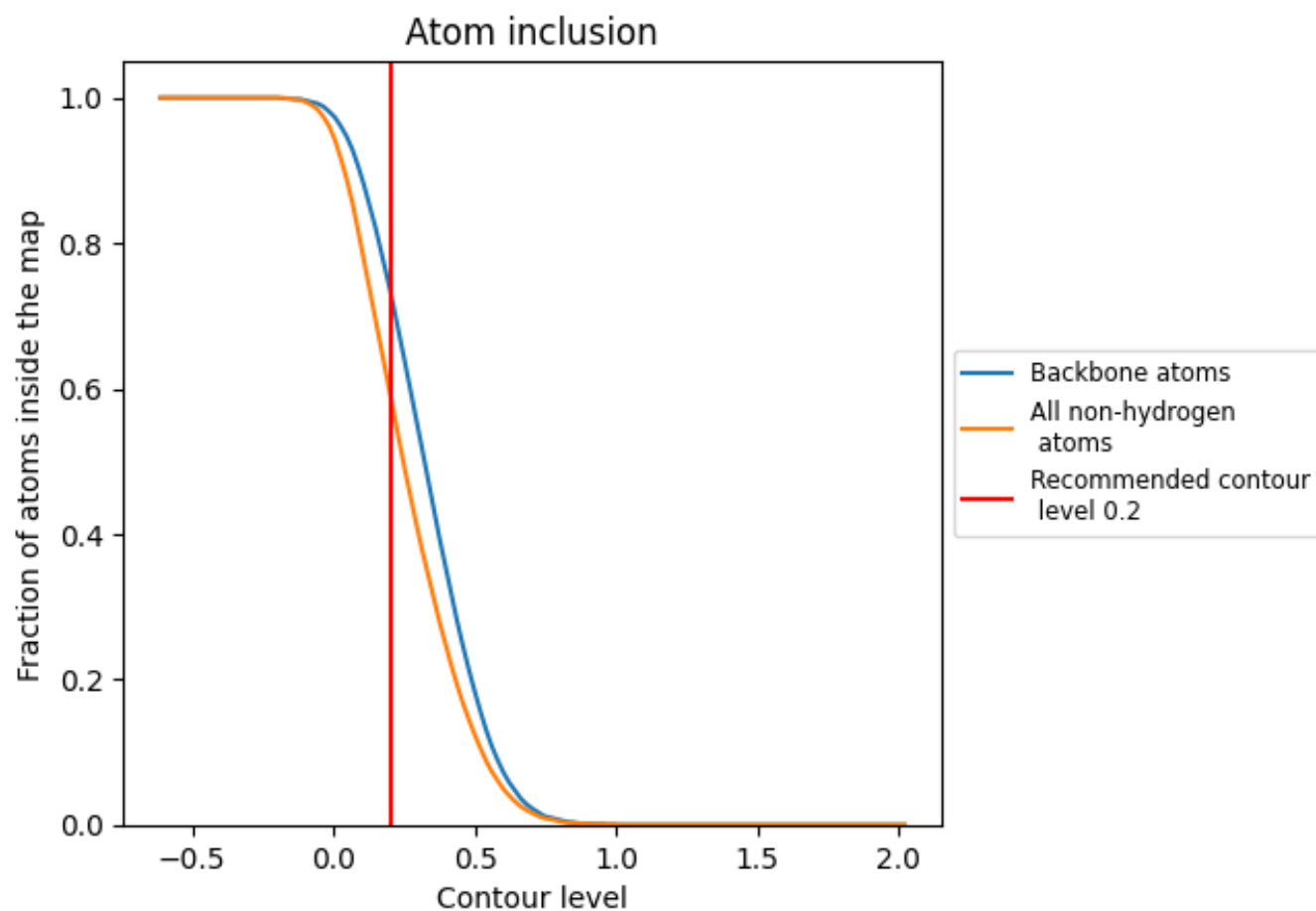
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ























The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5920	 0.2670
A	 0.4440	 0.1710
B	 0.6120	 0.2540
C	 0.5590	 0.2030
D	 0.5700	 0.2150
E	 0.6730	 0.2690
F	 0.6160	 0.2130
G	 0.6580	 0.2860
H	 0.4920	 0.1790
I	 0.6250	 0.2360
J	 0.5320	 0.2400
K	 0.5400	 0.2520
L	 0.7670	 0.4830
M	 0.6640	 0.3410
N	 0.5760	 0.2420
O	 0.4330	 0.1360
P	 0.5390	 0.2640
Q	 0.6080	 0.2820
R	 0.6580	 0.3150
S	 0.5830	 0.2620
T	 0.4370	 0.2570
U	 0.6160	 0.3150
V	 0.4340	 0.1260
W	 0.5720	 0.2720
X	 0.4950	 0.1220
Z	 0.4810	 0.1170
a	 0.5050	 0.1400
b	 0.4070	 0.1180
c	 0.4120	 0.0950
d	 0.4470	 0.1550
e	 0.5550	 0.1840
f	 0.4660	 0.1840
g	 0.5520	 0.2220
h	 0.5700	 0.2400
j	 0.6340	 0.4210



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.5970	 0.3920
l	 0.7240	 0.4150
m	 0.6520	 0.3910
n	 0.6620	 0.3400
o	 0.6980	 0.3670
p	 0.6520	 0.2870
q	 0.6110	 0.2510
s	 0.6390	 0.2590
t	 0.6160	 0.4050
u	 0.5440	 0.3040
v	 0.4910	 0.1550