



# wwPDB EM Validation Summary Report ⓘ

Jan 17, 2023 – 06:38 PM JST

PDB ID : 7W2K  
EMDB ID : EMD-32263  
Title : Deactive state CI from Rotenone-NADH dataset, Subclass 1  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-24  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

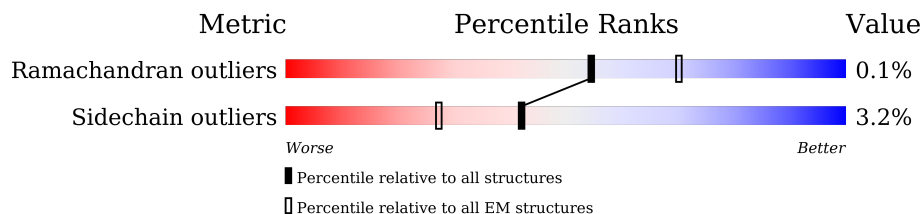
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 2.90 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.



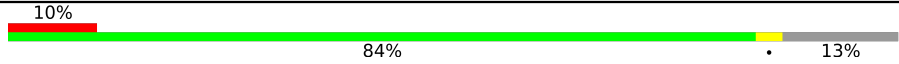

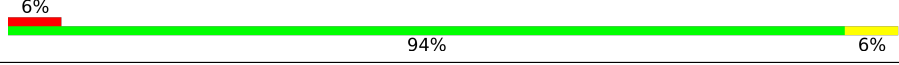
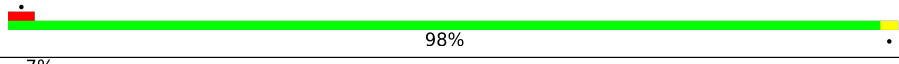
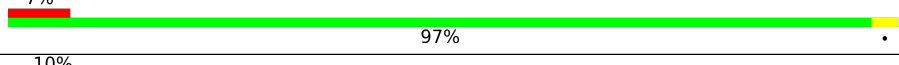
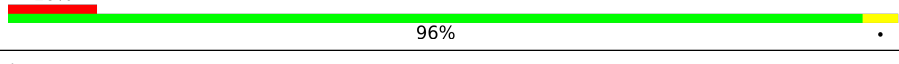
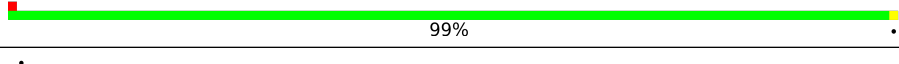
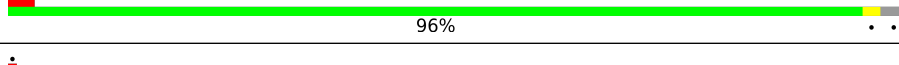
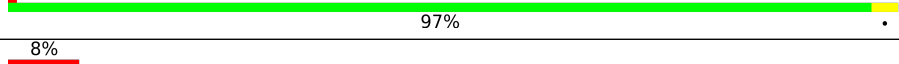
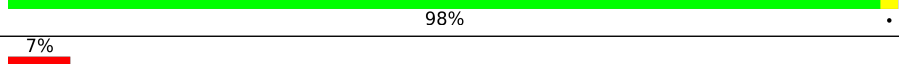
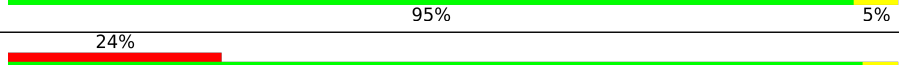
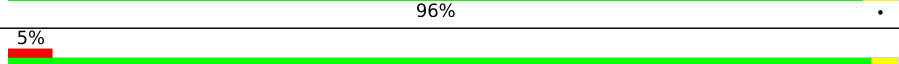
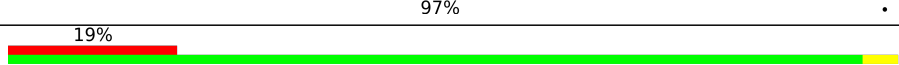
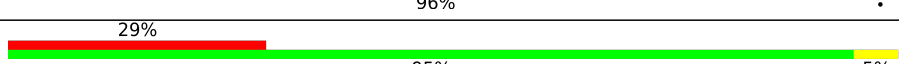
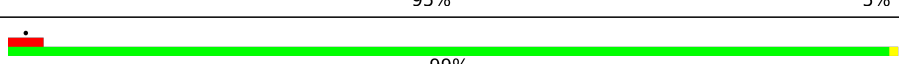
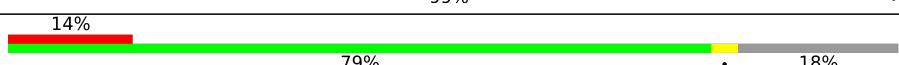
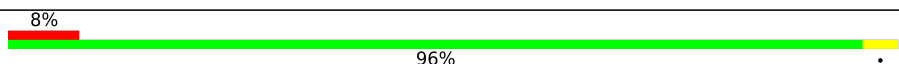
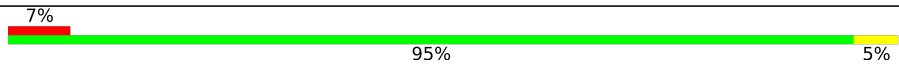
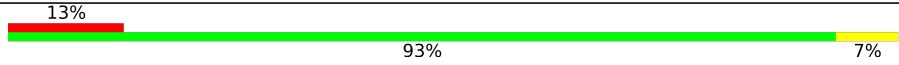
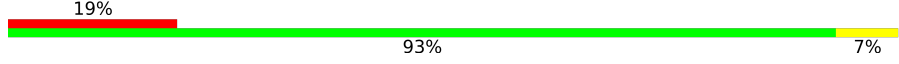
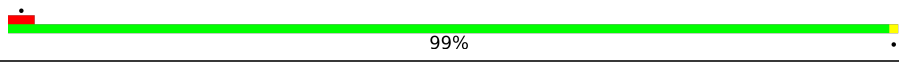
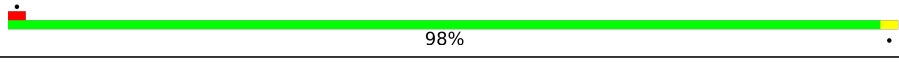
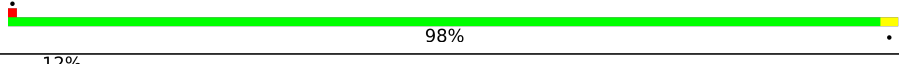


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	A	431	97%
2	B	176	98%
3	C	156	96%
4	E	115	10% 97%
5	F	86	13% 98%
6	G	88	52% 94% 6%
6	X	88	6% 97%
7	H	112	5% 99%
8	I	112	9% 83% 13%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	342	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	131	
44	w	320	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66522 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1235	788	221	212	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	965	616	176	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	688	433	129	124	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			762	479	144	136	3		

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2352	1511	420	413	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	377	VAL	ILE	conflict	UNP F1SL07

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5293	3319	923	1012	39	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	144	1204	770	218	212	4	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1648	1054	277	308	9	0	0

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1738	1124	298	314	2	0	0

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3364	2153	574	613	24	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	567	364	104	94	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	96	741	452	140	146	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1161	749	197	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			583	386	98	98	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1152	754	196	199	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			875	571	158	145	1		



- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1315	853	213	241	8	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	175	1461	916	265	272	8	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	890	568	145	173	4	0	0

- Molecule 29 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	342	225	58	59	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	121	1000	650	173	171	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	105	867	550	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2706	1779	419	462	46	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	99	800	545	118	132	5	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	98	748	493	113	128	14	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4782	3171	741	820	50	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	948	636	138	166	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	456	295	83	77	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1058	688	181	189	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	178	1534	982	279	265	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3631	2412	572	609	38	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2394	1607	369	397	21	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	171	1398	887	250	251	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1020	637	189	185	9	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1
v	126	ALA	GLN	conflict	UNP F1SCH1
v	128	ALA	PRO	conflict	UNP F1SCH1
v	130	ALA	GLU	conflict	UNP F1SCH1
v	131	ALA	VAL	conflict	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

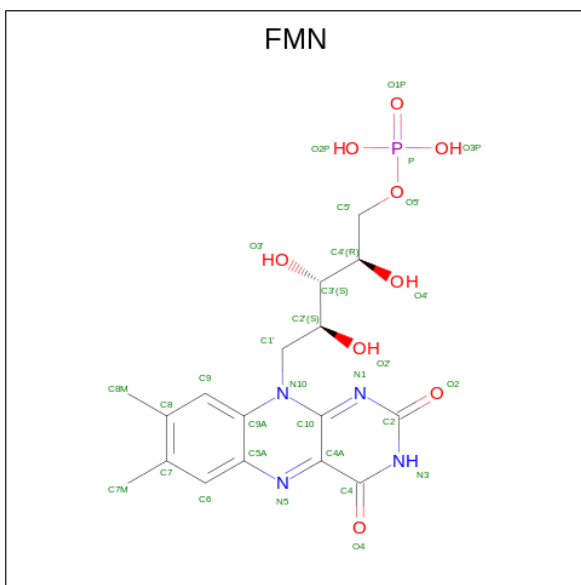
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2574	1638	437	489	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



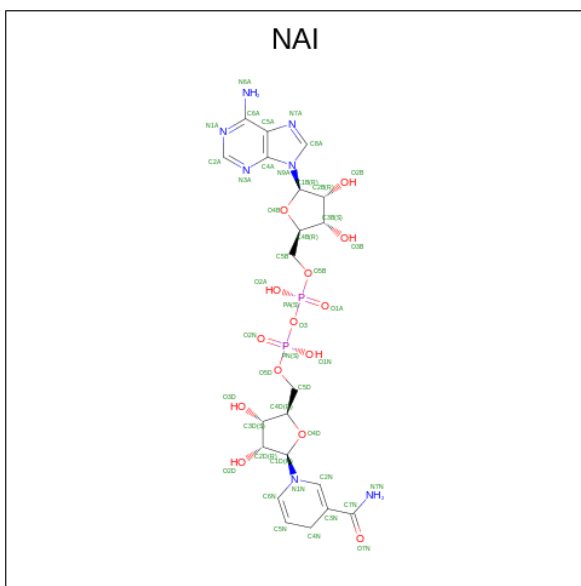
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



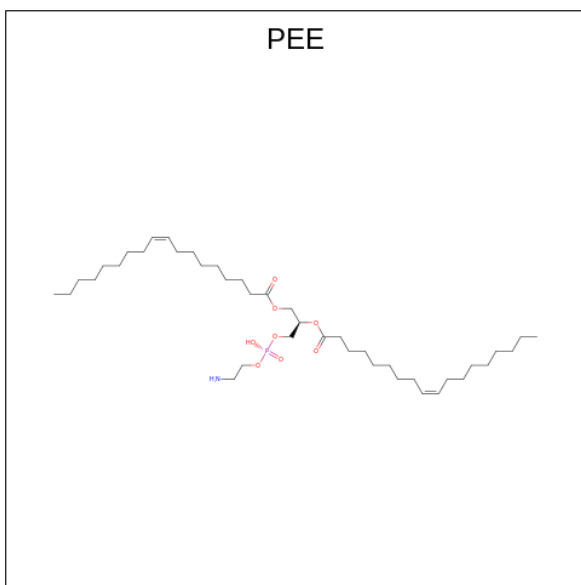
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



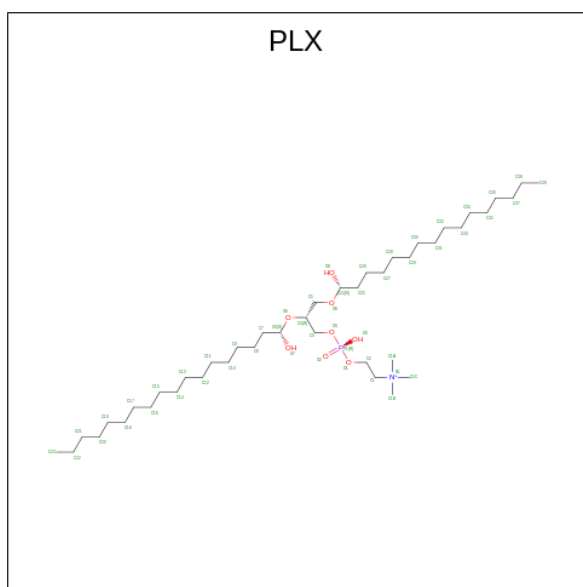
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



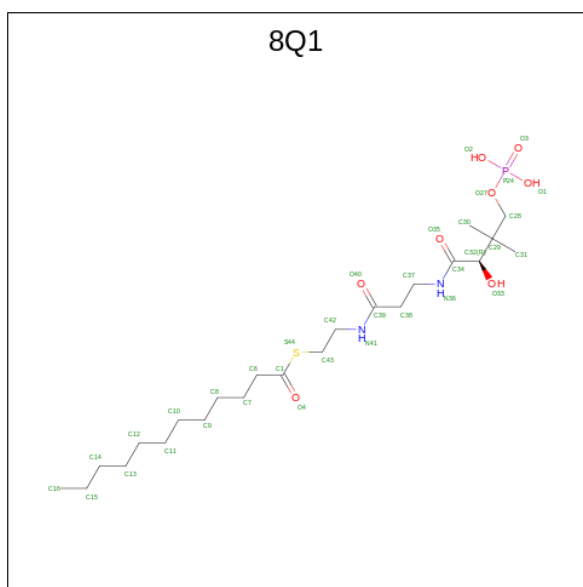
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total 51	41	1	8	1	0
48	C	1	Total 47	37	1	8	1	0
48	Q	1	Total 47	37	1	8	1	0
48	b	1	Total 46	36	1	8	1	0
48	j	1	Total 51	41	1	8	1	0
48	l	1	Total 46	36	1	8	1	0
48	r	1	Total 51	41	1	8	1	0
48	s	1	Total 41	31	1	8	1	0

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



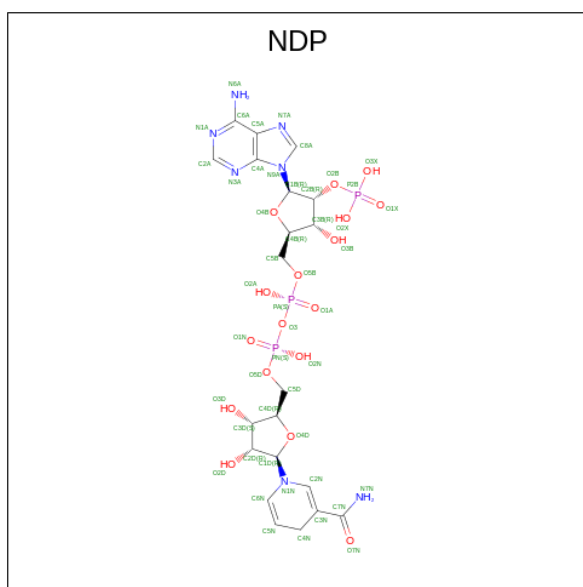
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	Total 52	42	1	8	1	0
49	a	1	Total 52	42	1	8	1	0
49	e	1	Total 52	42	1	8	1	0
49	g	1	Total 52	42	1	8	1	0
49	j	1	Total 52	42	1	8	1	0
49	r	1	Total 52	42	1	8	1	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
50	G	1	35	23	2	8	1	1	0
50	X	1	35	23	2	8	1	1	0

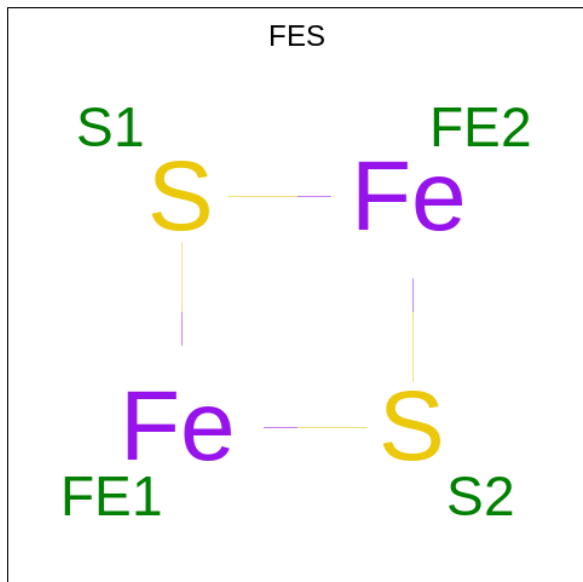
- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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



- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
52	M	1	4	2	2	0
52	O	1	4	2	2	0

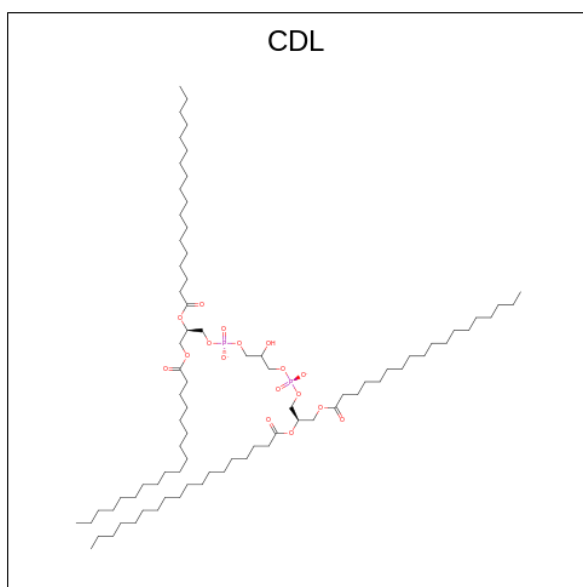
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	M	1	1	1	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

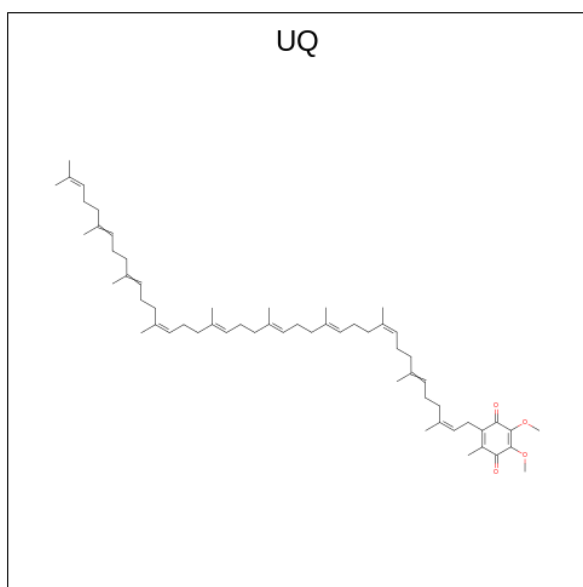
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	T	1	1	1	0

- Molecule 55 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



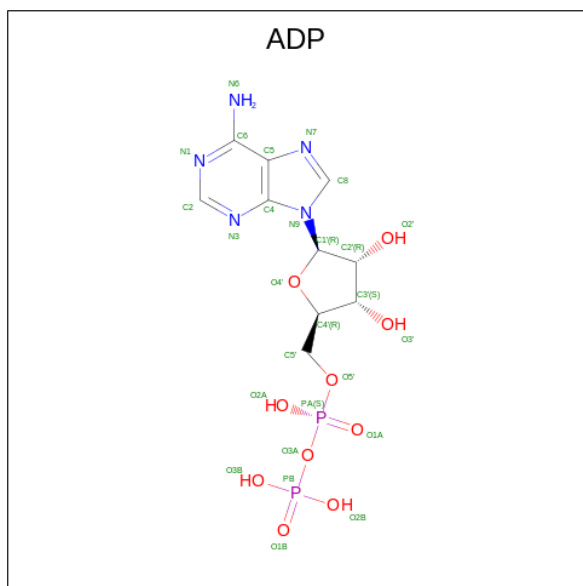
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
55	a	1	Total 91	C 72	O 17	P 2	0
55	i	1	Total 66	C 47	O 17	P 2	0
55	l	1	Total 199	C 161	O 34	P 4	0
55	l	1	Total 199	C 161	O 34	P 4	0
55	r	1	Total 100	C 81	O 17	P 2	0
55	u	1	Total 78	C 59	O 17	P 2	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	s	1	28	24	4	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

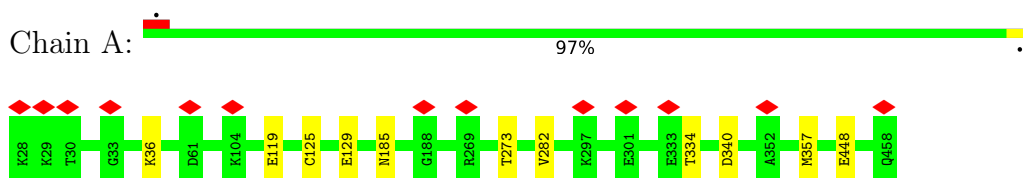


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

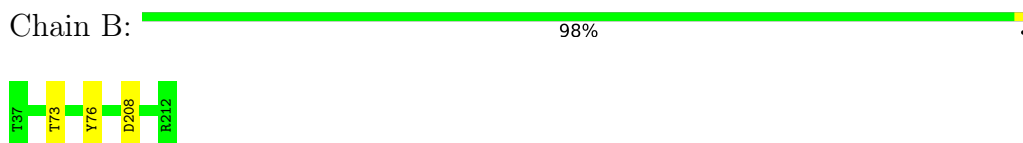
### 3 Residue-property plots [i](#)

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

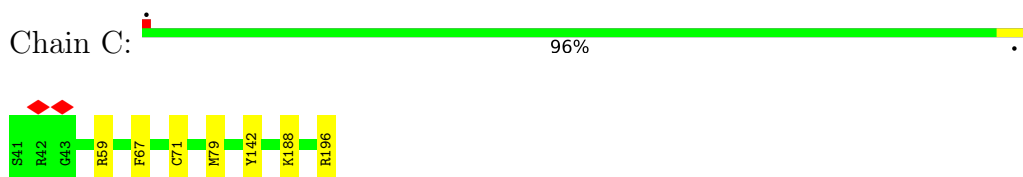
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



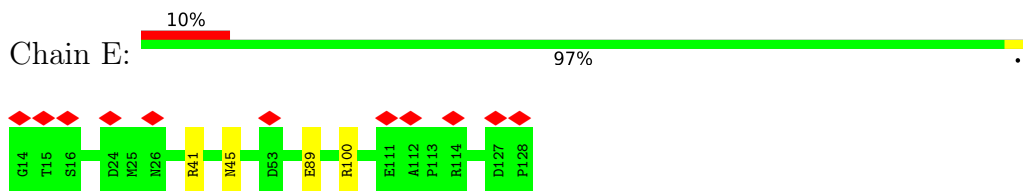
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



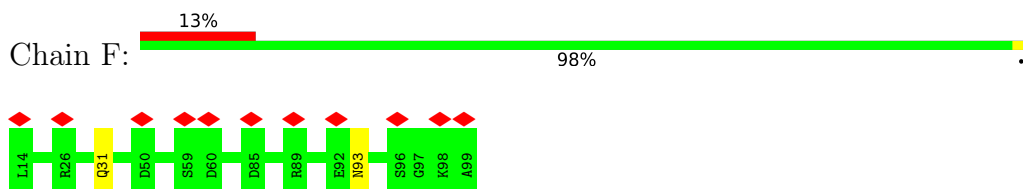
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



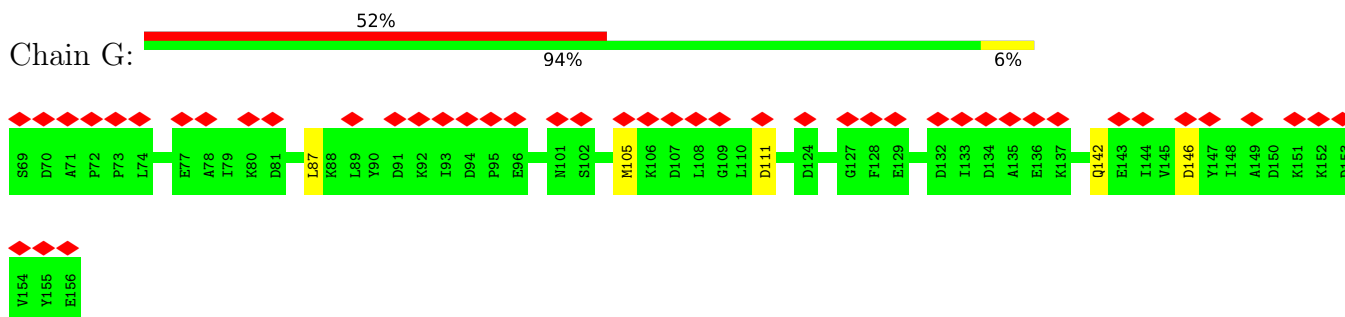
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



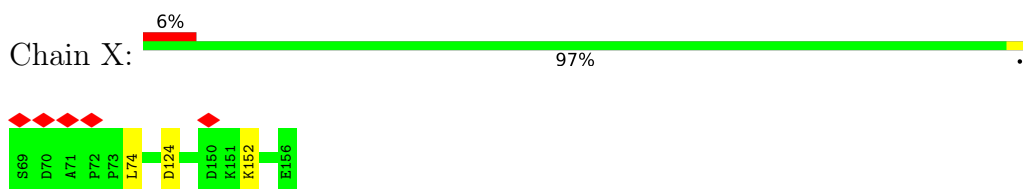
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



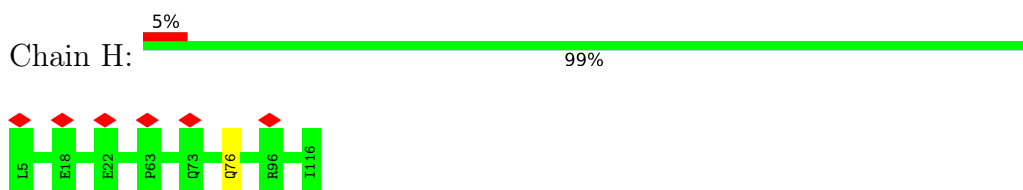
- Molecule 6: Acyl carrier protein



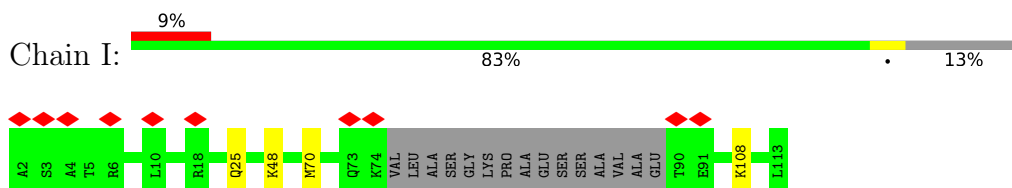
- Molecule 6: Acyl carrier protein



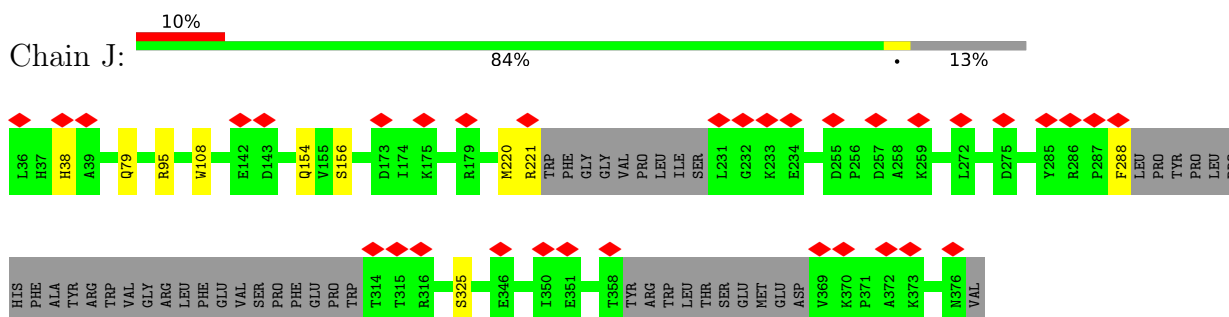
- Molecule 7: Complex I subunit B13



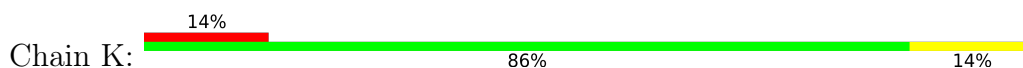
- Molecule 8: Complex I-B14.5a



- Molecule 9: NADH:ubiquinone oxidoreductase subunit A9

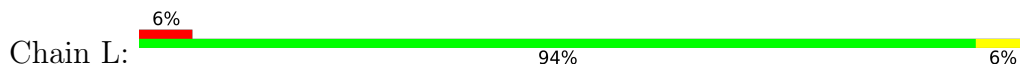


- Molecule 10: Complex I-9kD

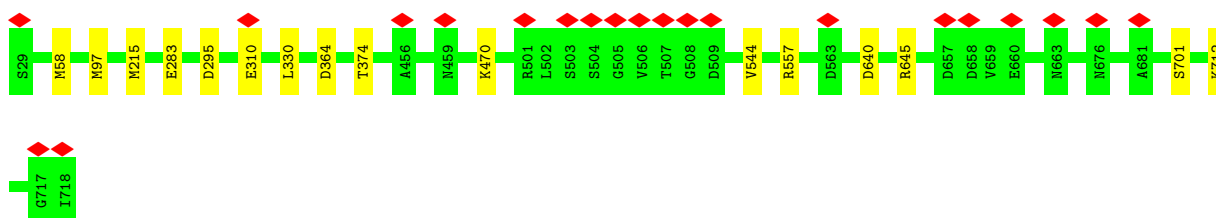




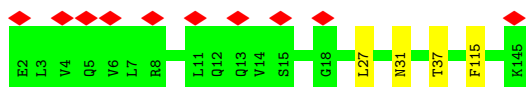
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



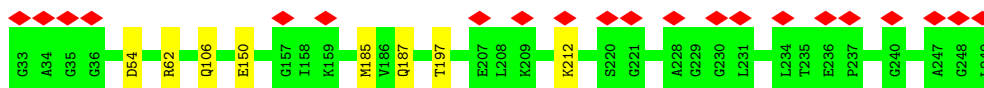
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



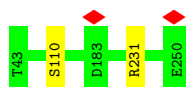
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

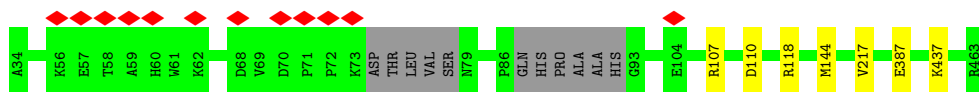


- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

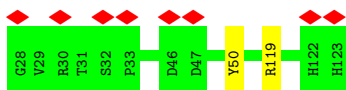




- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



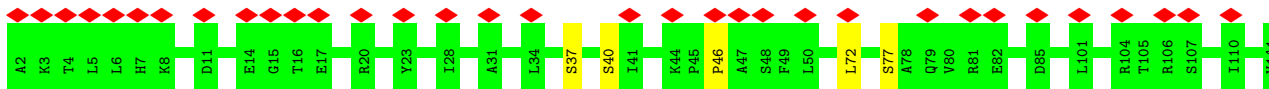
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



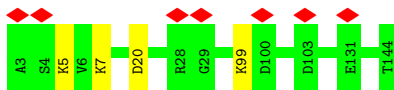
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



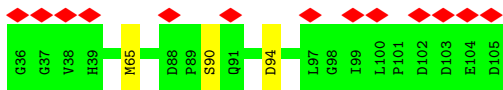
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: Complex I-B16.6



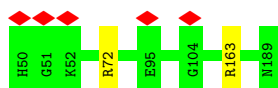
- Molecule 22: Complex I-AGGG



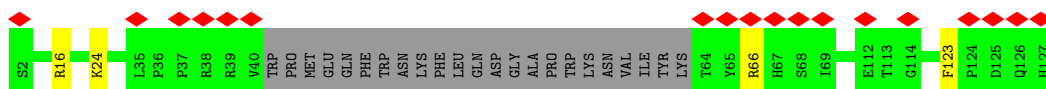
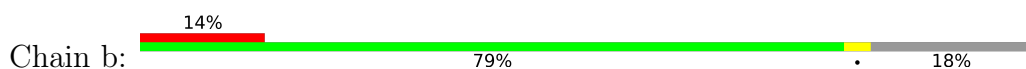
- Molecule 23: Complex I-B12



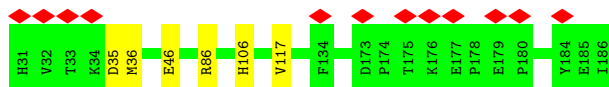
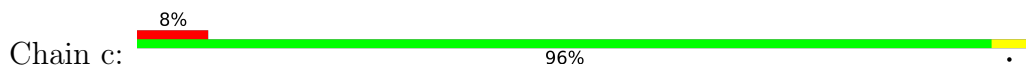
- Molecule 24: Complex I-SGDH



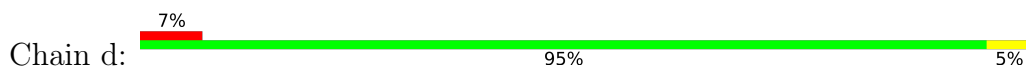
- Molecule 25: Complex I-B17



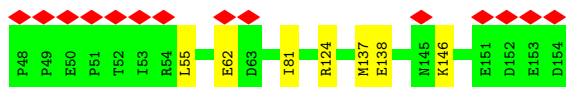
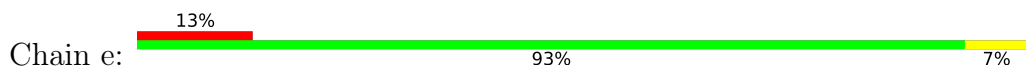
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



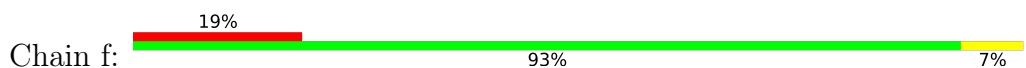
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



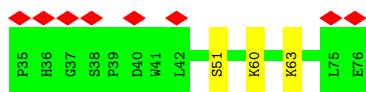
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 29: Complex I-KFYI



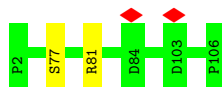




- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



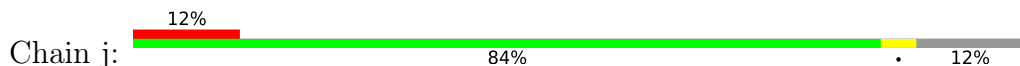
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



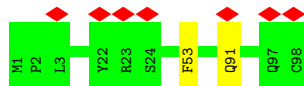
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



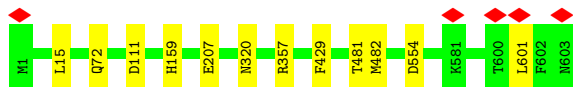
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



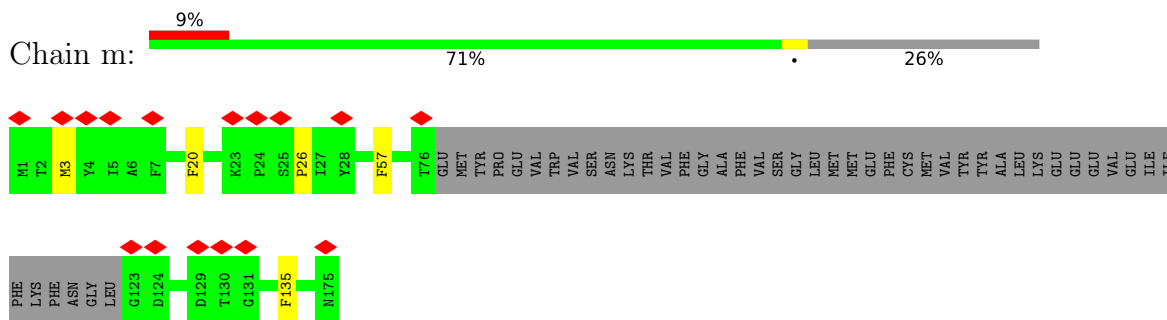
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



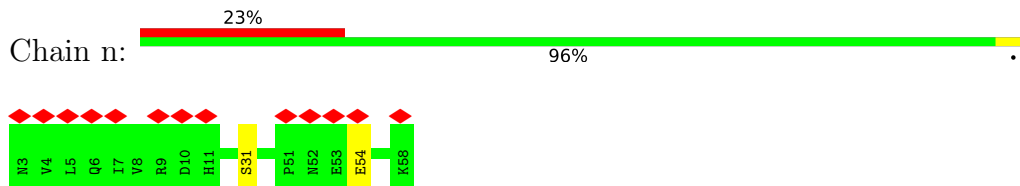
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



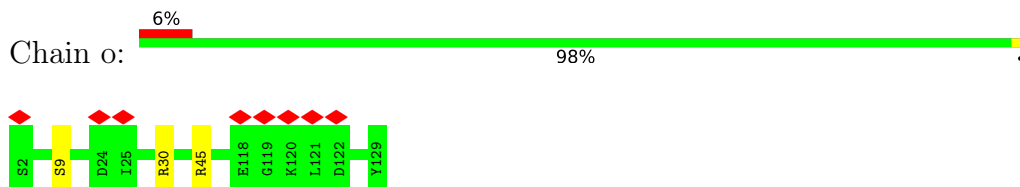
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



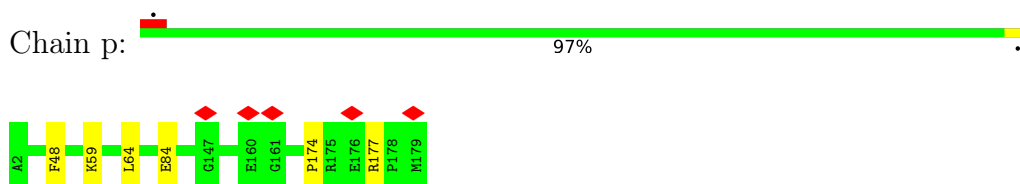
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



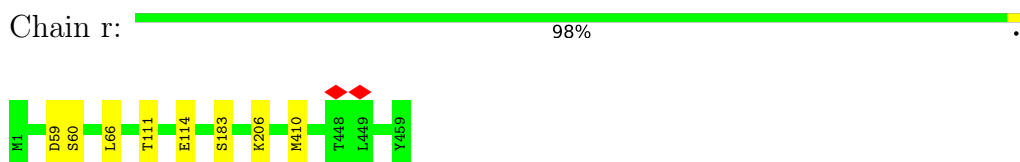
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



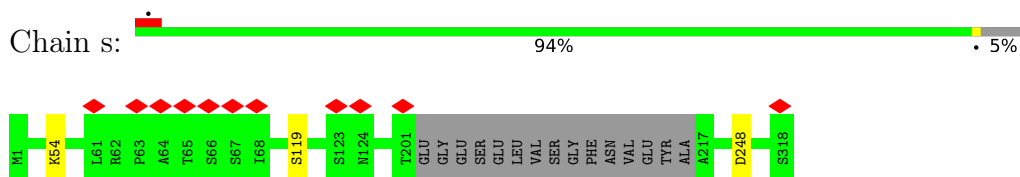
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

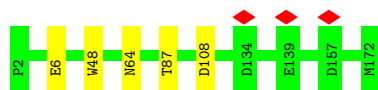


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

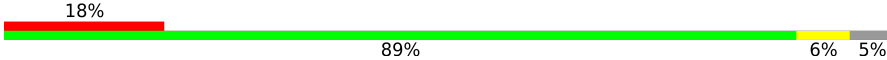


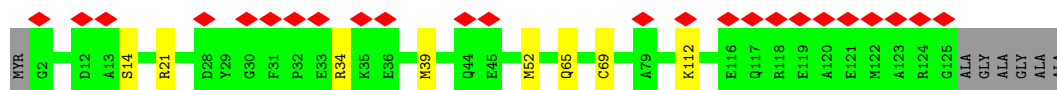
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  97%



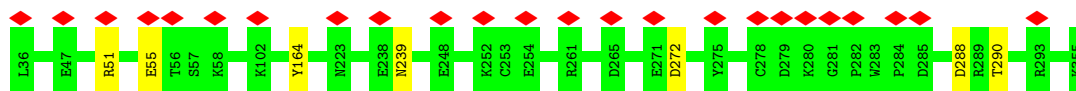
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  18% 89% 6% 5%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  8% 98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0279	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CDL, SF4, 8Q1, UQ, 2MR, NAI, PLX, FMN, MG, NDP, FES, ZN, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/3393	0.50	0/4584
2	B	0.26	0/1443	0.50	0/1952
3	C	0.26	0/1266	0.51	0/1715
4	E	0.27	0/989	0.52	0/1333
5	F	0.26	0/699	0.59	0/941
6	G	0.27	0/705	0.47	0/956
6	X	0.25	0/708	0.44	0/959
7	H	0.24	0/929	0.43	0/1258
8	I	0.25	0/780	0.53	0/1059
9	J	0.25	0/2404	0.49	0/3245
10	K	0.24	0/365	0.49	0/493
11	L	0.25	0/1039	0.51	0/1403
12	M	0.25	0/5381	0.50	0/7291
13	N	0.25	0/1245	0.51	0/1694
14	O	0.26	0/1688	0.50	0/2301
15	P	0.27	0/1789	0.51	0/2436
16	Q	0.27	0/3437	0.50	0/4656
17	S	0.26	0/582	0.47	0/783
18	T	0.24	0/755	0.51	0/1018
19	U	0.25	0/664	0.45	0/912
20	V	0.27	0/1042	0.48	0/1411
21	W	0.26	0/1192	0.47	0/1610
22	Y	0.26	0/609	0.47	0/835
23	Z	0.26	0/695	0.53	1/939 (0.1%)
24	a	0.26	0/1185	0.48	0/1606
25	b	0.26	0/902	0.52	0/1227
26	c	0.27	0/1371	0.51	0/1875
27	d	0.25	0/1494	0.49	0/2015
28	e	0.26	0/916	0.49	0/1246
29	f	0.28	0/350	0.47	0/473
30	g	0.28	0/1031	0.51	0/1394
31	h	0.25	0/889	0.51	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.26	0/2769	0.45	0/3764
33	j	0.26	0/819	0.45	0/1117
34	k	0.26	0/759	0.46	0/1029
35	l	0.26	0/4911	0.45	0/6680
36	m	0.27	0/970	0.47	0/1316
37	n	0.23	0/468	0.48	0/633
38	o	0.27	0/1088	0.51	0/1477
39	p	0.26	0/1590	0.51	0/2155
40	r	0.26	0/3723	0.46	0/5078
41	s	0.26	0/2464	0.46	0/3369
42	u	0.24	0/1436	0.47	0/1938
43	v	0.28	0/1044	0.58	0/1403
44	w	0.26	0/2634	0.48	0/3571
All	All	0.26	0/66612	0.49	1/90340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	43	ASP	CB-CG-OD1	5.26	123.04	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	86 (100%)	0	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/342 (84%)	281 (97%)	7 (2%)	1 (0%)	41	71
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	21 (3%)	1 (0%)	51	82
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	54
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	25	58
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	95/113 (84%)	87 (92%)	8 (8%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	573 (95%)	27 (4%)	1 (0%)	47	78
36	m	125/175 (71%)	112 (90%)	12 (10%)	1 (1%)	19	51
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	166 (94%)	9 (5%)	1 (1%)	25	58
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	299/318 (94%)	290 (97%)	9 (3%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/131 (93%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8029/8316 (96%)	7731 (96%)	291 (4%)	7 (0%)	54	82

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
12	M	283	GLU
26	c	106	HIS
20	V	46	PRO
35	l	15	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	334 (97%)	11 (3%)	39	73
2	B	151/151 (100%)	148 (98%)	3 (2%)	55	82
3	C	129/132 (98%)	122 (95%)	7 (5%)	22	54

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	106/107 (99%)	102 (96%)	4 (4%)	33	67
5	F	75/76 (99%)	73 (97%)	2 (3%)	44	77
6	G	76/81 (94%)	71 (93%)	5 (7%)	16	44
6	X	77/81 (95%)	74 (96%)	3 (4%)	32	66
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	92
8	I	82/97 (84%)	78 (95%)	4 (5%)	25	57
9	J	253/296 (86%)	244 (96%)	9 (4%)	35	69
10	K	41/41 (100%)	35 (85%)	6 (15%)	3	9
11	L	113/113 (100%)	106 (94%)	7 (6%)	18	47
12	M	579/580 (100%)	564 (97%)	15 (3%)	46	77
13	N	130/130 (100%)	126 (97%)	4 (3%)	40	74
14	O	176/183 (96%)	168 (96%)	8 (4%)	27	61
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	92
16	Q	358/370 (97%)	352 (98%)	6 (2%)	60	86
17	S	58/58 (100%)	56 (97%)	2 (3%)	37	71
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	78
19	U	69/69 (100%)	65 (94%)	4 (6%)	20	50
20	V	101/101 (100%)	97 (96%)	4 (4%)	31	65
21	W	121/123 (98%)	117 (97%)	4 (3%)	38	72
22	Y	58/63 (92%)	55 (95%)	3 (5%)	23	55
23	Z	65/65 (100%)	62 (95%)	3 (5%)	27	60
24	a	119/122 (98%)	117 (98%)	2 (2%)	60	86
25	b	97/119 (82%)	93 (96%)	4 (4%)	30	64
26	c	141/141 (100%)	136 (96%)	5 (4%)	36	70
27	d	155/155 (100%)	146 (94%)	9 (6%)	20	50
28	e	99/99 (100%)	92 (93%)	7 (7%)	14	40
29	f	35/38 (92%)	32 (91%)	3 (9%)	10	30
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	93
31	h	93/93 (100%)	91 (98%)	2 (2%)	52	81
32	i	310/311 (100%)	302 (97%)	8 (3%)	46	77
33	j	88/99 (89%)	84 (96%)	4 (4%)	27	61

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	79
35	l	536/537 (100%)	525 (98%)	11 (2%)	53	81
36	m	98/141 (70%)	94 (96%)	4 (4%)	30	64
37	n	46/53 (87%)	44 (96%)	2 (4%)	29	62
38	o	112/113 (99%)	109 (97%)	3 (3%)	44	77
39	p	159/159 (100%)	154 (97%)	5 (3%)	40	74
40	r	410/410 (100%)	402 (98%)	8 (2%)	55	82
41	s	263/275 (96%)	260 (99%)	3 (1%)	73	92
42	u	153/153 (100%)	148 (97%)	5 (3%)	38	72
43	v	103/111 (93%)	95 (92%)	8 (8%)	12	34
44	w	279/283 (99%)	272 (98%)	7 (2%)	47	78
All	All	7020/7235 (97%)	6798 (97%)	222 (3%)	42	73

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	Y	94	ASP
44	w	290	THR
28	e	137	MET
44	w	272	ASP
41	s	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
35	l	135	ASN
35	l	199	GLN
44	w	202	HIS
44	w	127	ASN
44	w	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.05	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.64	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.37	131.60	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.01	130.51	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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
55	CDL	a	201	-	90,90,99	1.14	8 (8%)	96,102,111	0.92	4 (4%)
48	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
49	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.95	19 (45%)	47,73,73	1.31	7 (14%)
49	PLX	e	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
55	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	0.97	4 (5%)
56	UQ	s	402	-	28,28,63	3.27	7 (25%)	34,37,79	2.79	10 (29%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
48	PEE	l	703	-	45,45,50	1.23	6 (13%)	48,50,55	0.99	2 (4%)
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
48	PEE	Q	501	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.21	8 (16%)
49	PLX	C	303	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
55	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
57	ADP	w	401	-	24,29,29	3.11	6 (25%)	29,45,45	1.43	4 (13%)
52	FES	M	803	12	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
50	8Q1	X	201	-	31,34,34	1.71	6 (19%)	40,43,43	1.60	6 (15%)
55	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	C	301	16,3	0,12,12	-	-	-		
49	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
55	CDL	r	503	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
55	CDL	u	201	-	77,77,99	1.20	9 (11%)	83,89,111	0.95	4 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
50	8Q1	G	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.52	6 (15%)
51	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	2.04	7 (13%)
52	FES	O	301	14	0,4,4	-	-	-		
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.94	2 (4%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)

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
55	CDL	a	201	-	-	49/101/101/110	-
48	PEE	j	201	-	-	21/54/54/54	-
48	PEE	r	501	-	-	23/54/54/54	-
49	PLX	g	201	-	-	28/55/55/55	-
47	NAI	A	503	-	-	7/25/72/72	0/5/5/5
45	SF4	B	302	2	-	-	0/6/5/5
49	PLX	e	201	-	-	33/55/55/55	-
55	CDL	i	401	-	-	35/76/76/110	-
56	UQ	s	402	-	-	8/21/45/87	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	l	703	-	-	21/49/49/54	-
48	PEE	b	201	-	-	22/49/49/54	-
48	PEE	Q	501	-	-	25/50/50/54	-
49	PLX	r	502	-	-	21/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
49	PLX	C	303	-	-	24/55/55/55	-
55	CDL	l	701	-	-	50/109/109/110	-
57	ADP	w	401	-	-	3/12/32/32	0/3/3/3
52	FES	M	803	12	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	s	401	-	-	16/44/44/54	-
50	8Q1	X	201	-	-	20/41/41/41	-
55	CDL	l	702	-	-	58/110/110/110	-
45	SF4	C	301	16,3	-	-	0/6/5/5
49	PLX	a	202	-	-	31/55/55/55	-
55	CDL	r	503	-	-	71/110/110/110	-
55	CDL	u	201	-	-	41/88/88/110	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	B	303	-	-	22/54/54/54	-
50	8Q1	G	201	6	-	18/41/41/41	-
51	NDP	J	401	-	-	7/30/77/77	0/4/5/5
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	C	302	-	-	24/50/50/54	-
49	PLX	j	202	-	-	32/55/55/55	-

The worst 5 of 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.20	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.42	1.30	1.53
51	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
51	J	401	NDP	C6N-C5N	12.54	1.55	1.33
51	J	401	NDP	O4D-C4D	10.71	1.68	1.45

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	402	UQ	C7-C8-C9	-9.19	111.50	126.79
51	J	401	NDP	C3N-C2N-N1N	-9.10	110.12	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.61	110.11	121.11
50	X	201	8Q1	C6-C1-S44	6.17	120.64	113.46
56	s	402	UQ	C12-C13-C14	-5.94	113.36	127.66

There are no chirality outliers.

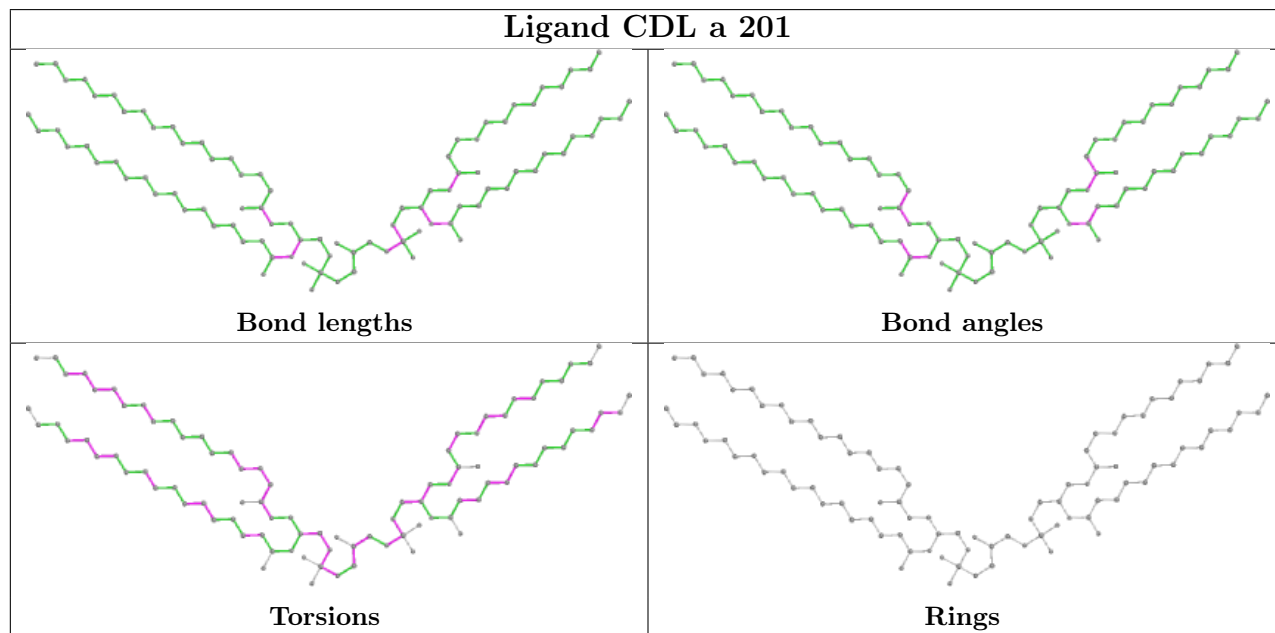
5 of 718 torsion outliers are listed below:

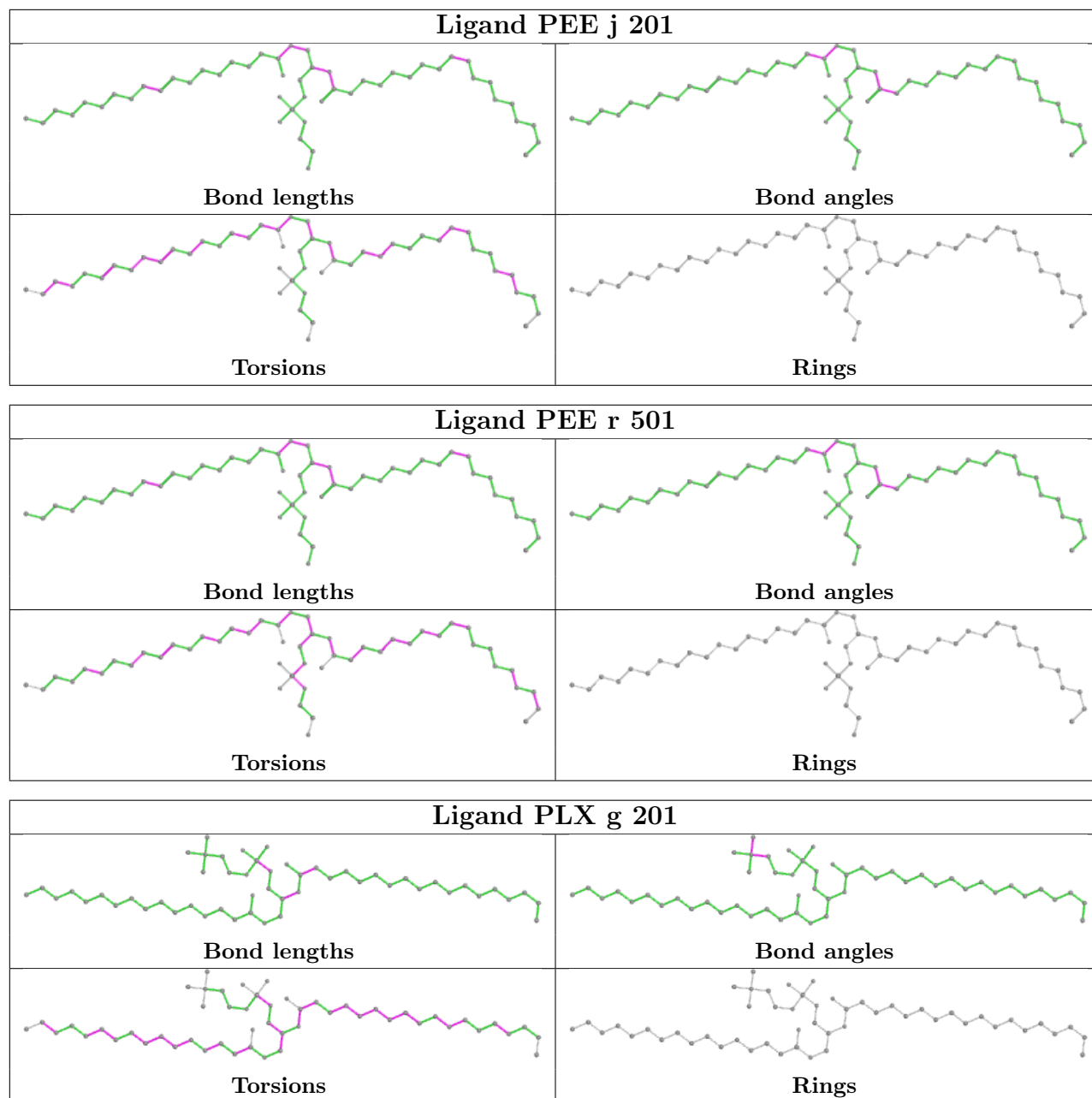
Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C3'-C4'-C5'-O5'
47	A	503	NAI	C5D-O5D-PN-O3

There are no ring outliers.

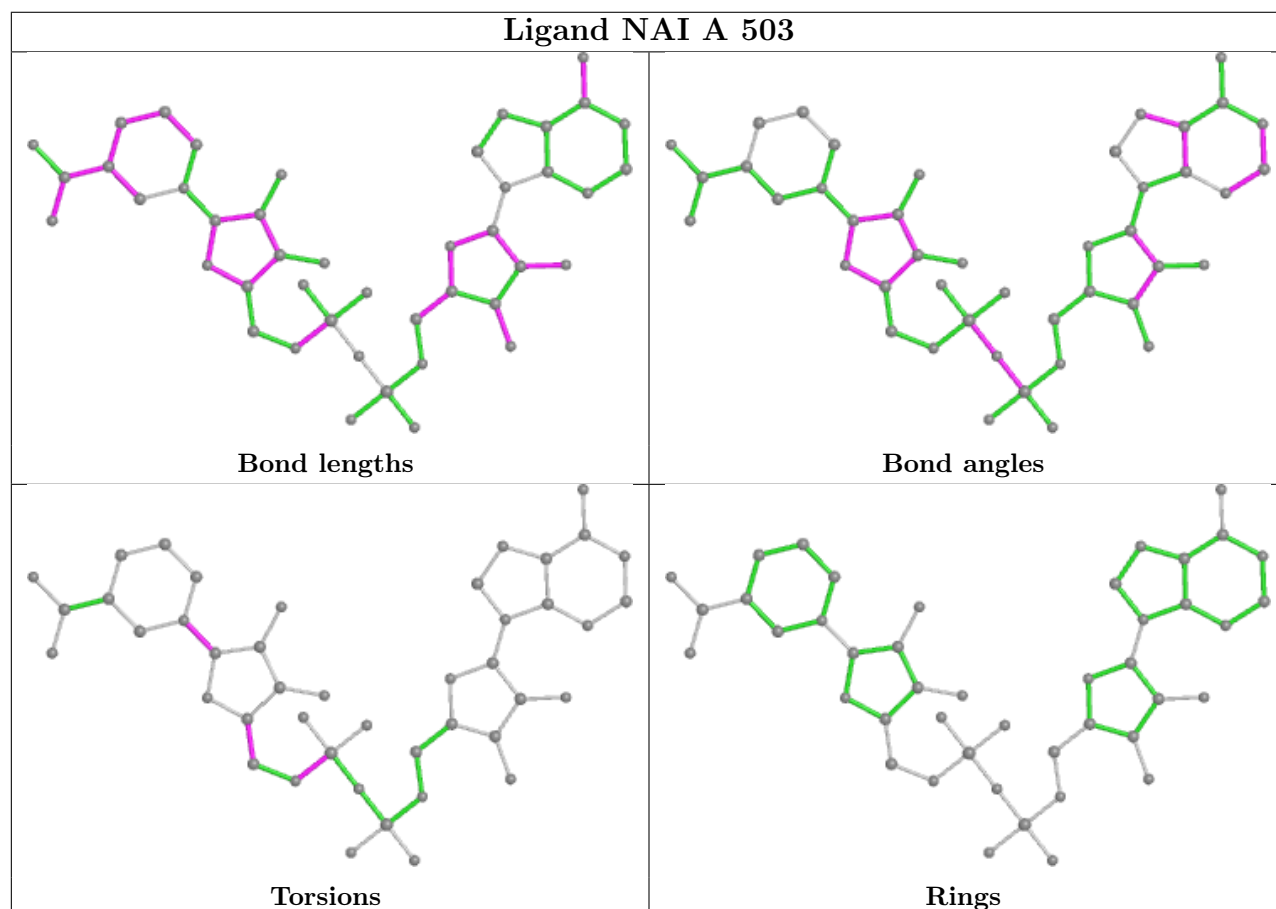
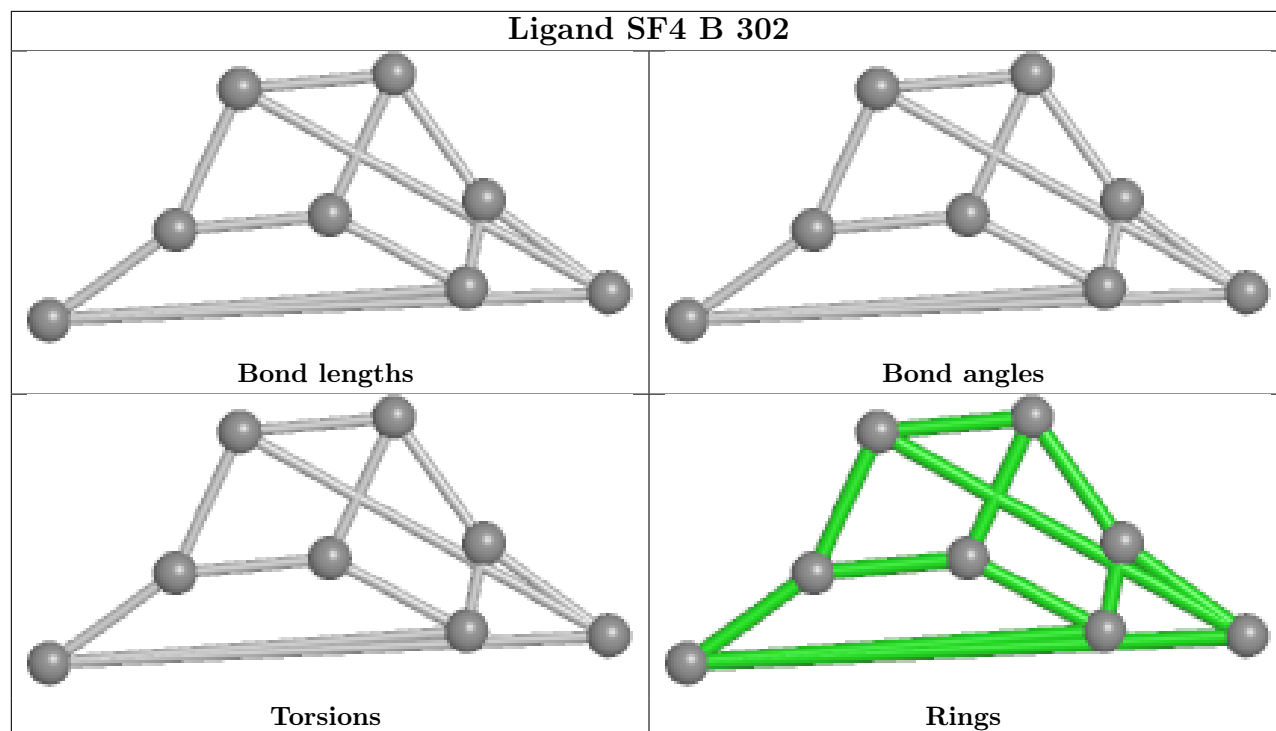
No monomer is involved in short contacts.

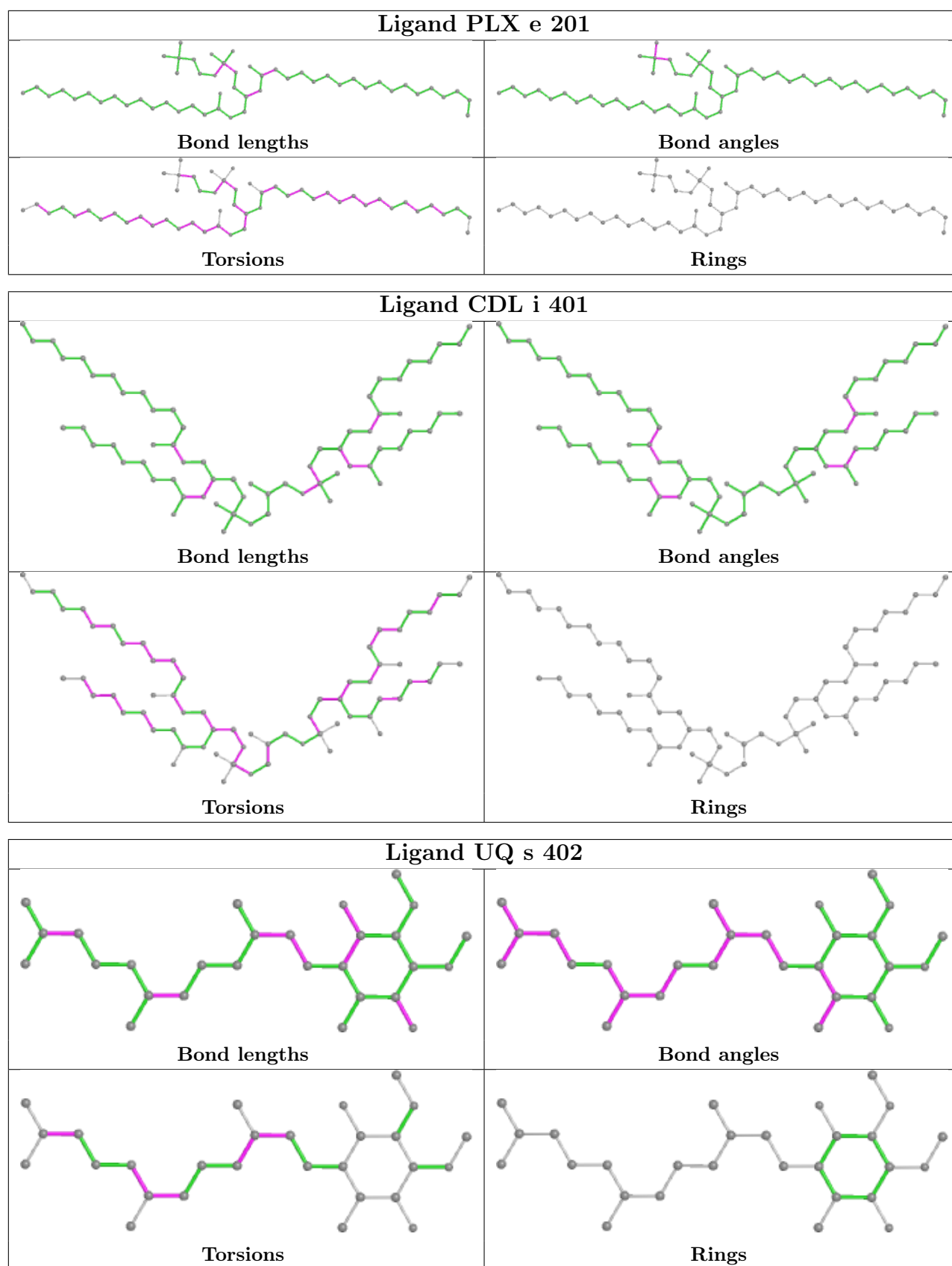
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

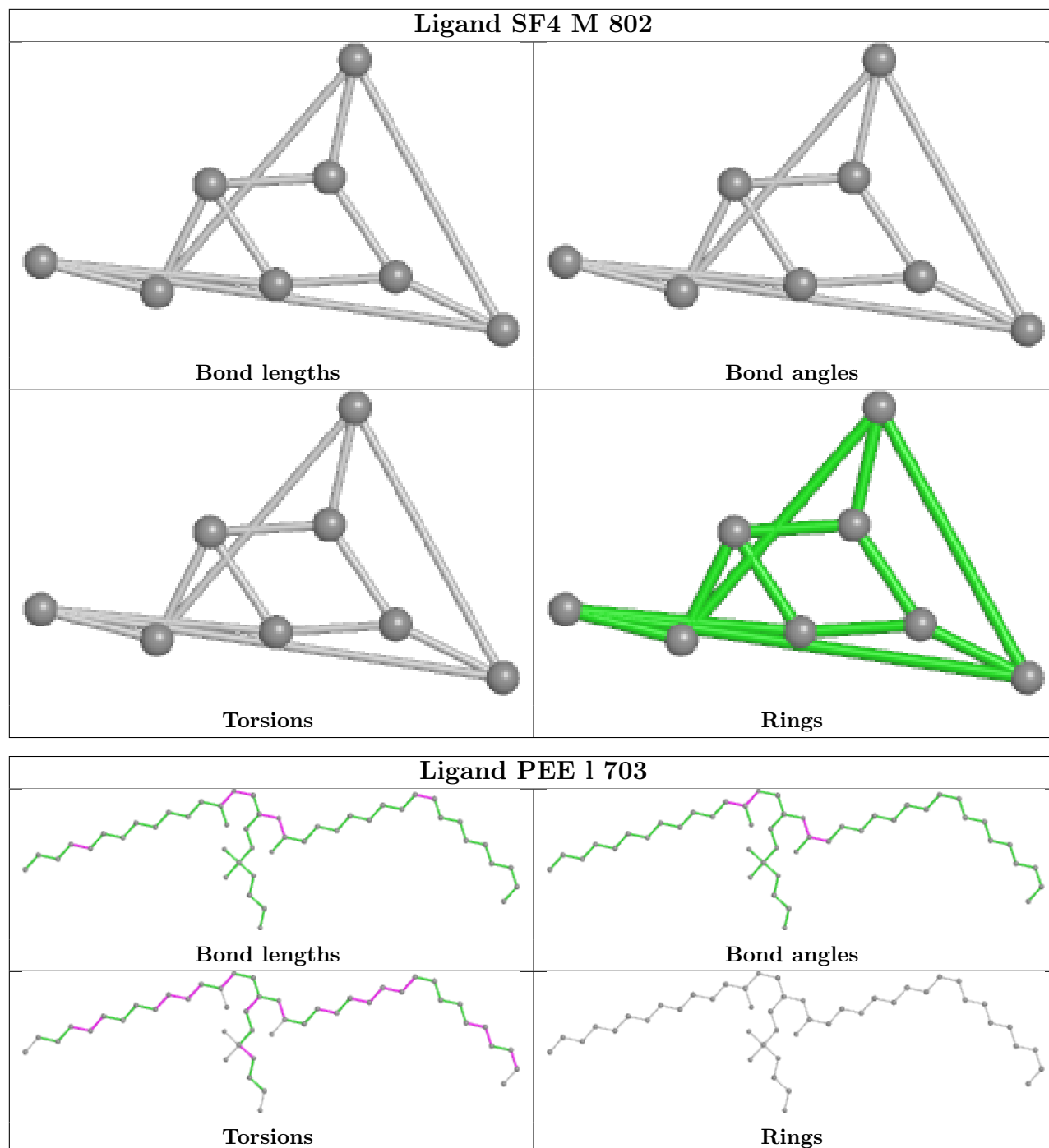


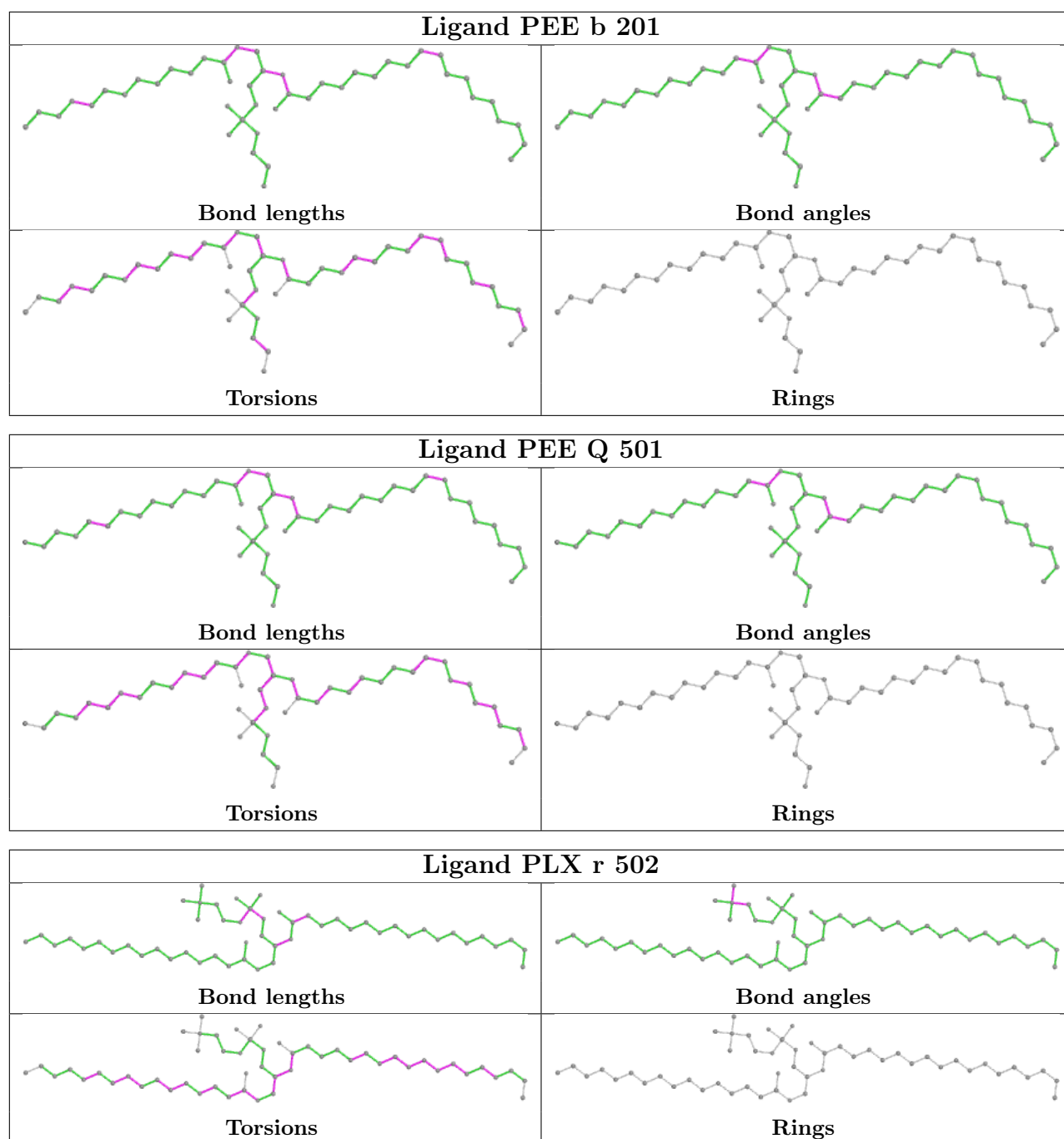


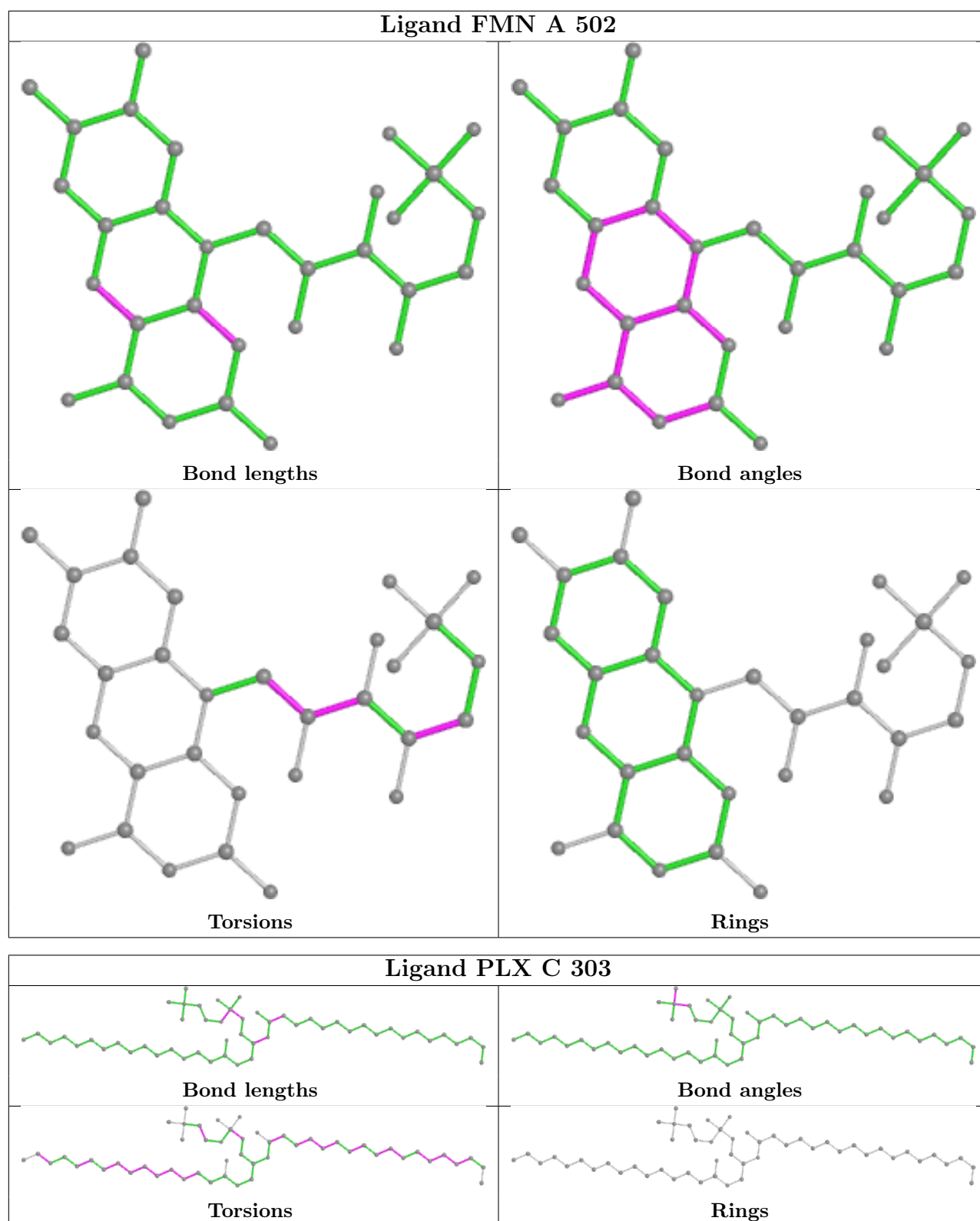


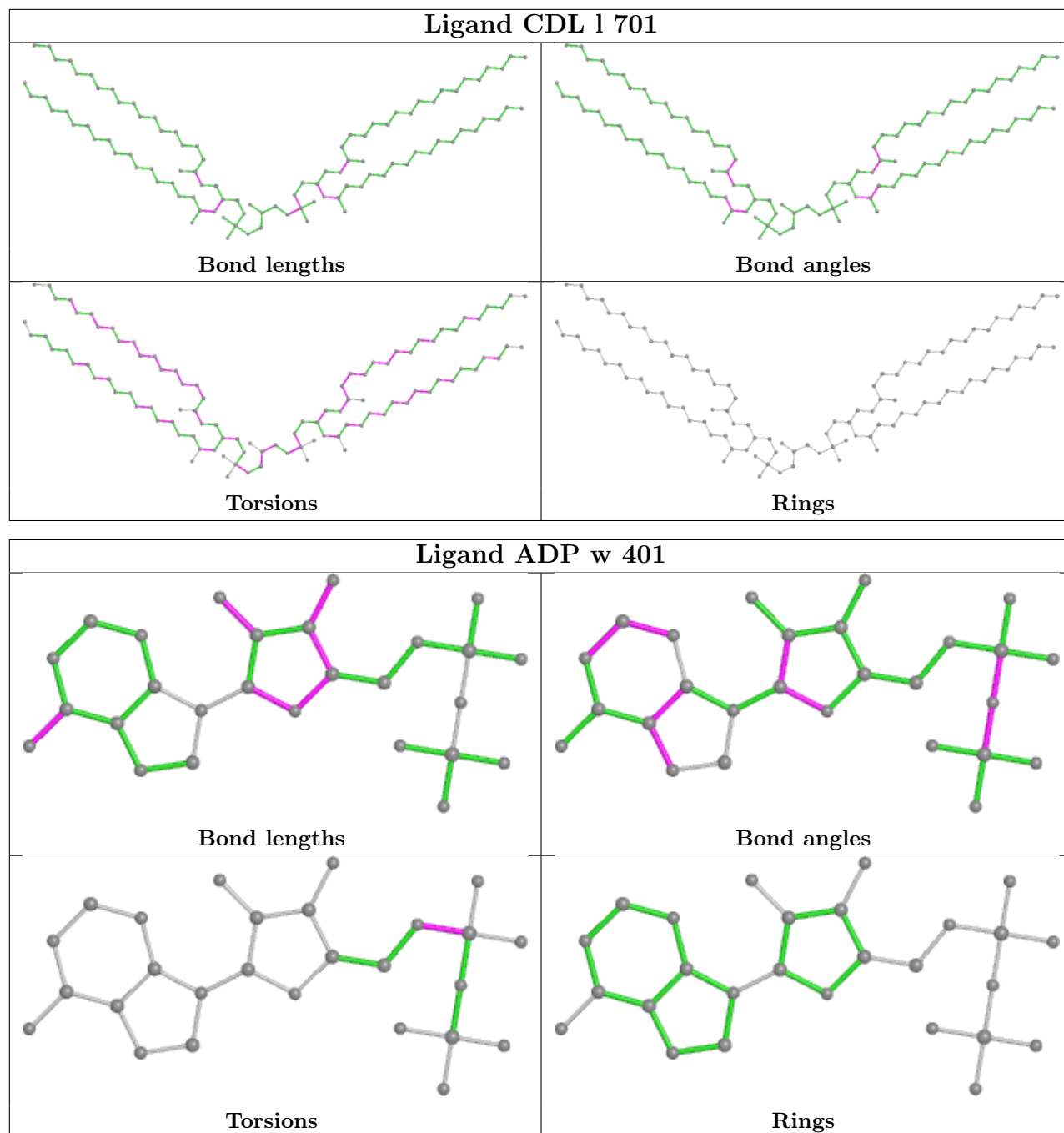


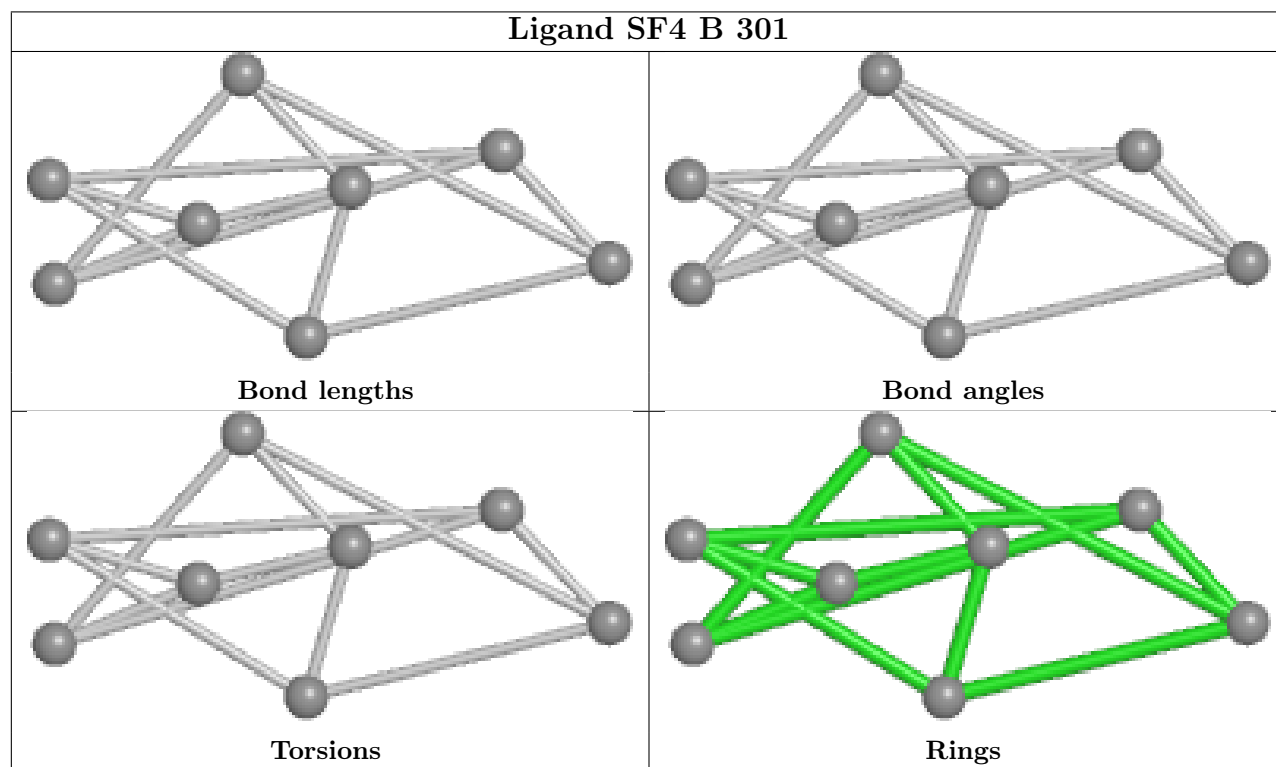
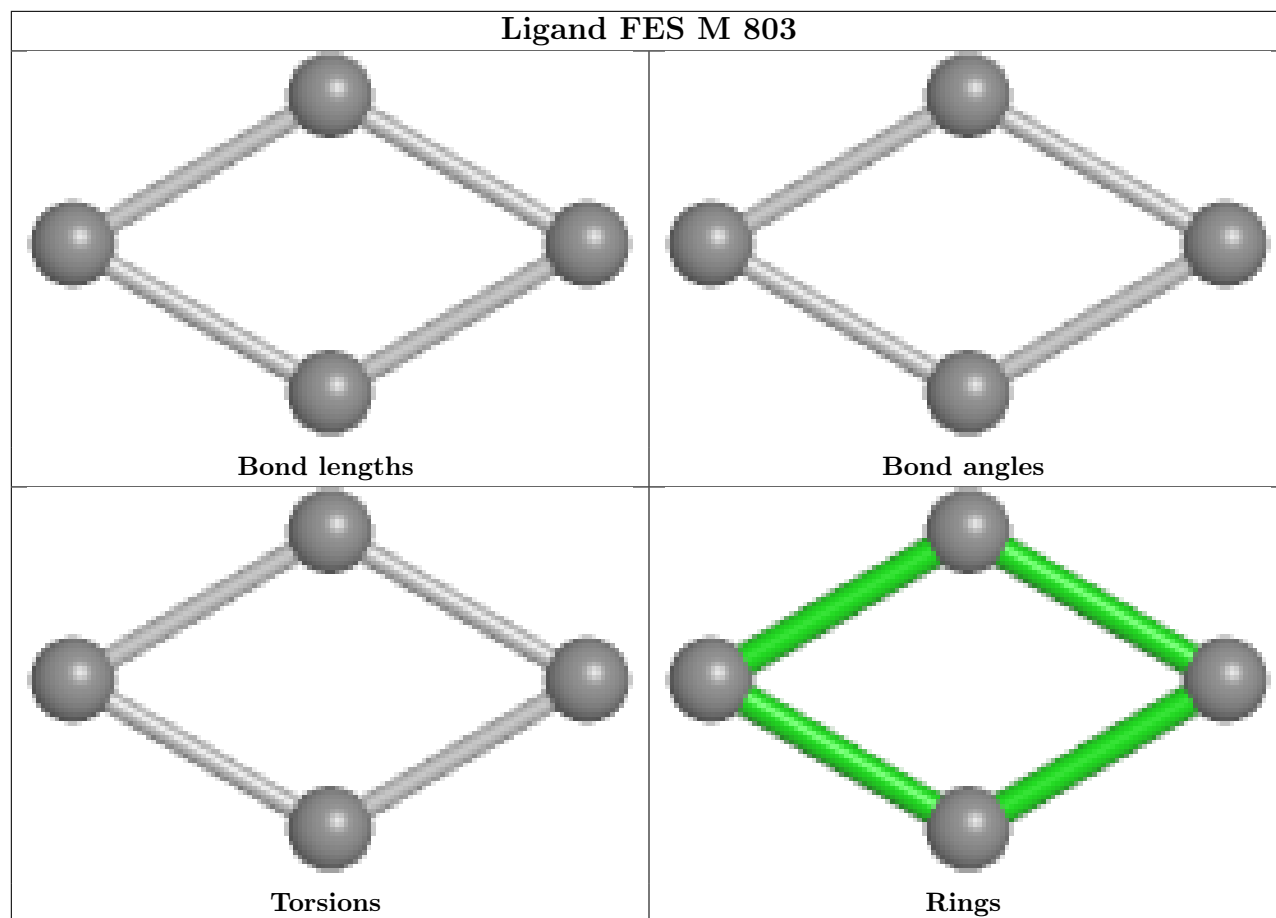


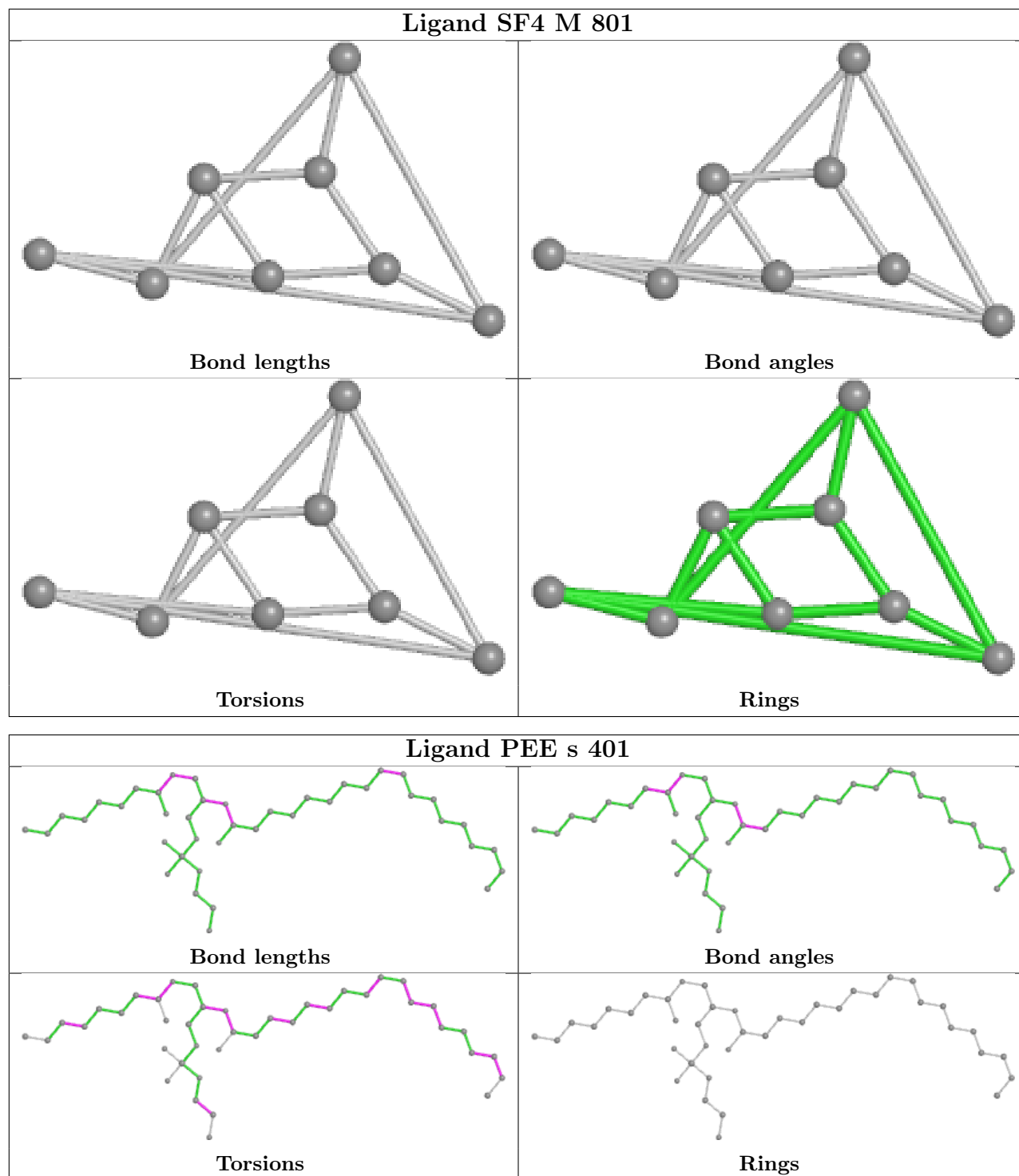




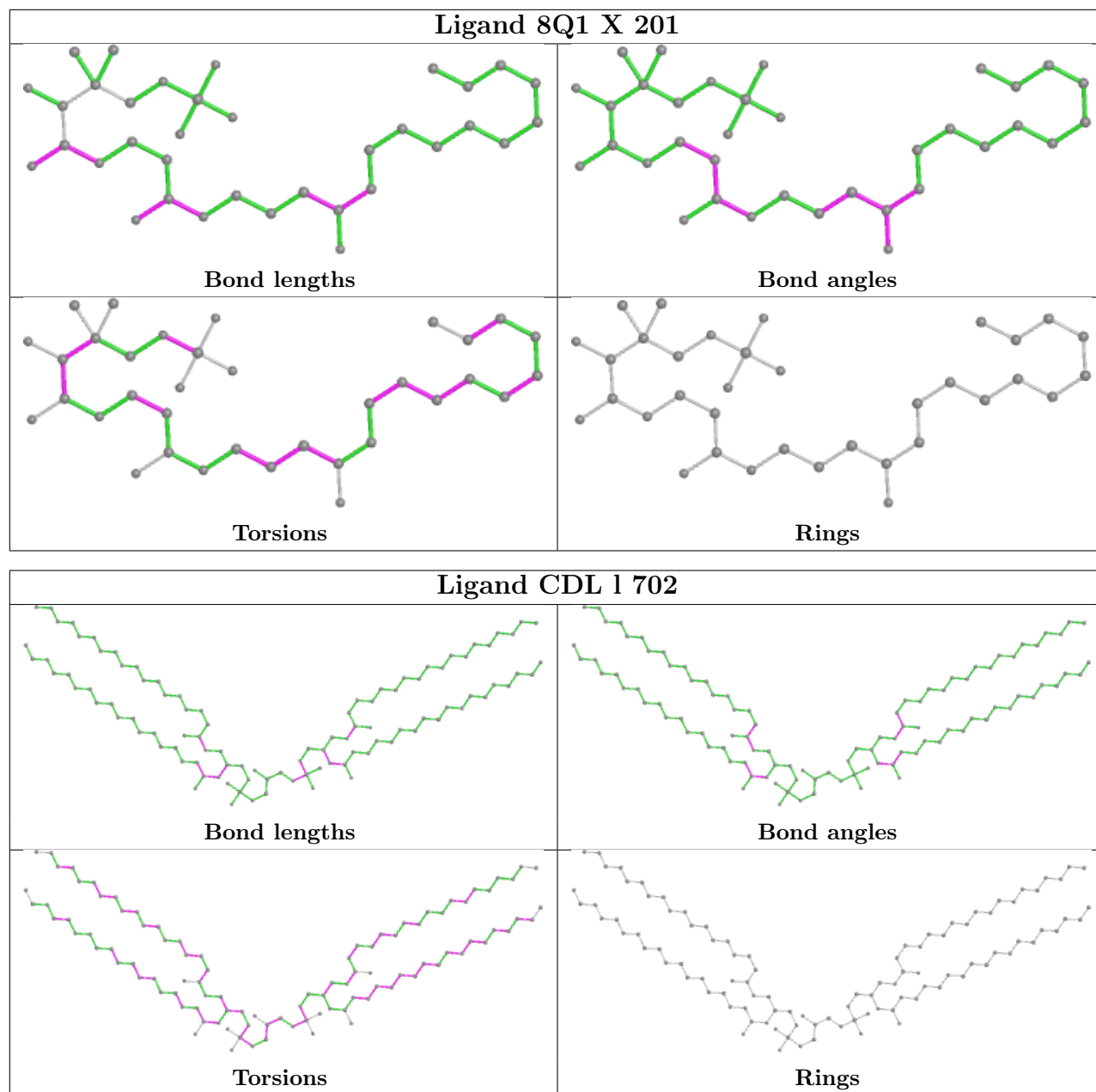


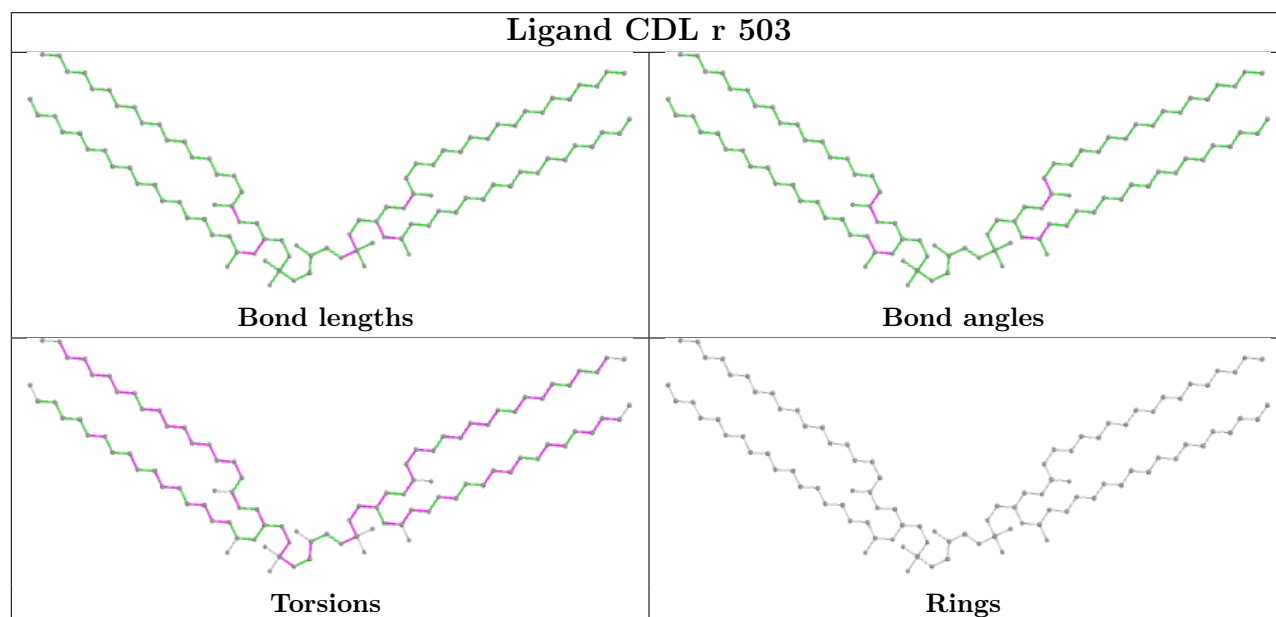
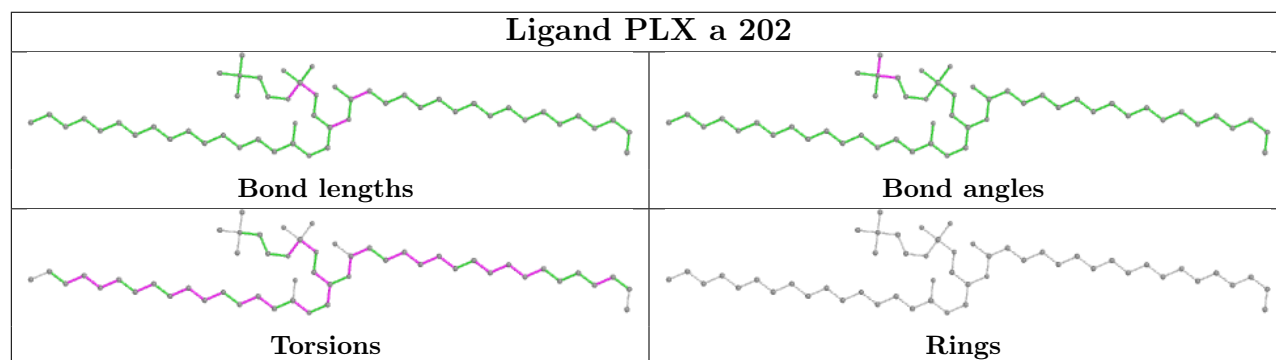
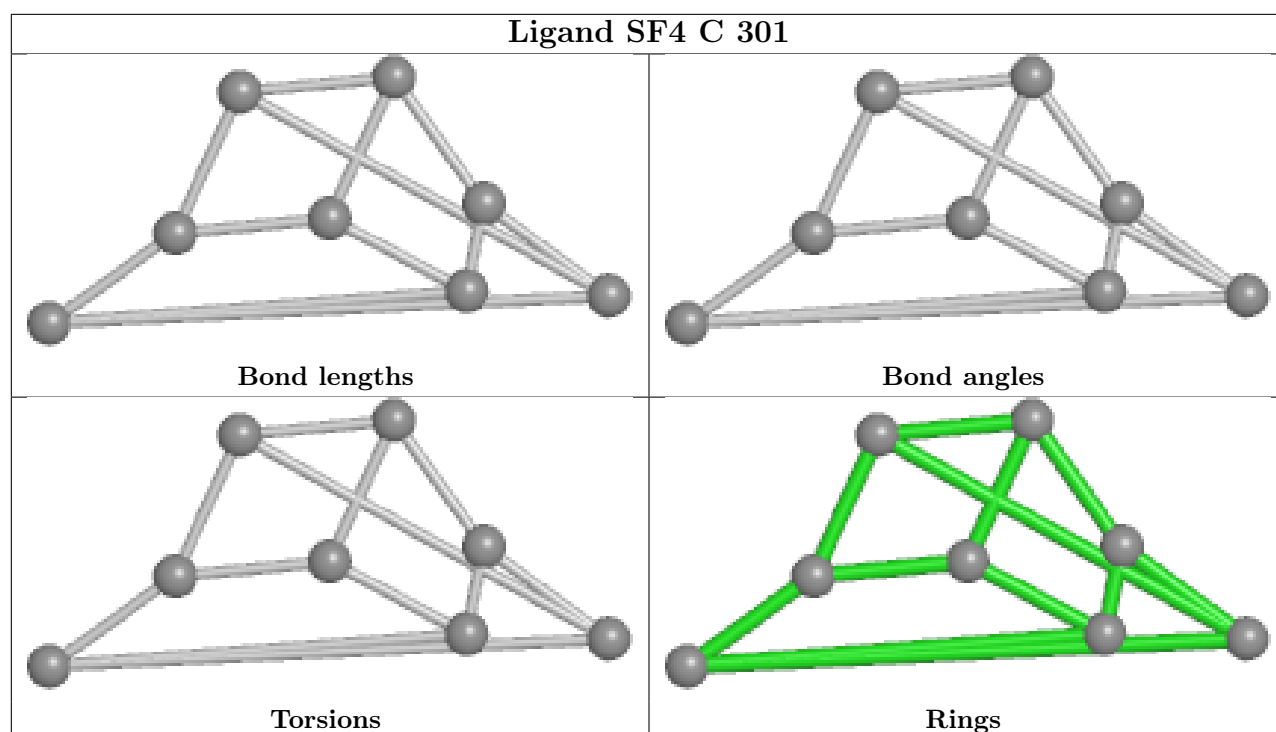


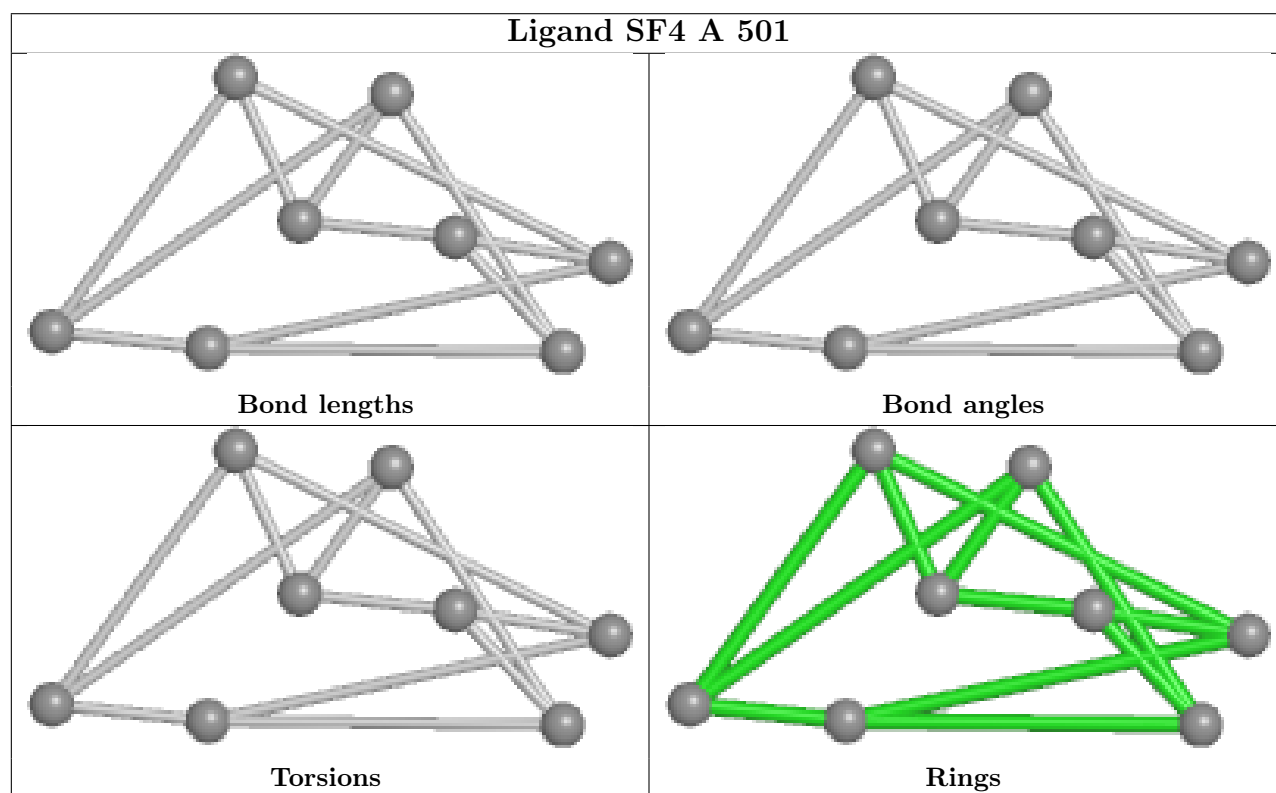
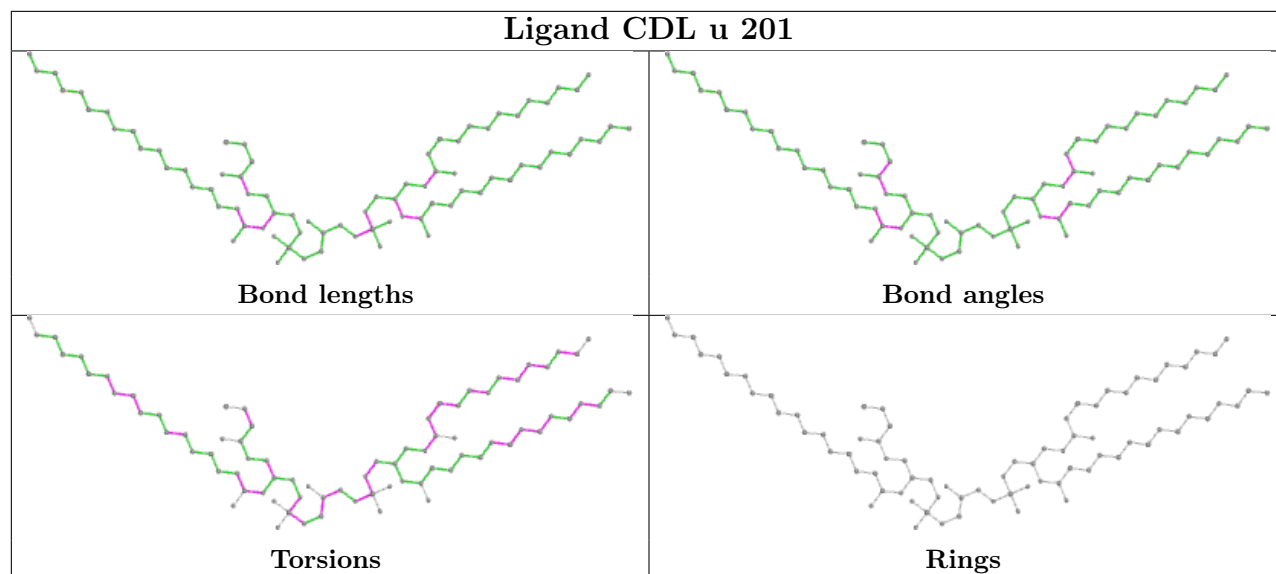


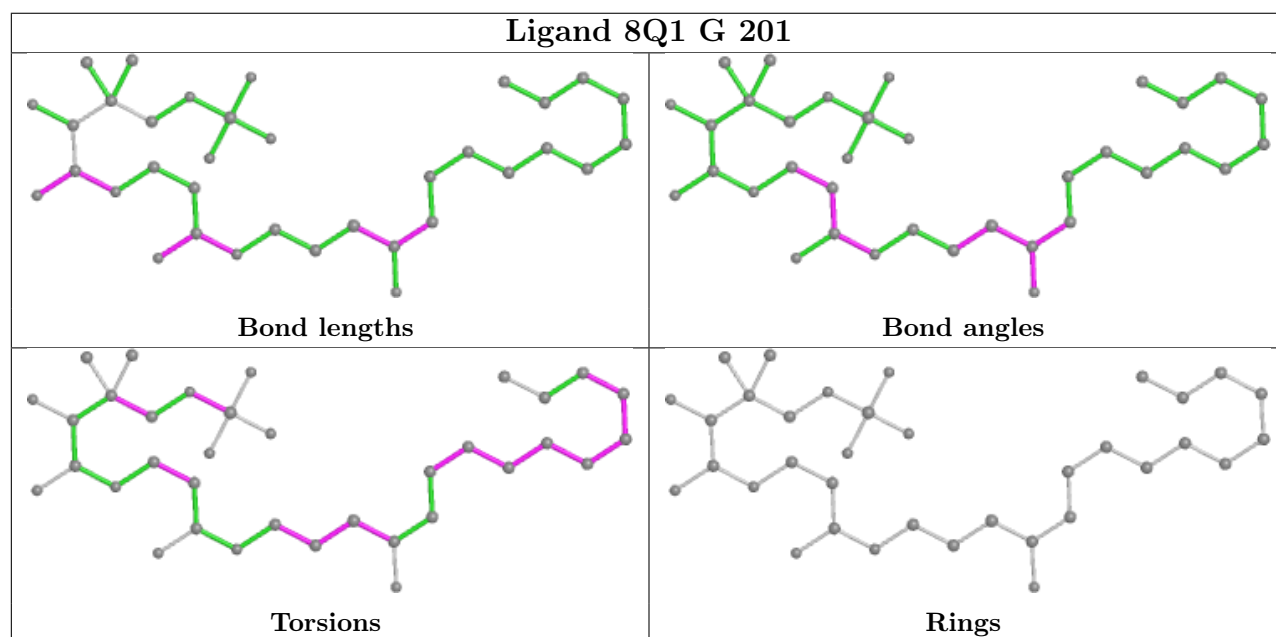
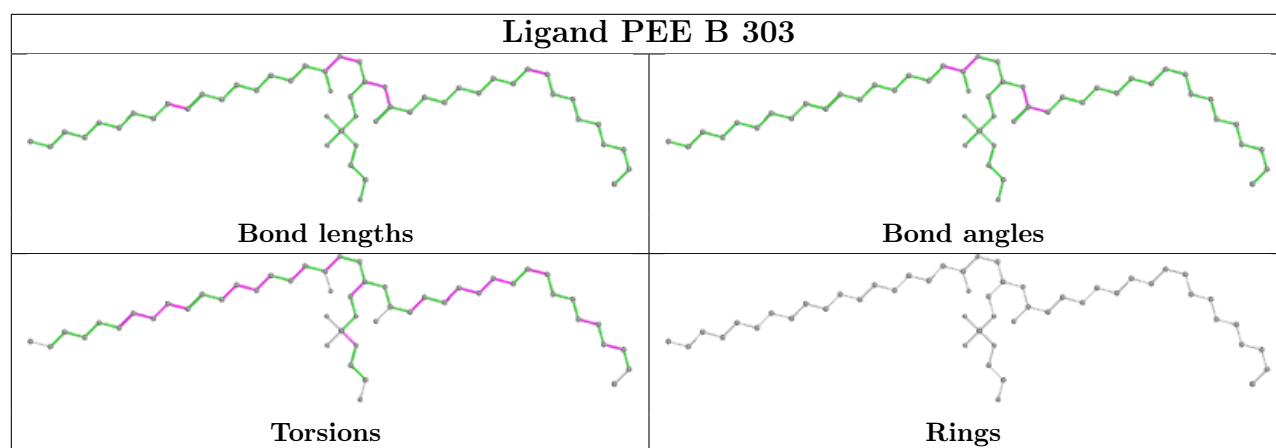


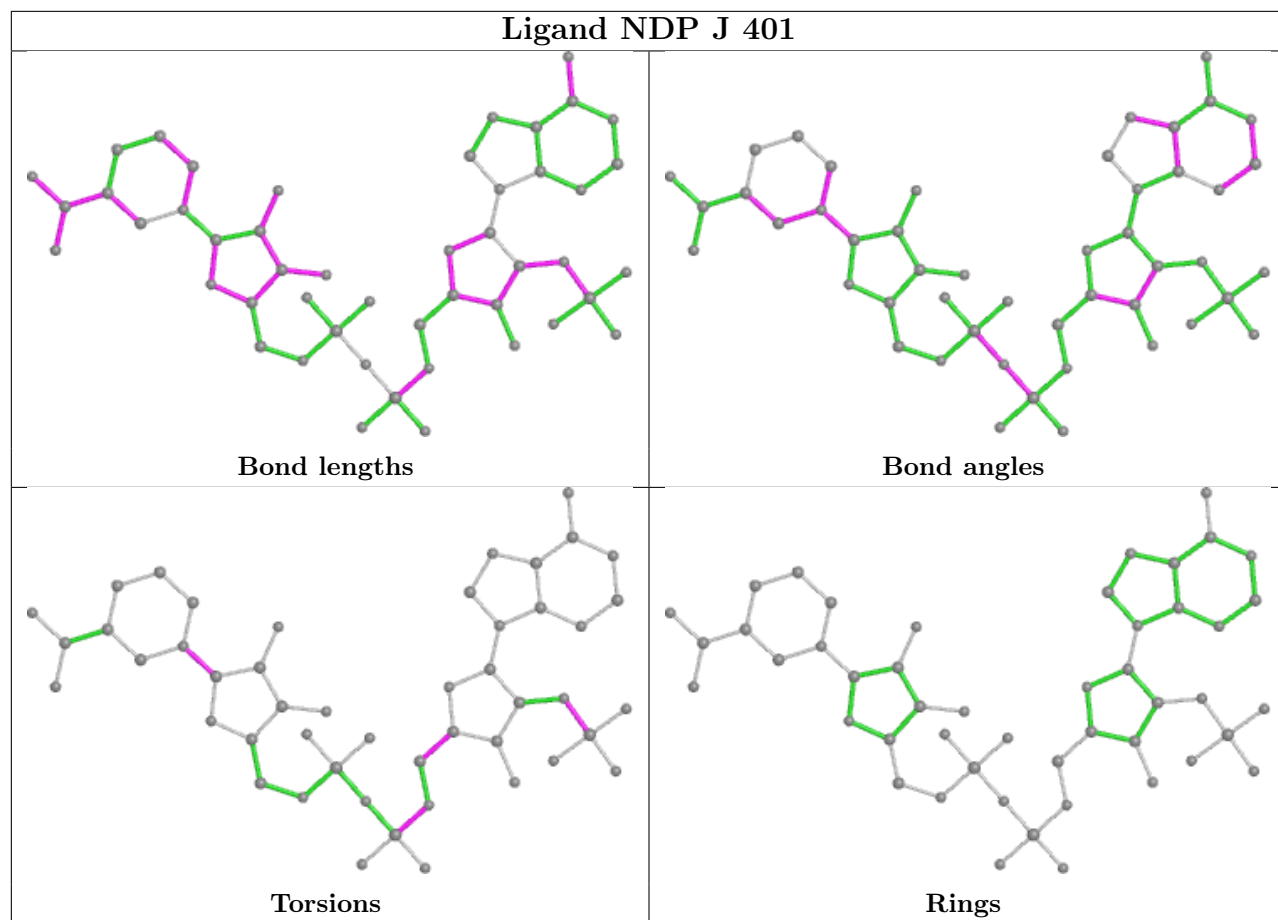


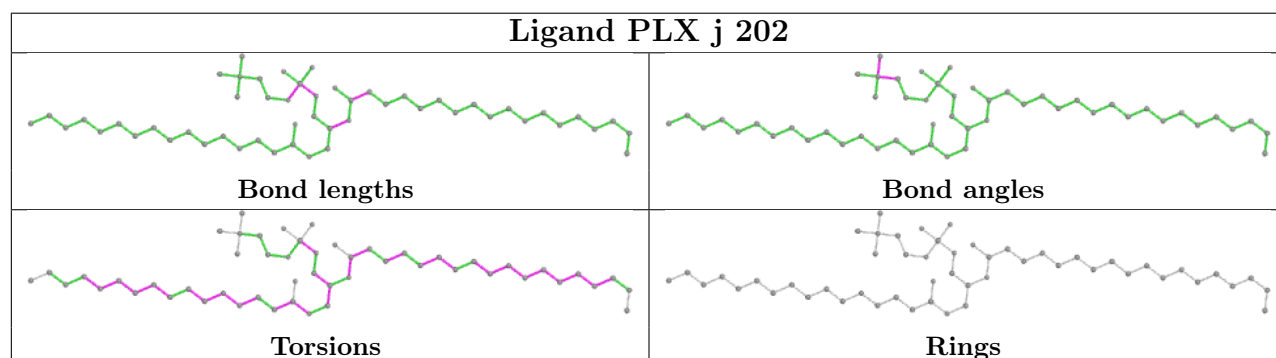
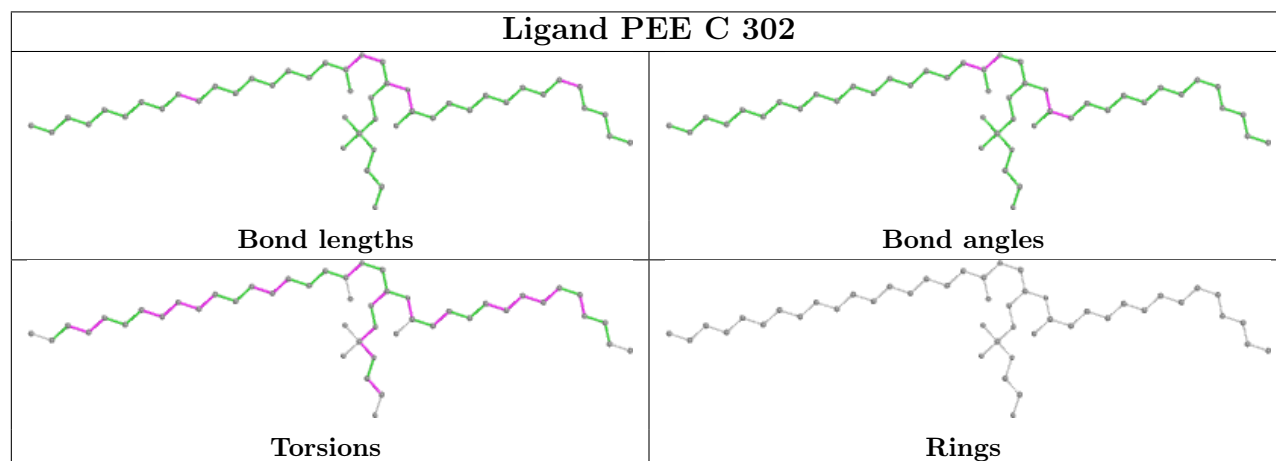
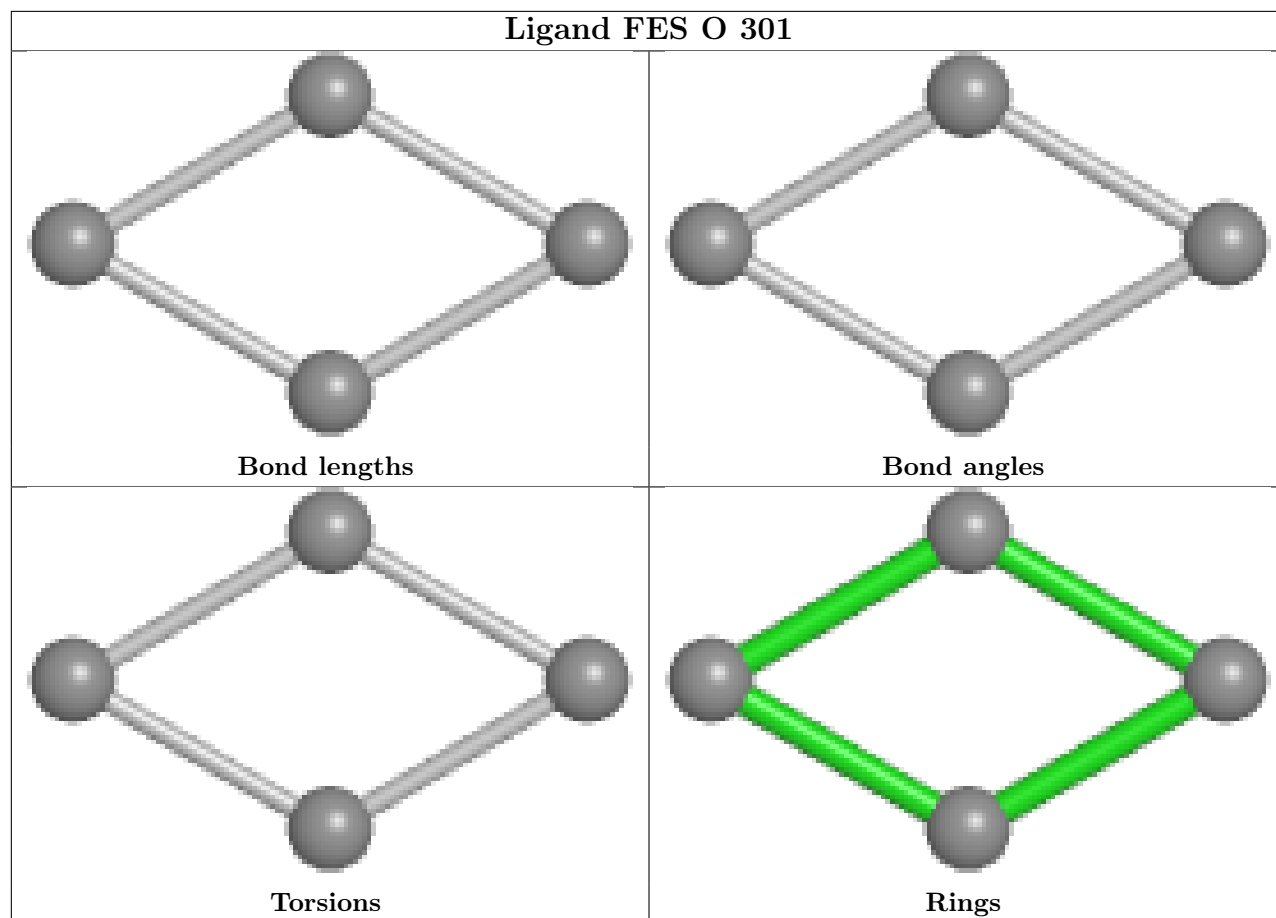












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

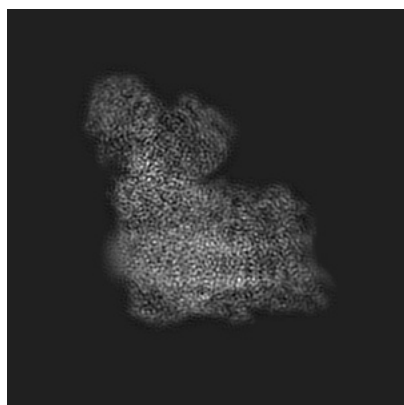
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32263. These allow visual inspection of the internal detail of the map and identification of artifacts.

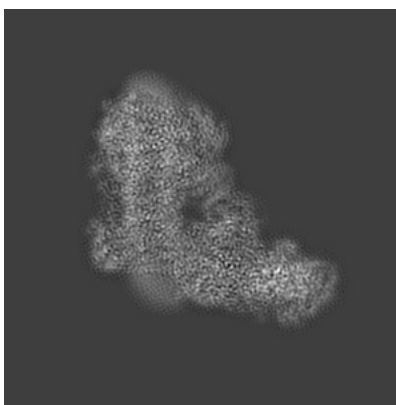
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

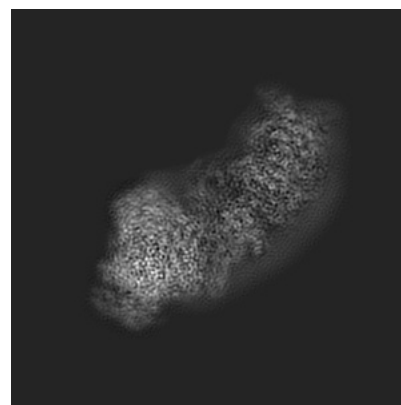
#### 6.1.1 Primary map



X



Y

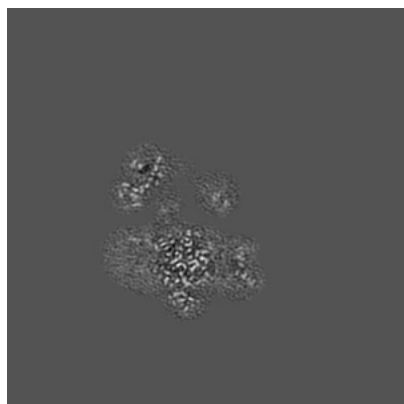


Z

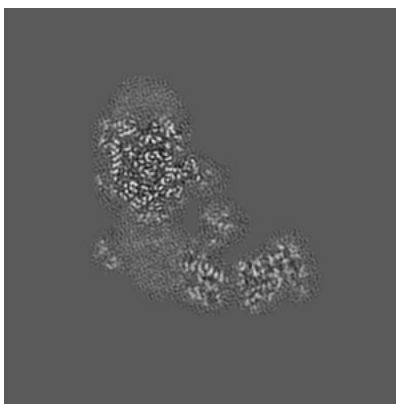
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

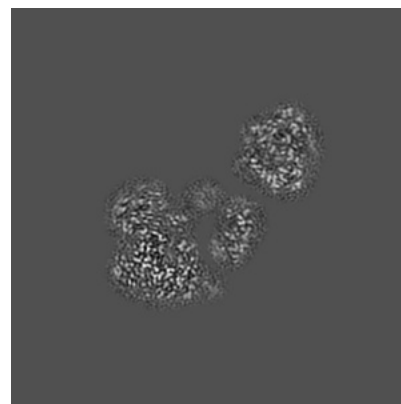
#### 6.2.1 Primary map



X Index: 155



Y Index: 155



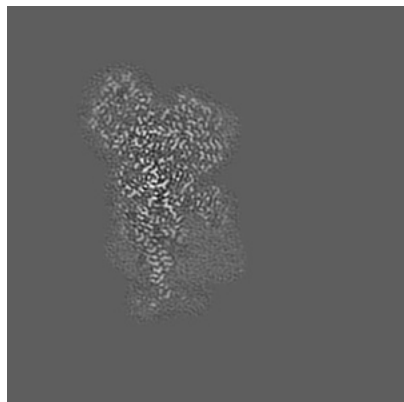
Z Index: 155



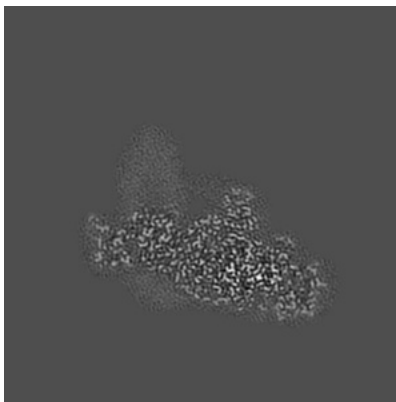
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

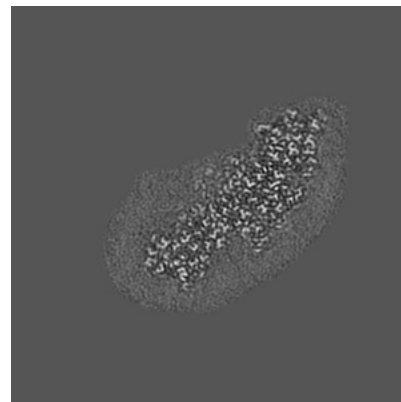
### 6.3.1 Primary map



X Index: 106



Y Index: 109

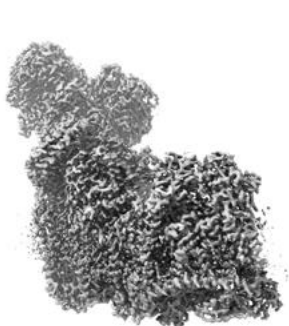


Z Index: 120

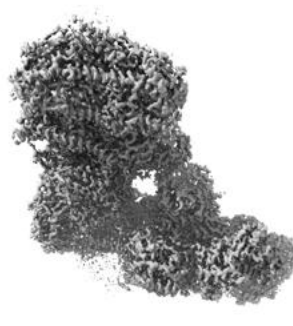
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

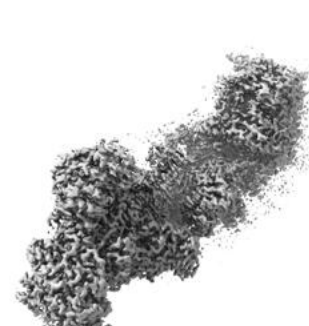
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0279. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

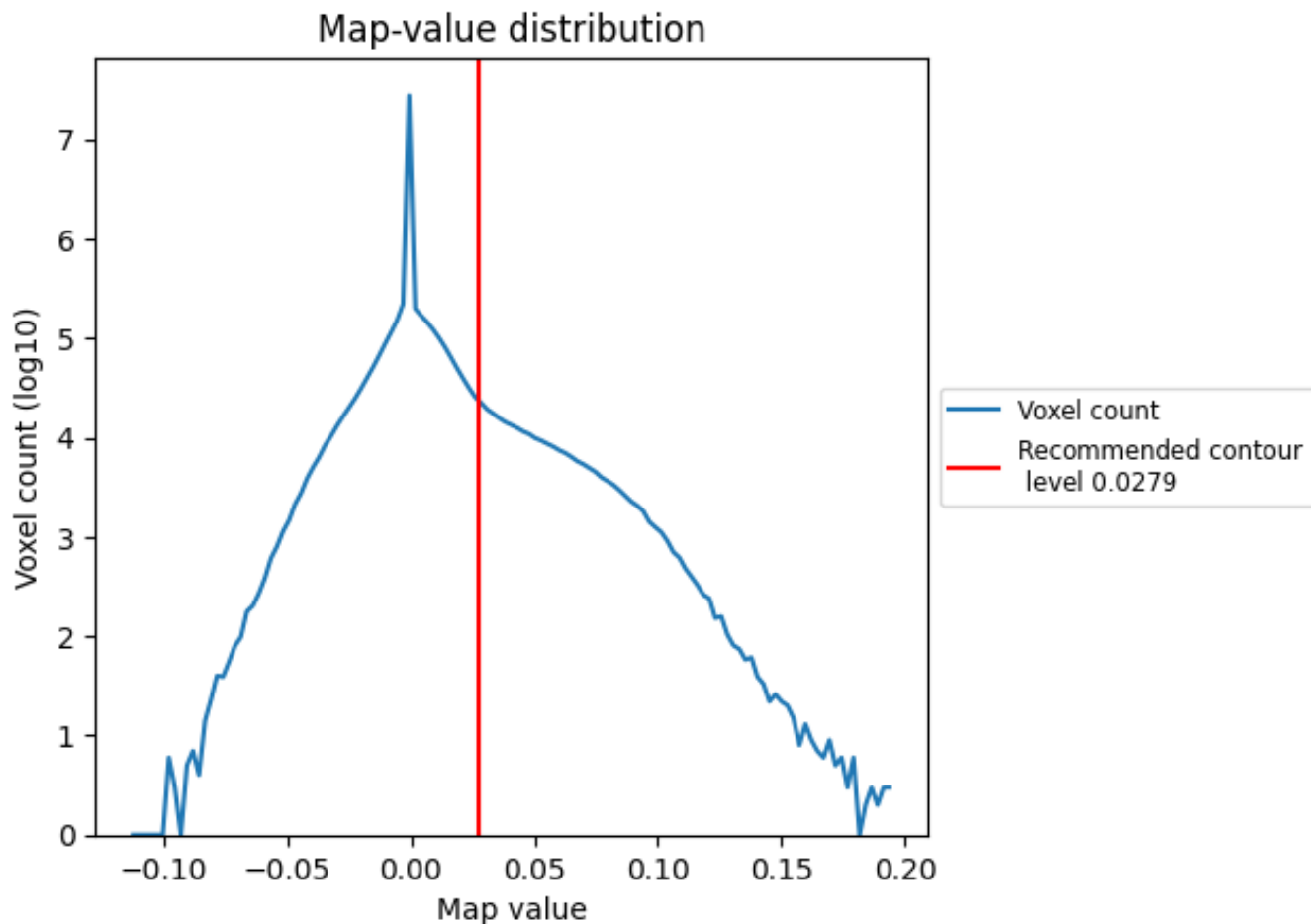
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

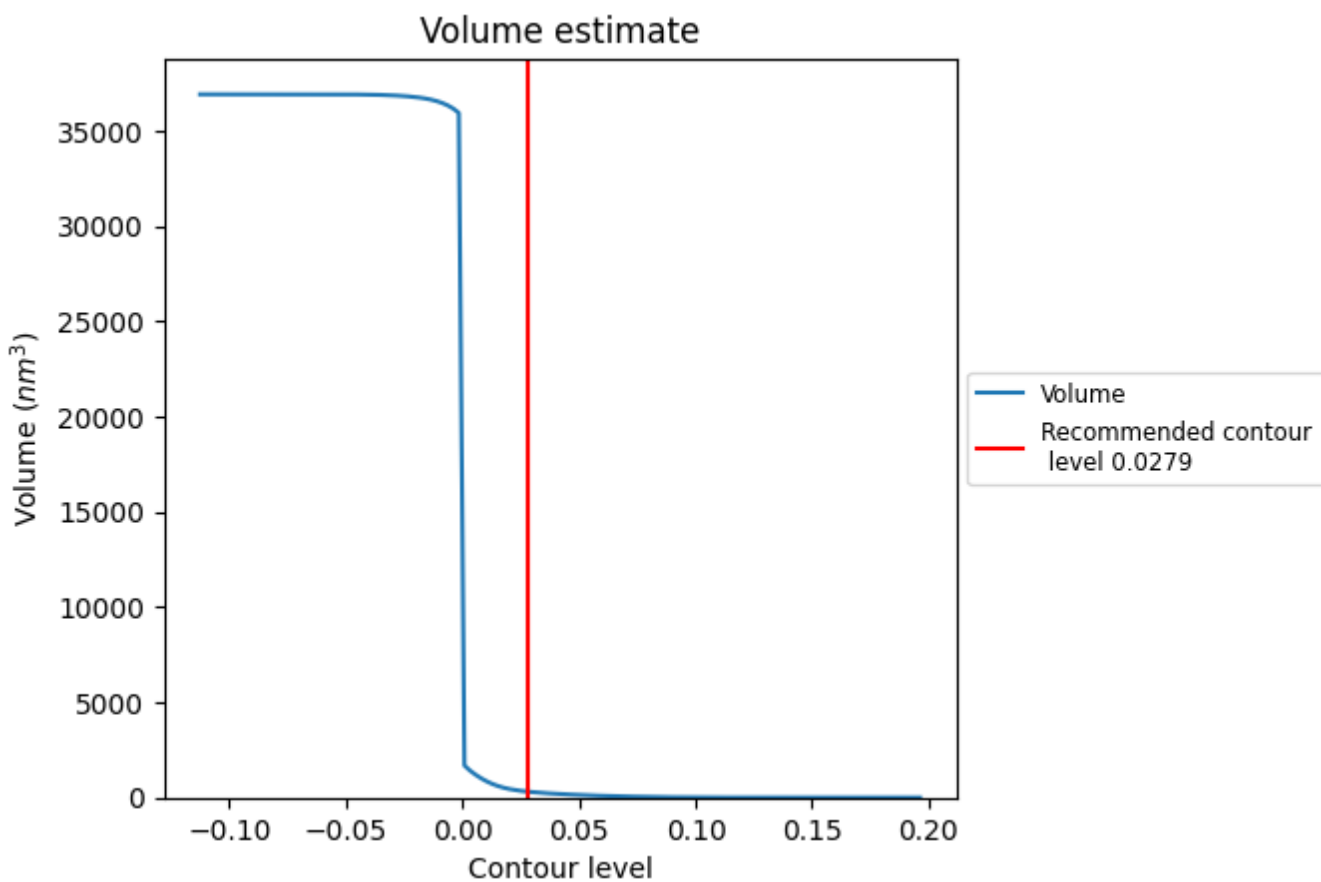
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

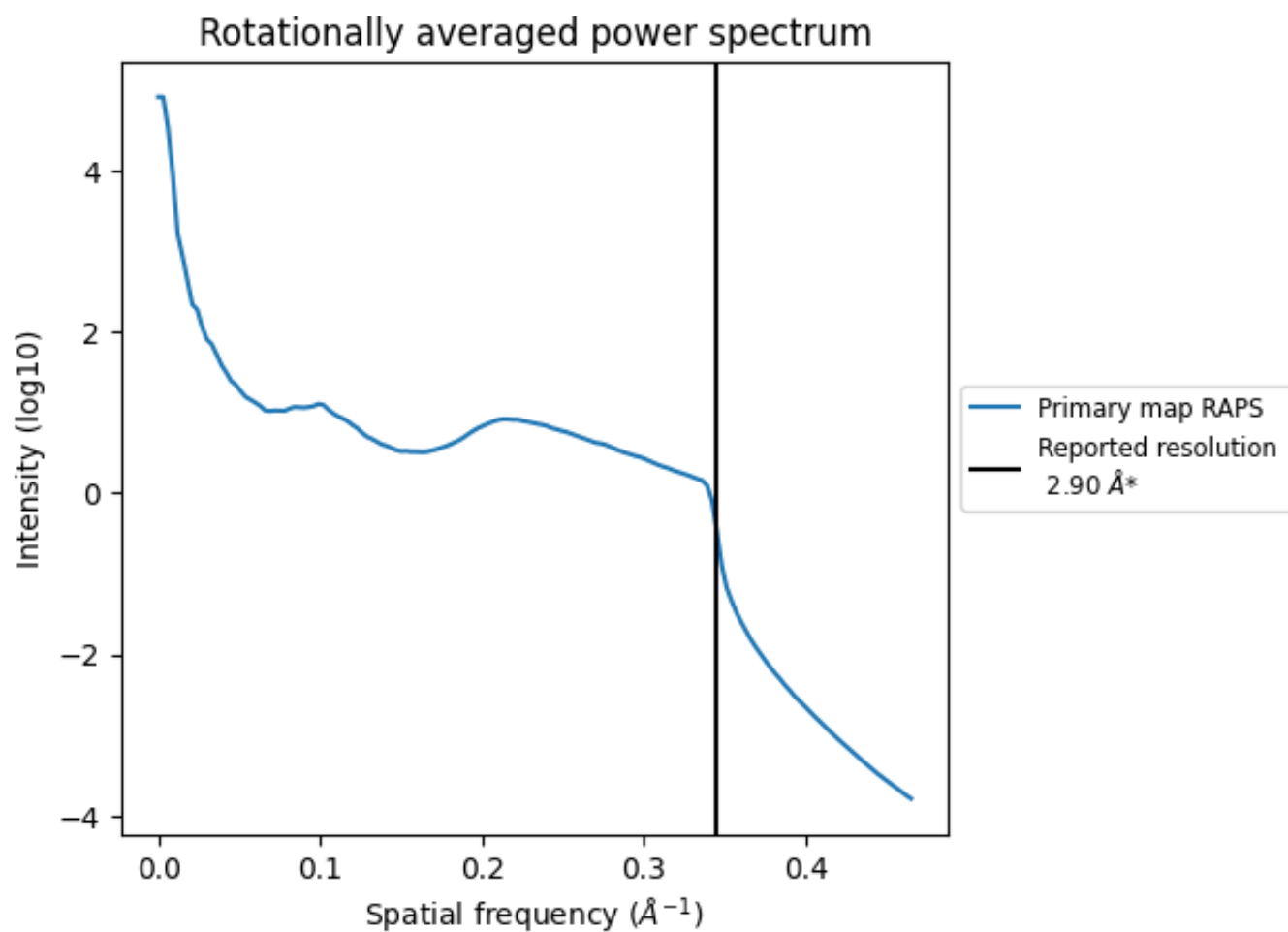
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm<sup>3</sup>; this corresponds to an approximate mass of 282 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.345 \text{\AA}^{-1}$

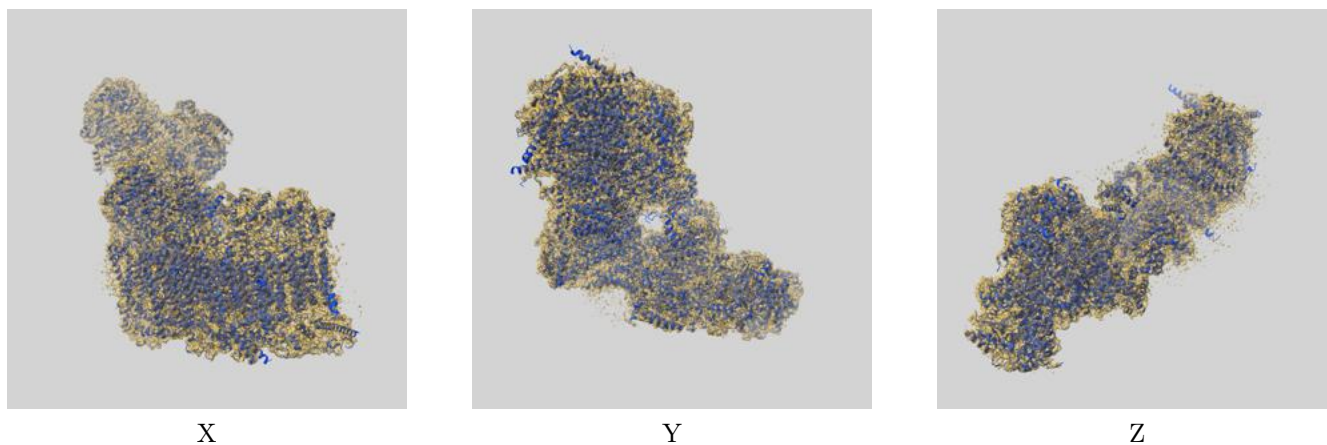
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

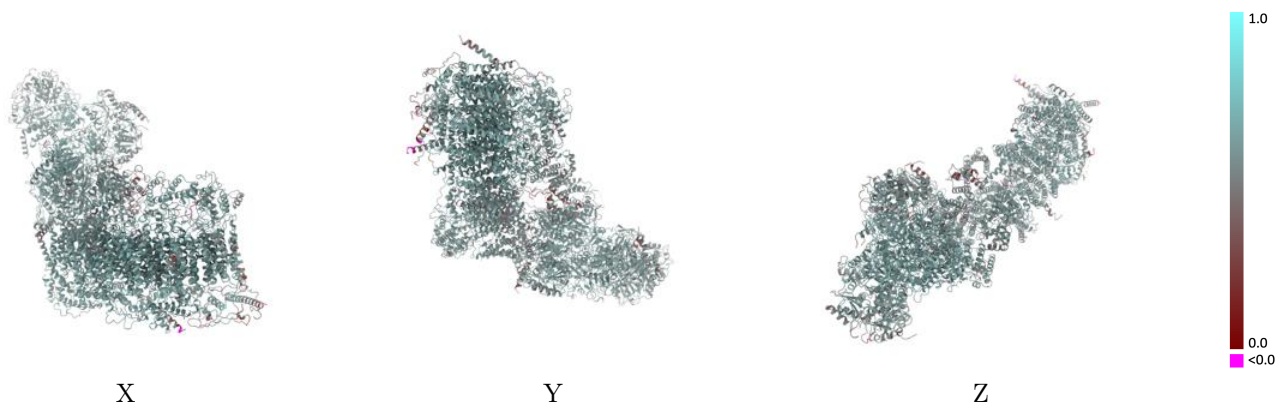
This section contains information regarding the fit between EMDB map EMD-32263 and PDB model 7W2K. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



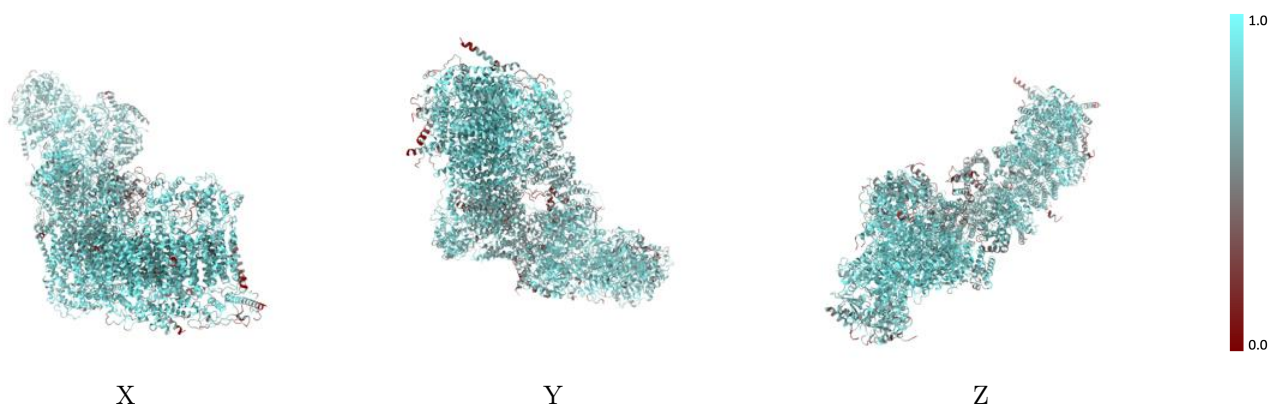
The images above show the 3D surface view of the map at the recommended contour level 0.0279 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

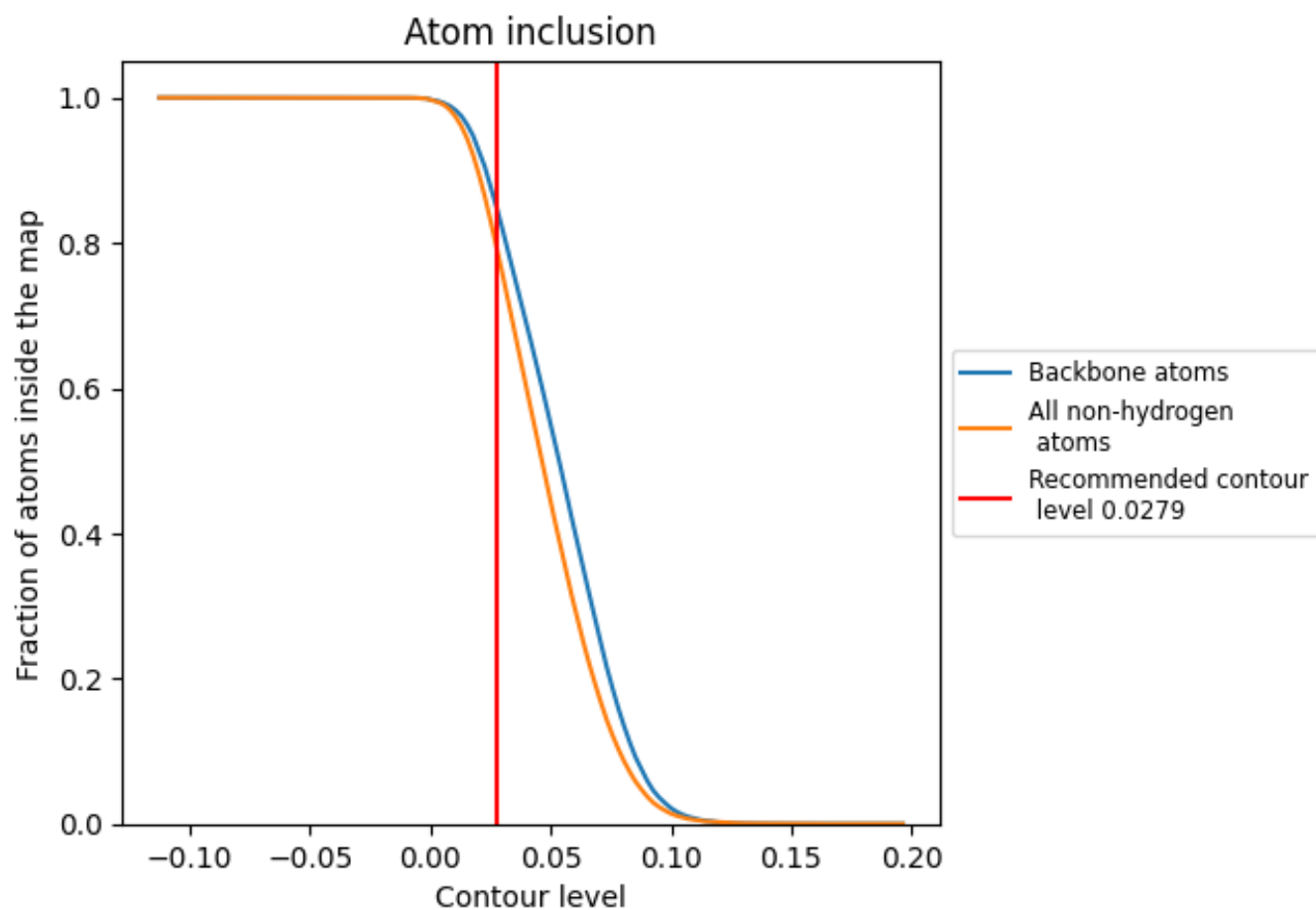
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0279).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.0279) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7888	 0.5830
A	 0.7719	 0.5670
B	 0.9181	 0.6290
C	 0.8490	 0.6110
E	 0.7431	 0.5680
F	 0.6398	 0.5080
G	 0.4404	 0.4210
H	 0.7531	 0.5670
I	 0.7466	 0.5830
J	 0.7203	 0.5600
K	 0.6890	 0.5540
L	 0.8300	 0.6020
M	 0.8201	 0.5880
N	 0.7648	 0.5930
O	 0.7330	 0.5490
P	 0.8995	 0.6210
Q	 0.8787	 0.6190
S	 0.8788	 0.6060
T	 0.8006	 0.5970
U	 0.7886	 0.5740
V	 0.5864	 0.5290
W	 0.8146	 0.5890
X	 0.7448	 0.5670
Y	 0.7025	 0.5440
Z	 0.5866	 0.4990
a	 0.8106	 0.6030
b	 0.6745	 0.5370
c	 0.7725	 0.5710
d	 0.7647	 0.5680
e	 0.7188	 0.5630
f	 0.6916	 0.5520
g	 0.8325	 0.6010
h	 0.8109	 0.5930
i	 0.8664	 0.6180
j	 0.6570	 0.5630



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
k	 0.7561	 0.5920
l	 0.8265	 0.6020
m	 0.7321	 0.5680
n	 0.6840	 0.5620
o	 0.7805	 0.5840
p	 0.7847	 0.5700
r	 0.8742	 0.6180
s	 0.8282	 0.5970
u	 0.8144	 0.5980
v	 0.6876	 0.5220
w	 0.7358	 0.5630