



wwPDB EM Validation Summary Report ⓘ

Jan 25, 2023 – 01:09 PM JST

PDB ID : 7W4C
EMDB ID : EMD-32300
Title : Active state CI from Q1-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-27
Resolution : 2.70 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

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:

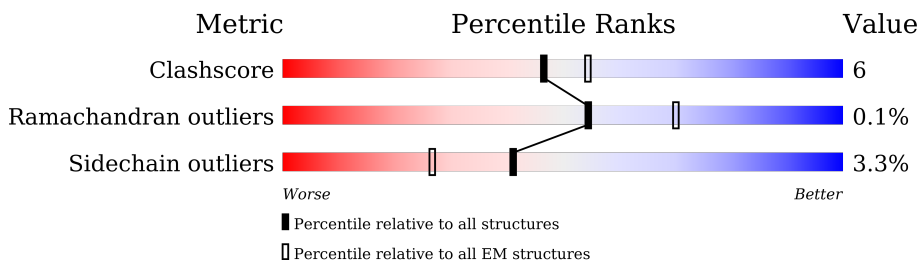
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.70 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)
Clashscore	158937	4297
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 ≥ 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	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	

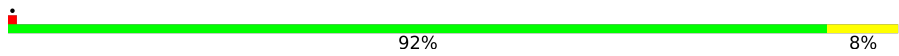
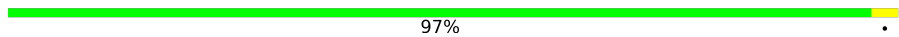
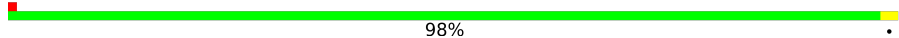
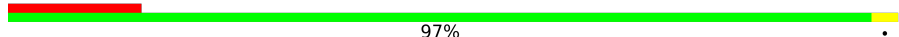
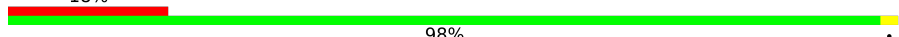
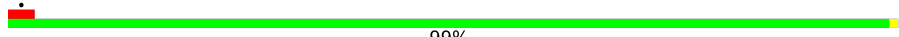
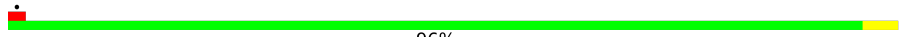



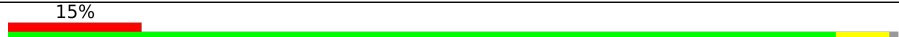

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	112	67% 20% 13%
9	J	342	85% 14%
10	K	43	19% 74% 26%
11	L	125	6% 89% 11%
12	M	690	85% 14%
13	N	144	88% 11%
14	O	217	8% 82% 17%
15	P	208	87% 13%
16	Q	430	84% 16%
17	S	70	83% 16%
18	T	96	6% 92% 7%
19	U	83	5% 88% 12%
20	V	140	83% 16%
21	W	142	6% 86% 14%
22	Y	70	10% 81% 13%
23	Z	84	13% 81% 12% 5%
24	a	140	96%
25	b	126	8% 75% 22%
26	c	156	97%
27	d	175	5% 95% 5%
28	e	107	9% 93%
29	f	49	29% 100%
30	g	122	95% 5%
31	h	105	6% 93% 7%
32	i	347	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	j	115	 92% 8%
34	k	98	 97%
35	l	606	 98%
36	m	175	 15% 97%
37	n	56	 18% 98%
38	o	128	 99%
39	p	178	 96%
40	r	459	 97%
41	s	318	 99%
42	u	171	 97%
43	v	125	 15% 93% 6%
44	w	320	 5% 98%

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
45	SF4	A	501	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68216 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	433	3330	2103	593	614	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	1248	794	227	213	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	971	619	179	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	687	432	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
			703	453	104	141	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
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	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
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- 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	1657	1054	280	313	10	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	430	3459	2212	594	629	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	566	364	103	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	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	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	1307	849	213	237	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	104	867	553	142	168	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	49	378	246	65	67	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	122	1005	653	174	172	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	863	548	161	148	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	2710	1782	420	462	46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1058	689	182	187		

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

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

- 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	3624	2406	572	608	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	318	2507	1678	385	423	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	1028	642	195	182	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

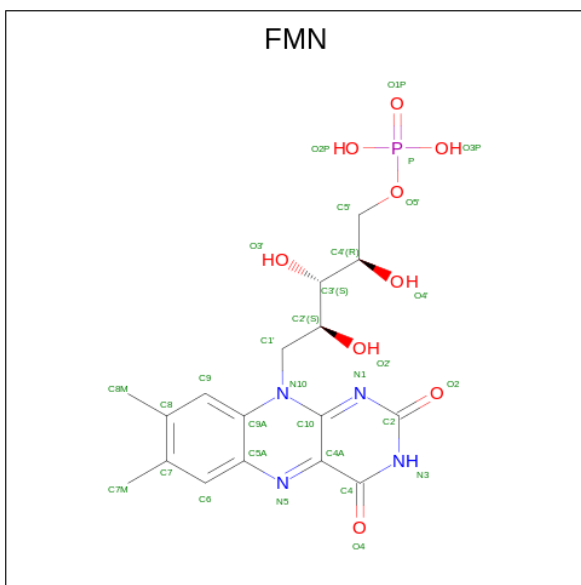
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2582	1643	438	491	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



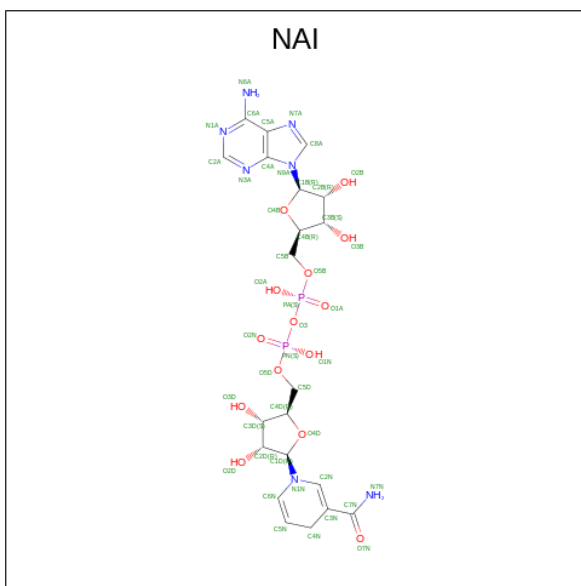
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



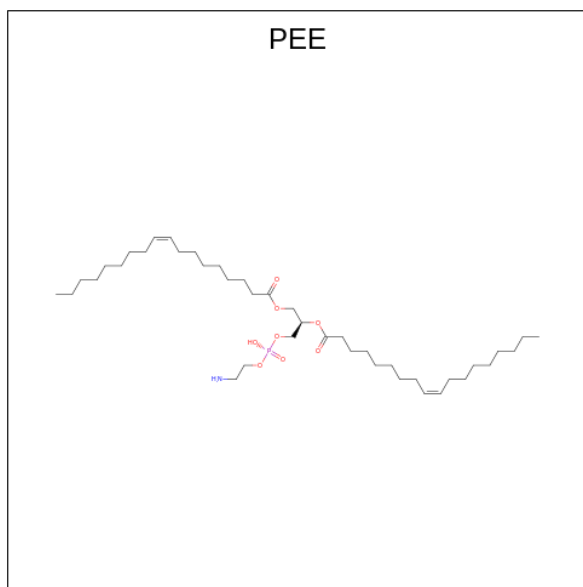
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (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: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



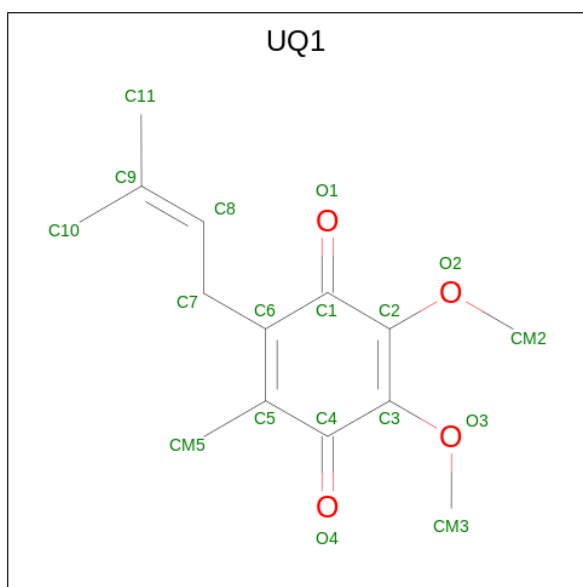
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
48	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
48	l	1	Total	C	N	O	P	0
			137	107	3	24	3	
48	s	1	Total	C	N	O	P	0
			41	31	1	8	1	

- 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-TRIOXANE-6,6,11-TRIOXANE (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



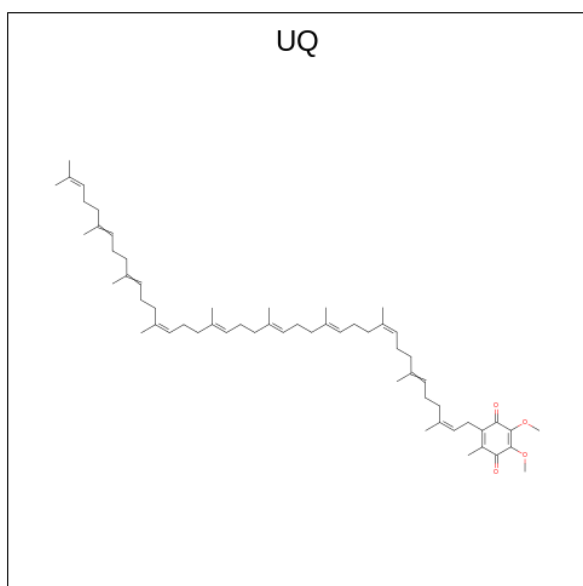
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	Total 52	42	1	8	1	0
49	J	1	Total 52	42	1	8	1	0
49	a	1	Total 52	42	1	8	1	0
49	e	1	Total 52	42	1	8	1	0
49	g	1	Total 52	42	1	8	1	0
49	j	1	Total 52	42	1	8	1	0
49	r	1	Total 52	42	1	8	1	0

- Molecule 50 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C₁₄H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			18	14	4	
50	Q	1	Total	C	O	0
			18	14	4	

- Molecule 51 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



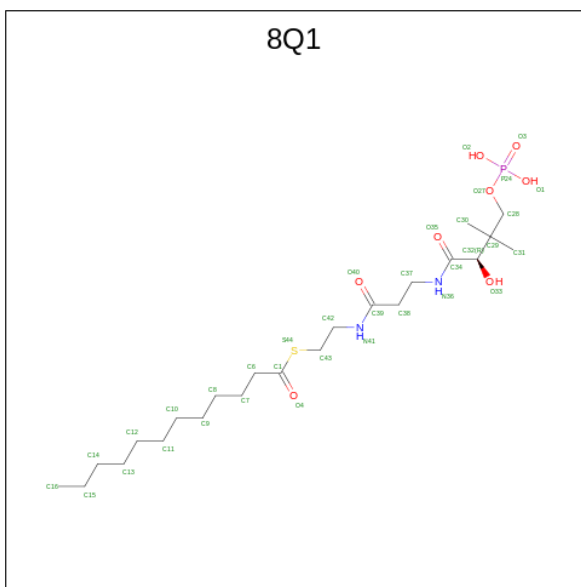
Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	C	O	0
			38	34	4	

Continued on next page...

Continued from previous page...

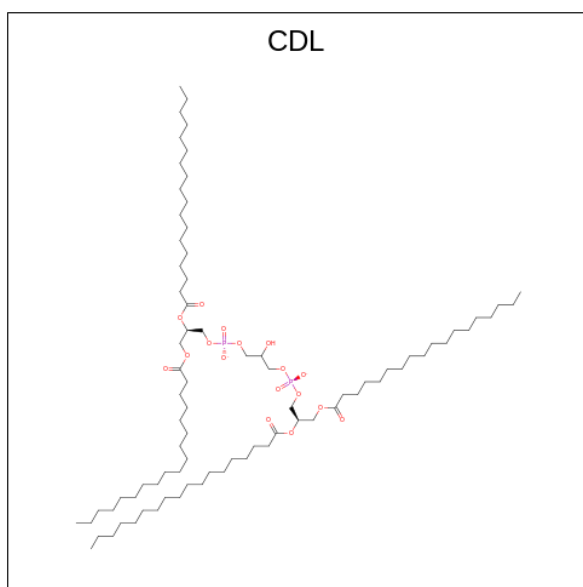
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	J	1	33	29	4	0

- Molecule 52 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



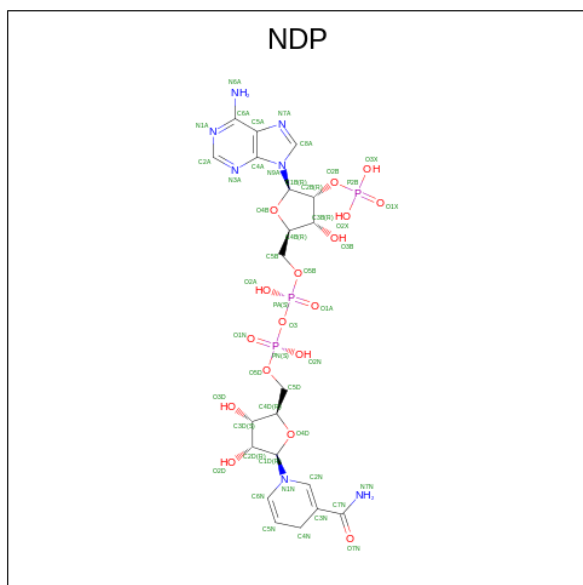
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
52	G	1	35	23	2	8	1	1	0
52	X	1	35	23	2	8	1	1	0

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



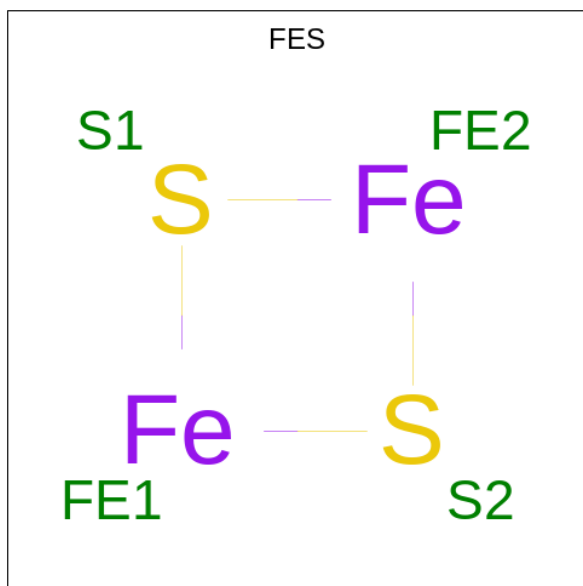
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	I	1	51	32	17	2	0
53	V	1	288	231	51	6	0
53	V	1	288	231	51	6	0
53	V	1	288	231	51	6	0
53	a	1	100	81	17	2	0
53	g	1	100	81	17	2	0
53	l	1	199	161	34	4	0
53	l	1	199	161	34	4	0
53	n	1	55	36	17	2	0
53	s	1	89	70	17	2	0

- Molecule 54 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	
54	J	1	48	21	7	17	3	0

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



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

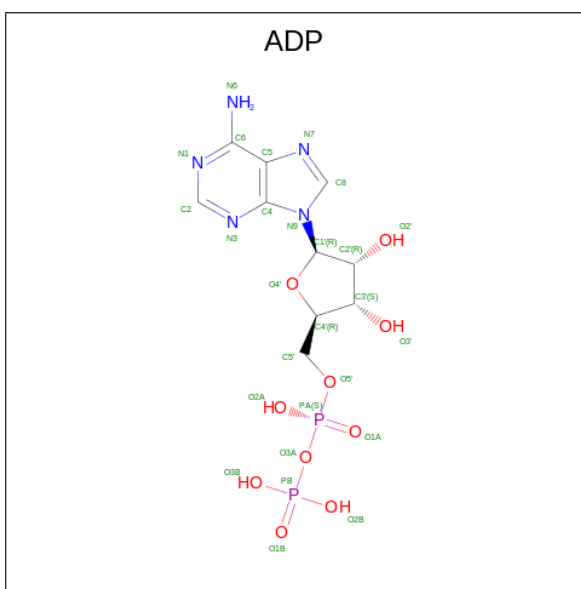
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

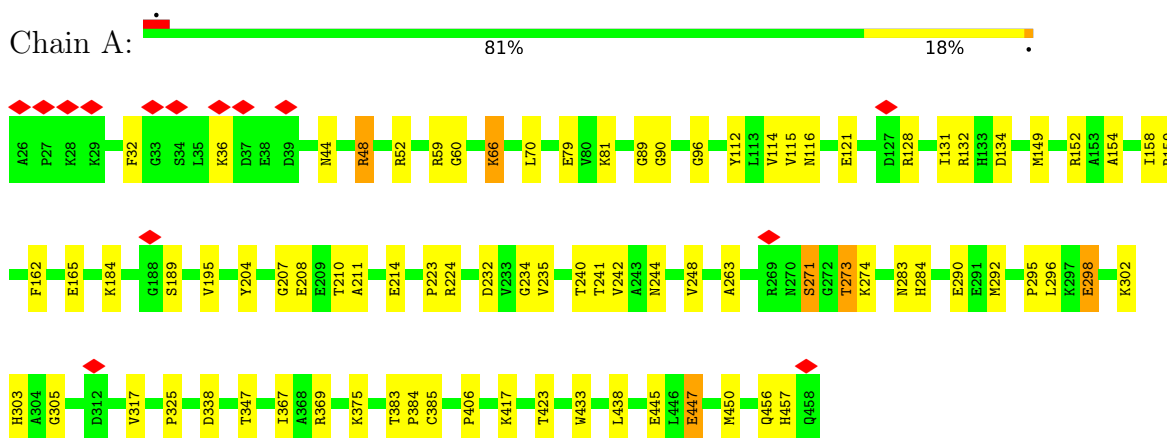


Mol	Chain	Residues	Atoms	AltConf
58	w	1	Total C N O P 27 10 5 10 2	0

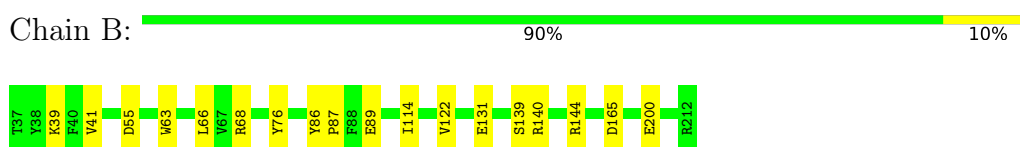
3 Residue-property plots [i](#)

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.

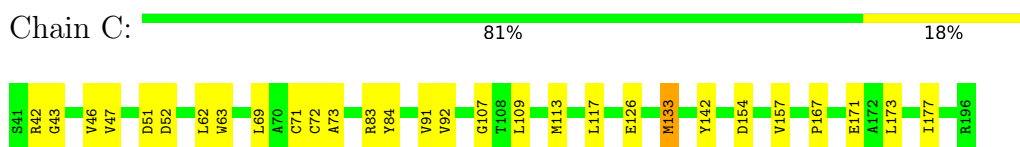
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



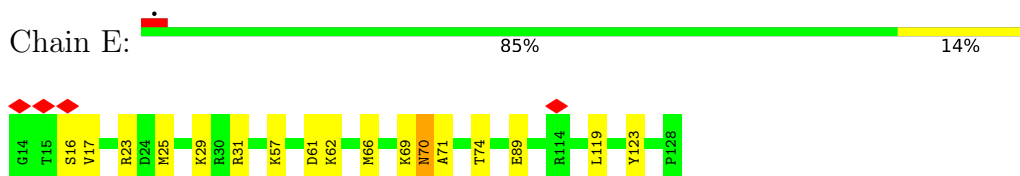
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



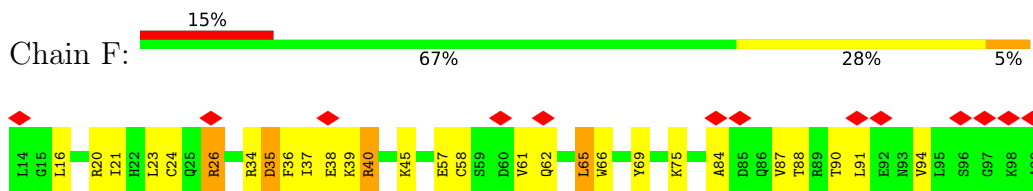
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



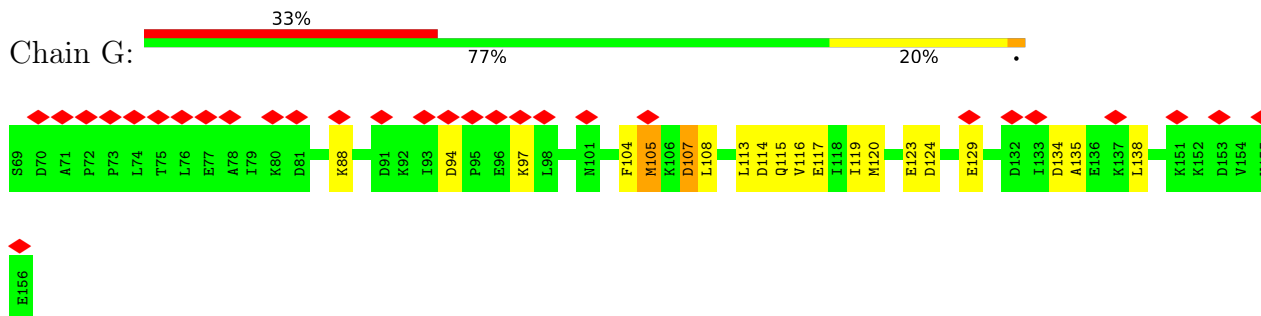
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



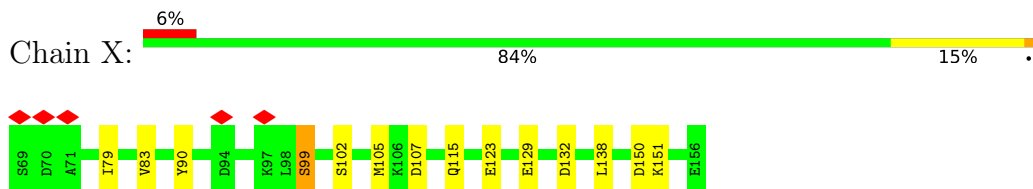
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



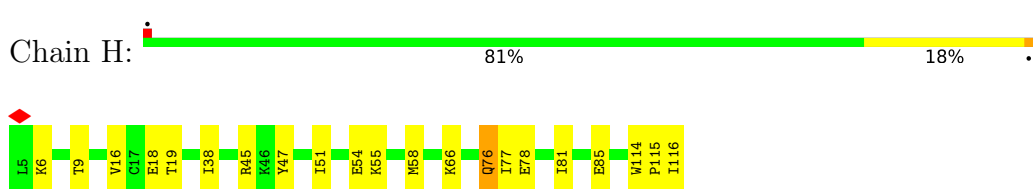
• Molecule 6: Acyl carrier protein



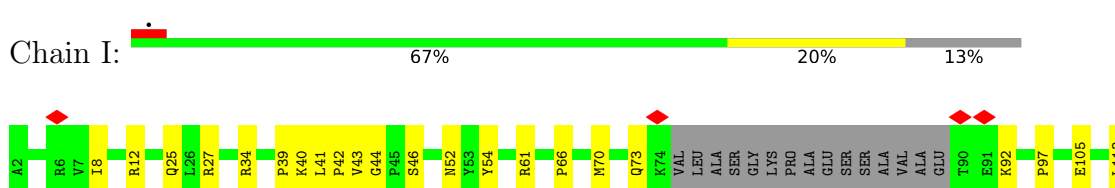
• Molecule 6: Acyl carrier protein



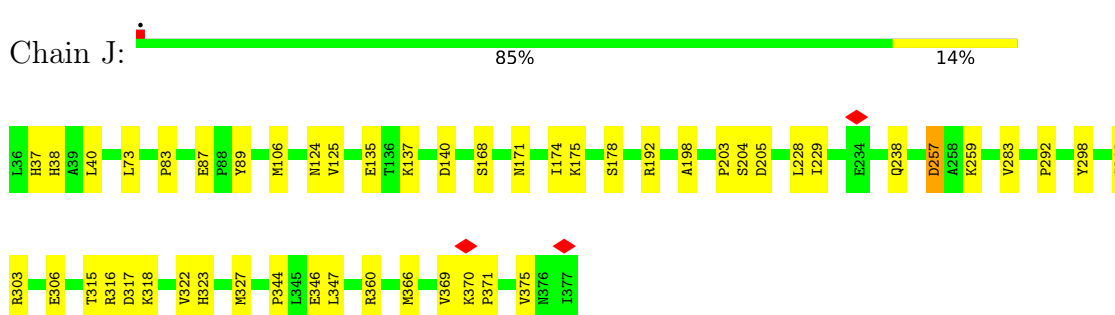
• Molecule 7: Complex I subunit B13



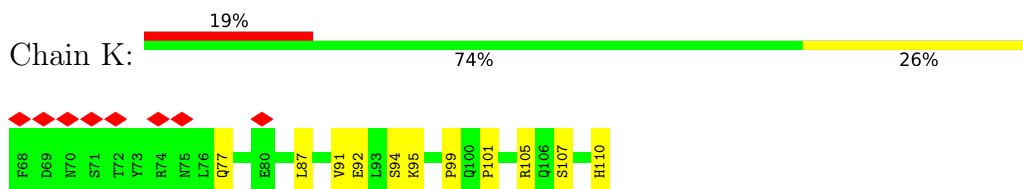
• Molecule 8: Complex I-B14.5a



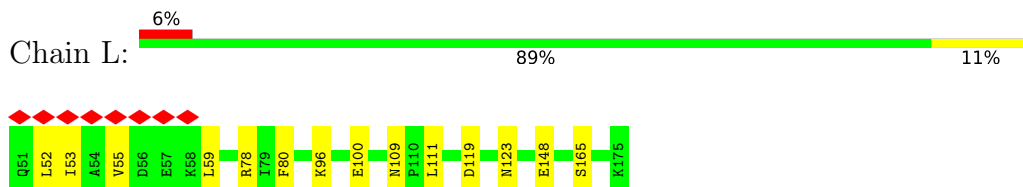
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



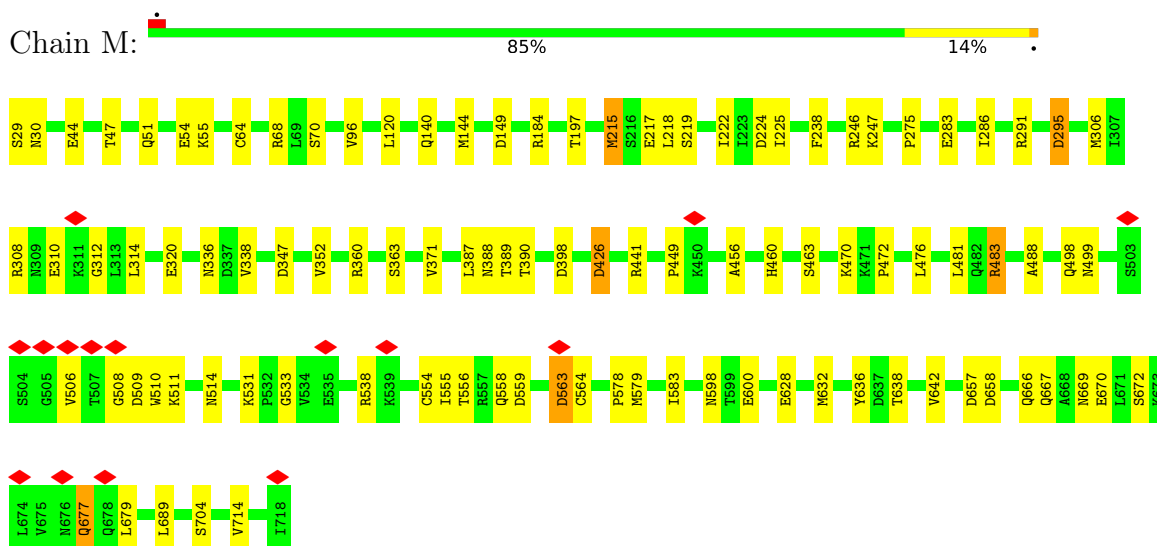
- Molecule 10: Complex I-9kD



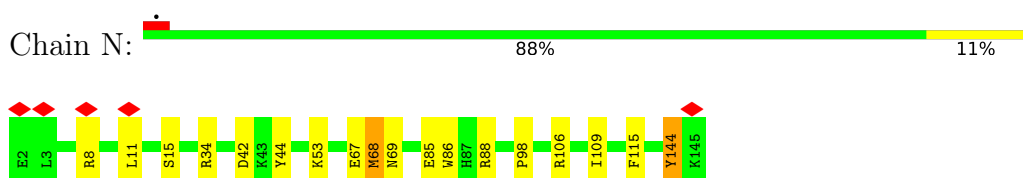
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



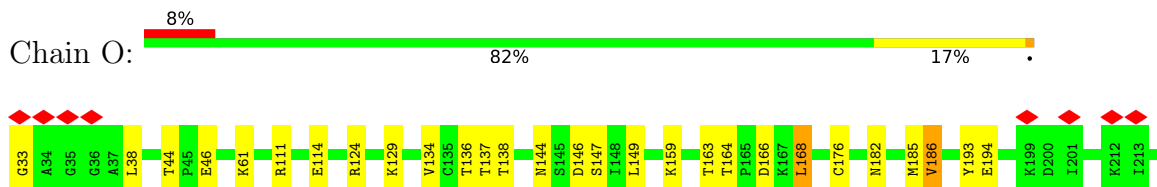
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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

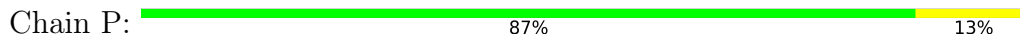


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

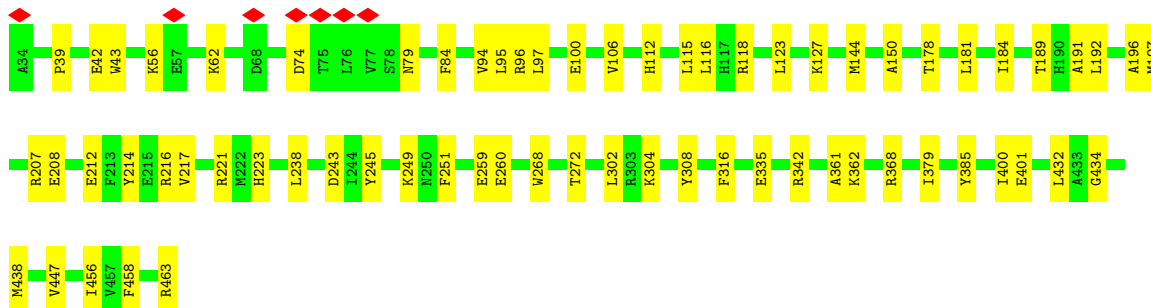
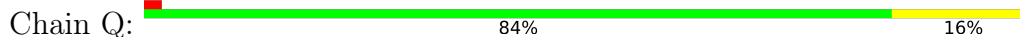




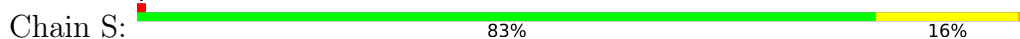
- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD



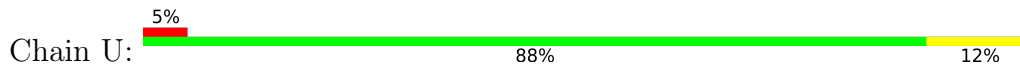
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1




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

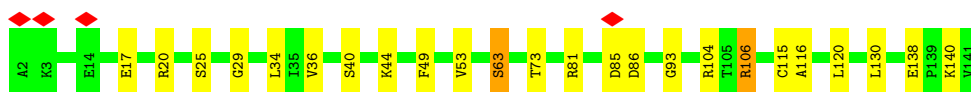


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3




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

Chain V:  83% 16%




- Molecule 21: Complex I-B16.6

Chain W:  6% 86% 14%




- Molecule 22: Complex I-AGGG

Chain Y:  10% 81% 13%



- Molecule 23: Complex I-B12

Chain Z:  13% 81% 12% 5%




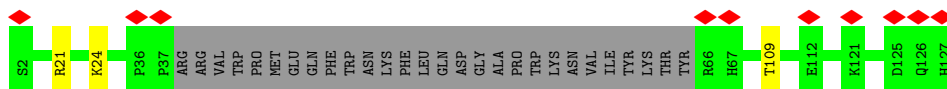
- Molecule 24: Complex I-SGDH

Chain a:  96%



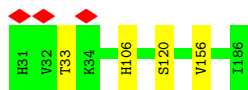
- Molecule 25: Complex I-B17

Chain b:  8% 75% 22%

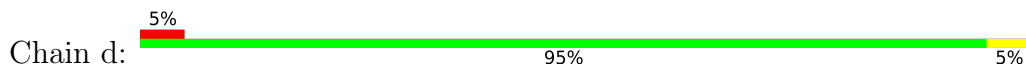


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

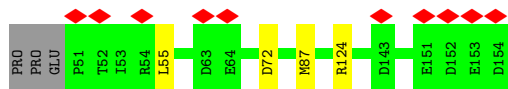
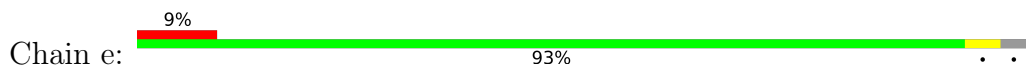
Chain c:  97%



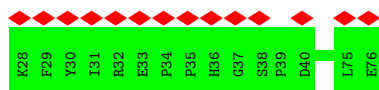
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



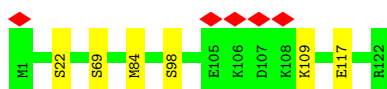
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



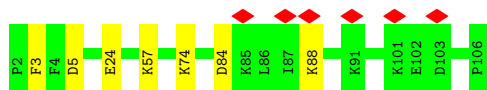
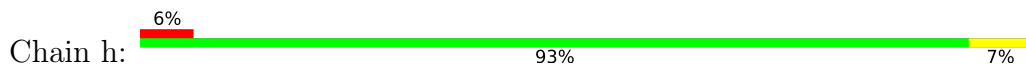
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



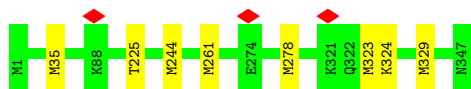
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



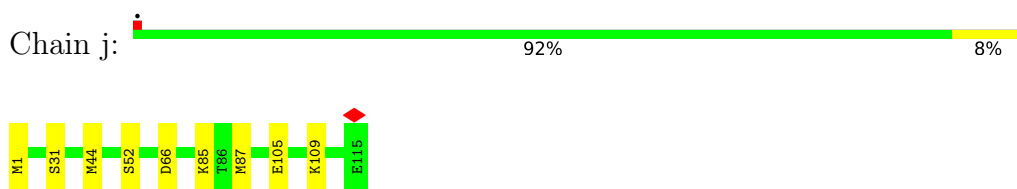
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



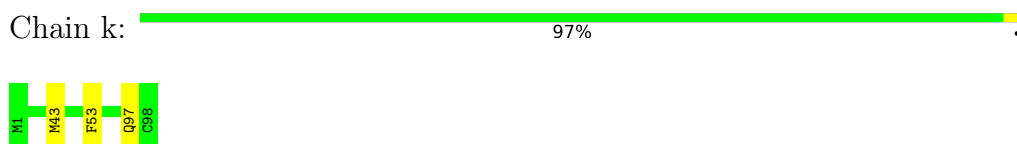
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



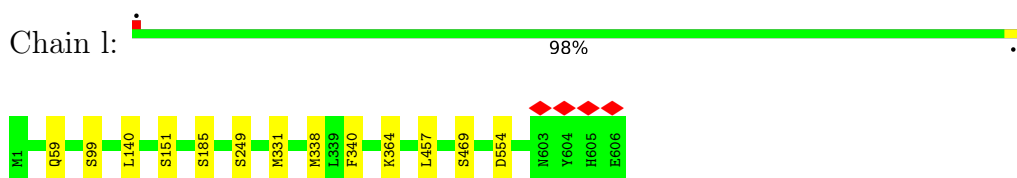
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



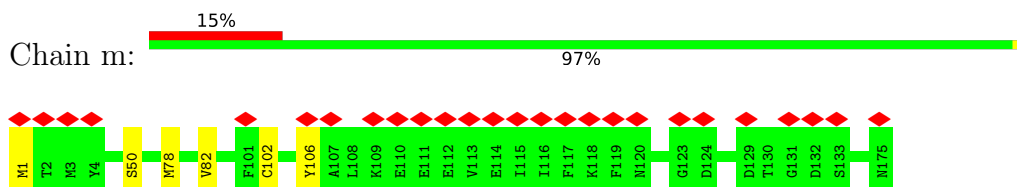
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



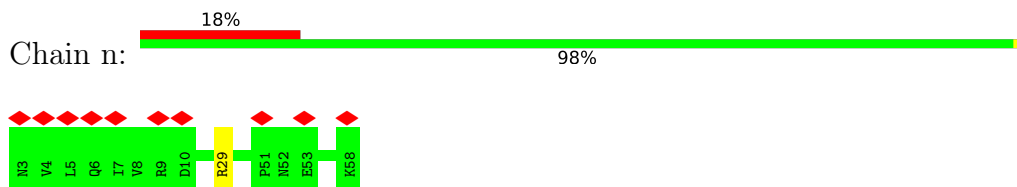
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



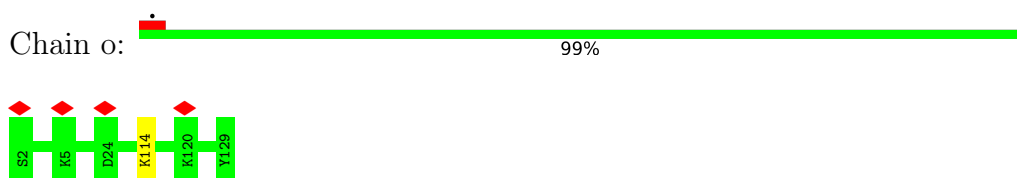
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



- 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





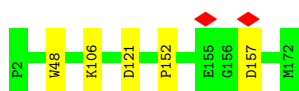
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



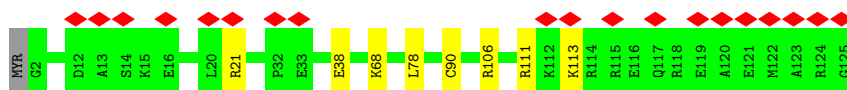
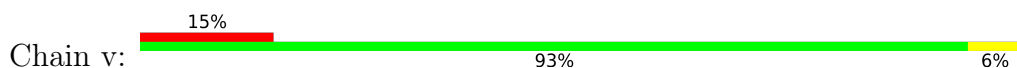
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92672	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	0.218	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0302	Depositor
Map size (\AA)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0979, 1.0979, 1.0979	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: 2MR, NAI, SF4, PLX, ZN, MG, NDP, PEE, UQ1, CDL, FES, UQ, ADP, FMN, 8Q1

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	0.25	0/3406	0.50	0/4603
2	B	0.26	0/1443	0.52	0/1952
3	C	0.25	0/1279	0.51	0/1730
4	E	0.25	0/995	0.49	0/1340
5	F	0.25	0/698	0.58	0/940
6	G	0.25	0/705	0.47	1/956 (0.1%)
6	X	0.24	0/715	0.41	0/967
7	H	0.25	0/929	0.46	0/1258
8	I	0.25	0/798	0.56	1/1079 (0.1%)
9	J	0.25	0/2828	0.48	0/3834
10	K	0.27	0/377	0.54	0/509
11	L	0.24	0/1039	0.49	0/1403
12	M	0.25	0/5384	0.50	1/7295 (0.0%)
13	N	0.25	0/1245	0.51	0/1694
14	O	0.25	0/1696	0.47	0/2310
15	P	0.26	0/1789	0.51	0/2436
16	Q	0.27	0/3538	0.50	0/4796
17	S	0.25	0/581	0.48	0/781
18	T	0.27	0/755	0.53	0/1018
19	U	0.25	0/664	0.44	0/912
20	V	0.25	0/1042	0.45	0/1411
21	W	0.26	0/1192	0.50	0/1610
22	Y	0.28	0/610	0.56	1/836 (0.1%)
23	Z	0.26	0/660	0.45	0/892
24	a	0.27	0/1184	0.47	0/1603
25	b	0.26	0/844	0.51	0/1149
26	c	0.27	0/1363	0.53	0/1865
27	d	0.26	0/1494	0.50	0/2015
28	e	0.25	0/891	0.49	0/1210
29	f	0.24	0/386	0.43	0/523
30	g	0.27	0/1036	0.48	0/1401
31	h	0.24	0/885	0.52	0/1185

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.25	0/2773	0.44	0/3768
33	j	0.25	0/938	0.45	0/1281
34	k	0.26	0/759	0.43	0/1029
35	l	0.26	0/4947	0.45	0/6728
36	m	0.27	0/1325	0.46	0/1800
37	n	0.24	0/491	0.51	0/663
38	o	0.26	0/1088	0.50	0/1476
39	p	0.25	0/1590	0.51	0/2155
40	r	0.25	0/3715	0.45	0/5067
41	s	0.27	0/2580	0.45	0/3528
42	u	0.26	0/1436	0.48	0/1938
43	v	0.26	0/1052	0.55	0/1411
44	w	0.26	0/2642	0.49	0/3580
All	All	0.26	0/67787	0.49	4/91937 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	70	MET	CB-CG-SD	5.96	130.27	112.40
12	M	563	ASP	CB-CG-OD1	5.74	123.47	118.30
22	Y	88	ASP	CB-CG-OD1	5.24	123.01	118.30
6	G	124	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	59	0
2	B	1412	0	1363	15	0
3	C	1248	0	1254	19	0
4	E	971	0	975	20	0
5	F	687	0	700	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	693	0	671	12	0
6	X	703	0	693	6	0
7	H	910	0	950	16	0
8	I	780	0	808	14	0
9	J	2751	0	2773	27	0
10	K	366	0	338	7	0
11	L	1016	0	1016	8	0
12	M	5296	0	5326	60	0
13	N	1204	0	1162	12	0
14	O	1657	0	1651	34	0
15	P	1738	0	1693	16	0
16	Q	3459	0	3396	42	0
17	S	566	0	561	6	0
18	T	741	0	702	4	0
19	U	643	0	642	7	0
20	V	1021	0	1025	14	0
21	W	1161	0	1144	12	0
22	Y	584	0	529	7	0
23	Z	641	0	620	10	0
24	a	1151	0	1164	0	0
25	b	819	0	835	0	0
26	c	1307	0	1200	0	0
27	d	1461	0	1429	0	0
28	e	867	0	817	0	0
29	f	378	0	356	0	0
30	g	1005	0	999	0	0
31	h	863	0	867	0	0
32	i	2710	0	2874	0	0
33	j	914	0	951	0	0
34	k	748	0	799	0	0
35	l	4816	0	4955	0	0
36	m	1292	0	1261	0	0
37	n	479	0	486	0	0
38	o	1058	0	1068	0	0
39	p	1534	0	1470	0	0
40	r	3624	0	3832	0	0
41	s	2507	0	2604	0	0
42	u	1398	0	1374	0	0
43	v	1028	0	982	0	0
44	w	2582	0	2531	0	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	27	5	0
48	B	51	0	82	3	0
48	C	47	0	71	2	0
48	U	51	0	82	3	0
48	V	51	0	82	3	0
48	W	41	0	59	1	0
48	i	47	0	71	0	0
48	l	137	0	205	0	0
48	s	41	0	59	0	0
49	C	52	0	88	2	0
49	J	52	0	88	2	0
49	a	52	0	88	0	0
49	e	52	0	88	0	0
49	g	52	0	88	0	0
49	j	52	0	88	0	0
49	r	52	0	88	0	0
50	C	18	0	18	3	0
50	Q	18	0	18	1	0
51	C	38	0	47	5	0
51	J	33	0	39	1	0
52	G	35	0	0	11	0
52	X	35	0	0	0	0
53	I	51	0	46	0	0
53	V	288	0	435	11	0
53	a	100	0	156	0	0
53	g	100	0	156	0	0
53	l	199	0	307	0	0
53	n	55	0	54	0	0
53	s	89	0	125	0	0
54	J	48	0	25	1	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	0	0
All	All	68216	0	68948	420	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 6.

The worst 5 of 420 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)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.26
54:J:401:NDP:O4D	54:J:401:NDP:C4D	1.68	1.13
4:E:70:ASN:HD21	52:G:201:8Q1:C43	1.87	0.86
1:A:60:GLY:HA2	14:O:241:PRO:HB3	1.59	0.84
13:N:68:MET:HG3	13:N:69:ASN:H	1.42	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	417 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	32
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	17	40
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	41	66
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	670 (97%)	18 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29	54
15	P	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
16	Q	427/430 (99%)	414 (97%)	13 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	65/70 (93%)	60 (92%)	5 (8%)	0	100	100
23	Z	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
24	a	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	147 (96%)	6 (4%)	1 (1%)	25	50
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/107 (95%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
32	i	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
33	j	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	l	604/606 (100%)	584 (97%)	20 (3%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	25	50
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	66
42	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	25	50
43	v	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8175/8326 (98%)	7890 (96%)	277 (3%)	8 (0%)	54 78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	77	ILE
14	O	243	PHE
41	s	208	VAL
9	J	38	HIS
26	c	106	HIS

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	346/346 (100%)	332 (96%)	14 (4%)	31 60
2	B	151/151 (100%)	148 (98%)	3 (2%)	55 81
3	C	132/132 (100%)	128 (97%)	4 (3%)	41 70
4	E	107/107 (100%)	103 (96%)	4 (4%)	34 63
5	F	75/76 (99%)	70 (93%)	5 (7%)	16 37
6	G	76/81 (94%)	72 (95%)	4 (5%)	22 48
6	X	79/81 (98%)	74 (94%)	5 (6%)	18 40
7	H	99/99 (100%)	98 (99%)	1 (1%)	76 91
8	I	87/97 (90%)	83 (95%)	4 (5%)	27 54
9	J	296/296 (100%)	289 (98%)	7 (2%)	49 77
10	K	42/42 (100%)	40 (95%)	2 (5%)	25 53
11	L	113/113 (100%)	110 (97%)	3 (3%)	44 74
12	M	580/580 (100%)	561 (97%)	19 (3%)	38 67
13	N	130/130 (100%)	125 (96%)	5 (4%)	33 62
14	O	180/183 (98%)	172 (96%)	8 (4%)	28 56
15	P	190/190 (100%)	188 (99%)	2 (1%)	73 90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	370/370 (100%)	365 (99%)	5 (1%)	67	86
17	S	57/58 (98%)	54 (95%)	3 (5%)	22	48
18	T	79/79 (100%)	75 (95%)	4 (5%)	24	50
19	U	69/69 (100%)	68 (99%)	1 (1%)	67	86
20	V	101/101 (100%)	96 (95%)	5 (5%)	24	51
21	W	121/123 (98%)	115 (95%)	6 (5%)	24	51
22	Y	62/63 (98%)	61 (98%)	1 (2%)	62	85
23	Z	62/65 (95%)	58 (94%)	4 (6%)	17	38
24	a	121/122 (99%)	118 (98%)	3 (2%)	47	76
25	b	90/119 (76%)	87 (97%)	3 (3%)	38	67
26	c	139/141 (99%)	136 (98%)	3 (2%)	52	79
27	d	155/155 (100%)	146 (94%)	9 (6%)	20	43
28	e	96/99 (97%)	92 (96%)	4 (4%)	30	58
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	102 (94%)	6 (6%)	21	45
31	h	92/93 (99%)	85 (92%)	7 (8%)	13	30
32	i	311/311 (100%)	303 (97%)	8 (3%)	46	75
33	j	100/100 (100%)	91 (91%)	9 (9%)	9	22
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	65
35	l	540/540 (100%)	527 (98%)	13 (2%)	49	77
36	m	129/141 (92%)	123 (95%)	6 (5%)	26	54
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	82
38	o	112/113 (99%)	111 (99%)	1 (1%)	78	92
39	p	159/159 (100%)	152 (96%)	7 (4%)	28	56
40	r	409/410 (100%)	397 (97%)	12 (3%)	42	71
41	s	274/275 (100%)	272 (99%)	2 (1%)	84	94
42	u	153/153 (100%)	149 (97%)	4 (3%)	46	75
43	v	104/111 (94%)	96 (92%)	8 (8%)	13	30
44	w	281/283 (99%)	273 (97%)	8 (3%)	43	73
All	All	7151/7249 (99%)	6915 (97%)	236 (3%)	41	67

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Z	14	MET
43	v	38	GLU
30	g	84	MET
42	u	157	ASP
39	p	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
43	v	85	HIS
35	l	200	GLN
21	W	61	GLN
12	M	30	ASN
27	d	107	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.97	1 (10%)	5,13,15	5.97	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	12.26	130.72	119.48
16	Q	118	2MR	CD-NE-CZ	4.09	131.07	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.16	130.85	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 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.23	8 (16%)
48	PEE	l	704	-	50,50,50	1.16	6 (12%)	53,55,55	0.93	2 (3%)
53	CDL	V	203	-	99,99,99	1.09	8 (8%)	105,111,111	0.88	4 (3%)
50	UQ1	C	304	-	18,18,18	2.39	7 (38%)	22,25,25	1.95	6 (27%)
47	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.31	7 (14%)
48	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
53	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
53	CDL	n	101	-	54,54,99	1.36	8 (14%)	60,66,111	1.11	4 (6%)
48	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	i	401	-	46,46,50	1.20	6 (13%)	49,51,55	1.02	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
53	CDL	l	702	-	98,98,99	0.92	4 (4%)	104,110,111	1.08	7 (6%)
54	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	1.95	6 (11%)
49	PLX	e	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.52	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
45	SF4	M	802	12	0,12,12	-	-	-	-	-
48	PEE	l	705	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
48	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
52	8Q1	G	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.74	6 (15%)
51	UQ	C	305	-	38,38,63	3.55	10 (26%)	46,49,79	2.83	17 (36%)
58	ADP	w	401	-	24,29,29	3.13	6 (25%)	29,45,45	1.41	3 (10%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
52	8Q1	X	201	-	31,34,34	1.71	6 (19%)	40,43,43	1.54	5 (12%)
48	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
51	UQ	J	402	-	33,33,63	3.45	8 (24%)	40,43,79	2.82	13 (32%)
49	PLX	r	501	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
53	CDL	l	703	-	99,99,99	1.09	8 (8%)	105,111,111	0.90	4 (3%)
49	PLX	j	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.64	1 (1%)
55	FES	M	803	12	0,4,4	-	-	-	-	-
53	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.86	4 (4%)
49	PLX	C	303	-	51,51,51	1.15	3 (5%)	55,59,59	0.60	1 (1%)
48	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.06	2 (4%)
53	CDL	g	202	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	V	204	-	93,93,99	1.12	8 (8%)	99,105,111	0.86	4 (4%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
49	PLX	J	403	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
53	CDL	s	402	-	88,88,99	1.14	8 (9%)	94,100,111	0.89	4 (4%)
53	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.13	4 (7%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)
50	UQ1	Q	501	-	18,18,18	2.32	6 (33%)	22,25,25	1.60	4 (18%)

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
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
48	PEE	l	704	-	-	29/54/54/54	-
53	CDL	V	203	-	-	54/110/110/110	-
50	UQ1	C	304	-	-	4/9/33/33	0/1/1/1
47	NAI	A	503	-	-	4/25/72/72	0/5/5/5
48	PEE	V	202	-	-	26/54/54/54	-
49	PLX	g	201	-	-	31/55/55/55	-
53	CDL	a	201	-	-	57/110/110/110	-
53	CDL	n	101	-	-	28/65/65/110	-
48	PEE	U	101	-	-	24/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	i	401	-	-	19/50/50/54	-
53	CDL	l	702	-	-	42/109/109/110	-
45	SF4	C	301	3	-	-	0/6/5/5
54	NDP	J	401	-	-	8/30/77/77	0/4/5/5
49	PLX	e	201	-	-	33/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	s	401	-	-	24/44/44/54	-
48	PEE	l	705	-	-	16/49/49/54	-
52	8Q1	G	201	-	-	11/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	UQ	C	305	-	-	11/33/57/87	0/1/1/1
58	ADP	w	401	-	-	5/12/32/32	0/3/3/3
48	PEE	B	303	-	-	26/54/54/54	-
52	8Q1	X	201	-	-	10/41/41/41	-
48	PEE	W	201	-	-	19/44/44/54	-
51	UQ	J	402	-	-	11/27/51/87	0/1/1/1
49	PLX	r	501	-	-	31/55/55/55	-
53	CDL	l	703	-	-	66/110/110/110	-
49	PLX	j	201	-	-	23/55/55/55	-
55	FES	M	803	12	-	-	0/1/1/1
53	CDL	V	201	-	-	58/104/104/110	-
49	PLX	C	303	-	-	25/55/55/55	-
48	PEE	l	701	-	-	18/43/43/54	-
53	CDL	g	202	-	-	58/110/110/110	-
45	SF4	A	501	1	-	-	0/6/5/5
53	CDL	V	204	-	-	51/104/104/110	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	a	202	-	-	31/55/55/55	-
49	PLX	J	403	-	-	32/55/55/55	-
55	FES	O	301	14	-	-	0/1/1/1
53	CDL	s	402	-	-	49/99/99/110	-
53	CDL	I	201	-	-	26/61/61/110	-
48	PEE	C	302	-	-	28/50/50/54	-
50	UQ1	Q	501	-	-	1/9/33/33	0/1/1/1

The worst 5 of 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.13	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.50	1.30	1.53
54	J	401	NDP	C3B-C2B	-12.96	1.24	1.52
54	J	401	NDP	C6N-C5N	12.38	1.55	1.33
54	J	401	NDP	O4D-C4D	10.65	1.68	1.45

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	402	UQ	C7-C8-C9	-8.31	112.95	126.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C	305	UQ	C7-C8-C9	-7.85	113.73	126.79
54	J	401	NDP	C3N-C2N-N1N	-7.71	112.10	123.10
54	J	401	NDP	C1D-N1N-C2N	-7.21	109.11	121.11
52	G	201	8Q1	C6-C1-S44	7.06	121.68	113.46

There are no chirality outliers.

5 of 996 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	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P

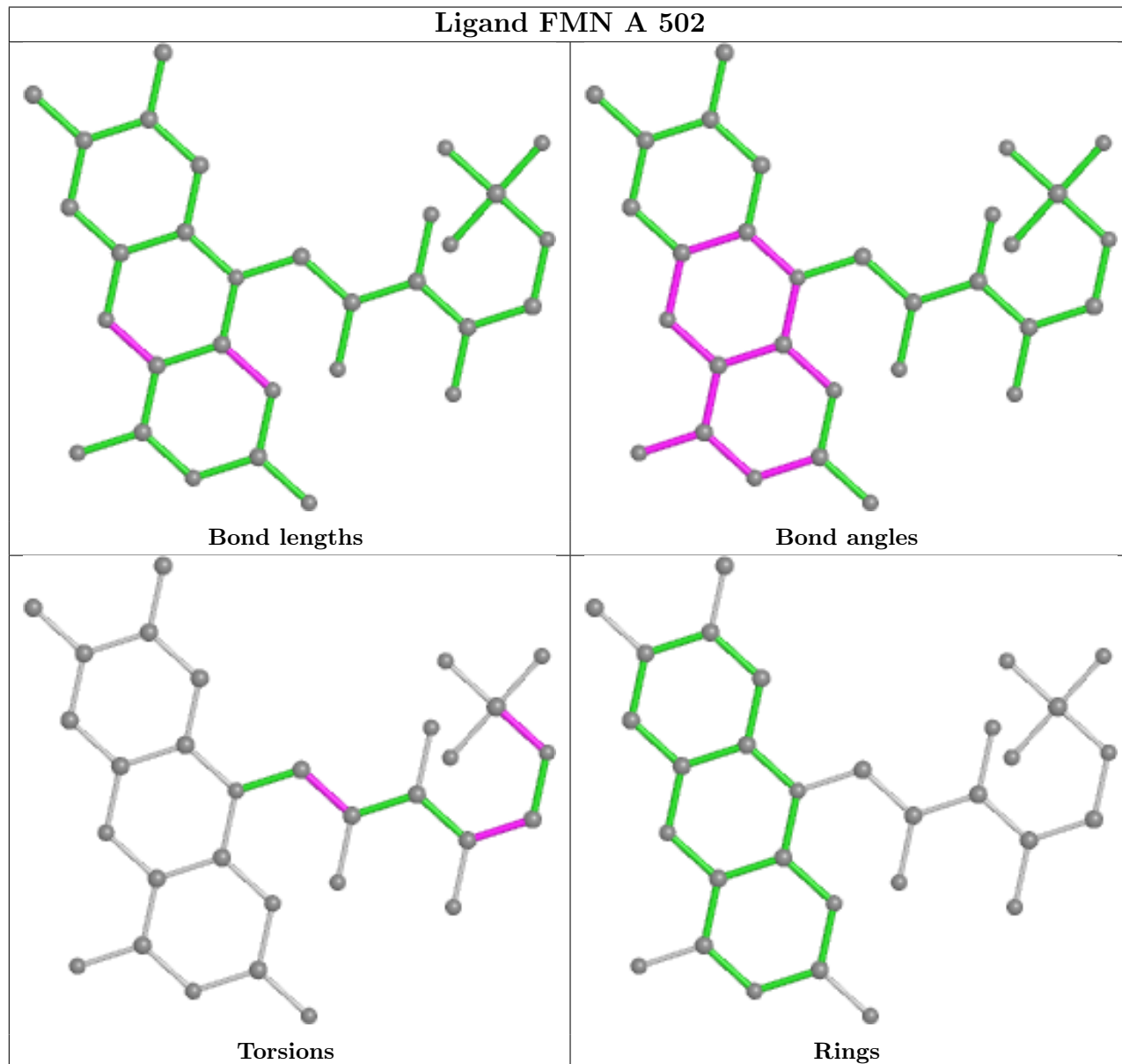
There are no ring outliers.

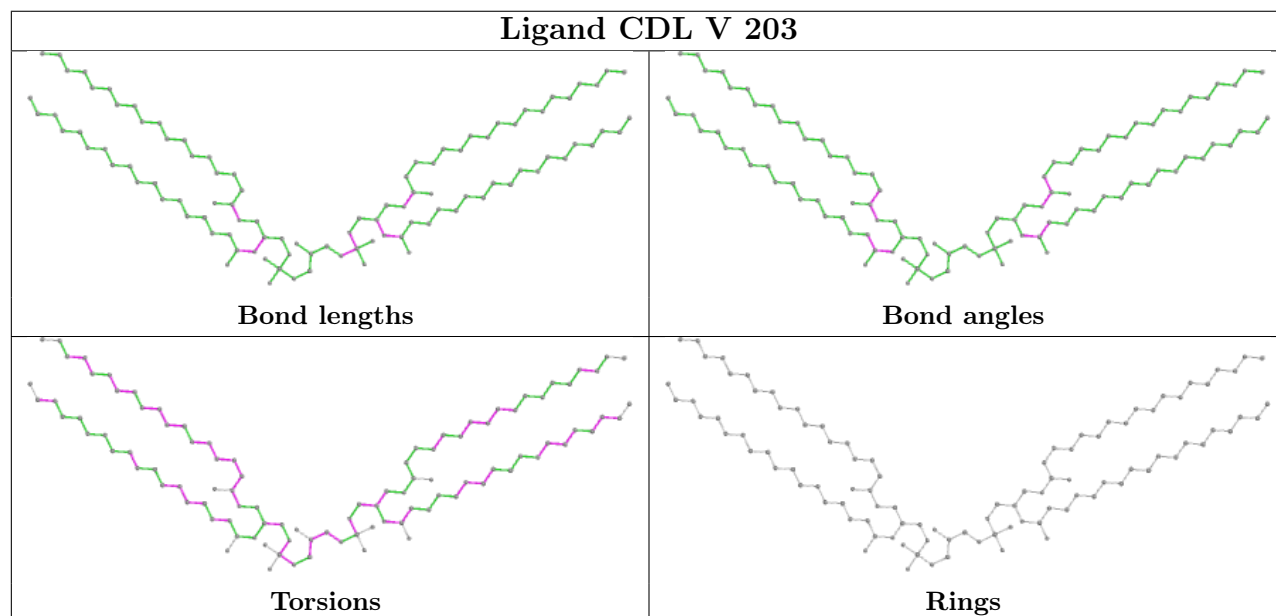
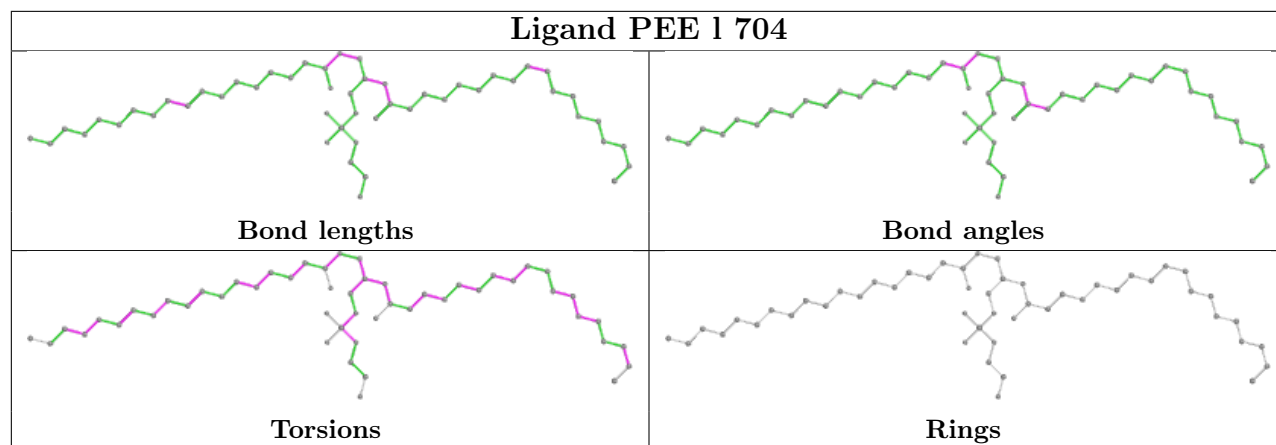
20 monomers are involved in 58 short contacts:

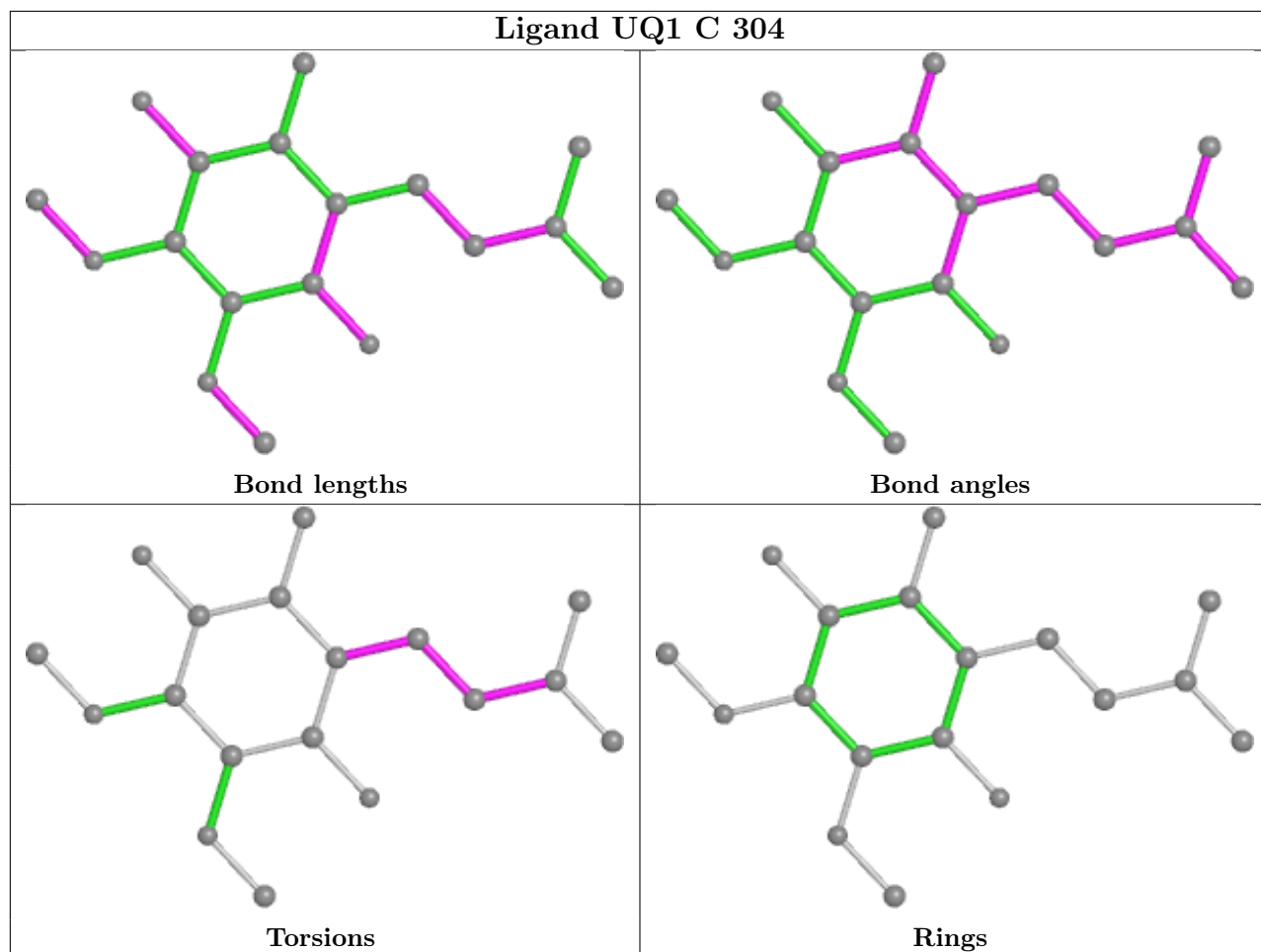
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	3	0
53	V	203	CDL	2	0
50	C	304	UQ1	3	0
47	A	503	NAI	5	0
48	V	202	PEE	3	0
48	U	101	PEE	3	0
45	C	301	SF4	1	0
54	J	401	NDP	1	0
52	G	201	8Q1	11	0
51	C	305	UQ	5	0
48	B	303	PEE	3	0
48	W	201	PEE	1	0
51	J	402	UQ	1	0
53	V	201	CDL	5	0
49	C	303	PLX	2	0
45	A	501	SF4	2	0
53	V	204	CDL	4	0
49	J	403	PLX	2	0
48	C	302	PEE	2	0
50	Q	501	UQ1	1	0

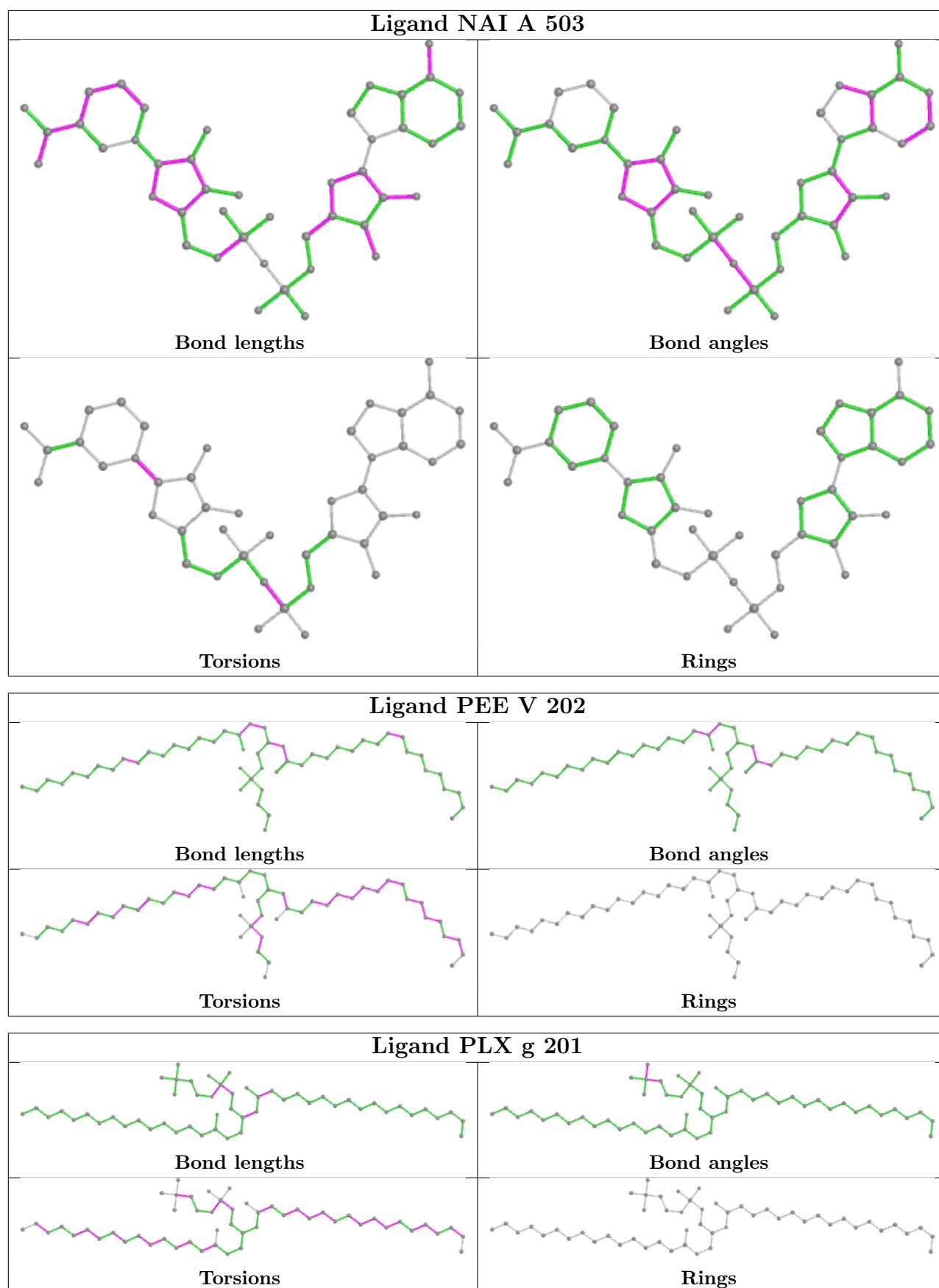
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

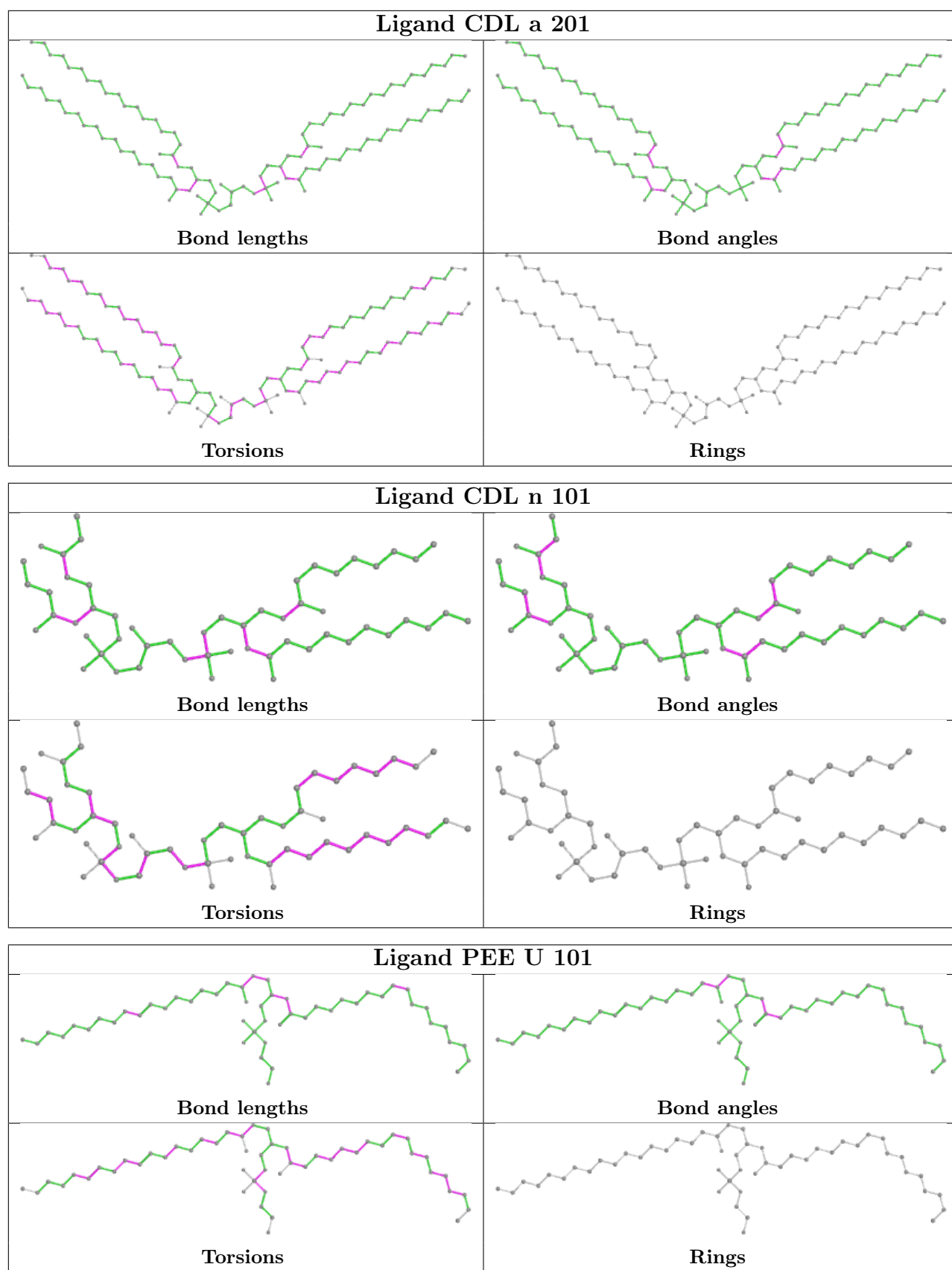
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

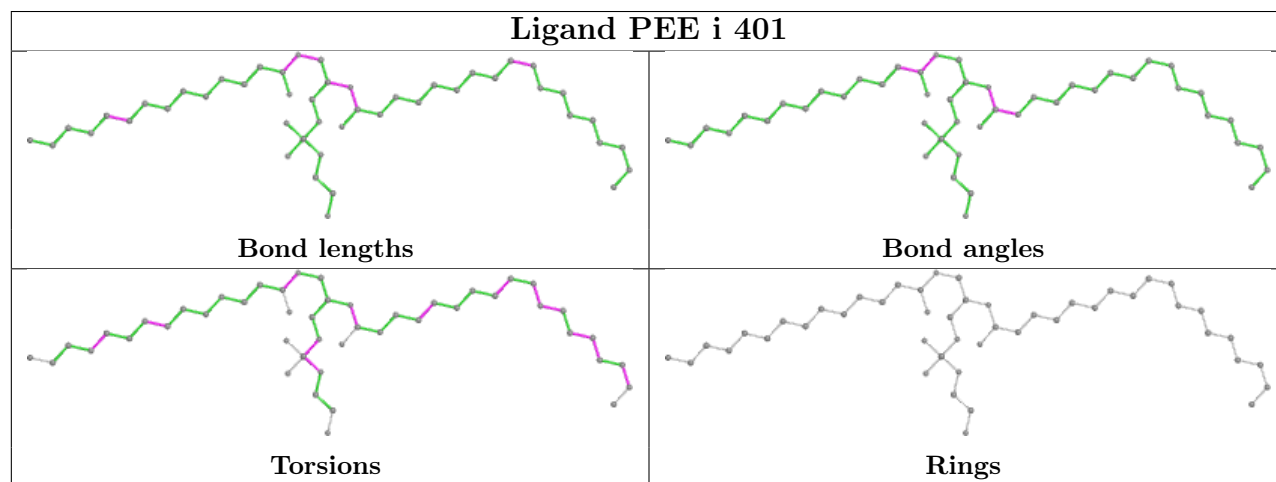
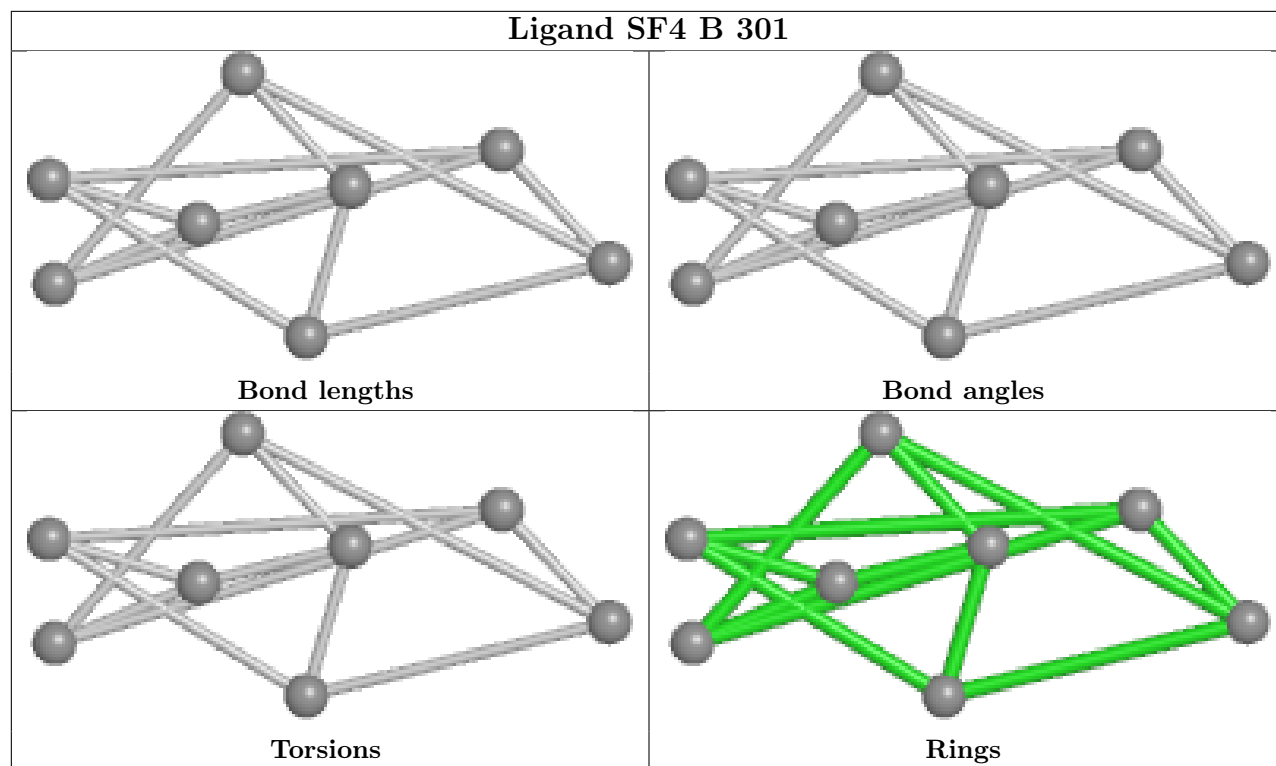


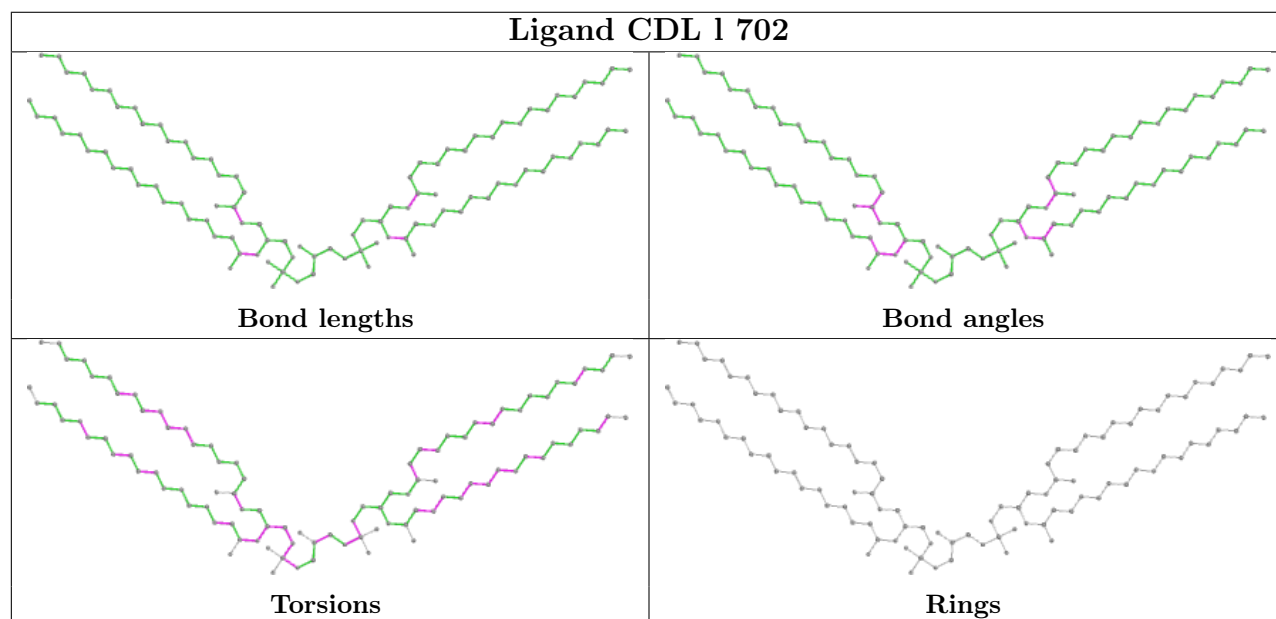
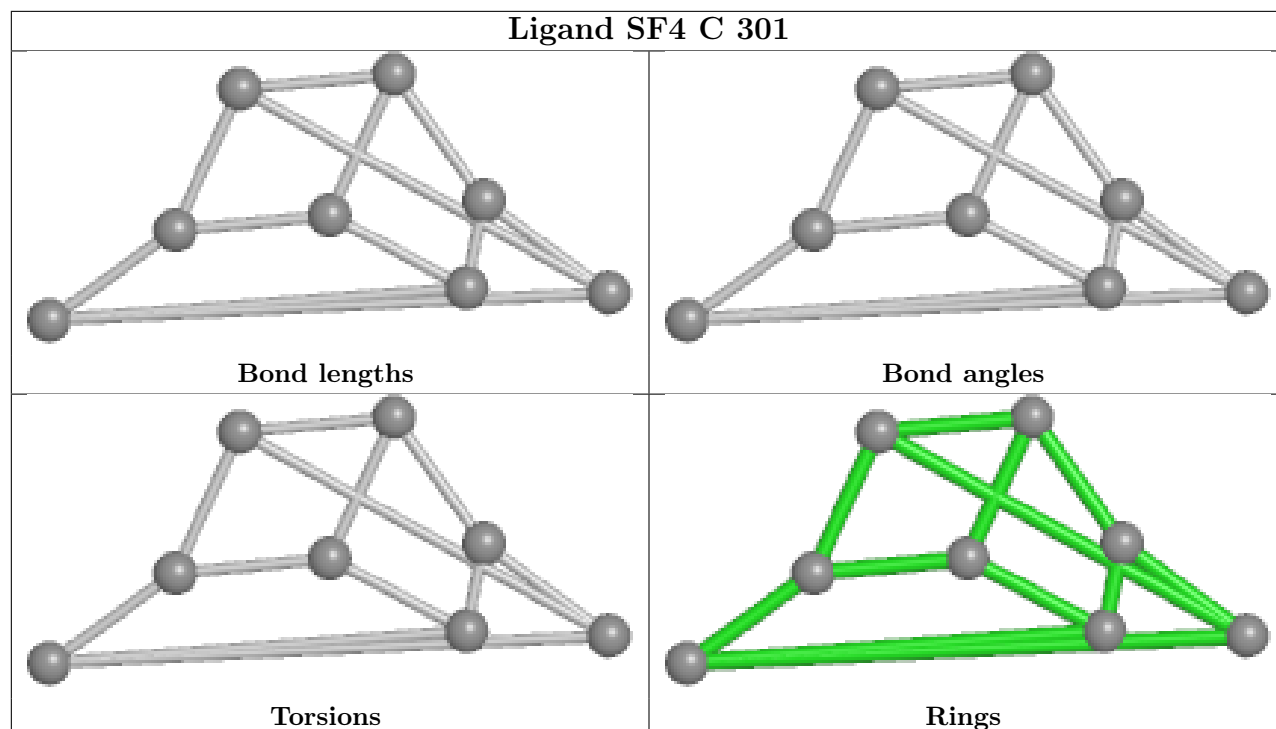


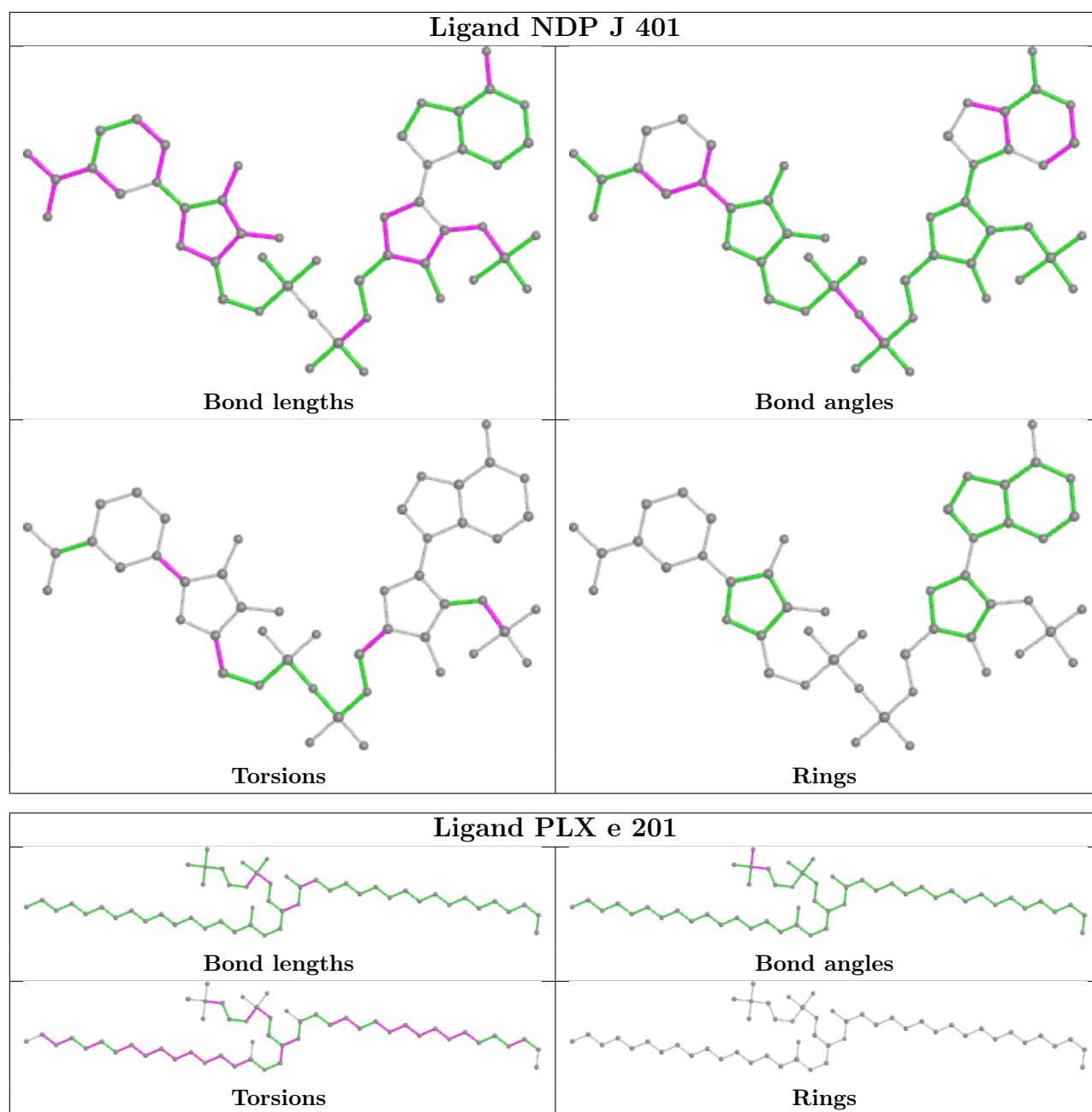


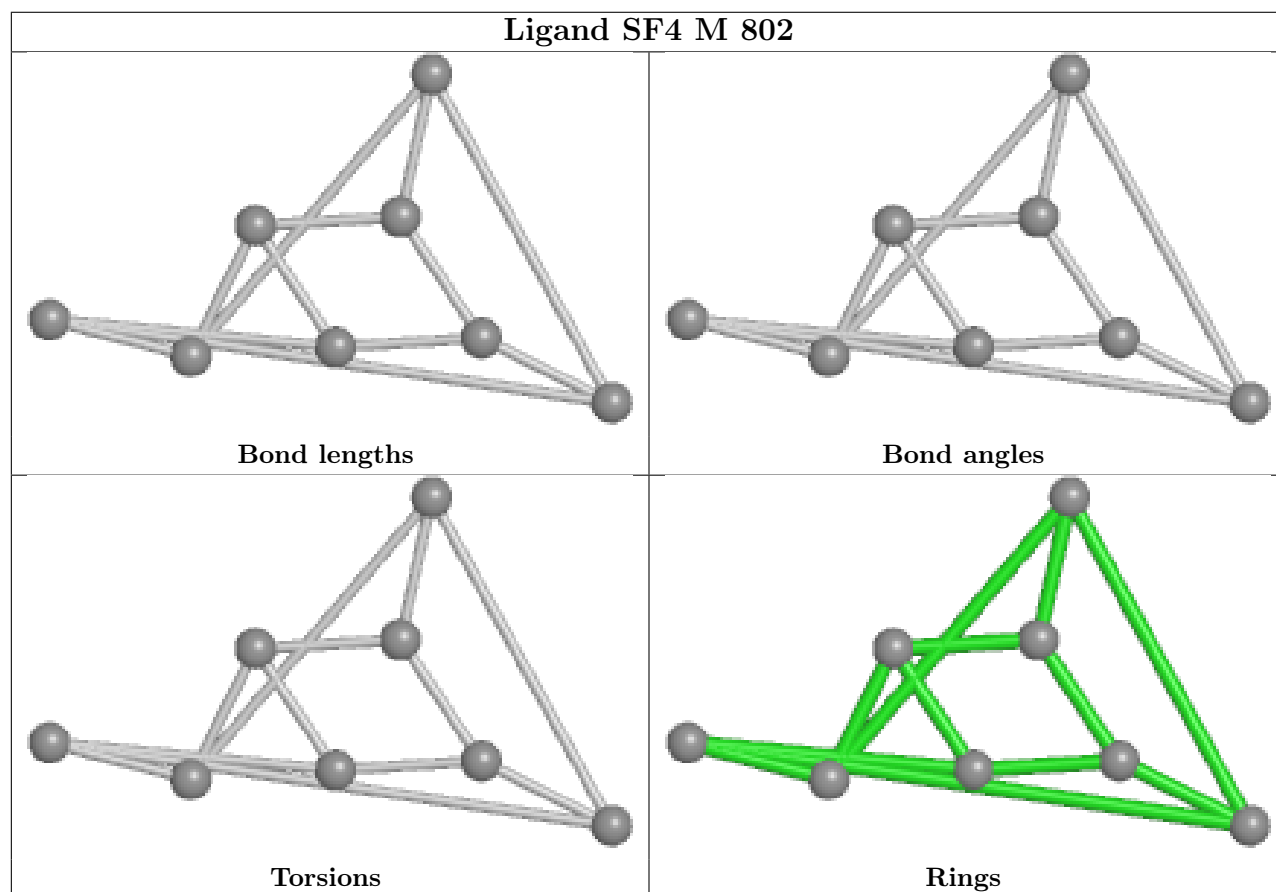
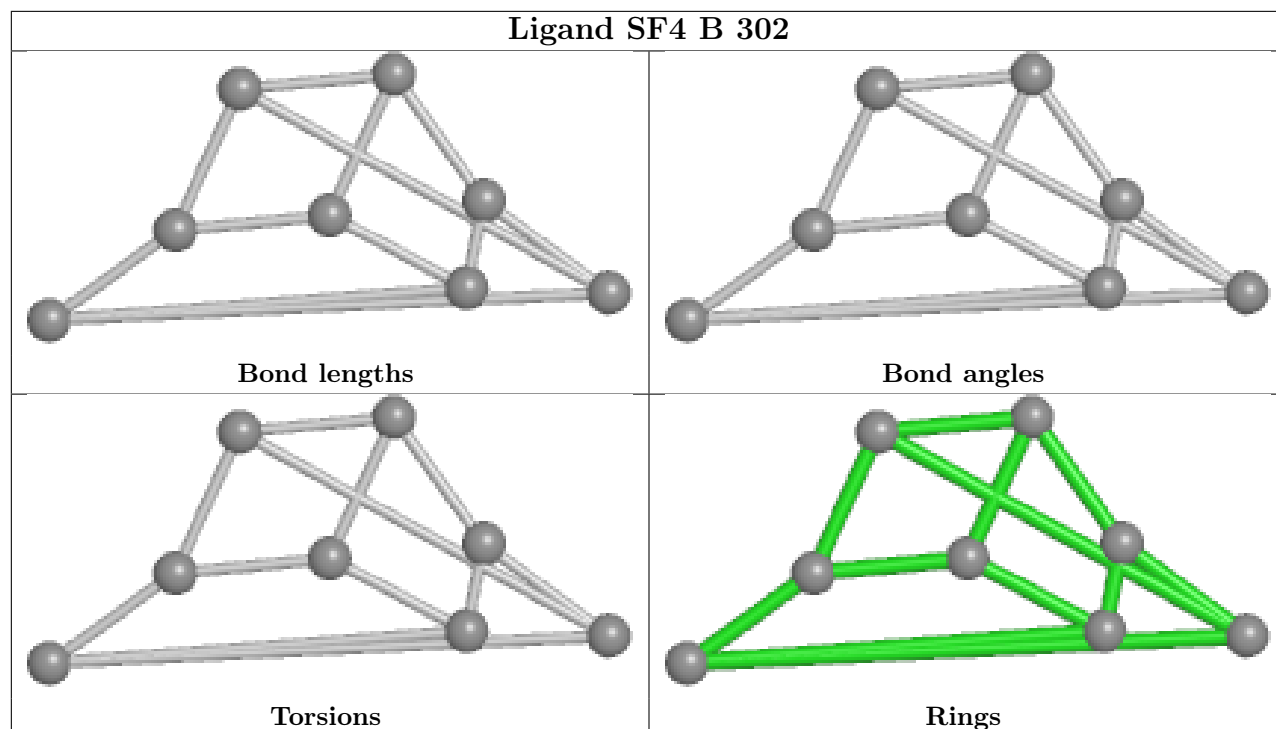


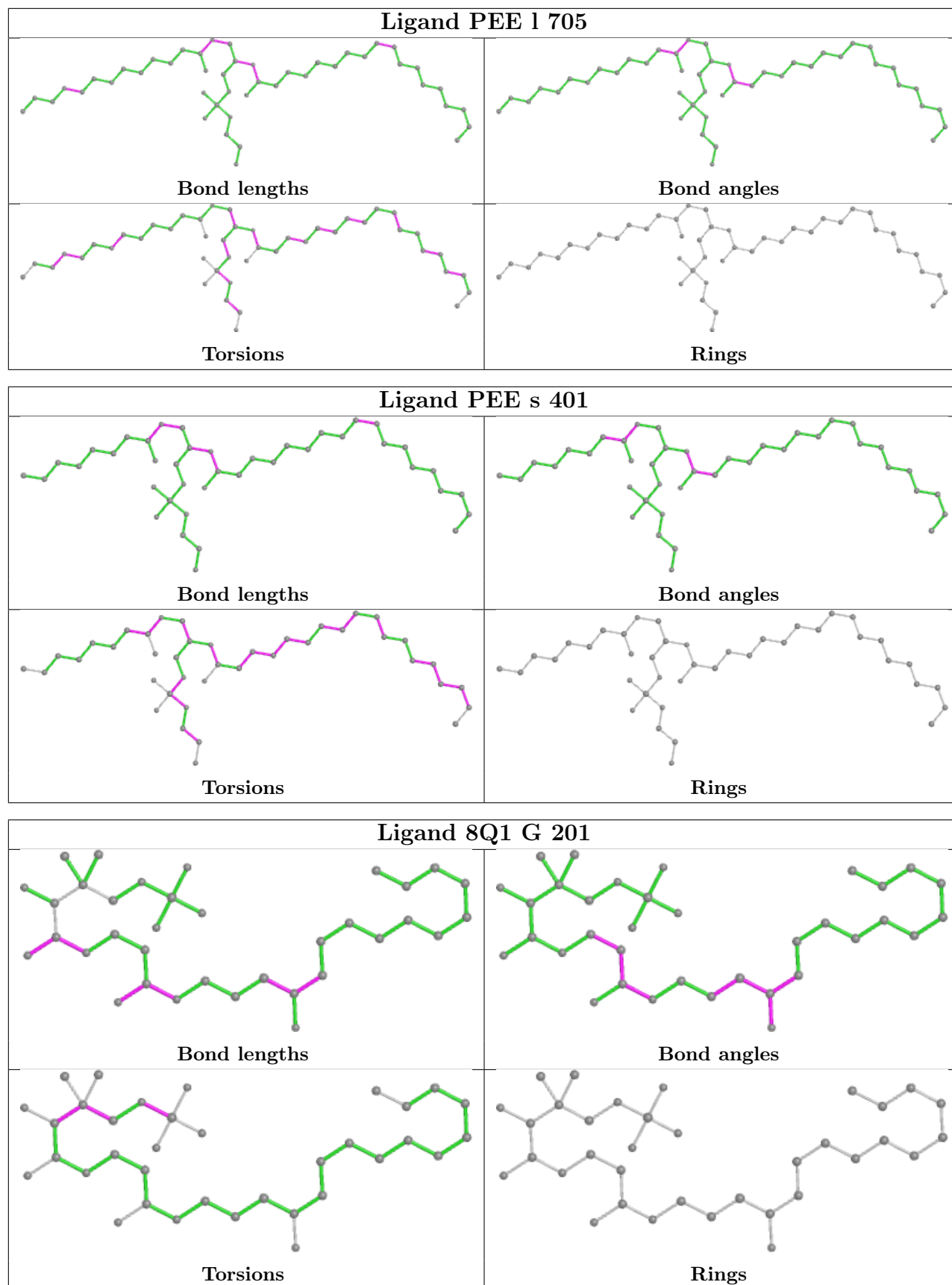


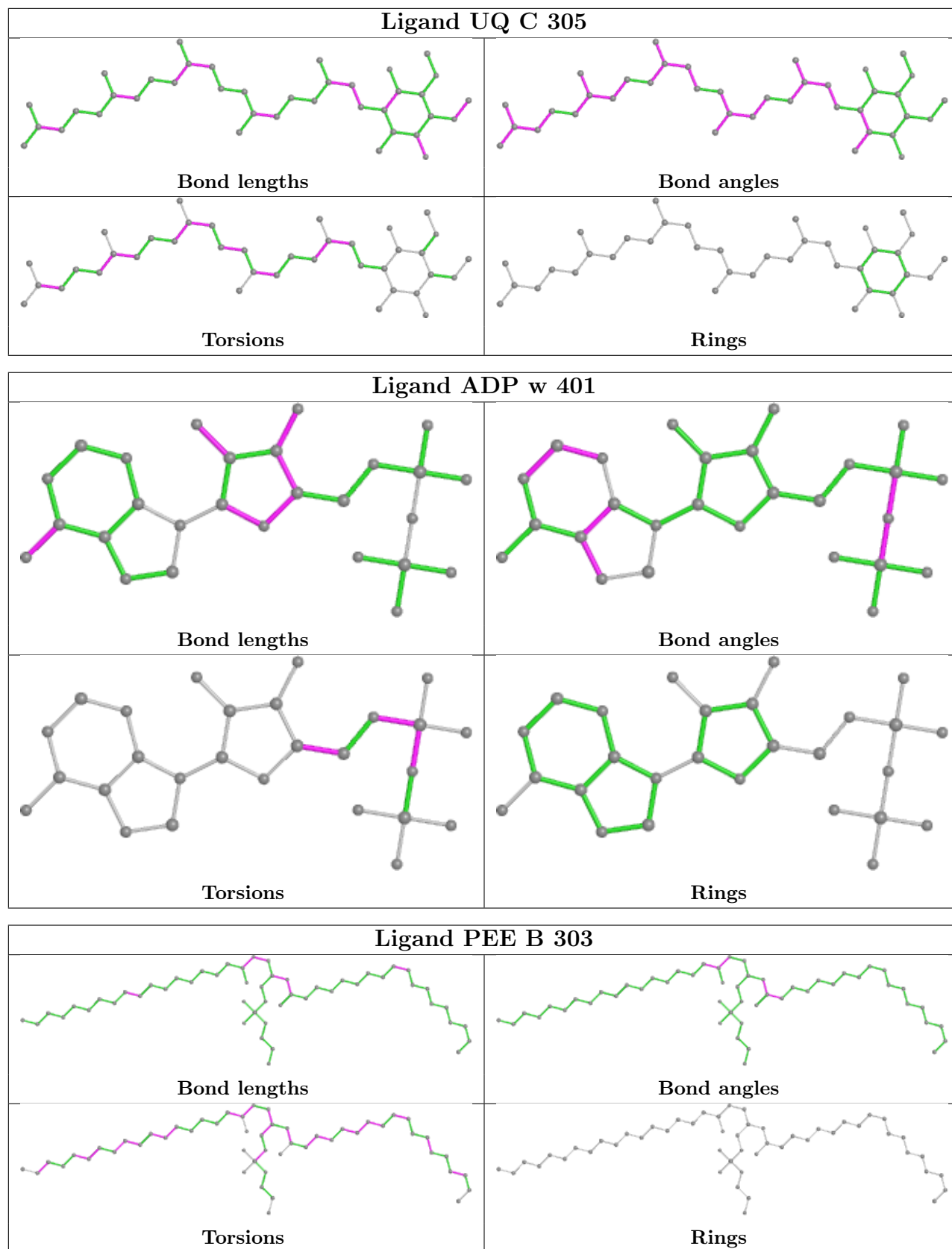


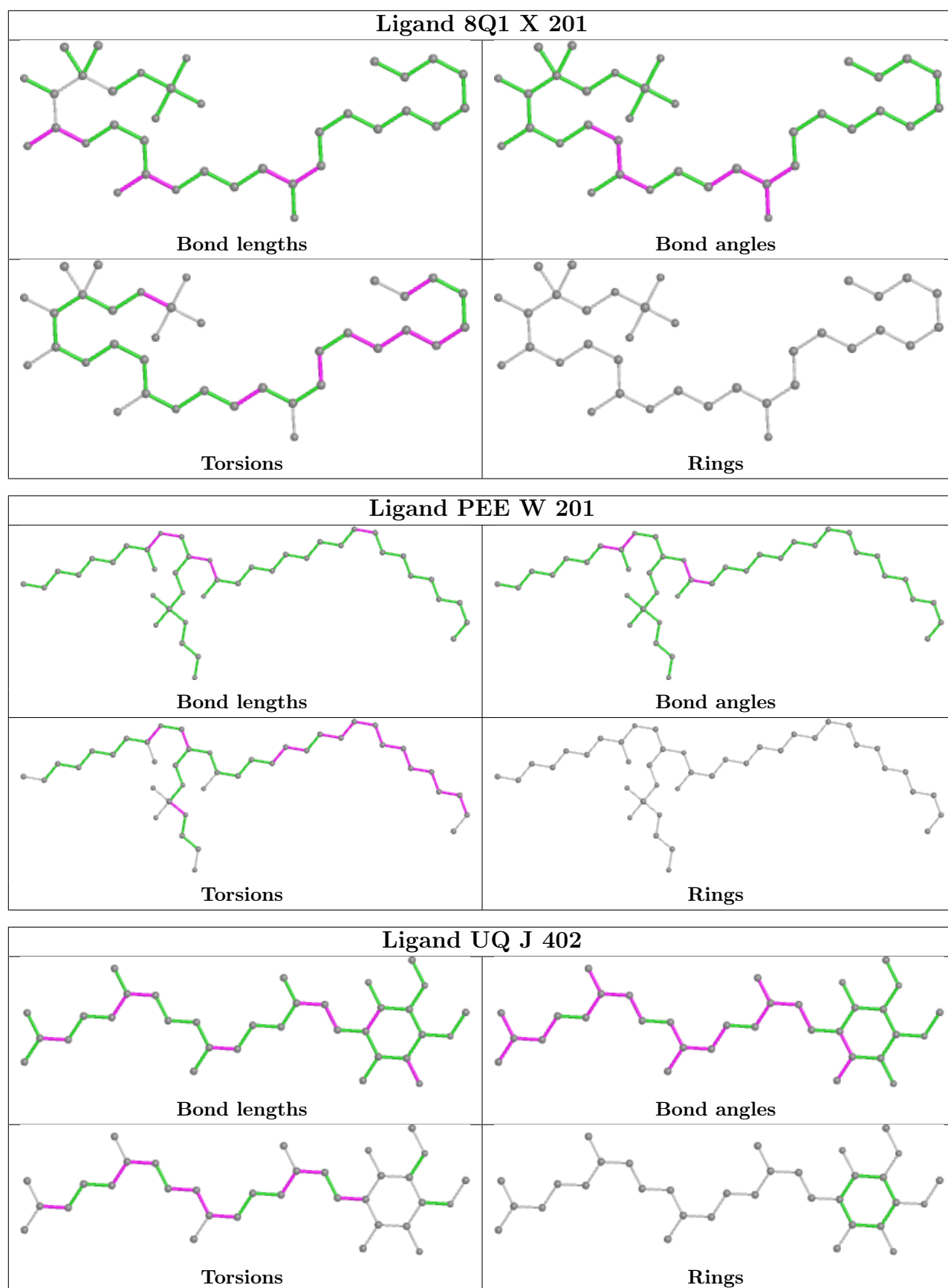


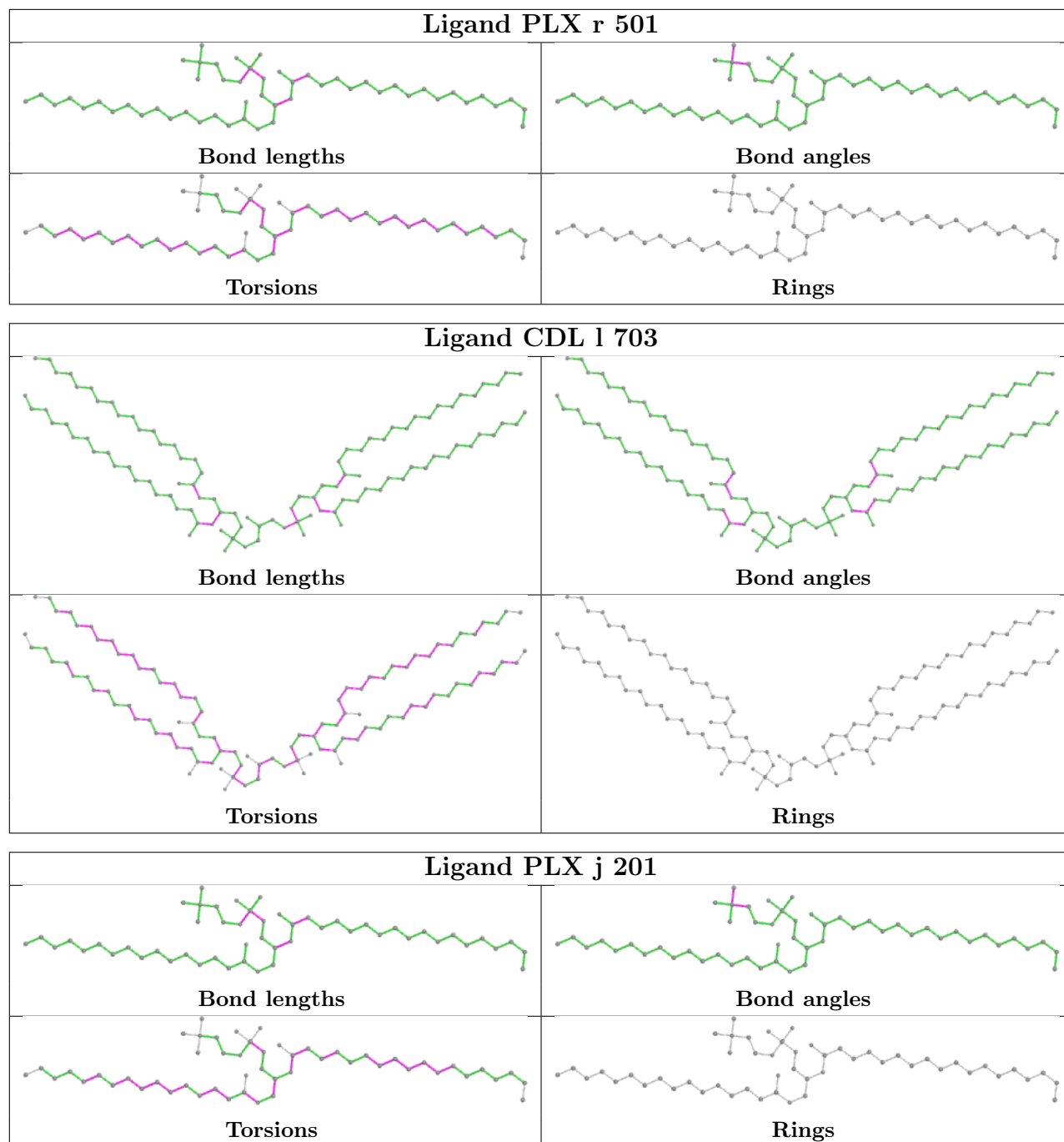


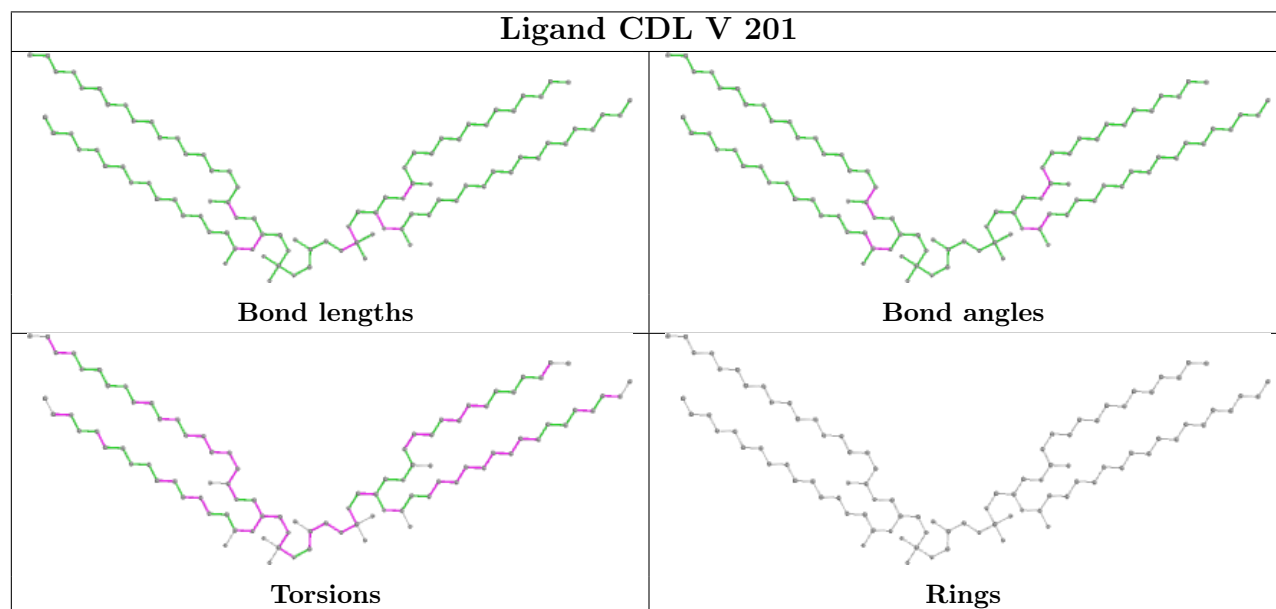
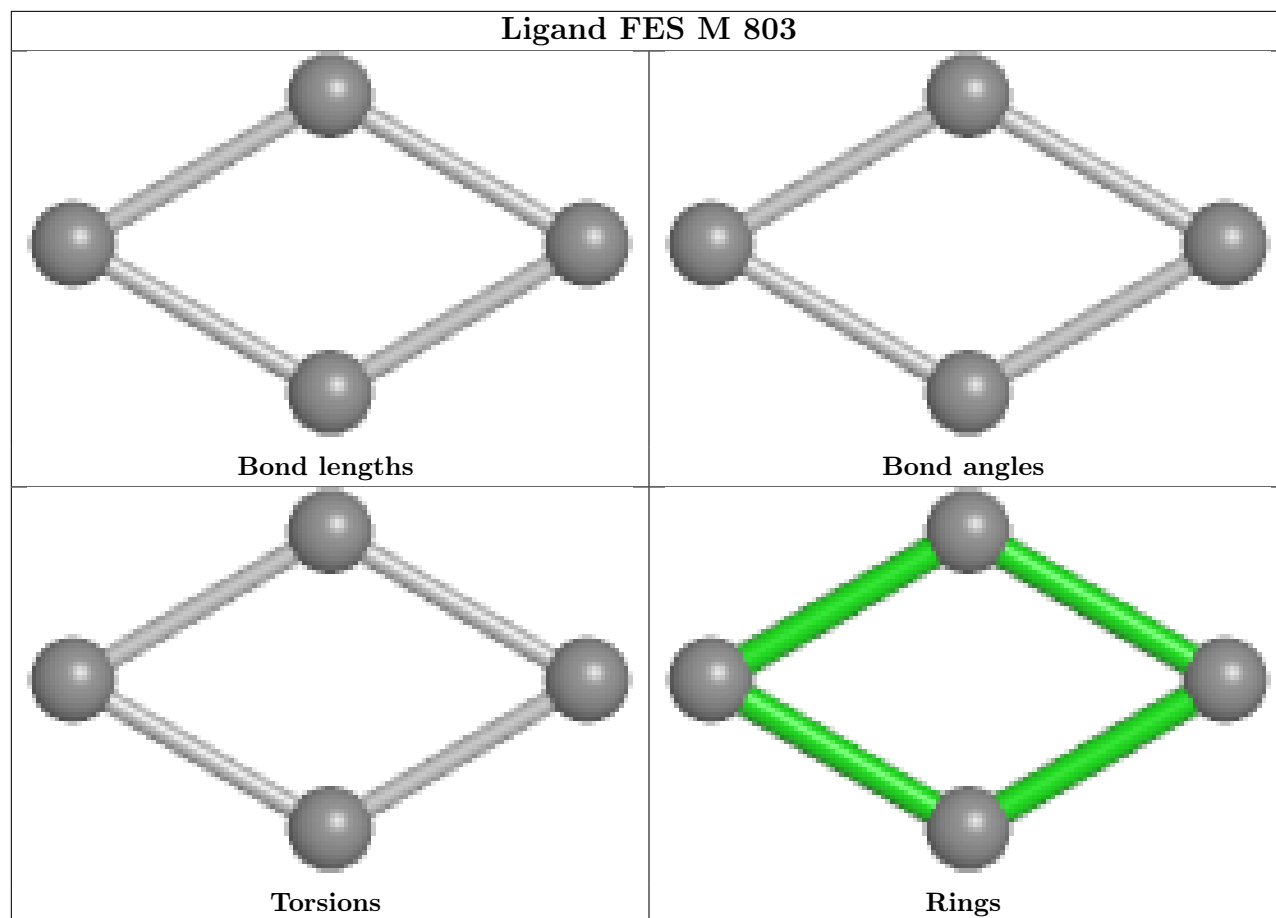


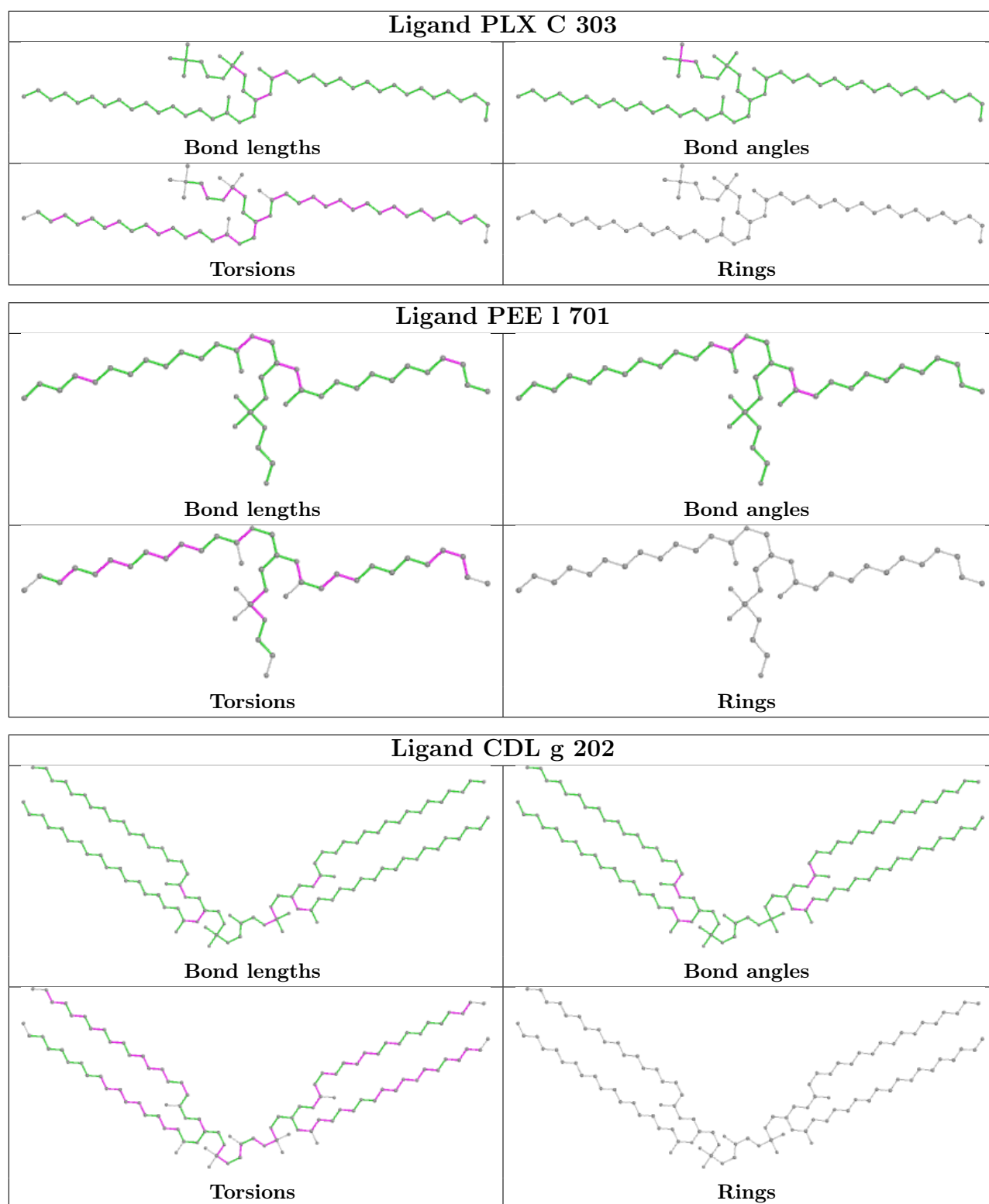


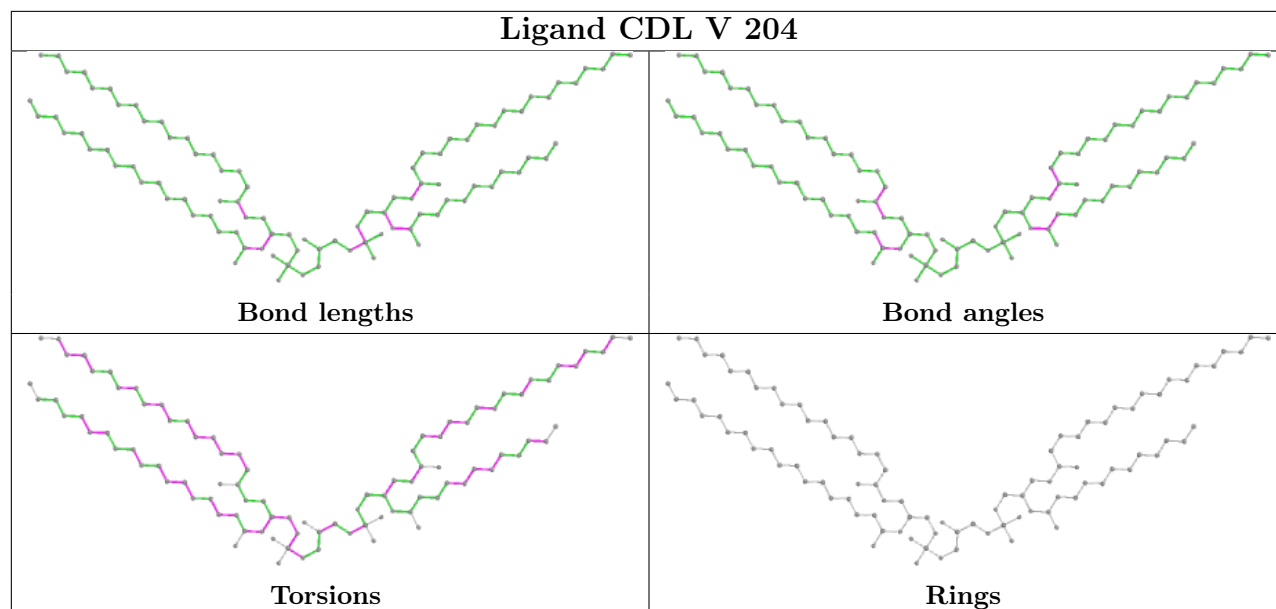
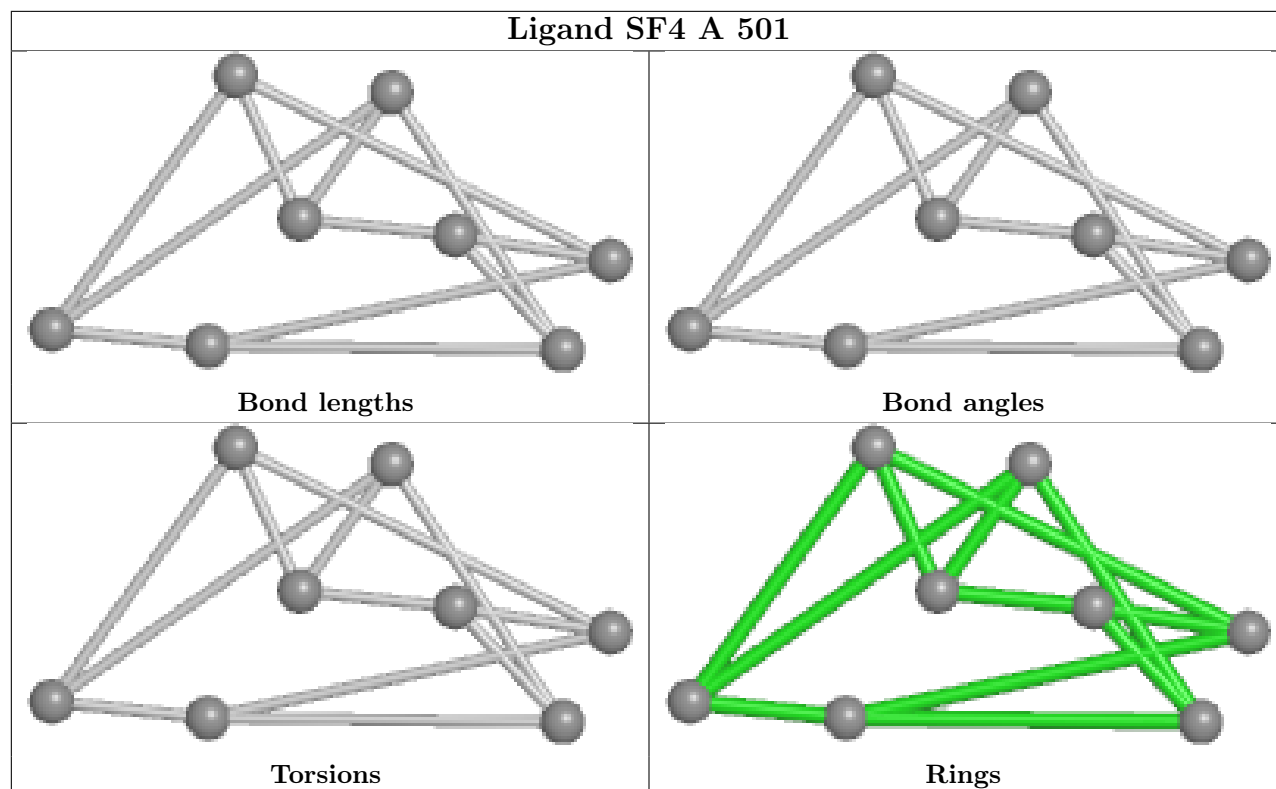


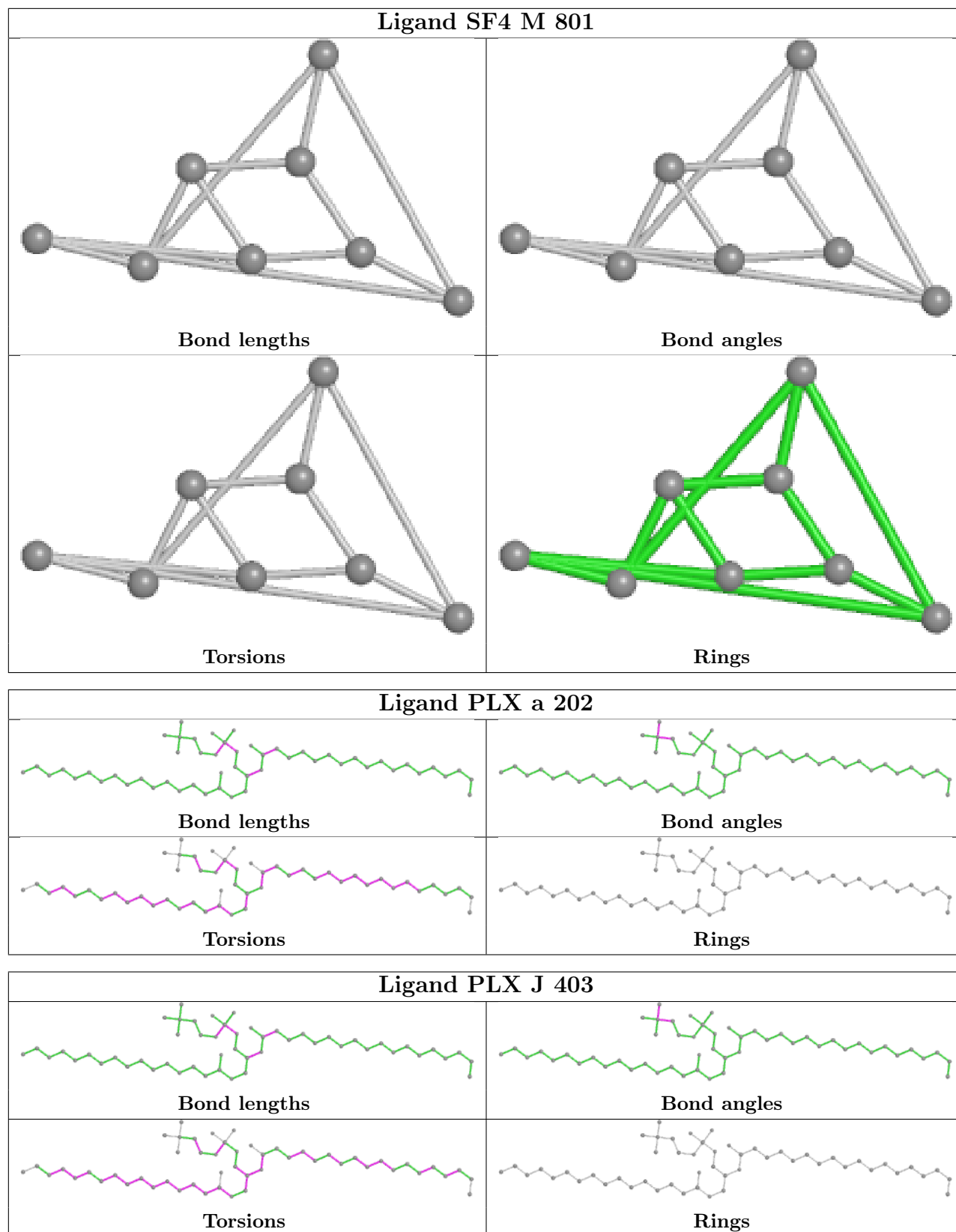


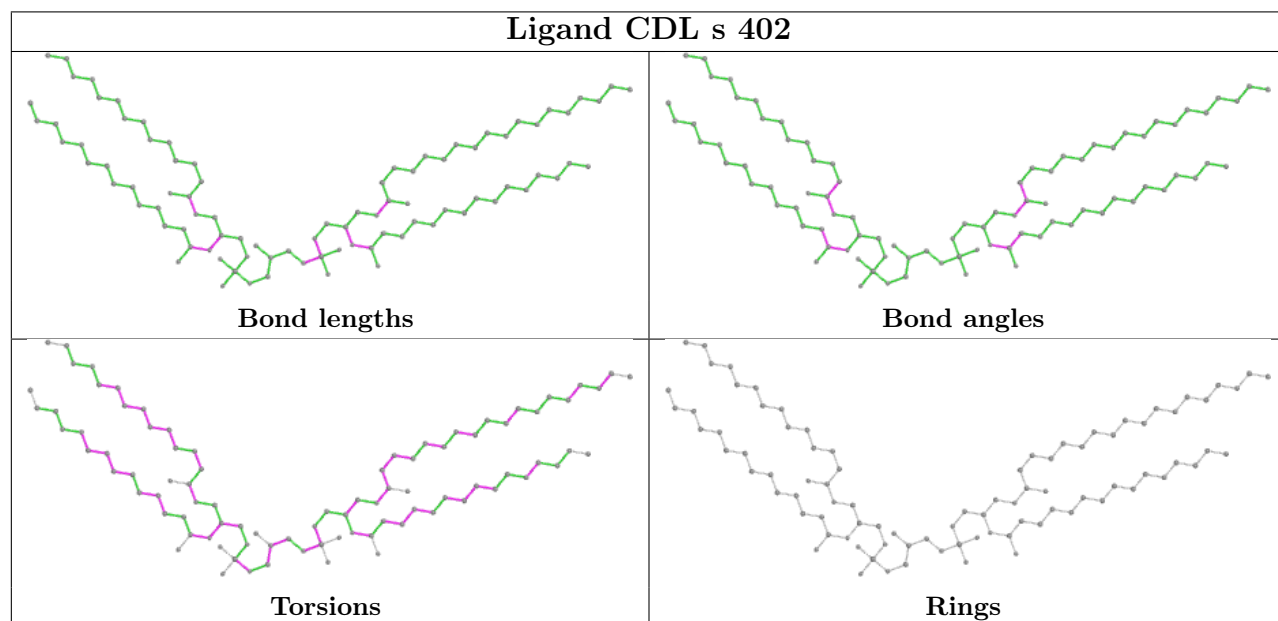
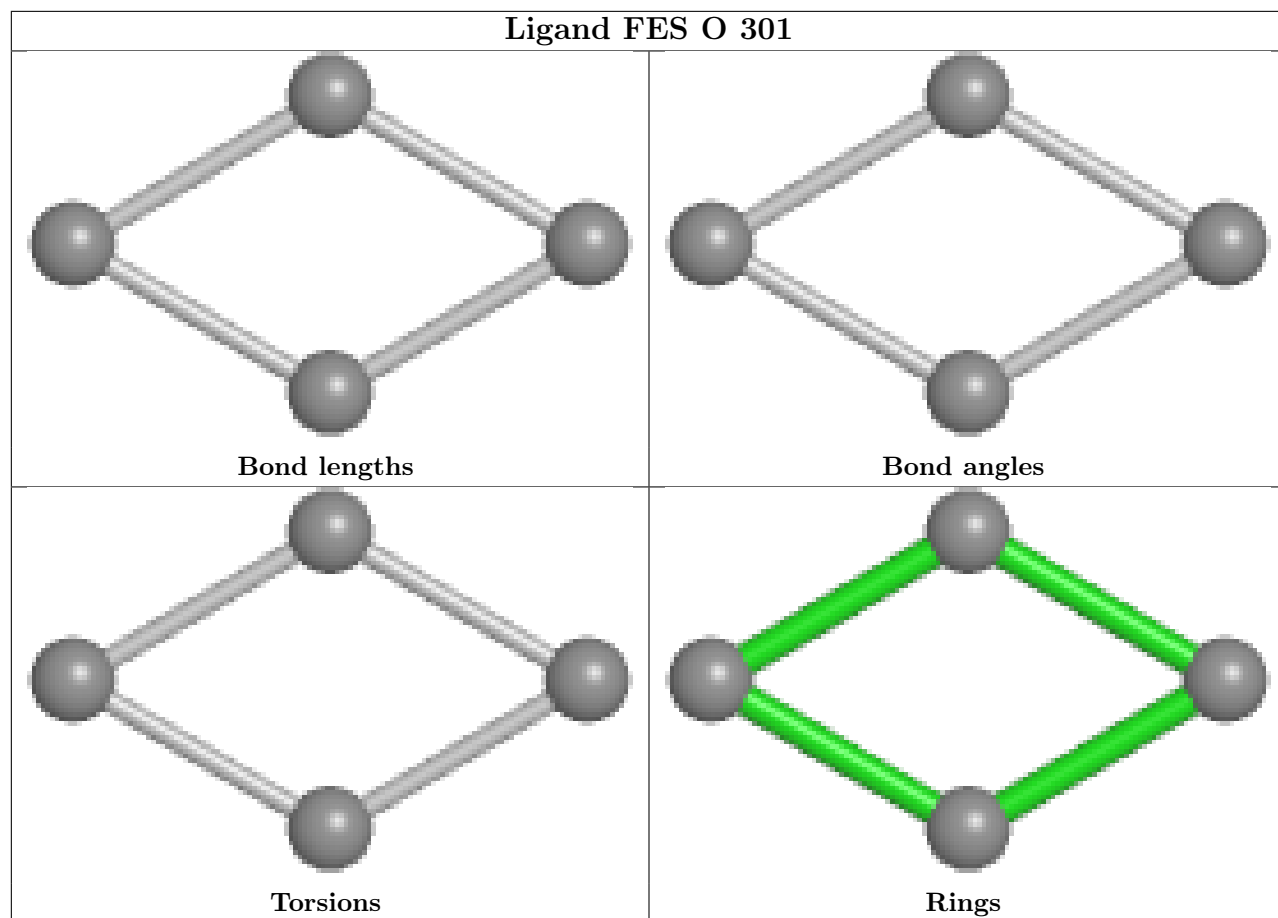


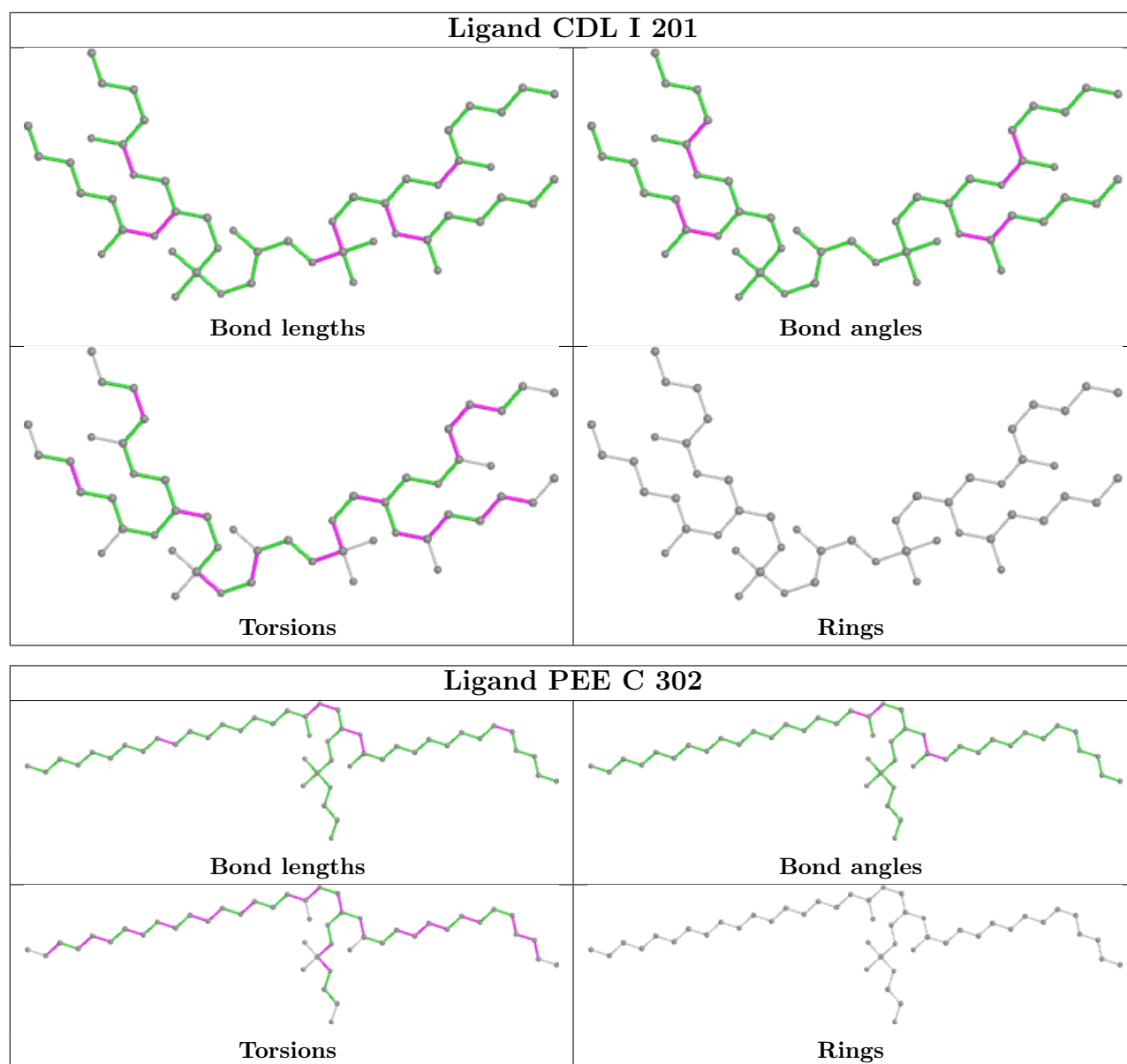


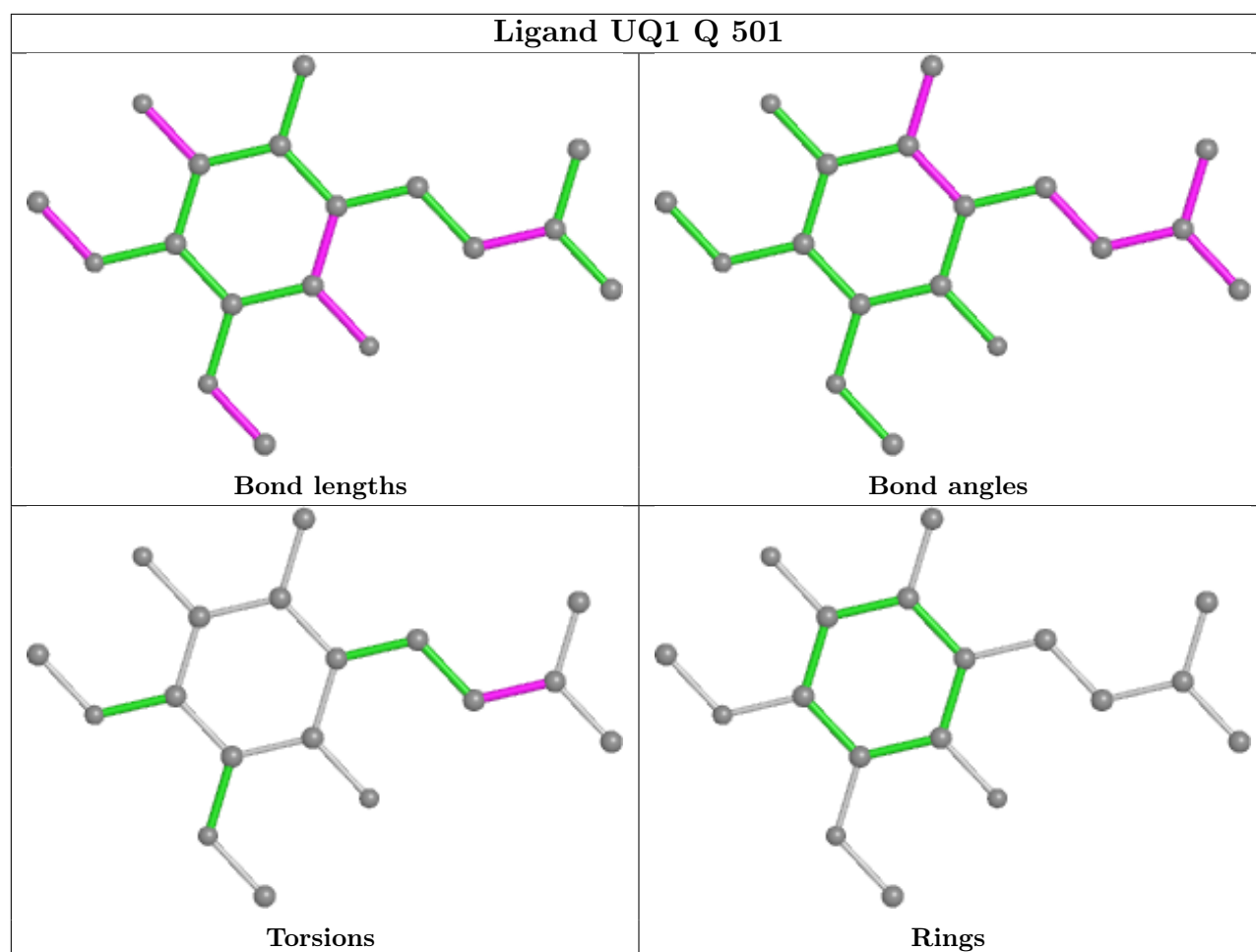












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

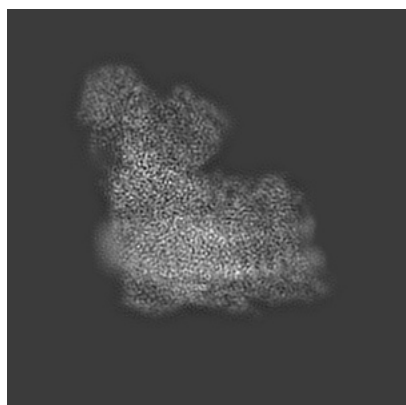
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32300. These allow visual inspection of the internal detail of the map and identification of artifacts.

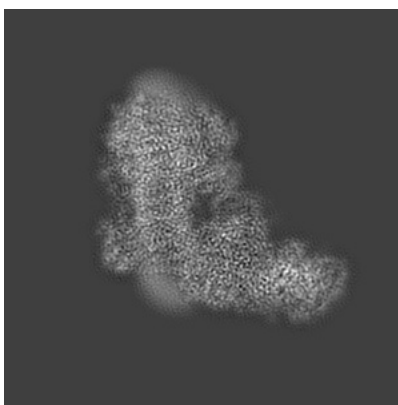
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

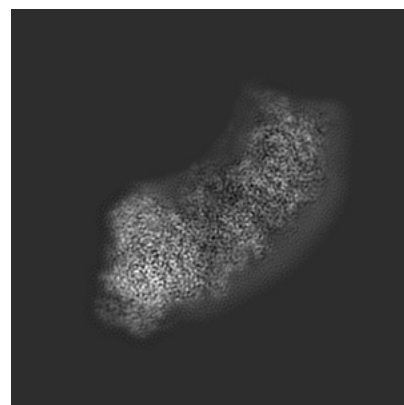
6.1.1 Primary map



X



Y

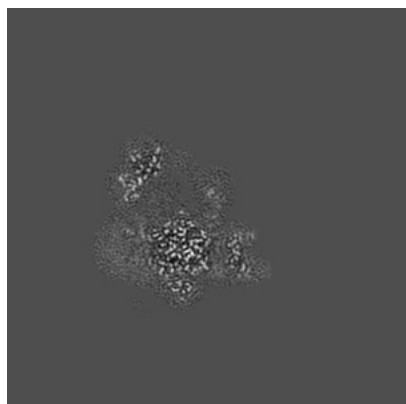


Z

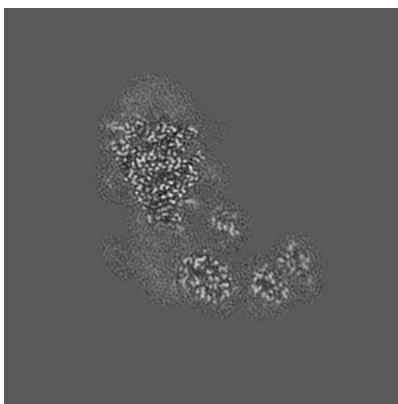
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

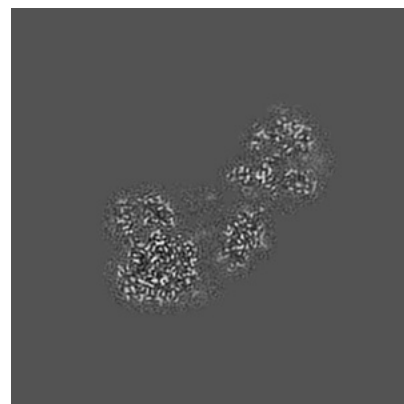
6.2.1 Primary map



X Index: 152



Y Index: 152

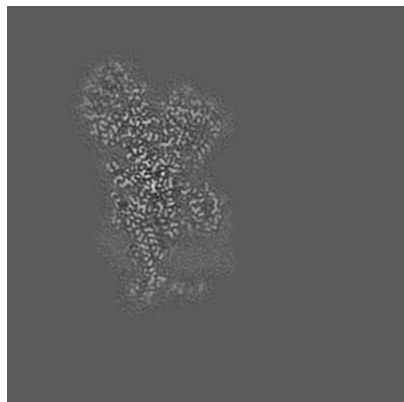


Z Index: 152

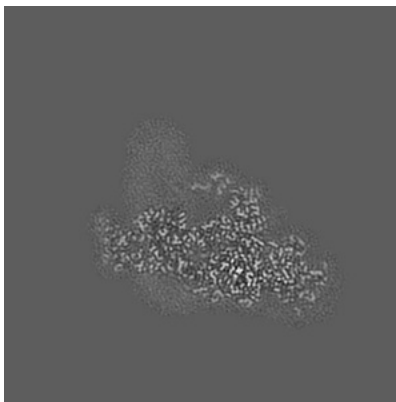
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

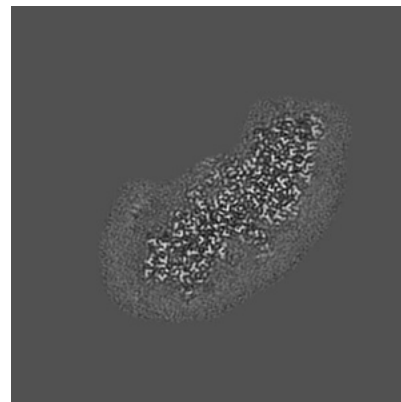
6.3.1 Primary map



X Index: 105



Y Index: 105

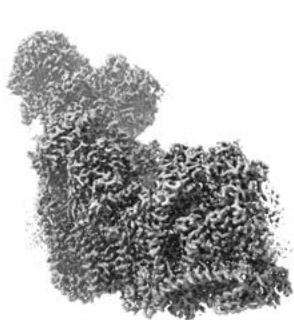


Z Index: 129

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

6.4 Orthogonal surface views [i](#)

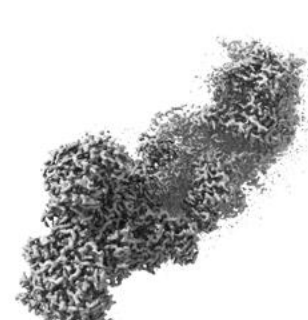
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

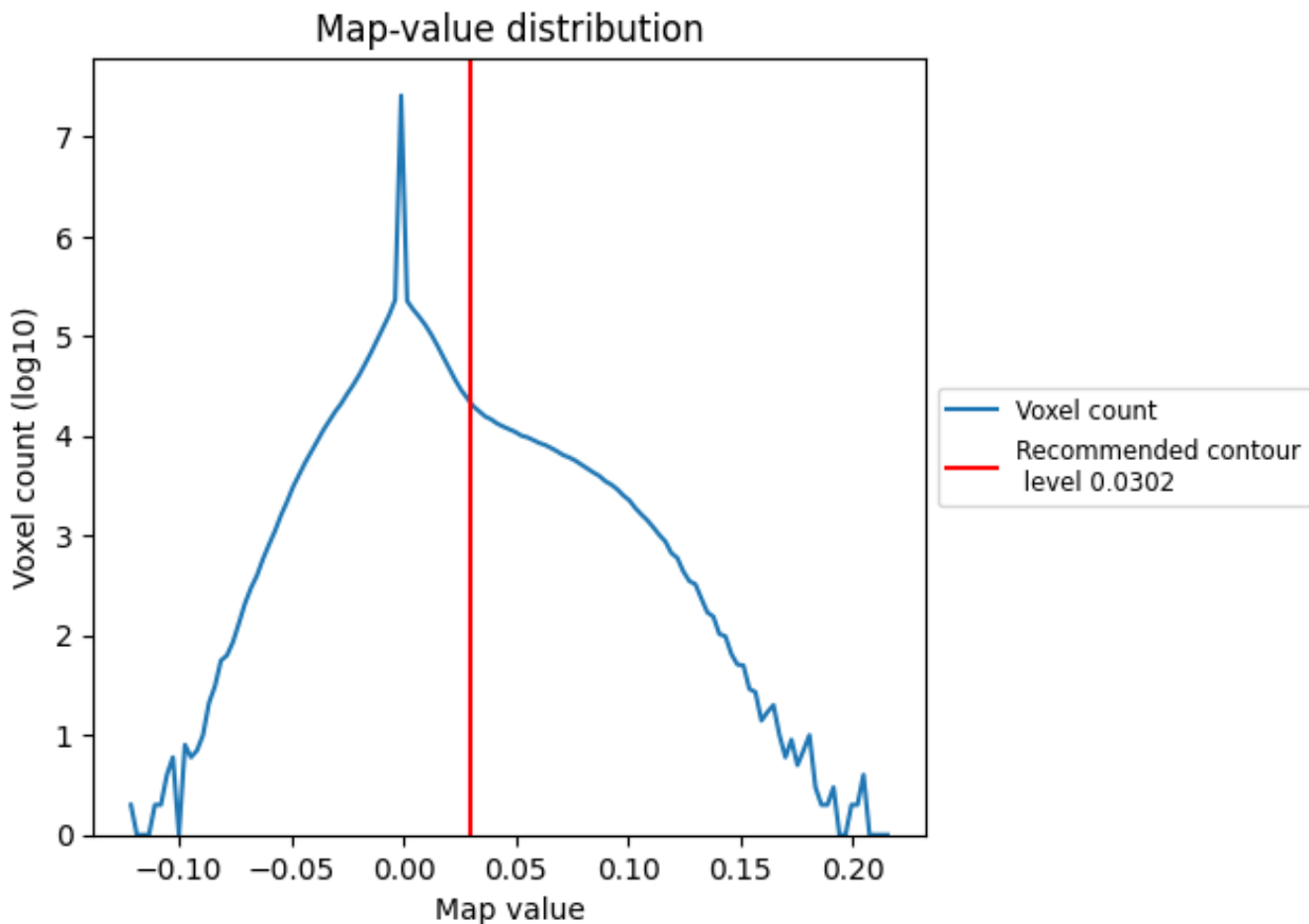
6.5 Mask visualisation

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

7 Map analysis [i](#)

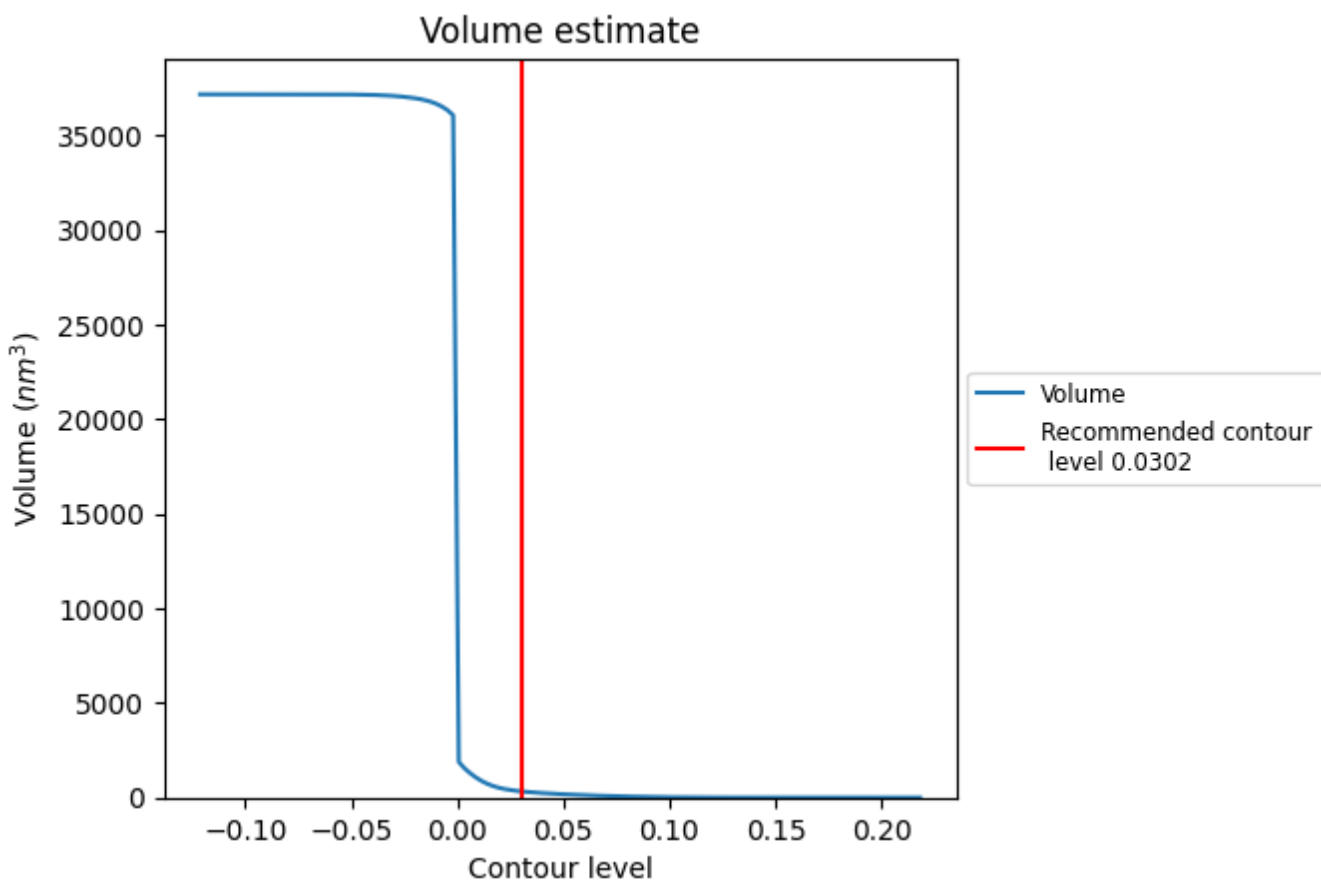
This section contains the results of statistical analysis of the map.

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.

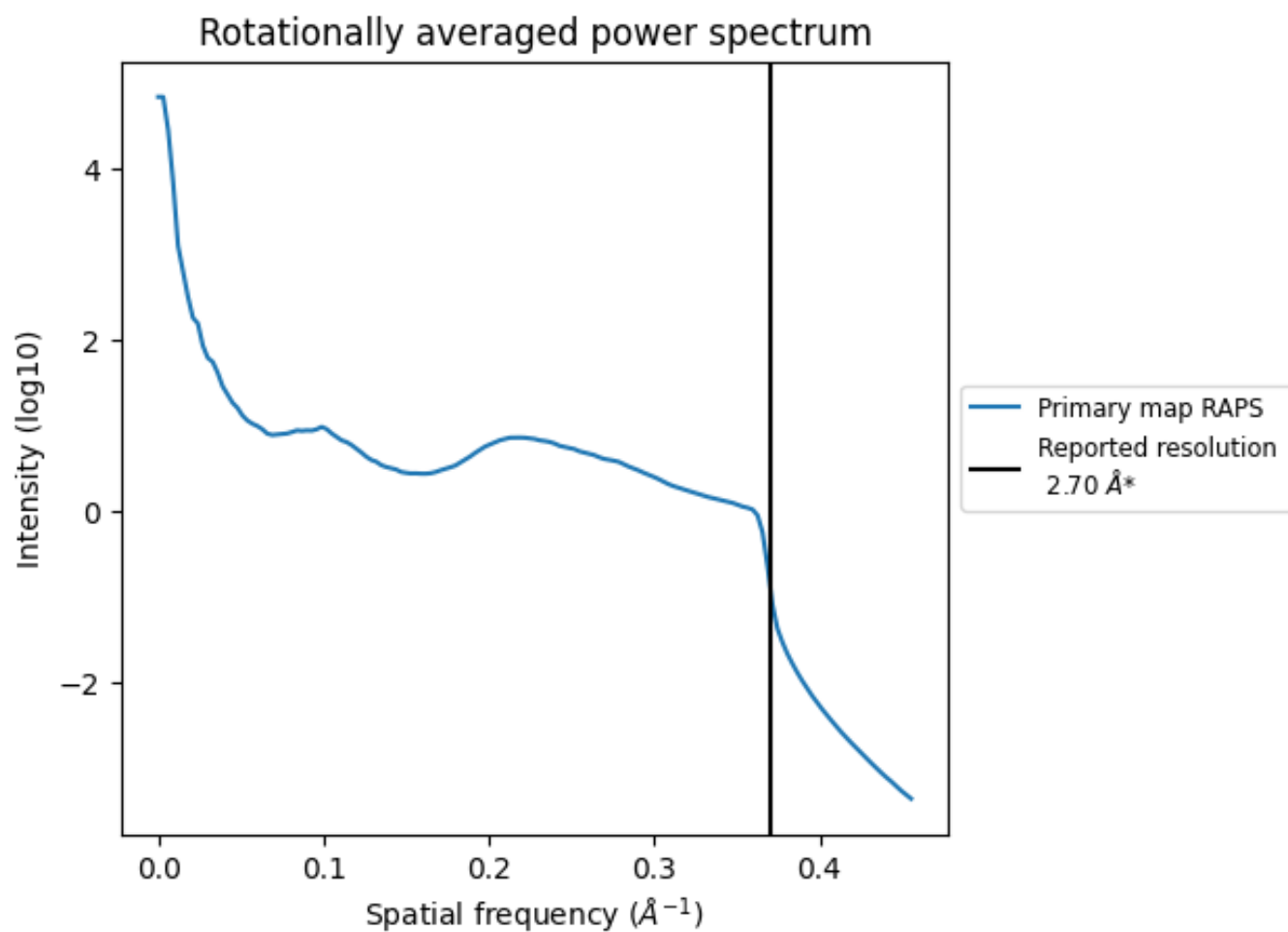
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 0.370 Å⁻¹

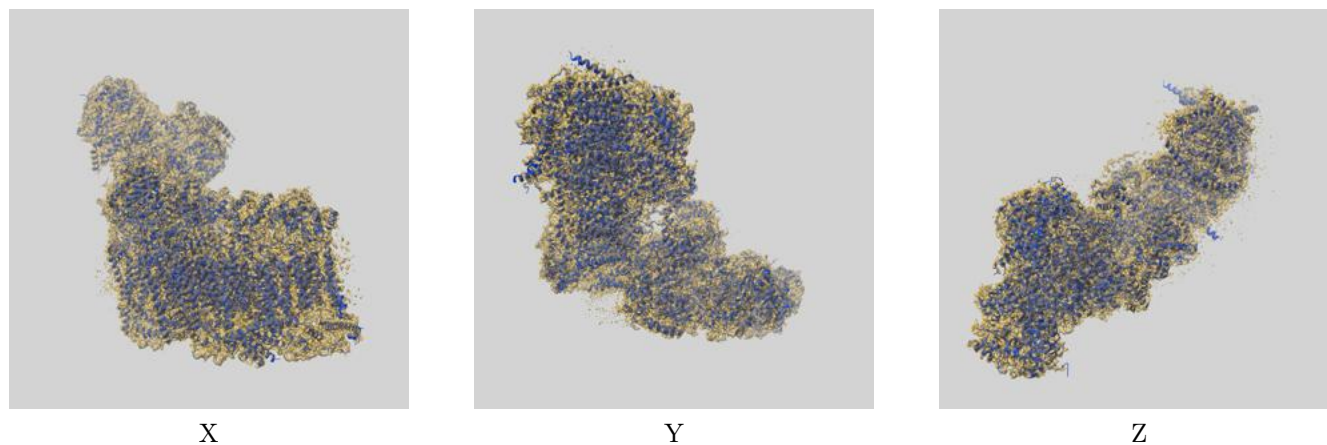
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

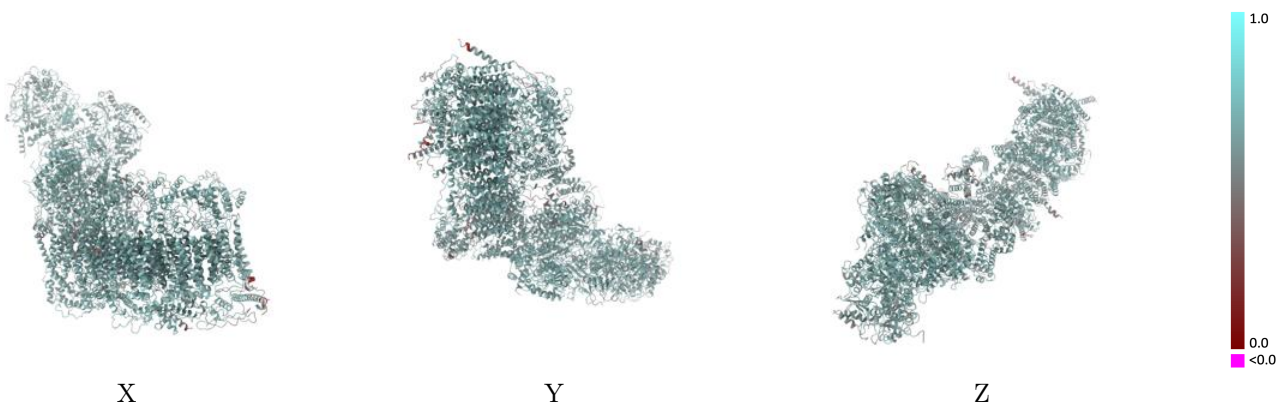
This section contains information regarding the fit between EMDB map EMD-32300 and PDB model 7W4C. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



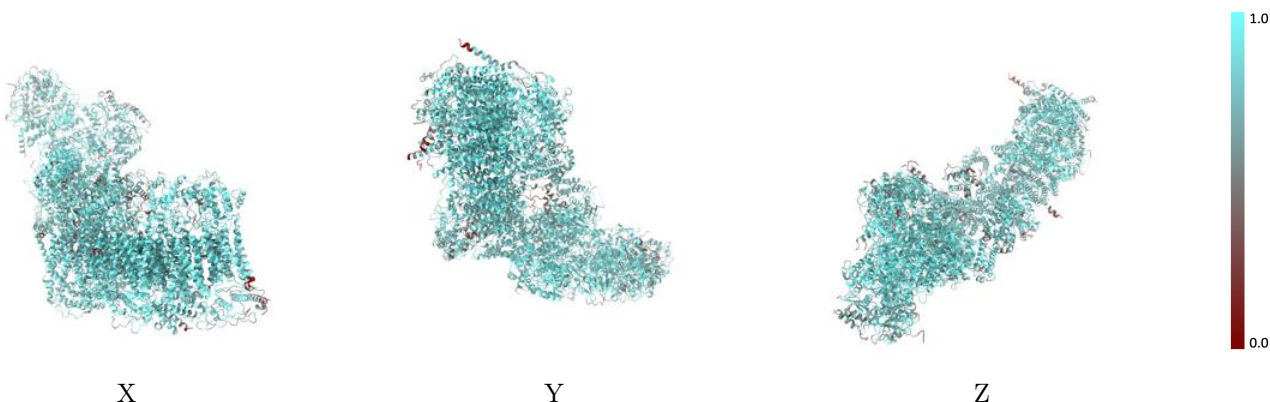
The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



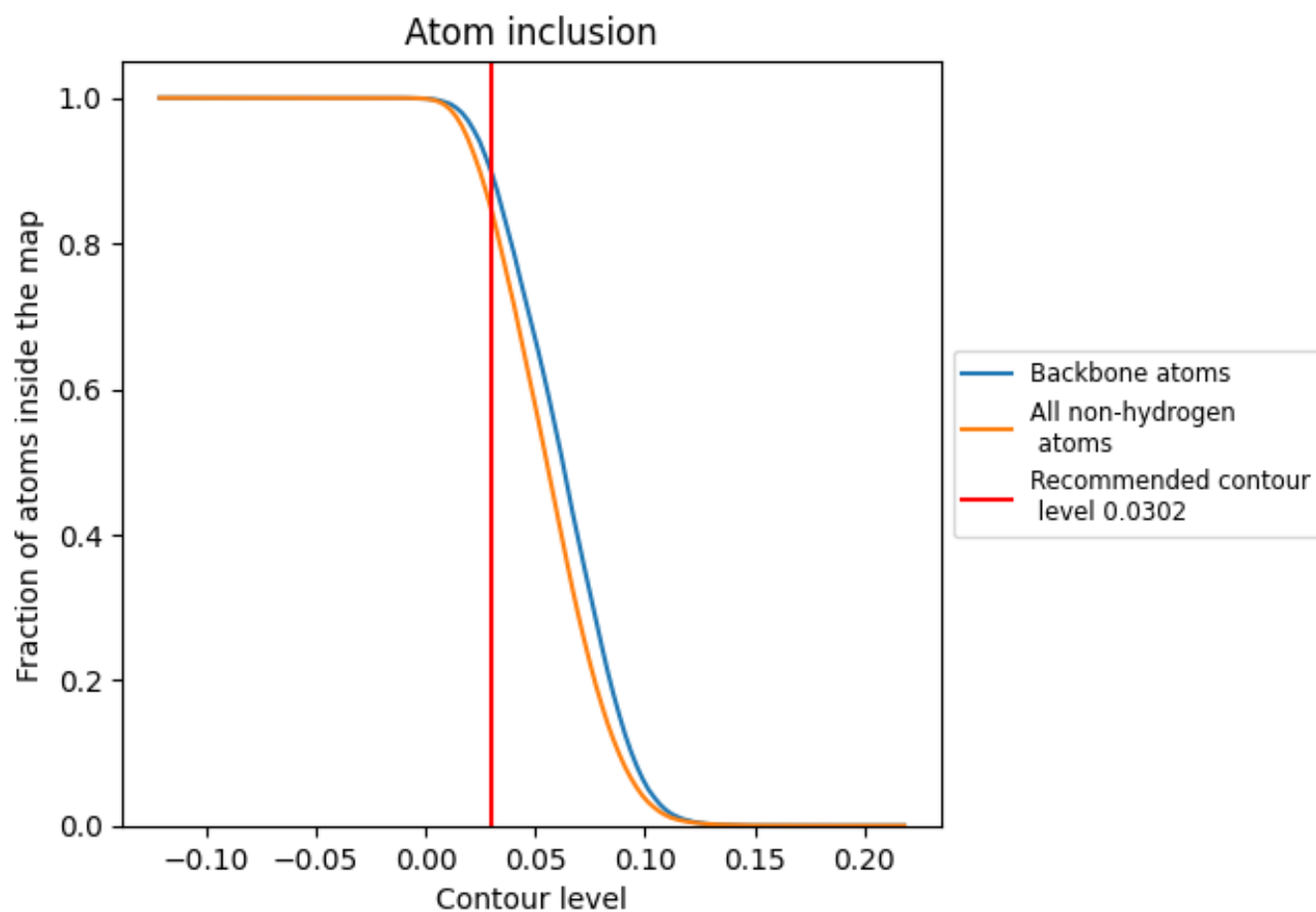
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0302).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.0302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8433	 0.6220
A	 0.7931	 0.6020
B	 0.9361	 0.6590
C	 0.9142	 0.6520
E	 0.8588	 0.6270
F	 0.6662	 0.5550
G	 0.5609	 0.5230
H	 0.8223	 0.6090
I	 0.8055	 0.6060
J	 0.8596	 0.6310
K	 0.6986	 0.5790
L	 0.8592	 0.6420
M	 0.8583	 0.6250
N	 0.8627	 0.6370
O	 0.7463	 0.5850
P	 0.9332	 0.6580
Q	 0.9323	 0.6550
S	 0.9094	 0.6370
T	 0.8352	 0.6340
U	 0.7941	 0.6100
V	 0.6978	 0.5990
W	 0.8279	 0.6130
X	 0.7746	 0.5990
Y	 0.7258	 0.5610
Z	 0.6816	 0.5540
a	 0.8394	 0.6350
b	 0.7746	 0.5870
c	 0.8387	 0.6220
d	 0.8000	 0.6120
e	 0.7695	 0.6000
f	 0.6270	 0.5450
g	 0.8188	 0.6220
h	 0.8266	 0.6110
i	 0.9381	 0.6510
j	 0.8610	 0.6350



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.9353	 0.6490
l	 0.8749	 0.6330
m	 0.7900	 0.5920
n	 0.6975	 0.5830
o	 0.8537	 0.6300
p	 0.8341	 0.6220
r	 0.9374	 0.6480
s	 0.9085	 0.6460
u	 0.8316	 0.6180
v	 0.7120	 0.5680
w	 0.8080	 0.6040