



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 03:09 AM JST

PDB ID : 6L7O / pdb_00006l7o
EMDB ID : EMD-0849
Title : cryo-EM structure of cyanobacteria Fd-NDH-1L complex
Authors : Zhang, C.; Shuai, J.; Wu, J.; Lei, M.
Deposited on : 2019-11-02
Resolution : 3.20 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:

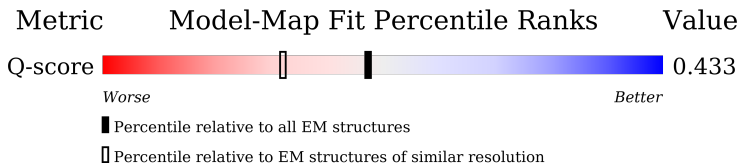
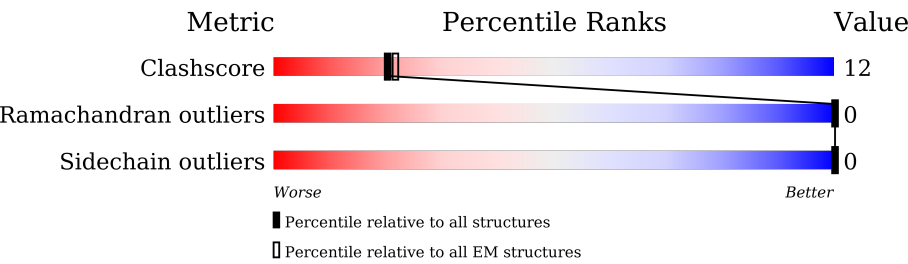
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	372	12% 81% 19%
2	B	515	• 79% 17% •
3	C	132	10% 72% 20% 8%
4	D	529	5% 74% 21% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	101	
6	F	656	
7	G	200	
8	H	394	
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	44	
17	Q	45	
18	R	98	
19	S	110	
20	V	146	

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
24	AJP	A	405	X	-	-	-
24	AJP	A	406	X	-	-	-
24	AJP	A	407	X	-	-	-
24	AJP	A	408	X	-	-	-
24	AJP	A	409	X	-	-	-
24	AJP	B	606	X	-	-	-
24	AJP	B	607	X	-	-	-
24	AJP	B	608	X	-	-	-
24	AJP	B	609	X	-	-	-
24	AJP	B	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	B	611	X	-	-	-
24	AJP	B	612	X	-	-	-
24	AJP	B	613	X	-	-	-
24	AJP	B	614	X	-	-	-
24	AJP	B	615	X	-	-	-
24	AJP	B	616	X	-	X	-
24	AJP	B	617	X	-	-	-
24	AJP	C	201	X	-	-	-
24	AJP	C	202	X	-	-	-
24	AJP	D	603	X	-	-	-
24	AJP	D	604	X	-	-	-
24	AJP	D	605	X	-	-	-
24	AJP	D	606	X	-	-	-
24	AJP	D	607	X	-	-	-
24	AJP	D	608	X	-	-	-
24	AJP	D	609	X	-	-	-
24	AJP	D	610	X	-	-	-
24	AJP	D	611	X	-	-	-
24	AJP	D	612	X	-	-	-
24	AJP	D	613	X	-	-	-
24	AJP	D	614	X	-	-	-
24	AJP	E	201	X	-	-	-
24	AJP	F	706	X	-	-	-
24	AJP	F	707	X	-	-	-
24	AJP	F	708	X	-	-	-
24	AJP	F	709	X	-	-	-
24	AJP	F	710	X	-	-	-
24	AJP	F	711	X	-	-	-
24	AJP	F	712	X	-	-	-
24	AJP	F	713	X	-	-	-
24	AJP	F	714	X	-	-	-
24	AJP	F	715	X	-	-	-
24	AJP	F	716	X	-	-	-
24	AJP	F	717	X	-	-	-
24	AJP	F	718	X	-	-	-
24	AJP	G	301	X	-	-	-
24	AJP	G	302	X	-	-	-
24	AJP	G	303	X	-	-	-
24	AJP	G	304	X	-	-	-
24	AJP	G	305	X	-	-	-
24	AJP	G	306	X	-	-	-
24	AJP	G	307	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	Q	101	X	-	-	-
24	AJP	Q	102	X	-	-	-
24	AJP	Q	103	X	-	-	-
24	AJP	Q	104	X	-	-	-
24	AJP	Q	105	X	-	-	-
24	AJP	Q	106	X	-	-	-
24	AJP	Q	107	X	-	-	-
24	AJP	Q	108	X	-	-	-
27	SF4	K	301	-	-	X	-
28	FES	R	101	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 35037 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2859	1919	444	486	10		

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	493	Total	C	N	O	S	0	0
			3732	2476	579	661	16		

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total	C	N	O	S	0	0
			978	669	150	155	4		

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	504	Total	C	N	O	S	0	0
			3896	2613	606	656	21		

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	101	Total	C	N	O	S	0	0
			783	517	128	134	4		

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	647	Total	C	N	O	S	0	0
			5004	3318	796	852	38		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	192	Total	C	N	O	S	0	0
			1463	974	229	256	4		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3177	2048	545	565	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1525	973	262	277	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	156	Total	C	N	O	S	0	0
			1278	817	218	238	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1597	1024	276	284	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	73	Total	C	N	O	S	0	0
			590	406	90	93	1		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			879	548	160	169	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1165	758	201	205	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	41	Total	C	N	O	S	0	0
			321	212	52	55	2		

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	44	Total	C	N	O	S	0	0
			332	221	53	56	2		

- Molecule 18 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	97	Total	C	N	O	S	0	0
			748	463	116	164	5		

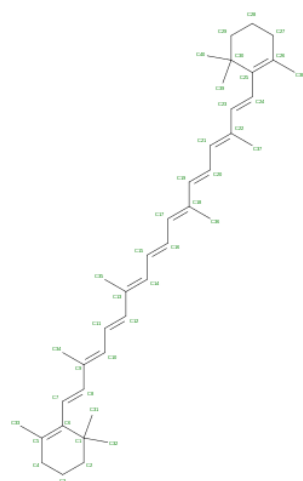
- Molecule 19 is a protein called Thr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	62	Total	C	N	O	S	0	0
			485	314	76	93	2		

- Molecule 20 is a protein called Thr0472 protein.

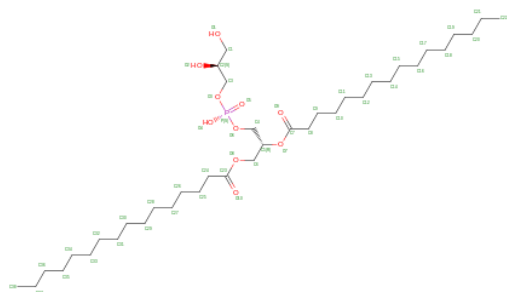
Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	103	Total	C	N	O	S	0	0
			797	517	133	143	4		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



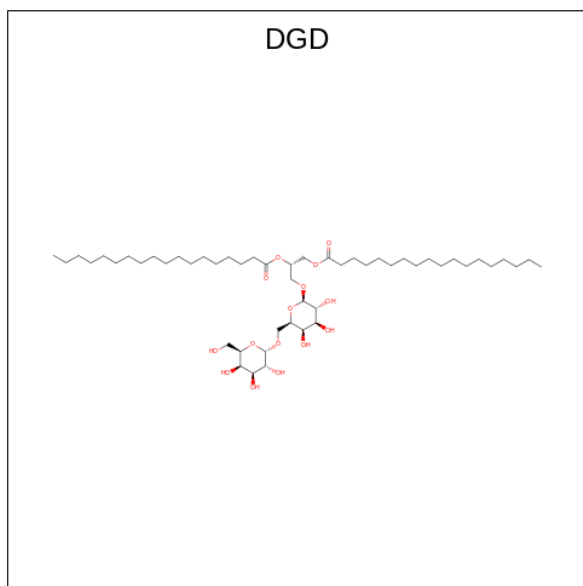
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	P	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



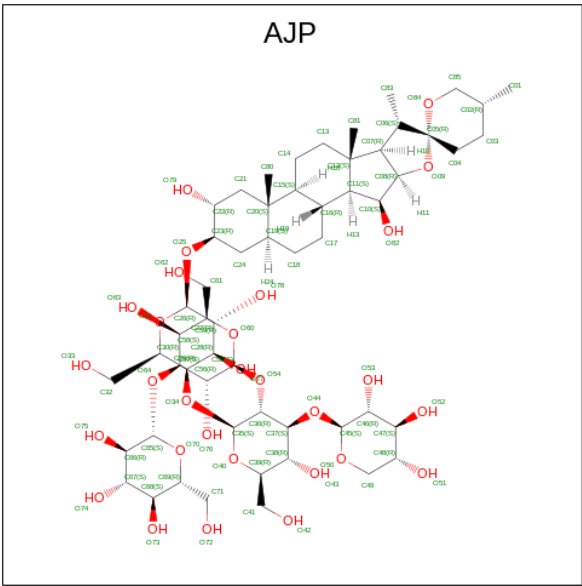
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	H	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			66	51	15	
23	A	1	Total	C	O	0
			66	51	15	

- Molecule 24 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			32	27	5	
24	A	1	Total	C	O	0
			32	27	5	
24	A	1	Total	C	O	0
			32	27	5	
24	A	1	Total	C	O	0
			32	27	5	
24	A	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	B	1	Total	C	O	0
			32	27	5	
24	C	1	Total	C	O	0
			32	27	5	
24	C	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	D	1	Total	C	O	0
			32	27	5	
24	E	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	

Continued on next page...

Continued from previous page...

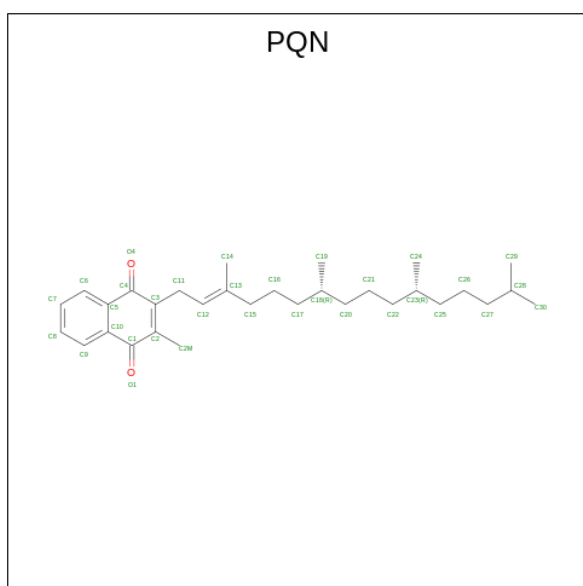
Mol	Chain	Residues	Atoms			AltConf
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	F	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	G	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	

Continued on next page...

Continued from previous page...

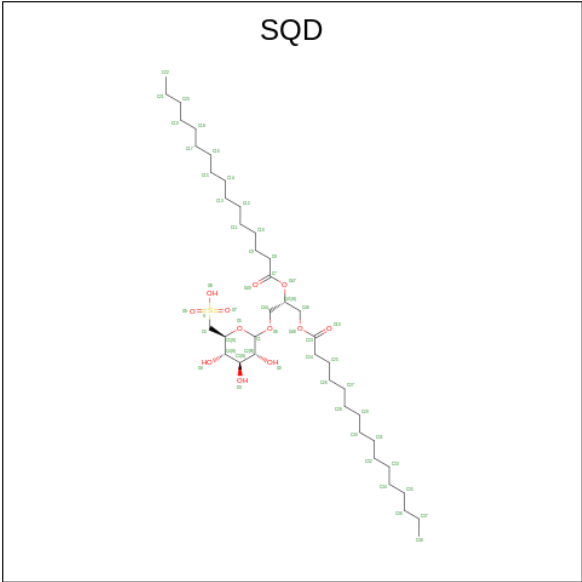
Mol	Chain	Residues	Atoms			AltConf
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	
24	Q	1	Total	C	O	0
			32	27	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



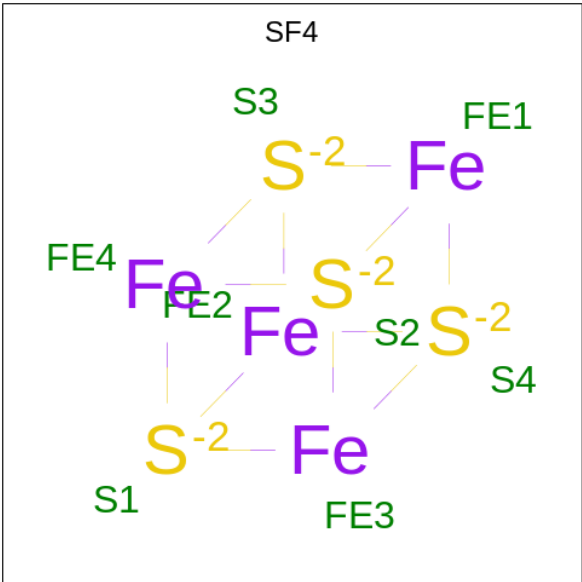
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



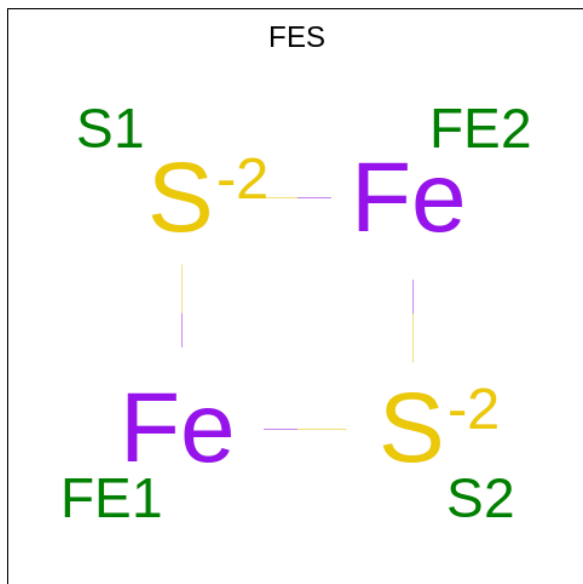
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	F	1	Total	C	O	S	0
			54	41	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
27	I	1	Total	Fe	S	0
			8	4	4	
27	I	1	Total	Fe	S	0
			8	4	4	
27	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

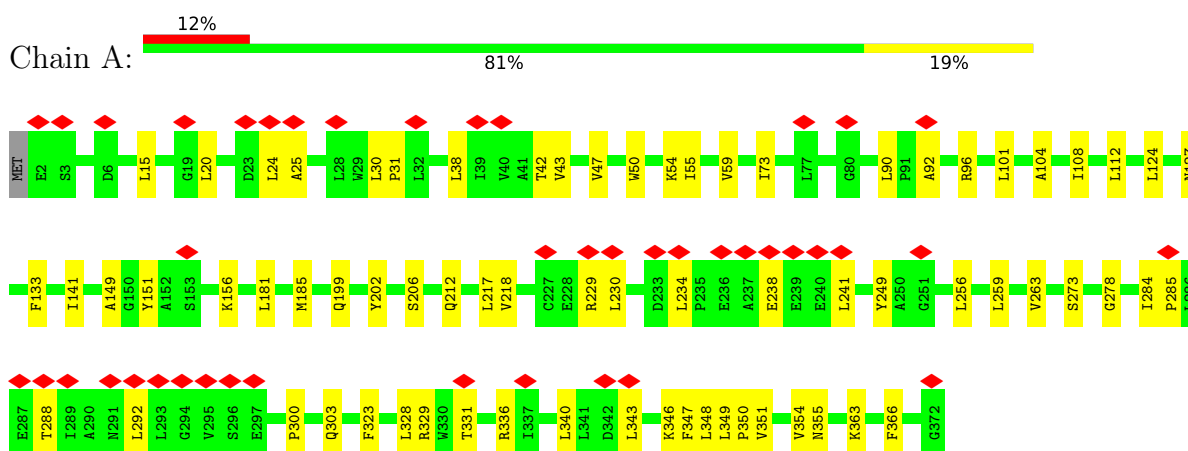


Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total	Fe	S	0
			4	2	2	

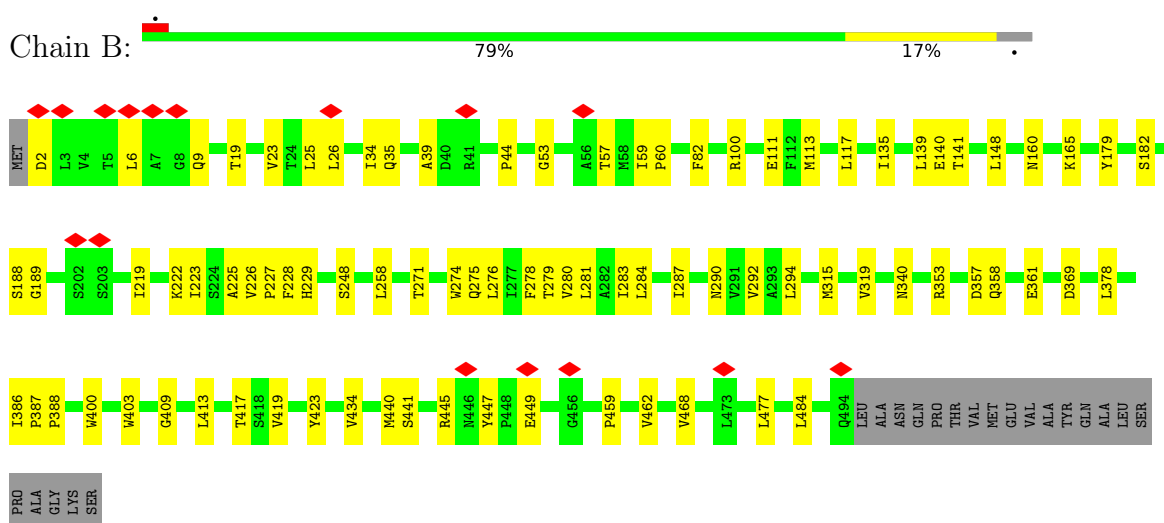
3 Residue-property plots

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: NAD(P)H-quinone oxidoreductase subunit 1

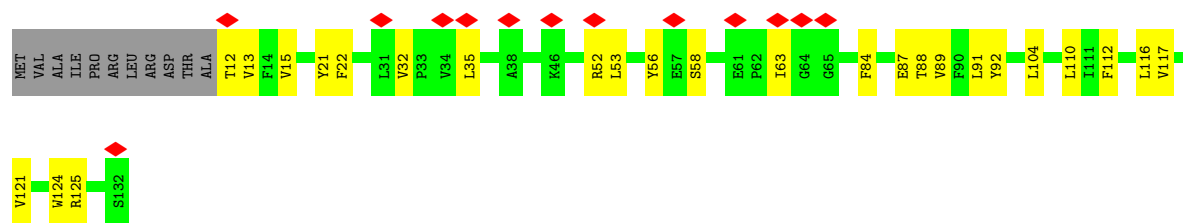


• Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

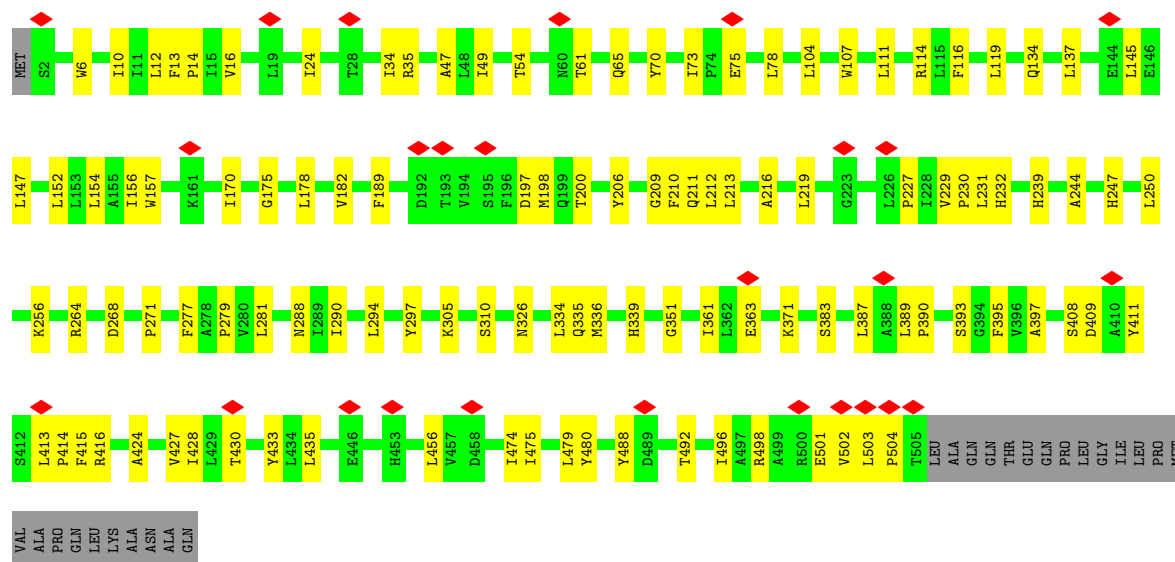
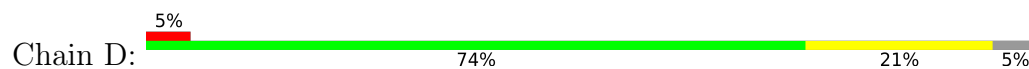


• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

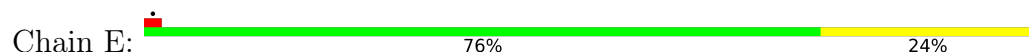




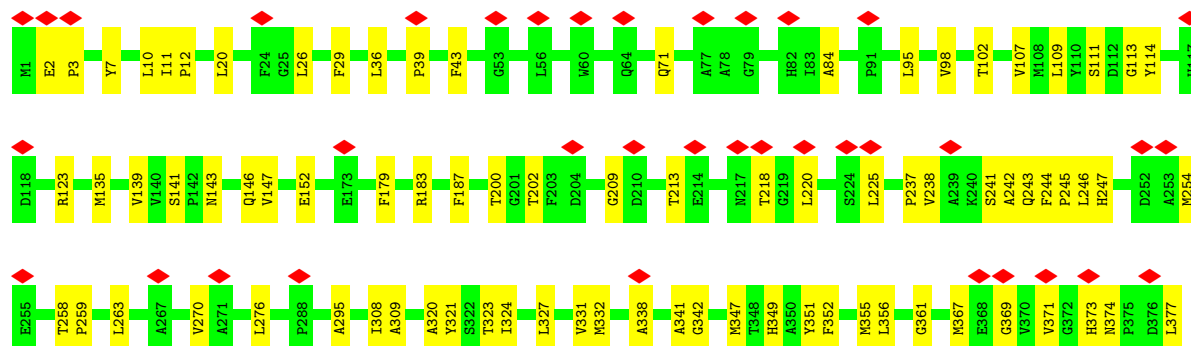
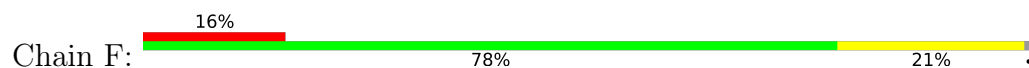
- Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

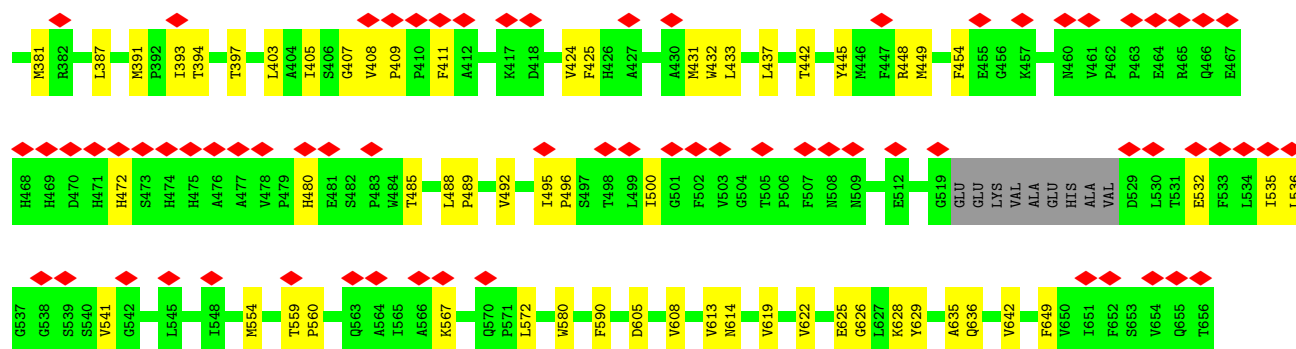


- Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

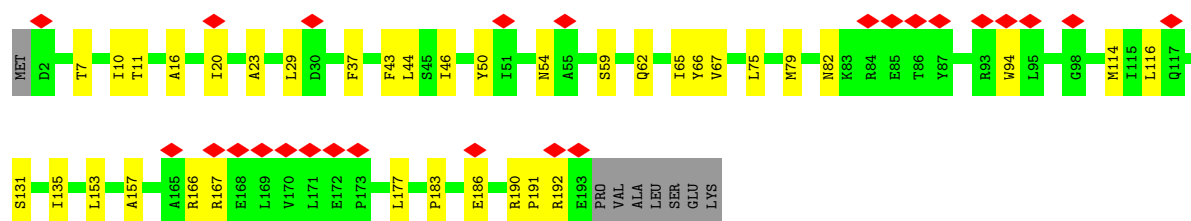
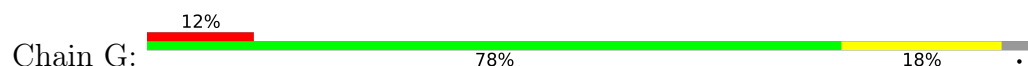


- Molecule 6: NADH dehydrogenase subunit 5

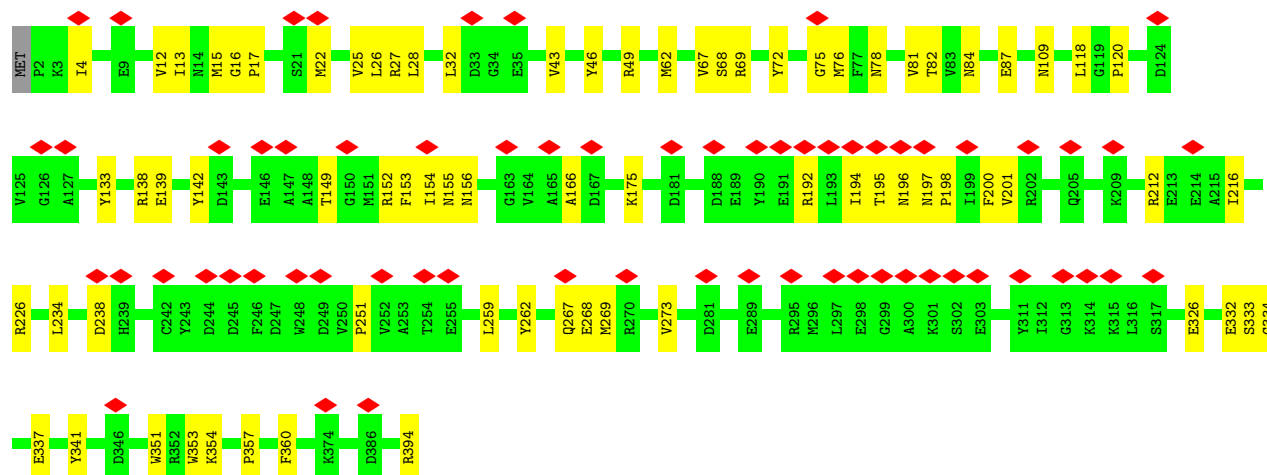
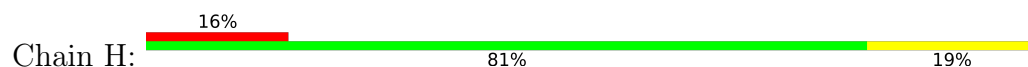




• Molecule 7: NADH-quinone oxidoreductase subunit J

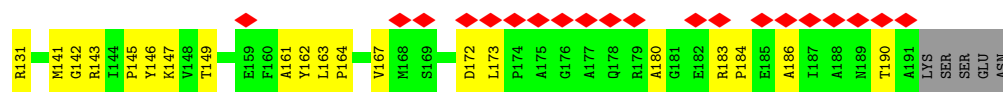


• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

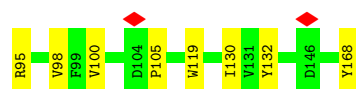
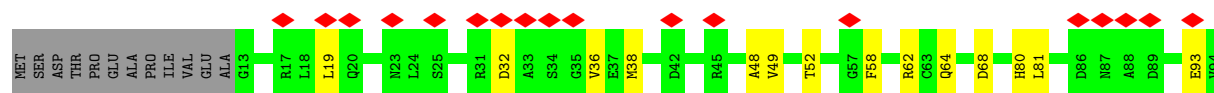
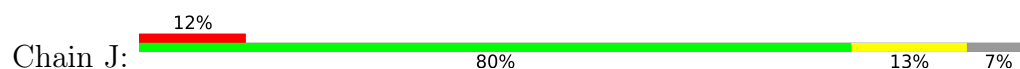


• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

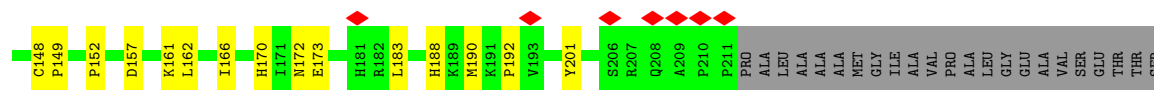
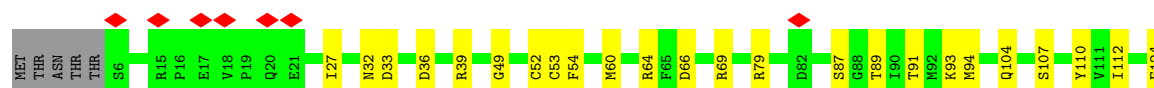




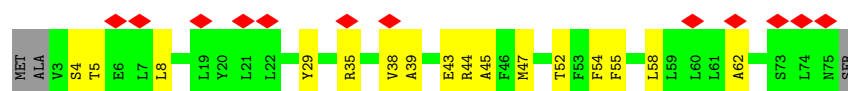
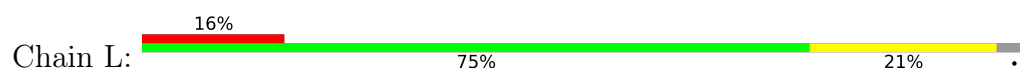
- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J



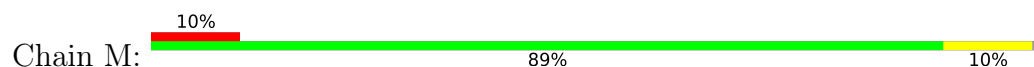
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit K



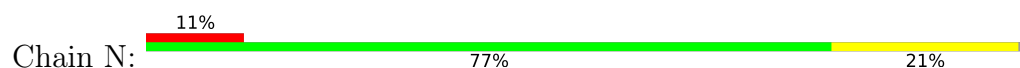
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

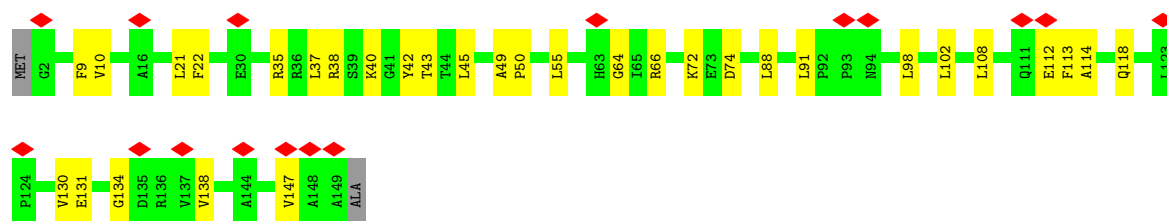


- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

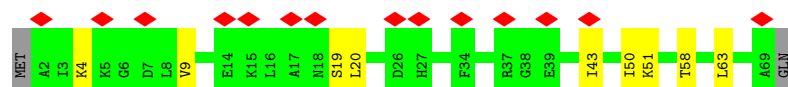
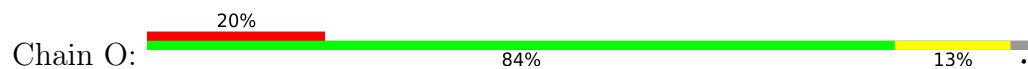


- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

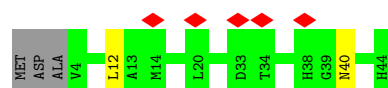
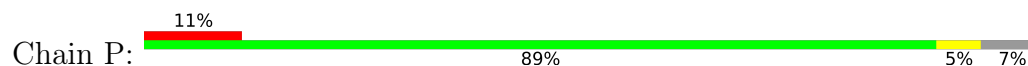




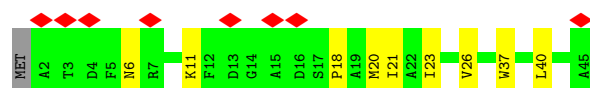
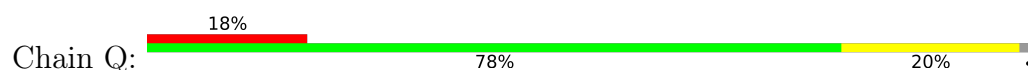
- Molecule 15: NAD(P)H-quinone oxidoreductase subunit O



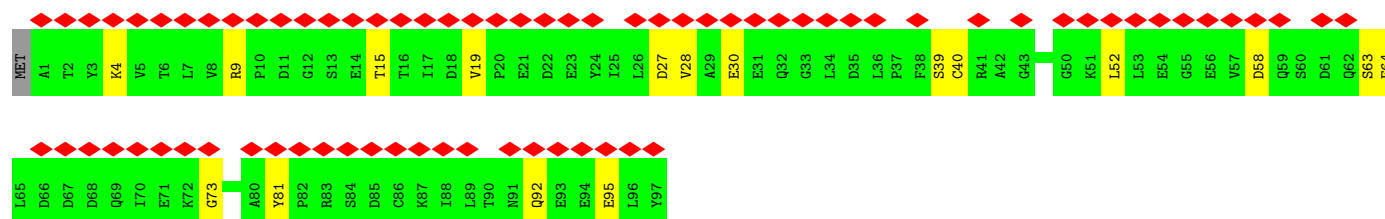
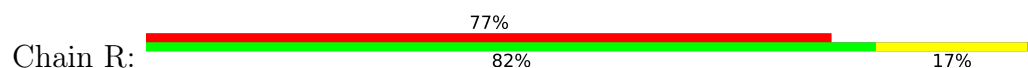
- Molecule 16: NAD(P)H-quinone oxidoreductase subunit P



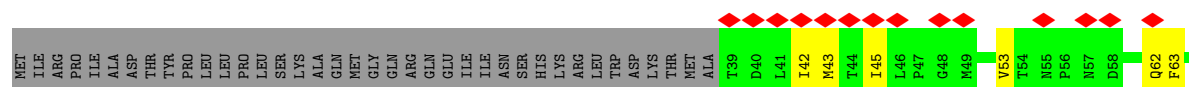
- Molecule 17: NAD(P)H-quinone oxidoreductase subunit Q

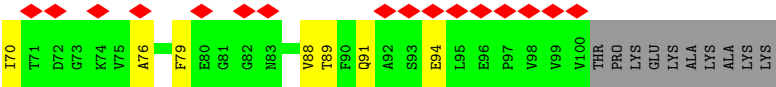


- Molecule 18: Ferredoxin-1

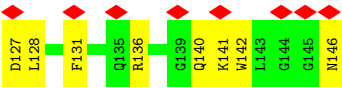
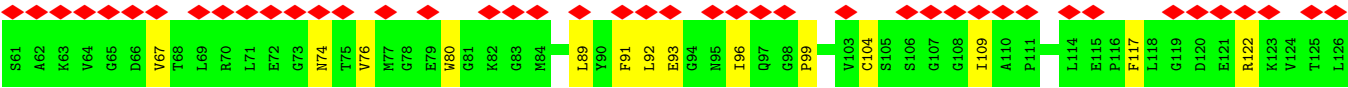
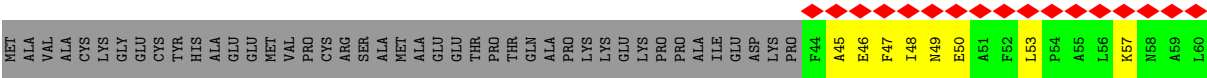


- Molecule 19: Thr0636 protein





• Molecule 20: Thr0472 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338822	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	327.0, 327.0, 327.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: DGD, SF4, PQN, SQD, AJP, LHG, BCR, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.13	0/2932	0.36	0/4008
2	B	0.11	0/3818	0.30	0/5209
3	C	0.14	0/1008	0.38	0/1375
4	D	0.11	0/4003	0.32	0/5464
5	E	0.10	0/793	0.29	0/1077
6	F	0.11	0/5153	0.30	0/7020
7	G	0.10	0/1495	0.28	0/2050
8	H	0.11	0/3260	0.32	0/4417
9	I	0.11	0/1563	0.32	0/2119
10	J	0.10	0/1314	0.28	0/1789
11	K	0.14	0/1638	0.33	0/2230
12	L	0.12	0/610	0.34	0/835
13	M	0.08	0/895	0.27	0/1214
14	N	0.10	0/1197	0.29	0/1628
15	O	0.10	0/550	0.31	0/748
16	P	0.14	0/330	0.46	0/448
17	Q	0.09	0/341	0.29	0/464
18	R	0.11	0/758	0.32	0/1029
19	S	0.10	0/494	0.33	0/674
20	V	0.15	0/814	0.47	1/1097 (0.1%)
All	All	0.11	0/32966	0.32	1/44895 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	96	ILE	N-CA-C	-6.53	107.51	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2859	0	2983	71	0
2	B	3732	0	3864	109	0
3	C	978	0	1008	43	0
4	D	3896	0	4041	129	0
5	E	783	0	837	20	0
6	F	5004	0	5033	128	0
7	G	1463	0	1546	52	0
8	H	3177	0	3155	58	0
9	I	1525	0	1500	32	0
10	J	1278	0	1233	15	0
11	K	1597	0	1628	35	0
12	L	590	0	602	12	0
13	M	879	0	860	9	0
14	N	1165	0	1176	28	0
15	O	538	0	549	7	0
16	P	321	0	317	2	0
17	Q	332	0	331	11	0
18	R	748	0	709	11	0
19	S	485	0	488	9	0
20	V	797	0	800	22	0
21	A	40	0	55	4	0
21	F	40	0	54	3	0
21	P	40	0	54	5	0
22	A	49	0	73	3	0
22	B	147	0	222	4	0
22	D	98	0	148	1	0
22	F	98	0	145	8	0
22	H	49	0	73	3	0
23	A	132	0	191	3	0
24	A	160	0	0	26	0
24	B	384	0	0	84	0
24	C	64	0	0	17	0
24	D	384	0	0	99	0
24	E	32	0	0	1	0
24	F	416	0	0	65	0
24	G	224	0	0	43	0
24	Q	256	0	0	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	33	0	44	0	0
26	B	54	0	78	3	0
26	F	108	0	156	6	0
26	L	54	0	77	1	0
27	I	16	0	0	0	0
27	K	8	0	0	3	0
28	R	4	0	0	2	0
All	All	35037	0	34030	840	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 12.

The worst 5 of 840 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)
4:D:413:LEU:HD21	24:D:608:AJP:C80	1.23	1.64
2:B:484:LEU:HD11	24:B:606:AJP:C13	1.27	1.60
2:B:287:ILE:CD1	24:B:616:AJP:C83	1.75	1.59
7:G:7:THR:HG22	24:G:302:AJP:C83	1.18	1.56
6:F:39:PRO:HB3	24:F:714:AJP:C83	1.23	1.55

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	369/372 (99%)	342 (93%)	27 (7%)	0	100	100
2	B	491/515 (95%)	472 (96%)	19 (4%)	0	100	100
3	C	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
4	D	502/529 (95%)	477 (95%)	25 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	F	643/656 (98%)	613 (95%)	30 (5%)	0	100	100
7	G	190/200 (95%)	183 (96%)	7 (4%)	0	100	100
8	H	391/394 (99%)	359 (92%)	32 (8%)	0	100	100
9	I	188/196 (96%)	177 (94%)	11 (6%)	0	100	100
10	J	154/168 (92%)	147 (96%)	7 (4%)	0	100	100
11	K	204/237 (86%)	193 (95%)	11 (5%)	0	100	100
12	L	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
13	M	108/111 (97%)	100 (93%)	8 (7%)	0	100	100
14	N	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
15	O	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
16	P	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
17	Q	42/45 (93%)	42 (100%)	0	0	100	100
18	R	95/98 (97%)	95 (100%)	0	0	100	100
19	S	60/110 (54%)	58 (97%)	2 (3%)	0	100	100
20	V	101/146 (69%)	93 (92%)	8 (8%)	0	100	100
All	All	4078/4350 (94%)	3863 (95%)	215 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/302 (99%)	300 (100%)	0	100	100
2	B	396/413 (96%)	396 (100%)	0	100	100
3	C	100/109 (92%)	100 (100%)	0	100	100
4	D	404/424 (95%)	404 (100%)	0	100	100
5	E	82/82 (100%)	82 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	519/527 (98%)	519 (100%)	0	100	100
7	G	159/166 (96%)	159 (100%)	0	100	100
8	H	337/338 (100%)	337 (100%)	0	100	100
9	I	166/172 (96%)	166 (100%)	0	100	100
10	J	138/148 (93%)	138 (100%)	0	100	100
11	K	175/196 (89%)	175 (100%)	0	100	100
12	L	61/63 (97%)	61 (100%)	0	100	100
13	M	95/96 (99%)	95 (100%)	0	100	100
14	N	119/120 (99%)	119 (100%)	0	100	100
15	O	57/59 (97%)	57 (100%)	0	100	100
16	P	35/37 (95%)	35 (100%)	0	100	100
17	Q	31/32 (97%)	31 (100%)	0	100	100
18	R	85/86 (99%)	85 (100%)	0	100	100
19	S	55/97 (57%)	55 (100%)	0	100	100
20	V	83/118 (70%)	83 (100%)	0	100	100
All	All	3397/3585 (95%)	3397 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	95	HIS
11	K	170	HIS
9	I	116	ASN
11	K	20	GLN
13	M	23	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

83 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	AJP	F	718	-	37,37,95	1.18	5 (13%)	58,62,149	2.29	16 (27%)
24	AJP	G	305	-	37,37,95	1.27	8 (21%)	58,62,149	2.19	17 (29%)
27	SF4	K	301	11	0,12,12	-	-	-		
24	AJP	F	710	-	37,37,95	1.34	4 (10%)	58,62,149	2.32	19 (32%)
24	AJP	F	715	-	37,37,95	1.17	5 (13%)	58,62,149	2.21	15 (25%)
24	AJP	Q	106	-	37,37,95	1.11	6 (16%)	58,62,149	2.16	17 (29%)
24	AJP	D	614	-	37,37,95	1.25	7 (18%)	58,62,149	2.22	18 (31%)
23	DGD	A	404	1	67,67,67	0.86	2 (2%)	81,81,81	1.42	11 (13%)
24	AJP	G	306	-	37,37,95	1.40	7 (18%)	58,62,149	2.23	19 (32%)
24	AJP	Q	105	-	37,37,95	1.16	5 (13%)	58,62,149	2.15	17 (29%)
27	SF4	I	201	9	0,12,12	-	-	-		
22	LHG	B	603	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
24	AJP	D	604	-	37,37,95	1.52	7 (18%)	58,62,149	2.45	20 (34%)
24	AJP	F	713	-	37,37,95	1.36	7 (18%)	58,62,149	2.24	18 (31%)
24	AJP	A	407	-	37,37,95	1.26	6 (16%)	58,62,149	2.25	17 (29%)
22	LHG	B	604	-	48,48,48	0.60	0	51,54,54	1.25	6 (11%)
24	AJP	F	707	-	37,37,95	1.39	8 (21%)	58,62,149	2.20	18 (31%)
24	AJP	C	202	-	37,37,95	1.37	8 (21%)	58,62,149	2.21	17 (29%)
24	AJP	D	608	-	37,37,95	1.30	6 (16%)	58,62,149	2.29	19 (32%)
24	AJP	D	613	24	37,37,95	1.22	5 (13%)	58,62,149	2.33	19 (32%)
22	LHG	F	702	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	B	609	-	37,37,95	1.27	7 (18%)	58,62,149	2.26	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	AJP	D	606	-	37,37,95	1.36	6 (16%)	58,62,149	2.23	18 (31%)
24	AJP	F	706	-	37,37,95	1.30	6 (16%)	58,62,149	2.15	19 (32%)
24	AJP	B	606	-	37,37,95	1.49	7 (18%)	58,62,149	2.38	19 (32%)
21	BCR	A	401	1	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
24	AJP	A	405	-	37,37,95	1.34	6 (16%)	58,62,149	2.22	16 (27%)
24	AJP	B	614	-	37,37,95	1.18	6 (16%)	58,62,149	2.11	16 (27%)
24	AJP	B	617	-	37,37,95	1.18	6 (16%)	58,62,149	2.19	18 (31%)
24	AJP	G	302	-	37,37,95	1.28	6 (16%)	58,62,149	2.22	18 (31%)
22	LHG	A	402	1	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
28	FES	R	101	18	0,4,4	-	-	-	-	-
24	AJP	B	610	-	37,37,95	1.28	8 (21%)	58,62,149	2.20	16 (27%)
24	AJP	A	408	-	37,37,95	1.32	8 (21%)	58,62,149	2.23	19 (32%)
22	LHG	B	602	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
24	AJP	F	708	-	37,37,95	1.33	7 (18%)	58,62,149	2.24	19 (32%)
24	AJP	B	613	-	37,37,95	1.32	7 (18%)	58,62,149	2.17	19 (32%)
24	AJP	D	611	-	37,37,95	1.24	6 (16%)	58,62,149	2.24	16 (27%)
24	AJP	F	717	-	37,37,95	1.26	7 (18%)	58,62,149	2.38	18 (31%)
24	AJP	D	607	-	37,37,95	1.26	5 (13%)	58,62,149	2.30	17 (29%)
21	BCR	F	701	6	41,41,41	1.07	2 (4%)	56,56,56	1.25	6 (10%)
22	LHG	D	602	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	F	709	-	37,37,95	1.30	6 (16%)	58,62,149	2.21	20 (34%)
24	AJP	A	409	-	37,37,95	1.21	5 (13%)	58,62,149	2.25	19 (32%)
24	AJP	G	304	-	37,37,95	1.34	8 (21%)	58,62,149	2.21	19 (32%)
21	BCR	P	101	16	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
24	AJP	Q	104	-	37,37,95	1.26	7 (18%)	58,62,149	2.13	19 (32%)
24	AJP	D	609	24	37,37,95	1.35	7 (18%)	58,62,149	2.34	13 (22%)
24	AJP	F	711	-	37,37,95	1.30	7 (18%)	58,62,149	2.24	17 (29%)
24	AJP	F	712	6	37,37,95	1.16	4 (10%)	58,62,149	2.14	16 (27%)
24	AJP	G	301	-	37,37,95	1.51	7 (18%)	58,62,149	2.32	20 (34%)
24	AJP	D	603	-	37,37,95	1.55	8 (21%)	58,62,149	2.26	20 (34%)
24	AJP	F	714	-	37,37,95	1.38	8 (21%)	58,62,149	2.24	18 (31%)
24	AJP	B	607	-	37,37,95	1.28	6 (16%)	58,62,149	2.17	17 (29%)
24	AJP	D	610	-	37,37,95	1.42	7 (18%)	58,62,149	2.26	21 (36%)
26	SQD	F	704	-	53,54,54	0.95	4 (7%)	62,65,65	1.49	9 (14%)
24	AJP	E	201	-	37,37,95	1.30	7 (18%)	58,62,149	2.23	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	F	705	-	53,54,54	0.96	5 (9%)	62,65,65	1.49	9 (14%)
24	AJP	C	201	-	37,37,95	1.30	7 (18%)	58,62,149	2.18	16 (27%)
27	SF4	I	202	9	0,12,12	-	-	-	-	-
24	AJP	Q	107	17	37,37,95	1.24	7 (18%)	58,62,149	2.18	18 (31%)
22	LHG	F	703	6	48,48,48	0.58	1 (2%)	51,54,54	1.24	6 (11%)
24	AJP	D	605	-	37,37,95	1.25	6 (16%)	58,62,149	2.19	18 (31%)
24	AJP	B	611	2	37,37,95	1.44	9 (24%)	58,62,149	2.40	19 (32%)
22	LHG	D	601	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
24	AJP	G	303	-	37,37,95	1.30	8 (21%)	58,62,149	2.42	16 (27%)
23	DGD	A	403	-	67,67,67	0.84	2 (2%)	81,81,81	1.42	12 (14%)
24	AJP	B	616	-	37,37,95	1.33	7 (18%)	58,62,149	2.24	18 (31%)
24	AJP	Q	108	-	37,37,95	1.24	7 (18%)	58,62,149	2.18	16 (27%)
25	PQN	B	601	2	34,34,34	2.84	9 (26%)	42,45,45	2.04	6 (14%)
24	AJP	F	716	-	37,37,95	1.54	8 (21%)	58,62,149	2.26	19 (32%)
24	AJP	A	406	-	37,37,95	1.27	3 (8%)	58,62,149	2.26	19 (32%)
24	AJP	Q	103	-	37,37,95	1.29	6 (16%)	58,62,149	2.24	18 (31%)
22	LHG	H	401	8	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
24	AJP	B	608	-	37,37,95	1.15	6 (16%)	58,62,149	2.13	16 (27%)
24	AJP	G	307	-	37,37,95	1.25	5 (13%)	58,62,149	2.23	15 (25%)
26	SQD	B	605	-	53,54,54	0.95	5 (9%)	62,65,65	1.48	9 (14%)
24	AJP	Q	102	-	37,37,95	1.47	7 (18%)	58,62,149	2.37	18 (31%)
24	AJP	B	612	-	37,37,95	1.29	6 (16%)	58,62,149	2.33	18 (31%)
24	AJP	B	615	-	37,37,95	1.17	6 (16%)	58,62,149	2.13	16 (27%)
24	AJP	D	612	-	37,37,95	1.26	5 (13%)	58,62,149	2.24	18 (31%)
26	SQD	L	101	12	53,54,54	0.96	5 (9%)	62,65,65	1.51	10 (16%)
24	AJP	Q	101	-	37,37,95	1.23	7 (18%)	58,62,149	2.15	16 (27%)

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
24	AJP	F	718	-	12/12/14/38	-	0/6/6/11
24	AJP	G	305	-	12/12/14/38	-	0/6/6/11
27	SF4	K	301	11	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	F	710	-	12/12/14/38	-	0/6/6/11
24	AJP	F	715	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	106	-	12/12/14/38	-	0/6/6/11
24	AJP	D	614	-	12/12/14/38	-	0/6/6/11
23	DGD	A	404	1	-	19/55/95/95	0/2/2/2
24	AJP	G	306	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	105	-	12/12/14/38	-	0/6/6/11
27	SF4	I	201	9	-	-	0/6/5/5
22	LHG	B	603	-	-	21/53/53/53	-
24	AJP	D	604	-	12/12/14/38	-	0/6/6/11
24	AJP	F	713	-	12/12/14/38	-	0/6/6/11
24	AJP	A	407	-	12/12/14/38	-	0/6/6/11
22	LHG	B	604	-	-	25/53/53/53	-
24	AJP	F	707	-	12/12/14/38	-	0/6/6/11
24	AJP	C	202	-	12/12/14/38	-	0/6/6/11
24	AJP	D	608	-	12/12/14/38	-	0/6/6/11
24	AJP	D	613	24	12/12/14/38	-	0/6/6/11
22	LHG	F	702	-	-	25/53/53/53	-
24	AJP	B	609	-	12/12/14/38	-	0/6/6/11
24	AJP	D	606	-	12/12/14/38	-	0/6/6/11
24	AJP	F	706	-	12/12/14/38	-	0/6/6/11
24	AJP	B	606	-	12/12/14/38	-	0/6/6/11
21	BCR	A	401	1	-	10/29/63/63	0/2/2/2
24	AJP	A	405	-	12/12/14/38	-	0/6/6/11
24	AJP	B	614	-	12/12/14/38	-	0/6/6/11
24	AJP	B	617	-	12/12/14/38	-	0/6/6/11
24	AJP	G	302	-	12/12/14/38	-	0/6/6/11
22	LHG	A	402	1	-	20/53/53/53	-
28	FES	R	101	18	-	-	0/1/1/1
24	AJP	B	610	-	12/12/14/38	-	0/6/6/11
24	AJP	A	408	-	12/12/14/38	-	0/6/6/11
24	AJP	F	708	-	12/12/14/38	-	0/6/6/11
22	LHG	B	602	-	-	27/53/53/53	-
24	AJP	B	613	-	12/12/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	D	611	-	12/12/14/38	-	0/6/6/11
24	AJP	F	717	-	12/12/14/38	-	0/6/6/11
24	AJP	D	607	-	12/12/14/38	-	0/6/6/11
21	BCR	F	701	6	-	11/29/63/63	0/2/2/2
22	LHG	D	602	-	-	21/53/53/53	-
24	AJP	F	709	-	12/12/14/38	-	0/6/6/11
24	AJP	A	409	-	12/12/14/38	-	0/6/6/11
24	AJP	G	304	-	12/12/14/38	-	0/6/6/11
21	BCR	P	101	16	-	14/29/63/63	0/2/2/2
24	AJP	Q	104	-	12/12/14/38	-	0/6/6/11
24	AJP	D	609	24	12/12/14/38	-	0/6/6/11
24	AJP	F	711	-	12/12/14/38	-	0/6/6/11
24	AJP	F	712	6	12/12/14/38	-	0/6/6/11
24	AJP	G	301	-	12/12/14/38	-	0/6/6/11
24	AJP	D	603	-	12/12/14/38	-	0/6/6/11
24	AJP	F	714	-	12/12/14/38	-	0/6/6/11
24	AJP	B	607	-	12/12/14/38	-	0/6/6/11
24	AJP	D	610	-	12/12/14/38	-	0/6/6/11
26	SQD	F	704	-	-	20/49/69/69	0/1/1/1
24	AJP	E	201	-	12/12/14/38	-	0/6/6/11
26	SQD	F	705	-	-	16/49/69/69	0/1/1/1
24	AJP	C	201	-	12/12/14/38	-	0/6/6/11
27	SF4	I	202	9	-	-	0/6/5/5
24	AJP	Q	107	17	12/12/14/38	-	0/6/6/11
24	AJP	D	605	-	12/12/14/38	-	0/6/6/11
22	LHG	F	703	6	-	24/53/53/53	-
24	AJP	B	611	2	12/12/14/38	-	0/6/6/11
22	LHG	D	601	-	-	17/53/53/53	-
24	AJP	G	303	-	12/12/14/38	-	0/6/6/11
24	AJP	B	616	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	108	-	12/12/14/38	-	0/6/6/11
23	DGD	A	403	-	-	18/55/95/95	0/2/2/2
25	PQN	B	601	2	-	7/23/43/43	0/2/2/2
24	AJP	F	716	-	12/12/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	A	406	-	12/12/14/38	-	0/6/6/11
24	AJP	Q	103	-	12/12/14/38	-	0/6/6/11
22	LHG	H	401	8	-	25/53/53/53	-
24	AJP	B	608	-	12/12/14/38	-	0/6/6/11
24	AJP	G	307	-	12/12/14/38	-	0/6/6/11
26	SQD	B	605	-	-	14/49/69/69	0/1/1/1
24	AJP	Q	102	-	12/12/14/38	-	0/6/6/11
24	AJP	B	612	-	12/12/14/38	-	0/6/6/11
24	AJP	B	615	-	12/12/14/38	-	0/6/6/11
24	AJP	D	612	-	12/12/14/38	-	0/6/6/11
26	SQD	L	101	12	-	19/49/69/69	0/1/1/1
24	AJP	Q	101	-	12/12/14/38	-	0/6/6/11

The worst 5 of 432 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	PQN	C12-C13	8.24	1.52	1.33
25	B	601	PQN	O4-C4	8.17	1.40	1.23
25	B	601	PQN	O1-C1	8.10	1.40	1.23
25	B	601	PQN	C2-C1	-4.20	1.39	1.48
24	B	606	AJP	C16-C11	-4.04	1.48	1.54

The worst 5 of 1197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	609	AJP	C12-C07-C08	-9.56	94.56	104.88
24	B	612	AJP	C12-C07-C08	-9.22	94.92	104.88
24	D	607	AJP	C12-C07-C08	-9.19	94.95	104.88
24	G	307	AJP	C12-C07-C08	-9.19	94.95	104.88
24	F	711	AJP	C12-C07-C08	-9.18	94.96	104.88

5 of 720 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	AJP	C11
24	A	405	AJP	C22
24	A	405	AJP	C16
24	A	405	AJP	C20
24	A	405	AJP	C15

5 of 353 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	BCR	C1-C6-C7-C8
21	A	401	BCR	C23-C24-C25-C30
21	F	701	BCR	C7-C8-C9-C34
21	F	701	BCR	C21-C22-C23-C24
21	P	101	BCR	C1-C6-C7-C8

There are no ring outliers.

78 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	718	AJP	12	0
24	G	305	AJP	10	0
27	K	301	SF4	3	0
24	F	710	AJP	5	0
24	F	715	AJP	2	0
24	Q	106	AJP	5	0
24	D	614	AJP	4	0
23	A	404	DGD	2	0
24	G	306	AJP	6	0
24	Q	105	AJP	2	0
22	B	603	LHG	2	0
24	D	604	AJP	9	0
24	F	713	AJP	2	0
24	A	407	AJP	10	0
22	B	604	LHG	2	0
24	F	707	AJP	11	0
24	C	202	AJP	12	0
24	D	608	AJP	13	0
24	D	613	AJP	18	0
22	F	702	LHG	1	0
24	B	609	AJP	3	0
24	D	606	AJP	6	0
24	F	706	AJP	2	0
24	B	606	AJP	19	0
21	A	401	BCR	4	0
24	A	405	AJP	1	0
24	B	614	AJP	9	0
24	B	617	AJP	8	0
24	G	302	AJP	6	0
22	A	402	LHG	3	0
28	R	101	FES	2	0

Continued on next page...

Continued from previous page...

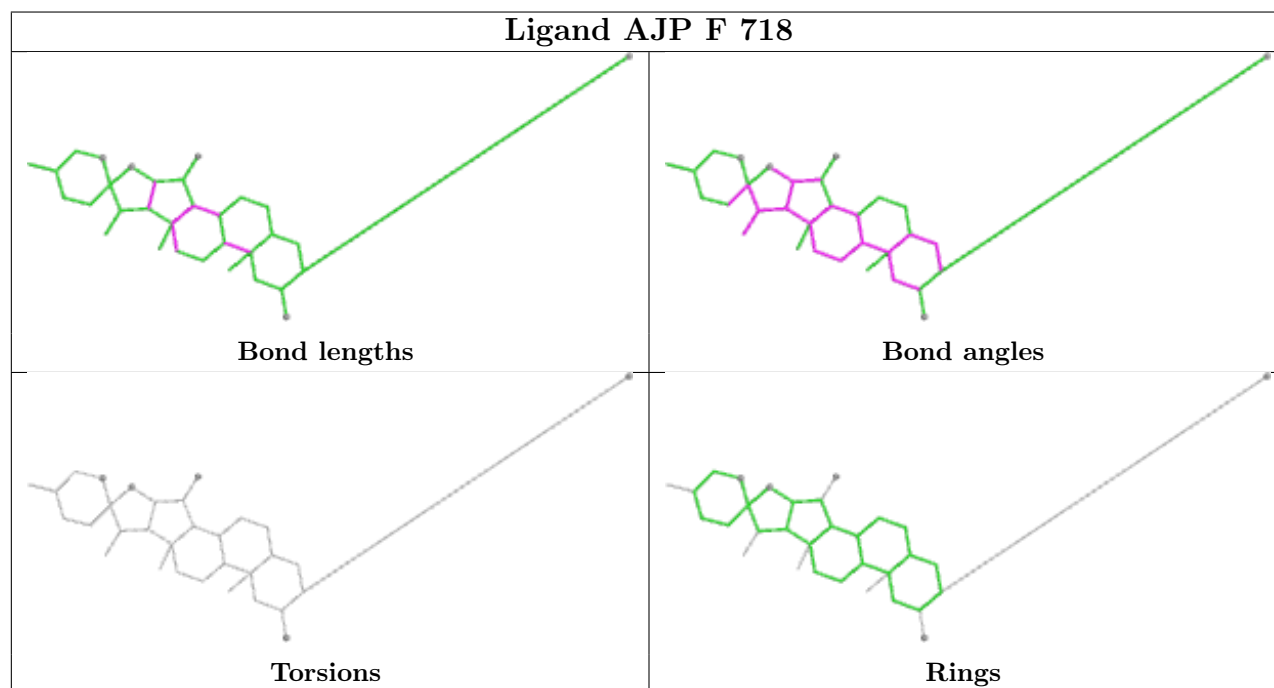
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	610	AJP	2	0
24	A	408	AJP	6	0
24	F	708	AJP	4	0
24	B	613	AJP	1	0
24	D	611	AJP	7	0
24	F	717	AJP	1	0
24	D	607	AJP	6	0
21	F	701	BCR	3	0
24	F	709	AJP	2	0
24	A	409	AJP	9	0
24	G	304	AJP	6	0
21	P	101	BCR	5	0
24	Q	104	AJP	1	0
24	D	609	AJP	9	0
24	F	711	AJP	8	0
24	F	712	AJP	11	0
24	G	301	AJP	10	0
24	D	603	AJP	4	0
24	F	714	AJP	8	0
24	B	607	AJP	5	0
24	D	610	AJP	10	0
26	F	704	SQD	5	0
24	E	201	AJP	1	0
26	F	705	SQD	1	0
24	C	201	AJP	5	0
24	Q	107	AJP	5	0
22	F	703	LHG	7	0
24	D	605	AJP	6	0
24	B	611	AJP	5	0
22	D	601	LHG	1	0
24	G	303	AJP	5	0
23	A	403	DGD	1	0
24	B	616	AJP	23	0
24	Q	108	AJP	1	0
24	F	716	AJP	3	0
24	A	406	AJP	2	0
24	Q	103	AJP	1	0
22	H	401	LHG	3	0
24	B	608	AJP	4	0
24	G	307	AJP	3	0
26	B	605	SQD	3	0
24	Q	102	AJP	7	0

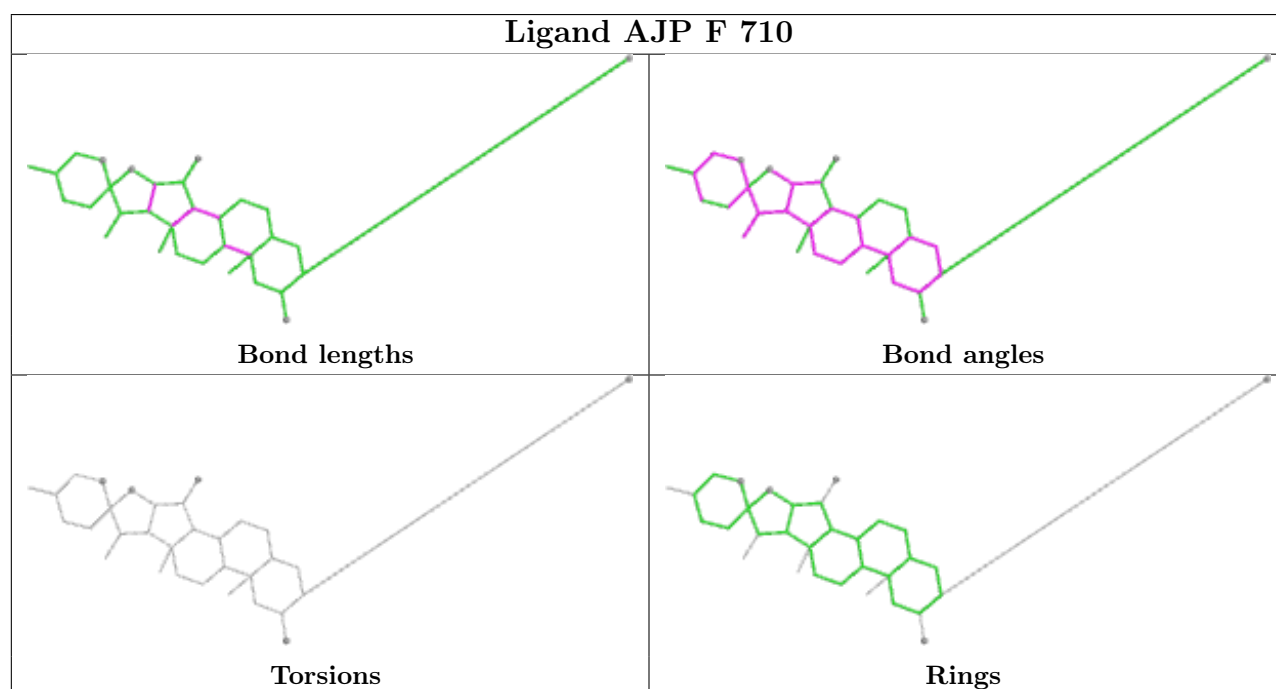
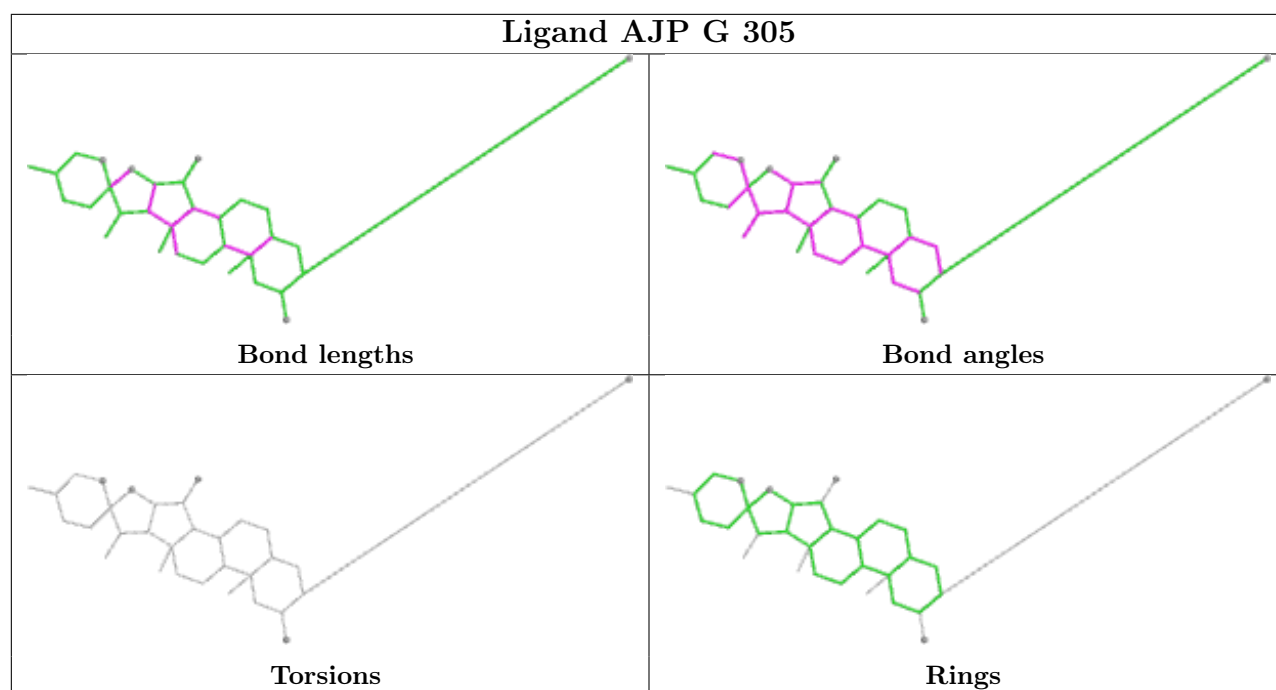
Continued on next page...

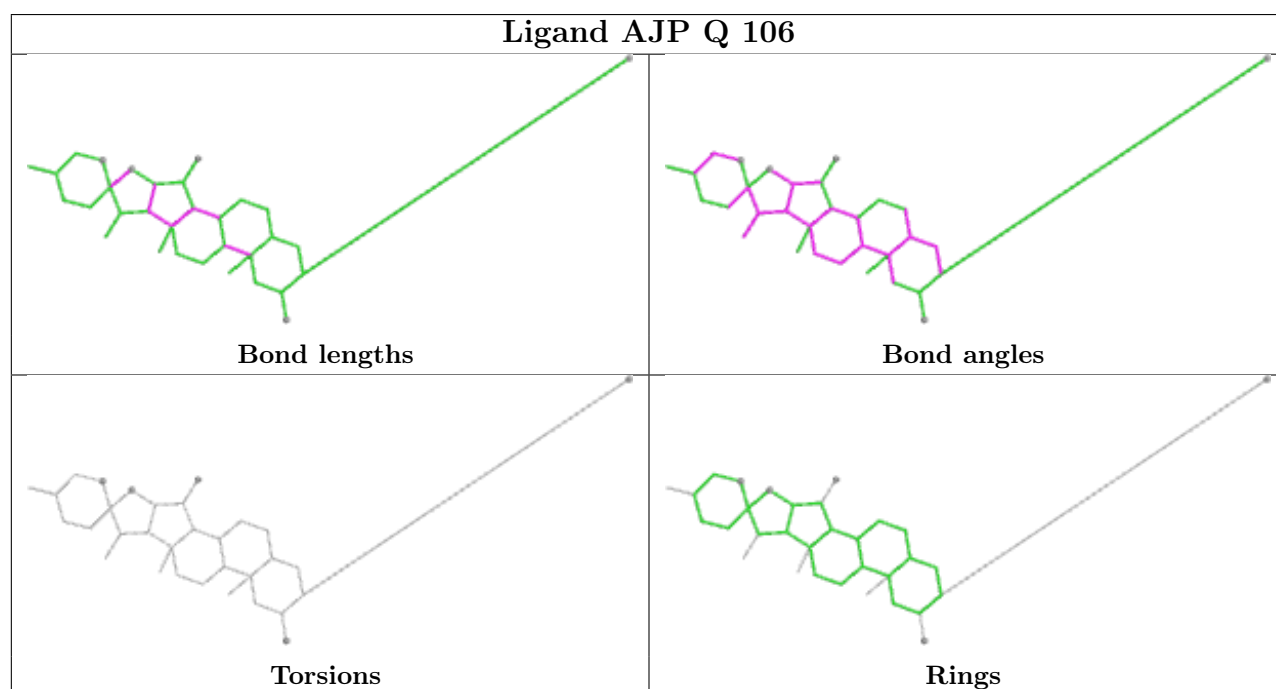
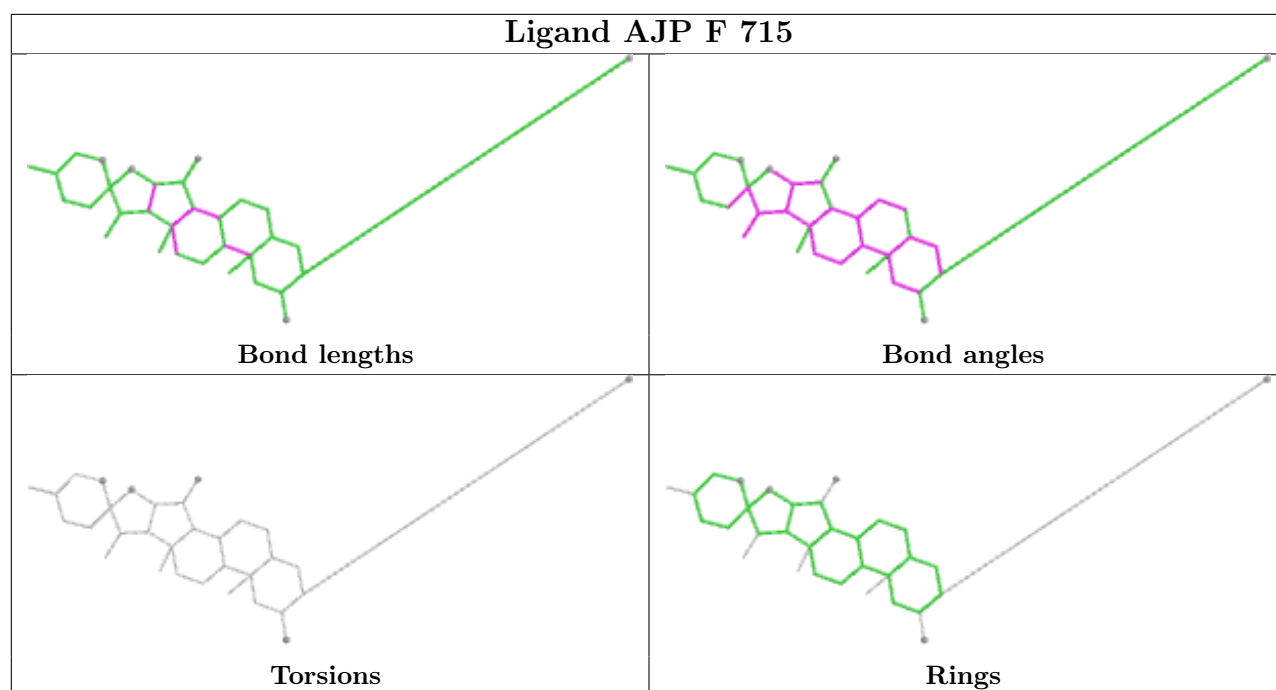
Continued from previous page...

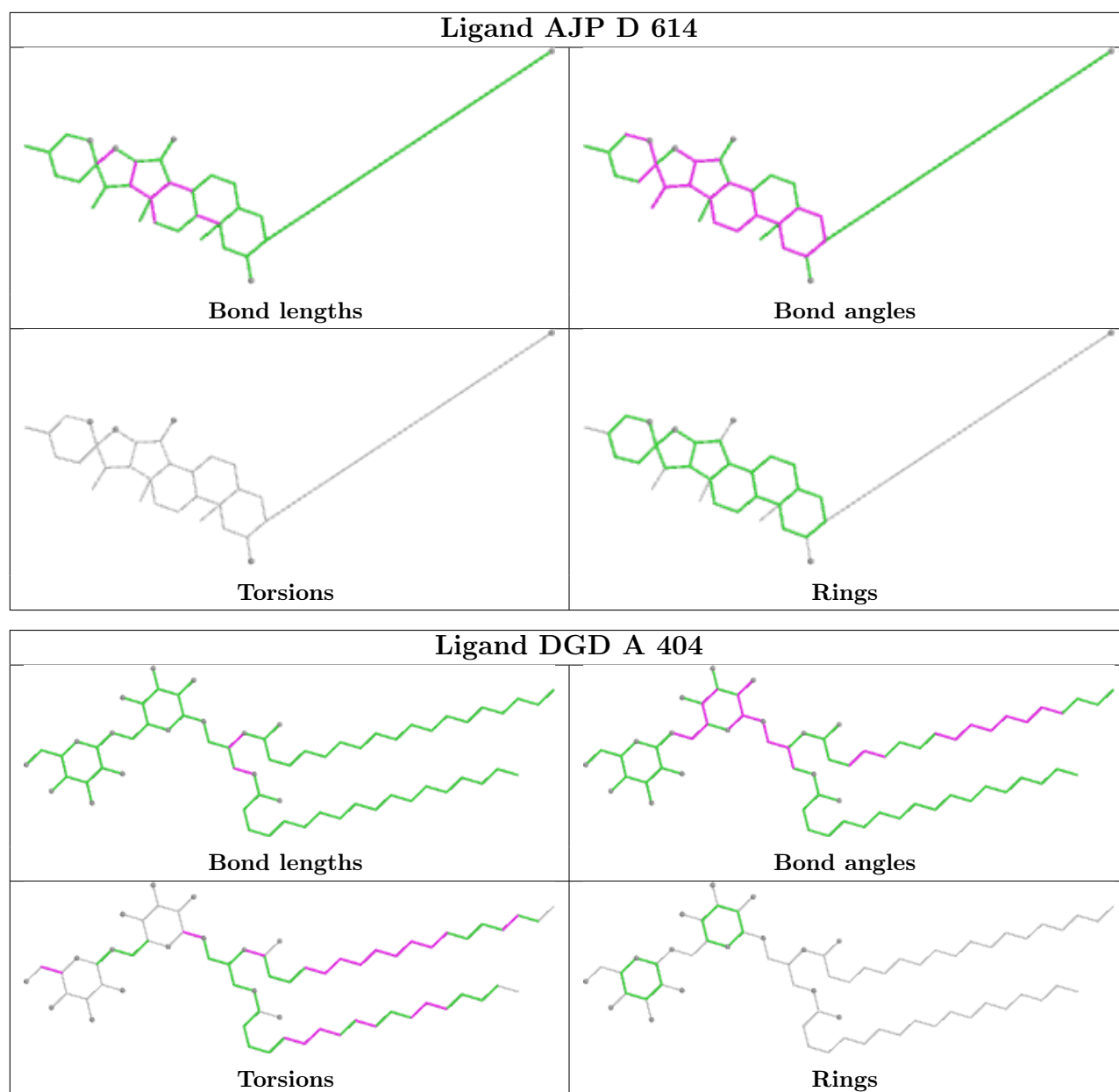
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	612	AJP	2	0
24	B	615	AJP	7	0
24	D	612	AJP	11	0
26	L	101	SQD	1	0
24	Q	101	AJP	3	0

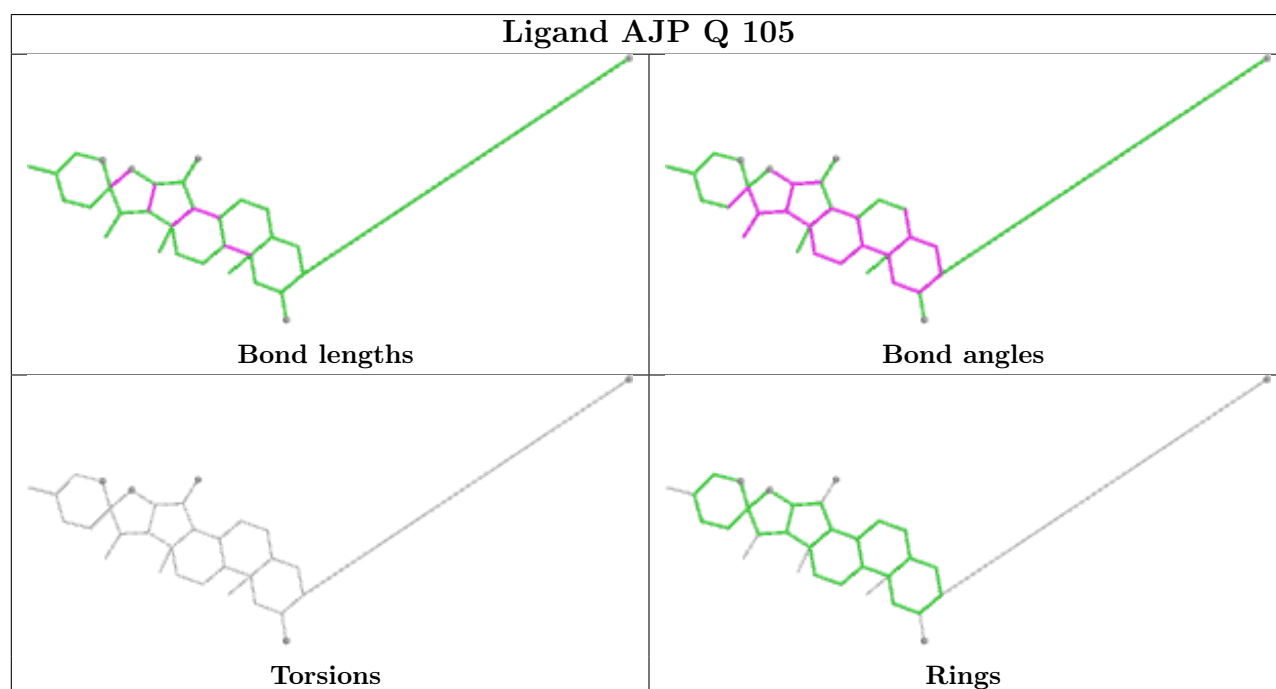
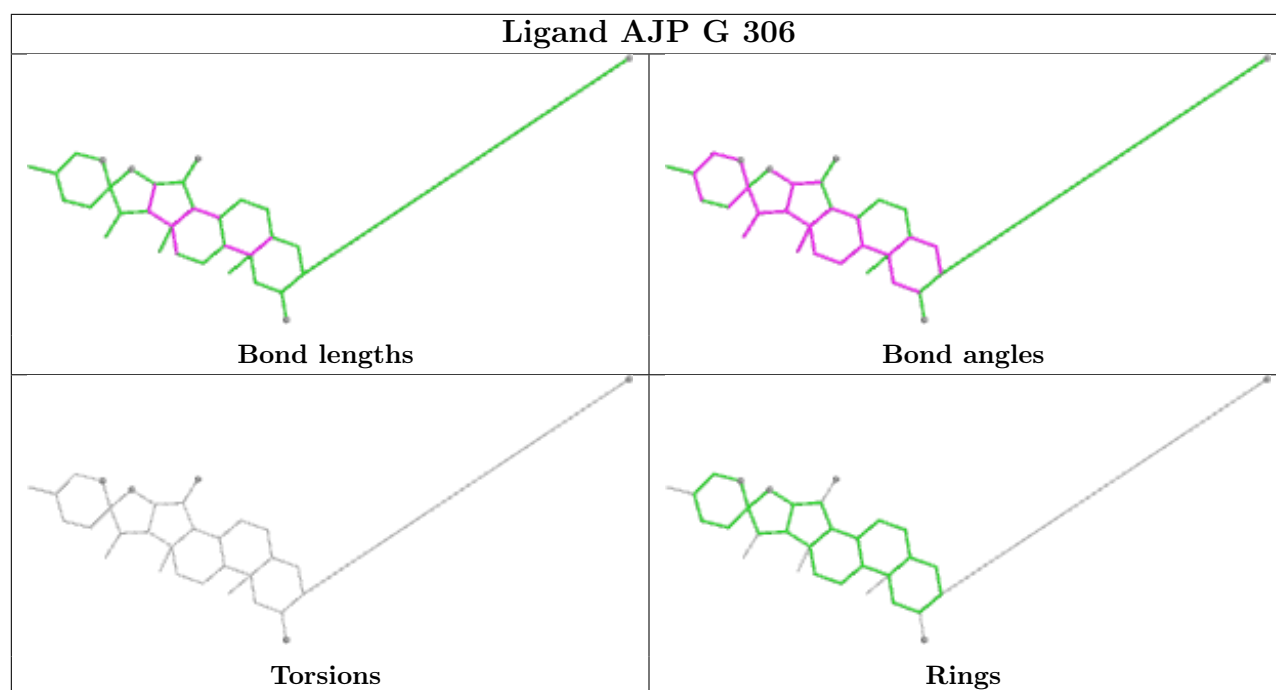
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

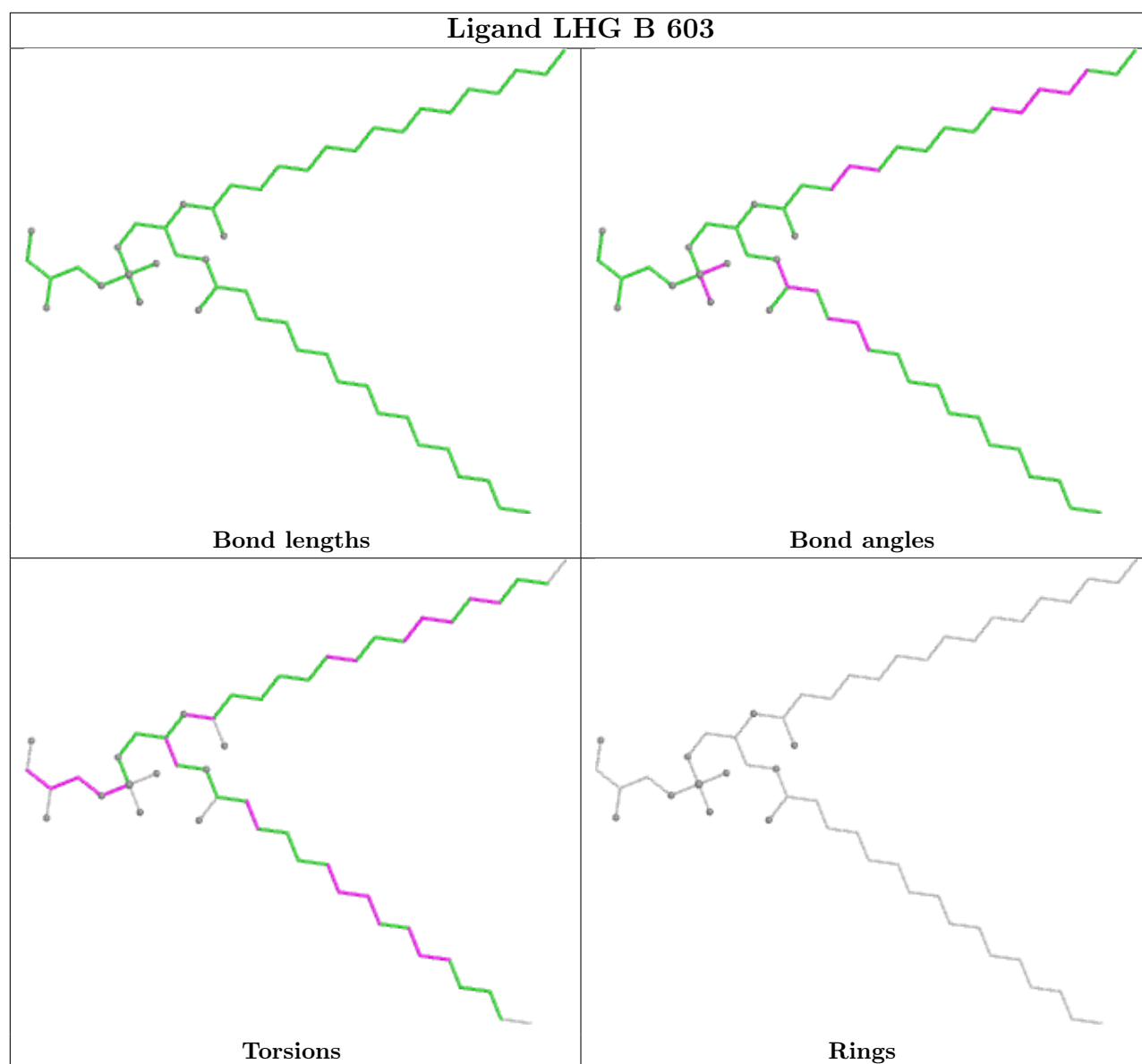


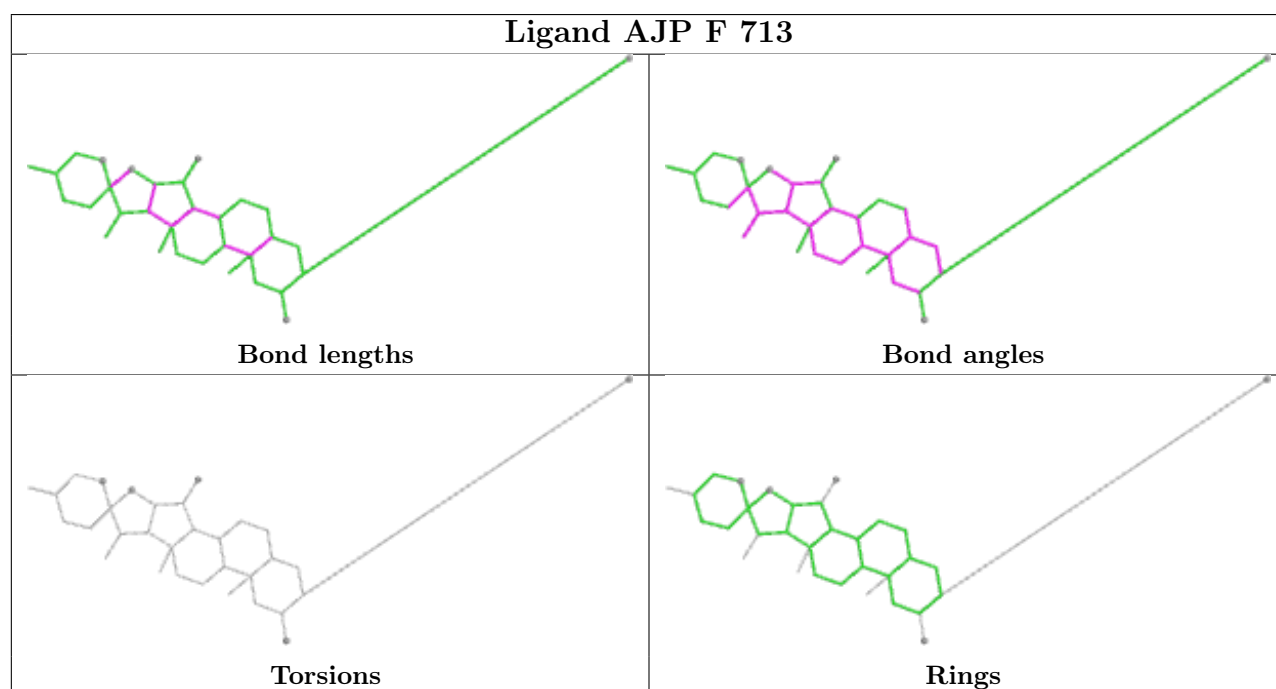
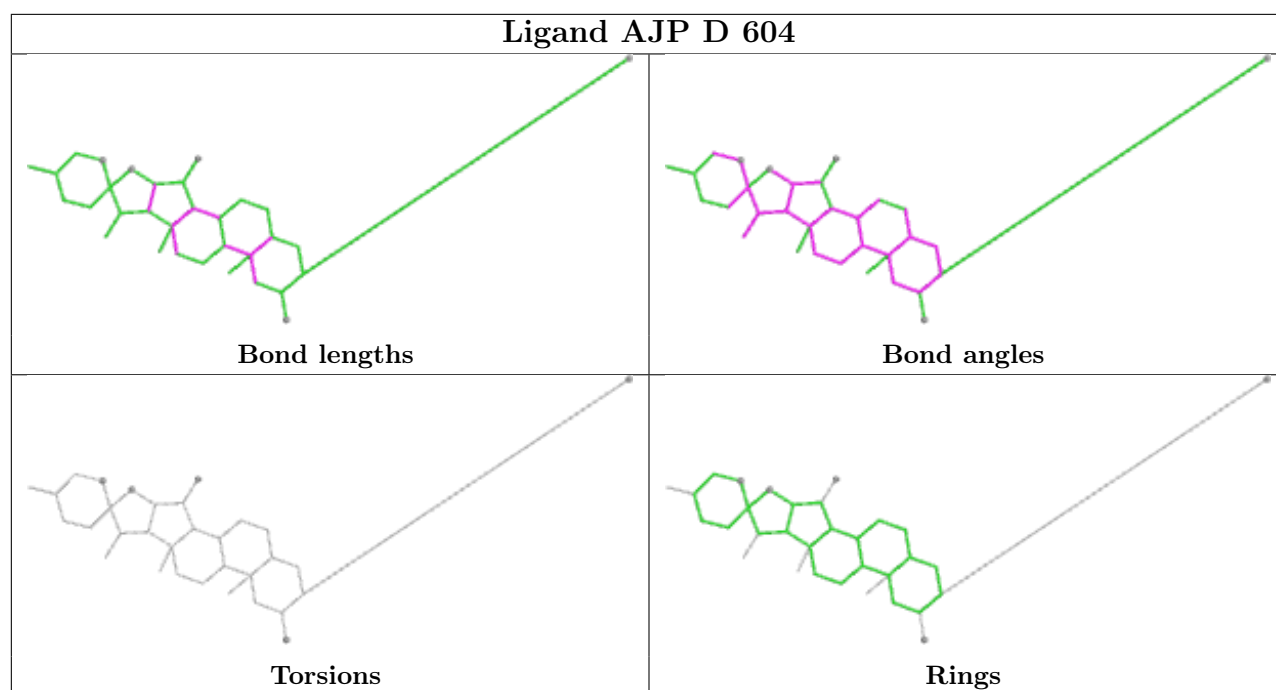


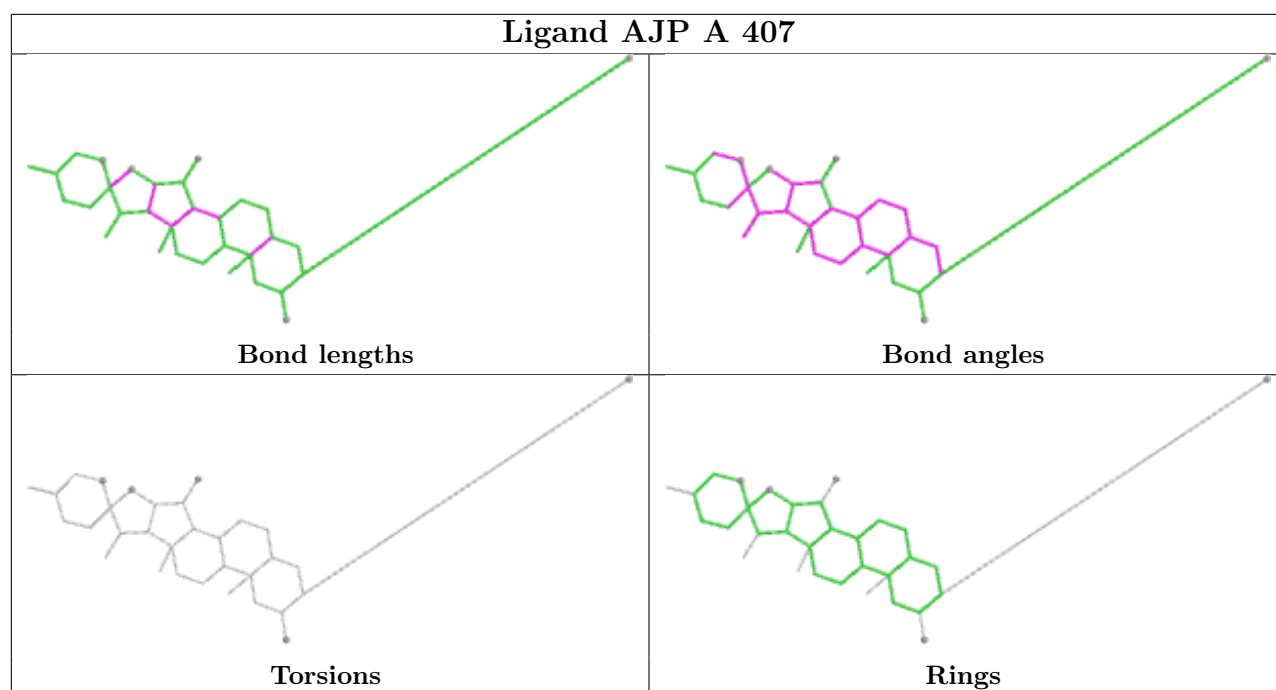


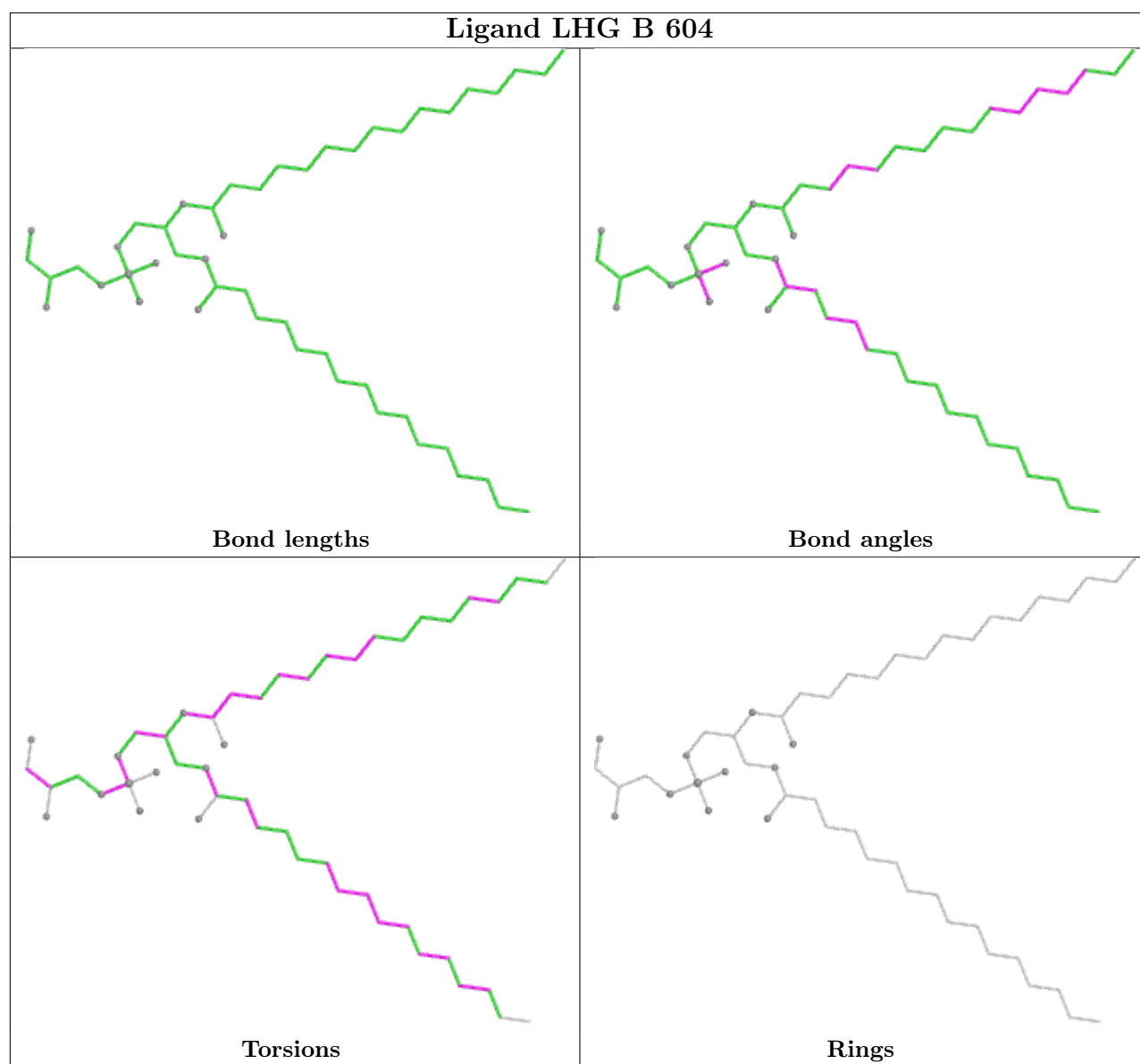


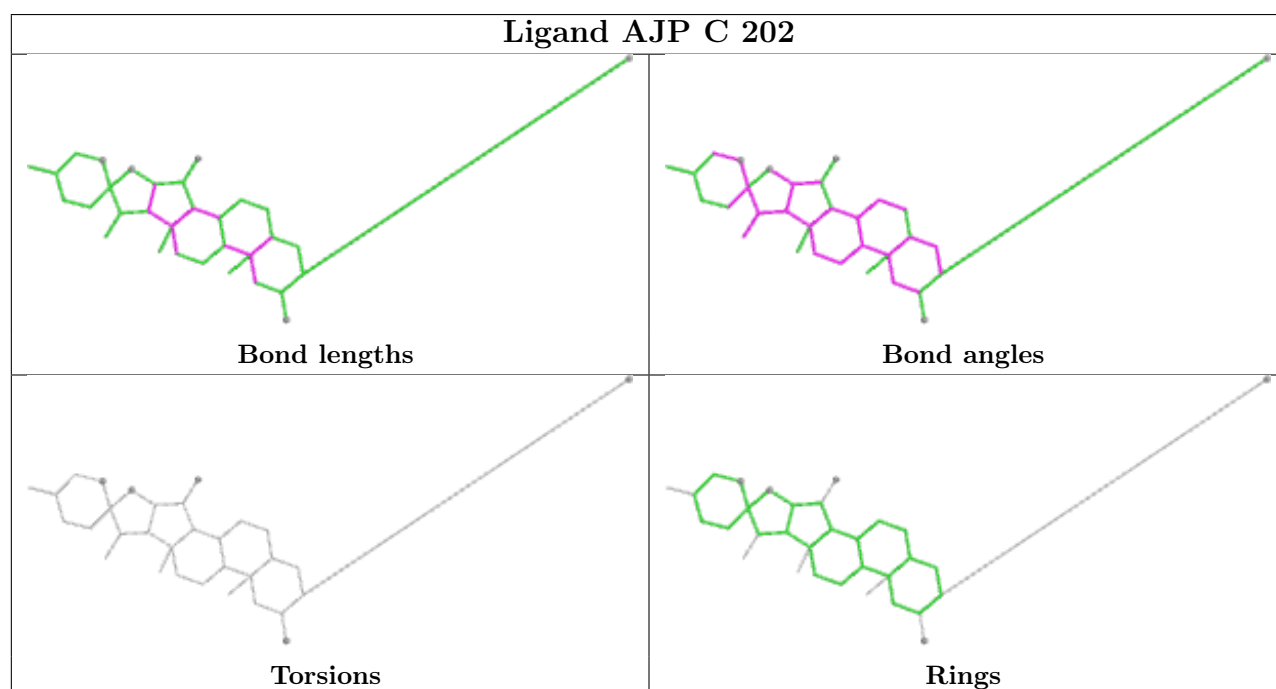
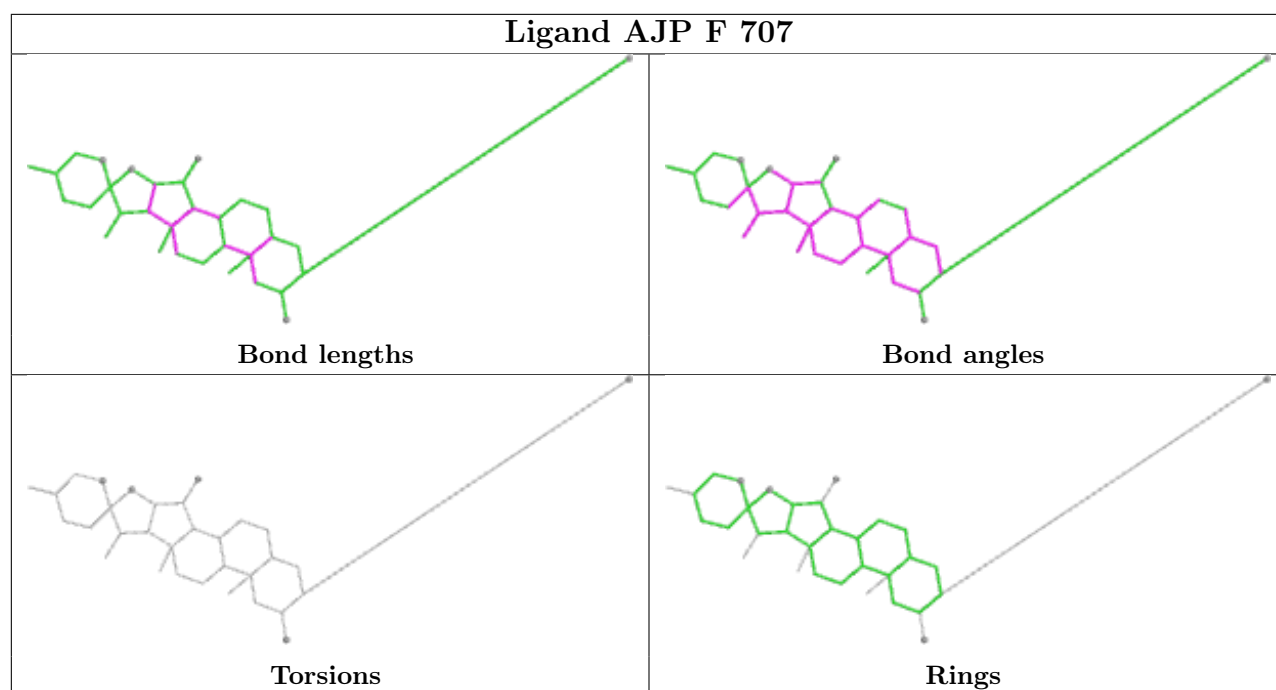


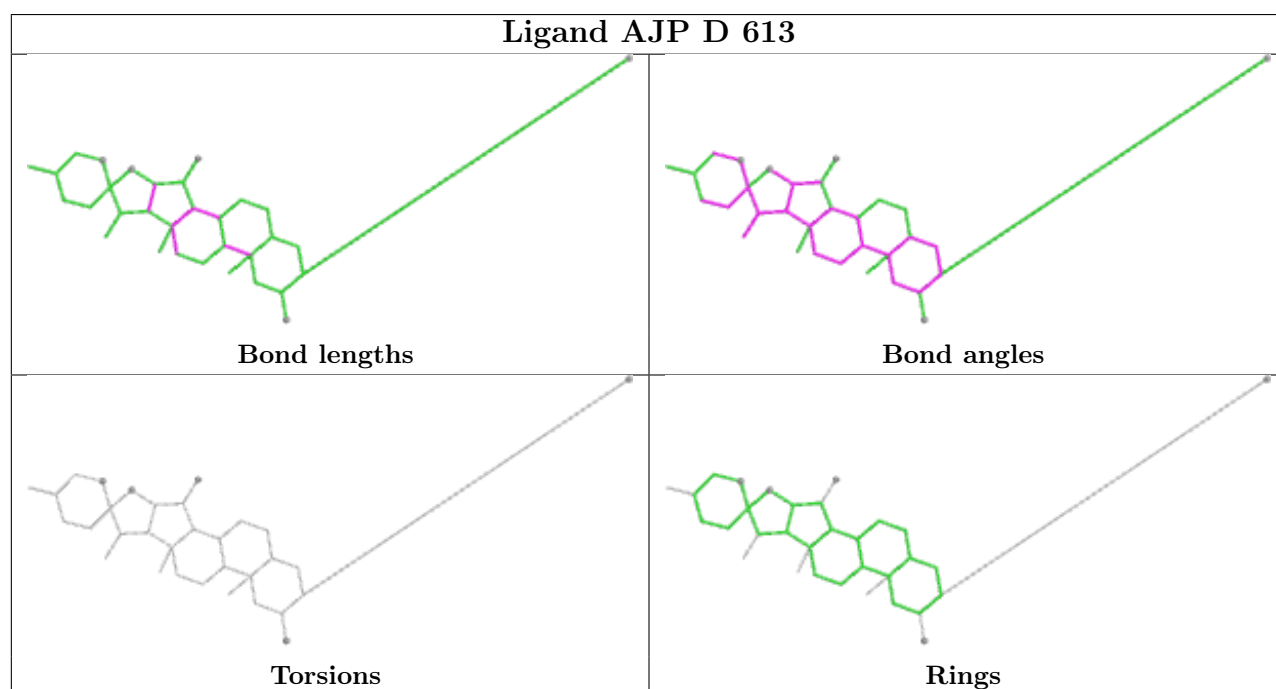
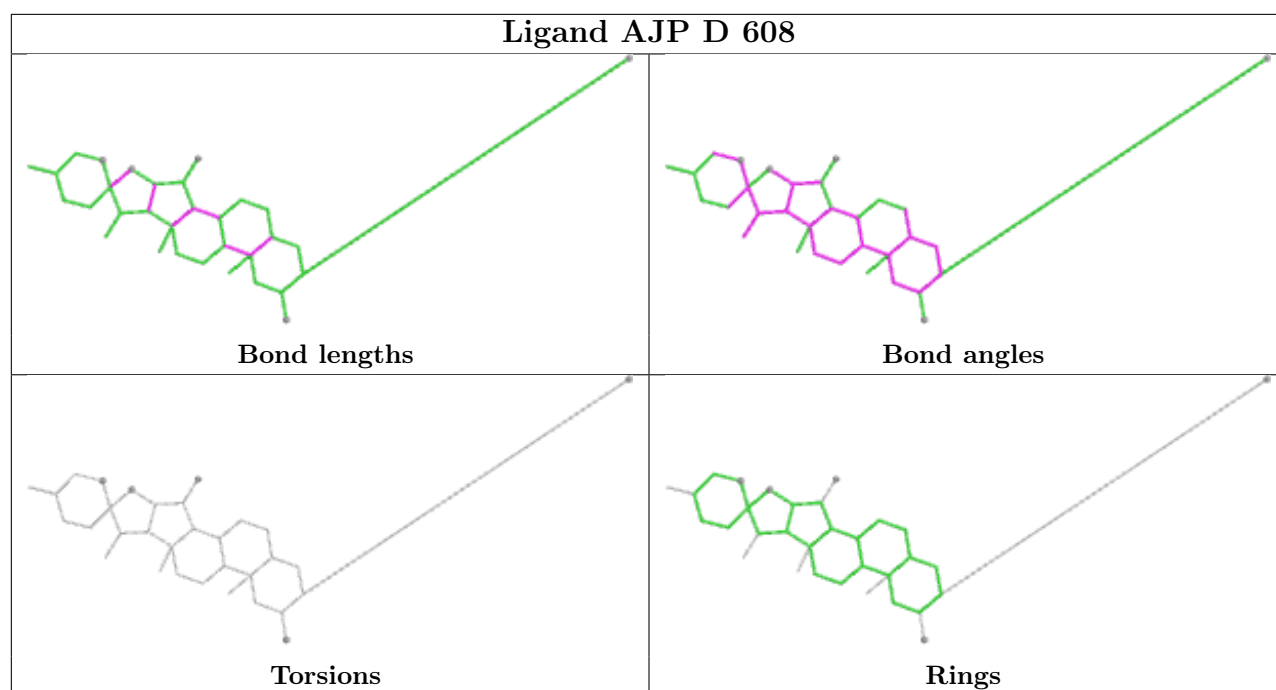


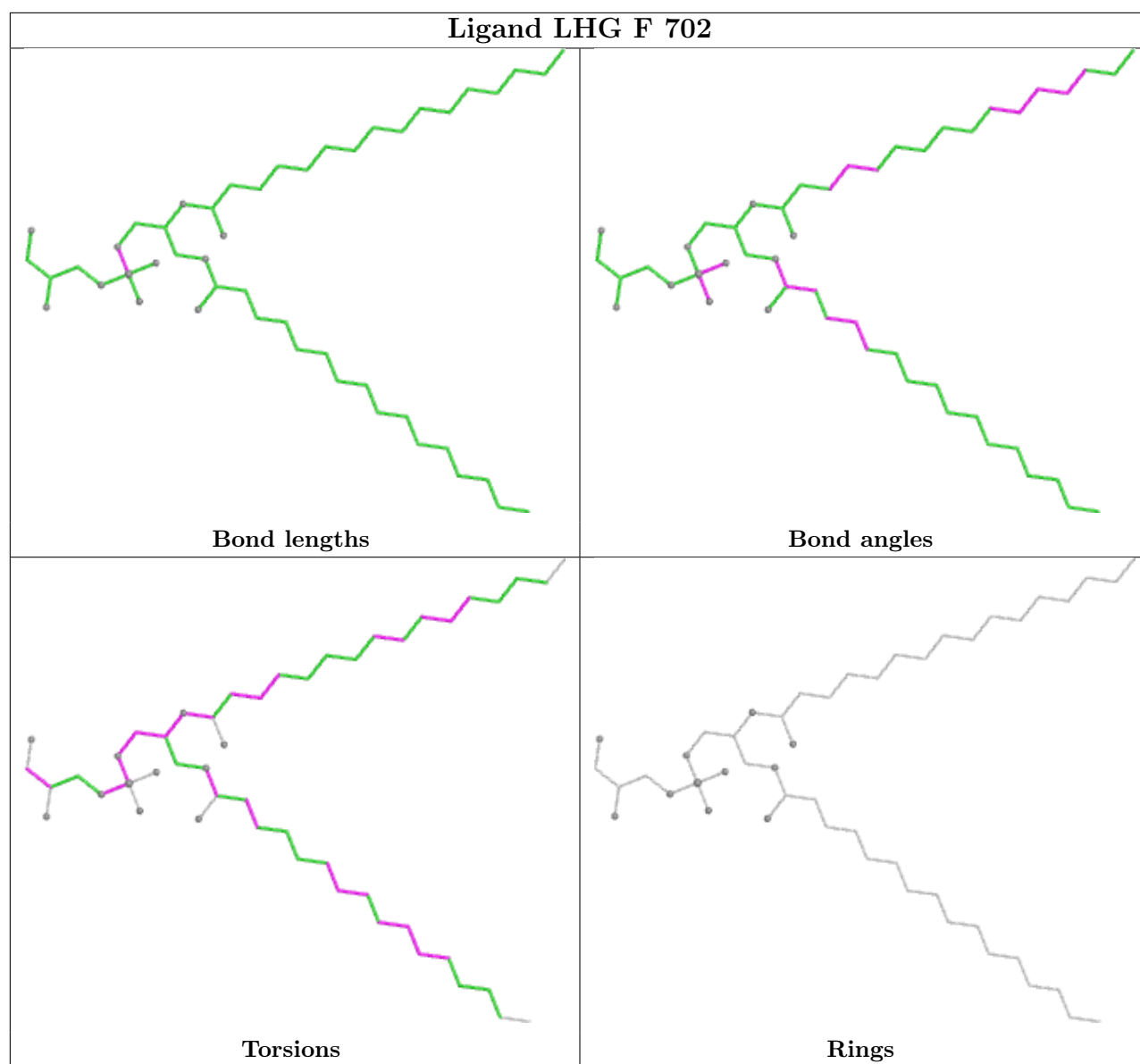


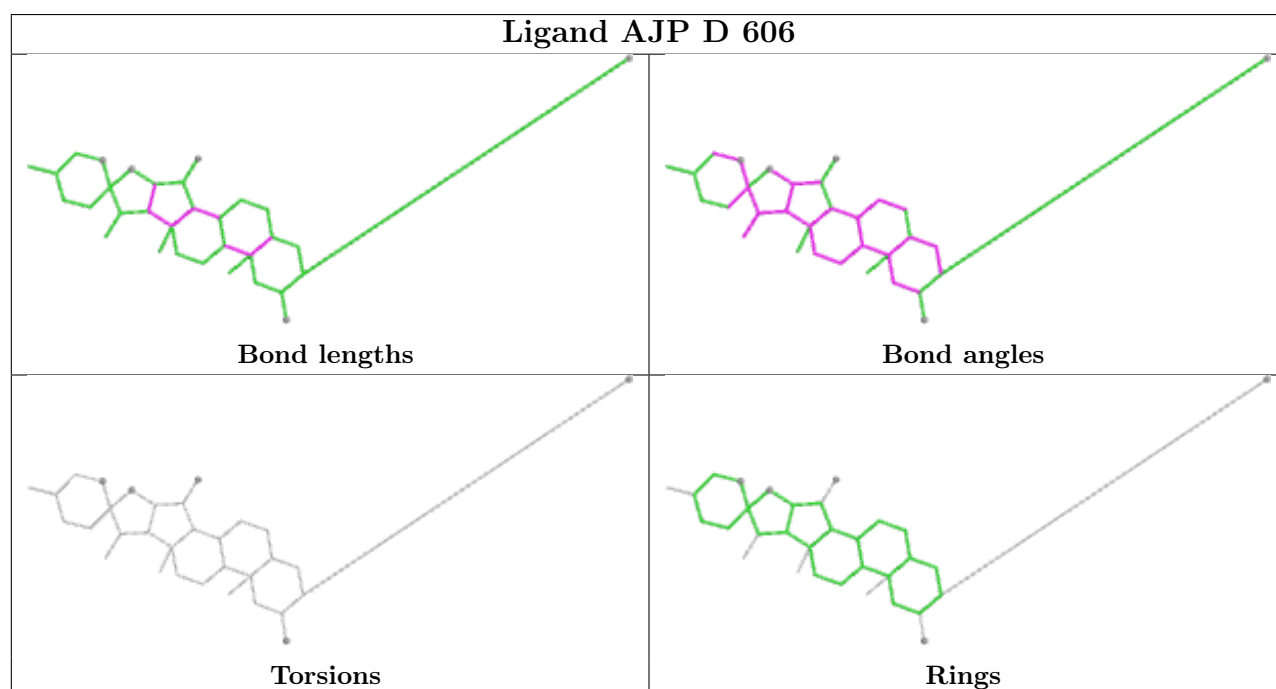
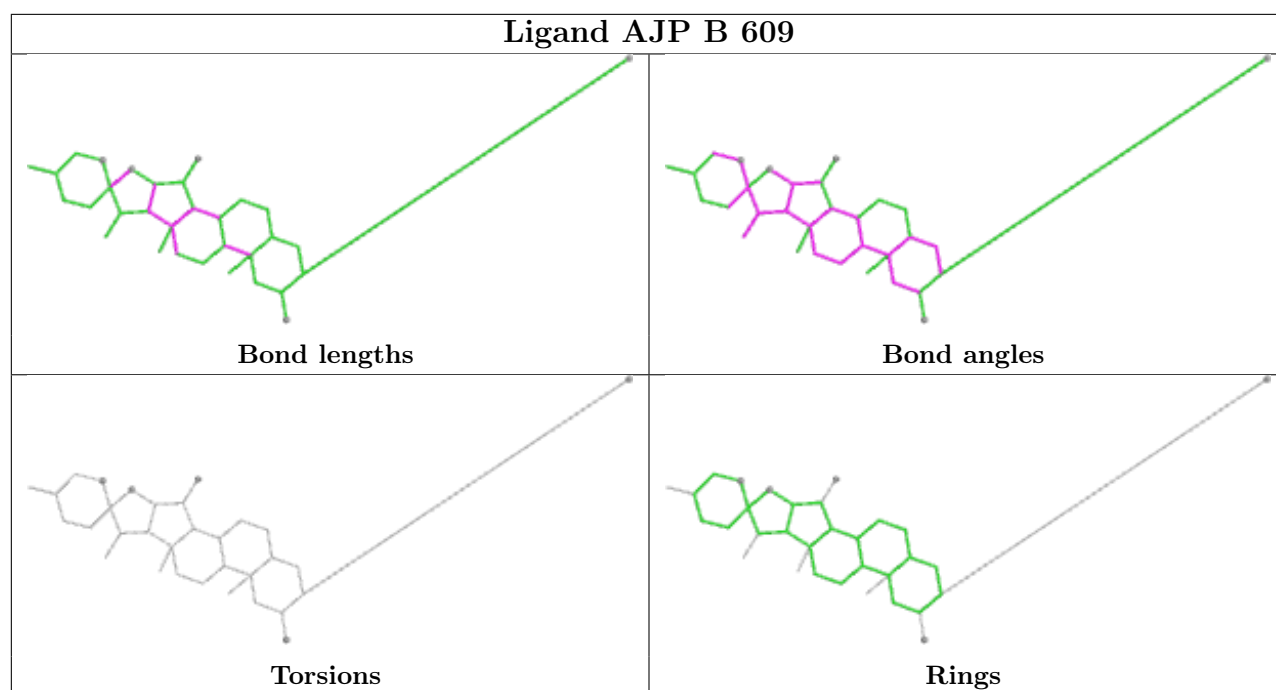


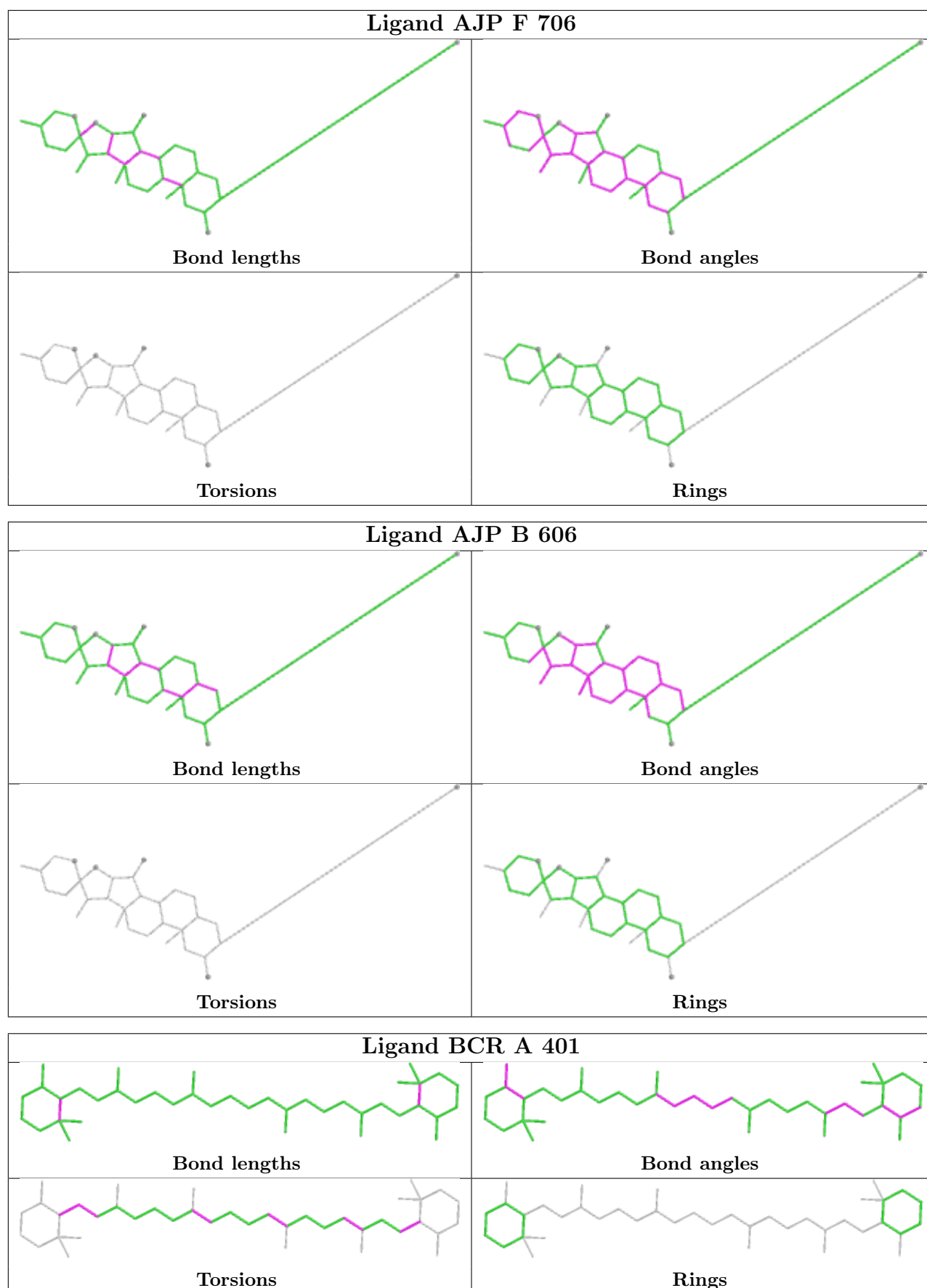


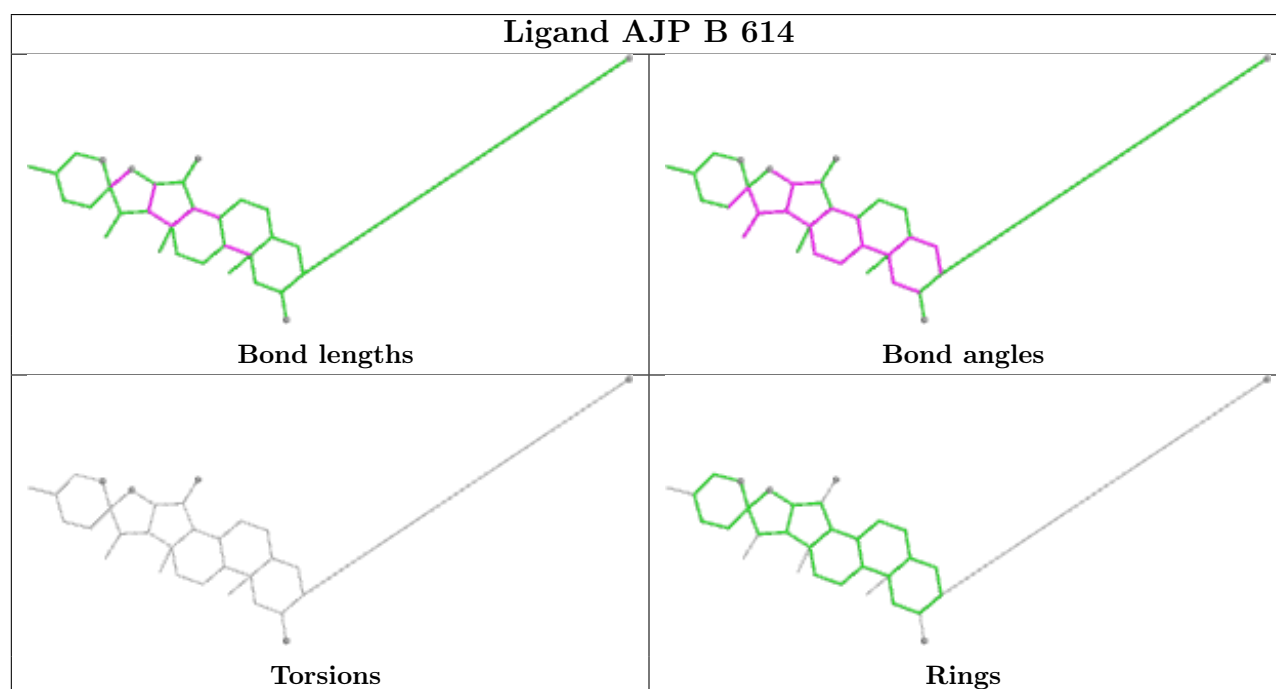
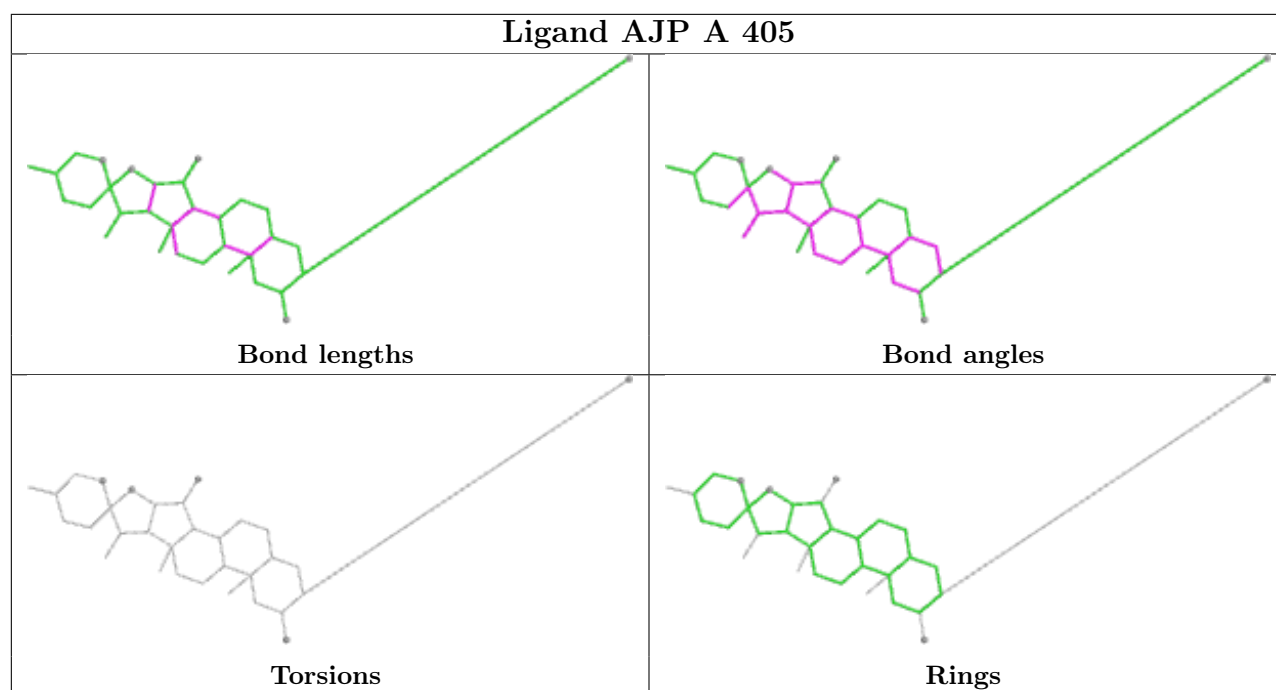


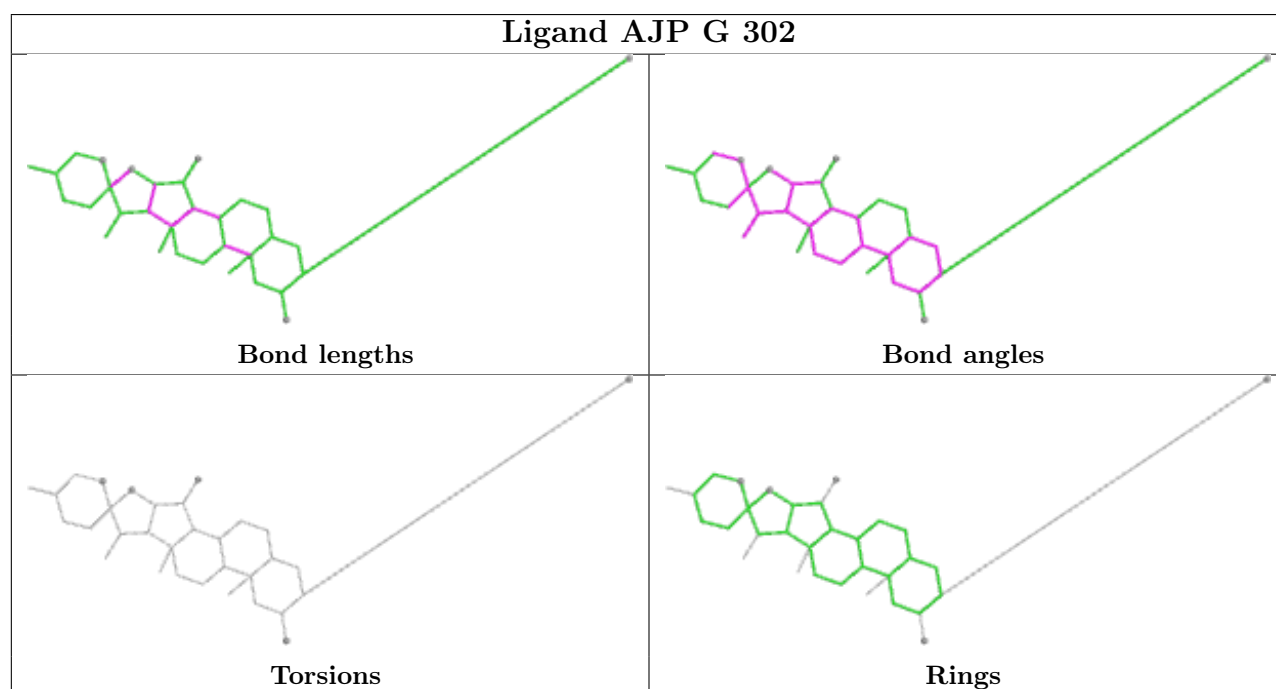
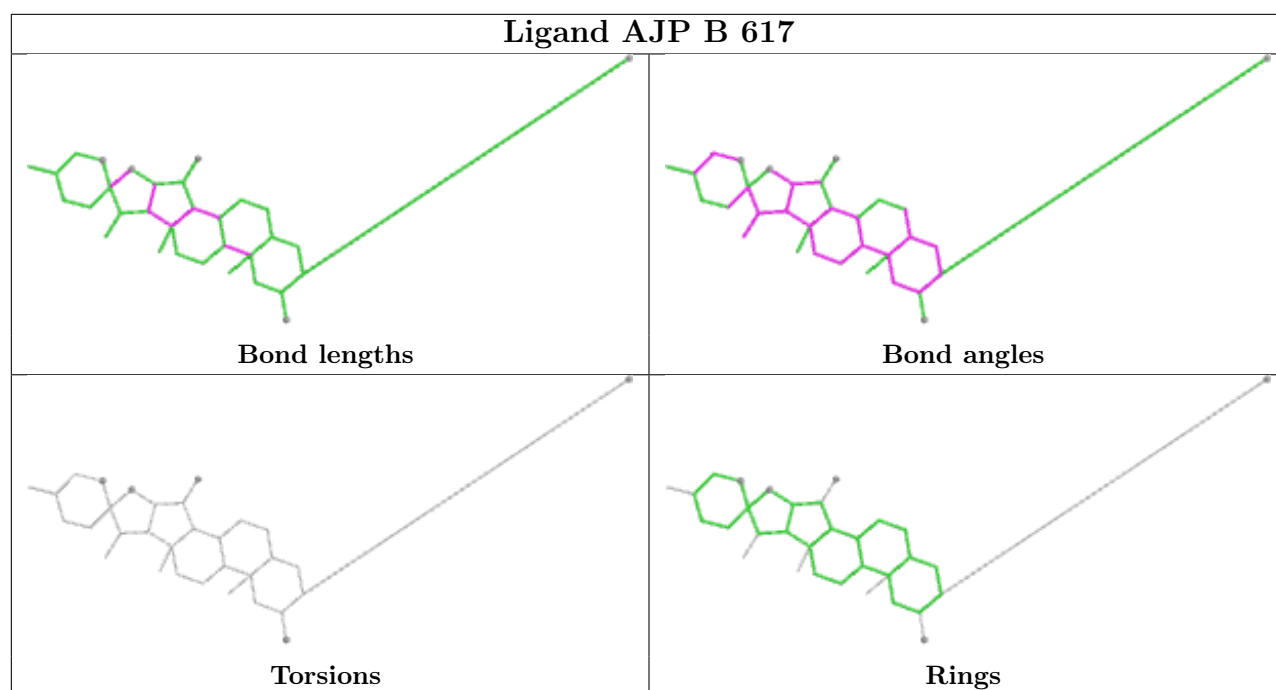


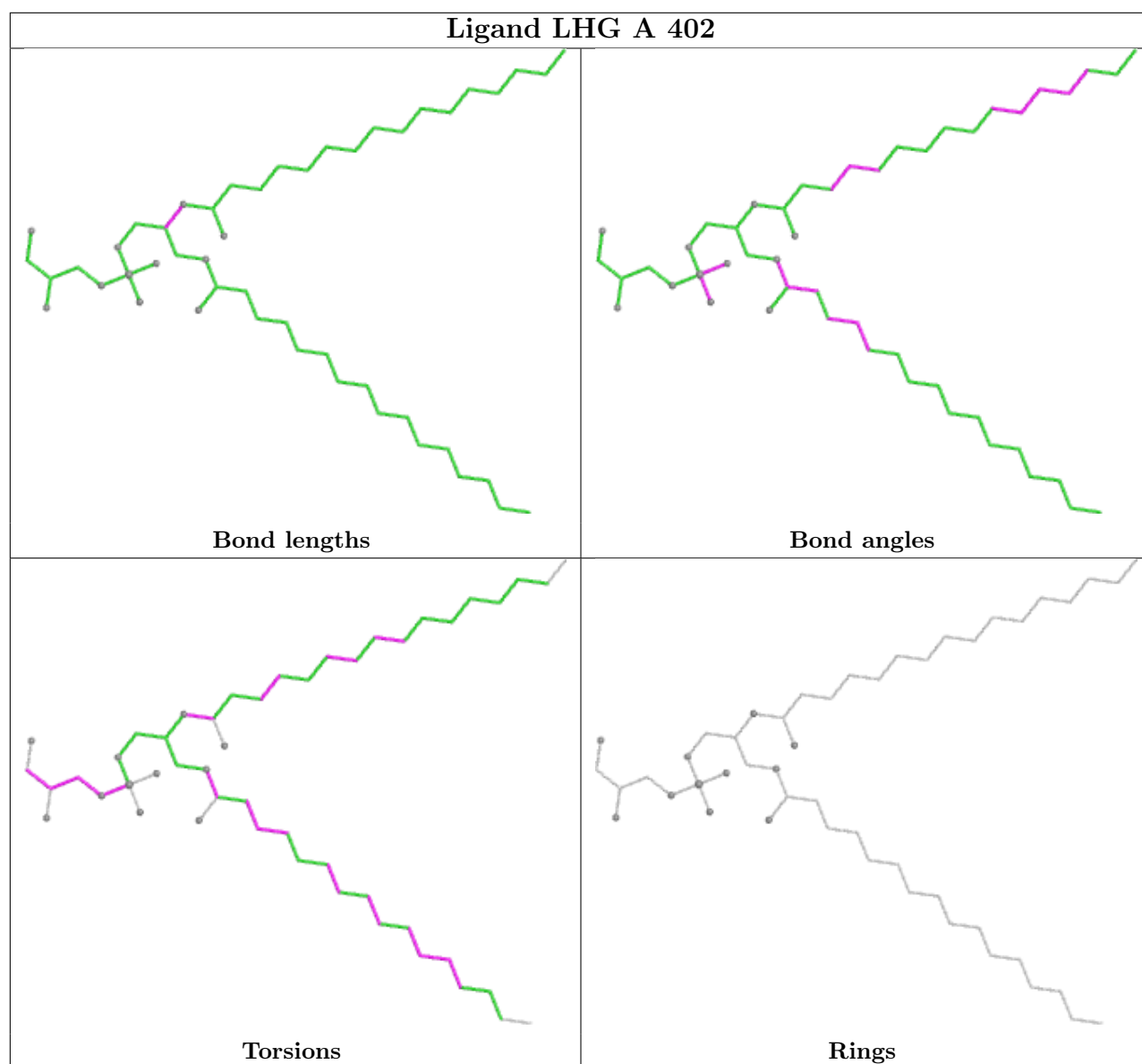


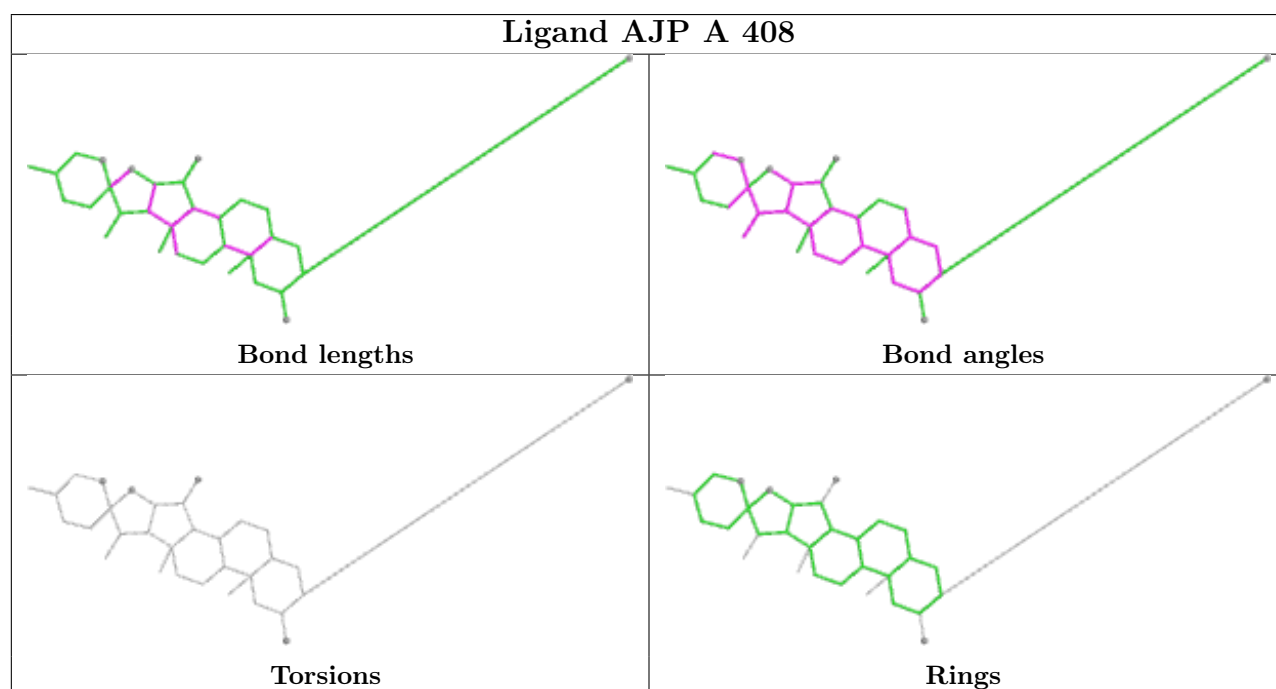
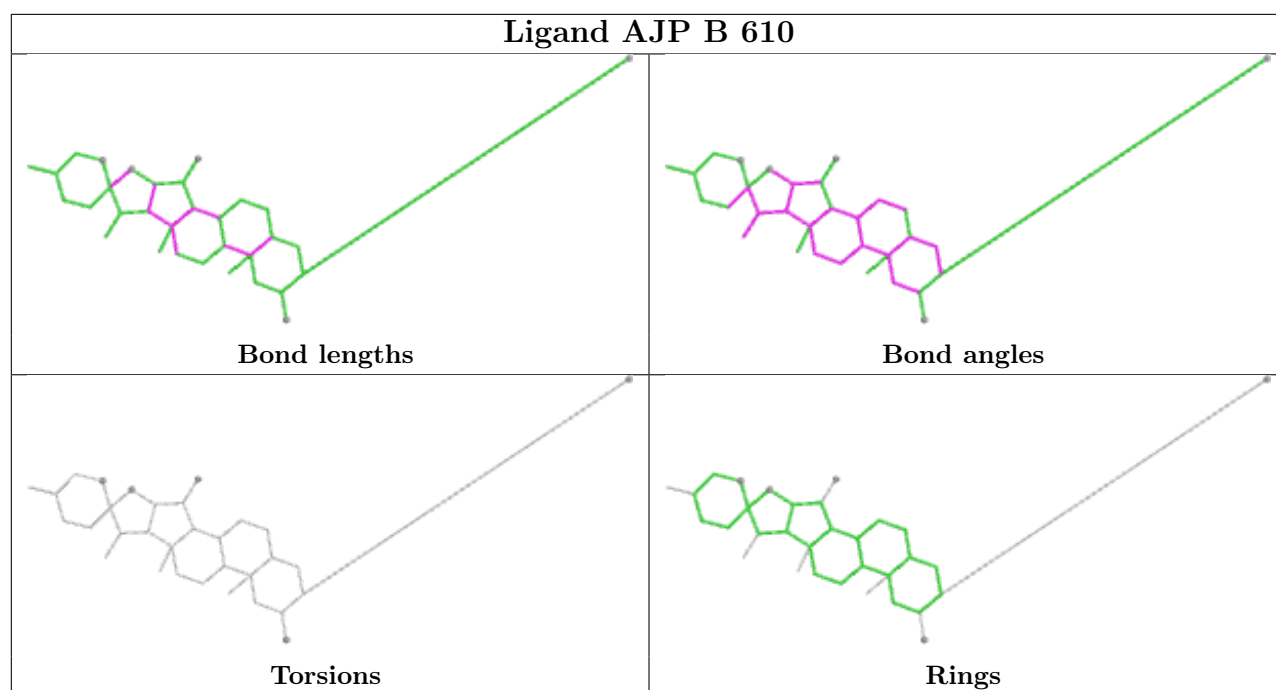


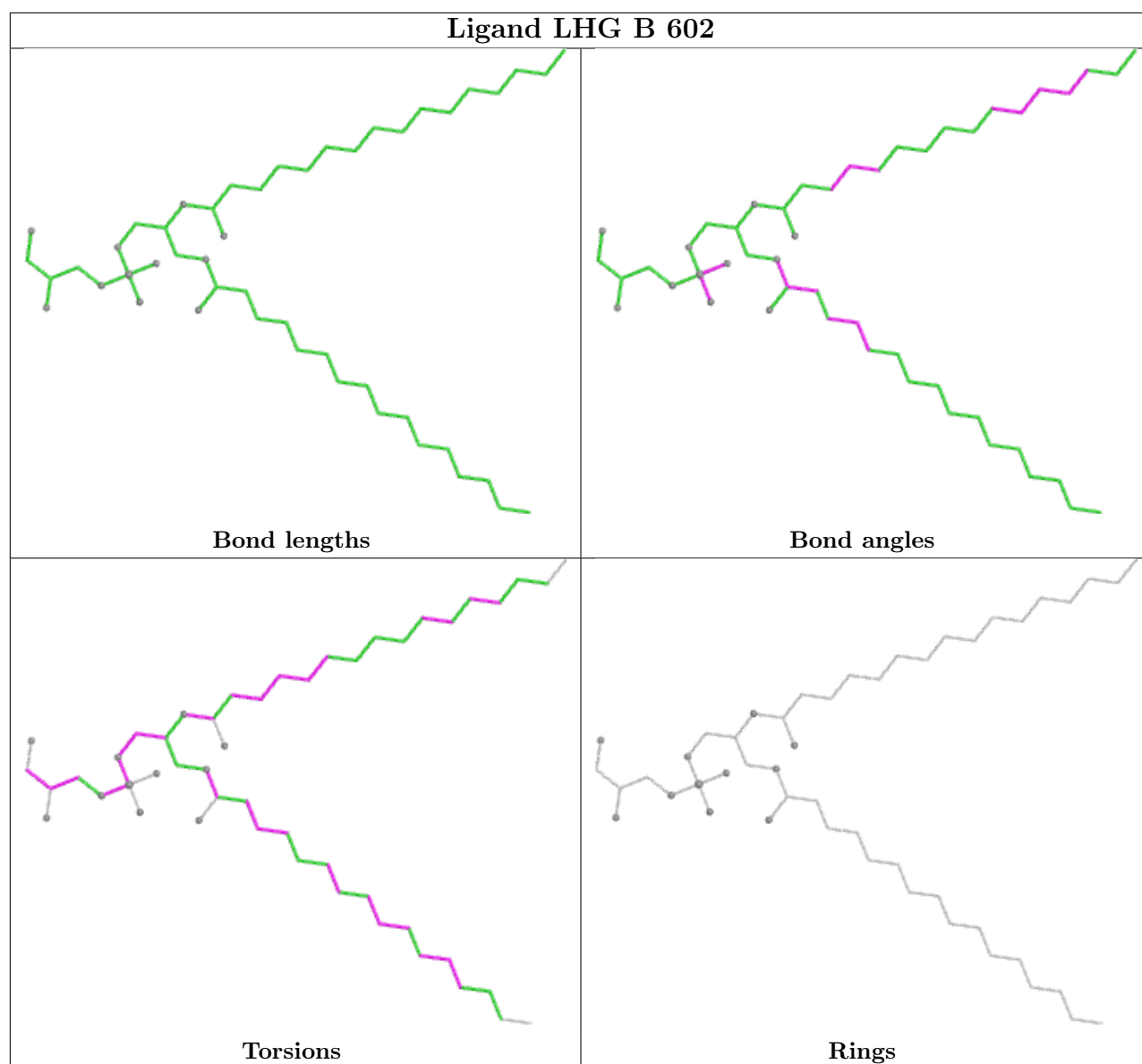


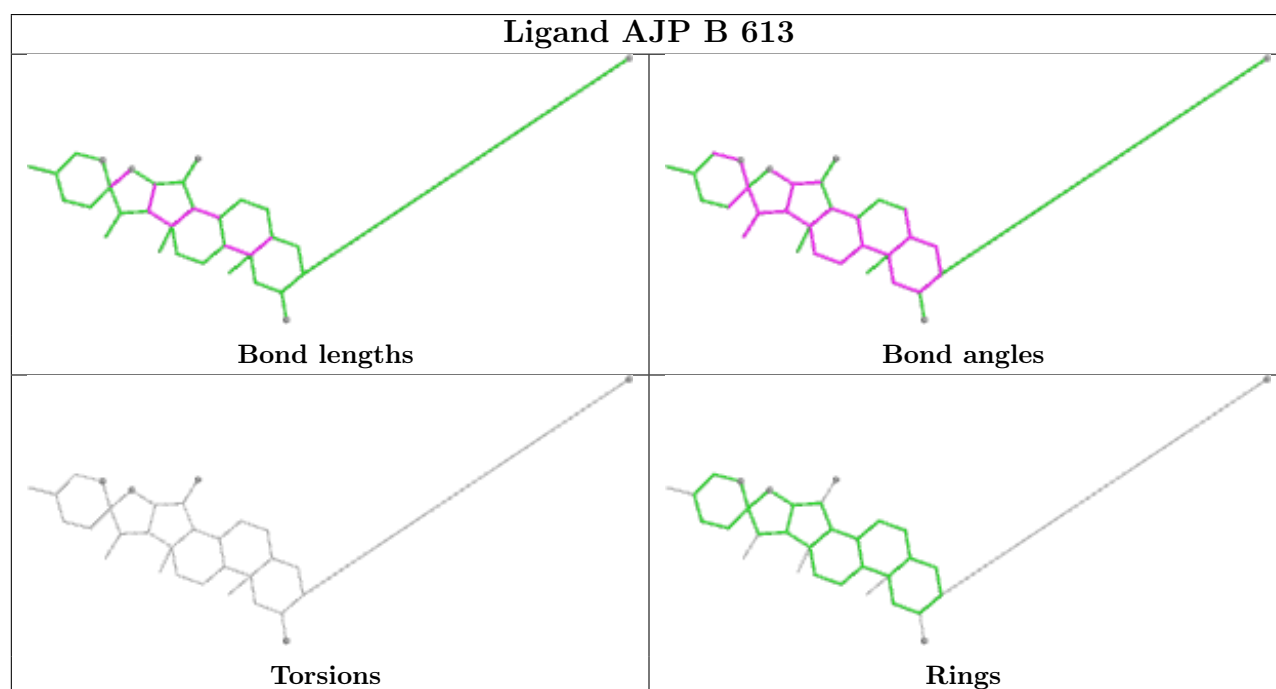
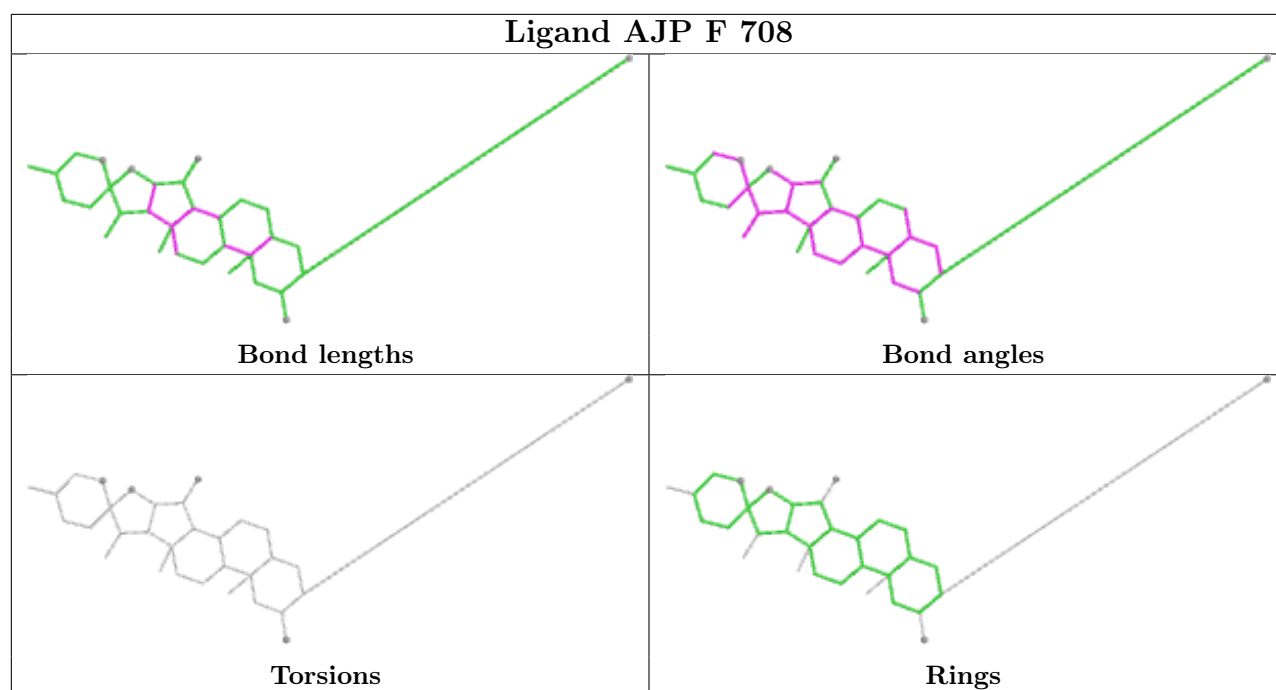


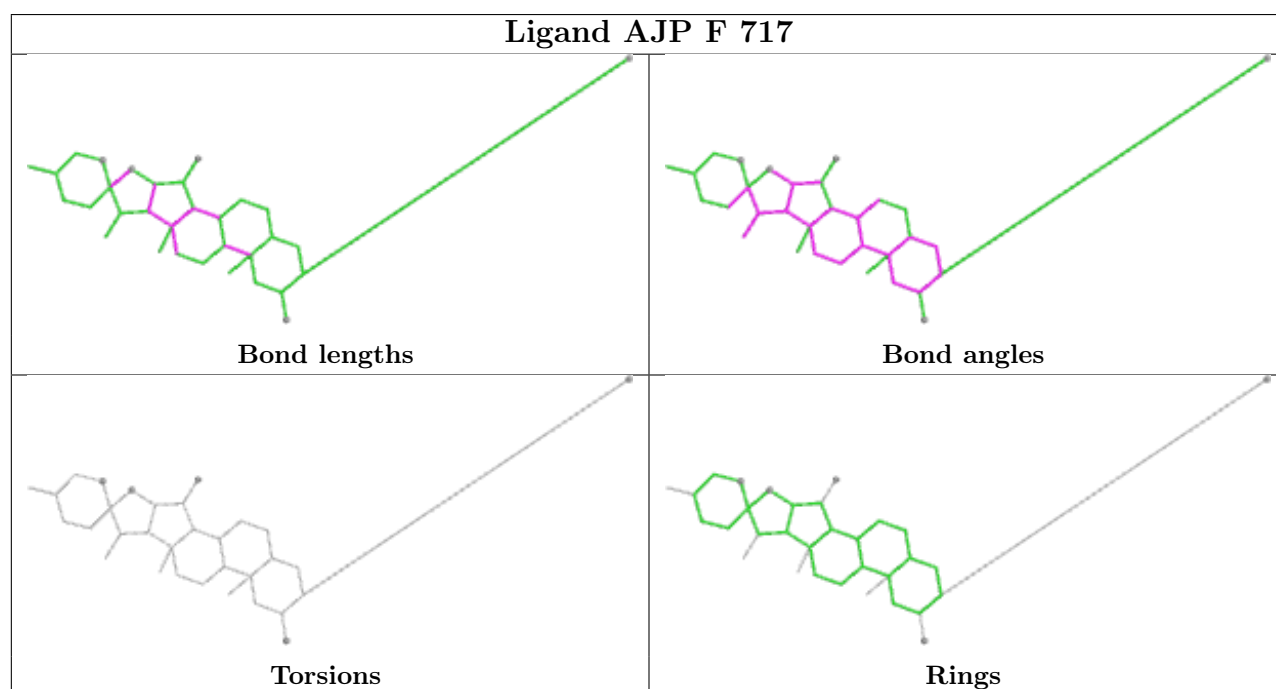
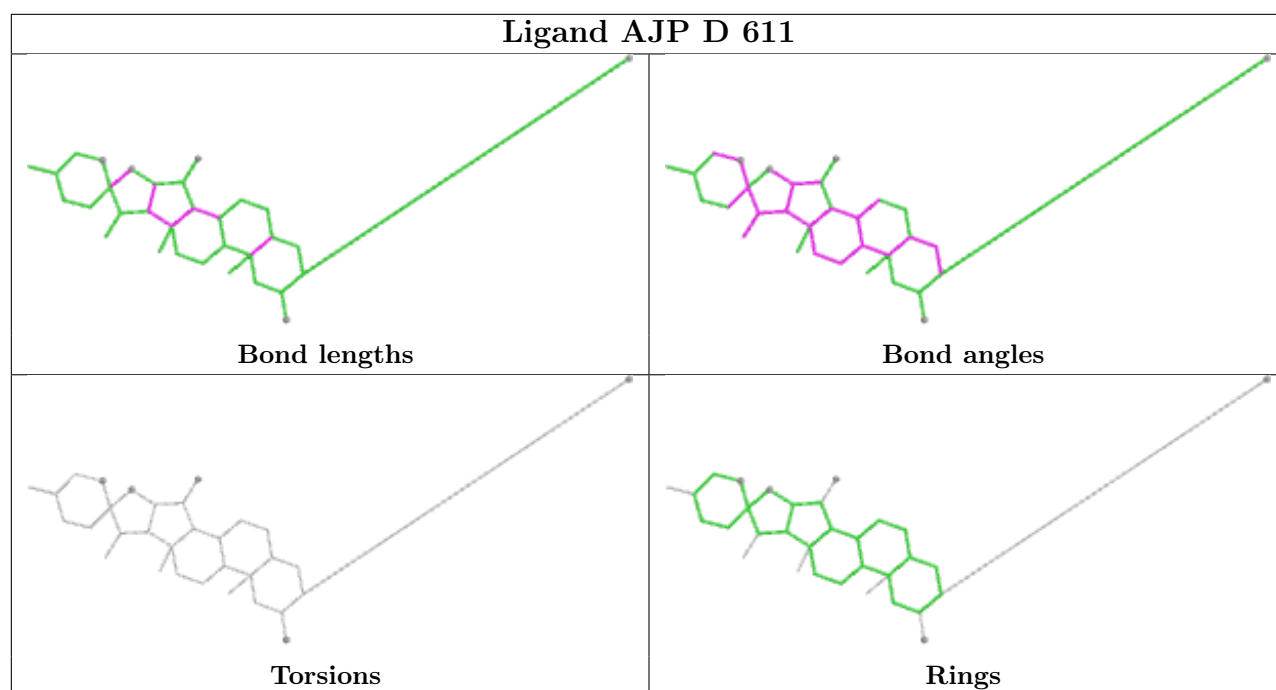


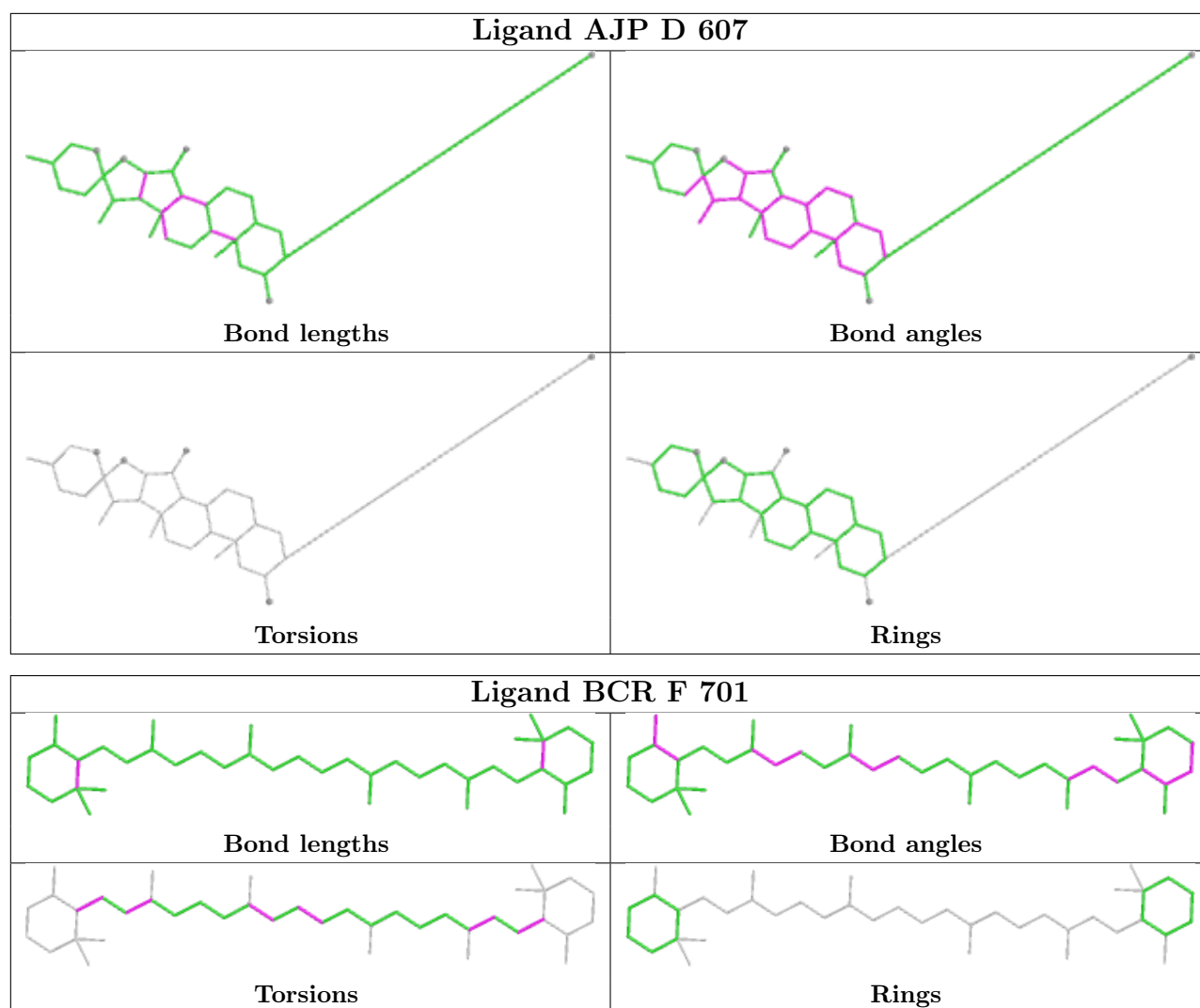


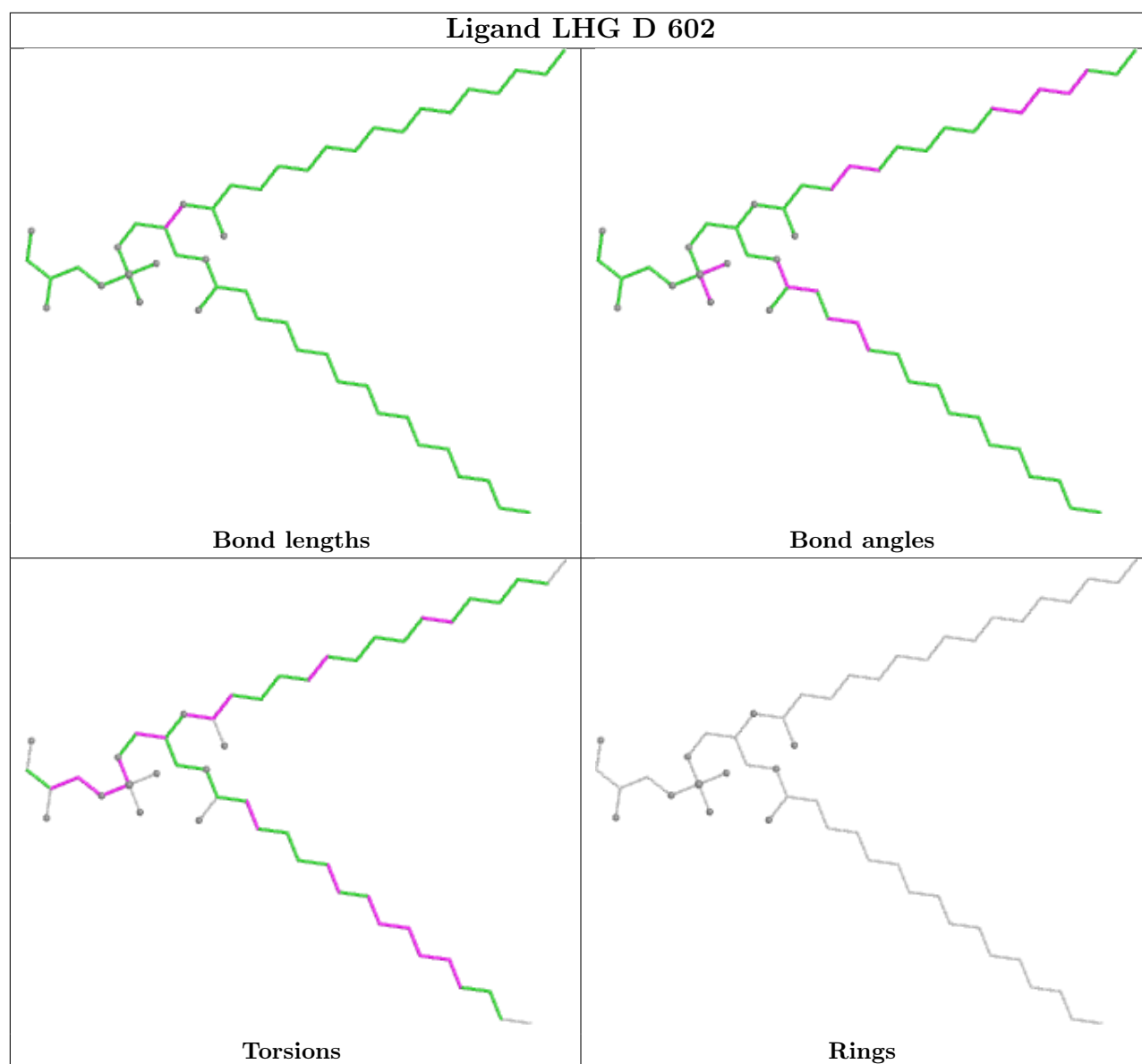


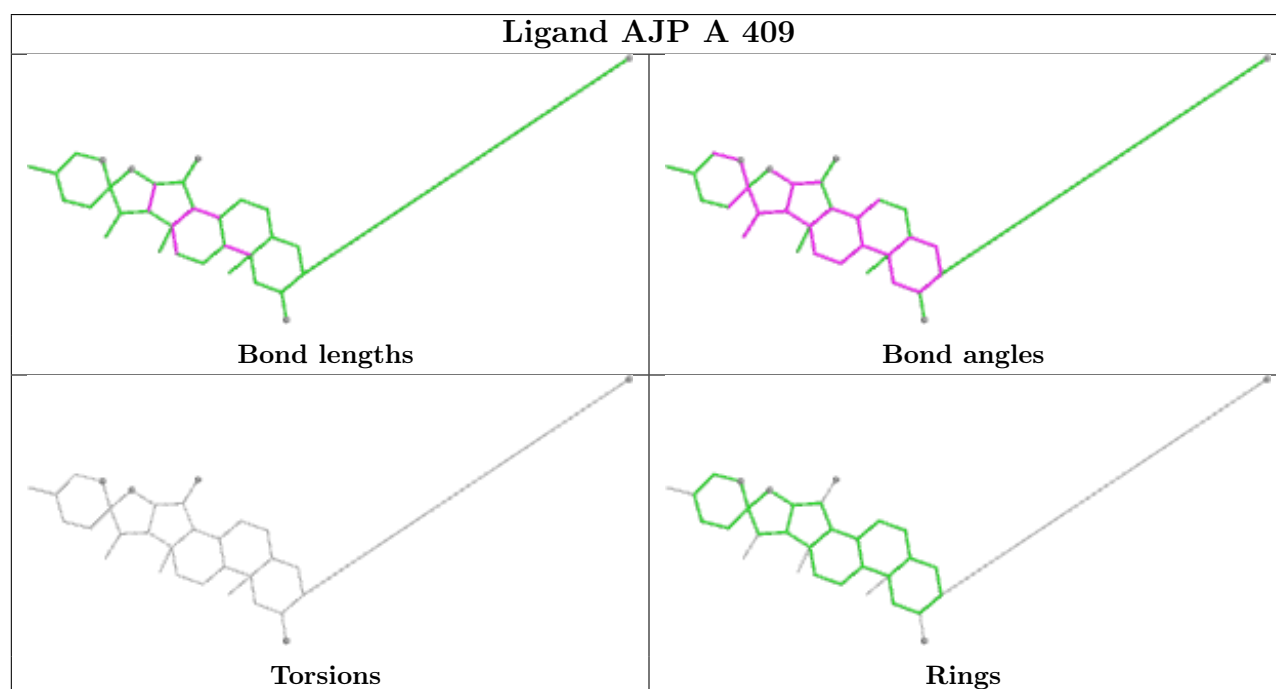
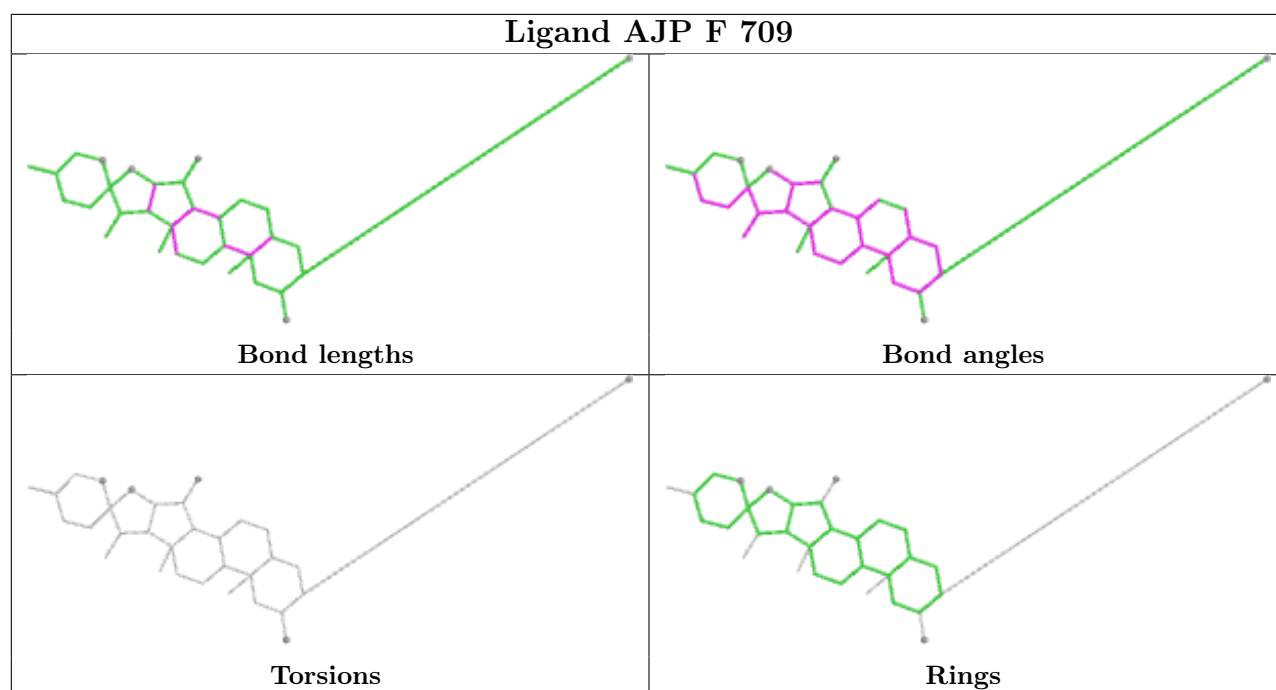


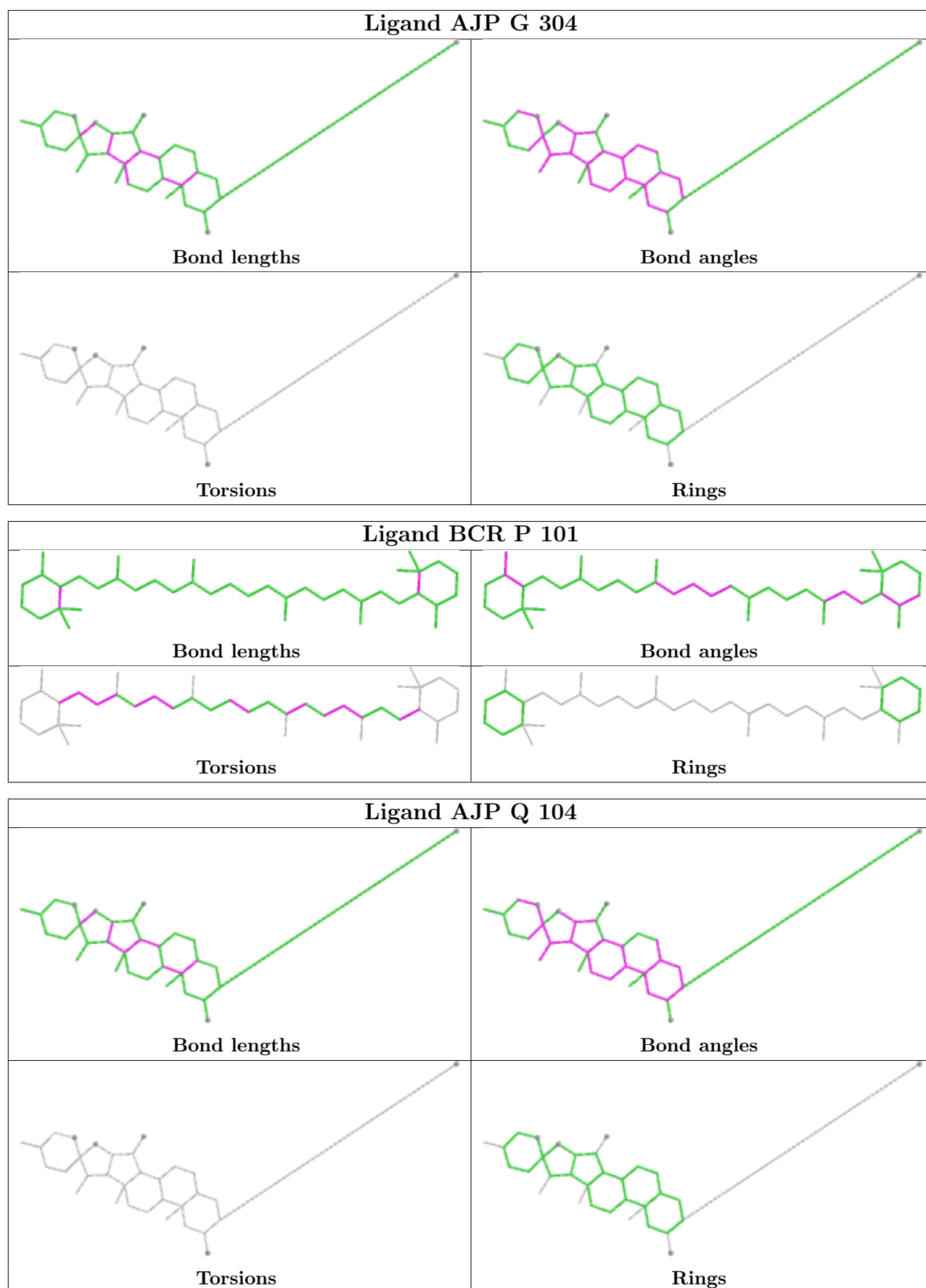


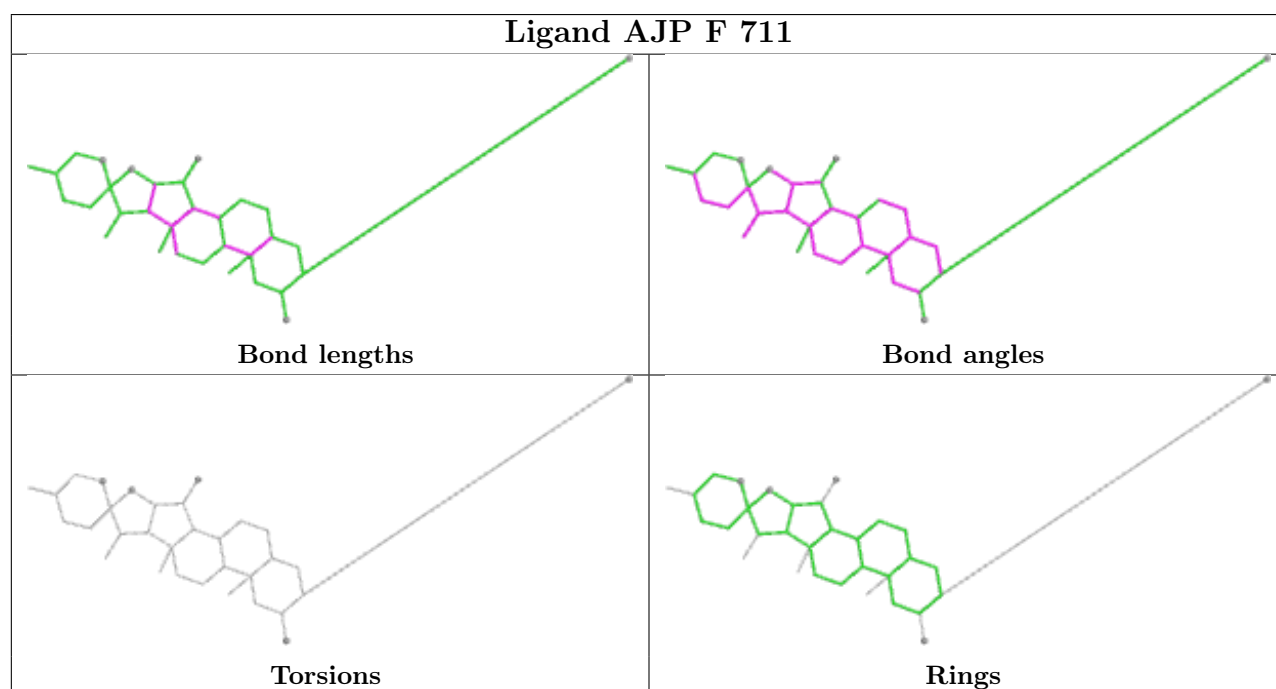
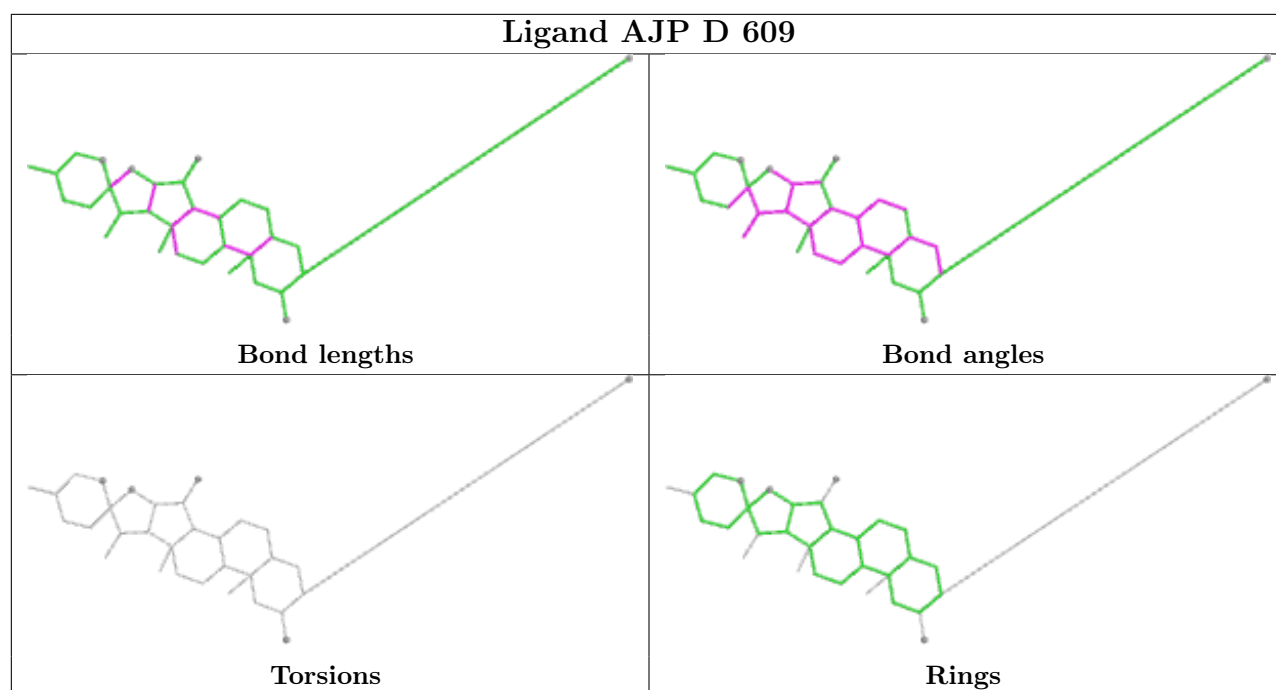


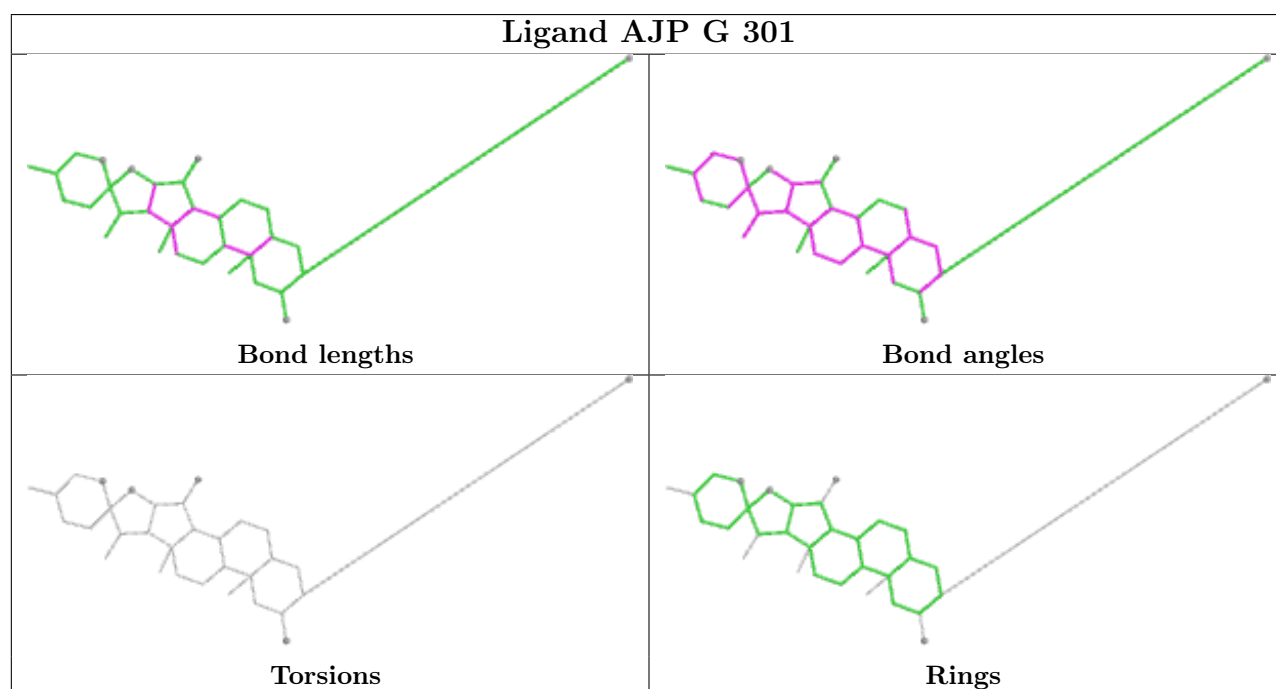
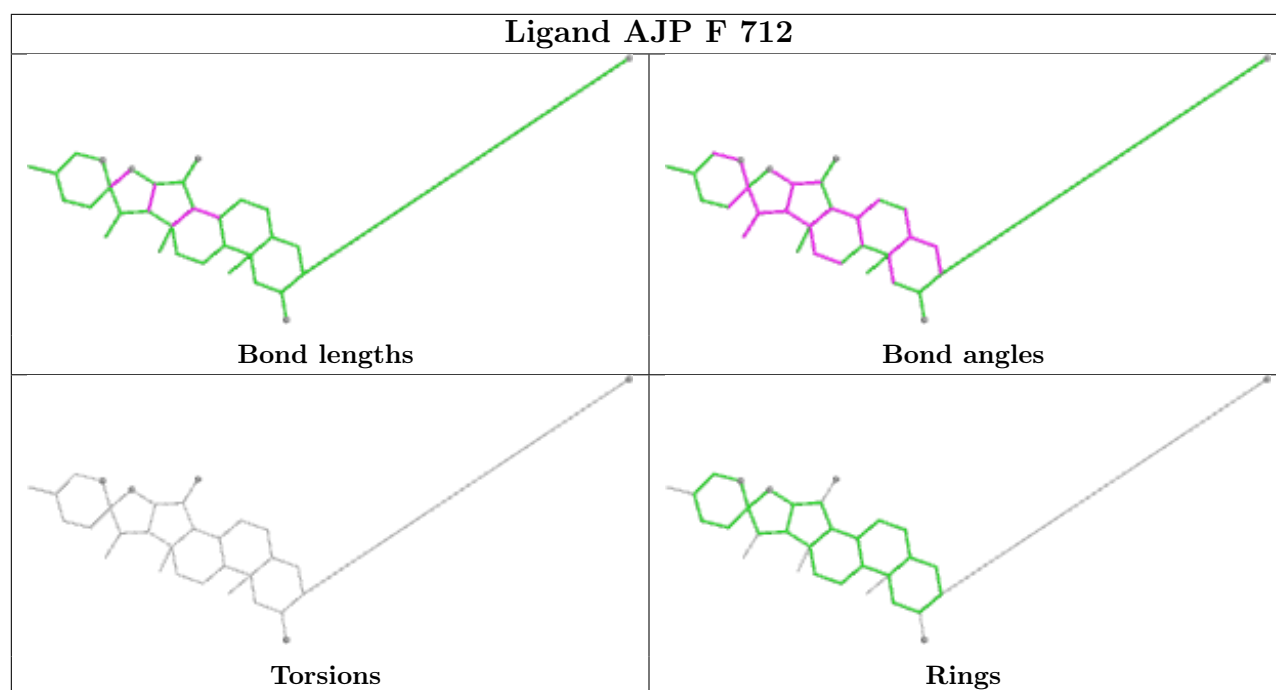


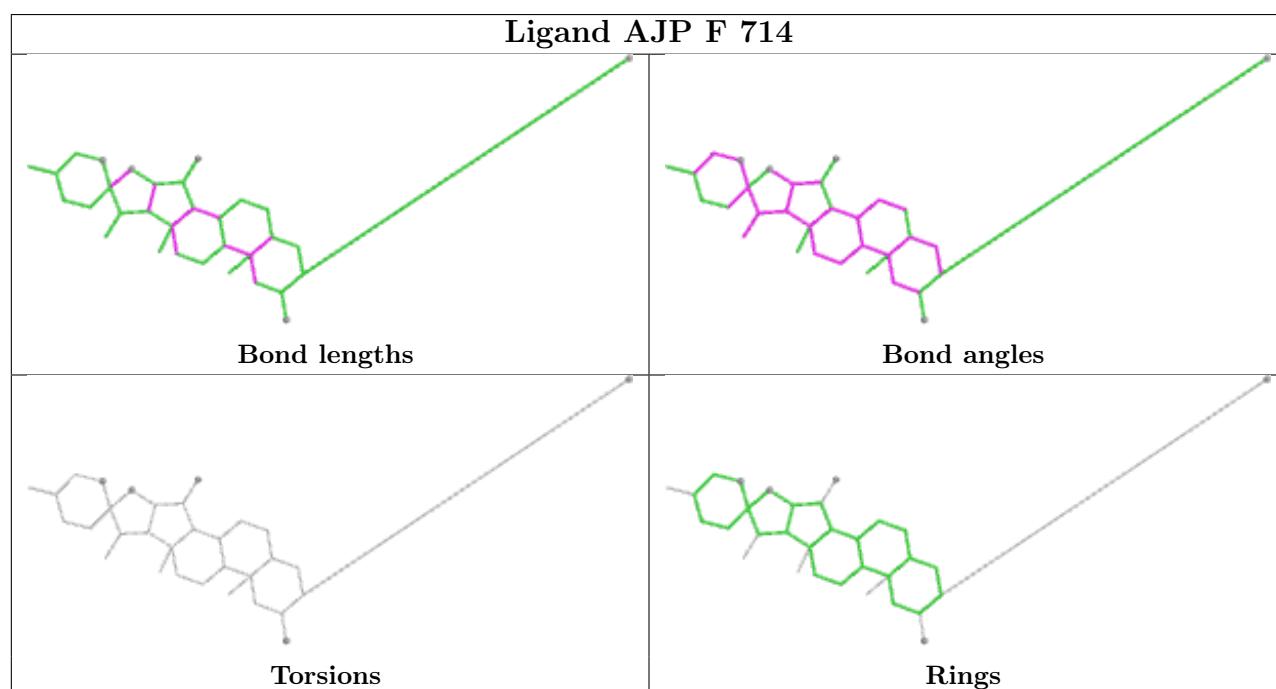
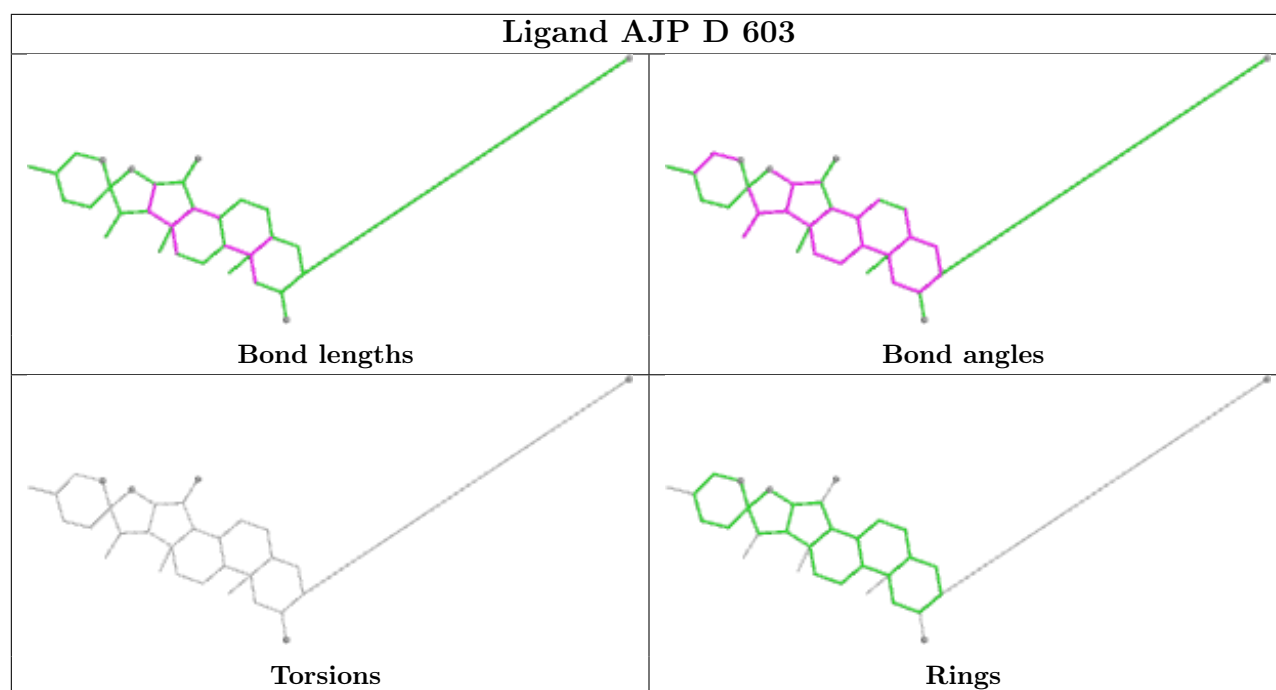


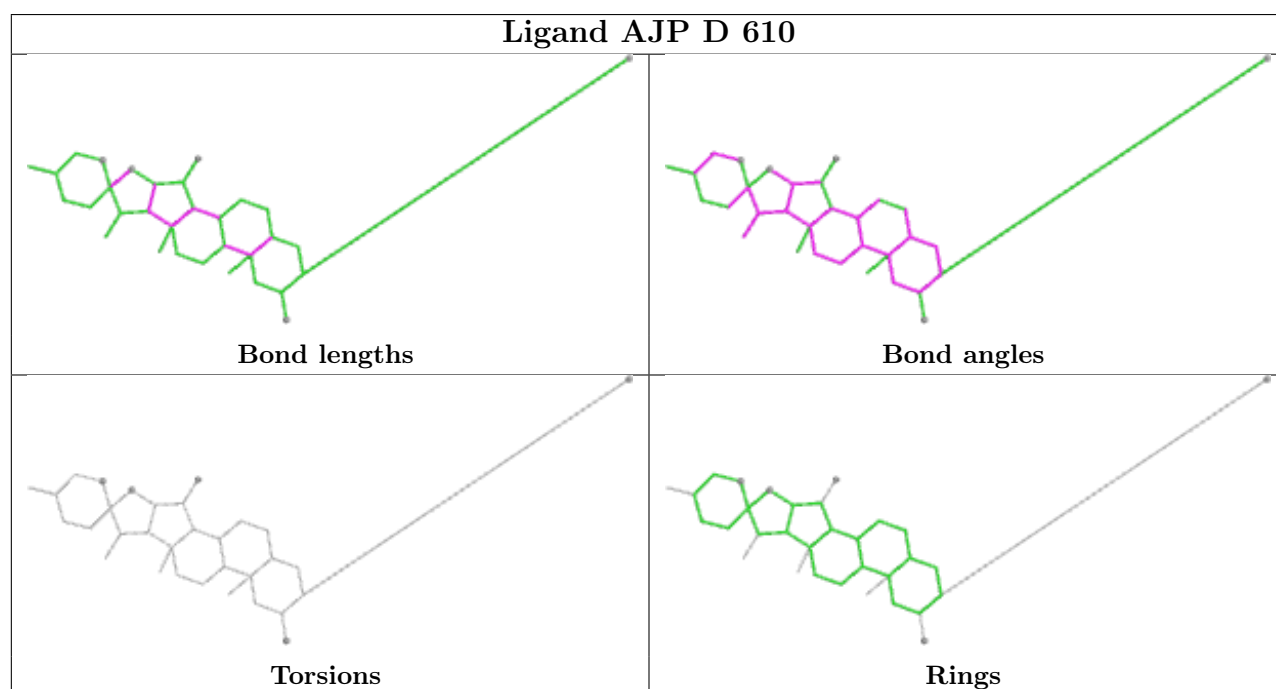
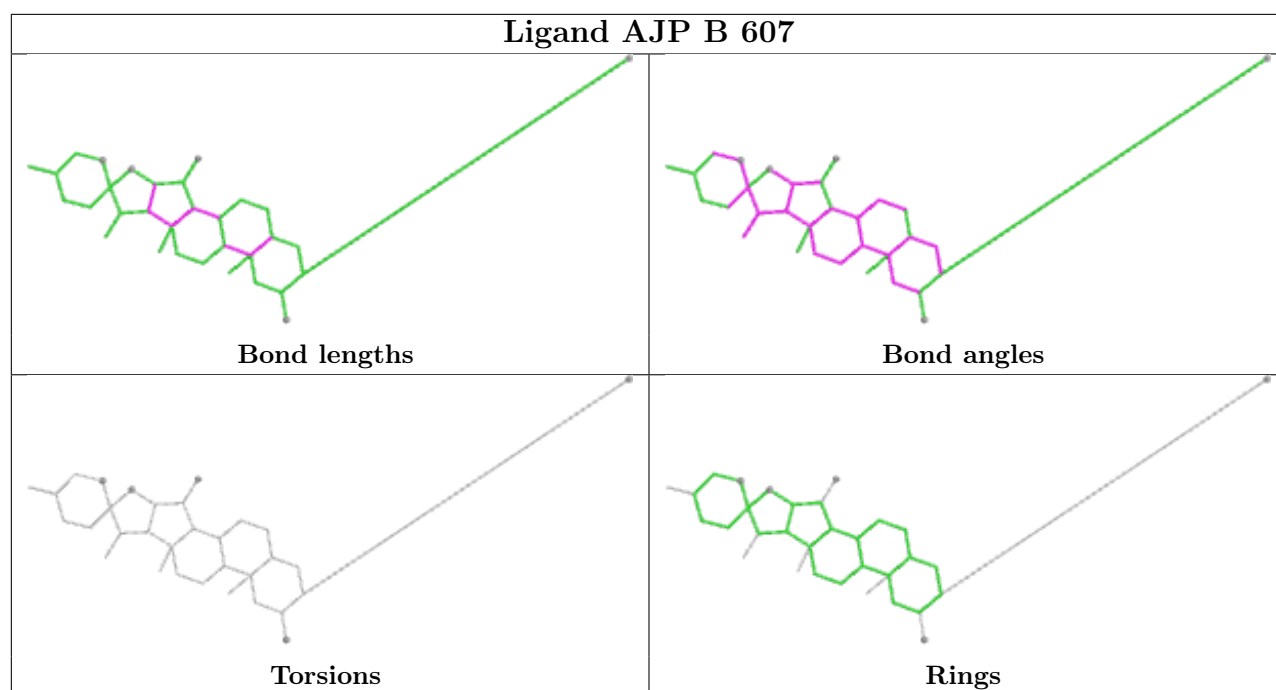


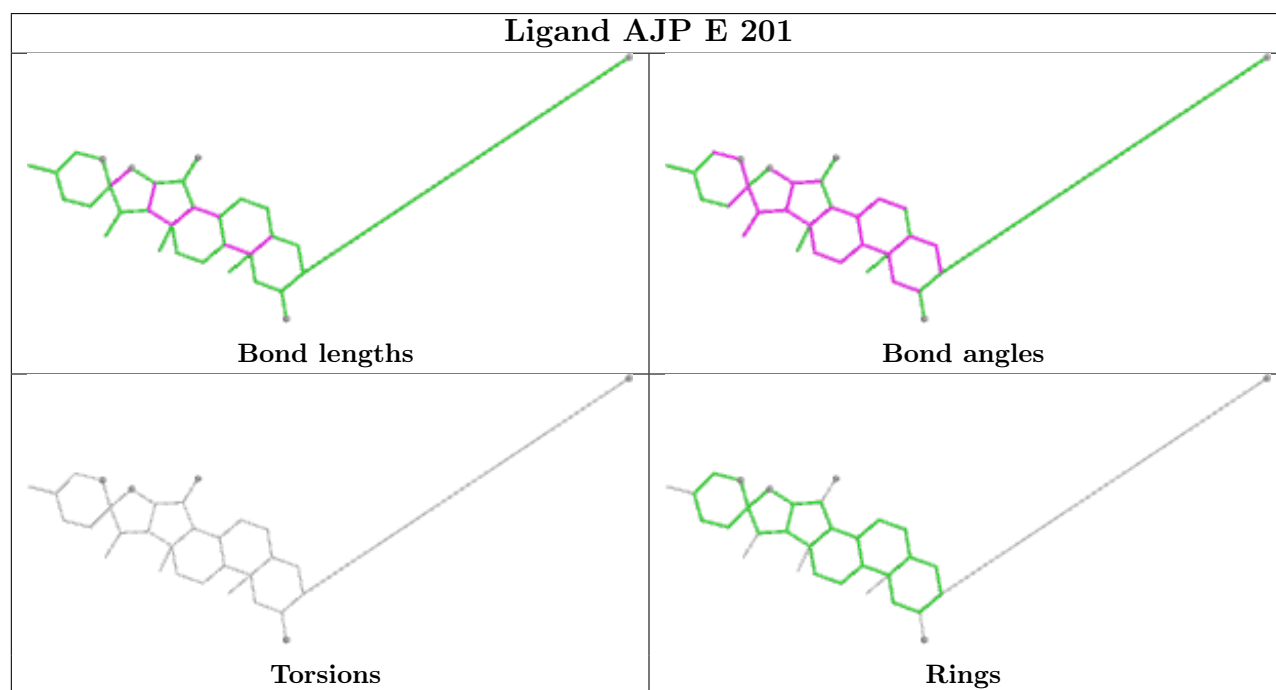
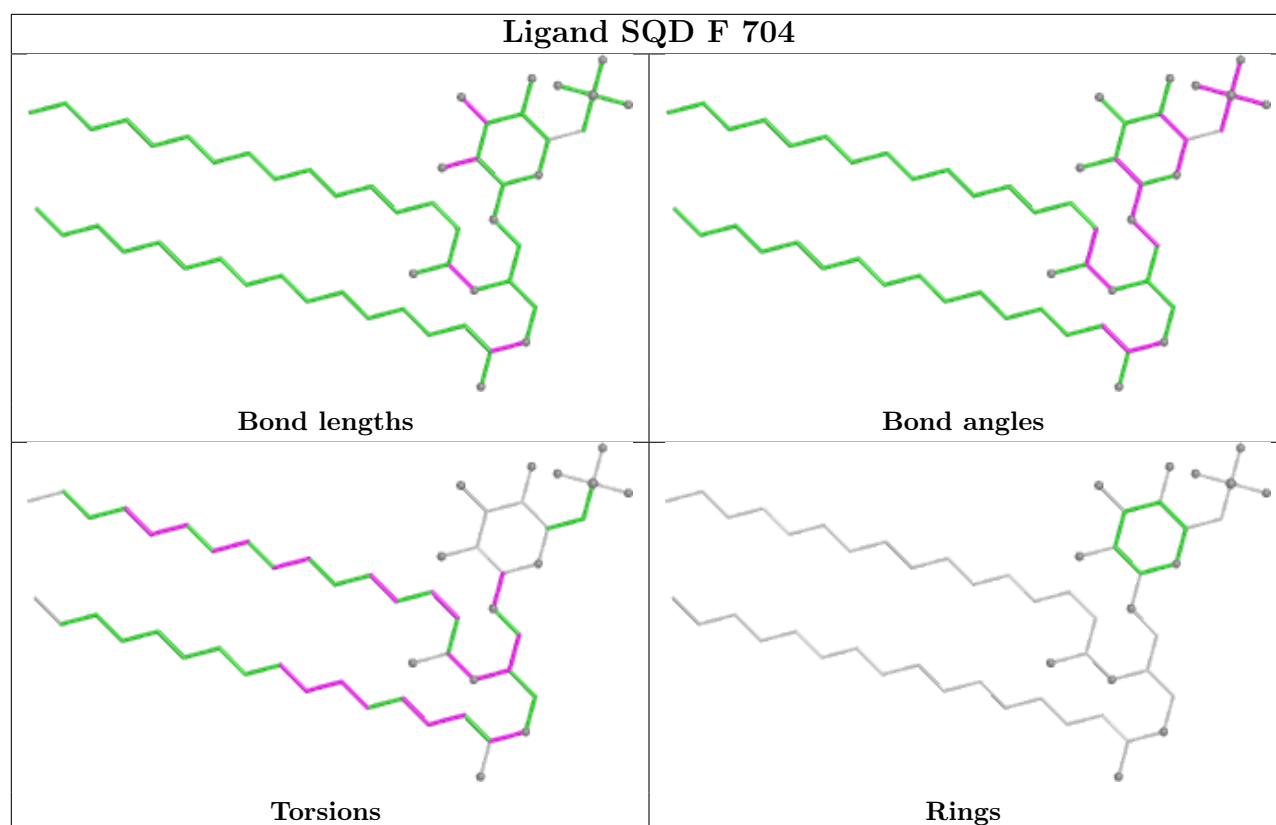


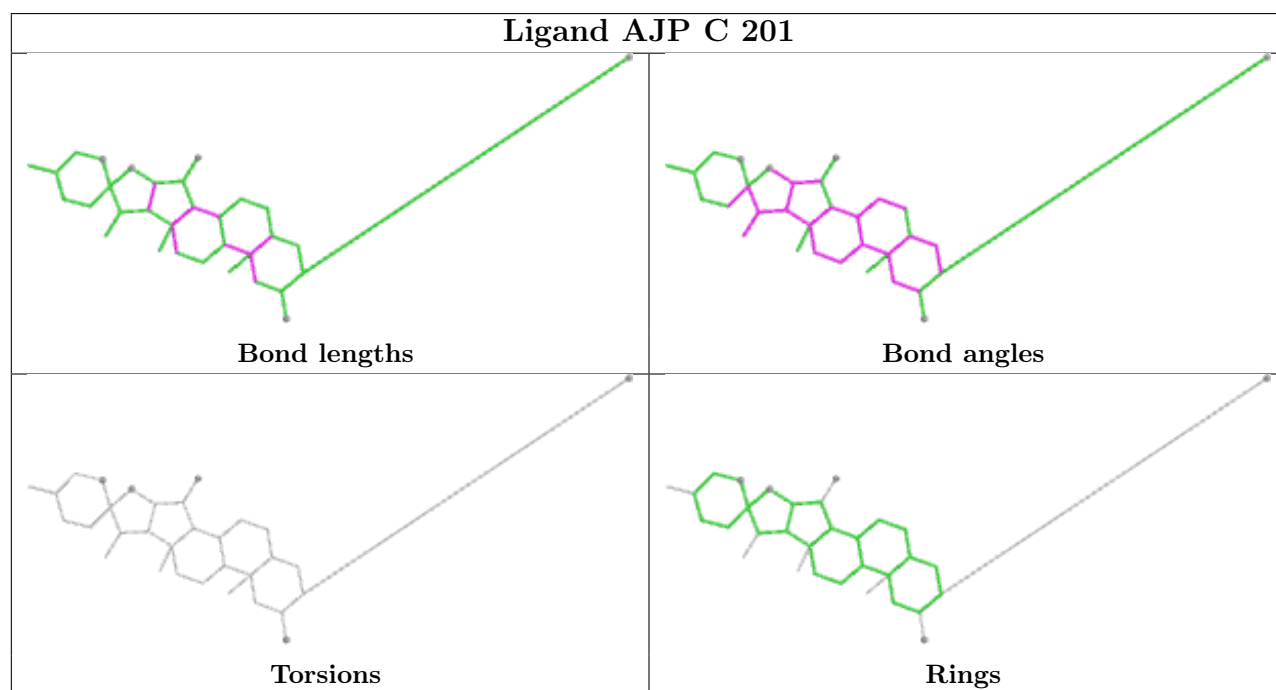
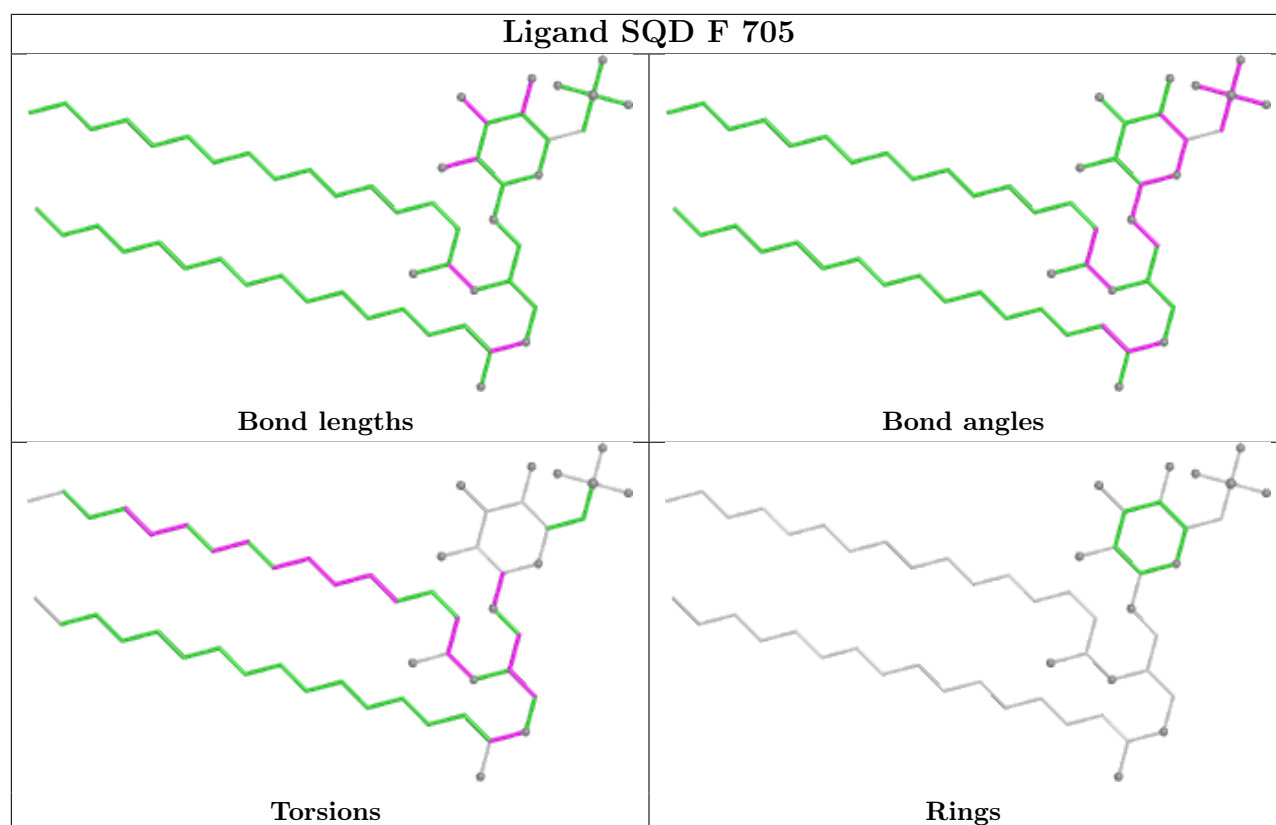


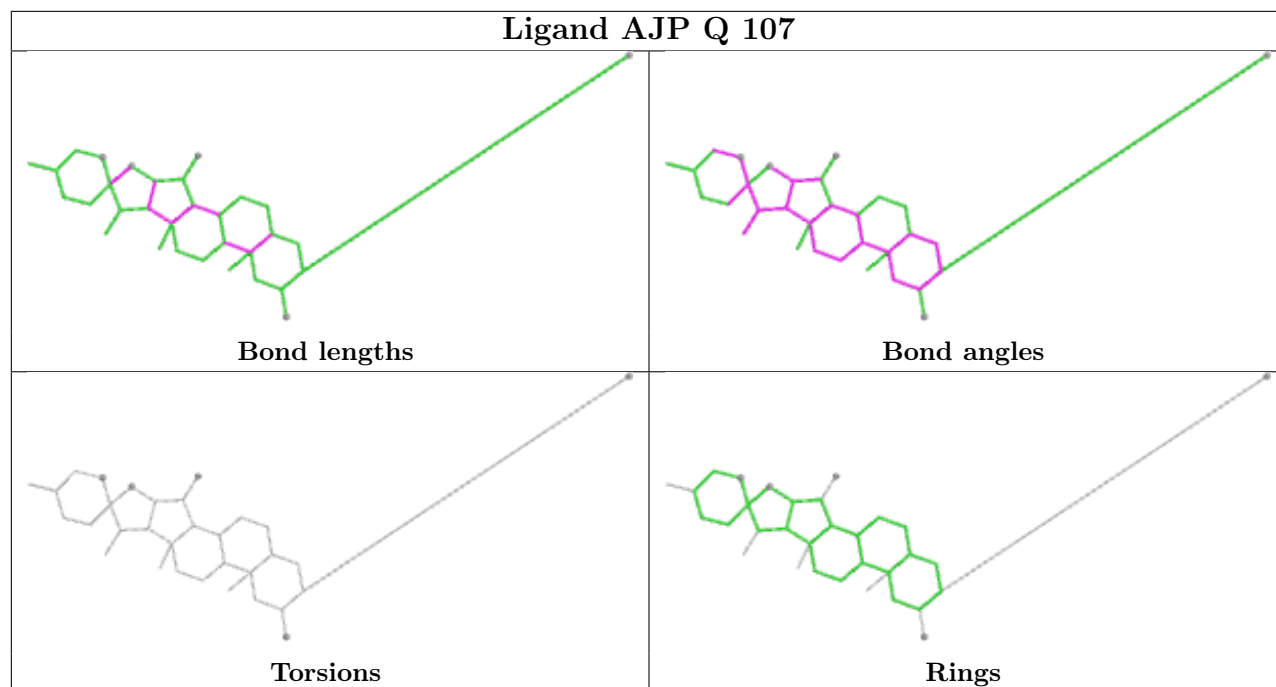


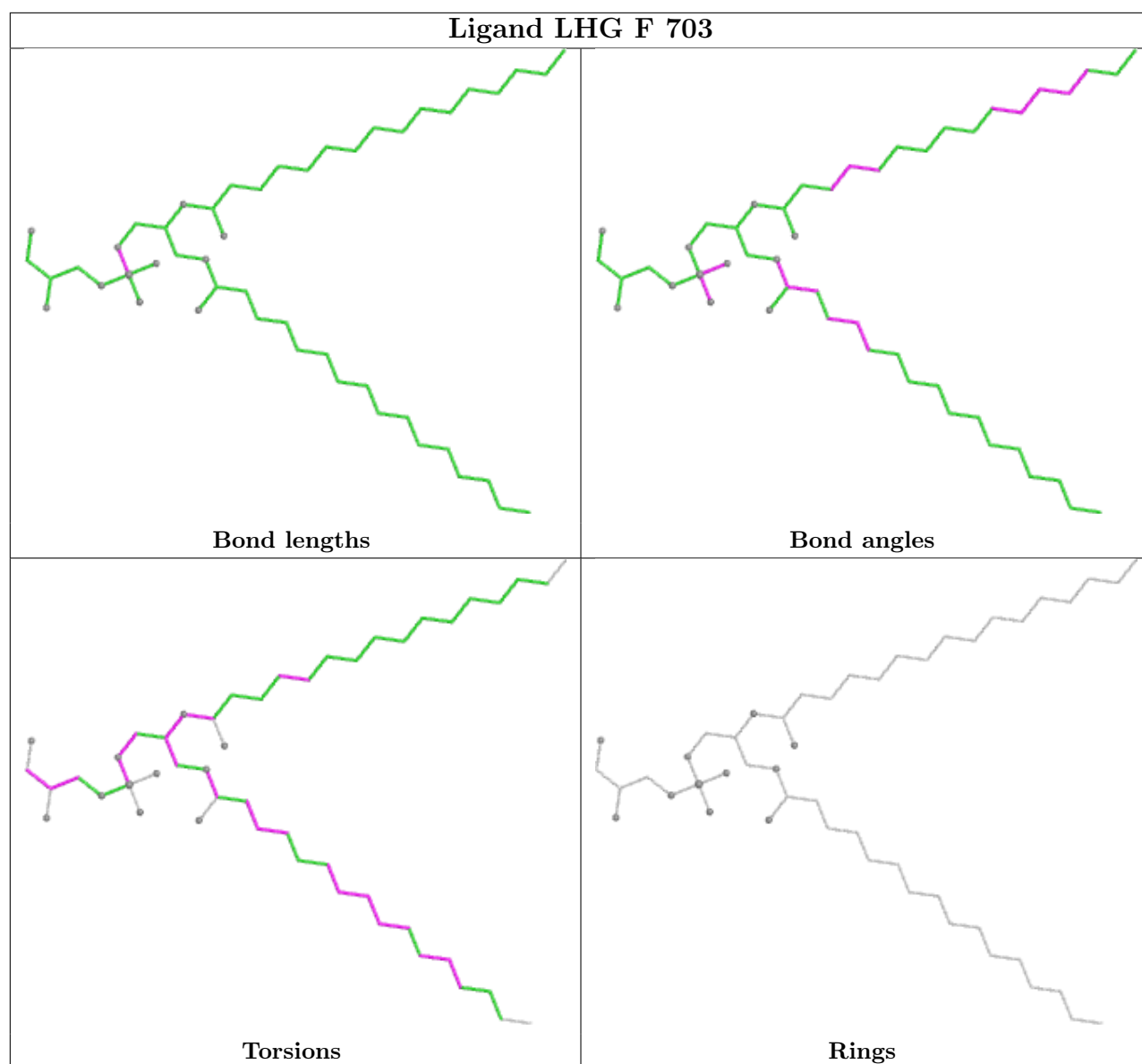


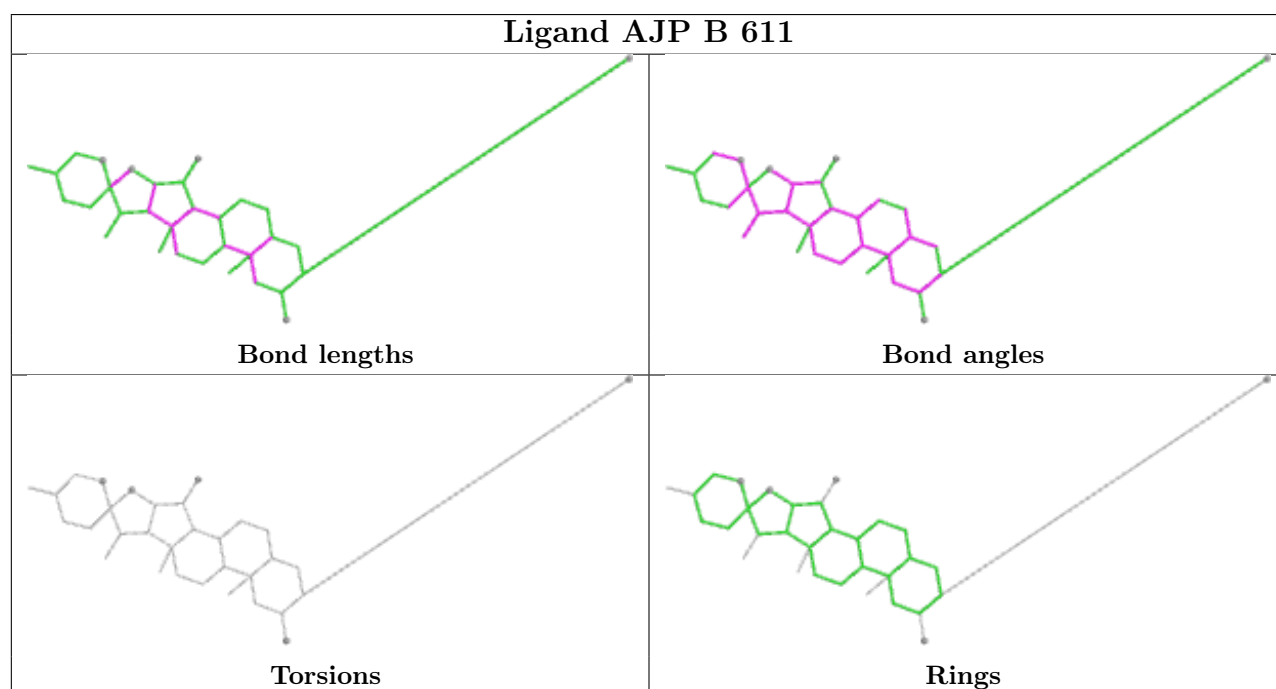
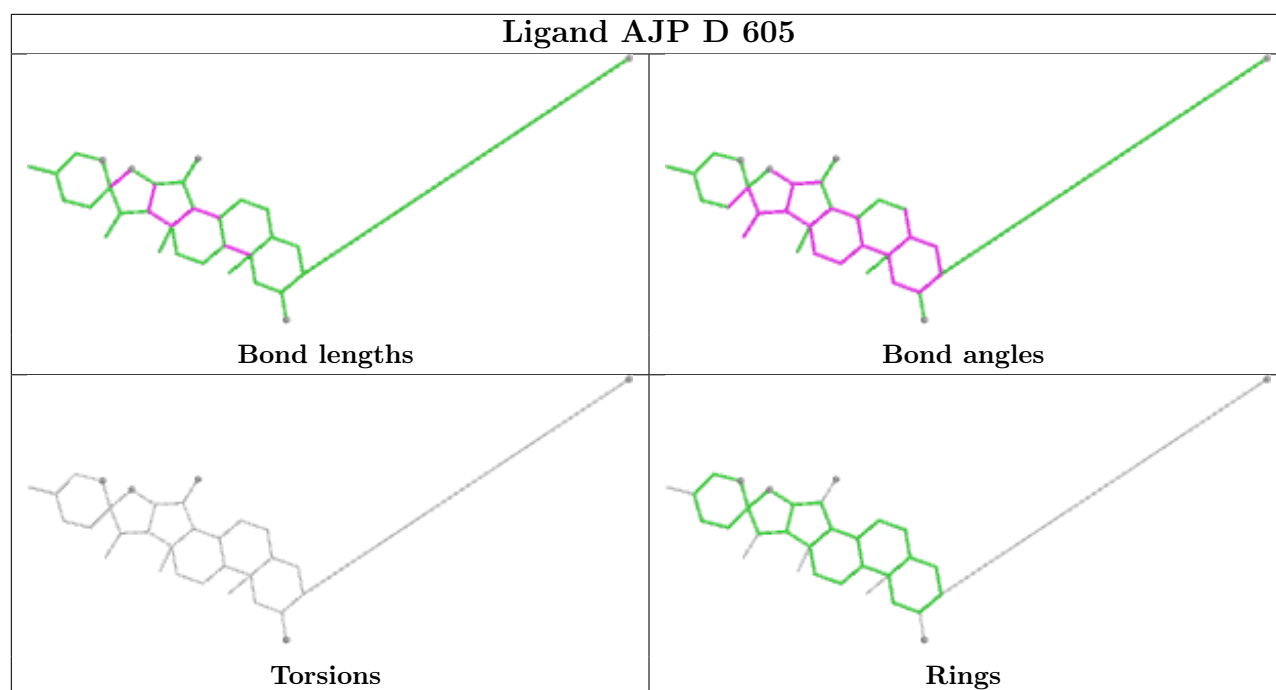


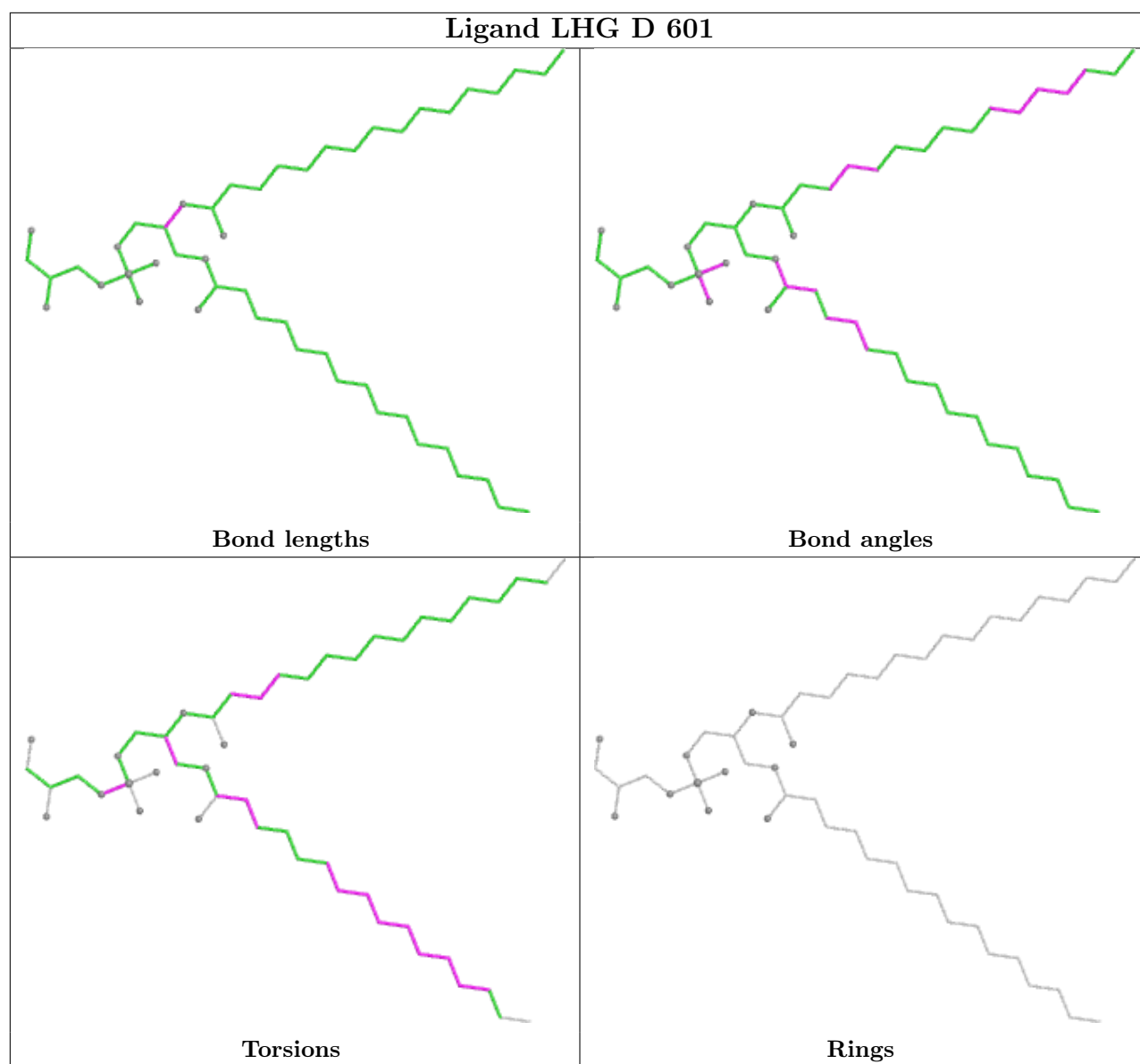


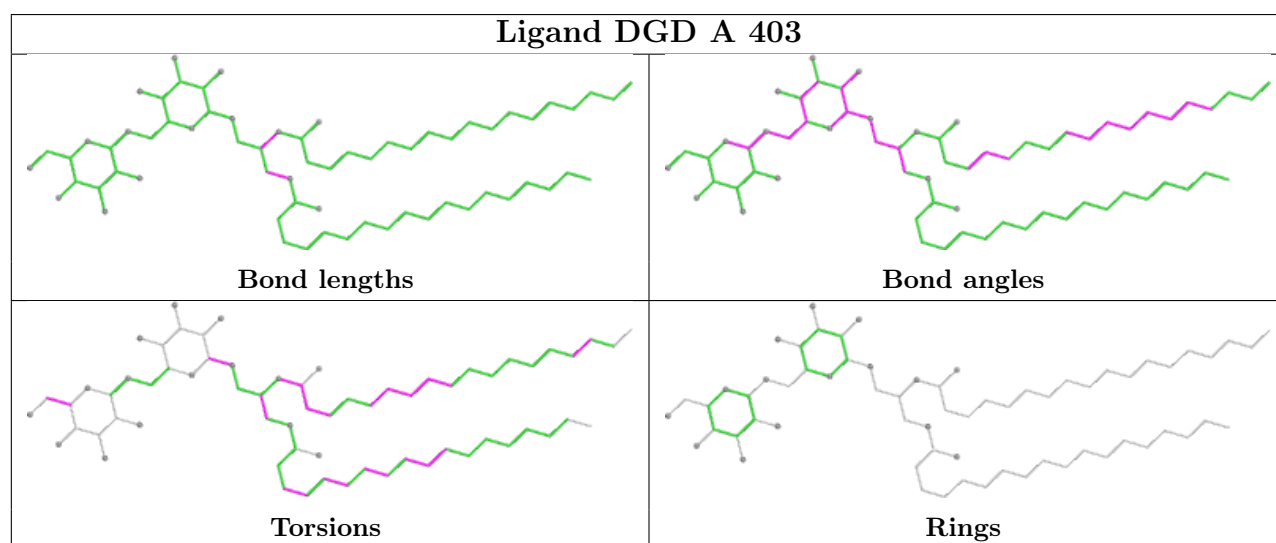
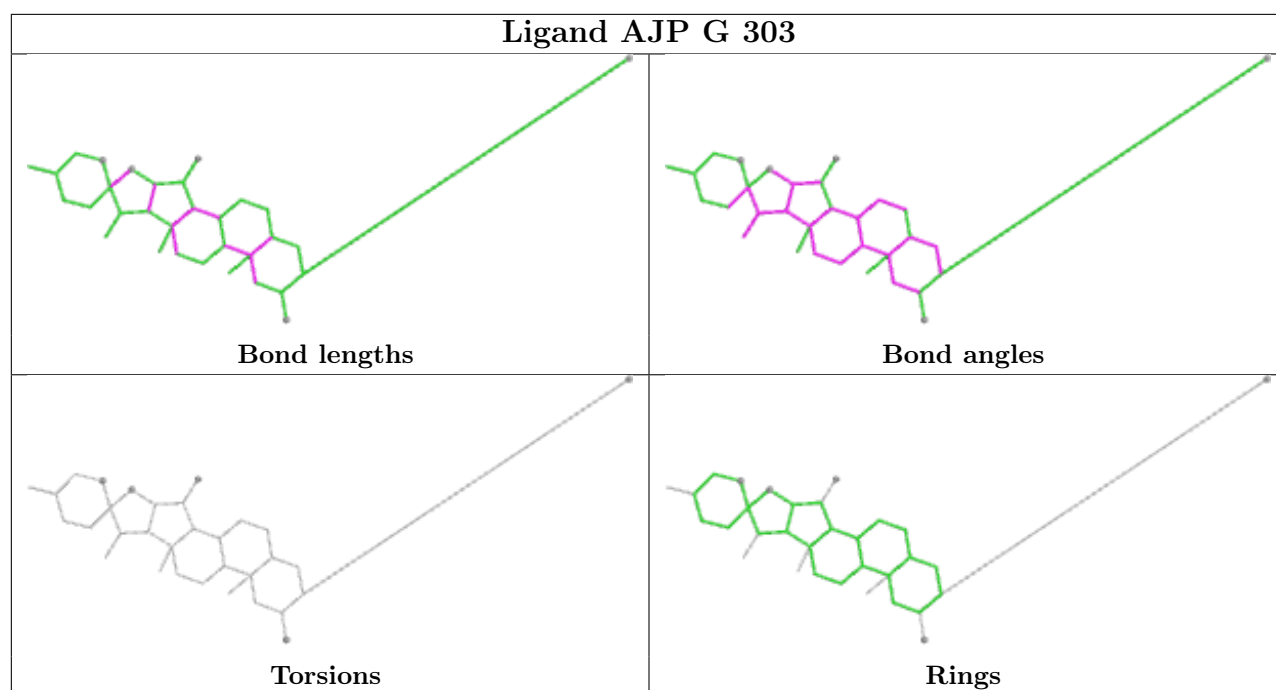


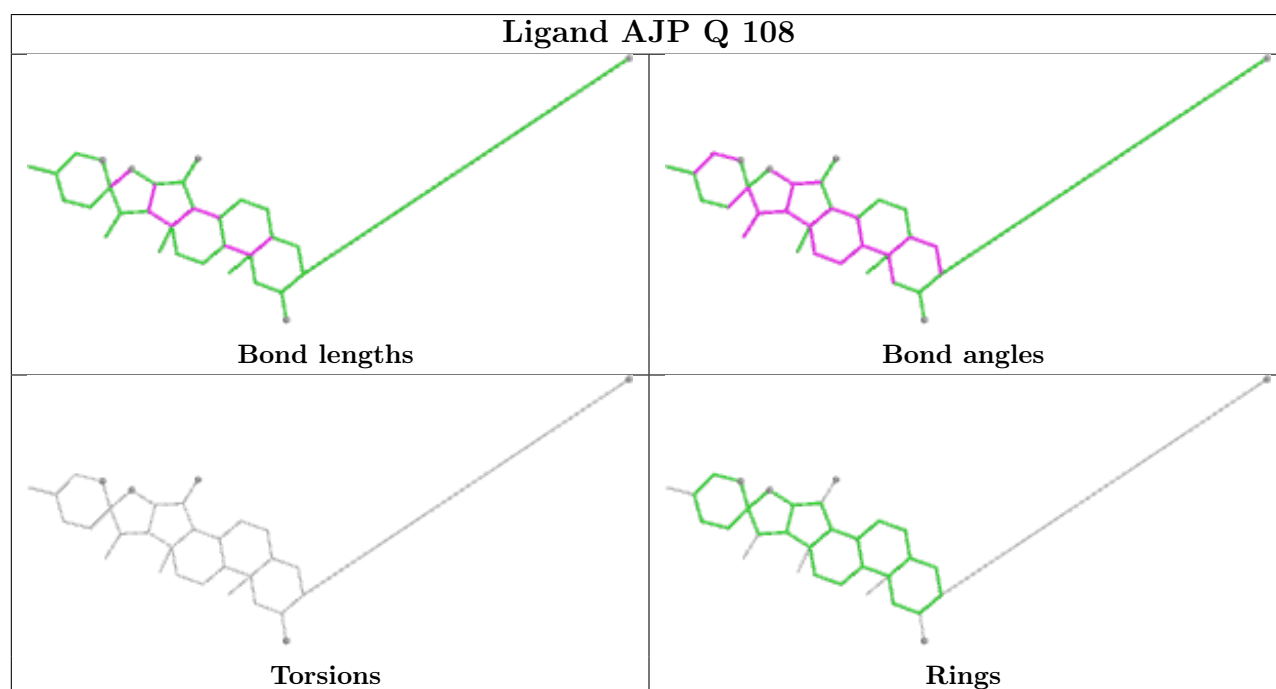
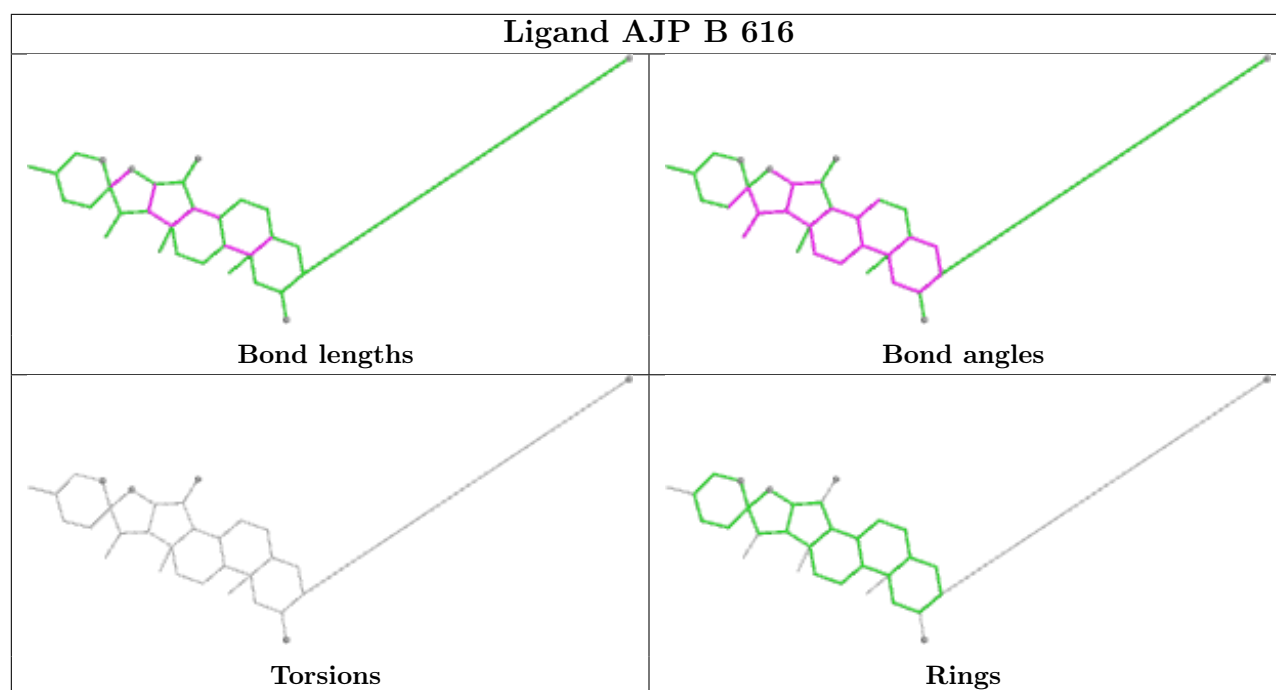


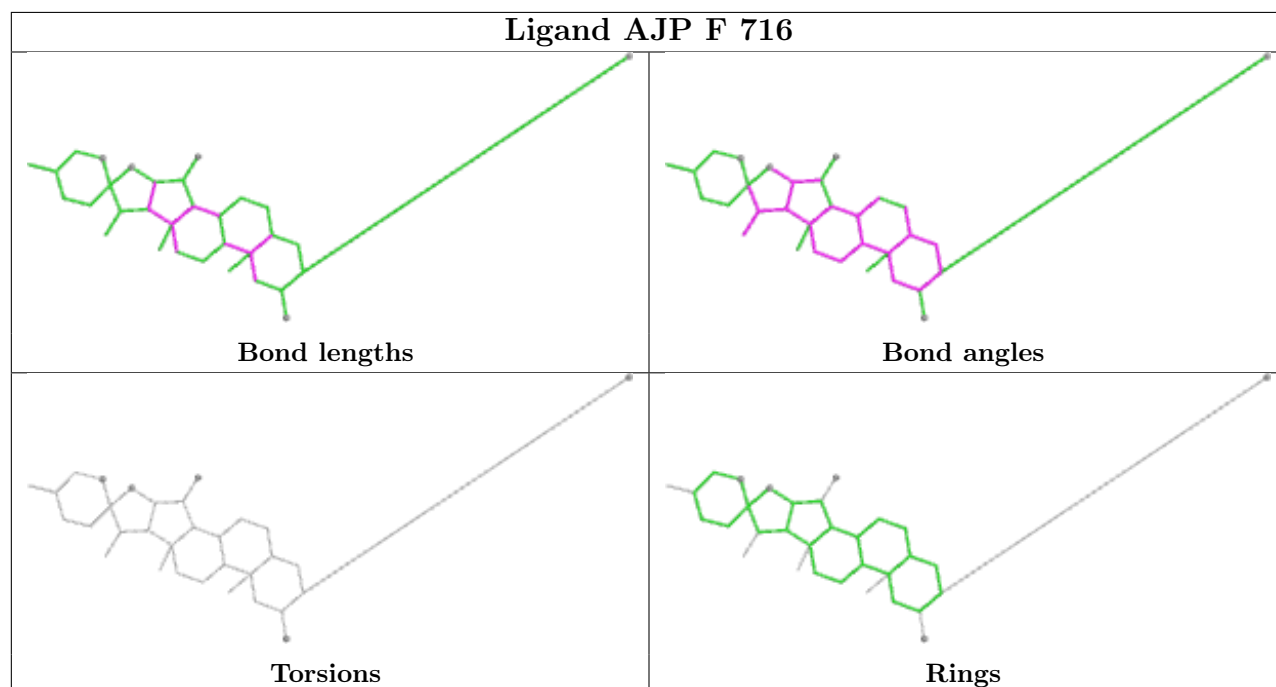
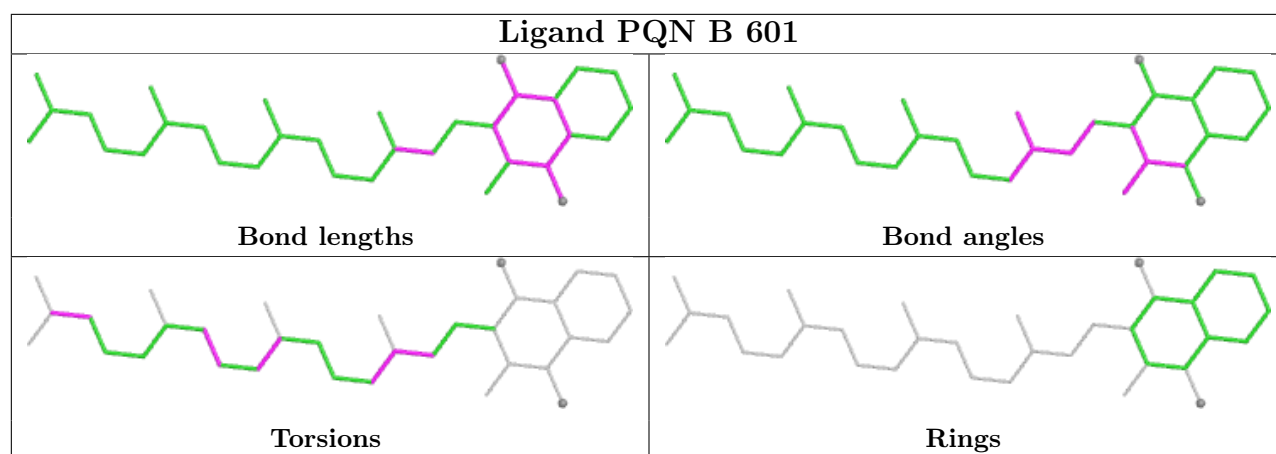


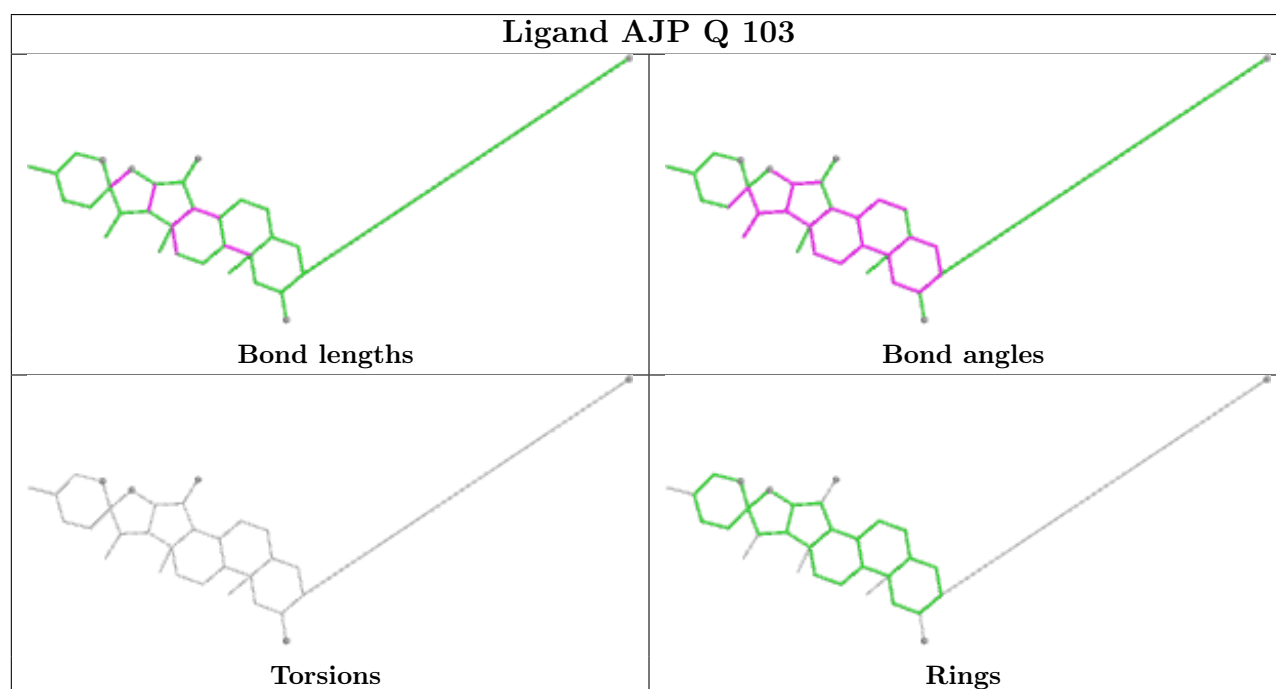
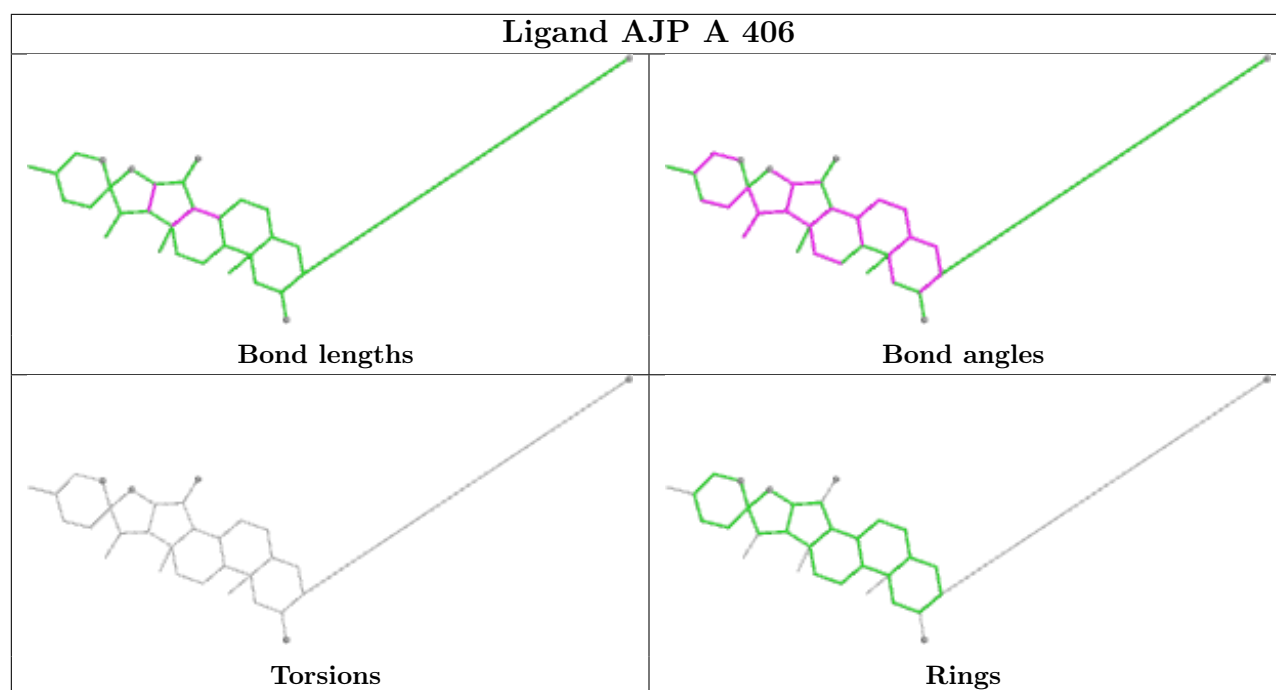


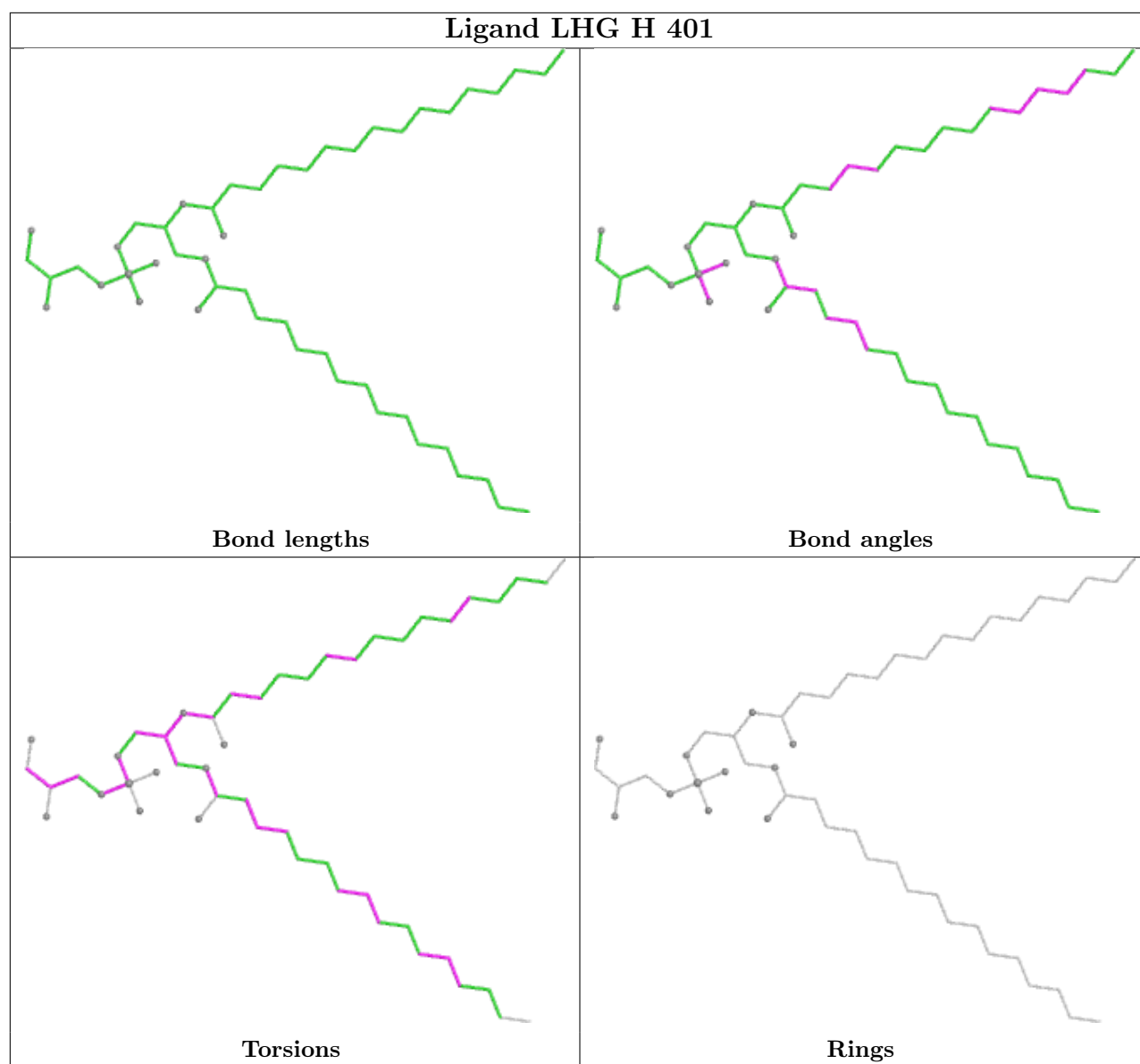


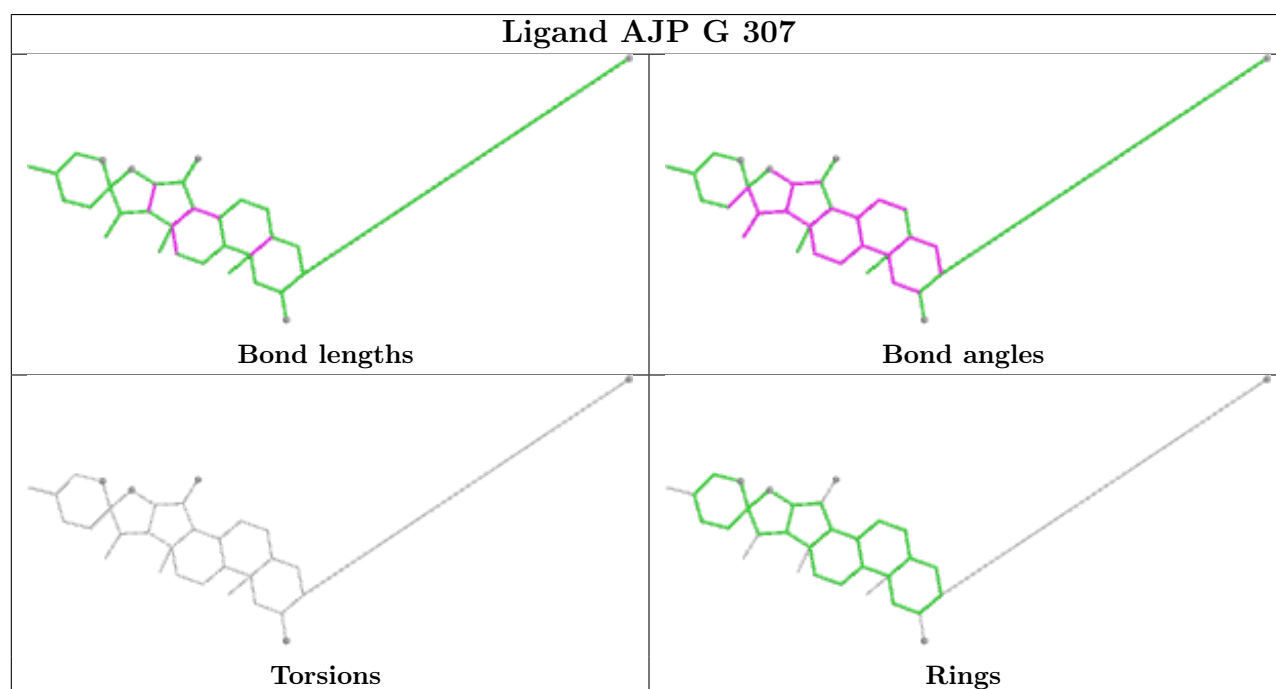
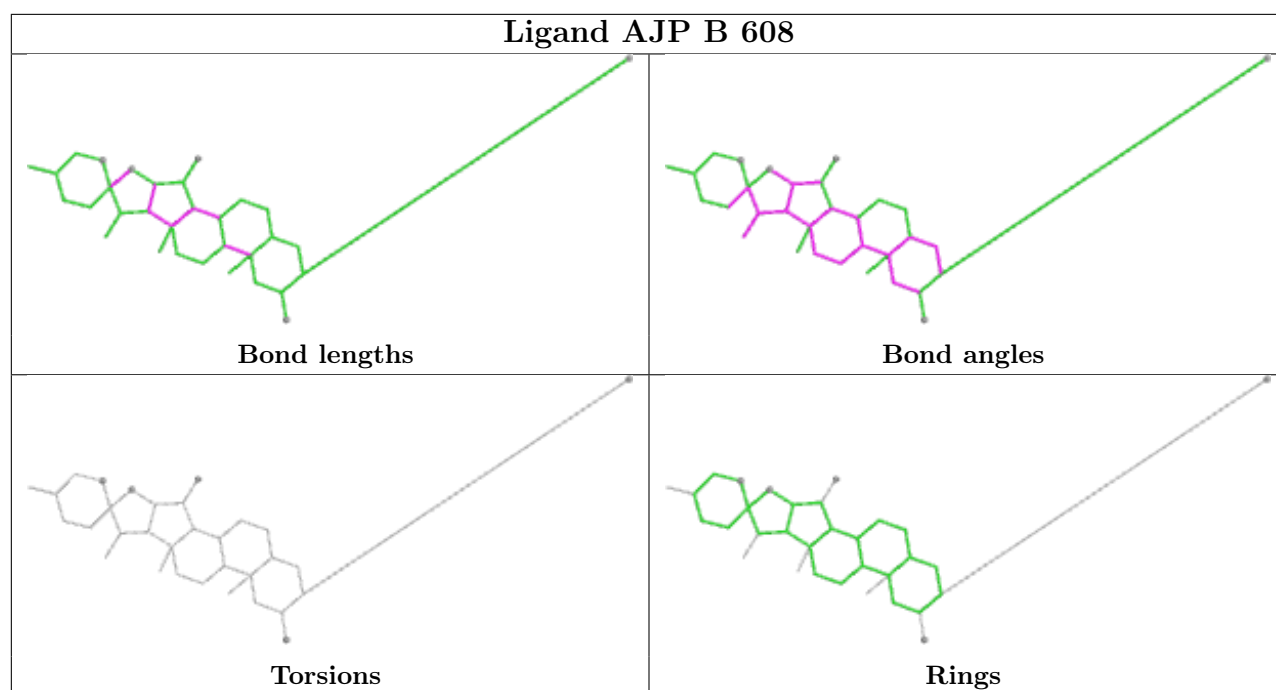


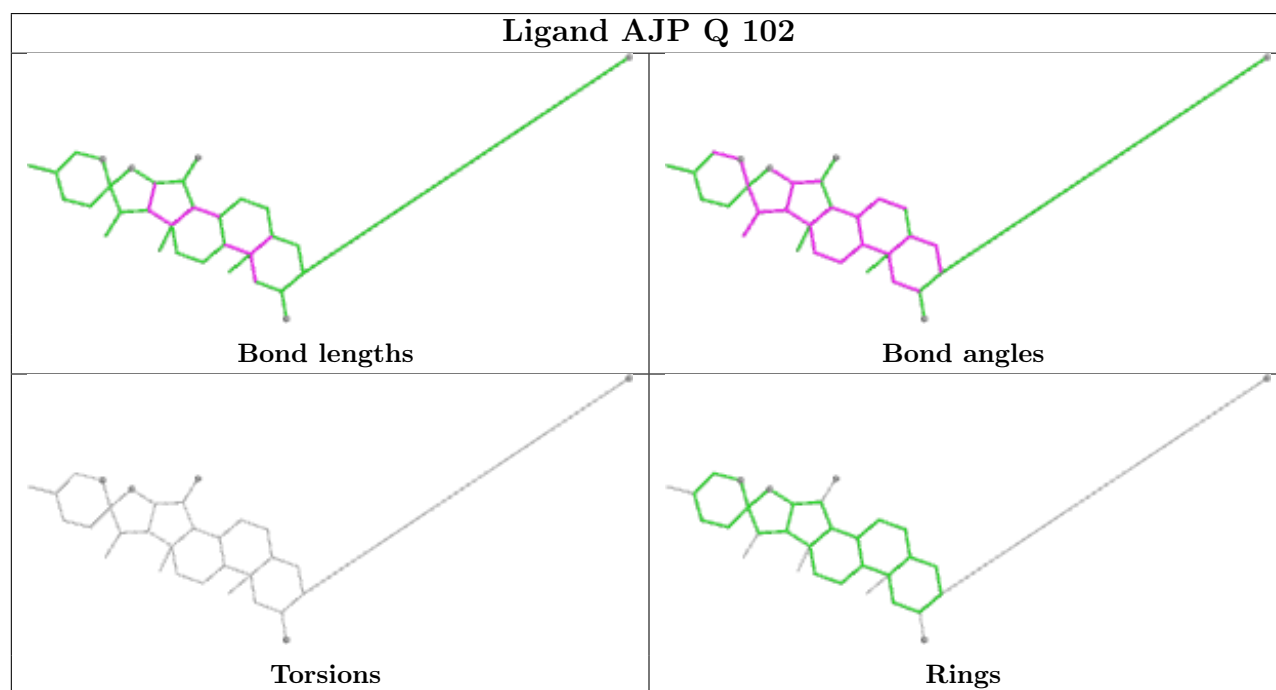
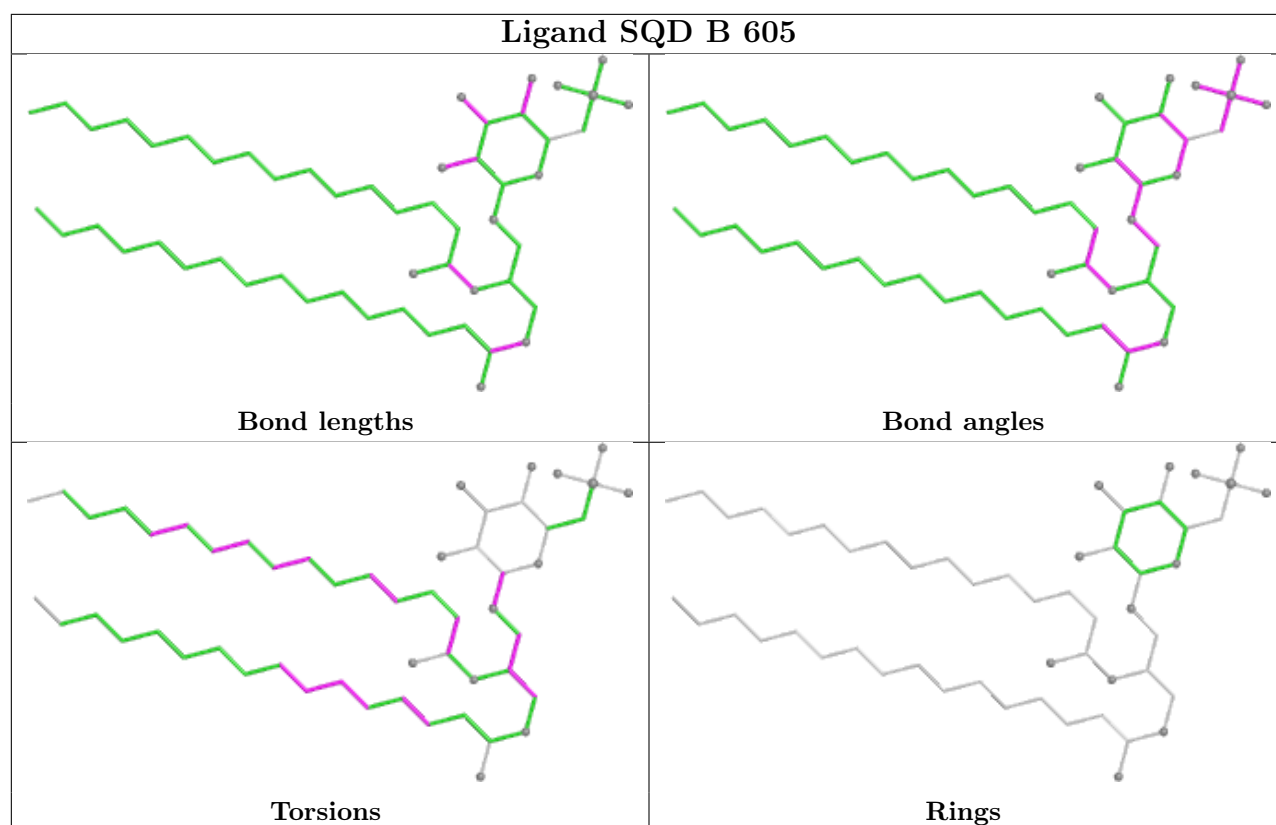


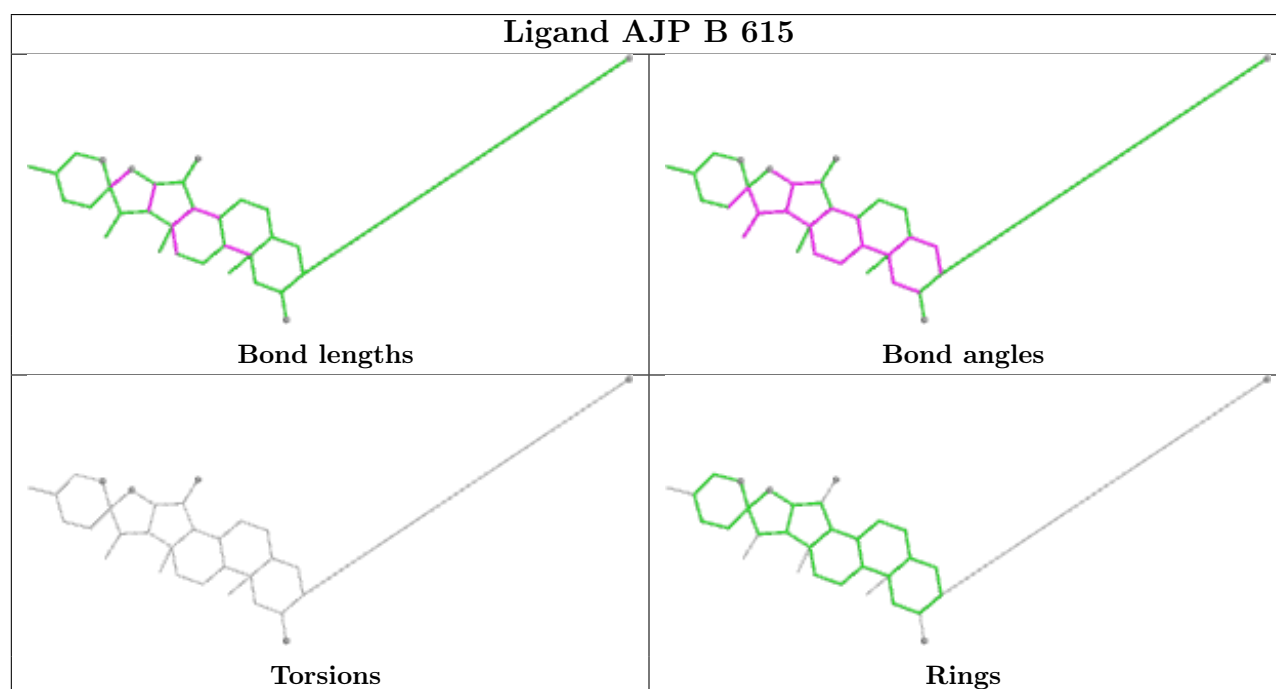
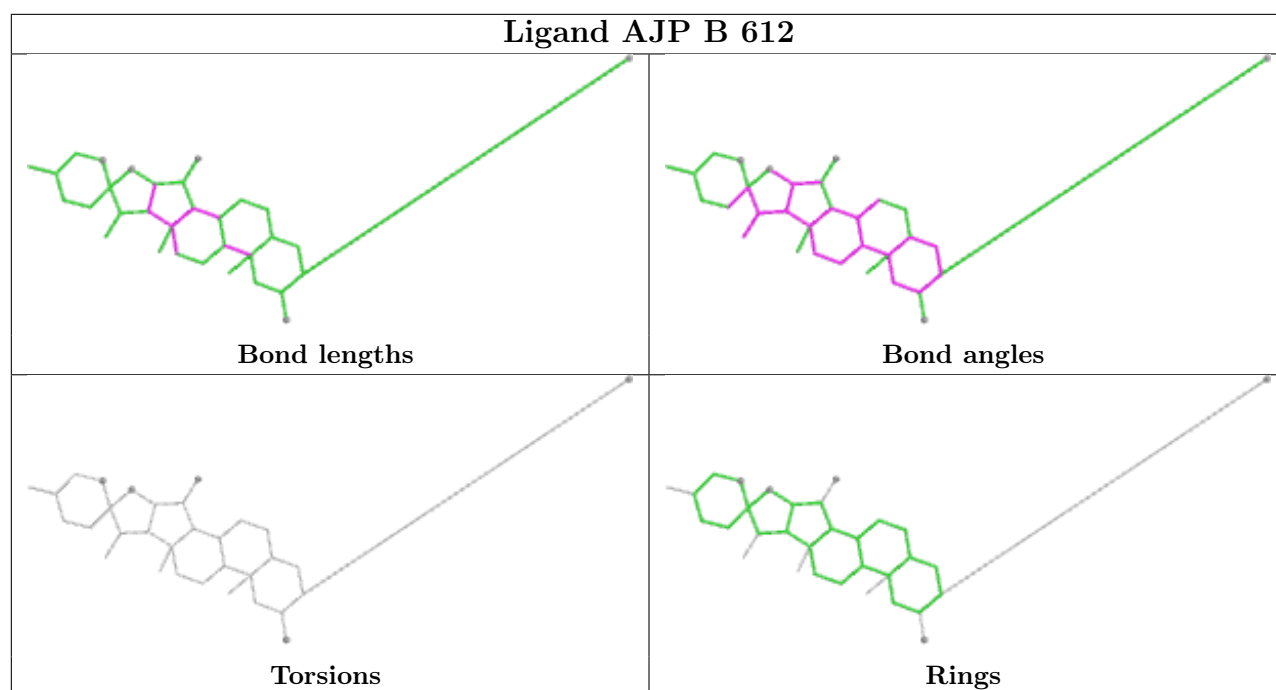


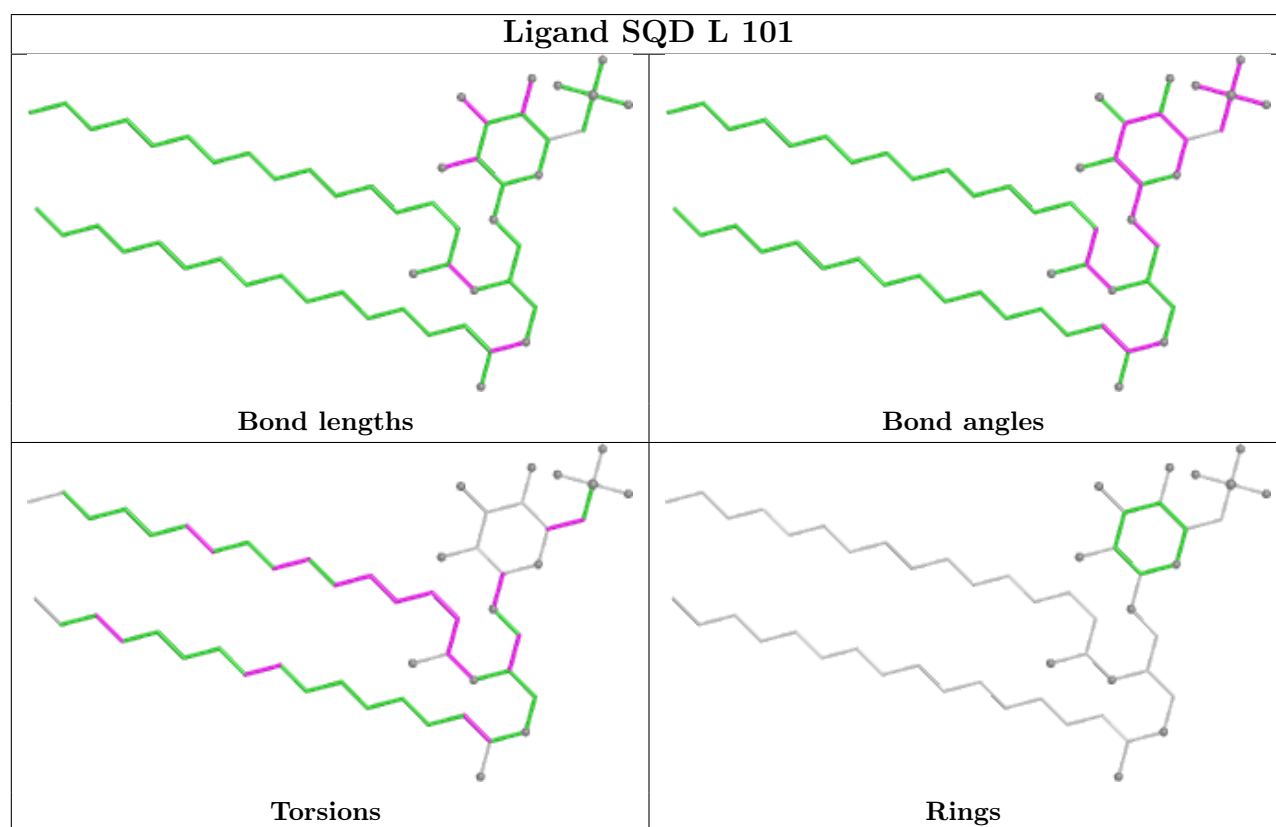
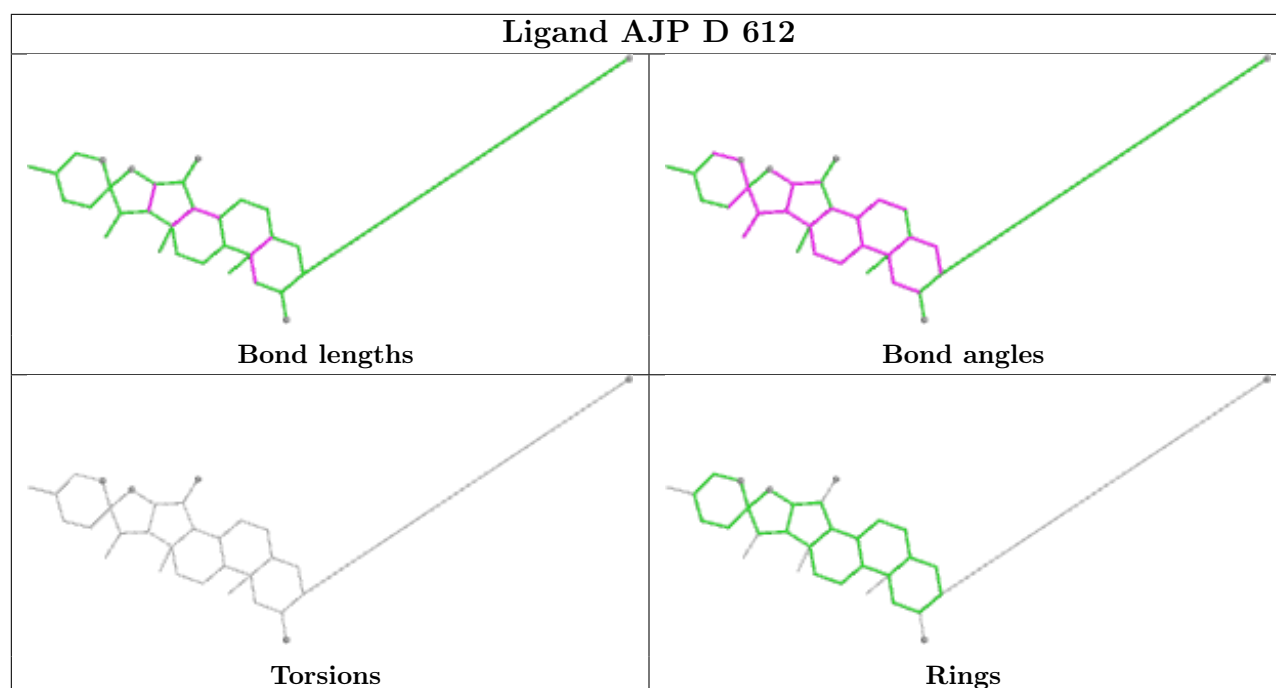


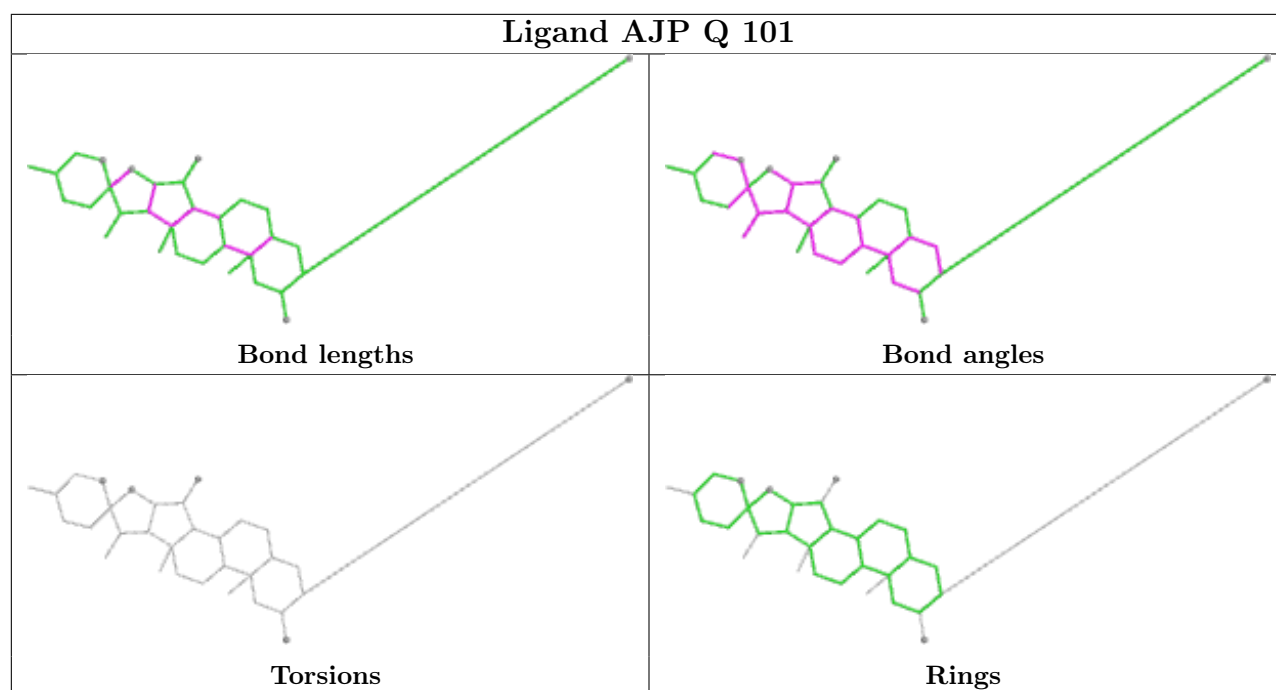












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

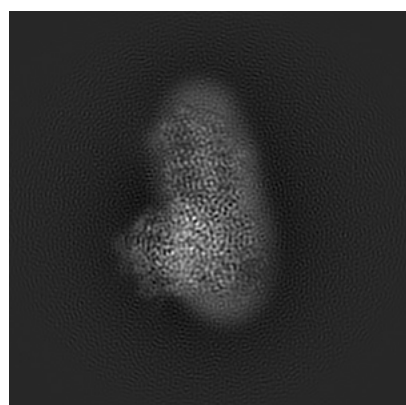
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0849. 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](#)

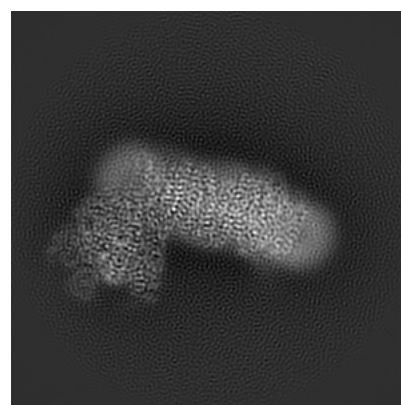
6.1.1 Primary map



X



Y

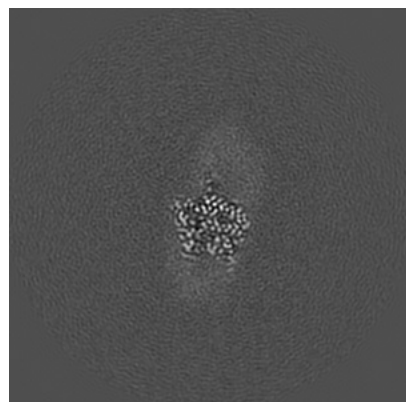


Z

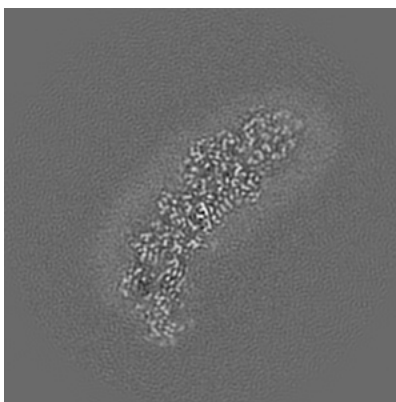
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

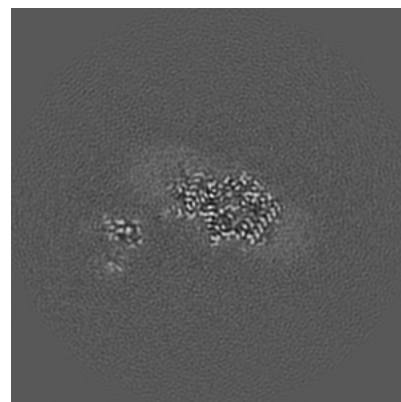
6.2.1 Primary map



X Index: 150



Y Index: 150

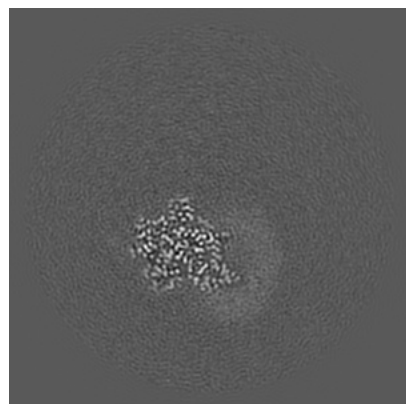


Z Index: 150

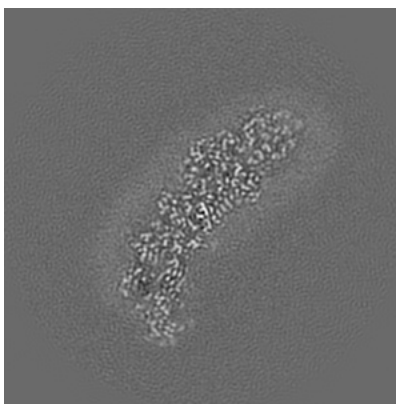
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

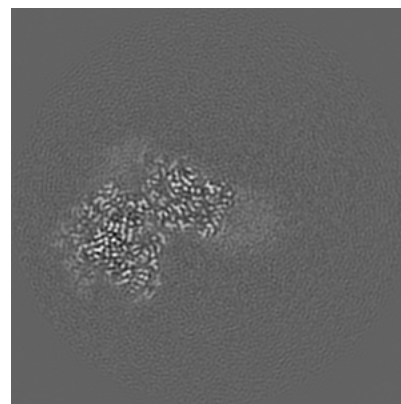
6.3.1 Primary map



X Index: 88



Y Index: 150

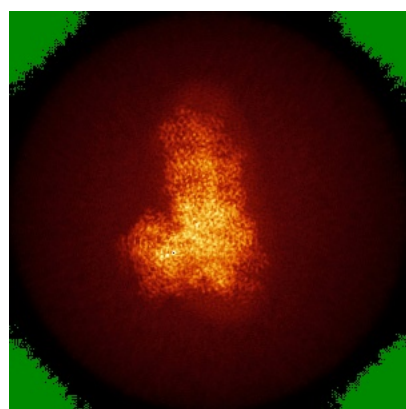


Z Index: 121

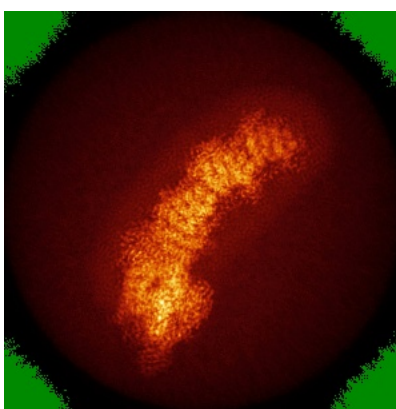
The images above show the largest variance slices of the map in three orthogonal directions.

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

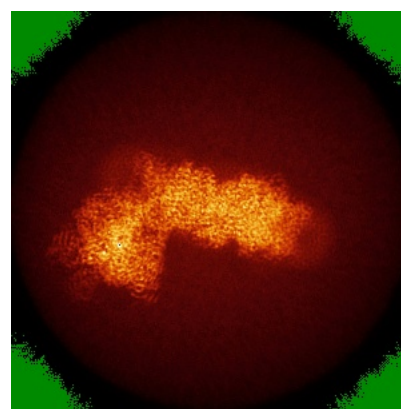
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

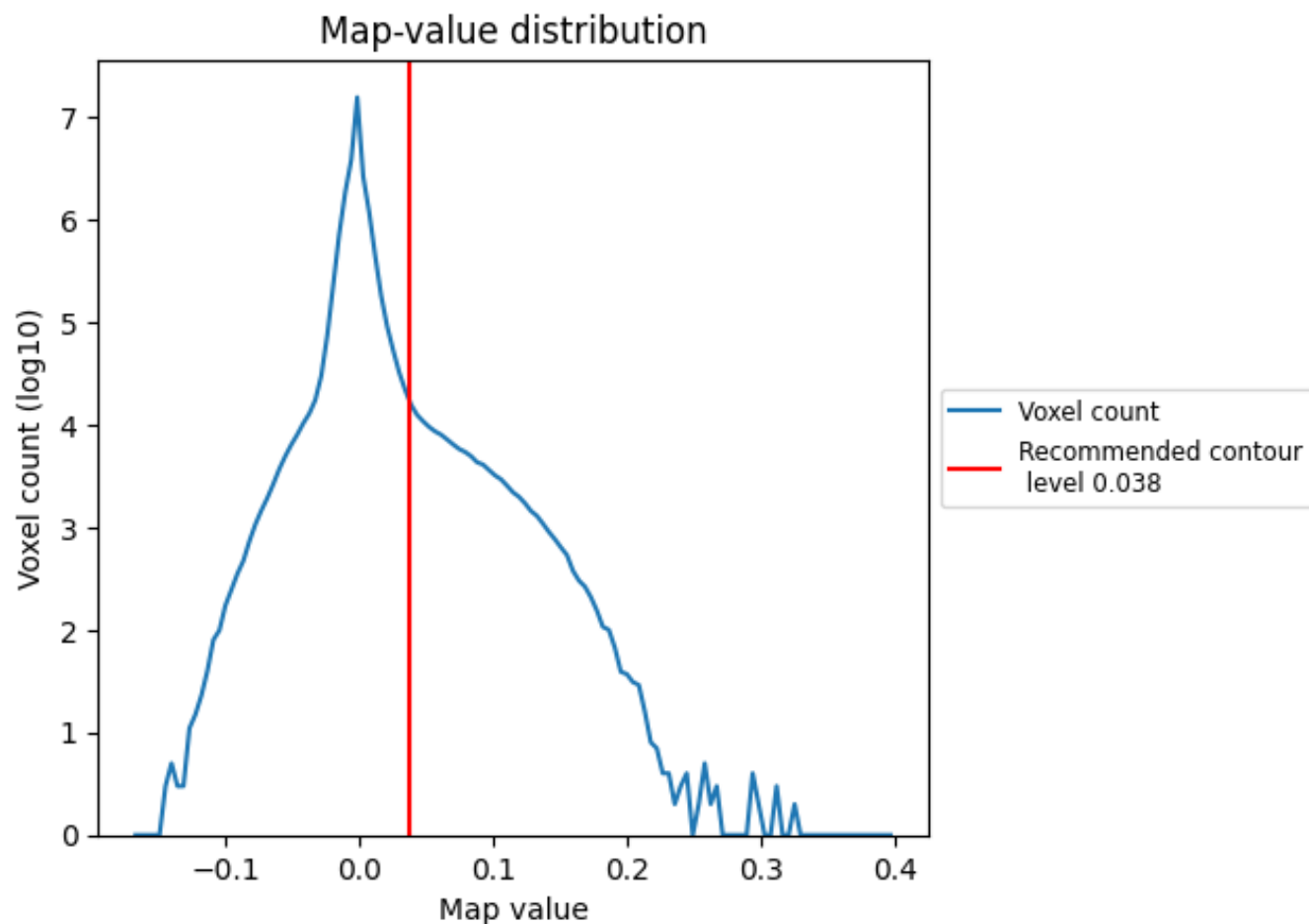
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

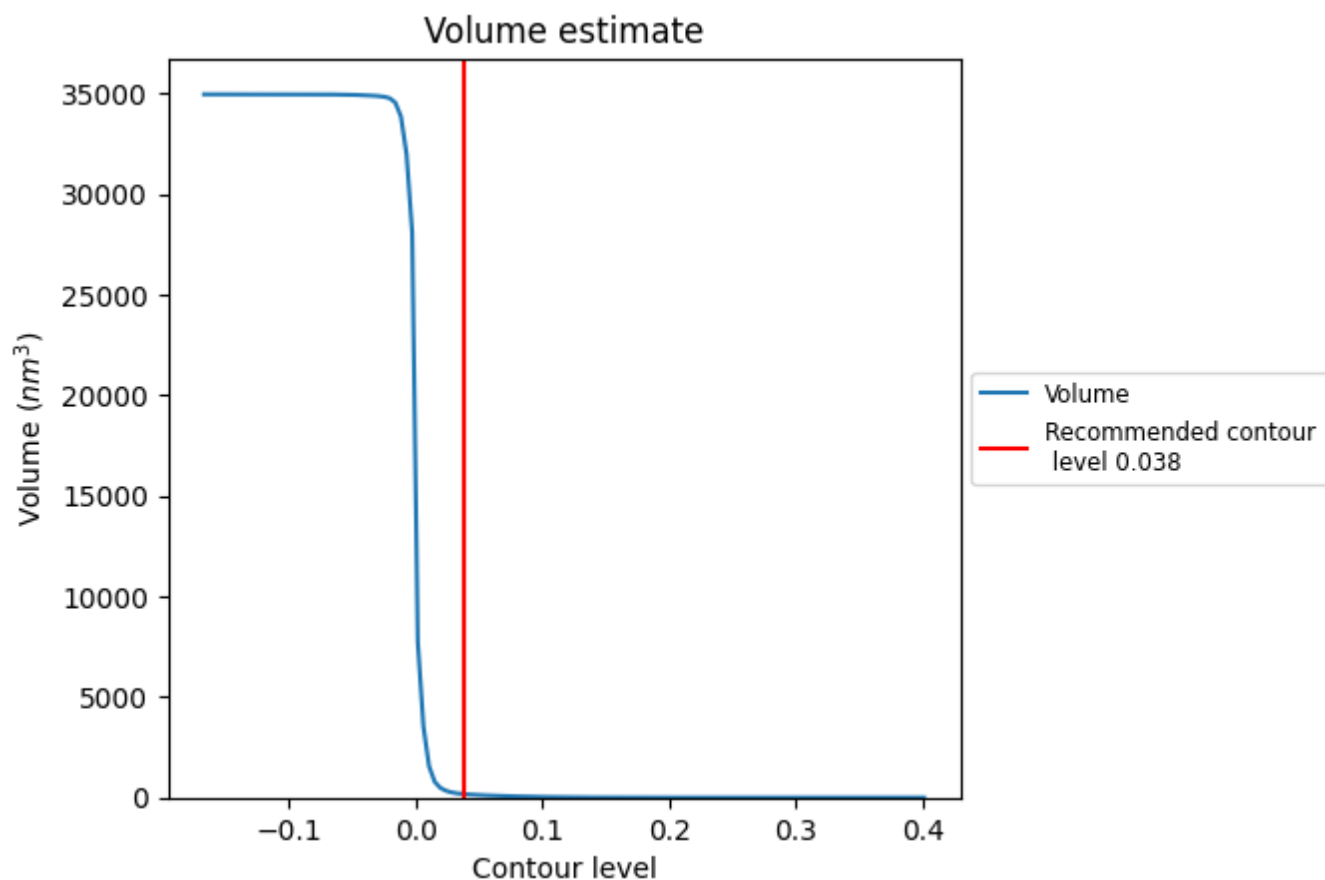
This section contains the results of statistical analysis of the map.

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.

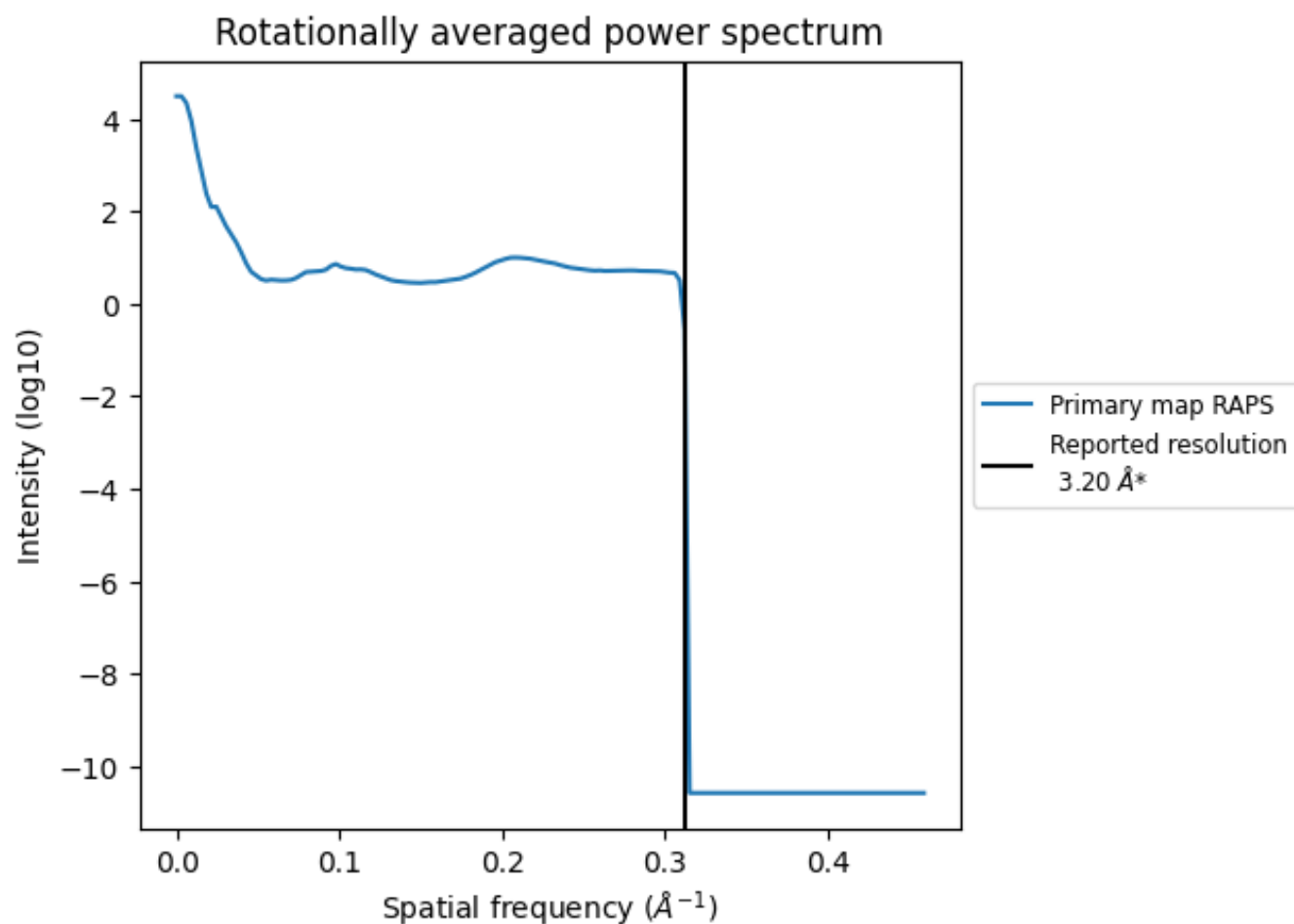
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

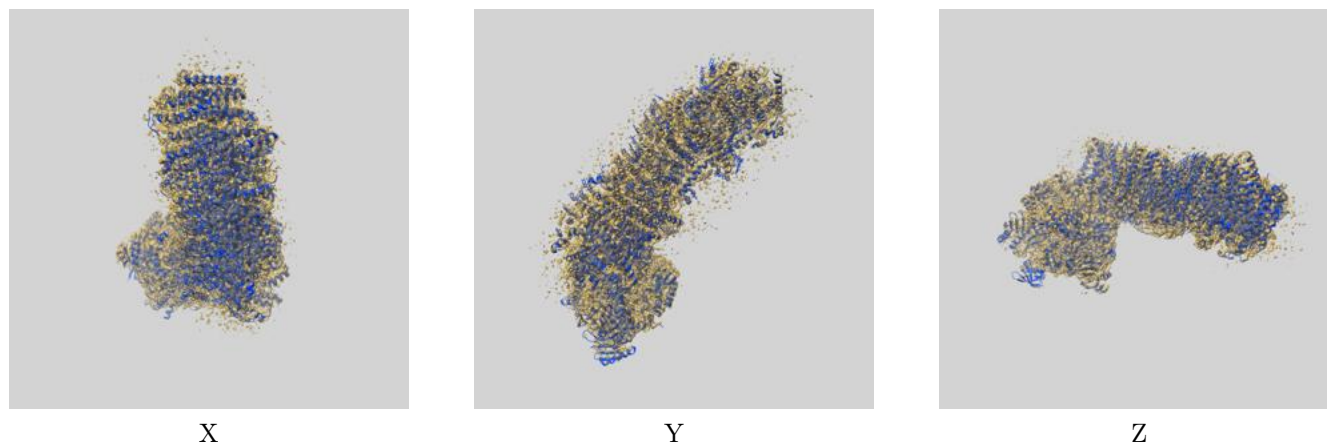
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

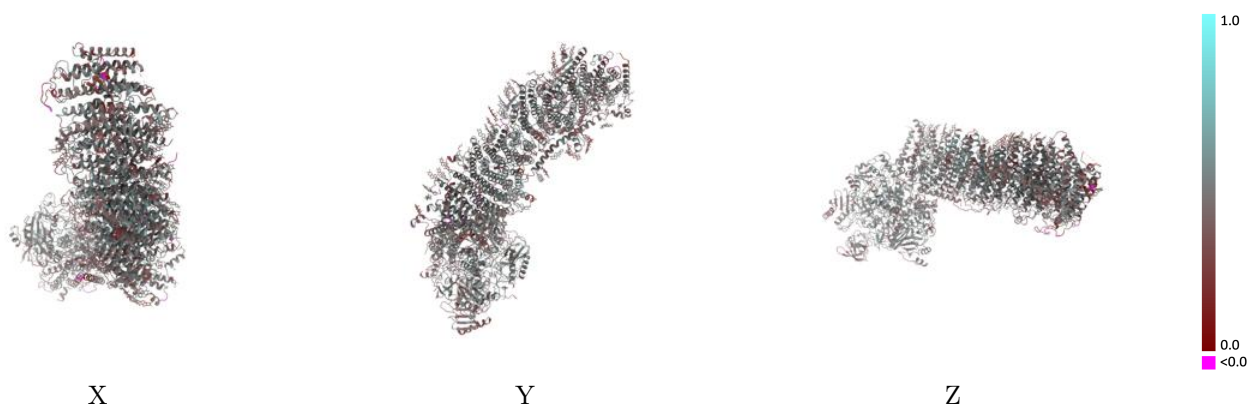
This section contains information regarding the fit between EMDB map EMD-0849 and PDB model 6L7O. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



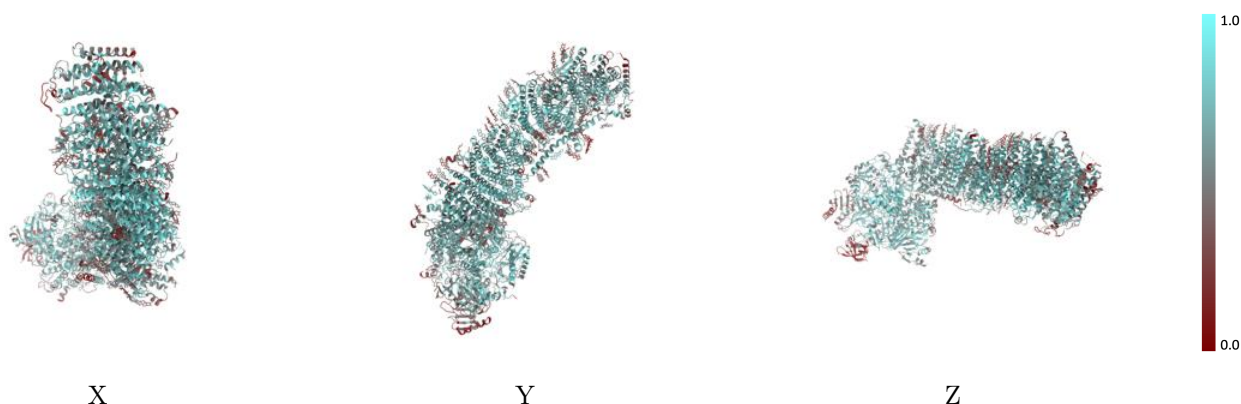
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



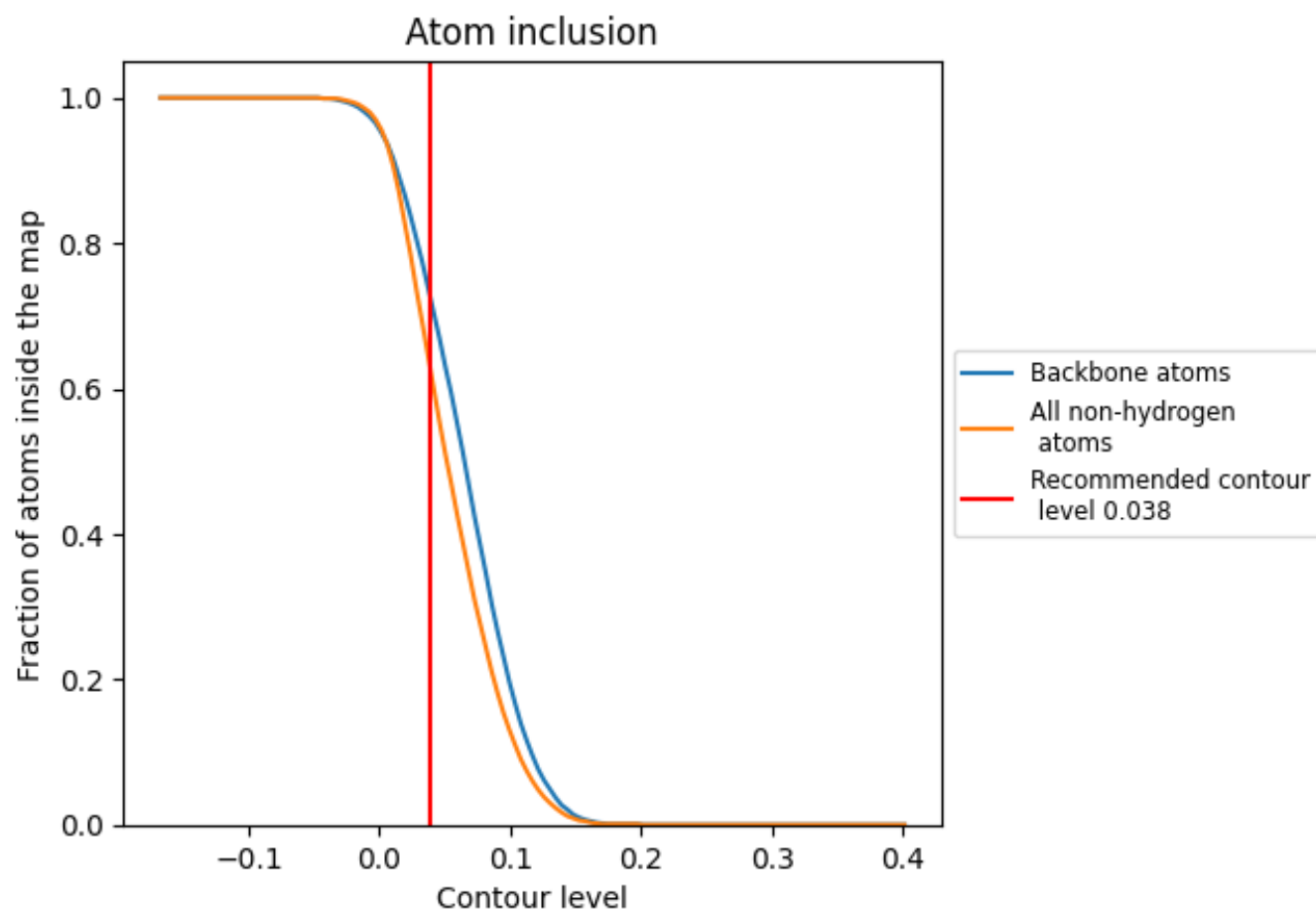
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.4330
A	 0.6510	 0.4290
B	 0.6920	 0.4540
C	 0.6580	 0.4240
D	 0.7160	 0.4480
E	 0.7290	 0.4560
F	 0.6000	 0.4130
G	 0.6320	 0.4350
H	 0.6380	 0.4150
I	 0.6330	 0.4280
J	 0.6950	 0.4530
K	 0.7290	 0.4760
L	 0.6120	 0.4340
M	 0.6940	 0.4610
N	 0.6480	 0.4380
O	 0.6220	 0.4420
P	 0.6410	 0.4420
Q	 0.4630	 0.3720
R	 0.1930	 0.3750
S	 0.4230	 0.4150
V	 0.3120	 0.3830

