



# wwPDB EM Validation Summary Report ⓘ

Jun 26, 2023 – 10:53 AM JST

PDB ID : 7X0S  
EMDB ID : EMD-32923  
Title : Human TRiC-tubulin-S3  
Authors : Cong, Y.; Liu, C.X.  
Deposited on : 2022-02-22  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

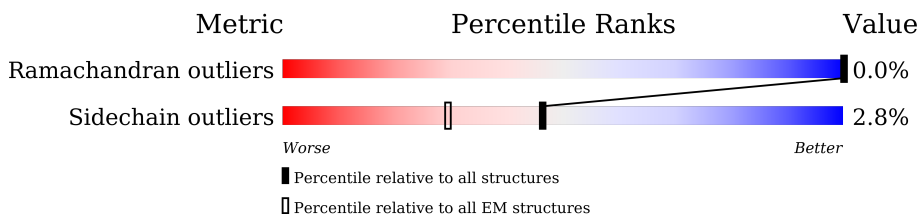
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	K	531	97%
1	z	531	98%
2	J	548	5% 93%
2	P	548	6% 93%
3	H	543	5% 94%
3	O	543	6% 95%
4	G	545	95%
4	N	545	94%
5	E	539	6% 97%

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Mol	Chain	Length	Quality of chain
5	e	539	 6% 97%
6	I	539	 94%
6	M	539	 94%
7	B	535	 5% 96%
7	L	535	 6% 96%
8	A	556	 7% 94%
8	a	556	 7% 94%
9	R	444	 47% 92%

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 68346 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 T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		
1	z	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	527	Total	C	N	O	S	0	0
			4008	2529	682	770	27		
2	P	527	Total	C	N	O	S	0	0
			4008	2529	682	770	27		

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	526	Total	C	N	O	S	0	0
			4037	2549	697	766	25		
3	O	526	Total	C	N	O	S	0	0
			4037	2549	697	766	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	290	SER	LEU	engineered mutation	UNP Q99832
O	290	SER	LEU	engineered mutation	UNP Q99832

- Molecule 4 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	526	Total	C	N	O	S	0	0
			4094	2552	727	785	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	526	Total	C	N	O	S	0	0
			4094	2552	727	785	30		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	535	Total	C	N	O	S	0	0
			4126	2583	718	795	30		
5	e	535	Total	C	N	O	S	0	0
			4126	2583	718	795	30		

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	521	Total	C	N	O	S	0	0
			3935	2459	687	766	23		
6	M	521	Total	C	N	O	S	0	0
			3935	2459	687	766	23		

- Molecule 7 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	523	Total	C	N	O	S	0	0
			3937	2463	696	759	19		
7	L	523	Total	C	N	O	S	0	0
			3937	2463	696	759	19		

- Molecule 8 is a protein called T-complex protein 1 subunit alpha.

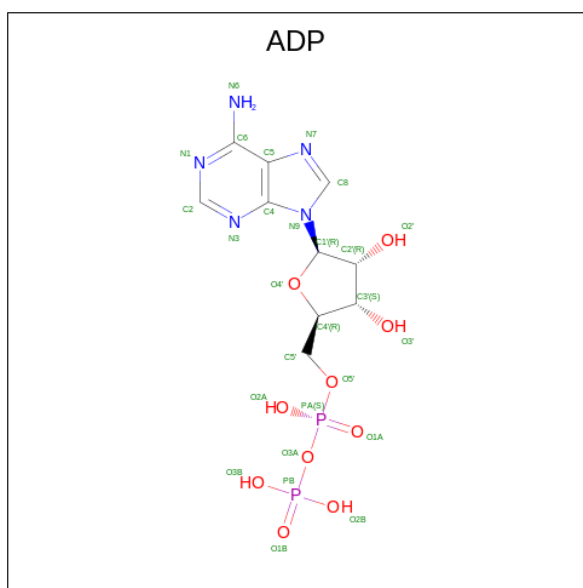
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		
8	a	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		

- Molecule 9 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	426	Total	C	N	O	S	0	0
			3346	2106	573	642	25		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	z	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

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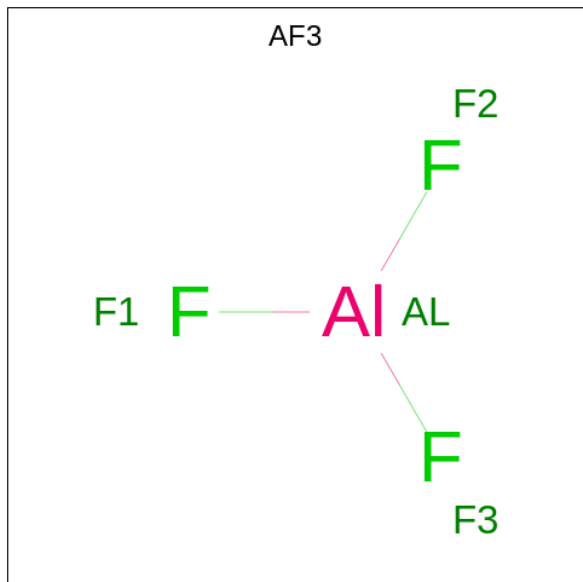
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	a	1	27	10	5	10	2	0
10	M	1	27	10	5	10	2	0
10	L	1	27	10	5	10	2	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total 1	Mg 1	0
11	J	1	Total 1	Mg 1	0
11	H	1	Total 1	Mg 1	0
11	G	1	Total 1	Mg 1	0
11	E	1	Total 1	Mg 1	0
11	I	1	Total 1	Mg 1	0
11	B	1	Total 1	Mg 1	0
11	A	1	Total 1	Mg 1	0
11	z	1	Total 1	Mg 1	0
11	P	1	Total 1	Mg 1	0
11	O	1	Total 1	Mg 1	0
11	N	1	Total 1	Mg 1	0
11	e	1	Total 1	Mg 1	0
11	a	1	Total 1	Mg 1	0
11	M	1	Total 1	Mg 1	0
11	L	1	Total 1	Mg 1	0

- Molecule 12 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $\text{AlF}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
12	K	1	4	1	3	0
12	J	1	4	1	3	0
12	H	1	4	1	3	0
12	G	1	4	1	3	0
12	E	1	4	1	3	0
12	I	1	4	1	3	0
12	B	1	4	1	3	0
12	A	1	4	1	3	0
12	z	1	4	1	3	0
12	P	1	4	1	3	0
12	O	1	4	1	3	0
12	N	1	4	1	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
12	e	1	4	1	3	0
12	a	1	4	1	3	0
12	M	1	4	1	3	0
12	L	1	4	1	3	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
13	K	1	1	1	0
13	J	1	1	1	0
13	H	1	1	1	0
13	G	1	1	1	0
13	E	1	1	1	0
13	I	1	1	1	0
13	B	1	1	1	0
13	A	1	1	1	0
13	z	1	1	1	0
13	P	1	1	1	0
13	O	1	1	1	0
13	N	1	1	1	0
13	e	1	1	1	0
13	a	1	1	1	0
13	M	1	1	1	0

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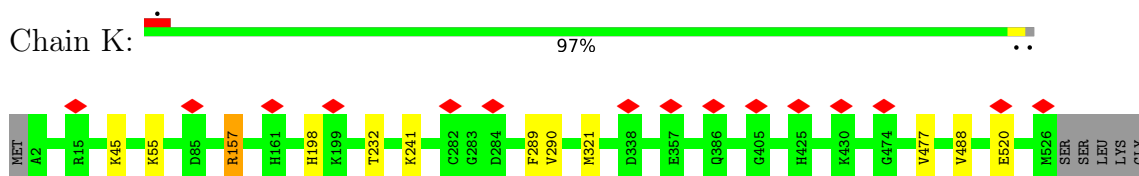
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Mol	Chain	Residues	Atoms		AltConf
13	L	1	Total	O	0
			1	1	

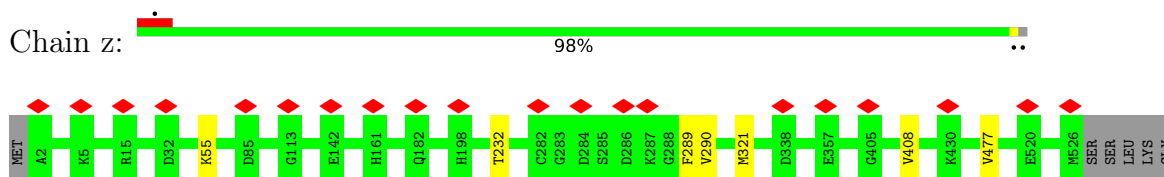
### 3 Residue-property plots

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.

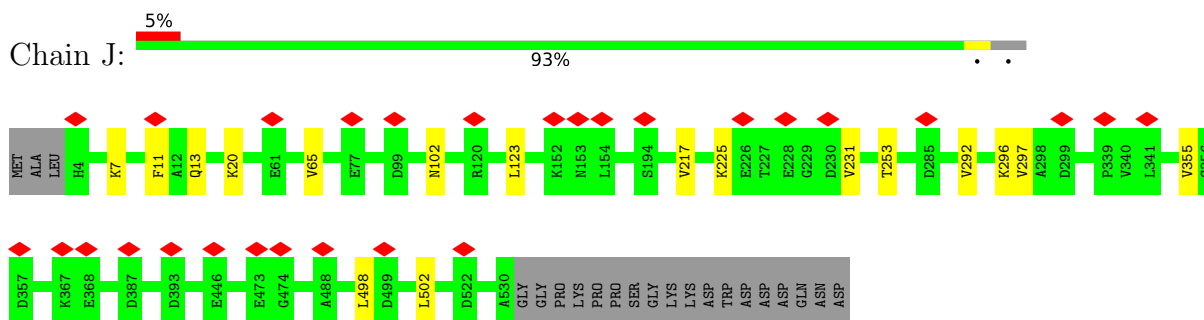
- Molecule 1: T-complex protein 1 subunit zeta



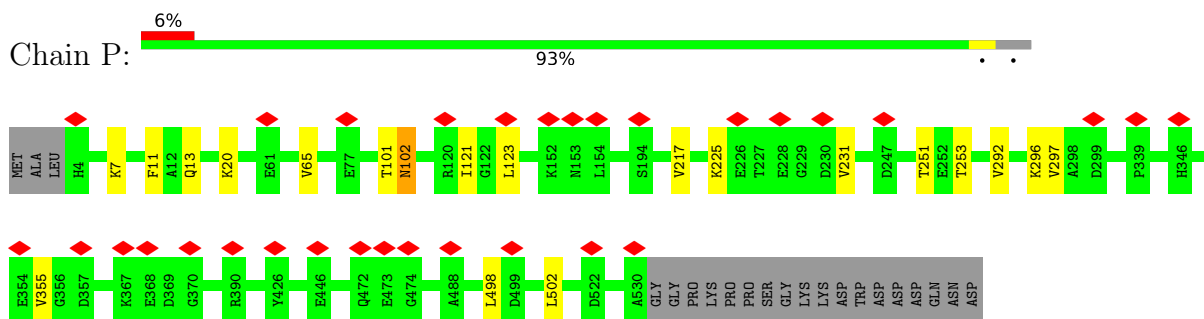
- Molecule 1: T-complex protein 1 subunit zeta



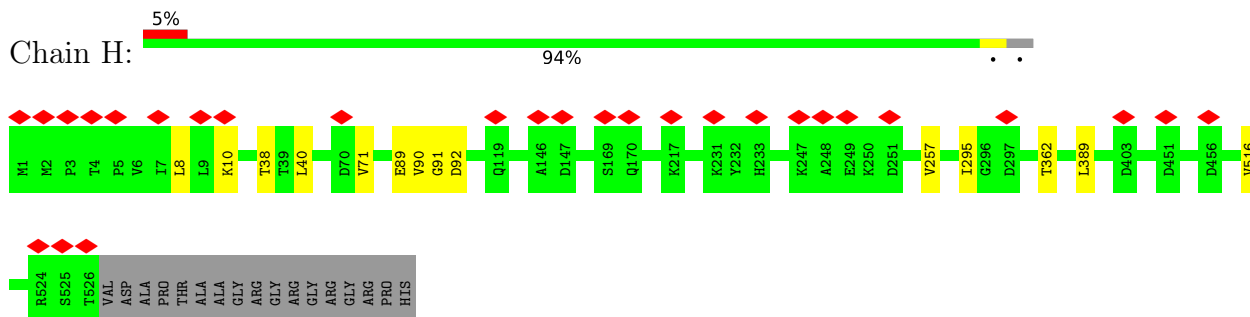
- Molecule 2: T-complex protein 1 subunit theta



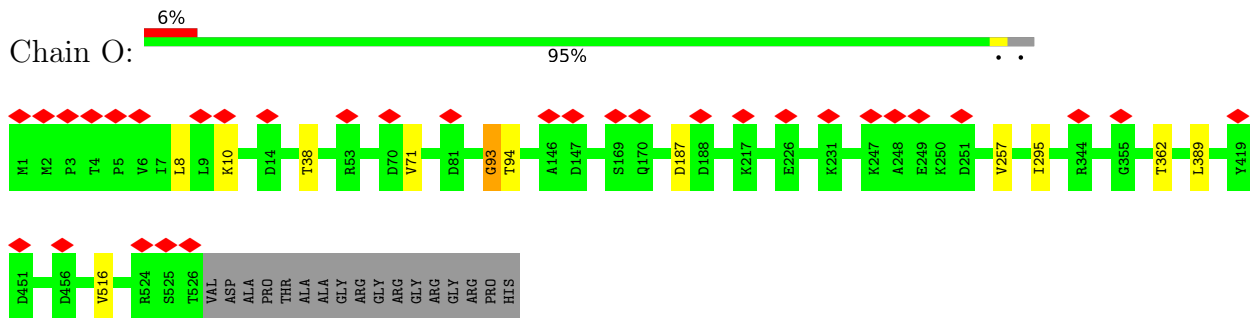
- Molecule 2: T-complex protein 1 subunit theta



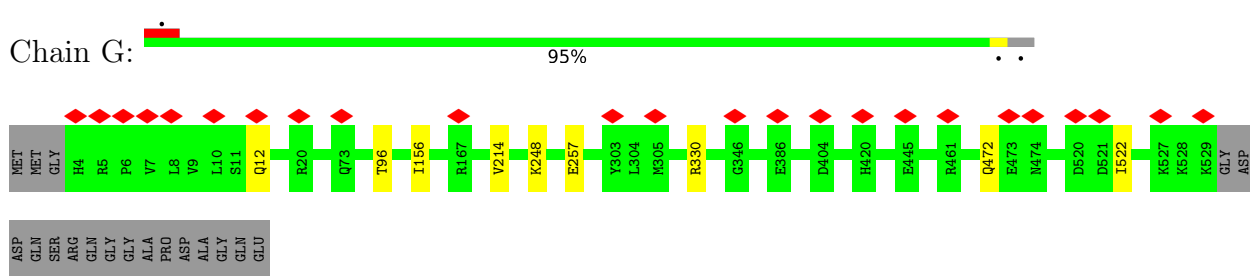
• Molecule 3: T-complex protein 1 subunit eta



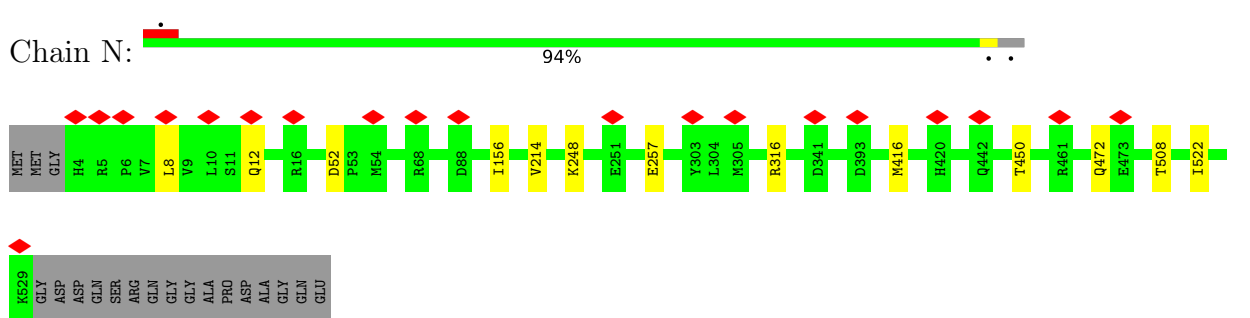
• Molecule 3: T-complex protein 1 subunit eta



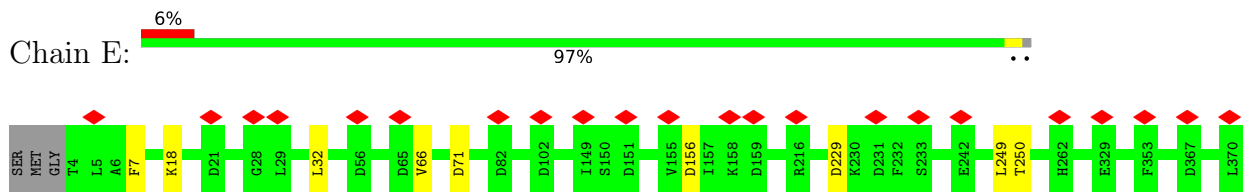
• Molecule 4: T-complex protein 1 subunit gamma

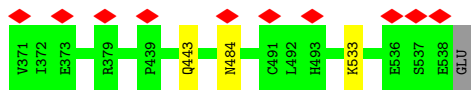


• Molecule 4: T-complex protein 1 subunit gamma

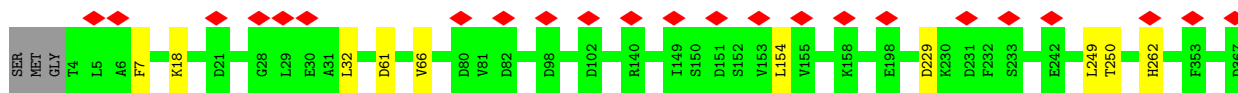


• Molecule 5: T-complex protein 1 subunit epsilon

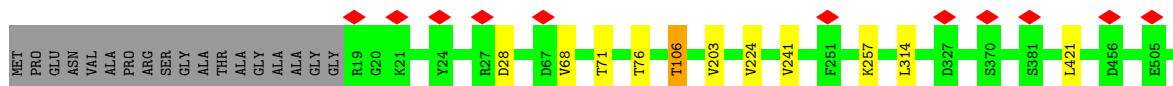




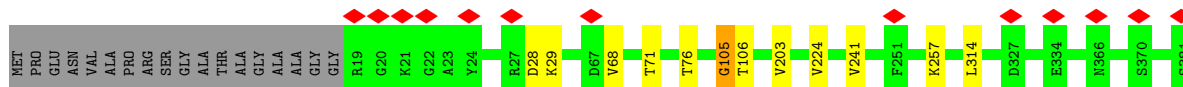
• Molecule 5: T-complex protein 1 subunit epsilon



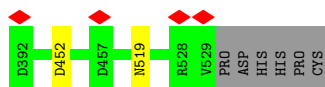
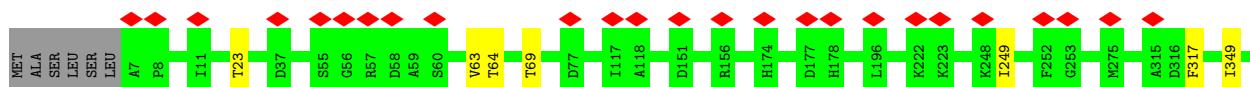
• Molecule 6: T-complex protein 1 subunit delta



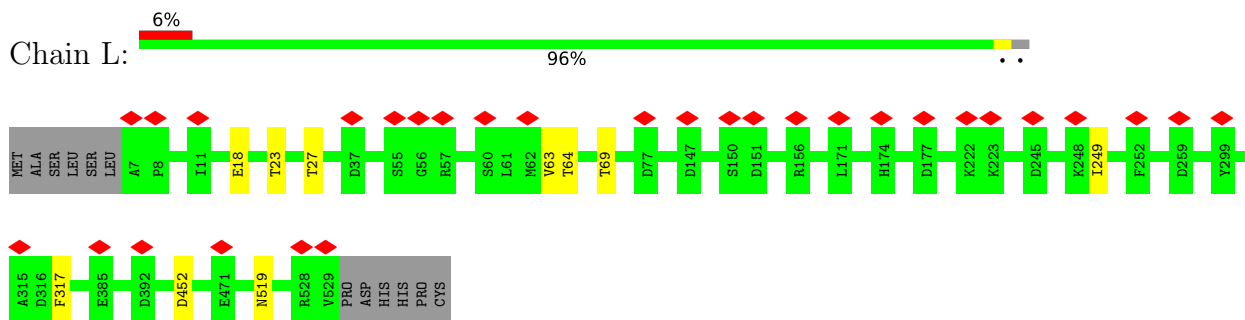
• Molecule 6: T-complex protein 1 subunit delta



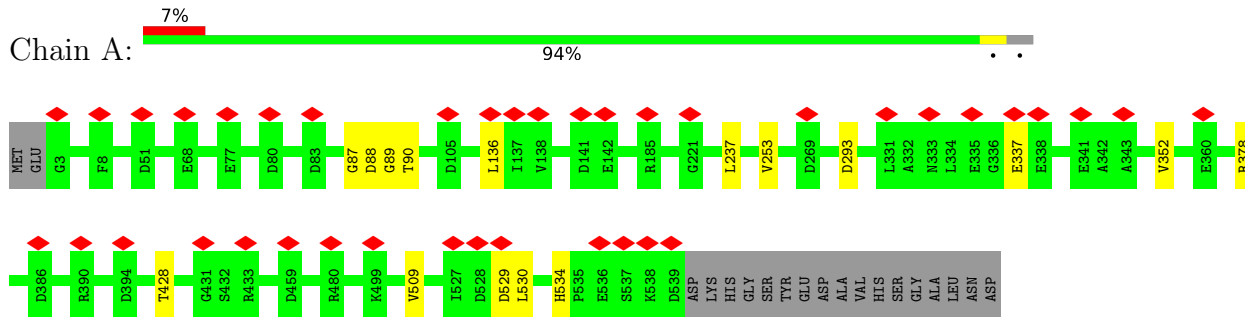
• Molecule 7: T-complex protein 1 subunit beta



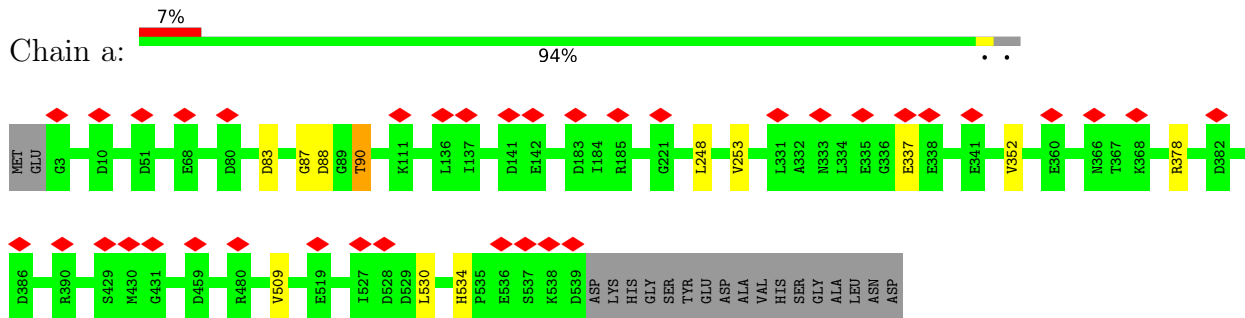
• Molecule 7: T-complex protein 1 subunit beta



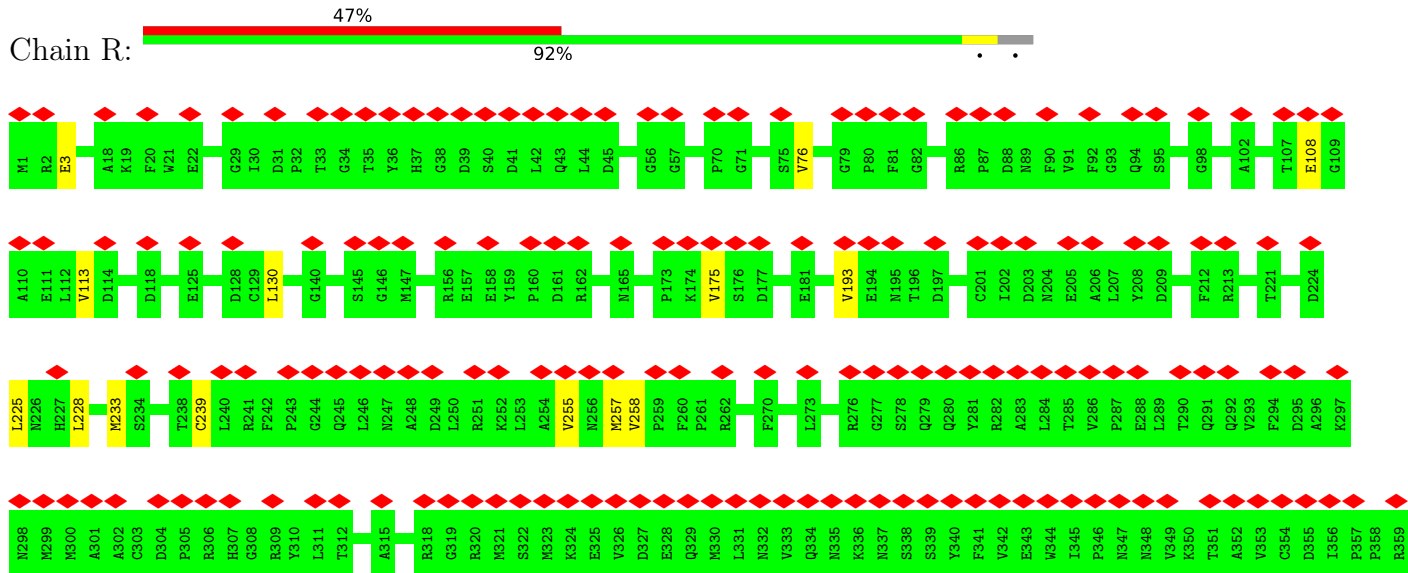
• Molecule 8: T-complex protein 1 subunit alpha

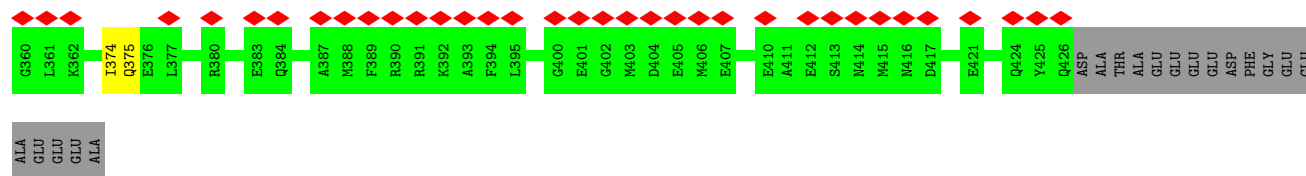


• Molecule 8: T-complex protein 1 subunit alpha



• Molecule 9: Tubulin beta chain





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103406	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 ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.603	Depositor
Minimum map value	-1.789	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.761	Depositor
Map size ( $\text{\AA}$ )	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.318, 1.318, 1.318	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AF3, MG

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	K	0.31	3/4069 (0.1%)	0.45	0/5486
1	z	0.28	0/4069	0.43	0/5486
2	J	0.24	0/4066	0.43	0/5498
2	P	0.28	1/4066 (0.0%)	0.44	0/5498
3	H	0.31	1/4094 (0.0%)	0.46	2/5526 (0.0%)
3	O	0.32	4/4094 (0.1%)	0.44	1/5526 (0.0%)
4	G	0.23	0/4141	0.42	0/5585
4	N	0.23	0/4141	0.42	0/5585
5	E	0.29	2/4176 (0.0%)	0.47	2/5626 (0.0%)
5	e	0.24	0/4176	0.42	0/5626
6	I	0.29	2/3967 (0.1%)	0.44	0/5352
6	M	0.31	3/3967 (0.1%)	0.44	1/5352 (0.0%)
7	B	0.24	0/3980	0.44	0/5365
7	L	0.24	0/3980	0.44	0/5365
8	A	0.33	1/4117 (0.0%)	0.50	3/5558 (0.1%)
8	a	0.32	3/4117 (0.1%)	0.45	1/5558 (0.0%)
9	R	0.24	0/3421	0.43	0/4637
All	All	0.28	20/68641 (0.0%)	0.44	10/92629 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	O	0	1
6	M	0	2
8	A	0	1
8	a	0	1
All	All	0	6

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	88	ASP	CB-CG	12.59	1.78	1.51
5	E	71	ASP	CB-CG	8.23	1.69	1.51
6	M	106	THR	C-O	-6.92	1.10	1.23
8	a	88	ASP	CB-CG	-6.67	1.37	1.51
1	K	157	ARG	C-O	-6.56	1.10	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	88	ASP	CB-CG-OD1	13.79	130.71	118.30
5	E	71	ASP	CB-CG-OD2	12.28	129.35	118.30
3	H	90	VAL	CG1-CB-CG2	-8.12	97.90	110.90
8	A	88	ASP	OD1-CG-OD2	-7.39	109.26	123.30
5	E	71	ASP	OD1-CG-OD2	-7.06	109.88	123.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A	90	THR	Peptide
6	M	29	LYS	Peptide
3	O	93	GLY	Mainchain
2	P	101	THR	Mainchain
8	a	90	THR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	523/531 (98%)	496 (95%)	27 (5%)	0	100	100
1	z	523/531 (98%)	493 (94%)	30 (6%)	0	100	100
2	J	525/548 (96%)	486 (93%)	39 (7%)	0	100	100
2	P	525/548 (96%)	490 (93%)	35 (7%)	0	100	100
3	H	524/543 (96%)	498 (95%)	26 (5%)	0	100	100
3	O	524/543 (96%)	500 (95%)	24 (5%)	0	100	100
4	G	524/545 (96%)	504 (96%)	20 (4%)	0	100	100
4	N	524/545 (96%)	501 (96%)	23 (4%)	0	100	100
5	E	533/539 (99%)	506 (95%)	27 (5%)	0	100	100
5	e	533/539 (99%)	508 (95%)	25 (5%)	0	100	100
6	I	519/539 (96%)	503 (97%)	16 (3%)	0	100	100
6	M	519/539 (96%)	503 (97%)	16 (3%)	0	100	100
7	B	521/535 (97%)	493 (95%)	28 (5%)	0	100	100
7	L	521/535 (97%)	496 (95%)	25 (5%)	0	100	100
8	A	535/556 (96%)	509 (95%)	25 (5%)	1 (0%)	47	79
8	a	535/556 (96%)	511 (96%)	23 (4%)	1 (0%)	47	79
9	R	424/444 (96%)	413 (97%)	11 (3%)	0	100	100
All	All	8832/9116 (97%)	8410 (95%)	420 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	a	90	THR
8	A	89	GLY

### 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	K	437/442 (99%)	425 (97%)	12 (3%)	44	74

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	z	437/442 (99%)	430 (98%)	7 (2%)	62	84
2	J	433/452 (96%)	416 (96%)	17 (4%)	32	65
2	P	433/452 (96%)	414 (96%)	19 (4%)	28	61
3	H	433/443 (98%)	421 (97%)	12 (3%)	43	73
3	O	433/443 (98%)	423 (98%)	10 (2%)	50	77
4	G	457/469 (97%)	448 (98%)	9 (2%)	55	80
4	N	457/469 (97%)	444 (97%)	13 (3%)	43	73
5	E	452/455 (99%)	441 (98%)	11 (2%)	49	76
5	e	452/455 (99%)	439 (97%)	13 (3%)	42	72
6	I	443/452 (98%)	430 (97%)	13 (3%)	42	72
6	M	443/452 (98%)	431 (97%)	12 (3%)	44	74
7	B	416/427 (97%)	407 (98%)	9 (2%)	52	78
7	L	416/427 (97%)	406 (98%)	10 (2%)	49	76
8	A	448/463 (97%)	436 (97%)	12 (3%)	44	74
8	a	448/463 (97%)	439 (98%)	9 (2%)	55	80
9	R	366/379 (97%)	350 (96%)	16 (4%)	28	61
All	All	7404/7585 (98%)	7200 (97%)	204 (3%)	46	73

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	z	321	MET
3	O	295	ILE
7	L	69	THR
2	P	11	PHE
2	P	253	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
8	a	242	GLN
8	a	492	ASN
6	M	486	GLN
8	A	56	ASN
8	A	21	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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
12	AF3	M	603	-	0,3,3	-	-	-		
10	ADP	L	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.49	5 (17%)
12	AF3	N	603	-	0,3,3	-	-	-		
10	ADP	a	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	O	603	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	A	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	M	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
12	AF3	z	603	-	0,3,3	-	-	-		
12	AF3	I	603	-	0,3,3	-	-	-		
10	ADP	I	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	N	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
12	AF3	O	602	-	0,3,3	-	-	-		
12	AF3	A	603	-	0,3,3	-	-	-		
12	AF3	P	603	-	0,3,3	-	-	-		
12	AF3	E	603	-	0,3,3	-	-	-		
12	AF3	B	603	-	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	AF3	K	603	-	0,3,3	-	-	-		
12	AF3	J	603	-	0,3,3	-	-	-		
10	ADP	z	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
12	AF3	H	603	-	0,3,3	-	-	-		
12	AF3	G	603	-	0,3,3	-	-	-		
10	ADP	P	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	B	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.50	5 (17%)
10	ADP	H	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
12	AF3	e	603	-	0,3,3	-	-	-		
10	ADP	E	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
12	AF3	L	603	-	0,3,3	-	-	-		
10	ADP	K	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
10	ADP	J	601	11	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	G	601	11	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
10	ADP	e	601	11	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
12	AF3	a	603	-	0,3,3	-	-	-		

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	a	601	11	-	1/12/32/32	0/3/3/3
10	ADP	E	601	11	-	2/12/32/32	0/3/3/3
10	ADP	A	601	11	-	2/12/32/32	0/3/3/3
10	ADP	O	603	11	-	1/12/32/32	0/3/3/3
10	ADP	M	601	11	-	1/12/32/32	0/3/3/3
10	ADP	K	601	11	-	0/12/32/32	0/3/3/3
10	ADP	P	601	11	-	1/12/32/32	0/3/3/3
10	ADP	I	601	11	-	2/12/32/32	0/3/3/3
10	ADP	N	601	11	-	1/12/32/32	0/3/3/3
10	ADP	J	601	11	-	2/12/32/32	0/3/3/3
10	ADP	B	601	11	-	2/12/32/32	0/3/3/3
10	ADP	L	601	11	-	1/12/32/32	0/3/3/3
10	ADP	G	601	11	-	2/12/32/32	0/3/3/3
10	ADP	H	601	11	-	2/12/32/32	0/3/3/3
10	ADP	e	601	11	-	1/12/32/32	0/3/3/3
10	ADP	z	601	11	-	2/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	601	ADP	C5-C4	2.37	1.47	1.40
10	A	601	ADP	C5-C4	2.35	1.47	1.40
10	L	601	ADP	C5-C4	2.35	1.47	1.40
10	G	601	ADP	C5-C4	2.35	1.47	1.40
10	B	601	ADP	C5-C4	2.35	1.47	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	601	ADP	PA-O3A-PB	-3.70	120.12	132.83
10	P	601	ADP	PA-O3A-PB	-3.70	120.12	132.83
10	E	601	ADP	PA-O3A-PB	-3.70	120.13	132.83
10	H	601	ADP	PA-O3A-PB	-3.70	120.14	132.83
10	O	603	ADP	PA-O3A-PB	-3.69	120.15	132.83

There are no chirality outliers.

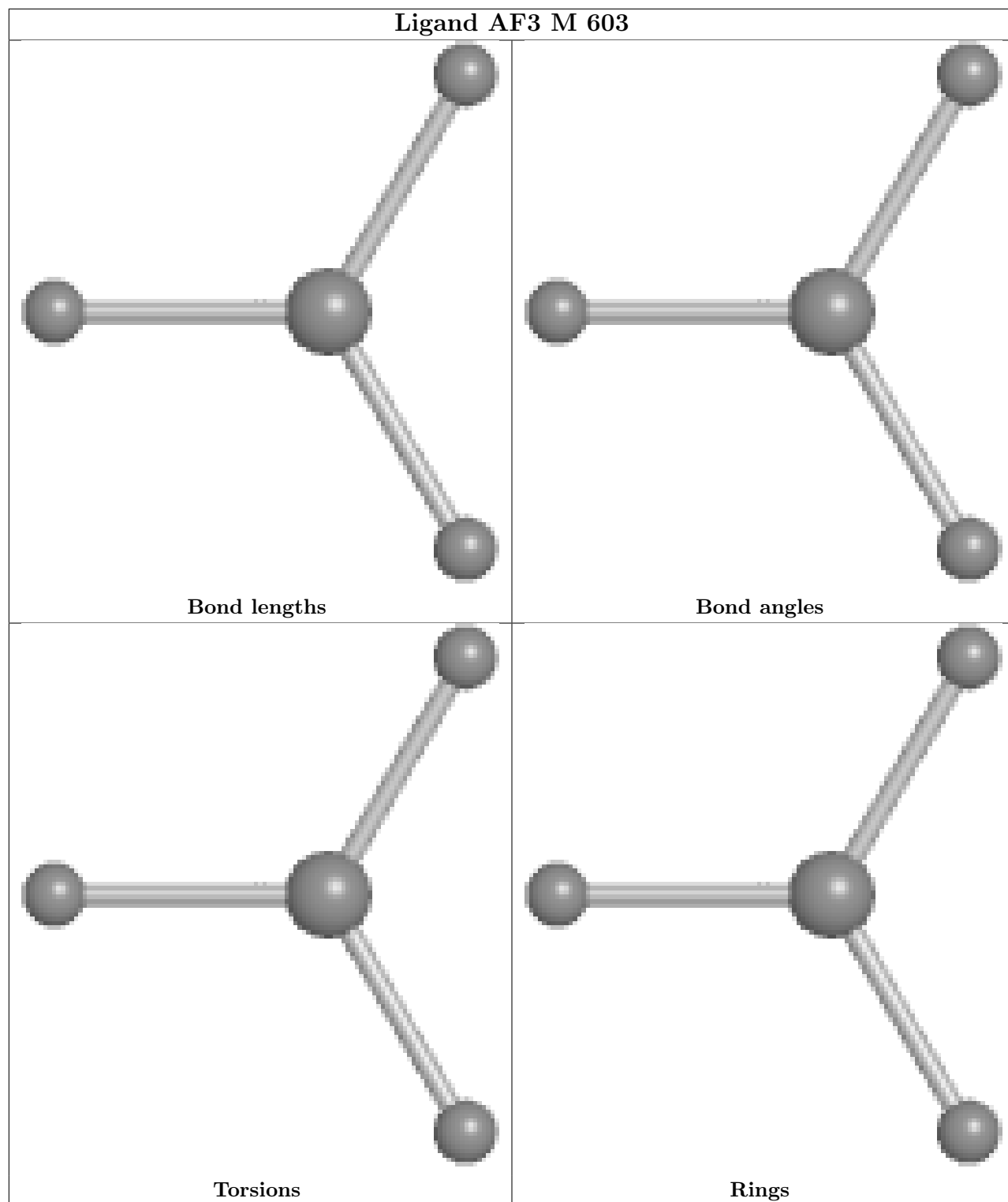
5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	601	ADP	C5'-O5'-PA-O1A
10	H	601	ADP	C5'-O5'-PA-O1A
10	G	601	ADP	C5'-O5'-PA-O1A
10	E	601	ADP	C5'-O5'-PA-O1A
10	I	601	ADP	C5'-O5'-PA-O1A

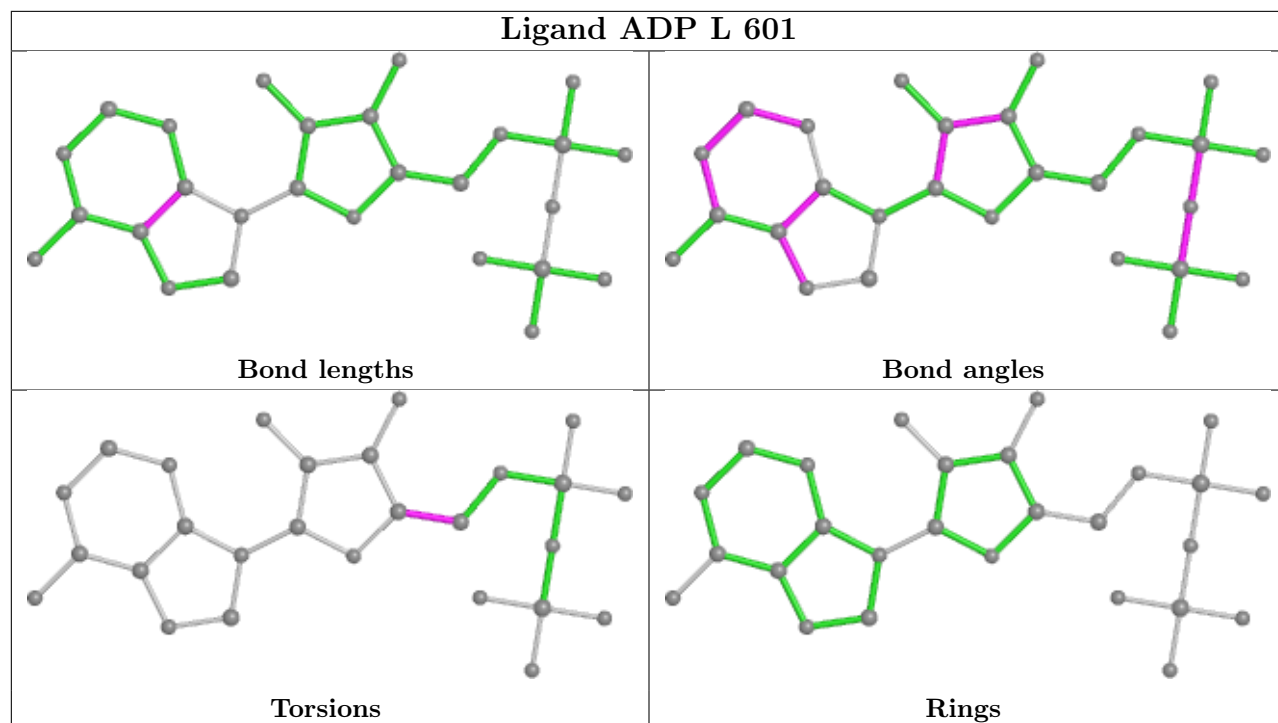
There are no ring outliers.

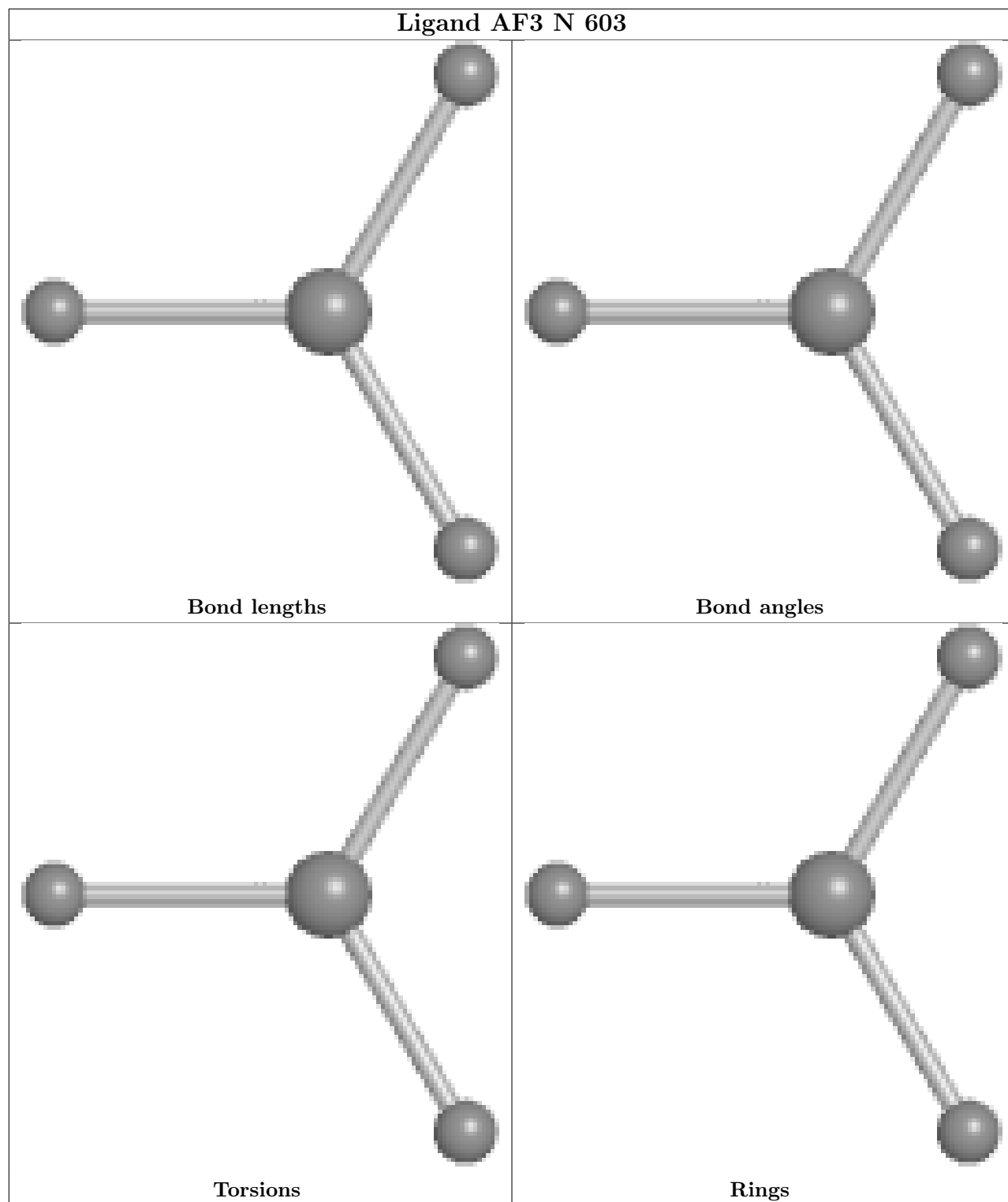
No monomer is involved in short contacts.

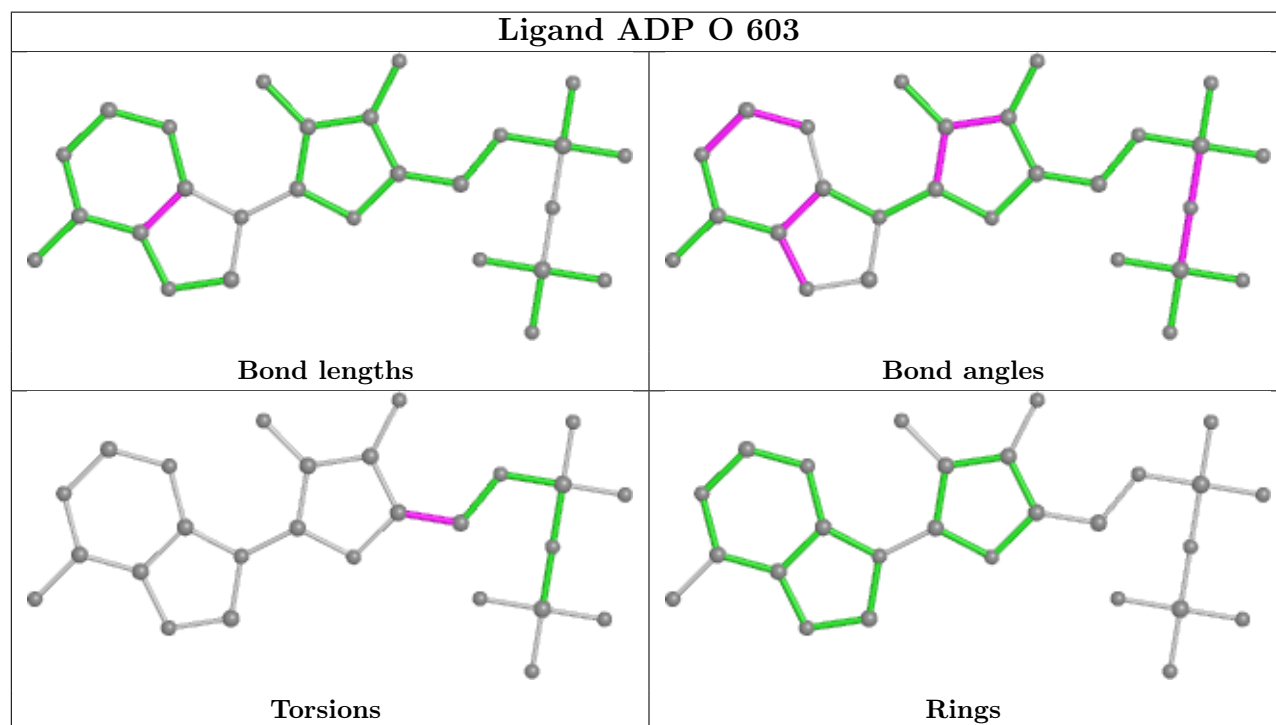
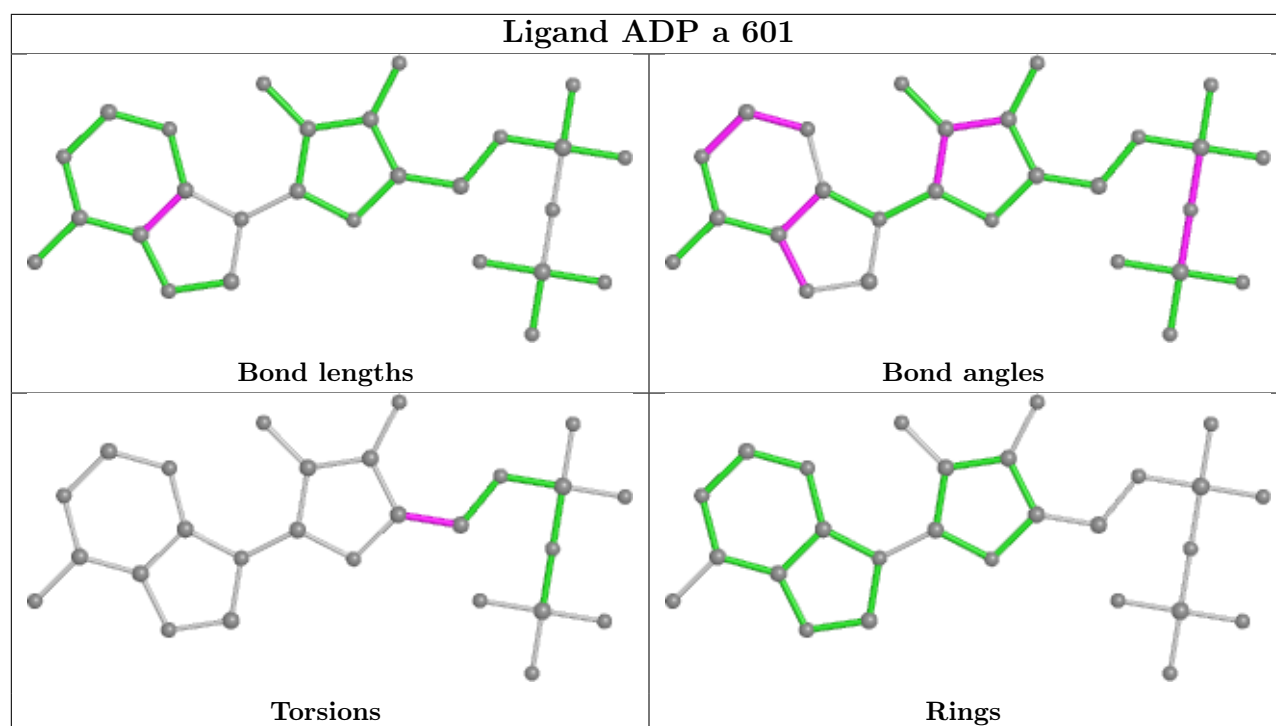
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

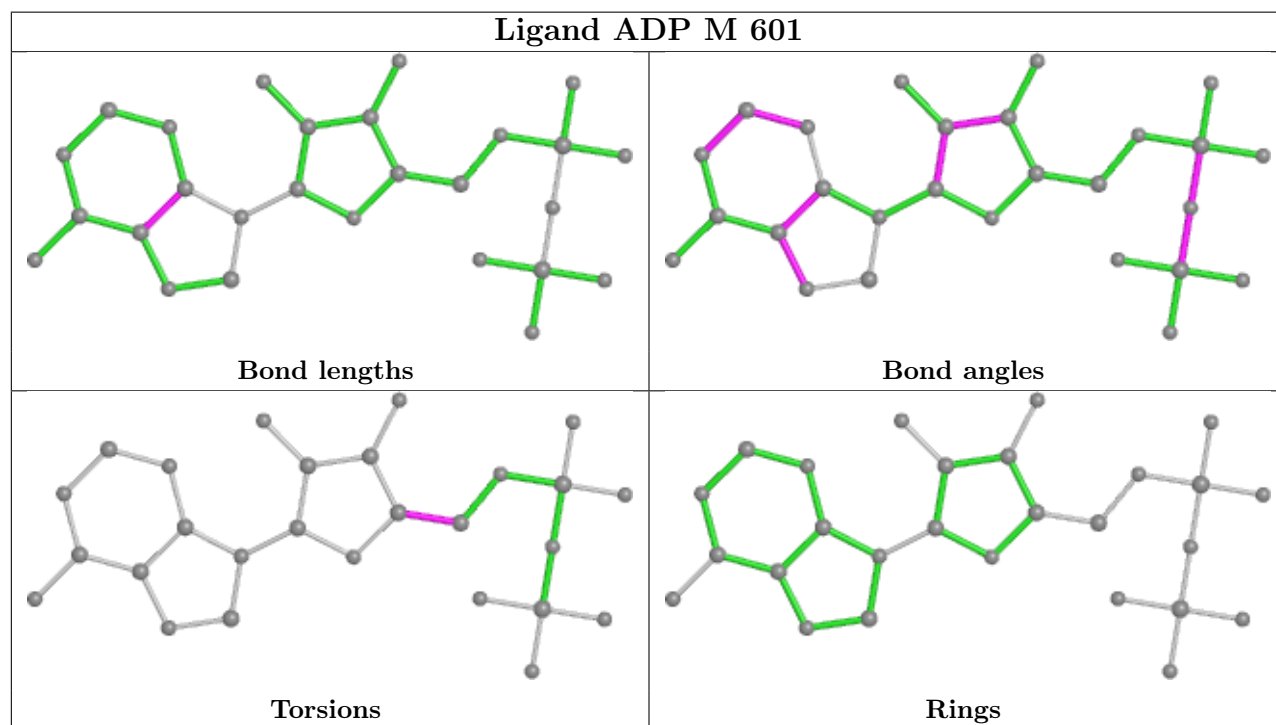
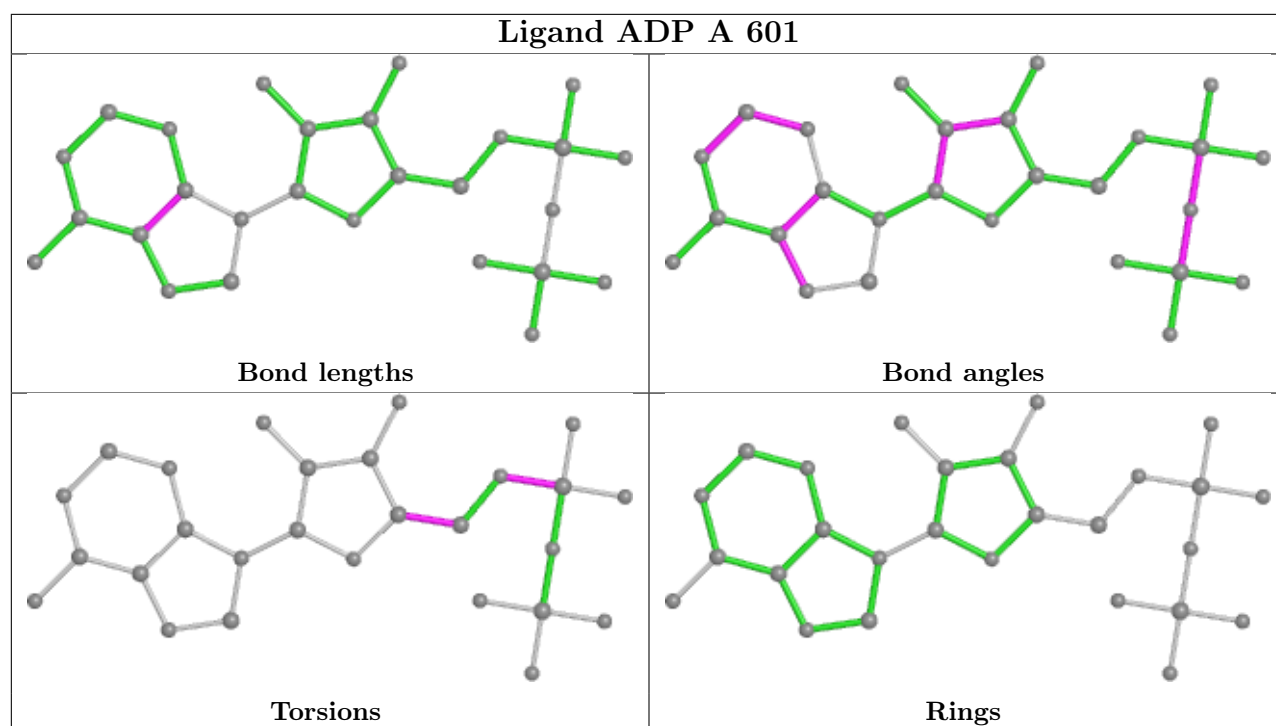


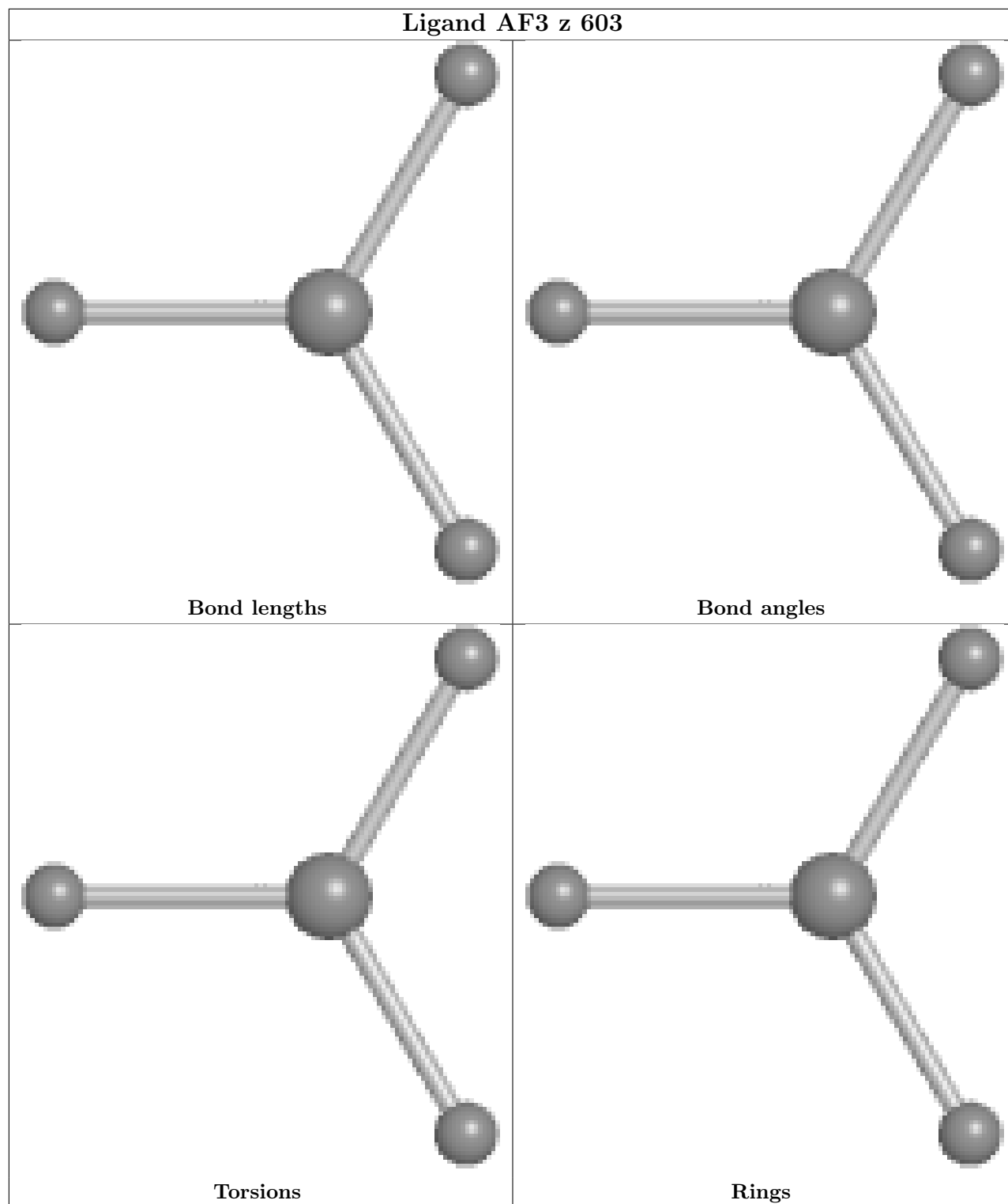


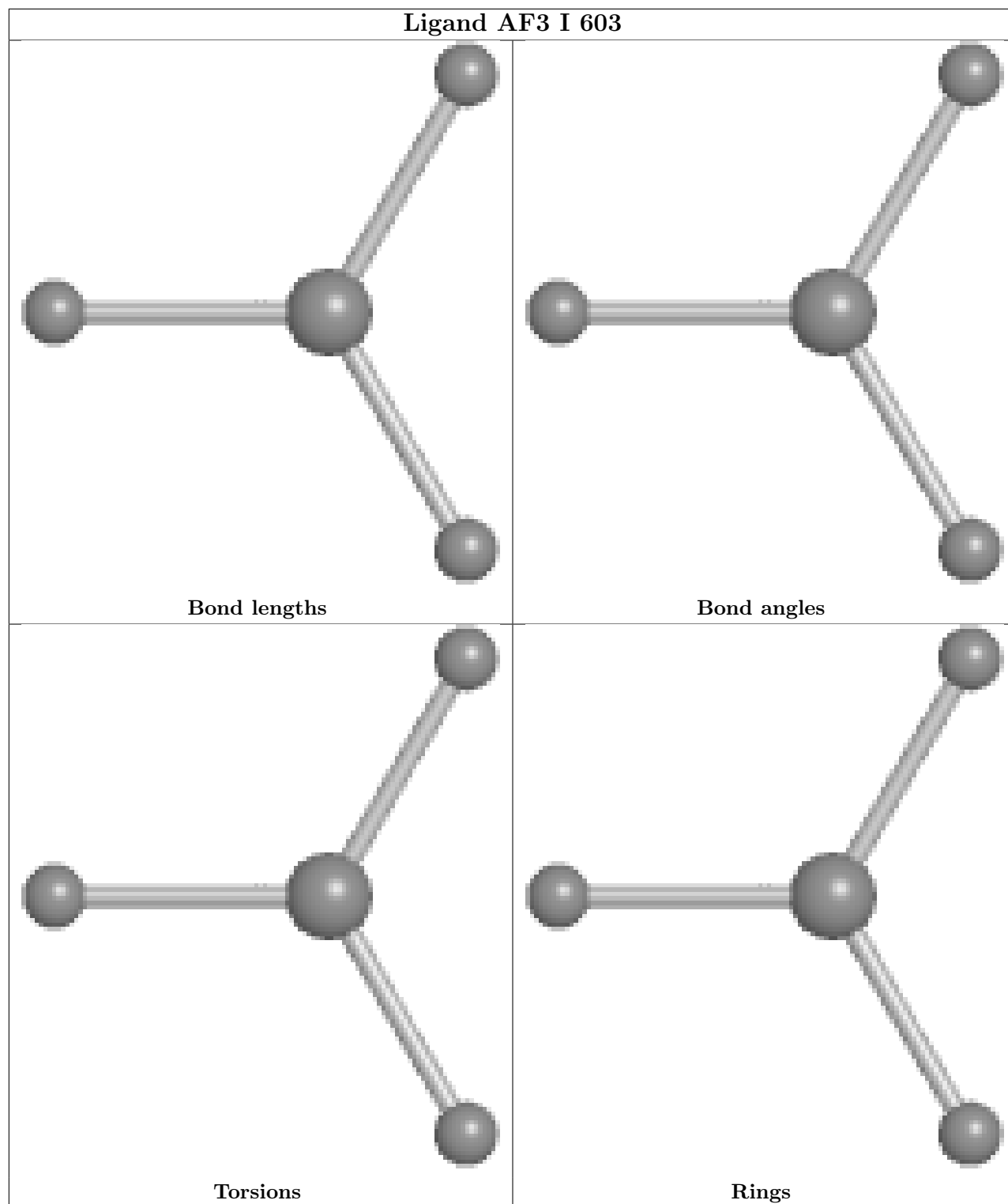


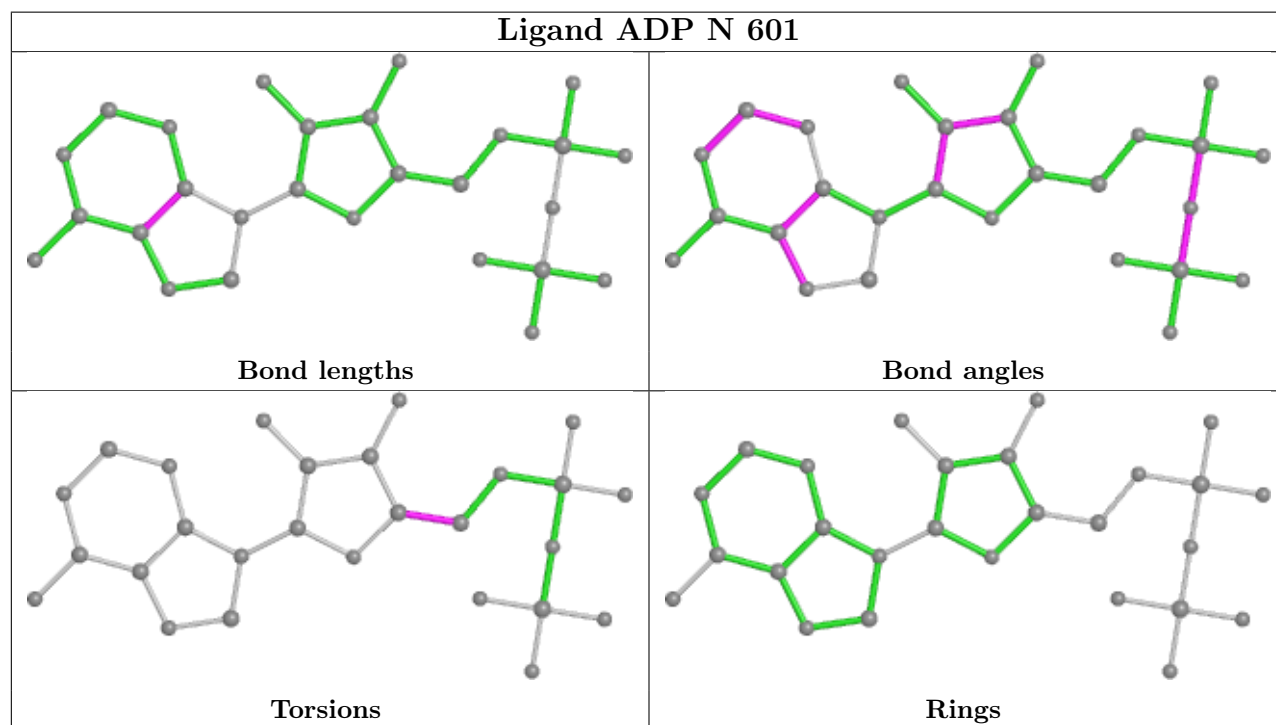
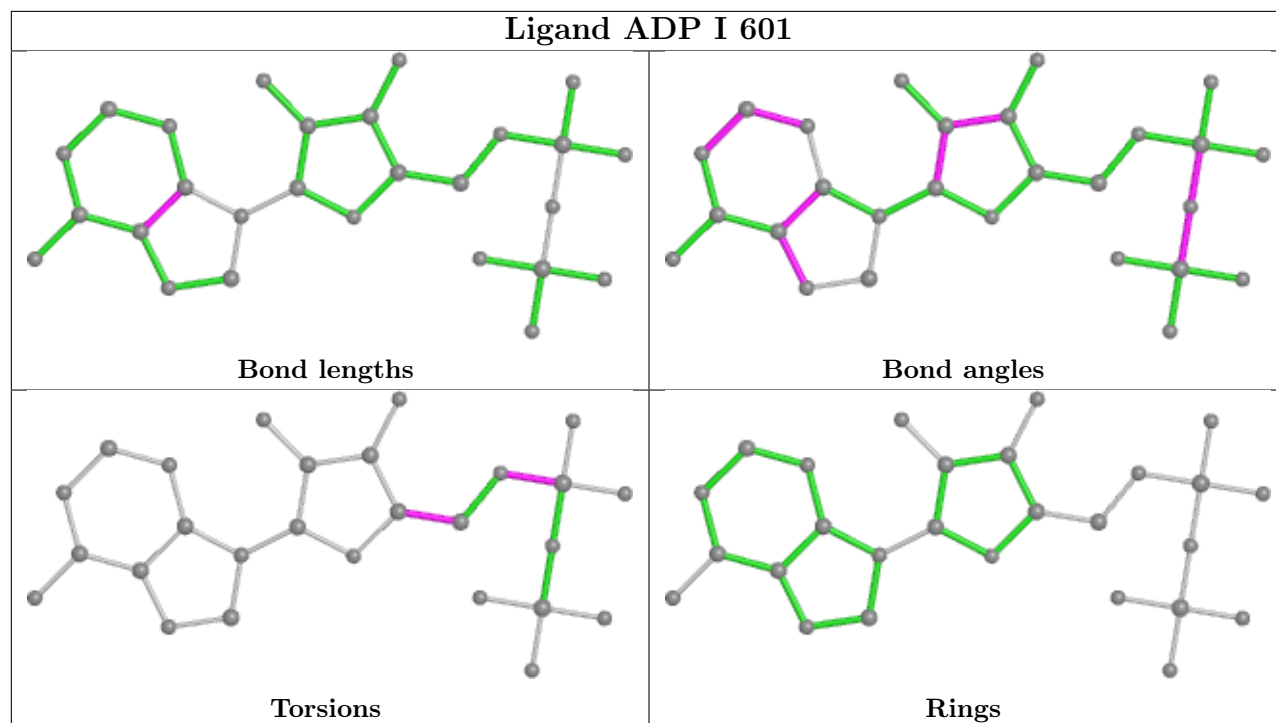


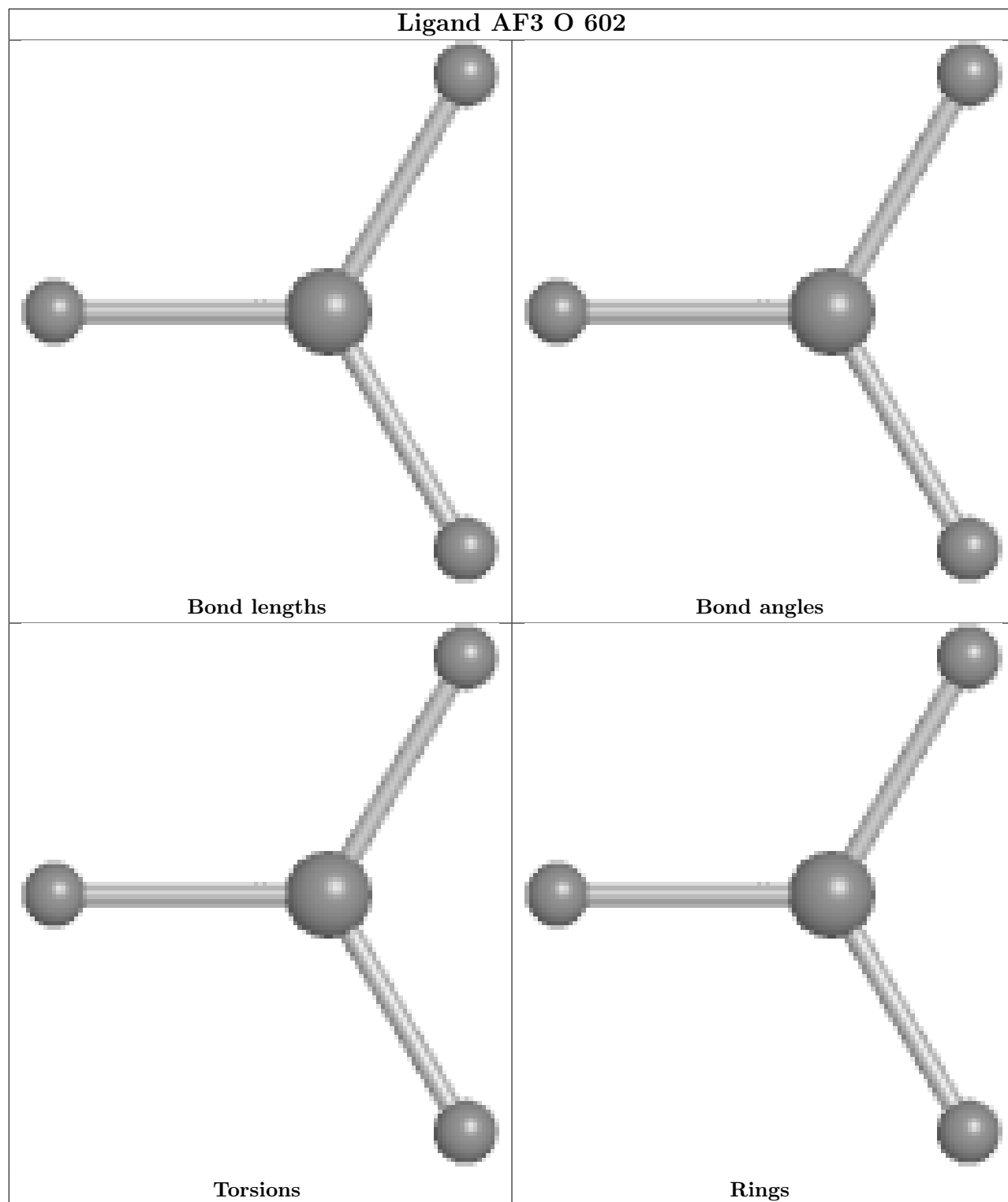




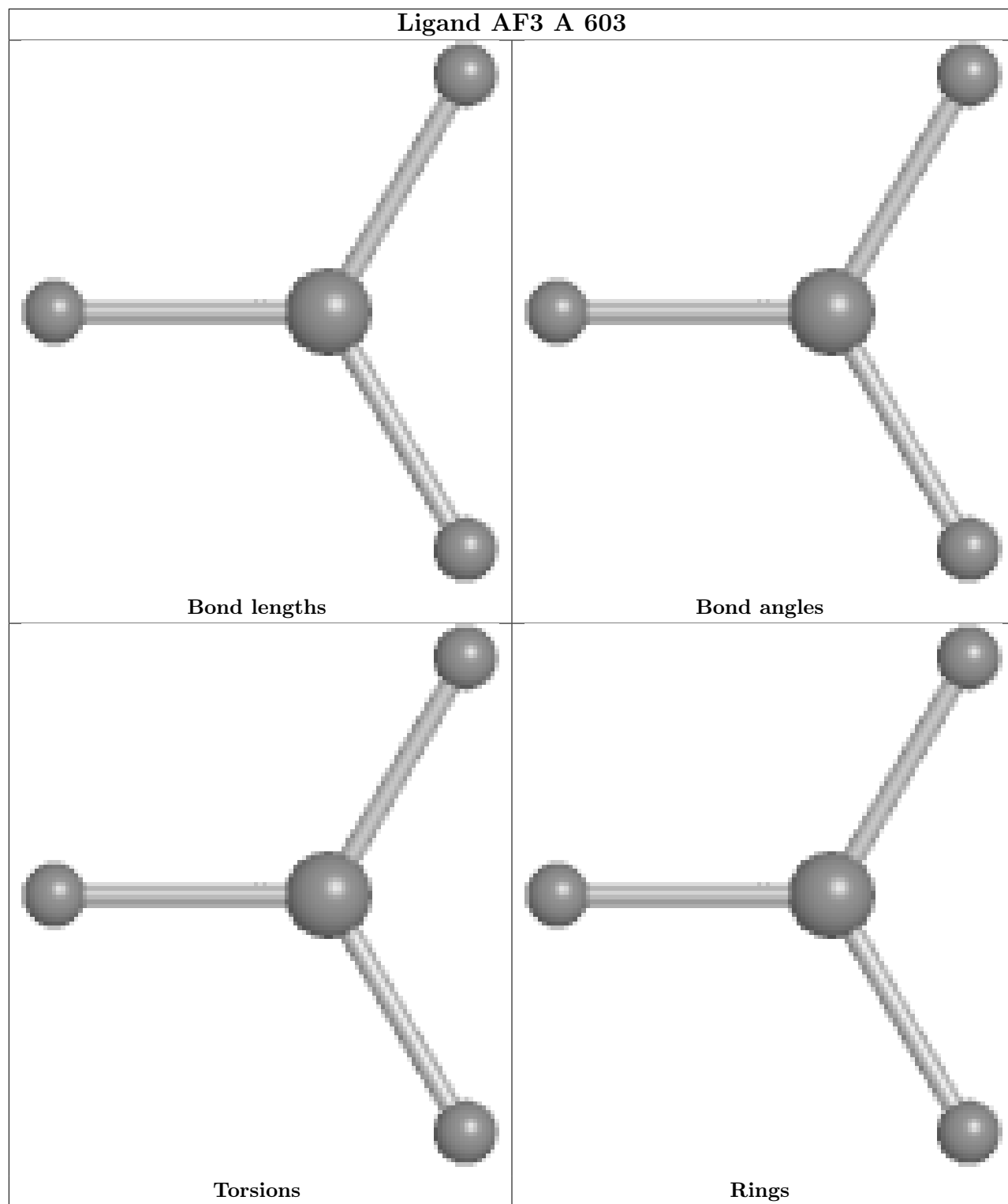


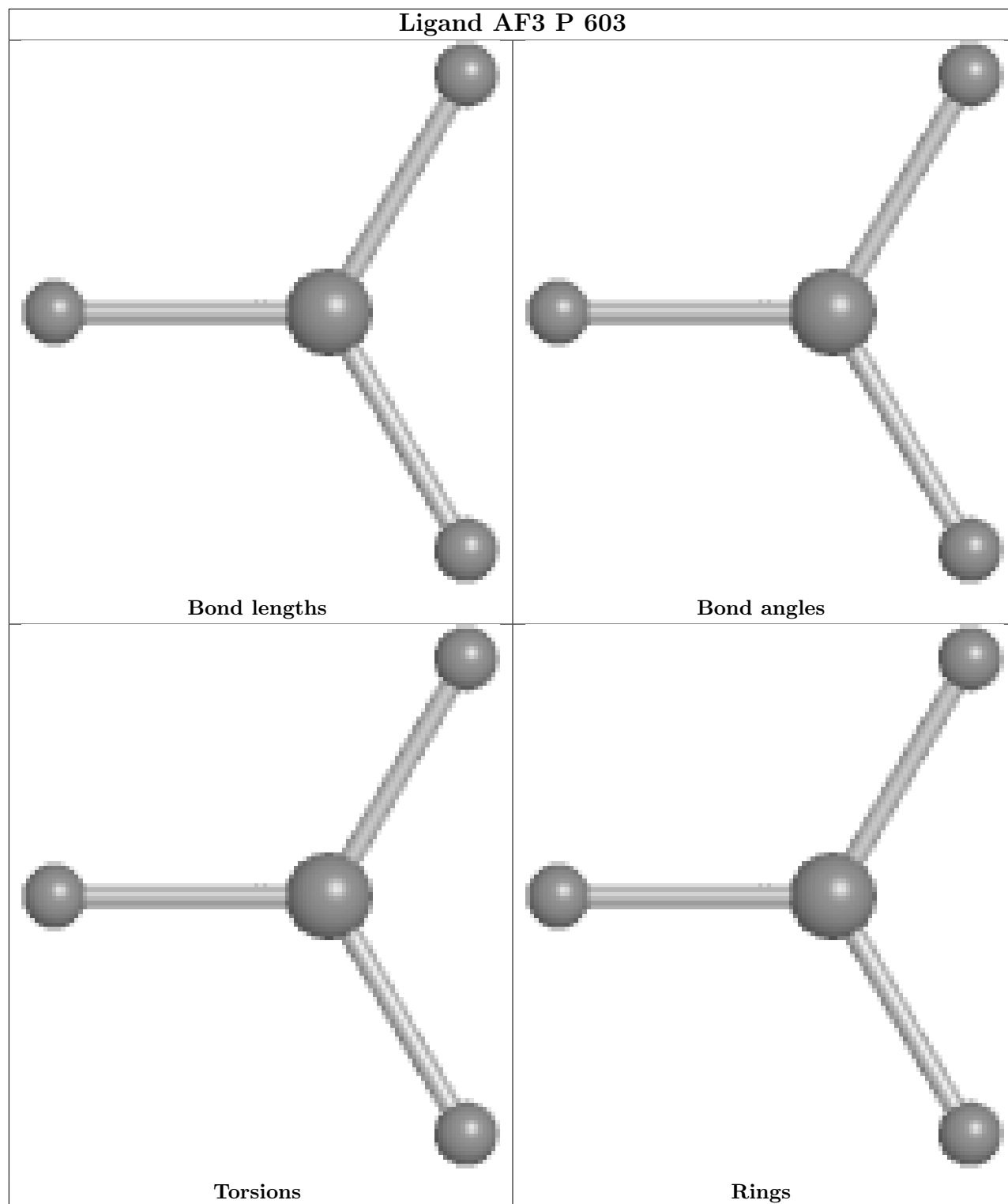


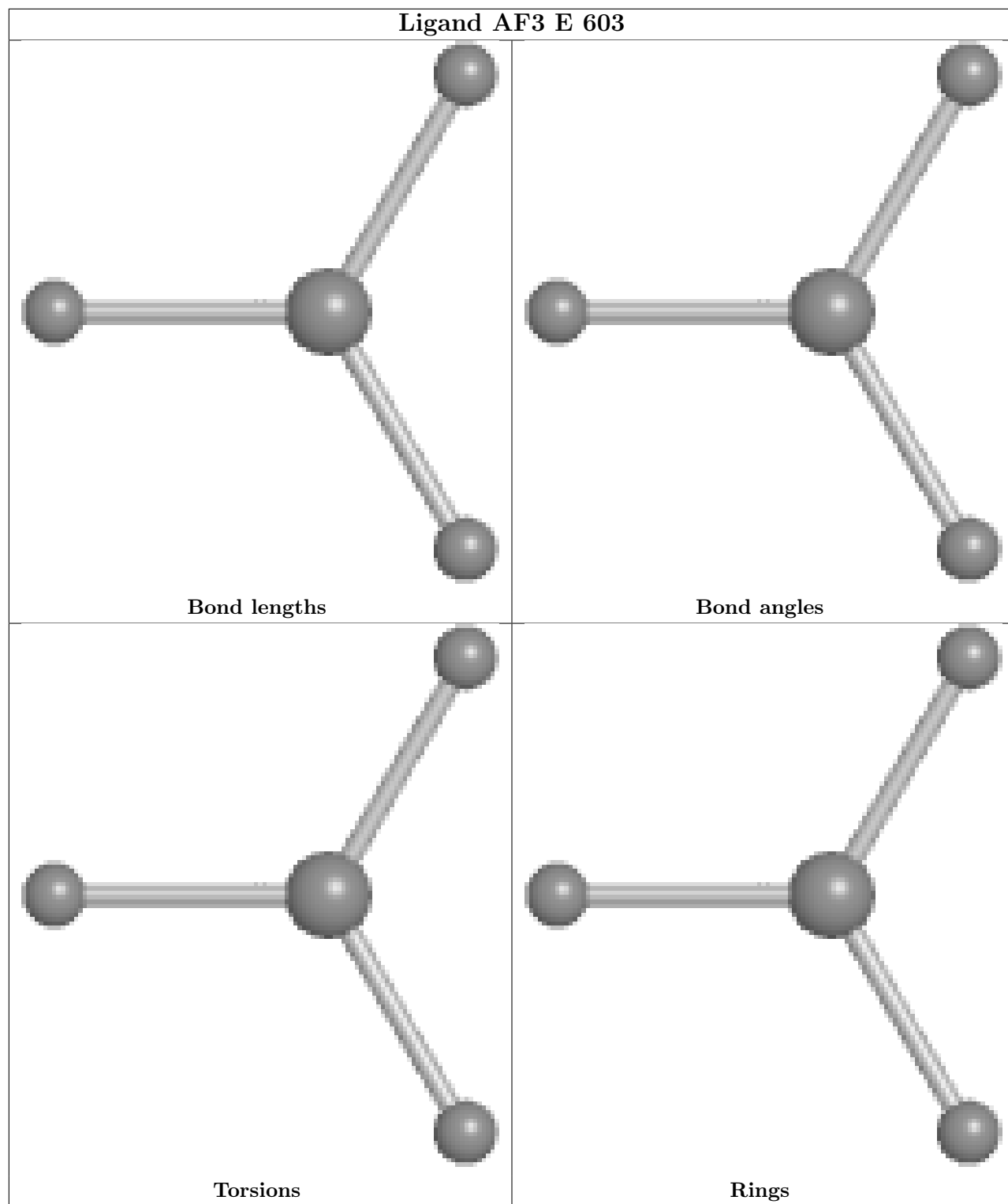


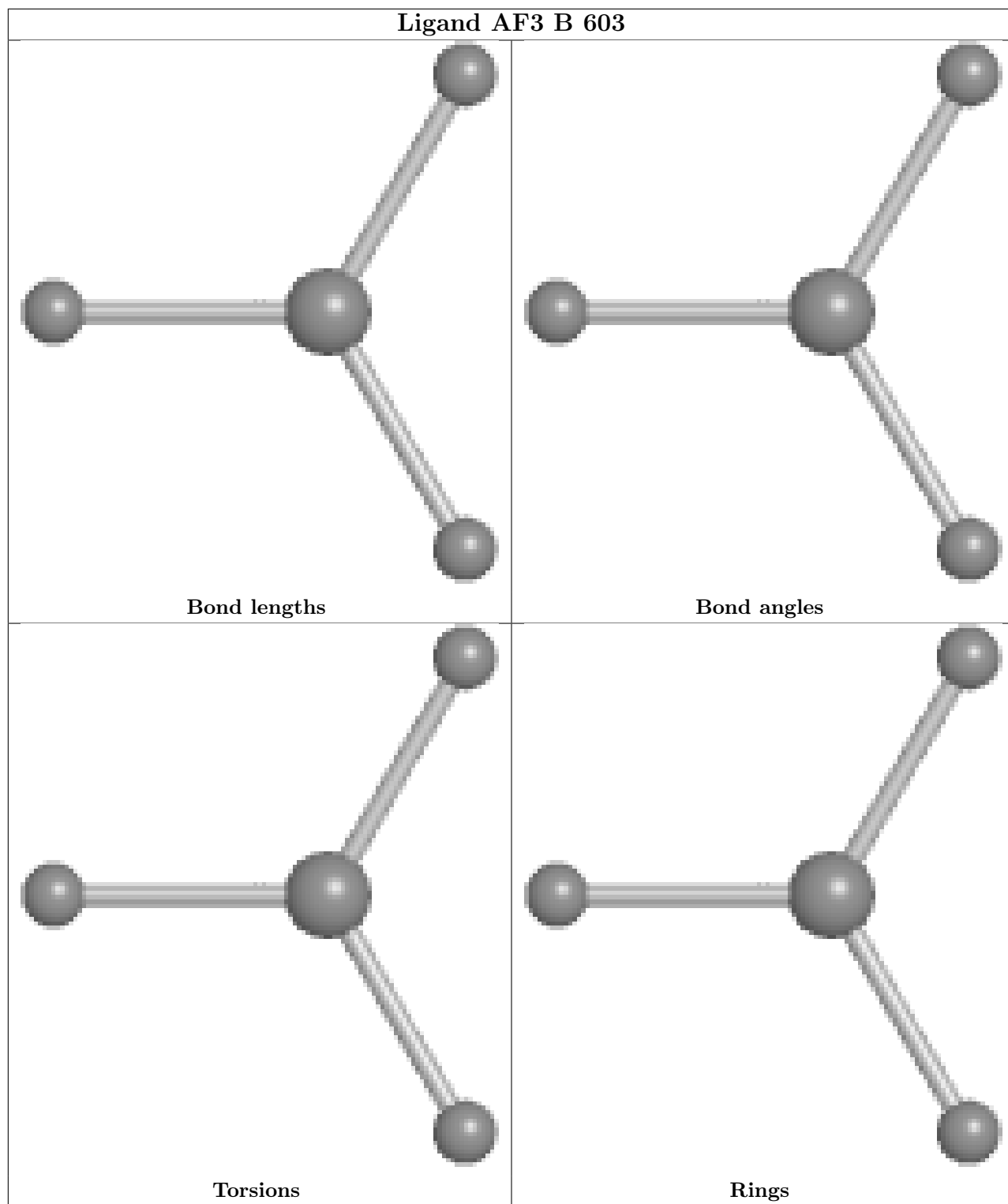


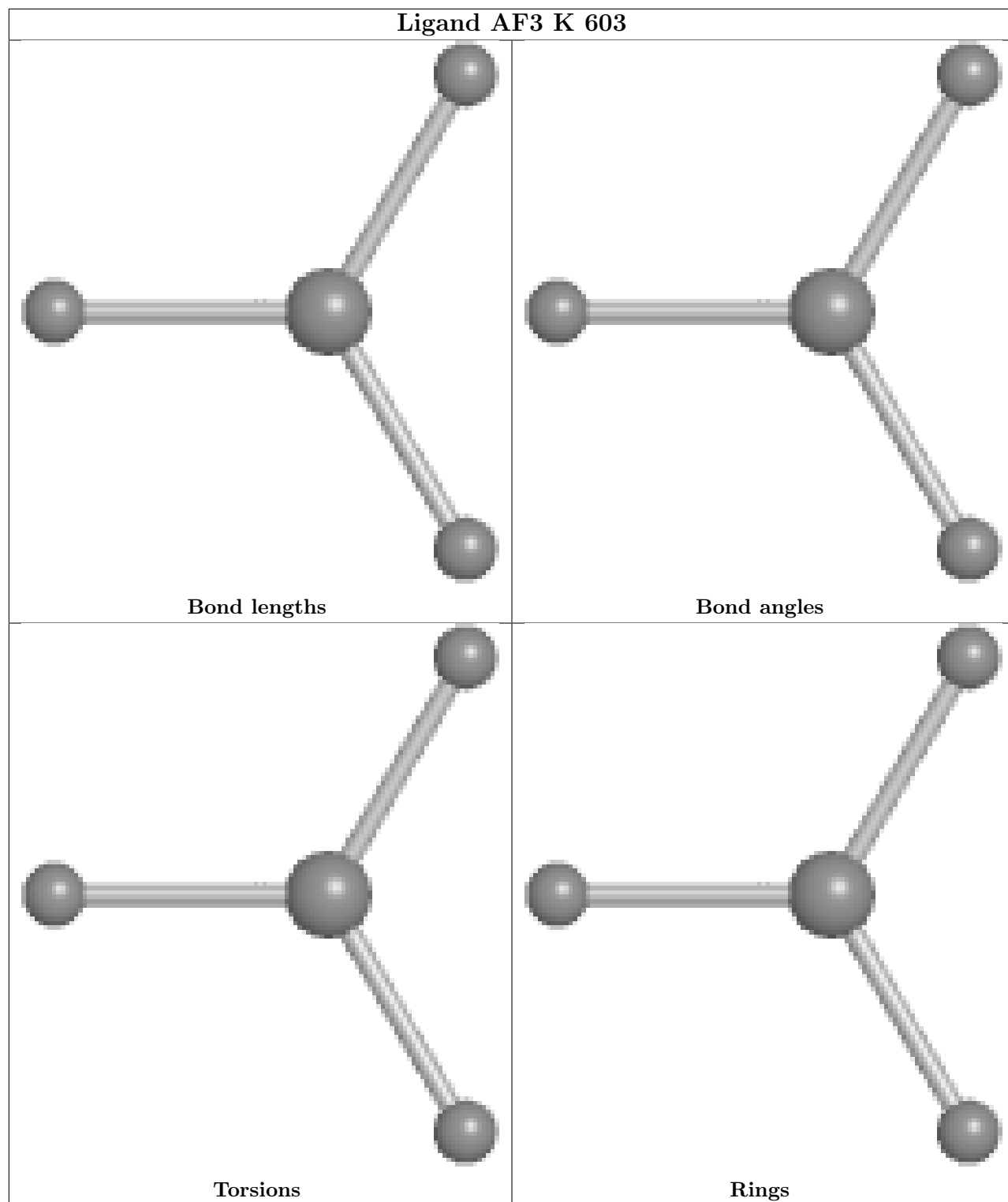


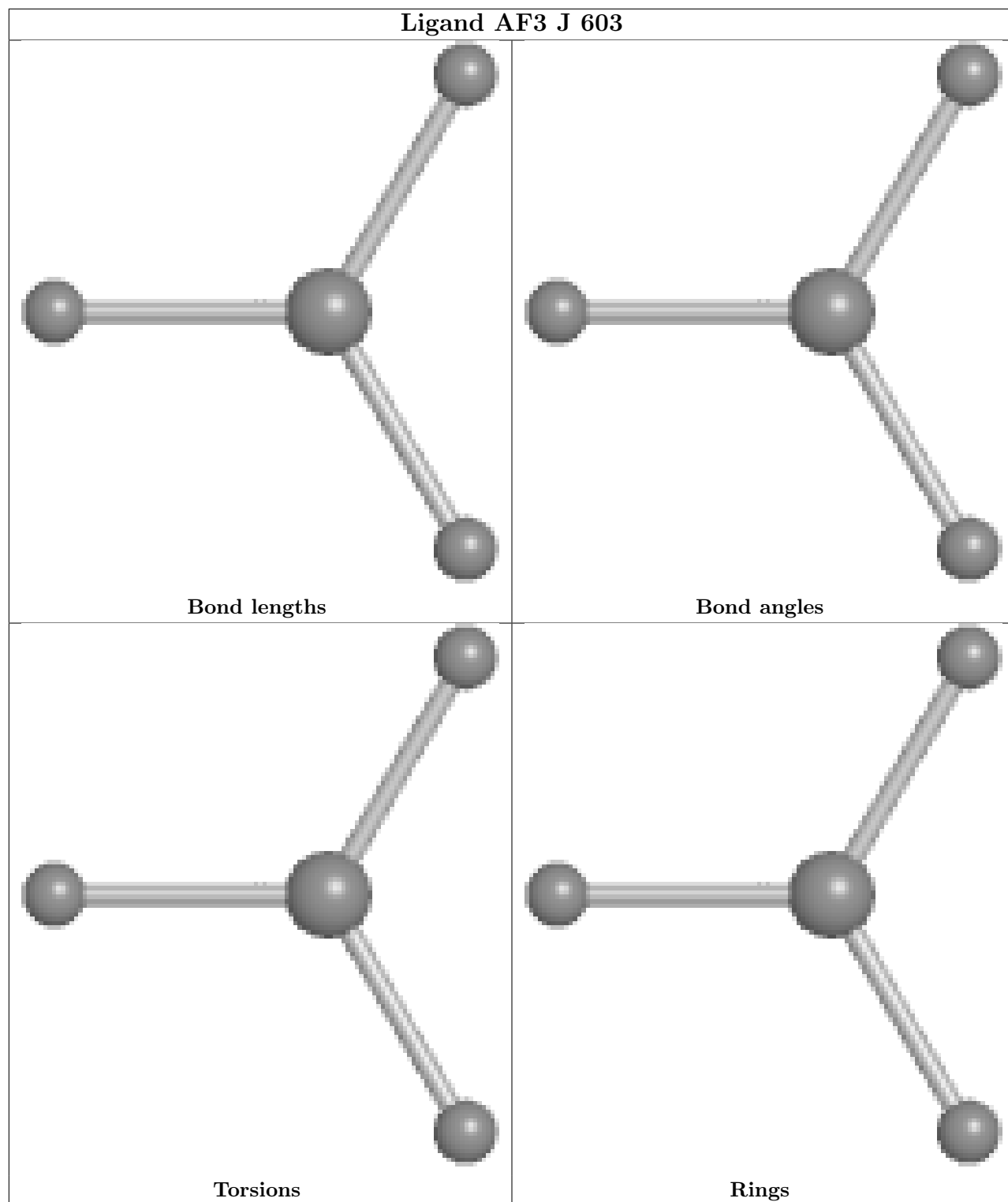


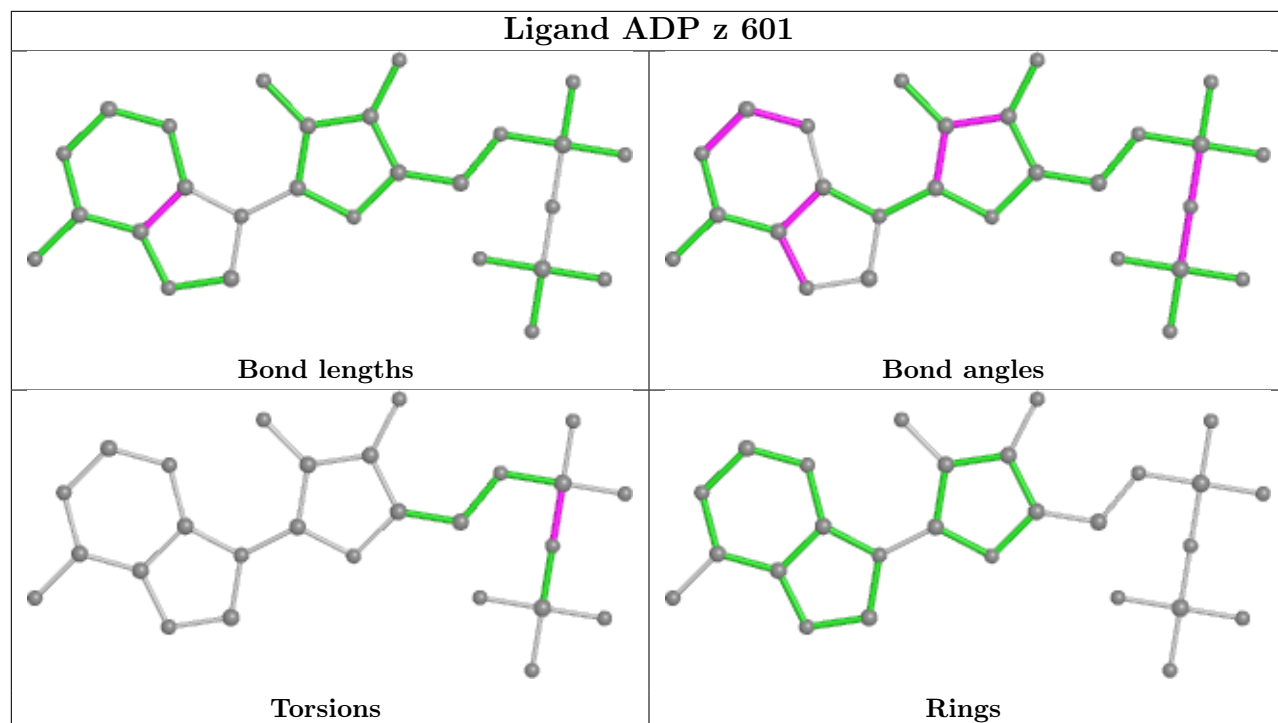


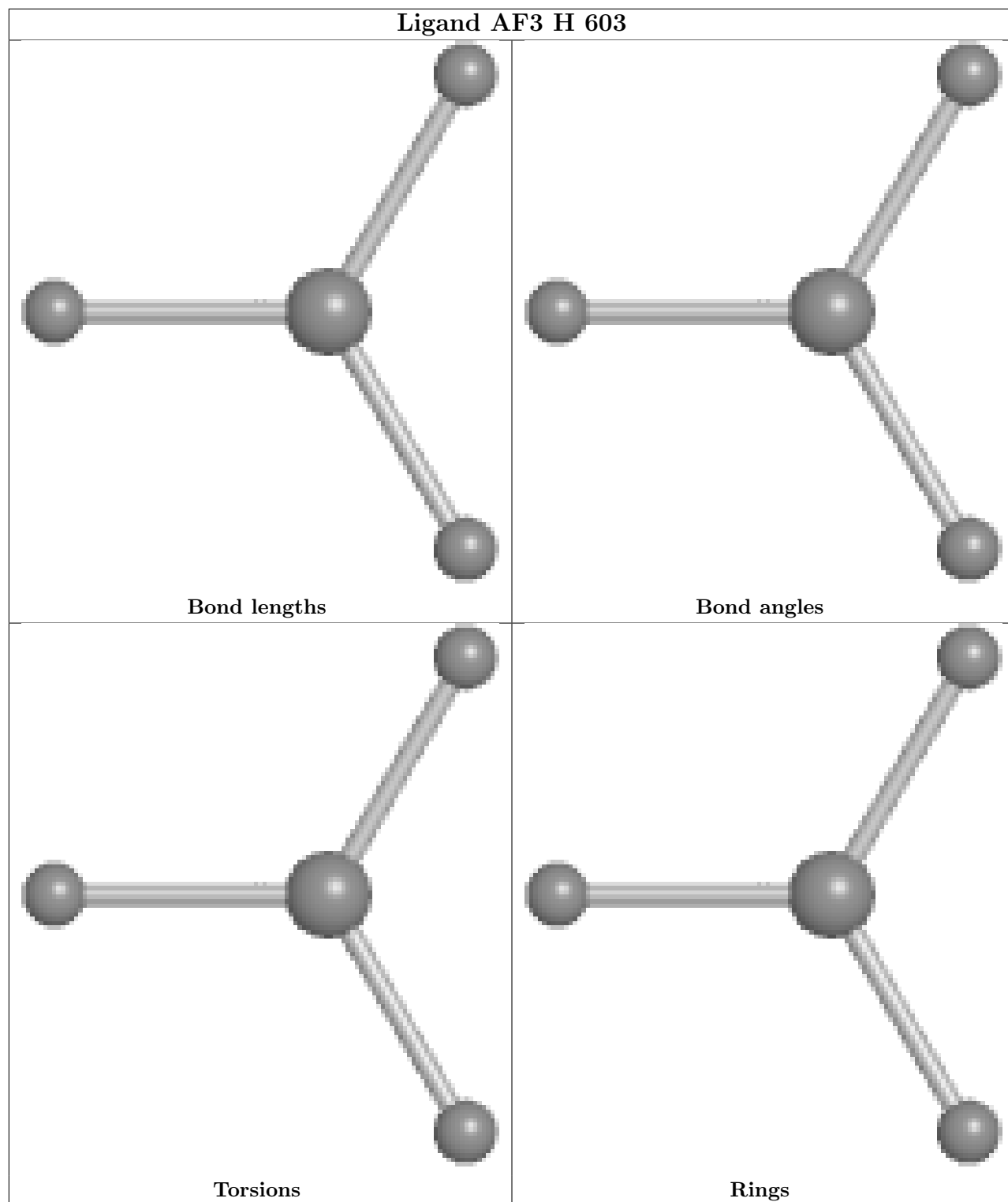




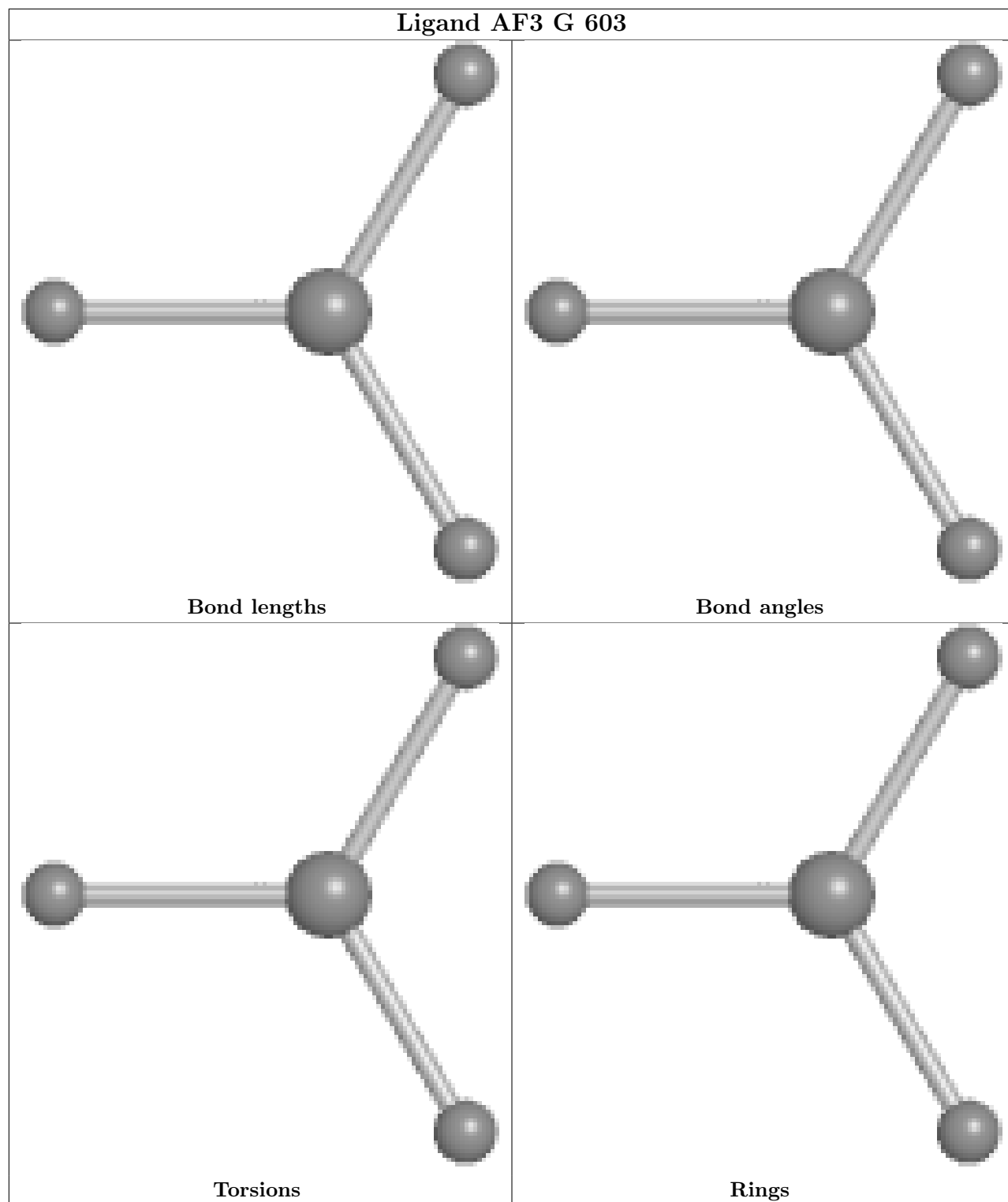


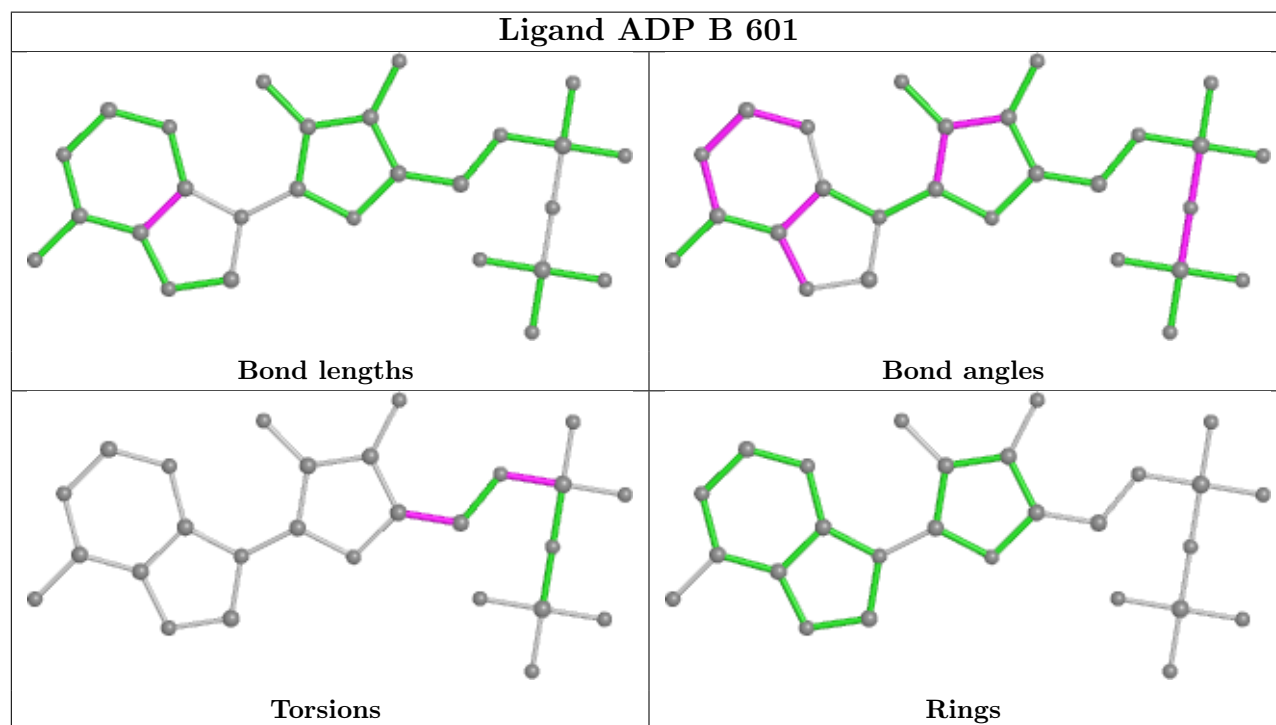
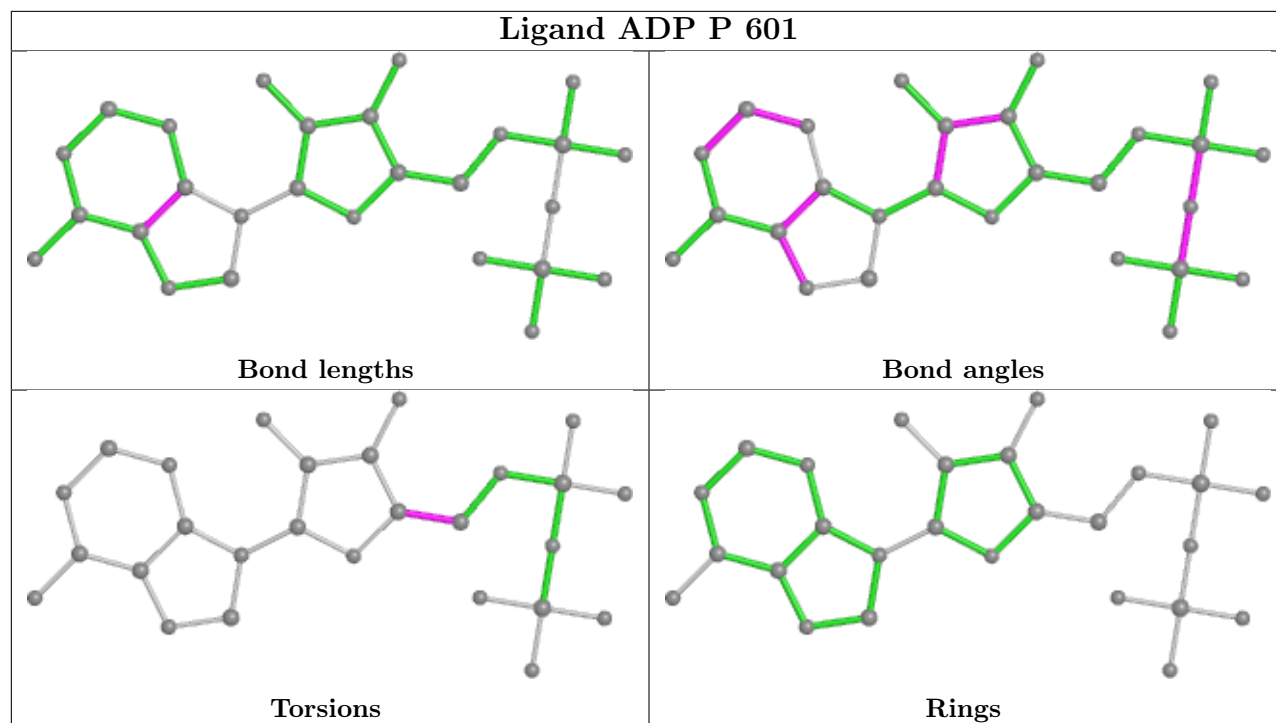


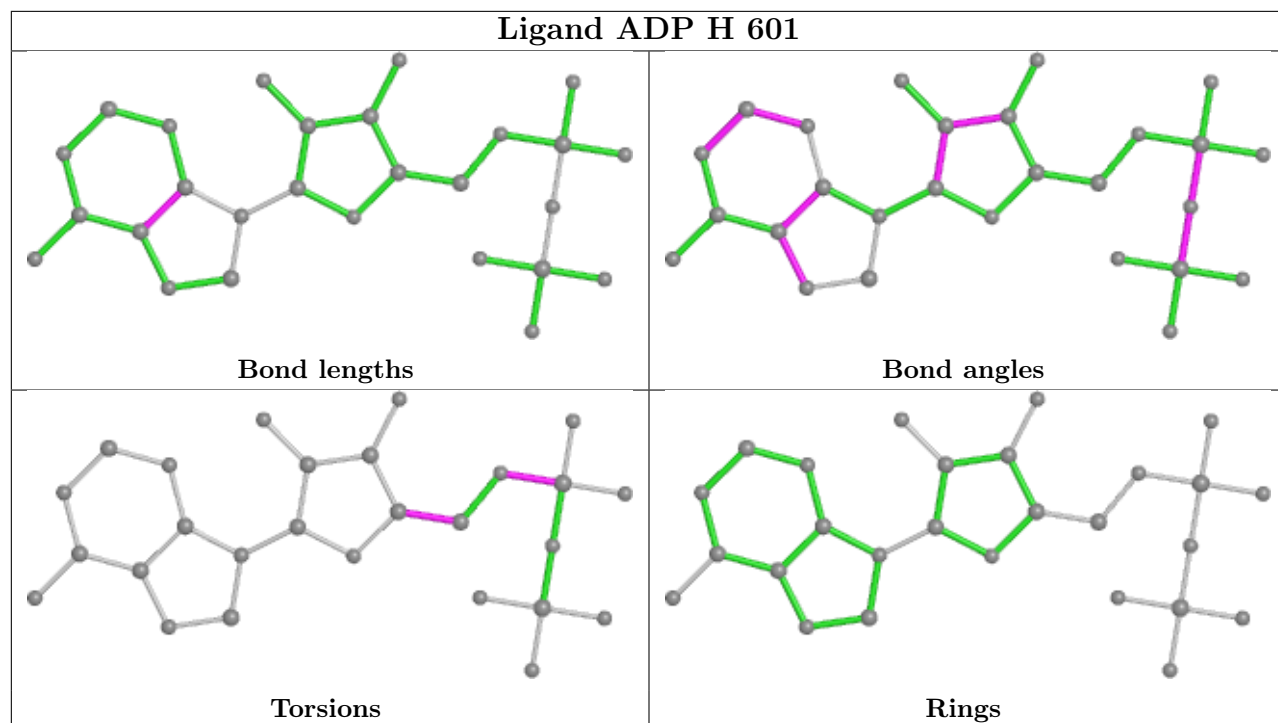


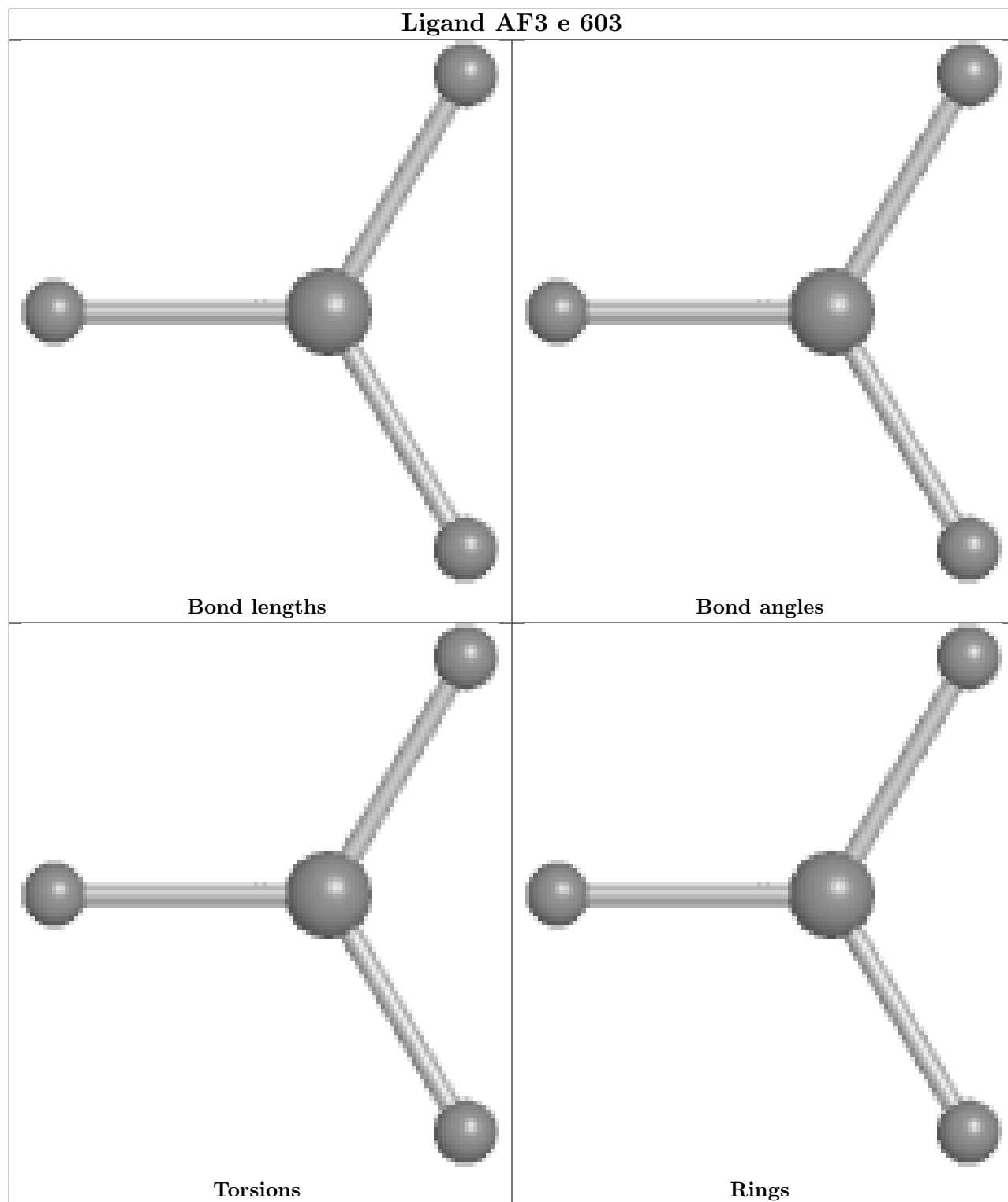


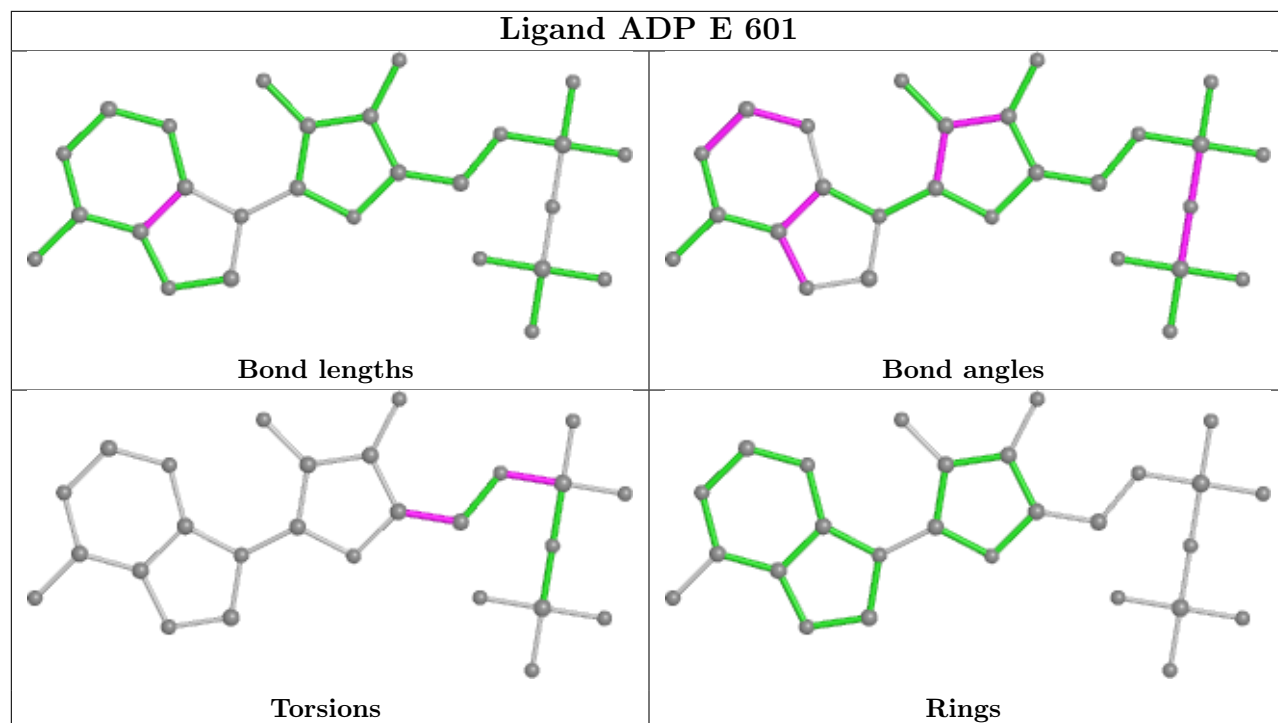


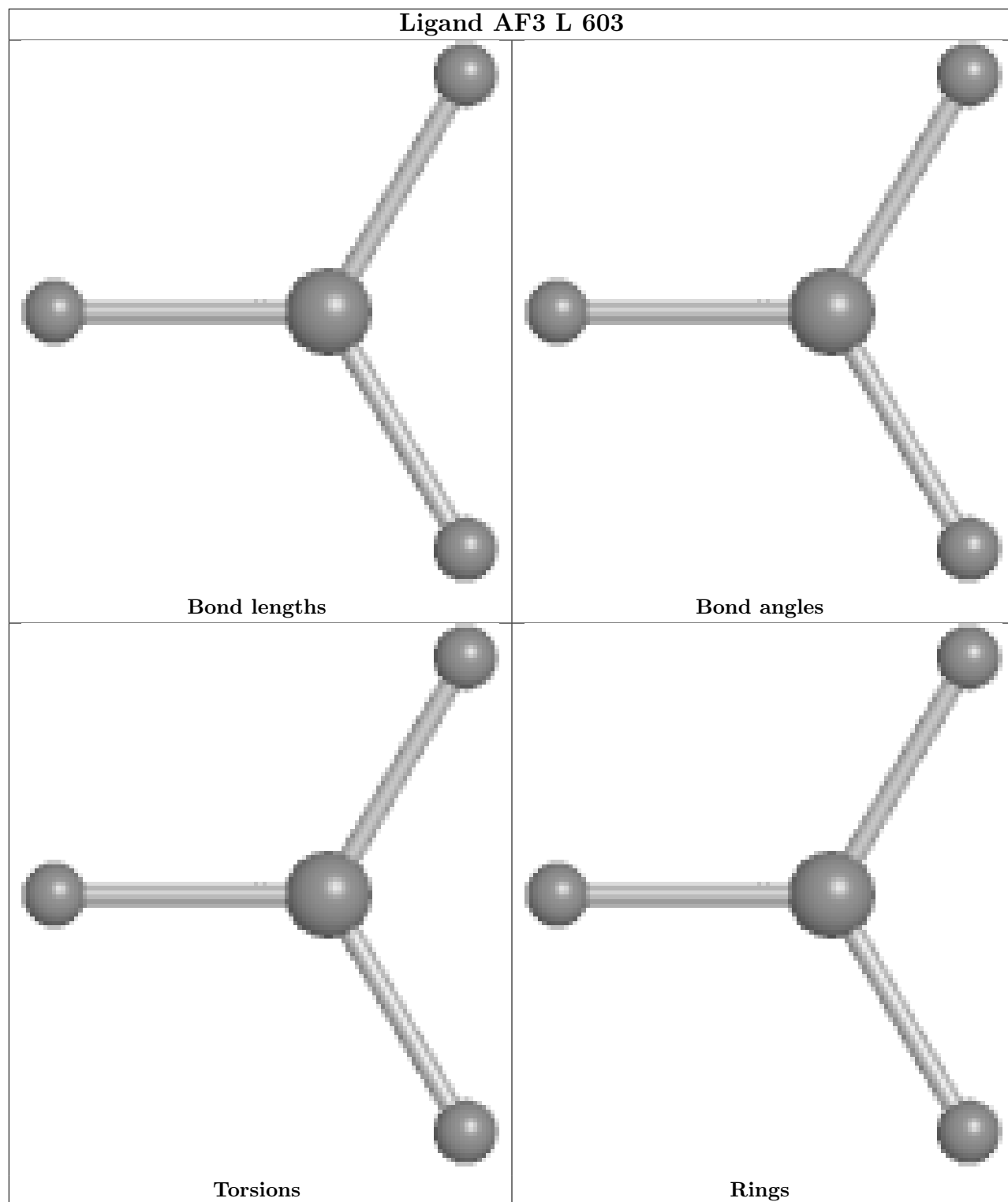


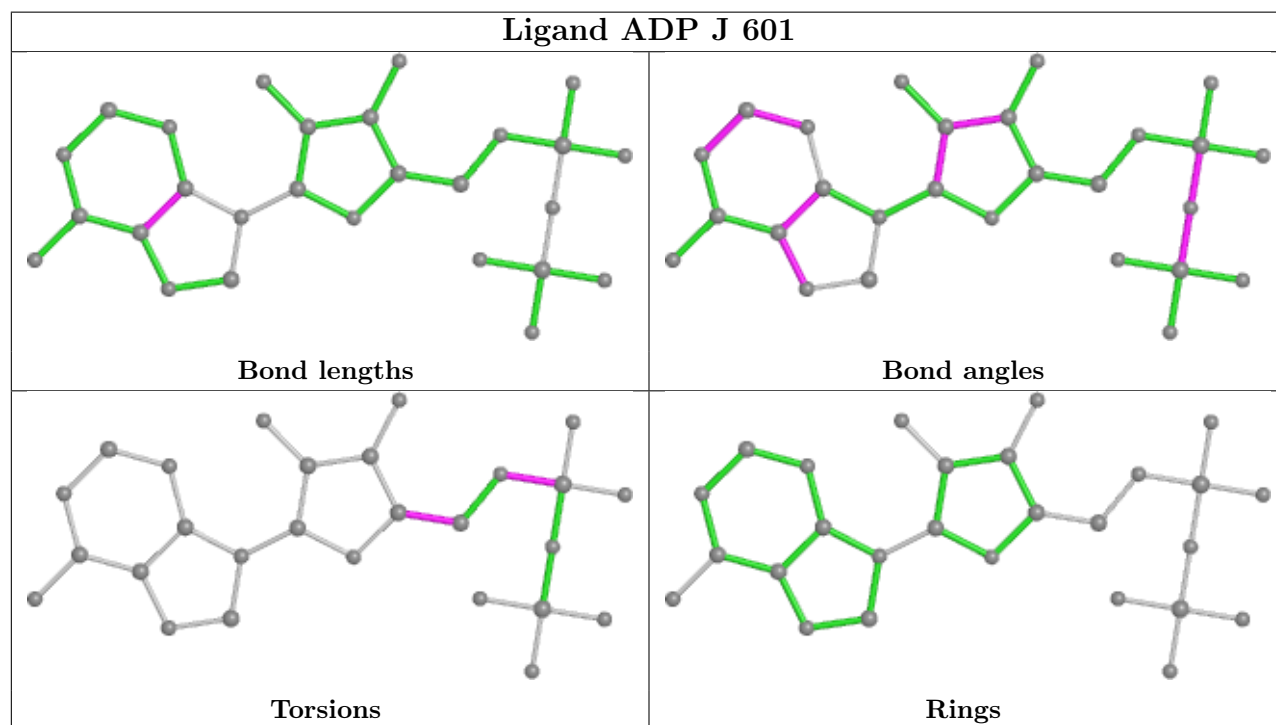
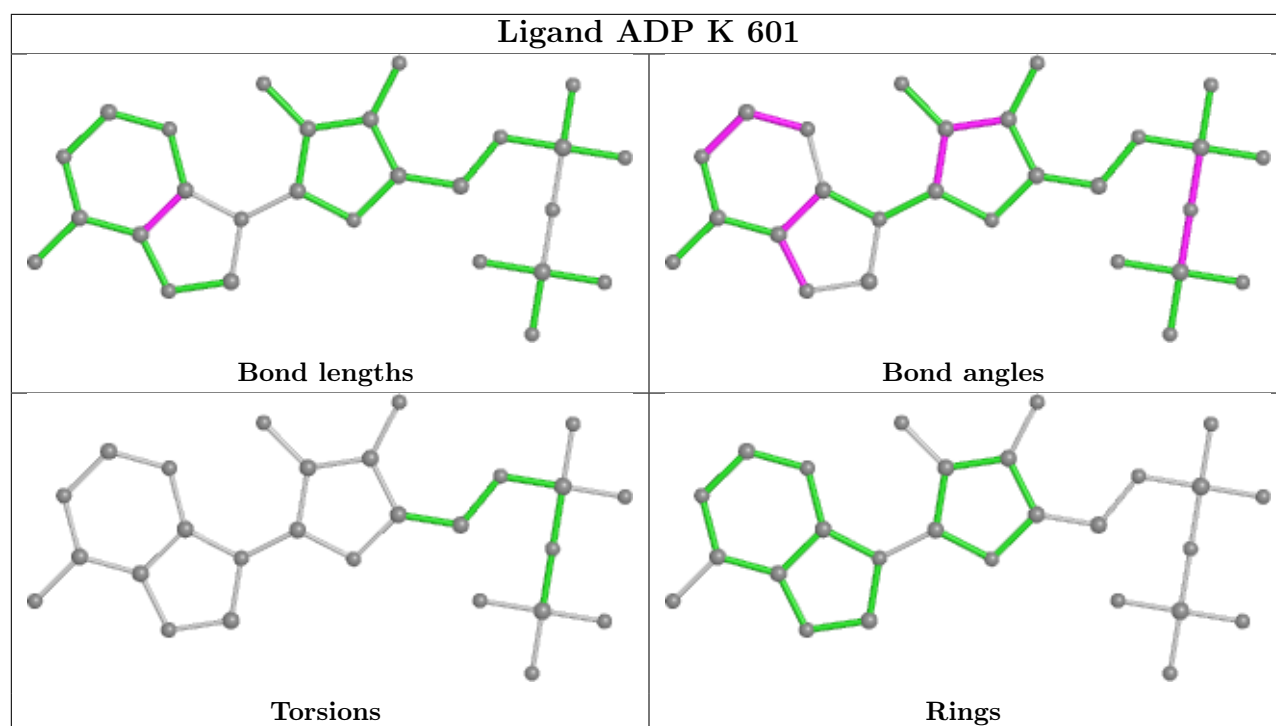


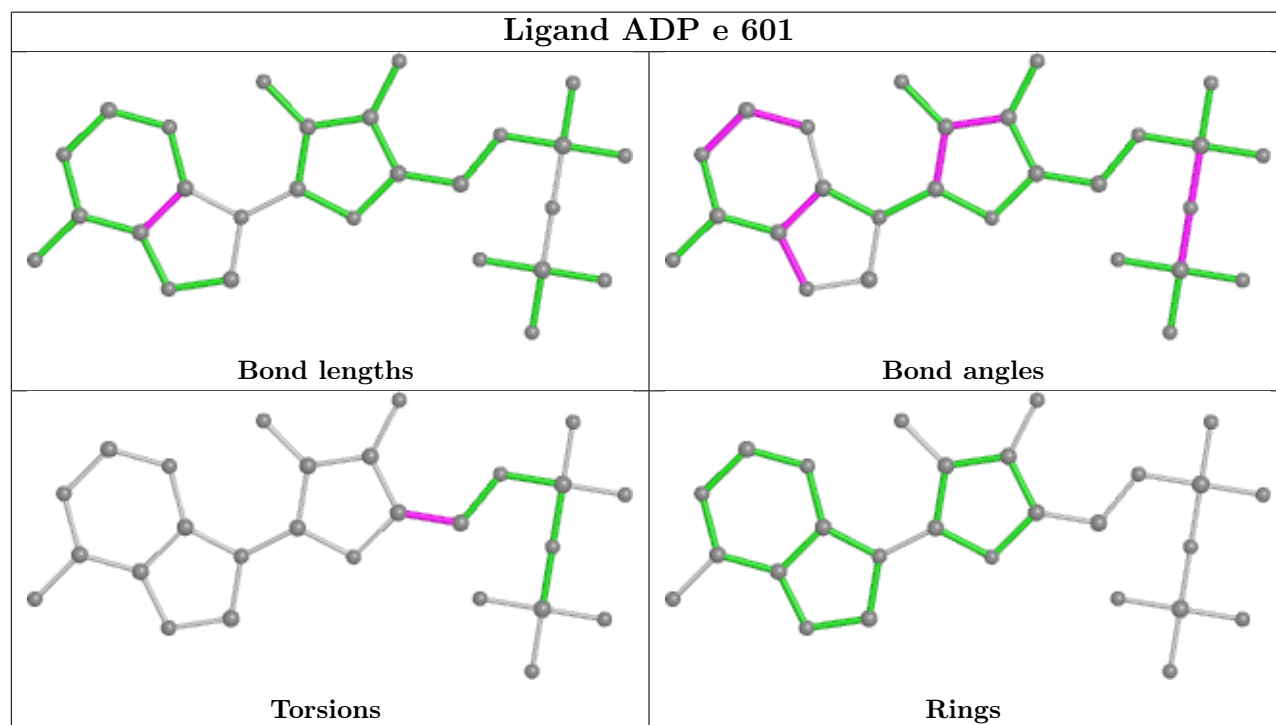
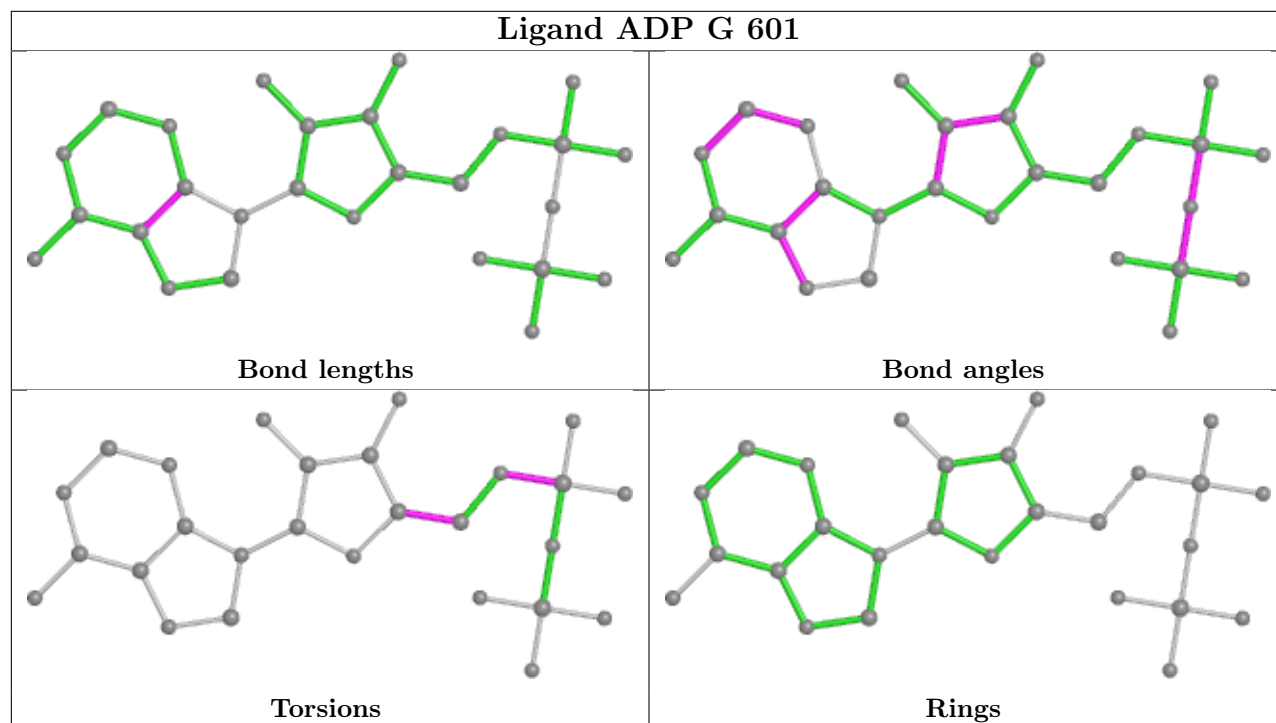




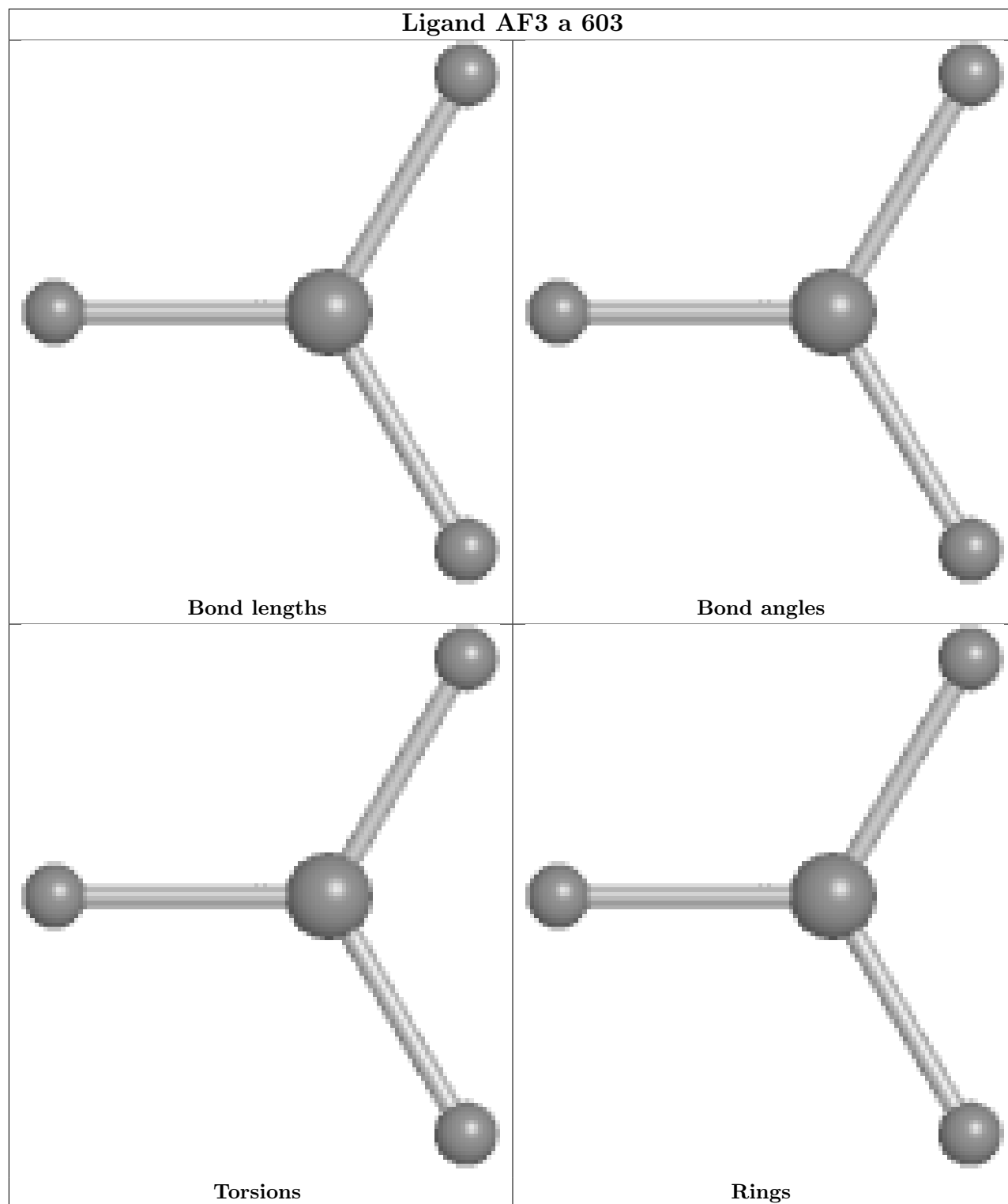












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

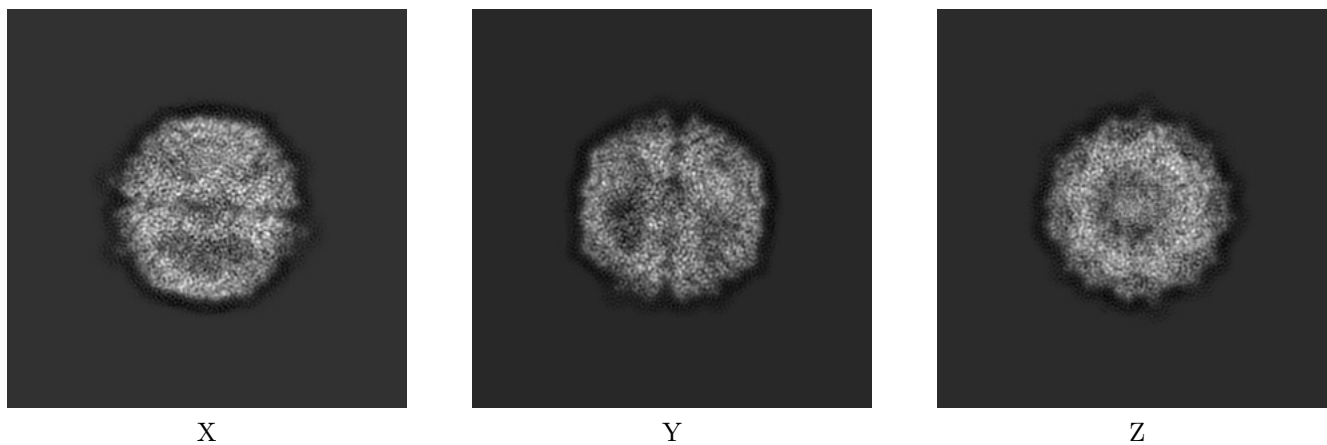
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32923. 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](#)

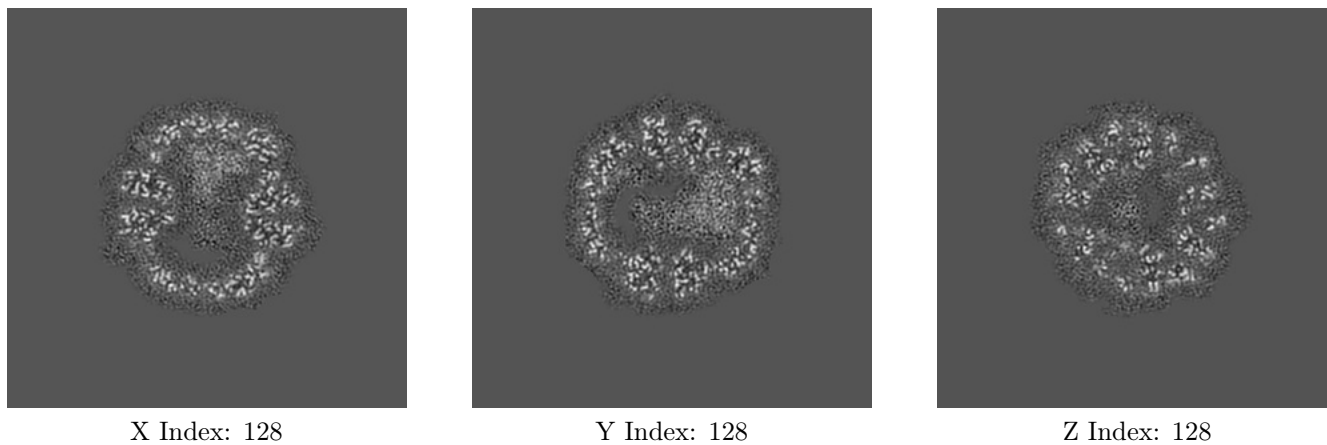
#### 6.1.1 Primary map



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

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

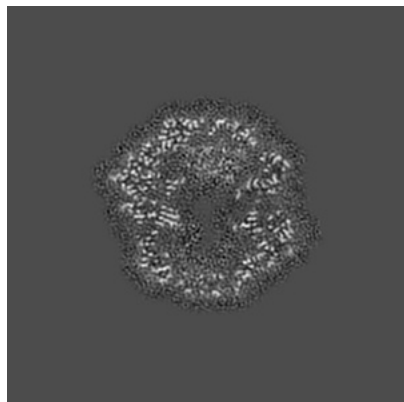
#### 6.2.1 Primary map



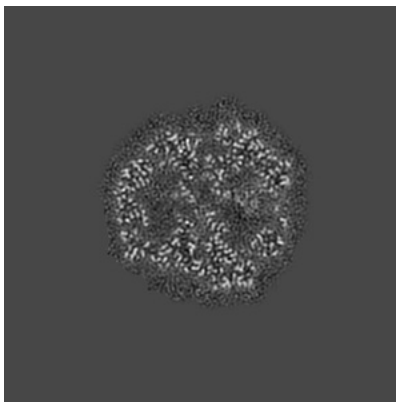
The images above show central slices of the map in three orthogonal directions.

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

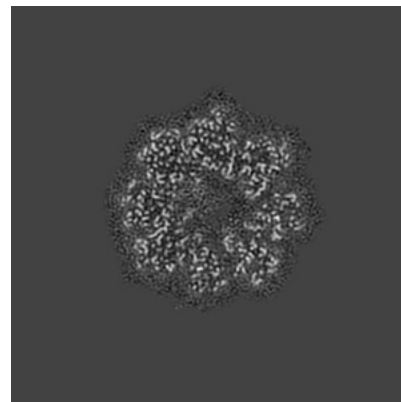
### 6.3.1 Primary map



X Index: 140



Y Index: 149

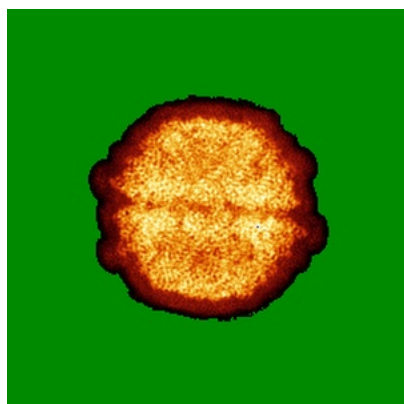


Z Index: 115

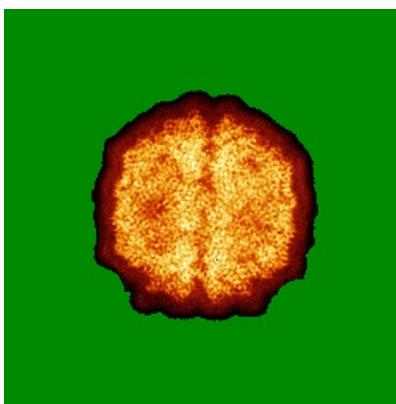
The images above show the largest variance slices of the map in three orthogonal directions.

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

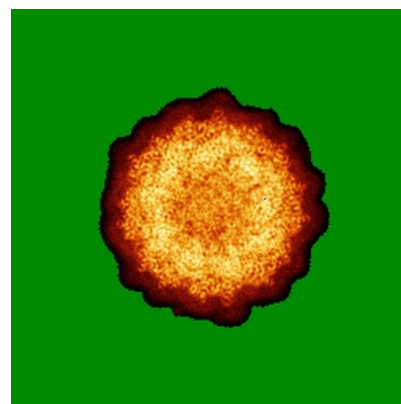
### 6.4.1 Primary map



X



Y



Z

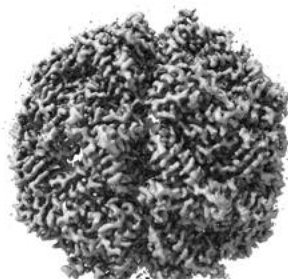
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.761. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

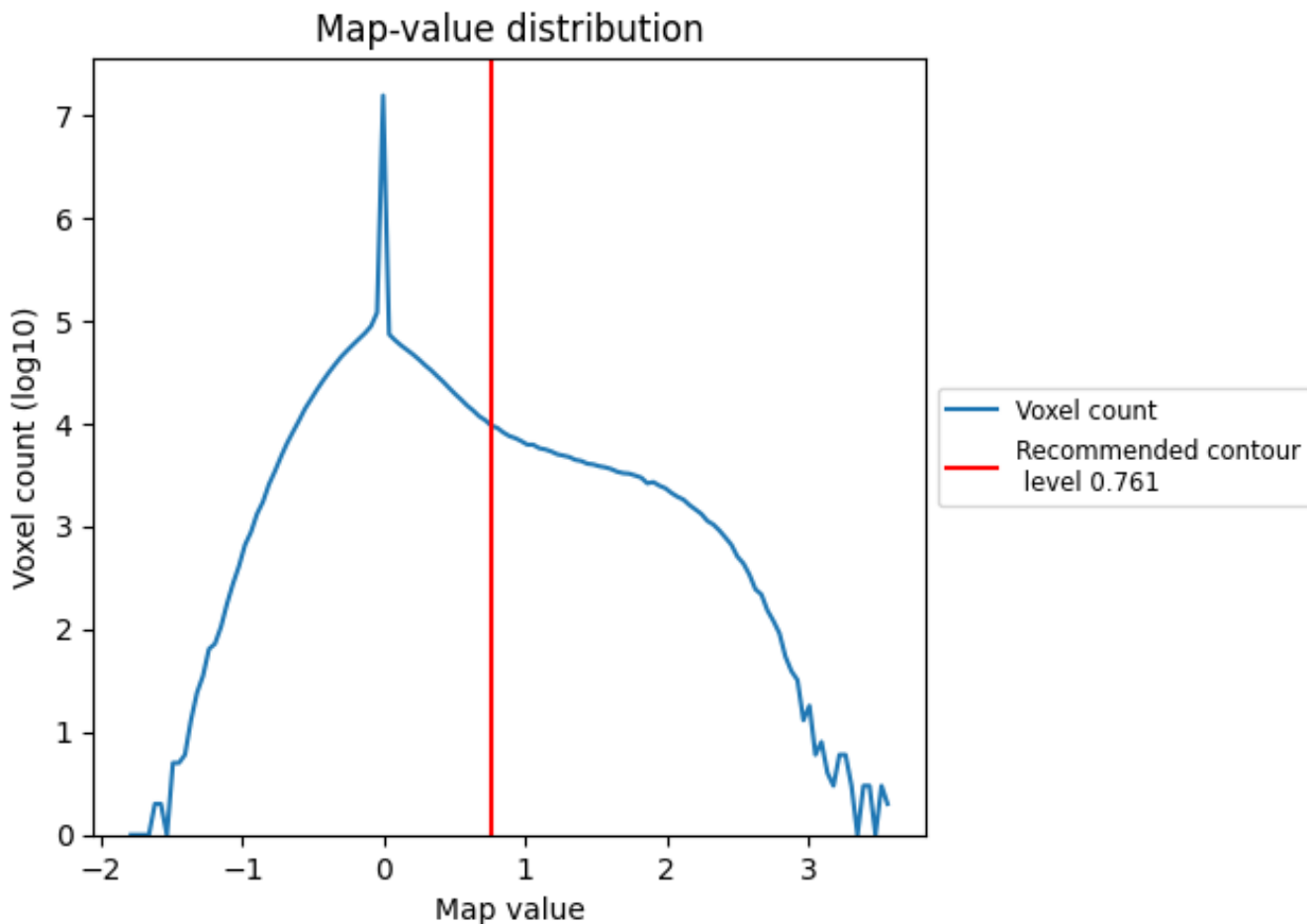
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

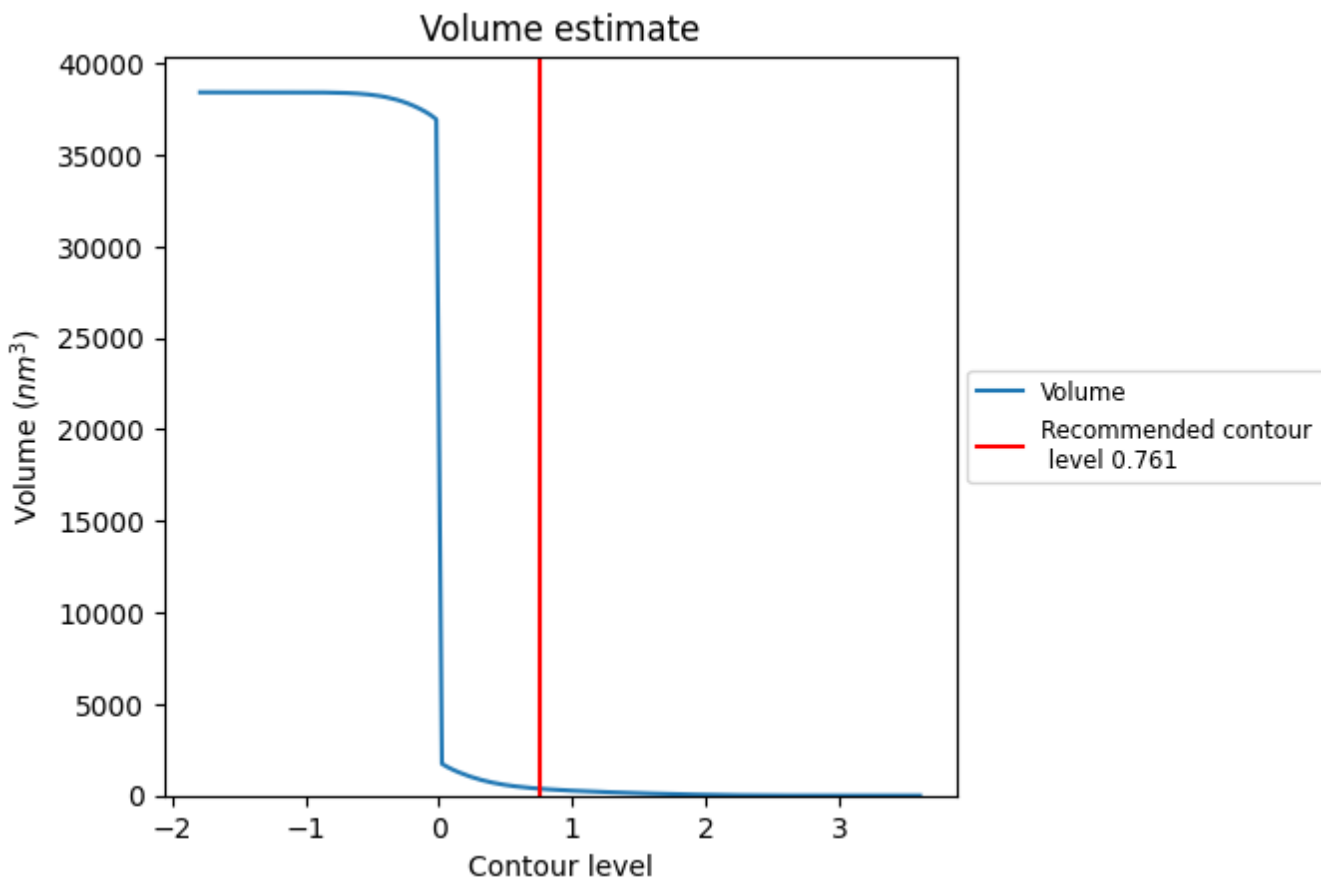
This section contains the results of statistical analysis of the map.

### 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.

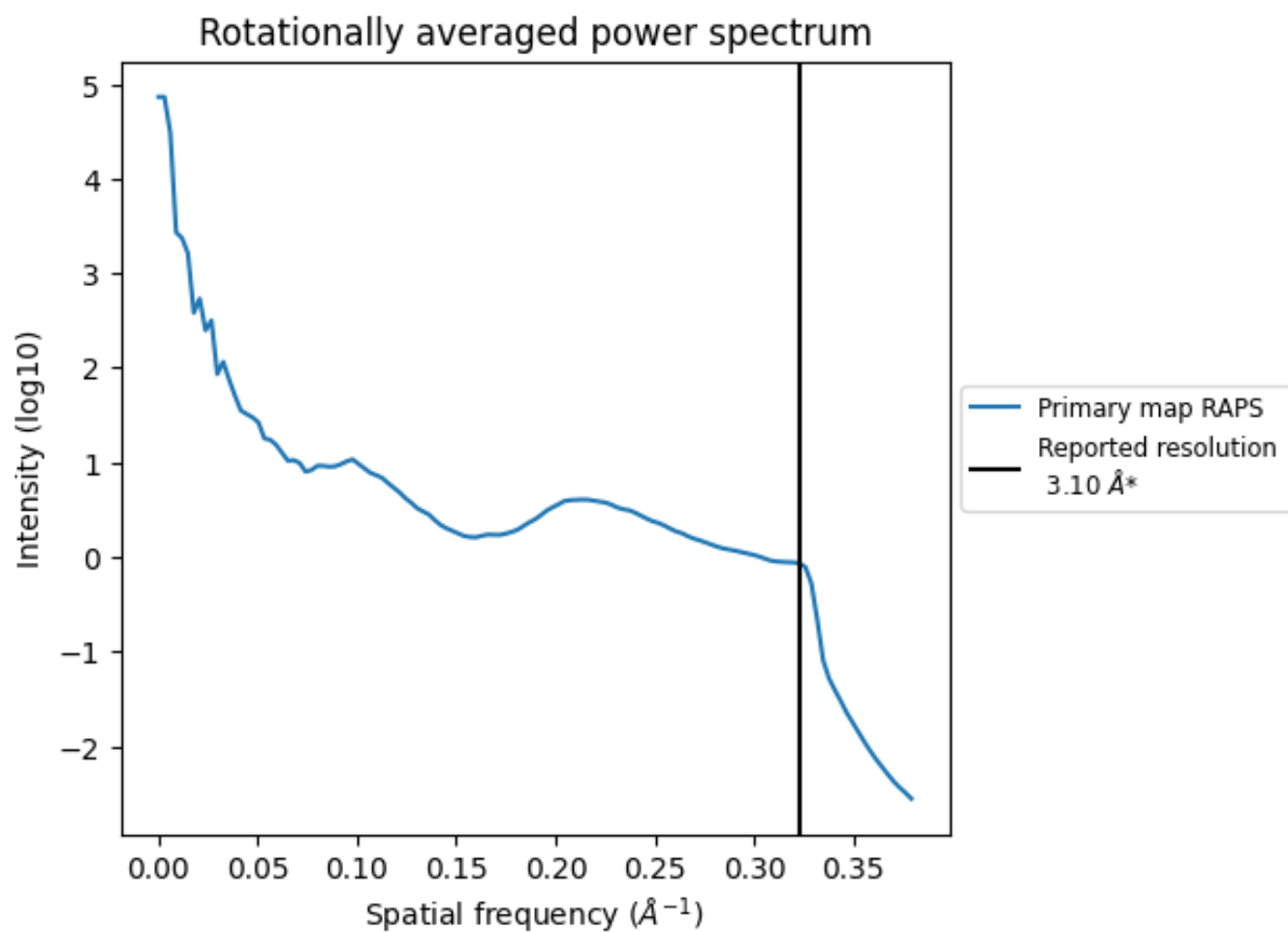
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 372 nm<sup>3</sup>; this corresponds to an approximate mass of 336 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 0.323 Å<sup>-1</sup>



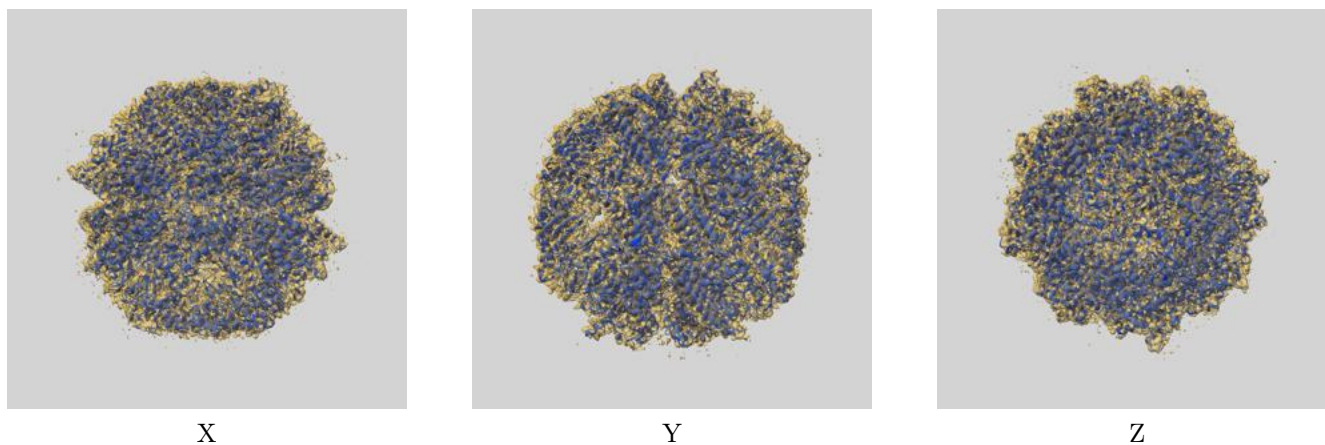
## 8 Fourier-Shell correlation

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

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

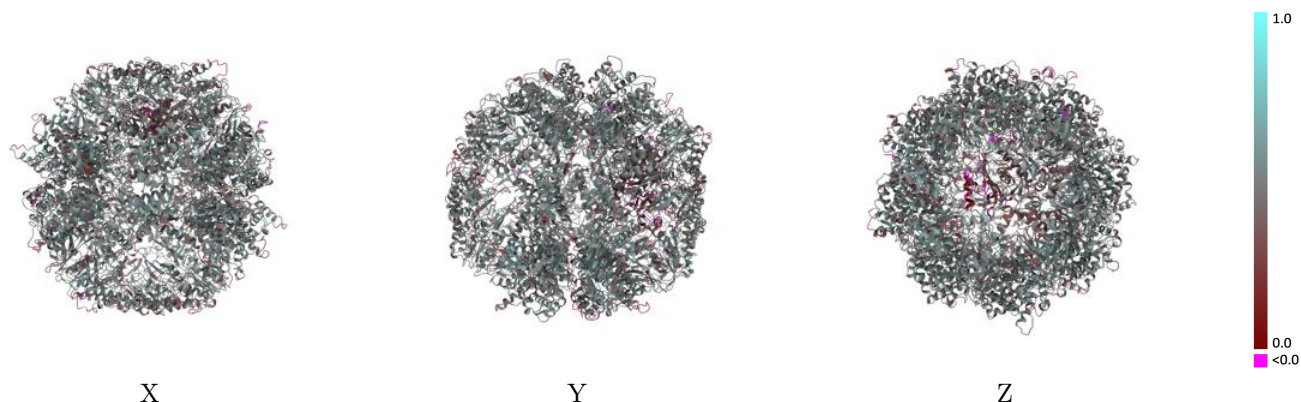
This section contains information regarding the fit between EMDB map EMD-32923 and PDB model 7X0S. Per-residue inclusion information can be found in section 3 on page 11.

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



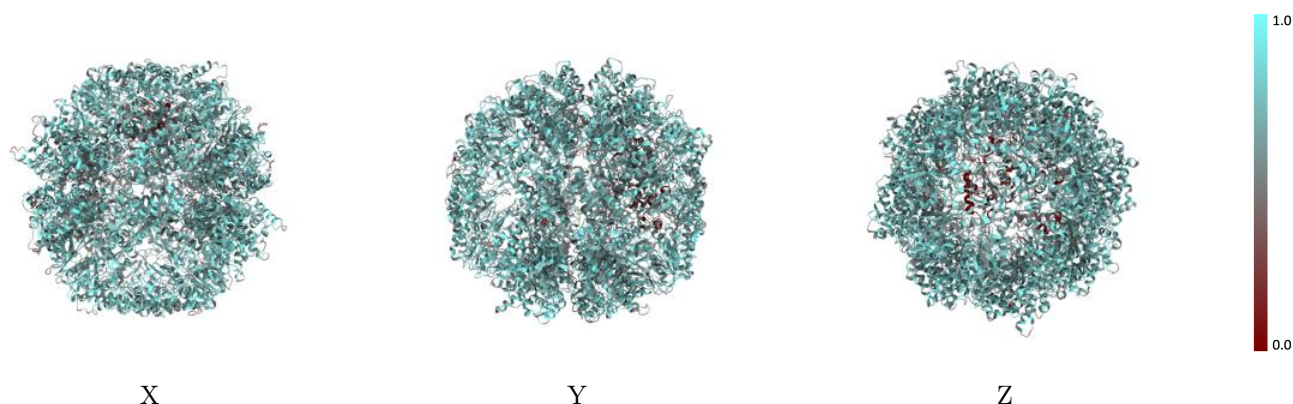
The images above show the 3D surface view of the map at the recommended contour level 0.761 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



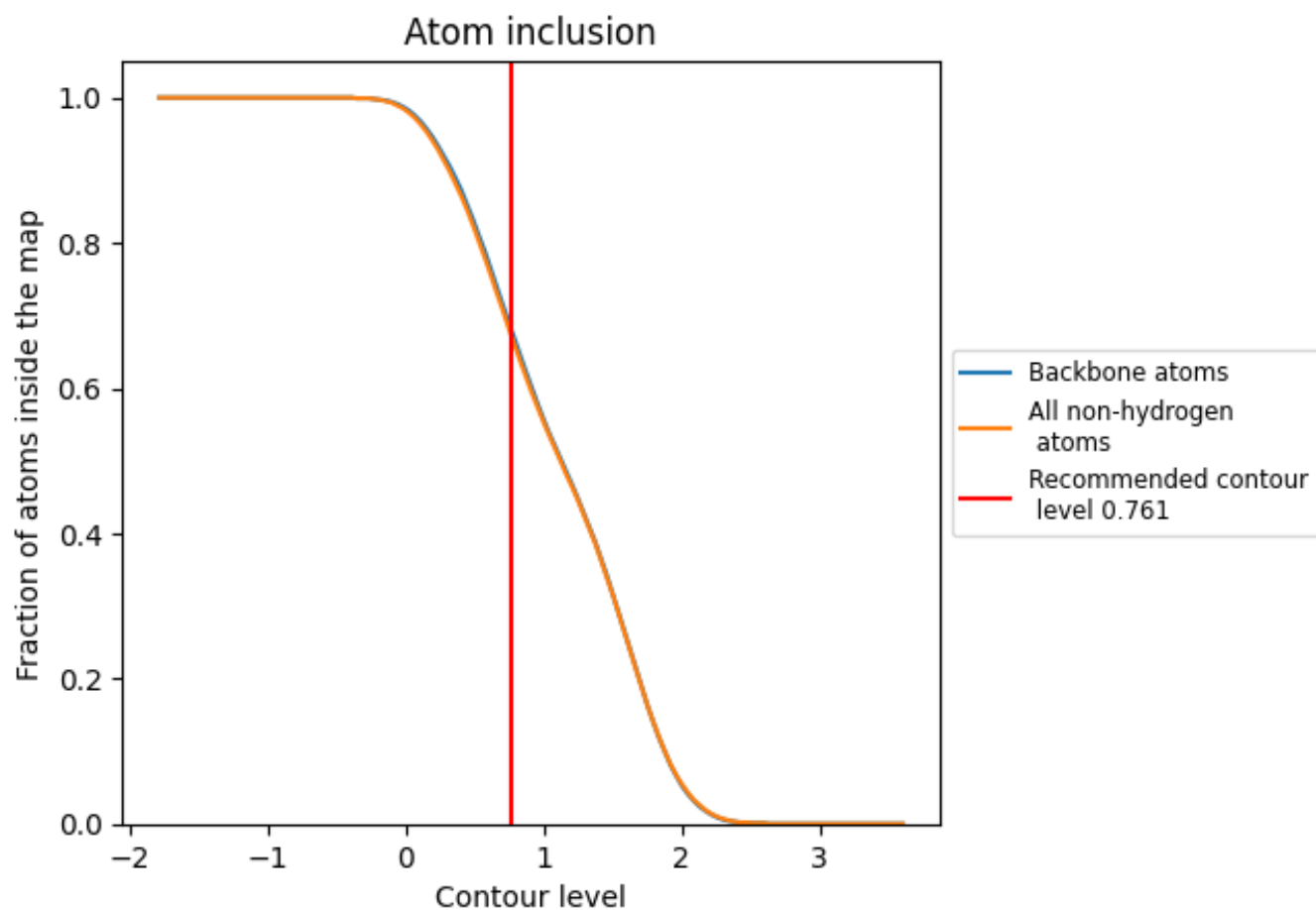
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.761).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.761) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6730	 0.4690
A	 0.6840	 0.4790
B	 0.6930	 0.4840
E	 0.6840	 0.4700
G	 0.7050	 0.4930
H	 0.6860	 0.4710
I	 0.6980	 0.4900
J	 0.6980	 0.4720
K	 0.7070	 0.4820
L	 0.6990	 0.4790
M	 0.6970	 0.4820
N	 0.7050	 0.4860
O	 0.6830	 0.4660
P	 0.7010	 0.4710
R	 0.4080	 0.3000
a	 0.6890	 0.4720
e	 0.6830	 0.4690
z	 0.7090	 0.4750

