



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:12 PM JST

PDB ID : 7X0S / pdb_00007x0s
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

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:

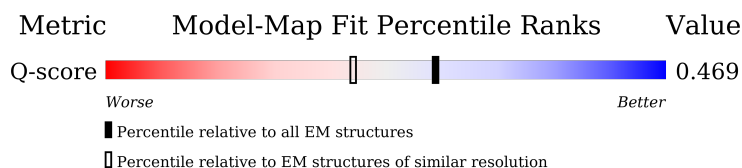
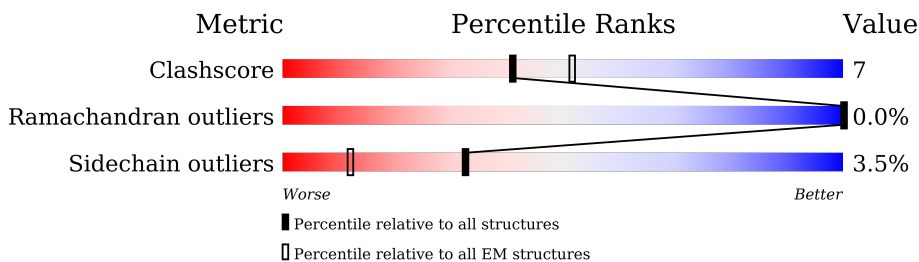
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	K	531	
1	z	531	
2	J	548	
2	P	548	

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Mol	Chain	Length	Quality of chain
3	H	543	
3	O	543	
4	G	545	
4	N	545	
5	E	539	
5	e	539	
6	I	539	
6	M	539	
7	B	535	
7	L	535	
8	A	556	
8	a	556	
9	R	444	

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
10	ADP	A	601	-	-	X	-
10	ADP	G	601	-	-	X	-
10	ADP	H	601	-	-	X	-
10	ADP	I	601	-	-	X	-
10	ADP	J	601	-	-	X	-
10	ADP	K	601	-	-	X	-
10	ADP	M	601	-	-	X	-
10	ADP	N	601	-	-	X	-
10	ADP	O	603	-	-	X	-
10	ADP	P	601	-	-	X	-
10	ADP	z	601	-	-	X	-
11	MG	K	602	-	-	X	-
11	MG	z	602	-	-	X	-
12	AF3	A	603	-	-	X	-
12	AF3	B	603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	AF3	E	603	-	-	X	-
12	AF3	G	603	-	-	X	-
12	AF3	H	603	-	-	X	-
12	AF3	J	603	-	-	X	-
12	AF3	K	603	-	-	X	-
12	AF3	L	603	-	-	X	-
12	AF3	N	603	-	-	X	-
12	AF3	O	602	-	-	X	-
12	AF3	P	603	-	-	X	-
12	AF3	a	603	-	-	X	-
12	AF3	e	603	-	-	X	-
12	AF3	z	603	-	-	X	-

2 Entry composition

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
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
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
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
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
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
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
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
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.

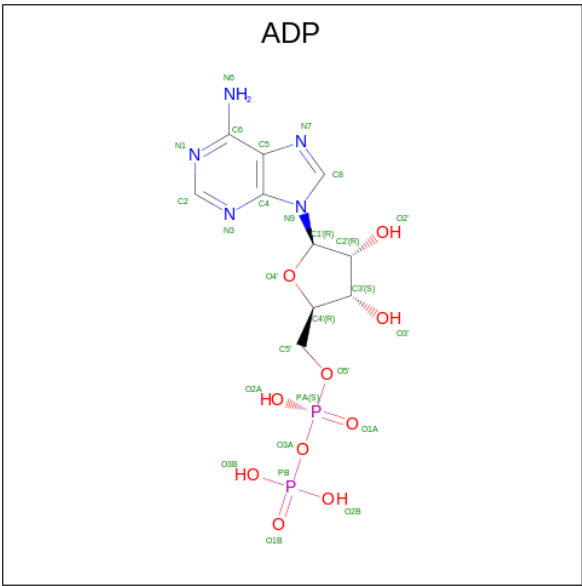
Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		
8	a	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		

- Molecule 9 is a protein called Tubulin beta chain.

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

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂)

(labeled as "Ligand of Interest" by depositor).



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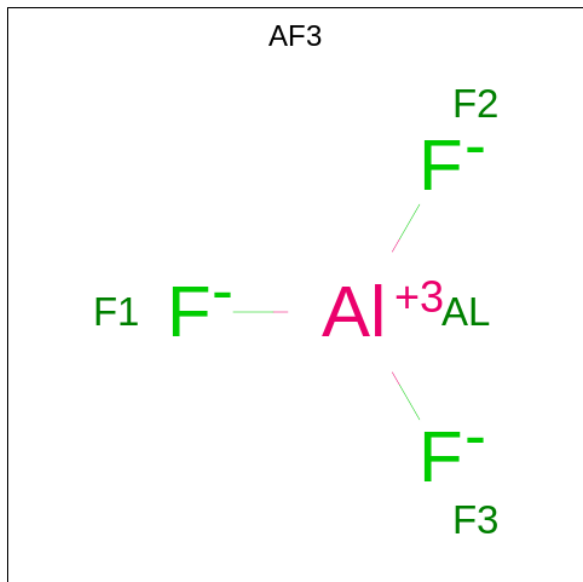
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Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

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

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 13 is water.

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

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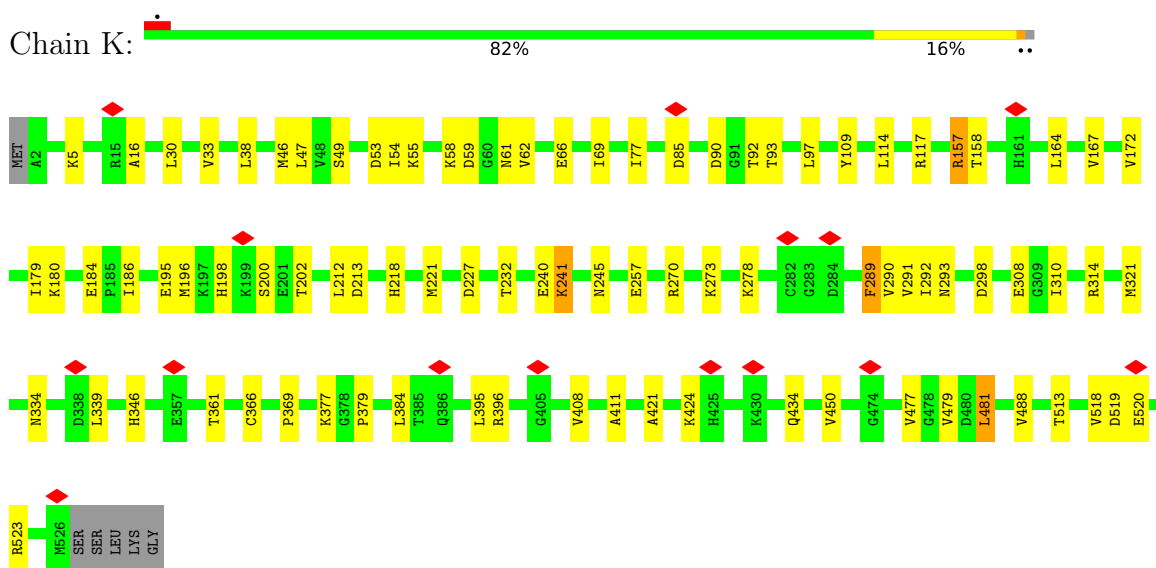
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Mol	Chain	Residues	Atoms		AltConf
13	L	1	Total	O	0
			1	1	

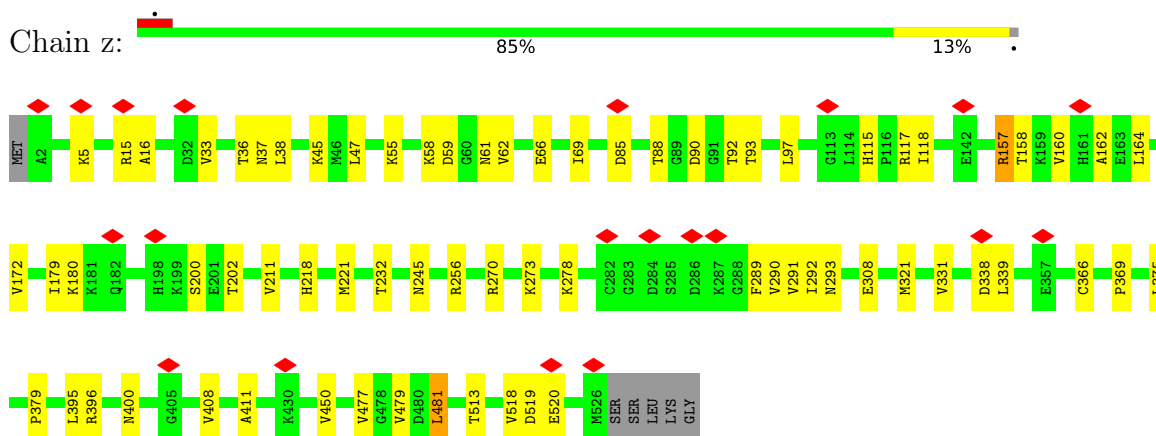
3 Residue-property plots

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.

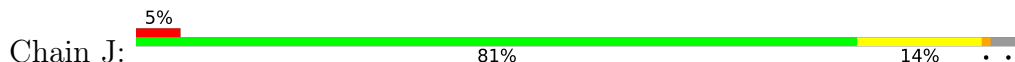
- Molecule 1: T-complex protein 1 subunit zeta

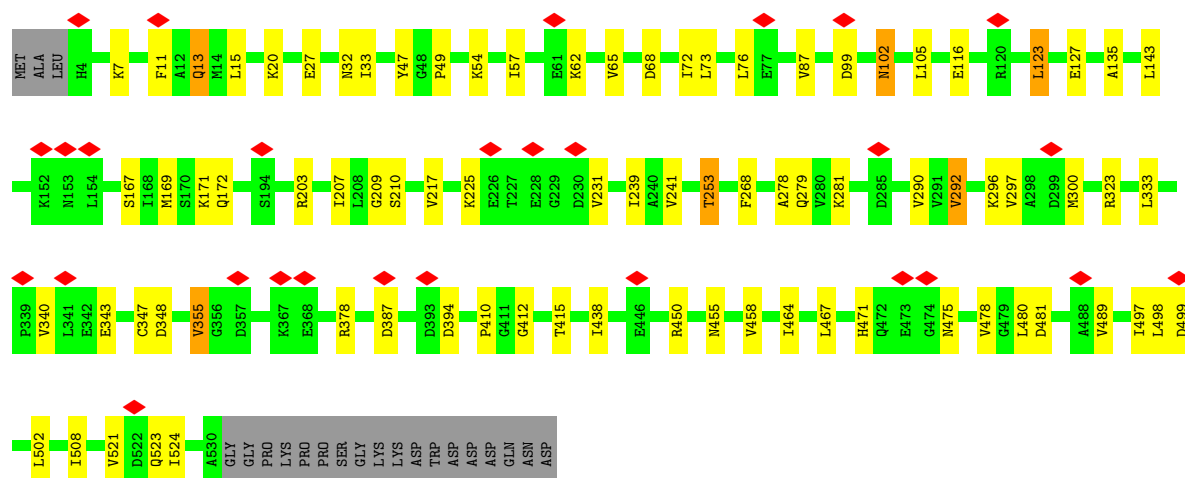


- Molecule 1: T-complex protein 1 subunit zeta

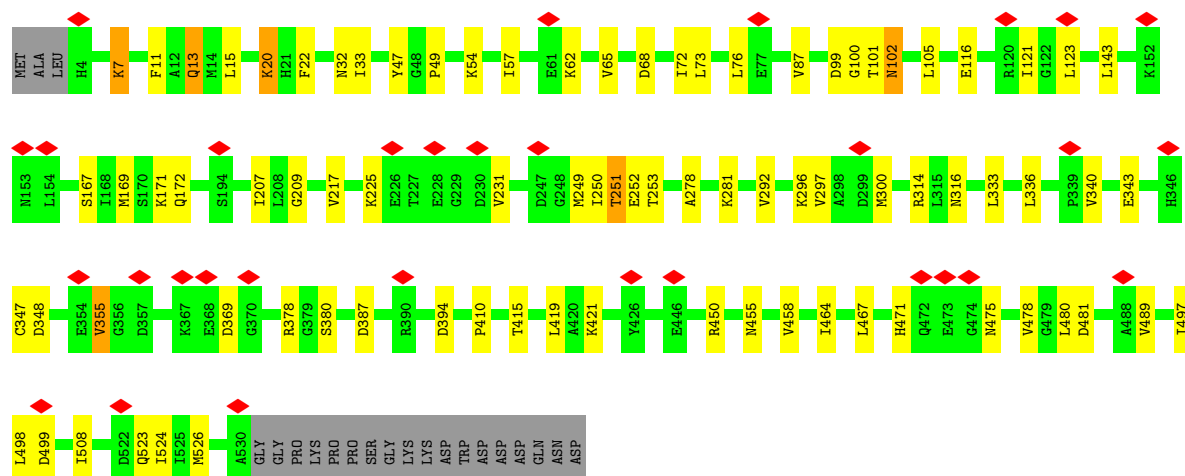
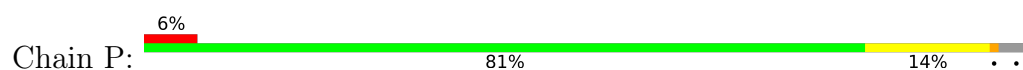


- Molecule 2: T-complex protein 1 subunit theta

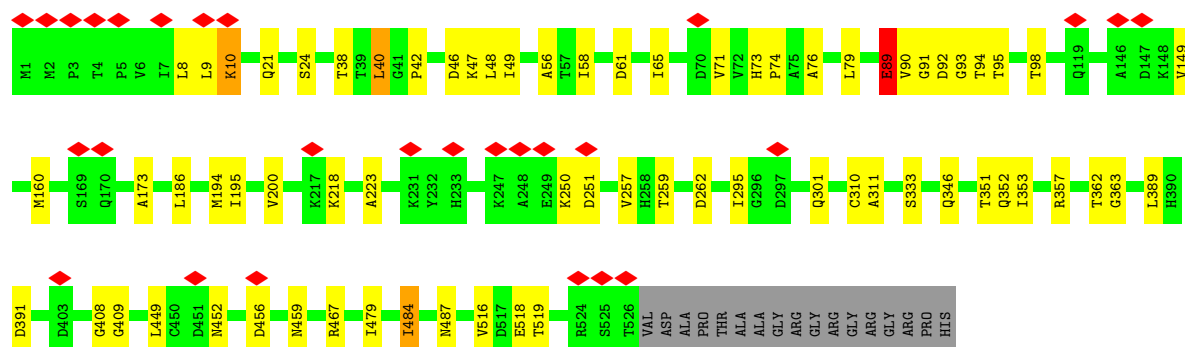
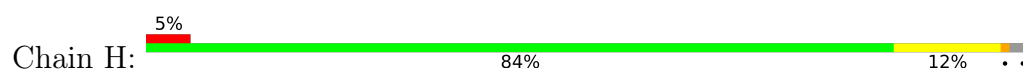




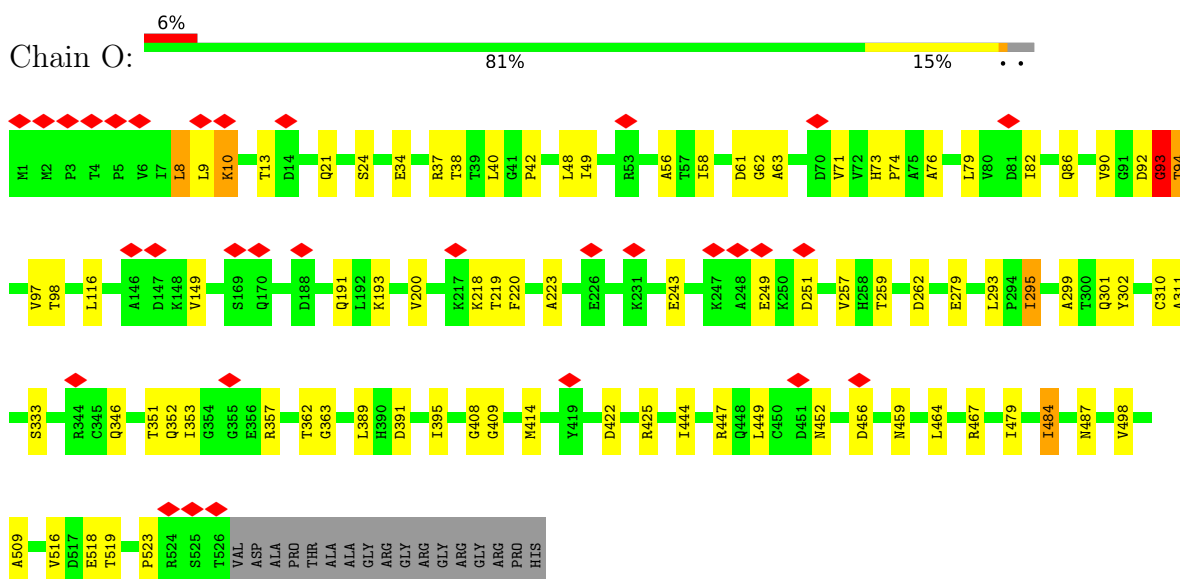
• Molecule 2: T-complex protein 1 subunit theta



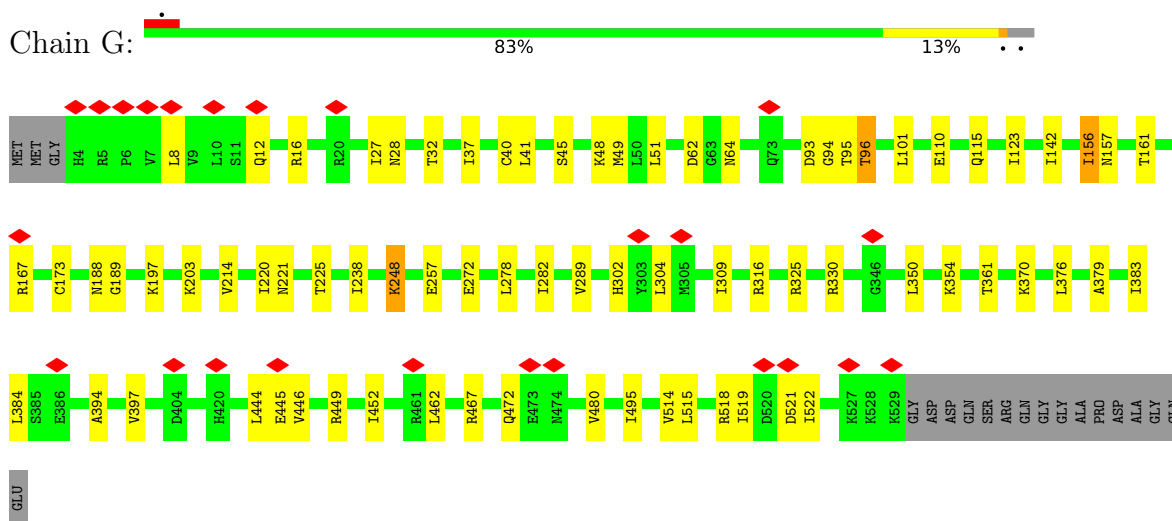
• Molecule 3: T-complex protein 1 subunit eta



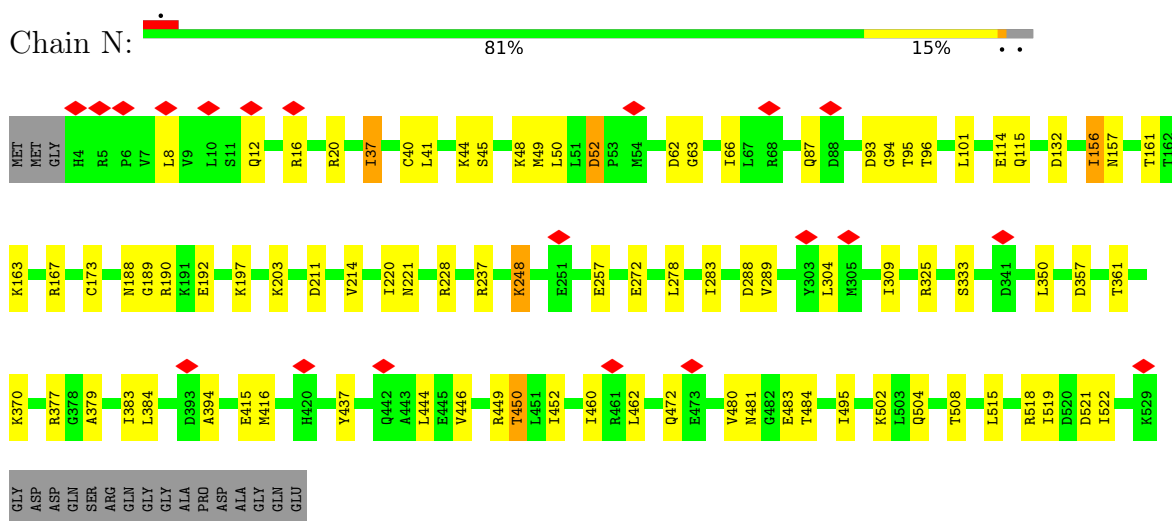
• Molecule 3: T-complex protein 1 subunit eta



• Molecule 4: T-complex protein 1 subunit gamma



• Molecule 4: T-complex protein 1 subunit gamma



Chain E:

6% 83% 15%

..

SER MET GLY T4 L5 A6 F7 K18 D19 Q20 D21 R22 G28 L29 L32 K33 L36 K40 G51 P52 D56 K57 M58 D63 G64 D65 V66 N70 D71 L76 D82 V90 D97 G101 D102 G103 T104 T105 L110 L114 L115 D123 R130 I143 I149 S150 D151 L154 V155 D156 I157 K158 D159 L171 G172 S173 V176 R216 V226 D229 K230 D231 F232 S233 H234 Q235 T236 V241 E242 K245 T246 L249 T250 H262 K263 I267 A295 R296 L297 V323 I328 E329 L330 I331 T335 F353 A354 G355 L356 V357 D357 L370 V371 I372 E373 Q374 R379 R398 D402 C405 M409 R415 G420 A435 D436 P439 E442 Q443 R447 L456 L460 I469 G470 T471 Q479 M483 A484 P485 I489 D490 C491 L492 H493 T496

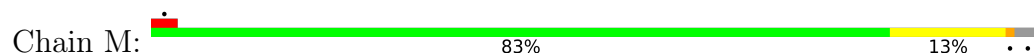
Chain e:

6% 83% 16%

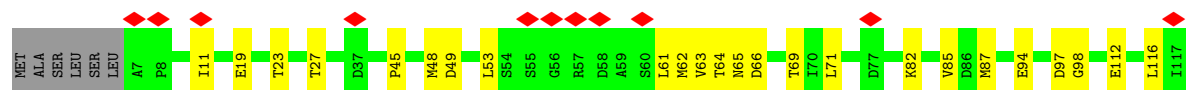
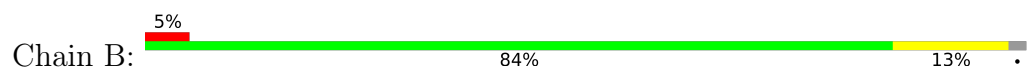
Chain I:



• Molecule 6: T-complex protein 1 subunit delta

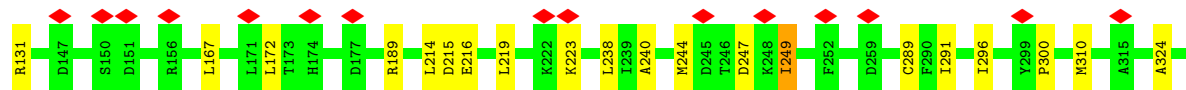
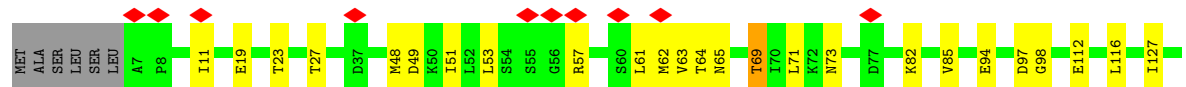
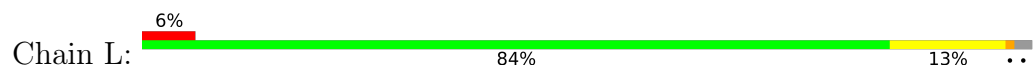


• Molecule 7: T-complex protein 1 subunit beta

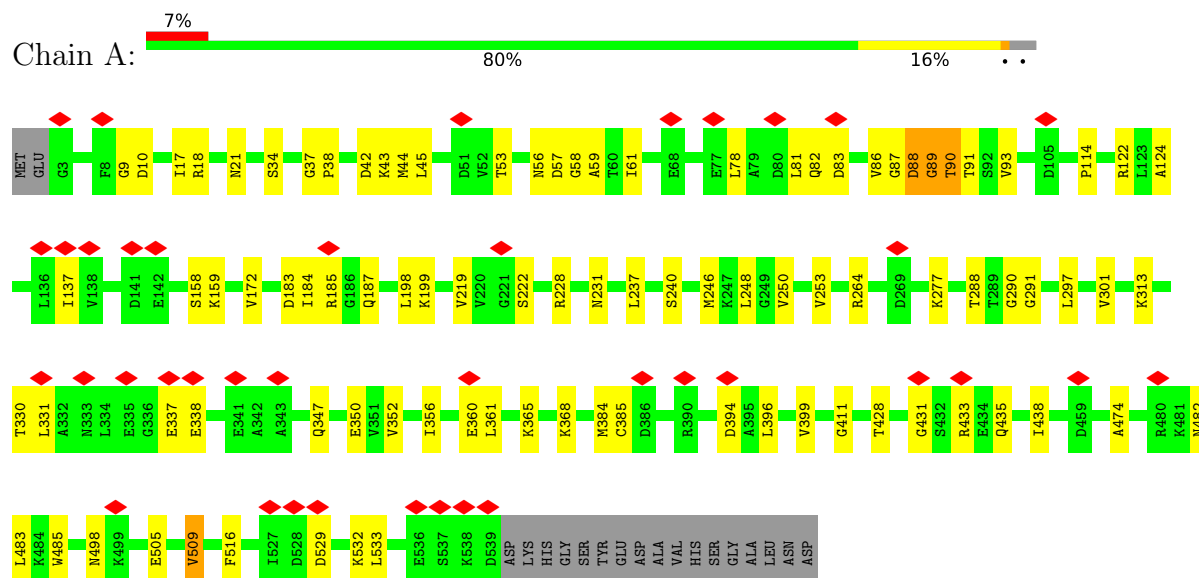


PRO
CYS

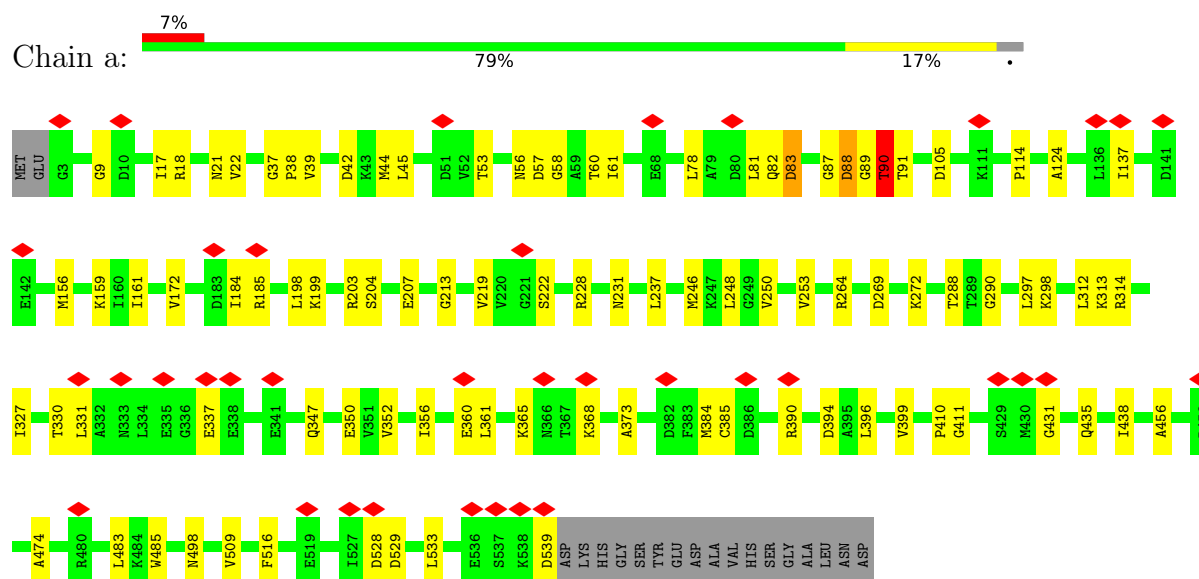
• Molecule 7: T-complex protein 1 subunit beta



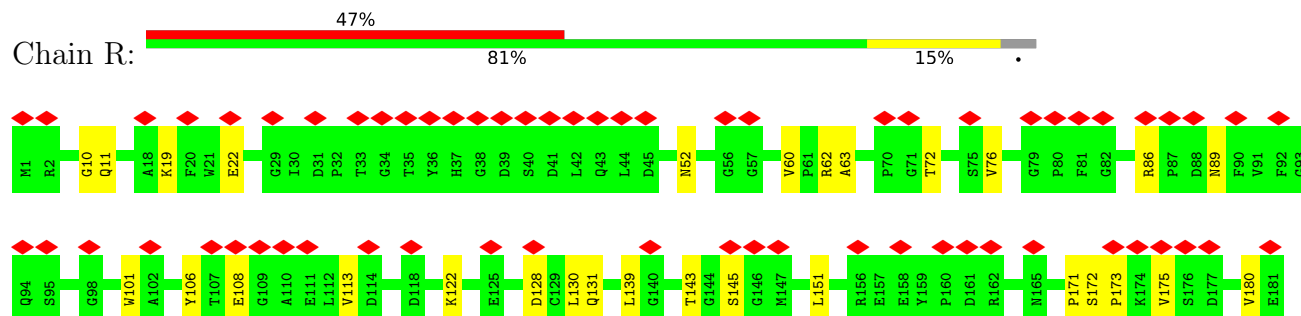
- Molecule 8: T-complex protein 1 subunit alpha

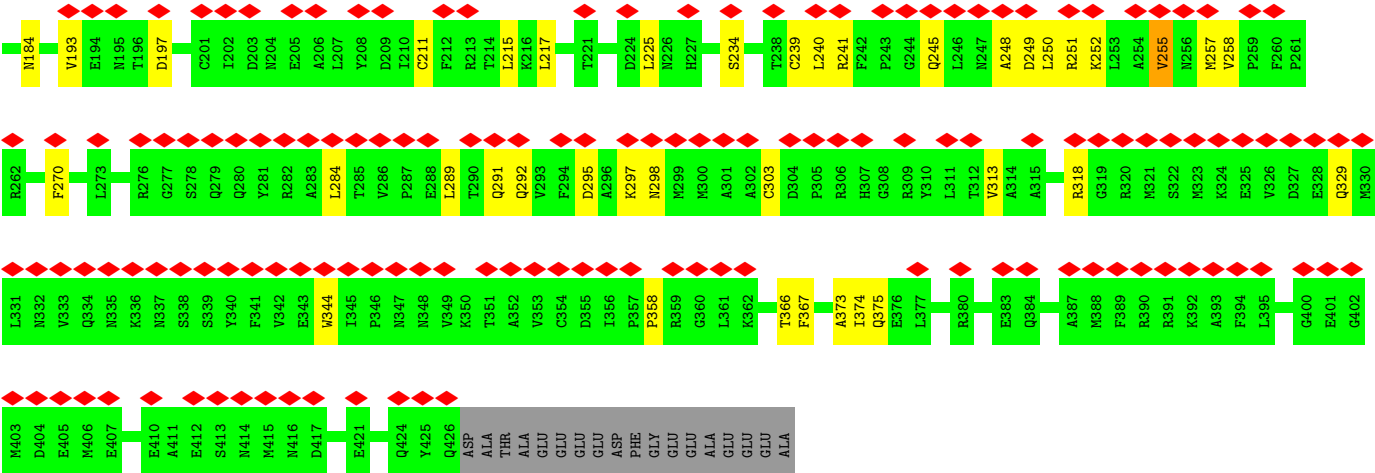


- Molecule 8: T-complex protein 1 subunit alpha



- 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, MG, AF3

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	4/4069 (0.1%)	0.34	1/5486 (0.0%)
1	z	0.23	2/4069 (0.0%)	0.33	0/5486
2	J	0.11	0/4066	0.33	0/5498
2	P	0.28	2/4066 (0.0%)	0.35	1/5498 (0.0%)
3	H	0.35	5/4094 (0.1%)	0.38	3/5526 (0.1%)
3	O	0.36	6/4094 (0.1%)	0.36	2/5526 (0.0%)
4	G	0.11	0/4141	0.31	0/5585
4	N	0.11	0/4141	0.31	0/5585
5	E	0.25	3/4176 (0.1%)	0.38	4/5626 (0.1%)
5	e	0.12	0/4176	0.33	0/5626
6	I	0.30	3/3967 (0.1%)	0.35	2/5352 (0.0%)
6	M	0.34	3/3967 (0.1%)	0.38	2/5352 (0.0%)
7	B	0.12	0/3980	0.34	0/5365
7	L	0.12	0/3980	0.35	0/5365
8	A	0.32	4/4117 (0.1%)	0.41	4/5558 (0.1%)
8	a	0.30	4/4117 (0.1%)	0.38	0/5558
9	R	0.11	0/3421	0.30	0/4637
All	All	0.25	36/68641 (0.1%)	0.35	19/92629 (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 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	106	THR	CA-C	-12.25	1.36	1.52
6	I	106	THR	CA-C	-11.78	1.38	1.52
3	O	94	THR	CA-C	-11.71	1.37	1.52
2	P	102	ASN	CA-C	-11.38	1.38	1.52
3	H	90	VAL	C-O	-10.99	1.12	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	87	GLY	O-C-N	-9.10	114.21	122.77
6	M	105	GLY	CA-C-N	-8.59	105.13	121.54
6	M	105	GLY	C-N-CA	-8.59	105.13	121.54
3	O	93	GLY	CA-C-N	-6.96	108.26	121.54
3	O	93	GLY	C-N-CA	-6.96	108.26	121.54

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](#)

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	K	4022	0	4161	60	0
1	z	4022	0	4161	60	0
2	J	4008	0	4067	68	0
2	P	4008	0	4068	61	0
3	H	4037	0	4140	51	0
3	O	4037	0	4141	80	0
4	G	4094	0	4233	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	4094	0	4234	81	0
5	E	4126	0	4236	50	0
5	e	4126	0	4236	51	0
6	I	3935	0	4144	61	0
6	M	3935	0	4144	61	0
7	B	3937	0	4055	45	0
7	L	3937	0	4055	43	0
8	A	4077	0	4235	77	0
8	a	4077	0	4235	71	0
9	R	3346	0	3239	32	0
10	A	27	0	12	18	0
10	B	27	0	11	7	0
10	E	27	0	12	7	0
10	G	27	0	12	30	0
10	H	27	0	12	14	0
10	I	27	0	12	15	0
10	J	27	0	12	18	0
10	K	27	0	12	11	0
10	L	27	0	11	7	0
10	M	27	0	12	13	0
10	N	27	0	12	28	0
10	O	27	0	12	17	0
10	P	27	0	12	13	0
10	a	27	0	12	7	0
10	e	27	0	12	6	0
10	z	27	0	12	16	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	3	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
11	O	1	0	0	0	0
11	P	1	0	0	0	0
11	a	1	0	0	0	0
11	e	1	0	0	0	0
11	z	1	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	4	0	0	2	0
12	B	4	0	0	4	0
12	E	4	0	0	2	0
12	G	4	0	0	2	0
12	H	4	0	0	2	0
12	I	4	0	0	1	0
12	J	4	0	0	6	0
12	K	4	0	0	5	0
12	L	4	0	0	3	0
12	M	4	0	0	1	0
12	N	4	0	0	4	0
12	O	4	0	0	6	0
12	P	4	0	0	5	0
12	a	4	0	0	4	0
12	e	4	0	0	3	0
12	z	4	0	0	5	0
13	A	1	0	0	2	0
13	B	1	0	0	4	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	3	0
13	I	1	0	0	0	0
13	J	1	0	0	3	0
13	K	1	0	0	0	0
13	L	1	0	0	3	0
13	M	1	0	0	0	0
13	N	1	0	0	0	0
13	O	1	0	0	2	0
13	P	1	0	0	2	0
13	a	1	0	0	4	0
13	e	1	0	0	0	0
13	z	1	0	0	0	0
All	All	68346	0	69974	954	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 7.

The worst 5 of 954 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)
8:A:88:ASP:CB	8:A:88:ASP:CG	1.78	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:102:ASN:ND2	10:J:601:ADP:O1A	1.58	1.35
8:A:89:GLY:CA	10:A:601:ADP:O3B	1.76	1.32
8:A:90:THR:N	10:A:601:ADP:O3B	1.63	1.30
6:I:105:GLY:HA2	10:I:601:ADP:O3B	1.30	1.30

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	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%)	43	73
8	a	535/556 (96%)	511 (96%)	23 (4%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	419 (96%)	18 (4%)	27	59
1	z	437/442 (99%)	424 (97%)	13 (3%)	36	65
2	J	433/452 (96%)	414 (96%)	19 (4%)	25	56
2	P	433/452 (96%)	414 (96%)	19 (4%)	25	56
3	H	433/443 (98%)	417 (96%)	16 (4%)	30	61
3	O	433/443 (98%)	421 (97%)	12 (3%)	38	66
4	G	457/469 (97%)	444 (97%)	13 (3%)	38	66
4	N	457/469 (97%)	442 (97%)	15 (3%)	33	63
5	E	452/455 (99%)	435 (96%)	17 (4%)	29	60
5	e	452/455 (99%)	433 (96%)	19 (4%)	26	58
6	I	443/452 (98%)	423 (96%)	20 (4%)	24	56
6	M	443/452 (98%)	425 (96%)	18 (4%)	27	59
7	B	416/427 (97%)	404 (97%)	12 (3%)	37	66
7	L	416/427 (97%)	404 (97%)	12 (3%)	37	66
8	A	448/463 (97%)	437 (98%)	11 (2%)	42	69
8	a	448/463 (97%)	436 (97%)	12 (3%)	39	67
9	R	366/379 (97%)	352 (96%)	14 (4%)	29	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7404/7585 (98%)	7144 (96%)	260 (4%)	32 62

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	M	42	LYS
6	M	203	VAL
6	I	314	LEU
6	I	241	VAL
6	M	328	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
9	R	137	HIS
1	z	434	GLN
7	L	502	GLN
8	a	242	GLN
9	R	292	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
10	ADP	B	601	11,12,7	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	e	603	10,5	0,3,3	-	-	-		
10	ADP	L	601	11,12,7	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	B	603	10,7	0,3,3	-	-	-		
12	AF3	z	603	10,1	0,3,3	-	-	-		
12	AF3	A	603	8,10	0,3,3	-	-	-		
10	ADP	O	603	11	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	M	603	6,10	0,3,3	-	-	-		
12	AF3	H	603	3,10	0,3,3	-	-	-		
10	ADP	N	601	11,12	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	J	601	11,2,12	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	K	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	P	603	10,2	0,3,3	-	-	-		
12	AF3	K	603	10,1	0,3,3	-	-	-		
10	ADP	I	601	11,12	27,29,29	1.32	4 (14%)	42,45,45	2.00	11 (26%)
12	AF3	a	603	8,10	0,3,3	-	-	-		
12	AF3	O	602	3	0,3,3	-	-	-		
10	ADP	E	601	11,12,5	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	M	601	11,12	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	A	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	2.02	11 (26%)
10	ADP	P	601	11,2,12	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	I	603	6,10	0,3,3	-	-	-		
12	AF3	J	603	10,2	0,3,3	-	-	-		
12	AF3	G	603	4,10	0,3,3	-	-	-		
12	AF3	L	603	10,7	0,3,3	-	-	-		
10	ADP	H	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	2.01	11 (26%)
12	AF3	E	603	10	0,3,3	-	-	-		
10	ADP	e	601	11,12,5	27,29,29	1.34	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	z	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	2.00	11 (26%)
10	ADP	a	601	11,8,12	27,29,29	1.33	4 (14%)	42,45,45	2.01	11 (26%)
10	ADP	G	601	11,12	27,29,29	1.33	4 (14%)	42,45,45	2.03	11 (26%)
12	AF3	N	603	4,10	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	N	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	M	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	K	601	11,12	-	0/16/32/32	0/3/3/3
10	ADP	B	601	11,12,7	-	2/16/32/32	0/3/3/3
10	ADP	e	601	11,12,5	-	1/16/32/32	0/3/3/3
10	ADP	A	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	a	601	11,8,12	-	1/16/32/32	0/3/3/3
10	ADP	P	601	11,2,12	-	1/16/32/32	0/3/3/3
10	ADP	L	601	11,12,7	-	1/16/32/32	0/3/3/3
10	ADP	I	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	H	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	z	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	J	601	11,2,12	-	2/16/32/32	0/3/3/3
10	ADP	O	603	11	-	1/16/32/32	0/3/3/3
10	ADP	G	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	E	601	11,12,5	-	2/16/32/32	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	601	ADP	C5-C4	4.38	1.47	1.39
10	A	601	ADP	C5-C4	4.36	1.47	1.39
10	L	601	ADP	C5-C4	4.35	1.47	1.39
10	G	601	ADP	C5-C4	4.35	1.47	1.39
10	B	601	ADP	C5-C4	4.35	1.47	1.39

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	601	ADP	C5-C4-N3	-6.24	118.61	126.75
10	A	601	ADP	C5-C4-N3	-6.23	118.62	126.75
10	G	601	ADP	C5-C4-N3	-6.20	118.66	126.75
10	J	601	ADP	C5-C4-N3	-6.17	118.70	126.75
10	z	601	ADP	C5-C4-N3	-6.16	118.71	126.75

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

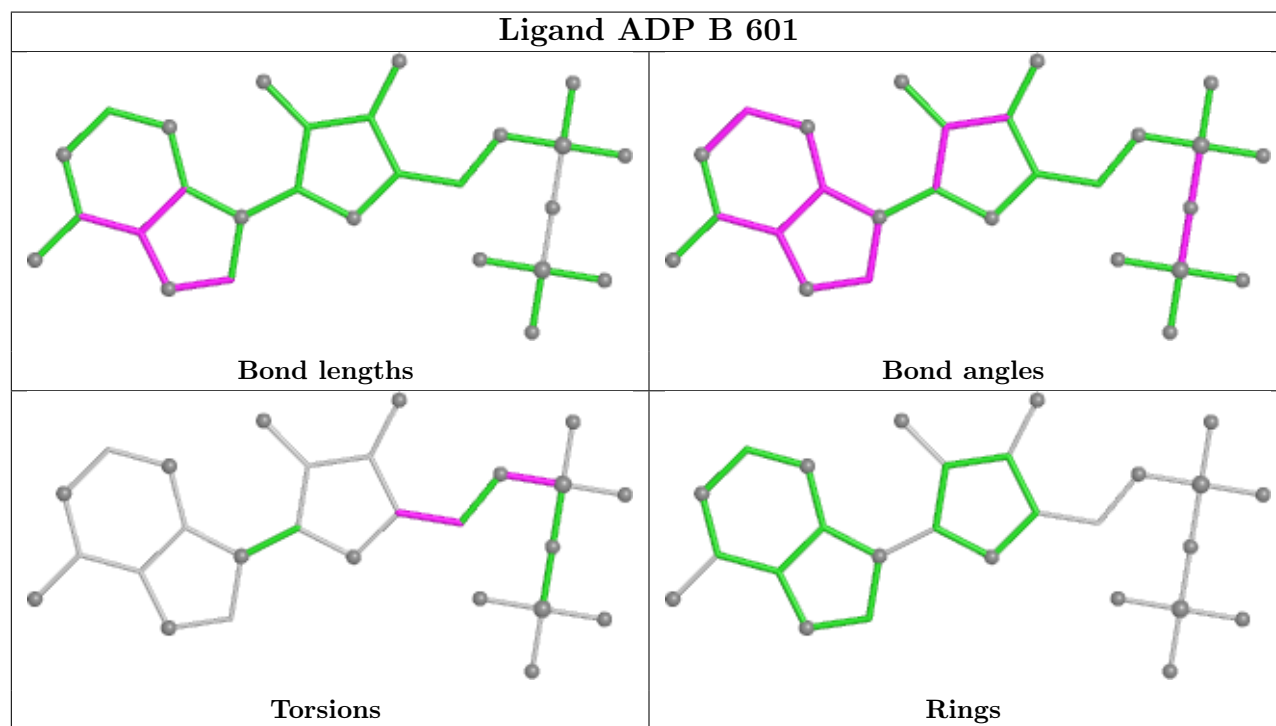
Mol	Chain	Res	Type	Atoms
10	J	601	ADP	C5'-O5'-PA-O1A
10	H	601	ADP	C5'-O5'-PA-O1A
10	G	601	ADP	C5'-O5'-PA-O1A
10	E	601	ADP	C5'-O5'-PA-O1A
10	I	601	ADP	C5'-O5'-PA-O1A

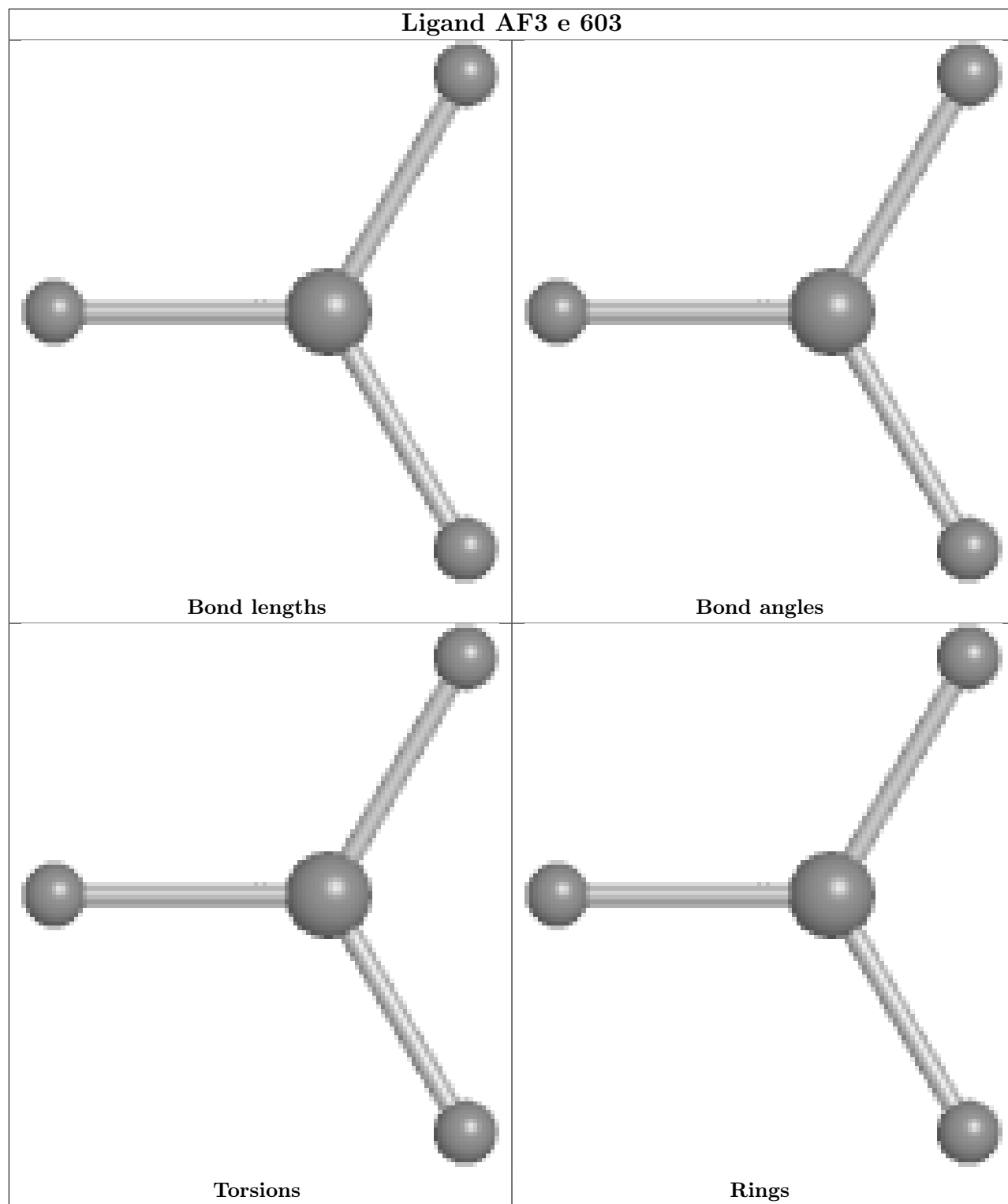
There are no ring outliers.

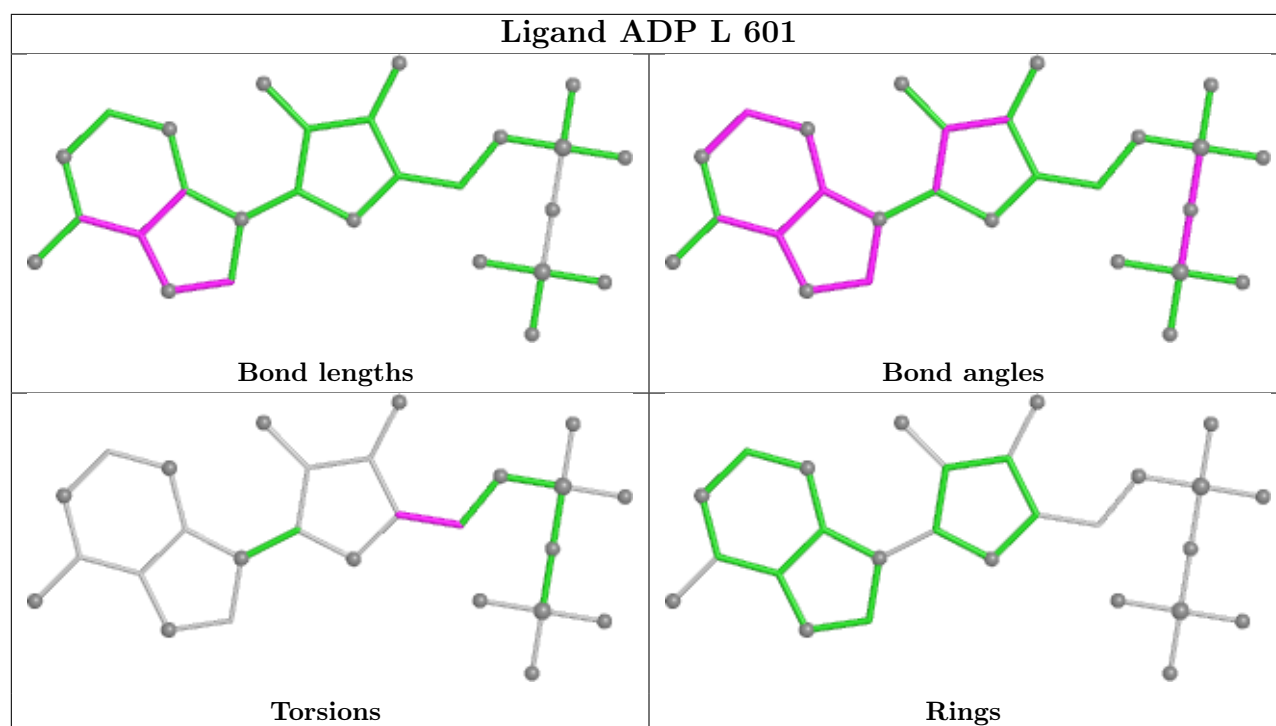
32 monomers are involved in 260 short contacts:

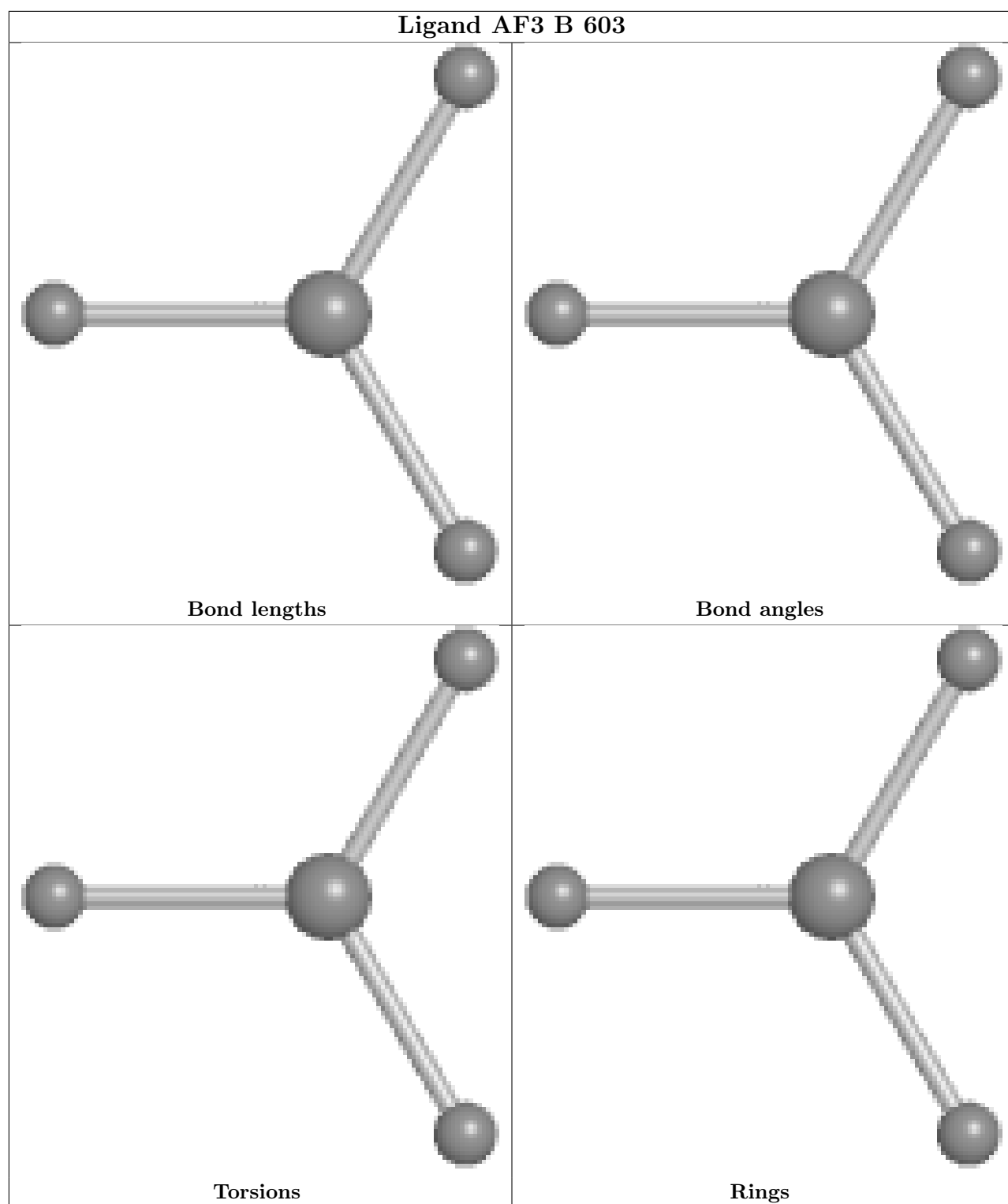
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	601	ADP	7	0
12	e	603	AF3	3	0
10	L	601	ADP	7	0
12	B	603	AF3	4	0
12	z	603	AF3	5	0
12	A	603	AF3	2	0
10	O	603	ADP	17	0
12	M	603	AF3	1	0
12	H	603	AF3	2	0
10	N	601	ADP	28	0
10	J	601	ADP	18	0
10	K	601	ADP	11	0
12	P	603	AF3	5	0
12	K	603	AF3	5	0
10	I	601	ADP	15	0
12	a	603	AF3	4	0
12	O	602	AF3	6	0
10	E	601	ADP	7	0
10	M	601	ADP	13	0
10	A	601	ADP	18	0
10	P	601	ADP	13	0
12	I	603	AF3	1	0
12	J	603	AF3	6	0
12	G	603	AF3	2	0
12	L	603	AF3	3	0
10	H	601	ADP	14	0
12	E	603	AF3	2	0
10	e	601	ADP	6	0
10	z	601	ADP	16	0
10	a	601	ADP	7	0
10	G	601	ADP	30	0
12	N	603	AF3	4	0

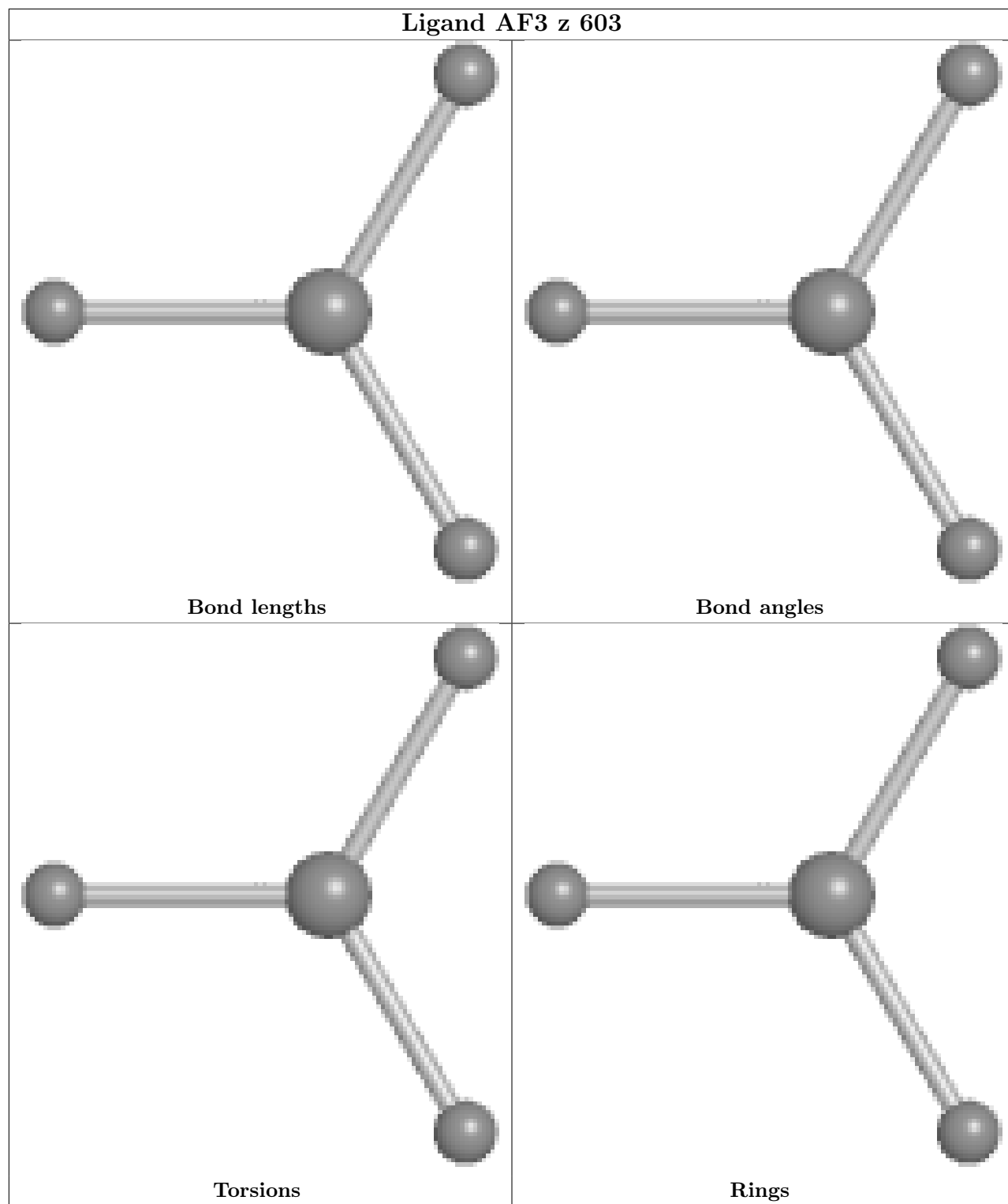
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

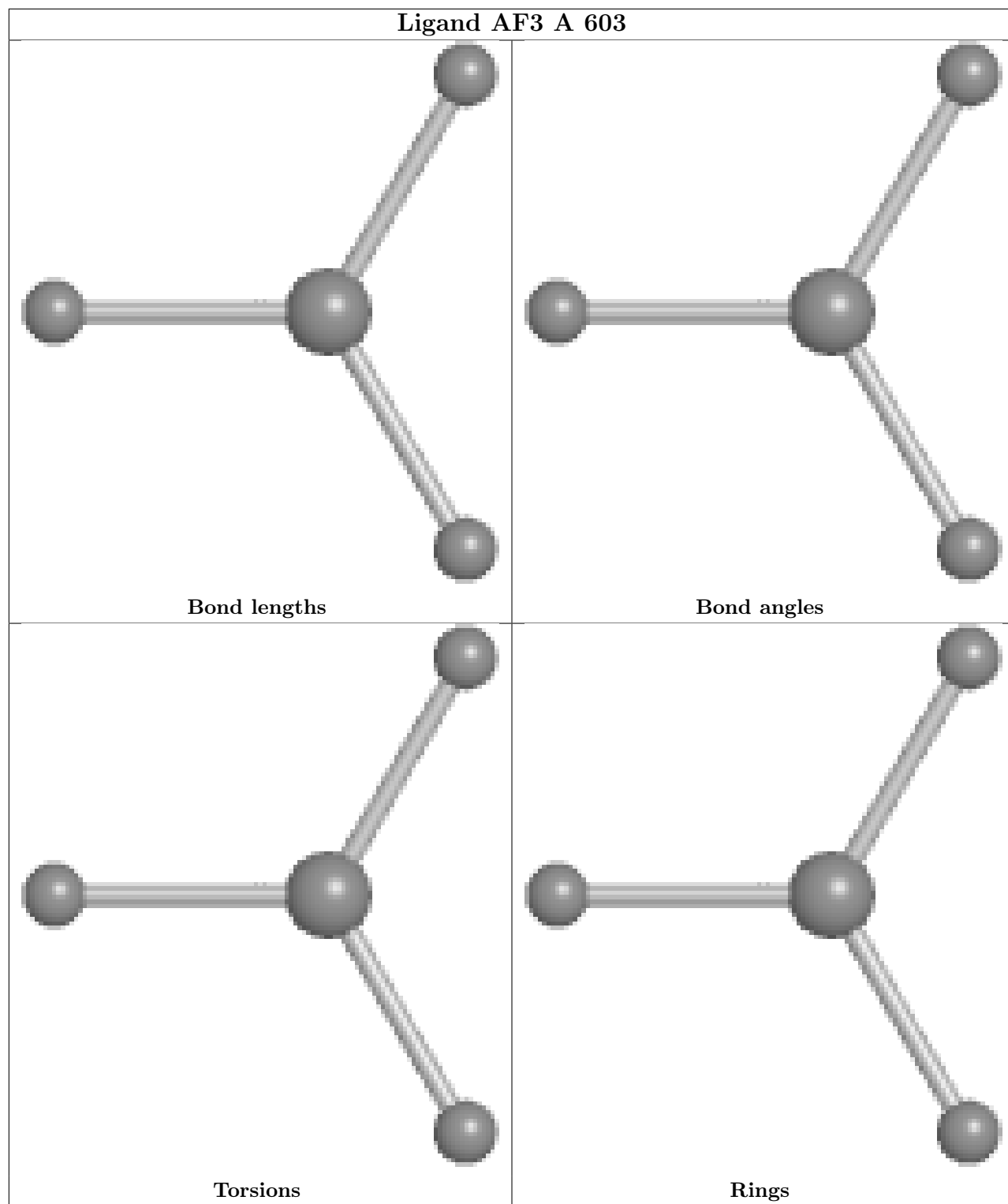


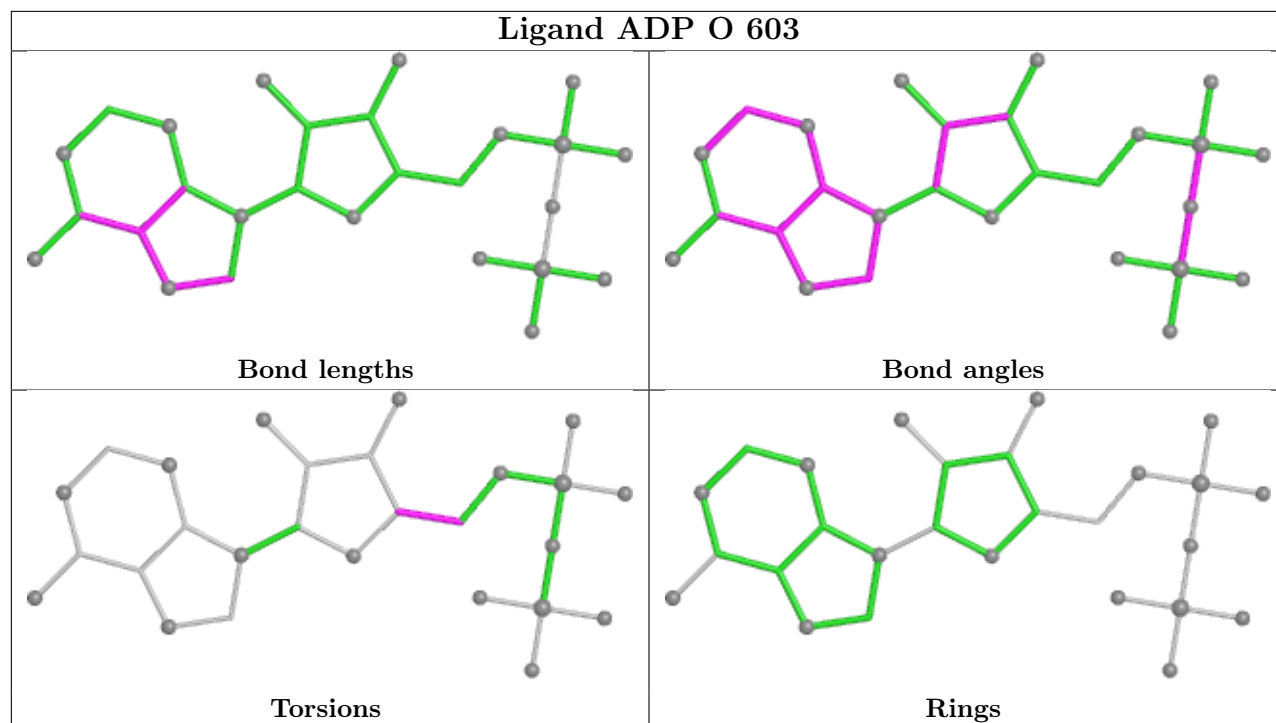


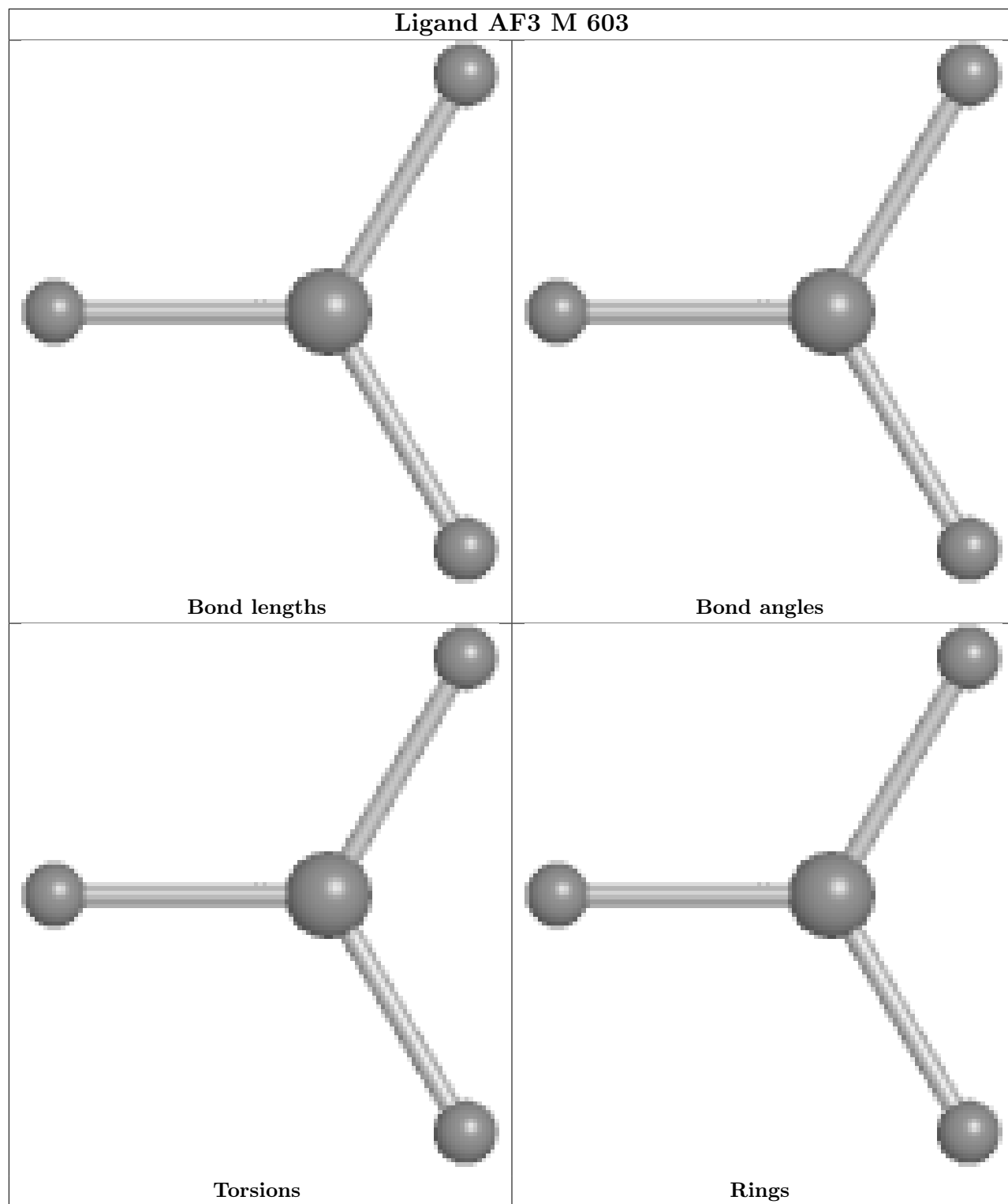


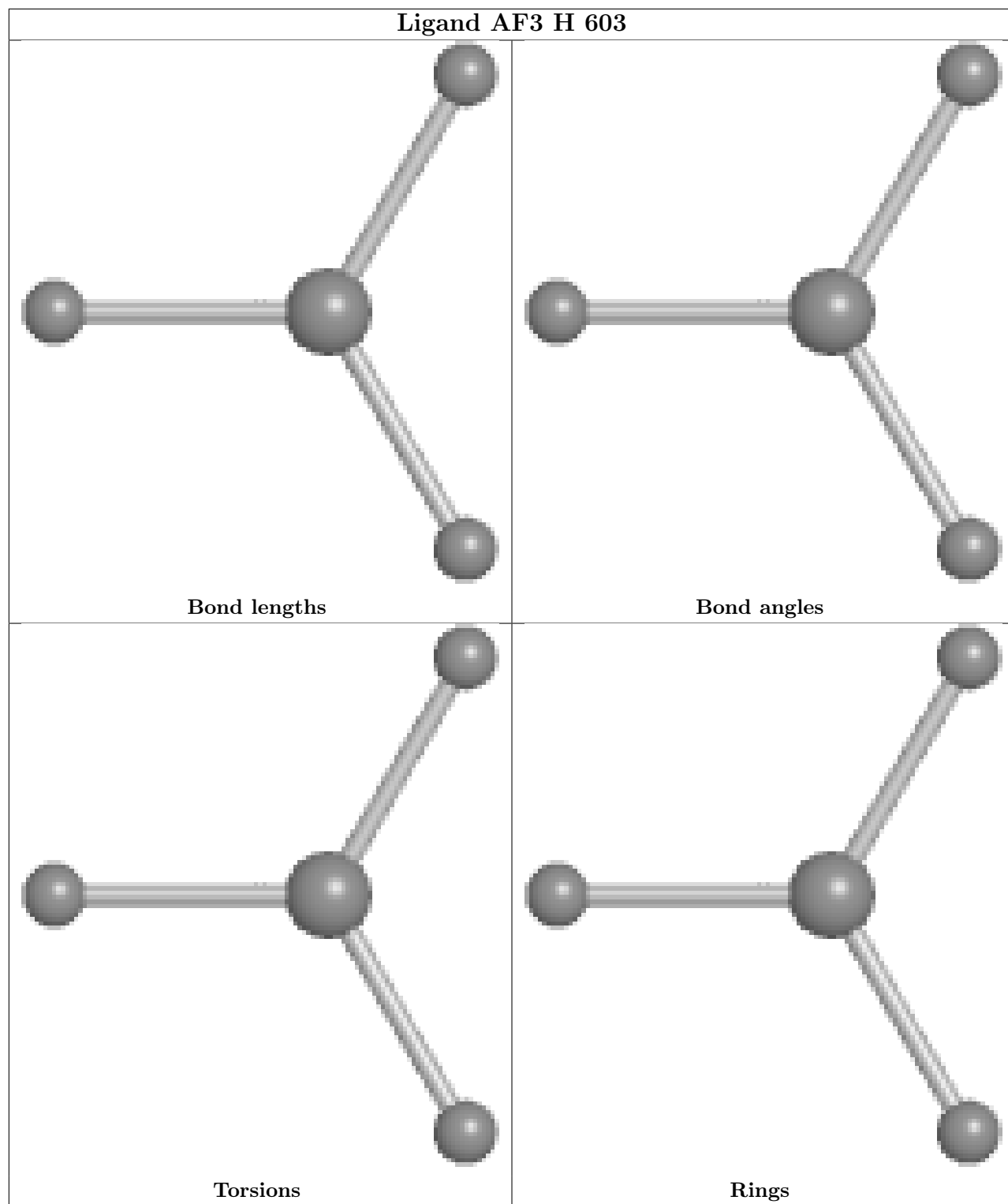


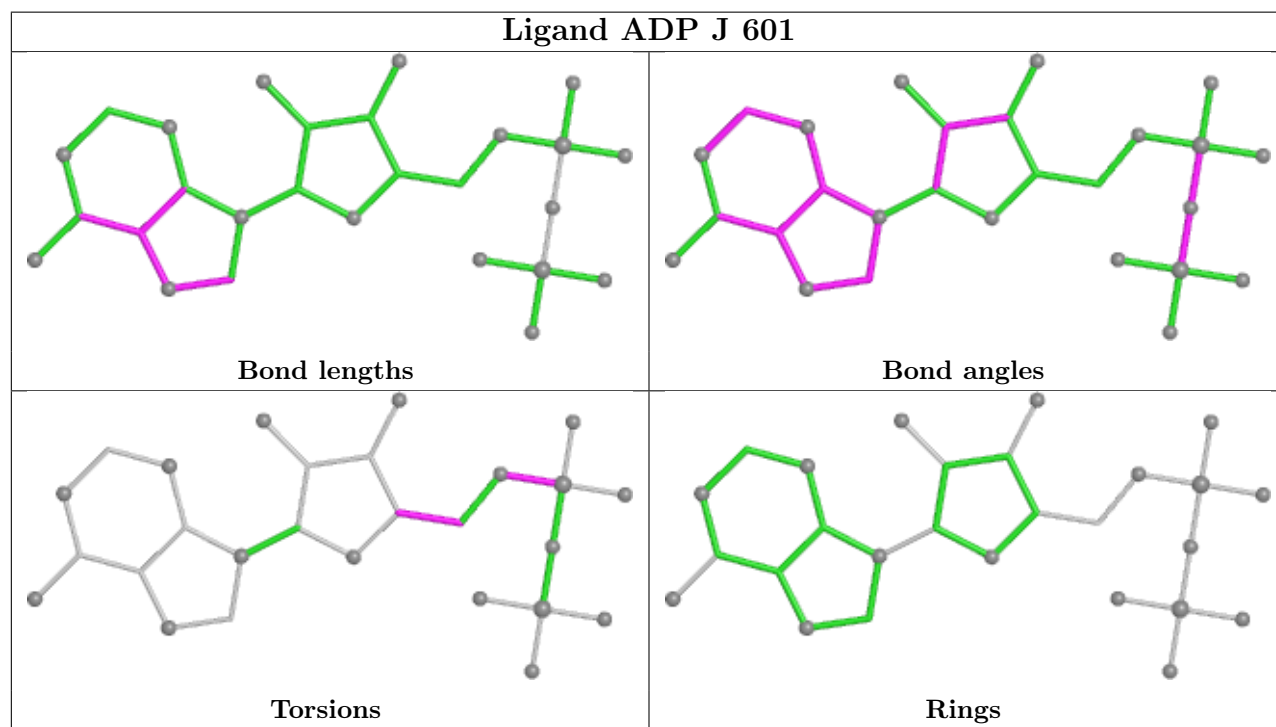
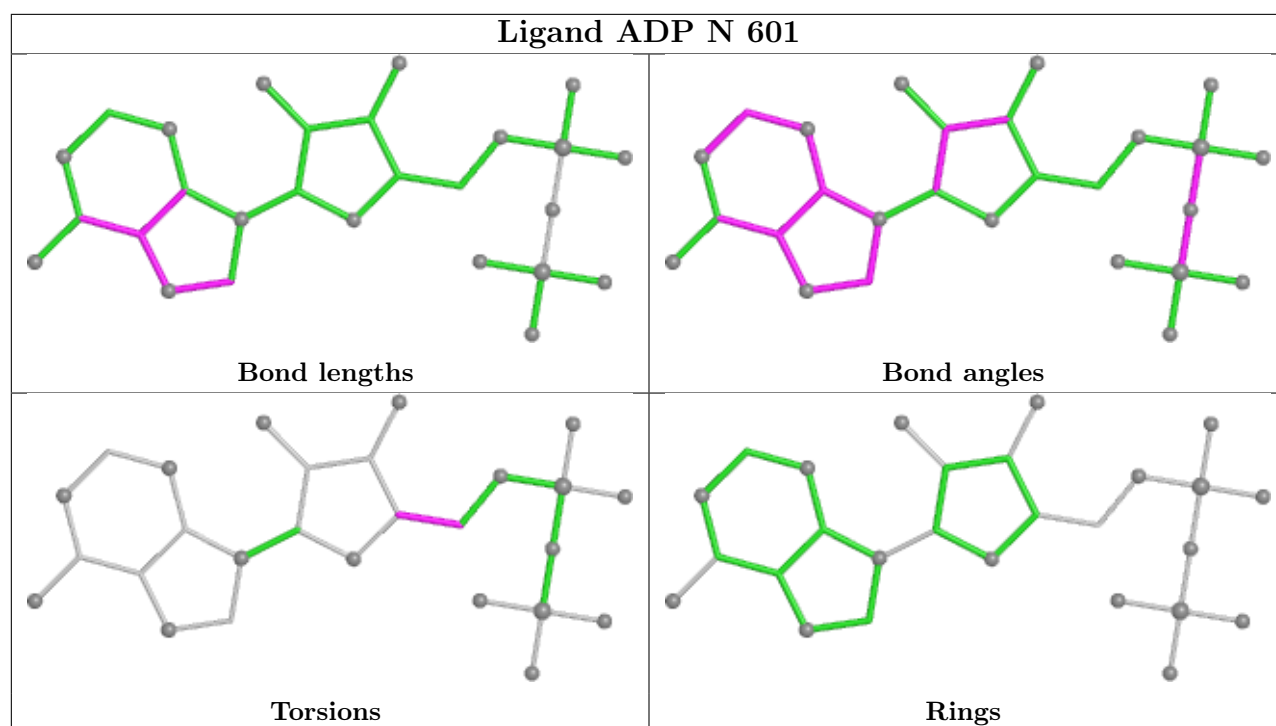


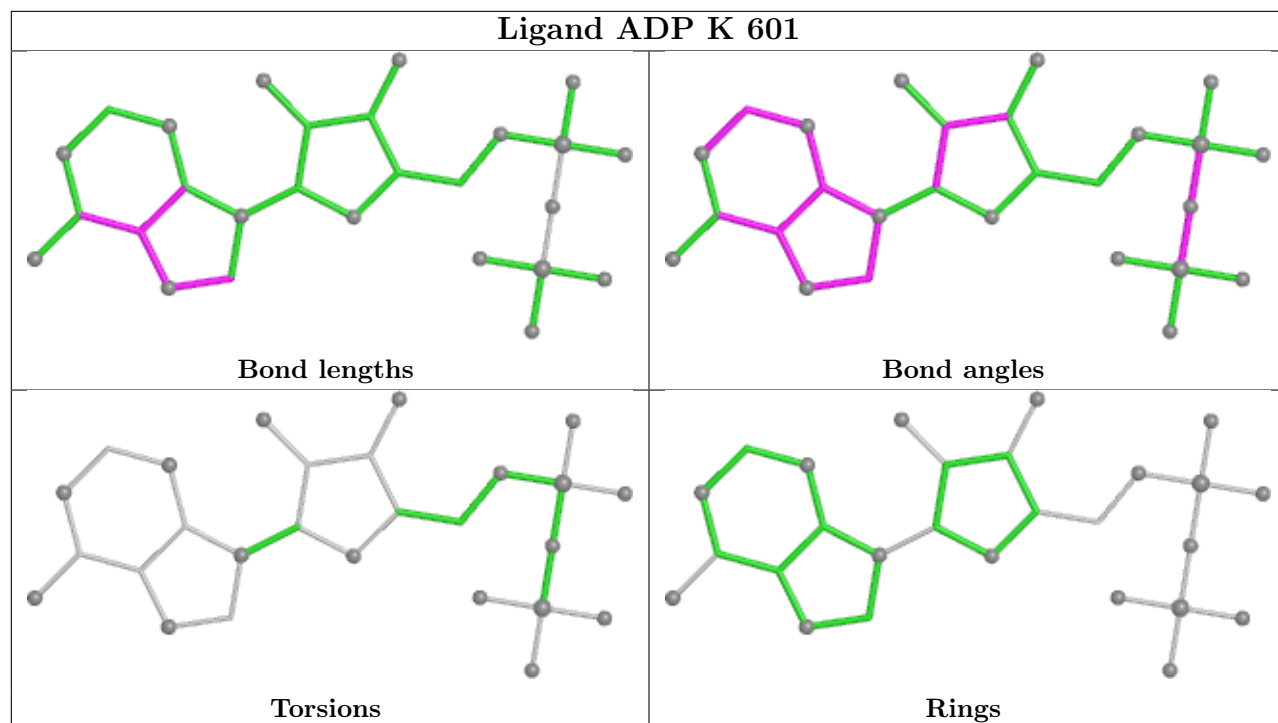


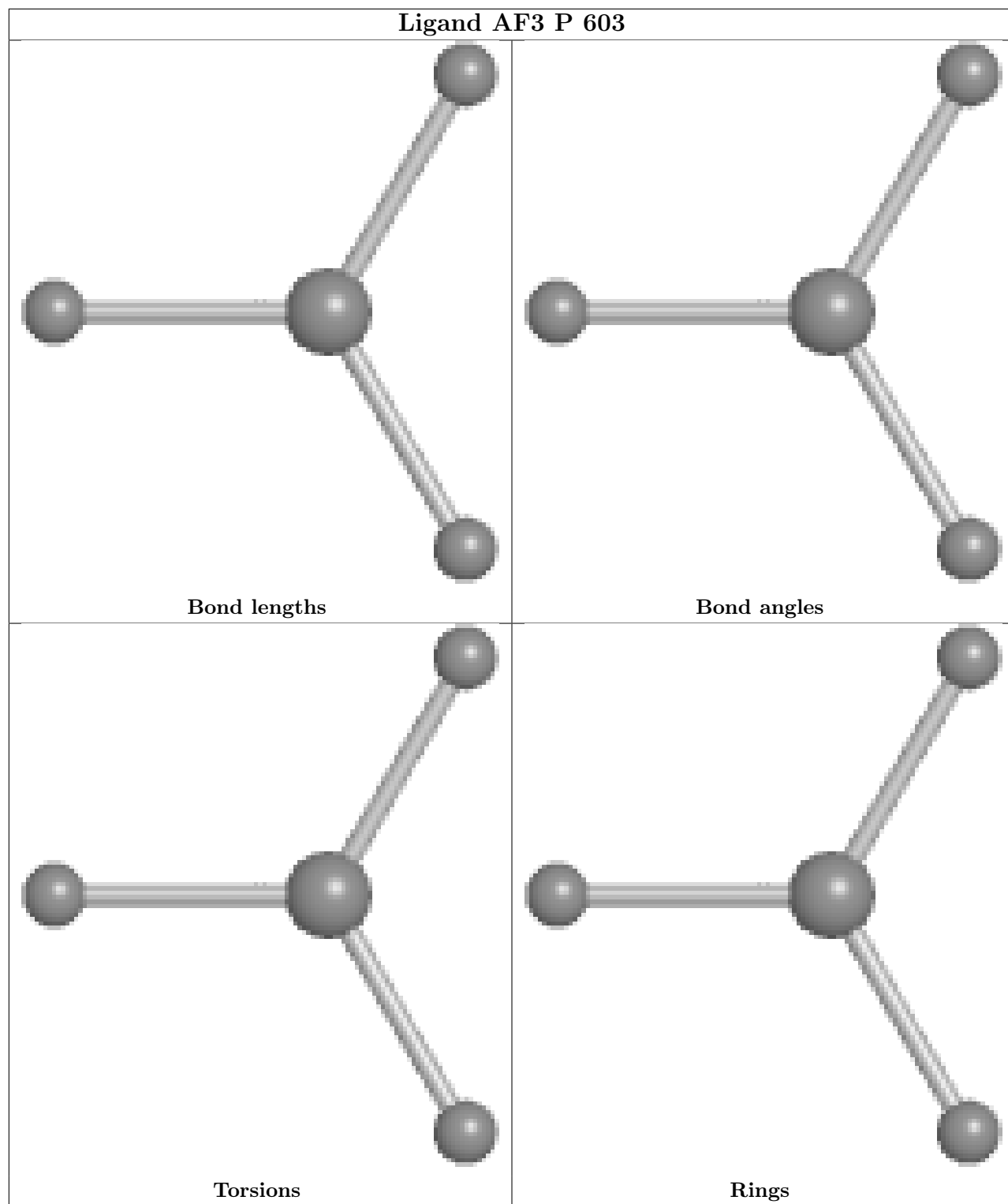


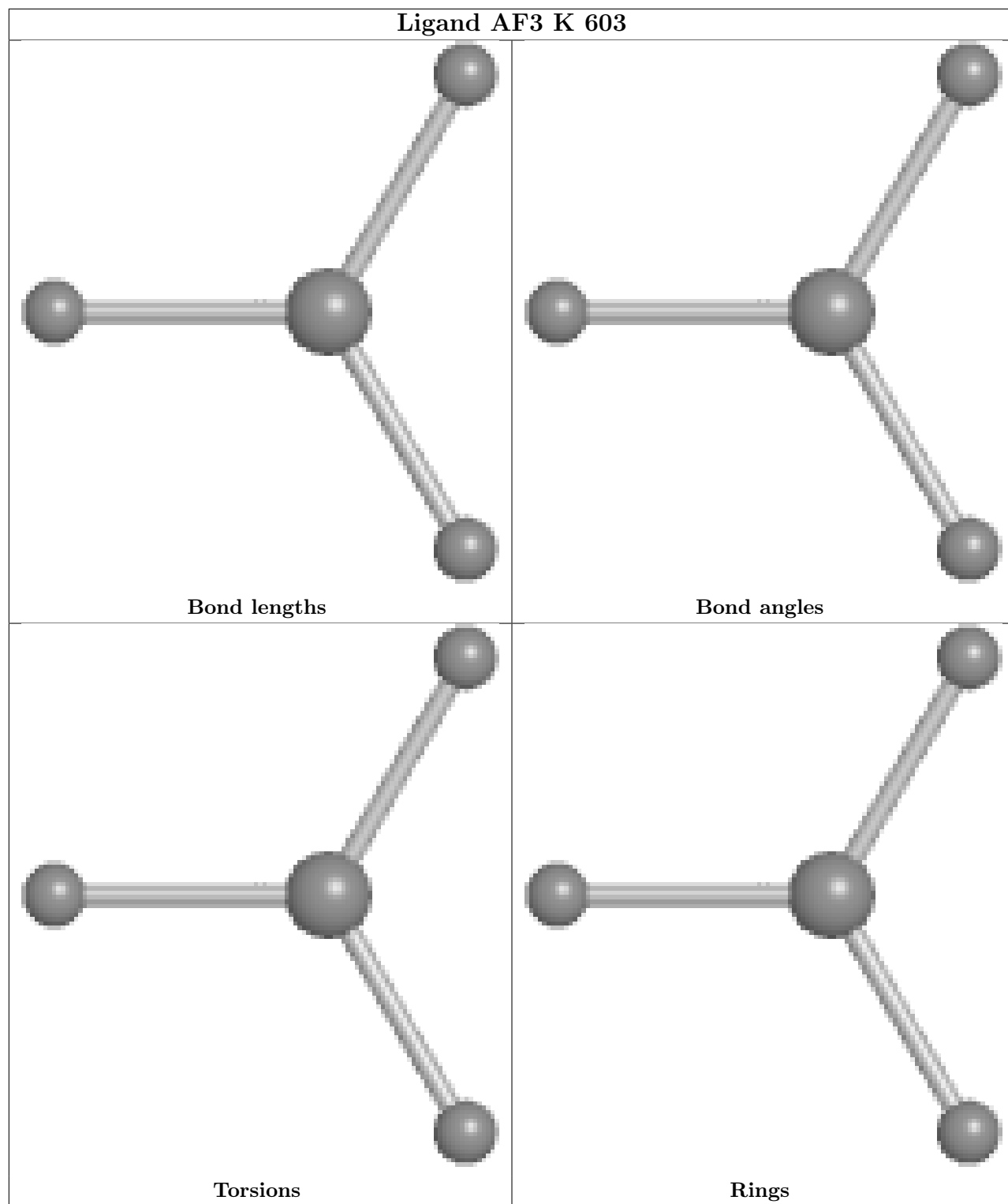


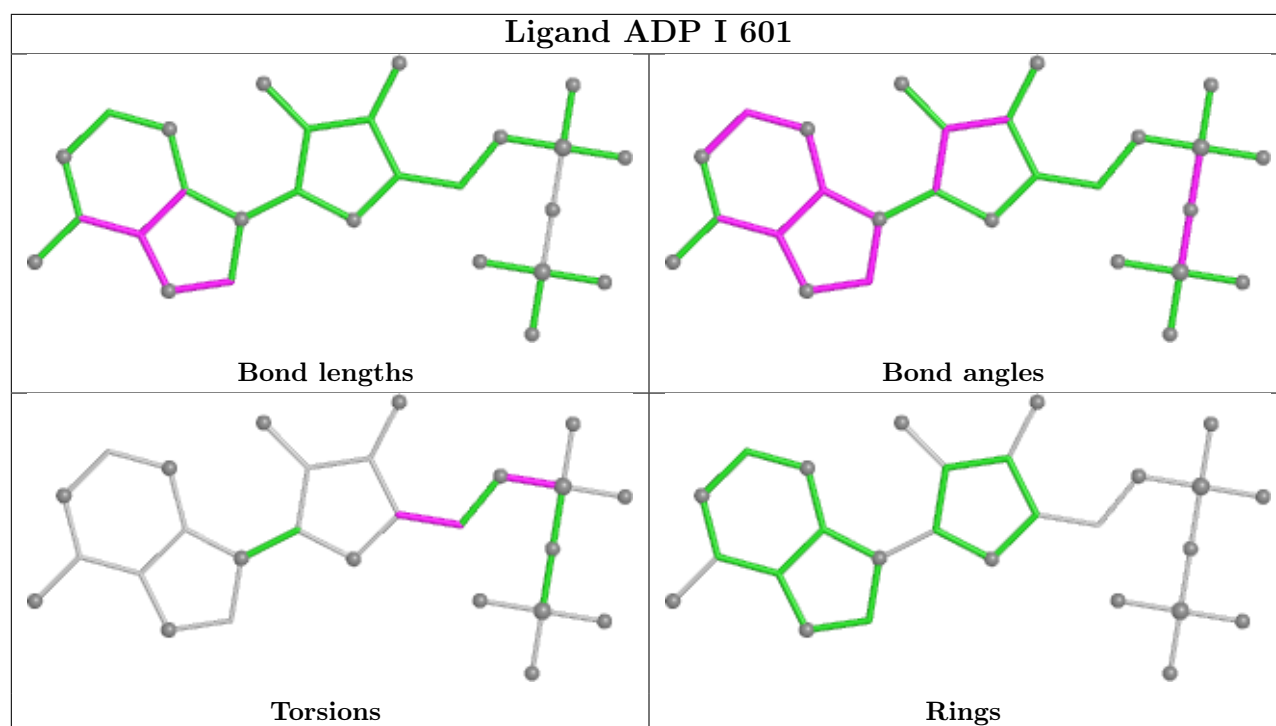


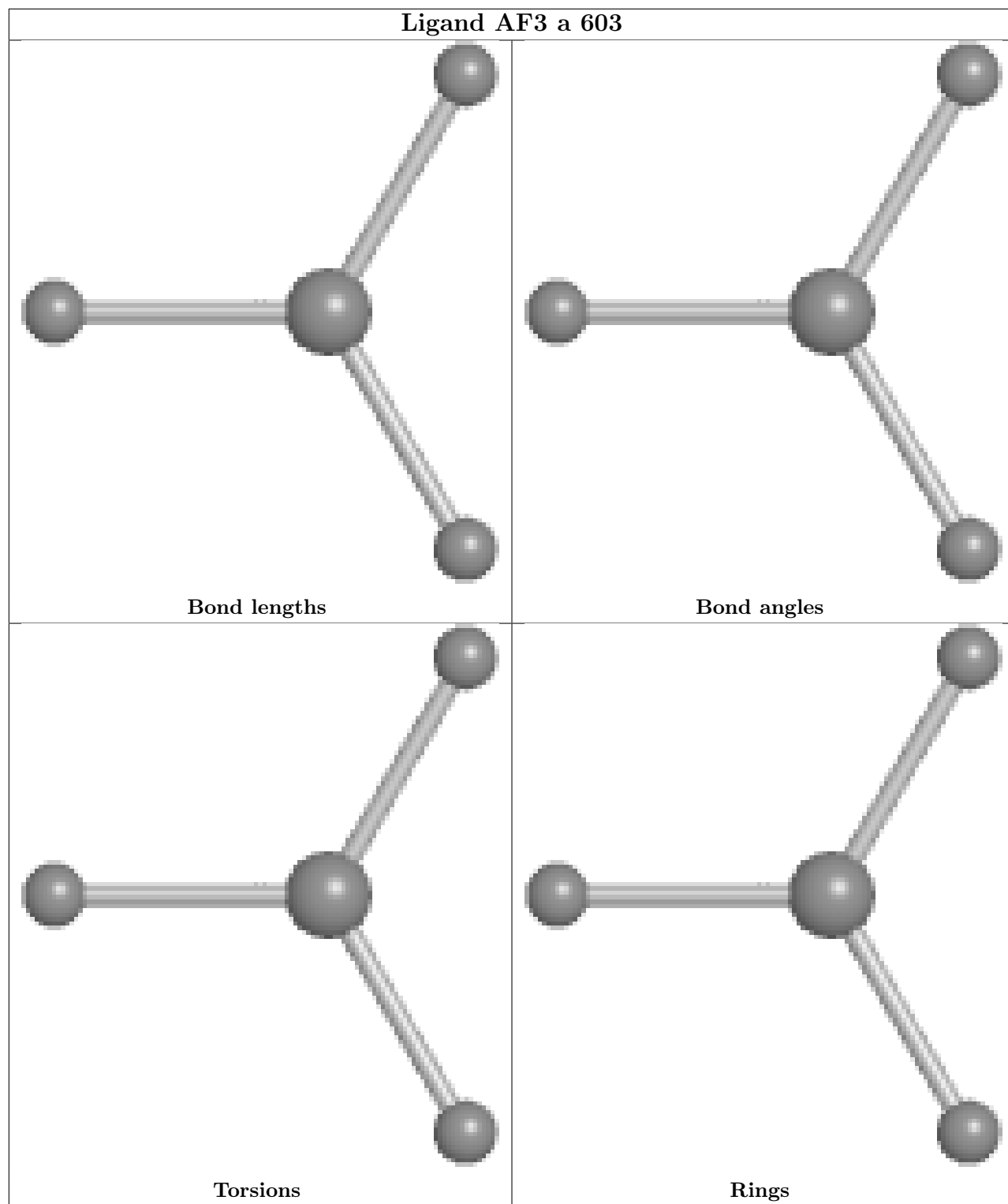


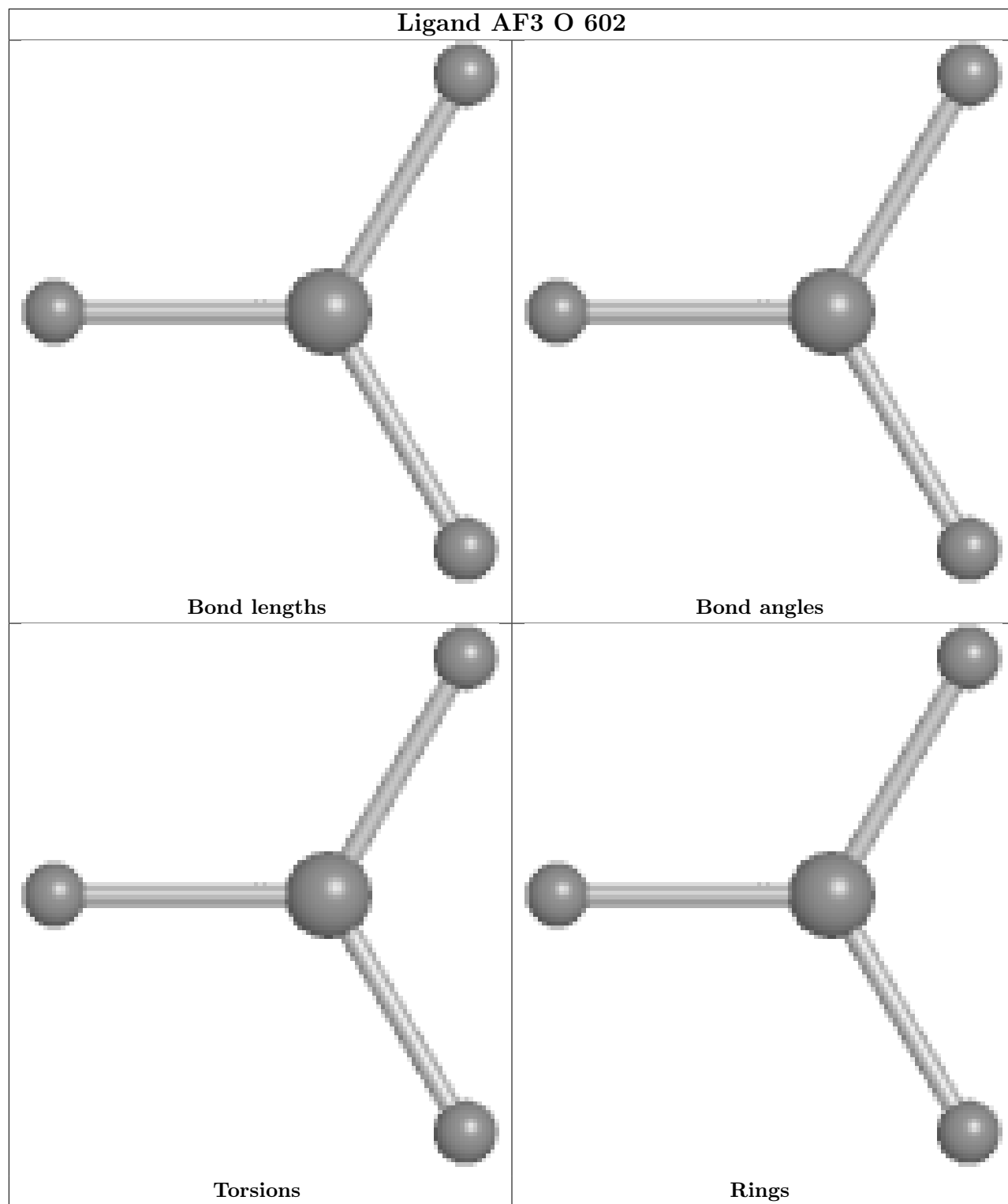


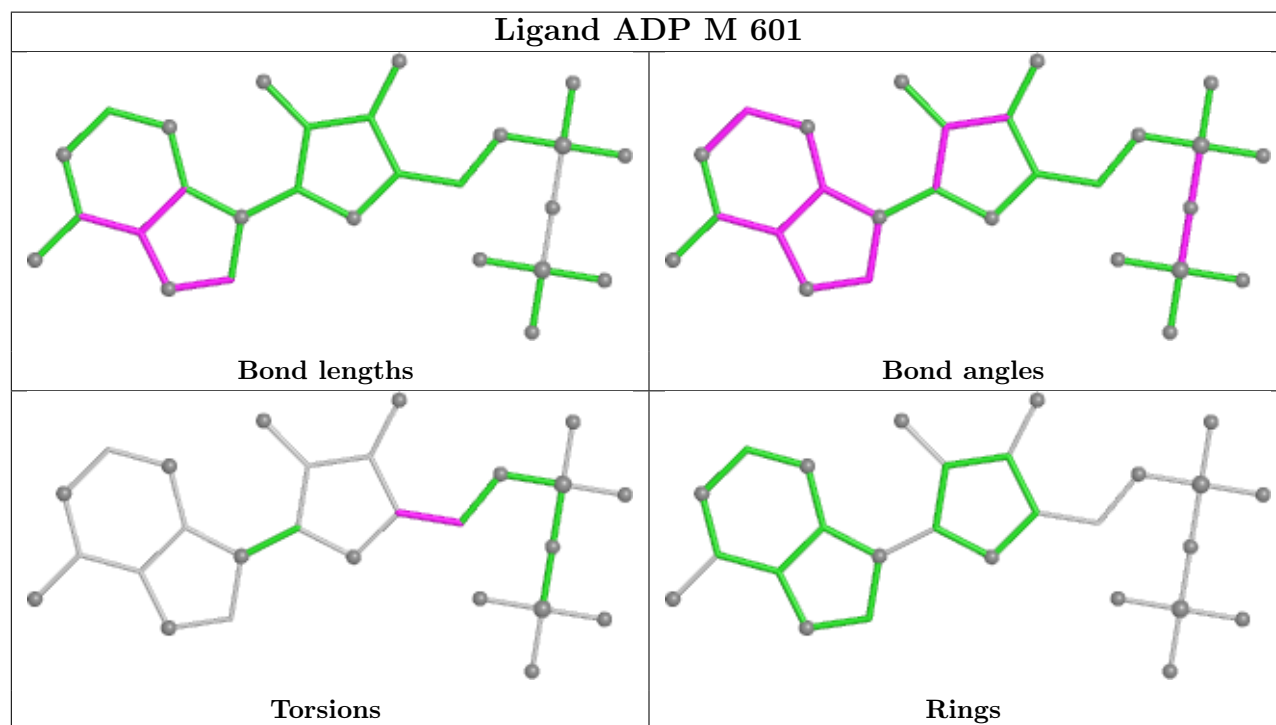
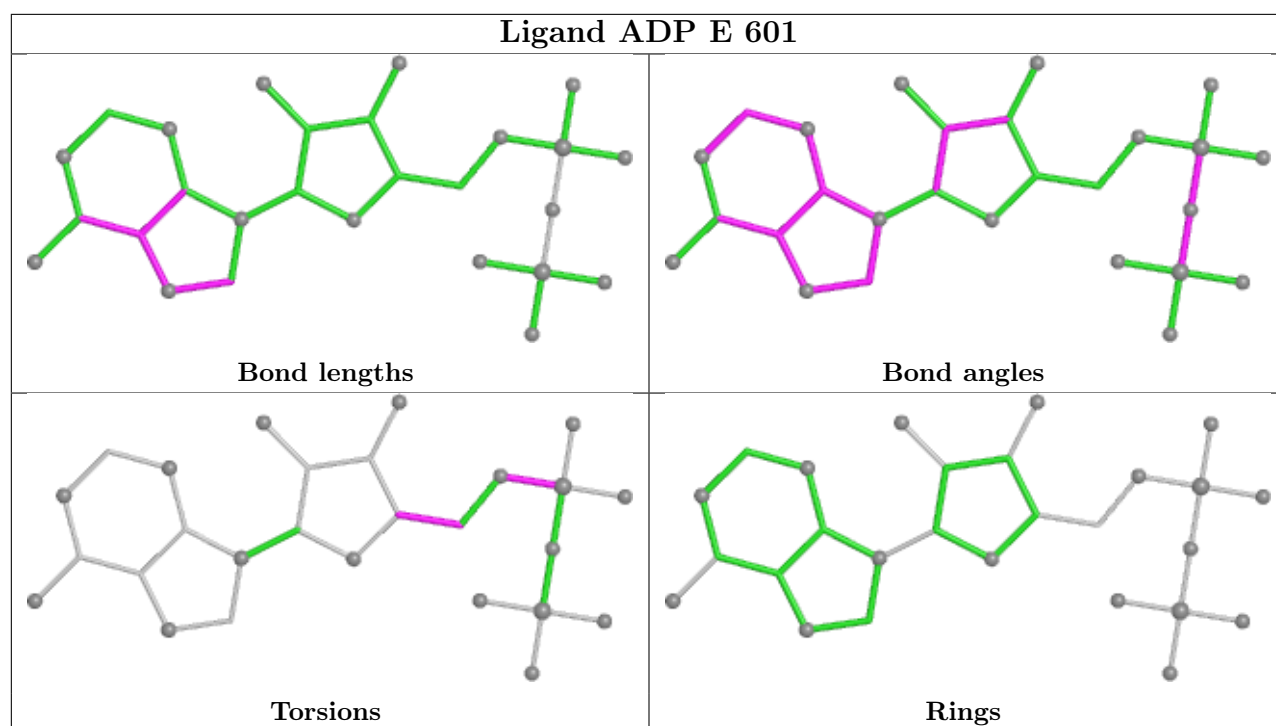


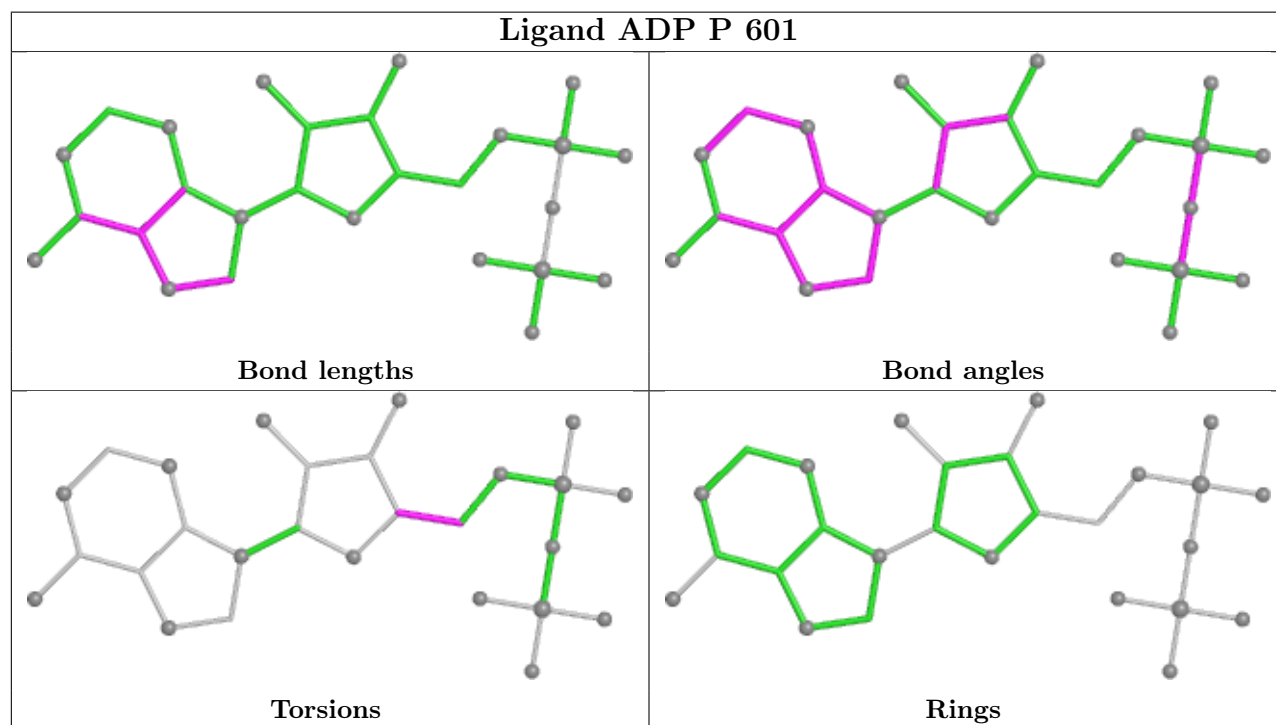
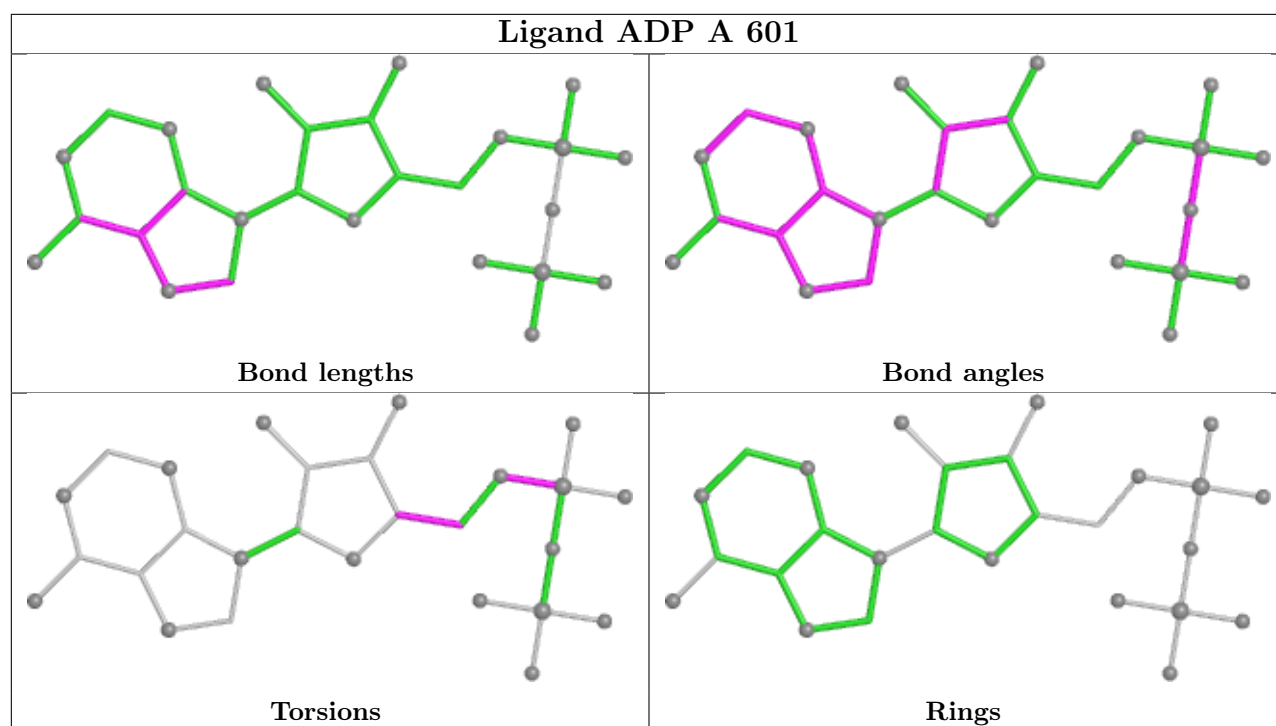


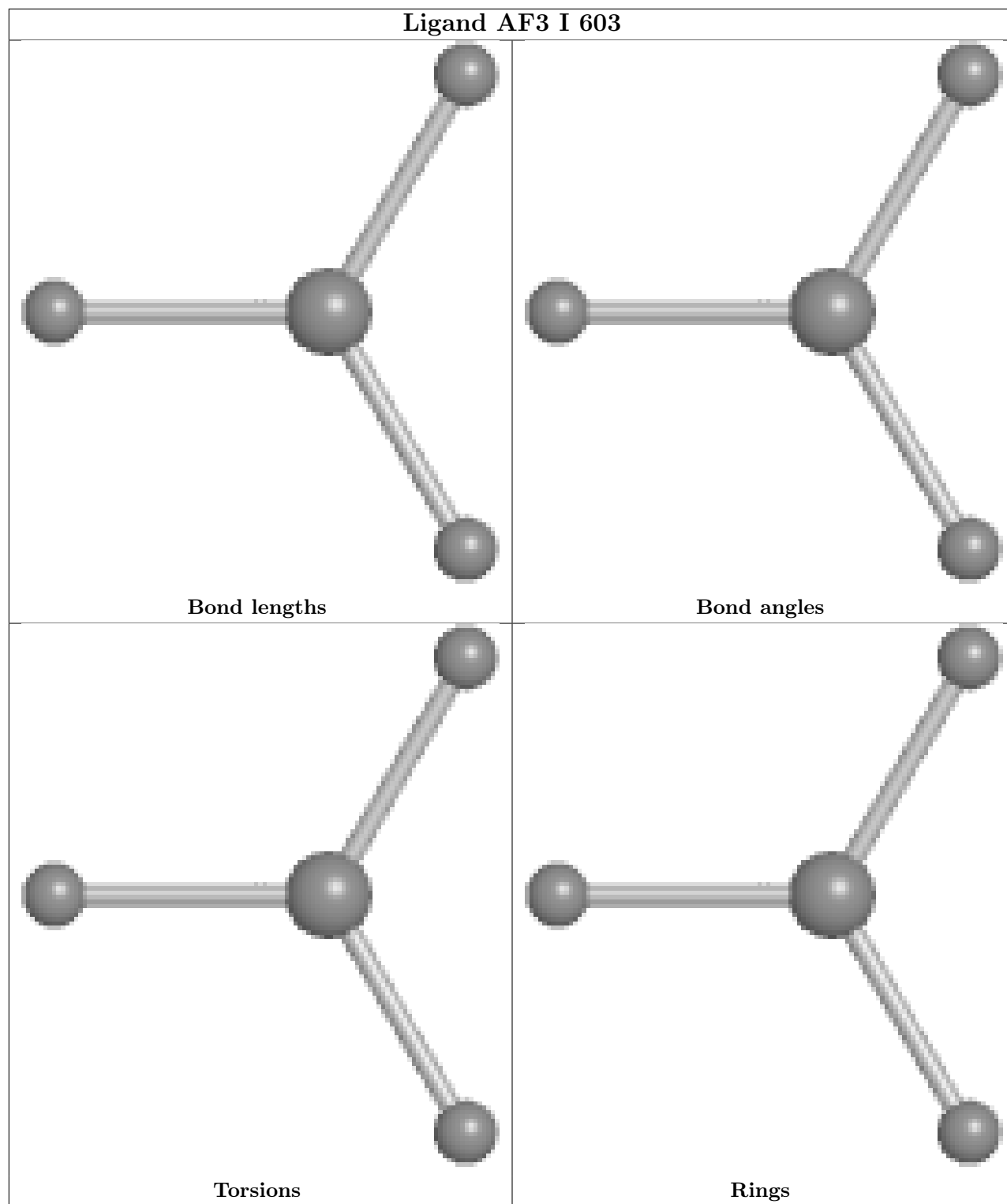


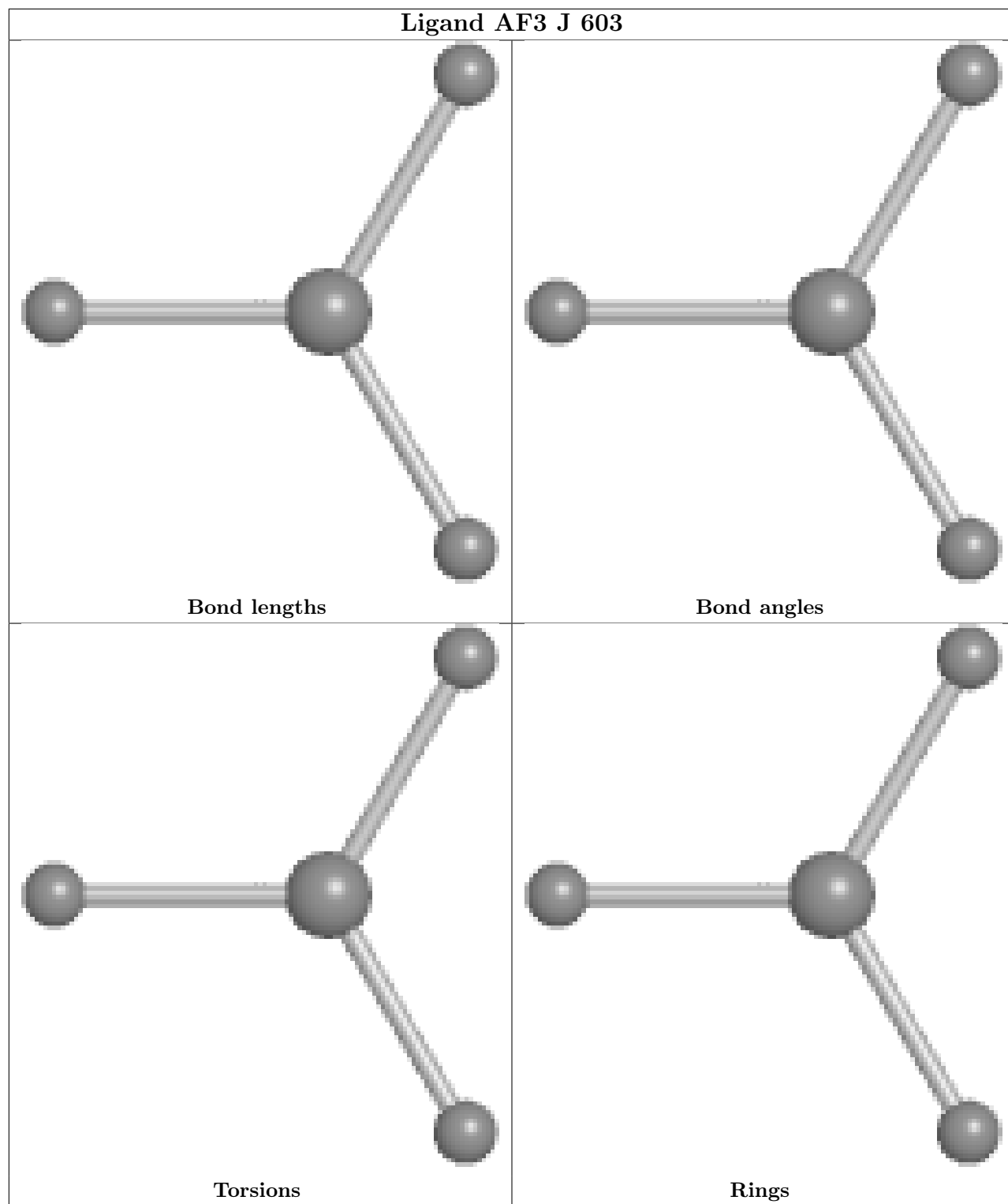


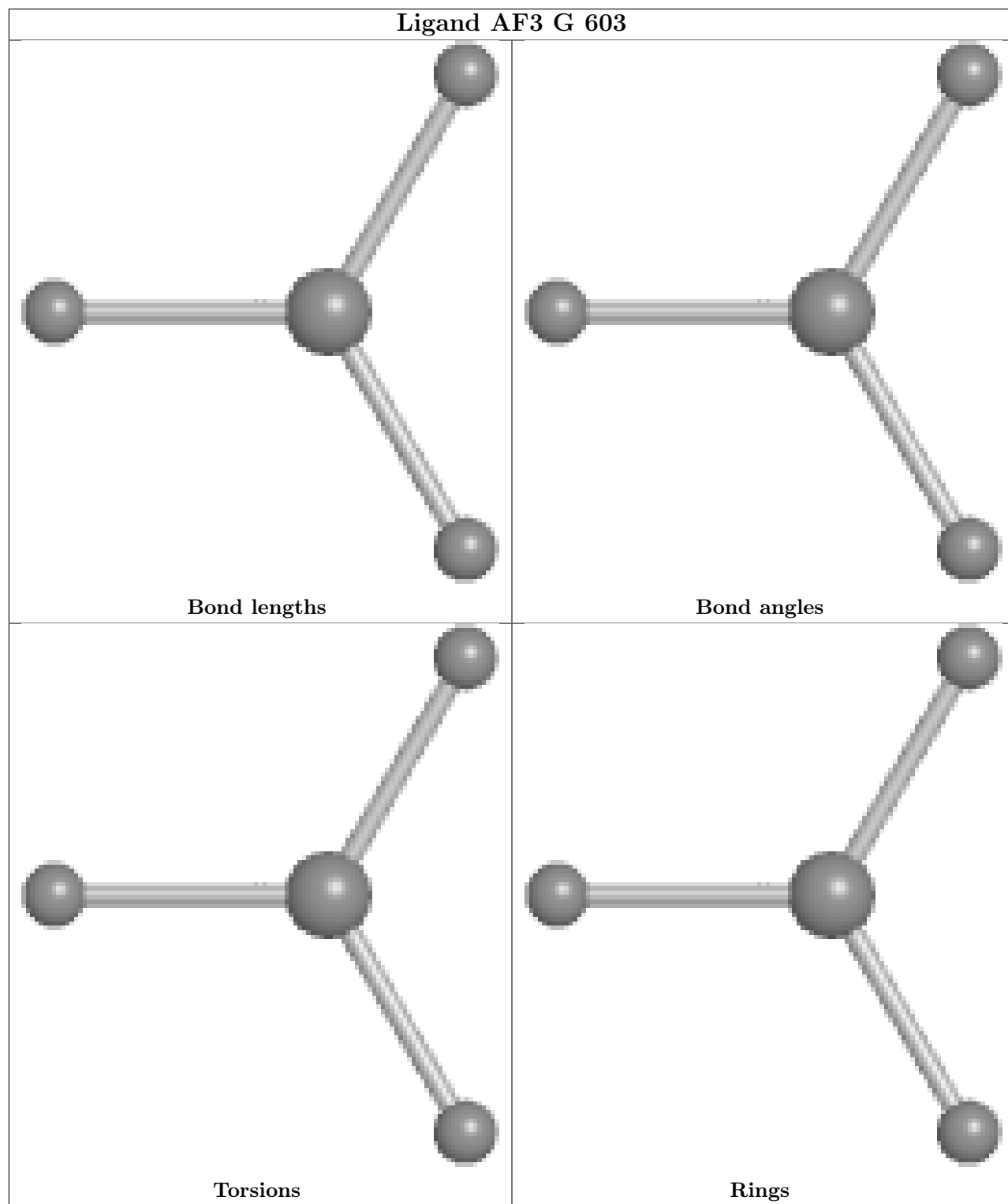


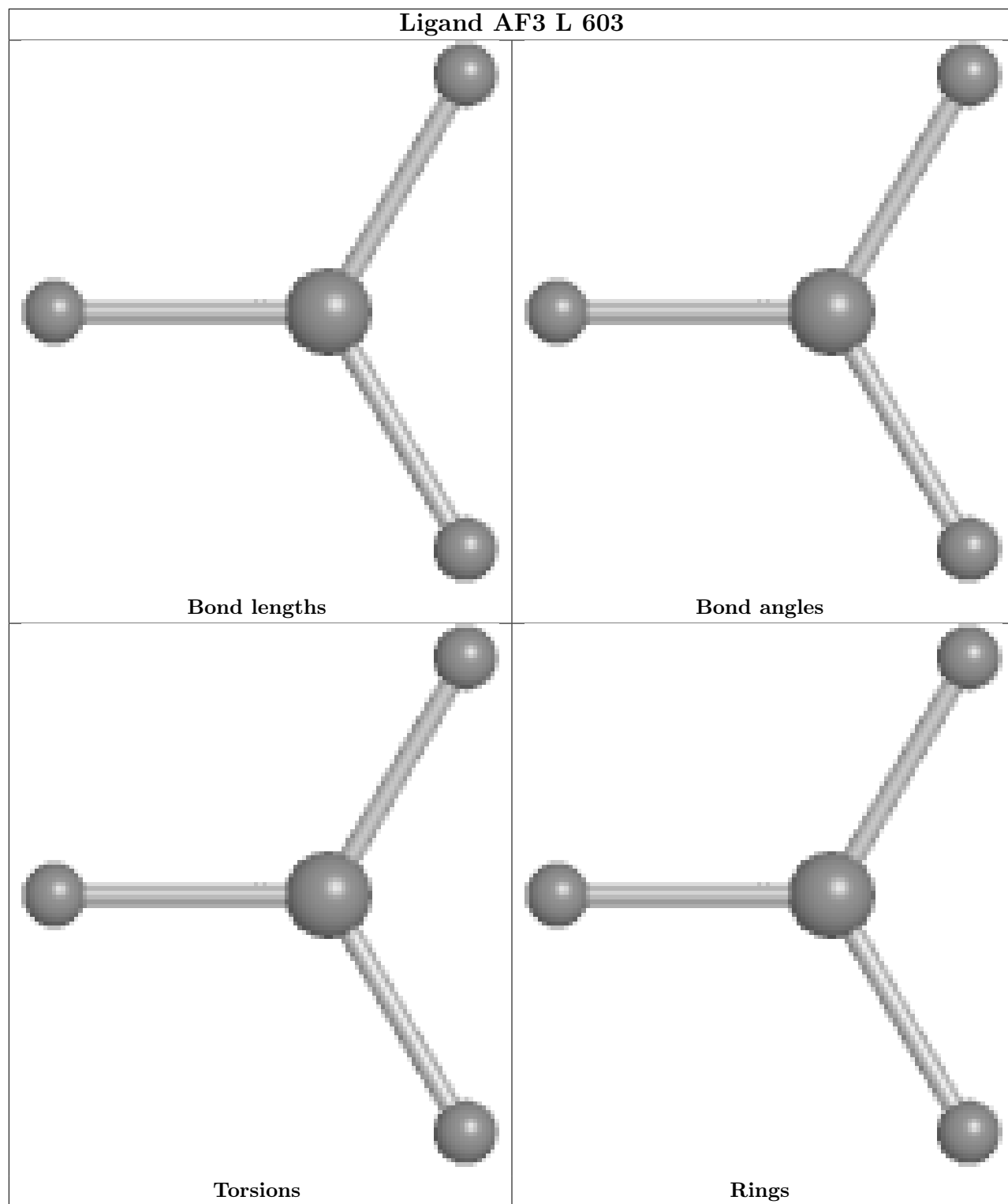


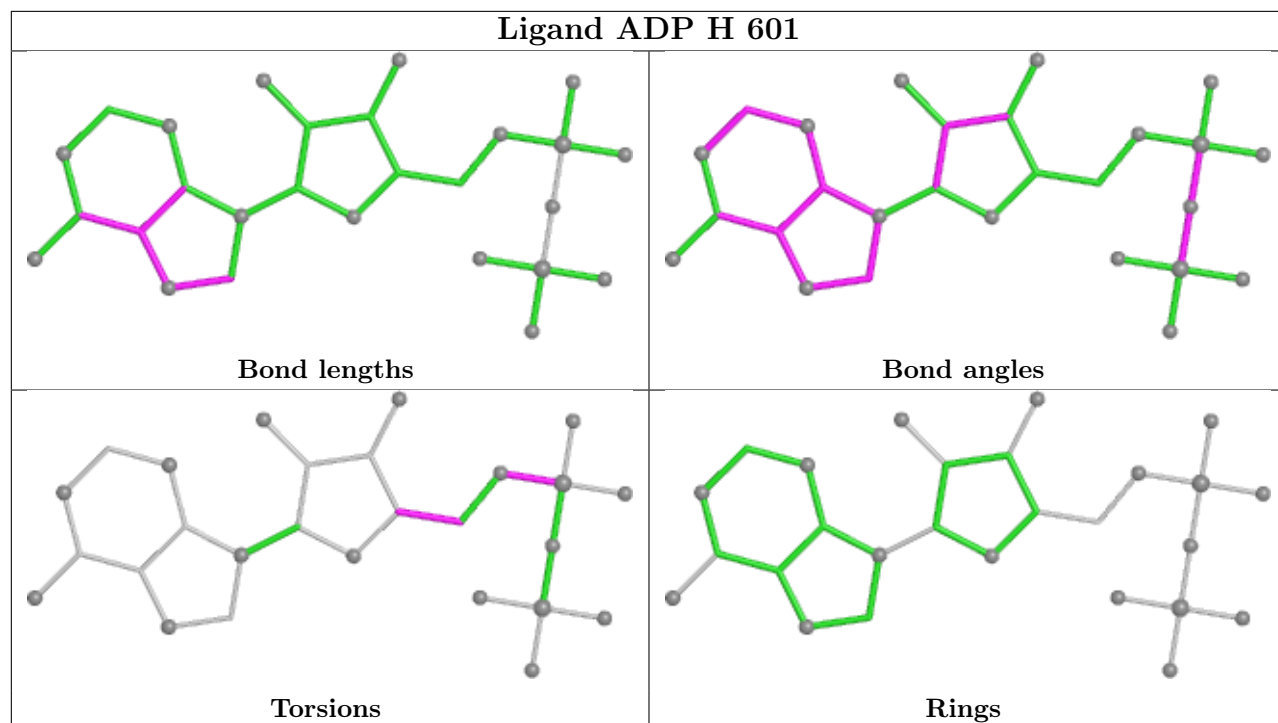


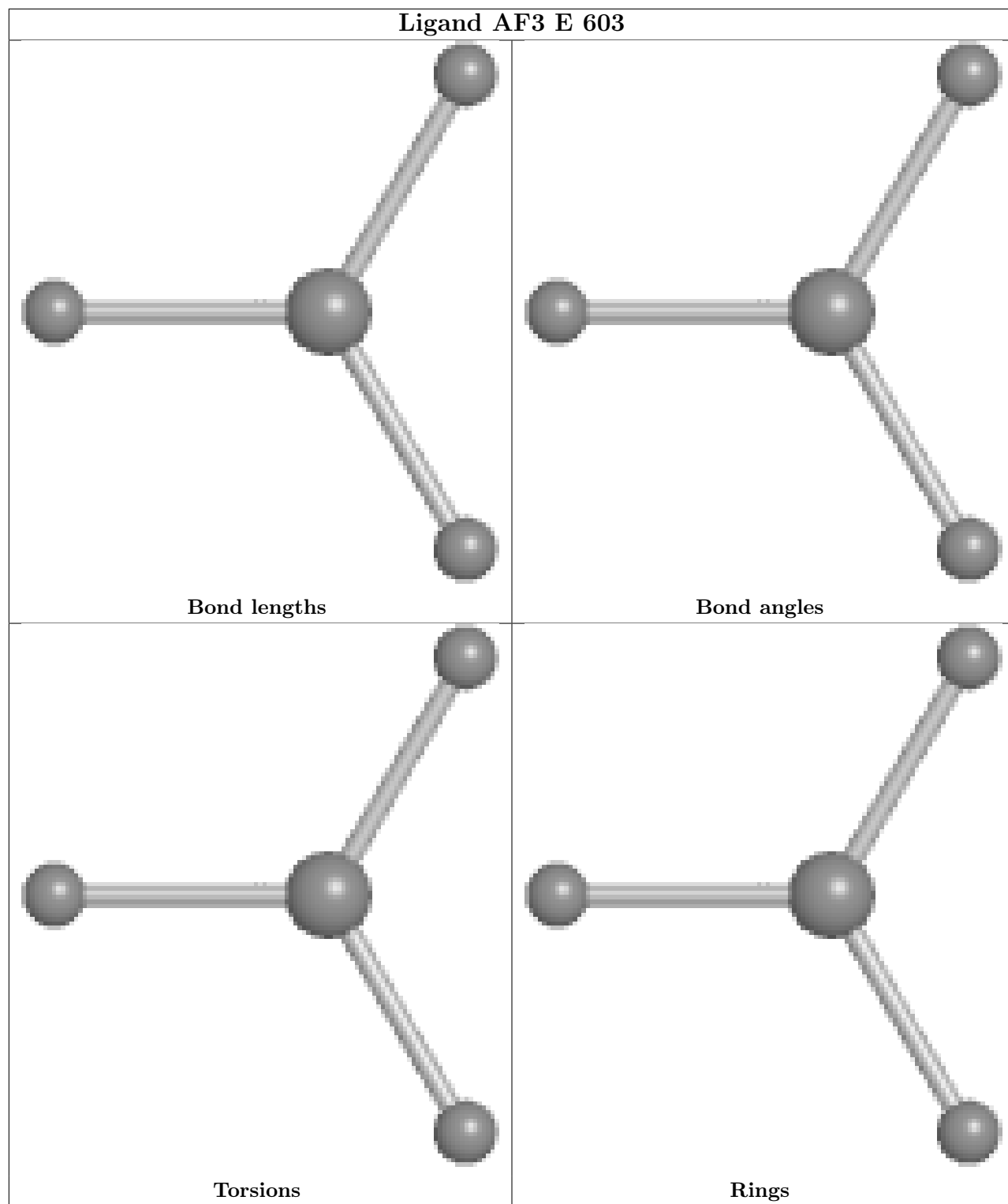


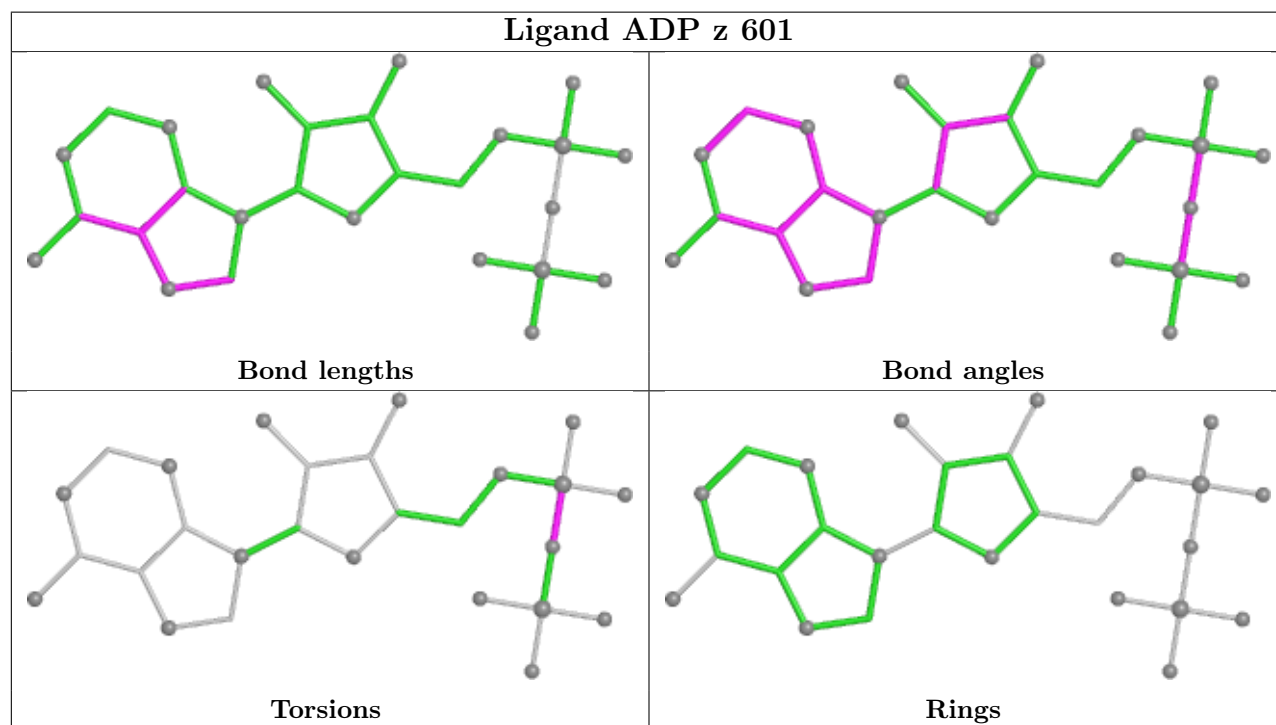
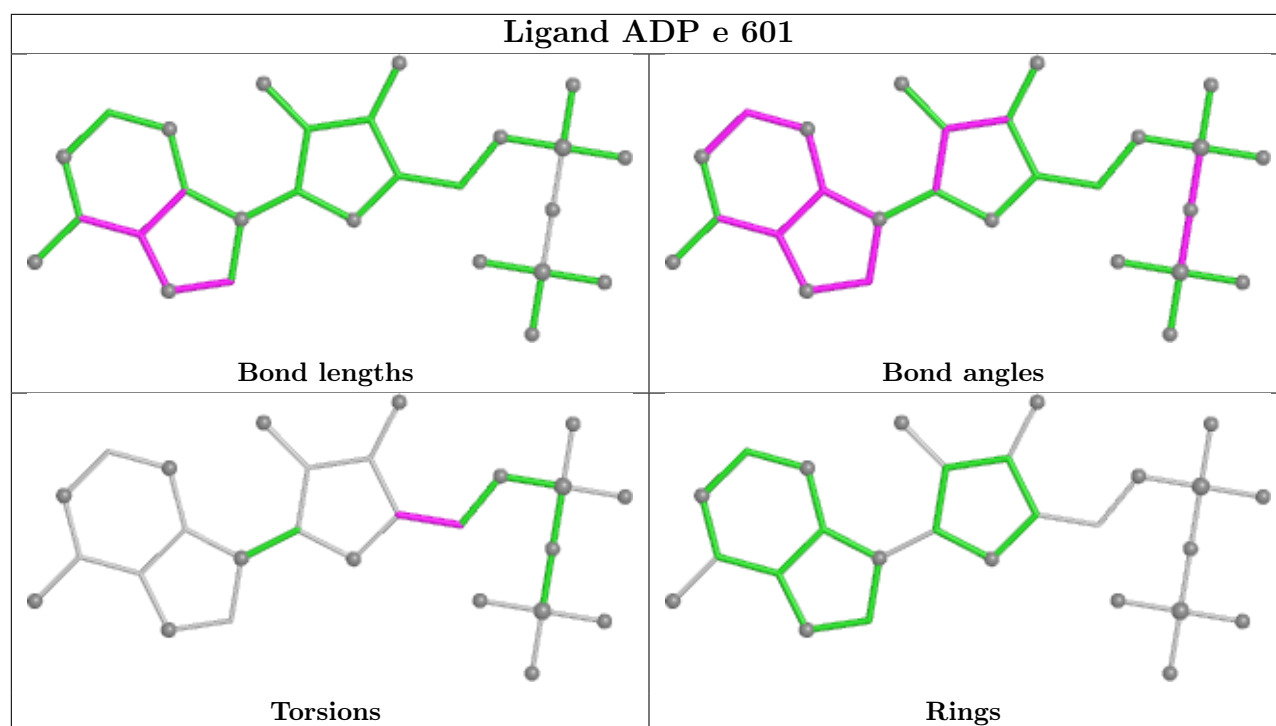


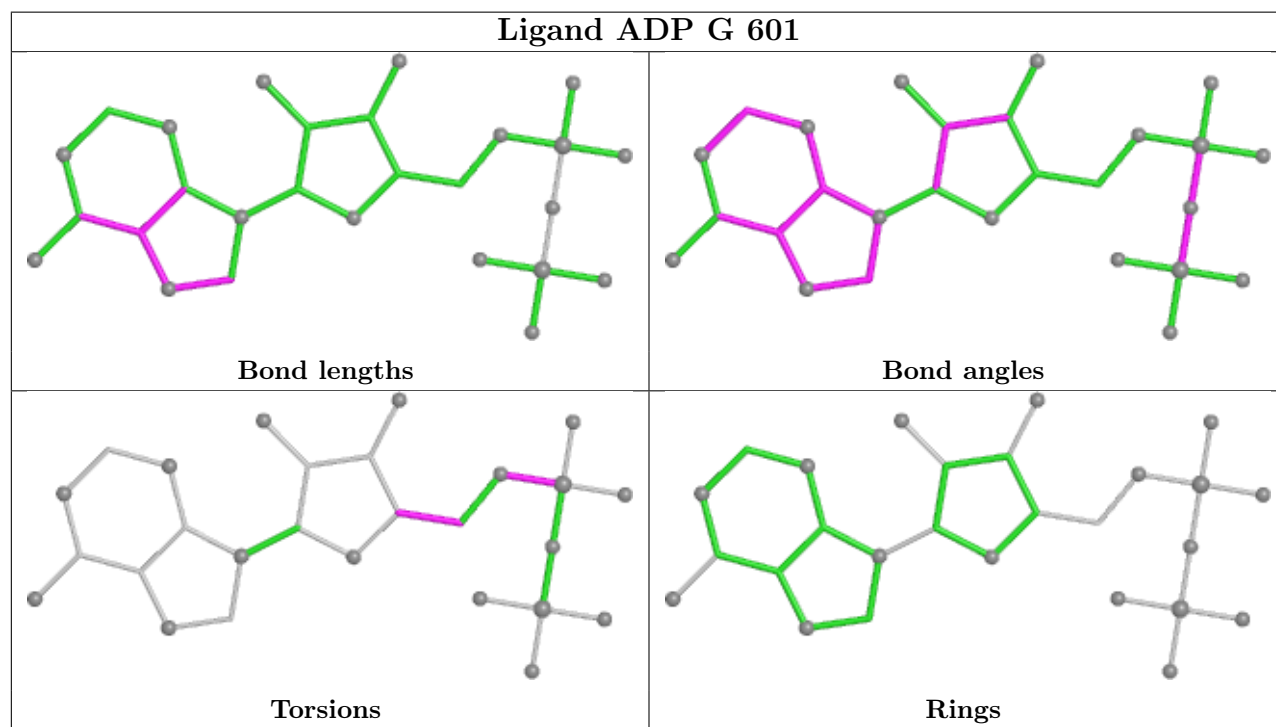
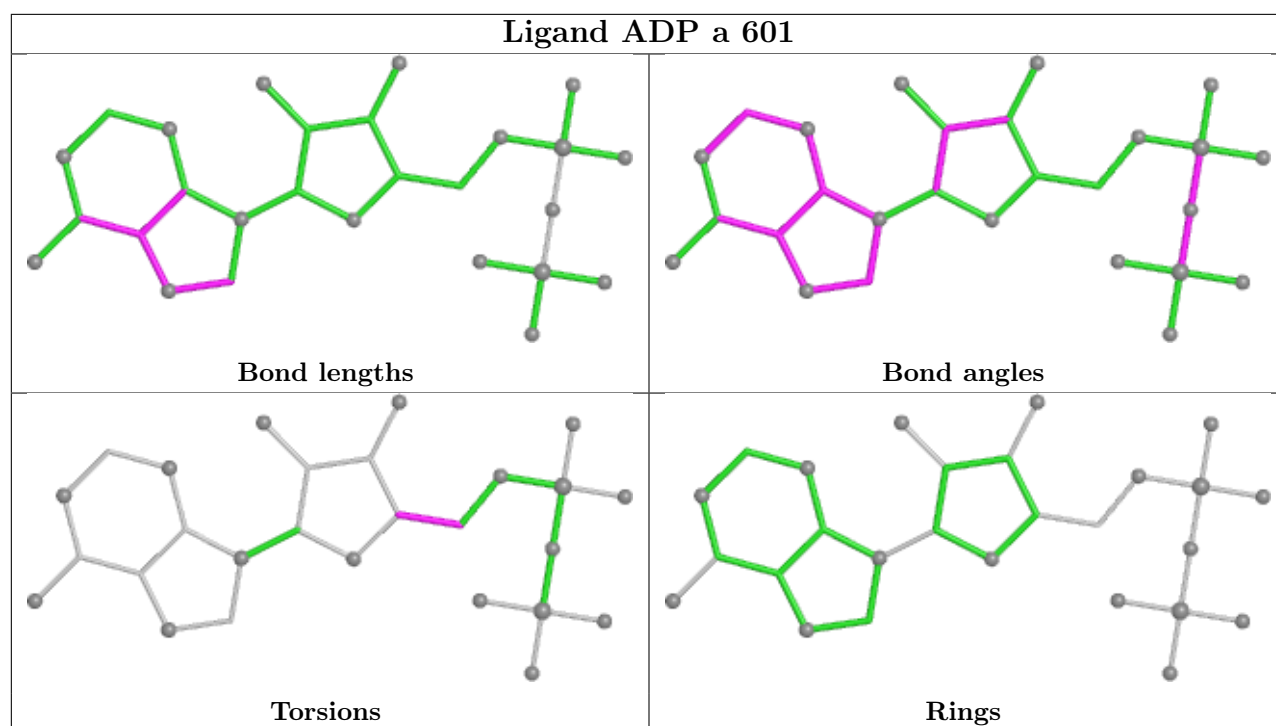


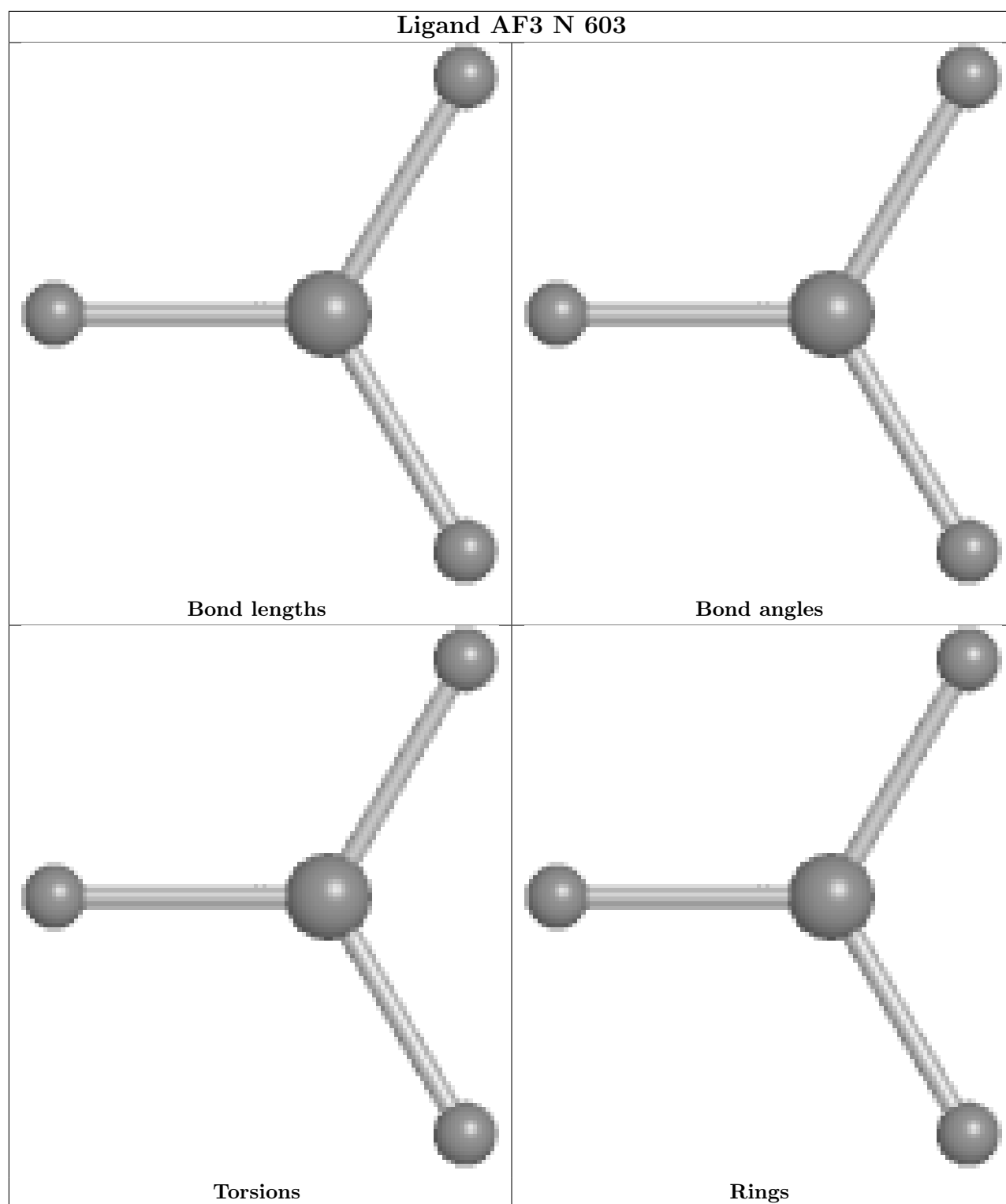












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

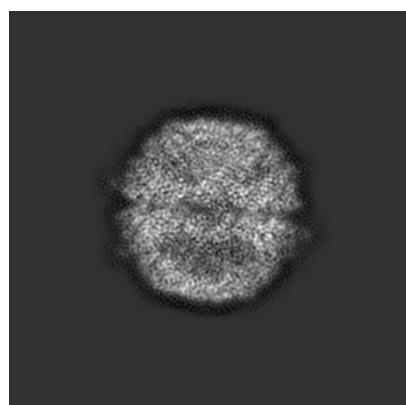
6 Map visualisation [i](#)

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.

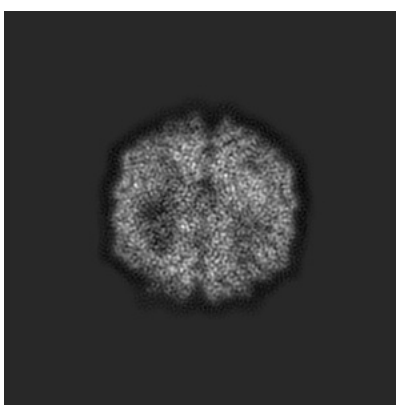
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

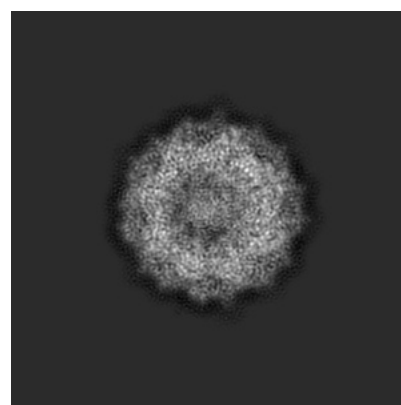
6.1.1 Primary map



X



Y

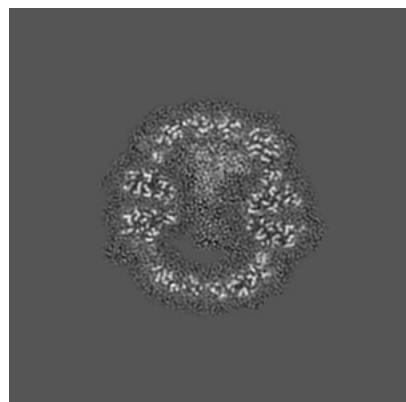


Z

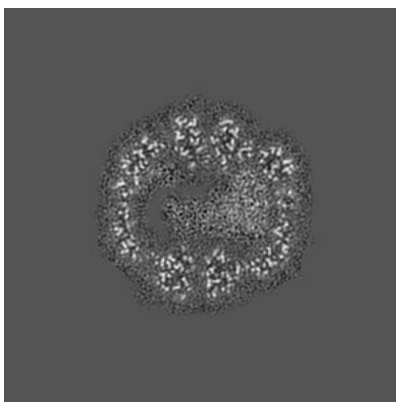
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

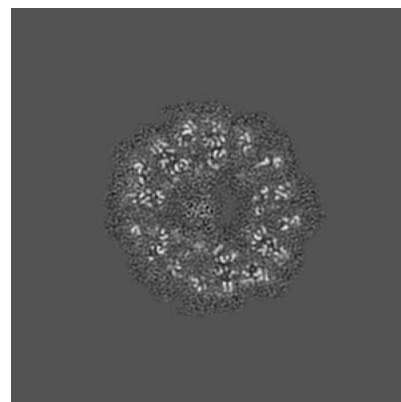
6.2.1 Primary map



X Index: 128



Y Index: 128

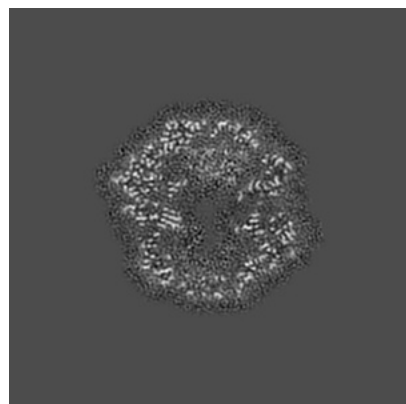


Z Index: 128

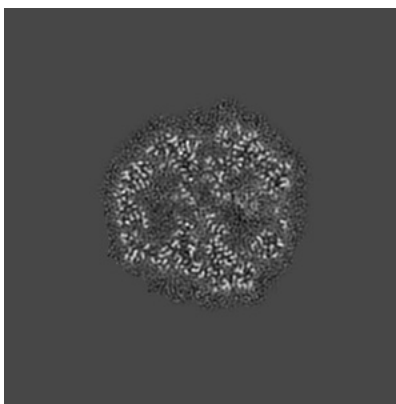
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

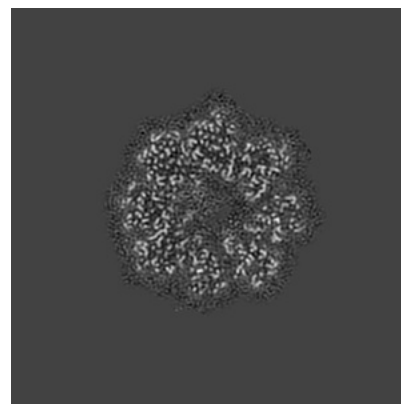
6.3.1 Primary map



X Index: 140



Y Index: 149

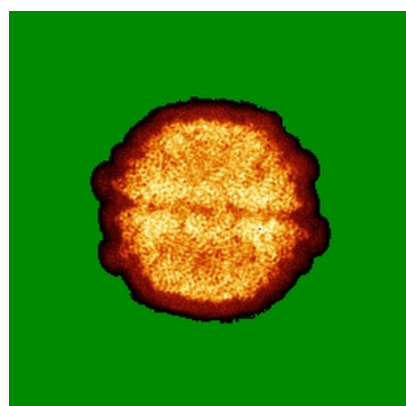


Z Index: 115

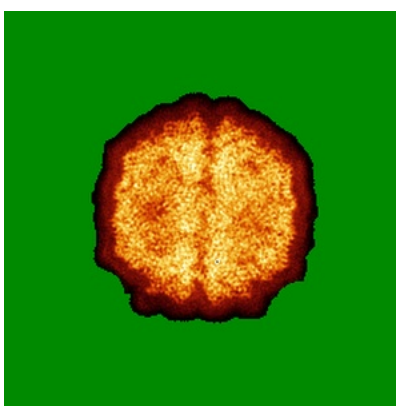
The images above show the largest variance slices of the map in three orthogonal directions.

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

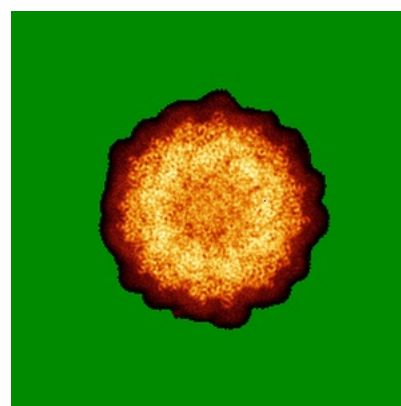
6.4.1 Primary map



X



Y



Z

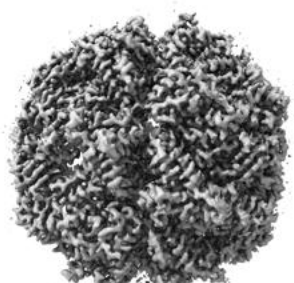
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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.

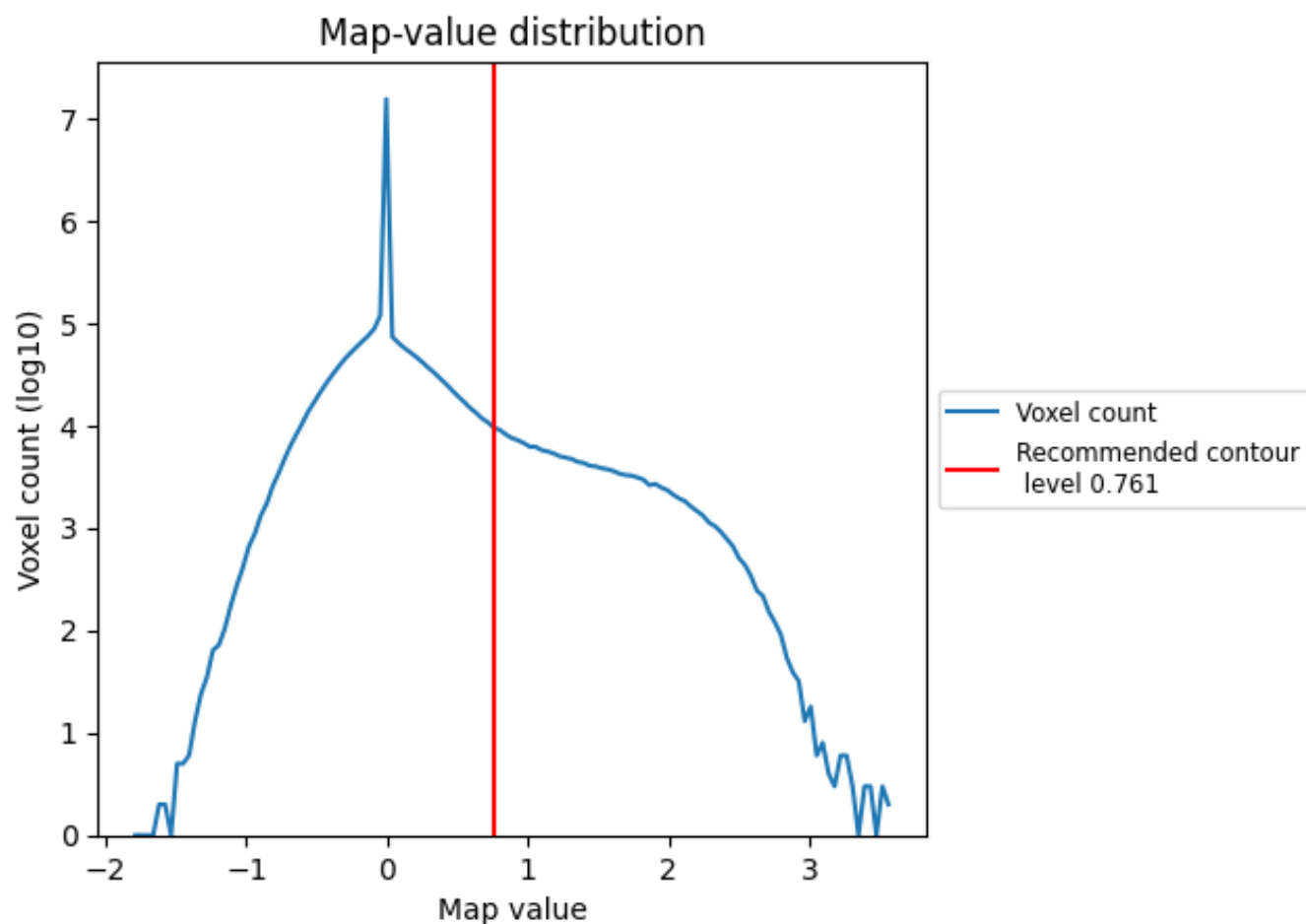
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

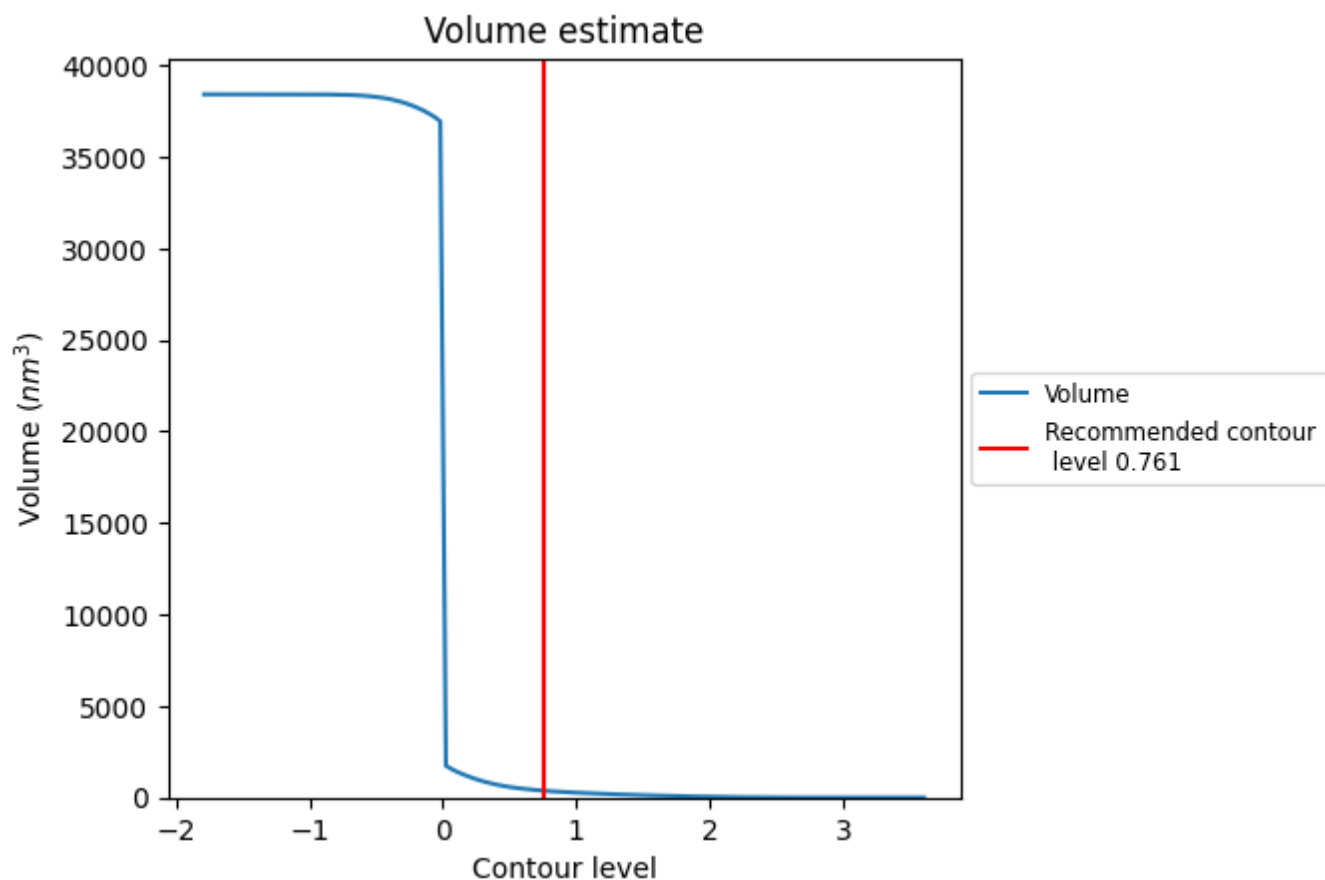
This section contains the results of statistical analysis of the map.

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.

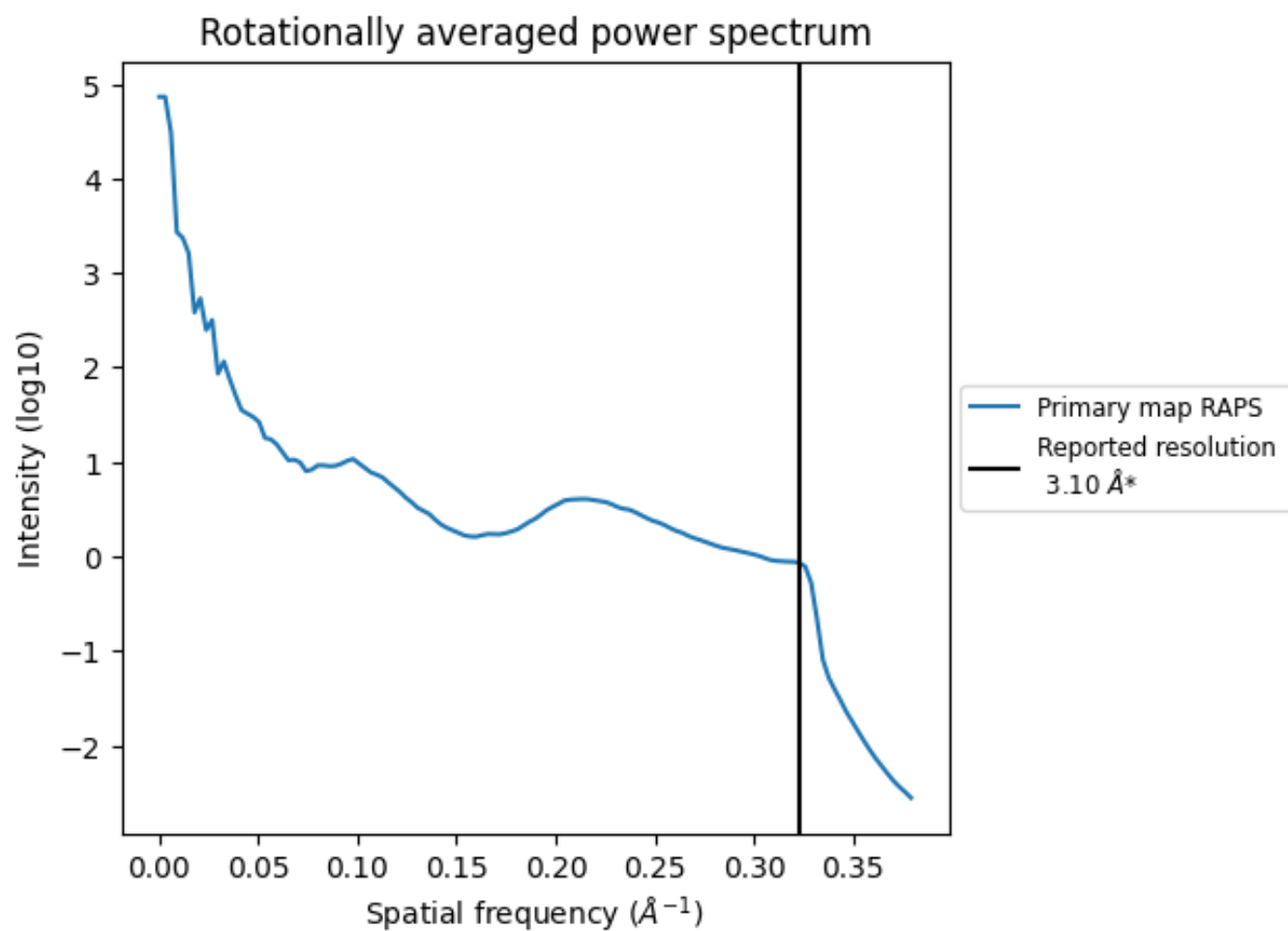
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

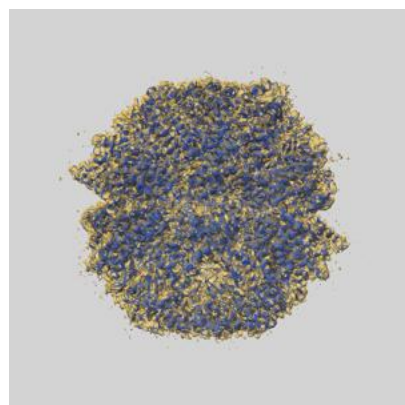
8 Fourier-Shell correlation

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

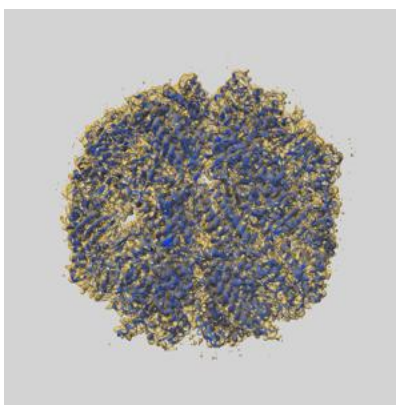
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32923 and PDB model 7X0S. Per-residue inclusion information can be found in section [3](#) on page [12](#).

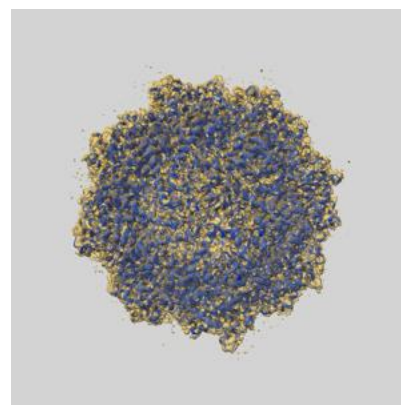
9.1 Map-model overlay [i](#)



X



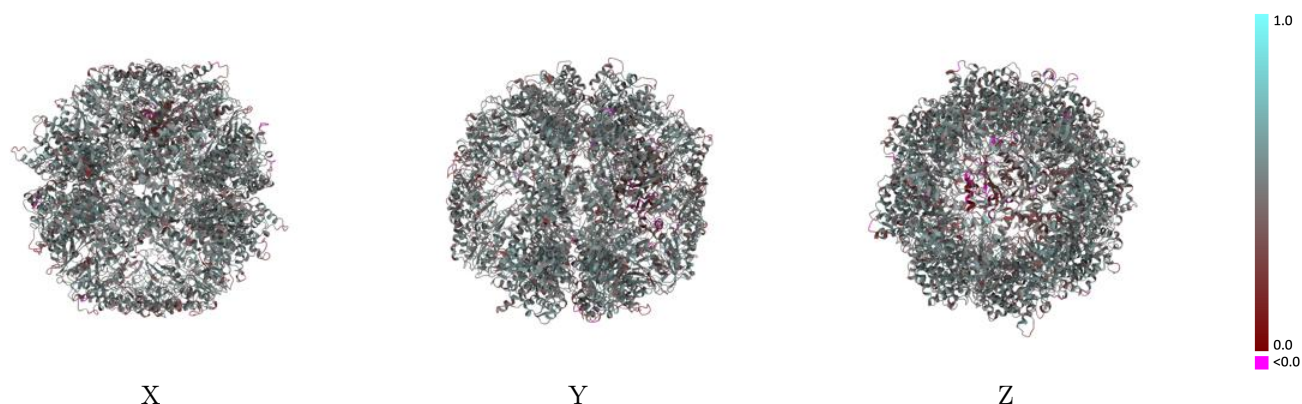
Y



Z

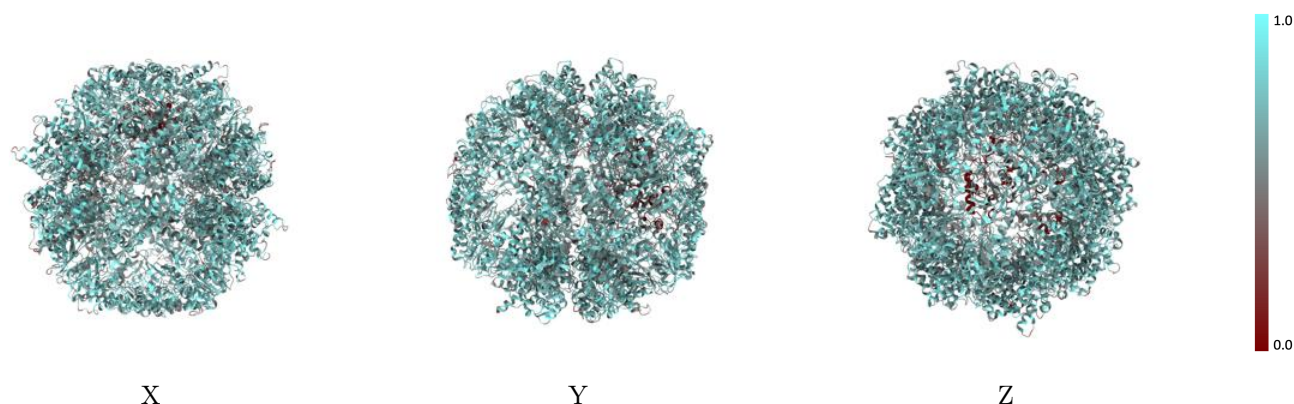
The images above show the 3D surface view of the map at the recommended contour level 0.761 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



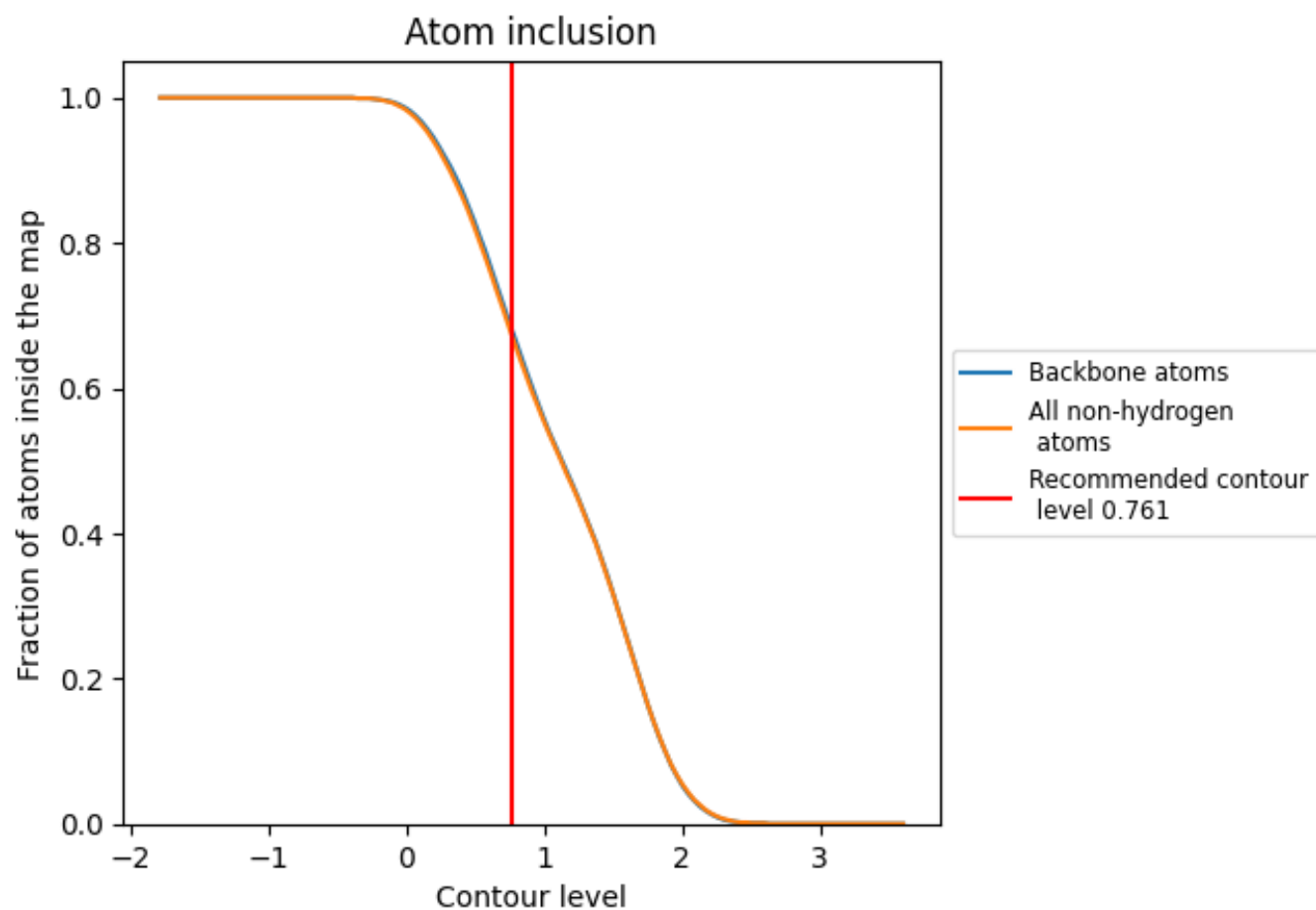
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

