



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2023 – 02:32 PM JST

PDB ID : 7YLW  
EMDB ID : EMD-33919  
Title : yeast TRiC-plp2-tubulin complex at S3 closed TRiC state  
Authors : Han, W.Y.  
Deposited on : 2022-07-27  
Resolution : 3.39 Å(reported)

This is a Full wwPDB EM Validation 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:

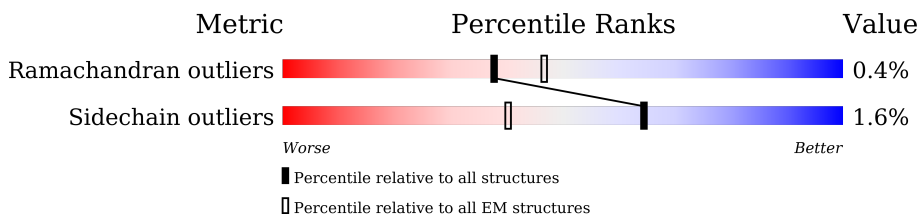
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 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 3.39 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	559	
1	a	559	
2	B	527	
2	b	527	
3	D	528	
3	d	528	
4	E	562	
4	e	562	
5	G	594	

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Mol	Chain	Length	Quality of chain
5	g	594	<p>5% 86% 12%</p>
6	H	550	<p>6% 93% 5%</p>
6	h	550	<p>93%</p>
7	Q	568	<p>8% 95%</p>
7	q	568	<p>8% 92% 5%</p>
8	T	457	<p>86% 10%</p>
9	Z	546	<p>7% 97%</p>
9	z	546	<p>6% 98%</p>
10	p	286	<p>24% 66% 33%</p>

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 70338 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	550	Total	C	N	O	S	0	0
			4158	2599	725	813	21		
1	a	546	Total	C	N	O	S	0	0
			4129	2582	721	806	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		
2	b	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	523	Total	C	N	O	S	0	0
			3998	2492	711	778	17		
3	d	524	Total	C	N	O	S	0	0
			4005	2497	712	779	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	536	Total	C	N	O	S	0	0
			4133	2595	710	806	22		
4	e	535	Total	C	N	O	S	0	0
			4124	2590	709	803	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	520	Total 4004	C 2510	N 703	O 764	S 27	0	0
5	g	520	Total 4003	C 2511	N 703	O 762	S 27	0	0

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	375	LEU	-	see sequence details	UNP P39077
G	376	GLU	-	see sequence details	UNP P39077
G	377	GLY	-	see sequence details	UNP P39077
G	378	SER	-	see sequence details	UNP P39077
G	379	GLY	-	see sequence details	UNP P39077
G	380	SER	-	see sequence details	UNP P39077
G	381	GLY	-	see sequence details	UNP P39077
G	382	TRP	-	see sequence details	UNP P39077
G	383	SER	-	see sequence details	UNP P39077
G	384	HIS	-	see sequence details	UNP P39077
G	385	PRO	-	see sequence details	UNP P39077
G	386	GLN	-	see sequence details	UNP P39077
G	387	PHE	-	see sequence details	UNP P39077
G	388	GLU	-	see sequence details	UNP P39077
G	389	LYS	-	see sequence details	UNP P39077
G	390	GLY	-	see sequence details	UNP P39077
G	391	SER	-	see sequence details	UNP P39077
G	392	GLY	-	see sequence details	UNP P39077
G	393	LYS	-	see sequence details	UNP P39077
G	394	ARG	-	see sequence details	UNP P39077
G	395	ARG	-	see sequence details	UNP P39077
G	396	TRP	-	see sequence details	UNP P39077
G	397	LYS	-	see sequence details	UNP P39077
G	398	LYS	-	see sequence details	UNP P39077
G	399	ASN	-	see sequence details	UNP P39077
G	400	PHE	-	see sequence details	UNP P39077
G	401	ILE	-	see sequence details	UNP P39077
G	402	ALA	-	see sequence details	UNP P39077
G	403	VAL	-	see sequence details	UNP P39077
G	404	SER	-	see sequence details	UNP P39077
G	405	ALA	-	see sequence details	UNP P39077
G	406	ALA	-	see sequence details	UNP P39077
G	407	ASN	-	see sequence details	UNP P39077
G	408	ARG	-	see sequence details	UNP P39077
G	409	PHE	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	410	LYS	-	see sequence details	UNP P39077
G	411	LYS	-	see sequence details	UNP P39077
G	412	ILE	-	see sequence details	UNP P39077
G	413	SER	-	see sequence details	UNP P39077
G	414	SER	-	see sequence details	UNP P39077
G	415	SER	-	see sequence details	UNP P39077
G	416	GLY	-	see sequence details	UNP P39077
G	417	ALA	-	see sequence details	UNP P39077
G	418	LEU	-	see sequence details	UNP P39077
G	419	GLY	-	see sequence details	UNP P39077
G	420	SER	-	see sequence details	UNP P39077
G	421	GLY	-	see sequence details	UNP P39077
G	422	HIS	-	see sequence details	UNP P39077
G	423	HIS	-	see sequence details	UNP P39077
G	424	HIS	-	see sequence details	UNP P39077
G	425	HIS	-	see sequence details	UNP P39077
G	426	HIS	-	see sequence details	UNP P39077
G	427	HIS	-	see sequence details	UNP P39077
G	428	HIS	-	see sequence details	UNP P39077
G	429	HIS	-	see sequence details	UNP P39077
G	430	GLY	-	see sequence details	UNP P39077
G	431	SER	-	see sequence details	UNP P39077
G	432	GLY	-	see sequence details	UNP P39077
G	433	LEU	-	see sequence details	UNP P39077
G	434	GLN	-	see sequence details	UNP P39077
G	435	LYS	-	see sequence details	UNP P39077
g	375	LEU	-	see sequence details	UNP P39077
g	376	GLU	-	see sequence details	UNP P39077
g	377	GLY	-	see sequence details	UNP P39077
g	378	SER	-	see sequence details	UNP P39077
g	379	GLY	-	see sequence details	UNP P39077
g	380	SER	-	see sequence details	UNP P39077
g	381	GLY	-	see sequence details	UNP P39077
g	382	TRP	-	see sequence details	UNP P39077
g	383	SER	-	see sequence details	UNP P39077
g	384	HIS	-	see sequence details	UNP P39077
g	385	PRO	-	see sequence details	UNP P39077
g	386	GLN	-	see sequence details	UNP P39077
g	387	PHE	-	see sequence details	UNP P39077
g	388	GLU	-	see sequence details	UNP P39077
g	389	LYS	-	see sequence details	UNP P39077
g	390	GLY	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	391	SER	-	see sequence details	UNP P39077
g	392	GLY	-	see sequence details	UNP P39077
g	393	LYS	-	see sequence details	UNP P39077
g	394	ARG	-	see sequence details	UNP P39077
g	395	ARG	-	see sequence details	UNP P39077
g	396	TRP	-	see sequence details	UNP P39077
g	397	LYS	-	see sequence details	UNP P39077
g	398	LYS	-	see sequence details	UNP P39077
g	399	ASN	-	see sequence details	UNP P39077
g	400	PHE	-	see sequence details	UNP P39077
g	401	ILE	-	see sequence details	UNP P39077
g	402	ALA	-	see sequence details	UNP P39077
g	403	VAL	-	see sequence details	UNP P39077
g	404	SER	-	see sequence details	UNP P39077
g	405	ALA	-	see sequence details	UNP P39077
g	406	ALA	-	see sequence details	UNP P39077
g	407	ASN	-	see sequence details	UNP P39077
g	408	ARG	-	see sequence details	UNP P39077
g	409	PHE	-	see sequence details	UNP P39077
g	410	LYS	-	see sequence details	UNP P39077
g	411	LYS	-	see sequence details	UNP P39077
g	412	ILE	-	see sequence details	UNP P39077
g	413	SER	-	see sequence details	UNP P39077
g	414	SER	-	see sequence details	UNP P39077
g	415	SER	-	see sequence details	UNP P39077
g	416	GLY	-	see sequence details	UNP P39077
g	417	ALA	-	see sequence details	UNP P39077
g	418	LEU	-	see sequence details	UNP P39077
g	419	GLY	-	see sequence details	UNP P39077
g	420	SER	-	see sequence details	UNP P39077
g	421	GLY	-	see sequence details	UNP P39077
g	422	HIS	-	see sequence details	UNP P39077
g	423	HIS	-	see sequence details	UNP P39077
g	424	HIS	-	see sequence details	UNP P39077
g	425	HIS	-	see sequence details	UNP P39077
g	426	HIS	-	see sequence details	UNP P39077
g	427	HIS	-	see sequence details	UNP P39077
g	428	HIS	-	see sequence details	UNP P39077
g	429	HIS	-	see sequence details	UNP P39077
g	430	GLY	-	see sequence details	UNP P39077
g	431	SER	-	see sequence details	UNP P39077
g	432	GLY	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	433	LEU	-	see sequence details	UNP P39077
g	434	GLN	-	see sequence details	UNP P39077
g	435	LYS	-	see sequence details	UNP P39077

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	520	Total	C	N	O	S	0	0
			3980	2510	678	773	19		
6	h	527	Total	C	N	O	S	0	0
			4032	2540	688	784	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	548	Total	C	N	O	S	0	0
			4163	2622	711	804	26		
7	q	541	Total	C	N	O	S	0	0
			4115	2592	703	794	26		

- Molecule 8 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	T	412	Total	C	N	O	S	0	0
			3221	2017	551	632	21		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

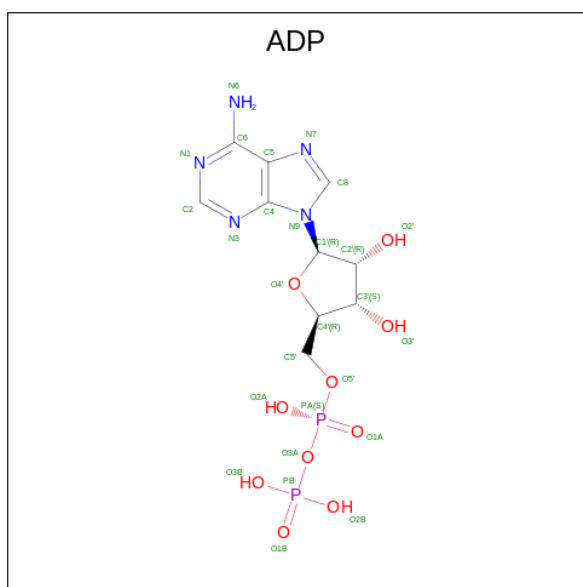
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		
9	z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		

- Molecule 10 is a protein called Phosducin-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	p	191	Total	C	N	O	S	0	0
			1571	983	272	310	6		

- Molecule 11 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	
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

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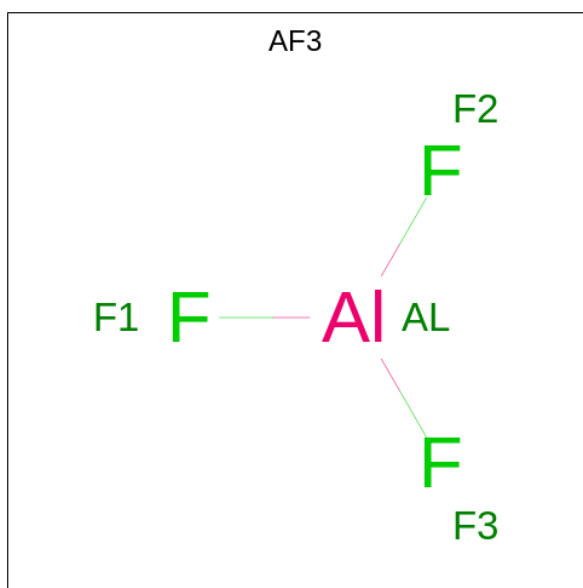
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	q	1	27	10	5	10	2	0
11	z	1	27	10	5	10	2	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total 1	Mg 1	0
12	B	1	Total 1	Mg 1	0
12	D	1	Total 1	Mg 1	0
12	E	1	Total 1	Mg 1	0
12	G	1	Total 1	Mg 1	0
12	H	1	Total 1	Mg 1	0
12	Q	1	Total 1	Mg 1	0
12	Z	1	Total 1	Mg 1	0
12	a	1	Total 1	Mg 1	0
12	b	1	Total 1	Mg 1	0
12	d	1	Total 1	Mg 1	0
12	e	1	Total 1	Mg 1	0
12	g	1	Total 1	Mg 1	0
12	h	1	Total 1	Mg 1	0
12	q	1	Total 1	Mg 1	0
12	z	1	Total 1	Mg 1	0

- Molecule 13 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF<sub>3</sub>) (labeled

as "Ligand of Interest" by depositor).



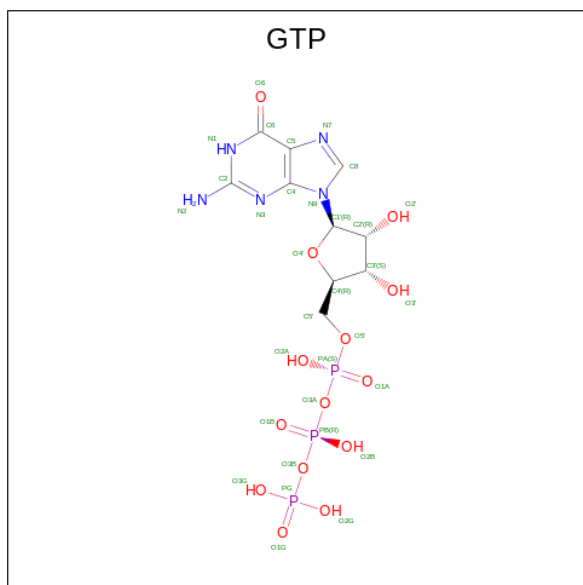
Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
13	A	1	4	1	3	0
13	B	1	4	1	3	0
13	D	1	4	1	3	0
13	E	1	4	1	3	0
13	G	1	4	1	3	0
13	H	1	4	1	3	0
13	Z	1	4	1	3	0
13	a	1	4	1	3	0
13	b	1	4	1	3	0
13	d	1	4	1	3	0
13	e	1	4	1	3	0
13	g	1	4	1	3	0
13	h	1	4	1	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
13	z	1	4	1	3	0

- Molecule 14 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	T	1	32	10	5	14	3	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
15	A	1	1	1	0
15	B	1	1	1	0
15	D	1	1	1	0
15	E	1	1	1	0
15	G	1	1	1	0
15	H	1	1	1	0
15	Z	1	1	1	0

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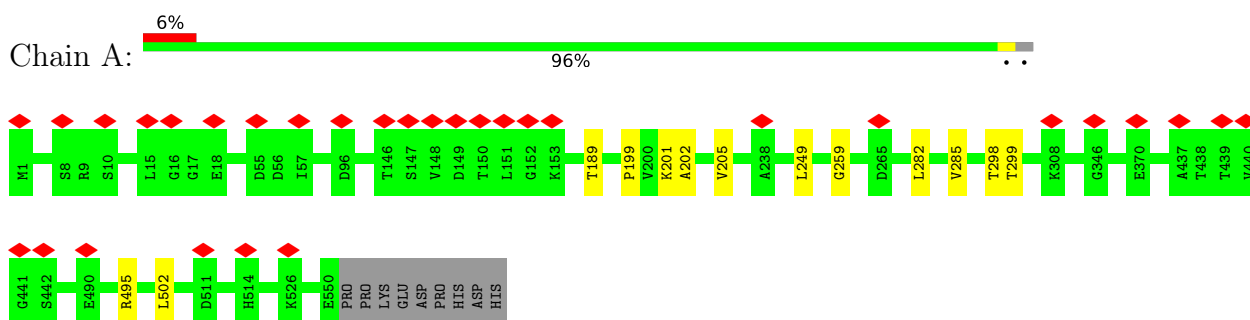
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
15	a	1	Total 1	O 1	0
15	b	1	Total 1	O 1	0
15	d	1	Total 1	O 1	0
15	e	1	Total 1	O 1	0
15	g	1	Total 1	O 1	0
15	h	1	Total 1	O 1	0
15	z	1	Total 1	O 1	0

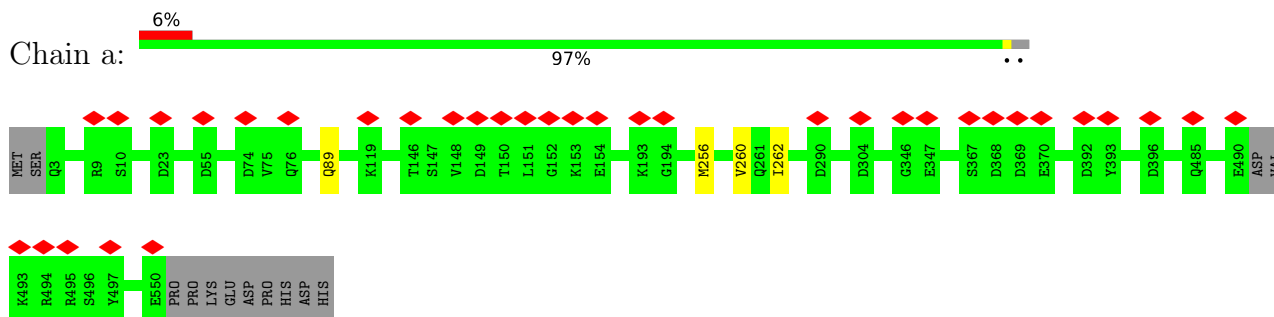
### 3 Residue-property plots [i](#)

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

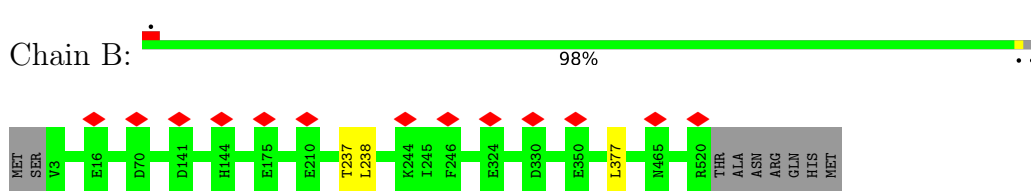
- Molecule 1: T-complex protein 1 subunit alpha



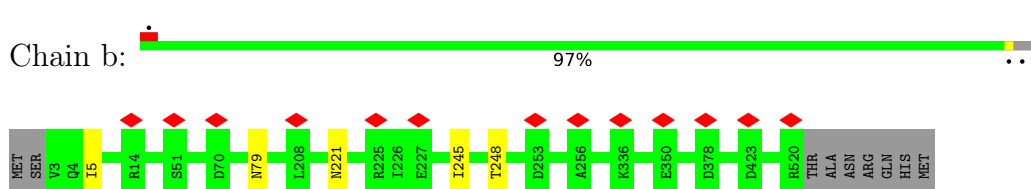
- Molecule 1: T-complex protein 1 subunit alpha



- Molecule 2: T-complex protein 1 subunit beta



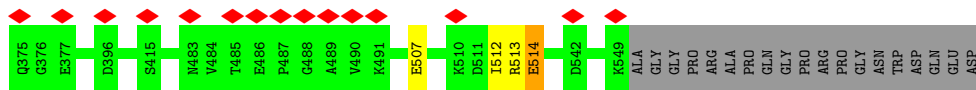
- Molecule 2: T-complex protein 1 subunit beta



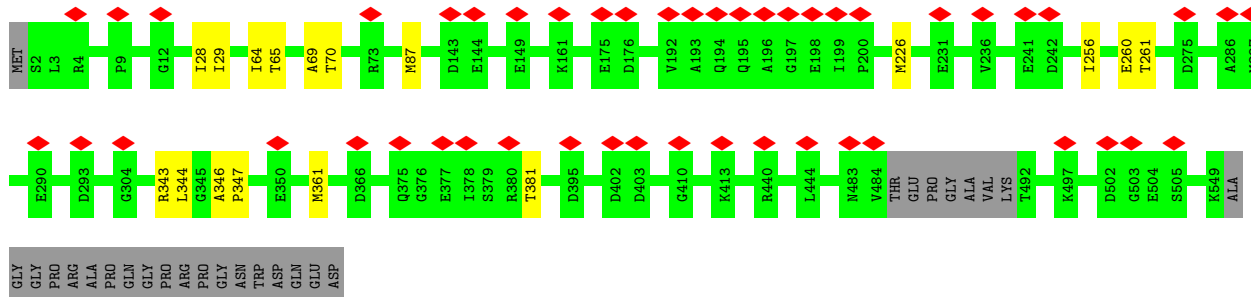
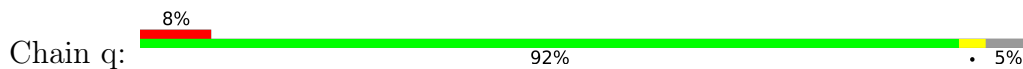




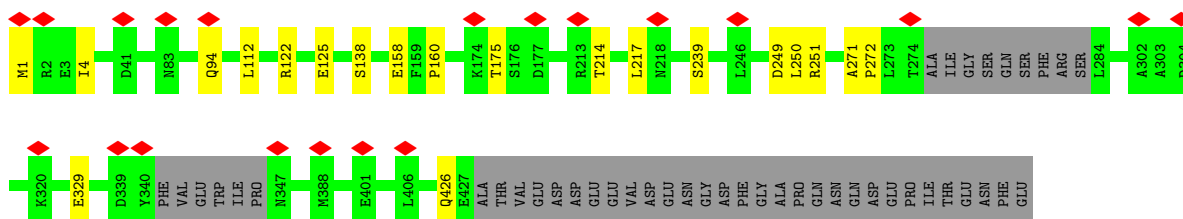
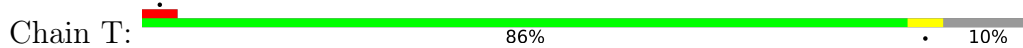




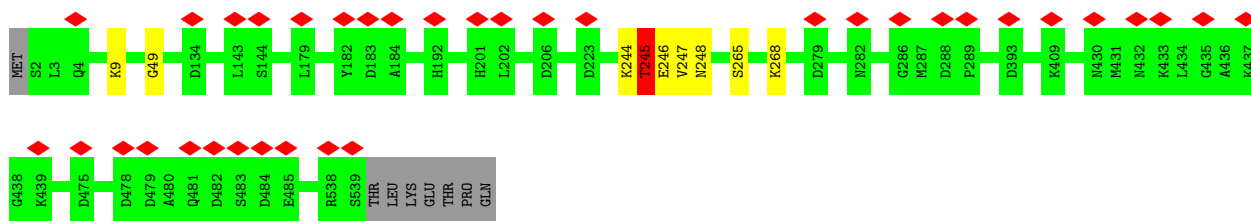
• Molecule 7: T-complex protein 1 subunit theta



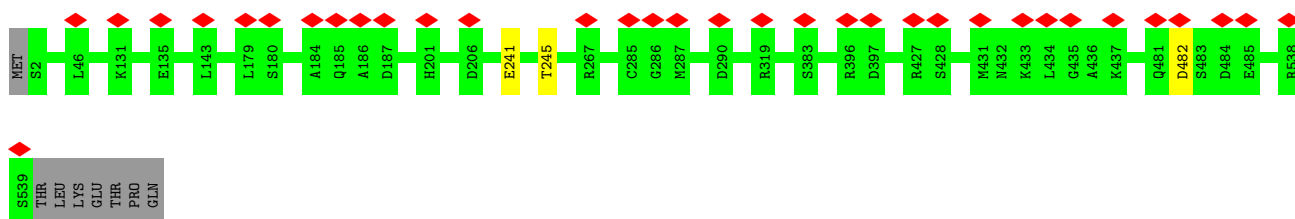
• Molecule 8: Tubulin beta chain



• Molecule 9: T-complex protein 1 subunit zeta



• Molecule 9: T-complex protein 1 subunit zeta





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28063	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	1.961	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.1	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: MG, ADP, AF3, GTP

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	0.42	0/4196	0.64	2/5661 (0.0%)
1	a	0.33	0/4166	0.60	0/5619
2	B	0.36	0/3976	0.58	0/5358
2	b	0.34	0/3976	0.60	0/5358
3	D	0.44	0/4036	0.65	0/5440
3	d	0.33	0/4043	0.60	0/5451
4	E	0.41	0/4184	0.61	0/5629
4	e	0.51	0/4175	0.64	0/5617
5	G	0.40	0/4048	0.66	1/5459 (0.0%)
5	g	0.33	0/4047	0.61	0/5460
6	H	0.43	0/4030	0.63	2/5440 (0.0%)
6	h	0.41	0/4083	0.61	2/5511 (0.0%)
7	Q	0.43	0/4214	0.63	0/5689
7	q	0.41	0/4164	0.63	1/5619 (0.0%)
8	T	0.65	0/3287	0.79	0/4448
9	Z	0.39	0/4191	0.63	1/5663 (0.0%)
9	z	0.35	0/4191	0.60	0/5663
10	p	0.38	0/1594	0.62	0/2134
All	All	0.41	0/70601	0.63	9/95219 (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
8	T	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	346	ALA	N-CA-C	-6.66	93.01	111.00
5	G	256	GLU	N-CA-C	5.66	126.28	111.00
6	H	432	ALA	N-CA-C	5.62	126.19	111.00
9	Z	245	THR	N-CA-C	5.54	125.95	111.00
6	h	245	ASN	N-CA-C	-5.50	96.15	111.00
1	A	201	LYS	N-CA-C	-5.37	96.49	111.00
1	A	202	ALA	N-CA-C	-5.32	96.64	111.00
6	H	118	GLU	N-CA-C	-5.20	96.96	111.00
6	h	254	LYS	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	T	271	ALA	Peptide
8	T	94	GLN	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	A	548/559 (98%)	522 (95%)	24 (4%)	2 (0%)	34	67
1	a	542/559 (97%)	518 (96%)	24 (4%)	0	100	100
2	B	516/527 (98%)	495 (96%)	21 (4%)	0	100	100
2	b	516/527 (98%)	501 (97%)	15 (3%)	0	100	100
3	D	521/528 (99%)	504 (97%)	17 (3%)	0	100	100
3	d	522/528 (99%)	508 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	534/562 (95%)	511 (96%)	22 (4%)	1 (0%)	47	78
4	e	533/562 (95%)	513 (96%)	19 (4%)	1 (0%)	47	78
5	G	514/594 (86%)	487 (95%)	26 (5%)	1 (0%)	47	78
5	g	514/594 (86%)	492 (96%)	21 (4%)	1 (0%)	47	78
6	H	516/550 (94%)	493 (96%)	20 (4%)	3 (1%)	25	57
6	h	525/550 (96%)	505 (96%)	16 (3%)	4 (1%)	19	51
7	Q	546/568 (96%)	514 (94%)	28 (5%)	4 (1%)	22	55
7	q	537/568 (94%)	501 (93%)	31 (6%)	5 (1%)	17	49
8	T	406/457 (89%)	370 (91%)	31 (8%)	5 (1%)	13	41
9	Z	536/546 (98%)	514 (96%)	17 (3%)	5 (1%)	17	49
9	z	536/546 (98%)	518 (97%)	17 (3%)	1 (0%)	47	78
10	p	187/286 (65%)	177 (95%)	10 (5%)	0	100	100
All	All	9049/9611 (94%)	8643 (96%)	373 (4%)	33 (0%)	38	67

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	25	GLN
6	H	432	ALA
7	Q	513	ARG
7	Q	514	GLU
9	Z	247	VAL
9	Z	268	LYS
7	q	70	THR
7	q	347	PRO
9	z	482	ASP
1	A	259	GLY
8	T	250	LEU
8	T	272	PRO
8	T	426	GLN
9	Z	49	GLY
9	Z	245	THR
6	h	257	ALA
6	h	258	GLU
7	q	260	GLU
1	A	199	PRO
5	G	311	LYS
7	Q	259	THR

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Mol	Chain	Res	Type
8	T	249	ASP
4	e	469	PHE
5	g	258	GLN
7	Q	260	GLU
6	h	221	LYS
7	q	69	ALA
7	q	261	THR
6	H	433	GLY
4	E	519	SER
8	T	160	PRO
9	Z	246	GLU
6	h	487	ASN

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	462/471 (98%)	453 (98%)	9 (2%)	57	78
1	a	458/471 (97%)	454 (99%)	4 (1%)	78	90
2	B	433/441 (98%)	430 (99%)	3 (1%)	84	92
2	b	433/441 (98%)	428 (99%)	5 (1%)	71	85
3	D	449/453 (99%)	438 (98%)	11 (2%)	49	74
3	d	450/453 (99%)	448 (100%)	2 (0%)	91	95
4	E	461/483 (95%)	457 (99%)	4 (1%)	78	90
4	e	460/483 (95%)	447 (97%)	13 (3%)	43	70
5	G	443/501 (88%)	434 (98%)	9 (2%)	55	77
5	g	443/501 (88%)	436 (98%)	7 (2%)	62	81
6	H	434/454 (96%)	428 (99%)	6 (1%)	67	83
6	h	440/454 (97%)	431 (98%)	9 (2%)	55	77
7	Q	458/473 (97%)	450 (98%)	8 (2%)	60	80
7	q	453/473 (96%)	442 (98%)	11 (2%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	T	353/392 (90%)	340 (96%)	13 (4%)	34	62
9	Z	455/463 (98%)	450 (99%)	5 (1%)	73	86
9	z	455/463 (98%)	453 (100%)	2 (0%)	91	95
10	p	173/251 (69%)	172 (99%)	1 (1%)	86	94
All	All	7713/8121 (95%)	7591 (98%)	122 (2%)	64	81

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	A	205	VAL
1	A	249	LEU
1	A	282	LEU
1	A	285	VAL
1	A	298	THR
1	A	299	THR
1	A	495	ARG
1	A	502	LEU
2	B	237	THR
2	B	238	LEU
2	B	377	LEU
3	D	161	LYS
3	D	226	PRO
3	D	240	GLN
3	D	248	THR
3	D	258	ARG
3	D	263	ILE
3	D	268	ARG
3	D	317	GLU
3	D	360	ILE
3	D	463	ILE
3	D	470	ARG
4	E	191	LYS
4	E	334	LEU
4	E	515	LEU
4	E	522	MET
5	G	104	LEU
5	G	251	GLU
5	G	253	LYS
5	G	256	GLU
5	G	278	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	G	291	ARG
5	G	306	GLN
5	G	308	TYR
5	G	563	GLU
6	H	68	THR
6	H	71	LYS
6	H	103	ILE
6	H	111	GLU
6	H	376	LEU
6	H	431	ILE
7	Q	43	LEU
7	Q	57	ASN
7	Q	256	ILE
7	Q	259	THR
7	Q	357	THR
7	Q	507	GLU
7	Q	512	ILE
7	Q	514	GLU
8	T	1	MET
8	T	4	ILE
8	T	112	LEU
8	T	122	ARG
8	T	125	GLU
8	T	138	SER
8	T	158	GLU
8	T	175	THR
8	T	214	THR
8	T	217	LEU
8	T	239	SER
8	T	251	ARG
8	T	329	GLU
9	Z	9	LYS
9	Z	244	LYS
9	Z	245	THR
9	Z	248	ASN
9	Z	265	SER
1	a	89	GLN
1	a	256	MET
1	a	260	VAL
1	a	262	ILE
2	b	5	ILE
2	b	79	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	221	ASN
2	b	245	ILE
2	b	248	THR
3	d	10	THR
3	d	60	ASP
4	e	84	THR
4	e	93	GLN
4	e	108	SER
4	e	151	ASP
4	e	156	LEU
4	e	274	CYS
4	e	282	LYS
4	e	283	THR
4	e	325	TRP
4	e	327	PHE
4	e	452	LEU
4	e	454	VAL
4	e	464	ILE
5	g	57	LEU
5	g	260	ASN
5	g	270	ASN
5	g	297	THR
5	g	490	LYS
5	g	492	LYS
5	g	494	LEU
6	h	1	MET
6	h	7	THR
6	h	47	LEU
6	h	60	THR
6	h	220	PHE
6	h	250	LEU
6	h	373	THR
6	h	422	LYS
6	h	479	TYR
10	p	186	CYS
7	q	28	ILE
7	q	29	ILE
7	q	64	ILE
7	q	65	THR
7	q	87	MET
7	q	226	MET
7	q	256	ILE

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Mol	Chain	Res	Type
7	q	343	ARG
7	q	344	LEU
7	q	361	MET
7	q	381	THR
9	z	241	GLU
9	z	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
3	D	240	GLN
3	D	303	HIS
4	E	85	ASN
4	E	253	GLN
4	E	299	GLN
4	E	486	ASN
5	G	106	GLN
5	G	231	HIS
5	G	258	GLN
5	G	260	ASN
5	G	281	GLN
6	H	231	GLN
6	H	232	GLN
6	H	245	ASN
6	H	256	ASN
6	H	305	GLN
7	Q	52	ASN
7	Q	58	HIS
7	Q	477	ASN
8	T	28	HIS
8	T	94	GLN
8	T	134	GLN
8	T	195	HIS
8	T	256	ASN
8	T	334	GLN
8	T	423	GLN
9	Z	67	GLN
9	Z	248	ASN
1	a	64	ASN
1	a	88	GLN
2	b	112	GLN

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Mol	Chain	Res	Type
2	b	375	GLN
4	e	142	HIS
4	e	543	GLN
5	g	326	ASN
5	g	465	ASN
5	g	568	GLN
6	h	173	ASN
6	h	174	ASN
6	h	245	ASN
7	q	27	GLN
7	q	52	ASN
7	q	219	ASN
7	q	472	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 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 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	$\# Z  > 2$
11	ADP	B	601	12	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	ADP	z	601	12	24,29,29	0.96	1 (4%)	29,45,45	1.48	5 (17%)
13	AF3	E	603	-	0,3,3	-	-	-	-	-
11	ADP	d	601	12	24,29,29	0.94	1 (4%)	29,45,45	1.50	5 (17%)
14	GTP	T	502	-	26,34,34	0.99	1 (3%)	32,54,54	1.46	4 (12%)
11	ADP	h	601	12	24,29,29	1.03	1 (4%)	29,45,45	1.81	4 (13%)
11	ADP	H	601	12	24,29,29	0.94	1 (4%)	29,45,45	1.36	4 (13%)
11	ADP	b	601	12	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
13	AF3	Z	603	-	0,3,3	-	-	-	-	-
13	AF3	d	603	-	0,3,3	-	-	-	-	-
11	ADP	Q	602	12	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
13	AF3	a	603	-	0,3,3	-	-	-	-	-
13	AF3	z	603	-	0,3,3	-	-	-	-	-
11	ADP	a	601	12	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
11	ADP	e	601	12	24,29,29	0.95	1 (4%)	29,45,45	1.56	4 (13%)
13	AF3	G	603	-	0,3,3	-	-	-	-	-
13	AF3	h	603	-	0,3,3	-	-	-	-	-
13	AF3	D	603	-	0,3,3	-	-	-	-	-
13	AF3	B	603	-	0,3,3	-	-	-	-	-
13	AF3	g	603	-	0,3,3	-	-	-	-	-
13	AF3	b	603	-	0,3,3	-	-	-	-	-
11	ADP	A	601	12	24,29,29	0.96	1 (4%)	29,45,45	1.39	5 (17%)
11	ADP	g	601	12	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
11	ADP	D	601	12	24,29,29	0.93	1 (4%)	29,45,45	1.58	4 (13%)
13	AF3	A	603	-	0,3,3	-	-	-	-	-
13	AF3	H	603	-	0,3,3	-	-	-	-	-
11	ADP	E	601	12	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
11	ADP	Z	601	12	24,29,29	0.96	1 (4%)	29,45,45	1.45	5 (17%)
11	ADP	q	601	12	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
11	ADP	G	601	12	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
13	AF3	e	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	b	601	12	-	0/12/32/32	0/3/3/3
11	ADP	d	601	12	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	Q	602	12	-	4/12/32/32	0/3/3/3
11	ADP	A	601	12	-	1/12/32/32	0/3/3/3
11	ADP	g	601	12	-	5/12/32/32	0/3/3/3
11	ADP	D	601	12	-	1/12/32/32	0/3/3/3
14	GTP	T	502	-	-	6/18/38/38	0/3/3/3
11	ADP	a	601	12	-	5/12/32/32	0/3/3/3
11	ADP	E	601	12	-	3/12/32/32	0/3/3/3
11	ADP	Z	601	12	-	5/12/32/32	0/3/3/3
11	ADP	B	601	12	-	3/12/32/32	0/3/3/3
11	ADP	q	601	12	-	3/12/32/32	0/3/3/3
11	ADP	h	601	12	-	4/12/32/32	0/3/3/3
11	ADP	z	601	12	-	2/12/32/32	0/3/3/3
11	ADP	H	601	12	-	0/12/32/32	0/3/3/3
11	ADP	G	601	12	-	2/12/32/32	0/3/3/3
11	ADP	e	601	12	-	4/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	502	GTP	C6-N1	-2.85	1.33	1.37
11	B	601	ADP	C5-C4	2.45	1.47	1.40
11	e	601	ADP	C5-C4	2.44	1.47	1.40
11	D	601	ADP	C5-C4	2.44	1.47	1.40
11	z	601	ADP	C5-C4	2.42	1.47	1.40
11	g	601	ADP	C5-C4	2.42	1.47	1.40
11	a	601	ADP	C5-C4	2.42	1.47	1.40
11	Q	602	ADP	C5-C4	2.42	1.47	1.40
11	G	601	ADP	C5-C4	2.41	1.47	1.40
11	A	601	ADP	C5-C4	2.41	1.47	1.40
11	q	601	ADP	C5-C4	2.41	1.47	1.40
11	Z	601	ADP	C5-C4	2.40	1.47	1.40
11	b	601	ADP	C5-C4	2.39	1.47	1.40
11	d	601	ADP	C5-C4	2.39	1.47	1.40
11	E	601	ADP	C5-C4	2.39	1.47	1.40
11	H	601	ADP	C5-C4	2.38	1.47	1.40
11	h	601	ADP	C2'-C1'	-2.28	1.50	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	h	601	ADP	PA-O3A-PB	-4.97	115.77	132.83
11	D	601	ADP	PA-O3A-PB	-4.28	118.15	132.83
11	h	601	ADP	C3'-C2'-C1'	4.21	107.31	100.98
14	T	502	GTP	PB-O3B-PG	-4.18	118.50	132.83
11	e	601	ADP	PA-O3A-PB	-4.08	118.83	132.83
11	B	601	ADP	PA-O3A-PB	-3.91	119.43	132.83
11	d	601	ADP	PA-O3A-PB	-3.83	119.68	132.83
11	G	601	ADP	N3-C2-N1	-3.71	122.88	128.68
11	H	601	ADP	N3-C2-N1	-3.69	122.91	128.68
11	A	601	ADP	N3-C2-N1	-3.69	122.91	128.68
11	b	601	ADP	N3-C2-N1	-3.69	122.92	128.68
11	z	601	ADP	N3-C2-N1	-3.66	122.95	128.68
11	Q	602	ADP	N3-C2-N1	-3.66	122.95	128.68
11	Z	601	ADP	N3-C2-N1	-3.66	122.96	128.68
11	d	601	ADP	N3-C2-N1	-3.65	122.98	128.68
11	q	601	ADP	N3-C2-N1	-3.64	122.98	128.68
11	a	601	ADP	N3-C2-N1	-3.64	122.99	128.68
11	E	601	ADP	N3-C2-N1	-3.62	123.02	128.68
11	e	601	ADP	N3-C2-N1	-3.61	123.03	128.68
11	g	601	ADP	N3-C2-N1	-3.60	123.06	128.68
11	B	601	ADP	N3-C2-N1	-3.59	123.07	128.68
11	b	601	ADP	PA-O3A-PB	-3.55	120.64	132.83
11	z	601	ADP	PA-O3A-PB	-3.52	120.74	132.83
11	Q	602	ADP	PA-O3A-PB	-3.51	120.77	132.83
11	D	601	ADP	N3-C2-N1	-3.48	123.23	128.68
11	a	601	ADP	PA-O3A-PB	-3.47	120.92	132.83
11	B	601	ADP	C3'-C2'-C1'	3.42	106.13	100.98
11	g	601	ADP	PA-O3A-PB	-3.40	121.16	132.83
11	e	601	ADP	C3'-C2'-C1'	3.36	106.04	100.98
11	Z	601	ADP	PA-O3A-PB	-3.36	121.29	132.83
11	g	601	ADP	C3'-C2'-C1'	3.33	106.00	100.98
14	T	502	GTP	PA-O3A-PB	-3.31	121.48	132.83
11	D	601	ADP	C3'-C2'-C1'	3.26	105.89	100.98
11	G	601	ADP	C3'-C2'-C1'	3.25	105.88	100.98
11	z	601	ADP	C3'-C2'-C1'	3.24	105.86	100.98
11	E	601	ADP	PA-O3A-PB	-3.24	121.71	132.83
11	q	601	ADP	PA-O3A-PB	-3.24	121.72	132.83
11	A	601	ADP	C3'-C2'-C1'	3.17	105.76	100.98
11	a	601	ADP	C3'-C2'-C1'	3.09	105.62	100.98
11	Q	602	ADP	C3'-C2'-C1'	3.08	105.61	100.98
11	b	601	ADP	C3'-C2'-C1'	3.00	105.49	100.98
11	d	601	ADP	C3'-C2'-C1'	2.98	105.46	100.98
11	H	601	ADP	C3'-C2'-C1'	2.97	105.45	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	q	601	ADP	C3'-C2'-C1'	2.94	105.41	100.98
11	E	601	ADP	C3'-C2'-C1'	2.94	105.40	100.98
11	h	601	ADP	N3-C2-N1	-2.93	124.10	128.68
11	h	601	ADP	C4-C5-N7	-2.92	106.36	109.40
11	b	601	ADP	C4-C5-N7	-2.84	106.44	109.40
11	z	601	ADP	C4-C5-N7	-2.84	106.44	109.40
11	Z	601	ADP	C3'-C2'-C1'	2.84	105.25	100.98
11	A	601	ADP	C4-C5-N7	-2.82	106.46	109.40
11	q	601	ADP	C4-C5-N7	-2.81	106.47	109.40
11	a	601	ADP	C4-C5-N7	-2.79	106.49	109.40
11	H	601	ADP	C4-C5-N7	-2.78	106.50	109.40
11	B	601	ADP	C4-C5-N7	-2.76	106.53	109.40
11	d	601	ADP	C4-C5-N7	-2.75	106.53	109.40
11	G	601	ADP	C4-C5-N7	-2.74	106.54	109.40
11	Z	601	ADP	C4-C5-N7	-2.74	106.54	109.40
11	E	601	ADP	C4-C5-N7	-2.74	106.55	109.40
11	g	601	ADP	C4-C5-N7	-2.71	106.58	109.40
11	D	601	ADP	C4-C5-N7	-2.69	106.59	109.40
11	e	601	ADP	C4-C5-N7	-2.68	106.60	109.40
11	Q	602	ADP	C4-C5-N7	-2.66	106.62	109.40
14	T	502	GTP	C5-C6-N1	2.37	118.14	113.95
11	G	601	ADP	PA-O3A-PB	-2.35	124.78	132.83
14	T	502	GTP	C8-N7-C5	2.20	107.18	102.99
11	A	601	ADP	PA-O3A-PB	-2.18	125.34	132.83
11	H	601	ADP	C2-N1-C6	2.03	122.22	118.75
11	d	601	ADP	C2-N1-C6	2.01	122.19	118.75
11	Z	601	ADP	C2-N1-C6	2.01	122.19	118.75
11	z	601	ADP	C2-N1-C6	2.01	122.19	118.75
11	A	601	ADP	C2-N1-C6	2.01	122.18	118.75

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	601	ADP	C5'-O5'-PA-O1A
11	E	601	ADP	C5'-O5'-PA-O2A
11	Q	602	ADP	C5'-O5'-PA-O1A
11	Q	602	ADP	C5'-O5'-PA-O2A
11	Z	601	ADP	C5'-O5'-PA-O3A
11	a	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	PB-O3A-PA-O5'
11	g	601	ADP	C5'-O5'-PA-O1A

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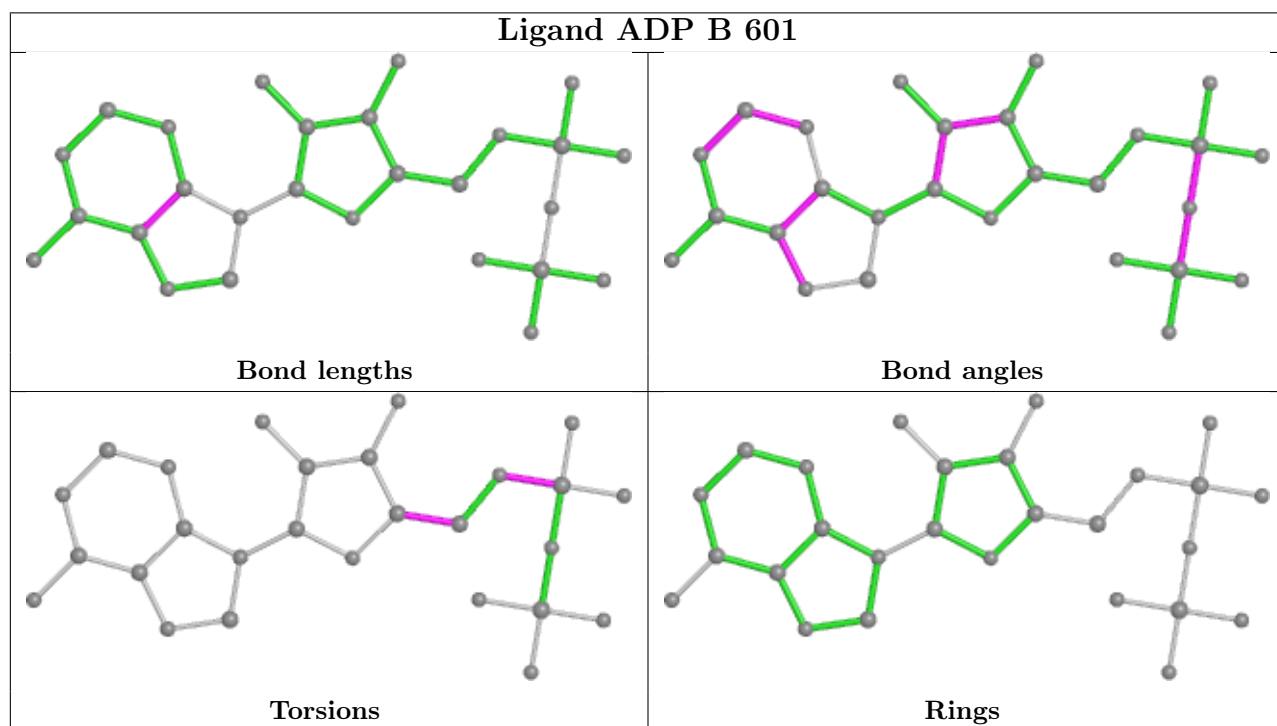
*Continued from previous page...*

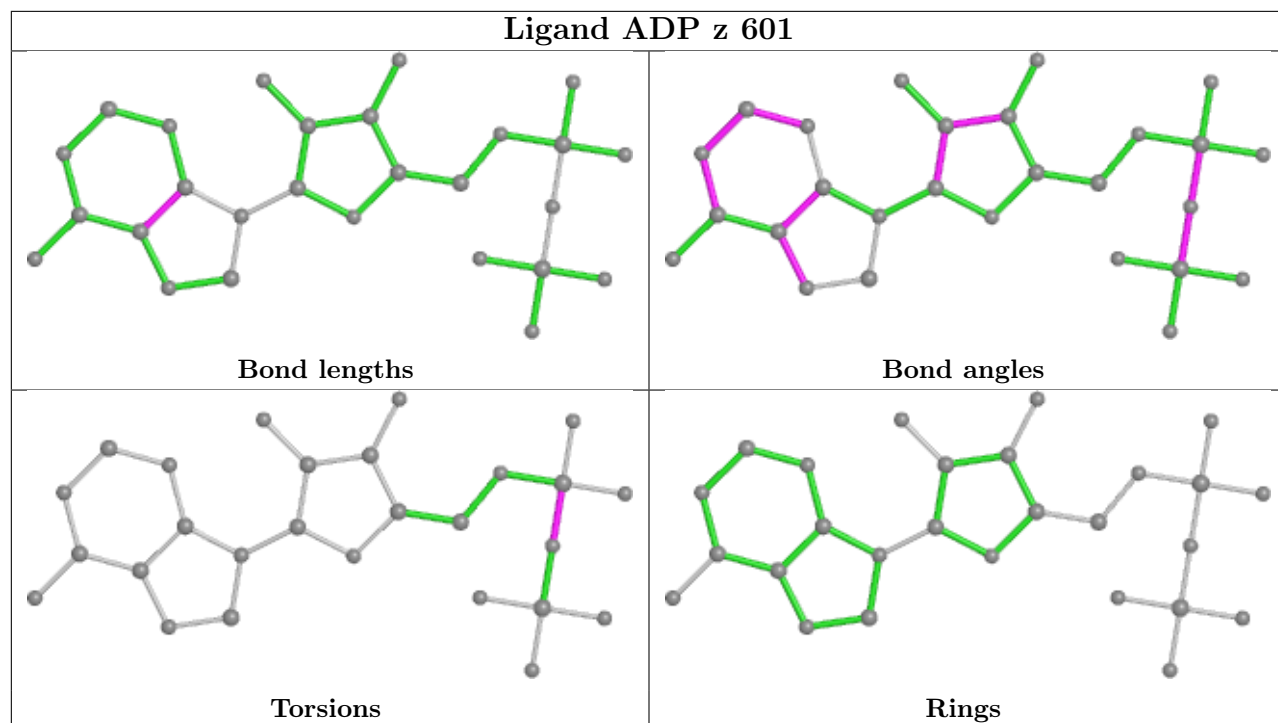
Mol	Chain	Res	Type	Atoms
11	h	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O3A
14	T	502	GTP	C5'-O5'-PA-O1A
14	T	502	GTP	C5'-O5'-PA-O2A
14	T	502	GTP	C3'-C4'-C5'-O5'
14	T	502	GTP	O4'-C4'-C5'-O5'
11	a	601	ADP	O4'-C4'-C5'-O5'
11	a	601	ADP	C3'-C4'-C5'-O5'
11	Z	601	ADP	PB-O3A-PA-O1A
11	Q	602	ADP	O4'-C4'-C5'-O5'
14	T	502	GTP	C4'-C5'-O5'-PA
11	g	601	ADP	O4'-C4'-C5'-O5'
11	E	601	ADP	C5'-O5'-PA-O3A
11	g	601	ADP	C5'-O5'-PA-O3A
14	T	502	GTP	C5'-O5'-PA-O3A
11	e	601	ADP	O4'-C4'-C5'-O5'
11	A	601	ADP	PB-O3A-PA-O2A
11	G	601	ADP	PB-O3A-PA-O2A
11	z	601	ADP	PB-O3A-PA-O2A
11	Z	601	ADP	C5'-O5'-PA-O1A
11	Z	601	ADP	C5'-O5'-PA-O2A
11	e	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	O4'-C4'-C5'-O5'
11	e	601	ADP	PB-O3A-PA-O1A
11	B	601	ADP	O4'-C4'-C5'-O5'
11	B	601	ADP	C5'-O5'-PA-O3A
11	Q	602	ADP	C5'-O5'-PA-O3A
11	a	601	ADP	C5'-O5'-PA-O3A
11	e	601	ADP	C5'-O5'-PA-O3A
11	h	601	ADP	C5'-O5'-PA-O3A
11	D	601	ADP	O4'-C4'-C5'-O5'
11	G	601	ADP	PB-O3A-PA-O1A
11	Z	601	ADP	PB-O3A-PA-O2A
11	z	601	ADP	PB-O3A-PA-O1A
11	B	601	ADP	C5'-O5'-PA-O2A
11	a	601	ADP	C5'-O5'-PA-O1A
11	q	601	ADP	O4'-C4'-C5'-O5'

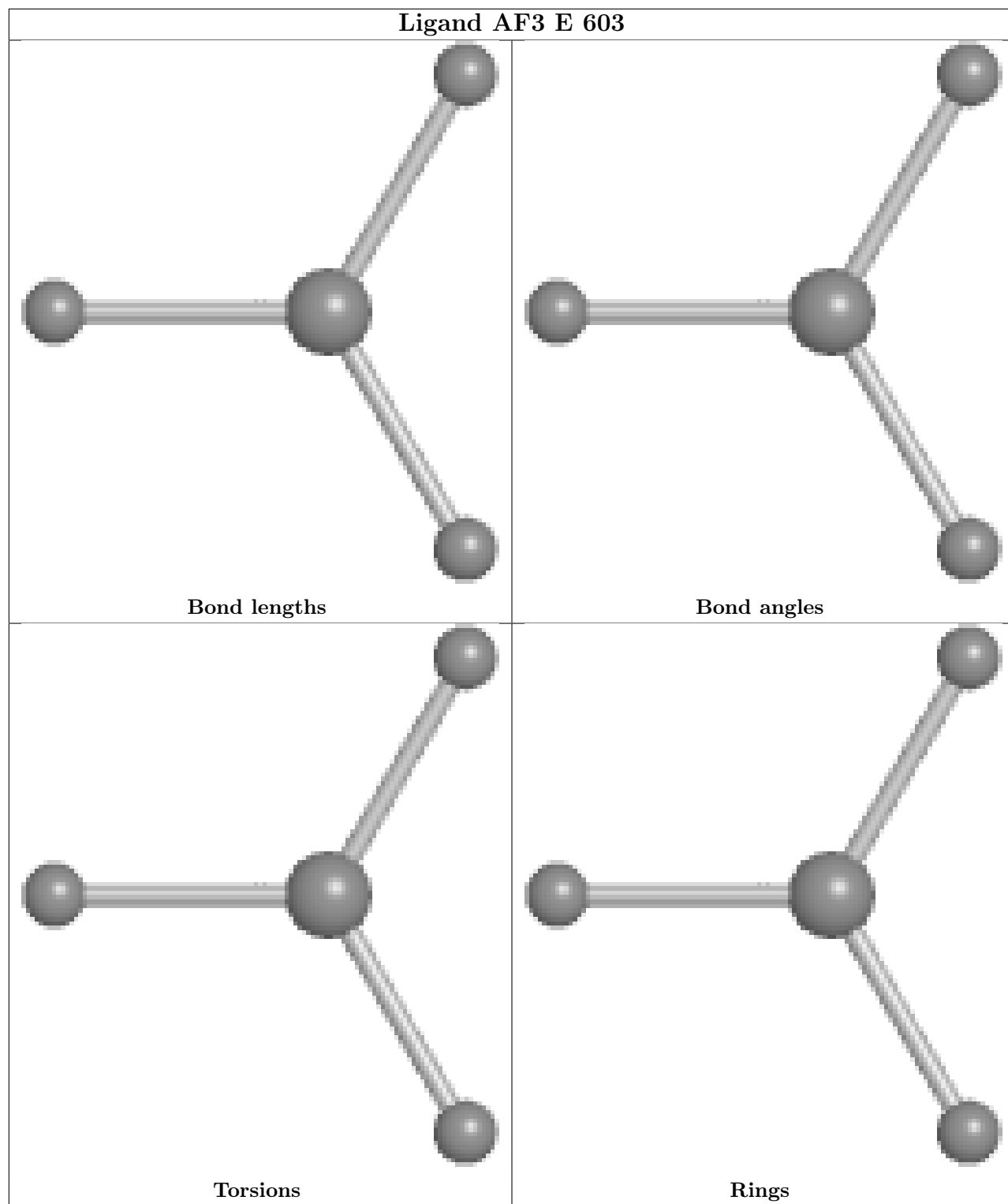
There are no ring outliers.

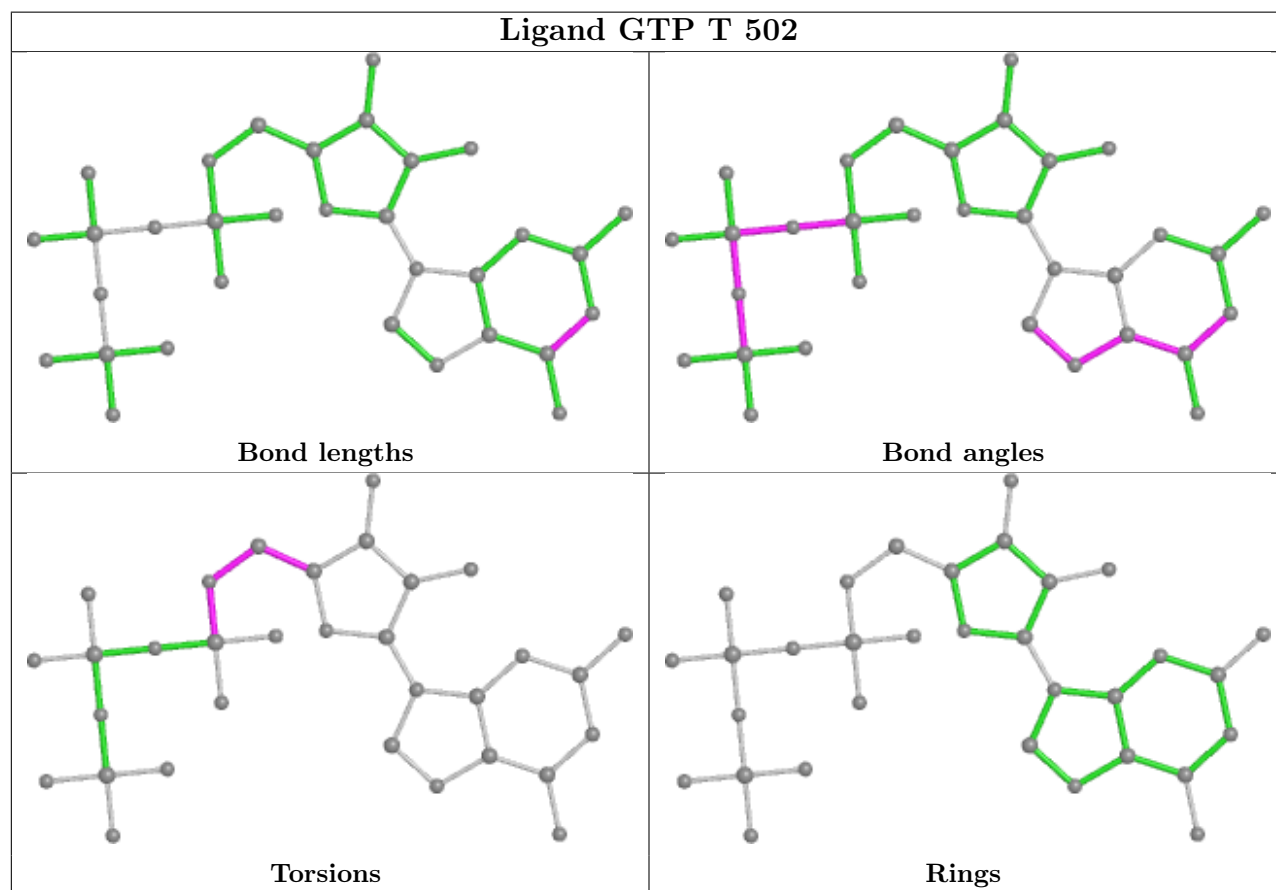
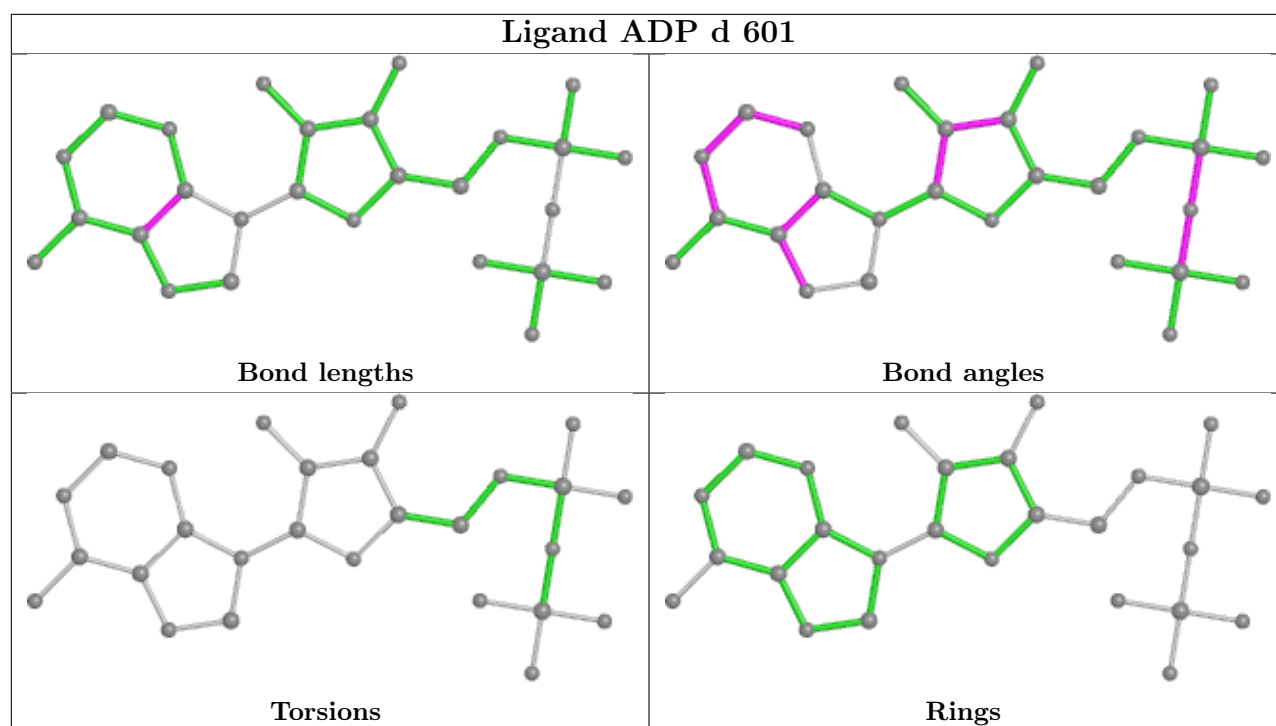
No monomer is involved in short contacts.

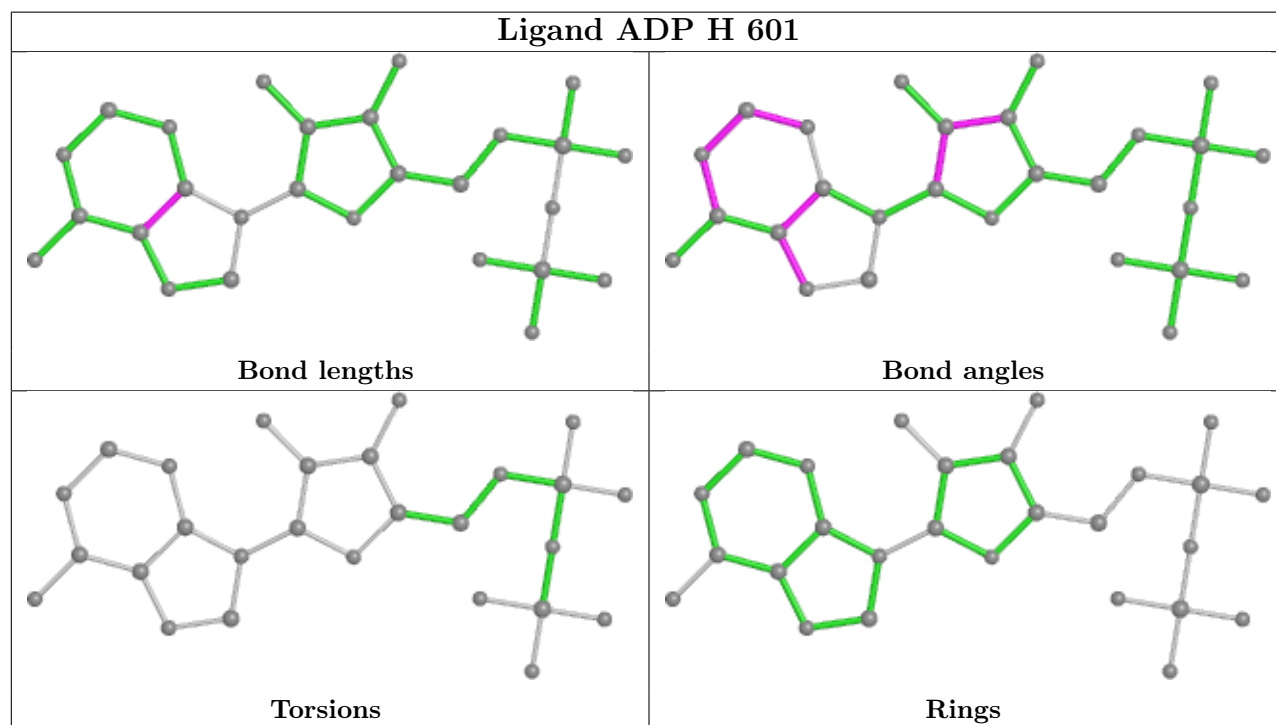
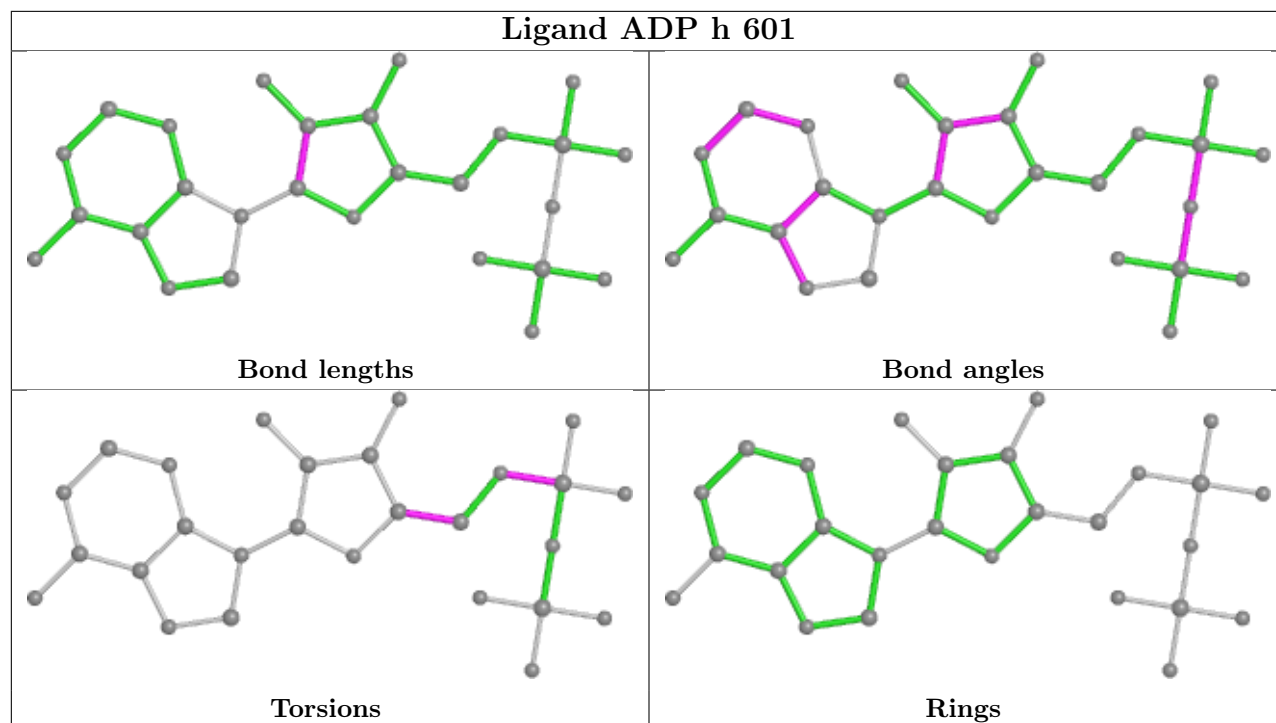
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

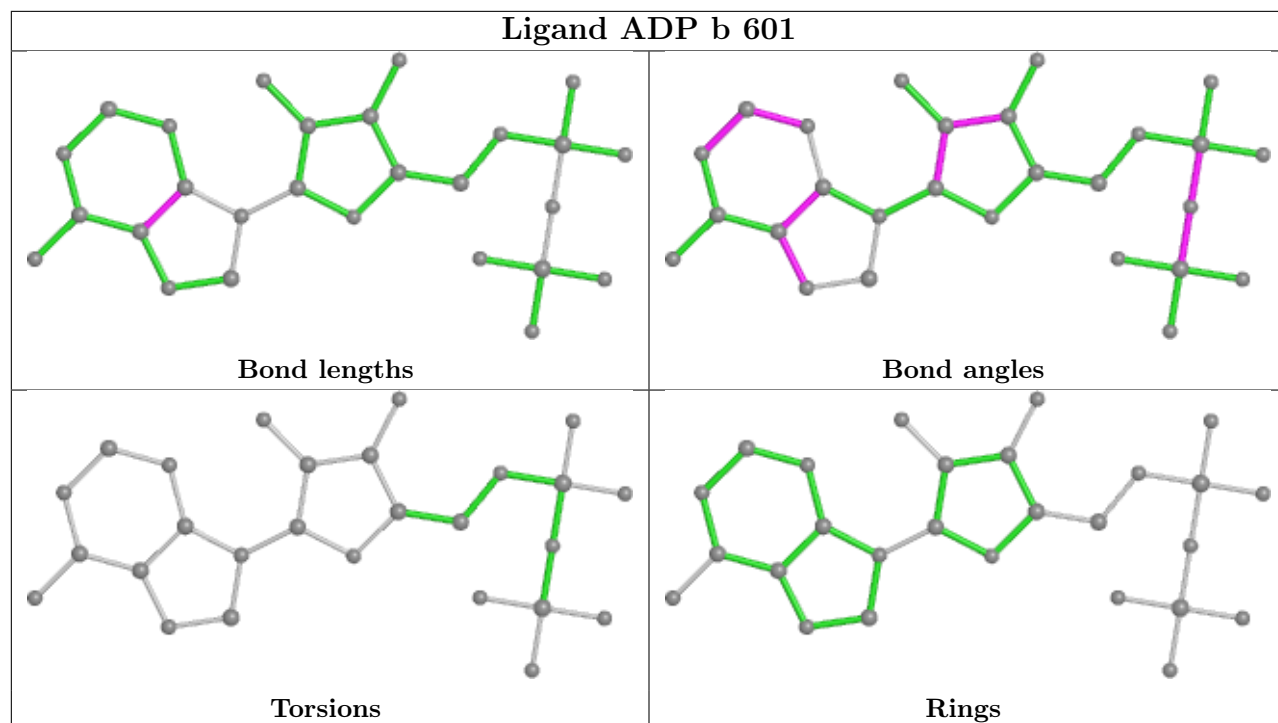


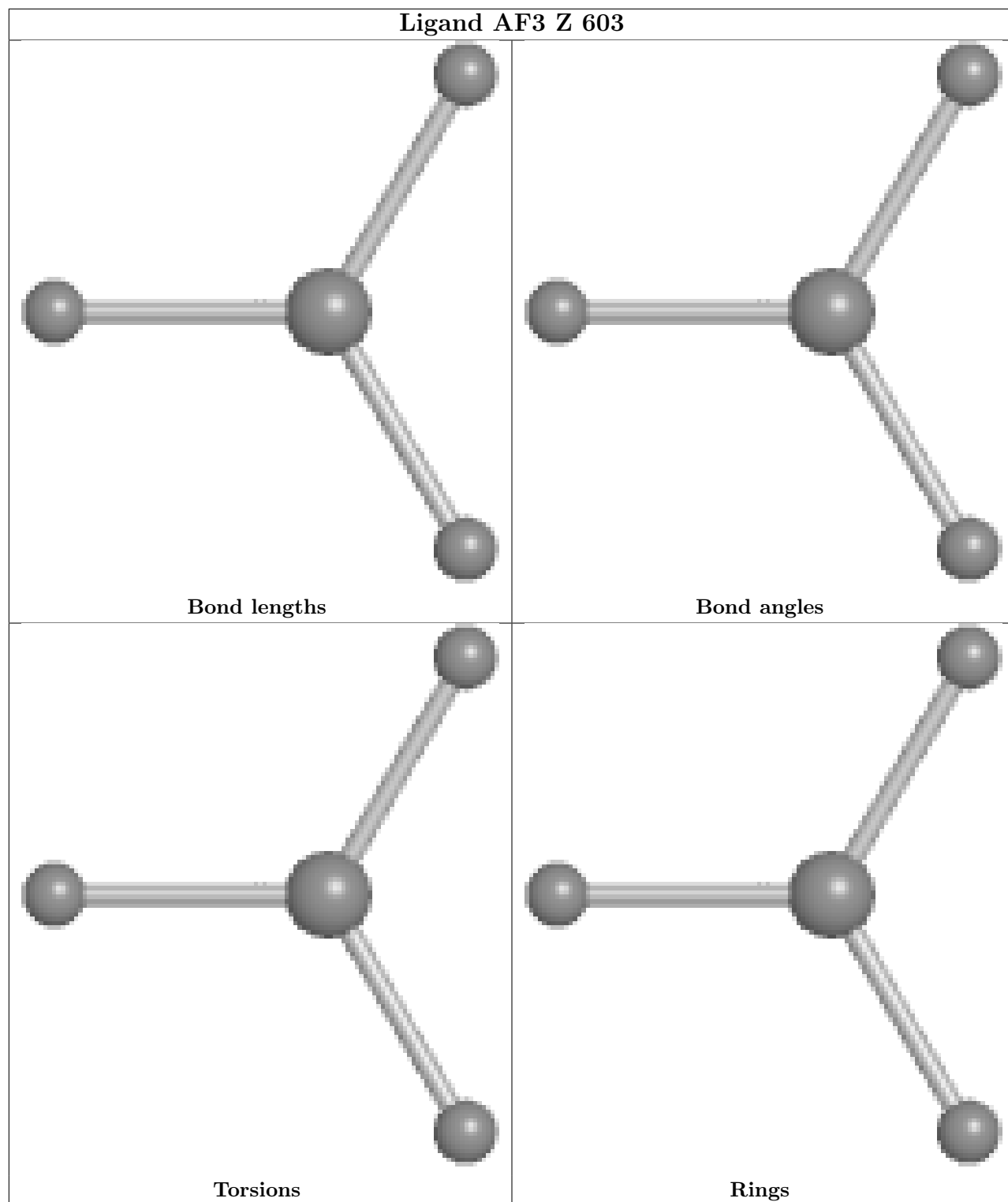




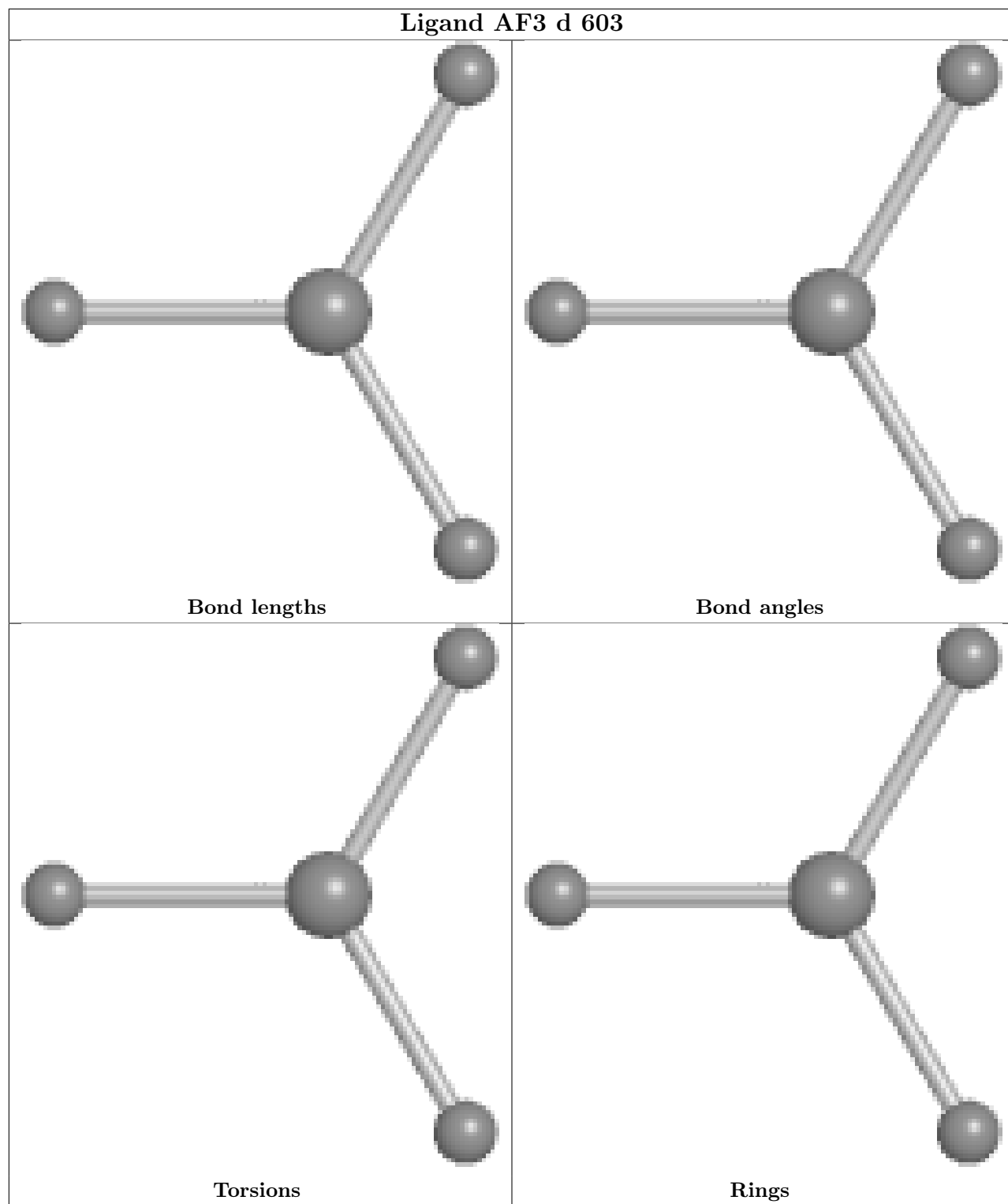


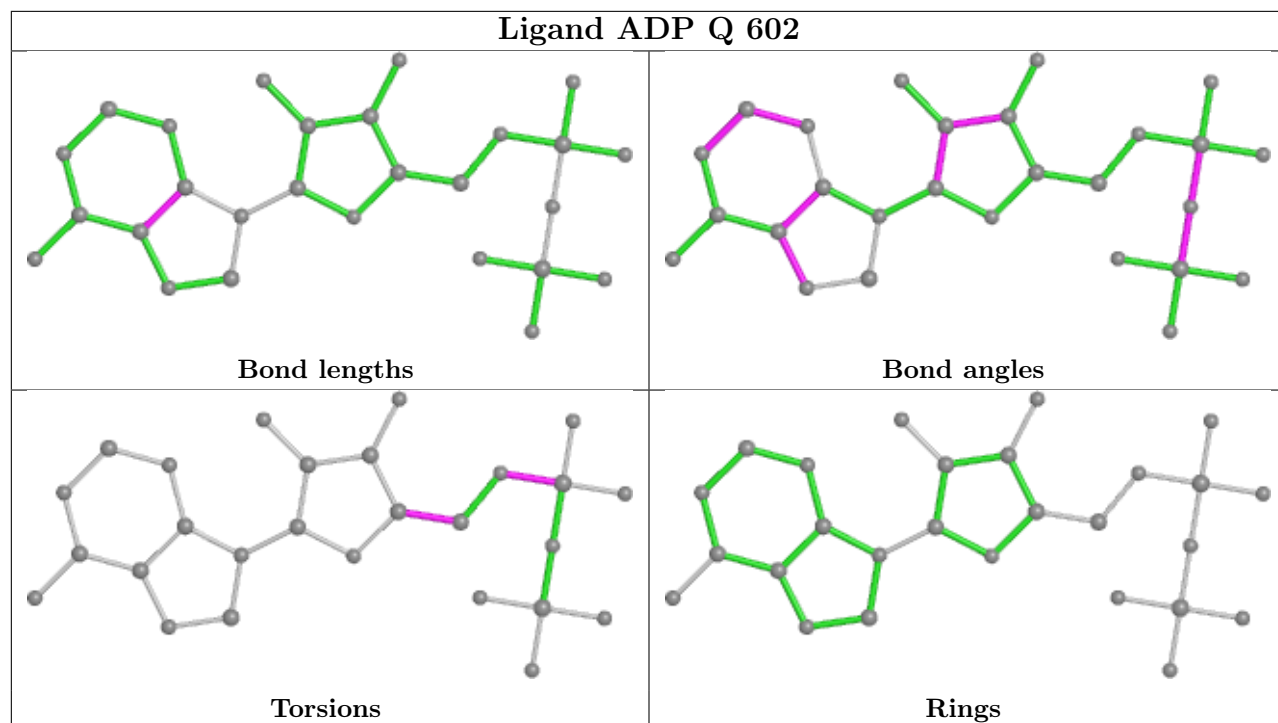


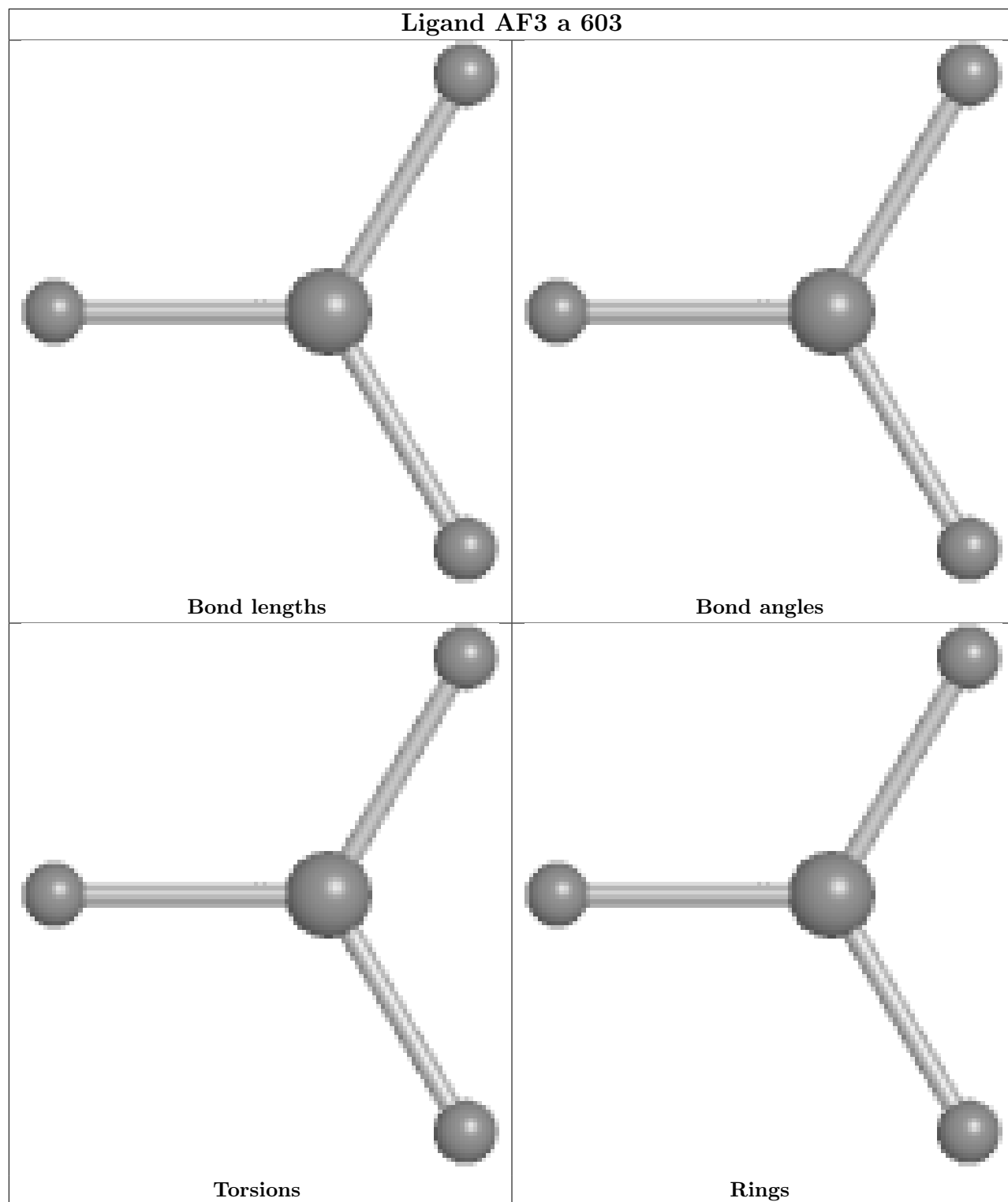


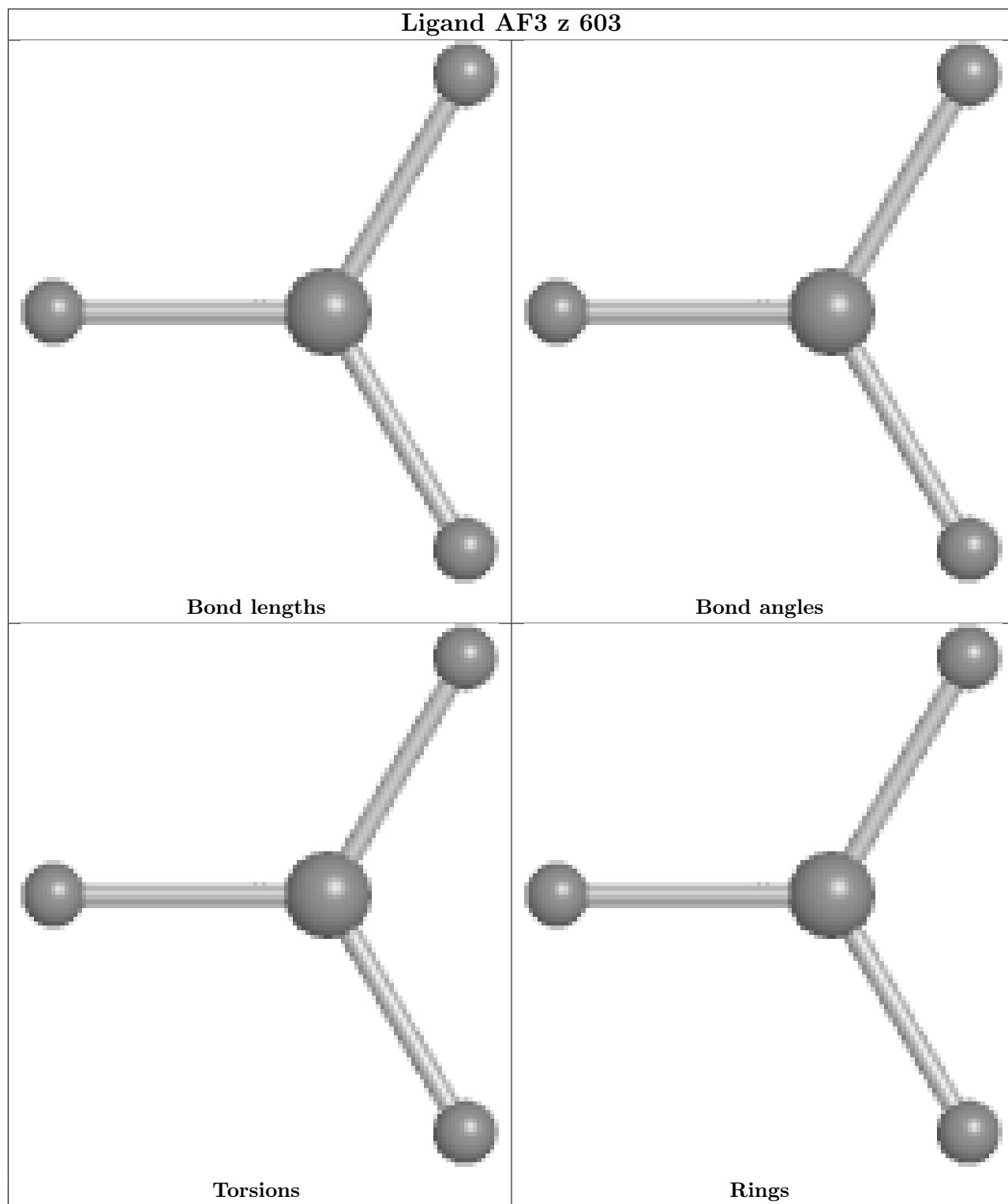


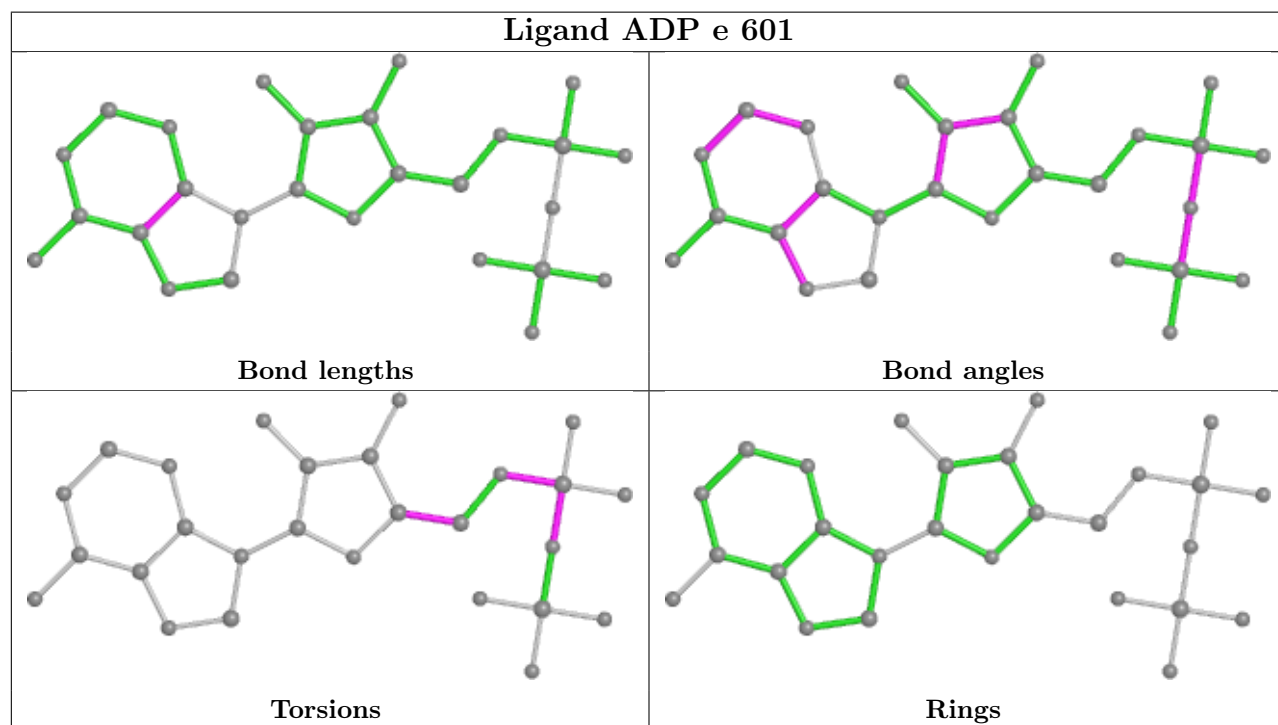
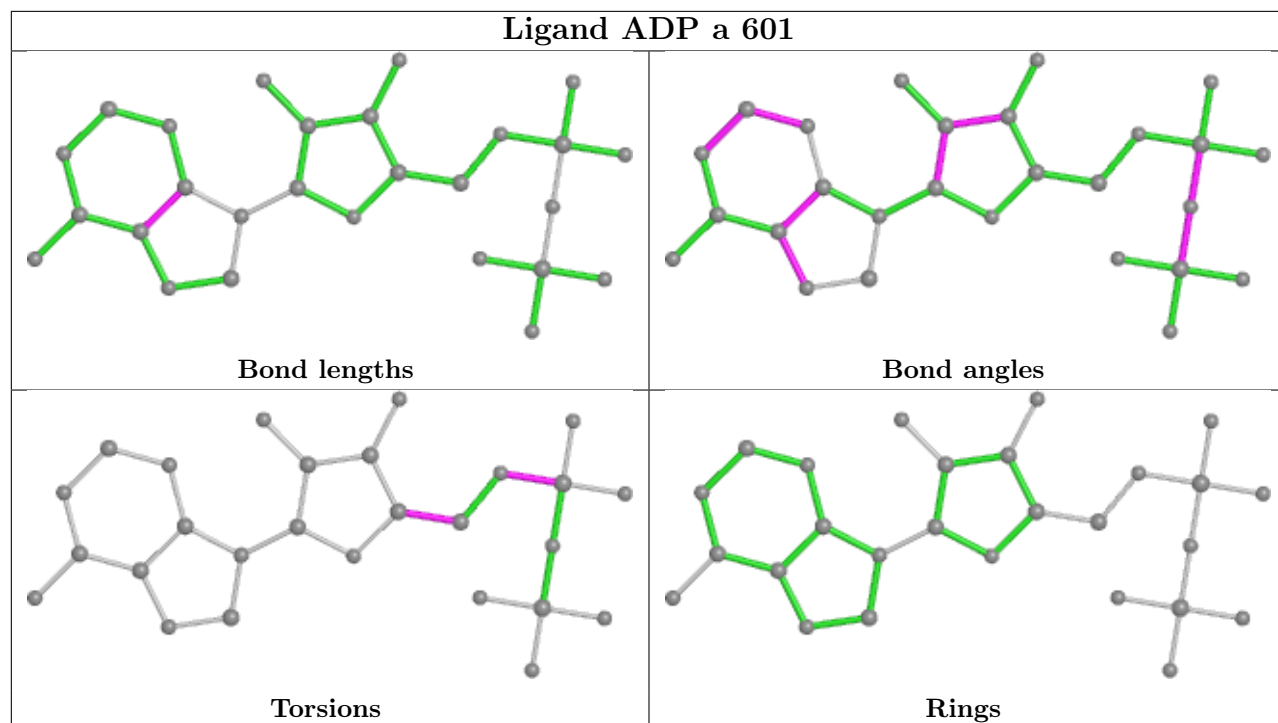


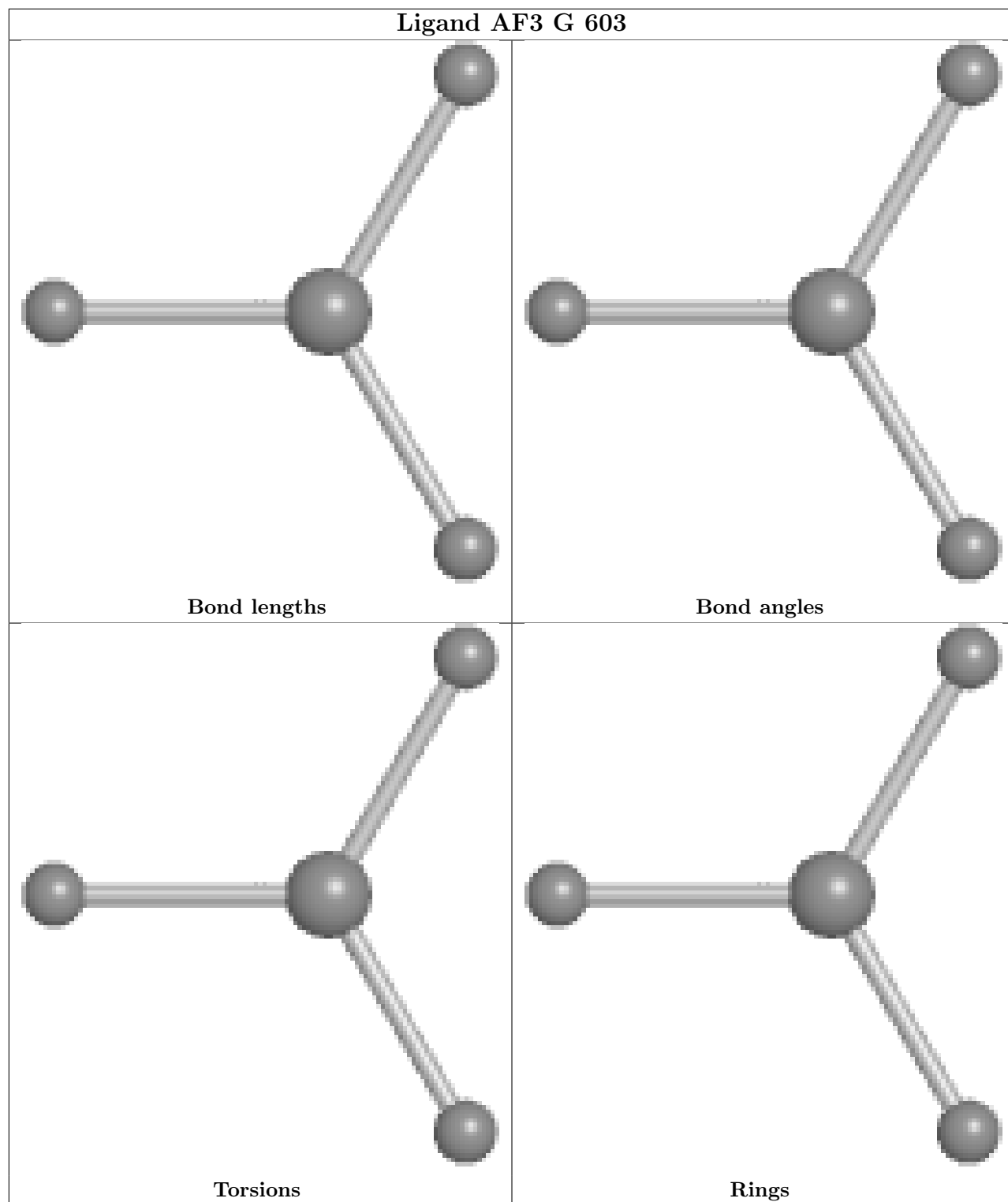


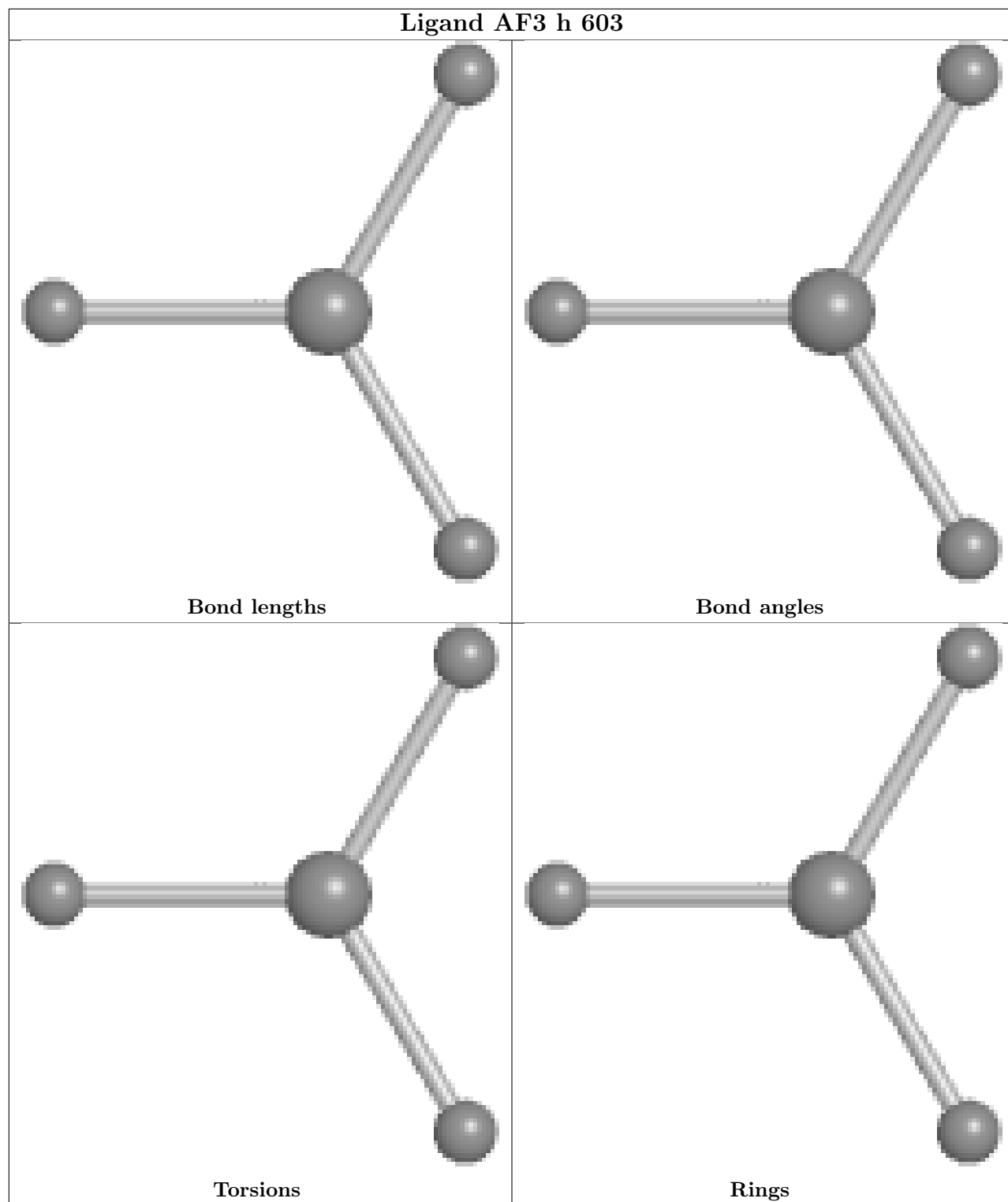


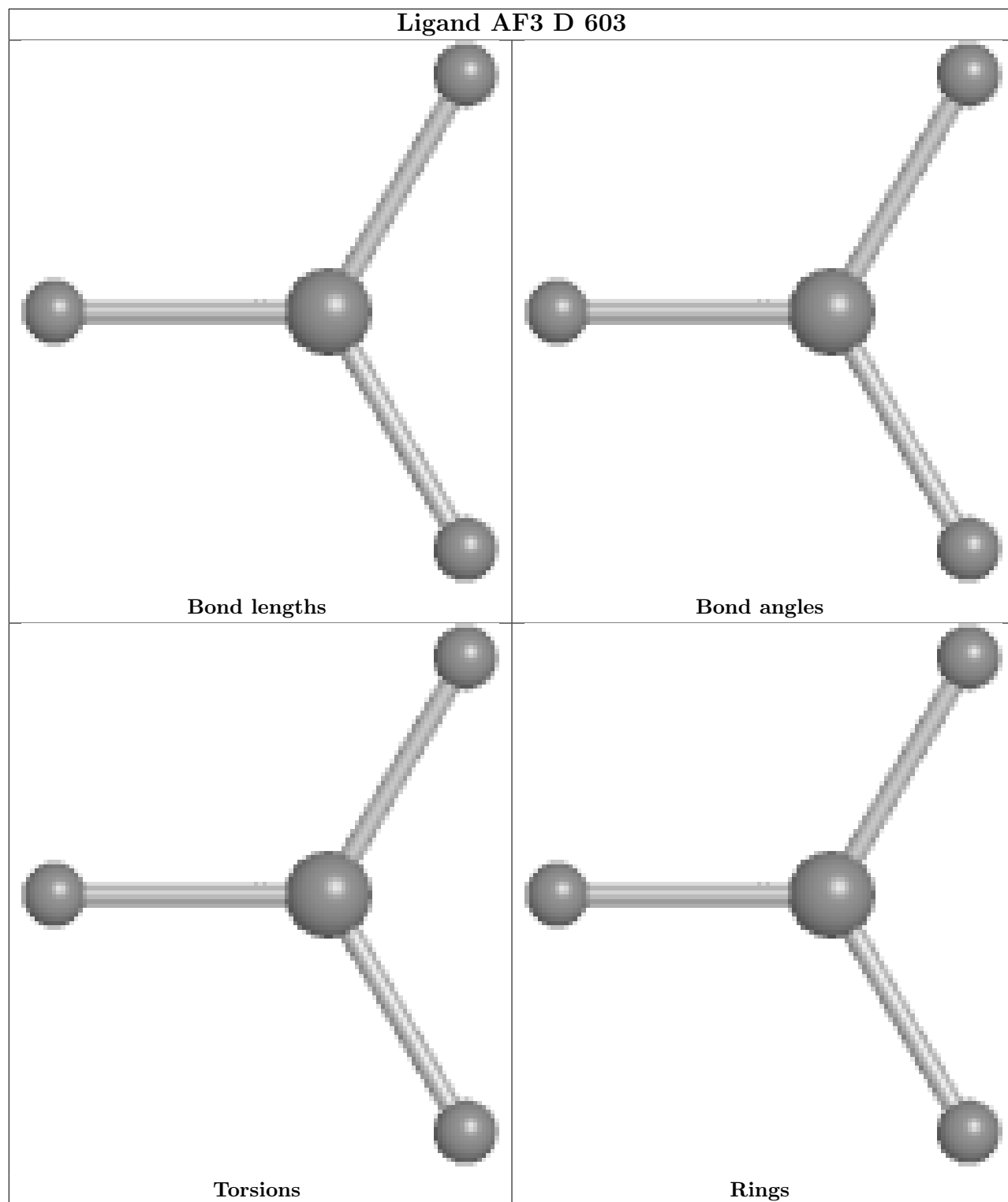




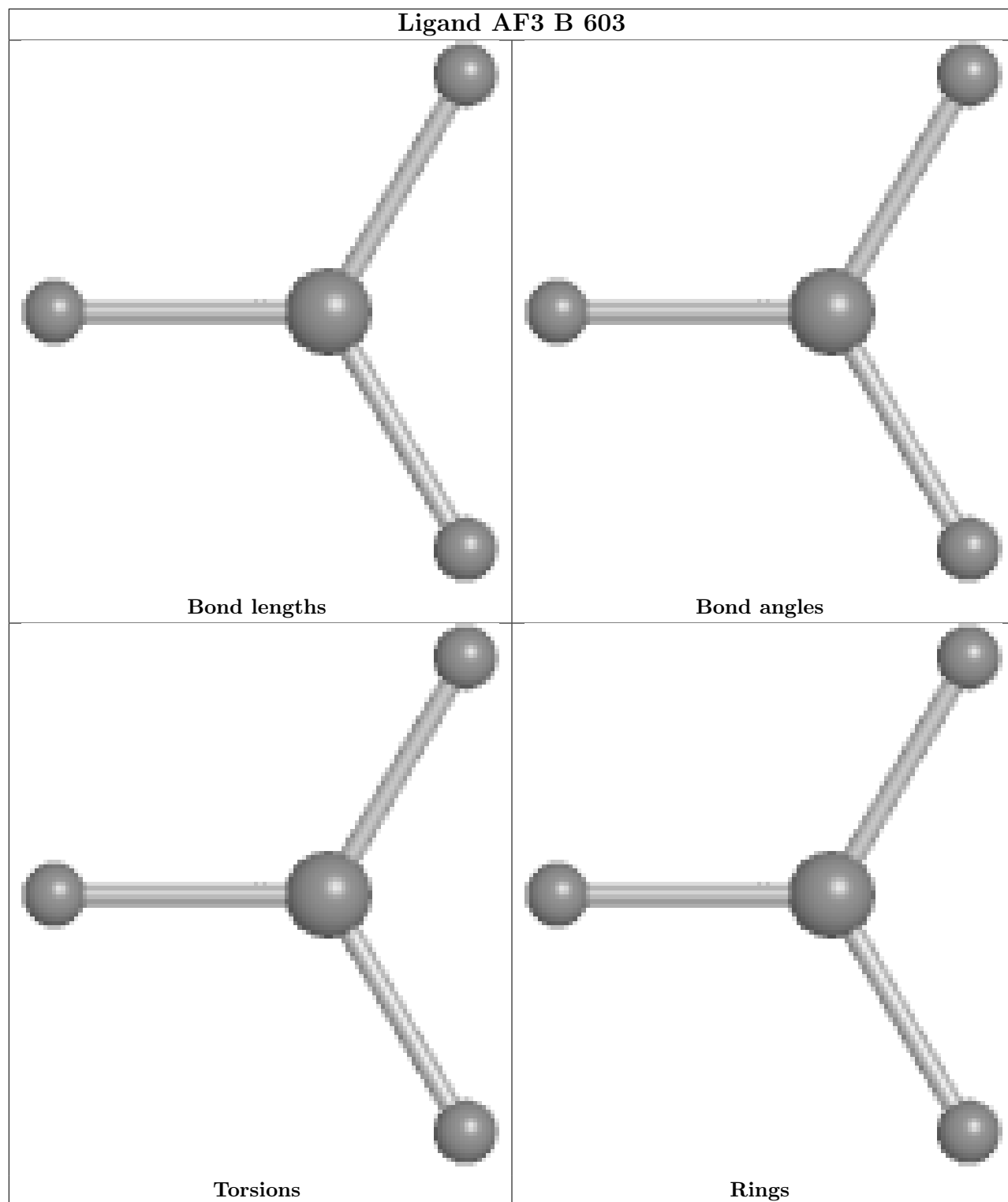


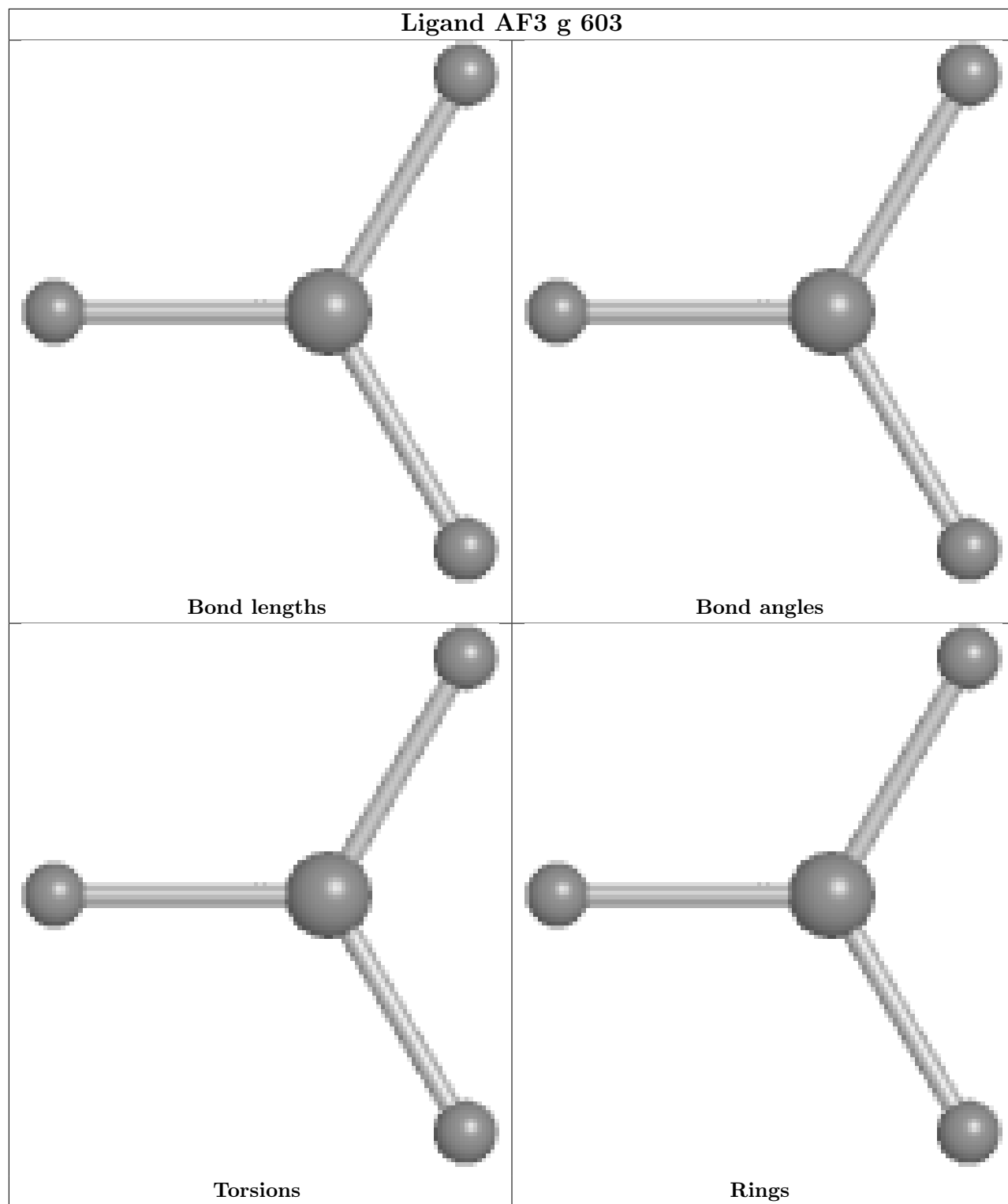


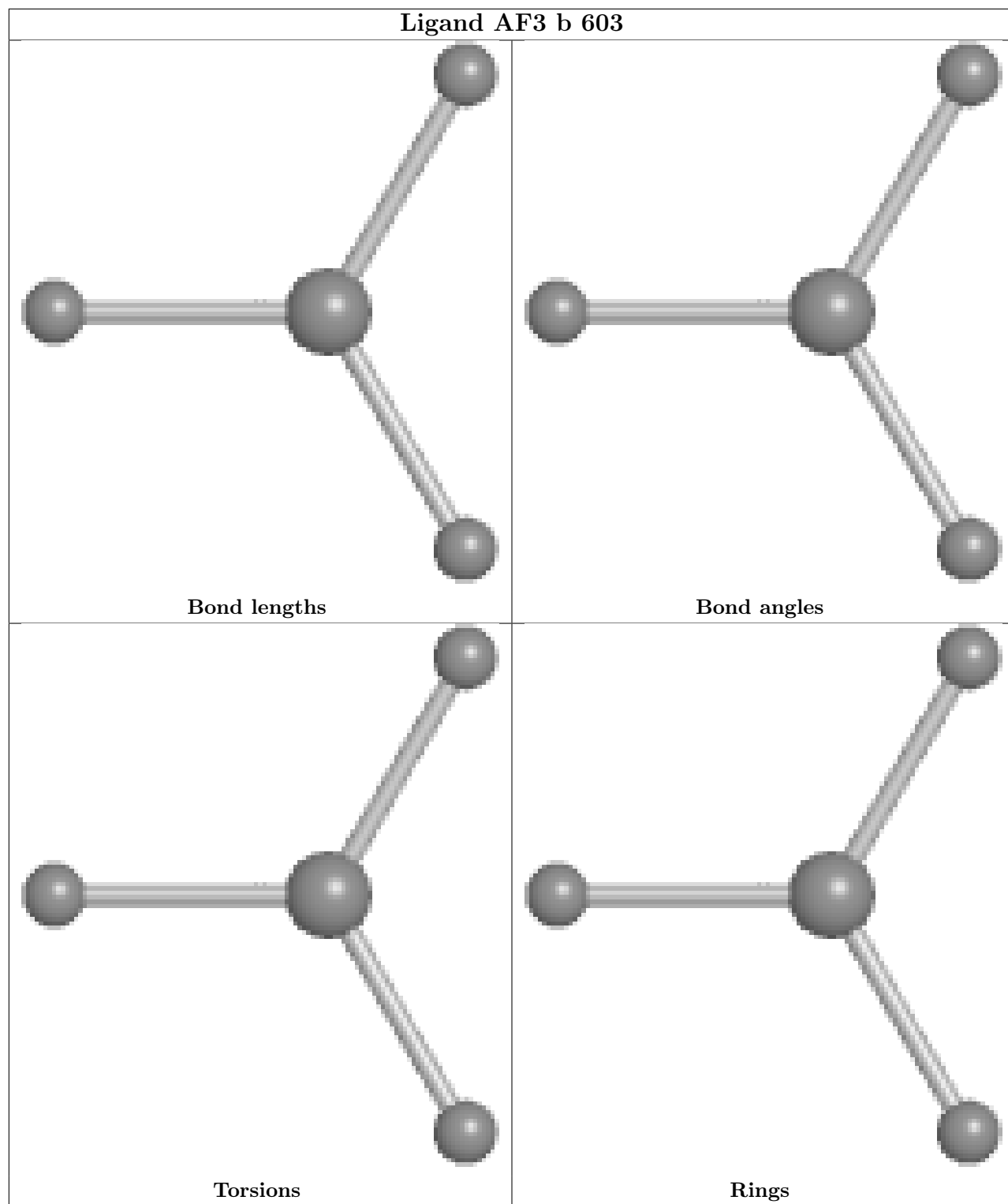


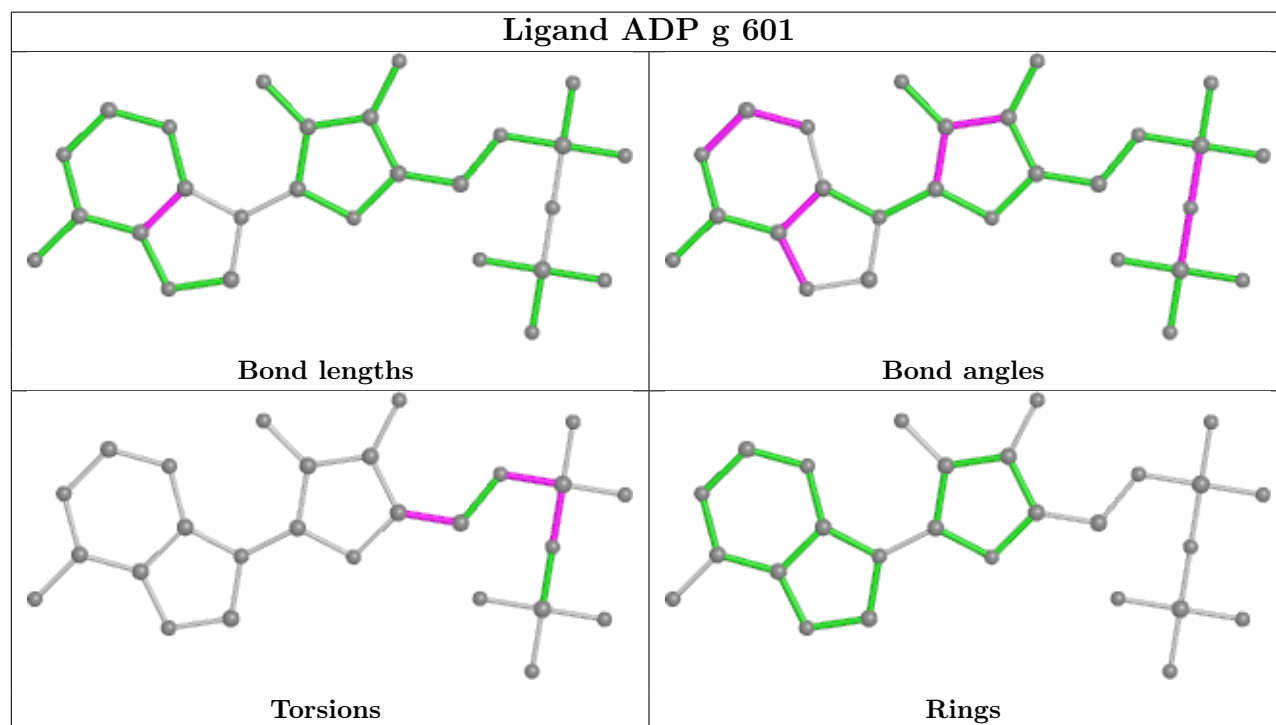
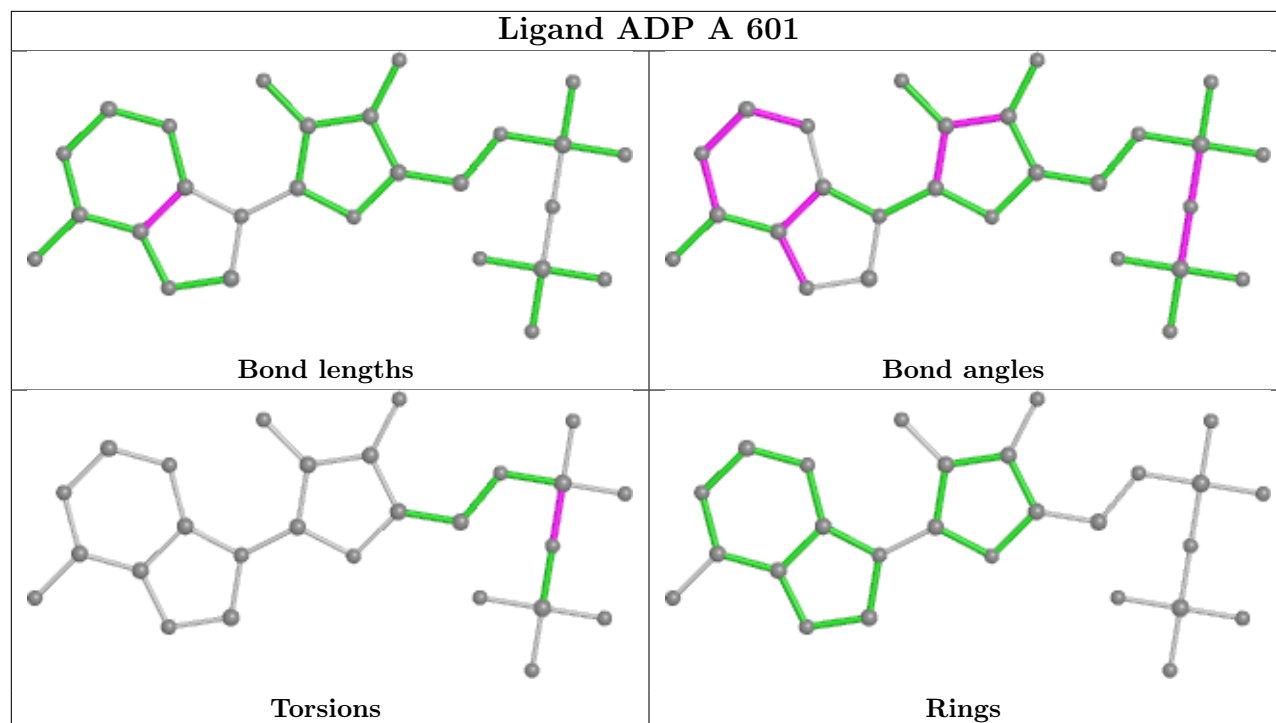


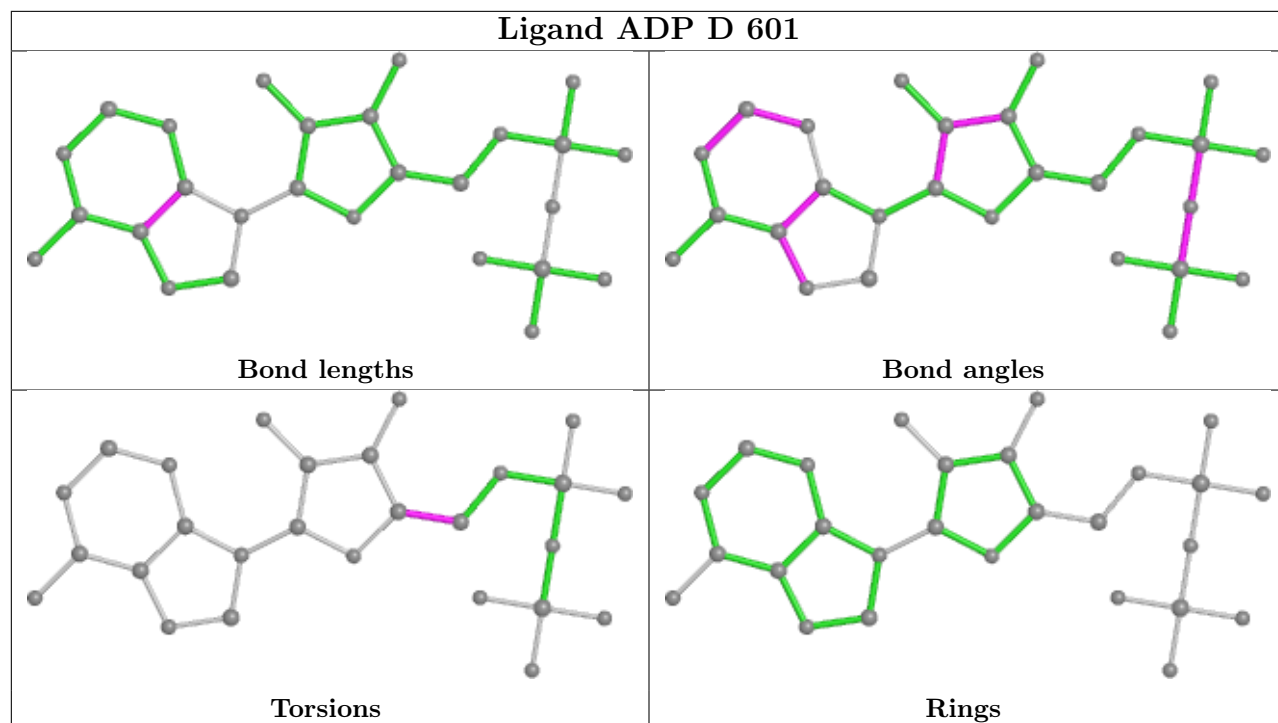


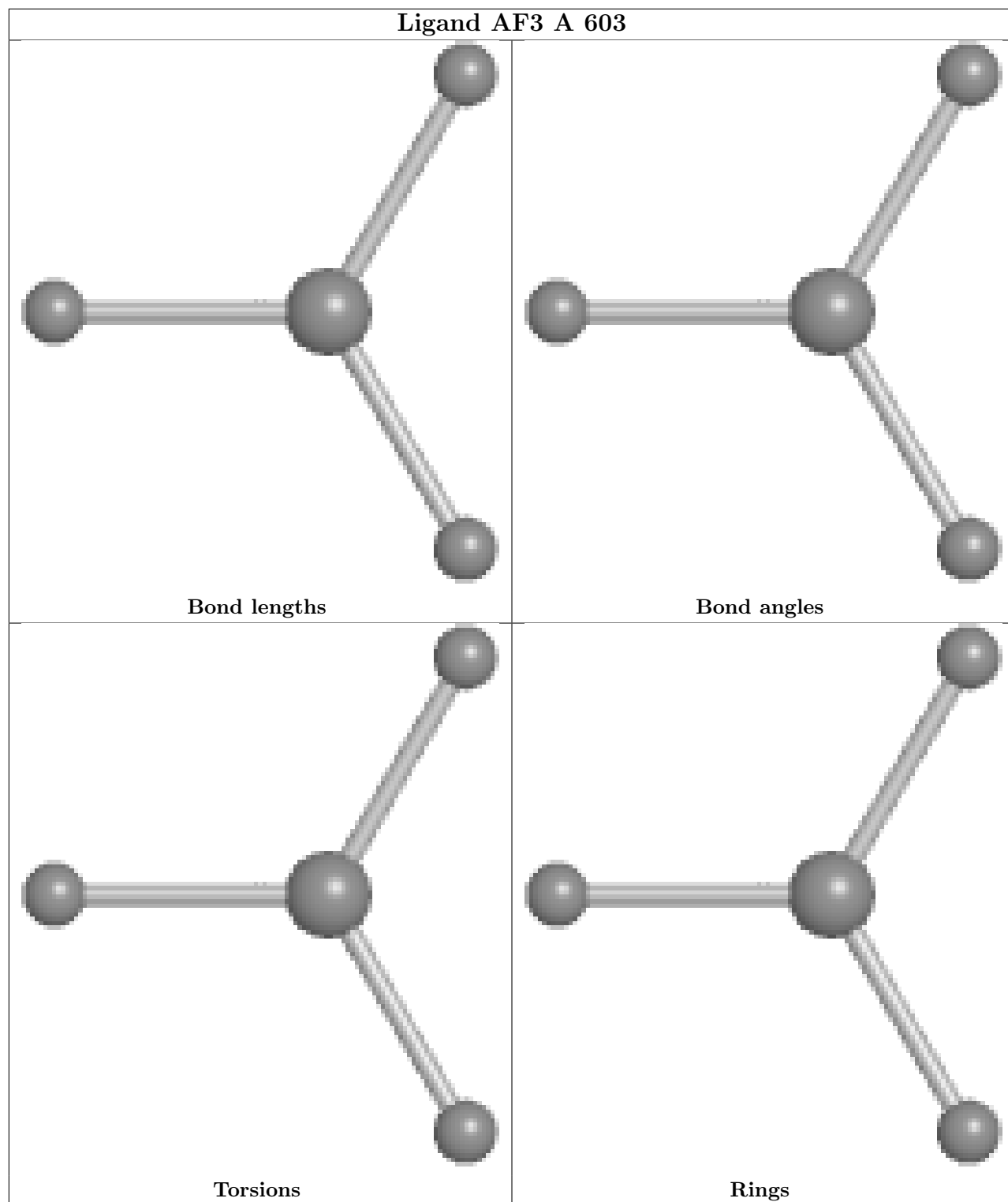


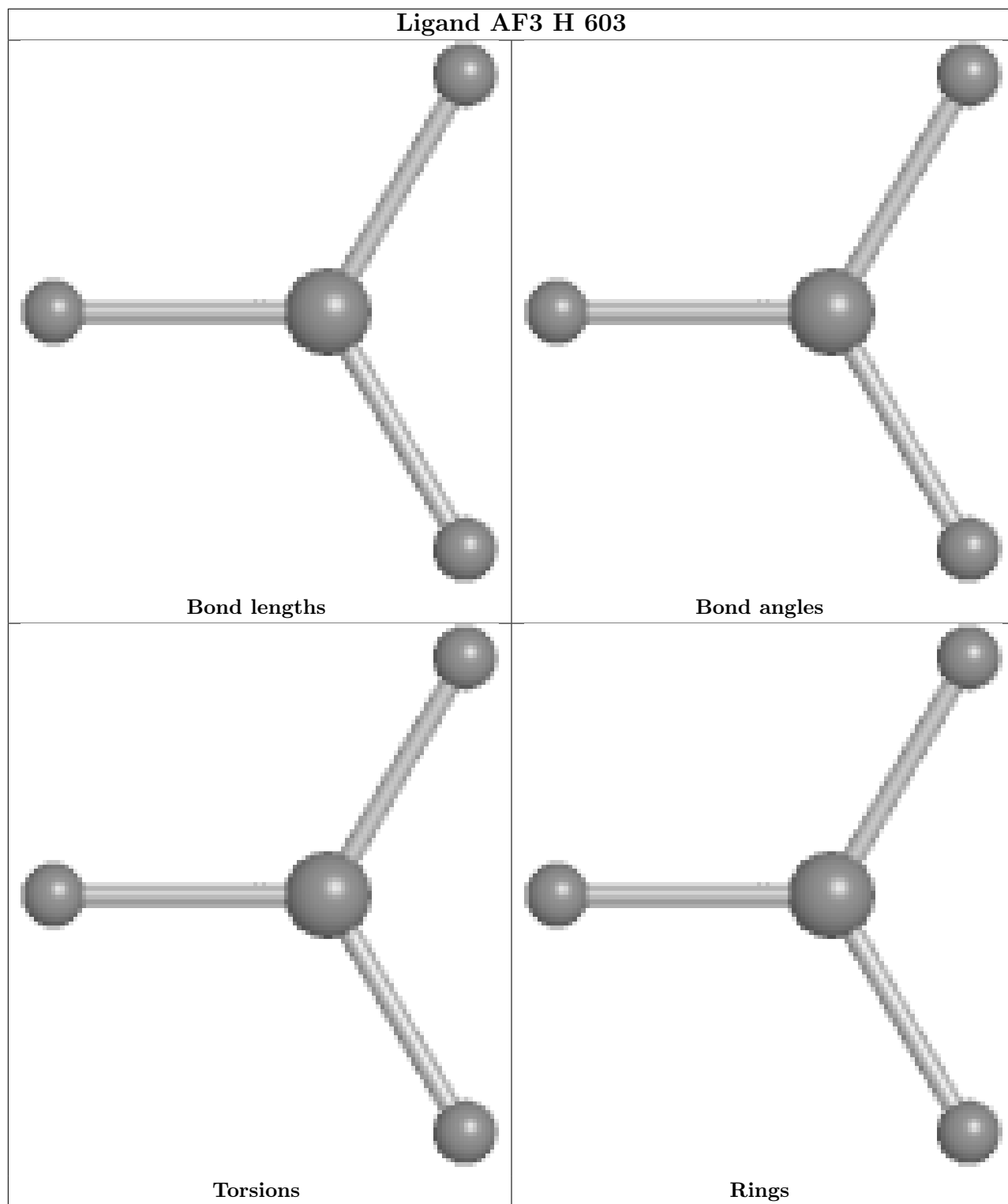


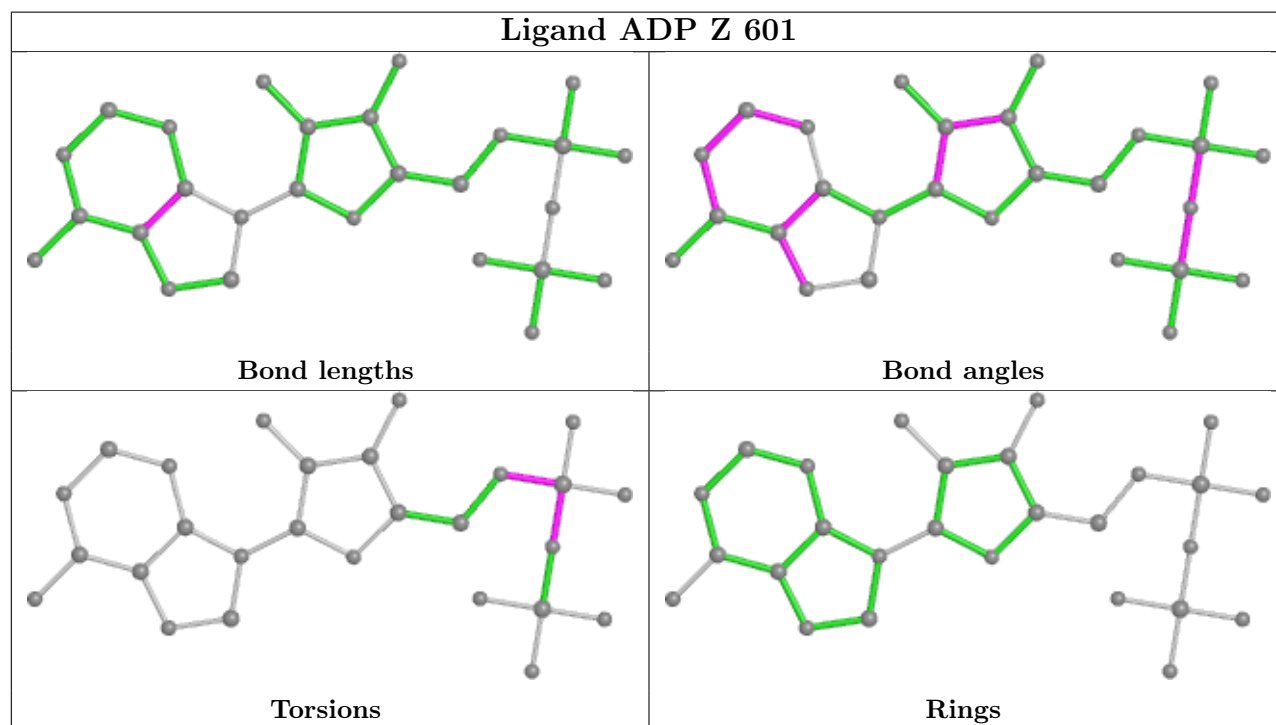
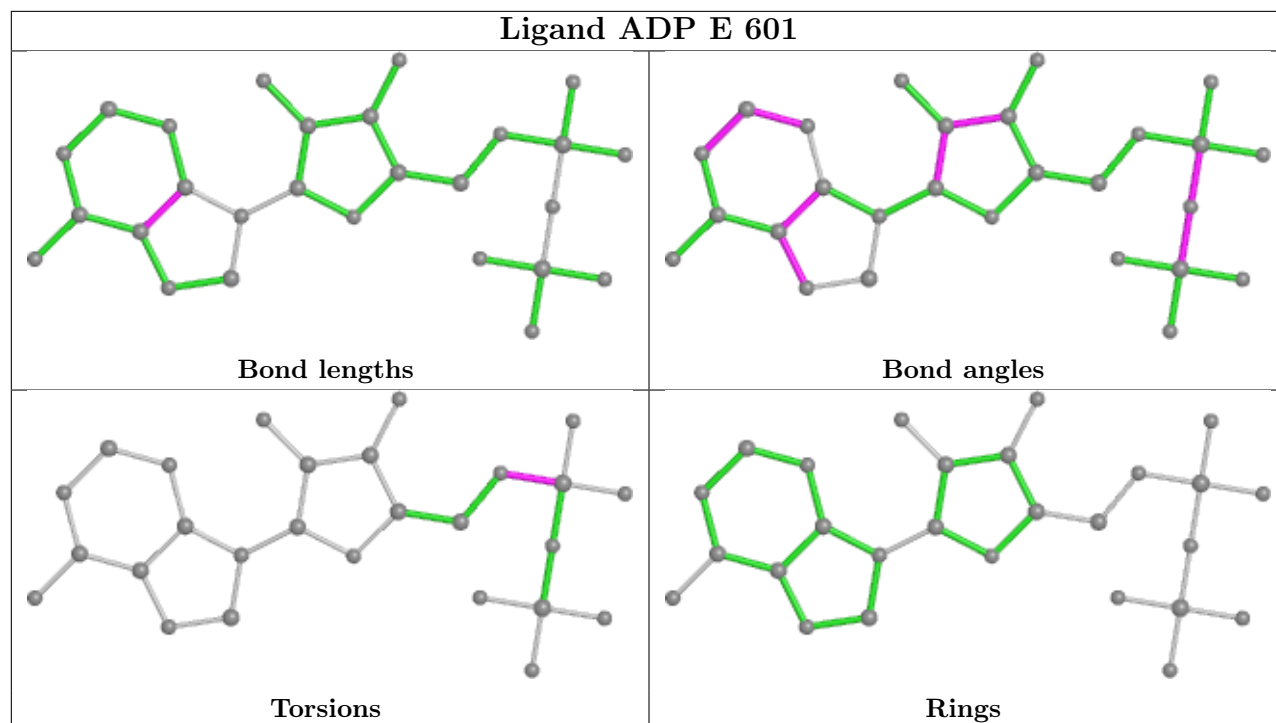




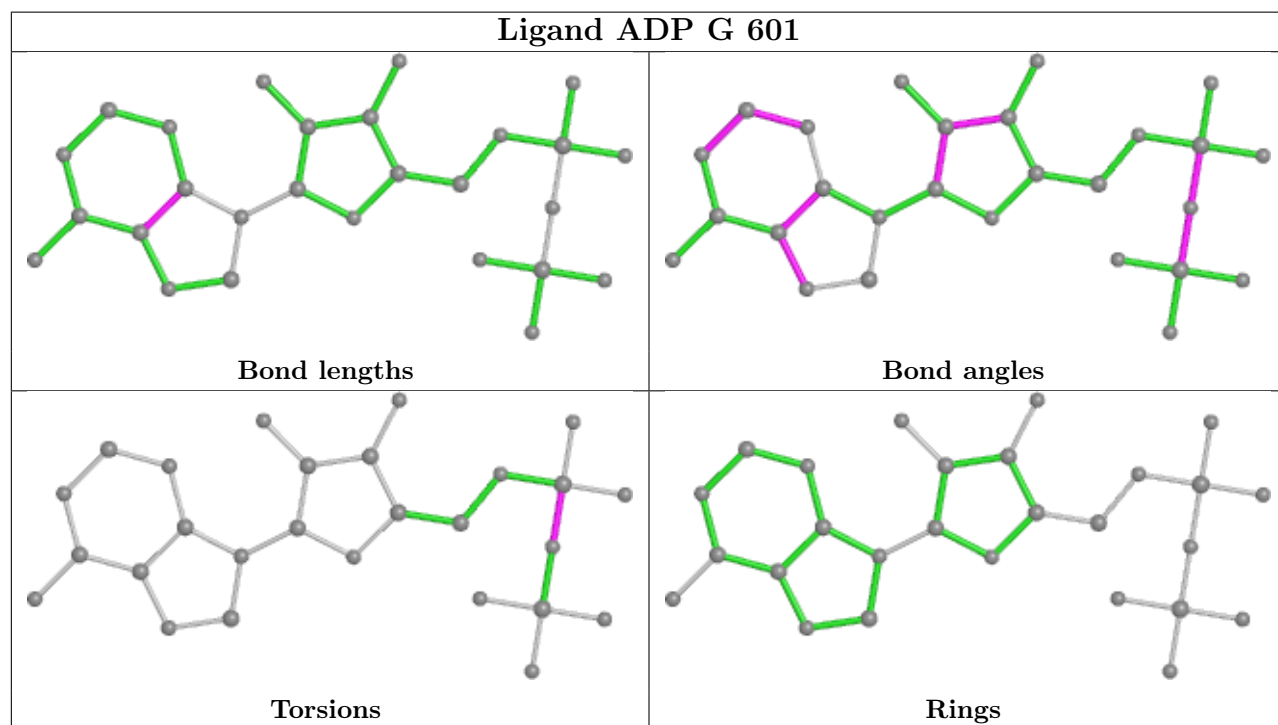
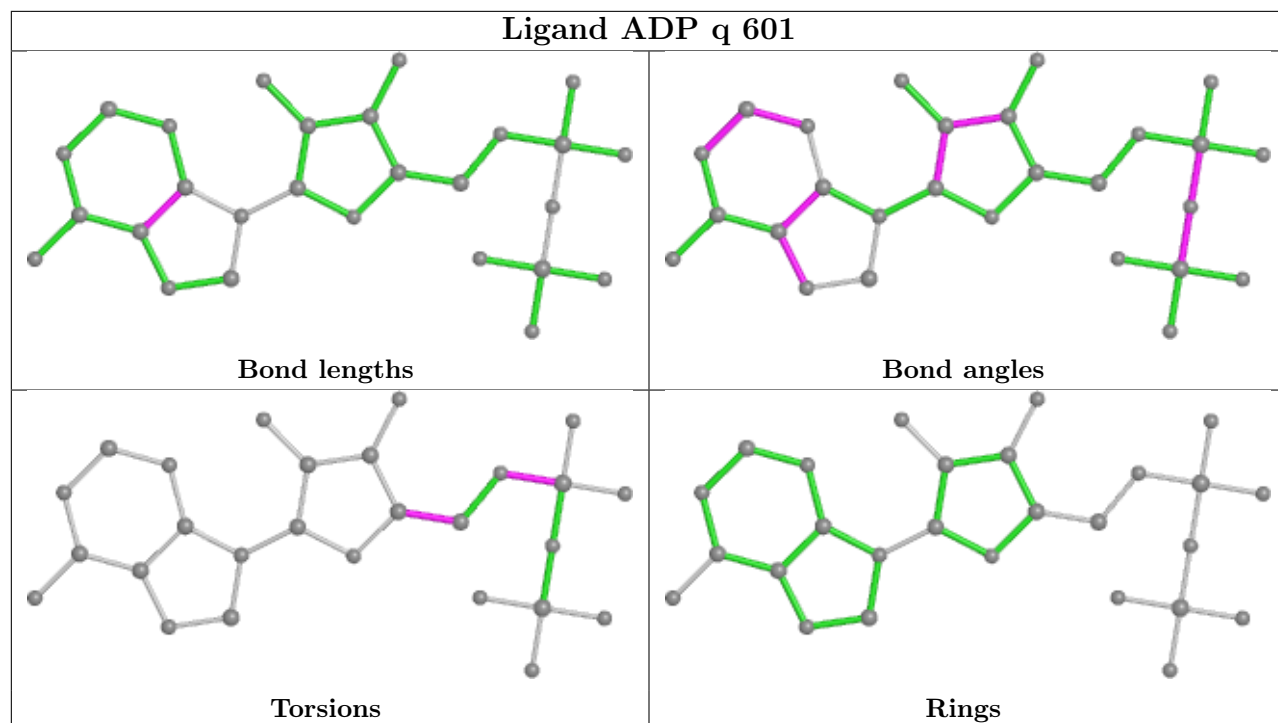


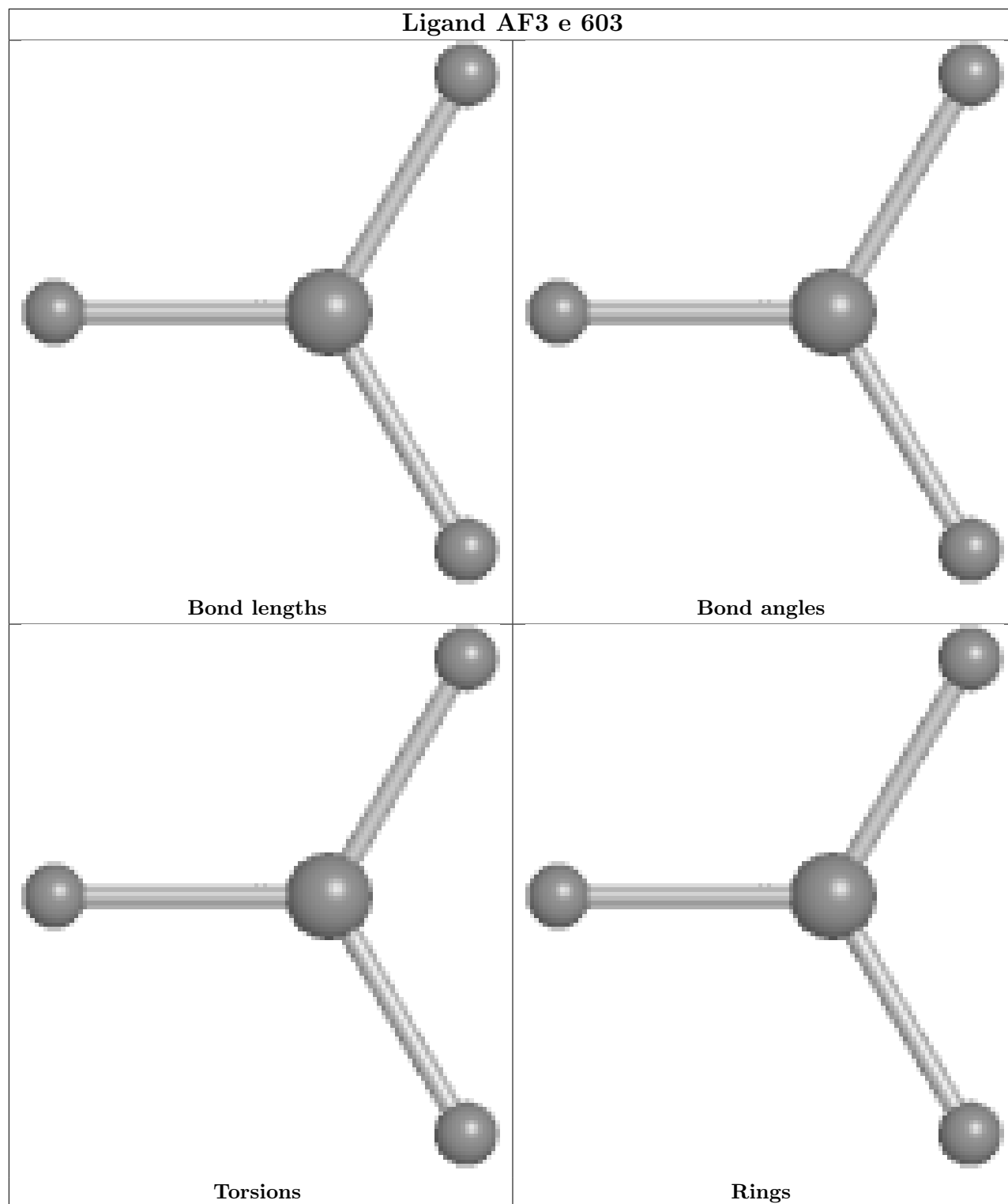












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

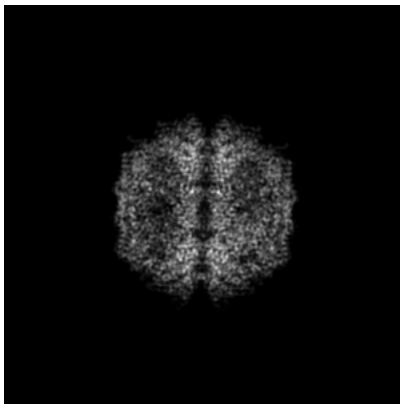
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33919. These allow visual inspection of the internal detail of the map and identification of artifacts.

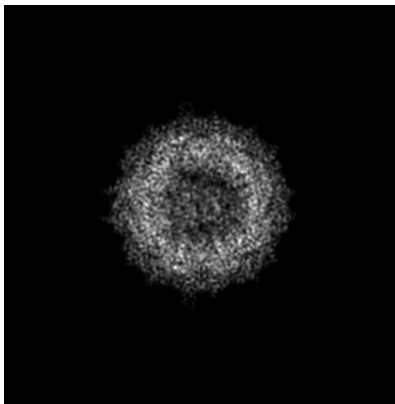
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

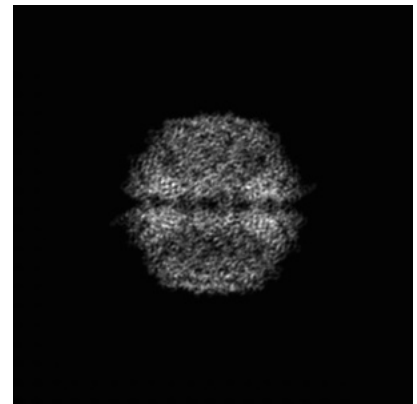
#### 6.1.1 Primary map



X

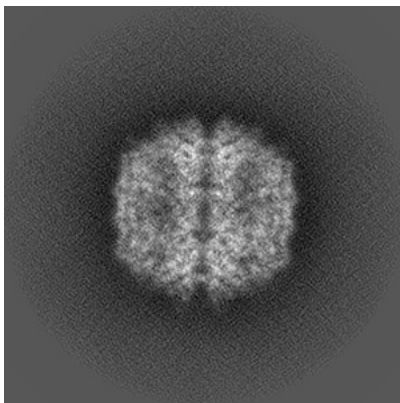


Y

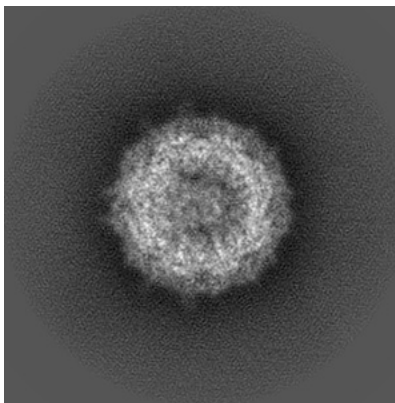


Z

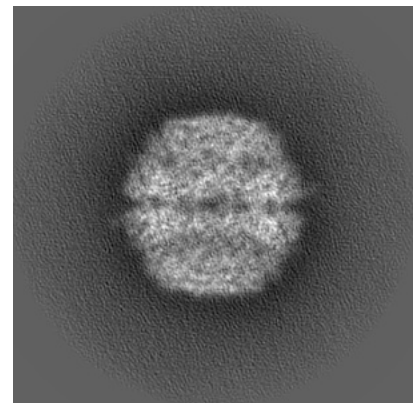
#### 6.1.2 Raw map



X



Y

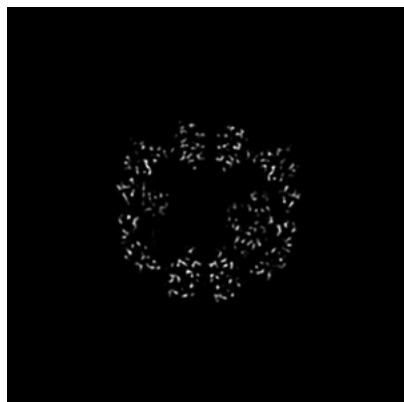


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 128

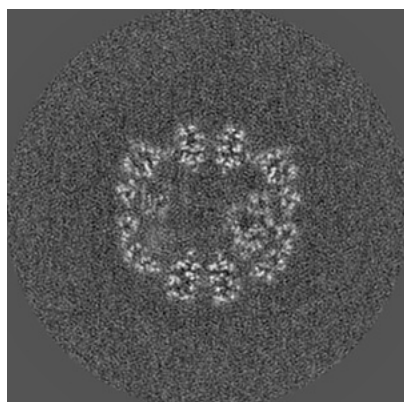


Y Index: 128

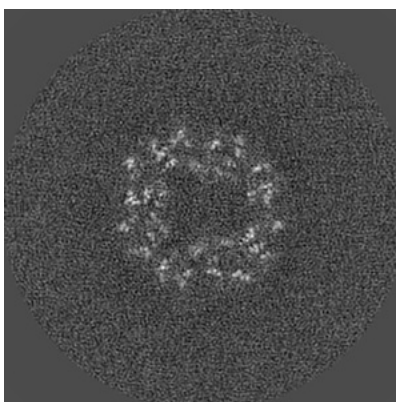


Z Index: 128

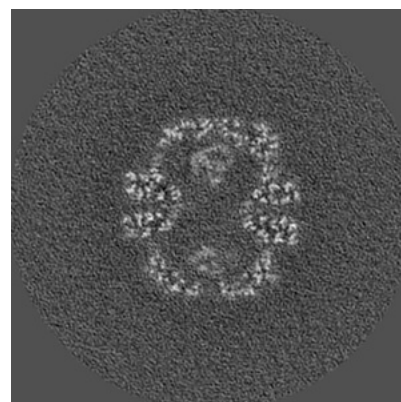
### 6.2.2 Raw map



X Index: 128



Y Index: 128

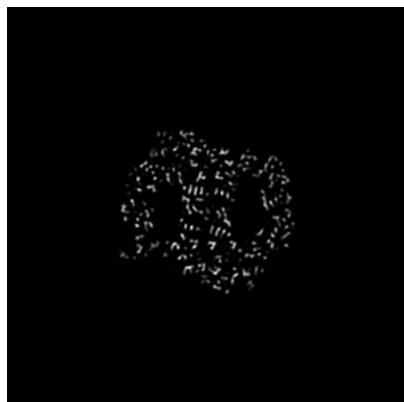


Z Index: 128

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: 154

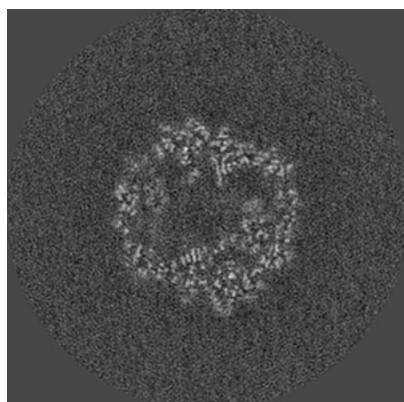


Y Index: 118

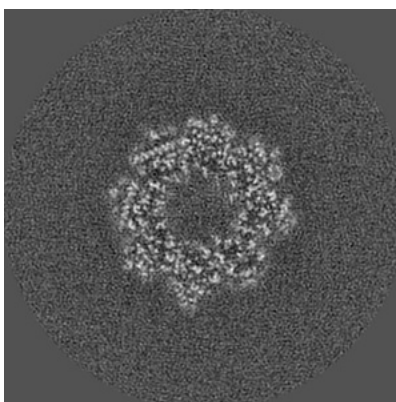


Z Index: 101

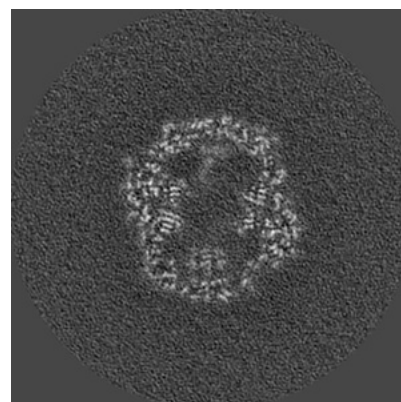
### 6.3.2 Raw map



X Index: 118



Y Index: 118

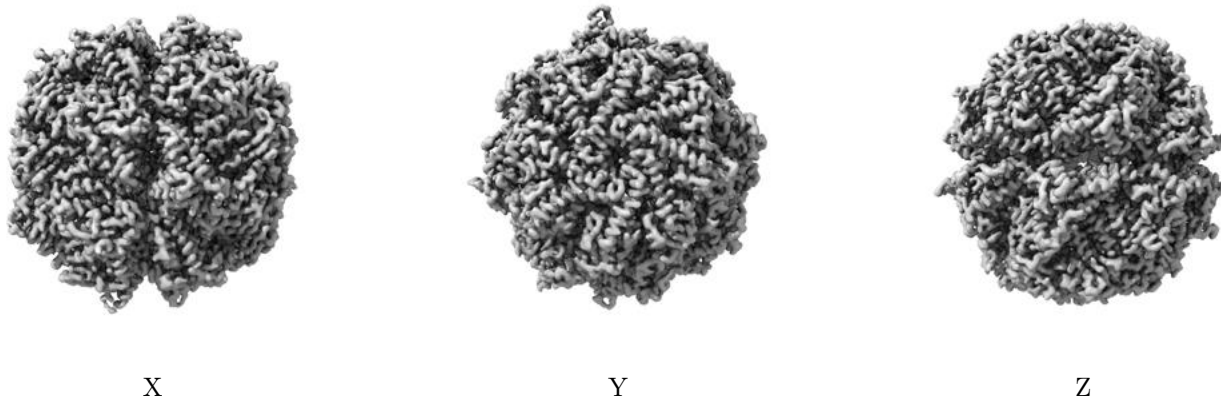


Z Index: 137

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

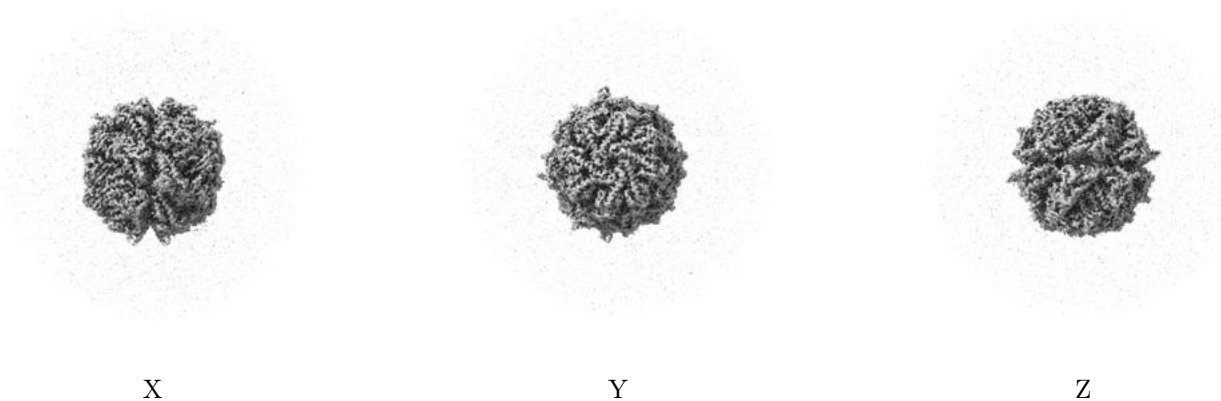
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

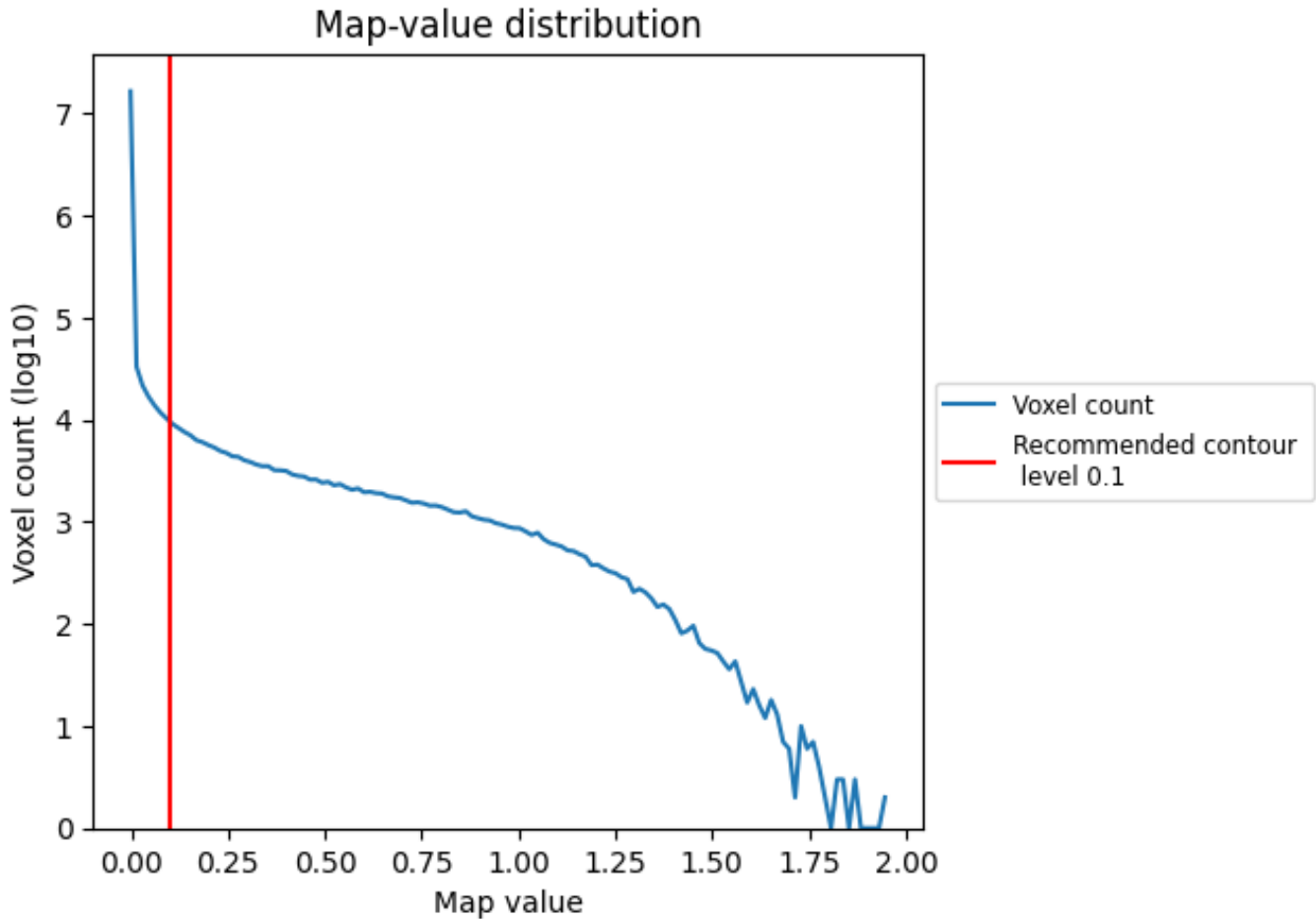
## 6.5 Mask visualisation [i](#)

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.

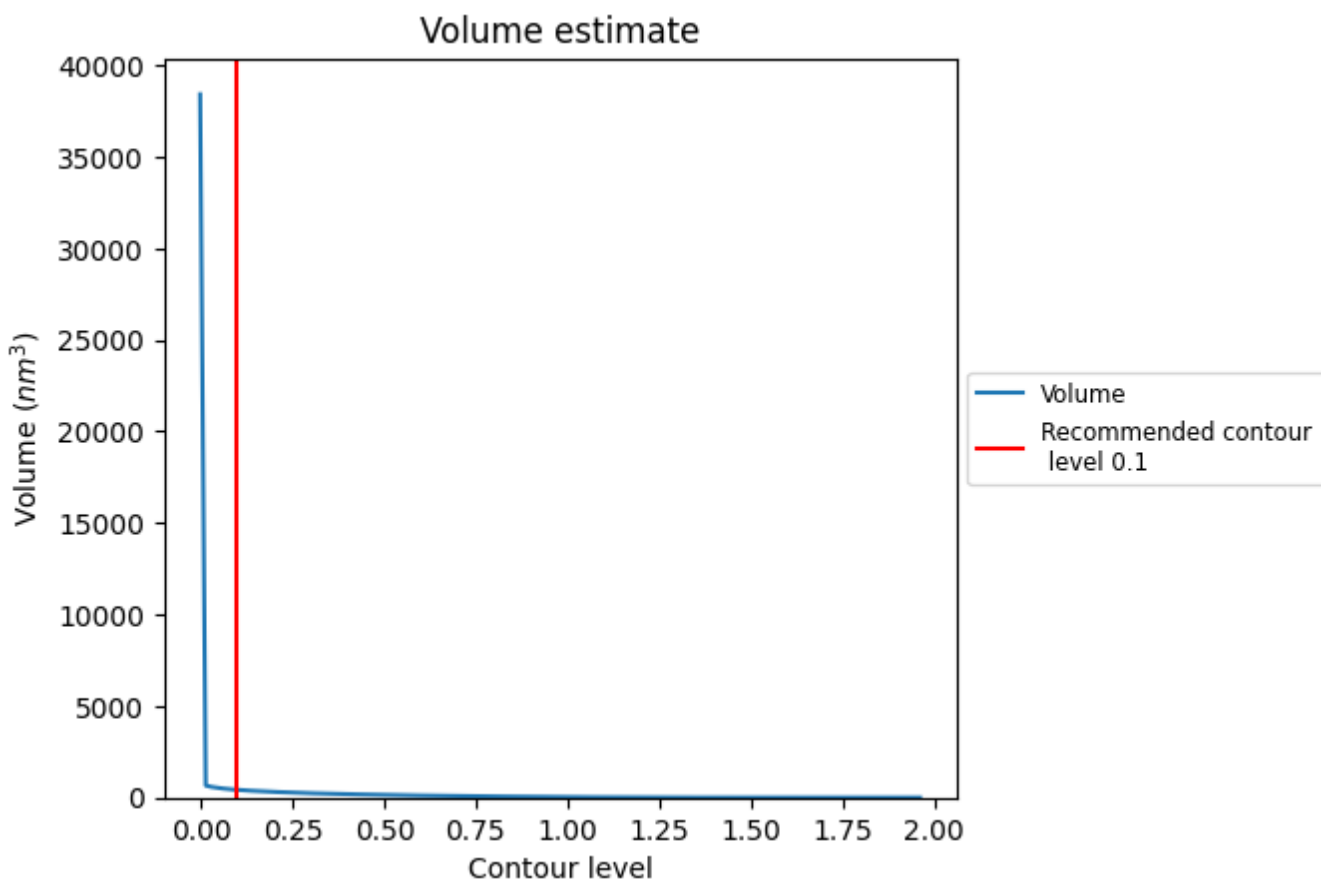
### 7.1 Map-value distribution [i](#)



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.



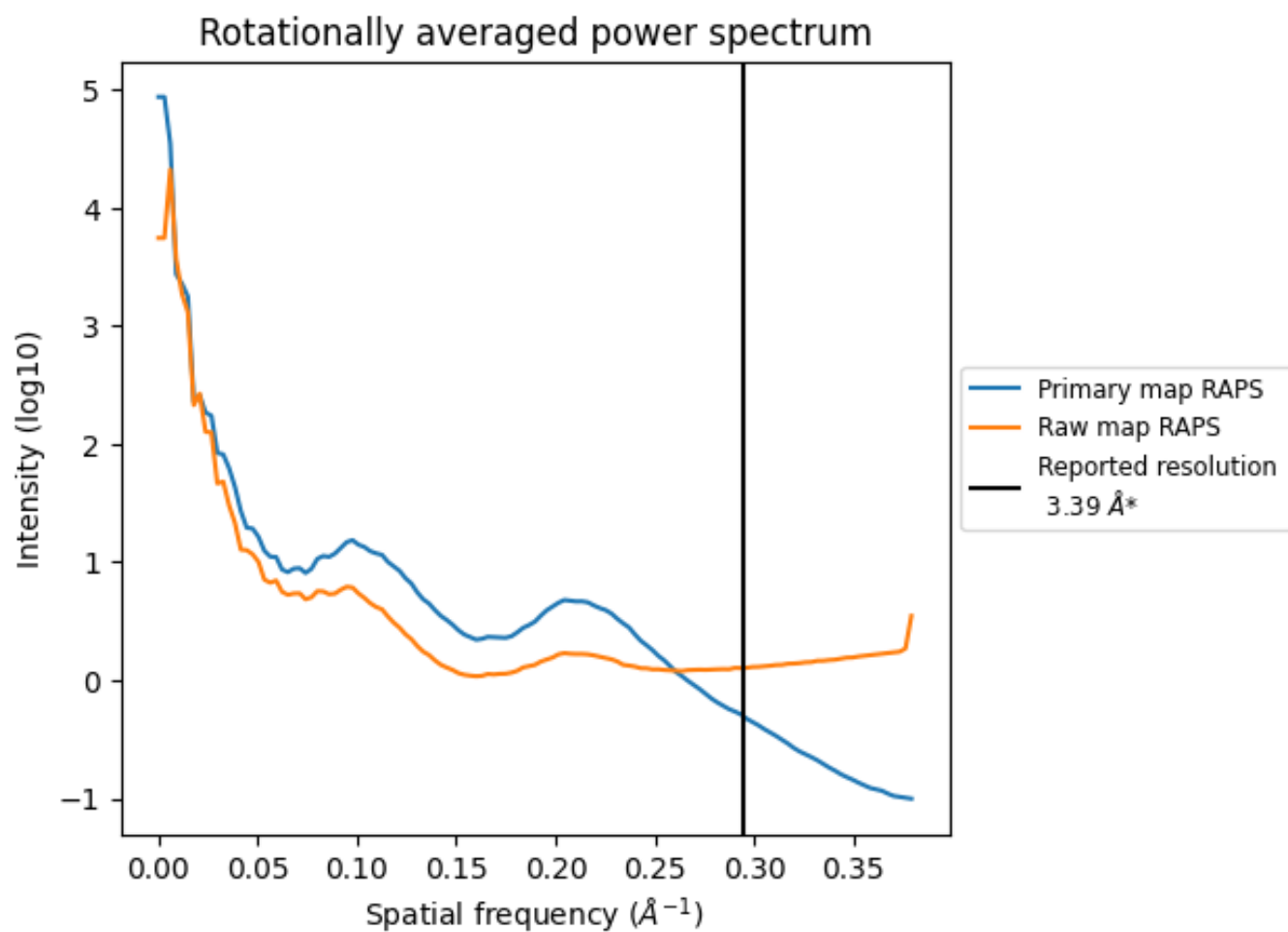
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm<sup>3</sup>; this corresponds to an approximate mass of 381 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

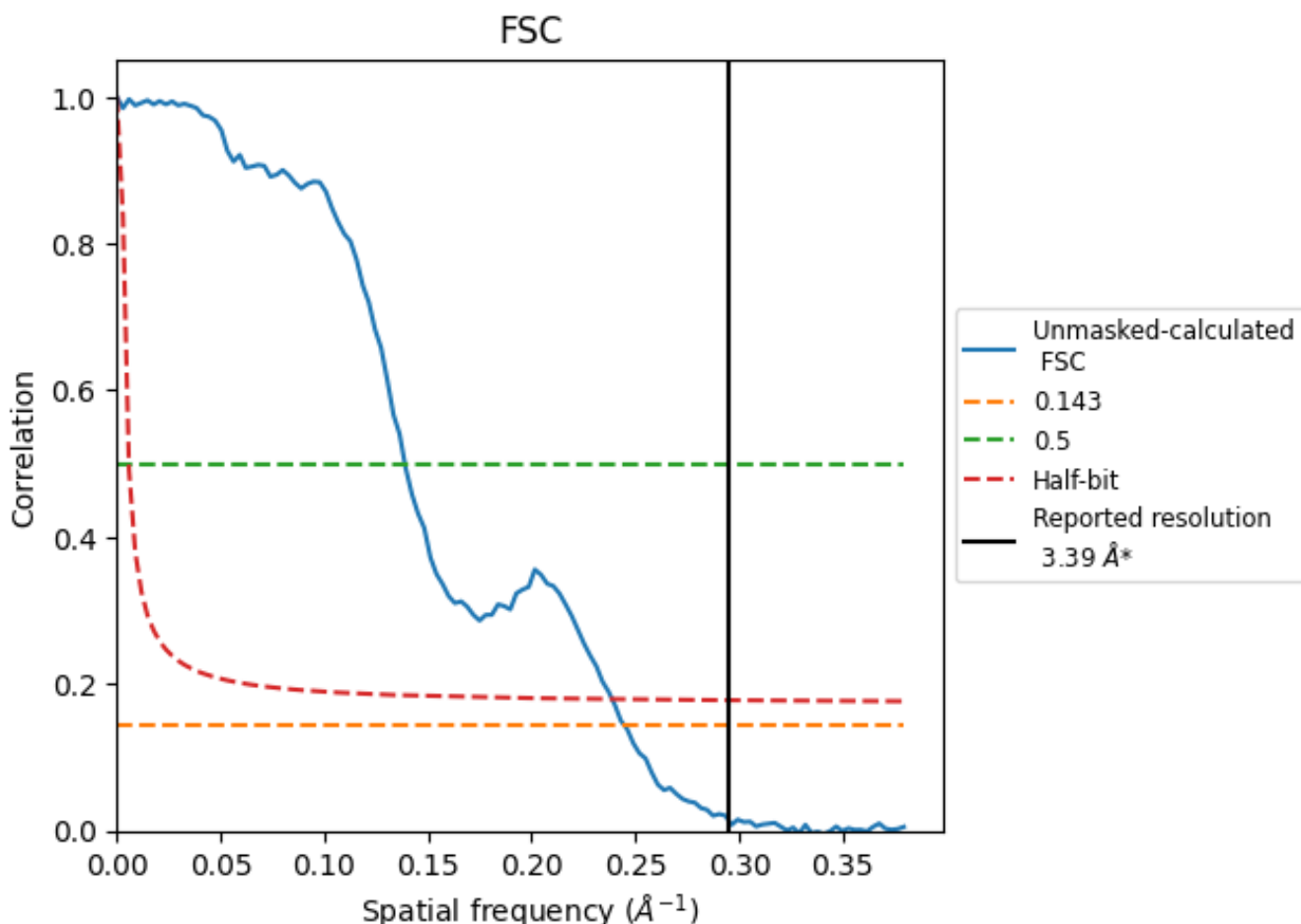


\*Reported resolution corresponds to spatial frequency of  $0.295 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.295 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

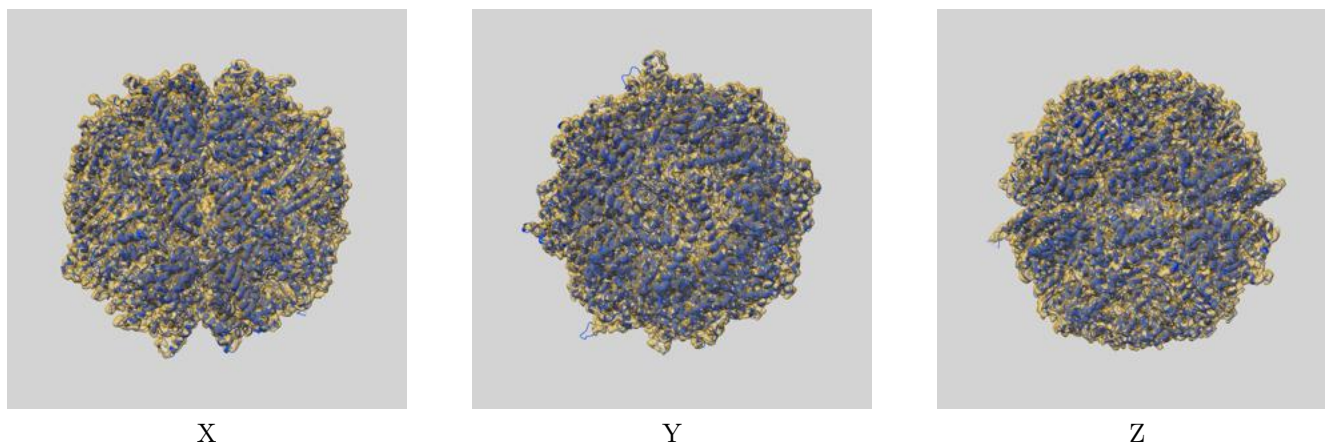
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	7.20	4.19

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.39 by more than 10 %

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

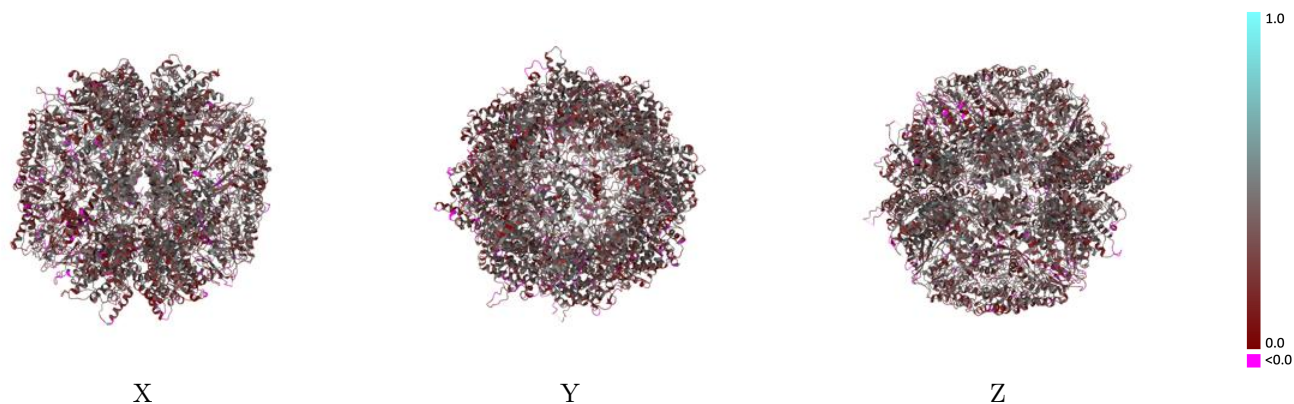
This section contains information regarding the fit between EMDB map EMD-33919 and PDB model 7YLW. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



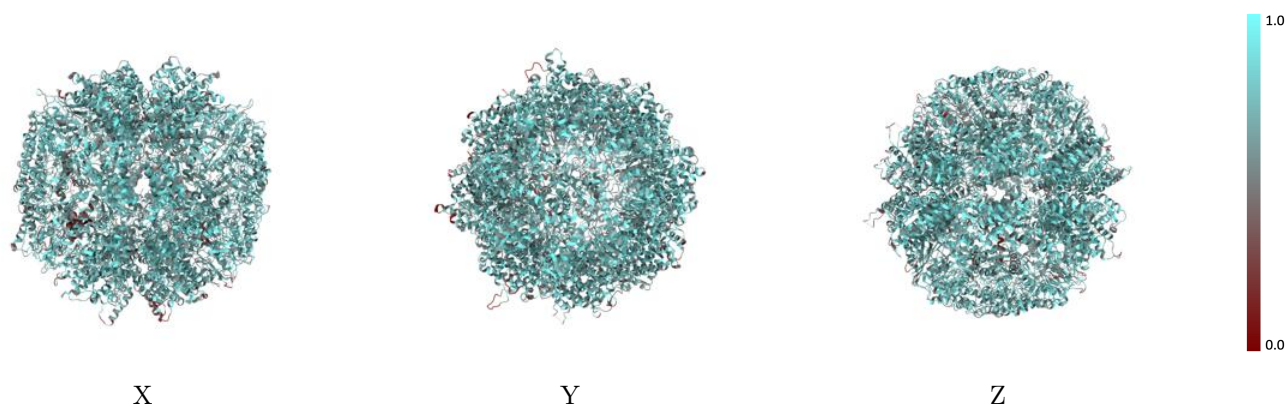
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



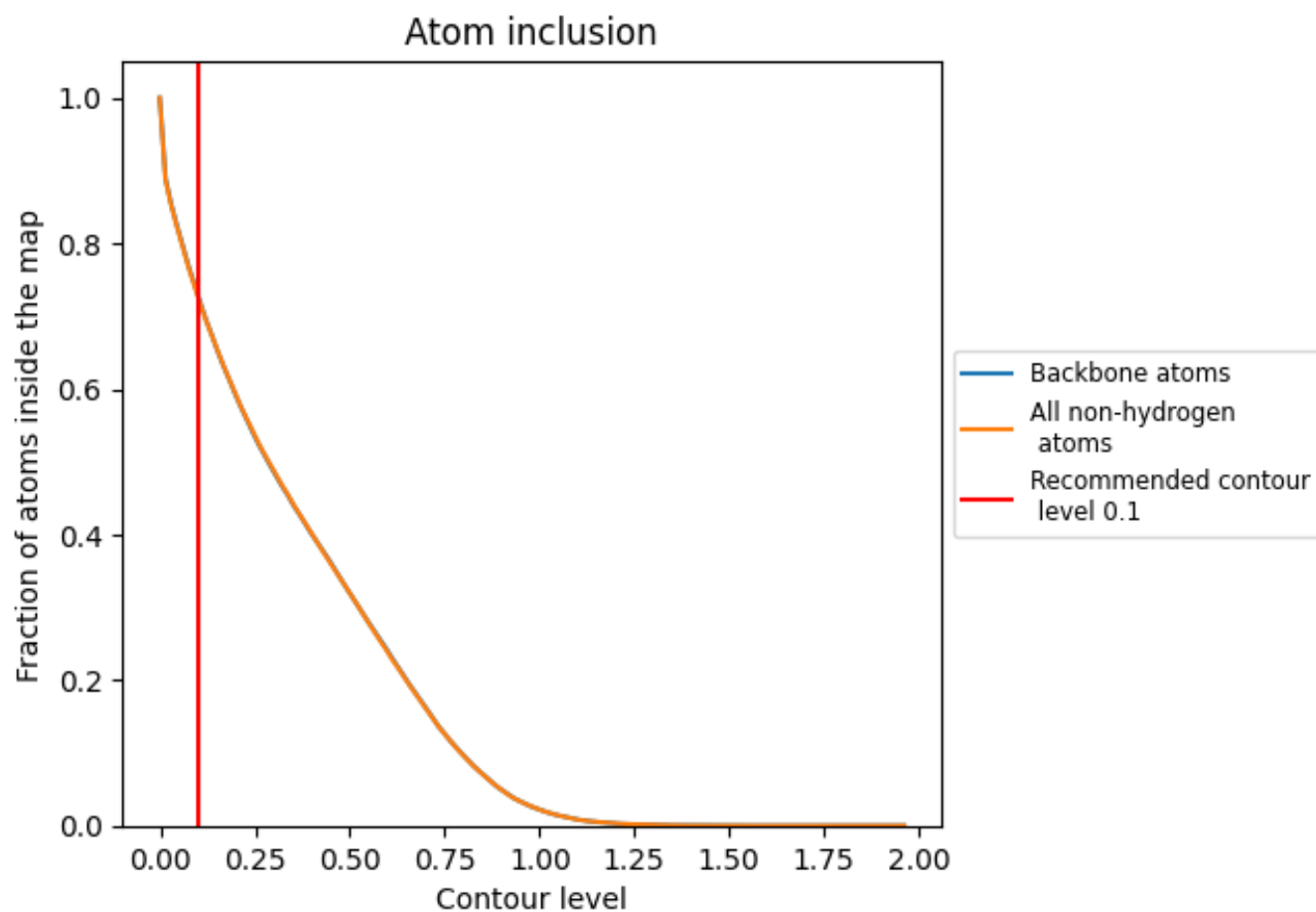
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7253	 0.3180
A	 0.7420	 0.3260
B	 0.7602	 0.3490
D	 0.7328	 0.3090
E	 0.7305	 0.3080
G	 0.7200	 0.3020
H	 0.7465	 0.3250
Q	 0.7271	 0.3210
T	 0.7377	 0.3590
Z	 0.7320	 0.3190
a	 0.7314	 0.3210
b	 0.7615	 0.3370
d	 0.7436	 0.3210
e	 0.7343	 0.3030
g	 0.7381	 0.3000
h	 0.7669	 0.3460
p	 0.4643	 0.2140
q	 0.7031	 0.2730
z	 0.7442	 0.3330

