



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 06:20 am BST

PDB ID : 9S72 / pdb_00009s72
EMDB ID : EMD-54634
Title : Human CCT in Closed Conformation
Authors : Gutierrez-Seijo, J.; Cuervo, A.; Cuellar, J.
Deposited on : 2025-08-02
Resolution : 2.71 Å(reported)
Based on initial model : .

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:

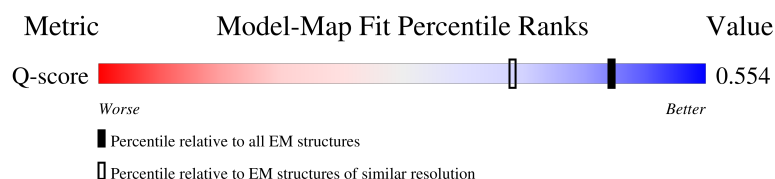
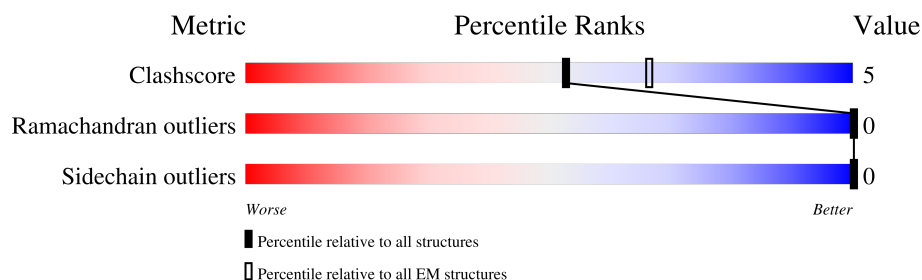
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.71 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	10297 (2.21 - 3.21)

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

Mol	Chain	Length	Quality of chain
1	A	556	
1	a	556	
2	B	535	
2	b	535	

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Mol	Chain	Length	Quality of chain
3	C	545	 85% 11% .
3	c	545	 84% 11% . .
4	D	539	 84% 12% .
4	d	539	 83% 13% .
5	E	541	 88% 11% .
5	e	541	 80% 19% .
6	F	531	 86% 12% .
6	f	531	 83% 15% .
7	G	543	 85% 11% .
7	g	543	 83% 13% .
8	H	548	 84% 12% .
8	h	548	 86% 10% .

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 131146 atoms, of which 66258 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
1	A	533	Total	C	H	N	O	S	0	0
			8254	2538	4204	708	781	23		
1	a	533	Total	C	H	N	O	S	0	0
			8254	2538	4204	708	781	23		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	526	Total	C	H	N	O	S	0	0
			7997	2473	4045	696	764	19		
2	B	526	Total	C	H	N	O	S	0	0
			7974	2473	4022	696	764	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	524	Total	C	H	N	O	S	0	0
			8281	2540	4208	720	783	30		
3	c	523	Total	C	H	N	O	S	0	0
			8259	2534	4195	718	782	30		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	517	Total	C	H	N	O	S	0	0
			8002	2439	4103	676	761	23		
4	d	518	Total	C	H	N	O	S	0	0
			8024	2445	4116	678	762	23		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	e	536	Total	C	H	N	O	S	0	0
			8313	2583	4188	719	792	31		
5	E	536	Total	C	H	N	O	S	0	0
			8313	2583	4188	719	792	31		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	525	Total	C	H	N	O	S	0	0
			8184	2528	4162	704	769	21		
6	f	525	Total	C	H	N	O	S	0	0
			8181	2528	4159	704	769	21		

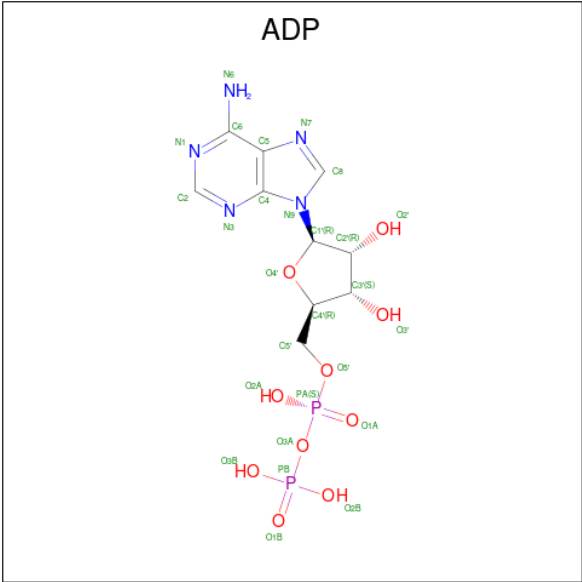
- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	g	524	Total	C	H	N	O	S	0	0
			8153	2543	4129	695	762	24		
7	G	525	Total	C	H	N	O	S	0	0
			8172	2548	4140	696	763	25		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	h	529	Total	C	H	N	O	S	0	0
			8129	2543	4100	685	774	27		
8	H	528	Total	C	H	N	O	S	0	0
			8119	2540	4095	684	773	27		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	h	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	f	1	Total	C	N	O	P	0
			27	10	5	10	2	

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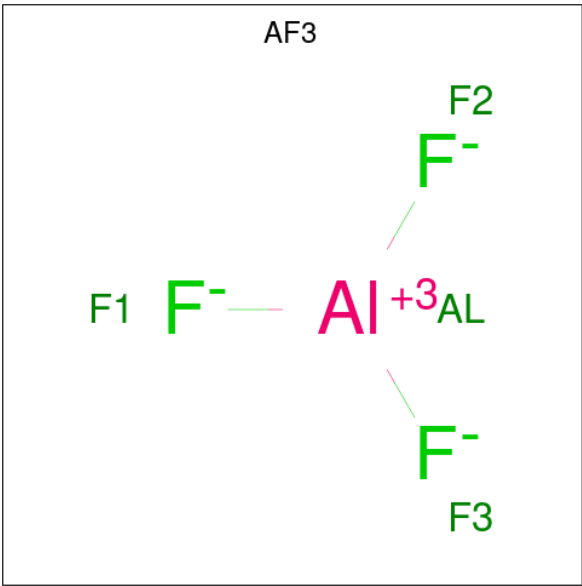
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	b	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	e	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	
10	g	1	Total	Mg	0
			1	1	
10	h	1	Total	Mg	0
			1	1	
10	a	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	c	1	Total	Mg	0
			1	1	
10	d	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	f	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	

- Molecule 11 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃) (labeled as "Lig-

and of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	Al	F	0
			4	1	3	
11	b	1	Total	Al	F	0
			4	1	3	
11	C	1	Total	Al	F	0
			4	1	3	
11	D	1	Total	Al	F	0
			4	1	3	
11	e	1	Total	Al	F	0
			4	1	3	
11	F	1	Total	Al	F	0
			4	1	3	
11	g	1	Total	Al	F	0
			4	1	3	
11	h	1	Total	Al	F	0
			4	1	3	
11	a	1	Total	Al	F	0
			4	1	3	
11	B	1	Total	Al	F	0
			4	1	3	
11	c	1	Total	Al	F	0
			4	1	3	
11	d	1	Total	Al	F	0
			4	1	3	
11	E	1	Total	Al	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms			AltConf
11	f	1	Total 4	Al 1	F 3	0
11	G	1	Total 4	Al 1	F 3	0
11	H	1	Total 4	Al 1	F 3	0

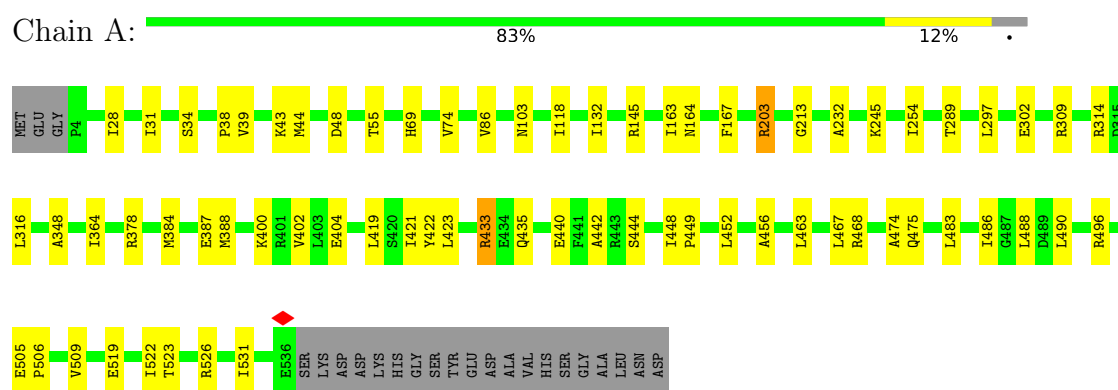
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total 2	O 2	0
12	b	2	Total 2	O 2	0
12	C	1	Total 1	O 1	0
12	D	1	Total 1	O 1	0
12	e	2	Total 2	O 2	0
12	F	1	Total 1	O 1	0
12	g	2	Total 2	O 2	0
12	h	1	Total 1	O 1	0
12	a	2	Total 2	O 2	0
12	B	3	Total 3	O 3	0
12	c	1	Total 1	O 1	0
12	d	1	Total 1	O 1	0
12	E	2	Total 2	O 2	0
12	f	1	Total 1	O 1	0
12	G	2	Total 2	O 2	0
12	H	1	Total 1	O 1	0

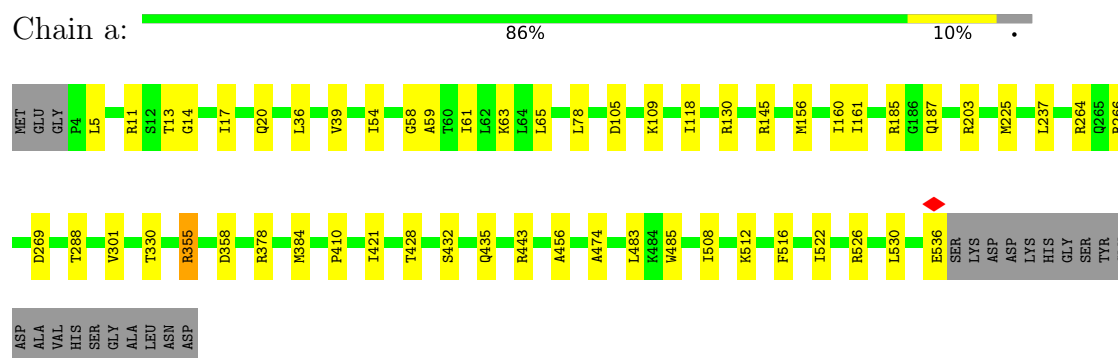
3 Residue-property plots

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.

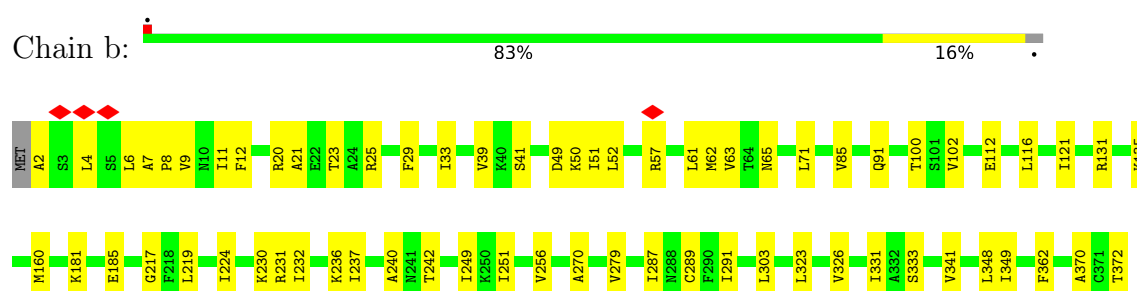
- Molecule 1: T-complex protein 1 subunit alpha

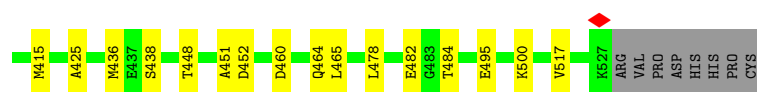


- Molecule 1: T-complex protein 1 subunit alpha

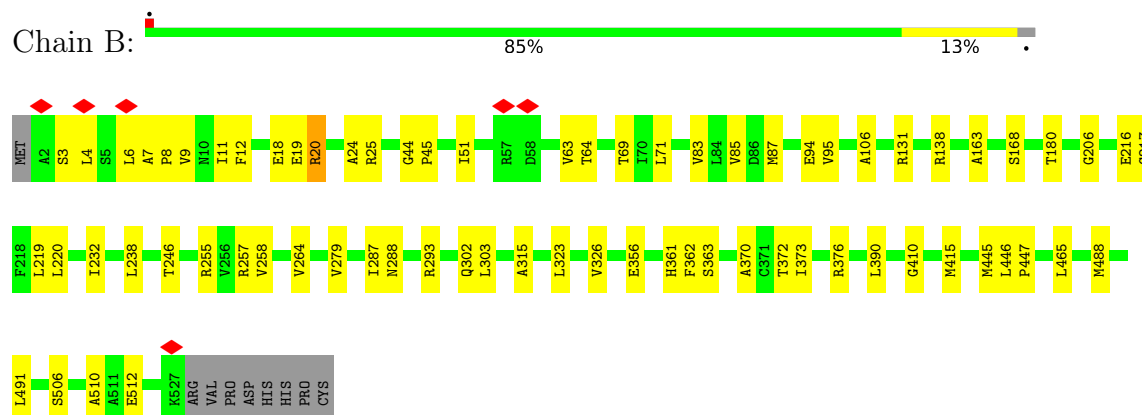


- Molecule 2: T-complex protein 1 subunit beta

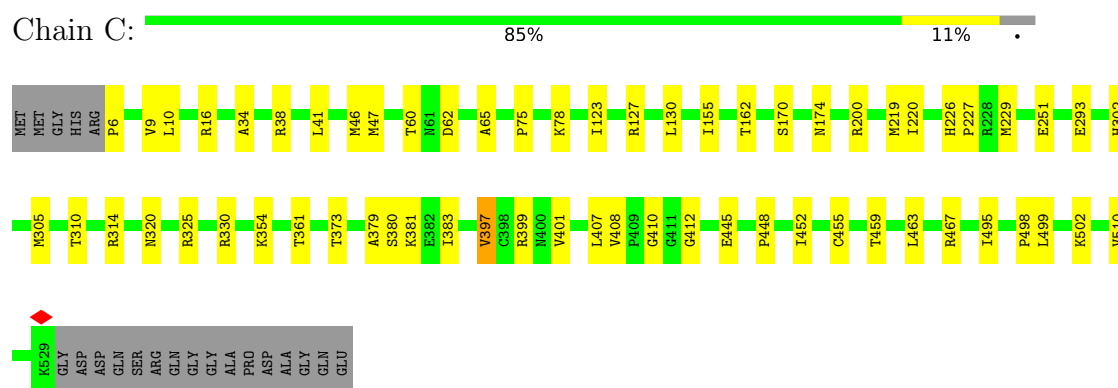




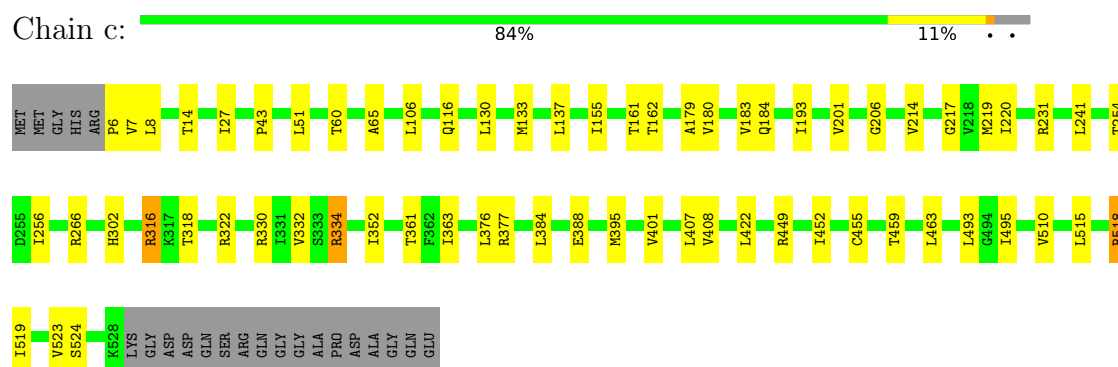
- Molecule 2: T-complex protein 1 subunit beta



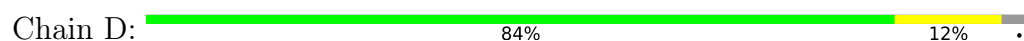
- Molecule 3: T-complex protein 1 subunit gamma



- Molecule 3: T-complex protein 1 subunit gamma



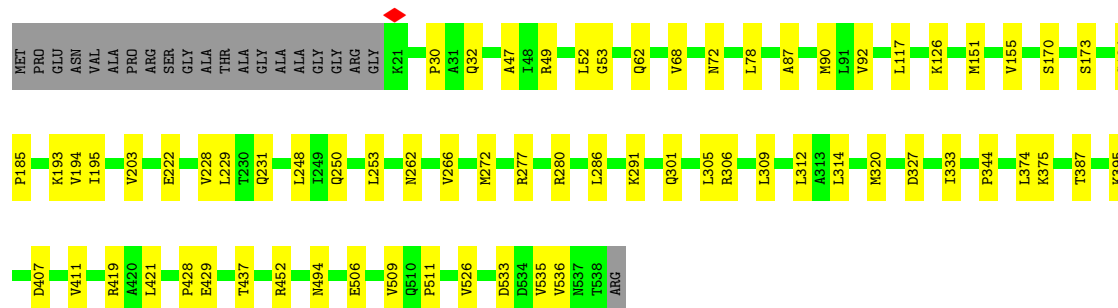
- Molecule 4: T-complex protein 1 subunit delta





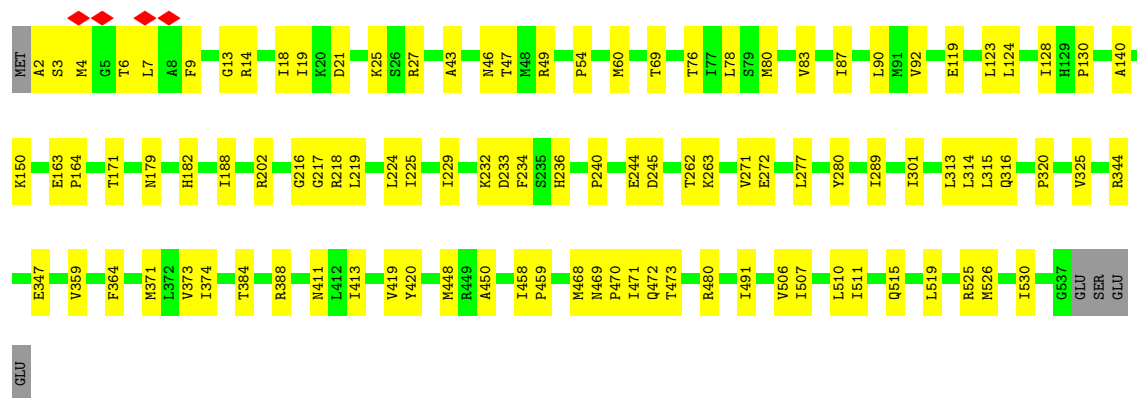
- Molecule 4: T-complex protein 1 subunit delta

Chain d: 83% 13% .



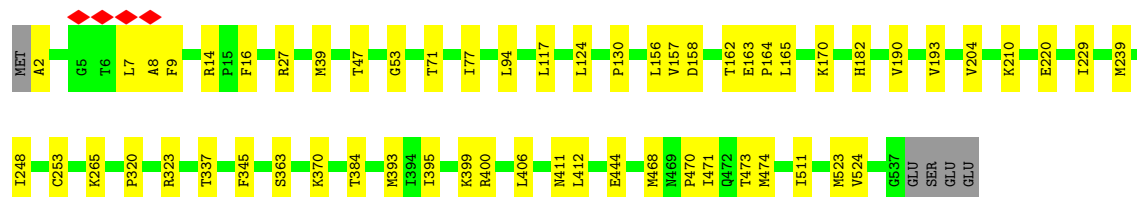
- Molecule 5: T-complex protein 1 subunit epsilon

Chain e: 80% 19% .



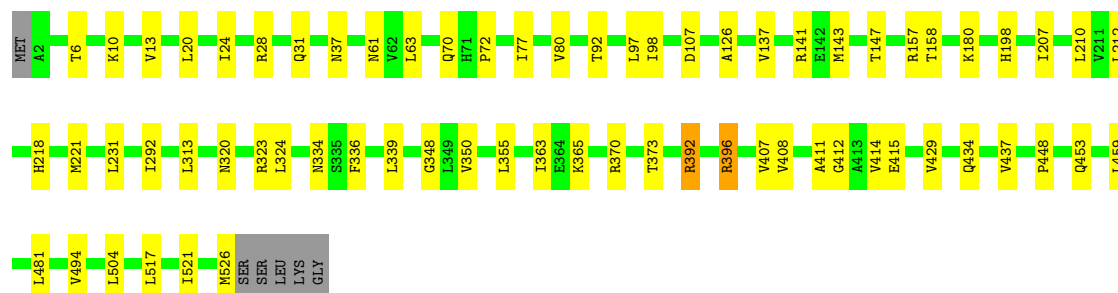
- Molecule 5: T-complex protein 1 subunit epsilon

Chain E: 88% 11% .



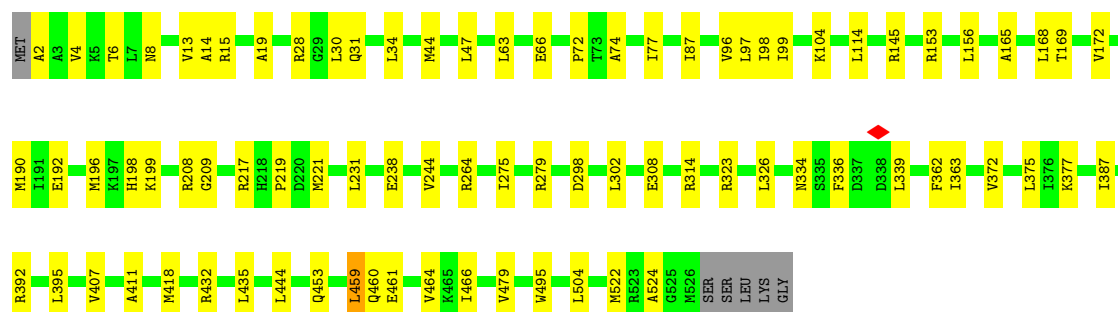
- Molecule 6: T-complex protein 1 subunit zeta

Chain F:  86% 12% .



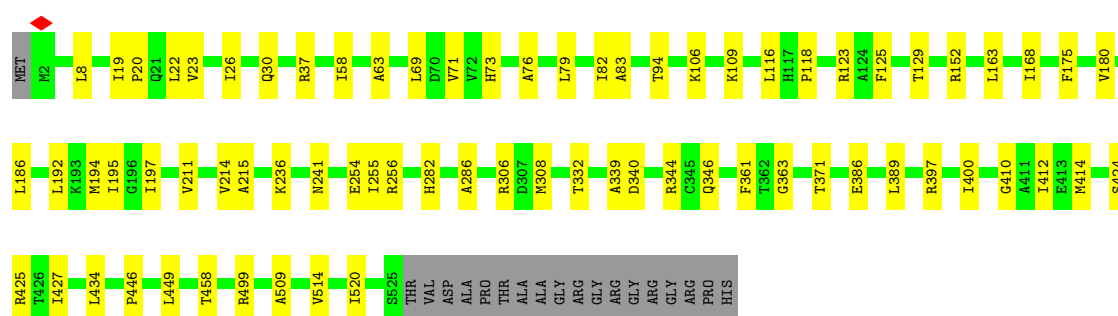
- Molecule 6: T-complex protein 1 subunit zeta

Chain f:  83% 15% .



- Molecule 7: T-complex protein 1 subunit eta

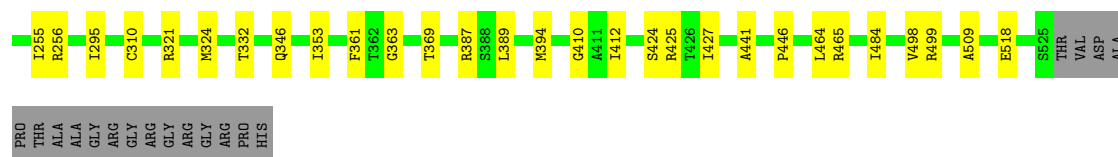
Chain g:  83% 13% .



- Molecule 7: T-complex protein 1 subunit eta

Chain G:  85% 11% .





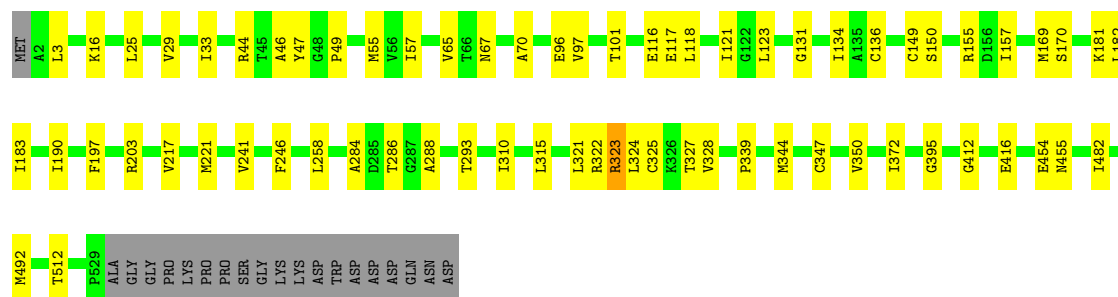
• Molecule 8: T-complex protein 1 subunit theta

Chain h: 86% 10% .



• Molecule 8: T-complex protein 1 subunit theta

Chain H: 84% 12% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105562	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.79	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.845	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.0371	Depositor
Map size (Å)	321.6, 321.6, 321.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/4090	0.86	4/5522 (0.1%)
1	a	0.54	0/4090	0.92	0/5522
2	B	0.43	0/3995	0.74	1/5386 (0.0%)
2	b	0.47	0/3995	0.80	2/5386 (0.0%)
3	C	0.54	0/4119	0.85	3/5555 (0.1%)
3	c	0.46	0/4110	0.84	3/5544 (0.1%)
4	D	0.45	0/3931	0.72	0/5308
4	d	0.53	0/3940	0.86	0/5319
5	E	0.49	0/4175	0.84	2/5624 (0.0%)
5	e	0.61	0/4175	0.95	1/5624 (0.0%)
6	F	0.57	0/4069	0.97	0/5486
6	f	0.54	0/4069	0.89	1/5486 (0.0%)
7	G	0.52	0/4089	0.91	0/5519
7	g	0.56	0/4081	0.94	0/5509
8	H	0.61	0/4082	0.96	0/5518
8	h	0.47	0/4087	0.81	0/5525
All	All	0.52	0/65097	0.87	17/87833 (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
1	A	0	4
1	a	0	8
2	B	0	4
2	b	0	2
3	C	0	5
3	c	0	4
4	D	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	4
5	E	0	1
5	e	0	4
6	F	0	5
6	f	0	7
7	G	0	4
7	g	0	3
8	H	0	5
8	h	0	1
All	All	0	67

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	6	THR	CA-CB-OG1	-9.25	95.72	109.60
3	C	397	VAL	N-CA-CB	7.26	121.47	110.58
2	B	20	ARG	CB-CA-C	-6.67	98.22	109.50
3	c	334	ARG	CB-CA-C	6.42	116.52	110.17
5	E	400	ARG	CB-CA-C	6.25	121.72	109.72

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	203	ARG	Sidechain
1	A	433	ARG	Sidechain
1	A	496	ARG	Sidechain
2	b	20	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4050	4204	4211	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	4050	4204	4211	34	0
2	B	3952	4022	4070	53	0
2	b	3952	4045	4070	64	0
3	C	4073	4208	4215	49	0
3	c	4064	4195	4202	54	0
4	D	3899	4103	4102	41	0
4	d	3908	4116	4115	52	0
5	E	4125	4188	4241	44	0
5	e	4125	4188	4241	86	0
6	F	4022	4162	4161	47	0
6	f	4022	4159	4161	50	0
7	G	4032	4140	4140	37	0
7	g	4024	4129	4128	49	0
8	H	4024	4095	4094	42	0
8	h	4029	4100	4099	38	0
9	A	27	0	12	1	0
9	B	27	0	12	1	0
9	C	27	0	12	7	0
9	D	27	0	12	1	0
9	E	27	0	12	1	0
9	F	27	0	12	5	0
9	G	27	0	12	2	0
9	H	27	0	12	3	0
9	a	27	0	12	1	0
9	b	27	0	12	0	0
9	c	27	0	12	5	0
9	d	27	0	12	5	0
9	e	27	0	12	1	0
9	f	27	0	12	2	0
9	g	27	0	12	1	0
9	h	27	0	12	4	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	a	1	0	0	0	0
10	b	1	0	0	0	0
10	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	d	1	0	0	0	0
10	e	1	0	0	0	0
10	f	1	0	0	0	0
10	g	1	0	0	0	0
10	h	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	C	4	0	0	0	0
11	D	4	0	0	0	0
11	E	4	0	0	0	0
11	F	4	0	0	0	0
11	G	4	0	0	0	0
11	H	4	0	0	0	0
11	a	4	0	0	0	0
11	b	4	0	0	0	0
11	c	4	0	0	0	0
11	d	4	0	0	1	0
11	e	4	0	0	1	0
11	f	4	0	0	1	0
11	g	4	0	0	0	0
11	h	4	0	0	1	0
12	A	2	0	0	0	0
12	B	3	0	0	3	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	E	2	0	0	0	0
12	F	1	0	0	0	0
12	G	2	0	0	0	0
12	H	1	0	0	0	0
12	a	2	0	0	0	0
12	b	2	0	0	0	0
12	c	1	0	0	0	0
12	d	1	0	0	0	0
12	e	2	0	0	0	0
12	f	1	0	0	0	0
12	g	2	0	0	0	0
12	h	1	0	0	0	0
All	All	64888	66258	66653	692	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 5.

The worst 5 of 692 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)
3:C:6:PRO:HB2	5:e:7:LEU:HD21	1.40	1.02
11:f:603:AF3:AL	11:f:603:AF3:F3	0.80	0.98
2:B:4:LEU:HG	2:B:11:ILE:HD11	1.49	0.93
4:d:195:ILE:HG21	4:d:203:VAL:HG22	1.51	0.90
4:D:283:ILE:HD12	4:D:312:LEU:HD23	1.55	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/556 (96%)	513 (97%)	18 (3%)	0	100	100
1	a	531/556 (96%)	514 (97%)	17 (3%)	0	100	100
2	B	524/535 (98%)	514 (98%)	10 (2%)	0	100	100
2	b	524/535 (98%)	510 (97%)	14 (3%)	0	100	100
3	C	522/545 (96%)	509 (98%)	13 (2%)	0	100	100
3	c	521/545 (96%)	511 (98%)	10 (2%)	0	100	100
4	D	515/539 (96%)	505 (98%)	10 (2%)	0	100	100
4	d	516/539 (96%)	507 (98%)	9 (2%)	0	100	100
5	E	534/541 (99%)	524 (98%)	10 (2%)	0	100	100
5	e	534/541 (99%)	521 (98%)	13 (2%)	0	100	100
6	F	523/531 (98%)	507 (97%)	16 (3%)	0	100	100
6	f	523/531 (98%)	514 (98%)	9 (2%)	0	100	100
7	G	523/543 (96%)	511 (98%)	12 (2%)	0	100	100
7	g	522/543 (96%)	509 (98%)	13 (2%)	0	100	100
8	H	526/548 (96%)	513 (98%)	13 (2%)	0	100	100
8	h	527/548 (96%)	516 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8396/8676 (97%)	8198 (98%)	198 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/463 (96%)	445 (100%)	0	100	100
1	a	445/463 (96%)	445 (100%)	0	100	100
2	B	418/427 (98%)	418 (100%)	0	100	100
2	b	418/427 (98%)	418 (100%)	0	100	100
3	C	455/469 (97%)	455 (100%)	0	100	100
3	c	454/469 (97%)	454 (100%)	0	100	100
4	D	440/452 (97%)	440 (100%)	0	100	100
4	d	441/452 (98%)	441 (100%)	0	100	100
5	E	451/456 (99%)	451 (100%)	0	100	100
5	e	451/456 (99%)	451 (100%)	0	100	100
6	F	437/442 (99%)	437 (100%)	0	100	100
6	f	437/442 (99%)	437 (100%)	0	100	100
7	G	432/443 (98%)	432 (100%)	0	100	100
7	g	431/443 (97%)	431 (100%)	0	100	100
8	H	436/452 (96%)	436 (100%)	0	100	100
8	h	436/452 (96%)	436 (100%)	0	100	100
All	All	7027/7208 (98%)	7027 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	494	ASN
7	G	501	ASN
5	E	46	ASN
6	f	503	GLN
8	H	95	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
9	ADP	b	601	-	27,29,29	0.54	0	42,45,45	0.52	0
11	AF3	b	603	-	0,3,3	-	-	-		
9	ADP	h	601	10	27,29,29	0.46	0	42,45,45	0.62	0
9	ADP	g	601	10	27,29,29	0.53	0	42,45,45	0.55	0
11	AF3	h	603	-	0,3,3	-	-	-		
9	ADP	B	601	10	27,29,29	0.53	0	42,45,45	0.52	0
11	AF3	G	603	9	0,3,3	-	-	-		
11	AF3	B	603	-	0,3,3	-	-	-		
9	ADP	A	601	11,10	27,29,29	0.54	0	42,45,45	0.51	0
9	ADP	c	601	11,10	27,29,29	0.57	0	42,45,45	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	AF3	A	603	1,9	0,3,3	-	-	-		
9	ADP	d	601	10	27,29,29	0.55	0	42,45,45	0.60	0
9	ADP	D	601	11,10	27,29,29	0.59	0	42,45,45	0.66	0
11	AF3	C	603	3	0,3,3	-	-	-		
11	AF3	e	603	-	0,3,3	-	-	-		
9	ADP	F	601	11,10	27,29,29	0.61	0	42,45,45	0.71	0
11	AF3	d	603	-	0,3,3	-	-	-		
9	ADP	f	601	11,10	27,29,29	0.68	1 (3%)	42,45,45	0.71	1 (2%)
11	AF3	F	603	6,9	0,3,3	-	-	-		
9	ADP	E	601	11,10	27,29,29	0.55	0	42,45,45	0.61	0
11	AF3	E	603	9	0,3,3	-	-	-		
11	AF3	g	603	-	0,3,3	-	-	-		
11	AF3	f	603	9	0,3,3	-	-	-		
11	AF3	H	603	-	0,3,3	-	-	-		
9	ADP	a	601	11,10	27,29,29	0.62	0	42,45,45	0.73	1 (2%)
11	AF3	c	603	9,3	0,3,3	-	-	-		
9	ADP	C	601	10	27,29,29	0.56	0	42,45,45	0.82	2 (4%)
9	ADP	e	601	10	27,29,29	0.56	0	42,45,45	0.78	1 (2%)
9	ADP	H	601	10	27,29,29	0.44	0	42,45,45	0.50	0
11	AF3	a	603	9	0,3,3	-	-	-		
11	AF3	D	603	9	0,3,3	-	-	-		
9	ADP	G	601	11,10	27,29,29	0.57	0	42,45,45	0.70	0

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
9	ADP	C	601	10	-	5/16/32/32	0/3/3/3
9	ADP	A	601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	e	601	10	-	0/16/32/32	0/3/3/3
9	ADP	b	601	-	-	4/16/32/32	0/3/3/3
9	ADP	c	601	11,10	-	8/16/32/32	0/3/3/3
9	ADP	H	601	10	-	2/16/32/32	0/3/3/3
9	ADP	d	601	10	-	5/16/32/32	0/3/3/3
9	ADP	f	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	h	601	10	-	3/16/32/32	0/3/3/3
9	ADP	g	601	10	-	1/16/32/32	0/3/3/3
9	ADP	E	601	11,10	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	B	601	10	-	3/16/32/32	0/3/3/3
9	ADP	D	601	11,10	-	5/16/32/32	0/3/3/3
9	ADP	a	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	G	601	11,10	-	6/16/32/32	0/3/3/3
9	ADP	F	601	11,10	-	0/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	601	ADP	PB-O2B	-2.21	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	601	ADP	PA-O3A-PB	-3.07	122.28	132.83
9	f	601	ADP	PA-O3A-PB	-2.33	124.84	132.83
9	e	601	ADP	C3'-C2'-C1'	-2.15	97.33	101.43
9	C	601	ADP	O4'-C4'-C3'	-2.08	101.01	105.11
9	C	601	ADP	PA-O3A-PB	-2.03	125.84	132.83

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	ADP	PA-O3A-PB-O2B
9	b	601	ADP	PB-O3A-PA-O5'
9	C	601	ADP	C5'-O5'-PA-O1A
9	C	601	ADP	C5'-O5'-PA-O3A
9	D	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

19 monomers are involved in 44 short contacts:

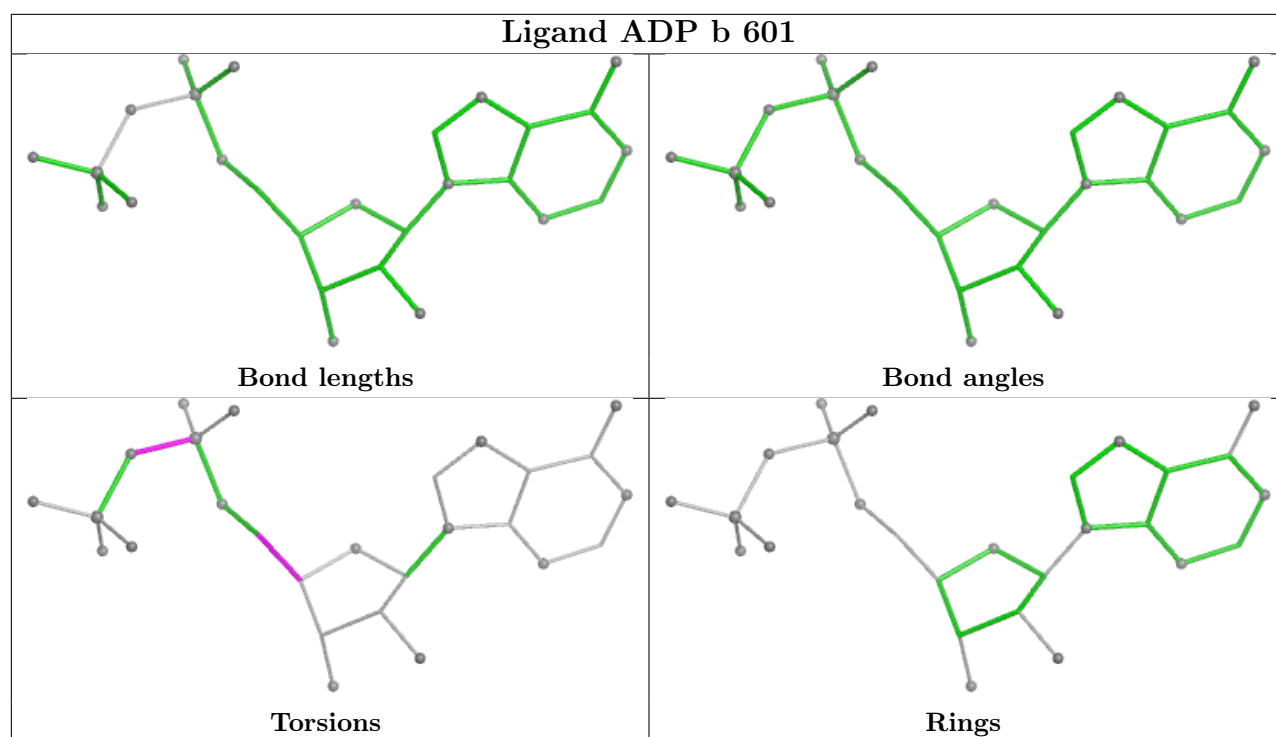
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	h	601	ADP	4	0
9	g	601	ADP	1	0
11	h	603	AF3	1	0
9	B	601	ADP	1	0
9	A	601	ADP	1	0
9	c	601	ADP	5	0

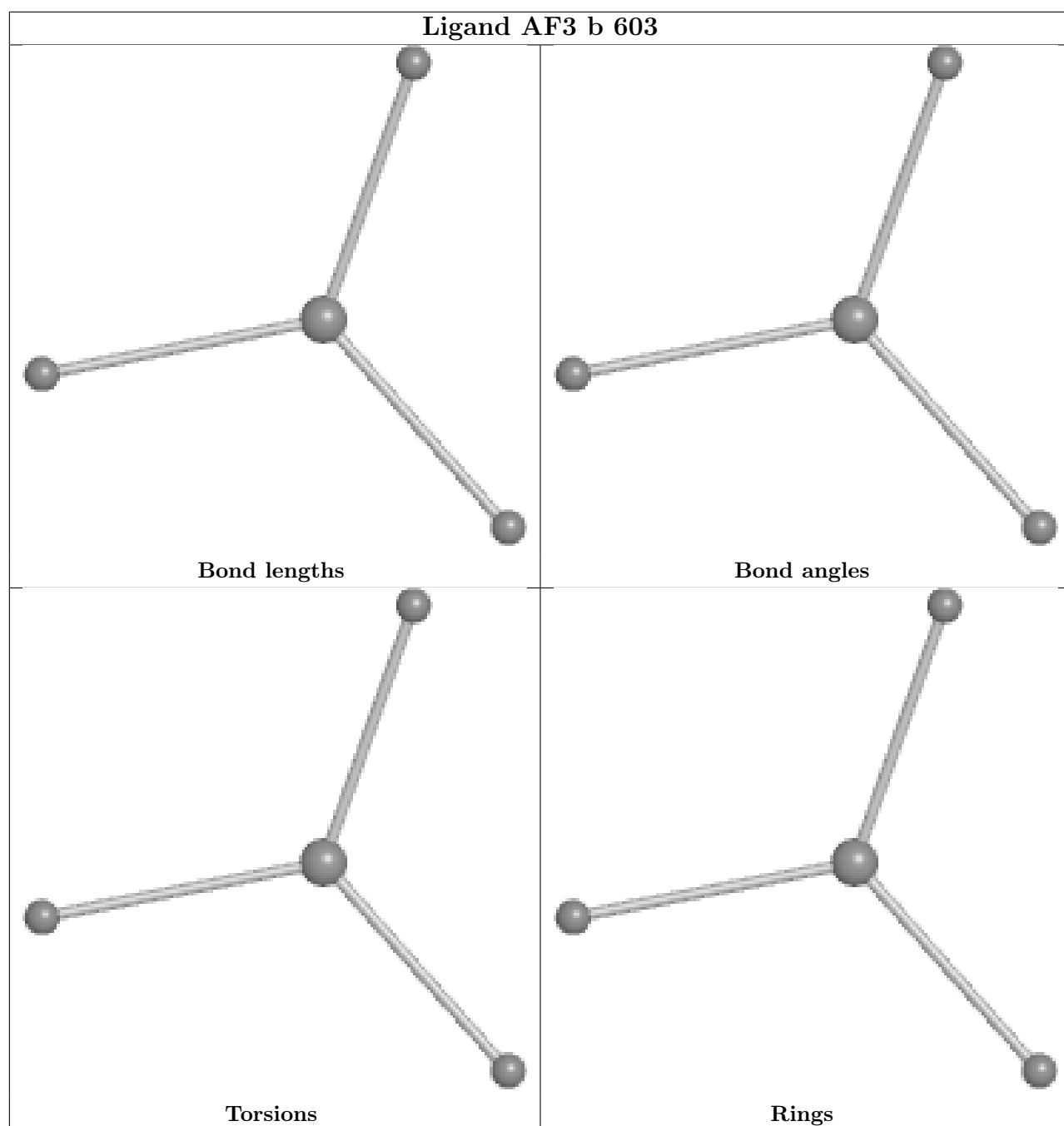
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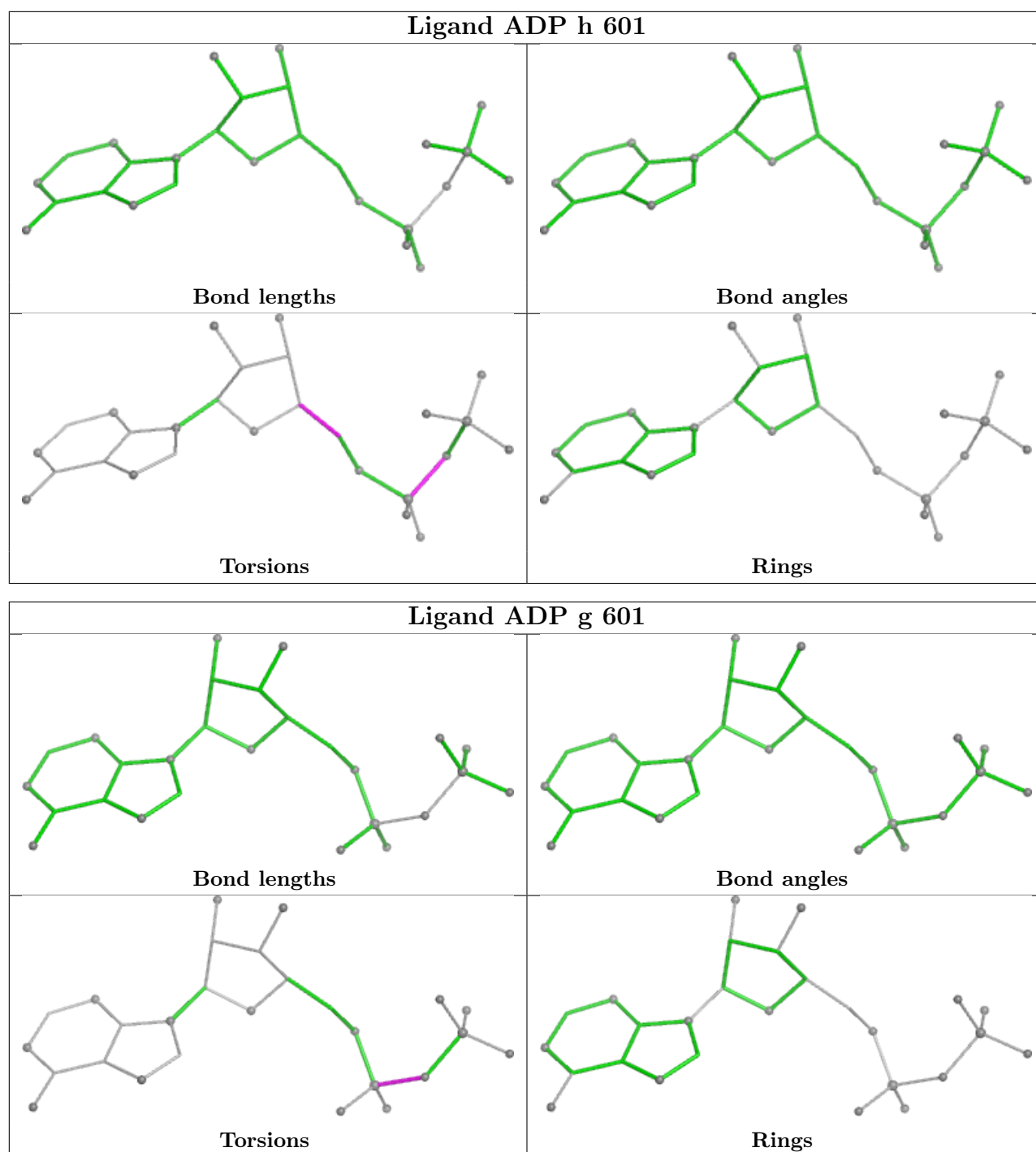
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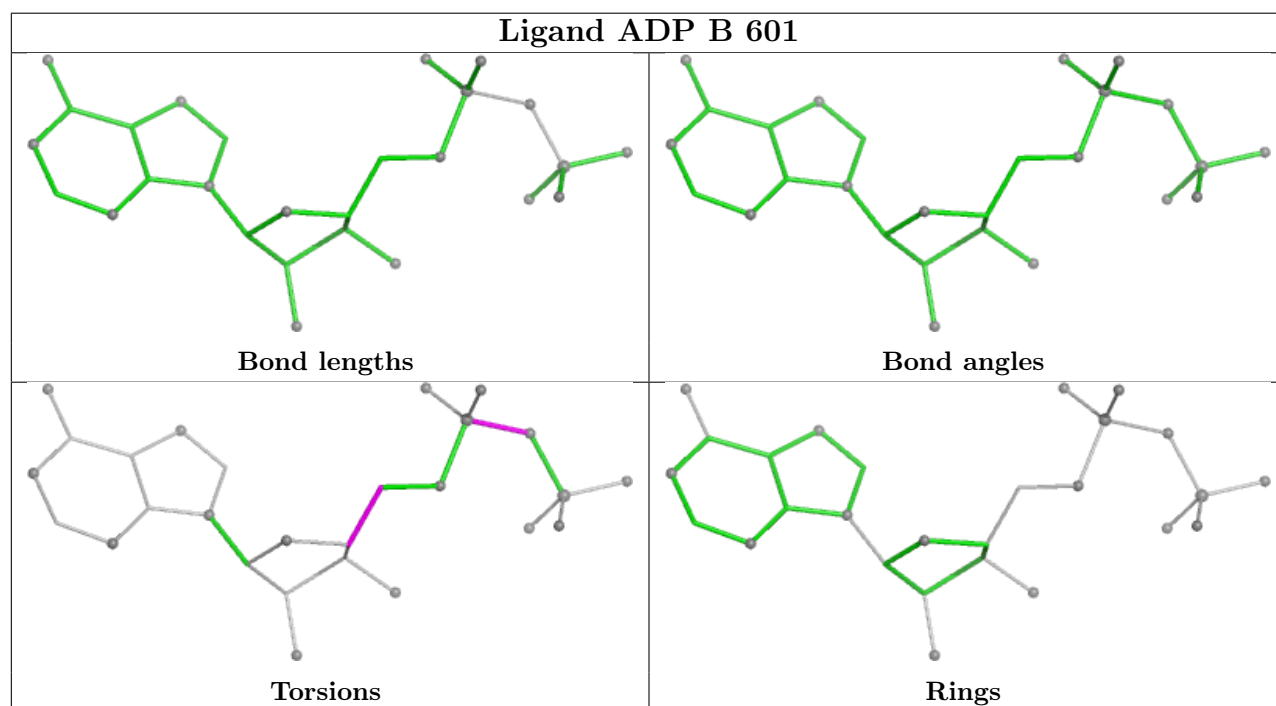
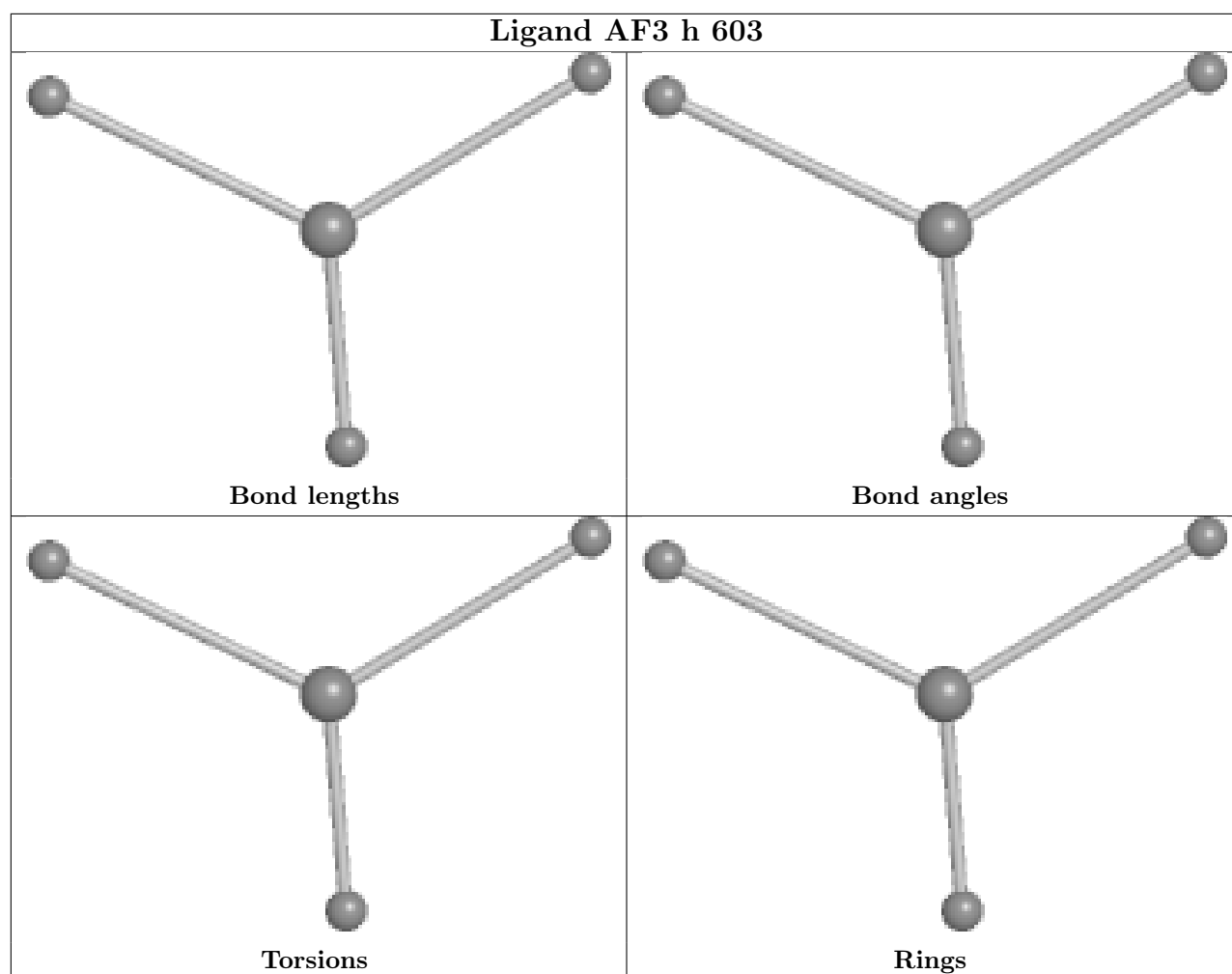
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	d	601	ADP	5	0
9	D	601	ADP	1	0
11	e	603	AF3	1	0
9	F	601	ADP	5	0
11	d	603	AF3	1	0
9	f	601	ADP	2	0
9	E	601	ADP	1	0
11	f	603	AF3	1	0
9	a	601	ADP	1	0
9	C	601	ADP	7	0
9	e	601	ADP	1	0
9	H	601	ADP	3	0
9	G	601	ADP	2	0

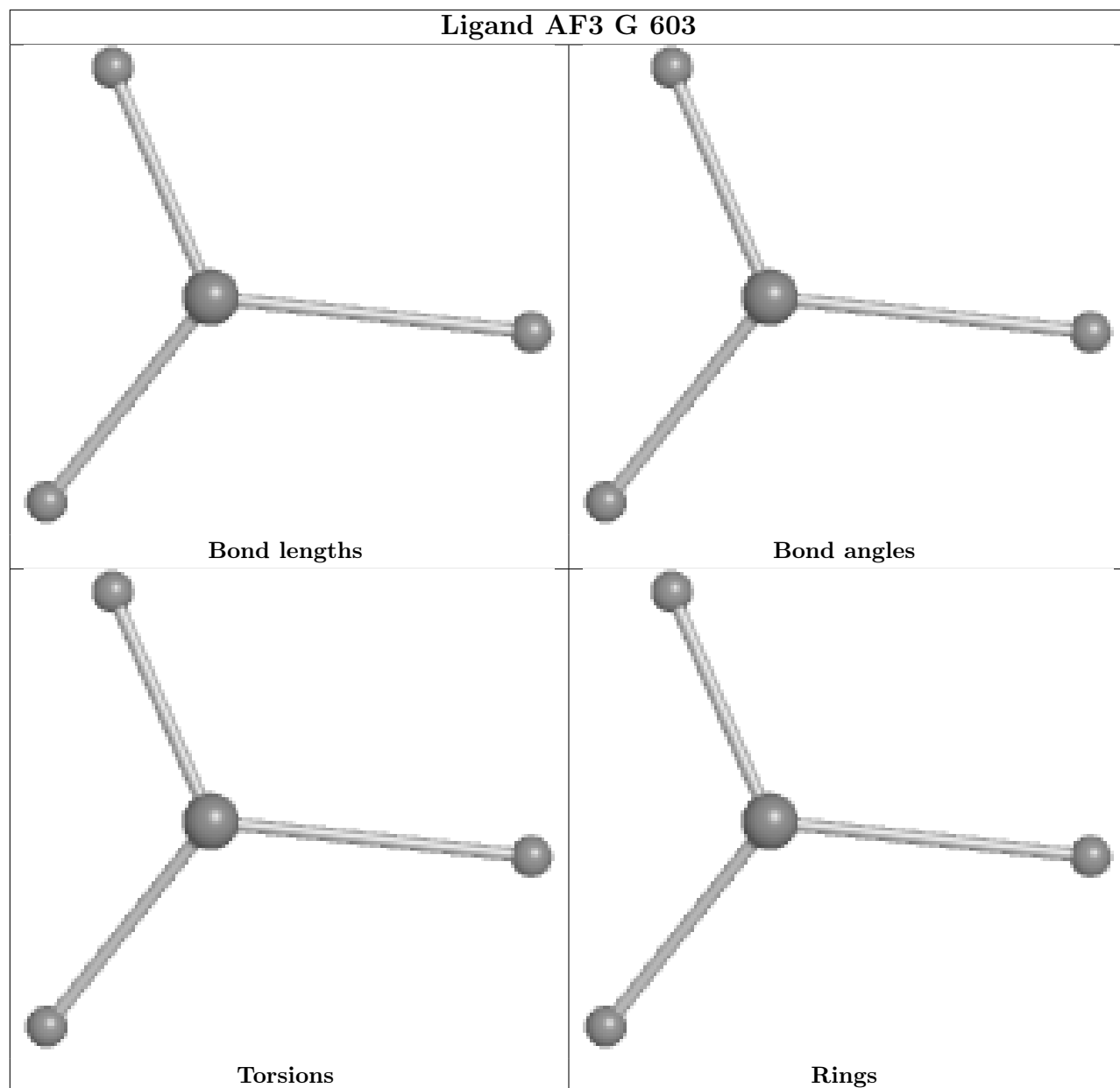
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

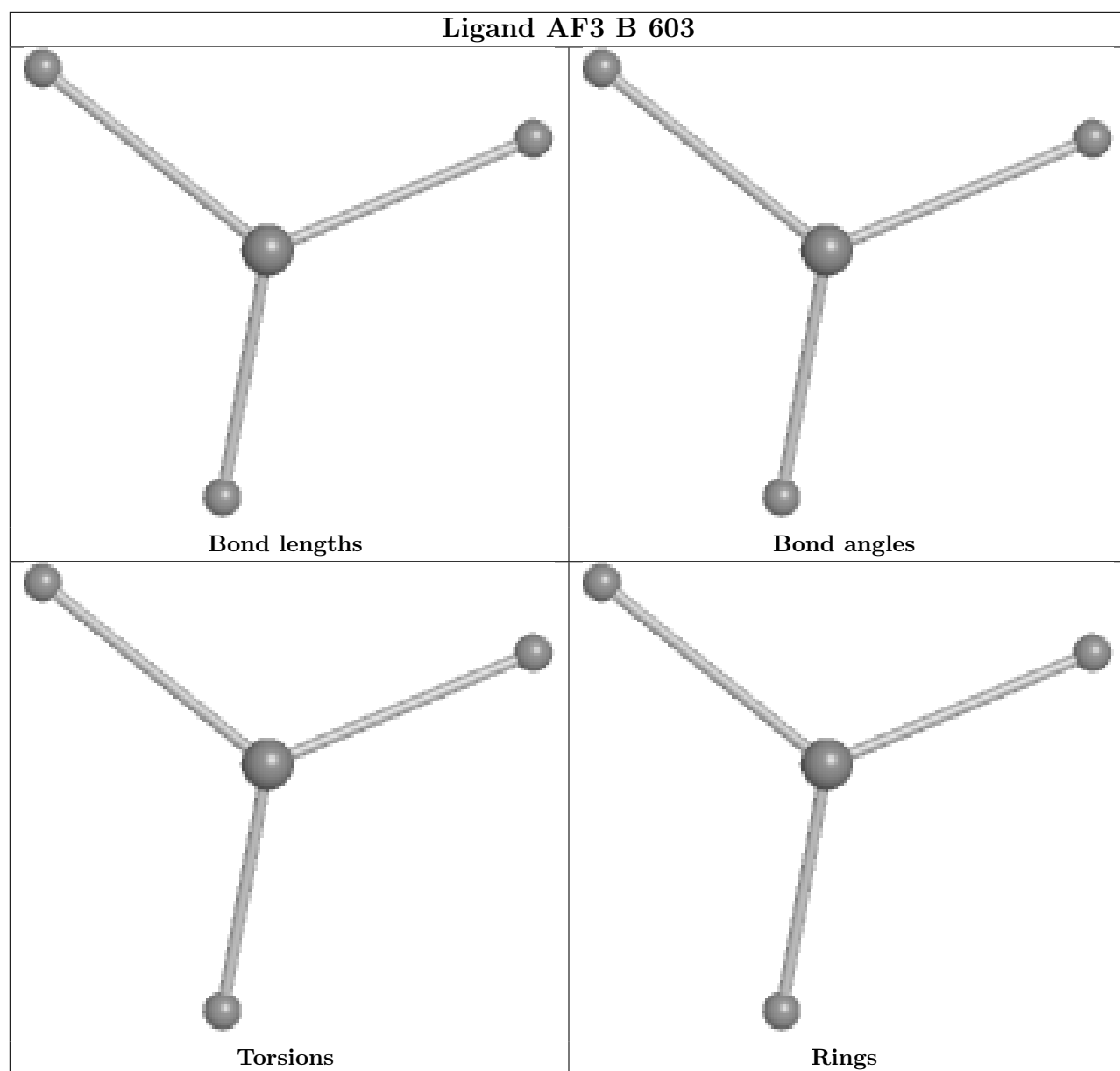


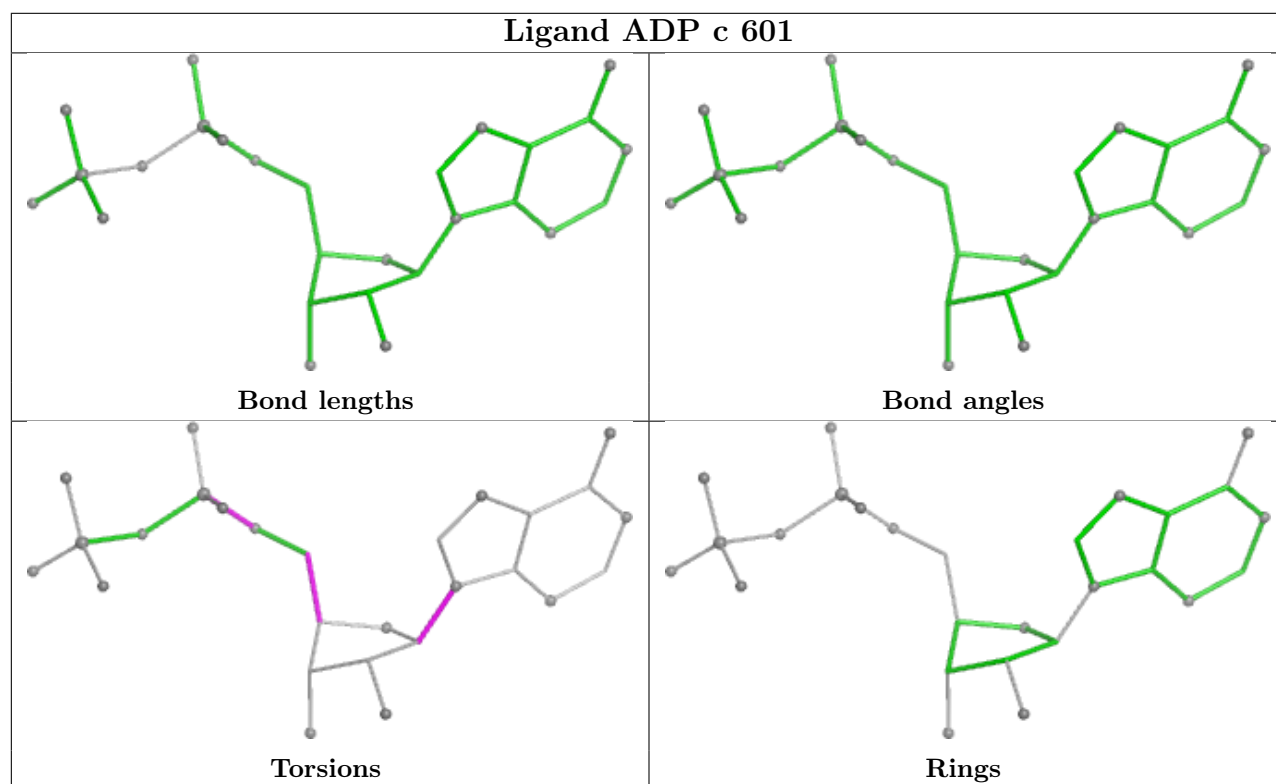
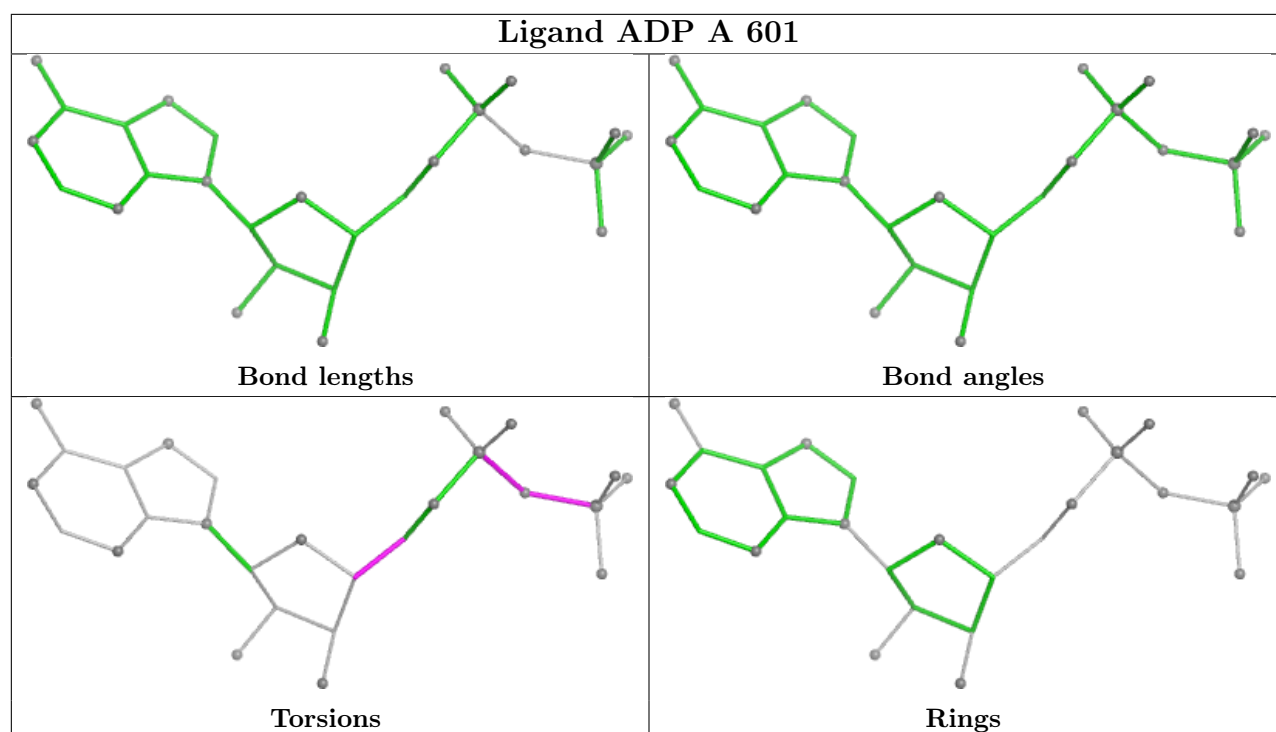


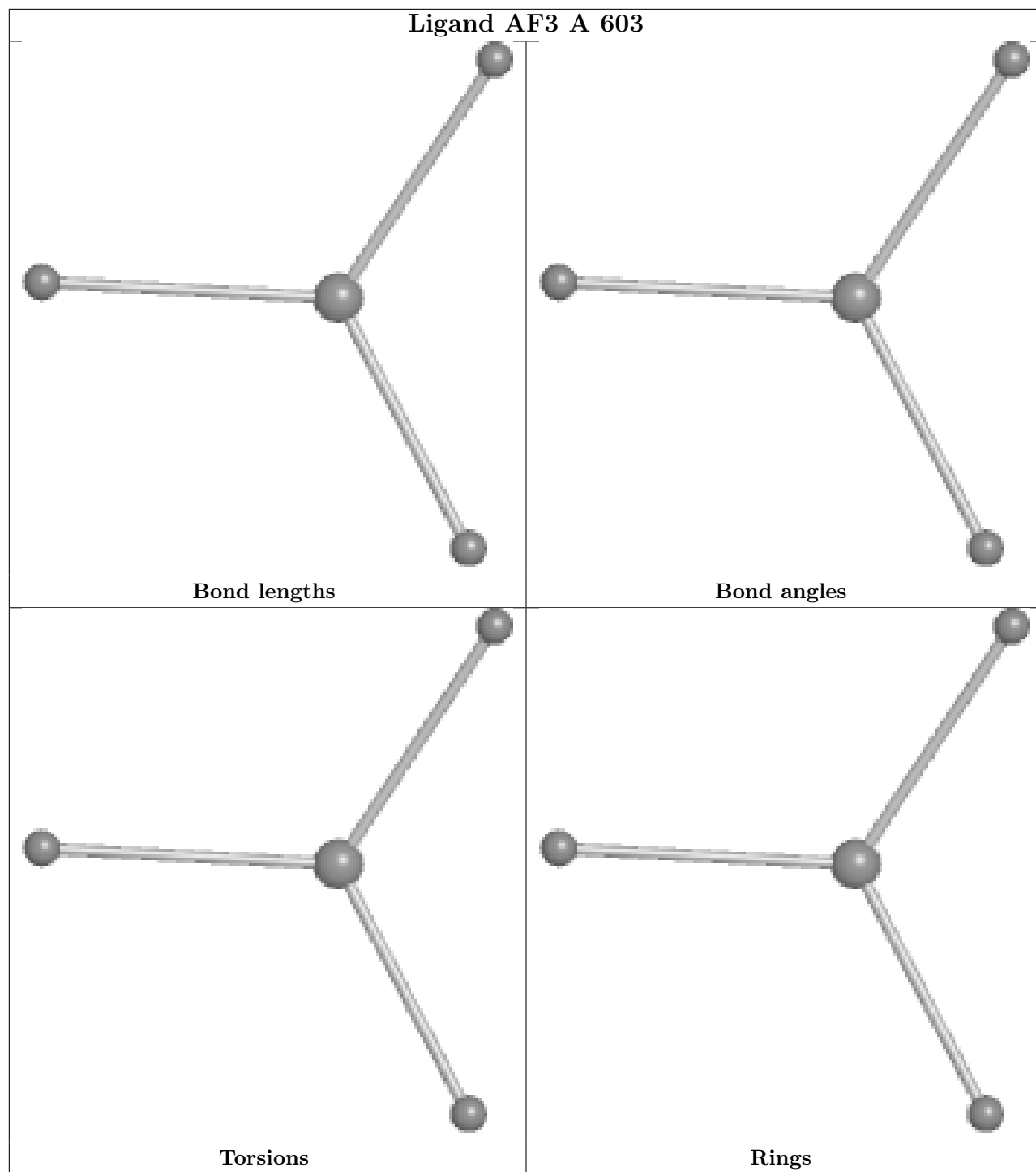


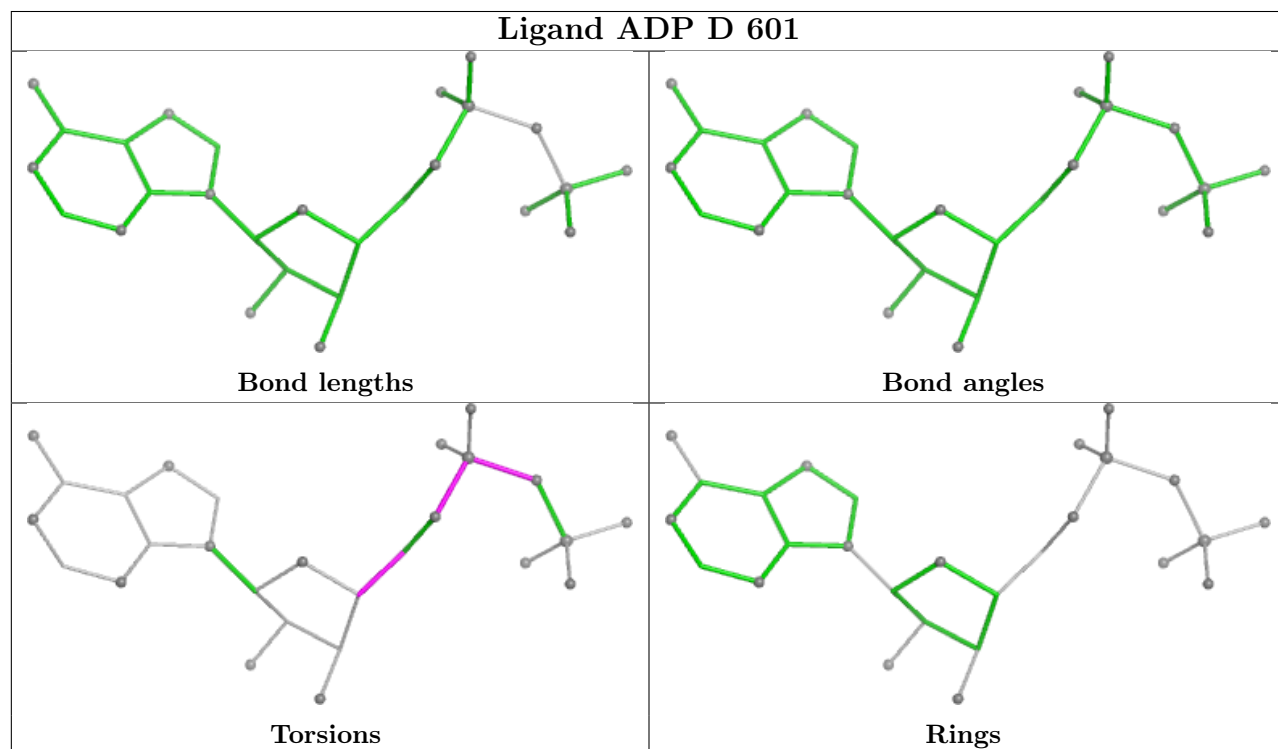
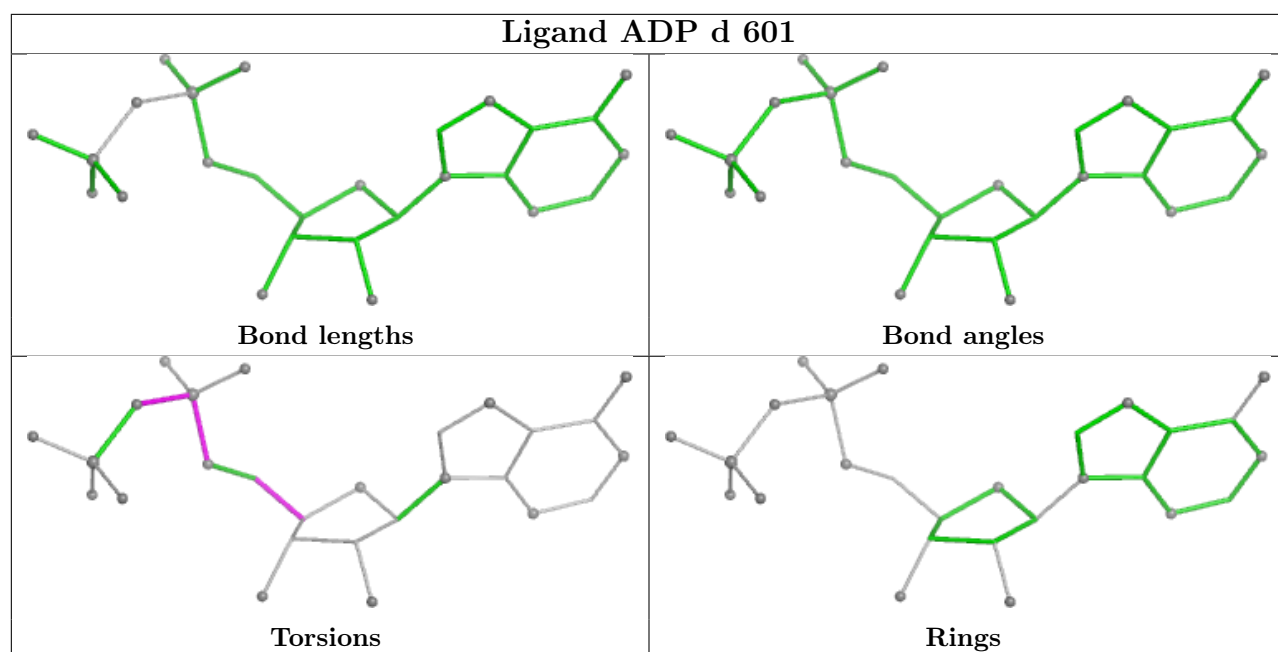


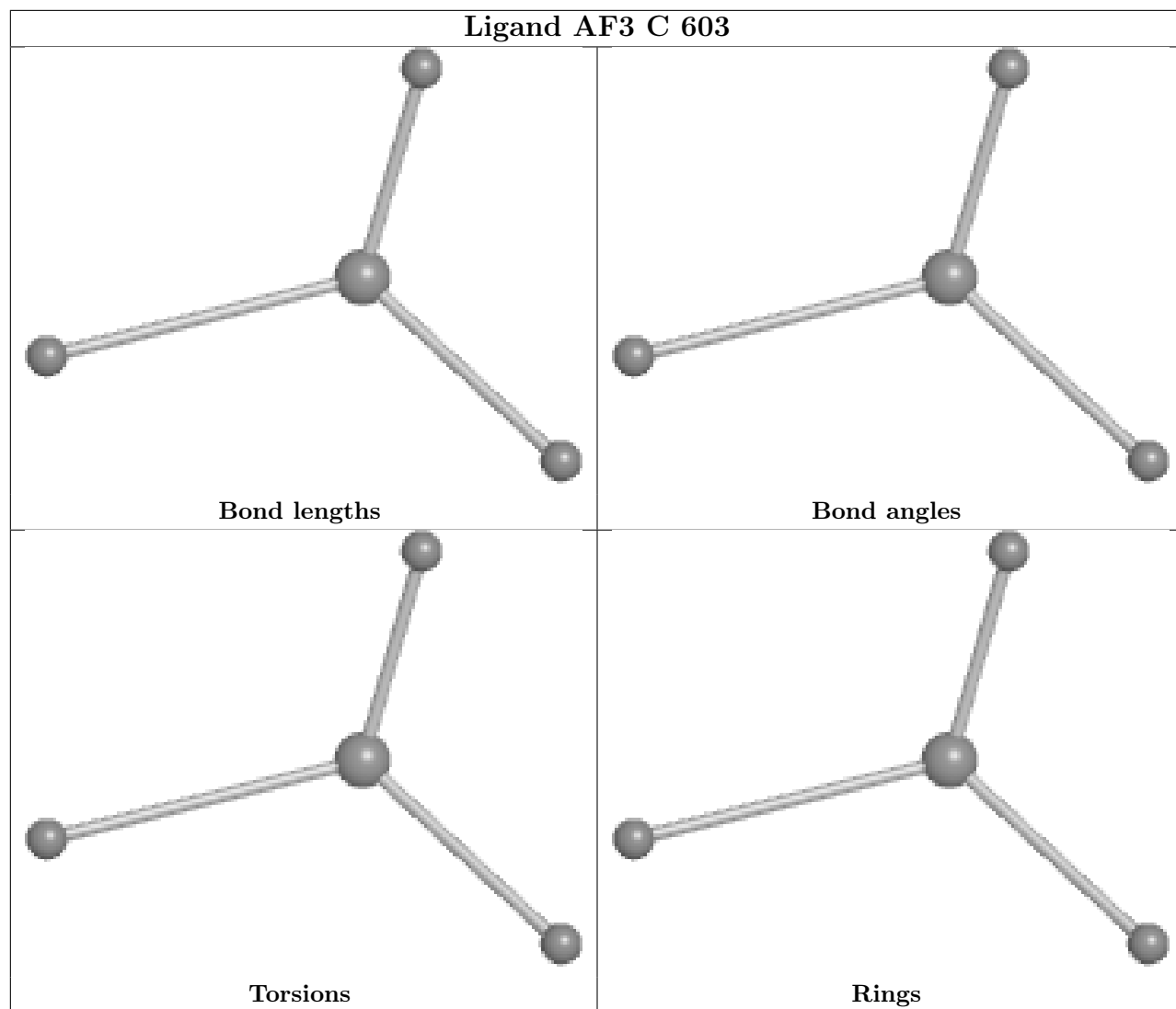


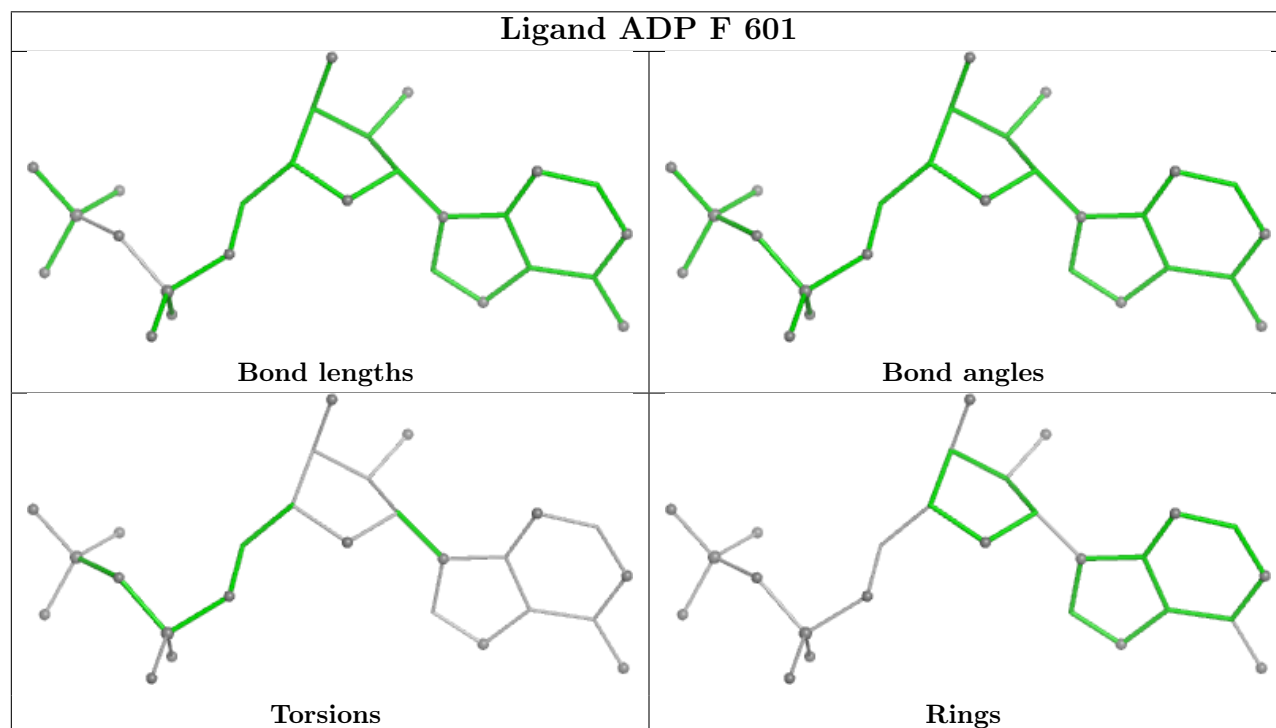
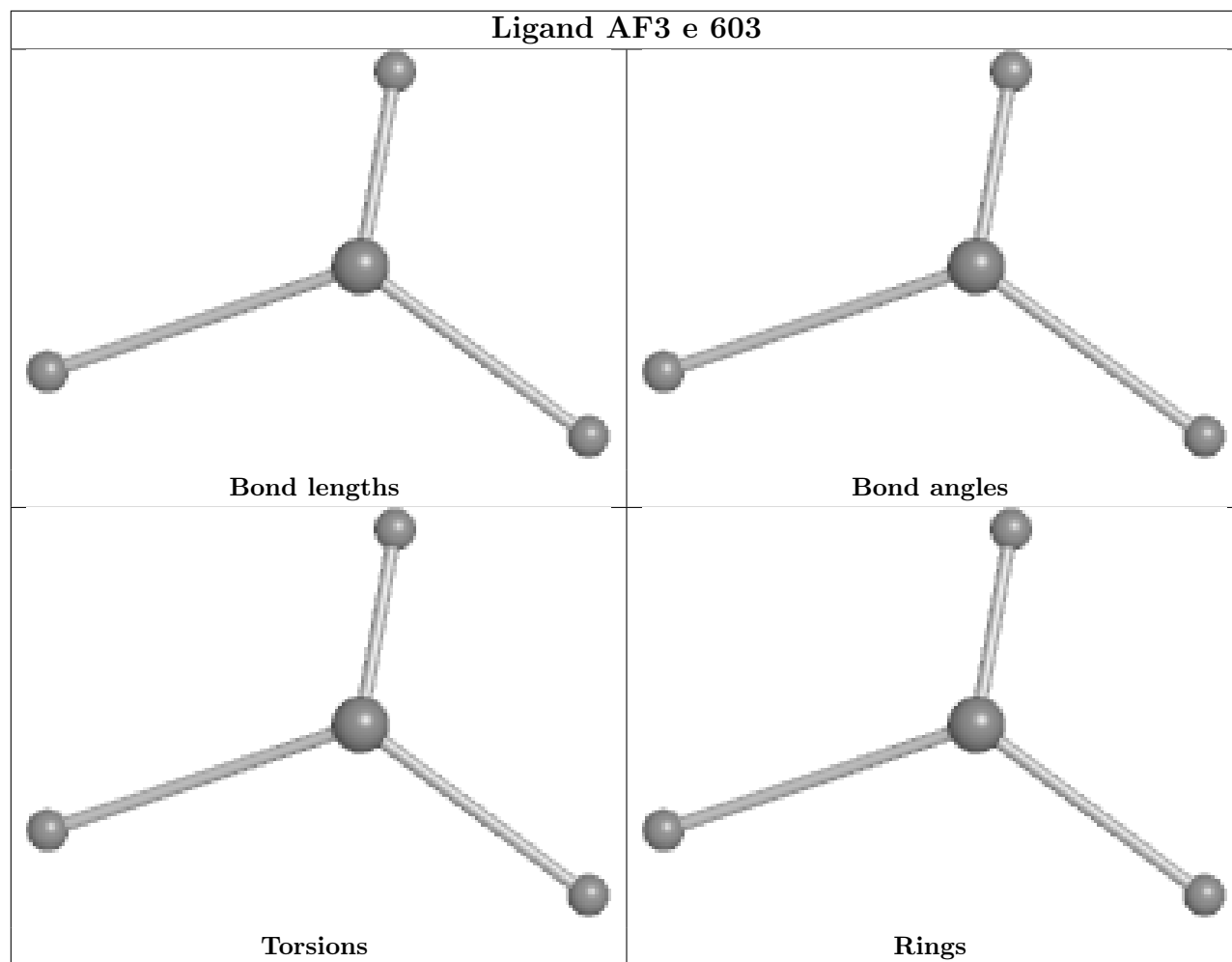


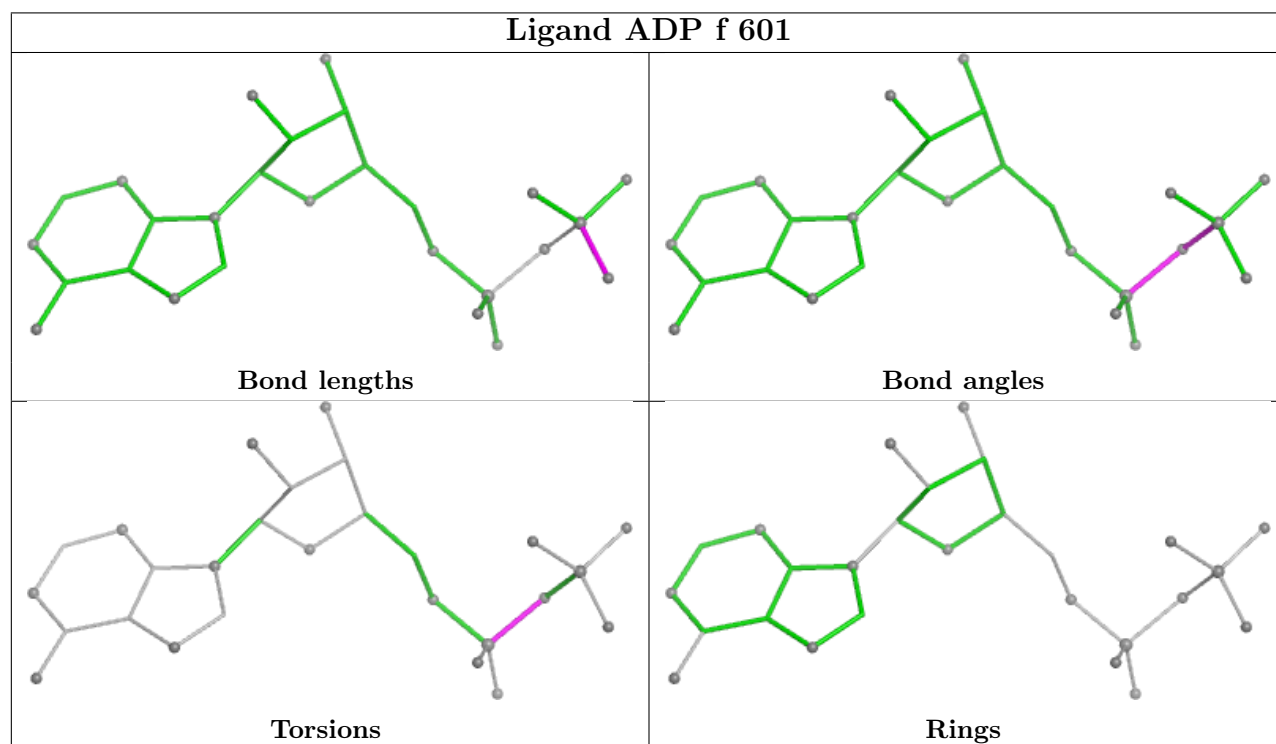
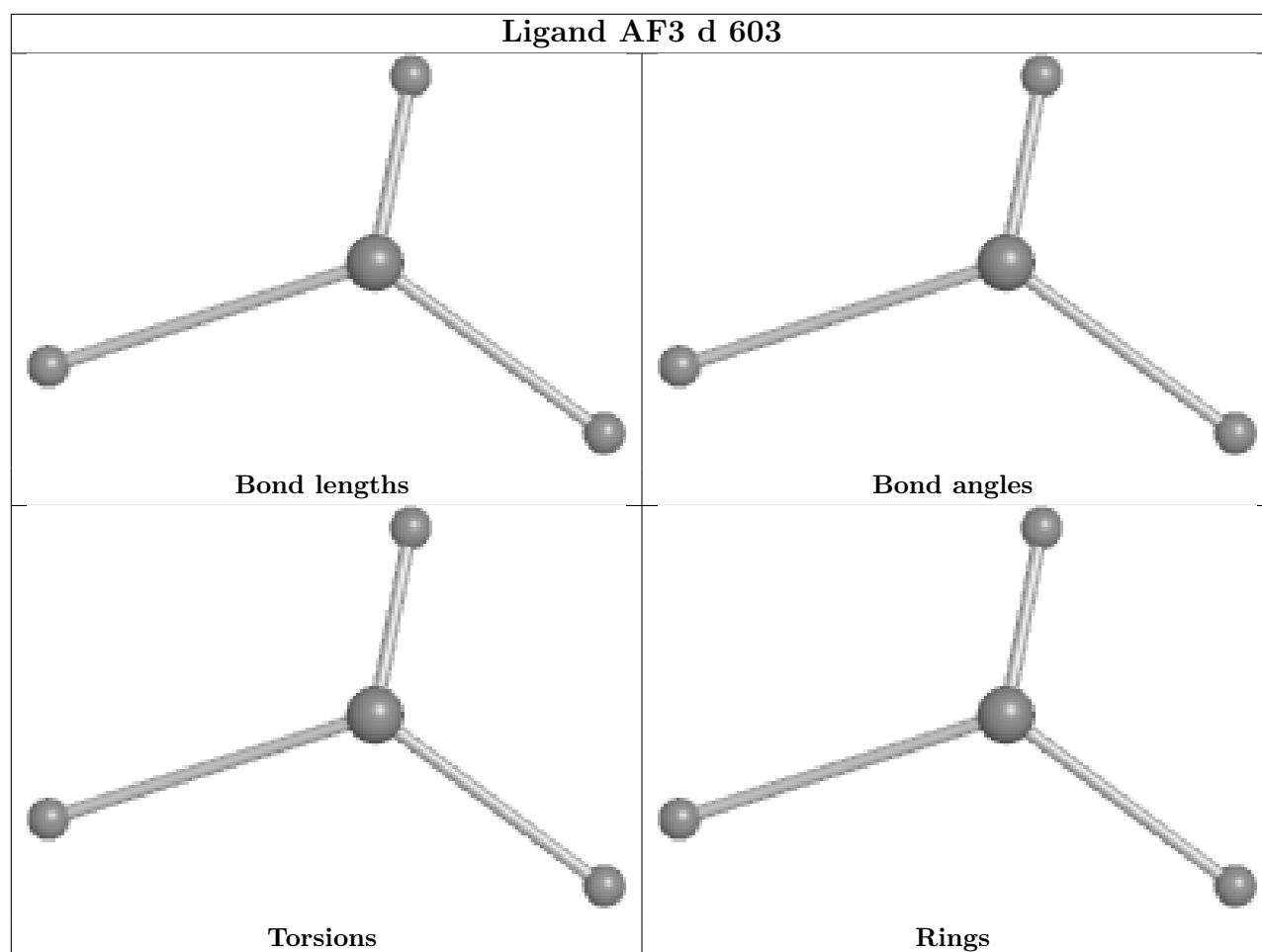


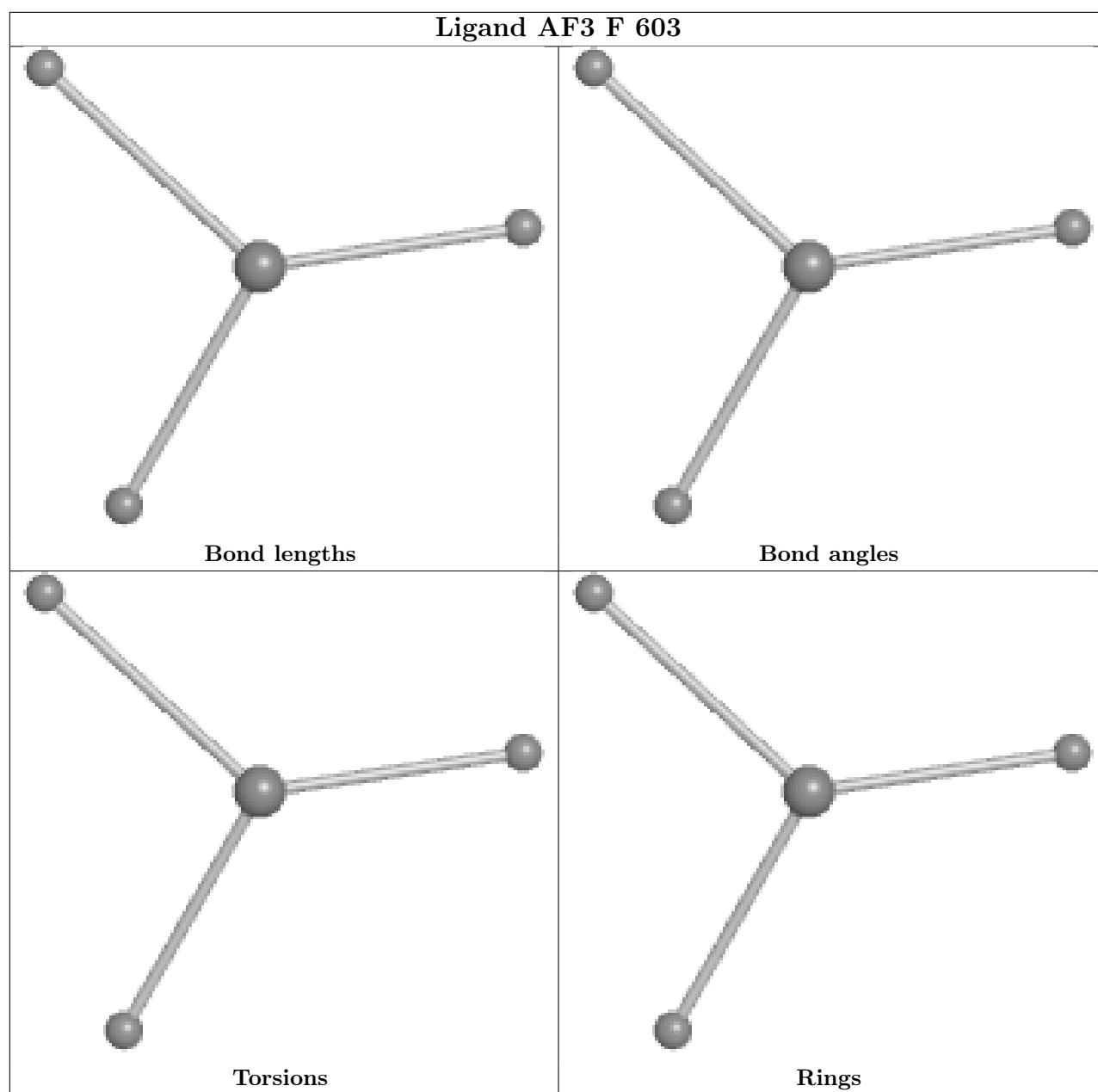


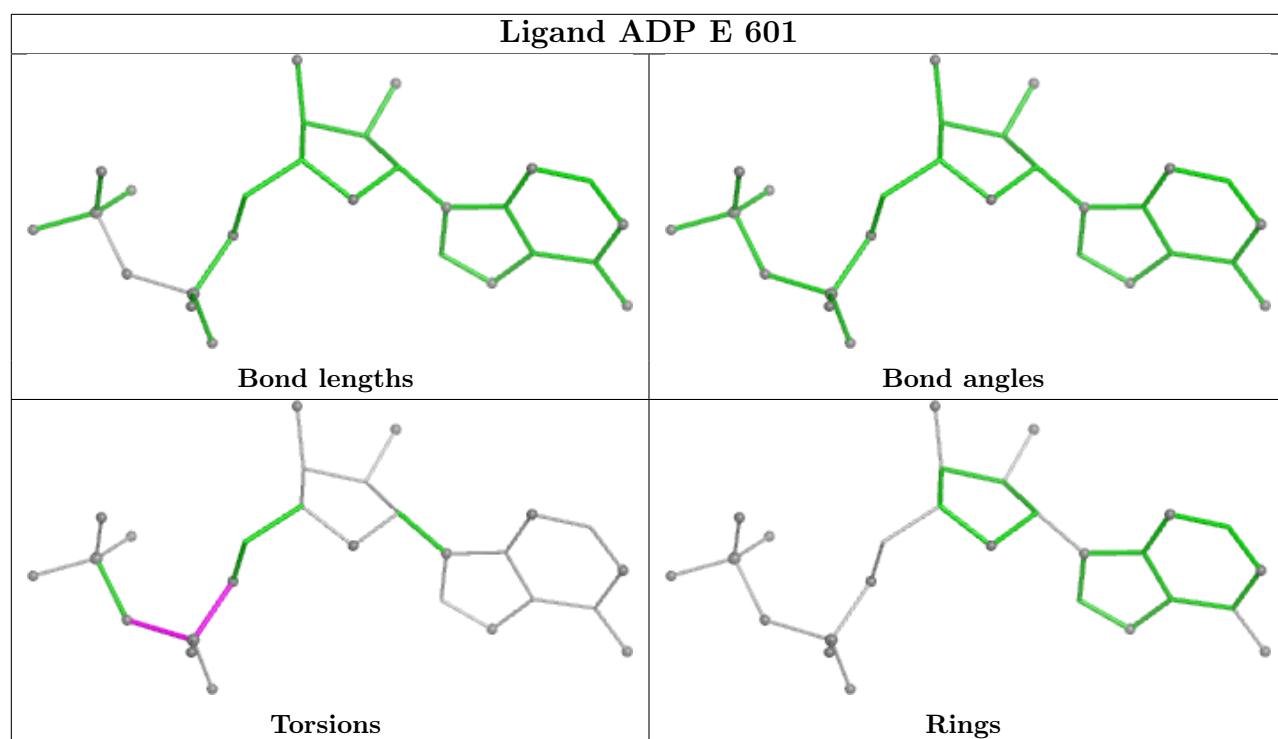


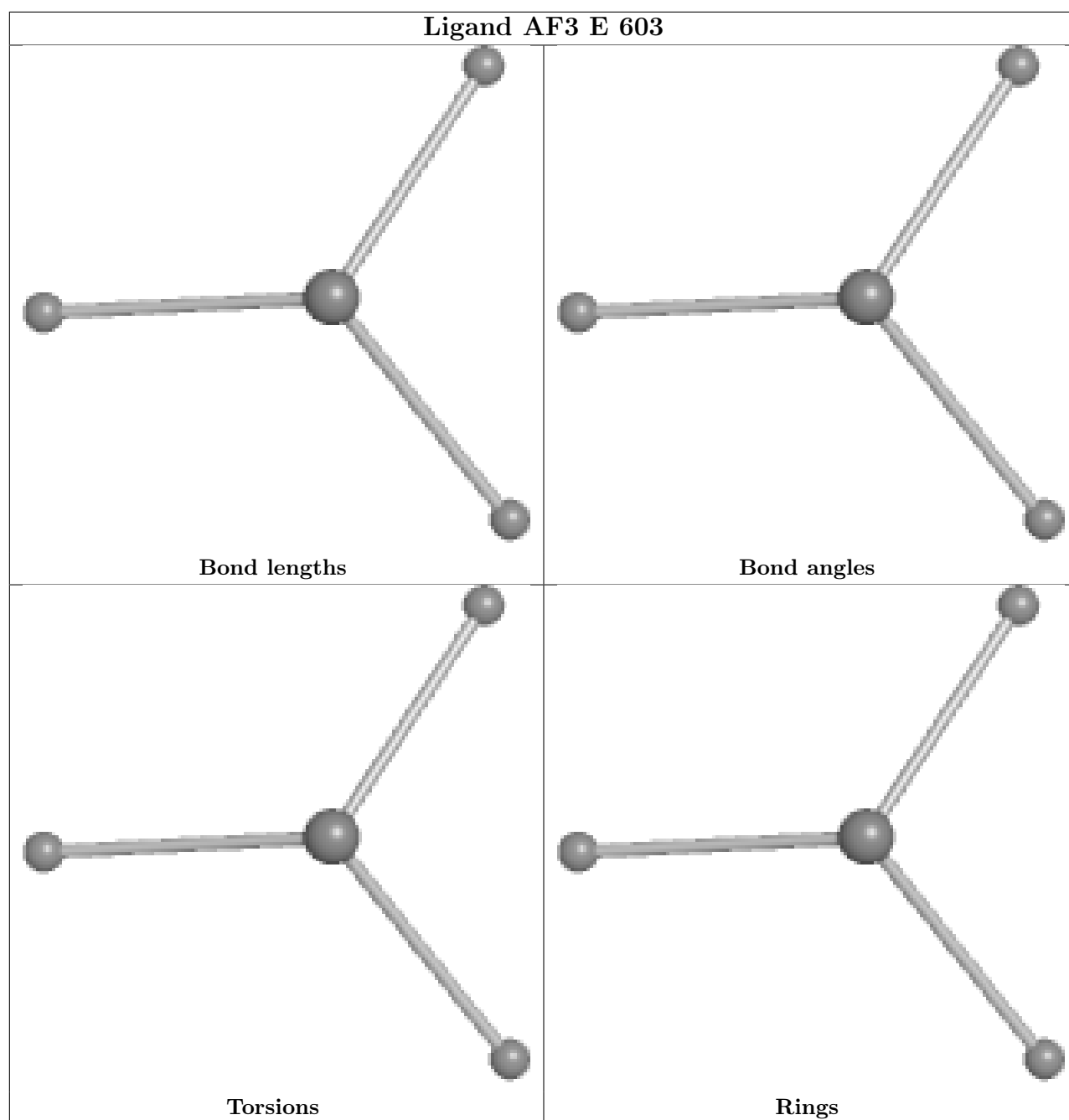


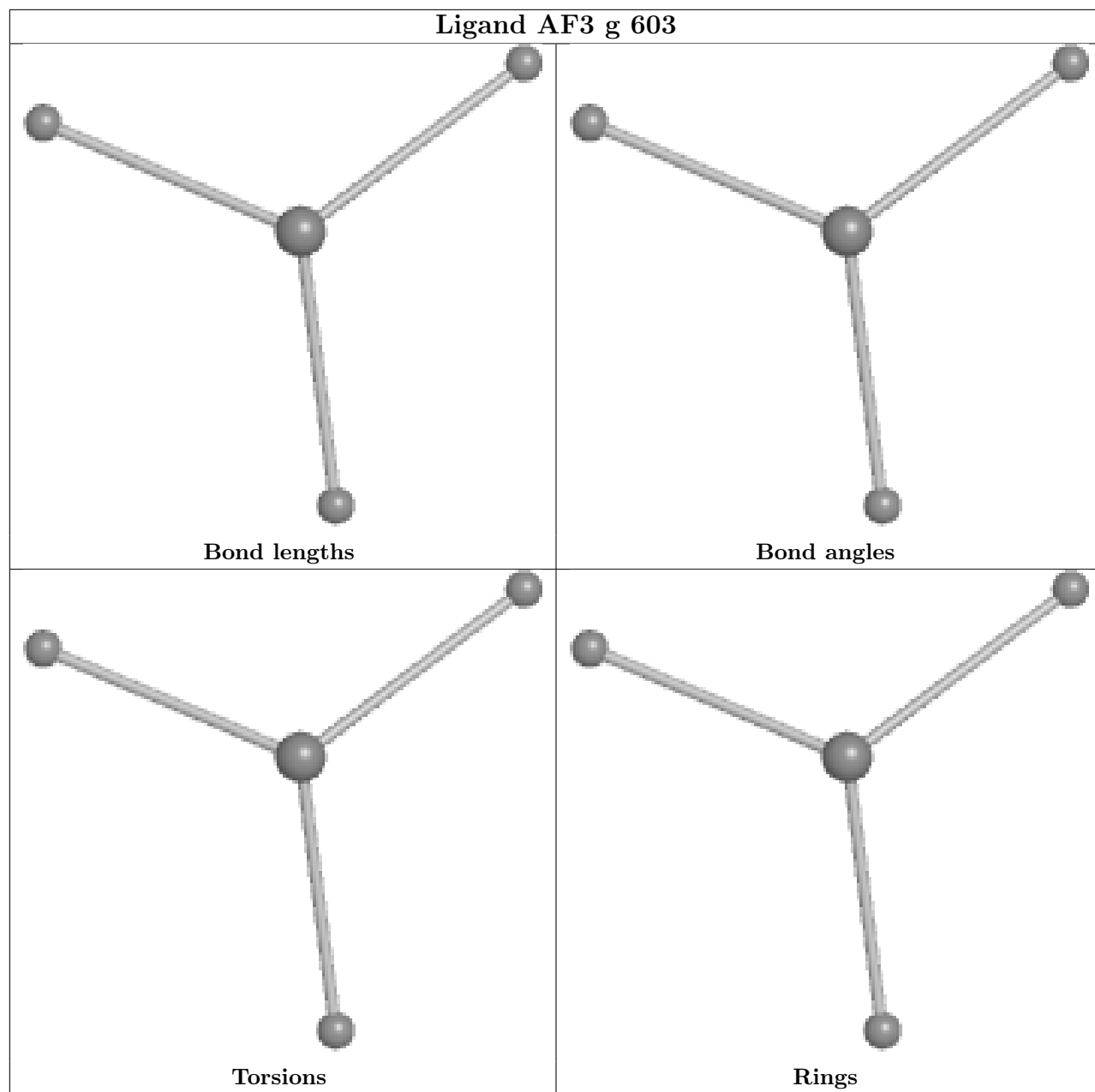


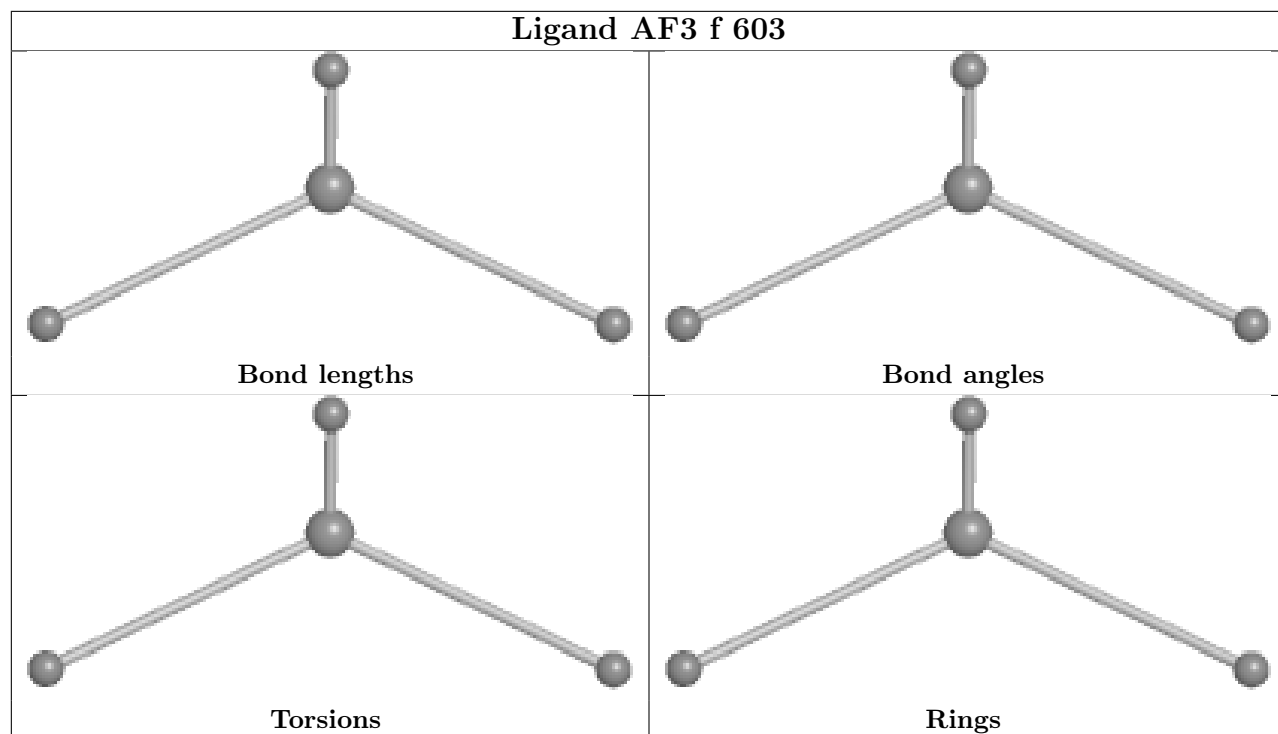


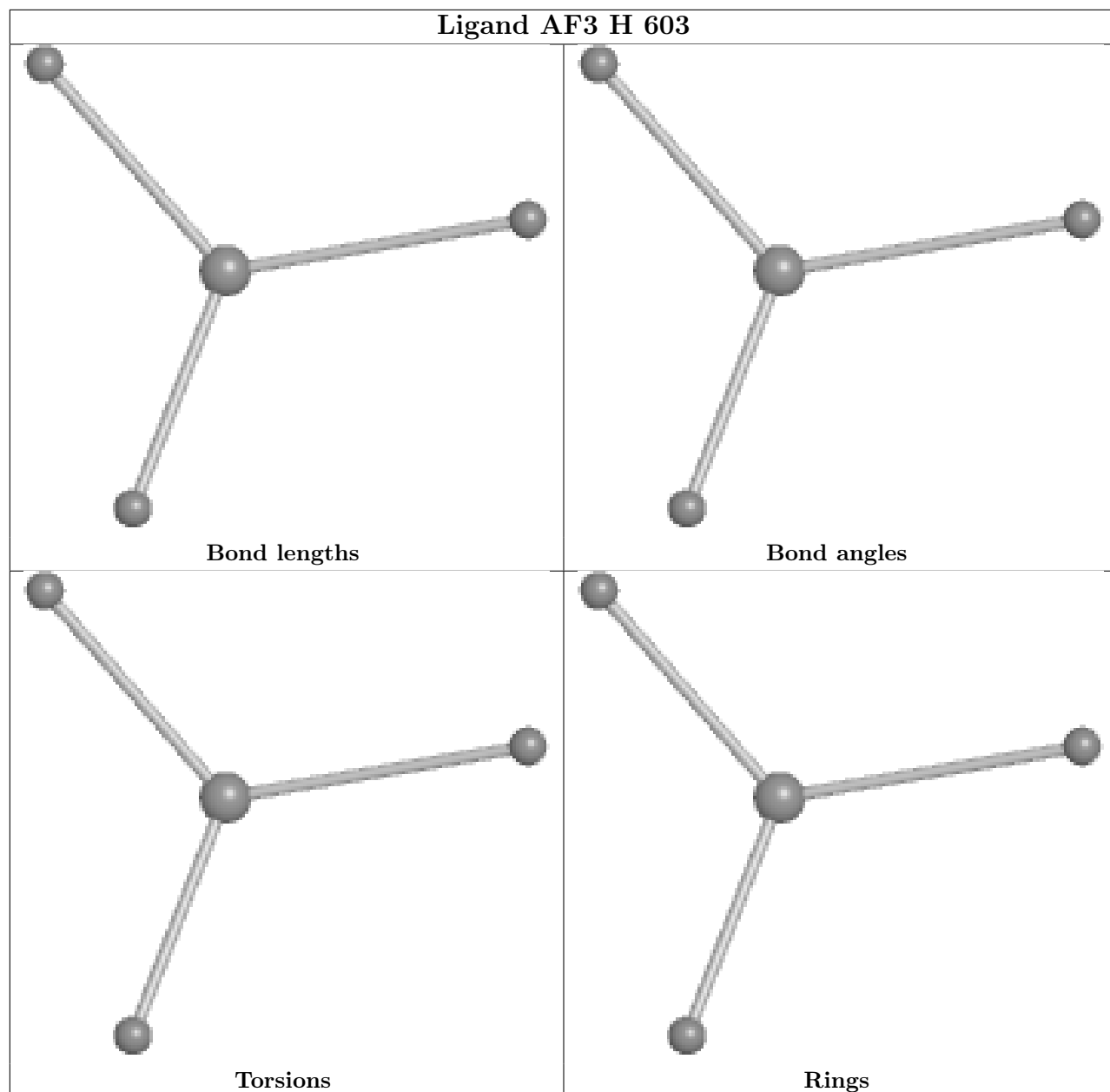


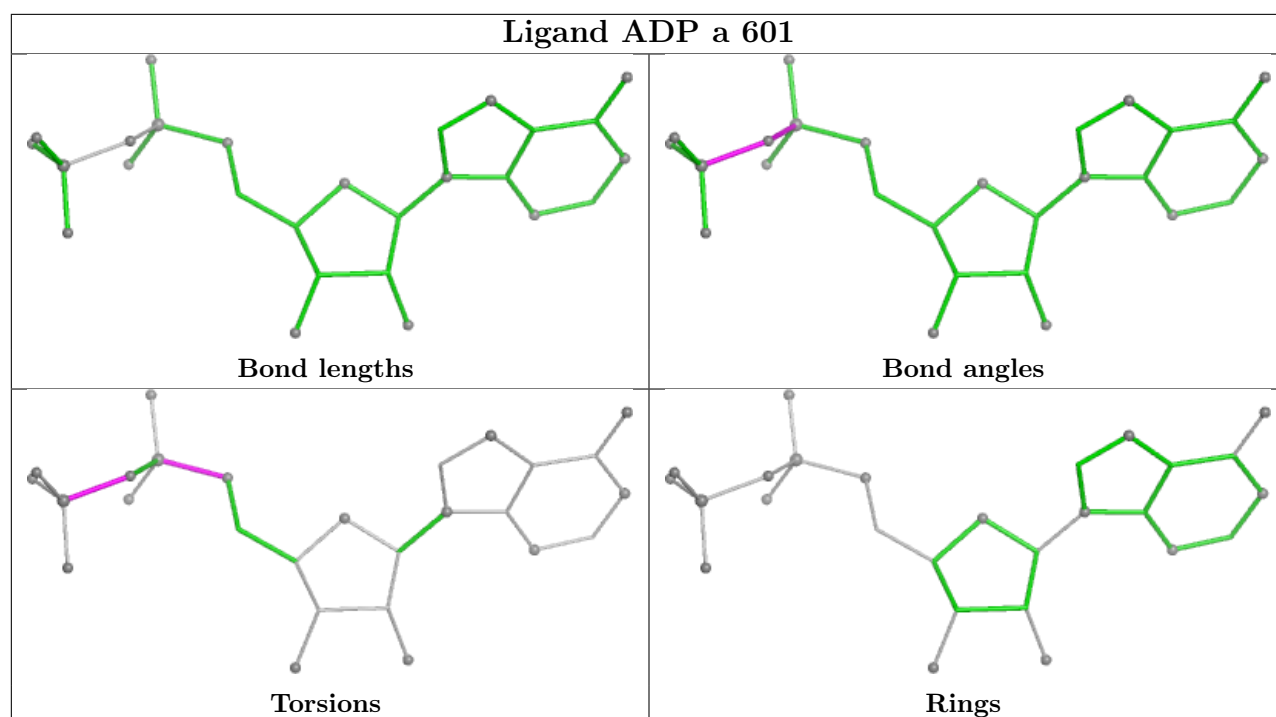


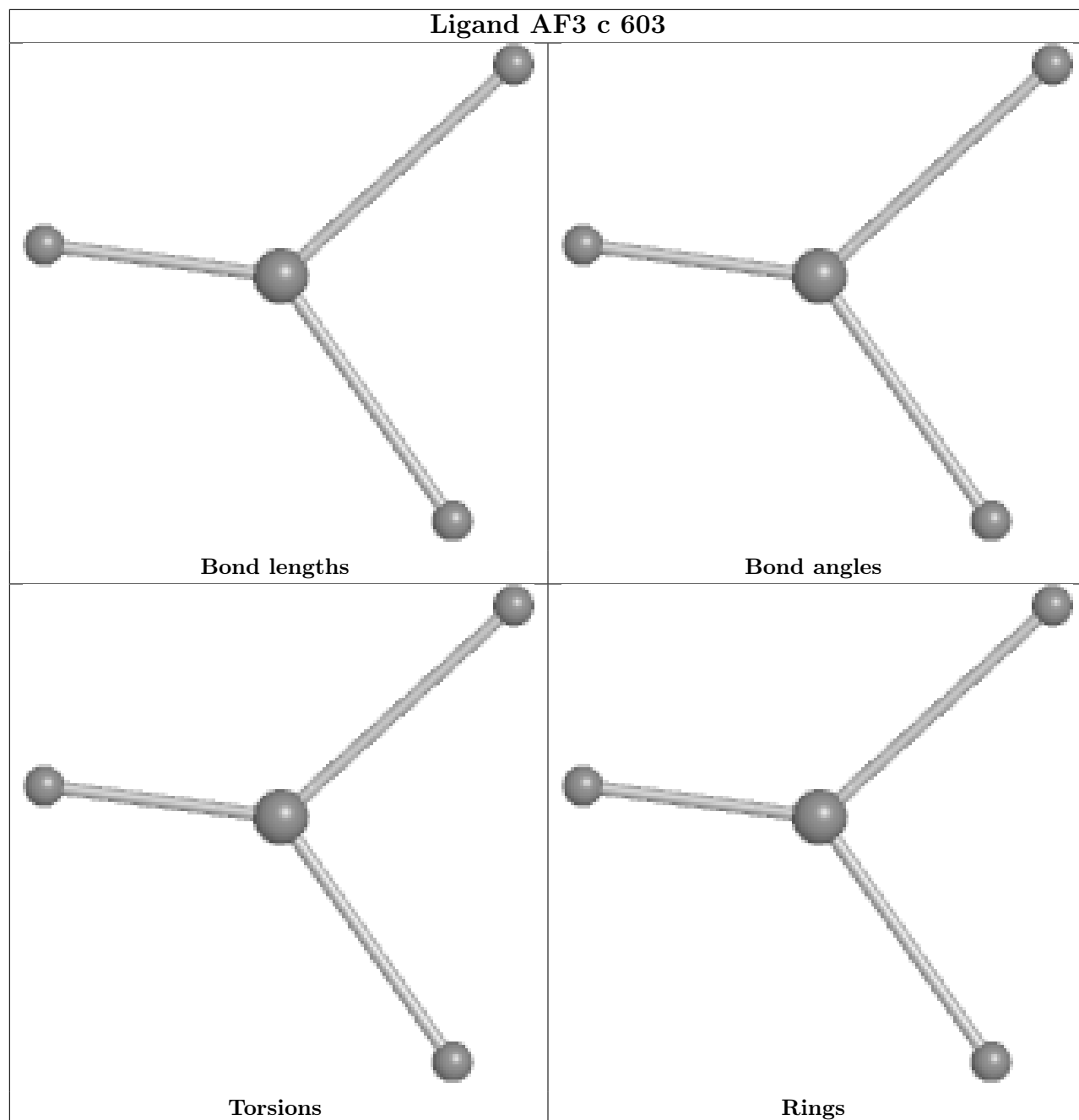


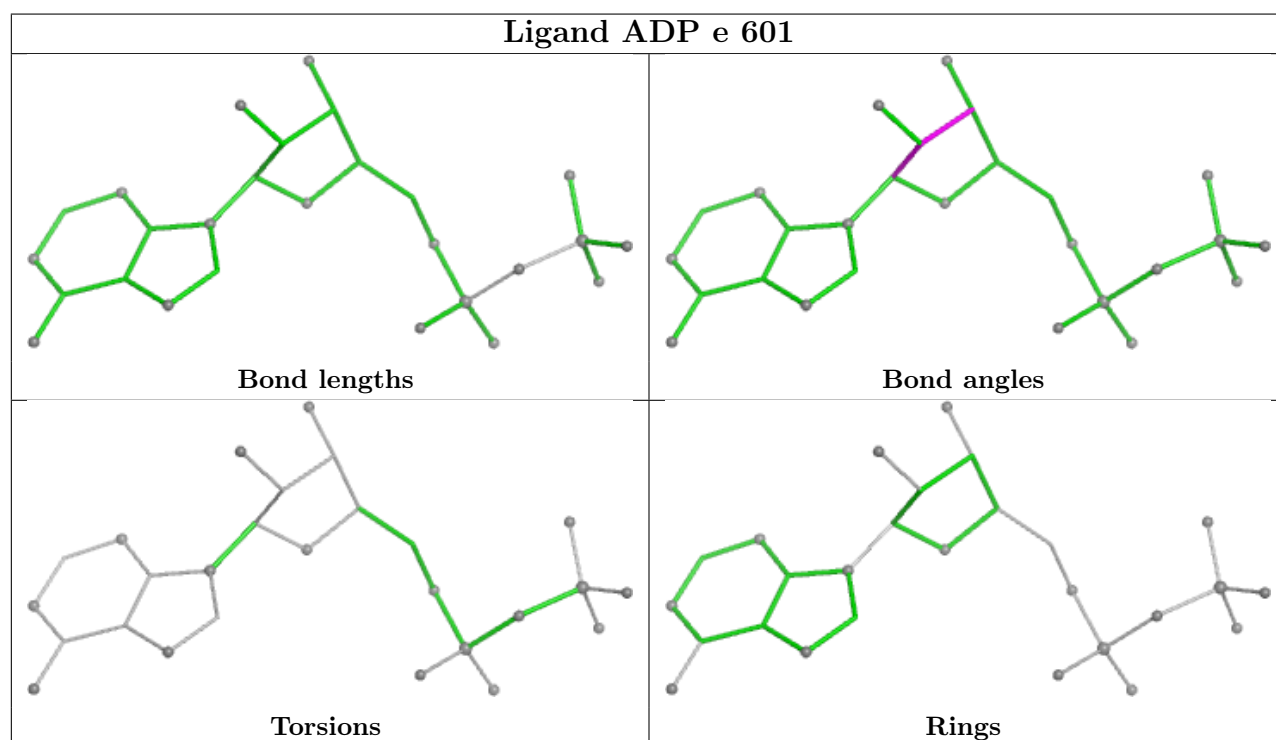
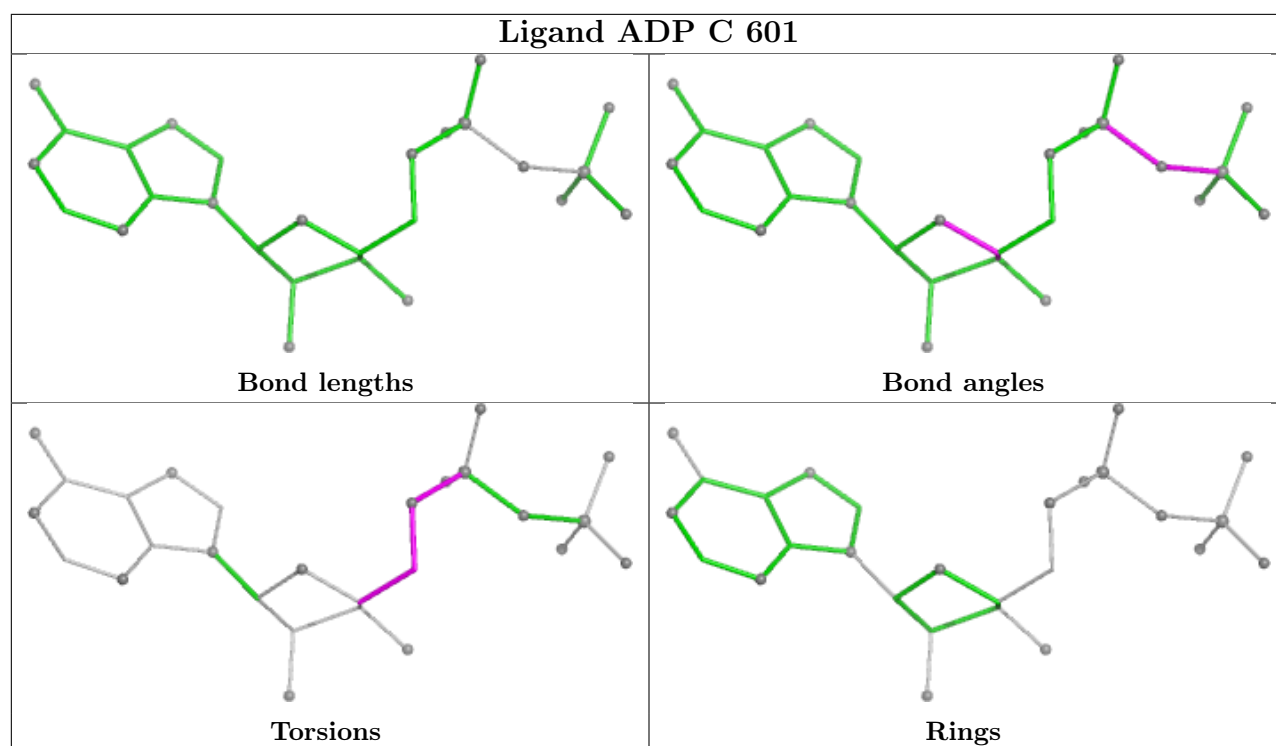


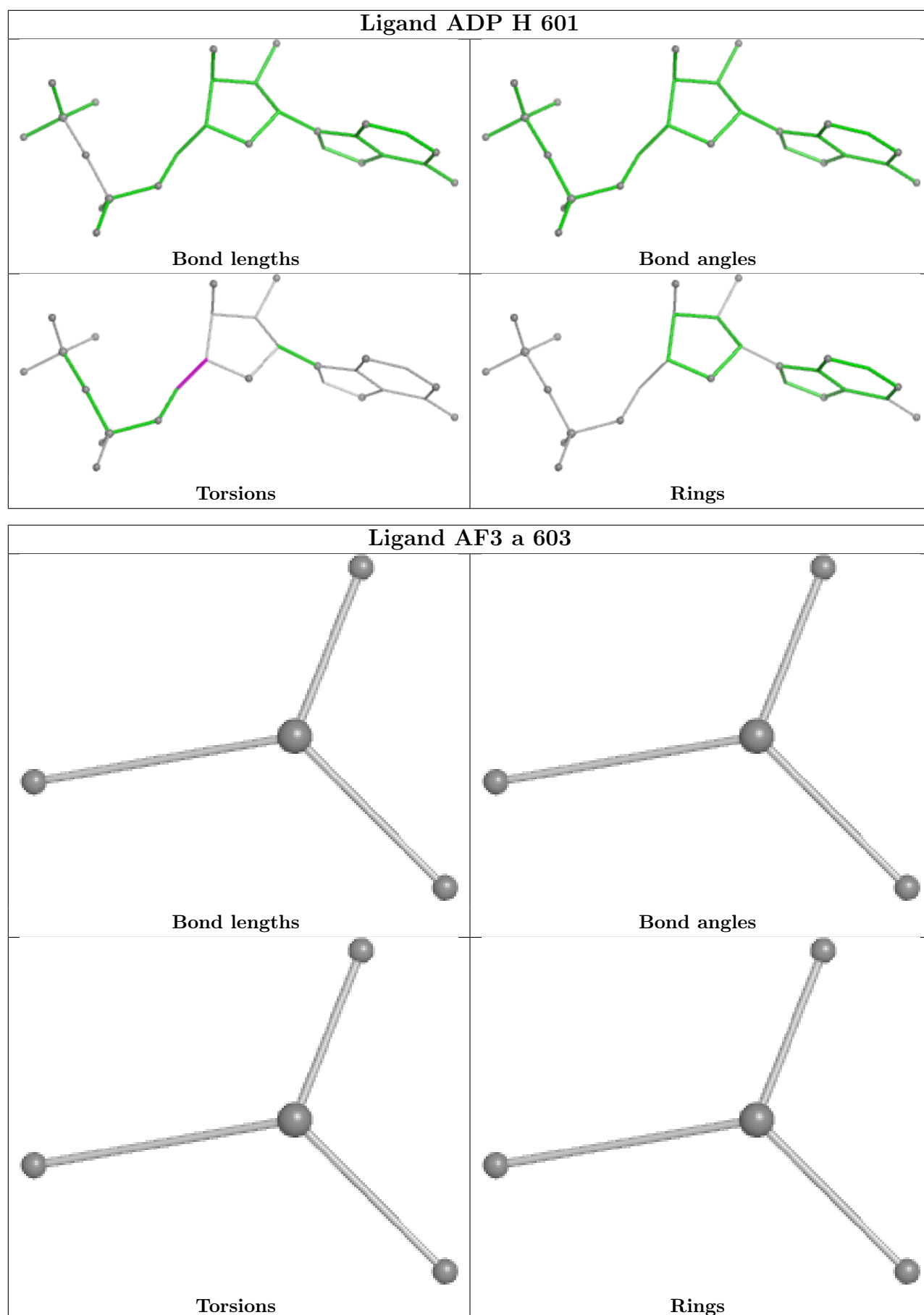


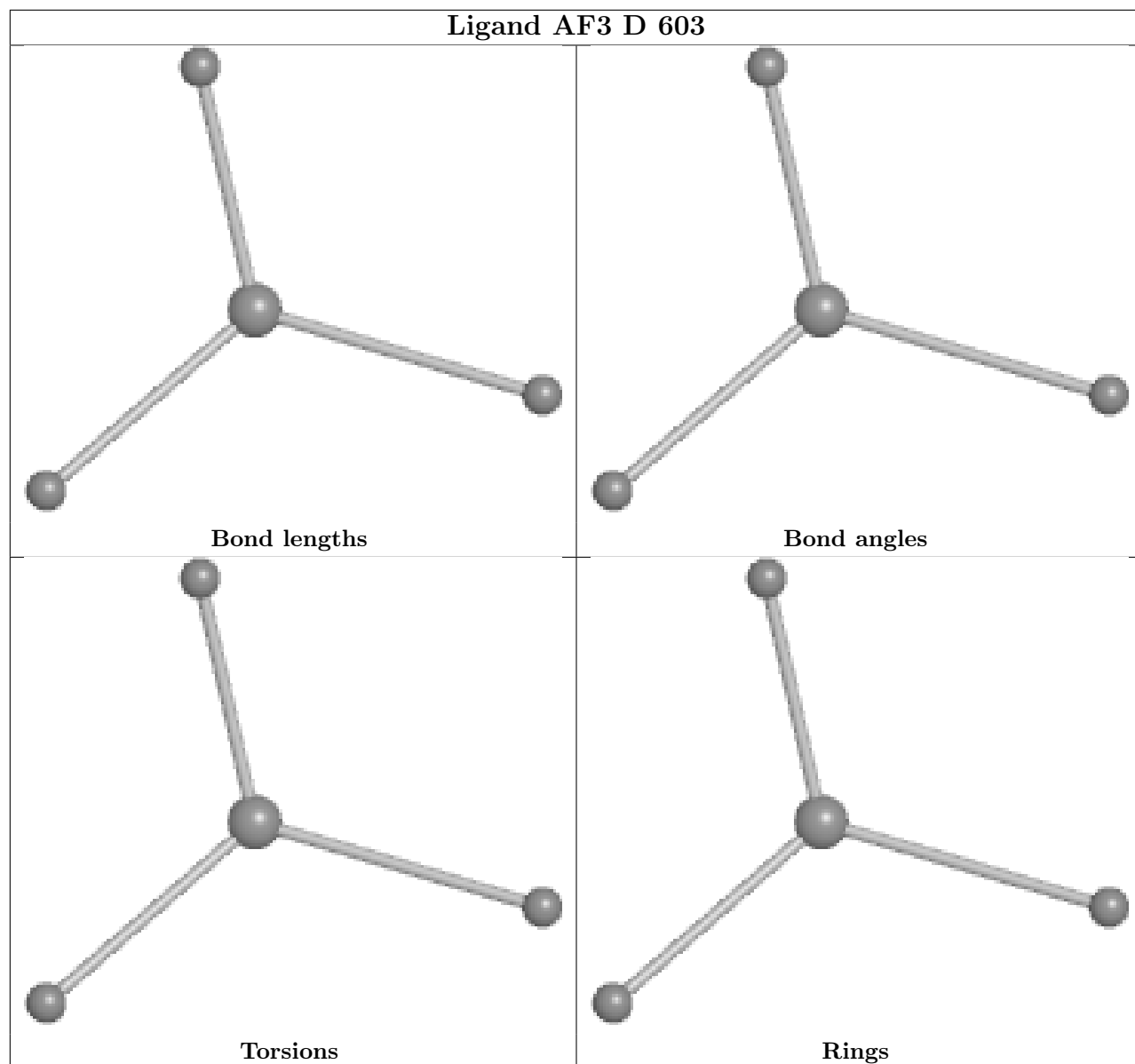


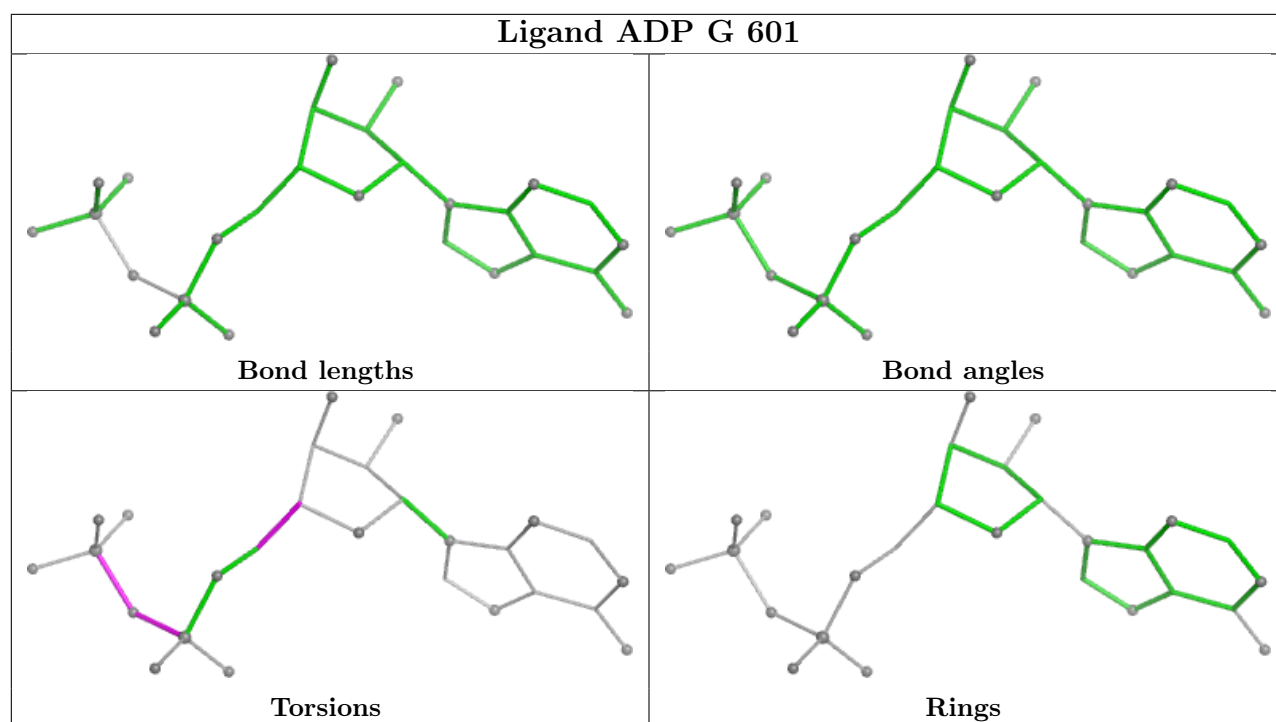












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

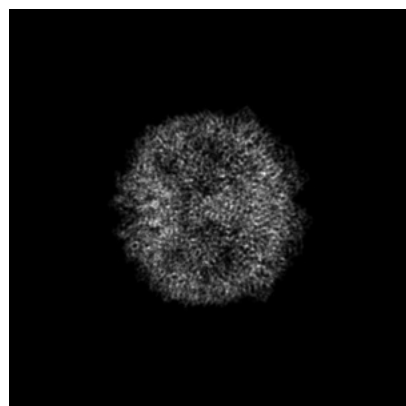
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54634. These allow visual inspection of the internal detail of the map and identification of artifacts.

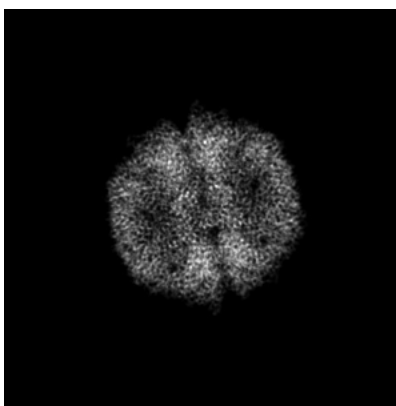
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

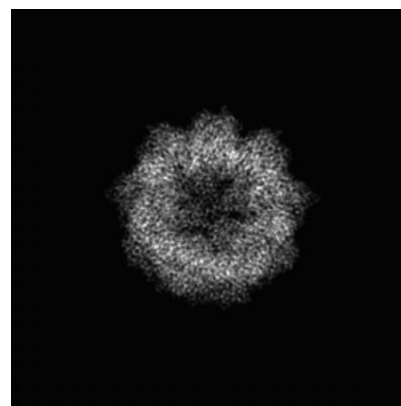
6.1.1 Primary map



X

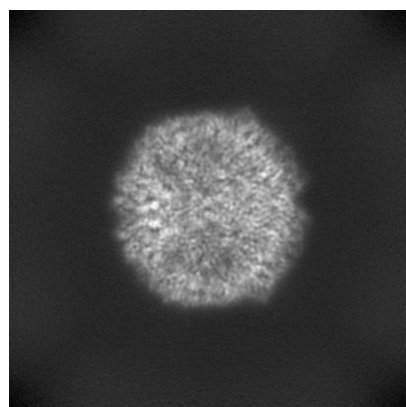


Y

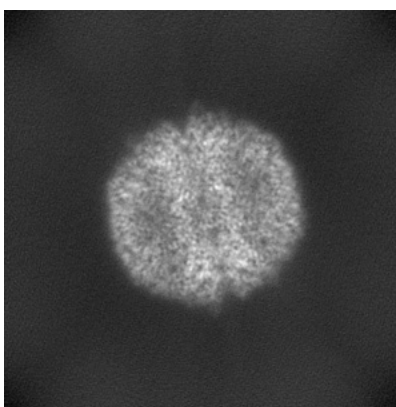


Z

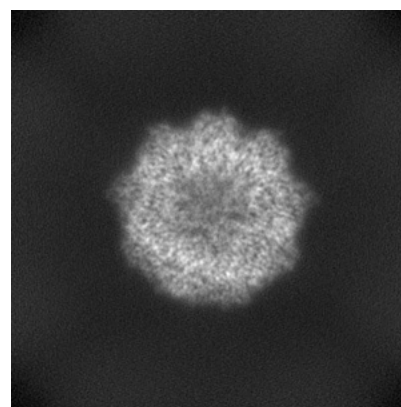
6.1.2 Raw map



X



Y

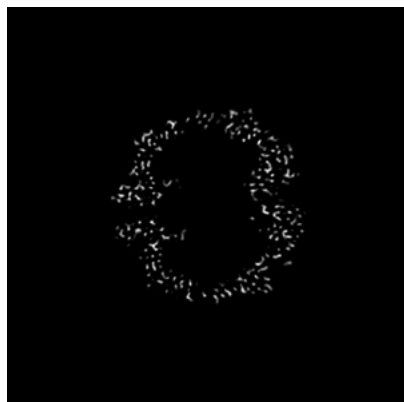


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

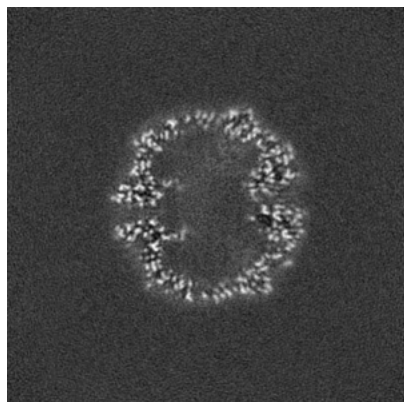


Y Index: 150

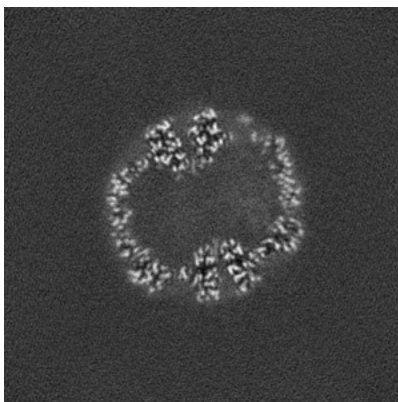


Z Index: 150

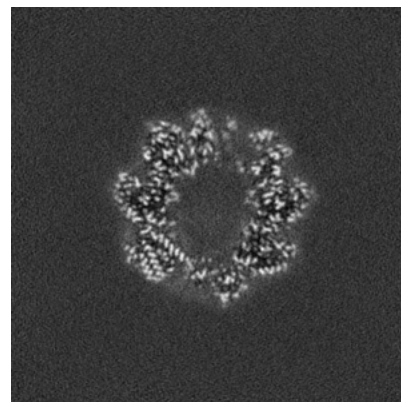
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 110

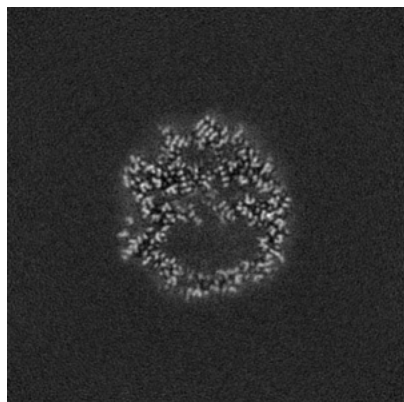


Y Index: 188

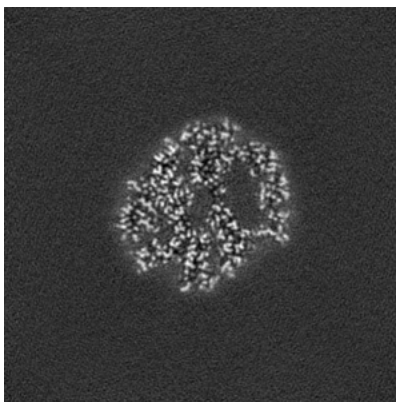


Z Index: 152

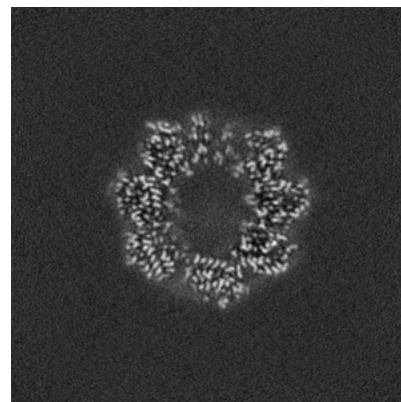
6.3.2 Raw map



X Index: 121



Y Index: 113

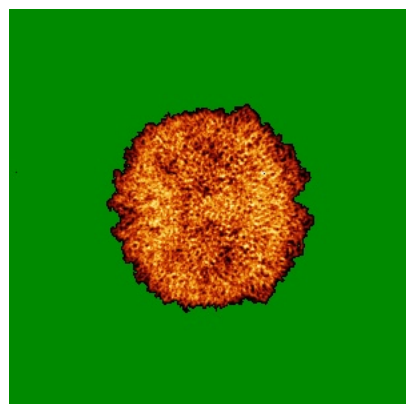


Z Index: 152

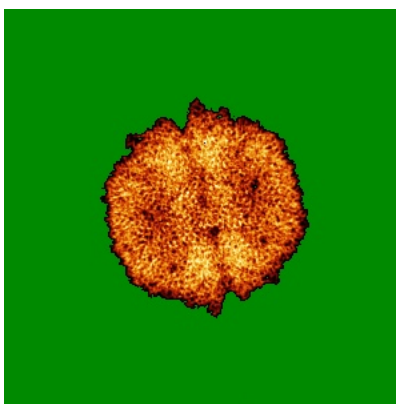
The images above show the largest variance slices of the map in three orthogonal directions.

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

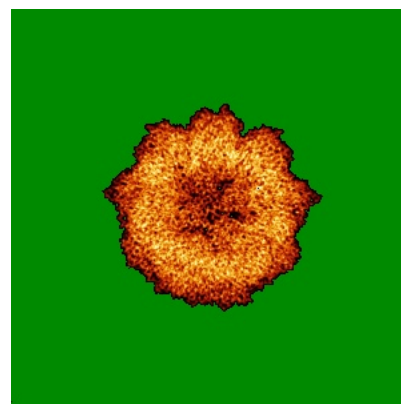
6.4.1 Primary map



X

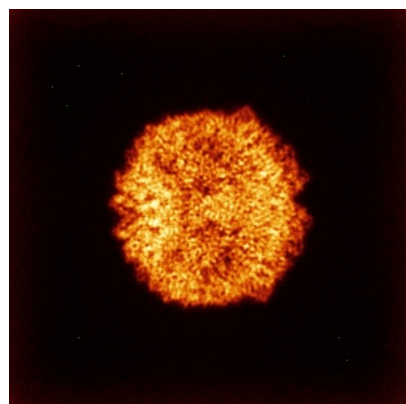


Y

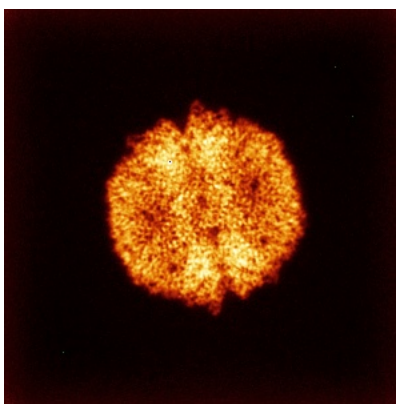


Z

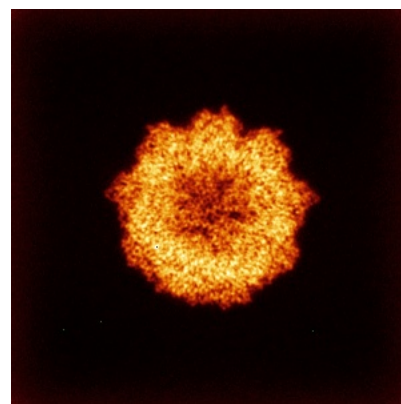
6.4.2 Raw map



X



Y

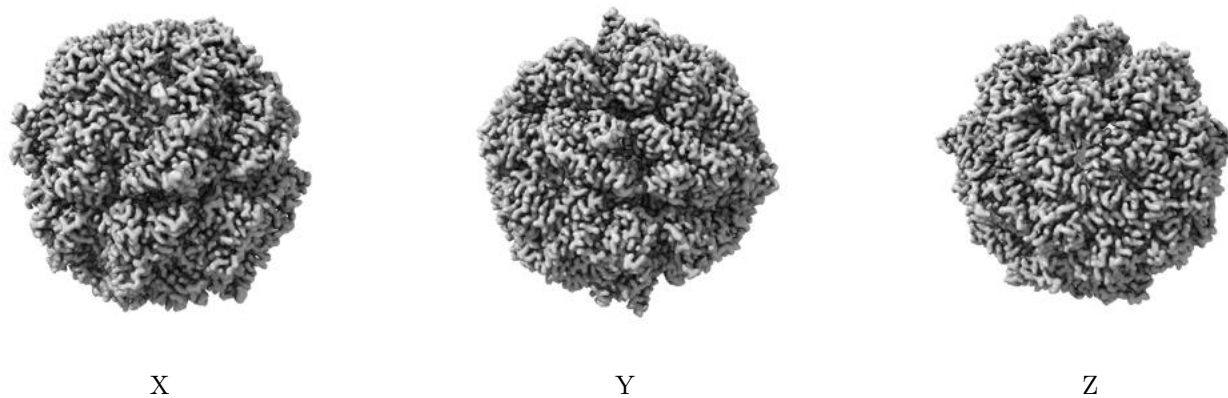


Z

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

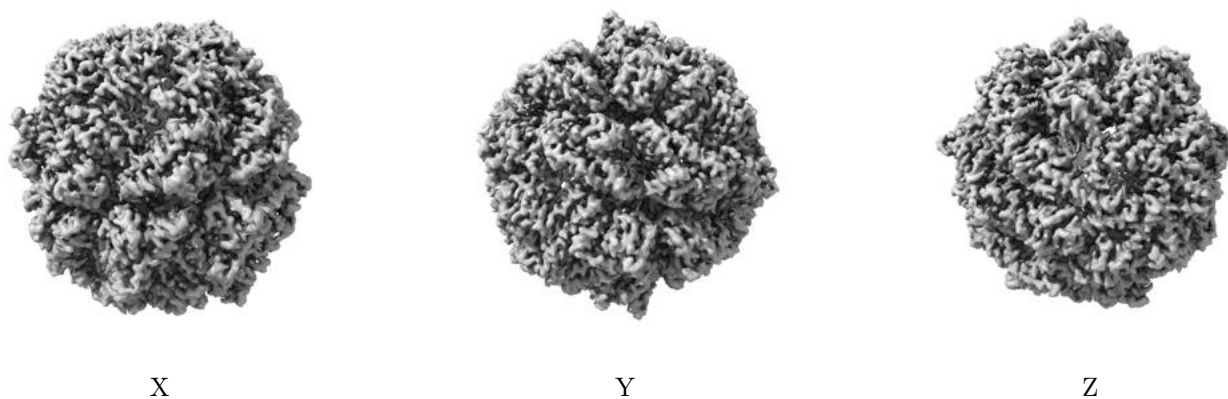
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0371. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

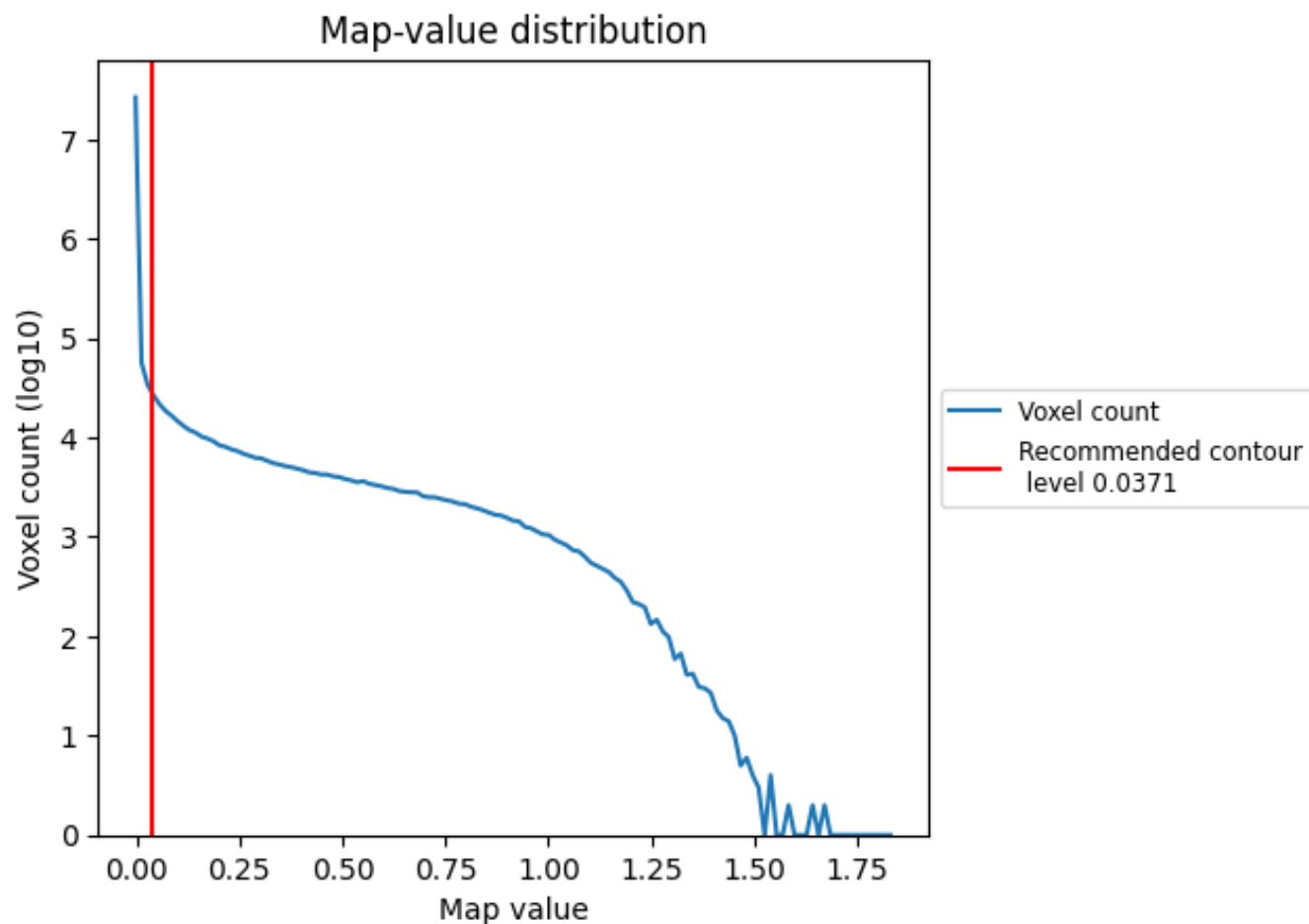
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

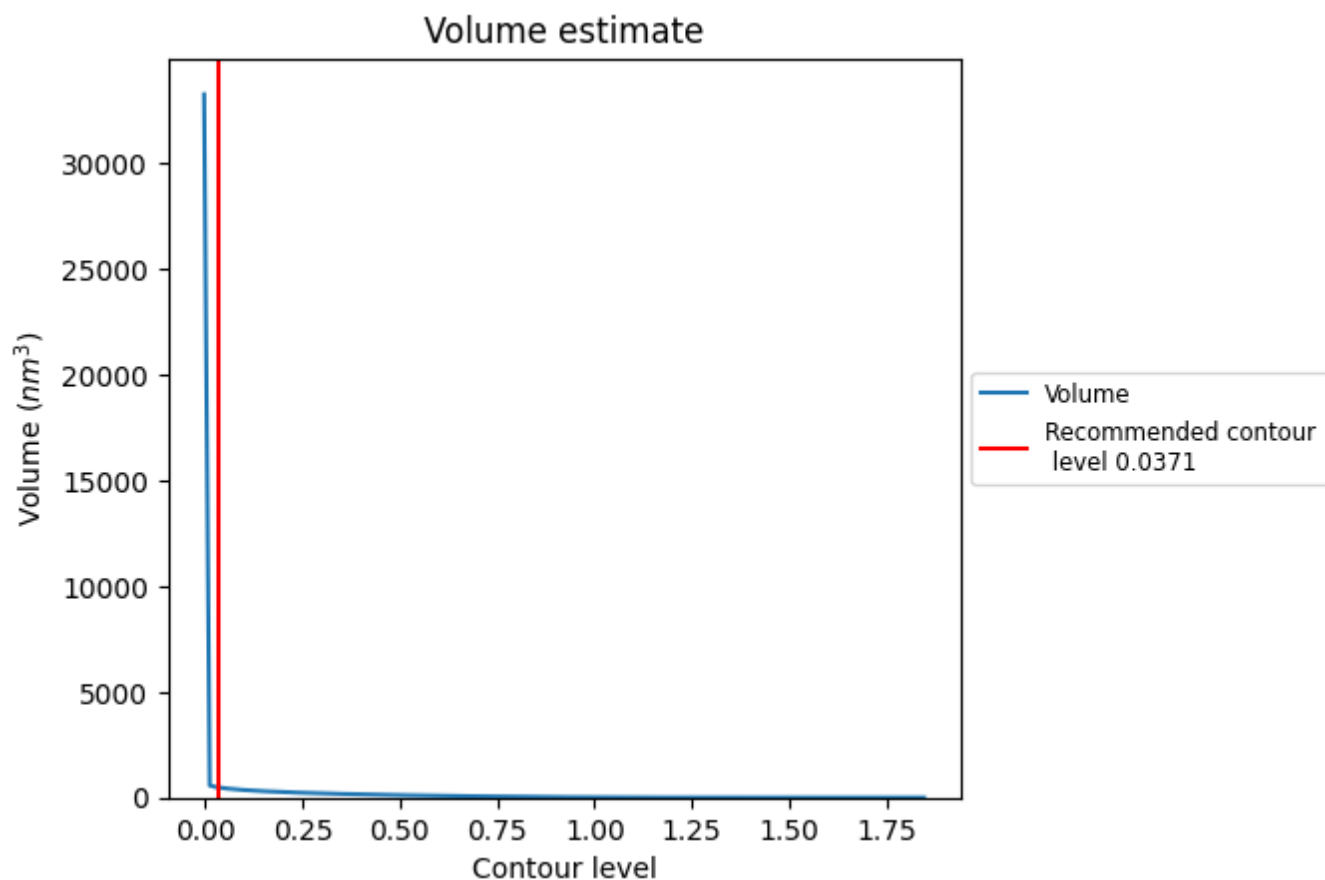
This section contains the results of statistical analysis of the map.

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.

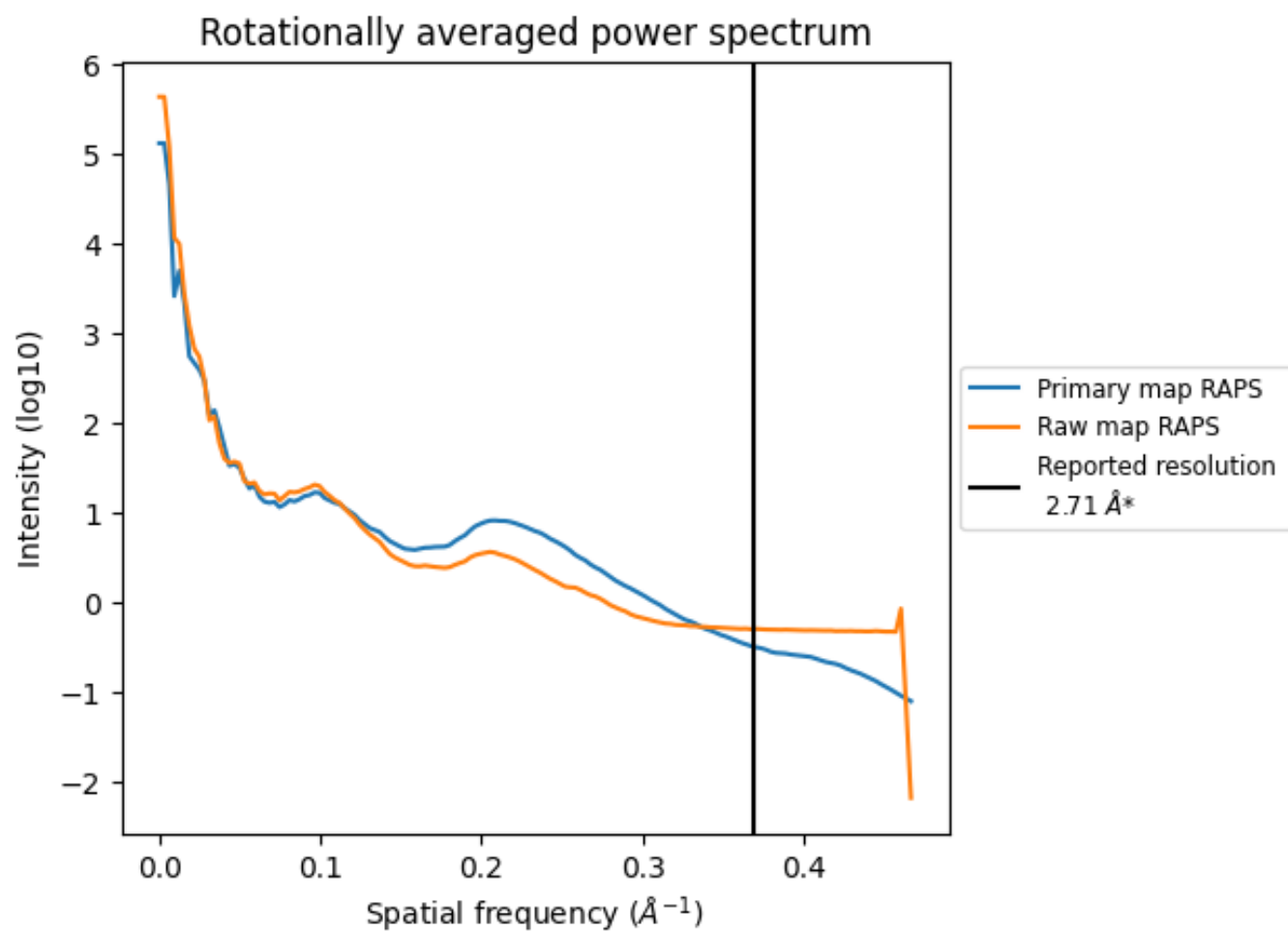
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 428 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 ⓘ

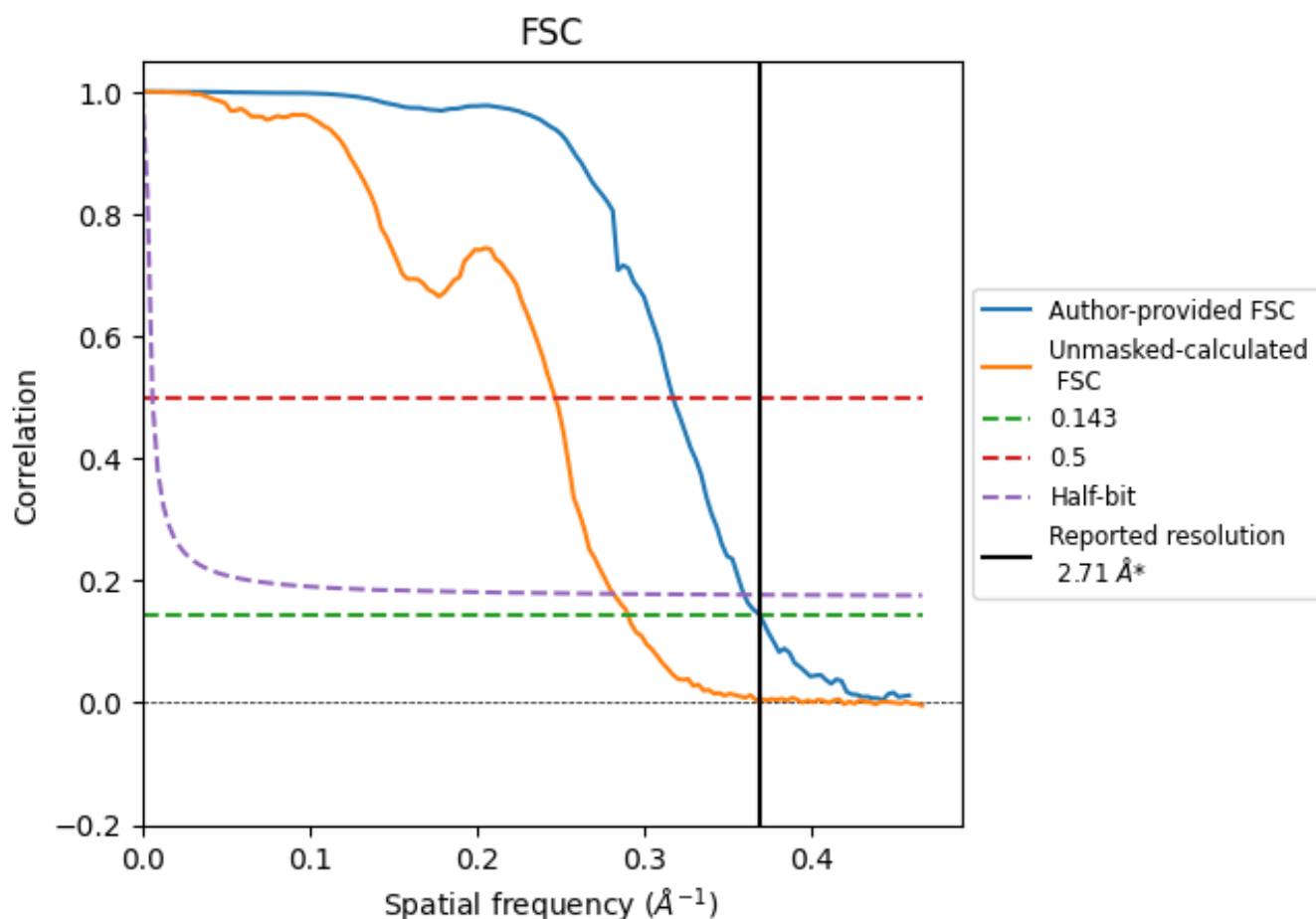


*Reported resolution corresponds to spatial frequency of 0.369 Å⁻¹

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 $0.369 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

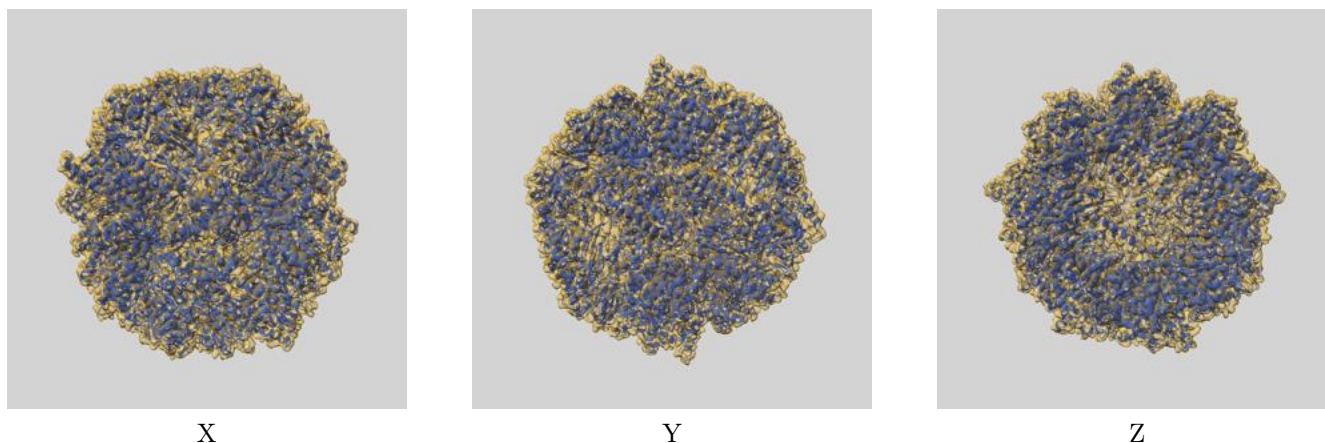
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.15	2.78
Unmasked-calculated*	3.44	4.05	3.55

*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 3.44 differs from the reported value 2.71 by more than 10 %

9 Map-model fit [i](#)

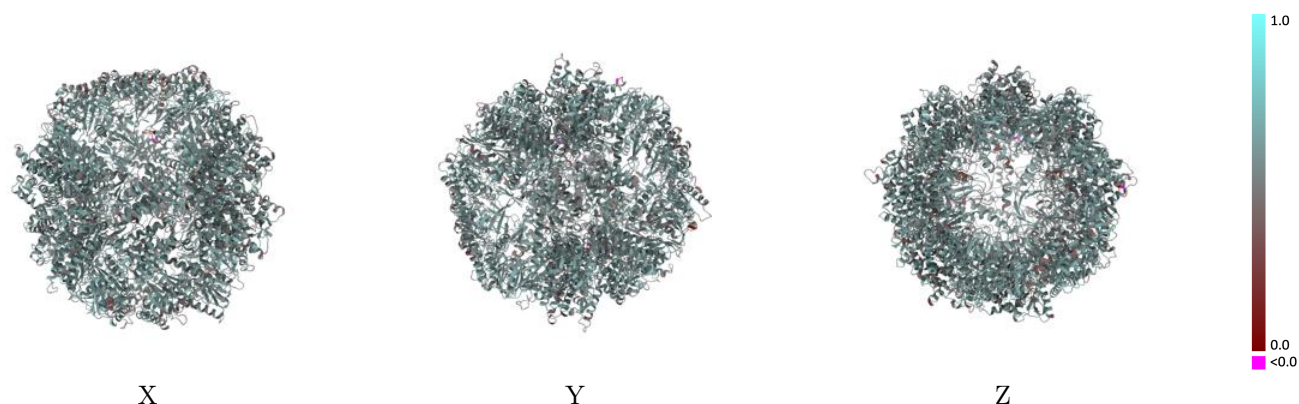
This section contains information regarding the fit between EMDB map EMD-54634 and PDB model 9S72. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



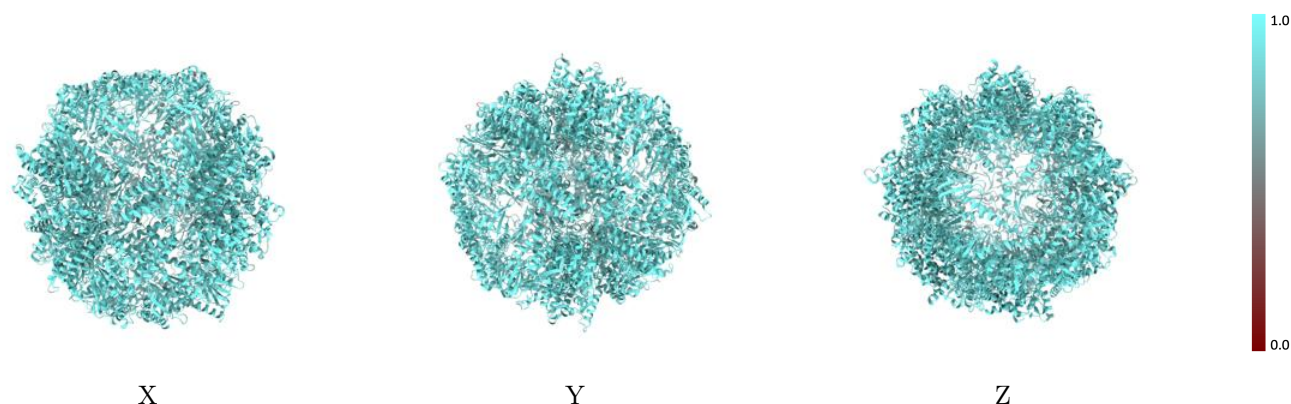
The images above show the 3D surface view of the map at the recommended contour level 0.0371 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



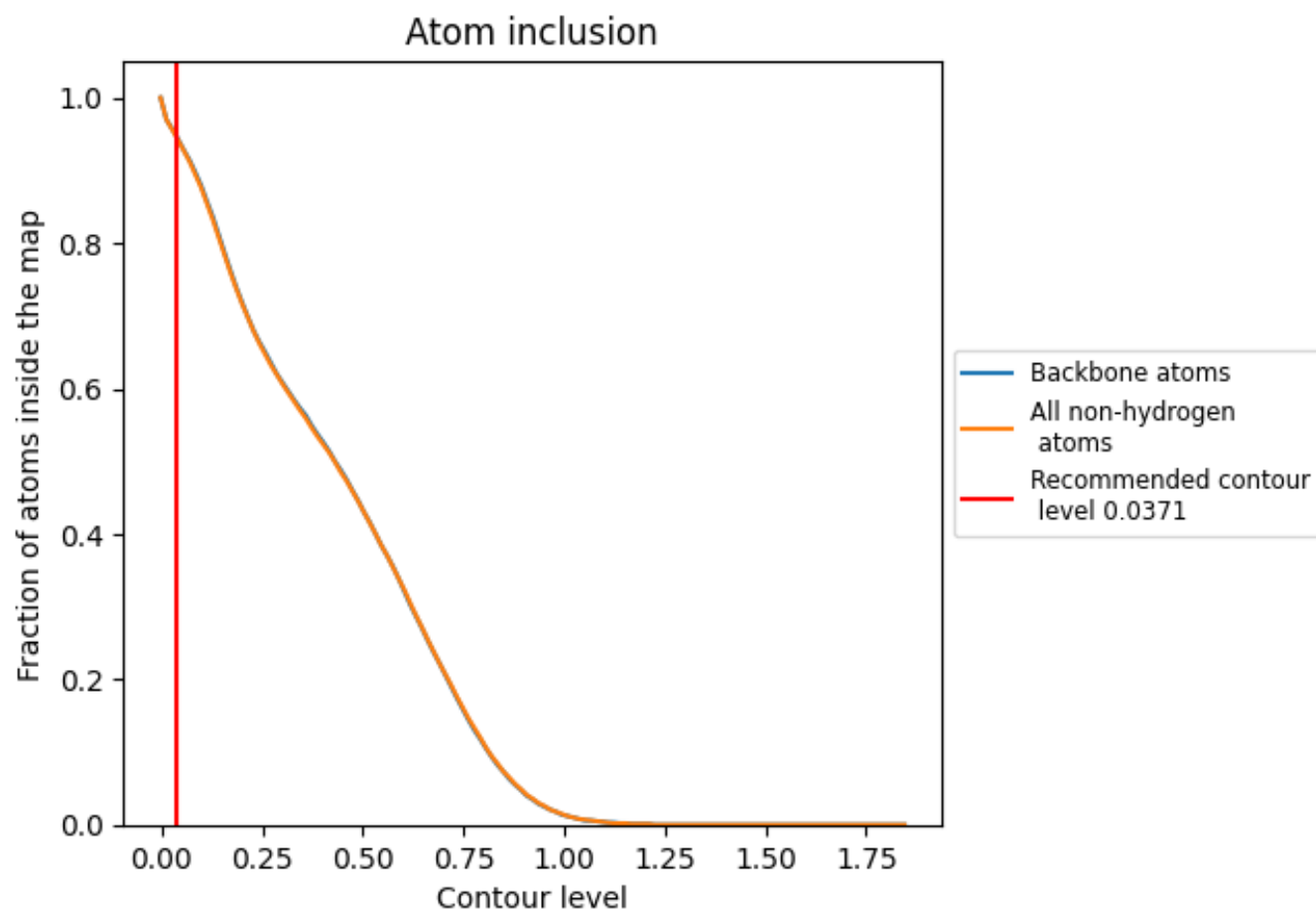
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0371).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.0371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.5540
A	 0.9470	 0.5480
B	 0.9500	 0.5650
C	 0.9540	 0.5580
D	 0.9550	 0.5600
E	 0.9480	 0.5650
F	 0.9460	 0.5410
G	 0.9530	 0.5670
H	 0.9480	 0.5490
a	 0.9430	 0.5420
b	 0.9470	 0.5580
c	 0.9490	 0.5530
d	 0.9550	 0.5600
e	 0.9390	 0.5450
f	 0.9400	 0.5370
g	 0.9530	 0.5630
h	 0.9500	 0.5480

