



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 07:51 PM UTC

PDB ID : 9YX4 / pdb_00009yx4
EMDB ID : EMD-73595
Title : Structure of the long chain acyl-CoA carboxylase complex from Mycobacterium smegmatis with ATP, bicarbonate, arachidoyl-CoA, and propionyl-CoA
Authors : Liang, Y.; Rubinstein, J.L.
Deposited on : 2025-10-26
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

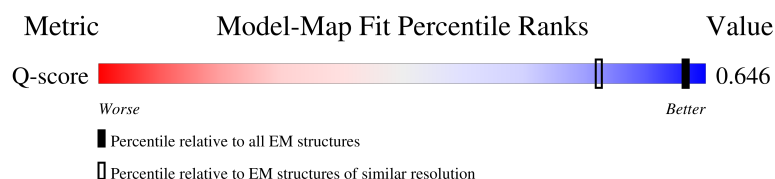
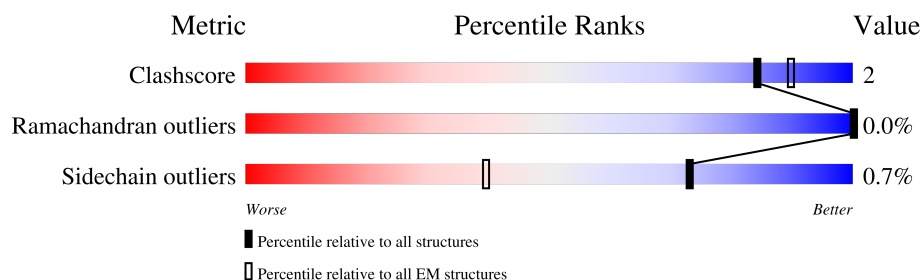
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

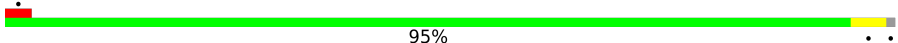
The reported resolution of this entry is 2.30 Å.

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.



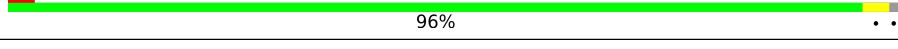
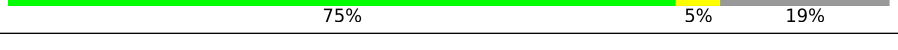
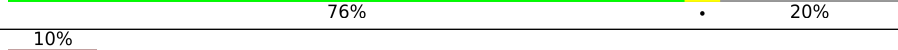
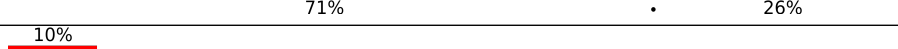
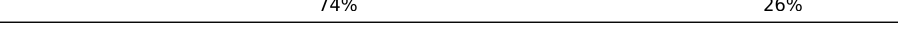
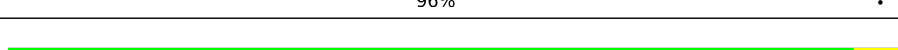
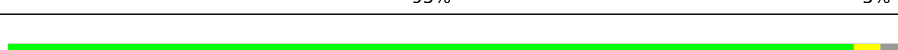
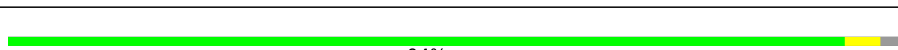
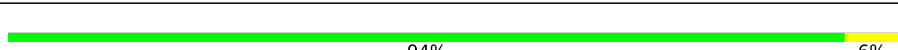
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	598	 95%
1	B	598	 77% 19%
1	C	598	 5% 74% 6% 19%
1	D	598	 72% 8% 20%

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Mol	Chain	Length	Quality of chain
1	I	598	
1	J	598	
1	K	598	
1	L	598	
1	Q	598	
1	R	598	
1	S	598	
1	T	598	
2	E	94	
2	P	94	
3	F	517	
3	O	517	
4	G	542	
4	H	542	
4	M	542	
4	N	542	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCT	B	603	-	-	X	-
6	BCT	Q	602	-	-	X	-
6	BCT	S	603	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 56623 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 Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O	S	0	0
			4251	2679	764	799	9		
1	I	69	Total	C	N	O	S	0	0
			431	272	74	82	3		
1	J	68	Total	C	N	O	S	0	0
			430	270	72	85	3		
1	K	69	Total	C	N	O	S	0	0
			457	286	77	91	3		
1	L	69	Total	C	N	O	S	0	0
			424	265	72	84	3		
1	Q	592	Total	C	N	O	S	0	0
			4278	2693	766	810	9		
1	B	482	Total	C	N	O	S	0	0
			3464	2196	619	643	6		
1	D	481	Total	C	N	O	S	0	0
			3430	2178	626	620	6		
1	C	482	Total	C	N	O	S	0	0
			3418	2166	625	622	5		
1	T	481	Total	C	N	O	S	0	0
			3547	2248	640	653	6		
1	R	482	Total	C	N	O	S	0	0
			3497	2218	631	642	6		
1	S	482	Total	C	N	O	S	0	0
			3471	2199	627	639	6		

- Molecule 2 is a protein called Acetyl-/propionyl-coenzyme A carboxylase AccE5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	70	Total	C	N	O	S	0	0
			539	339	105	91	4		
2	P	70	Total	C	N	O	S	0	0
			533	335	105	89	4		

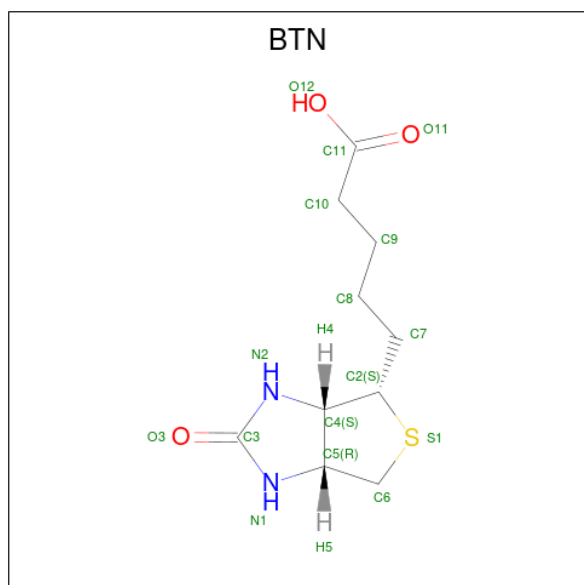
- Molecule 3 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	516	Total	C	N	O	S	0	0
			3870	2460	682	712	16		
3	O	516	Total	C	N	O	S	0	0
			3851	2451	677	707	16		

- Molecule 4 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	531	Total	C	N	O	S	0	0
			3972	2517	686	754	15		
4	H	540	Total	C	N	O	S	0	0
			4024	2550	698	761	15		
4	M	531	Total	C	N	O	S	0	0
			3975	2516	685	759	15		
4	N	540	Total	C	N	O	S	0	0
			4037	2555	698	770	14		

- Molecule 5 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



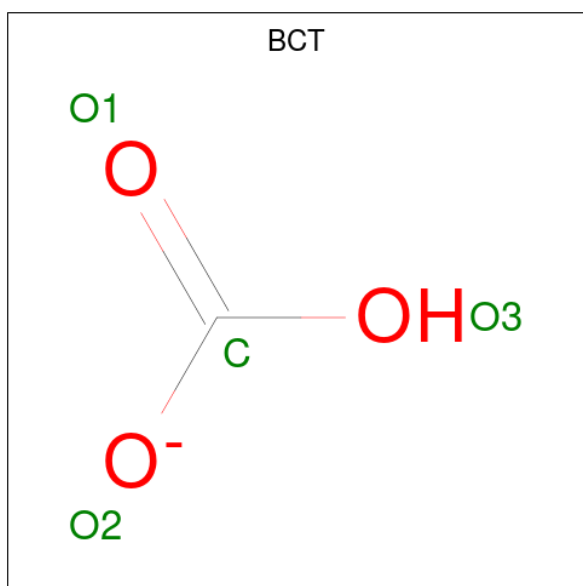
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	J	1	Total	C	N	O	S	0
			15	10	2	2	1	

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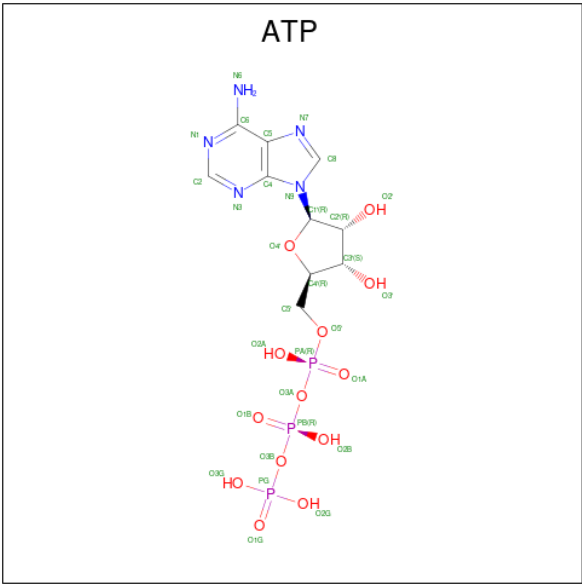
Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	L	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	Q	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			4	1	3	
6	Q	1	Total	C	O	0
			4	1	3	
6	B	1	Total	C	O	0
			4	1	3	
6	D	1	Total	C	O	0
			4	1	3	
6	C	1	Total	C	O	0
			4	1	3	
6	T	1	Total	C	O	0
			4	1	3	
6	R	1	Total	C	O	0
			4	1	3	
6	S	1	Total	C	O	0
			4	1	3	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	S	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

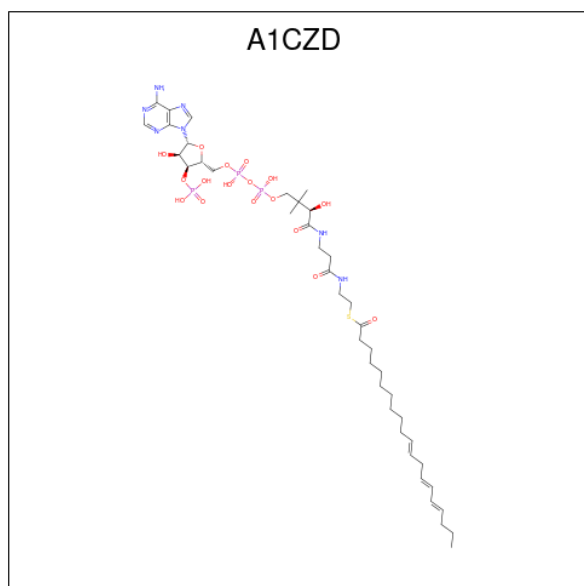
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	
8	Q	1	Total	Mg	0
			1	1	

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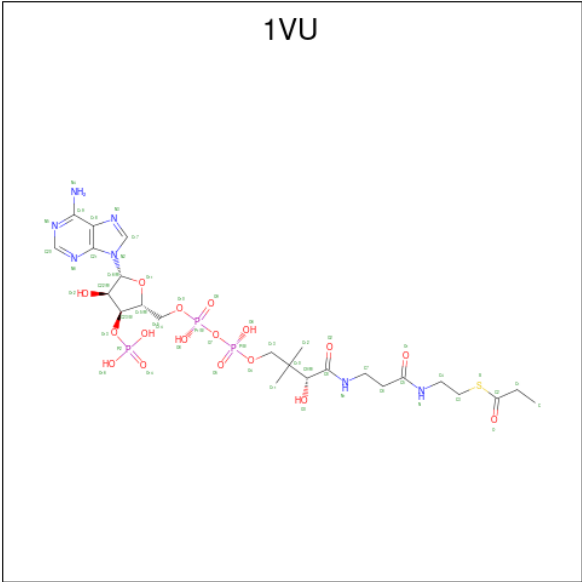
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	
8	T	1	Total	Mg	0
			1	1	
8	R	1	Total	Mg	0
			1	1	
8	S	1	Total	Mg	0
			1	1	

- Molecule 9 is S-{(3S,5S,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5,10,14-tetraoxo-2,4,6-trioxa-11,15-diazia-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (11E,14E,16E)-icosa-11,14,16-trienethioate (non-preferred name) (CCD ID: A1CZD) (formula: C₄₁H₆₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
9	F	1	Total 69	C 41	N 7	O 17	P 3	S 1	0
9	F	1	Total 69	C 41	N 7	O 17	P 3	S 1	0

- Molecule 10 is propionyl Coenzyme A (CCD ID: 1VU) (formula: C₂₄H₄₀N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).

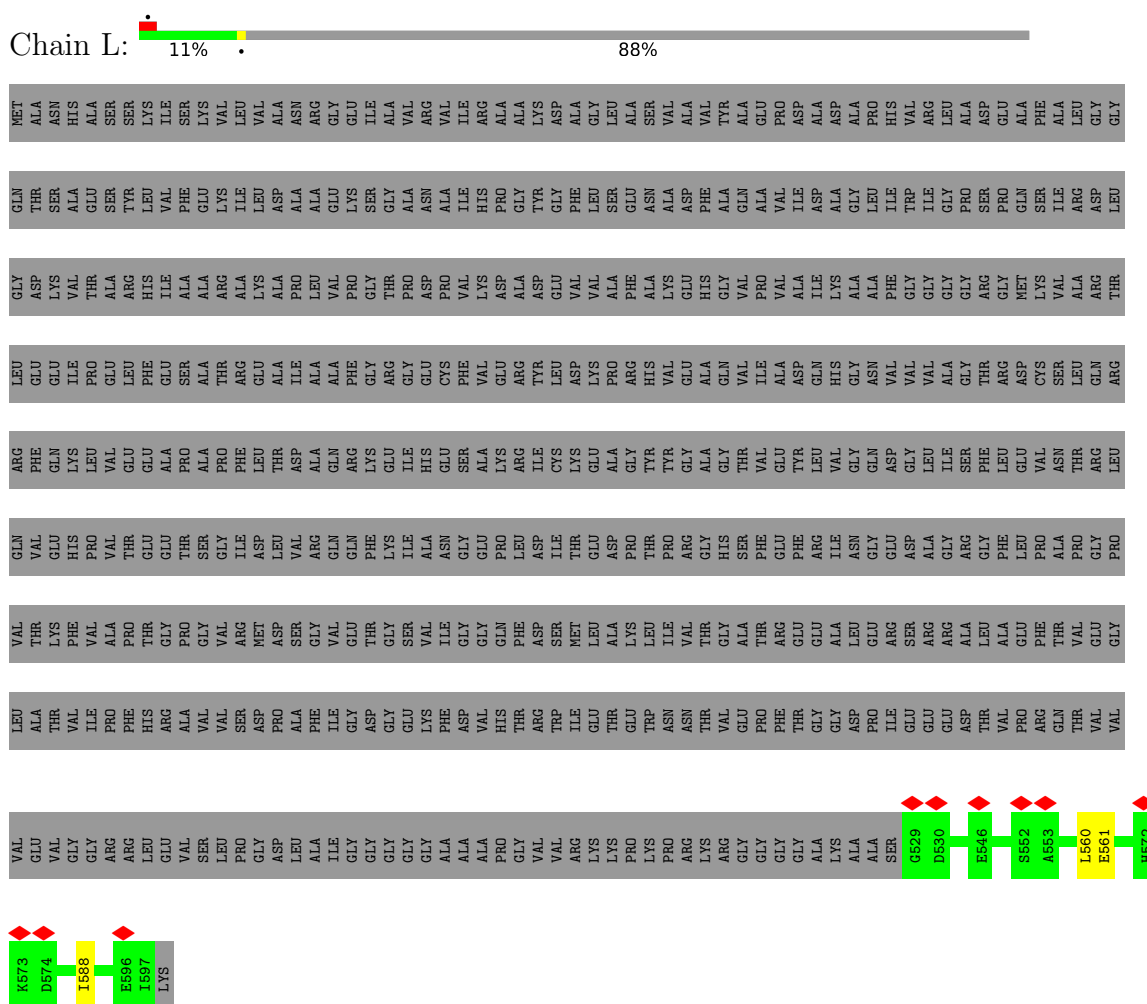


Mol	Chain	Residues	Atoms						AltConf
10	G	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	H	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	M	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	N	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	

89%

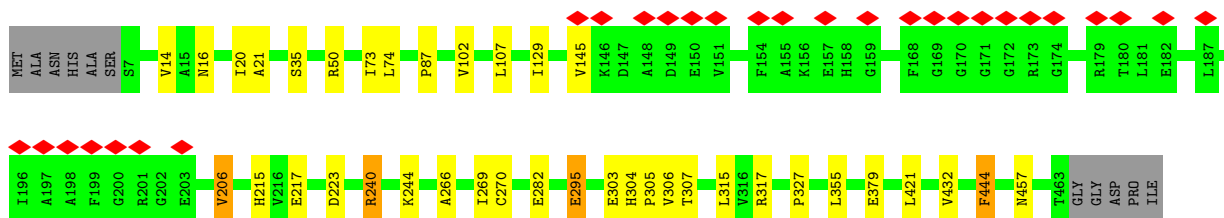
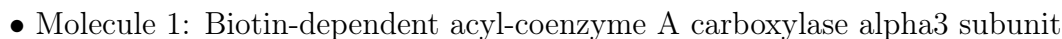
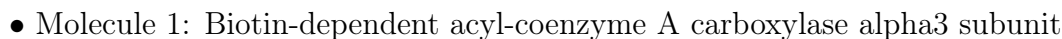
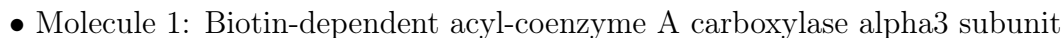
11%

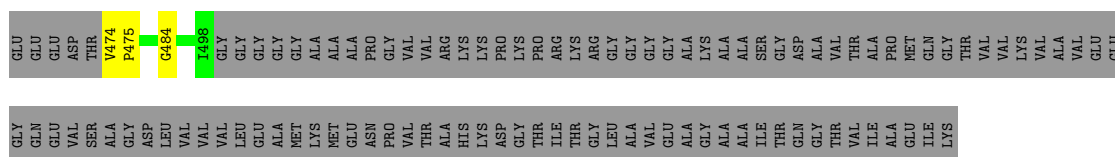
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

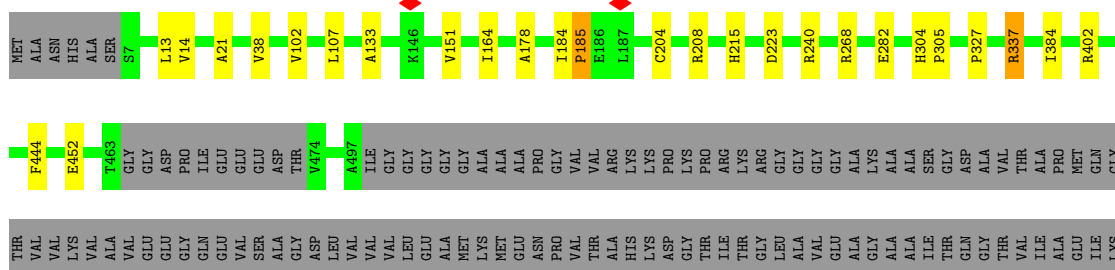






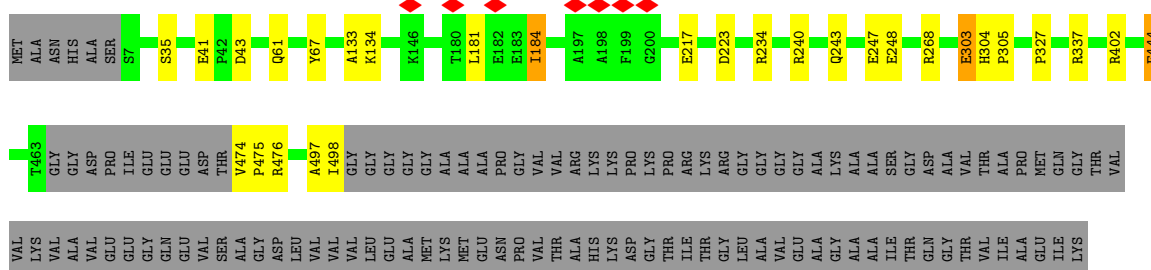
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain T: 76% 20%



- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain R: 76% 19%

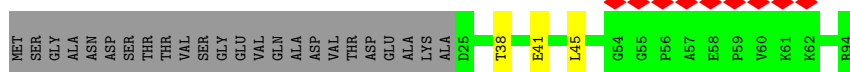


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

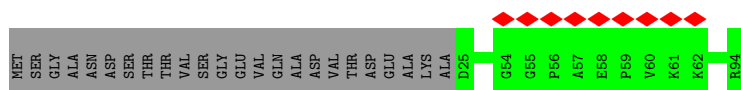
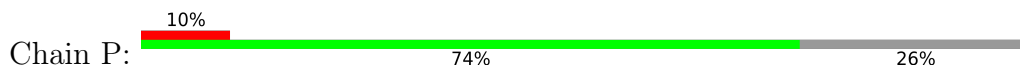
Chain S: 75% 5% 19%



- Molecule 2: Acetyl-/propionyl-coenzyme A carboxylase AccE5



- Molecule 2: Acetyl-/propionyl-coenzyme A carboxylase AccE5



- Molecule 3: Propionyl-CoA carboxylase beta chain



- Molecule 3: Propionyl-CoA carboxylase beta chain



- Molecule 4: Propionyl-CoA carboxylase beta chain



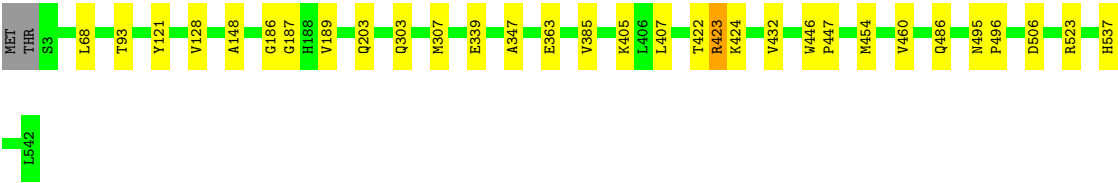
- Molecule 4: Propionyl-CoA carboxylase beta chain



- Molecule 4: Propionyl-CoA carboxylase beta chain



● Molecule 4: Propionyl-CoA carboxylase beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124481	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.299	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CZD, 1VU, MG, BTN, ATP, BCT

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	0.31	0/4331	0.43	0/5897
1	B	0.31	0/3536	0.45	1/4825 (0.0%)
1	C	0.31	0/3488	0.47	0/4763
1	D	0.32	0/3502	0.47	1/4783 (0.0%)
1	I	0.18	0/433	0.37	0/596
1	J	0.17	0/431	0.36	0/593
1	K	0.17	0/459	0.34	0/628
1	L	0.17	0/425	0.36	0/585
1	Q	0.32	0/4358	0.44	0/5930
1	R	0.33	0/3569	0.43	0/4863
1	S	0.30	0/3542	0.45	1/4831 (0.0%)
1	T	0.32	0/3620	0.44	0/4924
2	E	0.34	0/553	0.42	0/750
2	P	0.34	0/547	0.44	0/742
3	F	0.38	0/3950	0.56	3/5365 (0.1%)
3	O	0.37	0/3932	0.52	0/5346
4	G	0.38	0/4048	0.51	0/5509
4	H	0.38	0/4102	0.51	0/5585
4	M	0.39	0/4051	0.51	0/5515
4	N	0.40	0/4115	0.53	1/5603 (0.0%)
All	All	0.34	0/56992	0.48	7/77633 (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	D	0	1
1	R	0	2
1	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	2
3	F	0	1
4	H	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	440	LEU	N-CA-C	-8.22	102.28	111.07
3	F	438	GLN	N-CA-C	7.57	120.42	111.71
1	S	444	PHE	CA-CB-CG	6.10	119.90	113.80
4	N	424	LYS	N-CA-C	6.04	119.49	109.46
3	F	440	LEU	N-CA-CB	5.96	118.66	110.01

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	214	ARG	Sidechain
3	F	510	ARG	Sidechain
4	H	423	ARG	Sidechain
1	T	337	ARG	Sidechain
1	T	402	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4251	0	4175	22	0
1	B	3464	0	3324	14	0
1	C	3418	0	3272	29	0
1	D	3430	0	3292	31	0
1	I	431	0	416	0	0
1	J	430	0	419	1	0
1	K	457	0	458	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	424	0	397	1	0
1	Q	4278	0	4210	12	0
1	R	3497	0	3411	16	0
1	S	3471	0	3352	25	0
1	T	3547	0	3493	18	0
2	E	539	0	526	3	0
2	P	533	0	515	0	0
3	F	3870	0	3850	19	0
3	O	3851	0	3809	18	0
4	G	3972	0	3940	9	0
4	H	4024	0	3987	15	0
4	M	3975	0	3930	16	0
4	N	4037	0	3991	19	0
5	A	15	0	15	0	0
5	I	15	0	15	0	0
5	J	15	0	15	0	0
5	K	15	0	15	0	0
5	L	15	0	15	0	0
5	Q	15	0	15	0	0
6	A	4	0	1	0	0
6	B	4	0	1	2	0
6	C	4	0	1	0	0
6	D	4	0	1	0	0
6	Q	4	0	1	2	0
6	R	4	0	1	1	0
6	S	4	0	1	2	0
6	T	4	0	1	0	0
7	A	31	0	12	0	0
7	B	31	0	12	1	0
7	C	31	0	12	1	0
7	D	31	0	12	1	0
7	Q	31	0	12	1	0
7	R	31	0	12	0	0
7	S	31	0	12	0	0
7	T	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	1	0	0	0	0
9	F	138	0	0	8	0
10	G	52	0	38	2	0
10	H	52	0	38	6	0
10	M	52	0	38	6	0
10	N	52	0	38	7	0
All	All	56623	0	55113	262	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 2.

The worst 5 of 262 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:F:197:VAL:HG21	9:F:602:A1CZD:C35	1.73	1.17
3:F:197:VAL:CG2	9:F:602:A1CZD:C35	2.23	1.16
1:R:247:GLU:HG2	1:R:303:GLU:HG2	1.53	0.90
4:H:148:ALA:H	10:H:601:1VU:H37	1.41	0.85
4:N:186:GLY:HA3	10:N:601:1VU:O	1.78	0.81

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	590/598 (99%)	573 (97%)	17 (3%)	0	100	100
1	B	478/598 (80%)	457 (96%)	21 (4%)	0	100	100
1	C	478/598 (80%)	451 (94%)	27 (6%)	0	100	100
1	D	477/598 (80%)	455 (95%)	22 (5%)	0	100	100
1	I	67/598 (11%)	66 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	66/598 (11%)	64 (97%)	2 (3%)	0	100	100
1	K	67/598 (11%)	67 (100%)	0	0	100	100
1	L	67/598 (11%)	67 (100%)	0	0	100	100
1	Q	590/598 (99%)	569 (96%)	21 (4%)	0	100	100
1	R	478/598 (80%)	466 (98%)	12 (2%)	0	100	100
1	S	478/598 (80%)	459 (96%)	19 (4%)	0	100	100
1	T	477/598 (80%)	459 (96%)	17 (4%)	1 (0%)	43	55
2	E	68/94 (72%)	65 (96%)	3 (4%)	0	100	100
2	P	68/94 (72%)	66 (97%)	2 (3%)	0	100	100
3	F	514/517 (99%)	501 (98%)	13 (2%)	0	100	100
3	O	514/517 (99%)	497 (97%)	17 (3%)	0	100	100
4	G	529/542 (98%)	515 (97%)	14 (3%)	0	100	100
4	H	538/542 (99%)	521 (97%)	17 (3%)	0	100	100
4	M	529/542 (98%)	512 (97%)	17 (3%)	0	100	100
4	N	538/542 (99%)	524 (97%)	13 (2%)	1 (0%)	43	55
All	All	7611/10566 (72%)	7354 (97%)	255 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	423	ARG
1	T	185	PRO

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	411/453 (91%)	409 (100%)	2 (0%)	81	90
1	B	328/453 (72%)	325 (99%)	3 (1%)	70	84
1	C	314/453 (69%)	305 (97%)	9 (3%)	37	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	317/453 (70%)	312 (98%)	5 (2%)	55	73
1	I	36/453 (8%)	35 (97%)	1 (3%)	38	56
1	J	38/453 (8%)	38 (100%)	0	100	100
1	K	44/453 (10%)	44 (100%)	0	100	100
1	L	34/453 (8%)	33 (97%)	1 (3%)	37	55
1	Q	418/453 (92%)	415 (99%)	3 (1%)	76	87
1	R	337/453 (74%)	333 (99%)	4 (1%)	63	79
1	S	329/453 (73%)	326 (99%)	3 (1%)	70	84
1	T	349/453 (77%)	348 (100%)	1 (0%)	86	93
2	E	53/76 (70%)	53 (100%)	0	100	100
2	P	51/76 (67%)	51 (100%)	0	100	100
3	F	392/412 (95%)	391 (100%)	1 (0%)	86	93
3	O	387/412 (94%)	387 (100%)	0	100	100
4	G	411/436 (94%)	411 (100%)	0	100	100
4	H	415/436 (95%)	413 (100%)	2 (0%)	81	90
4	M	412/436 (94%)	411 (100%)	1 (0%)	87	94
4	N	418/436 (96%)	414 (99%)	4 (1%)	68	82
All	All	5494/8156 (67%)	5454 (99%)	40 (1%)	73	87

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	355	LEU
1	R	303	GLU
1	C	421	LEU
1	T	444	PHE
1	S	35	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	537	GLN
1	T	48	HIS
1	D	243	GLN
1	T	456	ASN

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Mol	Chain	Res	Type
4	H	397	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	$\# Z > 2$
7	ATP	R	601	8	32,33,33	0.38	0	48,52,52	0.72	2 (4%)
5	BTN	I	601	1	15,16,17	6.50	11 (73%)	20,21,23	2.90	8 (40%)
5	BTN	K	601	1	15,16,17	6.45	11 (73%)	20,21,23	2.66	8 (40%)
6	BCT	A	602	-	3,3,3	1.21	0	2,3,3	4.13	2 (100%)
7	ATP	D	601	8	32,33,33	0.59	1 (3%)	48,52,52	0.74	2 (4%)
6	BCT	C	603	-	3,3,3	1.15	0	2,3,3	4.26	2 (100%)
7	ATP	Q	603	8	32,33,33	0.62	1 (3%)	48,52,52	0.71	1 (2%)
6	BCT	Q	602	-	3,3,3	1.21	0	2,3,3	4.01	2 (100%)
10	1VU	H	601	-	52,54,54	0.47	0	73,80,80	0.91	3 (4%)
6	BCT	B	603	-	3,3,3	1.16	0	2,3,3	4.29	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	C	601	8	32,33,33	0.47	0	48,52,52	0.73	1 (2%)
5	BTN	A	601	1	15,16,17	6.50	11 (73%)	20,21,23	2.85	9 (45%)
6	BCT	D	603	-	3,3,3	1.34	0	2,3,3	3.36	1 (50%)
9	A1CZD	F	602	-	69,71,71	2.67	21 (30%)	90,97,97	1.64	13 (14%)
6	BCT	S	603	-	3,3,3	1.14	0	2,3,3	4.19	2 (100%)
7	ATP	S	601	8	32,33,33	0.74	2 (6%)	48,52,52	0.74	2 (4%)
7	ATP	A	603	8	32,33,33	0.40	0	48,52,52	0.72	1 (2%)
10	1VU	N	601	-	52,54,54	0.47	0	73,80,80	0.75	1 (1%)
6	BCT	T	602	-	3,3,3	1.18	0	2,3,3	4.15	2 (100%)
5	BTN	L	601	1	15,16,17	6.48	11 (73%)	20,21,23	2.83	9 (45%)
7	ATP	T	601	8	32,33,33	0.42	0	48,52,52	0.72	1 (2%)
7	ATP	B	601	8	32,33,33	0.55	0	48,52,52	0.72	1 (2%)
10	1VU	G	601	-	52,54,54	0.51	0	73,80,80	0.80	1 (1%)
6	BCT	R	603	-	3,3,3	1.22	0	2,3,3	4.14	2 (100%)
5	BTN	Q	601	1	15,16,17	6.47	11 (73%)	20,21,23	2.77	9 (45%)
5	BTN	J	601	1	15,16,17	6.53	11 (73%)	20,21,23	2.95	10 (50%)
9	A1CZD	F	601	-	69,71,71	2.81	22 (31%)	90,97,97	1.67	16 (17%)
10	1VU	M	601	-	52,54,54	0.47	0	73,80,80	0.84	2 (2%)

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
7	ATP	R	601	8	-	3/22/38/38	0/3/3/3
5	BTN	I	601	1	-	0/6/27/28	0/2/2/2
5	BTN	K	601	1	-	2/6/27/28	0/2/2/2
7	ATP	D	601	8	-	4/22/38/38	0/3/3/3
7	ATP	Q	603	8	-	4/22/38/38	0/3/3/3
10	1VU	H	601	-	-	23/53/69/69	0/3/3/3
7	ATP	C	601	8	-	4/22/38/38	0/3/3/3
5	BTN	A	601	1	-	3/6/27/28	0/2/2/2
9	A1CZD	F	602	-	-	31/70/86/86	0/3/3/3
7	ATP	S	601	8	-	2/22/38/38	0/3/3/3
7	ATP	A	603	8	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	1VU	N	601	-	-	9/53/69/69	0/3/3/3
5	BTN	L	601	1	-	2/6/27/28	0/2/2/2
7	ATP	T	601	8	-	6/22/38/38	0/3/3/3
7	ATP	B	601	8	-	3/22/38/38	0/3/3/3
10	1VU	G	601	-	-	11/53/69/69	0/3/3/3
5	BTN	Q	601	1	-	3/6/27/28	0/2/2/2
5	BTN	J	601	1	-	4/6/27/28	0/2/2/2
9	A1CZD	F	601	-	-	35/70/86/86	0/3/3/3
10	1VU	M	601	-	-	6/53/69/69	0/3/3/3

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	601	A1CZD	P65-O64	14.23	1.84	1.59
5	I	601	BTN	C6-S1	-13.42	1.44	1.81
5	Q	601	BTN	C6-S1	-13.35	1.44	1.81
5	J	601	BTN	C6-S1	-13.30	1.44	1.81
5	K	601	BTN	C6-S1	-13.29	1.44	1.81

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	BTN	C6-S1-C2	8.16	106.95	89.98
5	Q	601	BTN	C6-S1-C2	6.74	104.00	89.98
9	F	602	A1CZD	C19-C20-S22	6.63	121.31	113.40
5	K	601	BTN	C6-S1-C2	6.62	103.74	89.98
5	A	601	BTN	C6-S1-C2	6.10	102.66	89.98

There are no chirality outliers.

5 of 161 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	601	BTN	C9-C10-C11-O11
5	J	601	BTN	S1-C2-C7-C8
5	J	601	BTN	C4-C2-C7-C8
5	K	601	BTN	S1-C2-C7-C8
5	K	601	BTN	C4-C2-C7-C8

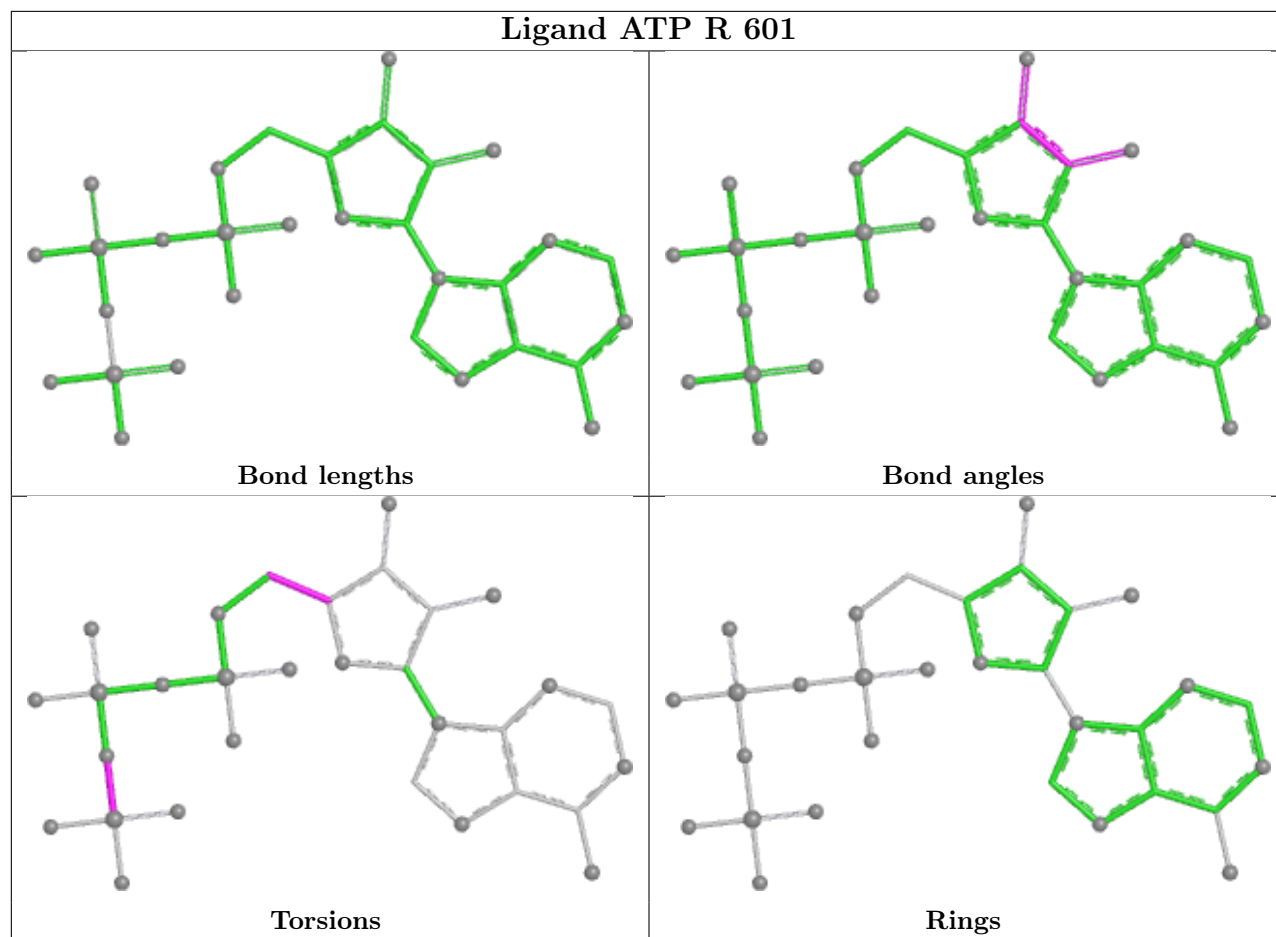
There are no ring outliers.

14 monomers are involved in 40 short contacts:

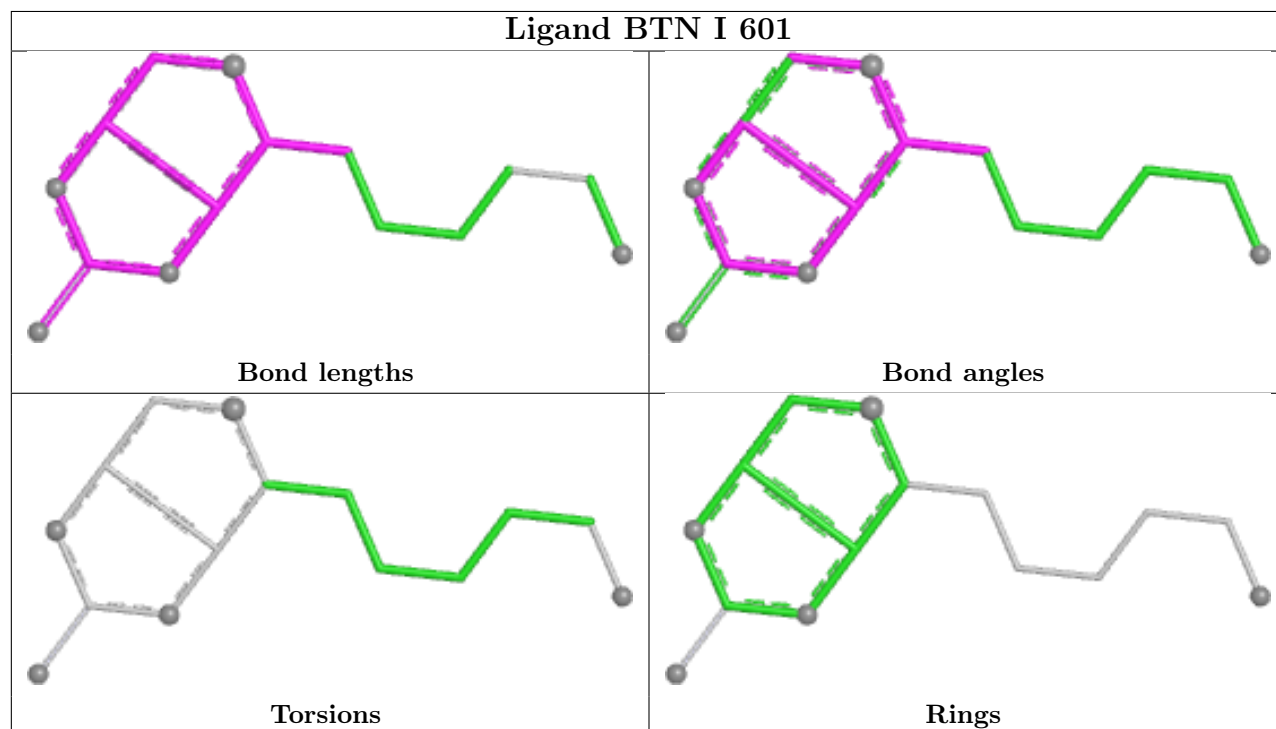
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	ATP	1	0
7	Q	603	ATP	1	0
6	Q	602	BCT	2	0
10	H	601	1VU	6	0
6	B	603	BCT	2	0
7	C	601	ATP	1	0
9	F	602	A1CZD	6	0
6	S	603	BCT	2	0
10	N	601	1VU	7	0
7	B	601	ATP	1	0
10	G	601	1VU	2	0
6	R	603	BCT	1	0
9	F	601	A1CZD	2	0
10	M	601	1VU	6	0

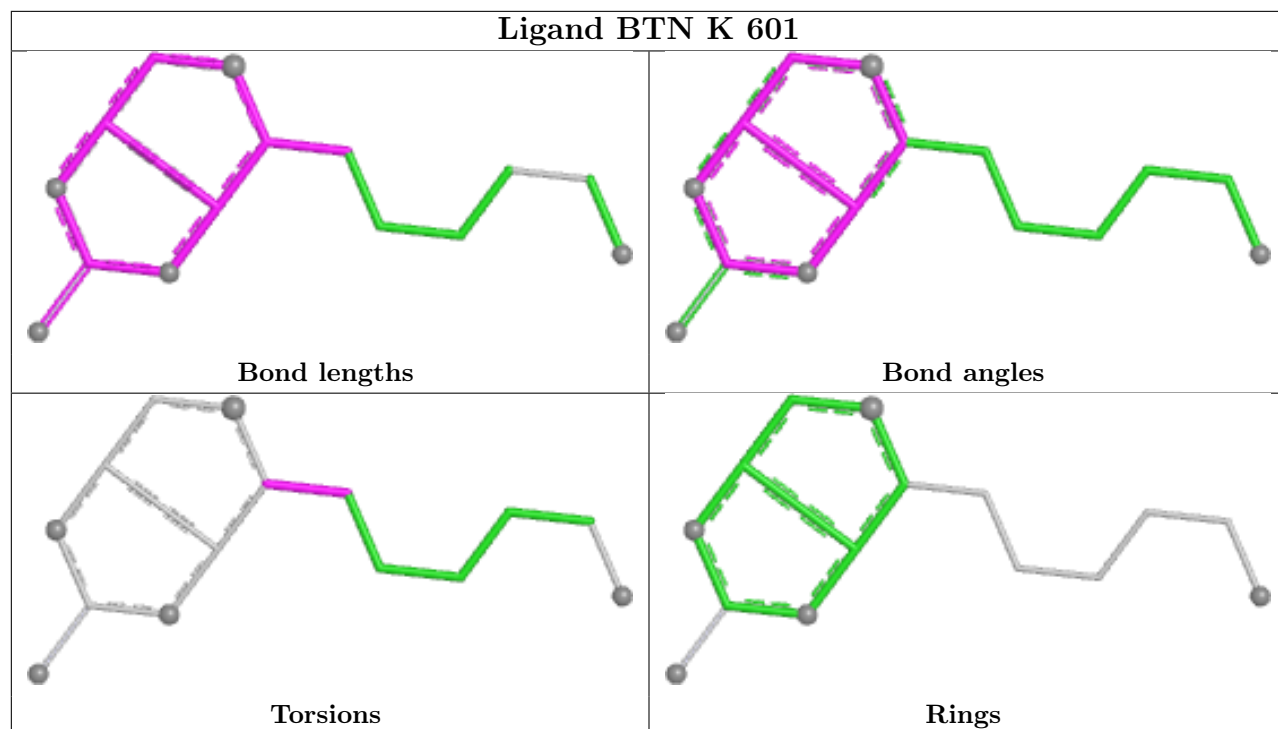
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

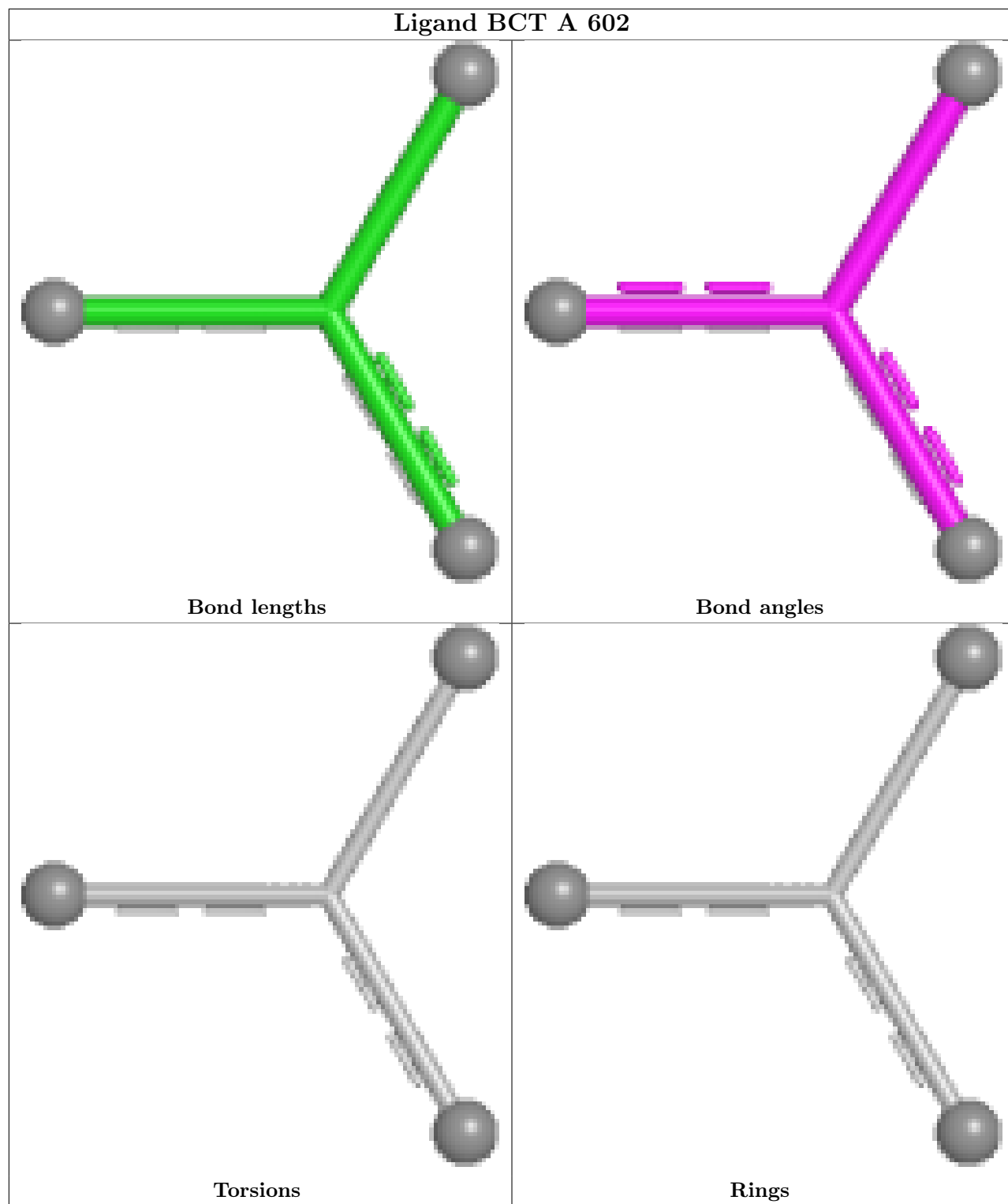
Ligand ATP R 601

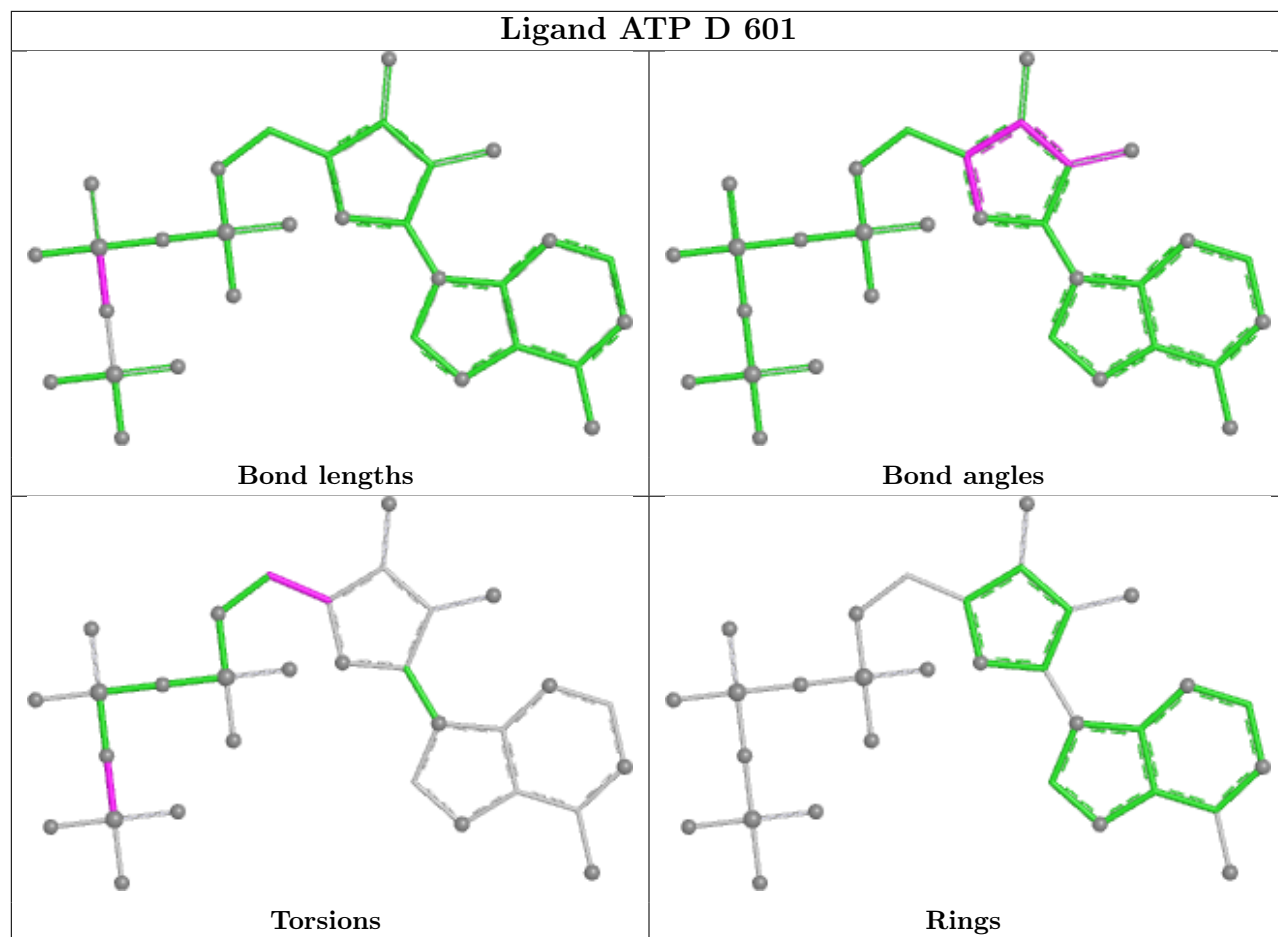


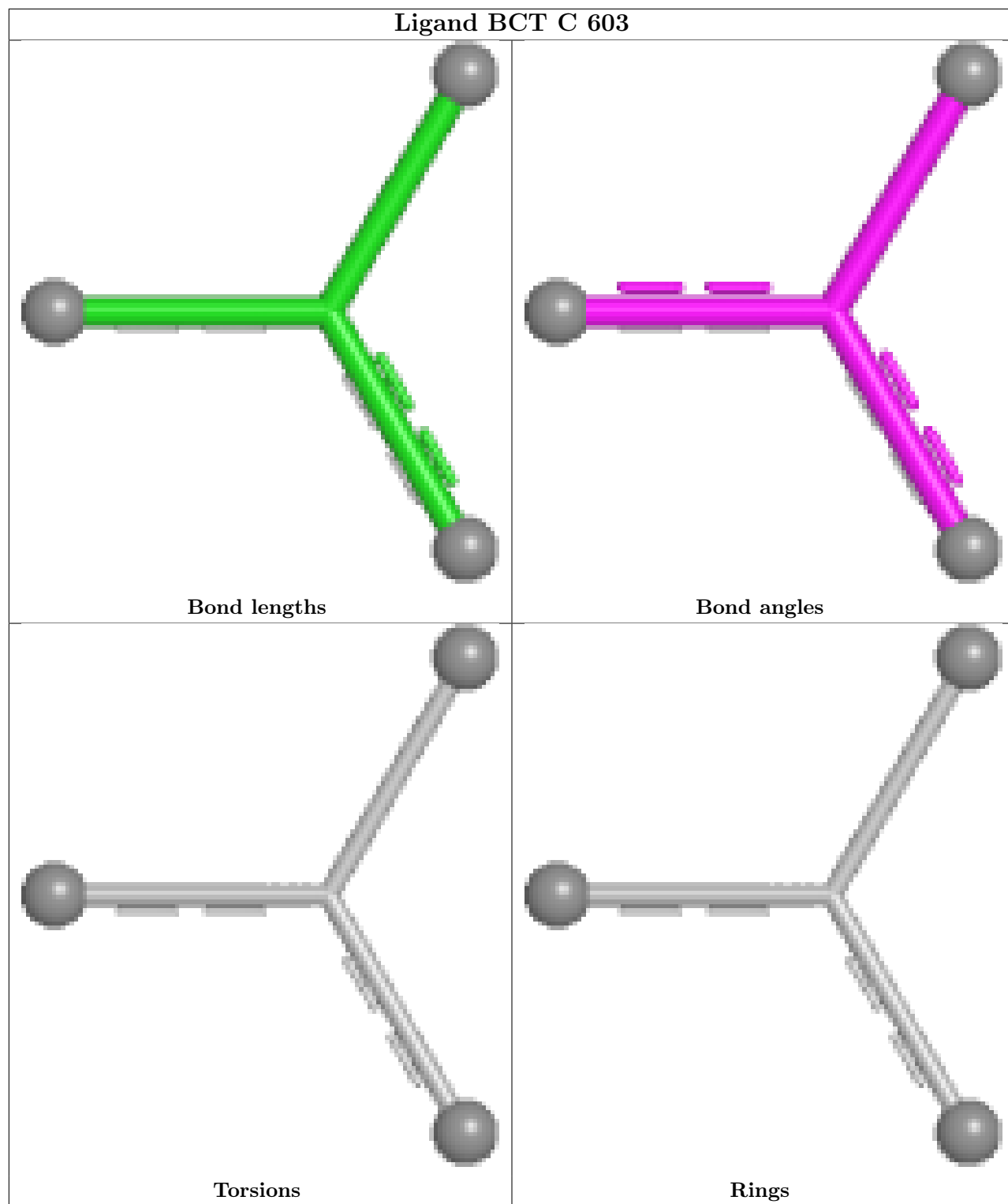
Ligand BTN I 601

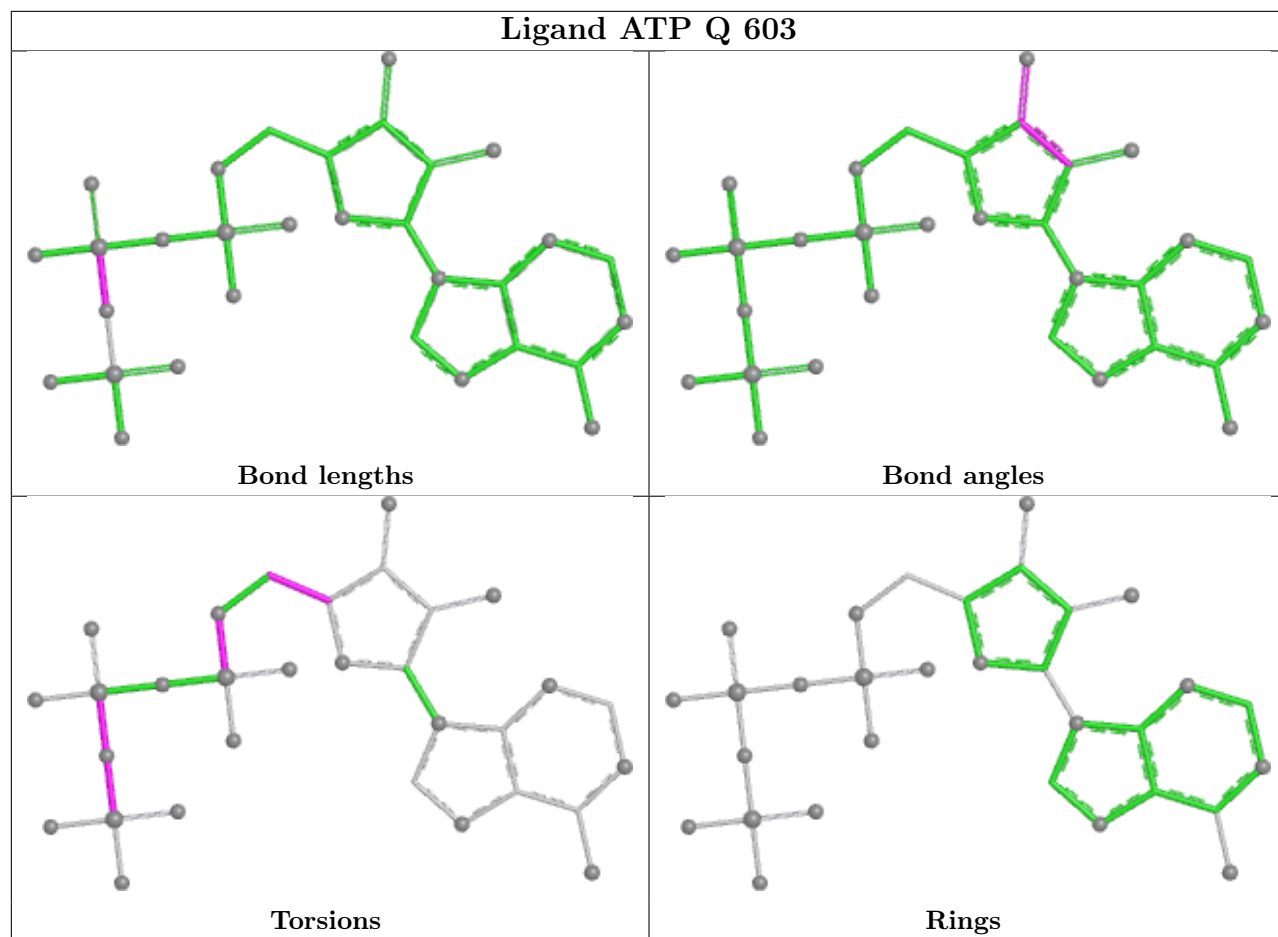


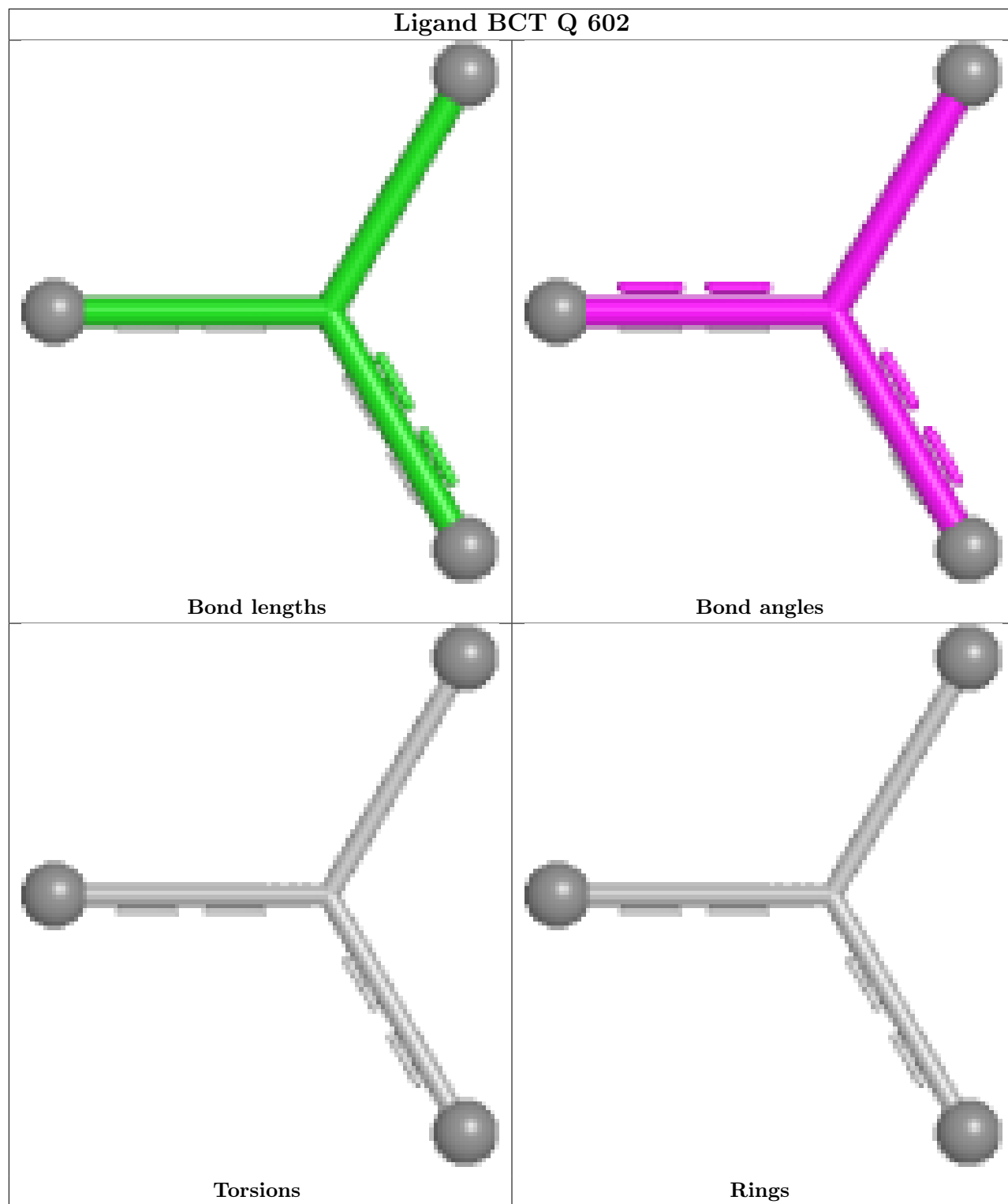


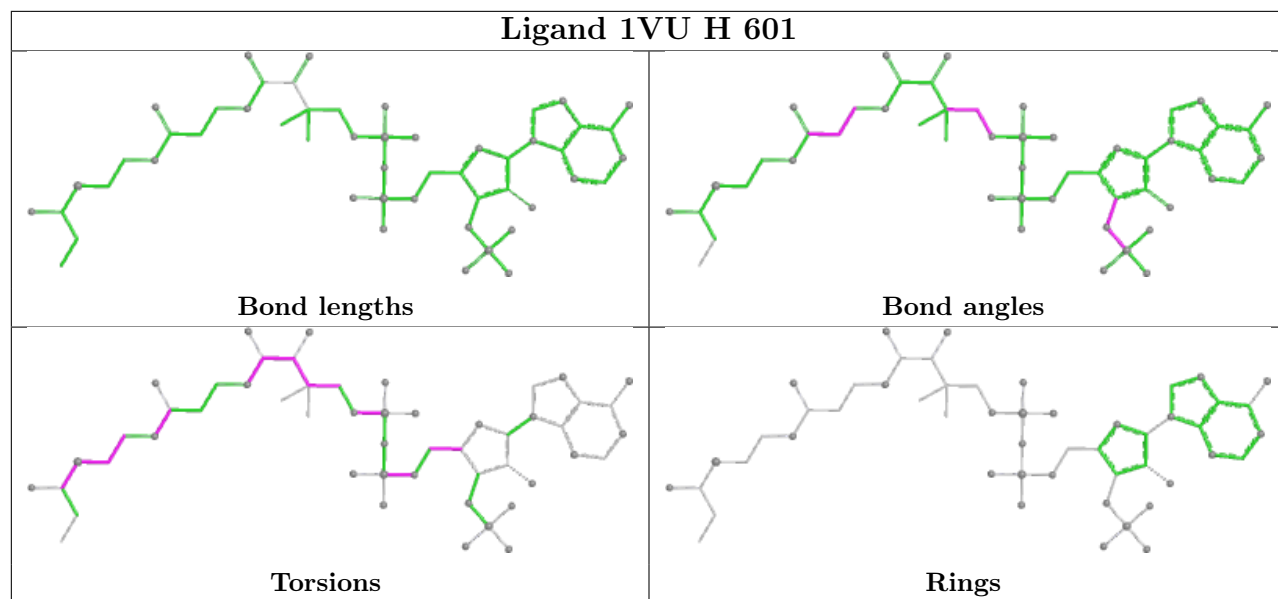


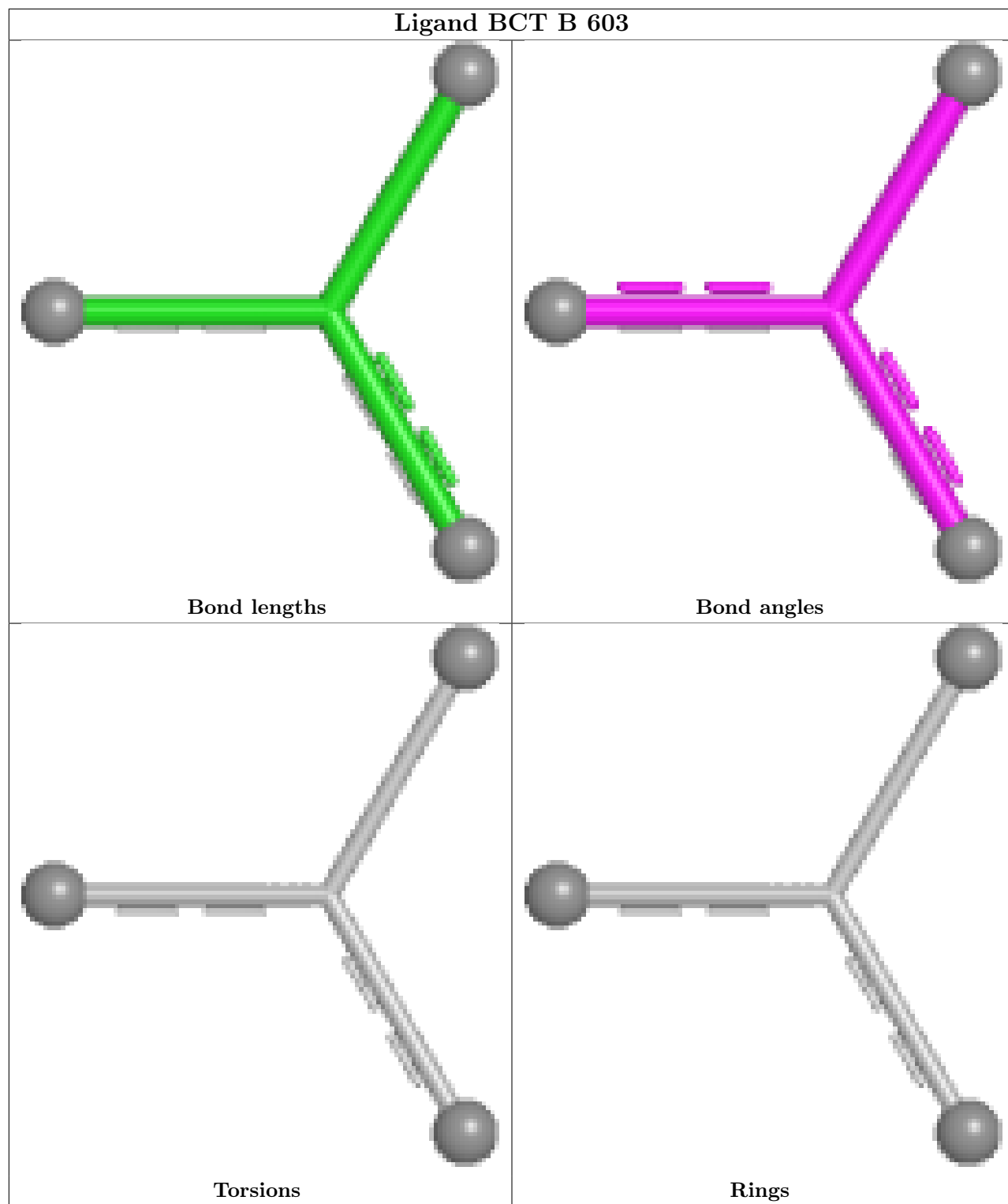




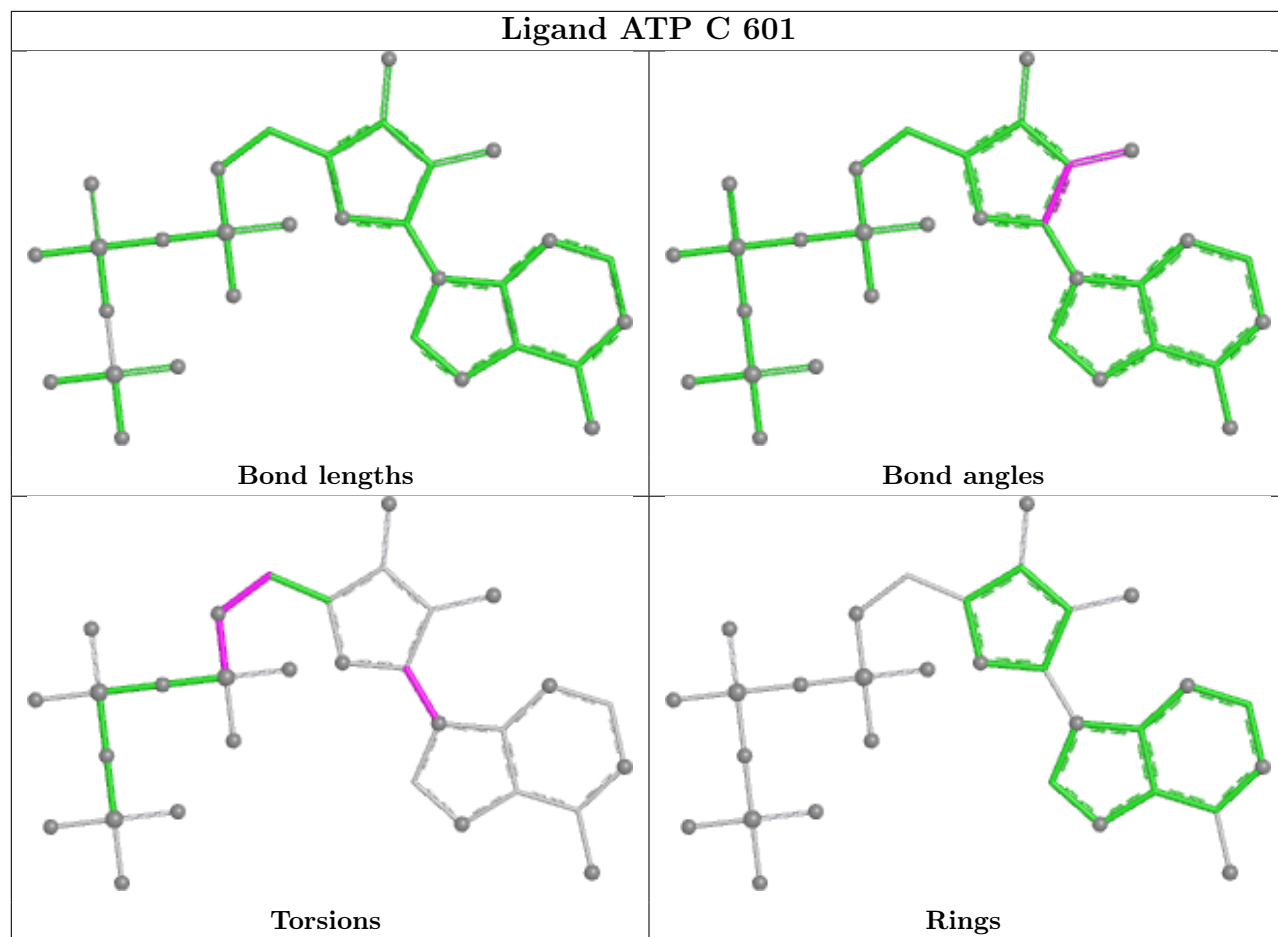




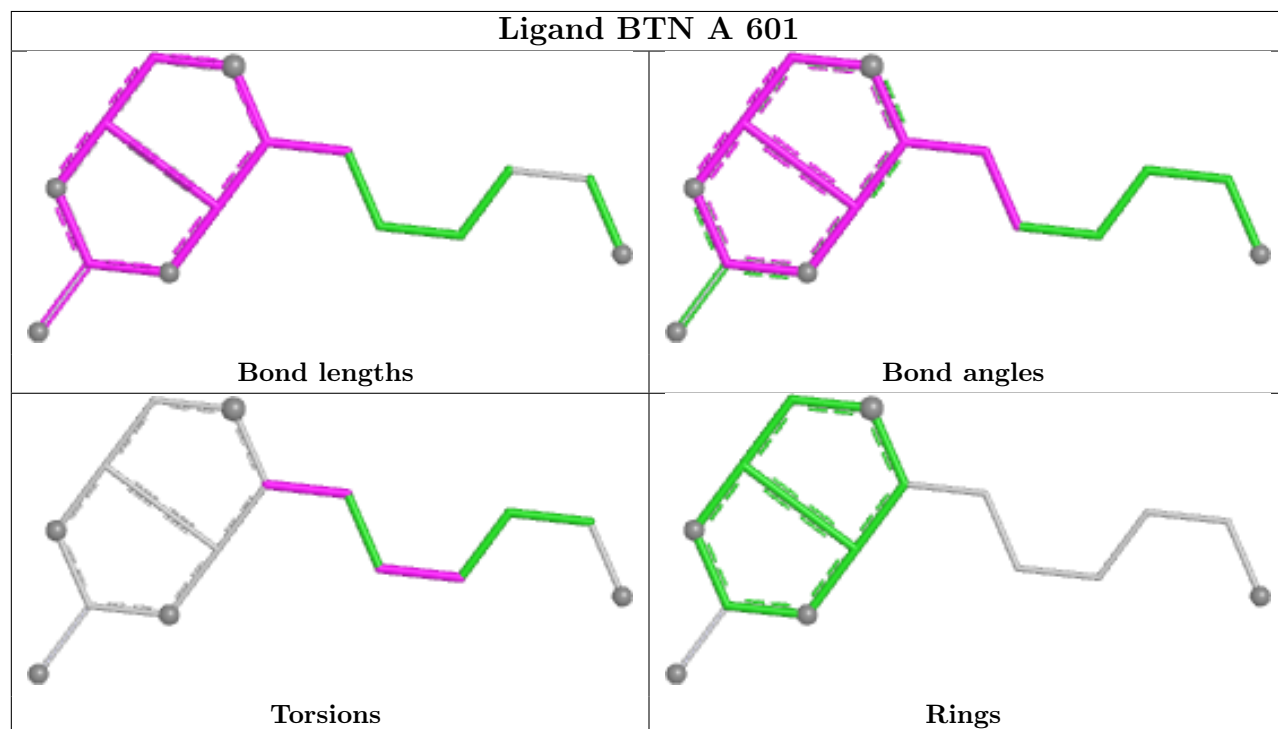


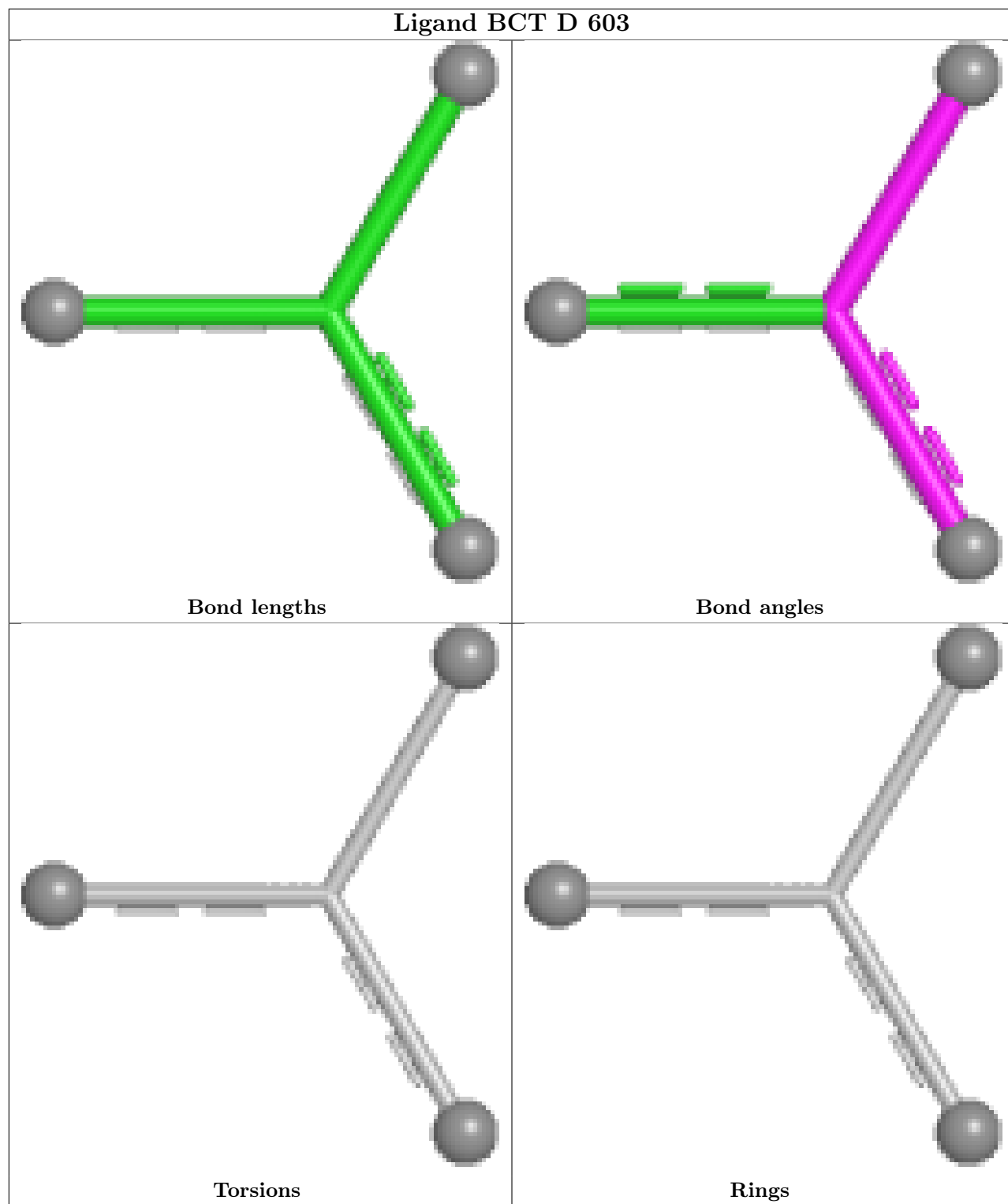


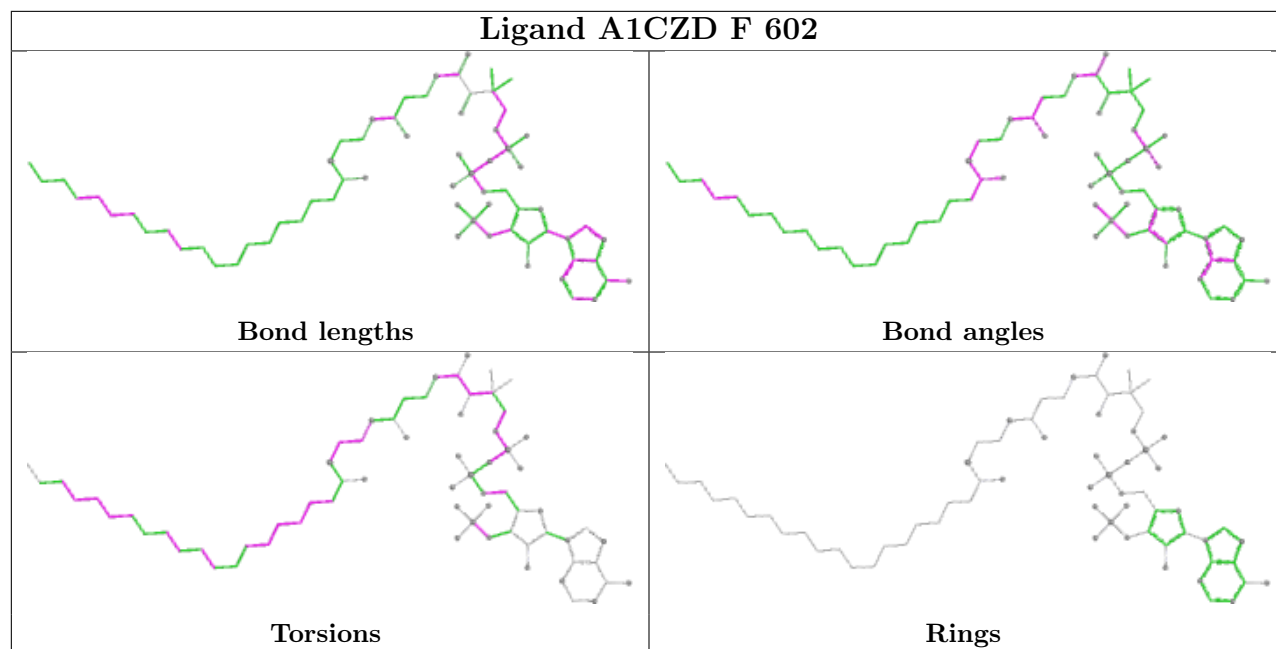
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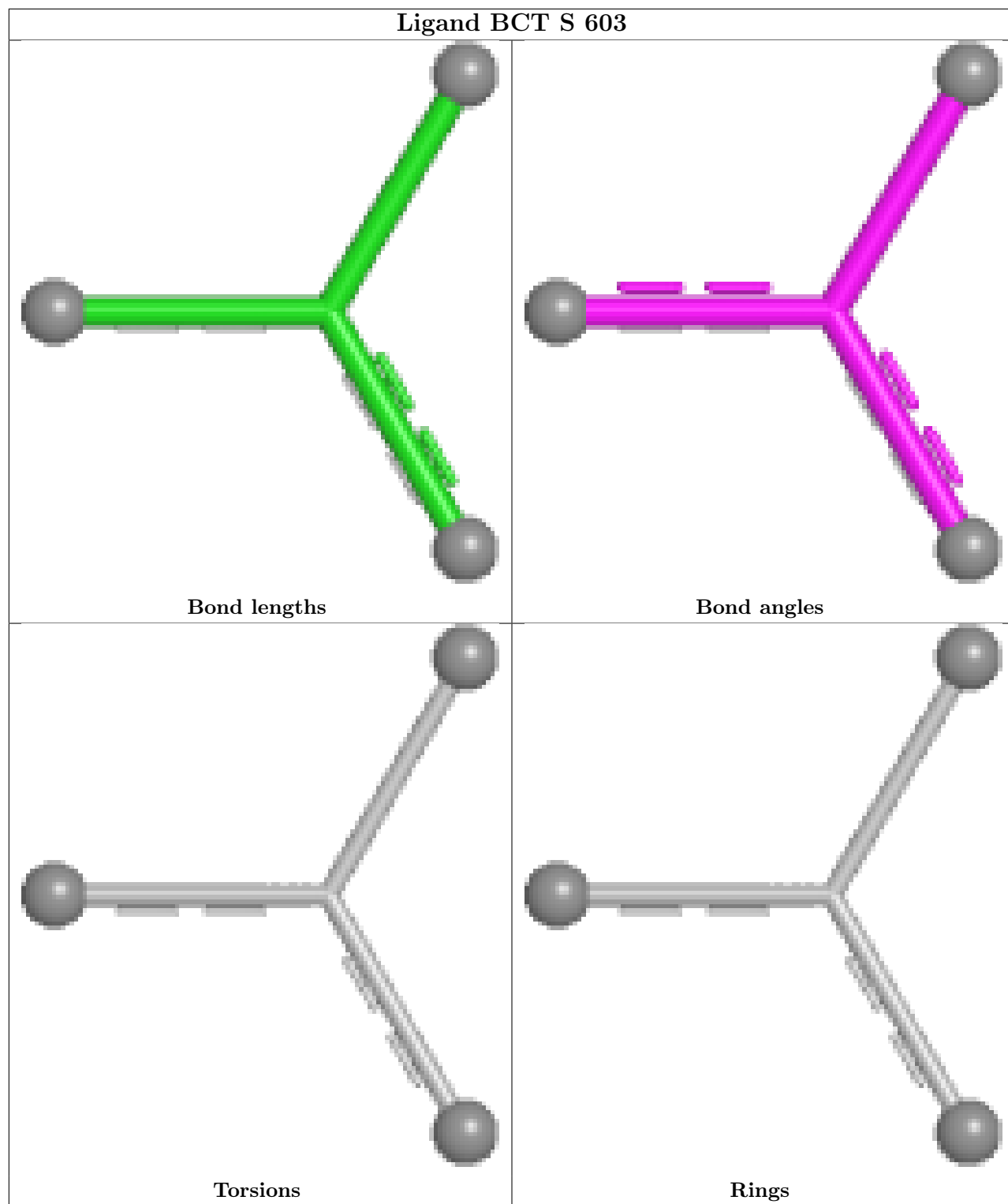


Ligand BTN A 601

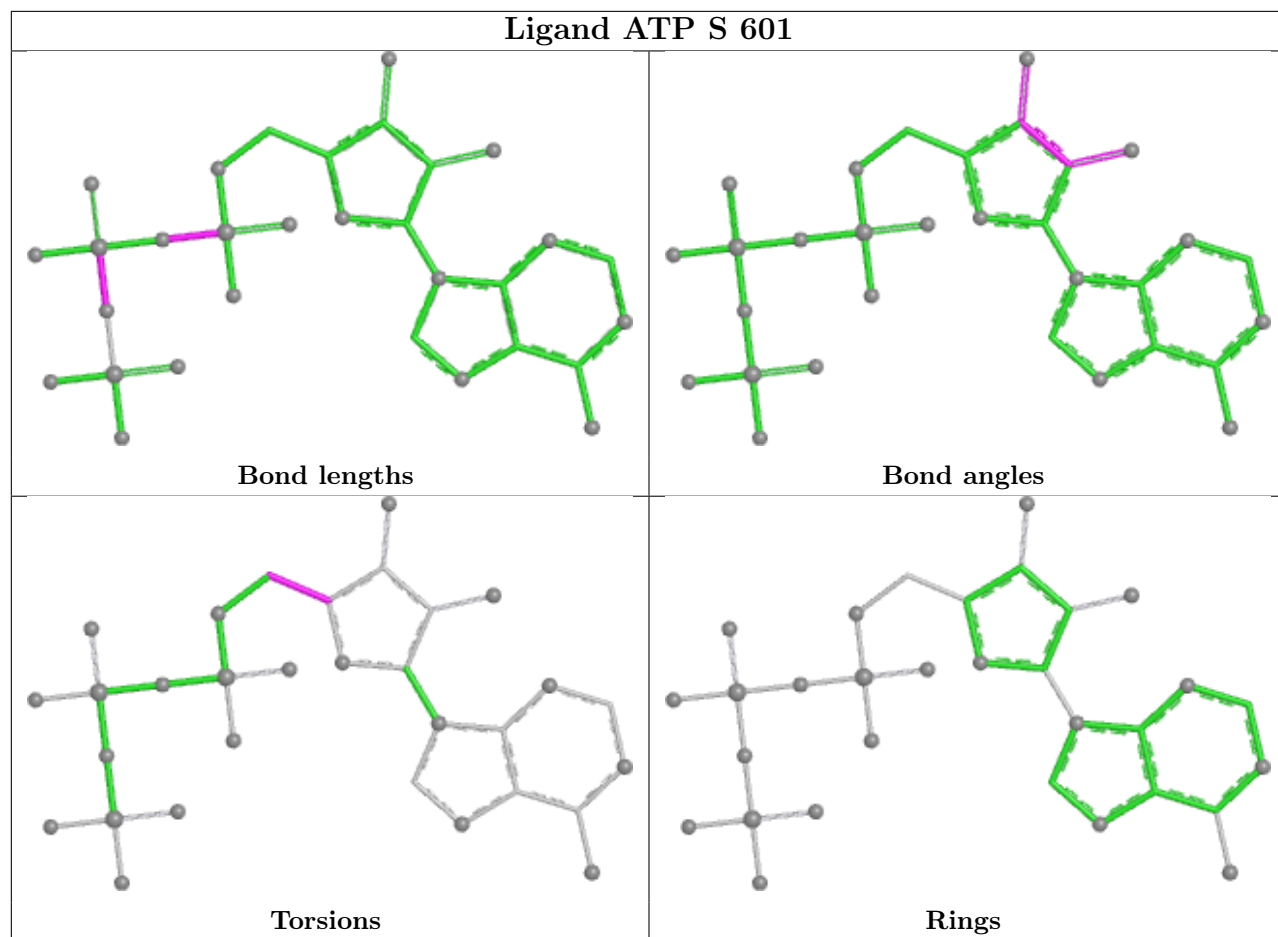


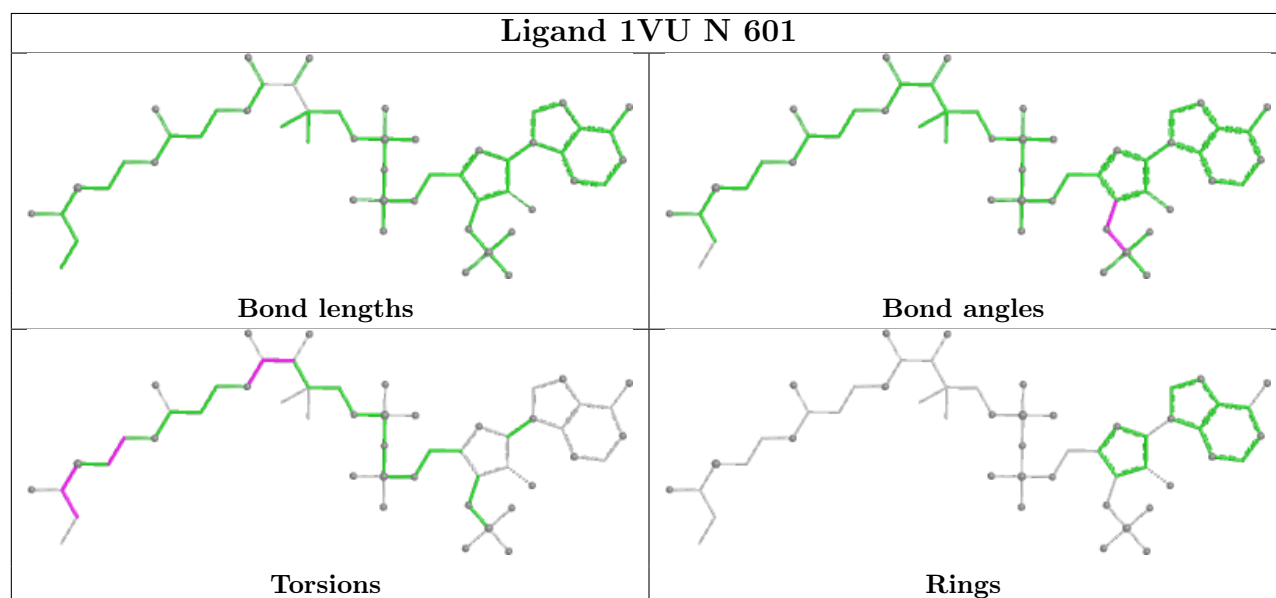
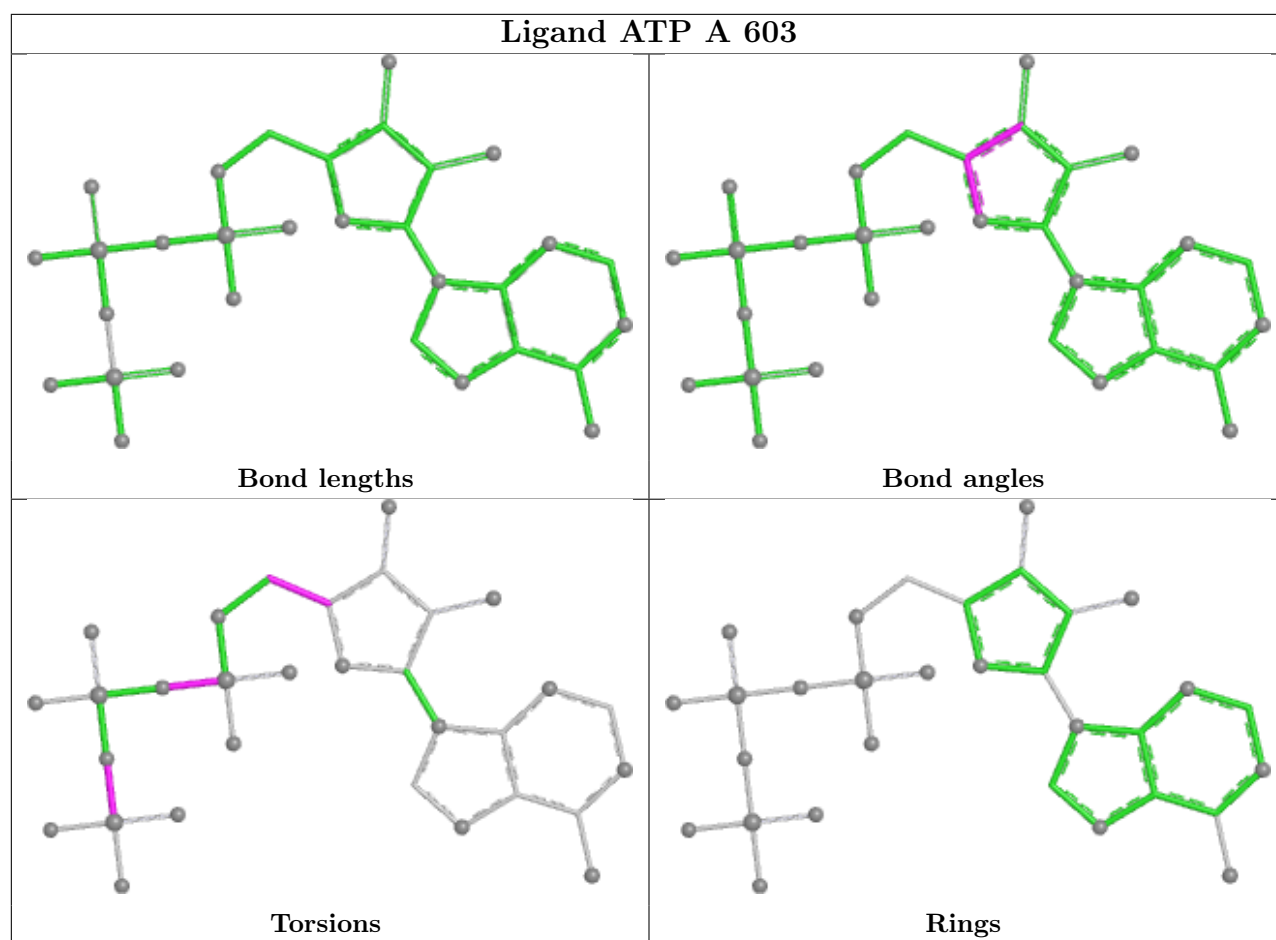


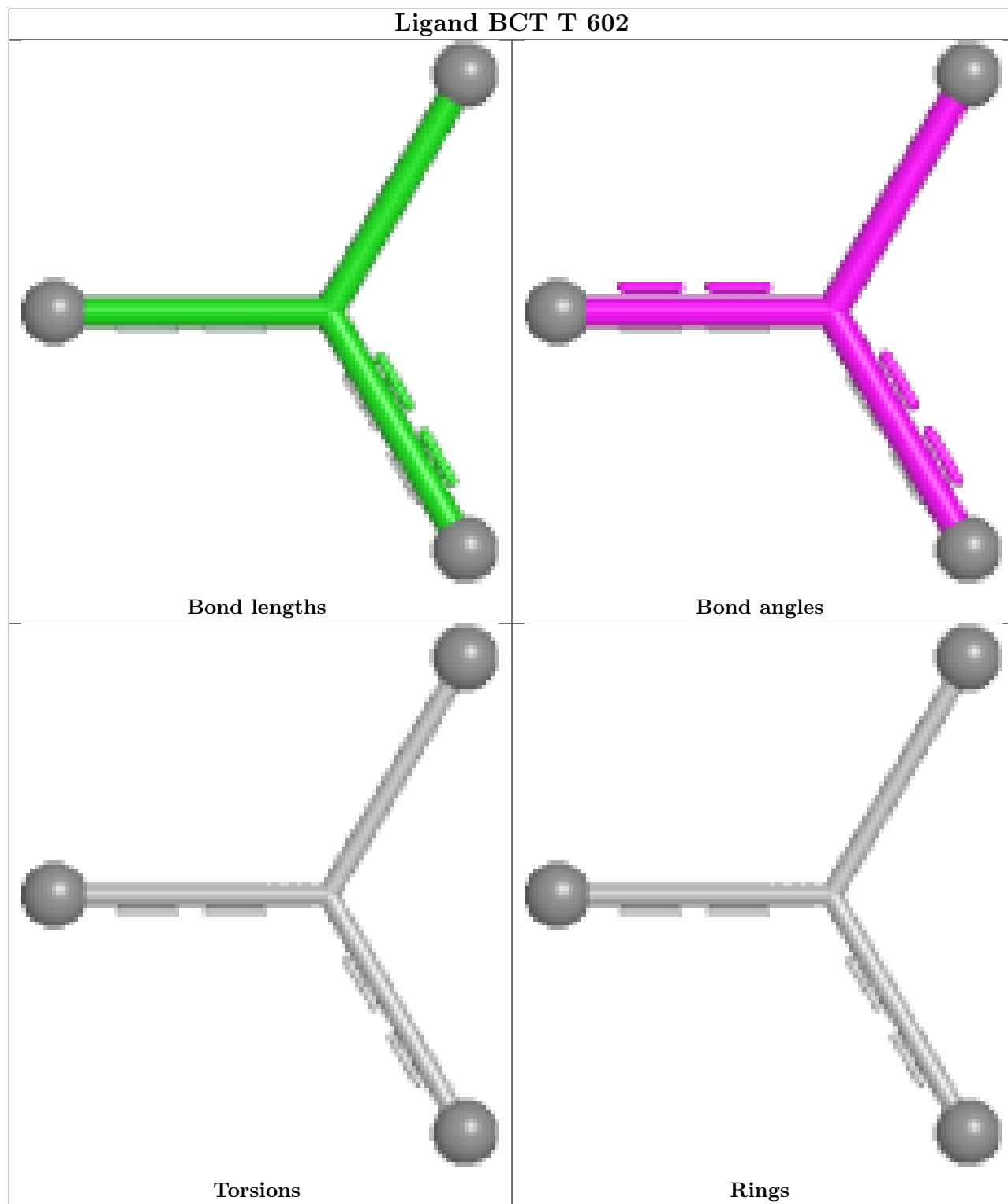


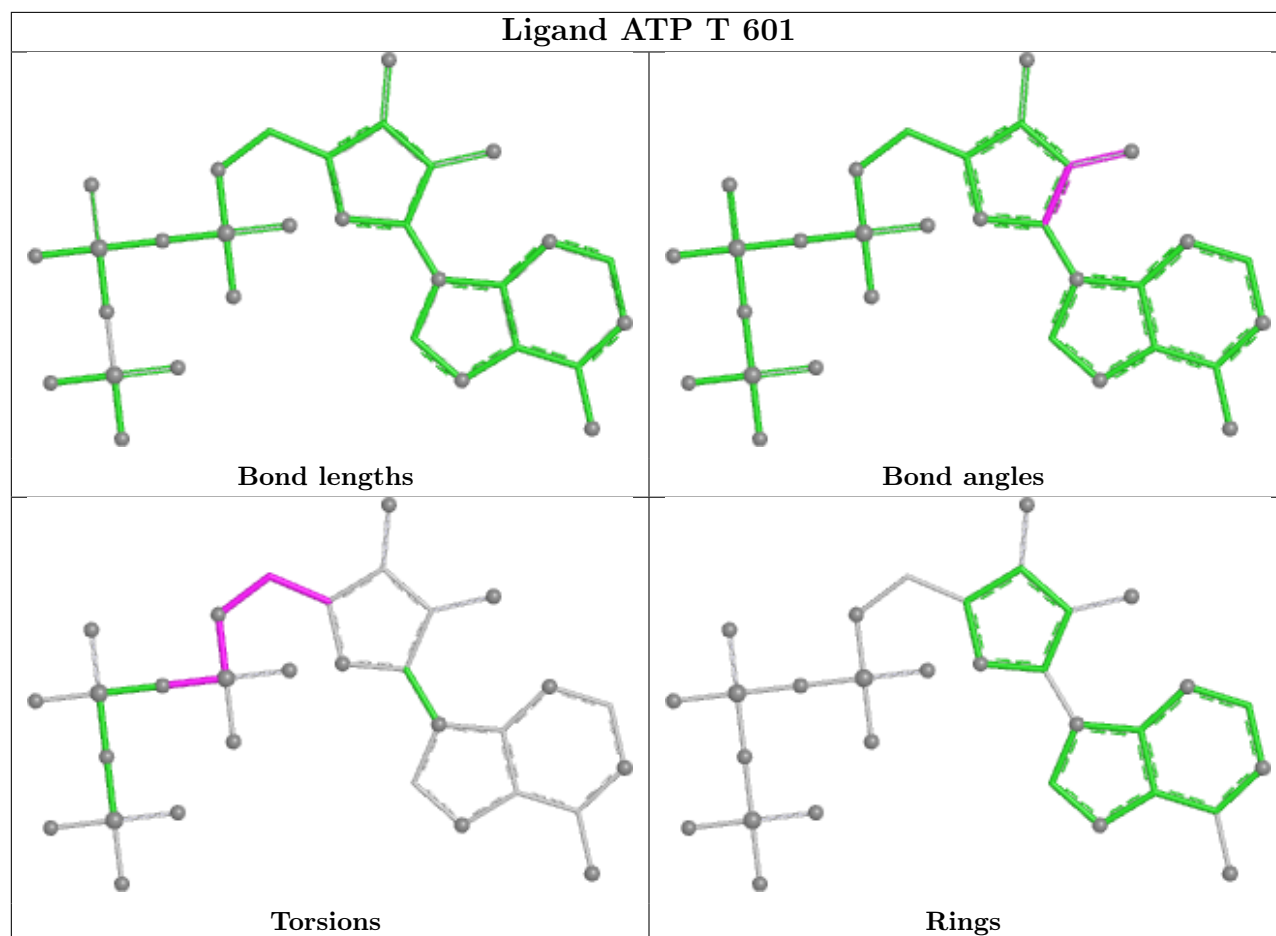
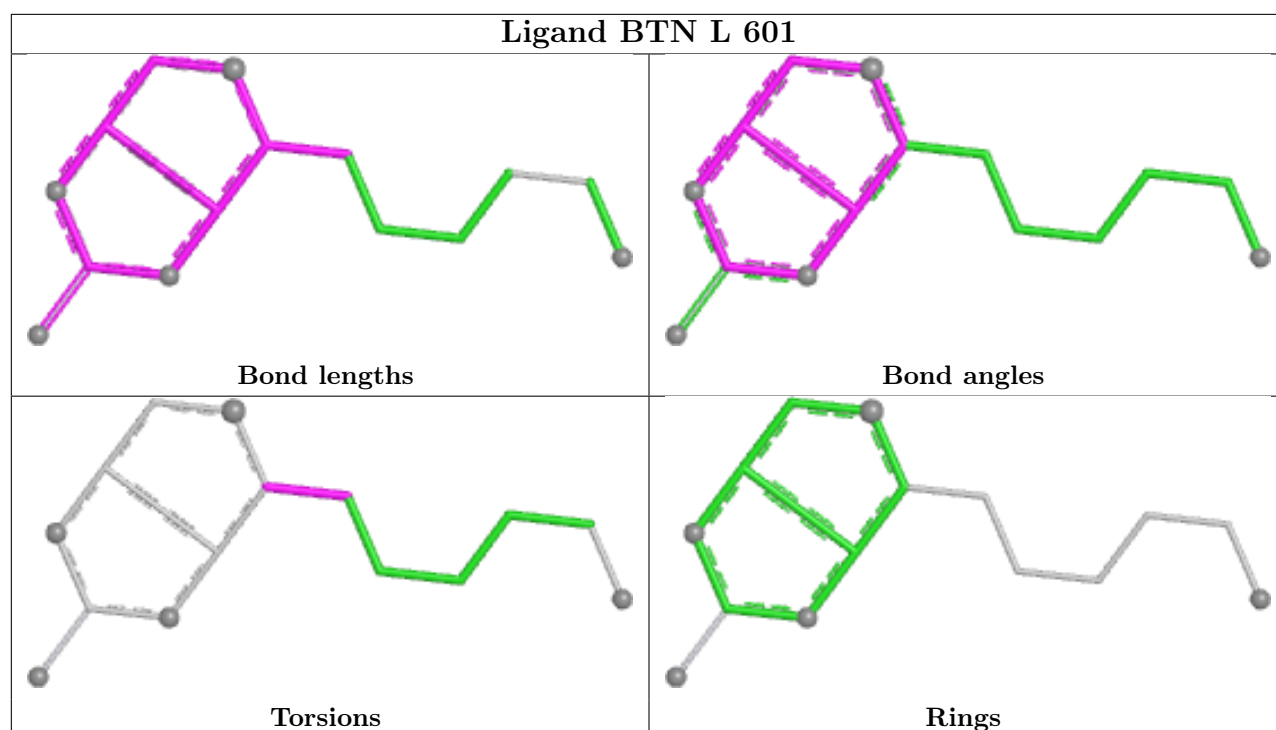


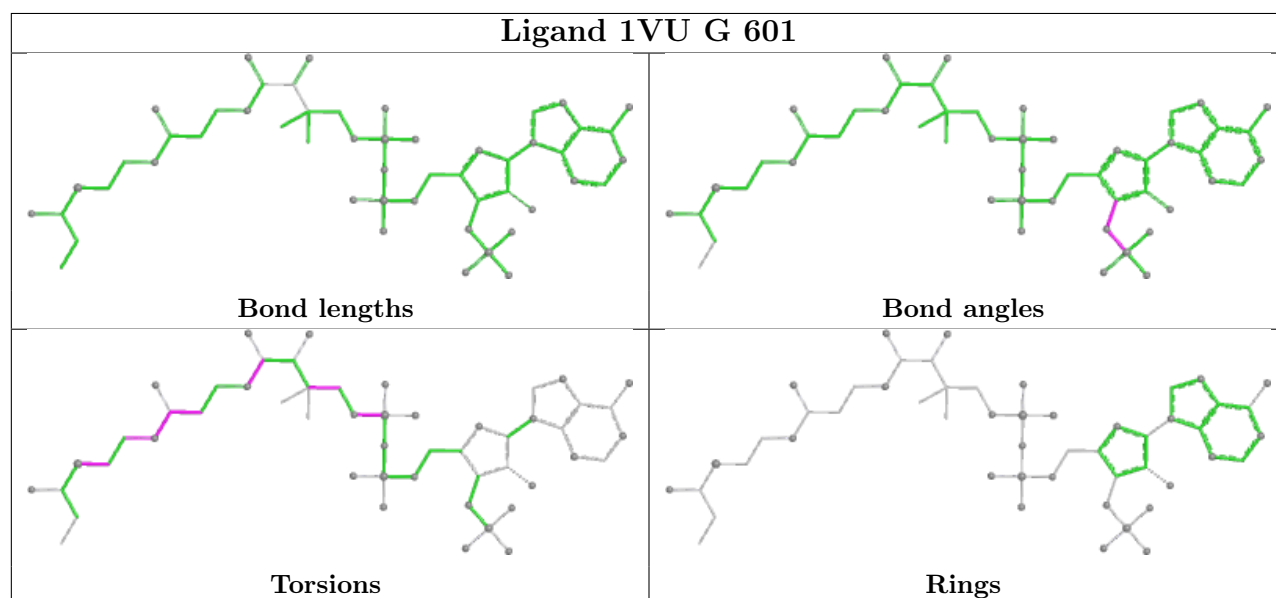
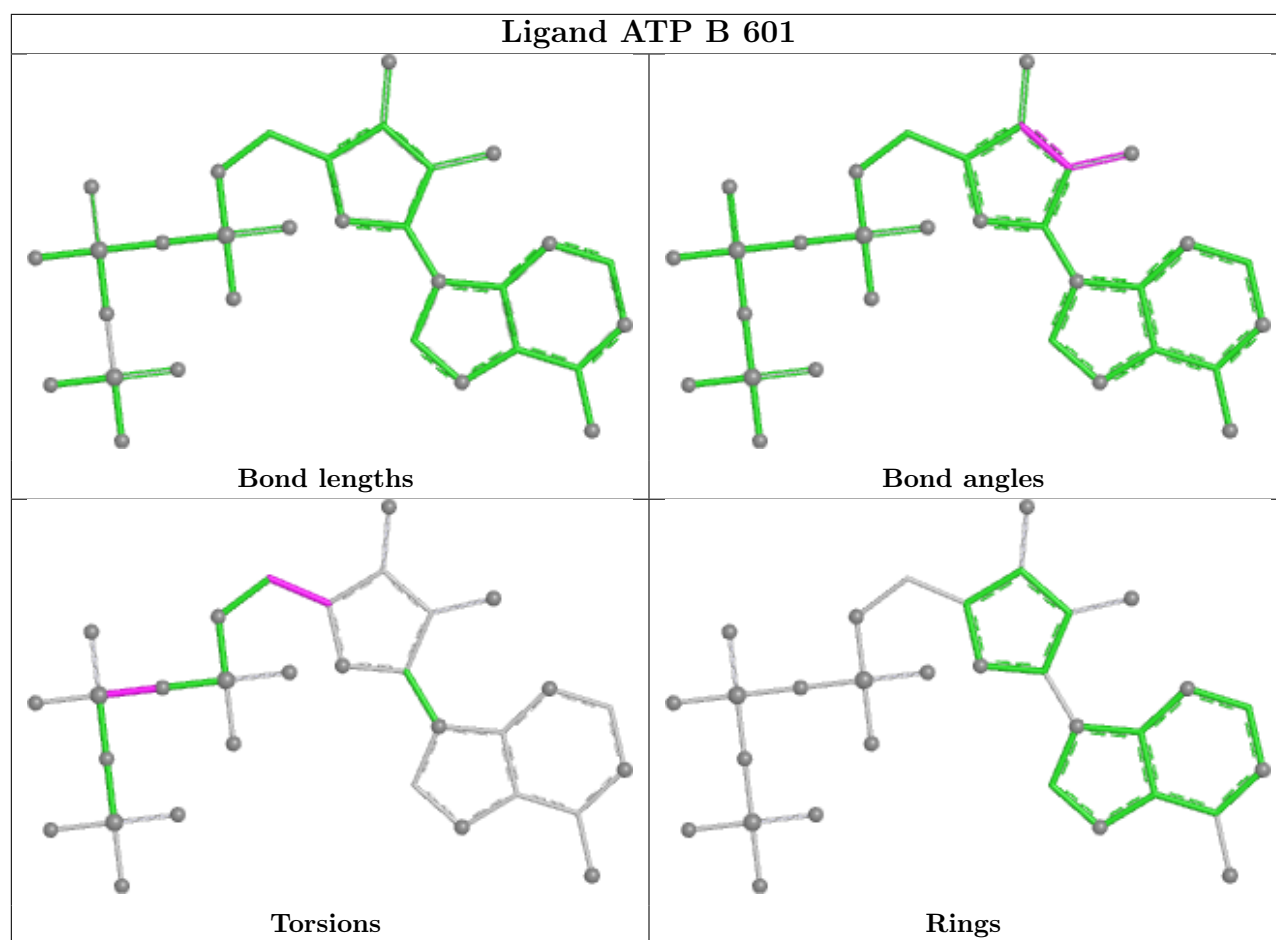
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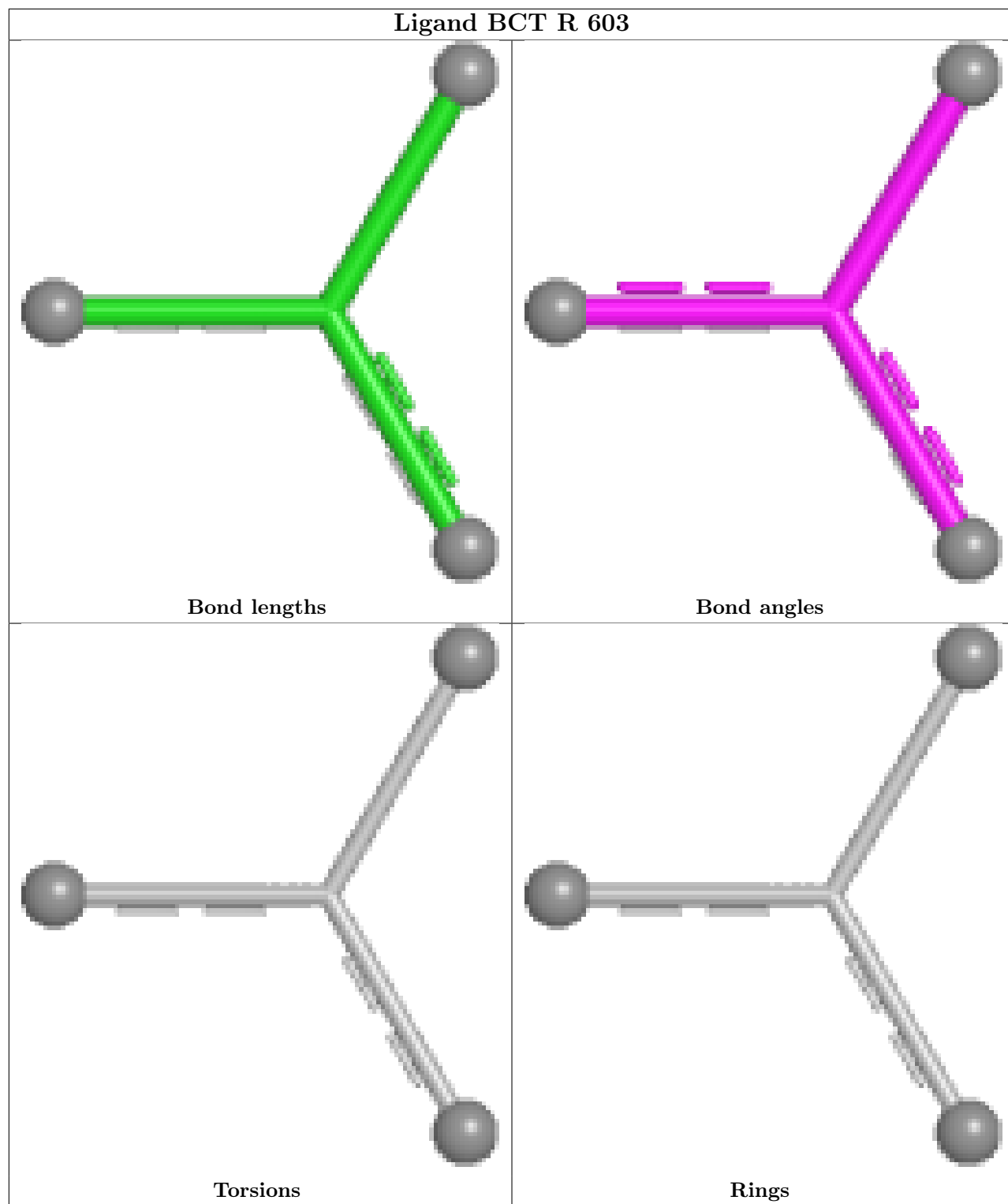


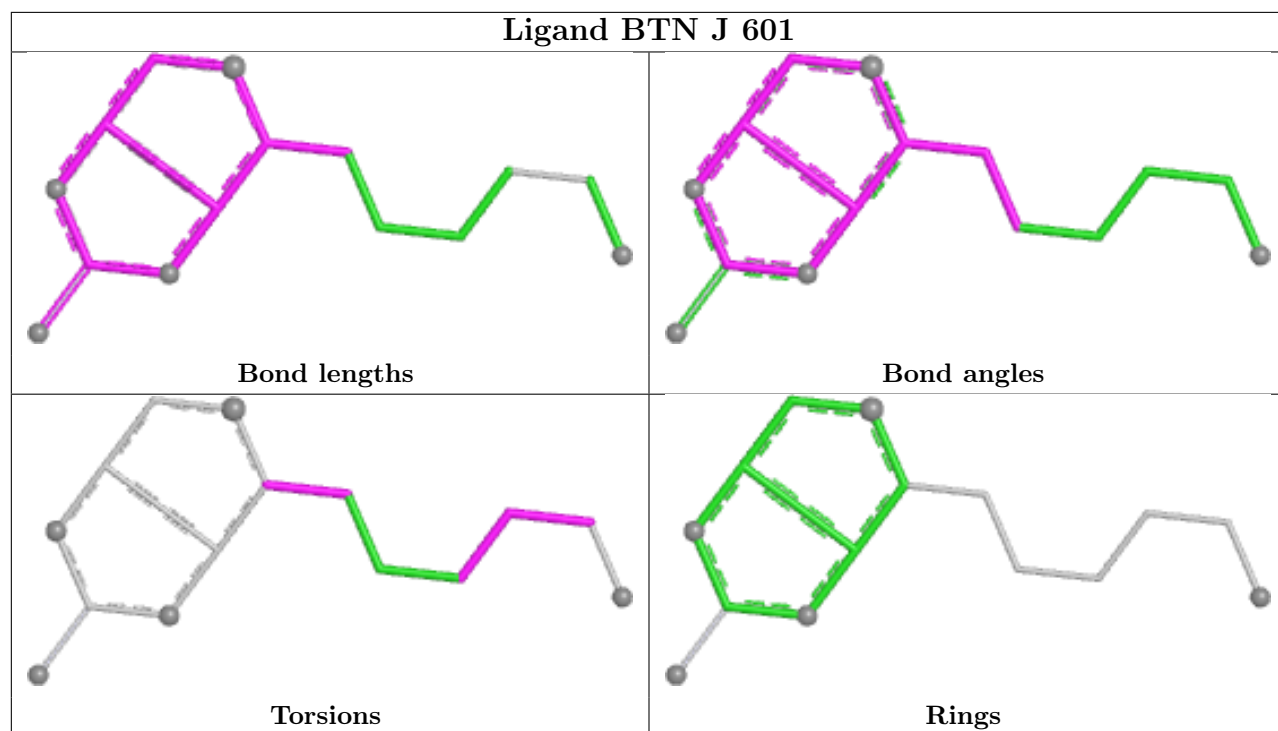
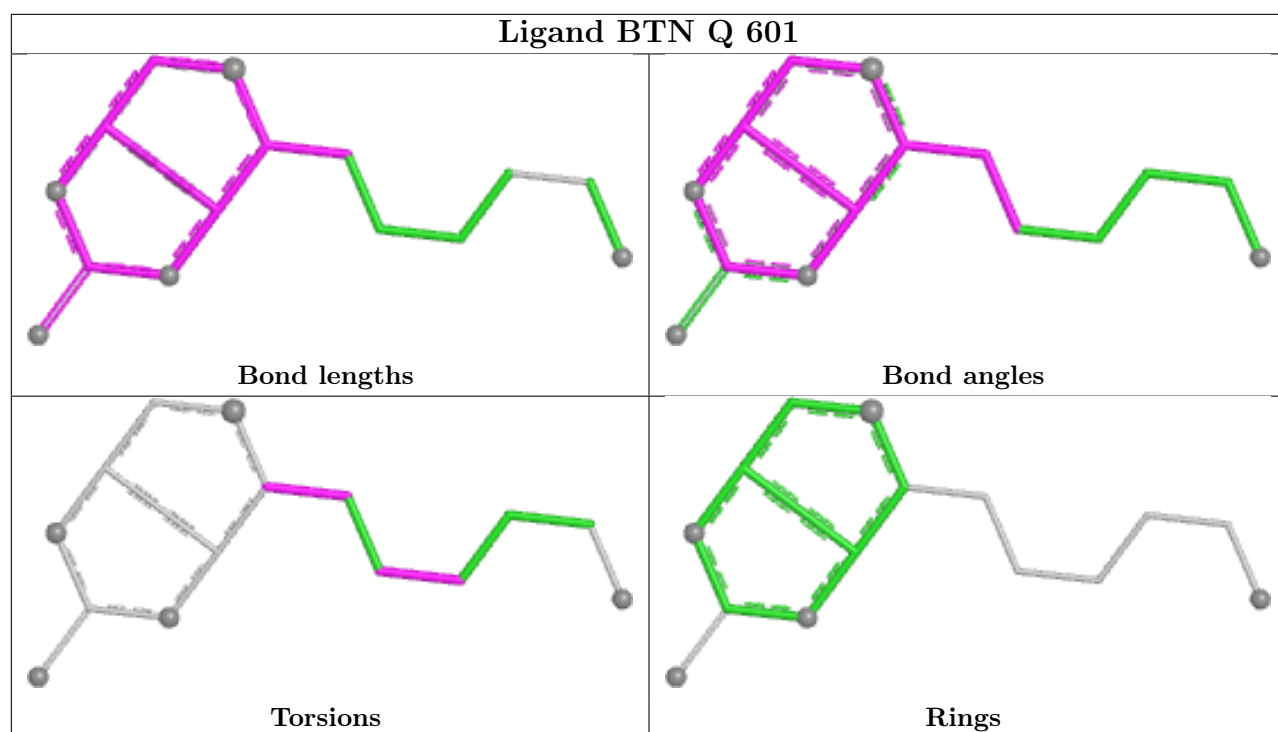


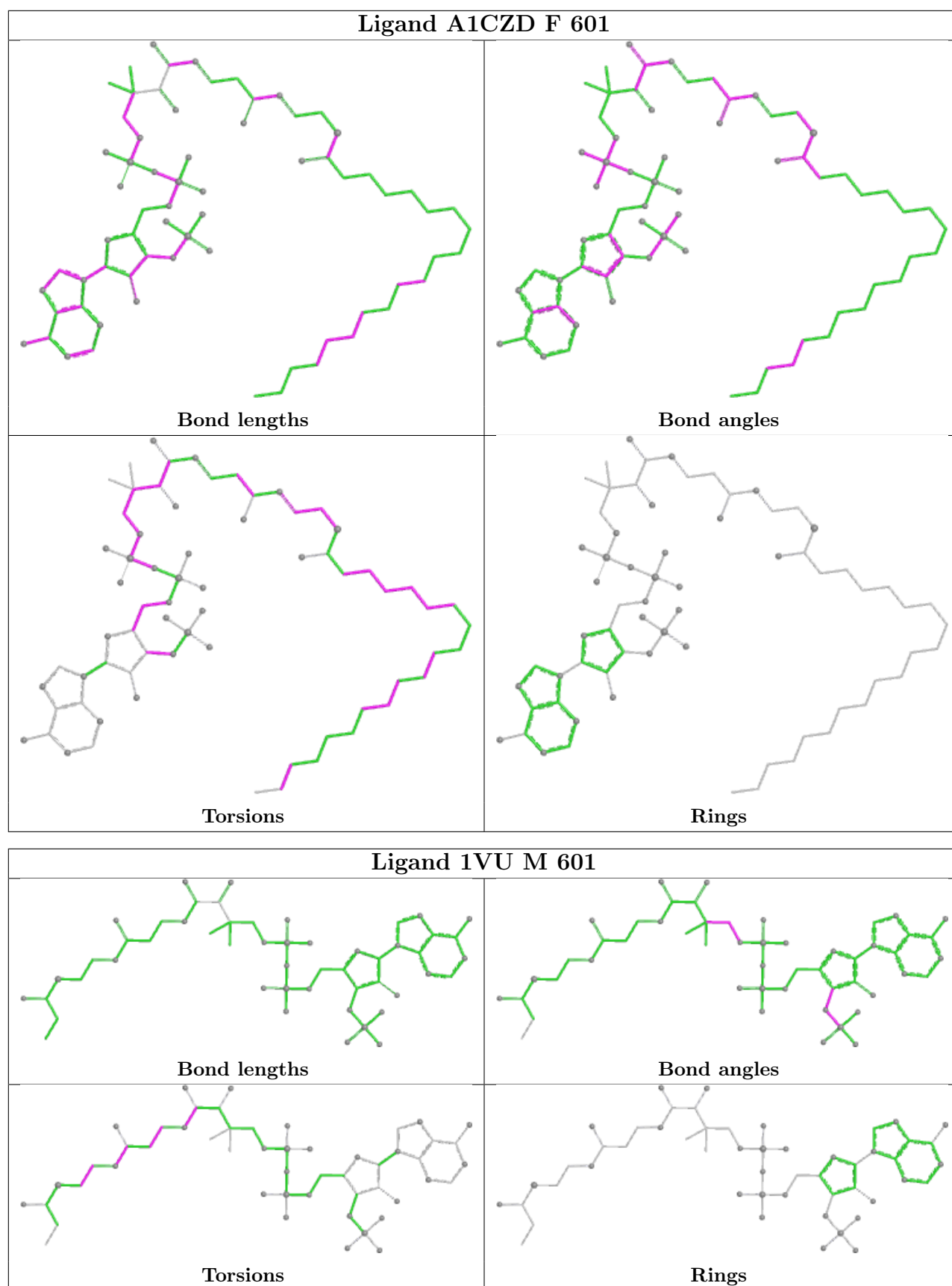












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

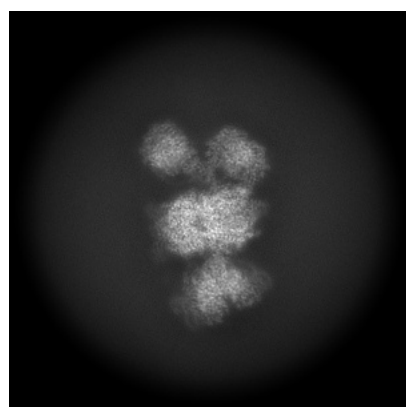
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73595. These allow visual inspection of the internal detail of the map and identification of artifacts.

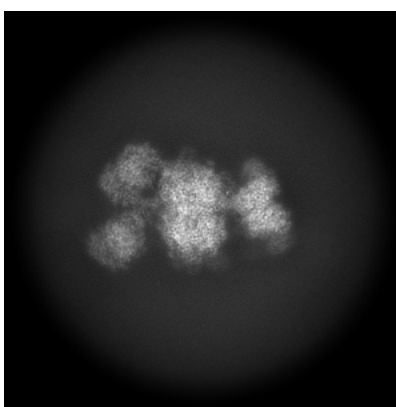
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

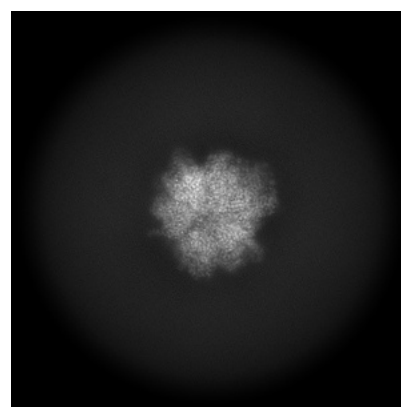
6.1.1 Primary map



X



Y

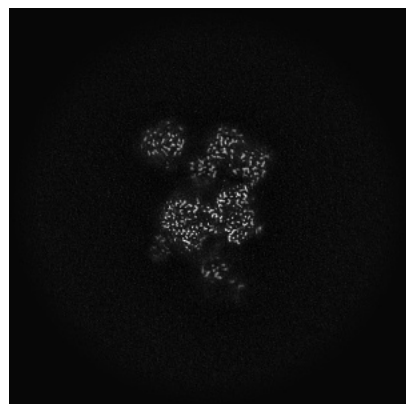


Z

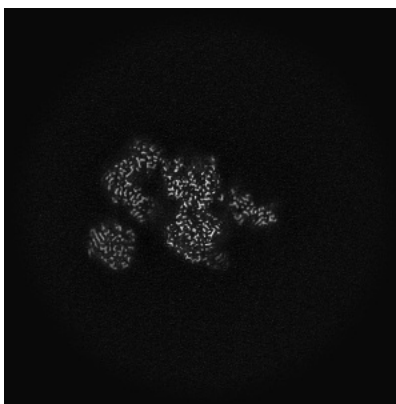
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

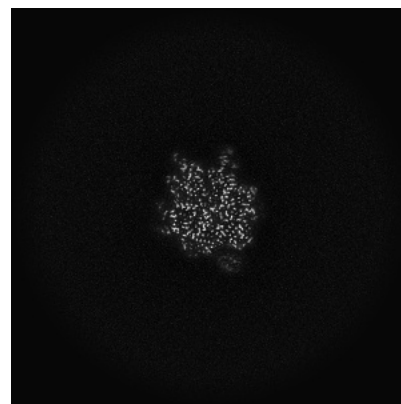
6.2.1 Primary map



X Index: 240



Y Index: 240

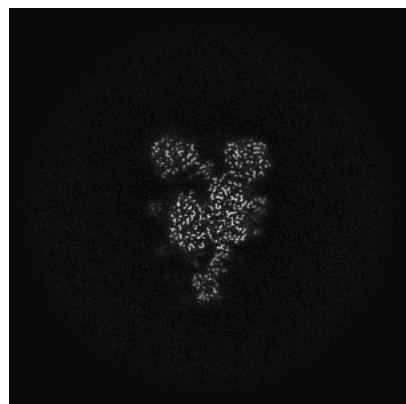


Z Index: 240

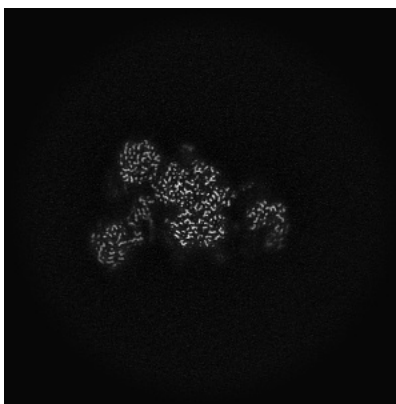
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

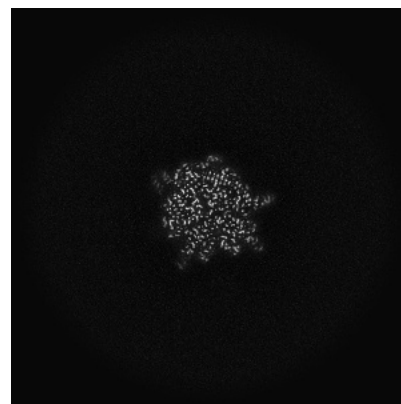
6.3.1 Primary map



X Index: 253



Y Index: 255

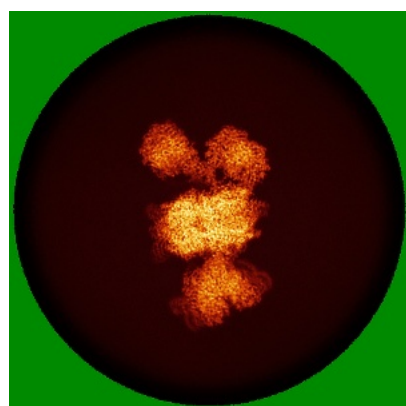


Z Index: 214

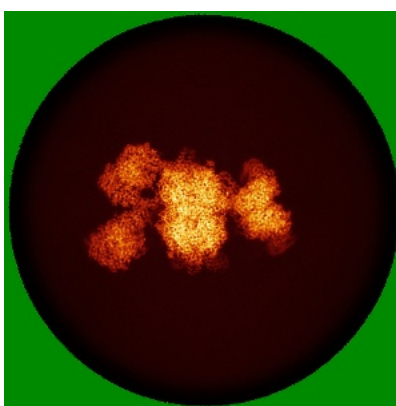
The images above show the largest variance slices of the map in three orthogonal directions.

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

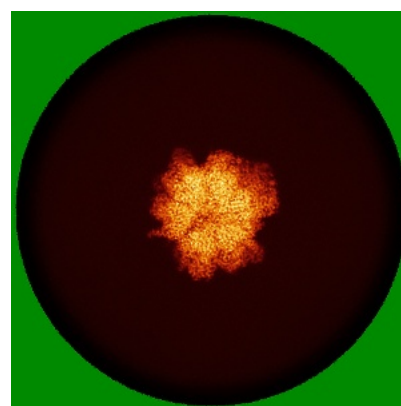
6.4.1 Primary map



X



Y

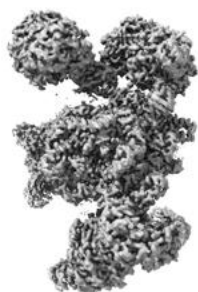


Z

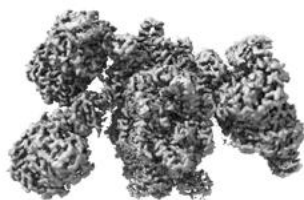
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

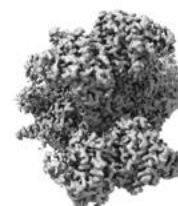
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

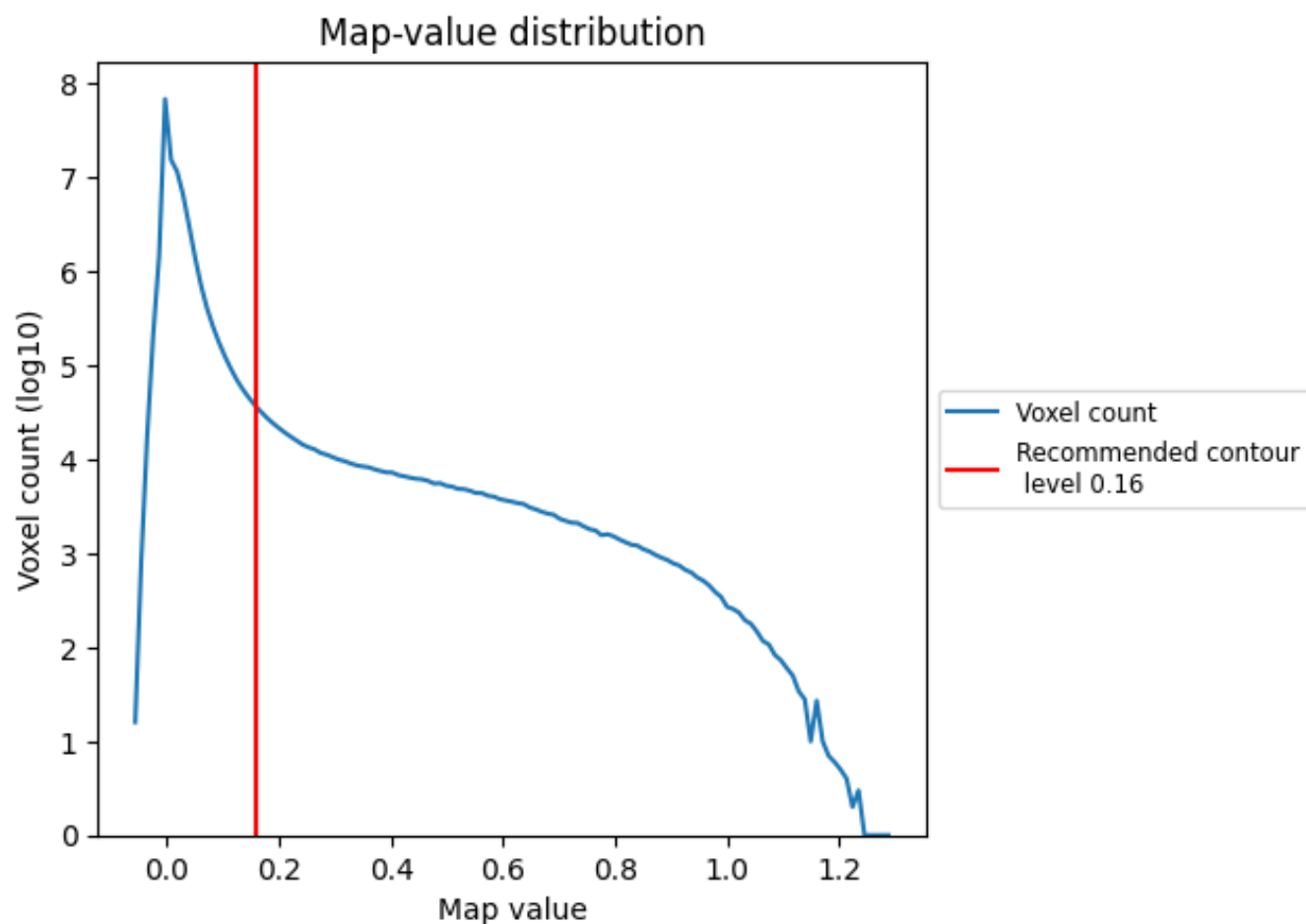
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

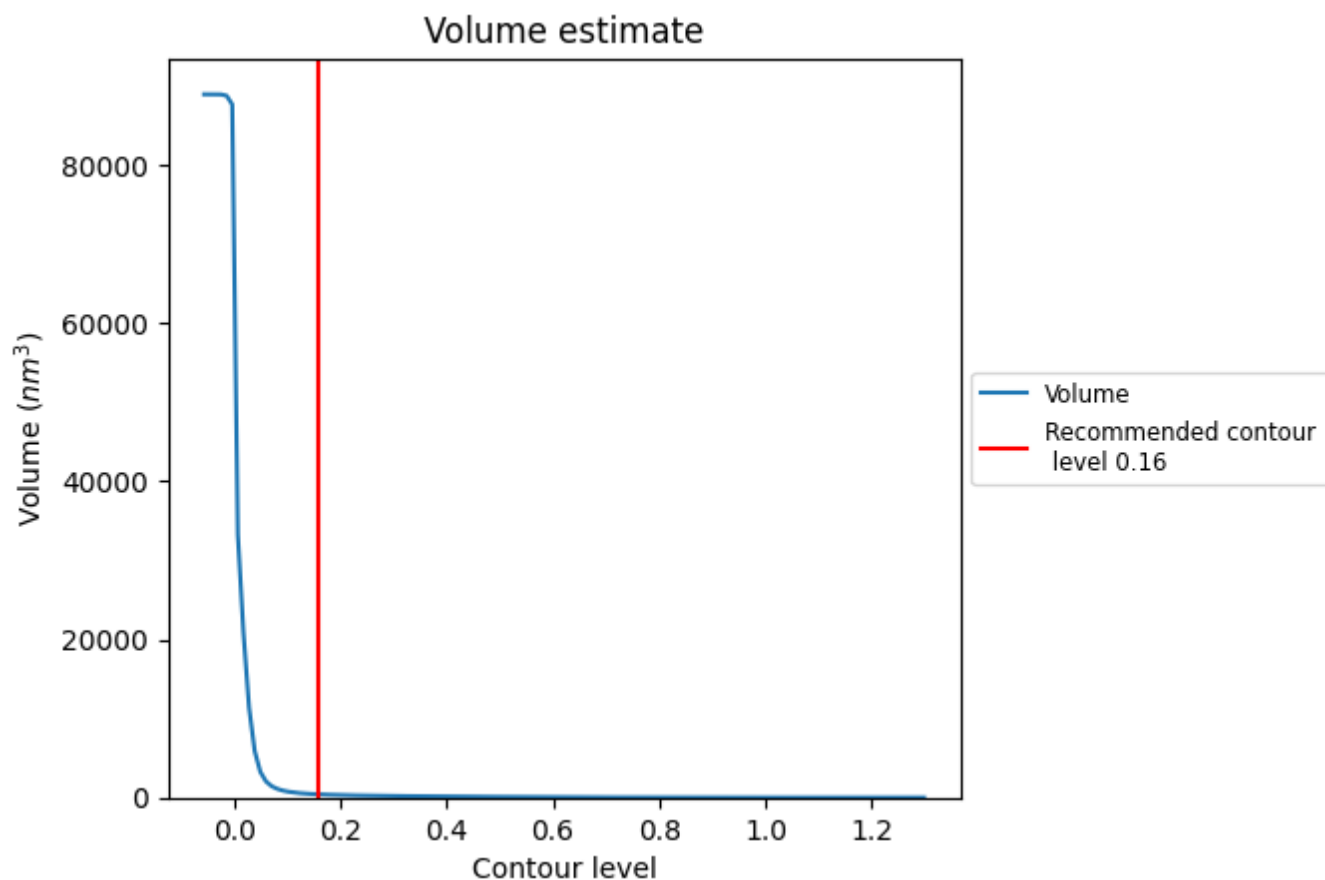
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

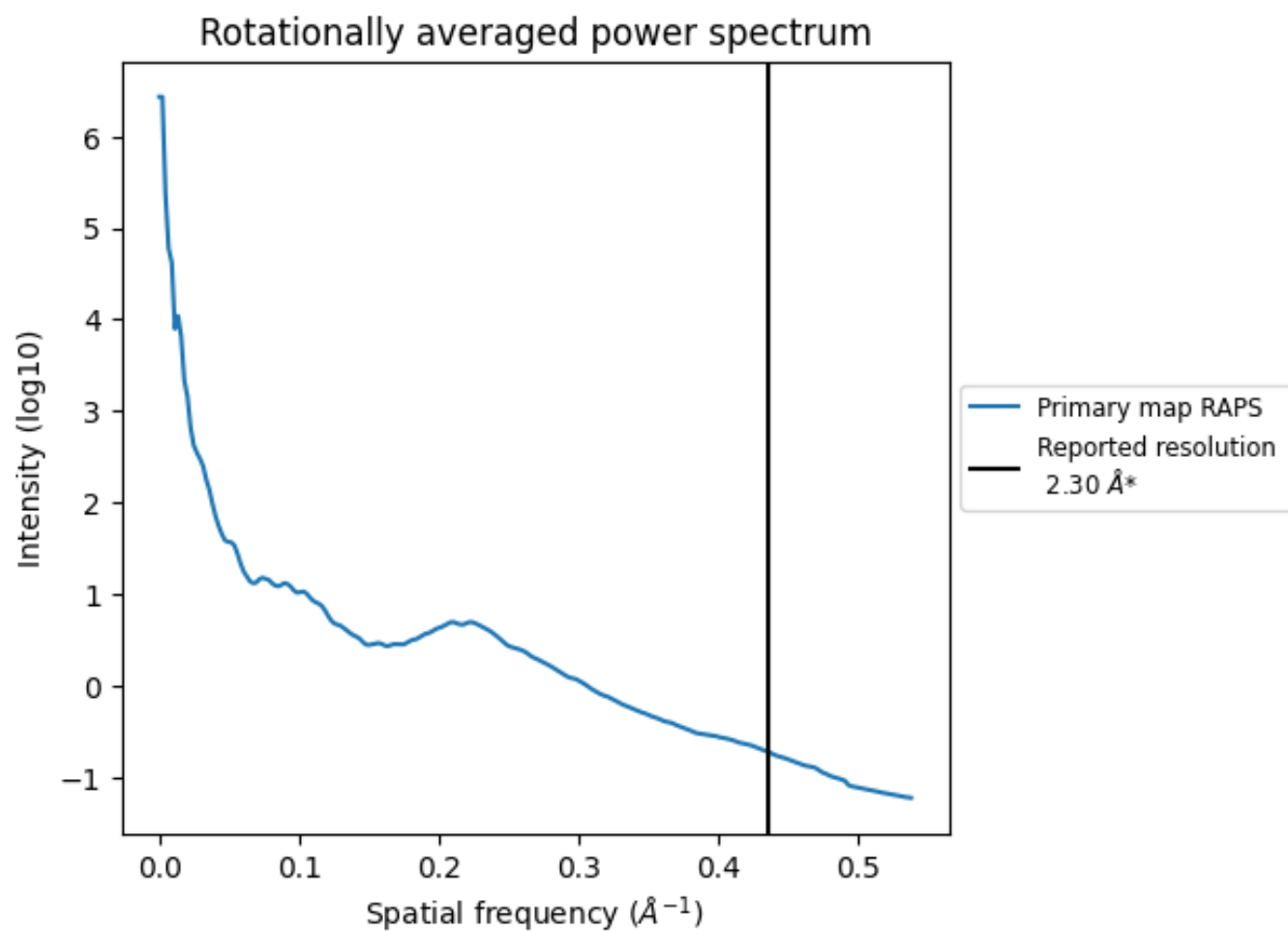
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm³; this corresponds to an approximate mass of 365 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 0.435 Å⁻¹

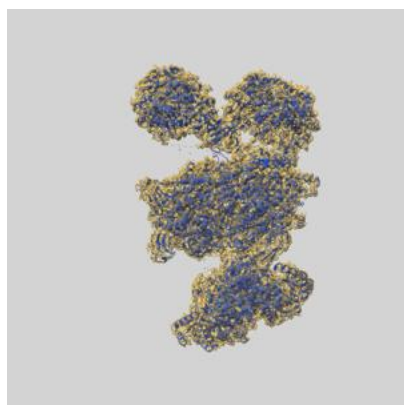
8 Fourier-Shell correlation

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

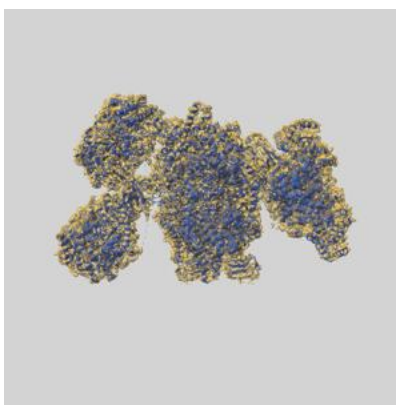
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73595 and PDB model 9YX4. Per-residue inclusion information can be found in section [3](#) on page [10](#).

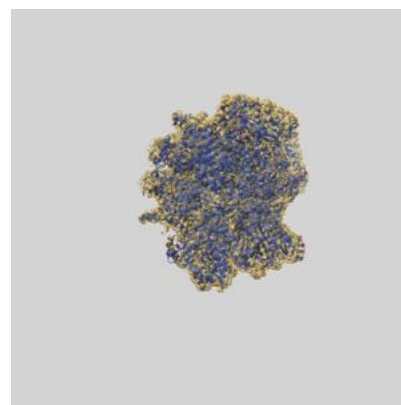
9.1 Map-model overlay [i](#)



X



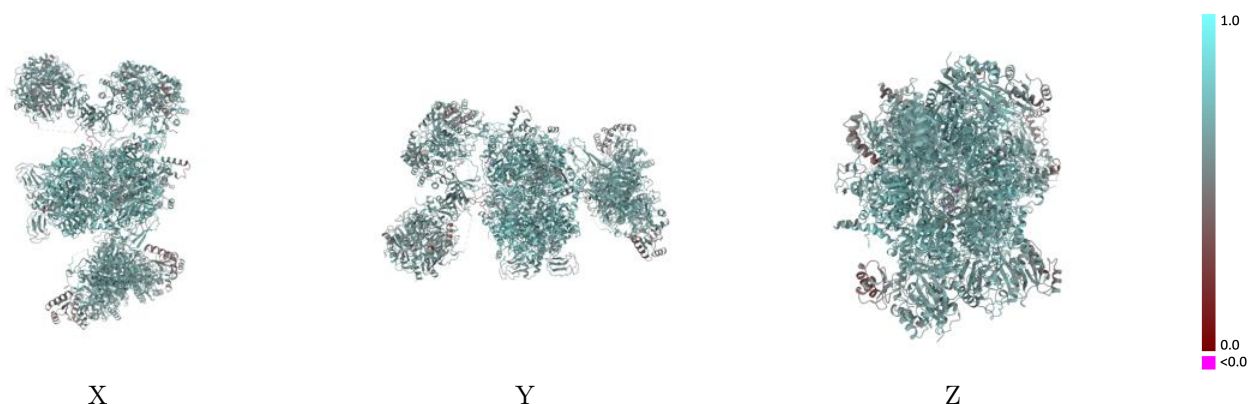
Y



Z

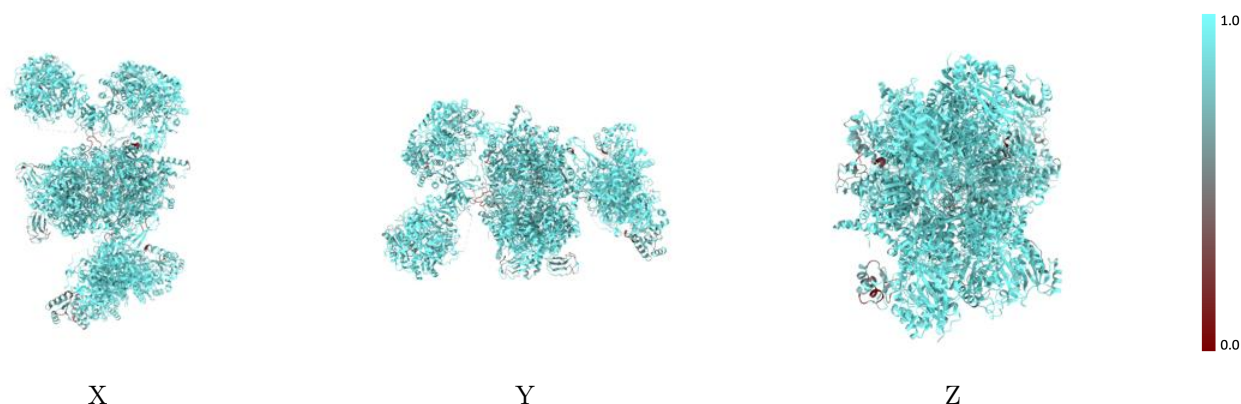
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



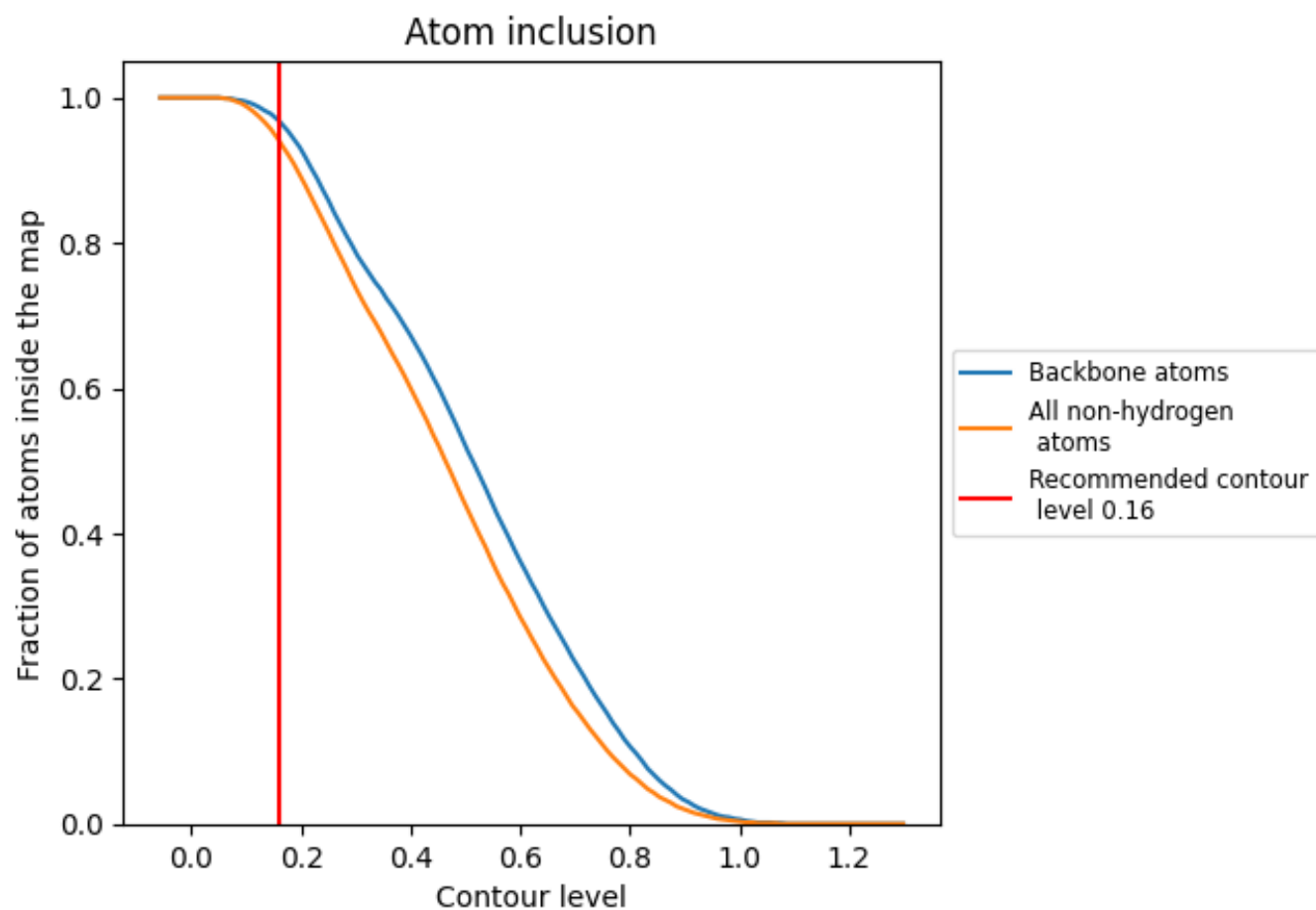
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.6460
A	 0.9300	 0.6100
B	 0.9190	 0.5950
C	 0.8850	 0.5660
D	 0.9370	 0.5810
E	 0.8790	 0.6360
F	 0.9590	 0.6970
G	 0.9840	 0.7160
H	 0.9800	 0.7100
I	 0.7820	 0.5900
J	 0.6920	 0.5890
K	 0.7500	 0.5940
L	 0.7150	 0.5870
M	 0.9830	 0.7160
N	 0.9800	 0.7110
O	 0.9750	 0.7030
P	 0.8880	 0.6340
Q	 0.9420	 0.6220
R	 0.9390	 0.6120
S	 0.9140	 0.5920
T	 0.9410	 0.6000

