



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 07:52 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 Full wwPDB EM Validation 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:

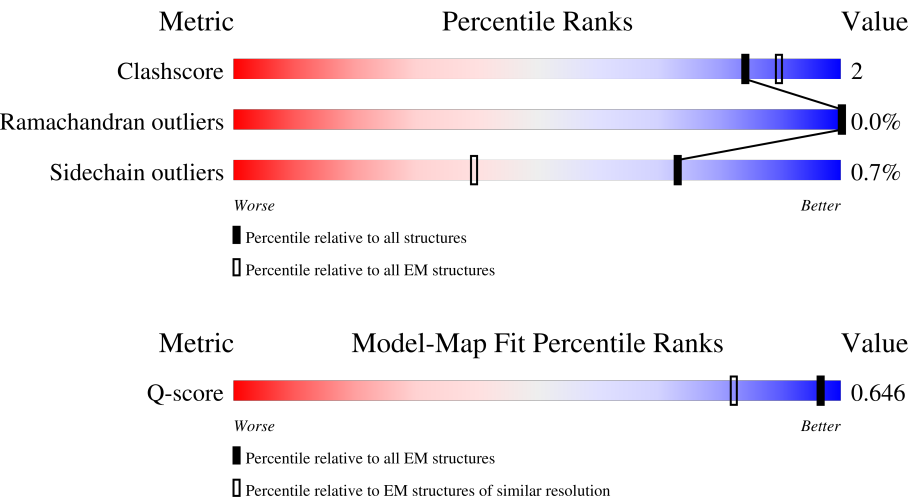
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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.



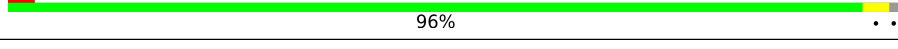
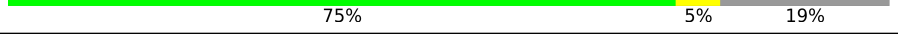
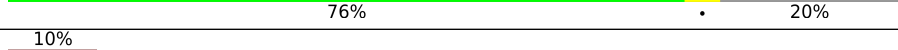
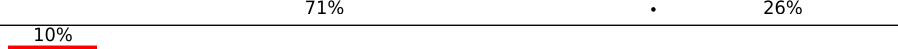
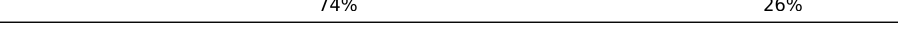
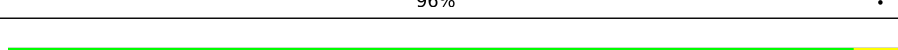
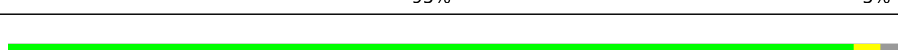
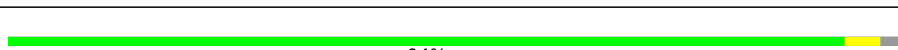
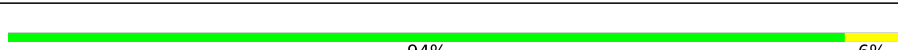
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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		

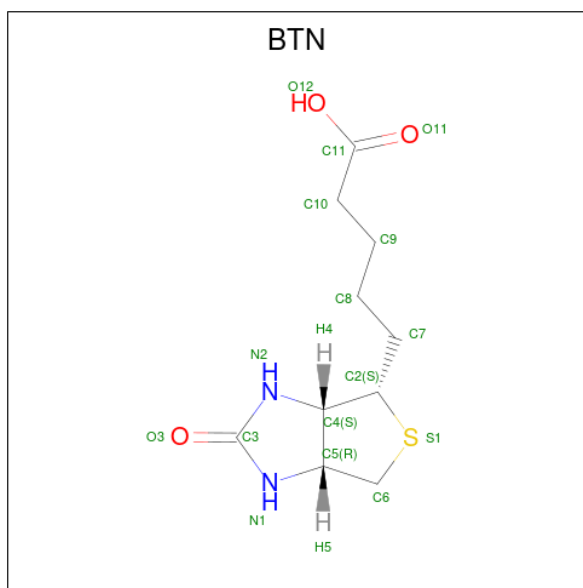
- Molecule 3 is a protein called Propionyl-CoA carboxylase beta chain.

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).



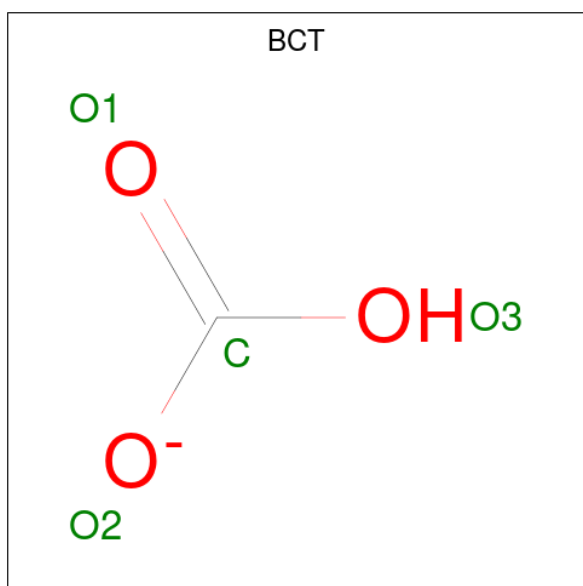
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	J	1	Total	C	N	O	S	0
			15	10	2	2	1	

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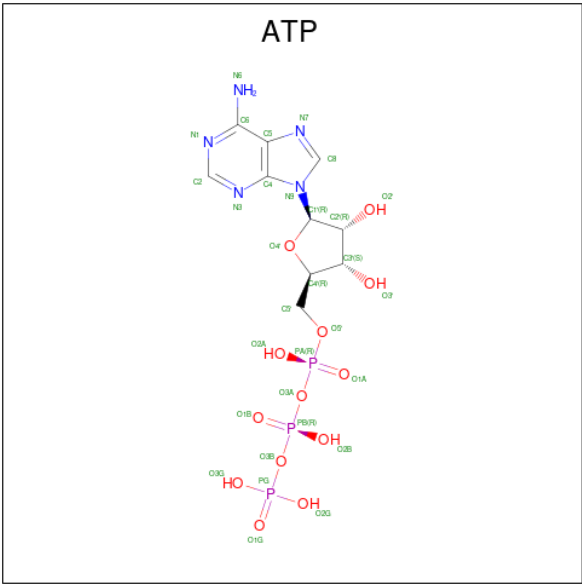
Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	L	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	Q	1	Total	C	N	O	S	0
			15	10	2	2	1	

- 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).

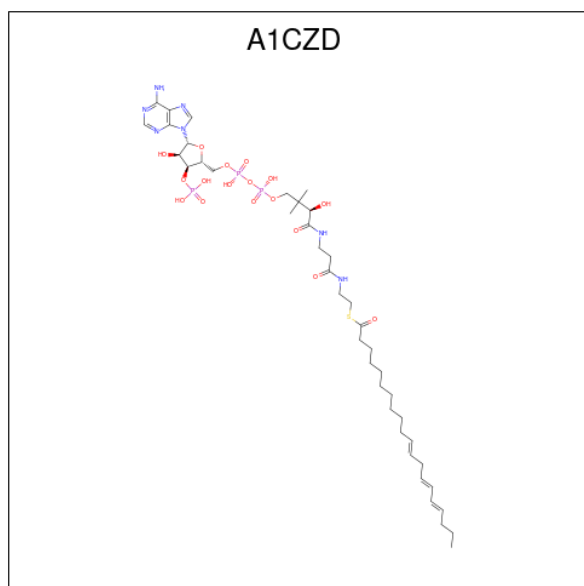
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	
8	Q	1	Total	Mg	0
			1	1	

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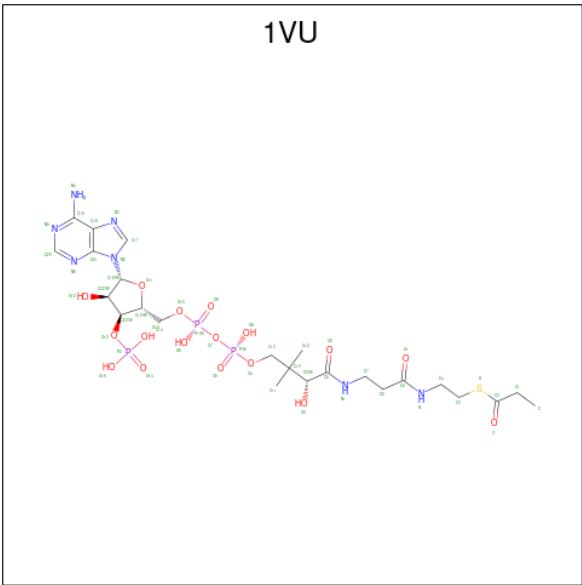
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	
8	T	1	Total	Mg	0
			1	1	
8	R	1	Total	Mg	0
			1	1	
8	S	1	Total	Mg	0
			1	1	

- 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).

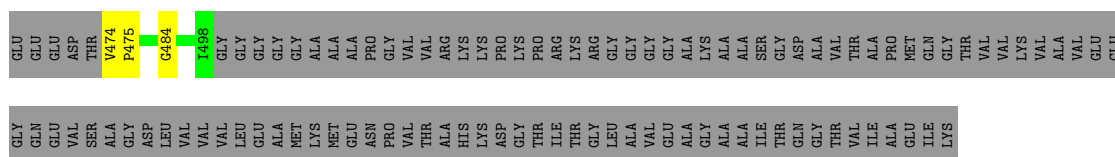


Mol	Chain	Residues	Atoms						AltConf
10	G	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	H	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	M	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	
10	N	1	Total	C	N	O	P	S	0
			52	24	7	17	3	1	

89%

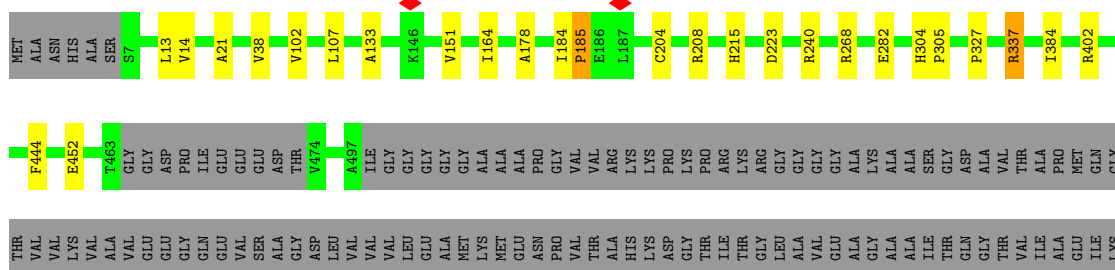
11%





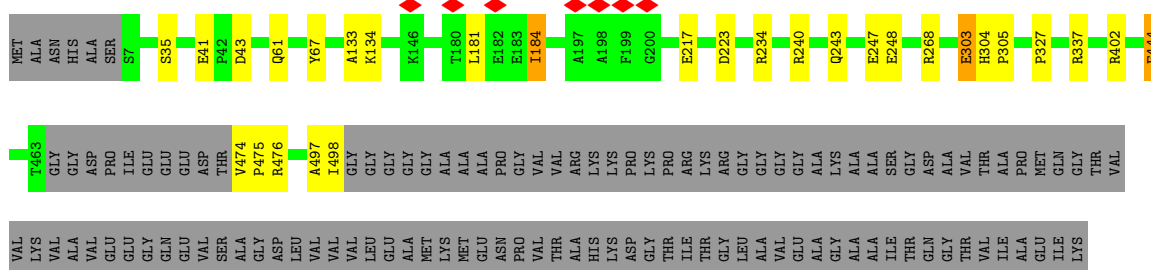
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain T: 76% 20%



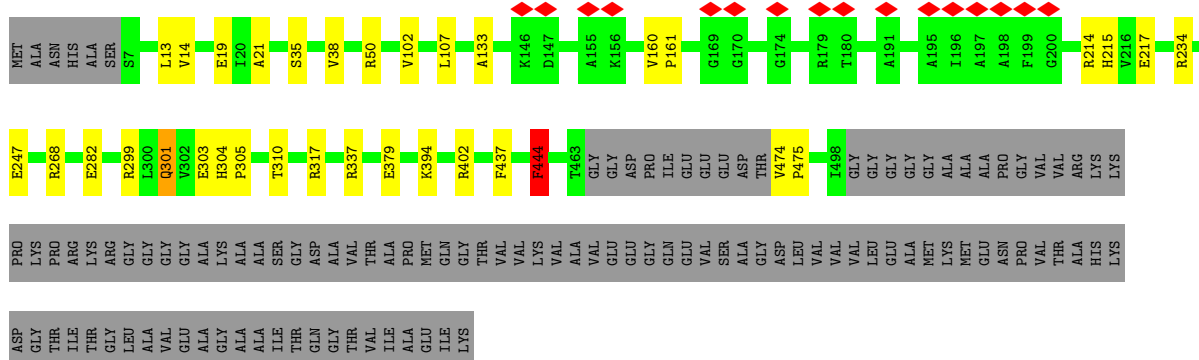
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain R: 76% 19%

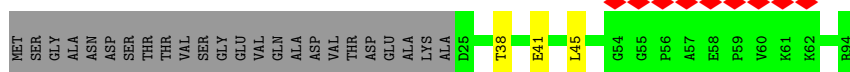


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

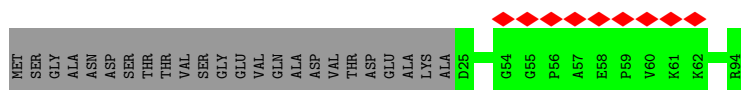
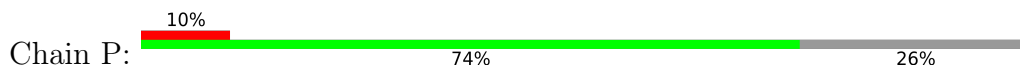
Chain S: 75% 5% 19%



- 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



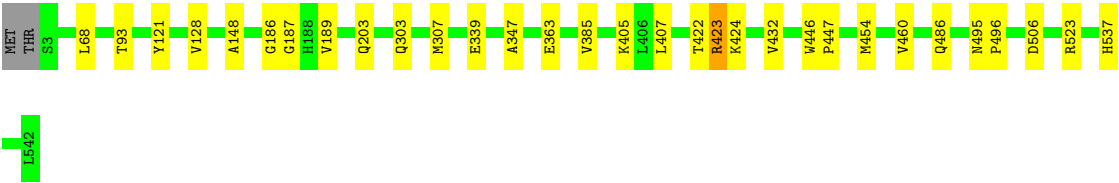
- Molecule 4: Propionyl-CoA carboxylase beta chain



- 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.

All (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
1	D	336	PRO	CB-CA-C	-5.54	104.31	111.46
1	B	439	GLY	CA-C-O	-5.05	118.19	122.29

There are no chirality outliers.

All (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	R	337	ARG	Sidechain
1	R	476	ARG	Sidechain
1	S	337	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:S:160:VAL:HG22	1:S:161:PRO:HA	1.73	0.71
1:D:247:GLU:HG2	1:D:303:GLU:HG2	1.74	0.70
4:M:148:ALA:H	10:M:601:1VU:H37	1.57	0.69
1:C:16:ASN:ND2	1:C:87:PRO:O	2.26	0.68
1:S:214:ARG:CD	1:S:444:PHE:HE2	2.07	0.68
1:D:127:ARG:NH2	1:D:141:THR:O	2.26	0.67
1:C:240:ARG:HG2	1:C:240:ARG:O	1.94	0.67
3:F:197:VAL:HG23	9:F:602:A1CZD:C35	2.24	0.66
9:F:601:A1CZD:C35	3:O:194:GLY:H	2.08	0.66
1:S:303:GLU:OE2	6:S:603:BCT:O3	2.14	0.66
1:S:214:ARG:HD2	1:S:444:PHE:CE2	2.31	0.65
10:H:601:1VU:H24	10:H:601:1VU:O9	1.97	0.64
4:H:97:THR:HG22	4:H:102:ASP:OD2	1.98	0.64
4:M:150:ILE:HD11	10:M:601:1VU:C4	2.28	0.64
1:R:248:GLU:OE2	1:R:402:ARG:NH1	2.26	0.64
1:B:241:ARG:NH2	1:B:348:GLU:OE2	2.33	0.62
3:F:430:VAL:HG21	3:O:136:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:184:ILE:N	1:T:185:PRO:HD2	2.15	0.61
1:D:303:GLU:HA	1:D:342:GLU:OE1	2.00	0.61
2:E:38:THR:HG22	2:E:41:GLU:CD	2.26	0.61
1:Q:240:ARG:NH2	1:Q:348:GLU:OE2	2.34	0.61
3:O:127:ASP:OD1	3:O:128:SER:N	2.33	0.60
1:Q:303:GLU:OE1	6:Q:602:BCT:O3	2.19	0.60
3:F:439:LEU:HD12	3:F:439:LEU:C	2.27	0.60
1:B:217:GLU:OE2	1:B:234:ARG:NH1	2.33	0.59
3:F:97:GLN:O	3:F:128:SER:OG	2.16	0.59
10:M:601:1VU:O1	10:M:601:1VU:N1	2.36	0.58
1:R:41:GLU:OE1	1:R:61:GLN:NE2	2.35	0.58
4:G:101:ARG:NH2	4:G:259:LEU:O	2.37	0.58
1:D:79:LYS:NZ	1:C:484:GLY:O	2.32	0.58
1:C:14:VAL:HG11	1:C:21:ALA:HA	1.84	0.58
1:S:214:ARG:HD2	1:S:444:PHE:HE2	1.67	0.58
10:H:601:1VU:H21	10:H:601:1VU:H28	1.84	0.58
1:A:578:THR:HG22	1:A:578:THR:O	2.02	0.57
1:T:133:ALA:O	1:T:268:ARG:NH1	2.37	0.57
1:D:59:GLY:O	1:D:72:LYS:NZ	2.36	0.57
4:M:101:ARG:NH2	4:M:259:LEU:O	2.38	0.57
1:Q:240:ARG:HH11	1:Q:240:ARG:HG2	1.70	0.57
1:C:20:ILE:O	1:C:21:ALA:HB3	2.05	0.56
1:Q:223:ASP:OD2	1:Q:327:PRO:HA	2.05	0.56
1:R:223:ASP:OD2	1:R:327:PRO:HA	2.06	0.56
1:A:181:LEU:HD22	1:A:181:LEU:H	1.71	0.56
4:N:363:GLU:OE2	4:N:405:LYS:NZ	2.30	0.56
1:T:337:ARG:NH2	1:S:310:THR:O	2.37	0.55
1:S:247:GLU:HG2	1:S:303:GLU:HG2	1.89	0.55
1:A:123:LYS:NZ	1:A:295:GLU:OE2	2.37	0.55
4:N:187:GLY:H	10:N:601:1VU:H36	1.72	0.55
1:D:133:ALA:O	1:D:268:ARG:NH1	2.38	0.55
4:G:307:MET:HG2	4:G:347:ALA:HB1	1.88	0.54
1:T:223:ASP:OD2	1:T:327:PRO:HA	2.08	0.54
3:F:135:ASP:OD2	3:F:138:THR:OG1	2.23	0.54
4:M:150:ILE:HD11	10:M:601:1VU:H32	1.89	0.54
1:R:217:GLU:OE2	1:R:234:ARG:NH1	2.40	0.54
1:R:247:GLU:CG	1:R:303:GLU:HG2	2.33	0.53
1:R:303:GLU:OE2	6:R:603:BCT:O3	2.25	0.53
1:C:50:ARG:NH2	1:C:379:GLU:OE2	2.38	0.53
1:C:223:ASP:OD2	1:C:327:PRO:HA	2.09	0.53
1:D:43:ASP:OD2	1:D:43:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:GLU:HB2	1:C:295:GLU:HG2	1.91	0.53
1:R:133:ALA:O	1:R:268:ARG:NH1	2.39	0.52
1:B:223:ASP:OD2	1:B:327:PRO:HA	2.09	0.52
4:M:346:VAL:HB	4:M:381:LEU:HD22	1.90	0.52
1:A:541:VAL:HG21	1:A:561:GLU:HB2	1.91	0.52
1:D:247:GLU:CG	1:D:303:GLU:HG2	2.40	0.52
1:A:76:ALA:HB2	4:H:5:THR:HG21	1.92	0.52
3:F:480:ASP:HB3	4:H:68:LEU:HD22	1.92	0.51
1:A:247:GLU:HG2	1:A:303:GLU:HG2	1.91	0.51
1:A:303:GLU:C	1:A:305:PRO:HD2	2.35	0.51
1:S:299:ARG:NH1	6:S:603:BCT:O2	2.39	0.51
10:G:601:1VU:H33	4:N:454:MET:HE1	1.92	0.51
4:N:460:VAL:HG21	4:N:486:GLN:HA	1.93	0.51
4:G:346:VAL:HB	4:G:381:LEU:HD22	1.93	0.51
1:J:532:VAL:O	1:J:594:ILE:N	2.39	0.51
4:H:285:THR:HG22	4:H:285:THR:O	2.11	0.50
1:D:233:THR:O	1:D:250:PRO:HA	2.12	0.50
1:S:234:ARG:NH1	1:S:301:GLN:OE1	2.38	0.50
1:S:215:HIS:NE2	1:S:282:GLU:OE1	2.40	0.50
1:Q:303:GLU:O	1:Q:306:VAL:HG22	2.12	0.50
1:T:102:VAL:HG13	1:T:107:LEU:HB2	1.94	0.50
1:B:133:ALA:O	1:B:268:ARG:NH1	2.42	0.50
1:S:474:VAL:N	1:S:475:PRO:CD	2.75	0.50
4:M:346:VAL:O	4:M:381:LEU:HA	2.12	0.49
3:O:340:ASP:OD2	3:O:379:ARG:NH1	2.37	0.49
1:D:303:GLU:CD	1:D:303:GLU:H	2.20	0.49
1:S:13:LEU:HD11	1:S:38:VAL:HG13	1.94	0.49
10:N:601:1VU:O2	10:N:601:1VU:H10	2.11	0.49
1:D:449:ARG:O	1:D:451:ILE:N	2.43	0.49
1:C:217:GLU:OE2	1:C:244:LYS:NZ	2.46	0.49
1:S:133:ALA:O	1:S:268:ARG:NH1	2.41	0.49
1:A:356:PRO:HD2	1:A:565:MET:HE2	1.95	0.48
3:O:387:ILE:HD11	3:O:411:GLY:HA2	1.95	0.48
1:D:65:GLU:O	1:D:72:LYS:NZ	2.33	0.48
1:R:43:ASP:OD2	1:R:67:TYR:OH	2.29	0.48
1:S:50:ARG:NH2	1:S:379:GLU:OE2	2.38	0.48
1:C:129:ILE:HG22	1:C:269:ILE:HD12	1.94	0.48
1:T:384:ILE:N	1:T:384:ILE:HD12	2.28	0.48
1:K:532:VAL:HG23	1:K:597:ILE:HD13	1.95	0.48
3:O:516:PRO:O	3:O:517:LEU:C	2.57	0.48
1:T:151:VAL:HG12	1:T:184:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:GLU:OE2	1:C:295:GLU:HG3	2.13	0.48
1:A:384:ILE:N	1:A:384:ILE:HD12	2.29	0.48
4:H:370:ARG:NH1	4:H:412:GLU:OE2	2.38	0.48
1:C:129:ILE:HG22	1:C:269:ILE:CD1	2.44	0.48
1:T:240:ARG:HG3	1:T:240:ARG:HH11	1.77	0.48
1:S:474:VAL:N	1:S:475:PRO:HD2	2.28	0.48
1:D:164:ILE:HD12	1:D:164:ILE:N	2.28	0.48
1:S:214:ARG:HD3	1:S:444:PHE:HE2	1.77	0.48
1:Q:299:ARG:NH1	6:Q:602:BCT:O2	2.36	0.48
4:N:307:MET:HG2	4:N:347:ALA:HB1	1.96	0.47
4:H:495:ASN:HB2	4:H:496:PRO:HD2	1.96	0.47
1:B:240:ARG:HH12	1:B:243:GLN:HB2	1.79	0.47
1:D:86:HIS:HD2	1:D:110:ILE:HG21	1.80	0.47
4:H:186:GLY:O	4:H:189:VAL:HG22	2.13	0.47
2:E:38:THR:HG22	2:E:41:GLU:OE1	2.15	0.47
4:N:339:GLU:OE1	4:N:523:ARG:NH1	2.41	0.47
1:D:17:ARG:NH1	1:D:43:ASP:OD1	2.46	0.47
1:C:145:VAL:CG2	1:C:206:VAL:HG23	2.45	0.47
1:C:266:ALA:HA	1:C:269:ILE:HG22	1.96	0.47
4:N:422:THR:HG22	4:N:446:TRP:CD2	2.49	0.47
1:D:13:LEU:HD11	1:D:38:VAL:HG13	1.97	0.47
4:N:148:ALA:H	10:N:601:1VU:H37	1.80	0.47
4:N:495:ASN:HB2	4:N:496:PRO:HD2	1.96	0.47
4:N:385:VAL:HG13	4:N:385:VAL:O	2.15	0.47
1:L:560:LEU:HD21	1:L:588:ILE:HD11	1.98	0.46
1:A:181:LEU:HD22	1:A:181:LEU:N	2.30	0.46
1:T:14:VAL:HG11	1:T:21:ALA:HA	1.97	0.46
1:D:140:GLY:HA2	1:D:207:GLU:HA	1.97	0.46
3:F:430:VAL:HG21	3:O:136:ALA:CB	2.44	0.46
4:H:307:MET:HG2	4:H:347:ALA:HB1	1.98	0.46
1:S:19:GLU:OE2	1:S:394:LYS:NZ	2.38	0.46
3:F:136:ALA:HB1	3:O:430:VAL:HG21	1.98	0.45
4:N:93:THR:HB	4:N:128:VAL:HG11	1.98	0.45
1:D:303:GLU:C	1:D:305:PRO:HD2	2.42	0.45
1:C:73:ILE:HG22	1:C:74:LEU:N	2.30	0.45
4:G:428:GLY:O	4:G:432:VAL:HG23	2.16	0.45
1:D:303:GLU:O	1:D:306:VAL:HG22	2.16	0.45
4:M:127:LYS:NZ	4:N:506:ASP:OD1	2.47	0.45
1:B:260:LYS:O	1:B:261:GLU:HB3	2.17	0.45
1:A:181:LEU:H	1:A:181:LEU:CD2	2.28	0.45
3:F:439:LEU:HD12	3:F:440:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ARG:NH1	3:F:283:ASP:OD2	2.48	0.45
9:F:602:A1CZD:C09	3:O:385:ASN:HA	2.46	0.45
3:O:439:LEU:C	3:O:439:LEU:HD23	2.41	0.45
1:C:73:ILE:HG22	1:C:74:LEU:H	1.82	0.45
4:G:495:ASN:HB2	4:G:496:PRO:HD2	1.98	0.45
1:D:89:TYR:CZ	1:D:302:VAL:HG22	2.52	0.45
1:T:151:VAL:CG1	1:T:184:ILE:HD12	2.47	0.45
1:Q:247:GLU:HG2	1:Q:303:GLU:HG2	1.99	0.45
1:T:240:ARG:O	1:T:452:GLU:HG3	2.17	0.45
3:F:197:VAL:HG11	9:F:602:A1CZD:O32	2.17	0.45
1:Q:578:THR:O	1:Q:578:THR:HG22	2.17	0.45
1:D:223:ASP:C	1:D:223:ASP:OD1	2.59	0.45
3:F:168:ALA:HA	3:F:191:PHE:O	2.17	0.44
4:N:68:LEU:HD22	3:O:480:ASP:HB3	1.99	0.44
1:D:407:GLU:OE1	1:C:317:ARG:NH1	2.43	0.44
1:Q:295:GLU:OE2	7:Q:603:ATP:O2A	2.36	0.44
4:N:407:LEU:HG	4:N:432:VAL:HG22	1.99	0.44
1:C:282:GLU:CD	1:C:295:GLU:HG3	2.43	0.44
1:S:402:ARG:NH2	1:S:437:PHE:O	2.41	0.44
4:M:339:GLU:OE1	4:M:523:ARG:NH1	2.49	0.44
1:D:300:LEU:HD11	1:D:316:VAL:HG22	2.00	0.44
1:S:102:VAL:HG13	1:S:107:LEU:HB2	2.00	0.44
1:A:481:VAL:HG11	2:E:45:LEU:HD13	2.00	0.44
1:S:217:GLU:OE2	1:S:234:ARG:NH1	2.51	0.44
4:M:307:MET:HG2	4:M:347:ALA:HB1	2.00	0.43
4:H:459:ALA:O	4:H:463:VAL:HG12	2.18	0.43
1:D:41:GLU:N	1:D:42:PRO:CD	2.80	0.43
1:R:240:ARG:HH12	1:R:243:GLN:HB2	1.83	0.43
4:M:495:ASN:HB2	4:M:496:PRO:HD2	2.00	0.43
3:O:190:MET:O	3:O:217:GLN:NE2	2.50	0.43
4:G:462:PHE:CZ	10:N:601:1VU:H29	2.54	0.43
4:H:395:GLU:HG3	4:M:228:LEU:HD11	2.00	0.43
3:O:280:MET:O	3:O:400:ARG:NH2	2.44	0.43
1:R:133:ALA:O	1:R:134:LYS:HB2	2.19	0.43
1:A:72:LYS:HE2	4:H:3:SER:OG	2.18	0.43
4:G:296:LEU:HD23	4:G:296:LEU:C	2.43	0.43
4:N:148:ALA:CB	10:N:601:1VU:H37	2.48	0.43
1:B:240:ARG:NH1	1:B:243:GLN:HB2	2.33	0.43
1:C:303:GLU:O	1:C:306:VAL:HG22	2.18	0.43
1:T:178:ALA:CB	1:T:184:ILE:HD13	2.49	0.43
1:D:240:ARG:NH1	1:D:348:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:HIS:NE2	1:C:282:GLU:OE1	2.38	0.43
1:T:208:ARG:HH11	1:T:208:ARG:HG3	1.83	0.43
1:T:304:HIS:N	1:T:305:PRO:CD	2.82	0.43
10:H:601:1VU:H29	10:H:601:1VU:H33	1.53	0.43
1:Q:193:ARG:O	1:Q:196:ILE:HG13	2.19	0.43
1:T:13:LEU:HD11	1:T:38:VAL:HG13	2.00	0.43
3:F:441:VAL:O	3:F:441:VAL:HG12	2.18	0.43
1:B:299:ARG:NH1	6:B:603:BCT:O3	2.48	0.43
1:T:164:ILE:HG22	1:T:204:CYS:SG	2.59	0.43
1:R:181:LEU:HA	1:R:184:ILE:HD13	2.01	0.43
1:A:122:ASP:OD1	1:A:122:ASP:C	2.61	0.42
7:C:601:ATP:O2A	7:C:601:ATP:H4'	2.18	0.42
1:S:160:VAL:CG2	1:S:161:PRO:HA	2.46	0.42
4:M:428:GLY:O	4:M:432:VAL:HG23	2.18	0.42
1:T:407:GLU:OE1	1:S:317:ARG:NH1	2.44	0.42
1:C:102:VAL:HG13	1:C:107:LEU:HB2	2.01	0.42
4:M:191:SER:HB3	4:M:192:PRO:HD3	2.01	0.42
1:D:240:ARG:O	1:D:241:ARG:C	2.61	0.42
1:D:330:ILE:O	1:D:332:GLU:N	2.47	0.42
1:C:304:HIS:N	1:C:305:PRO:CD	2.82	0.42
1:C:269:ILE:HG23	1:C:270:CYS:N	2.34	0.42
1:A:482:GLU:HA	1:A:486:ARG:O	2.20	0.42
1:A:578:THR:O	1:A:578:THR:CG2	2.67	0.42
10:M:601:1VU:H27	10:M:601:1VU:O3	2.19	0.42
1:S:214:ARG:HD2	1:S:444:PHE:CZ	2.55	0.42
1:C:266:ALA:O	1:C:269:ILE:HG22	2.20	0.42
1:C:444:PHE:CD1	1:C:444:PHE:C	2.97	0.42
1:R:444:PHE:C	1:R:444:PHE:CD1	2.97	0.42
9:F:601:A1CZD:O69	9:F:601:A1CZD:O41	2.38	0.42
10:H:601:1VU:H10	10:H:601:1VU:C14	2.50	0.42
1:A:444:PHE:CD1	1:A:444:PHE:C	2.97	0.42
1:B:299:ARG:NH2	6:B:603:BCT:O3	2.52	0.42
1:R:474:VAL:N	1:R:475:PRO:CD	2.83	0.42
4:G:191:SER:HB3	4:G:192:PRO:HD3	2.02	0.42
1:B:171:GLY:N	7:B:601:ATP:O1B	2.53	0.42
4:M:462:PHE:CE2	4:M:465:ARG:NH2	2.88	0.41
3:O:403:TYR:HA	3:O:429:ALA:O	2.20	0.41
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.89	0.41
10:N:601:1VU:H28	10:N:601:1VU:H24	1.89	0.41
1:C:304:HIS:CG	1:C:305:PRO:HD3	2.56	0.41
1:C:474:VAL:N	1:C:475:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:497:ALA:O	1:R:498:ILE:C	2.62	0.41
10:G:601:1VU:O2	10:G:601:1VU:H21	2.19	0.41
1:Q:304:HIS:CG	1:Q:305:PRO:HD3	2.55	0.41
3:F:500:ARG:HH11	3:F:500:ARG:HG3	1.86	0.41
9:F:602:A1CZD:C12	3:O:384:PHE:HB3	2.50	0.41
1:B:211:ASP:OD1	1:B:212:LYS:N	2.51	0.41
1:T:215:HIS:NE2	1:T:282:GLU:OE1	2.49	0.41
1:A:303:GLU:O	1:A:306:VAL:HG22	2.21	0.41
3:F:387:ILE:HD11	3:F:411:GLY:HA2	2.02	0.41
1:D:482:GLU:HA	1:D:486:ARG:O	2.21	0.41
1:Q:482:GLU:HA	1:Q:486:ARG:O	2.21	0.41
1:B:234:ARG:HD3	1:B:303:GLU:HB3	2.03	0.41
1:S:304:HIS:N	1:S:305:PRO:CD	2.84	0.41
4:N:186:GLY:O	4:N:189:VAL:HG22	2.21	0.40
1:C:432:VAL:O	1:C:432:VAL:HG12	2.21	0.40
1:A:486:ARG:HG2	1:B:56:PHE:CZ	2.57	0.40
4:H:462:PHE:CE2	10:M:601:1VU:H29	2.55	0.40
4:M:462:PHE:CD2	4:M:465:ARG:NH2	2.89	0.40
3:O:168:ALA:HA	3:O:191:PHE:O	2.20	0.40
1:A:70:PHE:N	1:A:70:PHE:CD1	2.90	0.40
10:H:601:1VU:O1	10:H:601:1VU:N1	2.53	0.40
4:M:25:LEU:HD22	4:N:447:PRO:HG3	2.03	0.40
3:F:91:HIS:CE1	3:F:129:ALA:HB2	2.56	0.40
4:H:191:SER:HB3	4:H:192:PRO:HD3	2.03	0.40
4:H:318:ASP:OD1	4:H:318:ASP:N	2.55	0.40
1:D:171:GLY:N	7:D:601:ATP:O1B	2.54	0.40
1:C:304:HIS:HB2	1:C:315:LEU:HD12	2.03	0.40
1:A:304:HIS:N	1:A:305:PRO:HD2	2.37	0.40
3:F:430:VAL:HG21	3:O:136:ALA:C	2.46	0.40
4:G:374:CYS:SG	4:N:537:HIS:CE1	3.15	0.40
3:O:28:ALA:HB1	3:O:94:THR:HB	2.02	0.40
1:D:50:ARG:NH2	1:D:379:GLU:OE2	2.40	0.40
1:D:335:THR:HA	1:D:336:PRO:HD2	1.90	0.40
1:R:304:HIS:CG	1:R:305:PRO:HD3	2.56	0.40
1:S:14:VAL:HG11	1:S:21:ALA:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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

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Mol	Chain	Res	Type
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
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

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	444	PHE
3	F	161	SER
4	H	22	LEU
4	H	318	ASP
1	I	536	MET
1	L	561	GLU
4	M	462	PHE
4	N	121	TYR
4	N	203	GLN
4	N	303	GLN
4	N	423	ARG
1	Q	138	VAL
1	Q	384	ILE
1	Q	444	PHE
1	B	421	LEU
1	B	444	PHE
1	B	457	ASN
1	D	35	SER
1	D	43	ASP
1	D	245	LEU
1	D	303	GLU
1	D	444	PHE
1	C	35	SER
1	C	206	VAL
1	C	240	ARG
1	C	295	GLU
1	C	307	THR
1	C	355	LEU
1	C	421	LEU
1	C	444	PHE
1	C	457	ASN
1	T	444	PHE
1	R	35	SER
1	R	184	ILE
1	R	303	GLU
1	R	444	PHE
1	S	35	SER
1	S	301	GLN
1	S	444	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
2	E	82	GLN
4	G	84	ASN
4	G	203	GLN
4	H	167	ASN
4	H	376	ASN
4	H	397	ASN
4	H	450	GLN
1	I	567	ASN
4	N	167	ASN
4	N	376	ASN
3	O	385	ASN
2	P	82	GLN
1	Q	243	GLN
1	Q	537	GLN
1	B	100	GLN
1	D	243	GLN
1	T	48	HIS
1	T	456	ASN
1	R	48	HIS
1	R	243	GLN
1	S	48	HIS

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%)
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
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

All (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
5	A	601	BTN	C6-S1	-13.25	1.44	1.81
5	L	601	BTN	C6-S1	-13.17	1.44	1.81
9	F	602	A1CZD	P65-O64	12.93	1.82	1.59
5	J	601	BTN	C3-N1	12.59	1.58	1.35
5	I	601	BTN	C3-N1	12.52	1.58	1.35
5	K	601	BTN	C3-N1	12.46	1.58	1.35
5	L	601	BTN	C3-N1	12.38	1.58	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	BTN	C3-N1	12.24	1.57	1.35
5	Q	601	BTN	C3-N1	12.19	1.57	1.35
5	L	601	BTN	C5-N1	-9.25	1.32	1.46
5	J	601	BTN	C5-N1	-9.08	1.32	1.46
5	I	601	BTN	C5-N1	-9.01	1.32	1.46
5	A	601	BTN	C5-N1	-8.99	1.32	1.46
5	K	601	BTN	C5-N1	-8.94	1.32	1.46
5	Q	601	BTN	C5-N1	-8.76	1.33	1.46
5	A	601	BTN	C3-N2	8.59	1.51	1.35
5	Q	601	BTN	C3-N2	8.43	1.50	1.35
5	J	601	BTN	C3-N2	8.41	1.50	1.35
5	L	601	BTN	C3-N2	8.34	1.50	1.35
5	I	601	BTN	C3-N2	8.28	1.50	1.35
5	K	601	BTN	C3-N2	8.25	1.50	1.35
5	A	601	BTN	C2-S1	-7.67	1.70	1.82
5	Q	601	BTN	C2-S1	-7.60	1.70	1.82
5	I	601	BTN	C2-S1	-7.54	1.70	1.82
5	J	601	BTN	C2-S1	-7.52	1.70	1.82
5	L	601	BTN	C2-S1	-7.16	1.71	1.82
5	K	601	BTN	C2-S1	-6.98	1.71	1.82
9	F	601	A1CZD	P39-O38	6.42	1.84	1.59
9	F	602	A1CZD	P39-O38	6.04	1.83	1.59
9	F	601	A1CZD	C05-C04	5.82	1.53	1.33
9	F	602	A1CZD	C05-C04	5.78	1.52	1.33
9	F	601	A1CZD	C06-C07	5.67	1.52	1.33
9	F	602	A1CZD	C06-C07	5.54	1.52	1.33
9	F	602	A1CZD	P43-O42	5.50	1.65	1.59
5	L	601	BTN	C6-C5	5.44	1.64	1.53
5	A	601	BTN	C6-C5	5.36	1.64	1.53
5	J	601	BTN	C6-C5	5.35	1.64	1.53
5	Q	601	BTN	C6-C5	5.34	1.64	1.53
9	F	601	A1CZD	C37-C34	5.32	1.61	1.52
5	K	601	BTN	C6-C5	5.31	1.64	1.53
5	I	601	BTN	C6-C5	5.05	1.63	1.53
9	F	601	A1CZD	C26-N25	4.68	1.44	1.33
5	K	601	BTN	C7-C2	4.62	1.64	1.52
5	Q	601	BTN	C7-C2	4.42	1.64	1.52
5	L	601	BTN	C7-C2	4.36	1.64	1.52
5	A	601	BTN	C7-C2	4.34	1.64	1.52
9	F	601	A1CZD	C31-N30	4.22	1.43	1.33
5	I	601	BTN	C4-N2	-4.21	1.38	1.45
9	F	602	A1CZD	C26-N25	4.18	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	BTN	C7-C2	4.15	1.63	1.52
5	Q	601	BTN	C4-N2	-4.10	1.38	1.45
5	J	601	BTN	C4-N2	-4.09	1.38	1.45
9	F	602	A1CZD	C37-C34	4.08	1.59	1.52
5	L	601	BTN	C4-N2	-4.01	1.38	1.45
5	A	601	BTN	C4-N2	-4.00	1.38	1.45
5	J	601	BTN	C7-C2	3.97	1.63	1.52
5	K	601	BTN	C4-N2	-3.95	1.38	1.45
5	L	601	BTN	C2-C4	-3.92	1.43	1.53
5	J	601	BTN	C2-C4	-3.90	1.43	1.53
9	F	602	A1CZD	C31-N30	3.83	1.42	1.33
5	A	601	BTN	C2-C4	-3.74	1.43	1.53
5	I	601	BTN	C2-C4	-3.70	1.43	1.53
9	F	601	A1CZD	P43-O46	3.70	1.73	1.59
5	Q	601	BTN	C2-C4	-3.70	1.43	1.53
9	F	601	A1CZD	C51-N53	3.70	1.56	1.46
9	F	601	A1CZD	C09-C10	3.66	1.52	1.31
9	F	601	A1CZD	C56-C61	3.55	1.45	1.39
5	K	601	BTN	C5-C4	3.55	1.65	1.55
5	K	601	BTN	C2-C4	-3.51	1.44	1.53
5	J	601	BTN	C5-C4	3.49	1.65	1.55
9	F	602	A1CZD	P43-O46	3.49	1.73	1.59
5	I	601	BTN	C5-C4	3.43	1.65	1.55
9	F	602	A1CZD	C56-C61	3.40	1.45	1.39
5	L	601	BTN	C5-C4	3.39	1.65	1.55
9	F	601	A1CZD	C20-S22	3.39	1.84	1.76
9	F	602	A1CZD	C09-C10	3.38	1.50	1.31
5	A	601	BTN	C5-C4	3.37	1.65	1.55
5	Q	601	BTN	C5-C4	3.35	1.65	1.55
9	F	602	A1CZD	P39-O42	3.10	1.62	1.59
9	F	602	A1CZD	C51-N53	2.95	1.54	1.46
9	F	602	A1CZD	O64-C49	-2.88	1.34	1.44
7	S	601	ATP	PA-O3A	-2.88	1.56	1.59
9	F	601	A1CZD	C50-C49	2.84	1.59	1.53
9	F	601	A1CZD	O64-C49	-2.80	1.34	1.44
9	F	601	A1CZD	C59-N58	2.75	1.38	1.33
9	F	601	A1CZD	C06-C05	2.75	1.52	1.44
9	F	601	A1CZD	P43-O42	2.69	1.62	1.59
7	Q	603	ATP	PB-O3B	-2.65	1.56	1.59
9	F	601	A1CZD	O38-C37	-2.64	1.35	1.43
9	F	602	A1CZD	C59-N58	2.59	1.38	1.33
9	F	601	A1CZD	C54-N53	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	602	A1CZD	O38-C37	-2.56	1.35	1.43
9	F	601	A1CZD	C57-N62	2.55	1.40	1.34
9	F	602	A1CZD	C54-N55	2.49	1.36	1.31
9	F	602	A1CZD	C54-N53	2.47	1.41	1.37
5	L	601	BTN	O3-C3	-2.41	1.18	1.23
5	K	601	BTN	O3-C3	-2.40	1.18	1.23
5	Q	601	BTN	O3-C3	-2.40	1.18	1.23
7	S	601	ATP	PB-O3B	-2.40	1.56	1.59
9	F	602	A1CZD	C06-C05	2.31	1.51	1.44
5	J	601	BTN	O3-C3	-2.31	1.18	1.23
9	F	602	A1CZD	C57-N62	2.30	1.40	1.34
5	A	601	BTN	O3-C3	-2.30	1.18	1.23
5	I	601	BTN	O3-C3	-2.20	1.18	1.23
9	F	601	A1CZD	C54-N55	2.19	1.35	1.31
9	F	602	A1CZD	C61-N60	2.06	1.38	1.34
9	F	601	A1CZD	O63-C50	-2.00	1.38	1.43
7	D	601	ATP	PB-O3B	-2.00	1.57	1.59

All (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
9	F	601	A1CZD	C19-C20-S22	6.02	120.58	113.40
5	J	601	BTN	C6-S1-C2	5.94	102.33	89.98
5	L	601	BTN	C4-C5-N1	5.78	108.85	102.43
5	A	601	BTN	C4-C5-N1	5.77	108.84	102.43
5	L	601	BTN	C6-S1-C2	5.70	101.83	89.98
6	B	603	BCT	O2-C-O1	5.69	134.22	119.68
6	C	603	BCT	O2-C-O1	5.66	134.15	119.68
5	Q	601	BTN	C4-C5-N1	5.61	108.66	102.43
5	K	601	BTN	C4-C5-N1	5.52	108.56	102.43
6	S	603	BCT	O2-C-O1	5.48	133.70	119.68
5	J	601	BTN	C4-C5-N1	5.43	108.46	102.43
5	I	601	BTN	C4-C5-N1	5.43	108.46	102.43
6	T	602	BCT	O2-C-O1	5.39	133.45	119.68
6	R	603	BCT	O2-C-O1	5.34	133.33	119.68
6	A	602	BCT	O2-C-O1	5.27	133.14	119.68
6	Q	602	BCT	O2-C-O1	5.22	133.04	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	601	BTN	C8-C7-C2	-5.13	102.25	114.04
10	H	601	1VU	P2-O13-C23	-4.93	110.27	123.43
5	J	601	BTN	C5-C4-N2	4.60	107.88	102.68
6	D	603	BCT	O2-C-O1	4.48	131.15	119.68
5	I	601	BTN	C5-C4-N2	4.39	107.63	102.68
10	N	601	1VU	P2-O13-C23	-4.38	111.73	123.43
9	F	601	A1CZD	O32-C31-N30	-4.29	113.91	122.98
10	M	601	1VU	P2-O13-C23	-4.28	112.00	123.43
5	L	601	BTN	C5-C4-N2	4.17	107.39	102.68
5	L	601	BTN	C6-C5-N1	-4.12	107.87	113.18
5	Q	601	BTN	C5-C4-N2	4.09	107.30	102.68
5	A	601	BTN	C5-C4-N2	4.09	107.30	102.68
5	K	601	BTN	C5-C4-N2	4.09	107.30	102.68
10	G	601	1VU	P2-O13-C23	-4.09	112.50	123.43
9	F	601	A1CZD	C23-S22-C20	3.99	113.63	101.84
5	J	601	BTN	C4-N2-C3	-3.86	107.77	112.56
5	L	601	BTN	C2-C4-C5	-3.83	104.20	108.89
5	A	601	BTN	C8-C7-C2	-3.78	105.35	114.04
9	F	602	A1CZD	O21-C20-C19	-3.77	119.64	123.98
9	F	602	A1CZD	C23-S22-C20	3.74	112.90	101.84
5	L	601	BTN	C4-N2-C3	-3.67	108.00	112.56
9	F	601	A1CZD	C28-C26-N25	3.64	122.98	116.34
5	J	601	BTN	C2-C4-C5	-3.64	104.44	108.89
9	F	602	A1CZD	C28-C26-N25	3.63	122.96	116.34
5	I	601	BTN	C4-N2-C3	-3.51	108.20	112.56
5	A	601	BTN	C4-N2-C3	-3.50	108.21	112.56
5	A	601	BTN	C2-C4-C5	-3.48	104.63	108.89
9	F	602	A1CZD	O32-C31-N30	-3.48	115.62	122.98
5	Q	601	BTN	C8-C7-C2	-3.43	106.15	114.04
5	K	601	BTN	C4-N2-C3	-3.38	108.36	112.56
5	A	601	BTN	C6-C5-N1	-3.36	108.85	113.18
9	F	602	A1CZD	O64-P65-O67	-3.36	97.37	109.33
5	Q	601	BTN	C4-N2-C3	-3.34	108.42	112.56
9	F	601	A1CZD	O21-C20-C19	-3.31	120.17	123.98
9	F	601	A1CZD	C56-C61-N60	-3.24	122.26	126.72
5	L	601	BTN	C5-N1-C3	-3.23	107.64	112.38
9	F	602	A1CZD	C56-C61-N60	-3.17	122.35	126.72
5	J	601	BTN	C5-N1-C3	-3.16	107.74	112.38
9	F	602	A1CZD	C50-C49-C48	-3.11	97.79	103.24
5	I	601	BTN	C5-N1-C3	-3.10	107.82	112.38
9	F	601	A1CZD	C33-C31-N30	3.10	122.37	116.48
5	A	601	BTN	C5-N1-C3	-3.10	107.82	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	601	A1CZD	O64-P65-O67	-3.09	98.31	109.33
5	Q	601	BTN	C5-N1-C3	-3.08	107.86	112.38
5	K	601	BTN	C5-N1-C3	-3.06	107.88	112.38
5	K	601	BTN	C2-C4-C5	-3.04	105.18	108.89
5	Q	601	BTN	C2-C4-C5	-2.86	105.39	108.89
9	F	602	A1CZD	O21-C20-S22	-2.85	119.05	122.68
9	F	602	A1CZD	O38-P39-O41	-2.79	97.89	108.94
5	I	601	BTN	C4-C2-S1	2.72	108.12	105.03
9	F	601	A1CZD	O21-C20-S22	-2.70	119.25	122.68
5	I	601	BTN	C7-C2-S1	-2.65	105.15	112.78
9	F	601	A1CZD	C50-C49-C48	-2.59	98.70	103.24
5	L	601	BTN	C2-C4-N2	2.58	116.07	113.34
6	A	602	BCT	O3-C-O1	-2.54	113.19	119.68
9	F	601	A1CZD	O27-C26-N25	-2.52	118.09	123.03
5	L	601	BTN	C6-C5-C4	-2.51	105.09	109.06
9	F	602	A1CZD	O27-C26-N25	-2.46	118.20	123.03
5	J	601	BTN	C6-C5-C4	-2.44	105.21	109.06
5	Q	601	BTN	C6-C5-N1	-2.43	110.05	113.18
5	A	601	BTN	C6-C5-C4	-2.41	105.25	109.06
6	R	603	BCT	O3-C-O1	-2.39	113.57	119.68
5	K	601	BTN	C2-C4-N2	2.37	115.85	113.34
6	T	602	BCT	O3-C-O1	-2.34	113.69	119.68
5	I	601	BTN	C2-C4-C5	-2.34	106.03	108.89
9	F	601	A1CZD	O38-P39-O41	-2.31	99.79	108.94
7	B	601	ATP	O2'-C2'-C3'	-2.27	104.53	111.82
6	S	603	BCT	O3-C-O1	-2.26	113.88	119.68
10	H	601	1VU	O4-C13-C10	-2.26	106.91	110.55
7	Q	603	ATP	O3'-C3'-C2'	-2.24	104.64	111.82
6	Q	602	BCT	O3-C-O1	-2.20	114.05	119.68
5	Q	601	BTN	C6-C5-C4	-2.20	105.58	109.06
5	K	601	BTN	C6-C5-C4	-2.15	105.66	109.06
10	H	601	1VU	C7-C6-C5	-2.15	108.81	112.39
7	T	601	ATP	O2'-C2'-C1'	-2.14	102.72	110.10
9	F	601	A1CZD	O40-P39-O41	2.14	122.40	112.44
5	J	601	BTN	C6-C5-N1	-2.13	110.43	113.18
6	B	603	BCT	O3-C-O1	-2.13	114.24	119.68
7	R	601	ATP	O3'-C3'-C2'	-2.12	105.03	111.82
9	F	601	A1CZD	C49-C50-C51	2.11	104.53	99.89
9	F	602	A1CZD	C56-C61-N53	2.10	108.10	105.81
7	R	601	ATP	O2'-C2'-C3'	-2.09	105.13	111.82
9	F	602	A1CZD	C03-C04-C05	-2.08	115.45	125.66
7	C	601	ATP	O2'-C2'-C1'	-2.08	102.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	603	BCT	O3-C-O1	-2.07	114.37	119.68
7	D	601	ATP	O4'-C4'-C3'	-2.07	101.05	105.15
7	A	603	ATP	O4'-C4'-C3'	-2.07	101.05	105.15
7	D	601	ATP	O2'-C2'-C3'	-2.04	105.29	111.82
5	J	601	BTN	C2-C4-N2	2.02	115.48	113.34
9	F	601	A1CZD	O40-P39-O42	2.02	112.72	107.27
10	M	601	1VU	O4-C13-C10	-2.01	107.31	110.55
7	S	601	ATP	O3'-C3'-C2'	-2.01	105.38	111.82
7	S	601	ATP	O2'-C2'-C3'	-2.01	105.39	111.82
9	F	601	A1CZD	C03-C04-C05	-2.01	115.80	125.66

There are no chirality outliers.

All (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
5	L	601	BTN	S1-C2-C7-C8
5	L	601	BTN	C4-C2-C7-C8
7	A	603	ATP	PB-O3B-PG-O3G
7	A	603	ATP	O4'-C4'-C5'-O5'
7	D	601	ATP	PB-O3B-PG-O2G
7	C	601	ATP	C4'-C5'-O5'-PA
7	C	601	ATP	O4'-C1'-N9-C8
7	C	601	ATP	O4'-C1'-N9-C4
7	T	601	ATP	C5'-O5'-PA-O3A
7	R	601	ATP	PB-O3B-PG-O3G
9	F	601	A1CZD	C17-C18-C19-C20
9	F	601	A1CZD	C24-C23-S22-C20
9	F	601	A1CZD	C01-C02-C03-C04
9	F	601	A1CZD	C06-C07-C08-C09
9	F	601	A1CZD	C23-C24-N25-C26
9	F	601	A1CZD	N30-C31-C33-C34
9	F	601	A1CZD	N30-C31-C33-O69
9	F	601	A1CZD	O32-C31-C33-C34
9	F	601	A1CZD	O32-C31-C33-O69
9	F	601	A1CZD	C31-C33-C34-C35
9	F	601	A1CZD	C31-C33-C34-C36
9	F	601	A1CZD	C31-C33-C34-C37

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Mol	Chain	Res	Type	Atoms
9	F	601	A1CZD	O69-C33-C34-C35
9	F	601	A1CZD	O69-C33-C34-C36
9	F	601	A1CZD	O69-C33-C34-C37
9	F	601	A1CZD	C33-C34-C37-O38
9	F	601	A1CZD	C35-C34-C37-O38
9	F	601	A1CZD	C36-C34-C37-O38
9	F	601	A1CZD	C34-C37-O38-P39
9	F	601	A1CZD	C37-O38-P39-O40
9	F	601	A1CZD	C37-O38-P39-O42
9	F	602	A1CZD	C17-C18-C19-C20
9	F	602	A1CZD	S22-C23-C24-N25
9	F	602	A1CZD	C23-C24-N25-C26
9	F	602	A1CZD	C33-C31-N30-C29
9	F	602	A1CZD	C31-C33-C34-C36
9	F	602	A1CZD	C31-C33-C34-C37
9	F	602	A1CZD	C48-C47-O46-P43
9	F	602	A1CZD	C37-O38-P39-O40
9	F	602	A1CZD	C37-O38-P39-O42
9	F	602	A1CZD	P43-O42-P39-O38
10	G	601	1VU	C13-O4-P-O5
10	H	601	1VU	C14-O10-P1-O8
10	H	601	1VU	C14-O10-P1-O9
10	H	601	1VU	C14-O10-P1-O7
10	H	601	1VU	O2-C8-C9-C10
10	H	601	1VU	N1-C8-C9-C10
10	H	601	1VU	N1-C8-C9-O3
10	H	601	1VU	C9-C8-N1-C7
10	H	601	1VU	C4-C3-S-C2
10	H	601	1VU	O-C2-S-C3
10	H	601	1VU	C1-C2-S-C3
10	M	601	1VU	C9-C8-N1-C7
10	M	601	1VU	O2-C8-N1-C7
10	M	601	1VU	C5-C6-C7-N1
10	M	601	1VU	C6-C5-N-C4
10	M	601	1VU	O1-C5-N-C4
10	N	601	1VU	C9-C8-N1-C7
10	N	601	1VU	O-C2-S-C3
10	N	601	1VU	C1-C2-S-C3
10	N	601	1VU	C-C1-C2-O
10	H	601	1VU	O2-C8-N1-C7
10	N	601	1VU	O2-C8-N1-C7
10	H	601	1VU	C6-C5-N-C4

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Mol	Chain	Res	Type	Atoms
9	F	602	A1CZD	C08-C09-C10-C11
9	F	602	A1CZD	O32-C31-N30-C29
7	B	601	ATP	C3'-C4'-C5'-O5'
10	H	601	1VU	O1-C5-N-C4
9	F	601	A1CZD	C48-C47-O46-P43
10	G	601	1VU	C6-C5-N-C4
7	B	601	ATP	O4'-C4'-C5'-O5'
7	S	601	ATP	C3'-C4'-C5'-O5'
10	G	601	1VU	O1-C5-N-C4
7	Q	603	ATP	O4'-C4'-C5'-O5'
7	T	601	ATP	C4'-C5'-O5'-PA
9	F	602	A1CZD	C03-C04-C05-C06
9	F	602	A1CZD	C05-C06-C07-C08
5	A	601	BTN	C7-C8-C9-C10
9	F	601	A1CZD	C14-C15-C16-C17
10	M	601	1VU	S-C3-C4-N
10	N	601	1VU	S-C3-C4-N
5	Q	601	BTN	C7-C8-C9-C10
9	F	601	A1CZD	C16-C17-C18-C19
7	A	603	ATP	C3'-C4'-C5'-O5'
7	T	601	ATP	O4'-C4'-C5'-O5'
7	T	601	ATP	C3'-C4'-C5'-O5'
7	R	601	ATP	O4'-C4'-C5'-O5'
9	F	601	A1CZD	C15-C16-C17-C18
9	F	602	A1CZD	C14-C15-C16-C17
9	F	602	A1CZD	C15-C16-C17-C18
7	S	601	ATP	O4'-C4'-C5'-O5'
9	F	602	A1CZD	O32-C31-C33-O69
10	H	601	1VU	O2-C8-C9-O3
10	N	601	1VU	O2-C8-C9-O3
9	F	601	A1CZD	O27-C26-C28-C29
9	F	602	A1CZD	C10-C11-C12-C13
9	F	602	A1CZD	C16-C17-C18-C19
10	H	601	1VU	O10-C14-C15-C23
10	G	601	1VU	C9-C8-N1-C7
9	F	602	A1CZD	O69-C33-C34-C35
9	F	602	A1CZD	O69-C33-C34-C36
10	H	601	1VU	S-C3-C4-N
9	F	602	A1CZD	C13-C14-C15-C16
10	G	601	1VU	O2-C8-N1-C7
10	G	601	1VU	O1-C5-C6-C7
9	F	601	A1CZD	C07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
9	F	601	A1CZD	N25-C26-C28-C29
5	A	601	BTN	S1-C2-C7-C8
7	T	601	ATP	PB-O3A-PA-O5'
5	A	601	BTN	C4-C2-C7-C8
5	Q	601	BTN	C4-C2-C7-C8
9	F	601	A1CZD	C48-C49-O64-P65
5	J	601	BTN	C11-C10-C9-C8
9	F	601	A1CZD	S22-C23-C24-N25
10	G	601	1VU	C11-C10-C13-O4
9	F	602	A1CZD	C24-C23-S22-C20
10	G	601	1VU	C4-C3-S-C2
7	Q	603	ATP	C5'-O5'-PA-O1A
7	C	601	ATP	C5'-O5'-PA-O1A
7	T	601	ATP	C5'-O5'-PA-O1A
9	F	602	A1CZD	O69-C33-C34-C37
10	H	601	1VU	C13-O4-P-O7
10	H	601	1VU	C13-O4-P-O6
10	H	601	1VU	O10-C14-C15-O11
7	A	603	ATP	PB-O3A-PA-O2A
7	B	601	ATP	PA-O3A-PB-O2B
9	F	602	A1CZD	C04-C05-C06-C07
10	N	601	1VU	N1-C8-C9-C10
9	F	601	A1CZD	C13-C14-C15-C16
9	F	601	A1CZD	C50-C49-O64-P65
10	G	601	1VU	C3-C4-N-C5
10	N	601	1VU	N1-C8-C9-O3
9	F	601	A1CZD	O46-C47-C48-O52
10	G	601	1VU	N-C5-C6-C7
9	F	602	A1CZD	C49-O64-P65-O67
7	A	603	ATP	PB-O3A-PA-O1A
5	Q	601	BTN	S1-C2-C7-C8
9	F	601	A1CZD	C09-C10-C11-C12
7	D	601	ATP	PB-O3B-PG-O1G
7	A	603	ATP	PB-O3B-PG-O2G
7	Q	603	ATP	PB-O3B-PG-O2G
7	D	601	ATP	PB-O3B-PG-O3G
7	R	601	ATP	PB-O3B-PG-O2G
9	F	602	A1CZD	C02-C03-C04-C05
9	F	602	A1CZD	C31-C33-C34-C35
10	H	601	1VU	C12-C10-C9-C8
9	F	601	A1CZD	P43-O42-P39-O41
9	F	602	A1CZD	P43-O42-P39-O40

Continued on next page...

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Mol	Chain	Res	Type	Atoms
9	F	602	A1CZD	C34-C37-O38-P39
10	G	601	1VU	C12-C10-C13-O4
10	H	601	1VU	C11-C10-C13-O4
10	H	601	1VU	C12-C10-C13-O4
10	H	601	1VU	C13-C10-C9-C8
7	D	601	ATP	O4'-C4'-C5'-O5'
9	F	602	A1CZD	N30-C31-C33-O69
7	Q	603	ATP	PG-O3B-PB-O2B

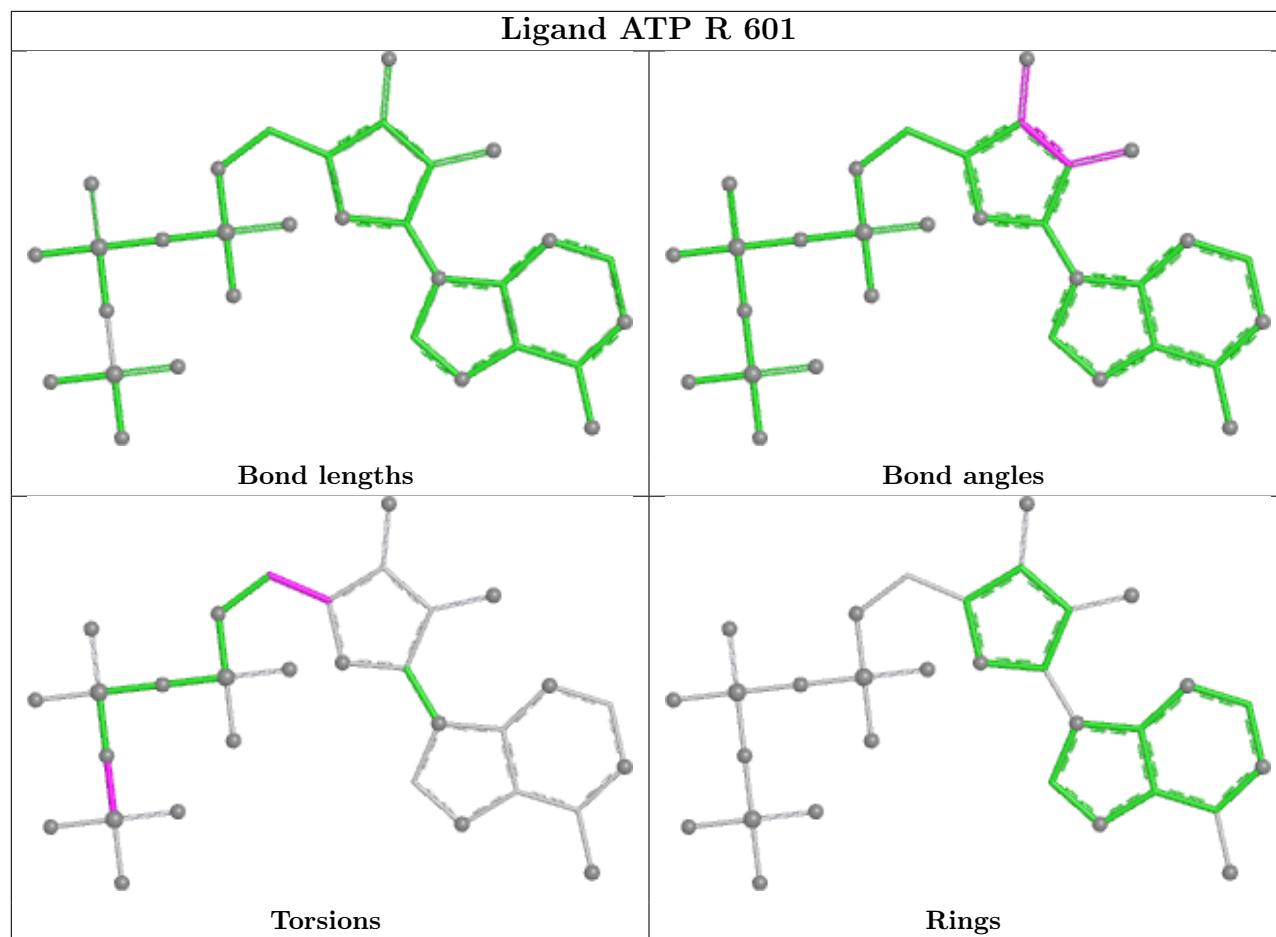
There are no ring outliers.

14 monomers are involved in 40 short contacts:

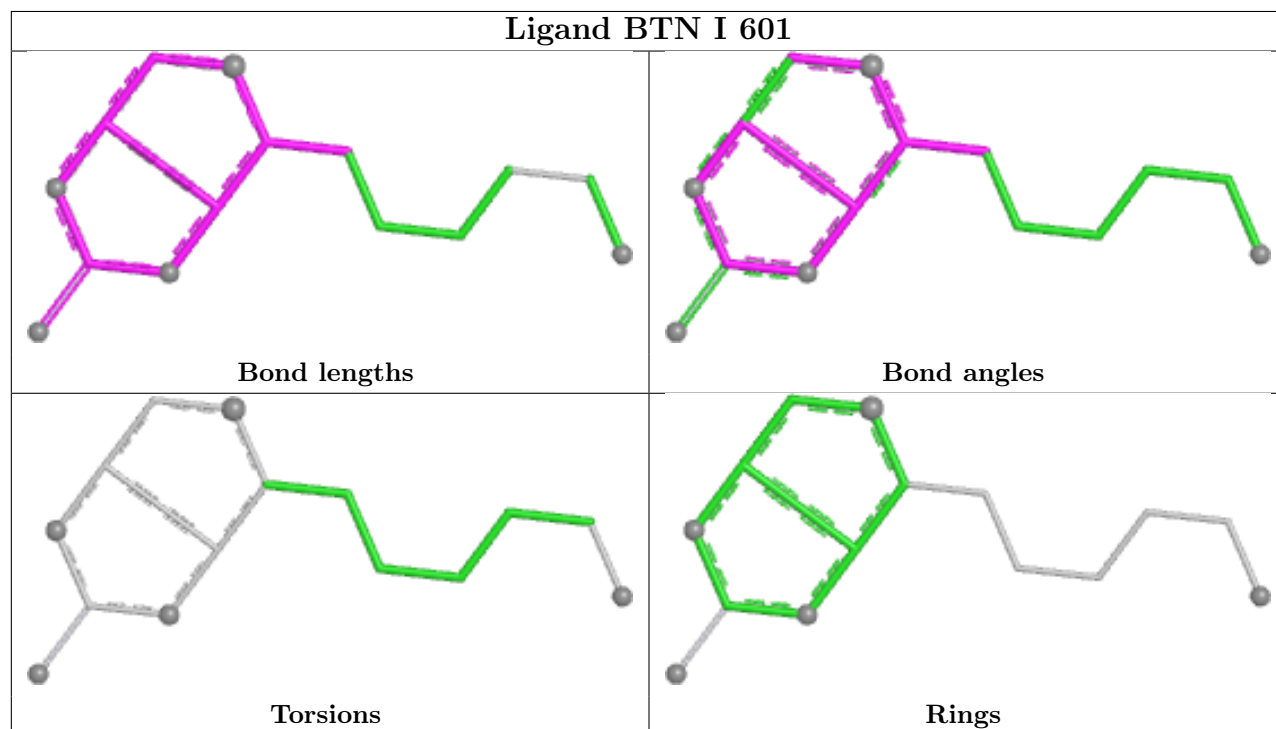
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	ATP	1	0
7	Q	603	ATP	1	0
6	Q	602	BCT	2	0
10	H	601	1VU	6	0
6	B	603	BCT	2	0
7	C	601	ATP	1	0
9	F	602	A1CZD	6	0
6	S	603	BCT	2	0
10	N	601	1VU	7	0
7	B	601	ATP	1	0
10	G	601	1VU	2	0
6	R	603	BCT	1	0
9	F	601	A1CZD	2	0
10	M	601	1VU	6	0

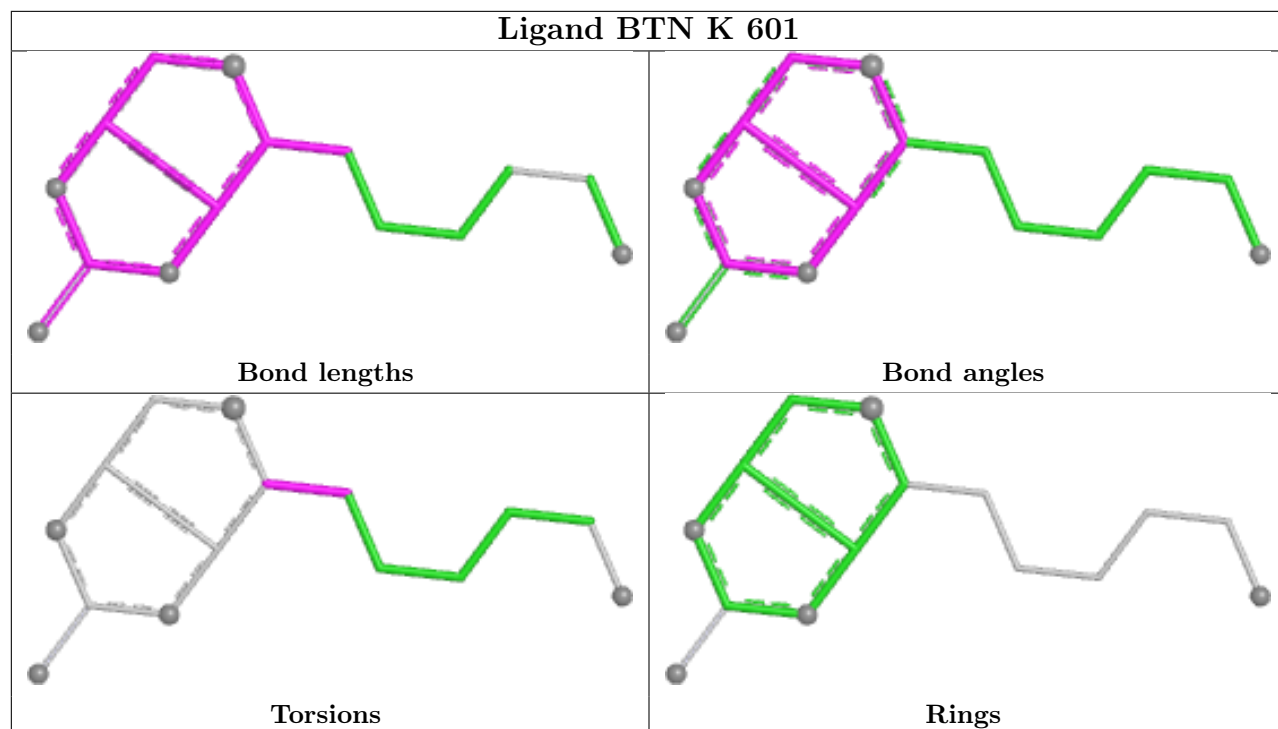
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

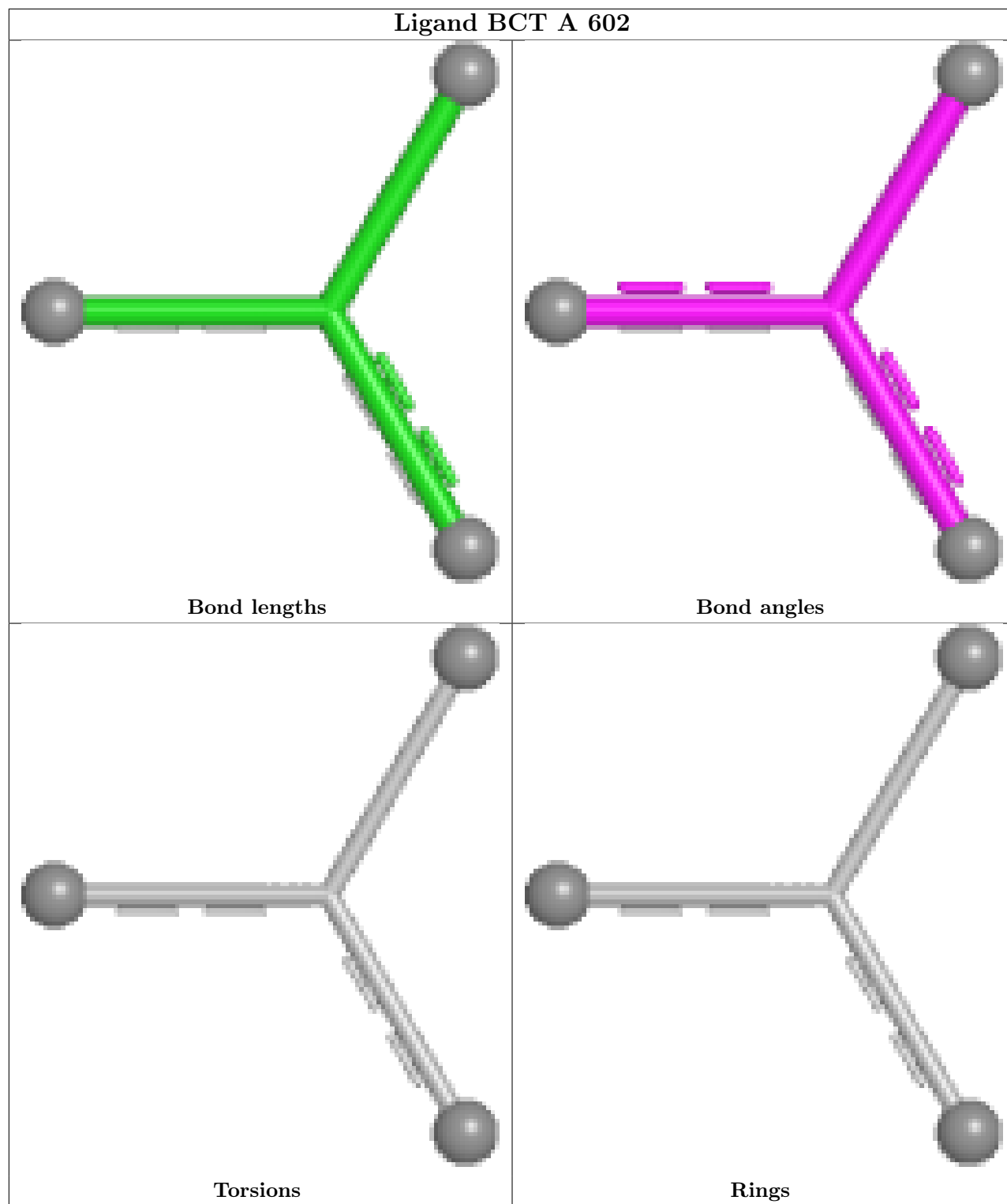
Ligand ATP R 601

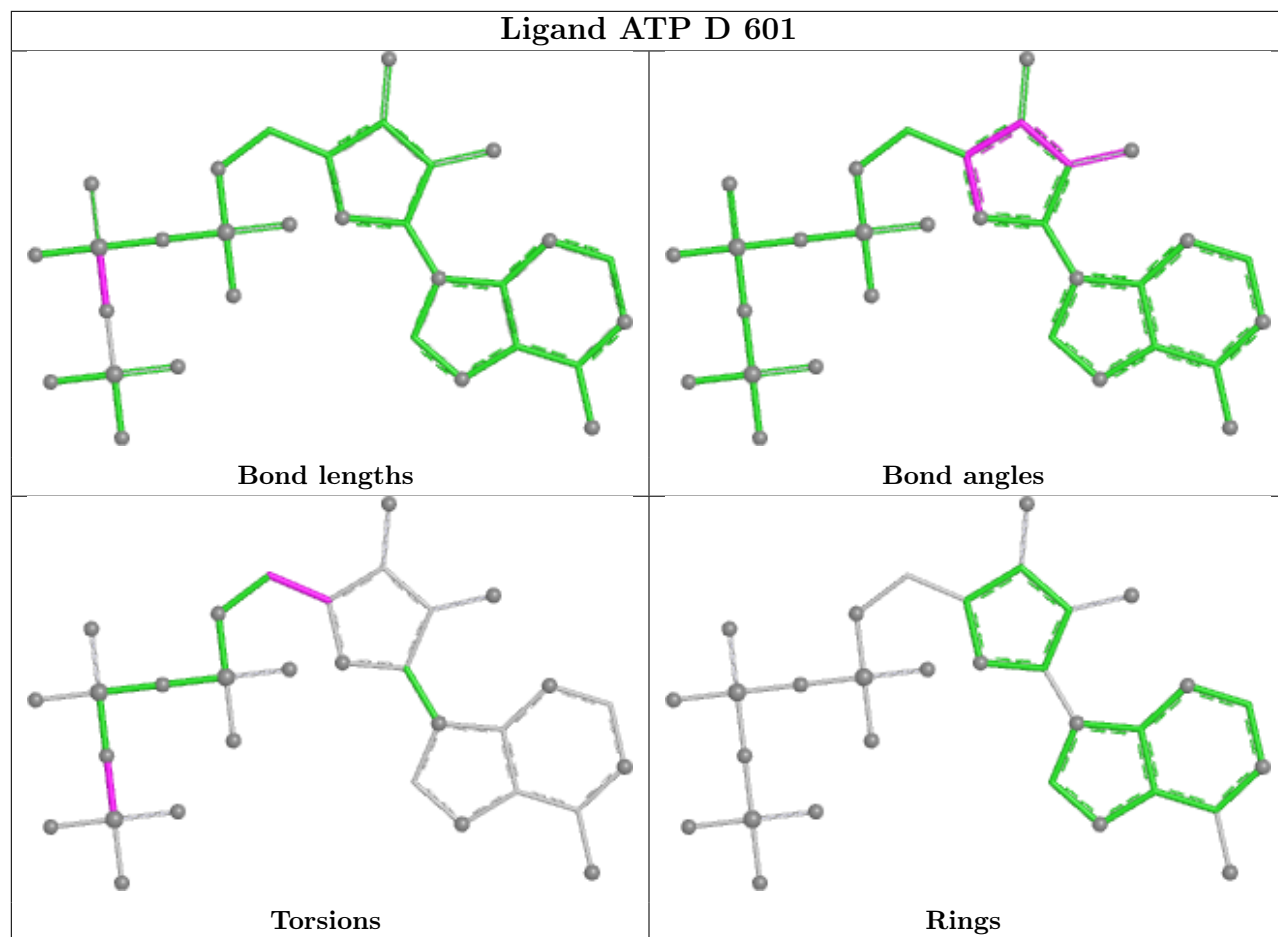


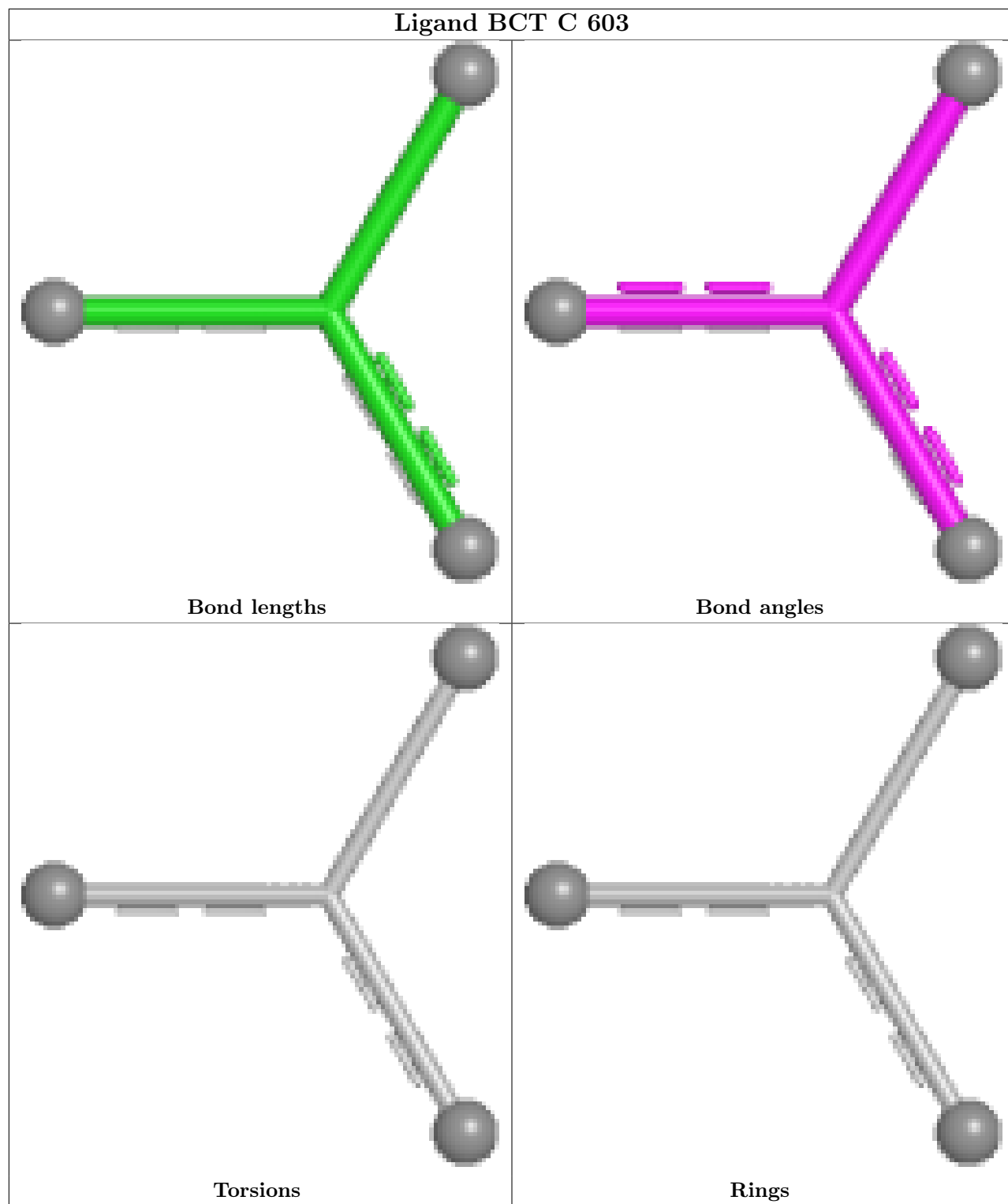
Ligand BTN I 601

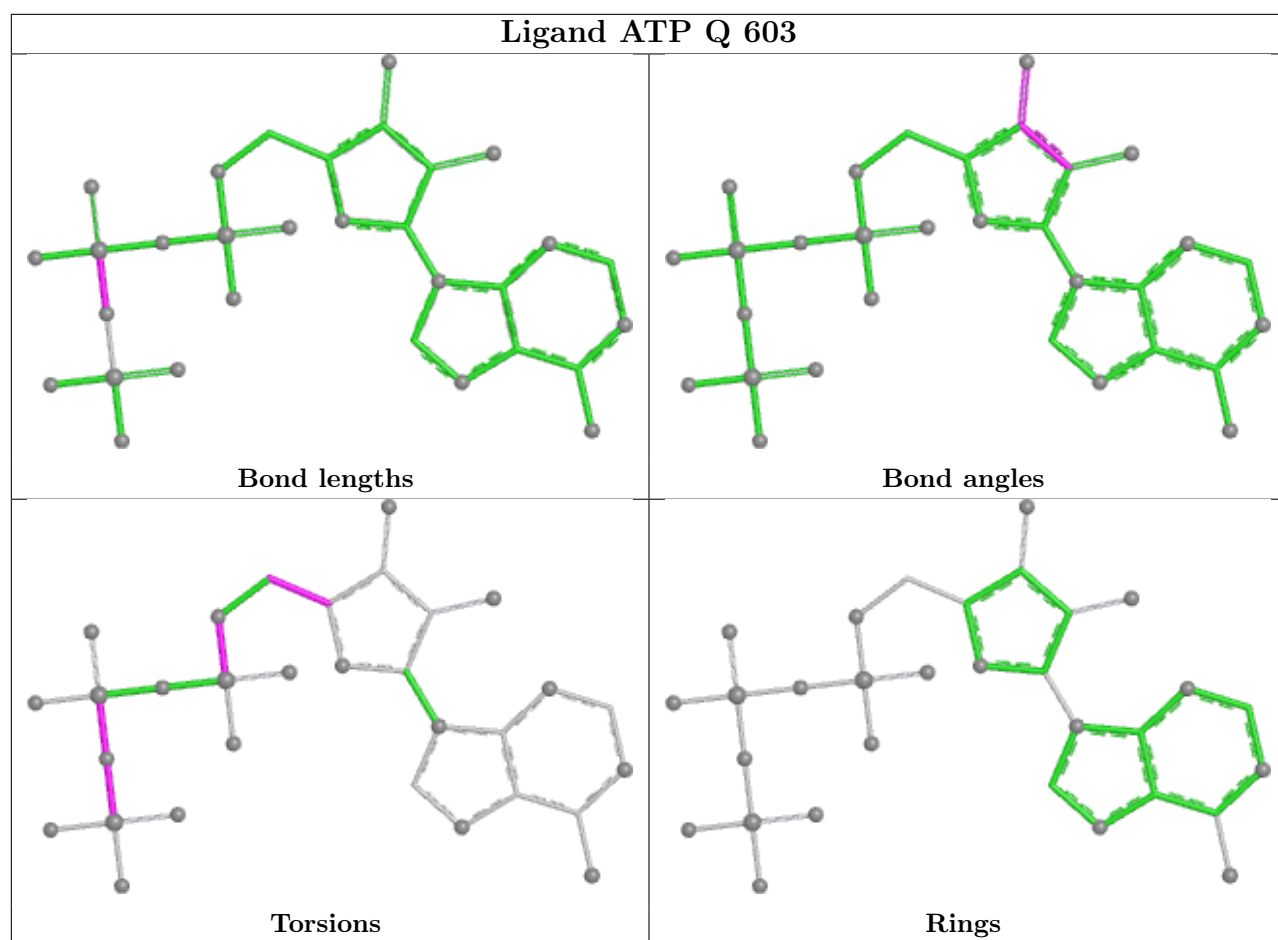


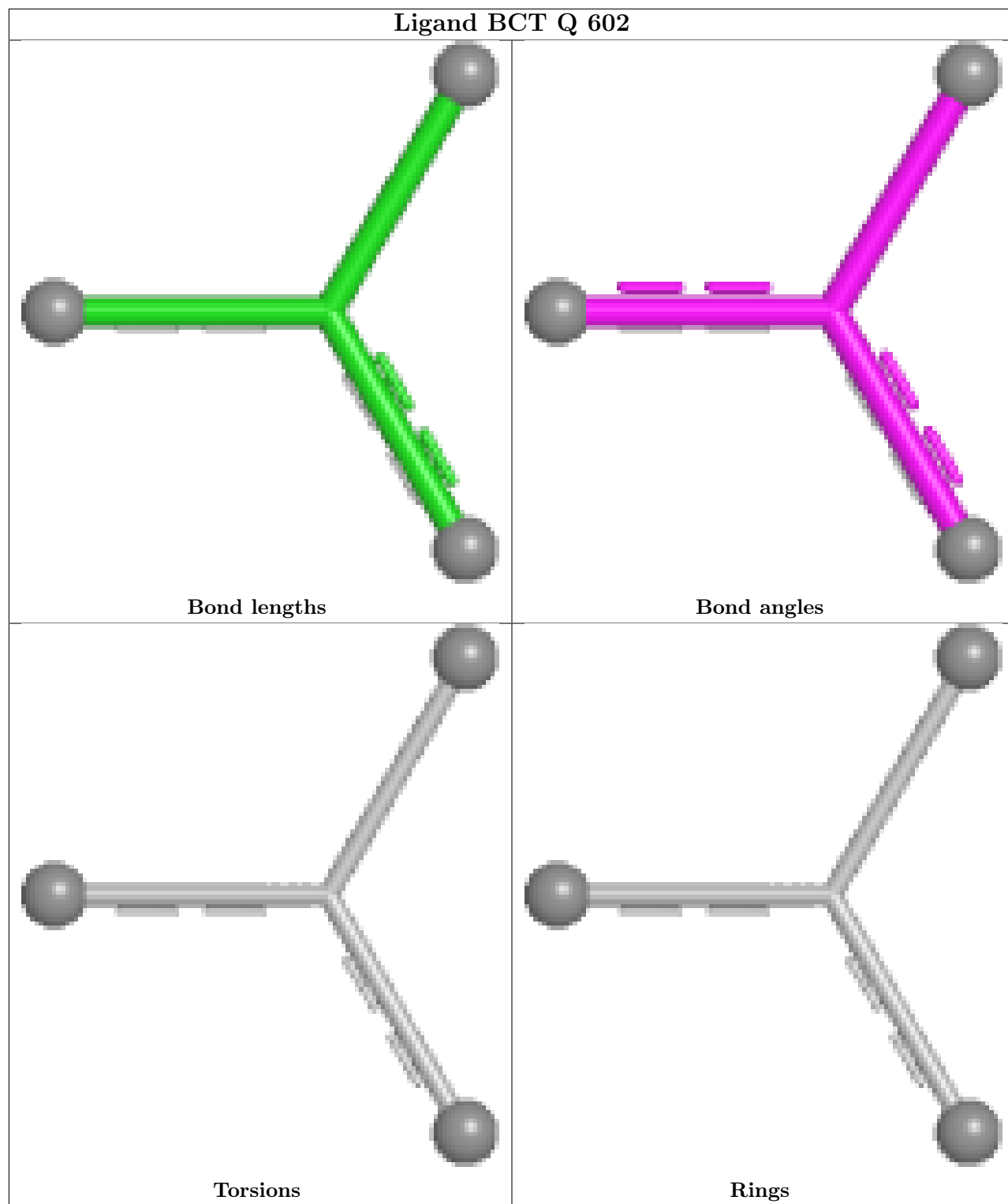


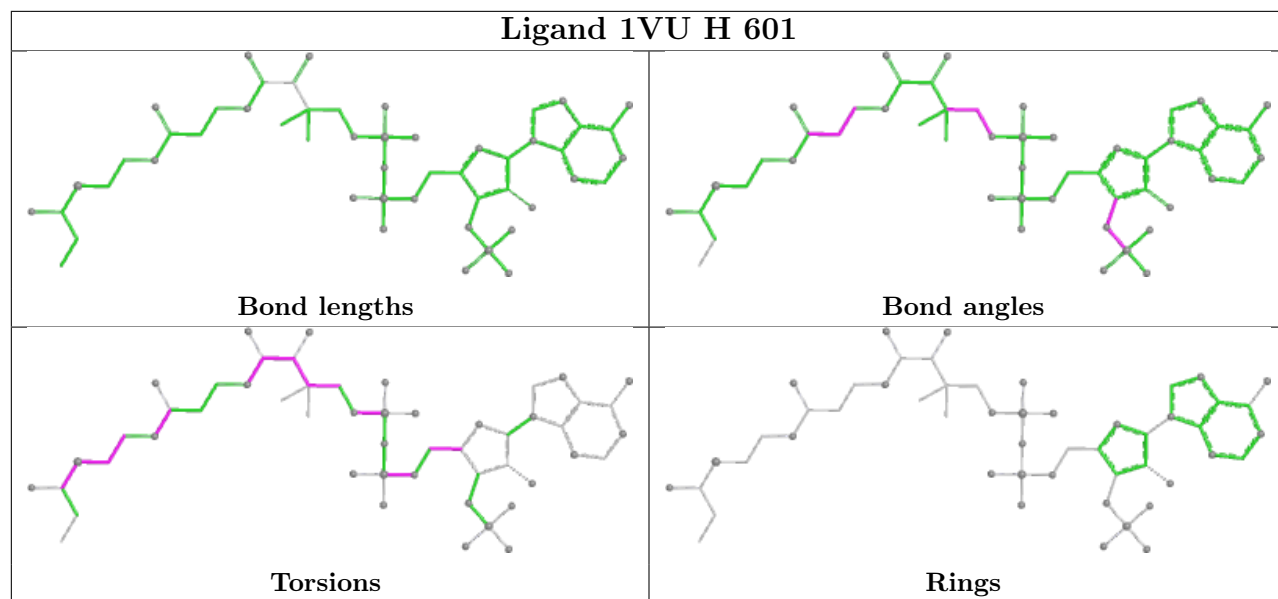


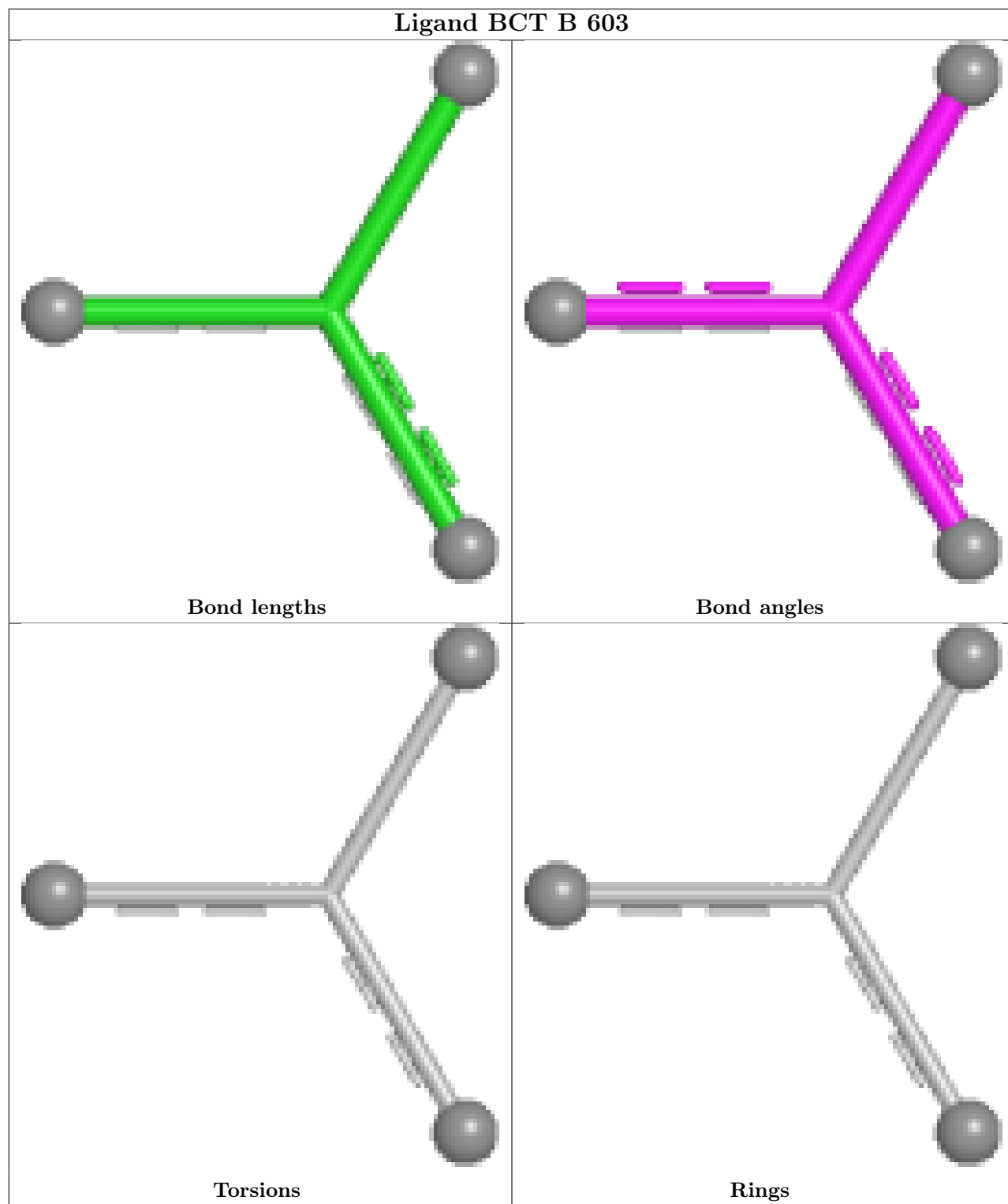




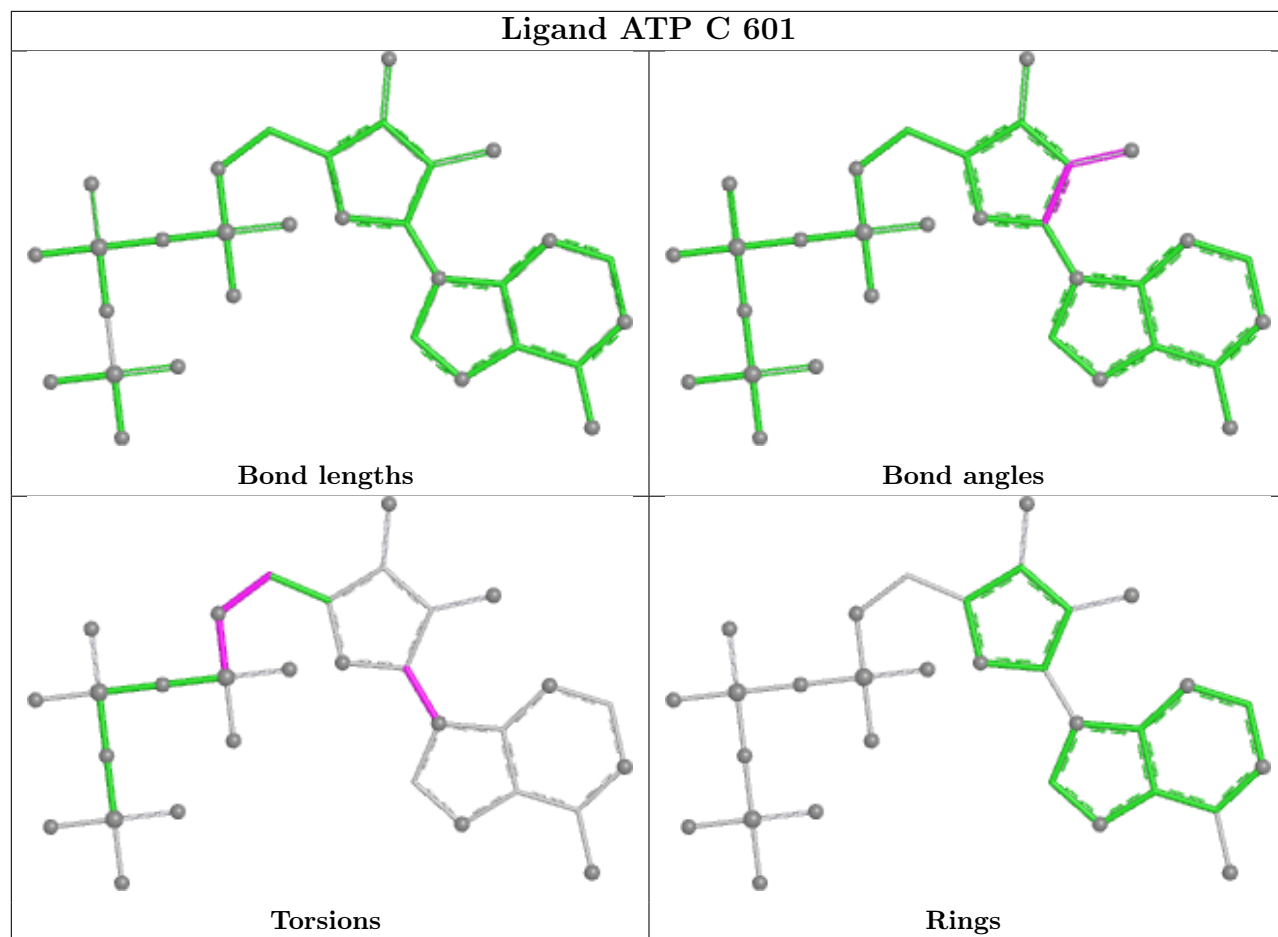




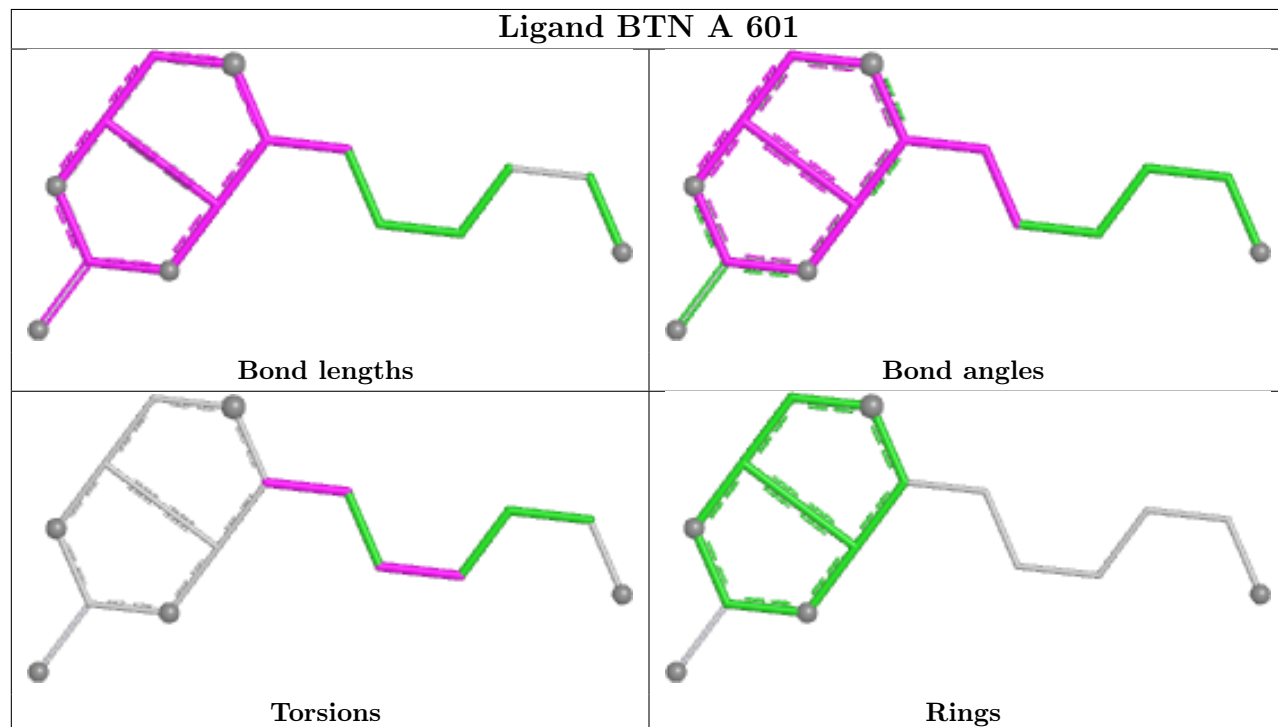


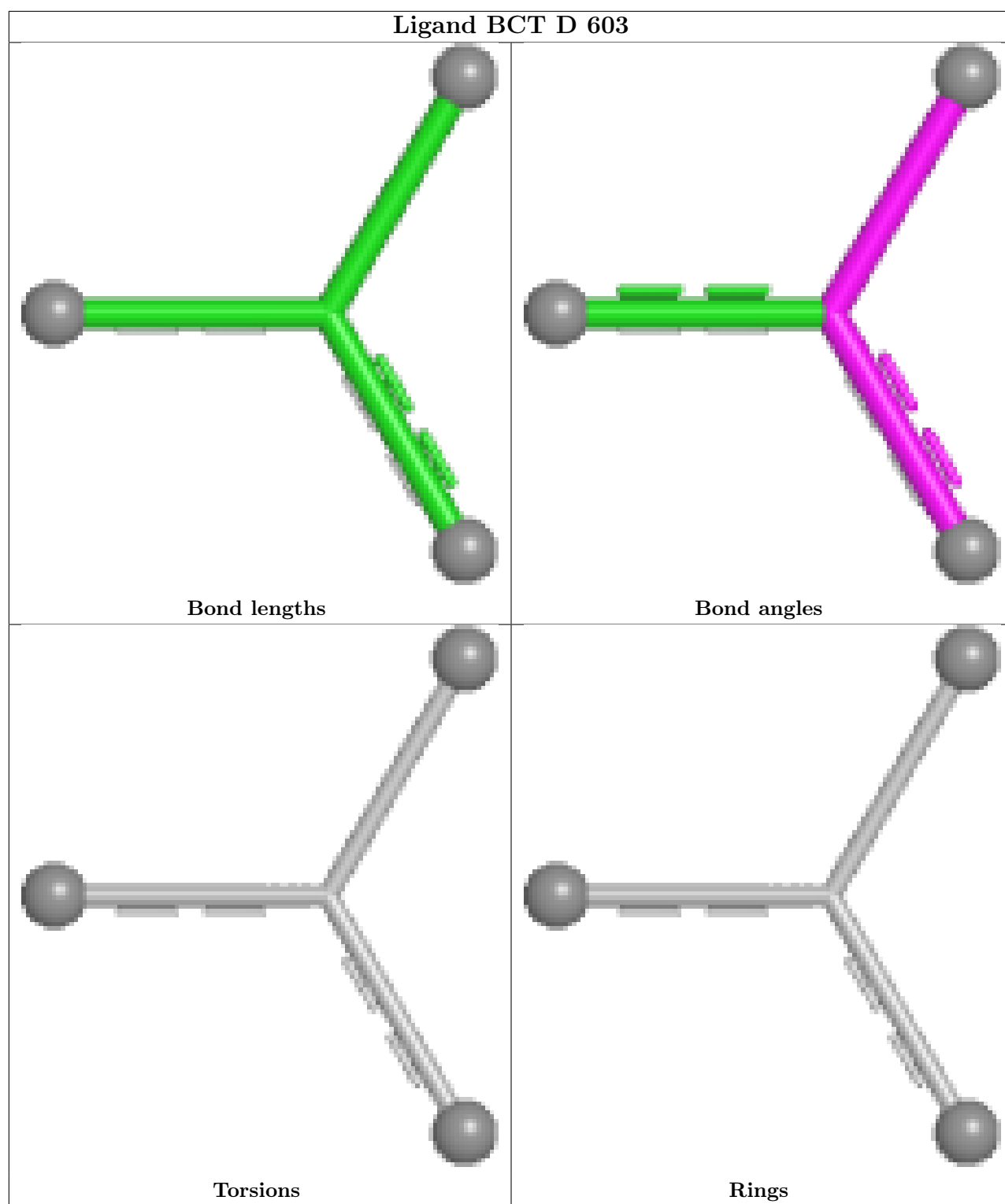


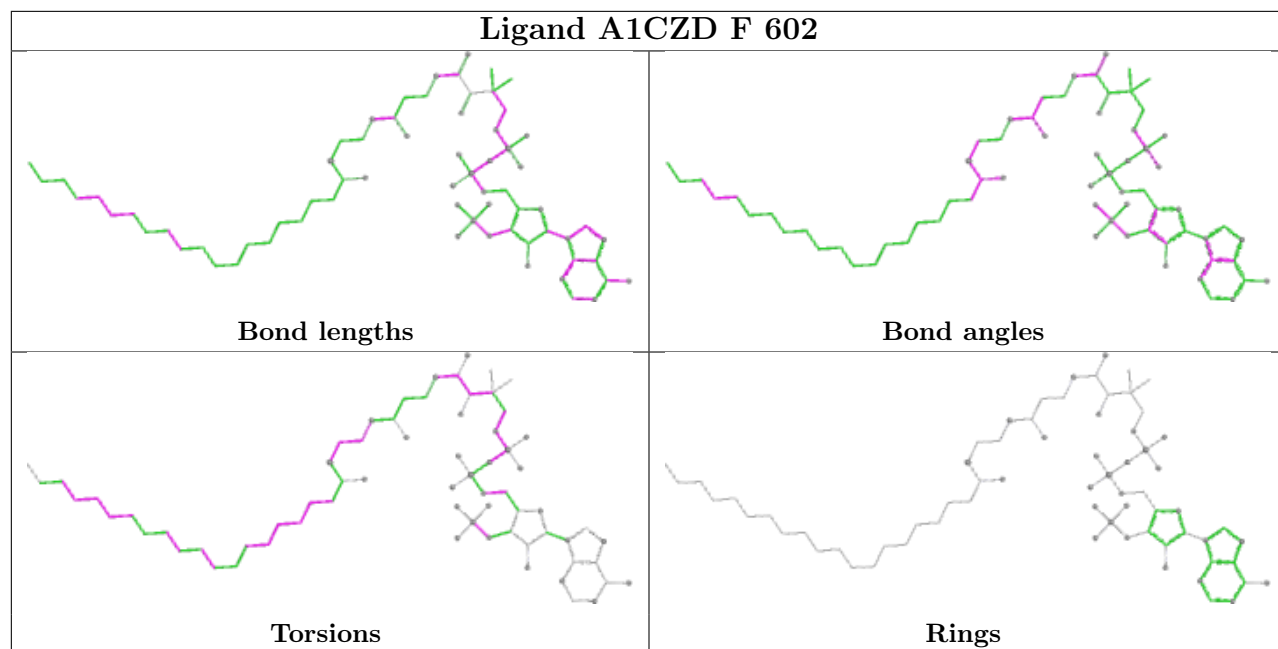
Ligand ATP C 601

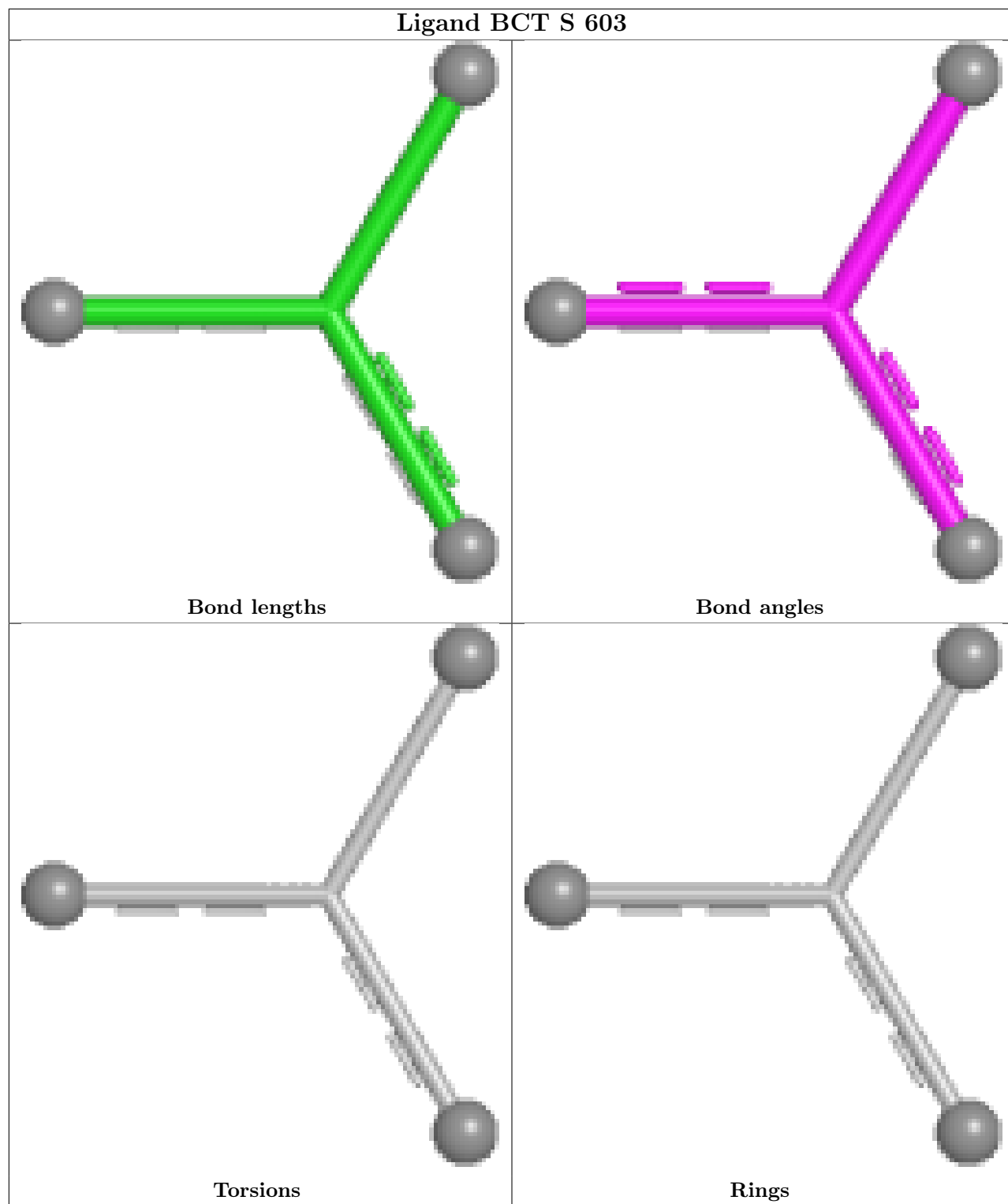


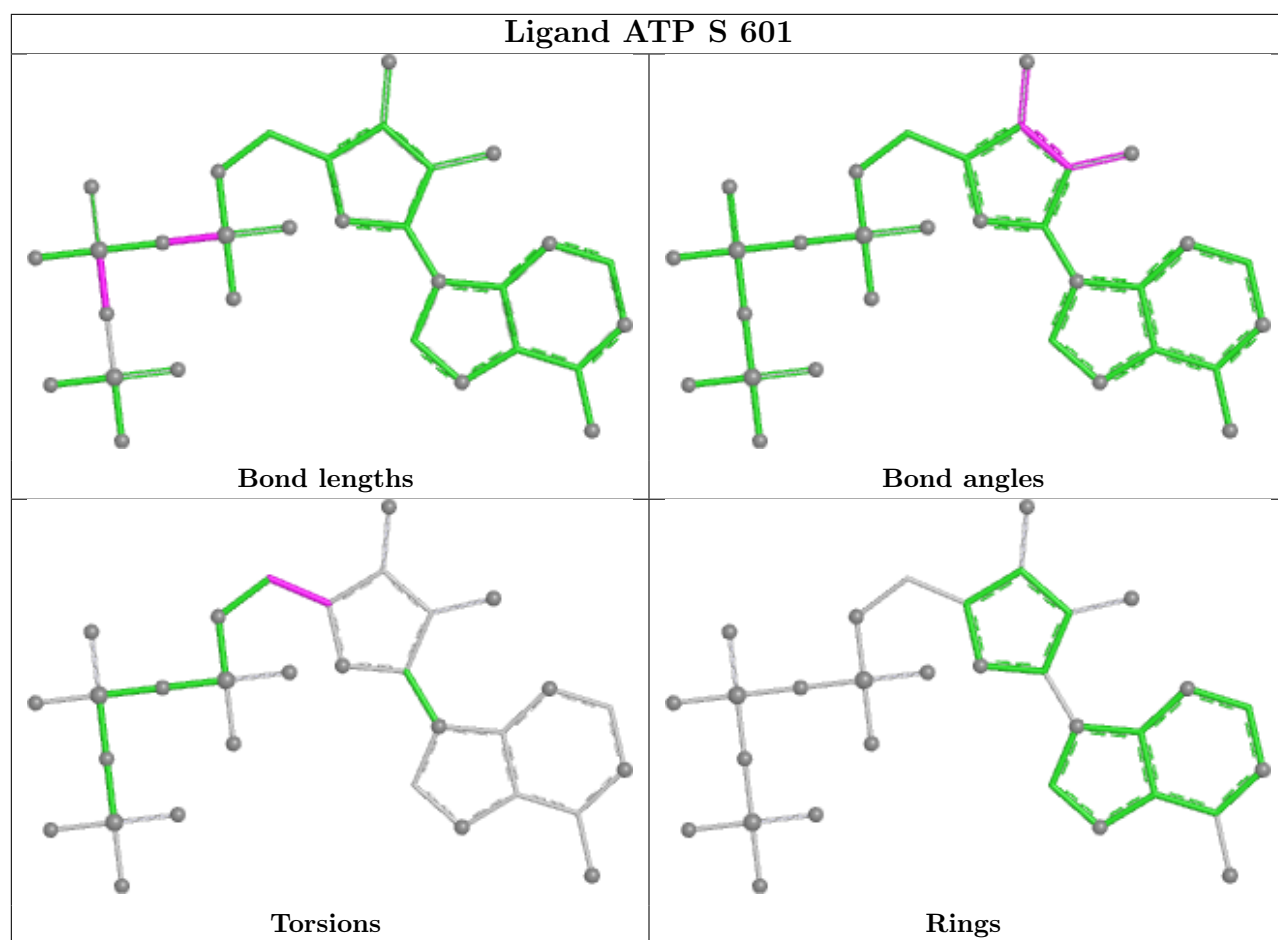
Ligand BTN A 601

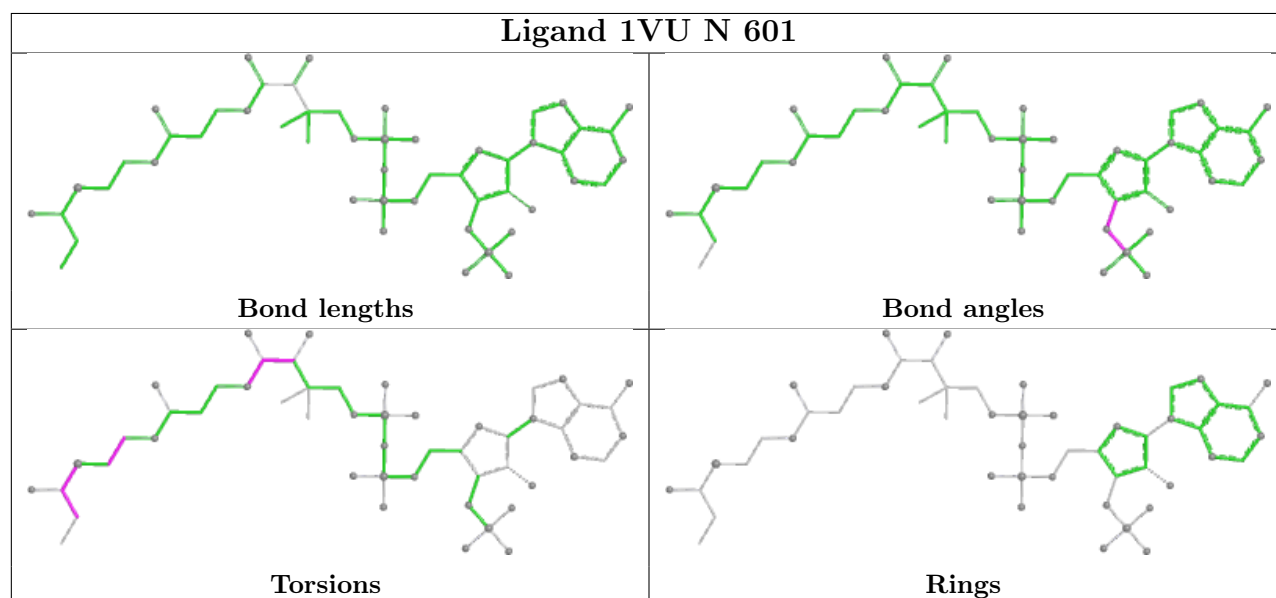
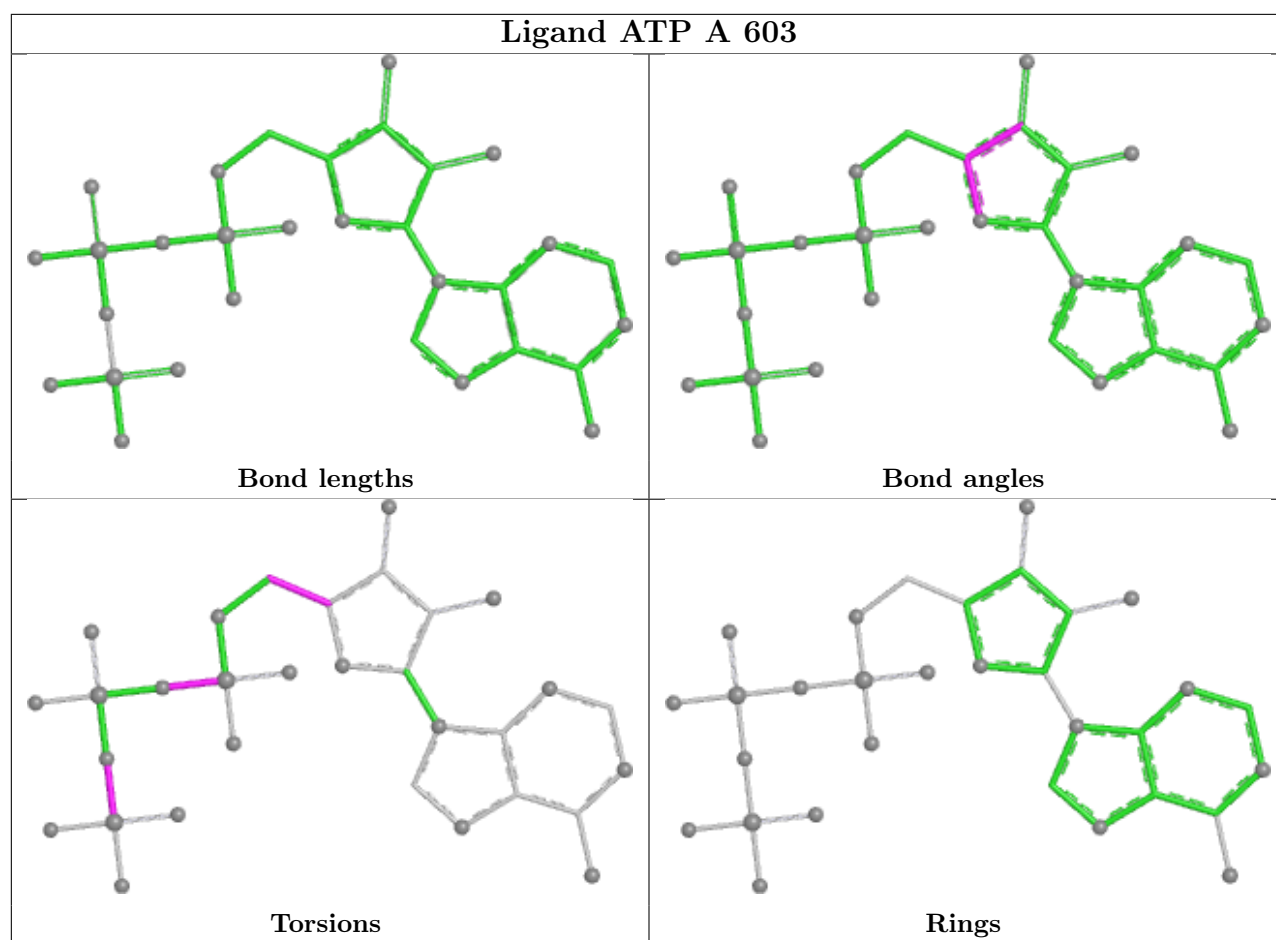


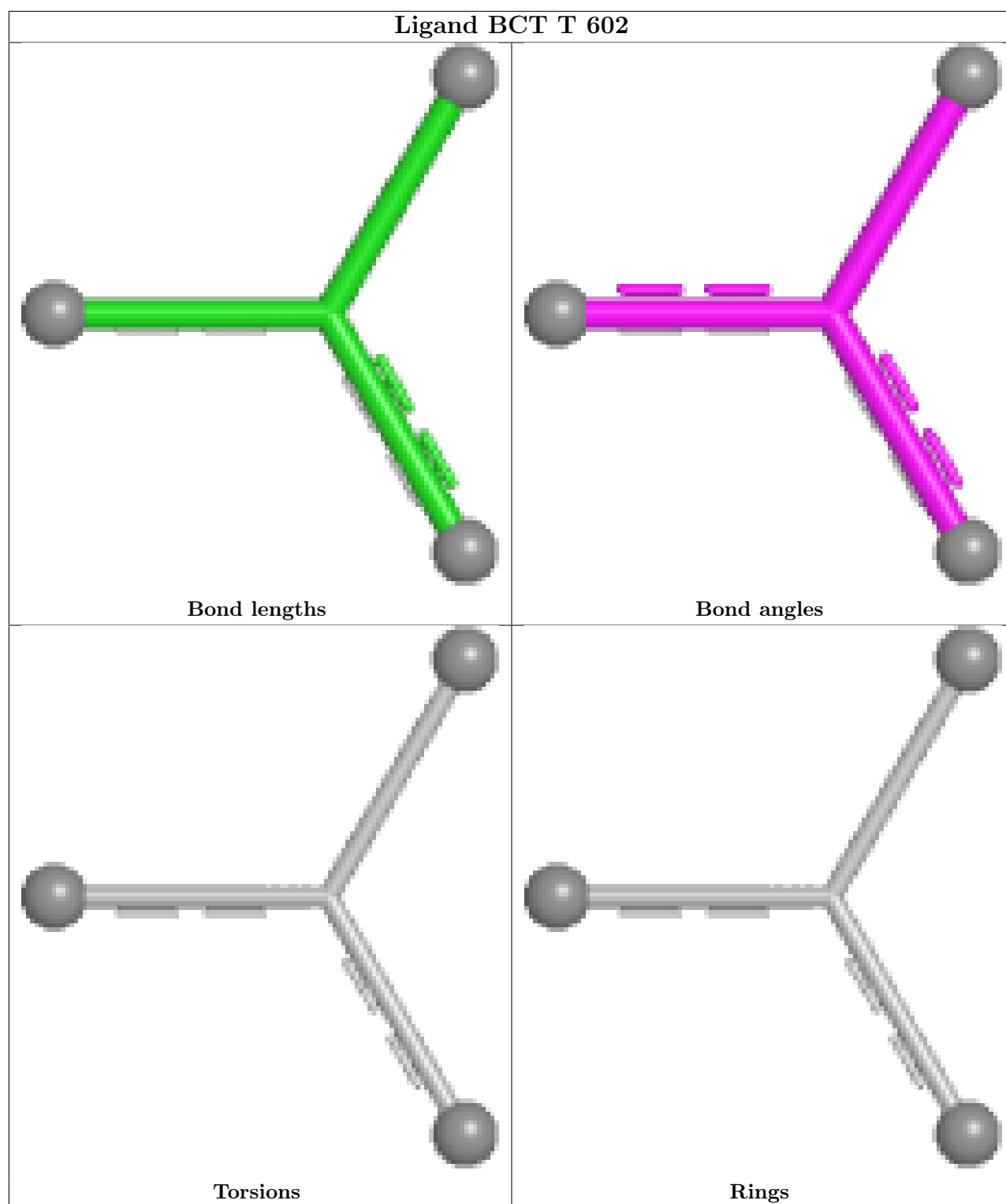


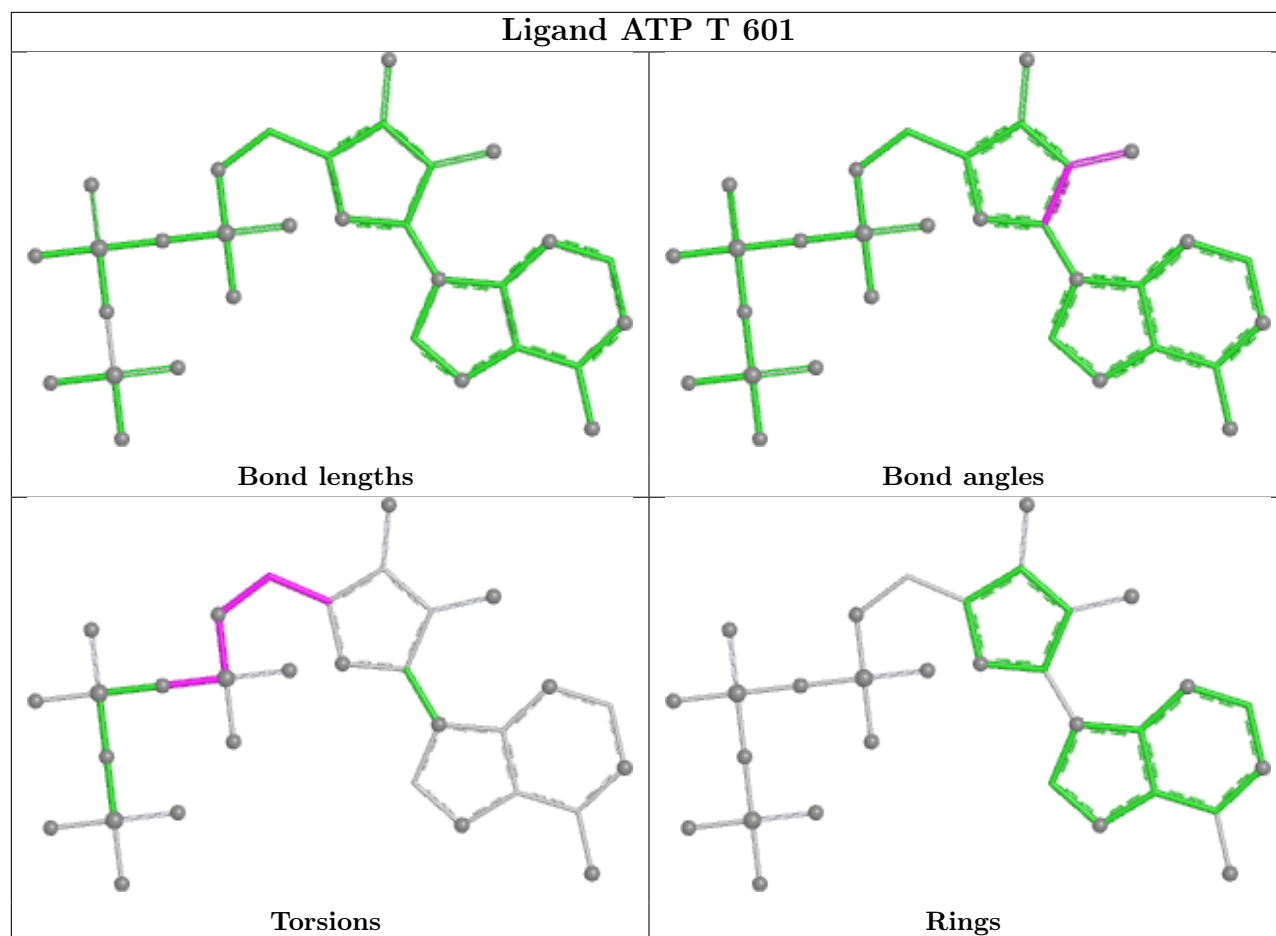
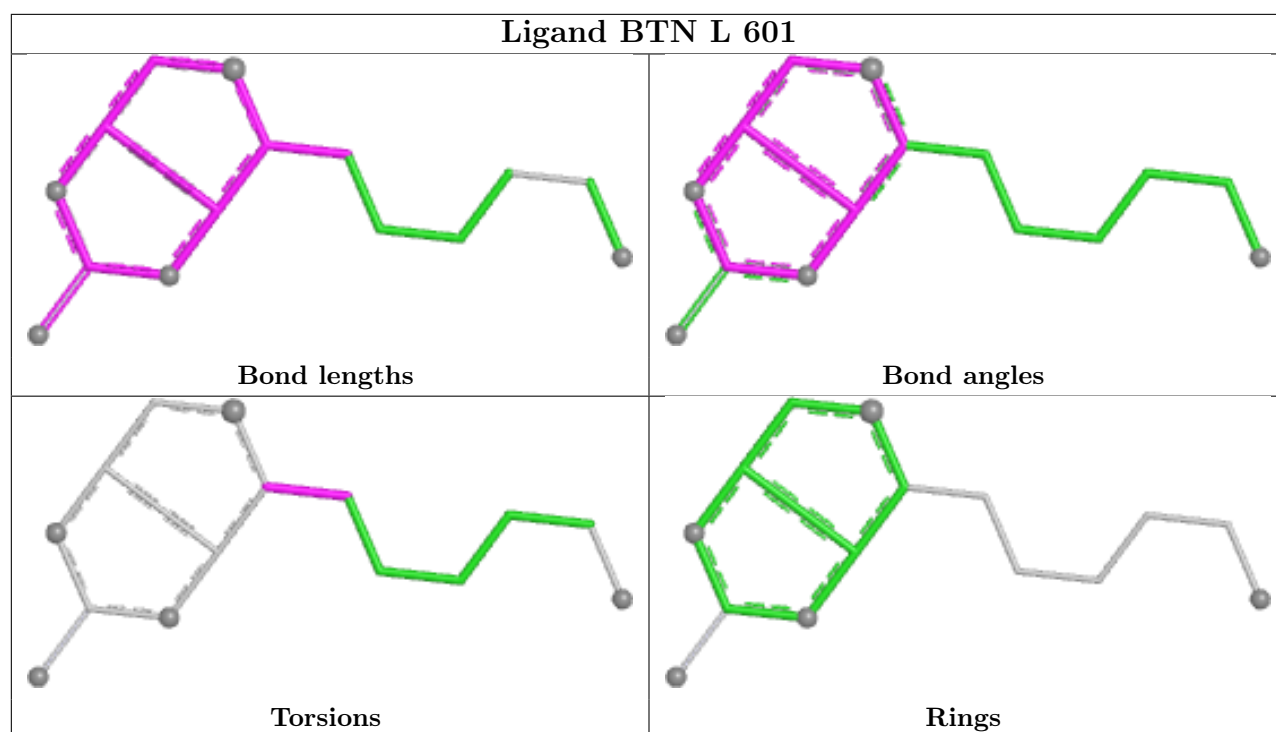




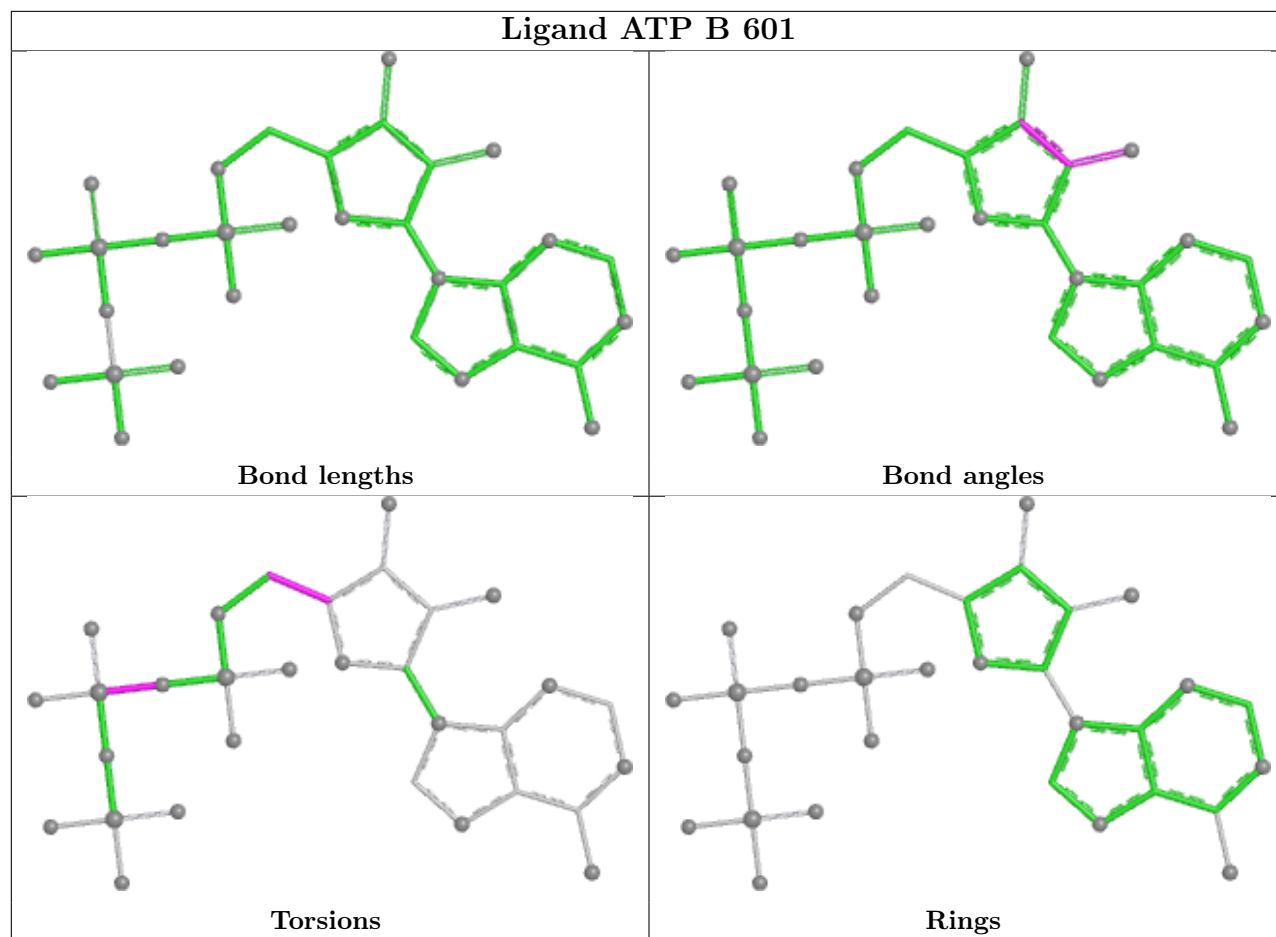




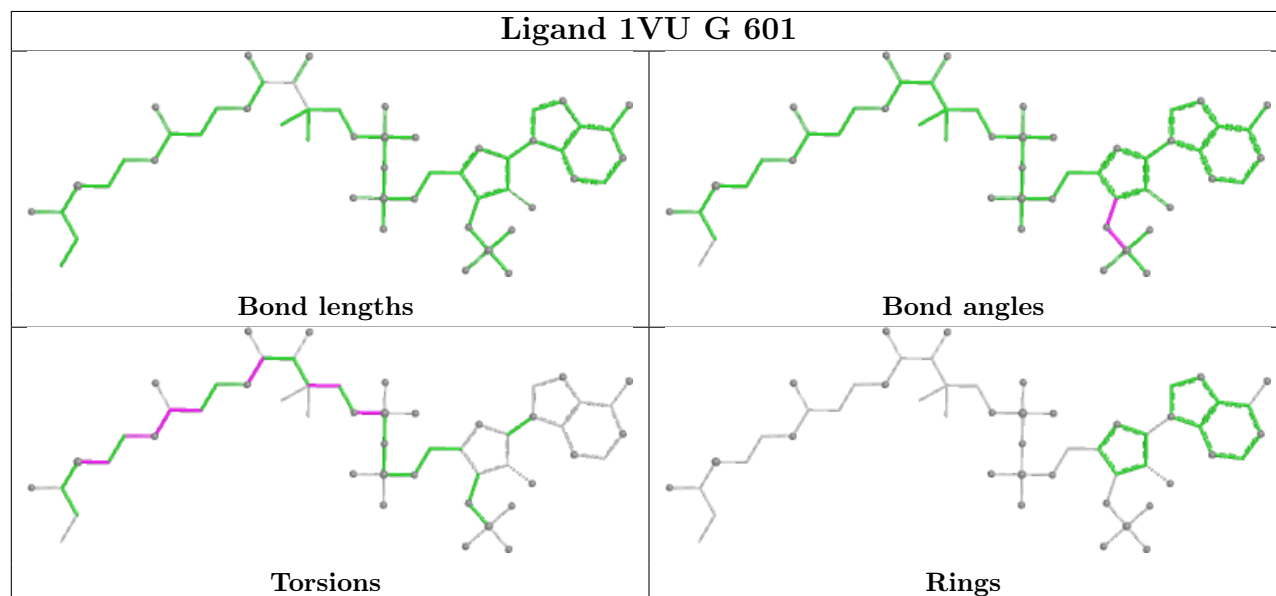


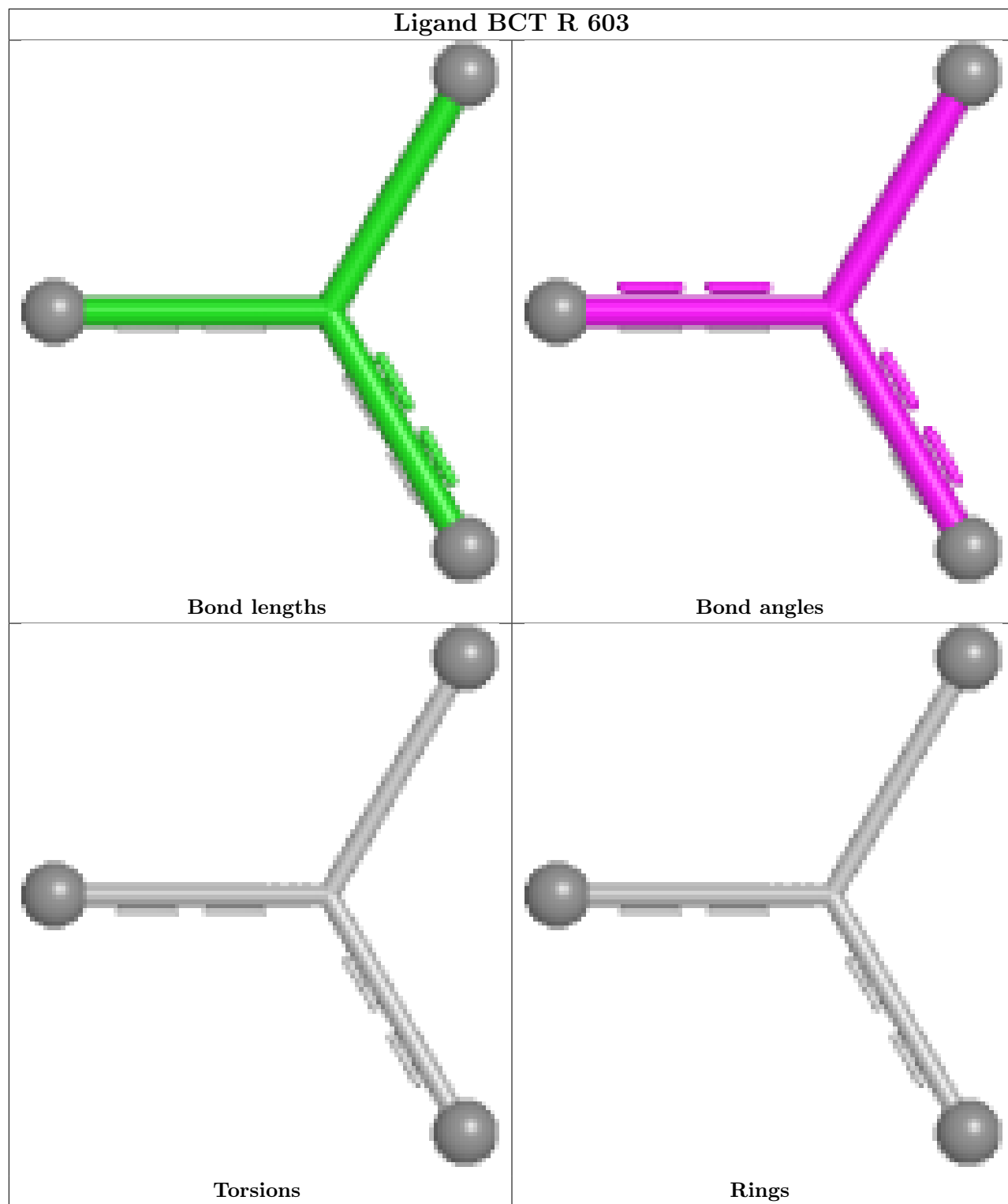


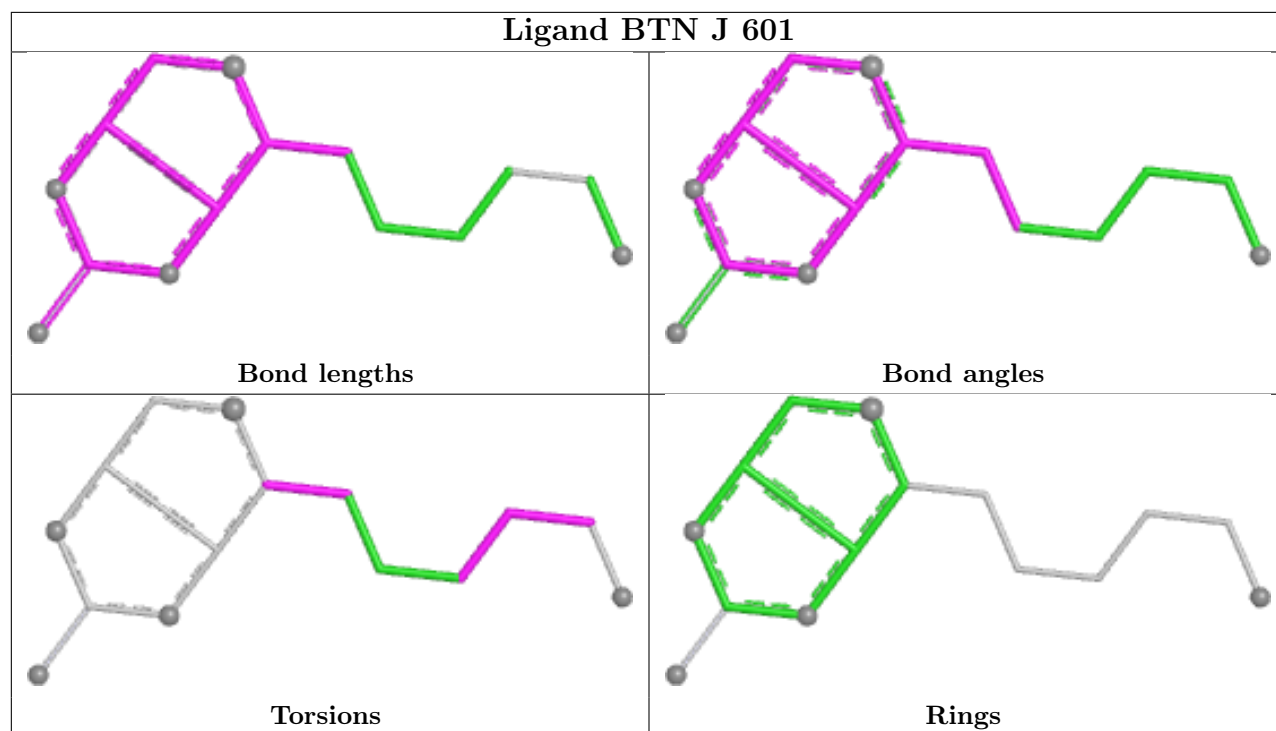
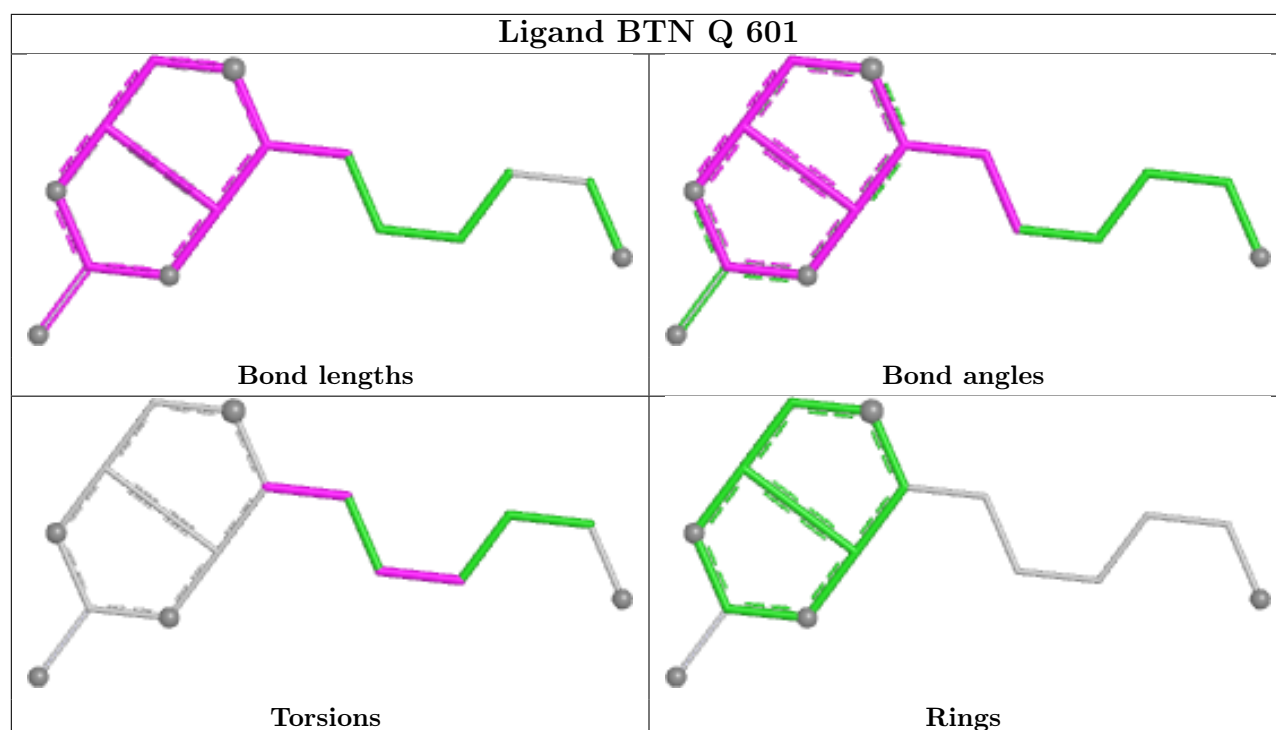
Ligand ATP B 601

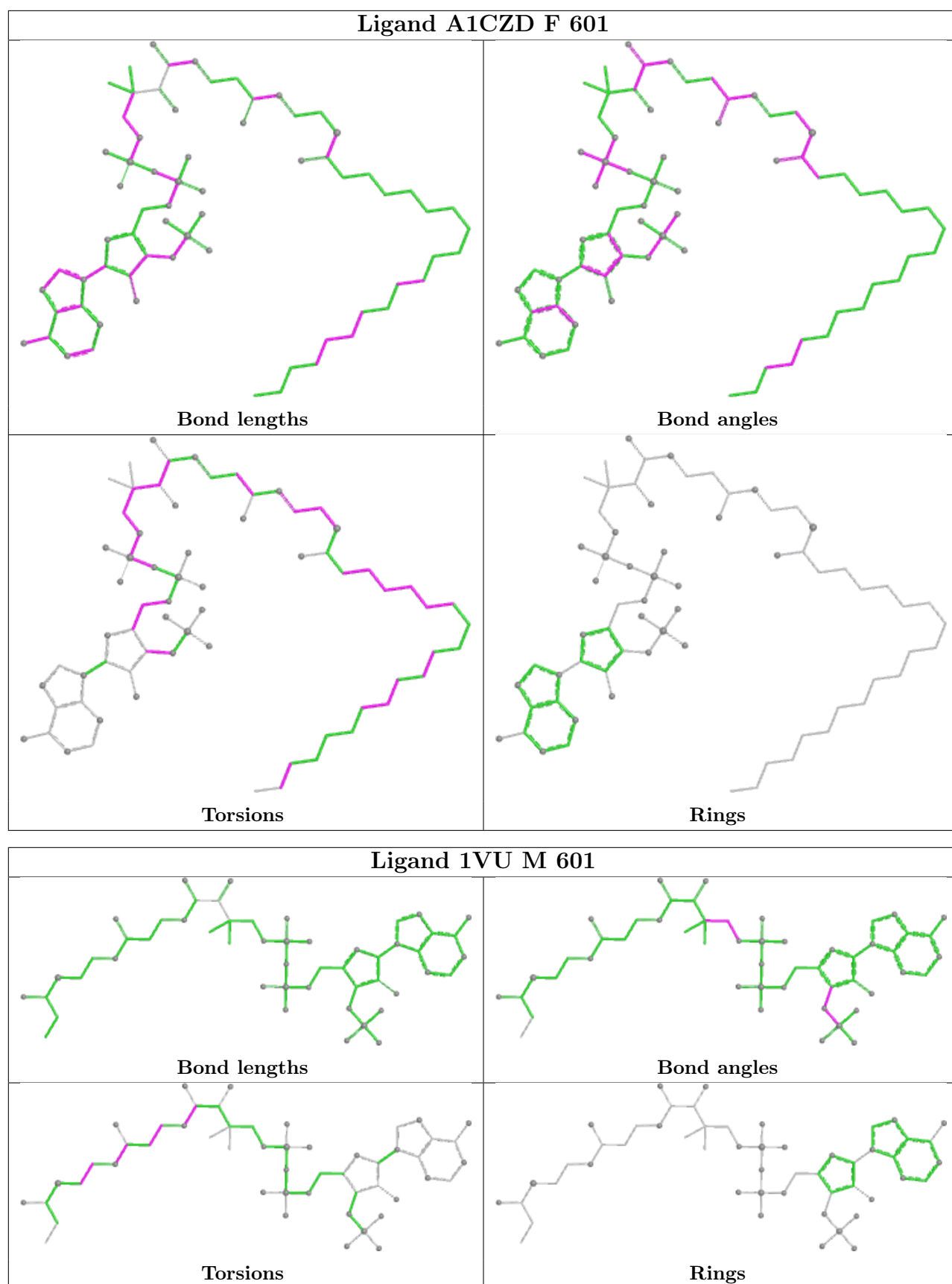


Ligand 1VU G 601









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

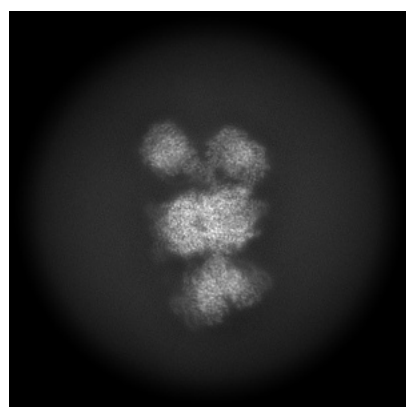
6 Map visualisation [i](#)

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

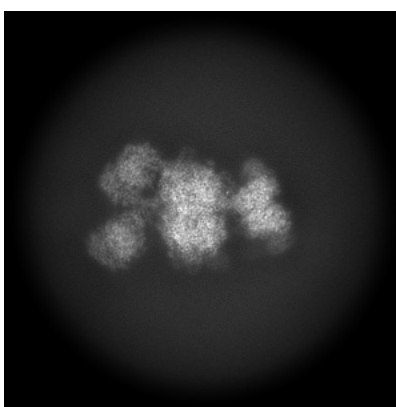
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

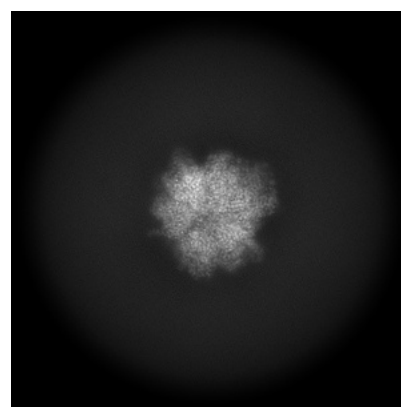
6.1.1 Primary map



X



Y

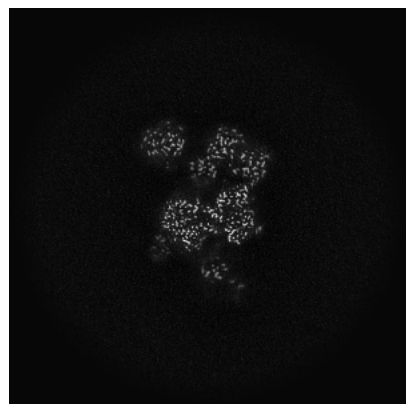


Z

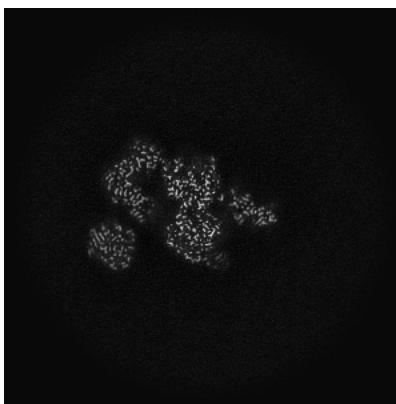
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

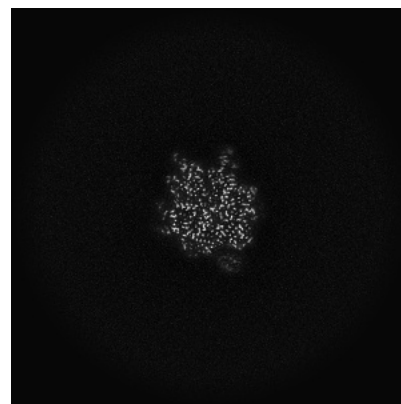
6.2.1 Primary map



X Index: 240



Y Index: 240

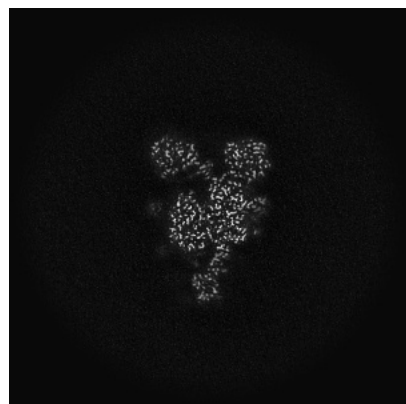


Z Index: 240

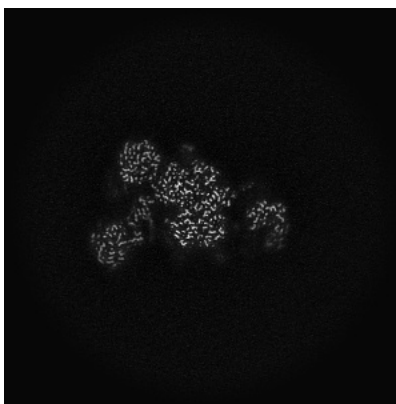
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

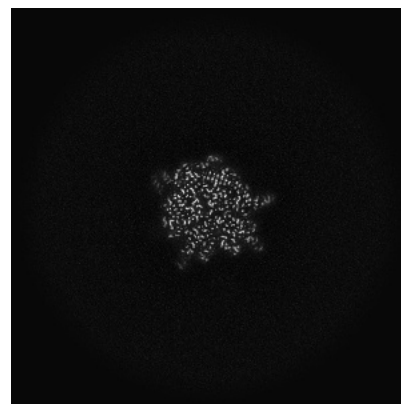
6.3.1 Primary map



X Index: 253



Y Index: 255

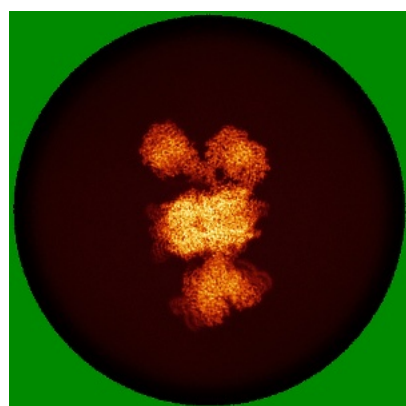


Z Index: 214

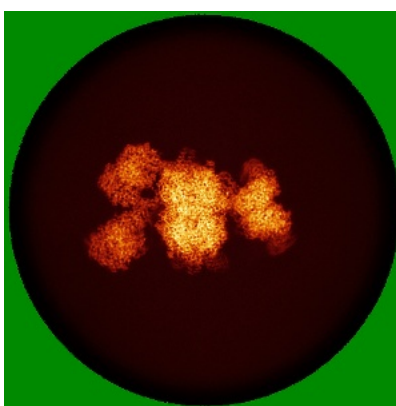
The images above show the largest variance slices of the map in three orthogonal directions.

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

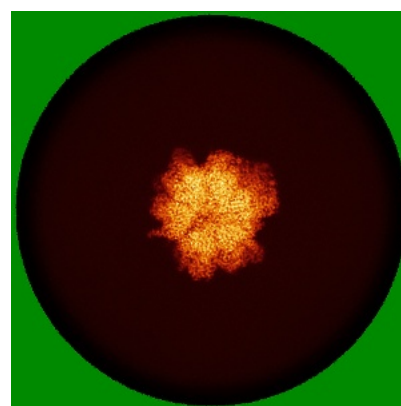
6.4.1 Primary map



X



Y

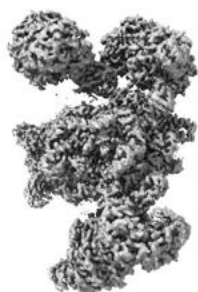


Z

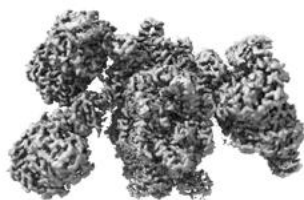
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

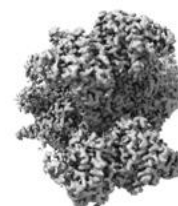
6.5.1 Primary map



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.

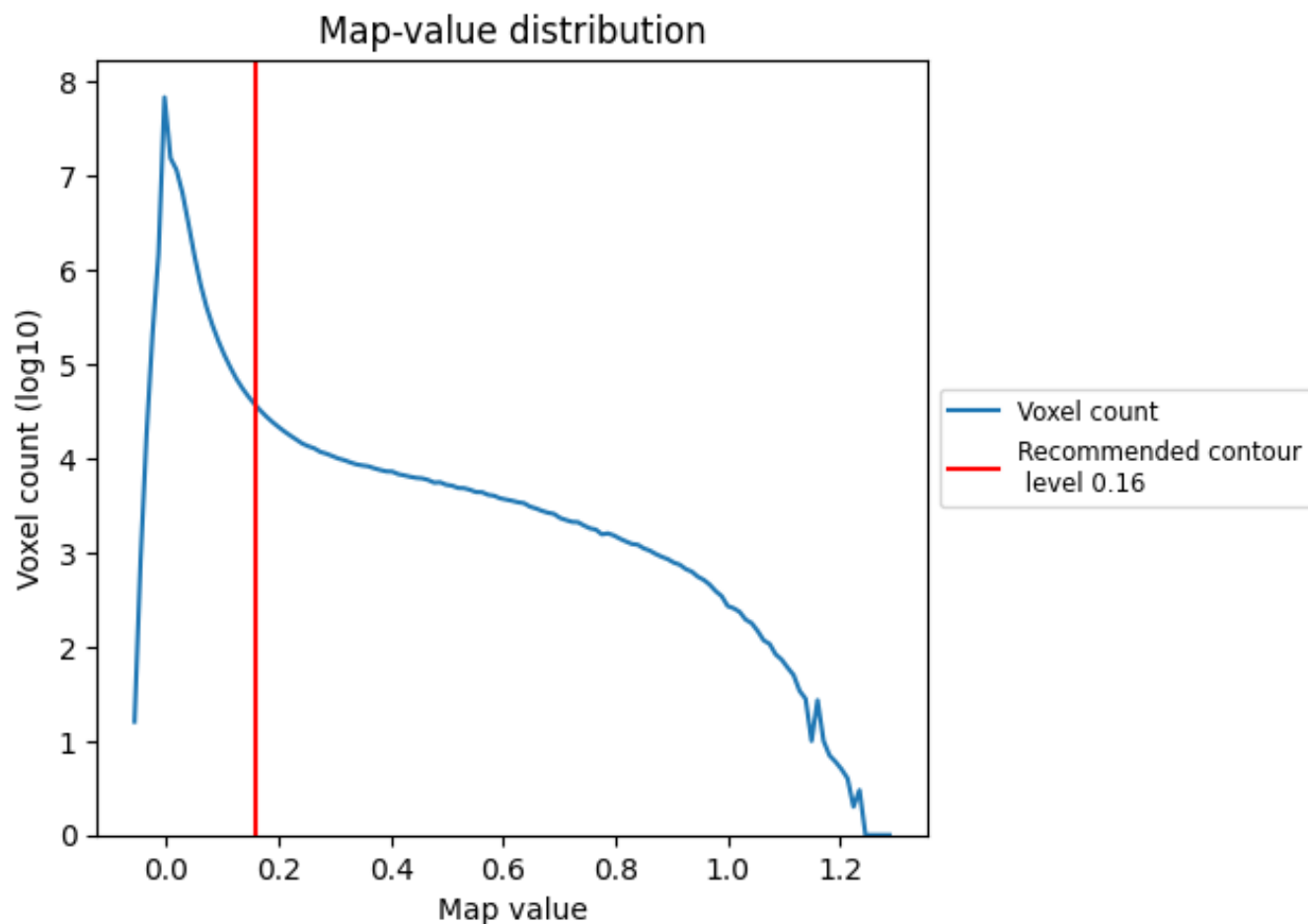
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

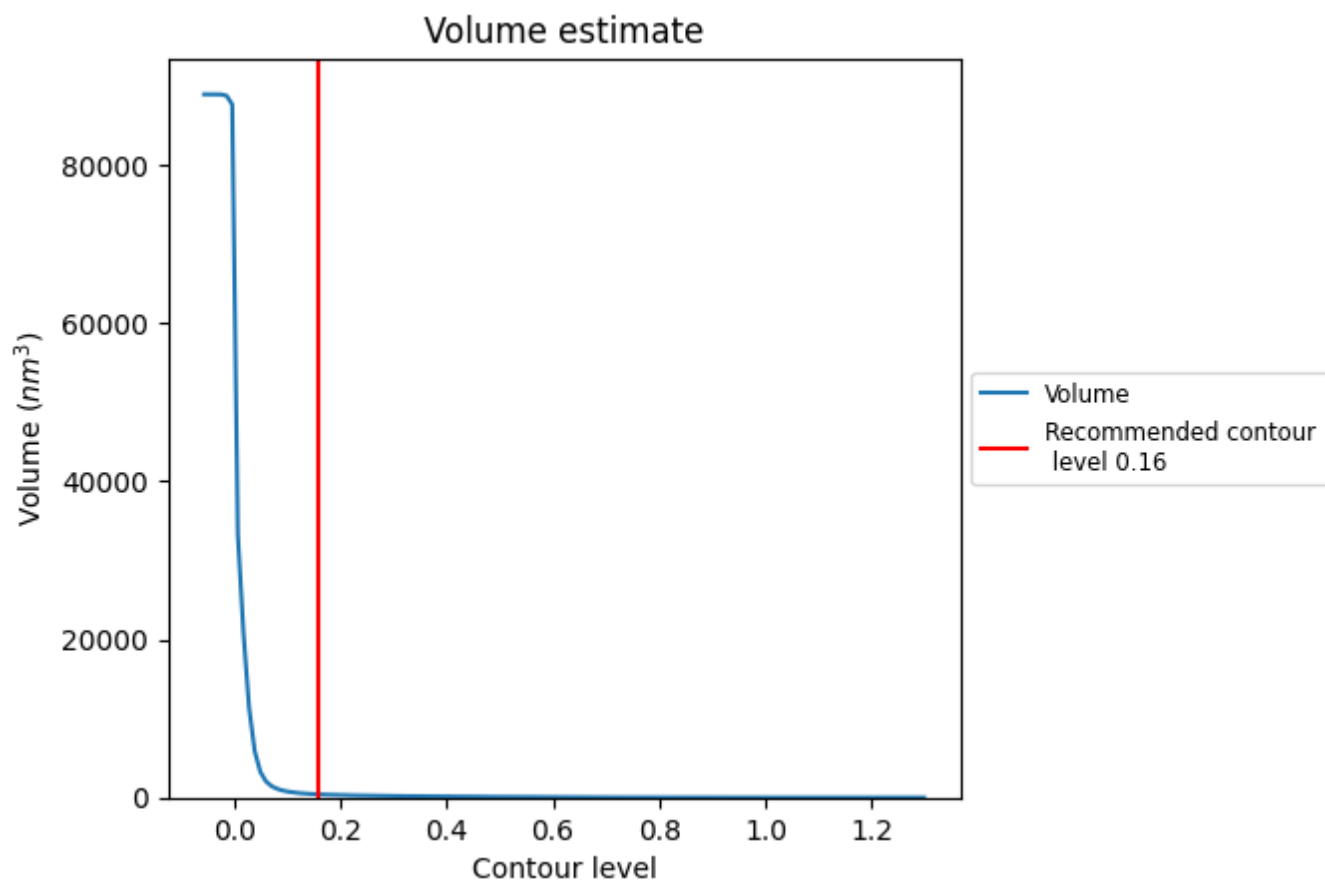
This section contains the results of statistical analysis of the map.

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.

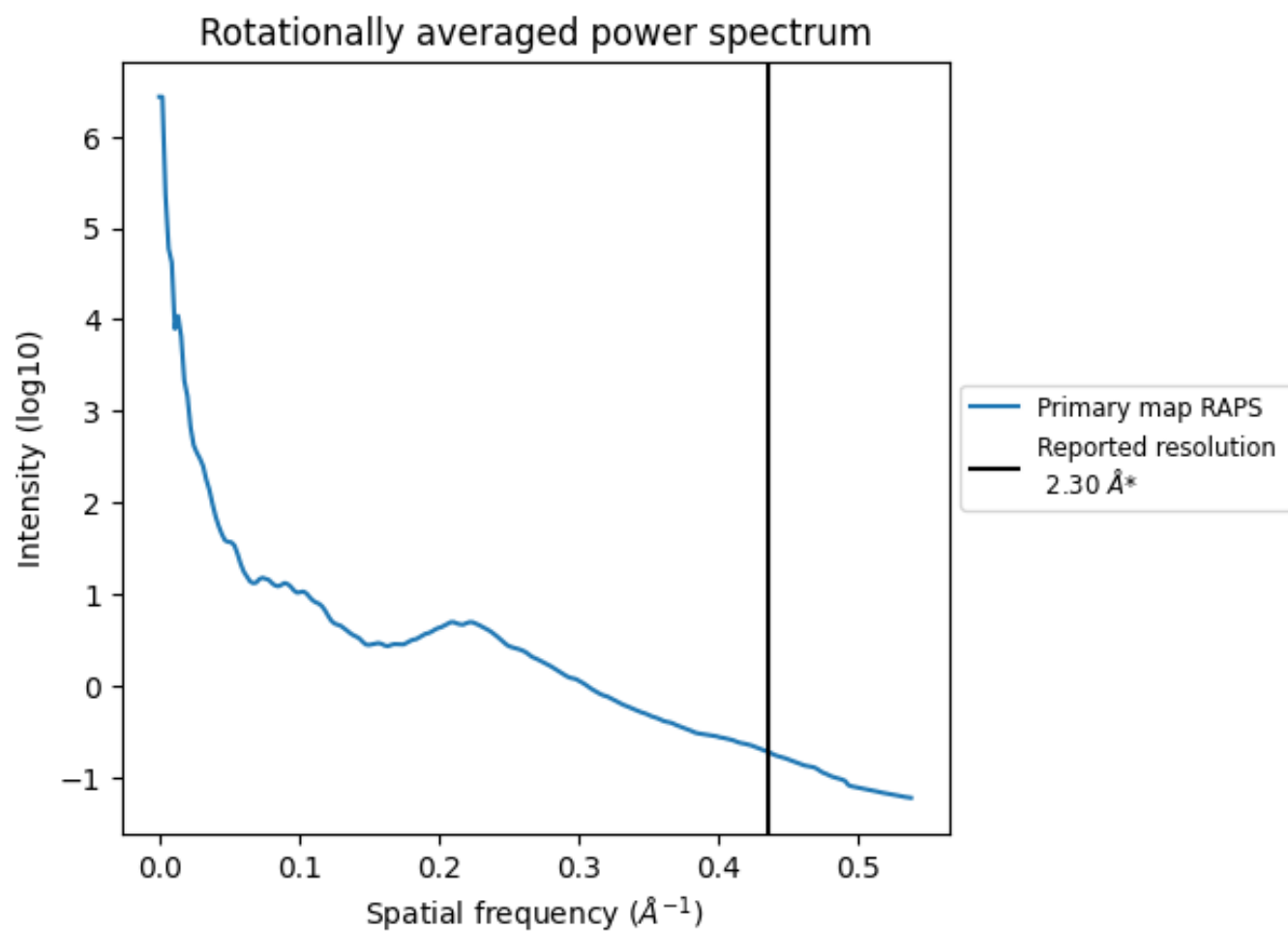
7.2 Volume estimate [i](#)



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

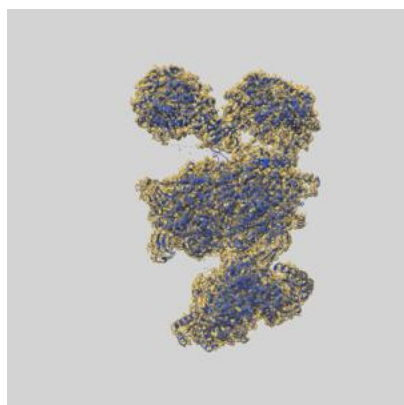
8 Fourier-Shell correlation ⓘ

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

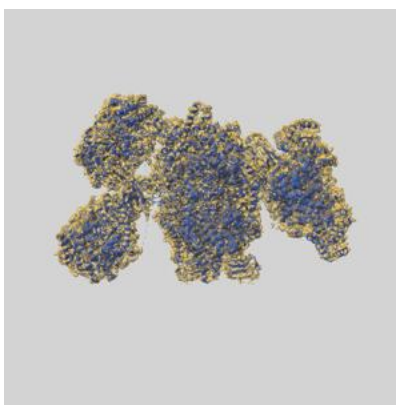
9 Map-model fit [i](#)

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](#).

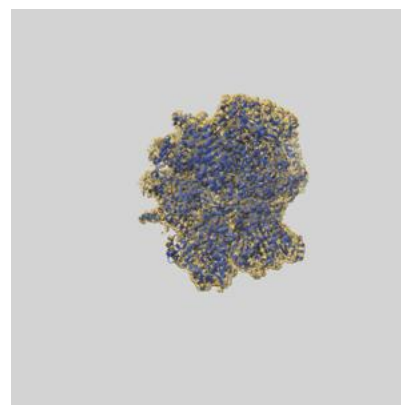
9.1 Map-model overlay [i](#)



X



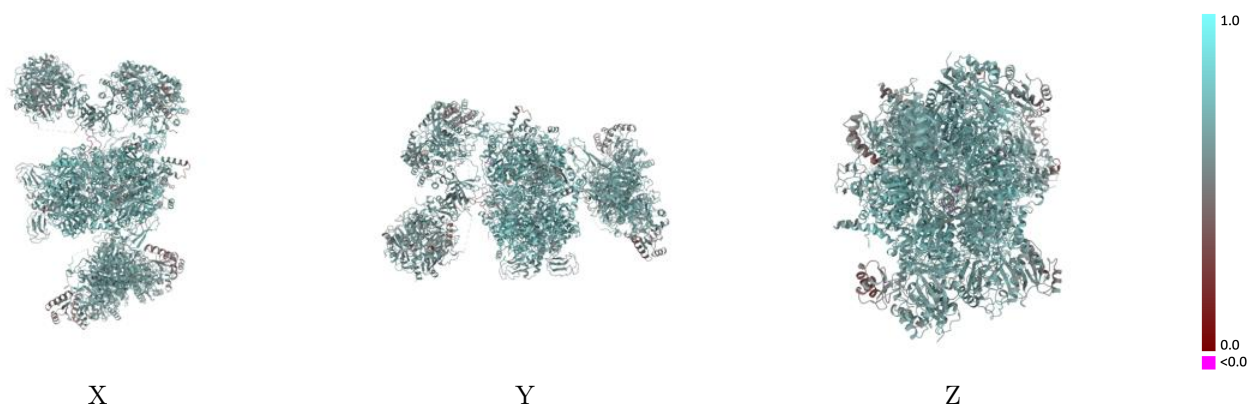
Y



Z

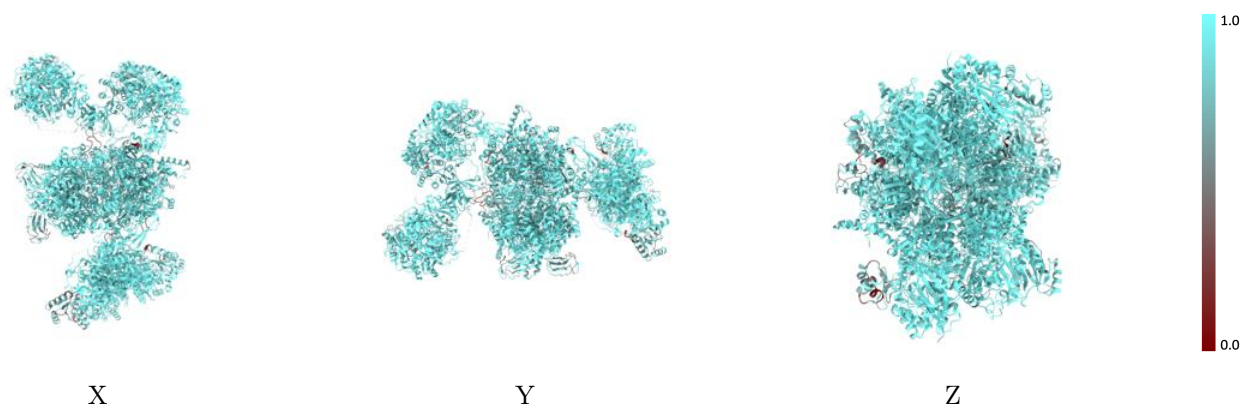
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



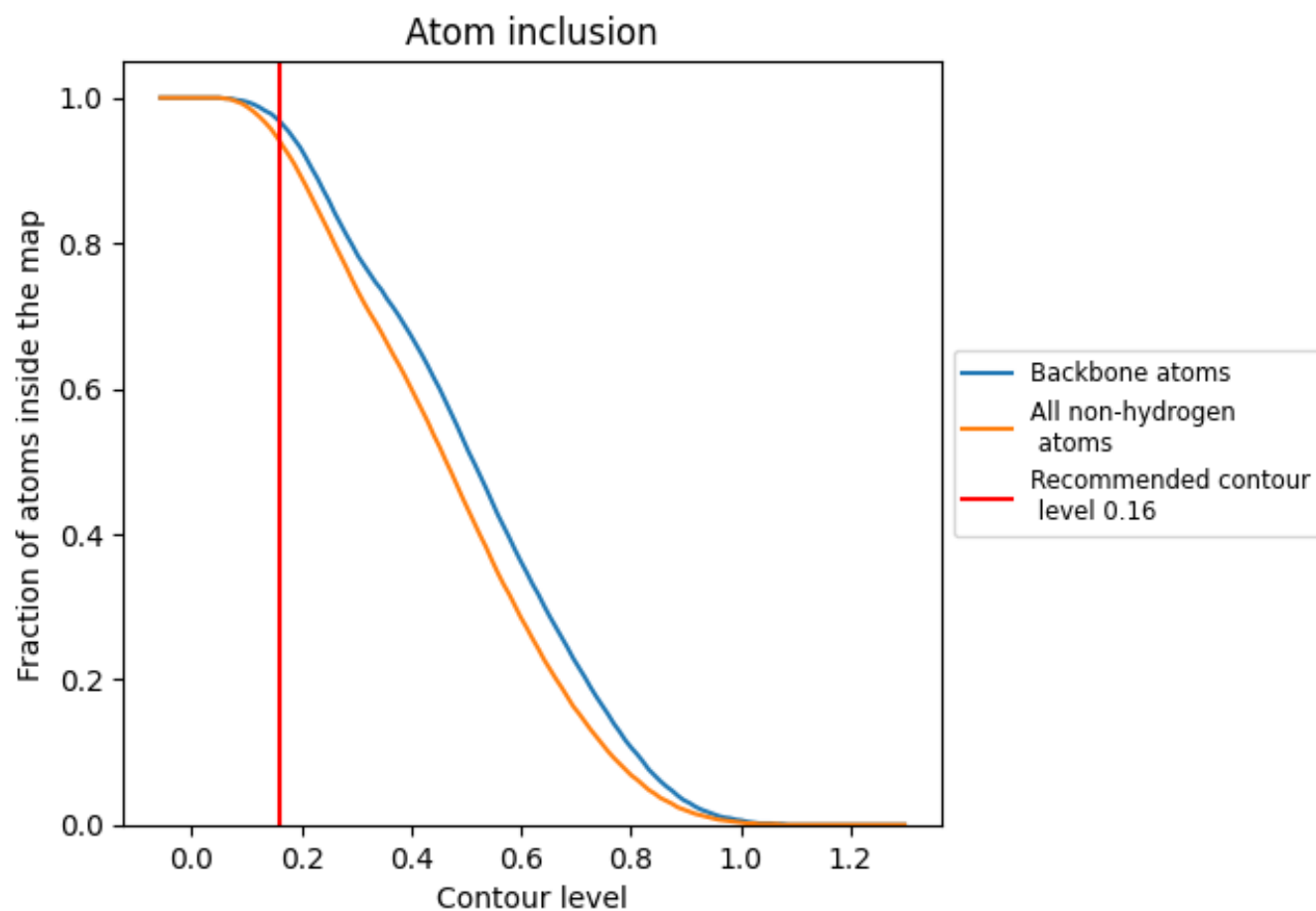
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

