



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:05 AM UTC

PDB ID : 8E71 / pdb\_00008e71  
Title : Staphylococcus aureus ClpP in complex with compound 3471  
Authors : Lee, R.E.; Griffith, E.C.  
Deposited on : 2022-08-23  
Resolution : 1.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

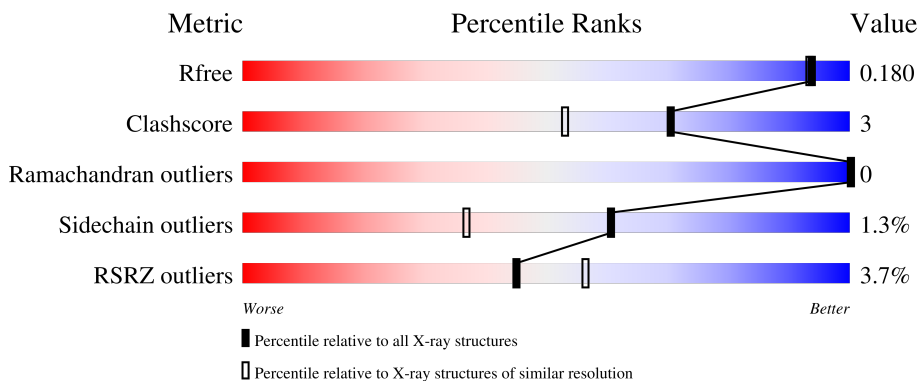
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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.



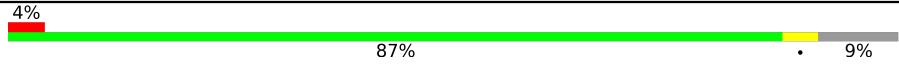

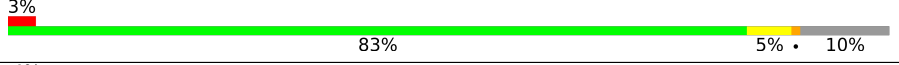



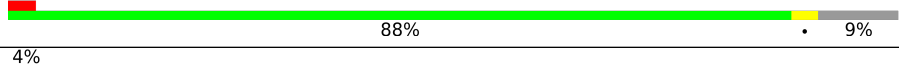

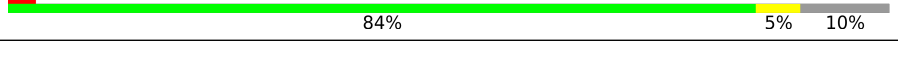
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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

Mol	Chain	Length	Quality of chain
1	A	203	
1	B	203	
1	C	203	
1	D	203	
1	E	203	

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Mol	Chain	Length	Quality of chain
1	F	203	 4% 87% 5% 4% 10%
1	G	203	 2% 86% 5% 7% 10%
1	I	203	 3% 83% 5% 9% 10%
1	K	203	 4% 85% 5% 6% 10%
1	L	203	 3% 84% 5% 10% 11%
1	M	203	 3% 86% 5% 6% 10%
1	N	203	 3% 88% 5% 4% 9%
1	S	203	 4% 87% 5% 6% 8%
1	T	203	 3% 84% 5% 10% 10%

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
2	MPD	C	301	-	-	X	-
2	MPD	E	301	-	-	X	-
2	MPD	G	302	-	-	X	-
2	MPD	I	301	-	-	X	-
2	MPD	K	301	-	-	X	-
2	MPD	L	301	-	-	X	-
2	MPD	M	301	-	-	X	-
2	MPD	N	301	-	-	X	-
2	MPD	S	301	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22593 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1397	883	237	271	6	0	0	0
1	B	182	1394	881	236	271	6	0	0	0
1	C	182	1391	878	236	271	6	0	0	0
1	D	181	1385	875	239	265	6	0	1	0
1	E	182	1390	878	235	271	6	0	0	0
1	F	185	1401	885	238	272	6	0	0	0
1	G	182	1405	887	240	272	6	0	1	0
1	I	182	1386	876	235	269	6	0	0	0
1	K	182	1391	878	236	271	6	0	0	0
1	L	181	1398	883	237	272	6	0	1	0
1	M	182	1394	881	236	271	6	0	0	0
1	N	185	1405	887	238	274	6	0	0	0
1	S	186	1410	890	239	275	6	0	0	0
1	T	182	1386	876	234	270	6	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	LEU	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	-	expression tag	UNP Q2G036
A	198	HIS	-	expression tag	UNP Q2G036
A	199	HIS	-	expression tag	UNP Q2G036
A	200	HIS	-	expression tag	UNP Q2G036
A	201	HIS	-	expression tag	UNP Q2G036
A	202	HIS	-	expression tag	UNP Q2G036
A	203	HIS	-	expression tag	UNP Q2G036
B	196	LEU	-	expression tag	UNP Q2G036
B	197	GLU	-	expression tag	UNP Q2G036
B	198	HIS	-	expression tag	UNP Q2G036
B	199	HIS	-	expression tag	UNP Q2G036
B	200	HIS	-	expression tag	UNP Q2G036
B	201	HIS	-	expression tag	UNP Q2G036
B	202	HIS	-	expression tag	UNP Q2G036
B	203	HIS	-	expression tag	UNP Q2G036
C	196	LEU	-	expression tag	UNP Q2G036
C	197	GLU	-	expression tag	UNP Q2G036
C	198	HIS	-	expression tag	UNP Q2G036
C	199	HIS	-	expression tag	UNP Q2G036
C	200	HIS	-	expression tag	UNP Q2G036
C	201	HIS	-	expression tag	UNP Q2G036
C	202	HIS	-	expression tag	UNP Q2G036
C	203	HIS	-	expression tag	UNP Q2G036
D	196	LEU	-	expression tag	UNP Q2G036
D	197	GLU	-	expression tag	UNP Q2G036
D	198	HIS	-	expression tag	UNP Q2G036
D	199	HIS	-	expression tag	UNP Q2G036
D	200	HIS	-	expression tag	UNP Q2G036
D	201	HIS	-	expression tag	UNP Q2G036
D	202	HIS	-	expression tag	UNP Q2G036
D	203	HIS	-	expression tag	UNP Q2G036
E	196	LEU	-	expression tag	UNP Q2G036
E	197	GLU	-	expression tag	UNP Q2G036
E	198	HIS	-	expression tag	UNP Q2G036
E	199	HIS	-	expression tag	UNP Q2G036
E	200	HIS	-	expression tag	UNP Q2G036
E	201	HIS	-	expression tag	UNP Q2G036
E	202	HIS	-	expression tag	UNP Q2G036
E	203	HIS	-	expression tag	UNP Q2G036
F	196	LEU	-	expression tag	UNP Q2G036
F	197	GLU	-	expression tag	UNP Q2G036
F	198	HIS	-	expression tag	UNP Q2G036

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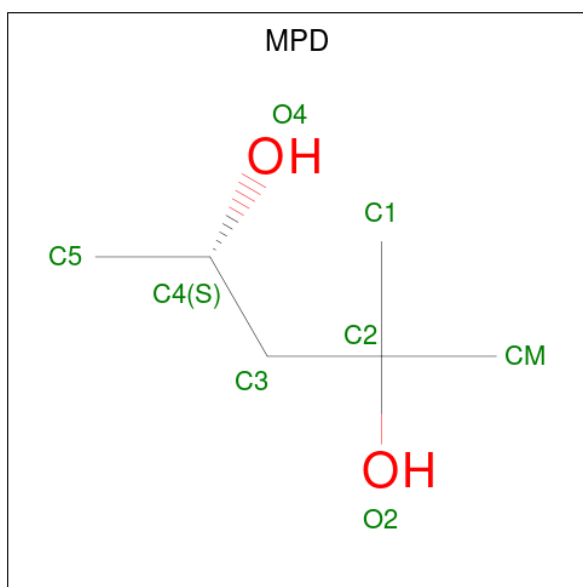
Chain	Residue	Modelled	Actual	Comment	Reference
F	199	HIS	-	expression tag	UNP Q2G036
F	200	HIS	-	expression tag	UNP Q2G036
F	201	HIS	-	expression tag	UNP Q2G036
F	202	HIS	-	expression tag	UNP Q2G036
F	203	HIS	-	expression tag	UNP Q2G036
G	196	LEU	-	expression tag	UNP Q2G036
G	197	GLU	-	expression tag	UNP Q2G036
G	198	HIS	-	expression tag	UNP Q2G036
G	199	HIS	-	expression tag	UNP Q2G036
G	200	HIS	-	expression tag	UNP Q2G036
G	201	HIS	-	expression tag	UNP Q2G036
G	202	HIS	-	expression tag	UNP Q2G036
G	203	HIS	-	expression tag	UNP Q2G036
I	196	LEU	-	expression tag	UNP Q2G036
I	197	GLU	-	expression tag	UNP Q2G036
I	198	HIS	-	expression tag	UNP Q2G036
I	199	HIS	-	expression tag	UNP Q2G036
I	200	HIS	-	expression tag	UNP Q2G036
I	201	HIS	-	expression tag	UNP Q2G036
I	202	HIS	-	expression tag	UNP Q2G036
I	203	HIS	-	expression tag	UNP Q2G036
K	196	LEU	-	expression tag	UNP Q2G036
K	197	GLU	-	expression tag	UNP Q2G036
K	198	HIS	-	expression tag	UNP Q2G036
K	199	HIS	-	expression tag	UNP Q2G036
K	200	HIS	-	expression tag	UNP Q2G036
K	201	HIS	-	expression tag	UNP Q2G036
K	202	HIS	-	expression tag	UNP Q2G036
K	203	HIS	-	expression tag	UNP Q2G036
L	196	LEU	-	expression tag	UNP Q2G036
L	197	GLU	-	expression tag	UNP Q2G036
L	198	HIS	-	expression tag	UNP Q2G036
L	199	HIS	-	expression tag	UNP Q2G036
L	200	HIS	-	expression tag	UNP Q2G036
L	201	HIS	-	expression tag	UNP Q2G036
L	202	HIS	-	expression tag	UNP Q2G036
L	203	HIS	-	expression tag	UNP Q2G036
M	196	LEU	-	expression tag	UNP Q2G036
M	197	GLU	-	expression tag	UNP Q2G036
M	198	HIS	-	expression tag	UNP Q2G036
M	199	HIS	-	expression tag	UNP Q2G036
M	200	HIS	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
M	201	HIS	-	expression tag	UNP Q2G036
M	202	HIS	-	expression tag	UNP Q2G036
M	203	HIS	-	expression tag	UNP Q2G036
N	196	LEU	-	expression tag	UNP Q2G036
N	197	GLU	-	expression tag	UNP Q2G036
N	198	HIS	-	expression tag	UNP Q2G036
N	199	HIS	-	expression tag	UNP Q2G036
N	200	HIS	-	expression tag	UNP Q2G036
N	201	HIS	-	expression tag	UNP Q2G036
N	202	HIS	-	expression tag	UNP Q2G036
N	203	HIS	-	expression tag	UNP Q2G036
S	196	LEU	-	expression tag	UNP Q2G036
S	197	GLU	-	expression tag	UNP Q2G036
S	198	HIS	-	expression tag	UNP Q2G036
S	199	HIS	-	expression tag	UNP Q2G036
S	200	HIS	-	expression tag	UNP Q2G036
S	201	HIS	-	expression tag	UNP Q2G036
S	202	HIS	-	expression tag	UNP Q2G036
S	203	HIS	-	expression tag	UNP Q2G036
T	196	LEU	-	expression tag	UNP Q2G036
T	197	GLU	-	expression tag	UNP Q2G036
T	198	HIS	-	expression tag	UNP Q2G036
T	199	HIS	-	expression tag	UNP Q2G036
T	200	HIS	-	expression tag	UNP Q2G036
T	201	HIS	-	expression tag	UNP Q2G036
T	202	HIS	-	expression tag	UNP Q2G036
T	203	HIS	-	expression tag	UNP Q2G036

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



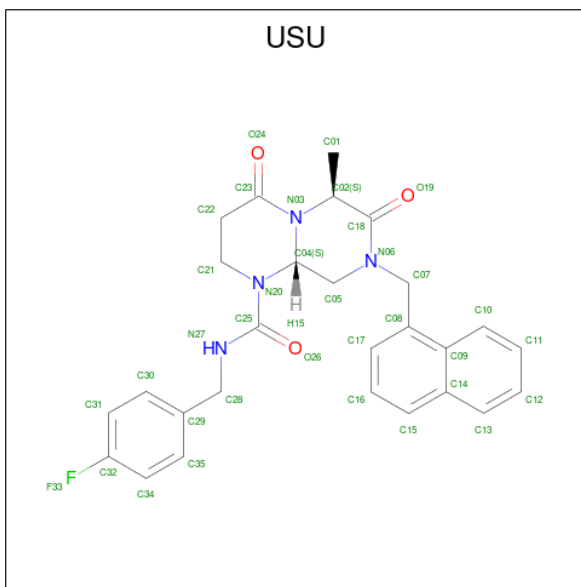
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0
2	M	1	Total C O 8 6 2	0	0
2	N	1	Total C O 8 6 2	0	0
2	S	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	C	O	0	0
			8	6	2		
2	T	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is (5S,6S,9aS)-N-[(4-fluorophenyl)methyl]-6-methyl-8-[(naphthalen-1-yl)methyl]-4,7-dioxohexahydro-2H-pyrazino[1,2-a]pyrimidine-1(6H)-carboxamide (CCD ID: USU) (formula: C<sub>27</sub>H<sub>27</sub>FN<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	B	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	C	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	D	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	E	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	F	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	G	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	I	1	Total	C	F	N	O	0	0
			35	27	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	L	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	M	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	N	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	S	1	Total	C	F	N	O	0	0
			35	27	1	4	3		
3	T	1	Total	C	F	N	O	0	0
			35	27	1	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	175	Total	O	0	0
			175	175		
4	C	144	Total	O	0	0
			144	144		
4	D	161	Total	O	0	0
			161	161		
4	E	170	Total	O	0	0
			170	170		
4	F	175	Total	O	0	0
			175	175		
4	G	191	Total	O	0	0
			191	191		
4	I	170	Total	O	0	0
			170	170		
4	K	172	Total	O	0	0
			172	172		
4	L	154	Total	O	0	0
			154	154		
4	M	160	Total	O	0	0
			160	160		
4	N	189	Total	O	0	0
			189	189		
4	S	186	Total	O	0	0
			186	186		

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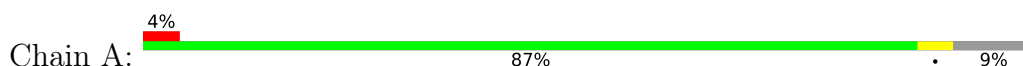
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	T	202	Total 202	O 202	0	0

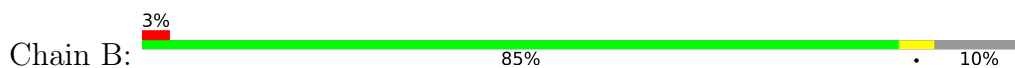
### 3 Residue-property plots [i](#)

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

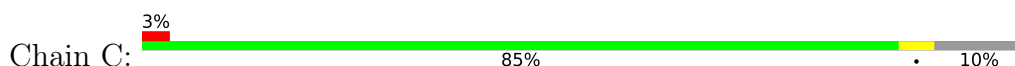
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



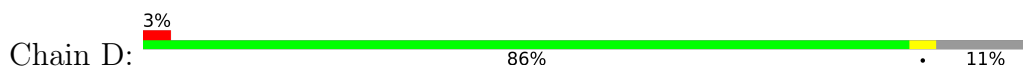
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



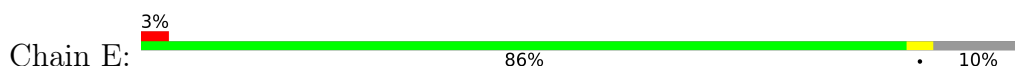
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



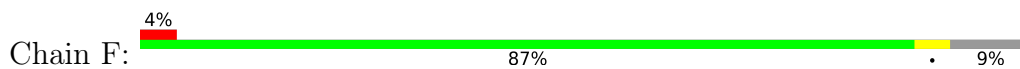
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



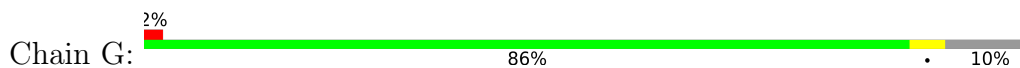
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



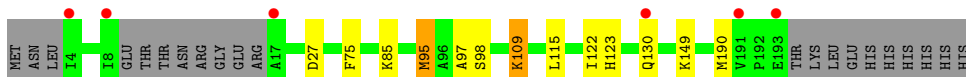
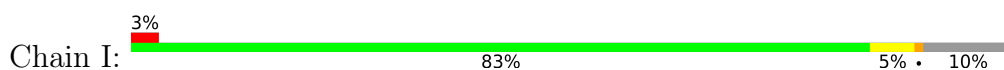
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



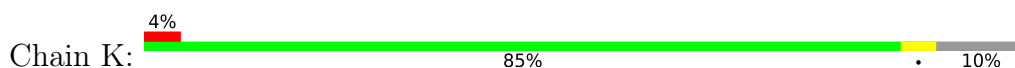
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



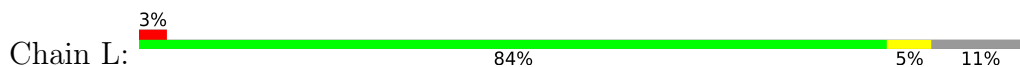
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



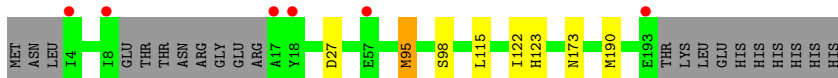
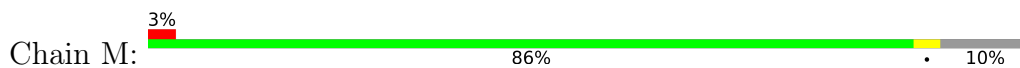
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



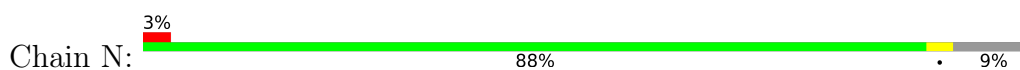
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



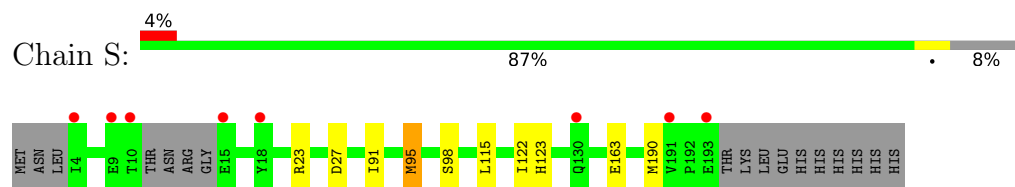
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



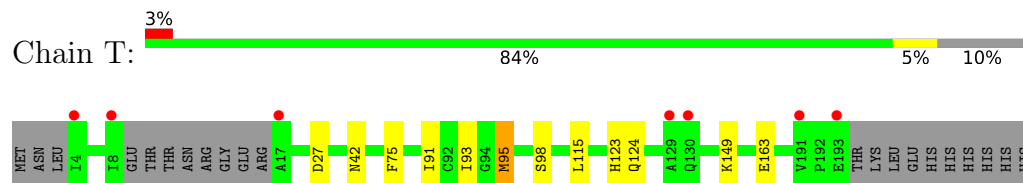
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.68Å 126.99Å 145.85Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	31.54 – 1.57 31.54 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.54-1.57) 99.5 (31.54-1.57)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 1.57Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.155 , 0.171 0.168 , 0.180	Depositor DCC
$R_{free}$ test set	23990 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, USU

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	1.09	1/1415 (0.1%)	1.15	1/1914 (0.1%)
1	B	1.10	0/1412	1.15	0/1907
1	C	1.04	0/1409	1.11	0/1903
1	D	1.09	0/1403	1.18	0/1895
1	E	1.03	0/1408	1.11	0/1903
1	F	1.07	0/1419	1.14	0/1919
1	G	1.08	0/1423	1.13	0/1921
1	I	1.08	1/1404 (0.1%)	1.11	0/1898
1	K	1.04	0/1409	1.10	1/1903 (0.1%)
1	L	1.07	0/1416	1.14	2/1912 (0.1%)
1	M	1.02	0/1412	1.10	0/1907
1	N	1.09	0/1423	1.12	0/1924
1	S	1.07	0/1428	1.15	1/1931 (0.1%)
1	T	1.14	0/1404	1.19	3/1898 (0.2%)
All	All	1.07	2/19785 (0.0%)	1.13	8/26735 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	130	GLN	C-O	6.02	1.30	1.23
1	A	53	ALA	C-O	5.52	1.30	1.24

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	163	GLU	CB-CG-CD	7.81	125.87	112.60
1	L	57	GLU	CB-CG-CD	6.69	123.98	112.60
1	L	182	GLU	CB-CG-CD	6.24	123.20	112.60
1	T	42	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	A	57	GLU	CB-CG-CD	5.49	121.94	112.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1397	0	1393	6	0
1	B	1394	0	1408	8	0
1	C	1391	0	1399	10	0
1	D	1385	0	1397	5	0
1	E	1390	0	1397	9	0
1	F	1401	0	1399	8	0
1	G	1405	0	1420	8	0
1	I	1386	0	1393	20	0
1	K	1391	0	1399	8	0
1	L	1398	0	1413	10	0
1	M	1394	0	1408	9	0
1	N	1405	0	1403	8	0
1	S	1410	0	1405	11	0
1	T	1386	0	1391	12	0
2	A	8	0	14	4	0
2	B	8	0	14	5	0
2	C	8	0	14	7	0
2	D	8	0	14	4	0
2	E	8	0	14	6	0
2	F	8	0	14	5	0
2	G	16	0	28	6	0
2	I	8	0	14	6	0
2	K	8	0	14	7	0
2	L	8	0	14	6	0
2	M	8	0	14	7	0
2	N	8	0	14	6	0
2	S	16	0	28	9	0
2	T	8	0	14	5	0
3	A	35	0	0	0	0
3	B	35	0	0	0	0
3	C	35	0	0	0	0
3	D	35	0	0	0	0
3	E	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	35	0	0	0	0
3	G	35	0	0	0	0
3	I	35	0	0	0	0
3	K	35	0	0	0	0
3	L	35	0	0	0	0
3	M	35	0	0	0	0
3	N	35	0	0	0	0
3	S	35	0	0	0	0
3	T	35	0	0	0	0
4	A	193	0	0	1	0
4	B	175	0	0	0	0
4	C	144	0	0	1	0
4	D	161	0	0	0	0
4	E	170	0	0	1	0
4	F	175	0	0	3	0
4	G	191	0	0	1	0
4	I	170	0	0	6	0
4	K	172	0	0	3	0
4	L	154	0	0	0	0
4	M	160	0	0	3	0
4	N	189	0	0	2	0
4	S	186	0	0	0	0
4	T	202	0	0	1	0
All	All	22593	0	19849	136	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 3.

The worst 5 of 136 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)
1:S:23:ARG:HH21	2:S:302:MPD:HM3	1.28	0.97
1:T:91:ILE:HD11	1:T:115:LEU:HD11	1.48	0.95
1:T:91:ILE:HD11	1:T:115:LEU:CD1	2.09	0.82
1:M:98:SER:HA	2:M:301:MPD:H11	1.78	0.64
1:T:123:HIS:H	2:T:301:MPD:C1	2.10	0.64

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 X-ray entries followed by that with respect to entries of similar resolution.

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	181/203 (89%)	179 (99%)	2 (1%)	0	100	100
1	B	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	C	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	D	178/203 (88%)	176 (99%)	2 (1%)	0	100	100
1	E	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	F	181/203 (89%)	178 (98%)	3 (2%)	0	100	100
1	G	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	I	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	K	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	L	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	M	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	N	181/203 (89%)	178 (98%)	3 (2%)	0	100	100
1	S	182/203 (90%)	179 (98%)	3 (2%)	0	100	100
1	T	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
All	All	2506/2842 (88%)	2466 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	146/171 (85%)	145 (99%)	1 (1%)	76	61
1	B	149/171 (87%)	147 (99%)	2 (1%)	61	37
1	C	148/171 (86%)	146 (99%)	2 (1%)	59	34
1	D	146/171 (85%)	144 (99%)	2 (1%)	59	34
1	E	148/171 (86%)	146 (99%)	2 (1%)	59	34
1	F	147/171 (86%)	146 (99%)	1 (1%)	76	61
1	G	150/171 (88%)	148 (99%)	2 (1%)	61	37
1	I	147/171 (86%)	144 (98%)	3 (2%)	48	20
1	K	148/171 (86%)	146 (99%)	2 (1%)	59	34
1	L	150/171 (88%)	148 (99%)	2 (1%)	61	37
1	M	149/171 (87%)	147 (99%)	2 (1%)	61	37
1	N	148/171 (86%)	147 (99%)	1 (1%)	76	61
1	S	148/171 (86%)	146 (99%)	2 (1%)	59	34
1	T	147/171 (86%)	145 (99%)	2 (1%)	59	34
All	All	2071/2394 (86%)	2045 (99%)	26 (1%)	61	37

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	109	LYS
1	L	27	ASP
1	T	27	ASP
1	K	95	MET
1	L	95	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	117	ASN
1	M	65	ASN
1	S	151	ASN
1	N	42	ASN
1	N	151	ASN

### 5.3.3 RNA

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](#)

30 ligands are modelled in this entry.

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
3	USU	G	303	-	38,39,39	2.09	7 (18%)	47,56,56	1.68	13 (27%)
3	USU	M	302	-	38,39,39	2.50	10 (26%)	47,56,56	2.23	18 (38%)
2	MPD	E	301	-	7,7,7	0.41	0	9,10,10	0.90	0
2	MPD	G	302	-	7,7,7	0.60	0	9,10,10	0.90	0
3	USU	S	303	-	38,39,39	2.36	12 (31%)	47,56,56	1.68	11 (23%)
2	MPD	K	301	-	7,7,7	0.37	0	9,10,10	0.72	0
2	MPD	S	301	-	7,7,7	0.53	0	9,10,10	1.01	0
3	USU	F	302	-	38,39,39	1.94	11 (28%)	47,56,56	1.97	14 (29%)
2	MPD	L	301	-	7,7,7	0.28	0	9,10,10	0.80	0
3	USU	T	302	-	38,39,39	1.97	8 (21%)	47,56,56	2.04	14 (29%)
3	USU	K	302	-	38,39,39	1.89	9 (23%)	47,56,56	1.85	12 (25%)
3	USU	E	302	-	38,39,39	2.35	8 (21%)	47,56,56	1.85	11 (23%)
2	MPD	T	301	-	7,7,7	0.48	0	9,10,10	1.05	1 (11%)
2	MPD	S	302	-	7,7,7	0.33	0	9,10,10	0.78	0
3	USU	C	302	-	38,39,39	1.92	9 (23%)	47,56,56	1.75	12 (25%)
3	USU	I	302	-	38,39,39	2.10	9 (23%)	47,56,56	1.54	8 (17%)
2	MPD	M	301	-	7,7,7	0.41	0	9,10,10	0.58	0
2	MPD	C	301	-	7,7,7	0.45	0	9,10,10	0.35	0
2	MPD	G	301	-	7,7,7	0.27	0	9,10,10	0.50	0
2	MPD	D	301	-	7,7,7	0.52	0	9,10,10	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	N	301	-	7,7,7	0.53	0	9,10,10	0.80	0
3	USU	L	302	-	38,39,39	1.93	8 (21%)	47,56,56	1.84	9 (19%)
2	MPD	B	301	-	7,7,7	0.58	0	9,10,10	1.17	1 (11%)
2	MPD	I	301	-	7,7,7	0.59	0	9,10,10	1.08	1 (11%)
3	USU	A	302	-	38,39,39	2.26	11 (28%)	47,56,56	1.78	13 (27%)
3	USU	B	302	-	38,39,39	2.21	11 (28%)	47,56,56	2.02	14 (29%)
2	MPD	F	301	-	7,7,7	0.84	1 (14%)	9,10,10	1.05	1 (11%)
2	MPD	A	301	-	7,7,7	0.43	0	9,10,10	1.05	0
3	USU	D	302	-	38,39,39	2.52	11 (28%)	47,56,56	1.77	7 (14%)
3	USU	N	302	-	38,39,39	2.04	7 (18%)	47,56,56	1.65	8 (17%)

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
3	USU	G	303	-	-	0/13/46/46	0/5/5/5
3	USU	M	302	-	-	0/13/46/46	0/5/5/5
2	MPD	E	301	-	-	0/5/5/5	-
2	MPD	G	302	-	-	0/5/5/5	-
3	USU	S	303	-	-	0/13/46/46	0/5/5/5
2	MPD	K	301	-	-	0/5/5/5	-
2	MPD	S	301	-	-	0/5/5/5	-
3	USU	F	302	-	-	0/13/46/46	0/5/5/5
2	MPD	L	301	-	-	0/5/5/5	-
3	USU	T	302	-	-	0/13/46/46	0/5/5/5
3	USU	K	302	-	-	0/13/46/46	0/5/5/5
3	USU	E	302	-	-	0/13/46/46	0/5/5/5
2	MPD	T	301	-	-	0/5/5/5	-
2	MPD	S	302	-	-	0/5/5/5	-
3	USU	C	302	-	-	0/13/46/46	0/5/5/5
3	USU	I	302	-	-	0/13/46/46	0/5/5/5
2	MPD	M	301	-	-	0/5/5/5	-
2	MPD	C	301	-	-	0/5/5/5	-
2	MPD	G	301	-	-	0/5/5/5	-
2	MPD	D	301	-	-	0/5/5/5	-
2	MPD	N	301	-	-	0/5/5/5	-
3	USU	L	302	-	-	0/13/46/46	0/5/5/5
2	MPD	B	301	-	-	0/5/5/5	-
2	MPD	I	301	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	USU	A	302	-	-	0/13/46/46	0/5/5/5
3	USU	B	302	-	-	0/13/46/46	0/5/5/5
2	MPD	F	301	-	-	0/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
3	USU	D	302	-	-	0/13/46/46	0/5/5/5
3	USU	N	302	-	-	0/13/46/46	0/5/5/5

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	302	USU	C23-N03	10.20	1.44	1.35
3	D	302	USU	C23-N03	9.44	1.43	1.35
3	E	302	USU	C23-N03	9.25	1.43	1.35
3	S	303	USU	C23-N03	8.44	1.42	1.35
3	A	302	USU	C23-N03	7.87	1.42	1.35

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	USU	O24-C23-N03	-6.67	113.62	122.36
3	I	302	USU	C01-C02-C18	-5.99	103.20	109.99
3	T	302	USU	C01-C02-C18	-5.73	103.50	109.99
3	E	302	USU	O24-C23-N03	-5.67	114.93	122.36
3	F	302	USU	O24-C23-N03	-5.67	114.93	122.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 83 short contacts:

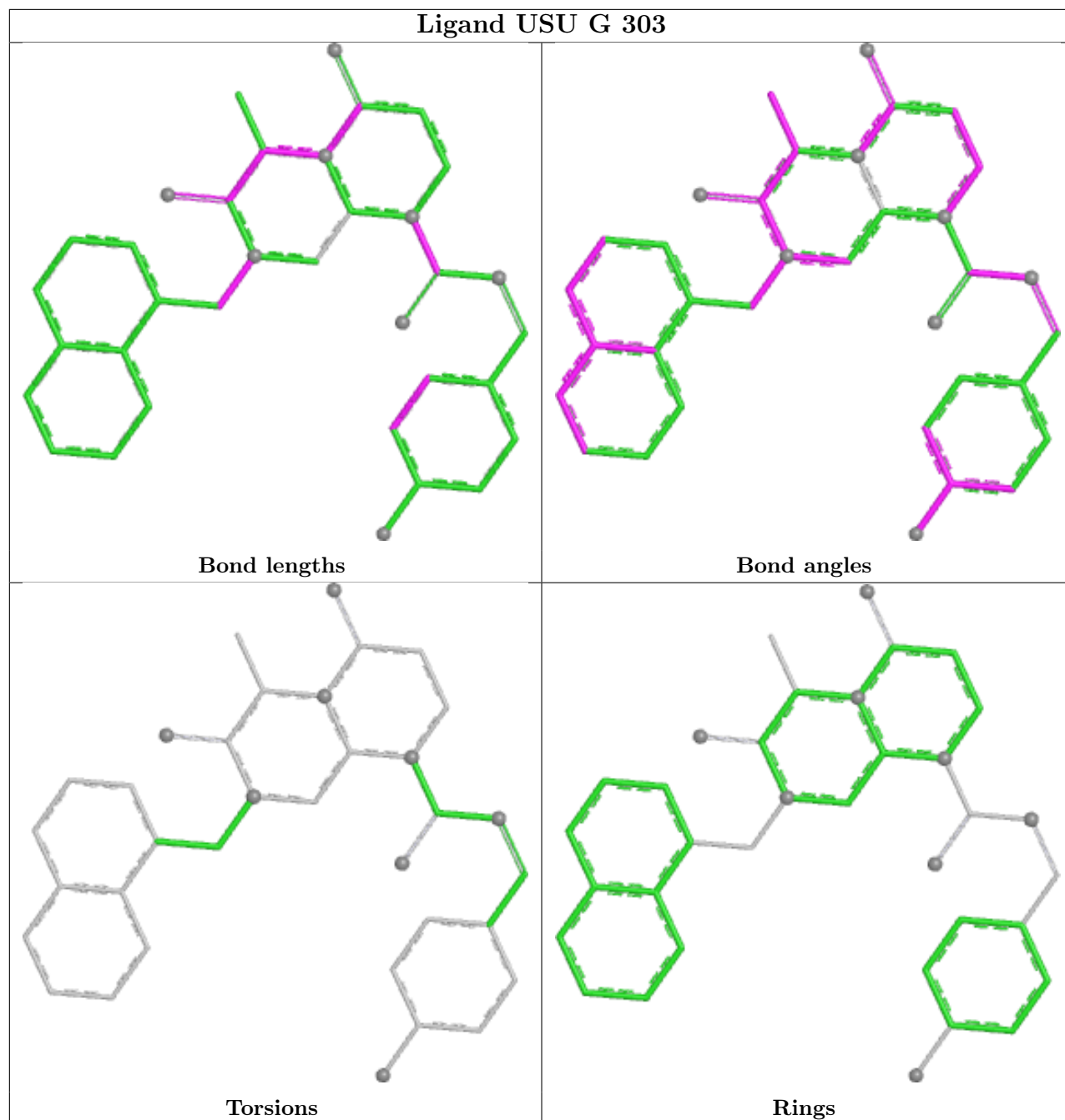
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	MPD	6	0
2	G	302	MPD	6	0
2	K	301	MPD	7	0
2	S	301	MPD	6	0
2	L	301	MPD	6	0
2	T	301	MPD	5	0
2	S	302	MPD	3	0
2	M	301	MPD	7	0
2	C	301	MPD	7	0
2	D	301	MPD	4	0

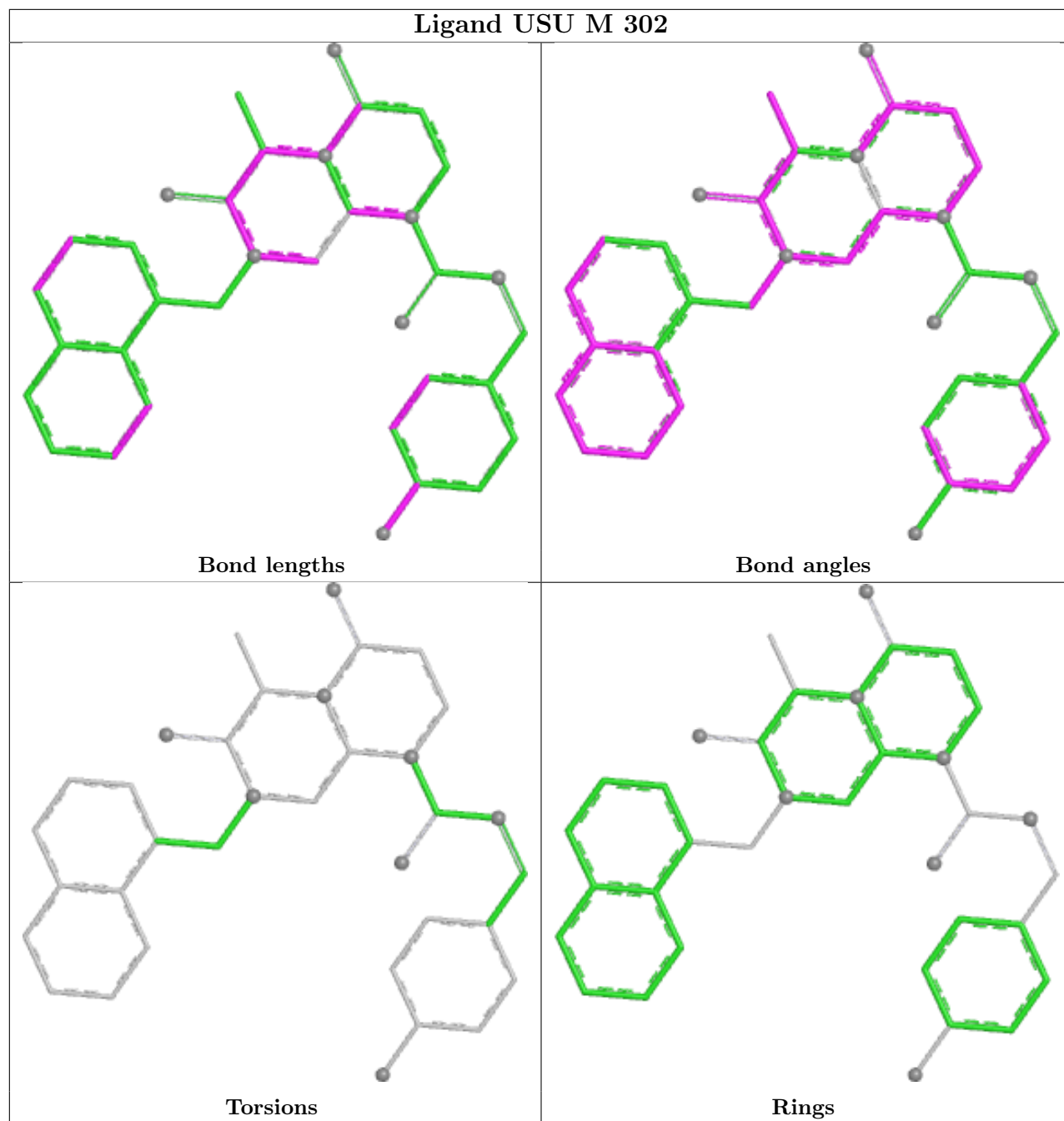
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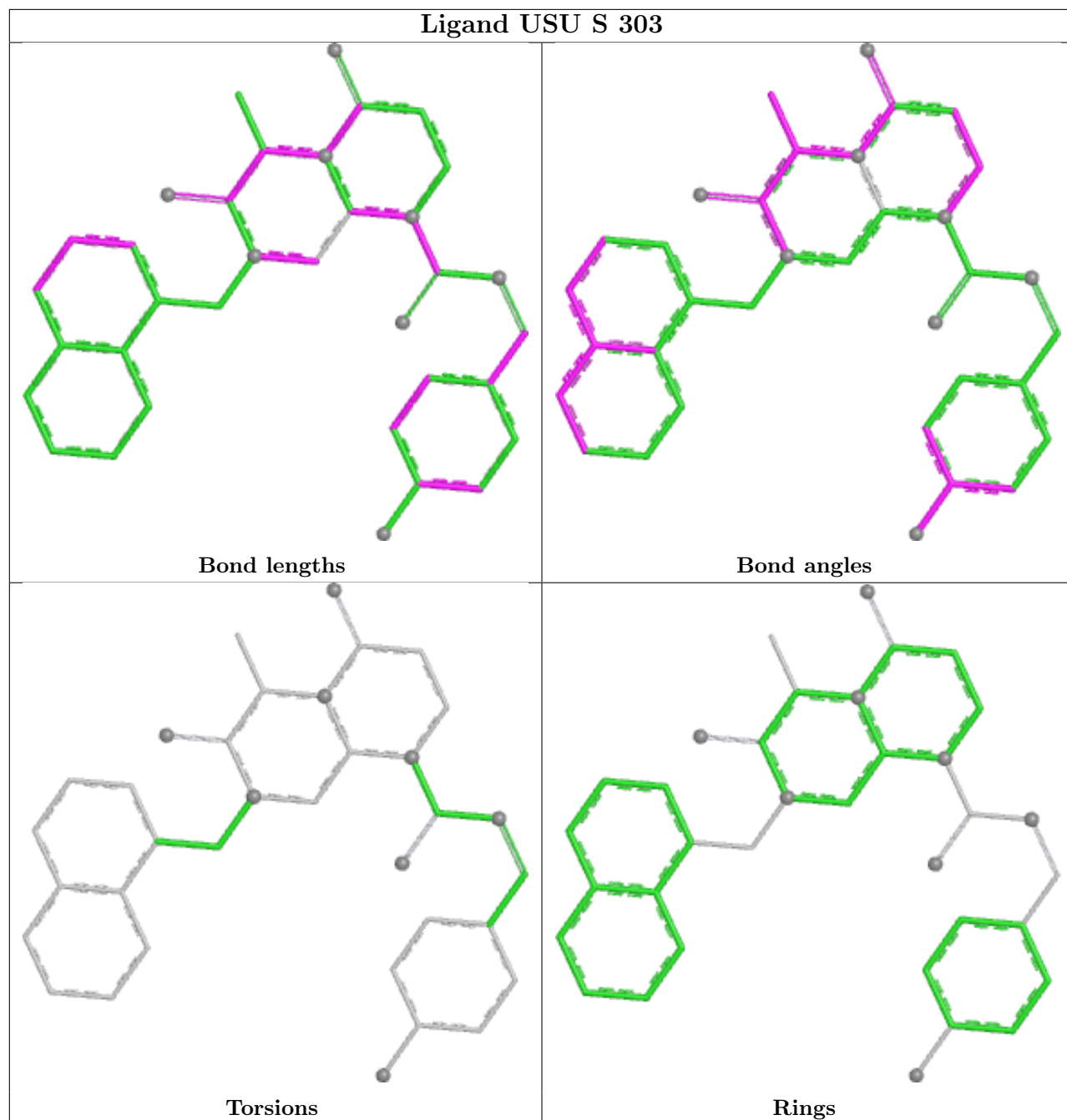
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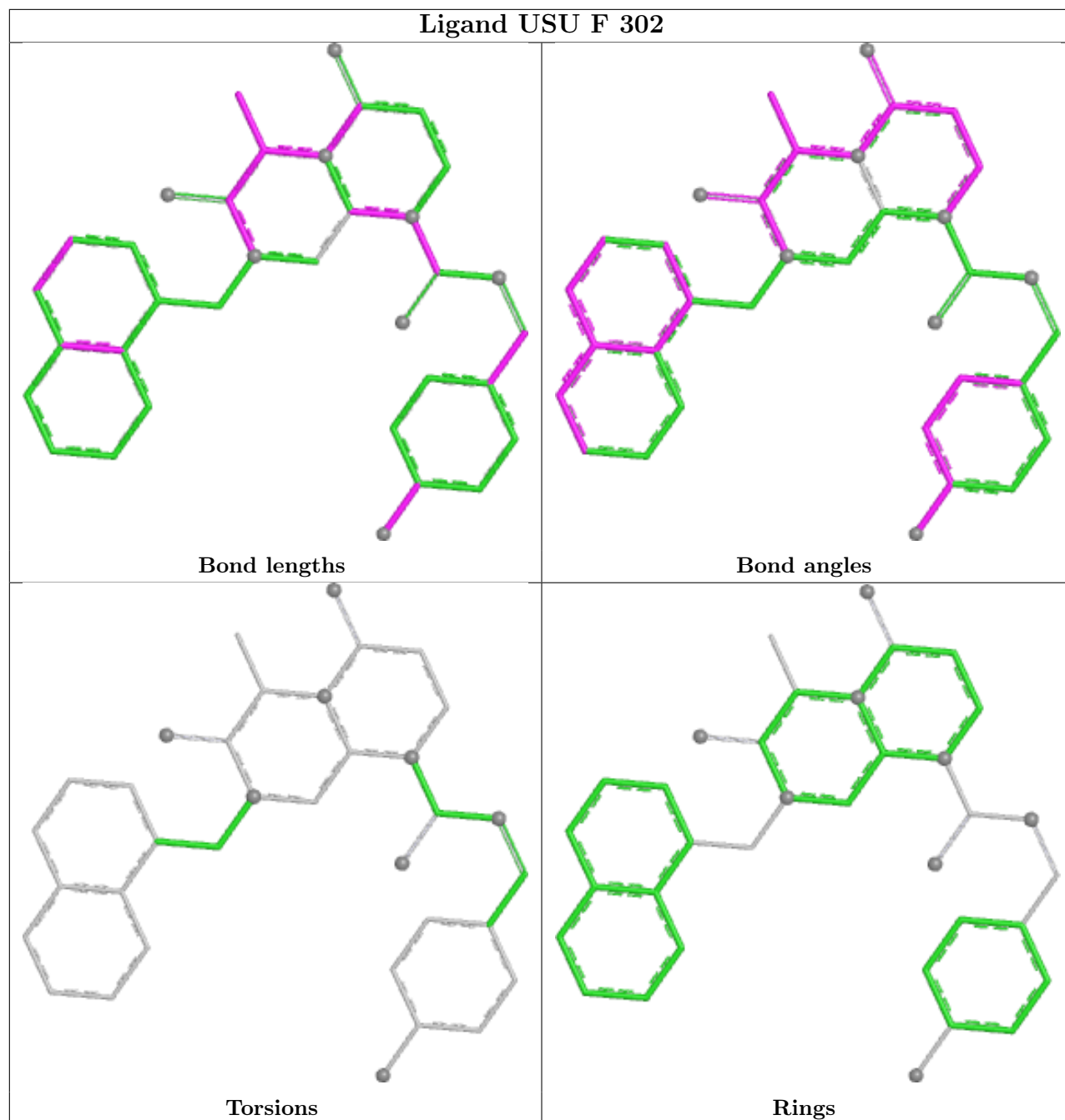
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	301	MPD	6	0
2	B	301	MPD	5	0
2	I	301	MPD	6	0
2	F	301	MPD	5	0
2	A	301	MPD	4	0

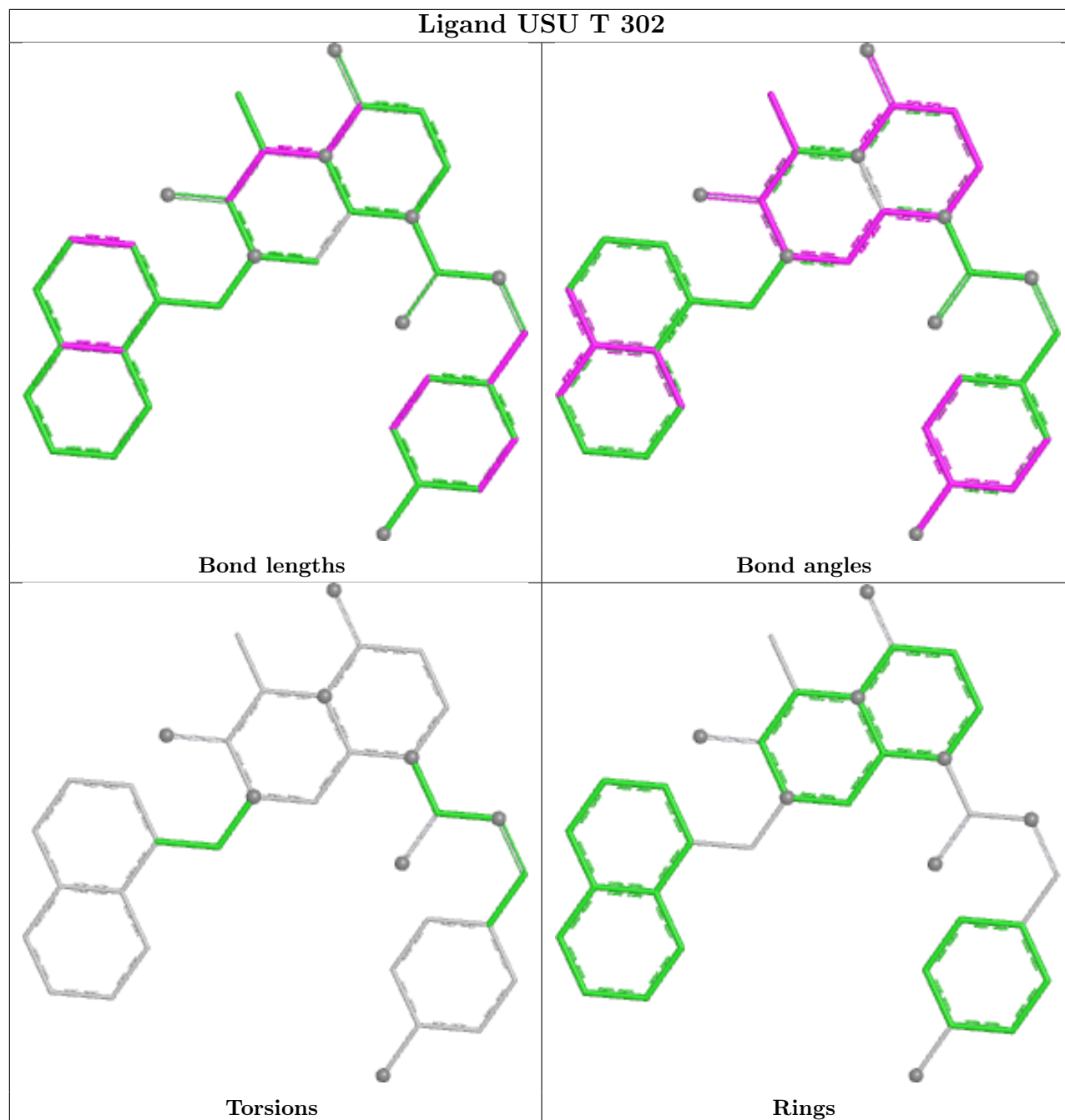
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

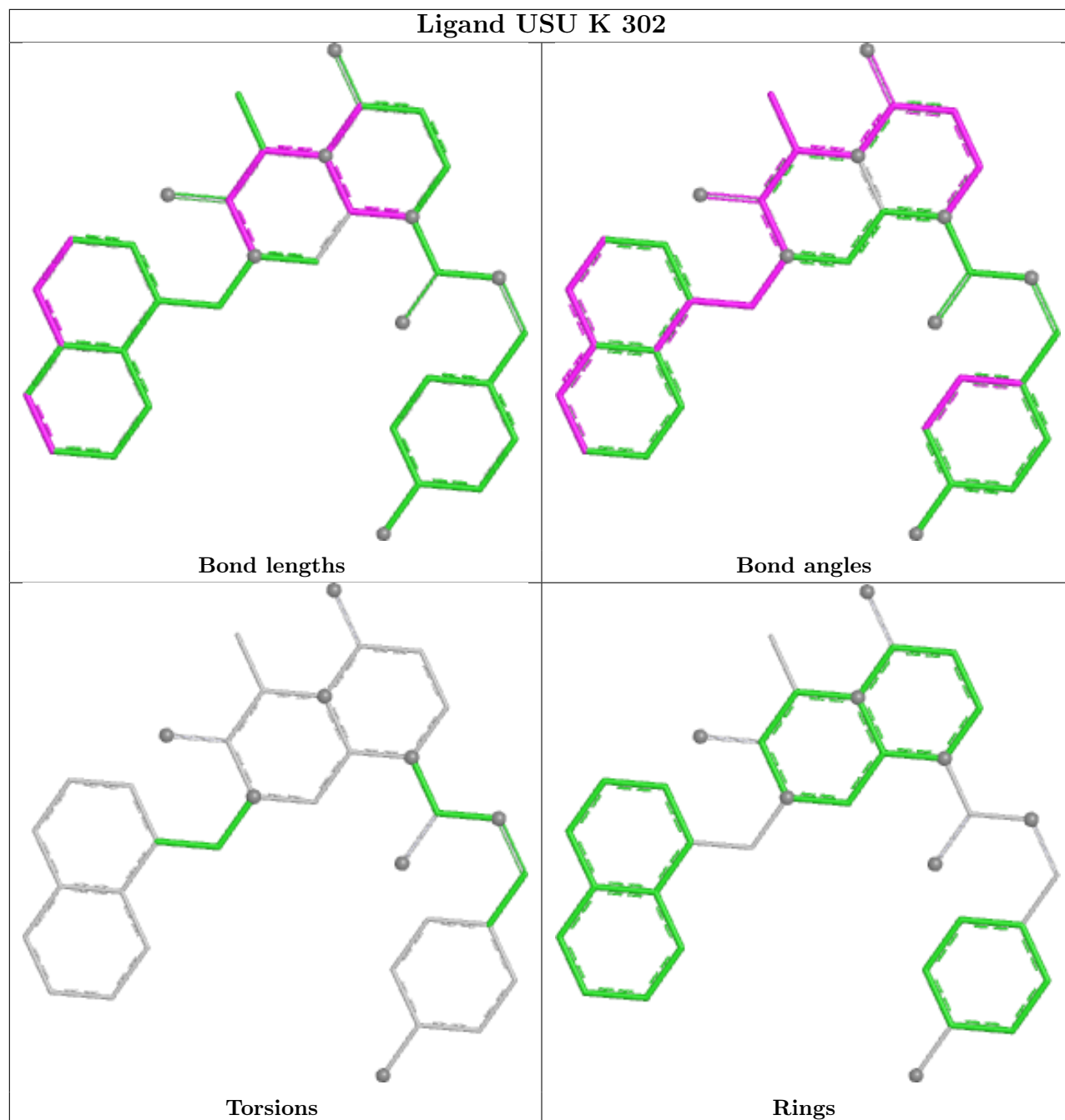


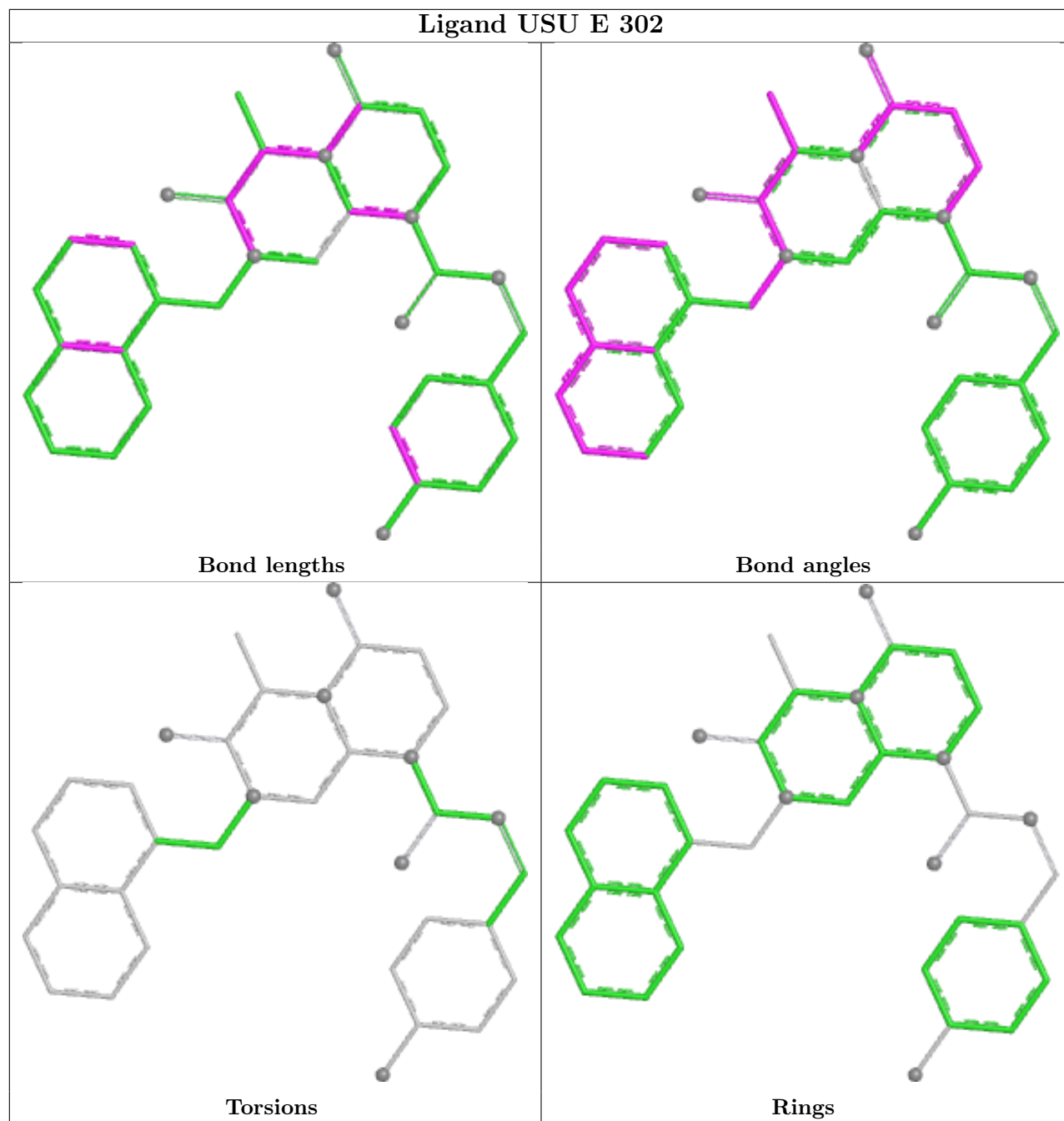


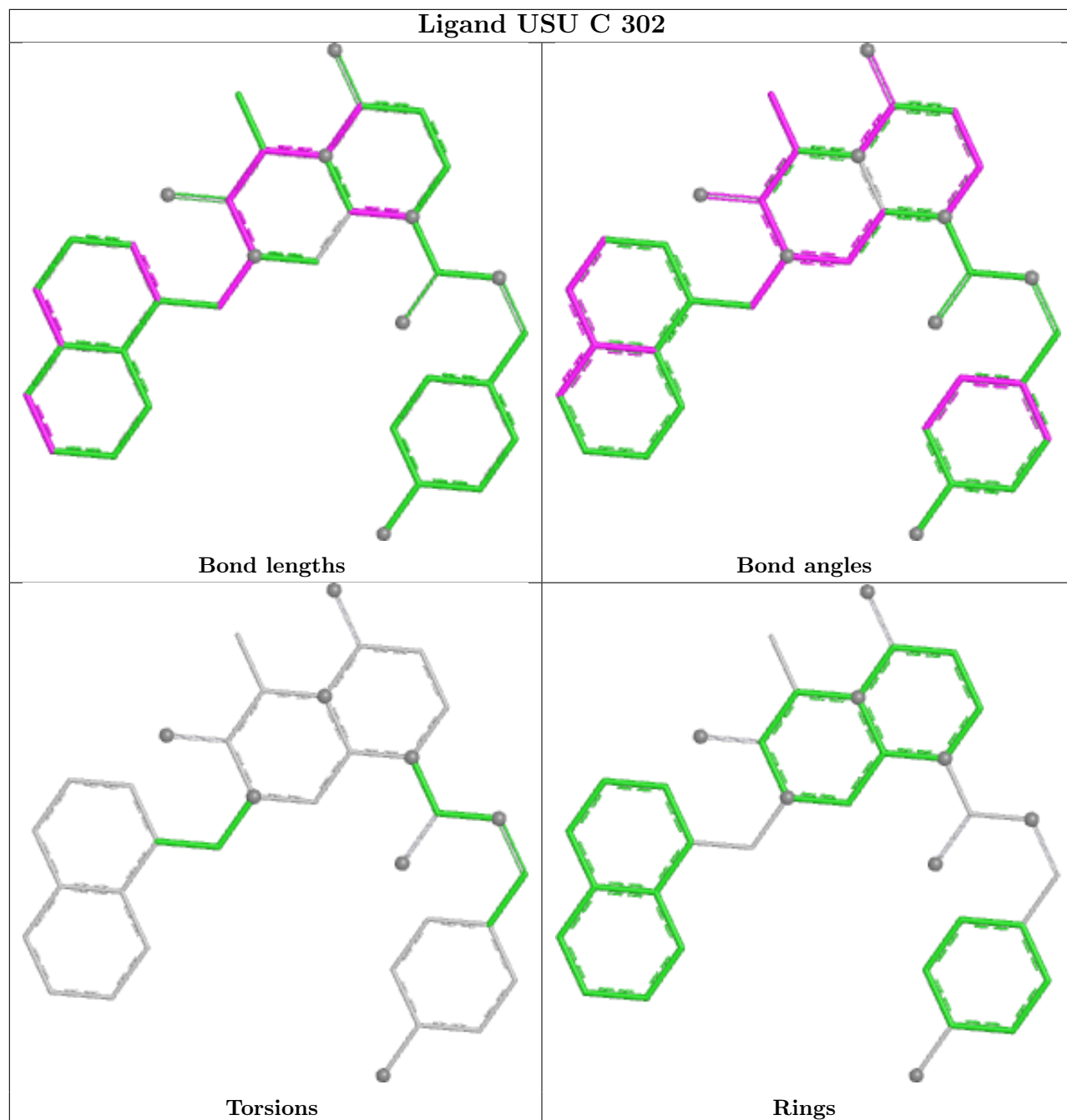


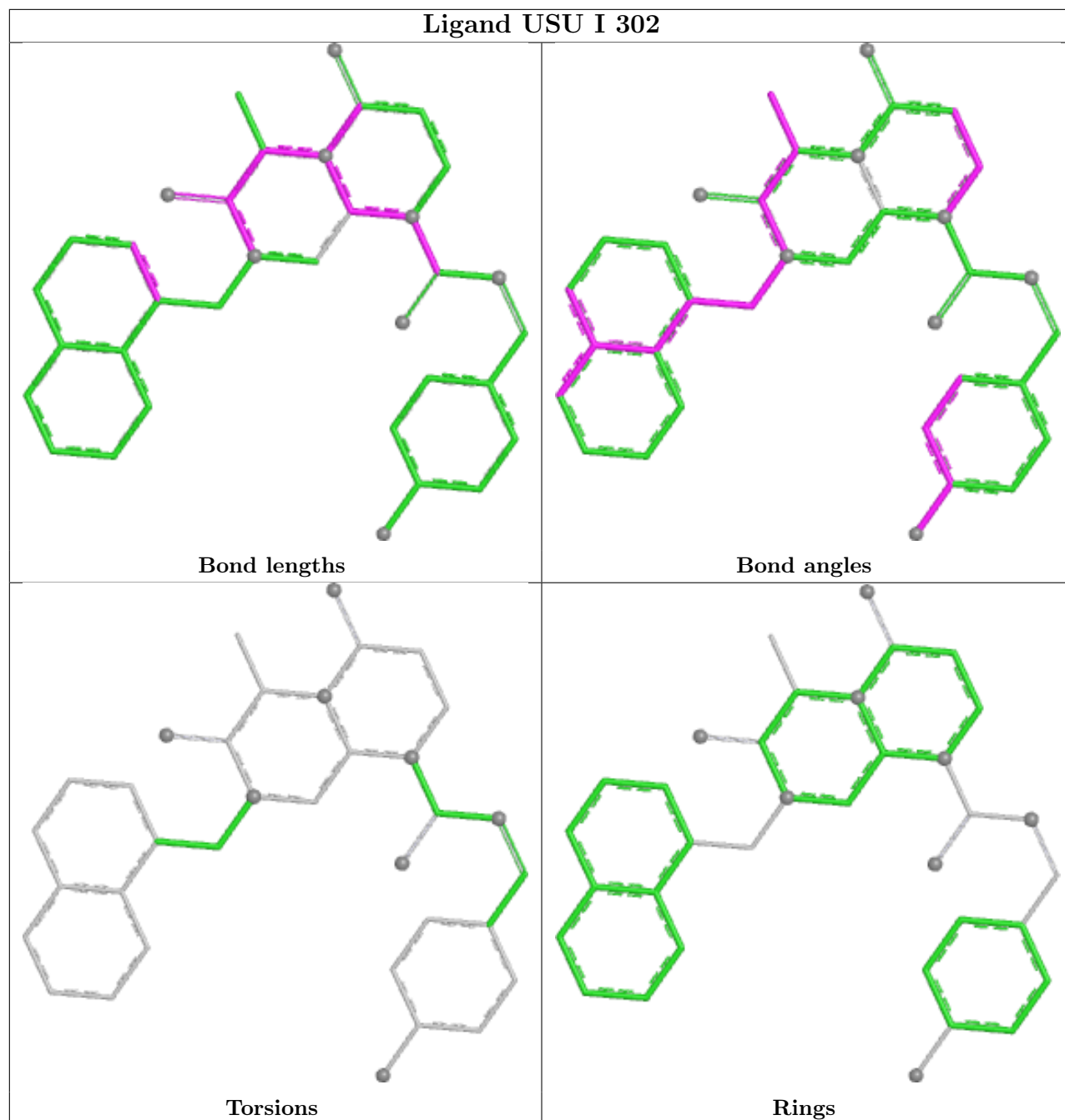


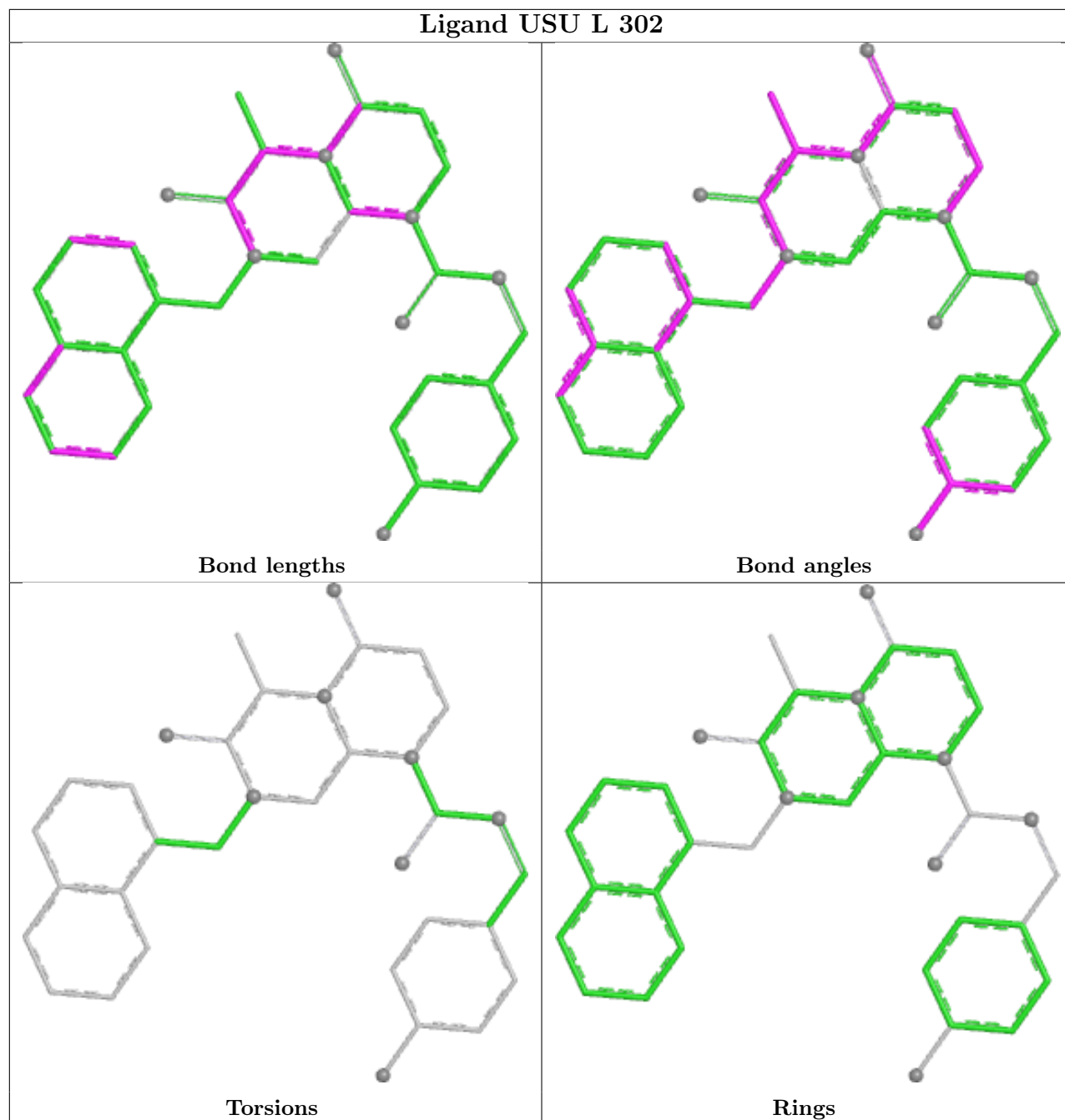


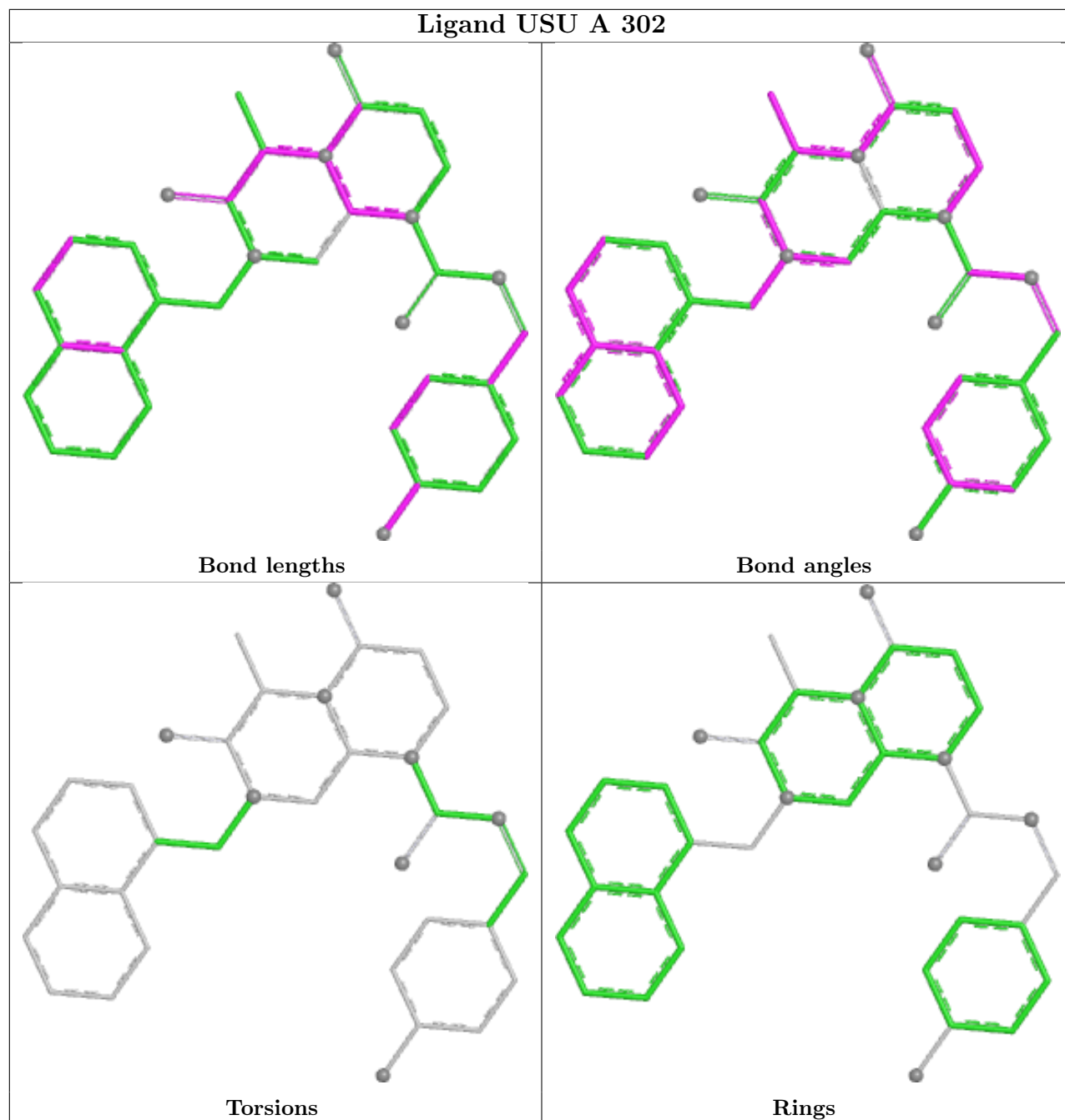


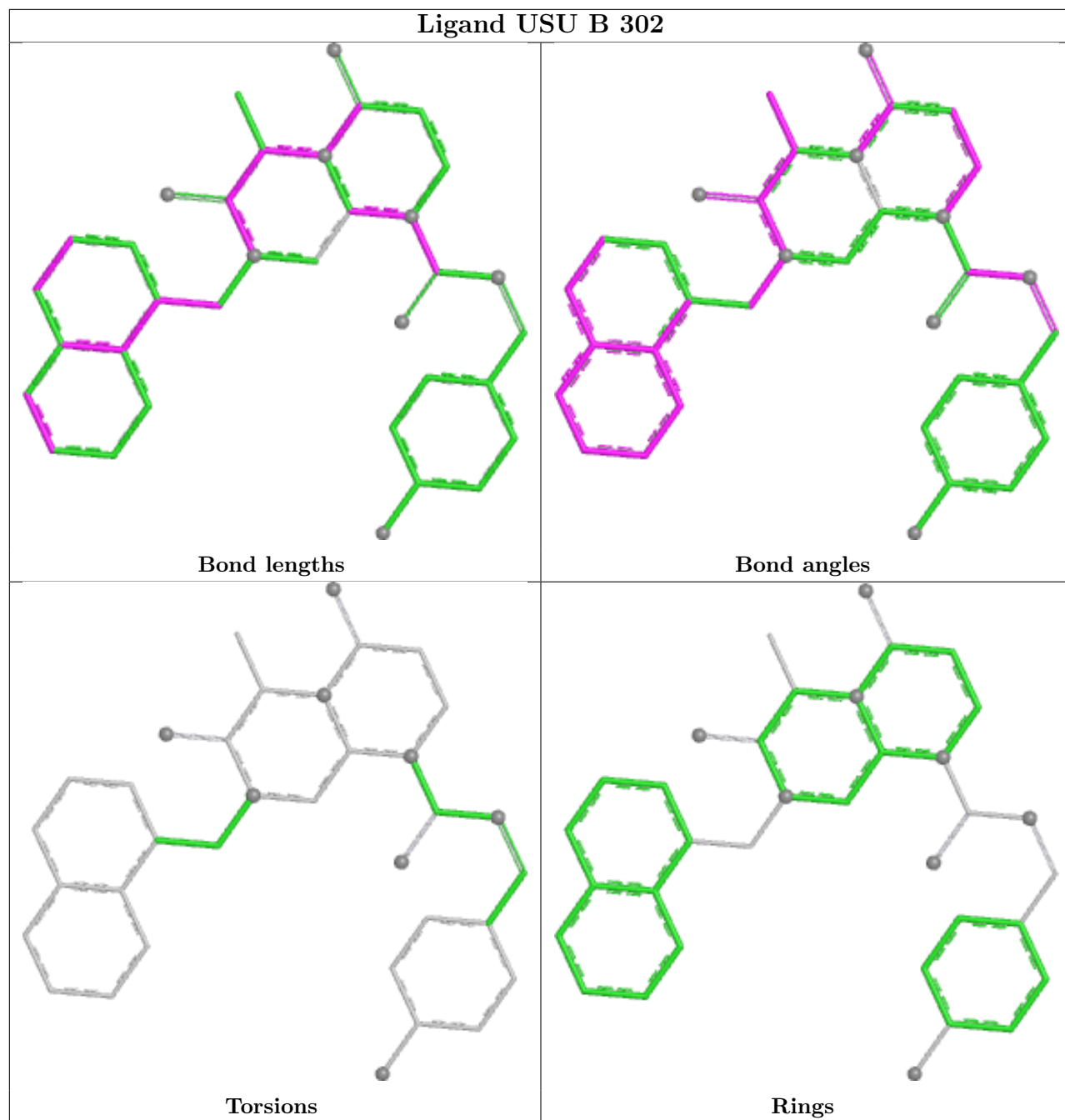


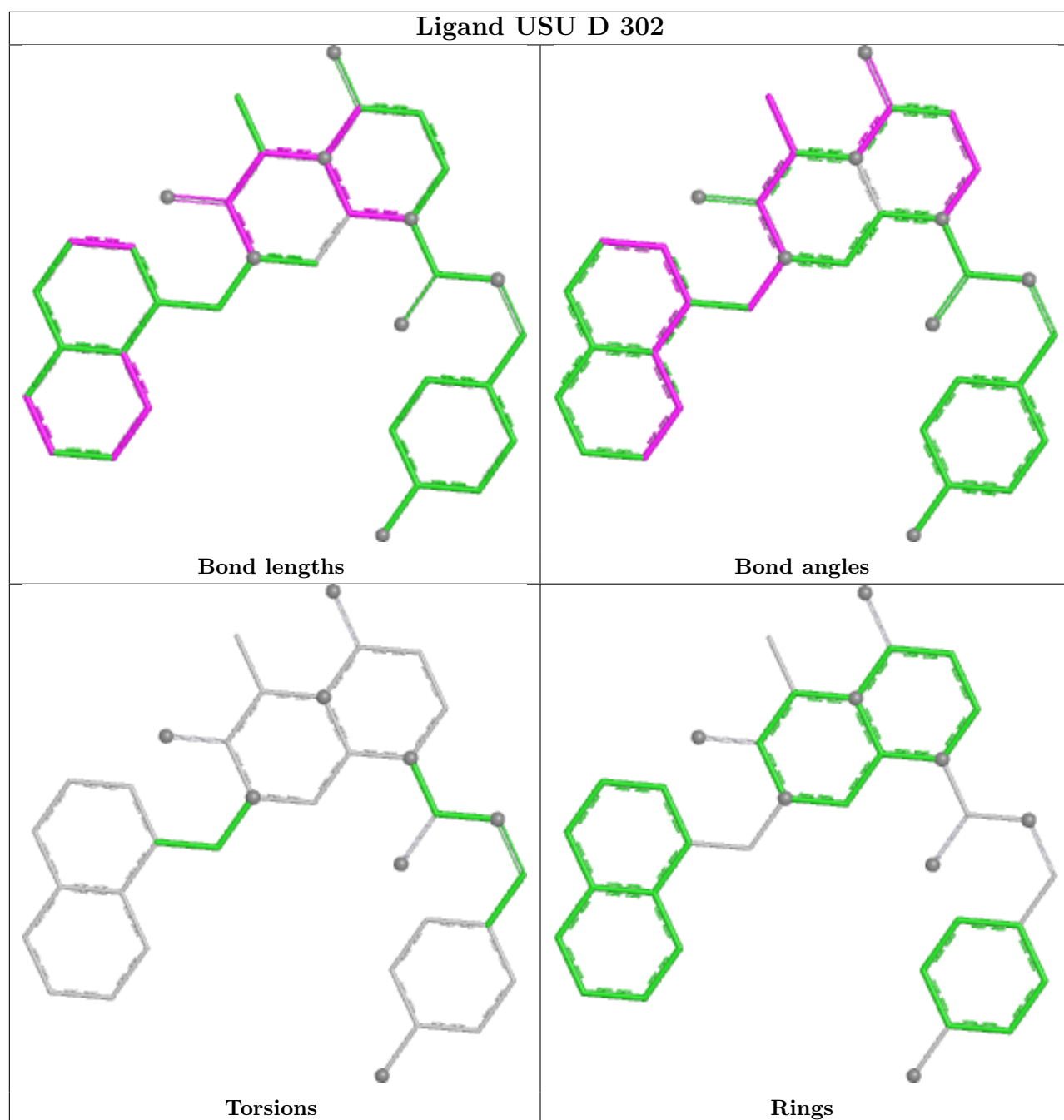


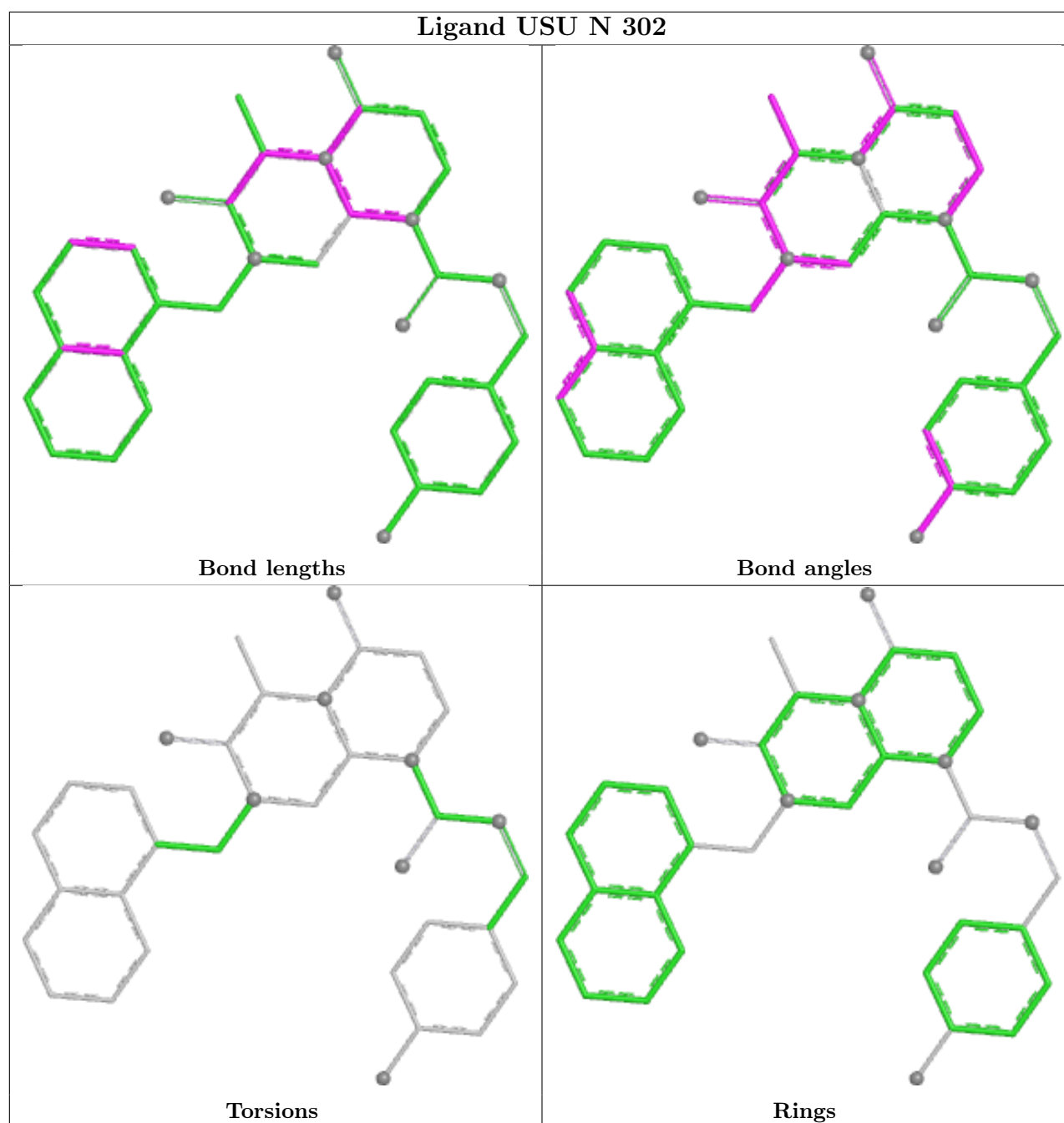












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	185/203 (91%)	0.04	8 (4%) 40 52	14, 19, 31, 51	0
1	B	182/203 (89%)	0.12	6 (3%) 49 62	15, 21, 35, 58	0
1	C	182/203 (89%)	0.40	7 (3%) 44 55	18, 24, 39, 50	0
1	D	181/203 (89%)	0.45	6 (3%) 49 62	17, 24, 36, 57	1 (0%)
1	E	182/203 (89%)	0.27	6 (3%) 49 62	18, 23, 36, 45	0
1	F	185/203 (91%)	0.03	8 (4%) 40 52	14, 19, 31, 55	0
1	G	182/203 (89%)	-0.03	5 (2%) 56 68	13, 18, 30, 41	1 (0%)
1	I	182/203 (89%)	-0.02	6 (3%) 49 62	14, 19, 32, 55	0
1	K	182/203 (89%)	0.17	8 (4%) 39 51	17, 22, 36, 46	0
1	L	181/203 (89%)	0.34	7 (3%) 43 55	13, 23, 37, 48	1 (0%)
1	M	182/203 (89%)	0.24	6 (3%) 49 62	18, 23, 37, 48	0
1	N	185/203 (91%)	0.05	6 (3%) 50 63	14, 20, 31, 48	0
1	S	186/203 (91%)	0.03	8 (4%) 40 52	14, 18, 32, 45	0
1	T	182/203 (89%)	0.02	7 (3%) 44 55	13, 18, 30, 48	0
All	All	2559/2842 (90%)	0.15	94 (3%) 45 56	13, 21, 35, 58	3 (0%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	ALA	6.0
1	I	193	GLU	5.7
1	C	8	ILE	5.5
1	K	8	ILE	5.4
1	D	193	GLU	4.3

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

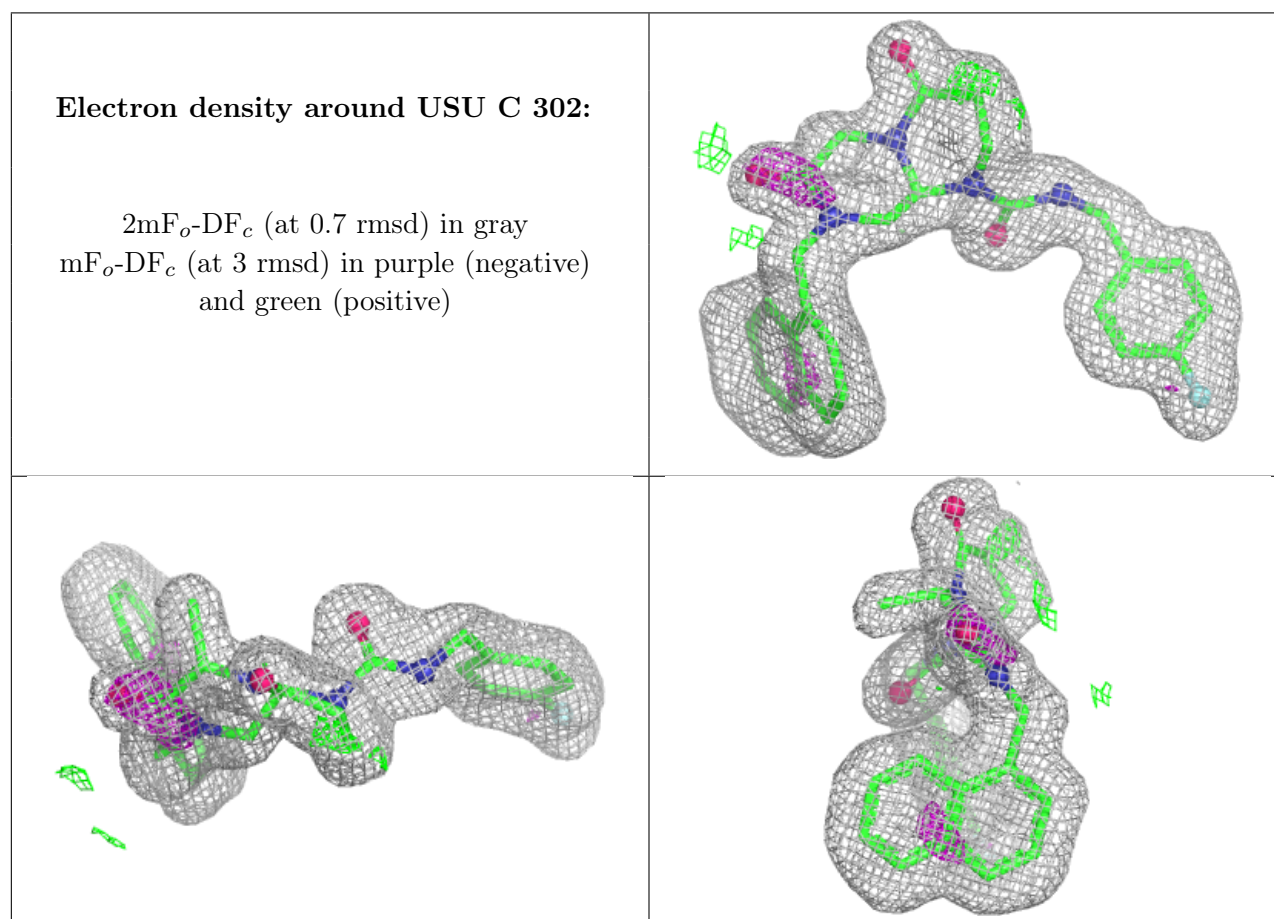
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPD	G	301	8/8	0.82	0.14	31,34,40,40	0
2	MPD	S	302	8/8	0.85	0.17	31,48,51,52	0
2	MPD	T	301	8/8	0.86	0.12	23,30,37,38	0
2	MPD	K	301	8/8	0.87	0.11	21,32,38,42	0
2	MPD	F	301	8/8	0.87	0.11	20,28,32,34	0
2	MPD	I	301	8/8	0.87	0.10	22,28,35,35	0
2	MPD	G	302	8/8	0.88	0.11	19,30,35,37	0
2	MPD	D	301	8/8	0.89	0.11	27,33,41,43	0
2	MPD	M	301	8/8	0.89	0.11	24,33,39,40	0
2	MPD	N	301	8/8	0.90	0.10	22,29,35,37	0
2	MPD	S	301	8/8	0.90	0.09	21,30,34,36	0
2	MPD	L	301	8/8	0.90	0.10	25,34,42,43	0
2	MPD	B	301	8/8	0.90	0.10	20,28,33,33	0
2	MPD	E	301	8/8	0.91	0.12	24,33,41,42	0
2	MPD	C	301	8/8	0.91	0.10	27,34,38,42	0
2	MPD	A	301	8/8	0.91	0.10	20,28,38,40	0
3	USU	C	302	35/35	0.93	0.08	22,25,31,35	0
3	USU	D	302	35/35	0.94	0.07	22,24,31,32	0
3	USU	N	302	35/35	0.94	0.07	19,21,27,28	0
3	USU	E	302	35/35	0.95	0.06	20,23,28,32	0
3	USU	G	303	35/35	0.95	0.07	17,19,25,26	0
3	USU	K	302	35/35	0.95	0.07	20,24,30,32	0
3	USU	M	302	35/35	0.95	0.07	21,23,28,31	0
3	USU	B	302	35/35	0.95	0.07	20,23,28,30	0
3	USU	L	302	35/35	0.96	0.06	20,24,32,32	0
3	USU	I	302	35/35	0.96	0.06	19,22,28,30	0
3	USU	F	302	35/35	0.96	0.06	18,21,27,29	0

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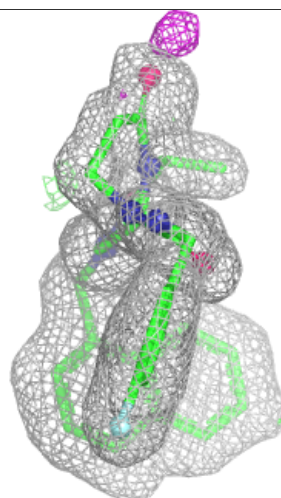
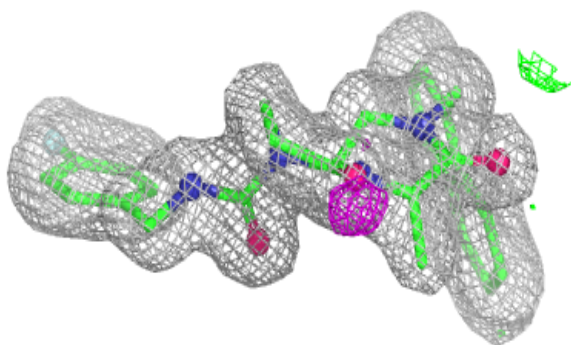
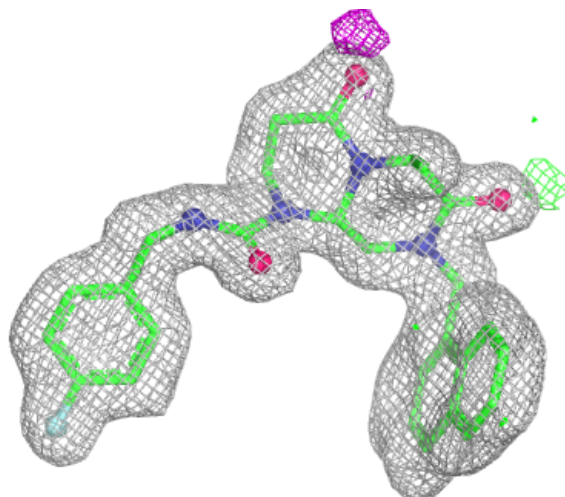
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	USU	S	303	35/35	0.96	0.06	16,18,25,27	0
3	USU	A	302	35/35	0.97	0.06	17,21,27,28	0
3	USU	T	302	35/35	0.97	0.05	17,20,27,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



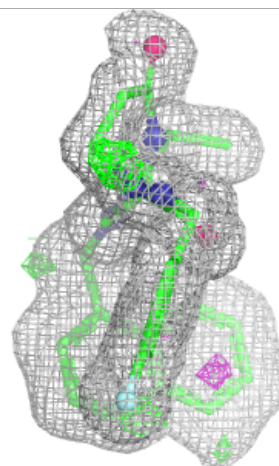
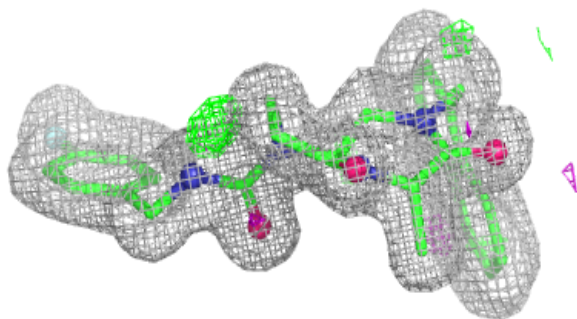
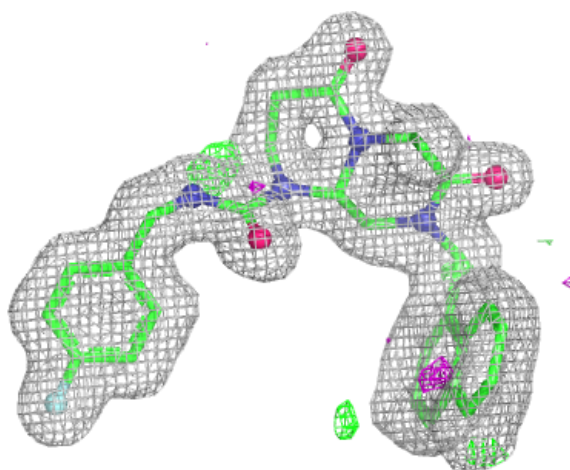
**Electron density around USU D 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



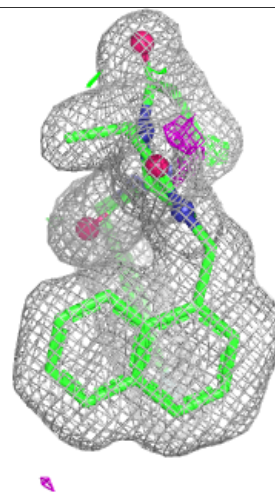
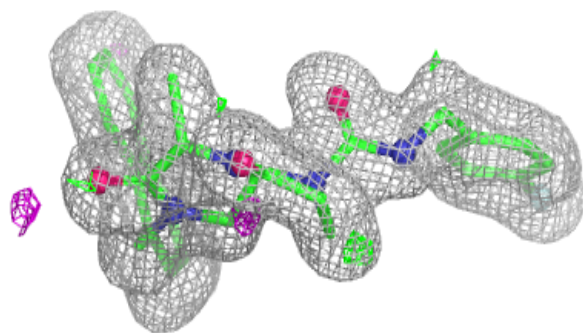
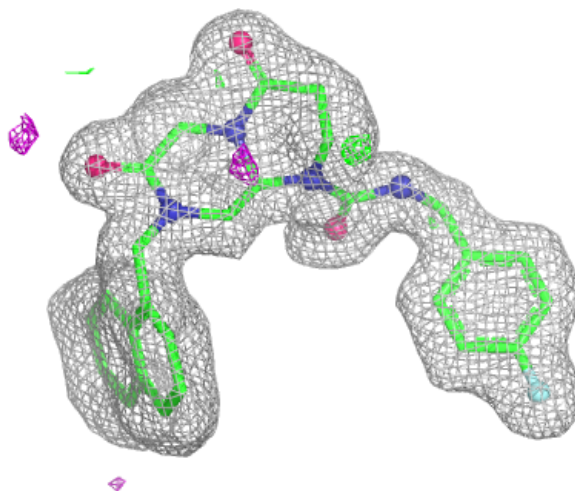
**Electron density around USU N 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



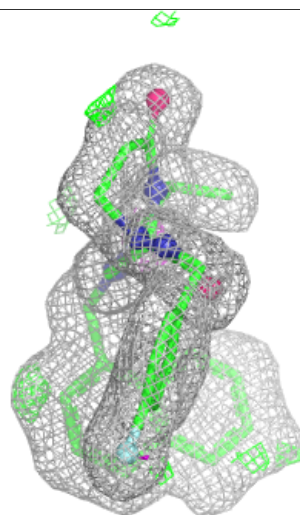
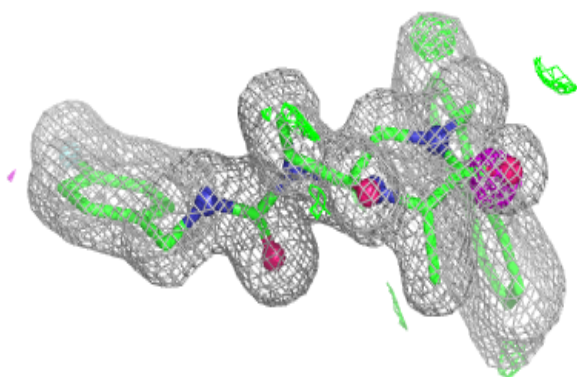
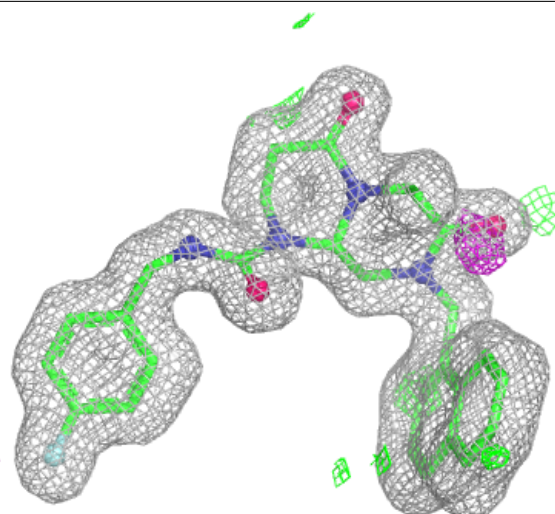
**Electron density around USU E 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



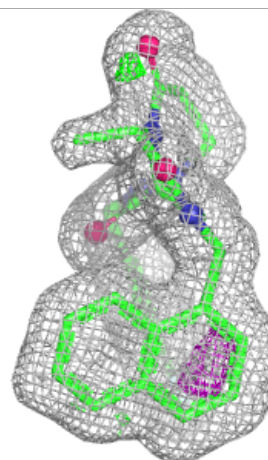
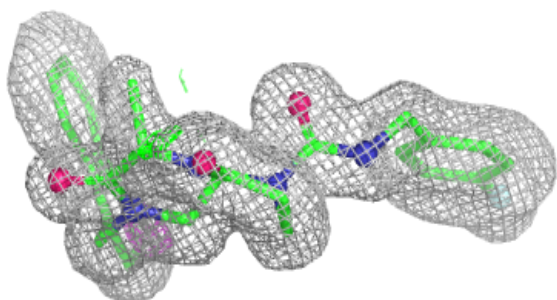
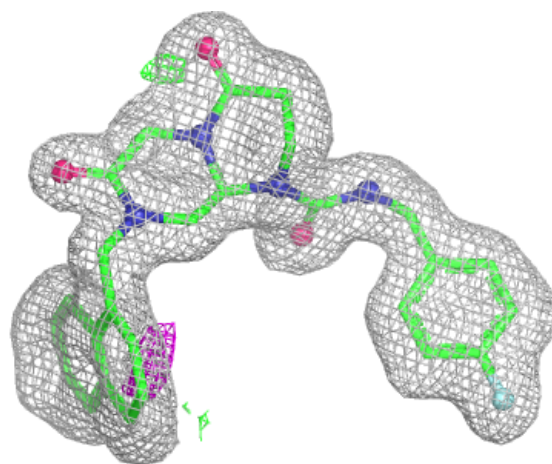
**Electron density around USU G 303:**

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and green (positive)



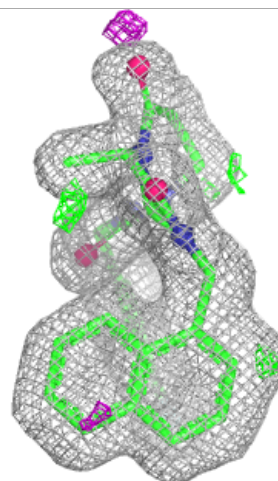
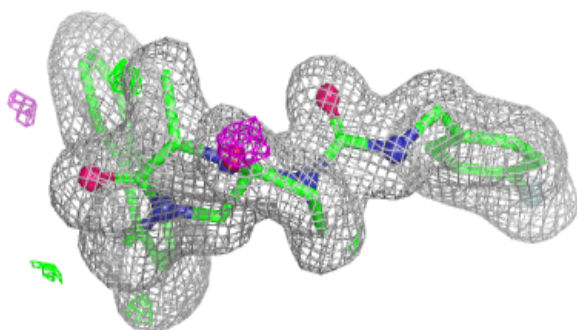
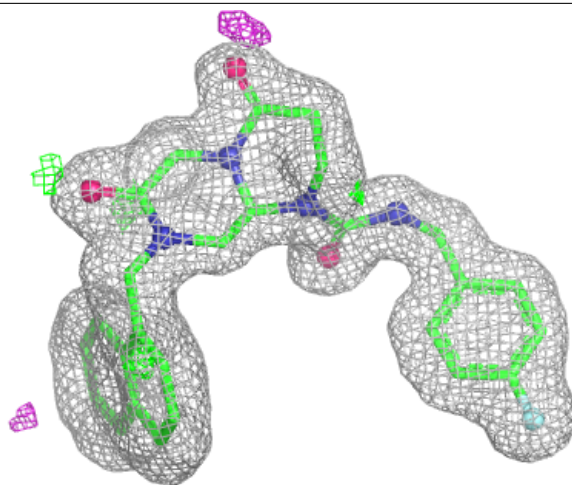
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and green (positive)



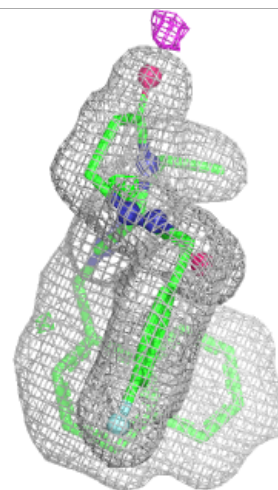
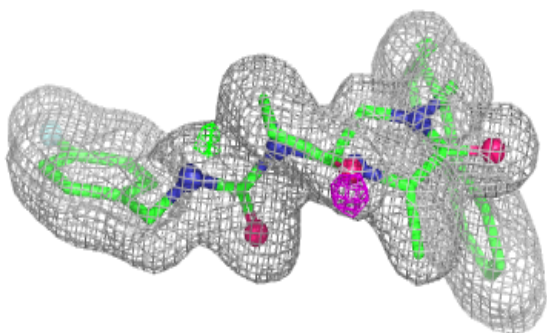
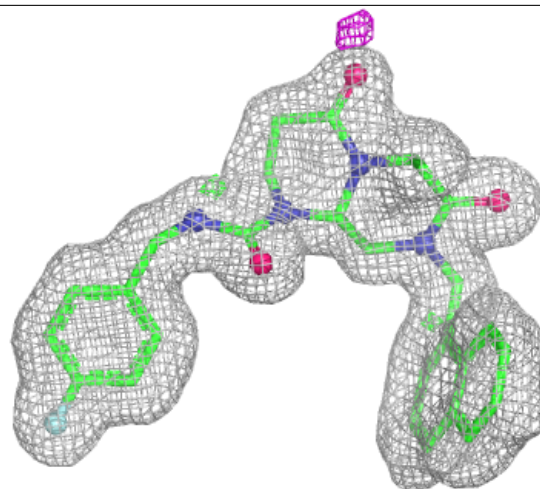
**Electron density around USU M 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



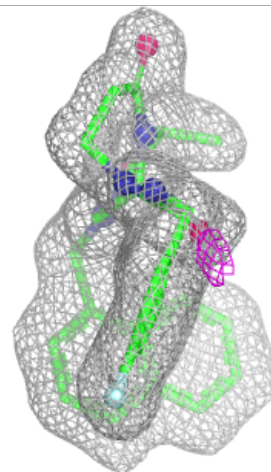
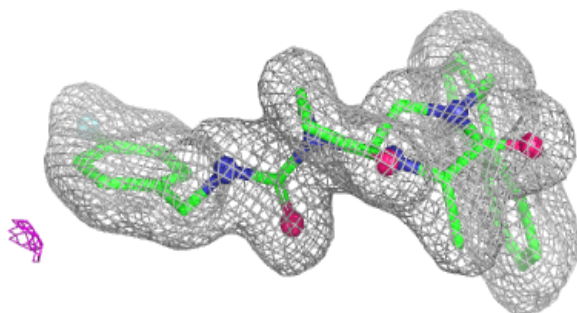
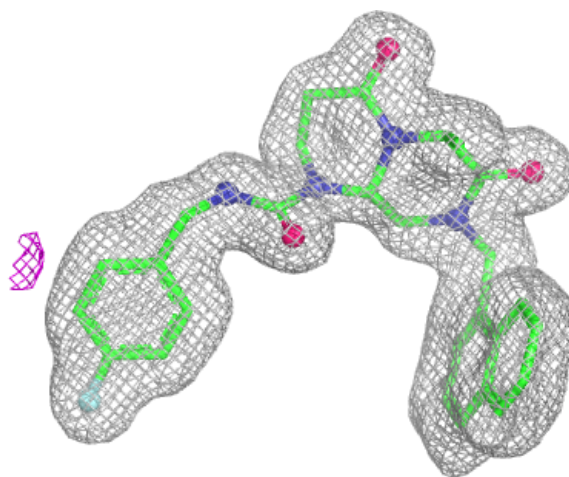
**Electron density around USU B 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



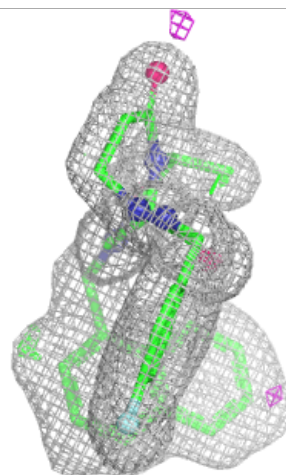
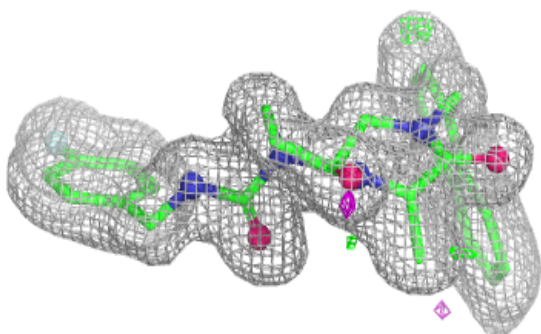
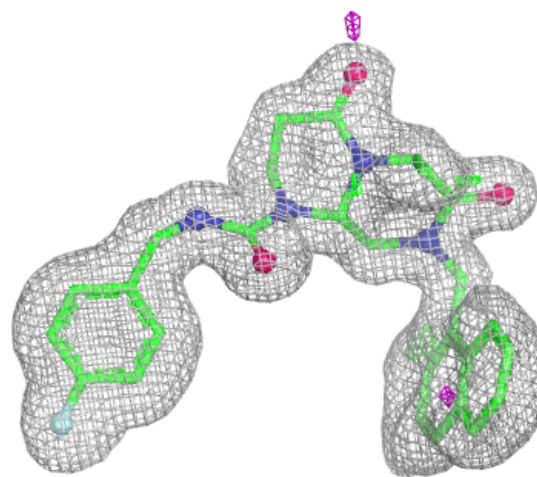
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and green (positive)



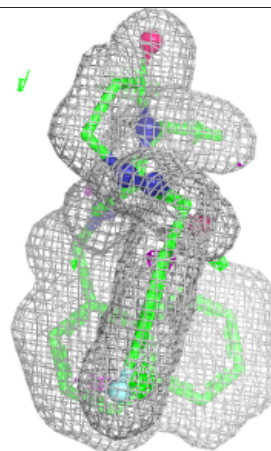
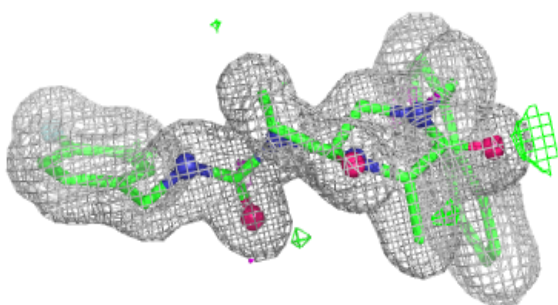
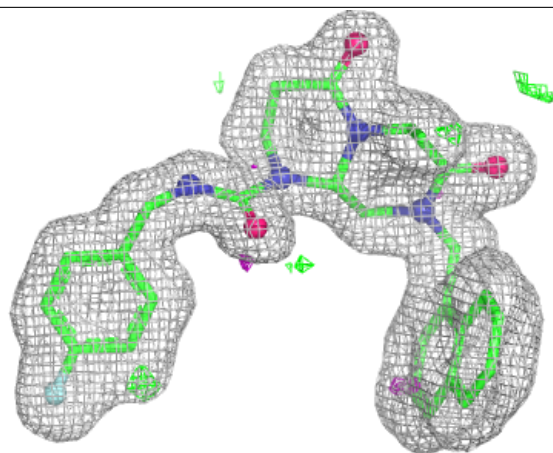
**Electron density around USU I 302:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



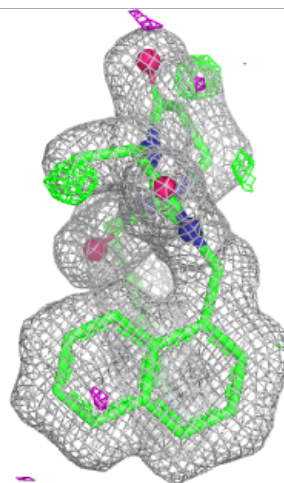
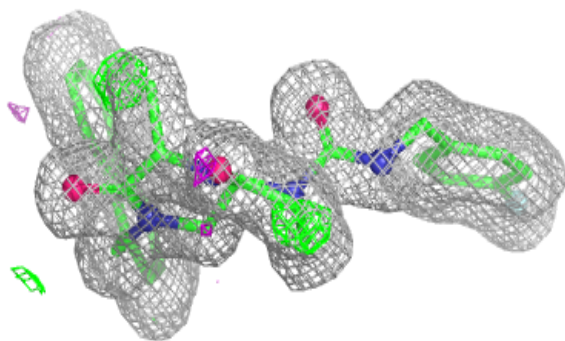
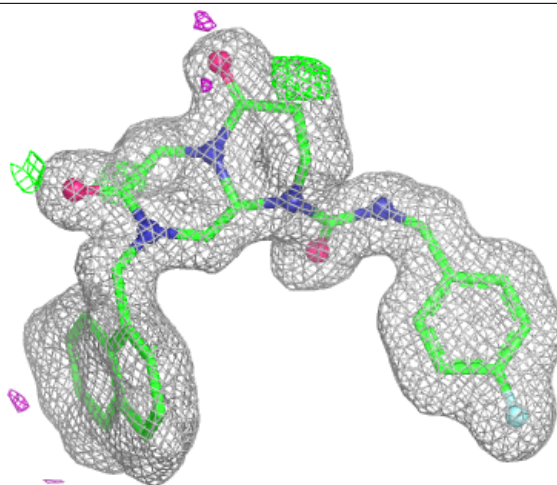
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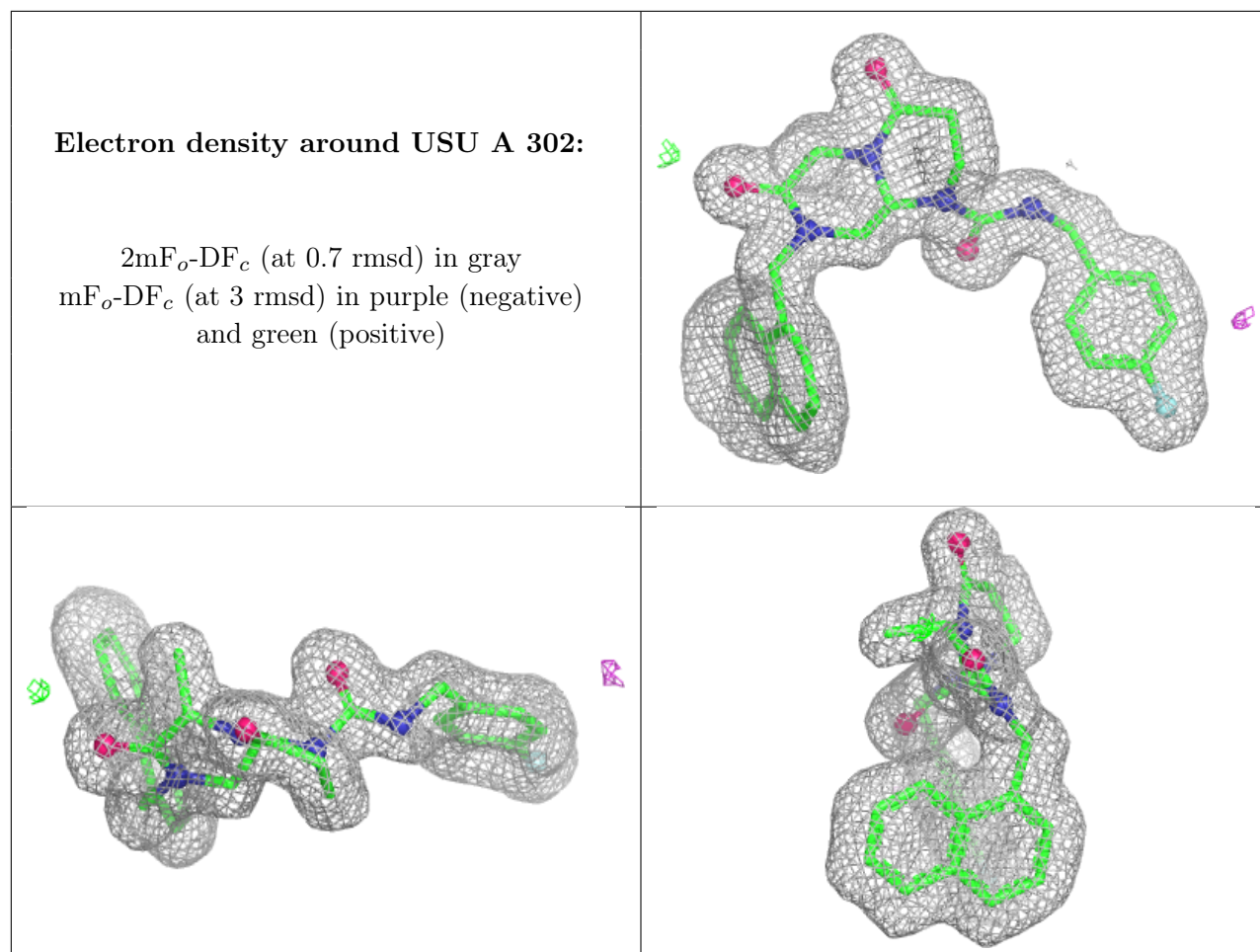
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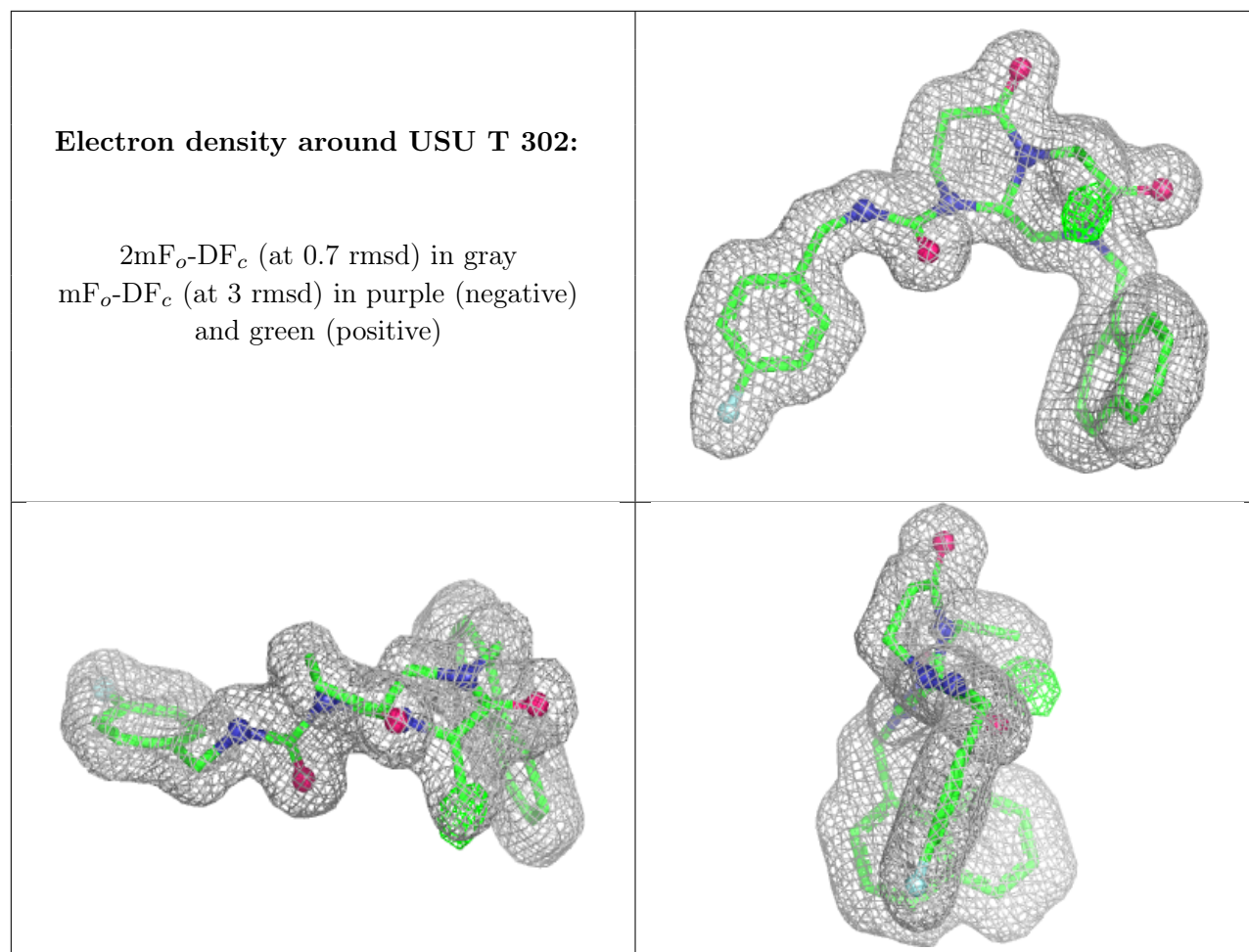


**Electron density around USU S 303:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.