



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:39 PM EDT

PDB ID : 8E7P  
Title : Staphylococcus aureus ClpP in complex with compound 3421  
Authors : Lee, R.E.; Griffith, E.C.  
Deposited on : 2022-08-24  
Resolution : 1.68 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

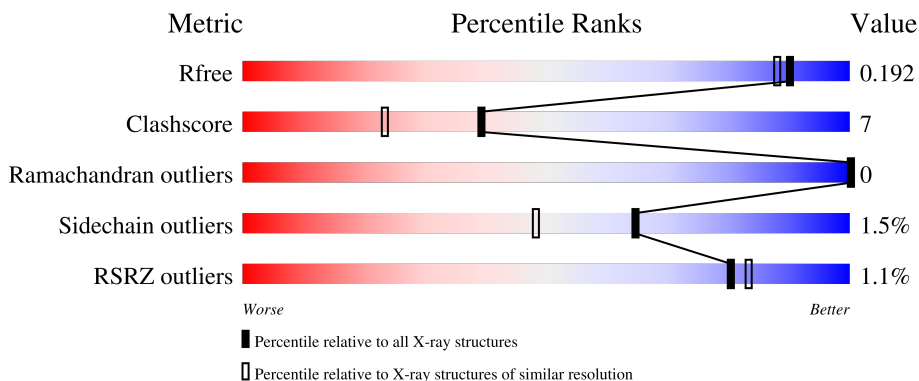
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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.



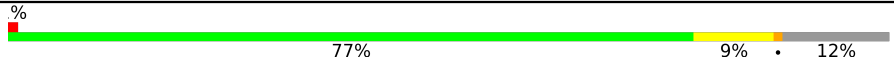

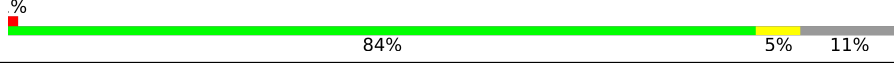



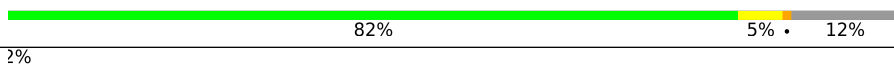


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	2% 81% 7% 11%
1	B	203	2% 81% 7% 11%
1	C	203	84% 6% 9%
1	D	203	84% 7% 8%
1	E	203	2% 83% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	I	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	
1	S	203	
1	T	203	

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	302	-	-	X	-
2	MPD	E	301	-	-	X	-
2	MPD	G	302	-	-	X	-
2	MPD	I	301	-	-	X	-
2	MPD	S	302	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22701 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	180	1424	894	245	278	7	0	5	0
1	B	180	1428	899	245	277	7	0	5	0
1	C	184	1451	915	246	283	7	0	5	0
1	D	186	1450	912	253	279	6	0	3	0
1	E	183	1435	905	244	279	7	0	4	0
1	F	178	1425	896	247	275	7	0	7	0
1	G	181	1455	915	251	282	7	0	8	0
1	I	181	1423	897	246	274	6	0	4	0
1	K	180	1417	893	241	276	7	0	4	0
1	L	183	1454	915	250	282	7	0	6	0
1	M	184	1453	914	249	283	7	0	6	0
1	N	179	1414	890	243	275	6	0	4	0
1	S	179	1408	885	242	275	6	0	4	0
1	T	179	1417	892	244	274	7	0	5	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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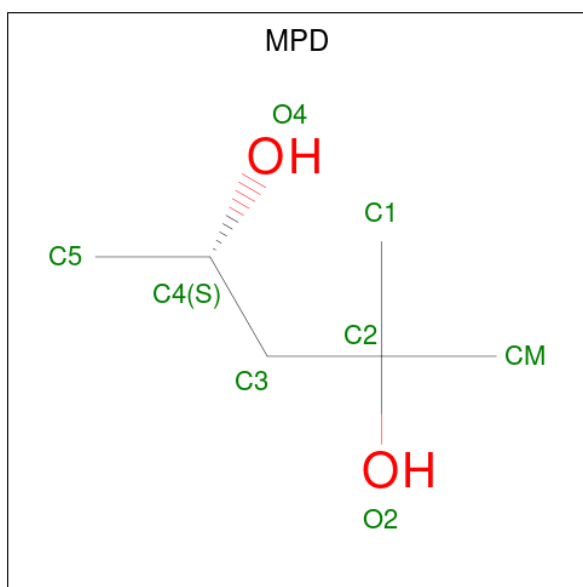
Chain	Residue	Modelled	Actual	Comment	Reference
F	199	HIS	-	expression tag	UNP Q2G036
F	200	HIS	-	expression tag	UNP Q2G036
F	201	HIS	-	expression tag	UNP Q2G036
F	202	HIS	-	expression tag	UNP Q2G036
F	203	HIS	-	expression tag	UNP Q2G036
G	196	LEU	-	expression tag	UNP Q2G036
G	197	GLU	-	expression tag	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 (three-letter code: 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	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	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

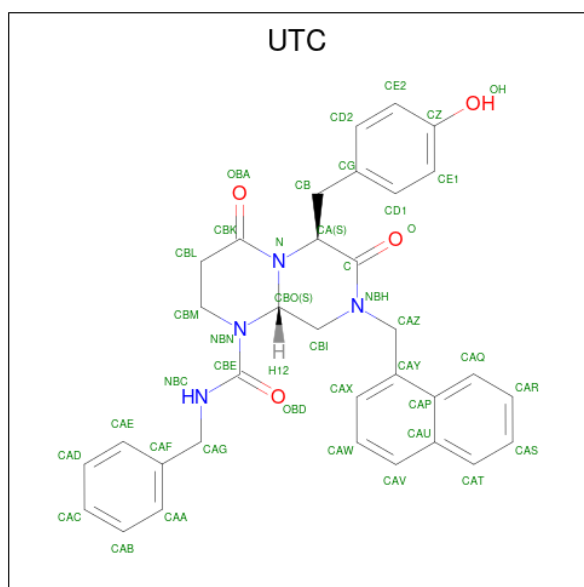
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	T	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is (5R,6S,9aS)-N-benzyl-6-[(4-hydroxyphenyl)methyl]-8-[(naphthalen-1-yl)methyl]-4,7-dioxohexahydro-2H-pyrazino[1,2-a]pyrimidine-1(6H)-carboxamide (three-letter code: UTC) (formula: C<sub>33</sub>H<sub>32</sub>N<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			41	33	4	4		
3	B	1	Total	C	N	O	0	0
			41	33	4	4		
3	C	1	Total	C	N	O	0	0
			41	33	4	4		
3	D	1	Total	C	N	O	0	0
			41	33	4	4		
3	F	1	Total	C	N	O	0	0
			41	33	4	4		
3	G	1	Total	C	N	O	0	0
			41	33	4	4		
3	I	1	Total	C	N	O	0	0
			41	33	4	4		
3	K	1	Total	C	N	O	0	0
			41	33	4	4		
3	L	1	Total	C	N	O	0	0
			41	33	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	M	1	41	33	4	4	0	0
3	N	1	41	33	4	4	0	0
3	S	1	41	33	4	4	0	0
3	S	1	41	33	4	4	0	0

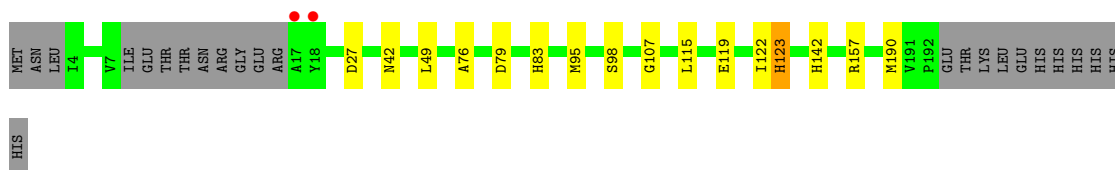
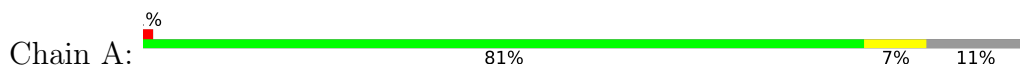
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total 120	O 120	0	0
4	B	127	Total 127	O 127	0	0
4	C	147	Total 147	O 147	0	0
4	D	163	Total 163	O 163	0	0
4	E	174	Total 174	O 174	0	0
4	F	145	Total 145	O 145	0	0
4	G	116	Total 116	O 116	0	0
4	I	113	Total 113	O 113	0	0
4	K	146	Total 146	O 146	0	0
4	L	167	Total 167	O 167	0	0
4	M	173	Total 173	O 173	0	0
4	N	144	Total 144	O 144	0	0
4	S	130	Total 130	O 130	0	0
4	T	129	Total 129	O 129	0	0

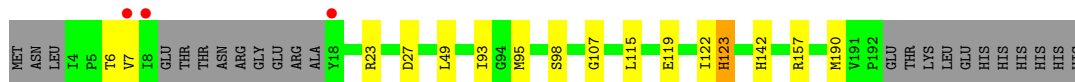
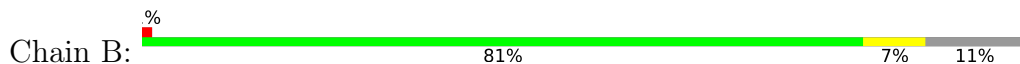
### 3 Residue-property plots [i](#)

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.

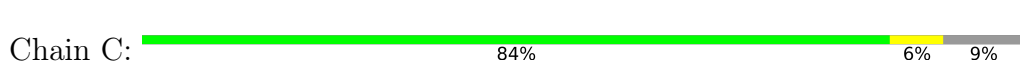
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



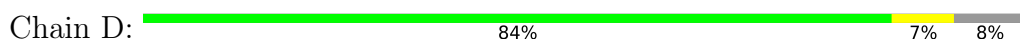
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



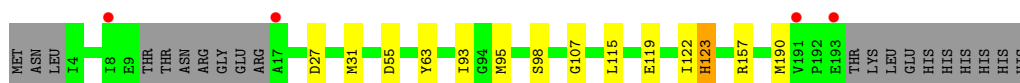
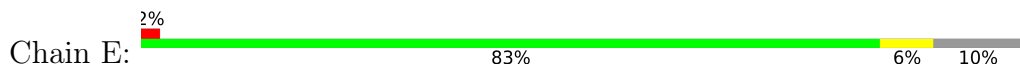
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



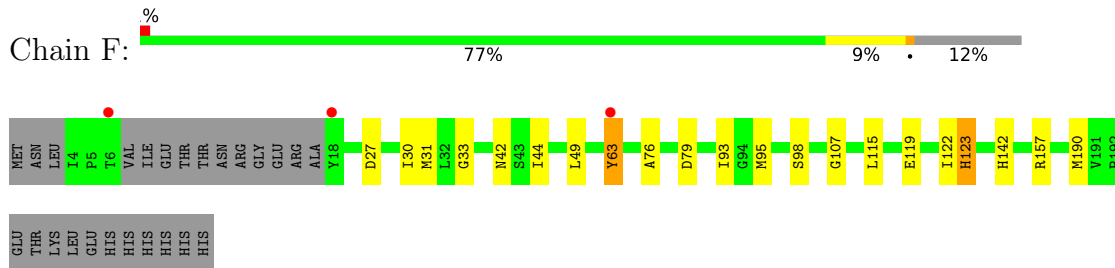
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



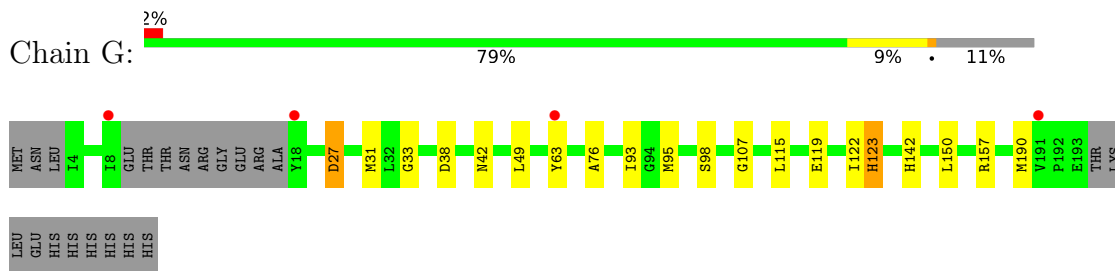
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



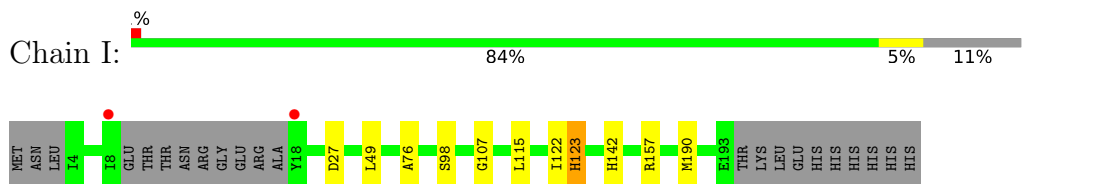
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



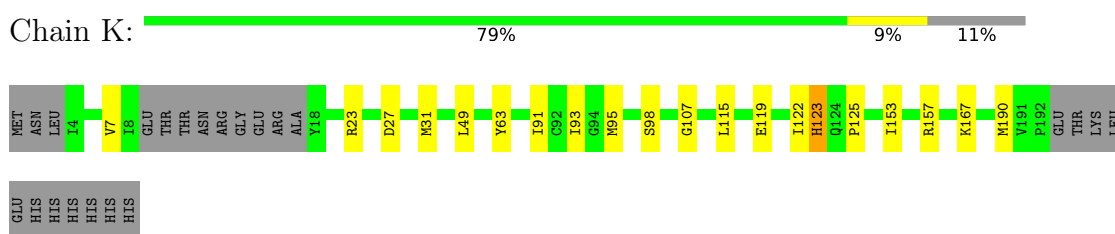
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



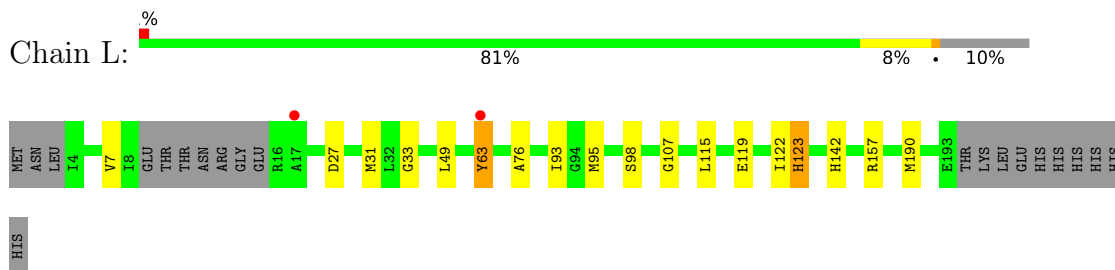
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



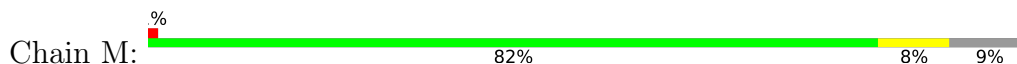
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

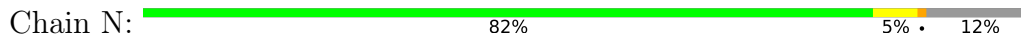


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

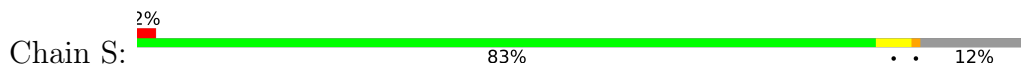




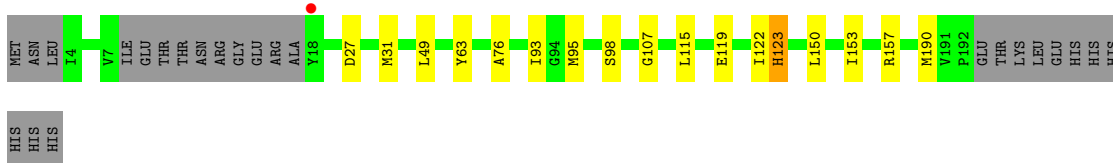
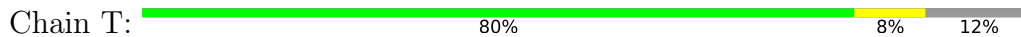
● Molecule 1: ATP-dependent Clp protease proteolytic subunit



● 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, $\alpha$ , $\beta$ , $\gamma$	94.07Å 126.14Å 145.47Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	49.90 – 1.68 49.85 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.90-1.68) 99.6 (49.85-1.68)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.68Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.166 , 0.182 0.177 , 0.192	Depositor DCC
$R_{free}$ test set	18992 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.4	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	0.96	EDS
Total number of atoms	22701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, UTC

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	0.77	0/1442	0.83	0/1947
1	B	0.73	0/1446	0.80	0/1951
1	C	0.73	0/1469	0.85	0/1984
1	D	0.81	0/1468	0.86	1/1981 (0.1%)
1	E	0.82	0/1453	0.89	1/1963 (0.1%)
1	F	0.76	0/1442	0.83	0/1945
1	G	0.74	0/1473	0.83	0/1988
1	I	0.72	0/1441	0.82	0/1946
1	K	0.77	0/1435	0.82	0/1937
1	L	0.77	0/1472	0.86	0/1987
1	M	0.85	1/1471 (0.1%)	0.87	1/1986 (0.1%)
1	N	0.78	0/1432	0.83	0/1933
1	S	0.72	0/1426	0.80	0/1926
1	T	0.74	0/1435	0.82	0/1936
All	All	0.77	1/20305 (0.0%)	0.84	3/27410 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	148	GLU	CD-OE1	11.54	1.38	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	M	55	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	D	171	ARG	NE-CZ-NH1	-6.32	117.14	120.30

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	1424	0	1421	30	0
1	B	1428	0	1434	22	0
1	C	1451	0	1454	33	0
1	D	1450	0	1456	21	0
1	E	1435	0	1441	23	0
1	F	1425	0	1439	35	0
1	G	1455	0	1455	42	0
1	I	1423	0	1433	16	0
1	K	1417	0	1422	25	0
1	L	1454	0	1457	32	0
1	M	1453	0	1448	29	0
1	N	1414	0	1422	22	0
1	S	1408	0	1404	19	0
1	T	1417	0	1421	24	0
2	A	8	0	14	5	0
2	B	8	0	14	4	0
2	C	8	0	14	6	0
2	D	16	0	28	5	0
2	E	8	0	14	7	0
2	F	8	0	14	4	0
2	G	8	0	14	6	0
2	I	8	0	14	6	0
2	K	8	0	14	4	0
2	L	8	0	14	5	0
2	M	8	0	14	4	0
2	N	8	0	14	5	0
2	S	8	0	14	6	0
2	T	8	0	14	5	0
3	A	41	0	0	6	0
3	B	41	0	0	6	0
3	C	41	0	0	6	0
3	D	41	0	0	0	0
3	F	41	0	0	5	0
3	G	41	0	0	6	0
3	I	41	0	0	4	0
3	K	41	0	0	7	0
3	L	41	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	41	0	0	6	0
3	N	41	0	0	8	0
3	S	82	0	0	15	0
4	A	120	0	0	0	0
4	B	127	0	0	1	0
4	C	147	0	0	0	0
4	D	163	0	0	0	0
4	E	174	0	0	3	0
4	F	145	0	0	0	0
4	G	116	0	0	1	0
4	I	113	0	0	0	0
4	K	146	0	0	0	0
4	L	167	0	0	0	0
4	M	173	0	0	1	0
4	N	144	0	0	1	0
4	S	130	0	0	0	0
4	T	129	0	0	0	0
All	All	22701	0	20317	305	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 7.

All (305) 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:M:49[B]:LEU:HD11	3:M:301:UTC:CAV	1.48	1.43
1:A:49:LEU:HD11	3:A:302:UTC:CAV	1.54	1.37
1:L:49[B]:LEU:HD11	3:L:301:UTC:CAV	1.54	1.35
1:G:49[B]:LEU:HD11	3:G:301:UTC:CAV	1.58	1.31
3:S:303:UTC:CAV	1:T:49[B]:LEU:HD11	1.62	1.29
1:C:49[B]:LEU:HD11	3:C:301:UTC:CAV	1.59	1.29
1:I:49[B]:LEU:HD11	3:I:302:UTC:CAV	1.67	1.25
1:S:49[B]:LEU:HD11	3:S:301:UTC:CAV	1.66	1.24
1:N:49[B]:LEU:HD11	3:N:301:UTC:CAV	1.70	1.22
1:B:49[B]:LEU:HD11	3:B:301:UTC:CAV	1.69	1.21
1:F:49[B]:LEU:HD11	3:F:301:UTC:CAV	1.70	1.21
1:K:49[B]:LEU:HD11	3:K:301:UTC:CAV	1.69	1.21
1:L:49[B]:LEU:CD1	3:L:301:UTC:CAV	2.28	1.12
1:M:49[B]:LEU:CD1	3:M:301:UTC:CAV	2.35	1.05
1:C:49[B]:LEU:CD1	3:C:301:UTC:CAV	2.36	1.04
1:C:33:GLY:HA3	1:D:42[B]:ASN:ND2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:303:UTC:CAV	1:T:49[B]:LEU:CD1	2.39	1.01
1:N:49[B]:LEU:CD1	3:N:301:UTC:CAV	2.39	1.00
1:A:49:LEU:CD1	3:A:302:UTC:CAV	2.40	0.99
1:G:49[B]:LEU:CD1	3:G:301:UTC:CAV	2.43	0.96
1:I:49[B]:LEU:CD1	3:I:302:UTC:CAV	2.44	0.96
3:S:303:UTC:CAU	1:T:49[B]:LEU:HD11	1.95	0.94
1:S:49[B]:LEU:CD1	3:S:301:UTC:CAV	2.45	0.94
1:F:49[B]:LEU:CD1	3:F:301:UTC:CAV	2.46	0.93
1:B:49[B]:LEU:CD1	3:B:301:UTC:CAV	2.46	0.92
1:F:49[B]:LEU:HD21	3:F:301:UTC:CAT	1.98	0.92
1:B:49[B]:LEU:HD11	3:B:301:UTC:CAU	2.01	0.91
1:K:49[B]:LEU:CD1	3:K:301:UTC:CAV	2.48	0.91
1:L:49[B]:LEU:HD21	3:L:301:UTC:CAT	2.00	0.90
1:M:49[B]:LEU:HD21	3:M:301:UTC:CAT	2.03	0.88
1:A:49:LEU:HD21	3:A:302:UTC:CAT	2.05	0.87
1:C:49[B]:LEU:HD21	3:C:301:UTC:CAT	2.04	0.87
1:L:49[B]:LEU:HD11	3:L:301:UTC:CAU	2.04	0.86
1:M:49[B]:LEU:HD11	3:M:301:UTC:CAU	2.04	0.86
1:G:49[B]:LEU:HD11	3:G:301:UTC:CAU	2.06	0.86
1:S:49[B]:LEU:HD21	3:S:301:UTC:CAT	2.07	0.85
1:K:49[B]:LEU:HD11	3:K:301:UTC:CAU	2.09	0.82
1:C:49[B]:LEU:HD11	3:C:301:UTC:CAU	2.10	0.80
1:E:95[A]:MET:CE	1:E:119[A]:GLU:HG2	2.11	0.80
1:A:95[A]:MET:HE1	1:A:119[A]:GLU:HG2	1.63	0.80
1:K:95[A]:MET:HE1	1:K:119[A]:GLU:HG2	1.62	0.80
1:M:95[A]:MET:HE1	1:M:119[A]:GLU:HG2	1.64	0.80
1:C:33:GLY:HA3	1:D:42[B]:ASN:HD21	1.47	0.79
1:G:49[B]:LEU:HD21	3:G:301:UTC:CAT	2.13	0.79
1:K:95[A]:MET:CE	1:K:119[A]:GLU:HG2	2.13	0.78
1:A:95[A]:MET:CE	1:A:119[A]:GLU:HG2	2.15	0.77
1:N:49[B]:LEU:HD11	3:N:301:UTC:CAU	2.15	0.77
1:E:119[A]:GLU:OE2	1:F:142:HIS:CE1	2.38	0.76
1:M:95[A]:MET:CE	1:M:119[A]:GLU:HG2	2.14	0.76
1:N:49[B]:LEU:HD21	3:N:301:UTC:CAT	2.17	0.75
1:C:33:GLY:CA	1:D:42[B]:ASN:HD21	2.01	0.73
1:E:95[A]:MET:HE1	1:E:119[A]:GLU:HG2	1.70	0.72
1:I:49[B]:LEU:HD11	3:I:302:UTC:CAU	2.19	0.72
1:C:33:GLY:CA	1:D:42[B]:ASN:ND2	2.53	0.72
1:K:49[B]:LEU:HD21	3:K:301:UTC:CAT	2.20	0.72
1:C:33:GLY:HA3	1:D:42[B]:ASN:CG	2.11	0.71
1:E:123:HIS:H	2:E:301:MPD:C1	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:27[B]:ASP:OD2	3:S:303:UTC:CAA	2.39	0.70
1:B:95[A]:MET:CE	1:B:119[A]:GLU:HG2	2.22	0.69
1:I:49[B]:LEU:HD21	3:I:302:UTC:CAT	2.23	0.69
1:S:27[B]:ASP:OD2	3:S:303:UTC:CAB	2.41	0.69
1:S:49[B]:LEU:HD11	3:S:301:UTC:CAU	2.22	0.68
1:T:95[A]:MET:CE	1:T:119[A]:GLU:HG2	2.25	0.67
1:B:95[A]:MET:HE1	1:B:119[A]:GLU:HG2	1.76	0.67
1:M:27[A]:ASP:OD2	3:N:301:UTC:CAA	2.42	0.66
1:L:119[A]:GLU:CD	1:M:142:HIS:HE1	1.98	0.66
1:L:119[A]:GLU:OE2	1:M:142:HIS:CE1	2.49	0.66
1:A:49:LEU:HD11	3:A:302:UTC:CAU	2.20	0.66
1:C:33:GLY:C	1:D:42[B]:ASN:HD21	1.99	0.66
1:M:119[A]:GLU:OE2	1:N:142:HIS:CE1	2.49	0.66
1:B:49[B]:LEU:HD11	3:B:301:UTC:CAT	2.26	0.65
1:C:33:GLY:O	1:D:42[B]:ASN:ND2	2.26	0.65
3:A:302:UTC:CAA	1:G:27[B]:ASP:OD2	2.45	0.65
1:E:119[A]:GLU:CD	1:F:142:HIS:HE1	1.99	0.65
1:E:123:HIS:H	2:E:301:MPD:H13	1.63	0.64
1:L:49[B]:LEU:HD11	3:L:301:UTC:CAT	2.29	0.63
1:L:49[B]:LEU:HD21	3:L:301:UTC:CAS	2.27	0.63
1:T:95[A]:MET:HE1	1:T:119[A]:GLU:HG2	1.81	0.63
1:E:119[A]:GLU:OE2	1:F:142:HIS:HE1	1.80	0.63
1:C:93[A]:ILE:HG22	1:D:76:ALA:HB1	1.81	0.63
1:G:122:ILE:HA	2:G:302:MPD:H13	1.81	0.62
1:E:107:GLY:O	1:E:157[B]:ARG:NH1	2.33	0.61
1:L:98:SER:HA	2:L:302:MPD:H12	1.82	0.61
3:S:303:UTC:CAT	1:T:49[B]:LEU:HD11	2.29	0.61
3:S:303:UTC:CAT	1:T:49[B]:LEU:HD21	2.31	0.61
1:G:150:LEU:HD13	2:G:302:MPD:H52	1.82	0.61
1:F:123:HIS:H	2:F:302:MPD:H11	1.66	0.60
1:L:95[A]:MET:CE	1:L:119[A]:GLU:HG2	2.31	0.60
1:B:119[A]:GLU:OE2	1:C:142:HIS:CE1	2.54	0.60
1:M:119[A]:GLU:OE2	1:N:142:HIS:HE1	1.84	0.60
1:N:123:HIS:H	2:N:302:MPD:H11	1.66	0.60
1:G:98:SER:HA	2:G:302:MPD:H12	1.84	0.59
1:S:123:HIS:H	2:S:302:MPD:C1	2.15	0.59
3:A:302:UTC:CAB	1:G:27[B]:ASP:OD2	2.50	0.59
1:I:123:HIS:H	2:I:301:MPD:C1	2.15	0.59
1:B:98:SER:HA	2:B:302:MPD:H12	1.84	0.59
1:G:93:ILE:HG12	1:G:115[B]:LEU:HD22	1.83	0.59
1:D:123:HIS:H	2:D:301:MPD:C1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:98:SER:HA	2:N:302:MPD:H12	1.85	0.58
1:F:95[A]:MET:CE	1:F:119[A]:GLU:HG2	2.32	0.58
1:N:27[B]:ASP:OD2	3:S:301:UTC:CAA	2.51	0.58
1:C:93[A]:ILE:HG22	1:D:76:ALA:CB	2.33	0.58
1:F:119[A]:GLU:OE2	1:G:142:HIS:CE1	2.57	0.58
1:E:123:HIS:O	2:E:301:MPD:H11	2.03	0.58
1:E:98:SER:HA	2:E:301:MPD:H12	1.85	0.57
1:M:119[A]:GLU:CD	1:N:142:HIS:HE1	2.08	0.57
1:M:123:HIS:H	2:M:302:MPD:H11	1.69	0.57
1:C:98:SER:HA	2:C:302:MPD:H12	1.86	0.57
1:L:122:ILE:HA	2:L:302:MPD:H13	1.87	0.57
1:L:95[A]:MET:HE1	1:L:119[A]:GLU:HG2	1.87	0.56
1:L:123:HIS:H	2:L:302:MPD:C1	2.17	0.56
1:N:122:ILE:HA	2:N:302:MPD:H13	1.87	0.56
1:F:93:ILE:HG12	1:F:115[B]:LEU:HD22	1.88	0.56
1:M:122:ILE:HA	2:M:302:MPD:H13	1.86	0.56
1:I:142:HIS:CE1	1:T:119[A]:GLU:OE2	2.58	0.56
1:C:122:ILE:HA	2:C:302:MPD:H13	1.87	0.55
1:A:42[B]:ASN:ND2	1:G:63:TYR:CE1	2.74	0.55
1:F:119[A]:GLU:CD	1:G:142:HIS:HE1	2.10	0.55
1:A:42[A]:ASN:OD1	1:G:33:GLY:HA3	2.06	0.55
1:S:98:SER:HA	2:S:302:MPD:H12	1.89	0.55
1:A:123:HIS:H	2:A:301:MPD:C1	2.19	0.55
1:N:123:HIS:H	2:N:302:MPD:C1	2.20	0.55
1:C:123:HIS:H	2:C:302:MPD:C1	2.20	0.55
1:G:95[A]:MET:HE1	1:G:119[A]:GLU:HG2	1.87	0.55
1:F:122:ILE:HA	2:F:302:MPD:H13	1.89	0.54
1:N:27[B]:ASP:OD2	3:S:301:UTC:CAB	2.56	0.54
1:G:95[A]:MET:CE	1:G:119[A]:GLU:HG2	2.37	0.54
3:S:303:UTC:CAU	1:T:49[B]:LEU:CD1	2.80	0.54
1:F:49[B]:LEU:HD11	3:F:301:UTC:CAU	2.35	0.54
1:D:122:ILE:HA	2:D:301:MPD:H13	1.88	0.54
1:D:123:HIS:H	2:D:301:MPD:H11	1.73	0.54
1:M:27[A]:ASP:OD2	3:N:301:UTC:CAB	2.55	0.54
1:I:98:SER:HA	2:I:301:MPD:H12	1.90	0.54
1:N:49[B]:LEU:HD11	3:N:301:UTC:CAT	2.37	0.54
1:I:142:HIS:HE1	1:T:119[A]:GLU:CD	2.11	0.53
1:M:115:LEU:HD23	1:M:190:MET:HB3	1.90	0.53
1:B:107:GLY:O	1:B:157[B]:ARG:NH1	2.41	0.53
1:E:115[A]:LEU:HD23	1:E:190:MET:HB3	1.90	0.53
1:B:119[A]:GLU:OE2	1:C:142:HIS:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:122:ILE:HA	2:T:301:MPD:H13	1.90	0.53
1:F:115[A]:LEU:HD23	1:F:190:MET:HB3	1.90	0.53
1:K:119[A]:GLU:CD	1:L:142:HIS:HE1	2.12	0.53
1:B:122:ILE:HA	2:B:302:MPD:H13	1.90	0.53
1:S:115:LEU:HD23	1:S:190:MET:HB3	1.91	0.53
1:C:49[B]:LEU:HD21	3:C:301:UTC:CAS	2.39	0.53
1:T:123:HIS:H	2:T:301:MPD:H11	1.72	0.52
1:F:30:ILE:CG2	1:F:44:ILE:CD1	2.86	0.52
1:G:123:HIS:H	2:G:302:MPD:C1	2.22	0.52
1:F:31:MET:HE3	1:F:63:TYR:CD1	2.44	0.52
1:K:119[A]:GLU:OE2	1:L:142:HIS:CE1	2.62	0.52
1:F:123:HIS:H	2:F:302:MPD:C1	2.22	0.52
1:B:119[A]:GLU:CD	1:C:142:HIS:HE1	2.13	0.52
1:D:9:GLU:O	1:D:15:GLU:HA	2.10	0.52
1:I:123:HIS:H	2:I:301:MPD:H11	1.75	0.52
1:D:107:GLY:O	1:D:157[B]:ARG:NH1	2.43	0.51
1:A:76:ALA:HA	1:G:93:ILE:HG22	1.93	0.51
1:A:98:SER:HA	2:A:301:MPD:H12	1.92	0.51
1:E:123:HIS:H	2:E:301:MPD:H11	1.76	0.51
1:L:33:GLY:HA3	1:M:42[A]:ASN:ND2	2.25	0.51
1:T:123:HIS:H	2:T:301:MPD:C1	2.23	0.51
1:I:122:ILE:HA	2:I:301:MPD:H13	1.92	0.51
1:T:115:LEU:HD23	1:T:190:MET:HB3	1.93	0.51
1:N:115:LEU:HD23	1:N:190:MET:HB3	1.93	0.51
1:K:123:HIS:H	2:K:302:MPD:H11	1.74	0.51
1:B:123:HIS:H	2:B:302:MPD:C1	2.23	0.50
1:F:95[A]:MET:HE1	1:F:119[A]:GLU:HG2	1.91	0.50
1:M:123:HIS:H	2:M:302:MPD:C1	2.23	0.50
1:C:123:HIS:H	2:C:302:MPD:H11	1.76	0.50
1:L:115:LEU:HD23	1:L:190:MET:HB3	1.92	0.50
1:S:107:GLY:O	1:S:157[B]:ARG:NH1	2.43	0.50
1:K:115:LEU:HD23	1:K:190:MET:HB3	1.93	0.50
1:D:115:LEU:HD23	1:D:190:MET:HB3	1.93	0.50
1:G:115[A]:LEU:HD23	1:G:190:MET:HB3	1.94	0.50
1:S:49[B]:LEU:HD21	3:S:301:UTC:CAS	2.42	0.50
1:T:98:SER:HA	2:T:301:MPD:H12	1.94	0.50
1:S:123:HIS:H	2:S:302:MPD:H11	1.76	0.50
1:K:49[B]:LEU:HD21	3:K:301:UTC:CAS	2.42	0.50
1:A:119[A]:GLU:OE2	1:B:142:HIS:CE1	2.65	0.50
1:K:49[B]:LEU:HD11	3:K:301:UTC:CAT	2.42	0.50
1:I:115:LEU:HD23	1:I:190:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49[B]:LEU:HD21	3:B:301:UTC:CAT	2.42	0.49
1:A:142:HIS:CE1	1:G:119[A]:GLU:OE2	2.65	0.49
1:B:115:LEU:HD23	1:B:190:MET:HB3	1.93	0.49
1:D:167:LYS:HE2	1:D:168:ASP:OD1	2.13	0.49
1:A:123:HIS:H	2:A:301:MPD:H11	1.77	0.49
1:E:31:MET:HE3	1:E:63:TYR:CD1	2.48	0.49
1:A:83:HIS:CE1	1:G:190:MET:CE	2.96	0.49
1:L:107:GLY:O	1:L:157[B]:ARG:NH1	2.46	0.49
1:D:98:SER:HA	2:D:301:MPD:H12	1.95	0.48
1:L:119[A]:GLU:OE2	1:M:142:HIS:HE1	1.91	0.48
1:B:6:THR:HB	4:B:449:HOH:O	2.13	0.48
1:C:49[B]:LEU:HD11	3:C:301:UTC:CAT	2.43	0.48
1:F:33:GLY:HA3	1:G:42[A]:ASN:ND2	2.29	0.48
1:L:49[B]:LEU:HD13	3:L:301:UTC:CAV	2.37	0.48
1:L:123:HIS:H	2:L:302:MPD:H11	1.78	0.48
1:A:115:LEU:HD23	1:A:190:MET:HB3	1.94	0.48
1:F:93:ILE:HG22	1:G:76:ALA:HB1	1.95	0.48
1:F:93:ILE:HG22	1:G:76:ALA:CB	2.44	0.48
1:A:119[A]:GLU:CD	1:B:142:HIS:HE1	2.17	0.48
1:A:142:HIS:HE1	1:G:119[A]:GLU:OE2	1.96	0.47
1:K:98:SER:HA	2:K:302:MPD:H12	1.95	0.47
1:K:107:GLY:O	1:K:157[B]:ARG:NH1	2.47	0.47
1:A:79:ASP:HB3	1:G:115[A]:LEU:HD13	1.96	0.47
1:C:93[B]:ILE:HG22	1:C:115:LEU:HD22	1.96	0.47
1:G:123:HIS:H	2:G:302:MPD:H11	1.80	0.47
1:M:98:SER:HA	2:M:302:MPD:H12	1.97	0.47
1:M:49[B]:LEU:HD21	3:M:301:UTC:CAS	2.45	0.47
1:N:153:ILE:O	1:N:157[B]:ARG:HG2	2.14	0.47
1:N:175:LEU:HD23	4:N:488:HOH:O	2.13	0.47
1:K:123:HIS:H	2:K:302:MPD:C1	2.27	0.47
1:E:95[B]:MET:CE	4:E:2361:HOH:O	2.62	0.47
1:M:107:GLY:O	1:M:157[B]:ARG:NH1	2.47	0.47
1:A:83:HIS:CE1	1:G:190:MET:HE2	2.50	0.47
1:M:4:ILE:HD11	4:M:406:HOH:O	2.14	0.47
1:I:142:HIS:HE1	1:T:119[A]:GLU:OE2	1.98	0.47
1:I:107:GLY:O	1:I:157[B]:ARG:NH1	2.48	0.46
1:F:119[A]:GLU:OE2	1:G:142:HIS:HE1	1.97	0.46
1:C:93[A]:ILE:CG2	1:D:76:ALA:HA	2.45	0.46
1:K:7:VAL:HG21	1:K:23:ARG:HG2	1.96	0.46
1:S:122:ILE:HA	2:S:302:MPD:H13	1.97	0.46
1:A:123:HIS:O	2:A:301:MPD:H11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:OE1	1:D:142:HIS:HE1	1.99	0.46
1:F:107:GLY:O	1:F:157[B]:ARG:NH1	2.48	0.46
1:G:31:MET:HE3	1:G:63:TYR:CD1	2.51	0.46
1:I:123:HIS:O	2:I:301:MPD:H11	2.16	0.46
1:T:31:MET:HE3	1:T:63:TYR:CD1	2.51	0.46
1:T:153:ILE:O	1:T:157[B]:ARG:HG2	2.16	0.46
1:C:63:TYR:CD1	1:C:93[A]:ILE:HD12	2.52	0.45
1:F:30:ILE:CG2	1:F:44:ILE:HD12	2.45	0.45
1:T:150:LEU:HD13	2:T:301:MPD:H52	1.99	0.45
1:B:7:VAL:HG21	1:B:23:ARG:HG2	1.99	0.45
1:C:93[B]:ILE:O	1:C:93[B]:ILE:HG13	2.15	0.45
1:E:95[B]:MET:HE2	4:E:2352:HOH:O	2.16	0.45
1:A:76:ALA:CB	1:G:93:ILE:HG22	2.46	0.45
1:F:49[B]:LEU:HD21	3:F:301:UTC:CAS	2.44	0.45
1:L:49[B]:LEU:CD2	3:L:301:UTC:CAT	2.86	0.45
1:L:119[A]:GLU:CD	1:M:142:HIS:CE1	2.84	0.45
1:A:122:ILE:HA	2:A:301:MPD:H13	1.99	0.45
1:K:31:MET:HE3	1:K:63:TYR:CD1	2.51	0.45
1:N:123:HIS:O	2:N:302:MPD:H11	2.16	0.45
1:L:7:VAL:HG11	1:M:50:PHE:CE1	2.52	0.45
1:S:123:HIS:O	2:S:302:MPD:H11	2.17	0.45
1:A:79:ASP:HB3	1:G:115[B]:LEU:HD23	1.99	0.45
1:L:93:ILE:HG22	1:M:76:ALA:HA	1.99	0.45
1:S:123:HIS:H	2:S:302:MPD:H13	1.81	0.45
1:L:123:HIS:H	2:L:302:MPD:H13	1.81	0.45
1:N:93:ILE:HG22	1:S:76:ALA:HB1	1.99	0.45
1:F:115[B]:LEU:HD12	1:F:190:MET:HB3	2.00	0.44
1:L:49[B]:LEU:CD1	3:L:301:UTC:CAU	2.80	0.44
1:K:49[B]:LEU:CD1	3:K:301:UTC:CAU	2.90	0.44
1:N:107:GLY:O	1:N:157[B]:ARG:NH1	2.51	0.44
1:B:123:HIS:H	2:B:302:MPD:H11	1.83	0.44
1:E:31:MET:HE3	1:E:63:TYR:CE1	2.52	0.44
1:K:95[A]:MET:CE	1:K:119[A]:GLU:CG	2.92	0.44
1:K:119[A]:GLU:CD	1:L:142:HIS:CE1	2.92	0.44
1:L:93:ILE:HG22	1:M:76:ALA:CB	2.48	0.44
1:C:93[A]:ILE:HG12	1:C:115:LEU:HD22	1.99	0.43
1:D:123:HIS:O	2:D:301:MPD:H11	2.18	0.43
1:E:115[B]:LEU:HD23	1:F:79:ASP:HB3	2.00	0.43
1:G:49[B]:LEU:HD21	3:G:301:UTC:CAS	2.48	0.43
1:E:119[A]:GLU:CD	1:F:142:HIS:CE1	2.84	0.43
2:C:302:MPD:H11	2:C:302:MPD:O4	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:49[B]:LEU:HD21	3:N:301:UTC:CAS	2.49	0.43
1:E:63:TYR:CE1	1:F:42[B]:ASN:OD1	2.72	0.43
1:F:31:MET:HE3	1:F:63:TYR:CE1	2.54	0.43
1:L:31:MET:HE3	1:L:63:TYR:CD1	2.54	0.43
1:S:93:ILE:HG22	1:T:76:ALA:HB1	2.00	0.43
1:A:107:GLY:O	1:A:157[B]:ARG:NH1	2.52	0.43
1:T:107:GLY:O	1:T:157[B]:ARG:NH1	2.51	0.43
1:E:115[A]:LEU:HD13	1:F:79:ASP:HB3	2.01	0.43
1:B:49[B]:LEU:HD21	3:B:301:UTC:CAS	2.49	0.42
1:E:122:ILE:HA	2:E:301:MPD:H13	2.01	0.42
1:M:49[B]:LEU:CD1	3:M:301:UTC:CAU	2.88	0.42
2:E:301:MPD:H11	2:E:301:MPD:O4	2.19	0.42
1:C:115:LEU:HD12	1:C:115:LEU:N	2.35	0.42
1:K:91:ILE:HG23	1:K:91:ILE:O	2.19	0.42
1:L:93:ILE:HG22	1:M:76:ALA:HB1	2.02	0.42
1:A:76:ALA:HA	1:G:93:ILE:CG2	2.48	0.42
1:G:150:LEU:CD1	2:G:302:MPD:H52	2.47	0.42
1:K:122:ILE:HA	2:K:302:MPD:H13	2.01	0.42
1:G:49[B]:LEU:CD1	3:G:301:UTC:CAU	2.90	0.42
1:K:93:ILE:HG22	1:L:76:ALA:HB1	2.01	0.42
1:G:107:GLY:O	1:G:157[B]:ARG:NH1	2.53	0.42
1:A:42[B]:ASN:HD21	1:G:31:MET:HB3	1.85	0.42
1:I:76:ALA:HB1	1:T:93:ILE:HG22	2.02	0.41
1:I:123:HIS:H	2:I:301:MPD:H13	1.82	0.41
1:F:98:SER:HA	2:F:302:MPD:H12	2.02	0.41
1:T:31:MET:HE3	1:T:63:TYR:CE1	2.56	0.41
1:F:95[B]:MET:HA	1:F:119[B]:GLU:O	2.21	0.41
1:C:123:HIS:O	2:C:302:MPD:H11	2.21	0.41
1:D:157[A]:ARG:HH11	1:D:157[A]:ARG:HD3	1.71	0.41
1:K:31:MET:HE3	1:K:63:TYR:CE1	2.56	0.41
1:S:93:ILE:HG22	1:T:76:ALA:CB	2.51	0.41
1:C:107:GLY:O	1:C:157[B]:ARG:NH1	2.54	0.41
1:A:76:ALA:HB1	1:G:93:ILE:HG22	2.01	0.41
1:F:95[A]:MET:HA	1:F:119[A]:GLU:O	2.21	0.41
1:K:153:ILE:O	1:K:157[B]:ARG:HG2	2.21	0.41
1:C:115:LEU:N	1:C:115:LEU:CD1	2.83	0.41
1:E:95[B]:MET:HE3	4:E:2361:HOH:O	2.20	0.41
1:A:83:HIS:CE1	1:G:190:MET:HE3	2.56	0.40
1:A:142:HIS:HE1	1:G:119[A]:GLU:CD	2.24	0.40
1:E:93:ILE:HG22	1:F:76:ALA:CB	2.51	0.40
1:G:38:ASP:OD2	4:G:401:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HG22	1:C:76:ALA:HB1	2.03	0.40
1:N:93:ILE:HG22	1:S:76:ALA:CB	2.52	0.40

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	181/203 (89%)	179 (99%)	2 (1%)	0	100	100
1	C	185/203 (91%)	182 (98%)	3 (2%)	0	100	100
1	D	185/203 (91%)	182 (98%)	3 (2%)	0	100	100
1	E	183/203 (90%)	181 (99%)	2 (1%)	0	100	100
1	F	181/203 (89%)	178 (98%)	3 (2%)	0	100	100
1	G	185/203 (91%)	182 (98%)	3 (2%)	0	100	100
1	I	181/203 (89%)	179 (99%)	2 (1%)	0	100	100
1	K	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
1	L	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
1	M	186/203 (92%)	183 (98%)	3 (2%)	0	100	100
1	N	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	S	179/203 (88%)	176 (98%)	3 (2%)	0	100	100
1	T	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
All	All	2551/2842 (90%)	2516 (99%)	35 (1%)	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	152/171 (89%)	150 (99%)	2 (1%)	69	54
1	B	153/171 (90%)	151 (99%)	2 (1%)	69	54
1	C	155/171 (91%)	152 (98%)	3 (2%)	57	38
1	D	153/171 (90%)	151 (99%)	2 (1%)	69	54
1	E	153/171 (90%)	151 (99%)	2 (1%)	69	54
1	F	153/171 (90%)	150 (98%)	3 (2%)	55	36
1	G	155/171 (91%)	152 (98%)	3 (2%)	57	38
1	I	152/171 (89%)	150 (99%)	2 (1%)	69	54
1	K	152/171 (89%)	148 (97%)	4 (3%)	46	25
1	L	155/171 (91%)	152 (98%)	3 (2%)	57	38
1	M	154/171 (90%)	153 (99%)	1 (1%)	86	79
1	N	152/171 (89%)	149 (98%)	3 (2%)	55	36
1	S	150/171 (88%)	147 (98%)	3 (2%)	55	36
1	T	151/171 (88%)	149 (99%)	2 (1%)	69	54
All	All	2140/2394 (89%)	2105 (98%)	35 (2%)	65	46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	123	HIS
1	B	27	ASP
1	B	123	HIS
1	C	27[A]	ASP
1	C	27[B]	ASP
1	C	123	HIS
1	D	27	ASP
1	D	123	HIS
1	E	27	ASP
1	E	123	HIS

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Mol	Chain	Res	Type
1	F	27	ASP
1	F	63	TYR
1	F	123	HIS
1	G	27[A]	ASP
1	G	27[B]	ASP
1	G	123	HIS
1	I	27	ASP
1	I	123	HIS
1	K	27	ASP
1	K	123	HIS
1	K	125	PRO
1	K	167	LYS
1	L	27	ASP
1	L	63	TYR
1	L	123	HIS
1	M	123	HIS
1	N	27[A]	ASP
1	N	27[B]	ASP
1	N	123	HIS
1	S	27[A]	ASP
1	S	27[B]	ASP
1	S	123	HIS
1	T	27	ASP
1	T	123	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

28 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
2	MPD	D	301	-	7,7,7	0.53	0	9,10,10	1.07	1 (11%)
2	MPD	G	302	-	7,7,7	0.27	0	9,10,10	0.66	0
2	MPD	S	302	-	7,7,7	0.25	0	9,10,10	0.66	0
2	MPD	T	301	-	7,7,7	0.29	0	9,10,10	0.93	1 (11%)
2	MPD	M	302	-	7,7,7	0.52	0	9,10,10	1.27	1 (11%)
2	MPD	A	301	-	7,7,7	0.22	0	9,10,10	0.91	1 (11%)
2	MPD	N	302	-	7,7,7	0.55	0	9,10,10	1.12	1 (11%)
3	UTC	K	301	-	44,46,46	1.79	8 (18%)	56,65,65	1.68	9 (16%)
3	UTC	S	301	-	44,46,46	1.51	6 (13%)	56,65,65	1.52	8 (14%)
3	UTC	N	301	-	44,46,46	1.75	9 (20%)	56,65,65	1.38	7 (12%)
3	UTC	L	301	-	44,46,46	1.73	11 (25%)	56,65,65	1.93	13 (23%)
2	MPD	I	301	-	7,7,7	0.27	0	9,10,10	1.35	1 (11%)
2	MPD	D	302	-	7,7,7	0.37	0	9,10,10	0.38	0
2	MPD	F	302	-	7,7,7	0.44	0	9,10,10	1.44	1 (11%)
2	MPD	E	301	-	7,7,7	0.41	0	9,10,10	1.10	1 (11%)
3	UTC	F	301	-	44,46,46	1.68	12 (27%)	56,65,65	1.61	8 (14%)
2	MPD	L	302	-	7,7,7	0.34	0	9,10,10	1.23	1 (11%)
2	MPD	K	302	-	7,7,7	0.29	0	9,10,10	0.91	1 (11%)
2	MPD	C	302	-	7,7,7	0.51	0	9,10,10	0.78	0
3	UTC	C	301	-	44,46,46	1.72	8 (18%)	56,65,65	1.57	11 (19%)
3	UTC	G	301	-	44,46,46	1.62	8 (18%)	56,65,65	1.73	13 (23%)
3	UTC	D	303	-	44,46,46	1.69	6 (13%)	56,65,65	1.54	9 (16%)
3	UTC	M	301	-	44,46,46	1.89	11 (25%)	56,65,65	1.68	11 (19%)
3	UTC	A	302	-	44,46,46	1.97	11 (25%)	56,65,65	1.67	13 (23%)
3	UTC	B	301	-	44,46,46	1.65	9 (20%)	56,65,65	1.39	9 (16%)
3	UTC	I	302	-	44,46,46	1.66	8 (18%)	56,65,65	1.63	8 (14%)
3	UTC	S	303	-	44,46,46	1.60	8 (18%)	56,65,65	1.51	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	B	302	-	7,7,7	0.39	0	9,10,10	0.99	1 (11%)

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
2	MPD	D	301	-	-	0/5/5/5	-
2	MPD	G	302	-	-	0/5/5/5	-
2	MPD	S	302	-	-	0/5/5/5	-
2	MPD	T	301	-	-	0/5/5/5	-
2	MPD	M	302	-	-	0/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
2	MPD	N	302	-	-	0/5/5/5	-
3	UTC	K	301	-	-	0/17/50/50	0/6/6/6
3	UTC	S	301	-	-	0/17/50/50	0/6/6/6
3	UTC	N	301	-	-	0/17/50/50	0/6/6/6
3	UTC	L	301	-	-	0/17/50/50	0/6/6/6
2	MPD	I	301	-	-	0/5/5/5	-
2	MPD	D	302	-	-	0/5/5/5	-
2	MPD	F	302	-	-	0/5/5/5	-
2	MPD	E	301	-	-	0/5/5/5	-
3	UTC	F	301	-	-	0/17/50/50	0/6/6/6
2	MPD	L	302	-	-	0/5/5/5	-
2	MPD	K	302	-	-	0/5/5/5	-
2	MPD	C	302	-	-	0/5/5/5	-
3	UTC	C	301	-	-	0/17/50/50	0/6/6/6
3	UTC	G	301	-	-	0/17/50/50	0/6/6/6
3	UTC	D	303	-	-	0/17/50/50	0/6/6/6
3	UTC	M	301	-	-	0/17/50/50	0/6/6/6
3	UTC	A	302	-	-	0/17/50/50	0/6/6/6
3	UTC	B	301	-	-	0/17/50/50	0/6/6/6
3	UTC	I	302	-	-	0/17/50/50	0/6/6/6
3	UTC	S	303	-	-	0/17/50/50	0/6/6/6
2	MPD	B	302	-	-	0/5/5/5	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	UTC	CA-C	-5.76	1.40	1.51
3	K	301	UTC	CA-C	-5.72	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	UTC	CBK-N	5.38	1.39	1.35
3	A	302	UTC	CA-C	-5.29	1.41	1.51
3	I	302	UTC	CA-C	-5.22	1.41	1.51
3	G	301	UTC	CA-C	-5.11	1.41	1.51
3	N	301	UTC	CA-C	-4.83	1.42	1.51
3	D	303	UTC	CAZ-NBH	4.75	1.54	1.46
3	M	301	UTC	CA-C	-4.67	1.42	1.51
3	M	301	UTC	CBK-N	4.63	1.39	1.35
3	S	303	UTC	CA-C	-4.51	1.43	1.51
3	I	302	UTC	CBK-N	4.51	1.39	1.35
3	B	301	UTC	CA-C	-4.44	1.43	1.51
3	A	302	UTC	CBM-NBN	4.31	1.54	1.47
3	S	303	UTC	CBK-N	4.31	1.39	1.35
3	D	303	UTC	CBL-CBK	-4.26	1.41	1.51
3	N	301	UTC	CBL-CBK	-4.23	1.41	1.51
3	L	301	UTC	CA-C	-4.16	1.43	1.51
3	A	302	UTC	CBL-CBK	-4.16	1.41	1.51
3	B	301	UTC	CBL-CBK	-4.03	1.41	1.51
3	K	301	UTC	CBL-CBK	-4.01	1.41	1.51
3	C	301	UTC	CBL-CBK	-3.91	1.42	1.51
3	D	303	UTC	CA-C	-3.91	1.44	1.51
3	F	301	UTC	CA-C	-3.89	1.44	1.51
3	D	303	UTC	CBK-N	3.86	1.38	1.35
3	N	301	UTC	CAZ-NBH	3.85	1.52	1.46
3	S	303	UTC	CBL-CBK	-3.80	1.42	1.51
3	L	301	UTC	CAZ-NBH	3.77	1.52	1.46
3	K	301	UTC	CAZ-NBH	3.77	1.52	1.46
3	G	301	UTC	CBK-N	3.70	1.38	1.35
3	N	301	UTC	CBO-NBN	-3.55	1.42	1.46
3	M	301	UTC	CAW-CAV	3.51	1.44	1.36
3	I	302	UTC	CBL-CBK	-3.48	1.43	1.51
3	F	301	UTC	CAD-CAE	-3.47	1.31	1.38
3	C	301	UTC	CAZ-NBH	3.47	1.52	1.46
3	S	301	UTC	CBO-NBN	-3.37	1.42	1.46
3	F	301	UTC	CBL-CBK	-3.36	1.43	1.51
3	K	301	UTC	CBK-N	3.34	1.38	1.35
3	C	301	UTC	CBK-N	3.30	1.38	1.35
3	N	301	UTC	CBK-N	3.29	1.38	1.35
3	S	301	UTC	CBL-CBK	-3.17	1.43	1.51
3	F	301	UTC	CBO-NBN	-3.16	1.43	1.46
3	K	301	UTC	CA-N	3.16	1.52	1.47
3	S	301	UTC	CBM-NBN	3.13	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	301	UTC	CAY-CAP	-3.10	1.35	1.42
3	L	301	UTC	CBI-NBH	3.10	1.50	1.46
3	S	301	UTC	CAZ-NBH	3.10	1.51	1.46
3	D	303	UTC	CAY-CAP	-3.08	1.35	1.42
3	B	301	UTC	CAZ-NBH	3.08	1.51	1.46
3	S	301	UTC	CA-C	-3.04	1.45	1.51
3	A	302	UTC	CAW-CAV	3.04	1.43	1.36
3	M	301	UTC	CAS-CAT	3.00	1.43	1.36
3	B	301	UTC	CAQ-CAP	-2.99	1.36	1.42
3	M	301	UTC	CAD-CAE	-2.96	1.32	1.38
3	G	301	UTC	CAY-CAP	-2.96	1.35	1.42
3	S	303	UTC	CAZ-NBH	2.96	1.51	1.46
3	F	301	UTC	CBK-N	2.91	1.37	1.35
3	M	301	UTC	CBM-NBN	2.89	1.52	1.47
3	B	301	UTC	CBK-N	2.89	1.37	1.35
3	L	301	UTC	CAW-CAV	2.88	1.43	1.36
3	A	302	UTC	CAY-CAP	-2.87	1.35	1.42
3	G	301	UTC	CAW-CAV	2.85	1.43	1.36
3	N	301	UTC	CA-N	2.84	1.52	1.47
3	B	301	UTC	CAY-CAP	-2.83	1.36	1.42
3	L	301	UTC	CAY-CAP	-2.76	1.36	1.42
3	F	301	UTC	CAZ-NBH	2.64	1.51	1.46
3	K	301	UTC	CBO-NBN	-2.59	1.43	1.46
3	S	303	UTC	CAY-CAP	-2.58	1.36	1.42
3	C	301	UTC	CBO-NBN	-2.57	1.43	1.46
3	L	301	UTC	CA-N	2.50	1.51	1.47
3	K	301	UTC	CAQ-CAP	-2.49	1.37	1.42
3	F	301	UTC	CAQ-CAP	-2.49	1.37	1.42
3	A	302	UTC	CAS-CAT	2.49	1.42	1.36
3	N	301	UTC	CAY-CAP	-2.47	1.36	1.42
3	G	301	UTC	CBM-NBN	2.47	1.51	1.47
3	L	301	UTC	CBL-CBK	-2.45	1.45	1.51
3	F	301	UTC	CAW-CAV	2.44	1.42	1.36
3	G	301	UTC	CAS-CAT	2.41	1.42	1.36
3	C	301	UTC	CAR-CAQ	2.40	1.42	1.36
3	I	302	UTC	CBM-NBN	2.39	1.51	1.47
3	L	301	UTC	CAP-CAU	-2.39	1.38	1.43
3	C	301	UTC	CAG-NBC	-2.37	1.41	1.46
3	B	301	UTC	CAZ-CAY	2.36	1.58	1.52
3	M	301	UTC	OBD-CBE	2.36	1.27	1.23
3	F	301	UTC	CA-N	2.35	1.51	1.47
3	S	301	UTC	CAS-CAT	2.33	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	UTC	CBO-NBN	-2.31	1.44	1.46
3	I	302	UTC	OBD-CBE	2.30	1.27	1.23
3	N	301	UTC	CAS-CAT	2.28	1.41	1.36
3	L	301	UTC	O-C	2.26	1.26	1.22
3	F	301	UTC	O-C	2.26	1.26	1.22
3	M	301	UTC	C-NBH	2.24	1.40	1.35
3	I	302	UTC	CBO-NBN	-2.22	1.44	1.46
3	D	303	UTC	CAW-CAV	2.20	1.41	1.36
3	G	301	UTC	OBD-CBE	2.18	1.27	1.23
3	B	301	UTC	CAR-CAQ	2.18	1.41	1.36
3	F	301	UTC	CAY-CAP	-2.17	1.37	1.42
3	L	301	UTC	CAX-CAY	2.13	1.41	1.37
3	C	301	UTC	CAW-CAV	2.13	1.41	1.36
3	I	302	UTC	O-C	2.12	1.26	1.22
3	I	302	UTC	C-NBH	2.12	1.39	1.35
3	K	301	UTC	CAG-CAF	-2.10	1.46	1.51
3	F	301	UTC	CAS-CAT	2.09	1.41	1.36
3	S	303	UTC	CAD-CAE	-2.07	1.34	1.38
3	G	301	UTC	CAX-CAY	2.07	1.41	1.37
3	N	301	UTC	CAQ-CAP	-2.06	1.38	1.42
3	A	302	UTC	CAR-CAQ	2.06	1.41	1.36
3	A	302	UTC	C-NBH	2.05	1.39	1.35
3	A	302	UTC	CBO-NBN	-2.03	1.44	1.46
3	L	301	UTC	CAR-CAQ	2.03	1.41	1.36
3	M	301	UTC	CE1-CZ	2.02	1.42	1.38
3	A	302	UTC	O-C	2.02	1.26	1.22
3	S	303	UTC	CA-N	2.02	1.50	1.47
3	M	301	UTC	CBL-CBK	-2.00	1.46	1.51
3	S	303	UTC	CAS-CAT	2.00	1.41	1.36

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	301	UTC	OBA-CBK-N	-6.50	113.99	122.28
3	L	301	UTC	CAG-NBC-CBE	5.76	126.03	120.84
3	L	301	UTC	OBA-CBK-N	-5.66	115.06	122.28
3	F	301	UTC	CAG-NBC-CBE	5.51	125.81	120.84
3	I	302	UTC	CBL-CBK-N	5.33	125.48	117.97
3	D	303	UTC	OBA-CBK-N	-5.31	115.50	122.28
3	I	302	UTC	OBA-CBK-N	-5.29	115.53	122.28
3	M	301	UTC	OBA-CBK-N	-5.11	115.77	122.28
3	N	301	UTC	OBA-CBK-N	-5.10	115.78	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	UTC	CBL-CBK-N	5.06	125.10	117.97
3	S	301	UTC	OBA-CBK-N	-4.96	115.95	122.28
3	S	301	UTC	CBL-CBK-N	4.66	124.53	117.97
3	G	301	UTC	OBA-CBK-N	-4.56	116.47	122.28
3	D	303	UTC	O-C-NBH	-4.52	117.15	122.49
3	L	301	UTC	CBL-CBK-N	4.48	124.28	117.97
3	C	301	UTC	O-C-NBH	-4.47	117.21	122.49
3	M	301	UTC	CBL-CBK-N	4.36	124.11	117.97
3	F	301	UTC	OBA-CBK-N	-4.19	116.93	122.28
3	K	301	UTC	CBL-CBK-N	4.17	123.84	117.97
3	K	301	UTC	O-C-NBH	-4.09	117.66	122.49
3	S	301	UTC	O-C-NBH	-4.08	117.66	122.49
3	D	303	UTC	CBL-CBK-N	4.06	123.69	117.97
3	G	301	UTC	CBL-CBK-N	4.06	123.69	117.97
3	M	301	UTC	O-C-NBH	-4.05	117.70	122.49
3	F	301	UTC	CBL-CBK-N	4.04	123.66	117.97
3	S	303	UTC	CBL-CBK-N	4.03	123.65	117.97
3	N	301	UTC	O-C-NBH	-4.02	117.74	122.49
3	M	301	UTC	CAX-CAY-CAP	3.96	124.70	119.08
3	B	301	UTC	CBL-CBK-N	3.94	123.52	117.97
3	L	301	UTC	CAZ-CAY-CAP	3.92	126.78	119.93
3	C	301	UTC	CBL-CBK-N	3.85	123.39	117.97
3	S	303	UTC	OBA-CBK-N	-3.80	117.43	122.28
3	G	301	UTC	CAX-CAY-CAP	3.74	124.38	119.08
3	C	301	UTC	OBA-CBK-N	-3.65	117.62	122.28
3	L	301	UTC	CAT-CAU-CAP	3.60	123.86	119.12
3	A	302	UTC	OBA-CBK-N	-3.55	117.75	122.28
2	I	301	MPD	O2-C2-C1	-3.50	96.86	108.08
3	N	301	UTC	CBL-CBK-N	3.45	122.83	117.97
3	A	302	UTC	CB-CA-C	-3.45	102.54	109.84
3	G	301	UTC	CAG-CAF-CAA	-3.40	113.86	120.91
3	B	301	UTC	OBA-CBK-N	-3.35	118.01	122.28
3	I	302	UTC	CBO-CBI-NBH	-3.30	106.82	111.02
3	S	303	UTC	CAZ-CAY-CAP	3.27	125.64	119.93
3	G	301	UTC	CBL-CBM-NBN	-3.20	101.07	111.61
3	M	301	UTC	CAW-CAX-CAY	-3.20	115.81	121.48
3	C	301	UTC	CBL-CBM-NBN	-3.16	101.20	111.61
3	F	301	UTC	O-C-NBH	-3.16	118.76	122.49
3	G	301	UTC	O-C-NBH	-3.08	118.84	122.49
2	F	302	MPD	O2-C2-C1	-3.01	98.43	108.08
2	L	302	MPD	O2-C2-C1	-2.96	98.58	108.08
3	F	301	UTC	CAV-CAW-CAX	-2.94	116.30	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	UTC	CB-CA-C	-2.94	103.61	109.84
3	K	301	UTC	CBL-CBM-NBN	-2.93	101.97	111.61
3	S	303	UTC	CAG-NBC-CBE	2.92	123.47	120.84
3	K	301	UTC	CBO-CBI-NBH	-2.83	107.42	111.02
3	G	301	UTC	CAE-CAF-CAA	2.80	122.56	118.17
3	L	301	UTC	CAZ-CAY-CAX	-2.77	111.61	119.62
3	C	301	UTC	CAG-NBC-CBE	2.75	123.32	120.84
3	L	301	UTC	CAZ-NBH-C	2.74	122.28	119.73
2	M	302	MPD	O2-C2-C1	-2.70	99.40	108.08
3	B	301	UTC	CBL-CBM-NBN	-2.68	102.77	111.61
3	L	301	UTC	O-C-NBH	-2.68	119.32	122.49
3	S	303	UTC	CAT-CAU-CAP	2.67	122.63	119.12
3	A	302	UTC	CD2-CG-CD1	2.66	122.34	118.17
3	M	301	UTC	CA-C-NBH	2.66	122.84	116.85
2	N	302	MPD	O2-C2-C1	-2.65	99.59	108.08
3	G	301	UTC	CAG-NBC-CBE	2.63	123.21	120.84
3	A	302	UTC	CBO-CBI-NBH	-2.63	107.67	111.02
3	K	301	UTC	CA-C-NBH	2.61	122.72	116.85
3	S	303	UTC	O-C-NBH	-2.60	119.41	122.49
3	B	301	UTC	O-C-NBH	-2.59	119.43	122.49
3	I	302	UTC	CAR-CAS-CAT	-2.58	116.82	120.44
3	D	303	UTC	CA-C-NBH	2.57	122.63	116.85
3	S	303	UTC	CAE-CAF-CAA	2.51	122.11	118.17
3	L	301	UTC	C-CA-N	-2.50	107.31	112.29
3	I	302	UTC	CA-C-NBH	2.49	122.47	116.85
3	C	301	UTC	CA-C-NBH	2.49	122.46	116.85
3	K	301	UTC	CAT-CAU-CAP	2.49	122.40	119.12
3	A	302	UTC	CBL-CBM-NBN	-2.48	103.45	111.61
3	A	302	UTC	CAG-NBC-CBE	2.47	123.07	120.84
3	F	301	UTC	CB-CA-C	-2.47	104.62	109.84
3	N	301	UTC	CAV-CAW-CAX	-2.46	117.07	120.99
3	I	302	UTC	CBL-CBM-NBN	-2.45	103.53	111.61
3	I	302	UTC	CB-CA-C	-2.44	104.67	109.84
3	A	302	UTC	CBI-CBO-NBN	2.43	116.75	112.59
3	L	301	UTC	CBL-CBM-NBN	-2.42	103.64	111.61
3	L	301	UTC	CAT-CAU-CAV	-2.42	117.54	123.19
3	S	301	UTC	CA-C-NBH	2.41	122.29	116.85
3	L	301	UTC	CBO-CBI-NBH	-2.39	107.97	111.02
3	A	302	UTC	CAX-CAY-CAP	2.39	122.47	119.08
3	A	302	UTC	CAR-CAS-CAT	-2.38	117.10	120.44
3	D	303	UTC	CAY-CAP-CAU	2.38	121.94	118.98
3	B	301	UTC	CA-C-NBH	2.38	122.21	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	301	UTC	CBL-CBM-NBN	-2.37	103.80	111.61
3	C	301	UTC	CB-CA-C	-2.37	104.83	109.84
3	A	302	UTC	CAR-CAQ-CAP	2.36	124.16	120.89
3	L	301	UTC	CA-C-NBH	2.35	122.14	116.85
3	I	302	UTC	C-CA-N	-2.34	107.64	112.29
3	S	303	UTC	CBL-CBM-NBN	-2.31	103.99	111.61
3	F	301	UTC	CAR-CAS-CAT	-2.31	117.19	120.44
2	D	301	MPD	O2-C2-C1	-2.29	100.73	108.08
2	E	301	MPD	O2-C2-C1	-2.29	100.73	108.08
3	K	301	UTC	CB-CA-C	-2.29	104.99	109.84
3	B	301	UTC	CAZ-CAY-CAP	2.29	123.93	119.93
3	C	301	UTC	CAC-CAD-CAE	2.28	123.67	120.19
3	C	301	UTC	CAT-CAU-CAP	2.26	122.09	119.12
2	A	301	MPD	O2-C2-C1	-2.25	100.87	108.08
3	D	303	UTC	CD2-CG-CD1	2.23	121.67	118.17
3	C	301	UTC	CD2-CG-CD1	2.23	121.67	118.17
3	S	303	UTC	CAB-CAA-CAF	-2.22	117.22	120.63
2	B	302	MPD	O2-C2-C1	-2.21	101.00	108.08
3	G	301	UTC	CD2-CG-CD1	2.20	121.62	118.17
3	B	301	UTC	CB-CA-C	-2.19	105.19	109.84
3	S	301	UTC	CD2-CG-CD1	2.19	121.61	118.17
3	N	301	UTC	CAC-CAD-CAE	2.19	123.52	120.19
3	G	301	UTC	CAT-CAU-CAP	2.19	122.00	119.12
3	M	301	UTC	CAR-CAS-CAT	-2.19	117.37	120.44
3	M	301	UTC	CBL-CBM-NBN	-2.17	104.46	111.61
3	G	301	UTC	CA-C-NBH	2.17	121.74	116.85
2	T	301	MPD	O2-C2-C1	-2.17	101.11	108.08
3	G	301	UTC	CAR-CAS-CAT	-2.16	117.41	120.44
3	D	303	UTC	CBL-CBM-NBN	-2.16	104.50	111.61
3	S	301	UTC	CAZ-CAY-CAP	2.15	123.69	119.93
3	M	301	UTC	CAZ-CAY-CAX	-2.13	113.44	119.62
3	M	301	UTC	CAT-CAU-CAP	2.13	121.92	119.12
2	K	302	MPD	O2-C2-C1	-2.13	101.26	108.08
3	D	303	UTC	CBO-CBI-NBH	-2.09	108.36	111.02
3	N	301	UTC	CA-C-NBH	2.09	121.56	116.85
3	B	301	UTC	CAZ-NBH-C	-2.08	117.79	119.73
3	M	301	UTC	CAR-CAQ-CAP	2.07	123.77	120.89
3	S	303	UTC	CAT-CAU-CAV	-2.07	118.36	123.19
3	K	301	UTC	C-CA-N	-2.07	108.18	112.29
3	F	301	UTC	CAX-CAY-CAP	2.06	122.01	119.08
3	S	303	UTC	CA-C-NBH	2.05	121.46	116.85
3	A	302	UTC	CBM-NBN-CBO	2.04	119.99	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	301	UTC	CB-CA-C	-2.04	105.52	109.84
3	D	303	UTC	C-CA-N	-2.04	108.23	112.29
3	A	302	UTC	CAZ-CAY-CAP	2.04	123.49	119.93
3	C	301	UTC	CAD-CAE-CAF	-2.04	117.51	120.63
3	B	301	UTC	CAR-CAS-CAT	-2.02	117.60	120.44
3	S	301	UTC	CAT-CAU-CAP	2.01	121.77	119.12

There are no chirality outliers.

There are no torsion outliers.

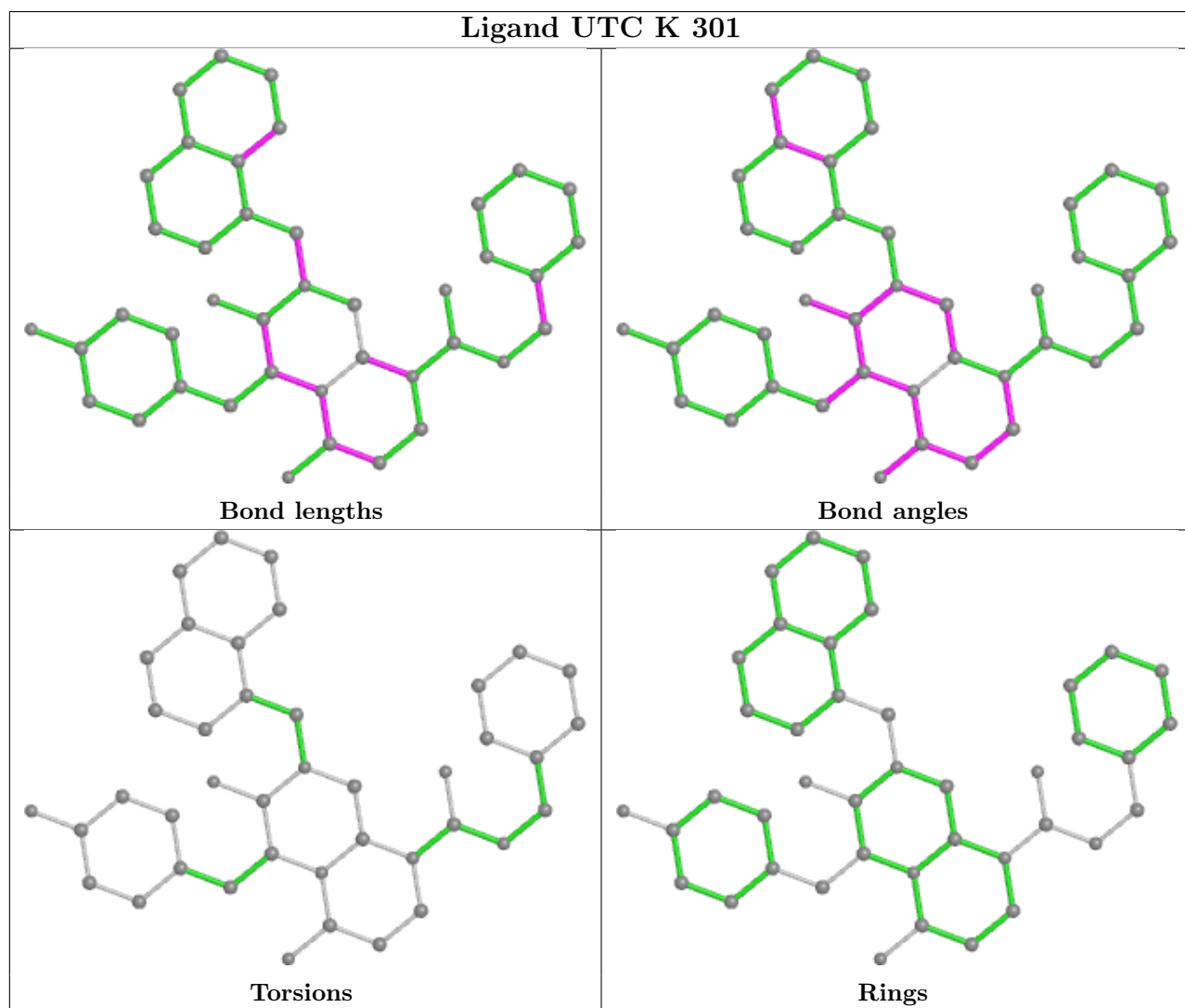
There are no ring outliers.

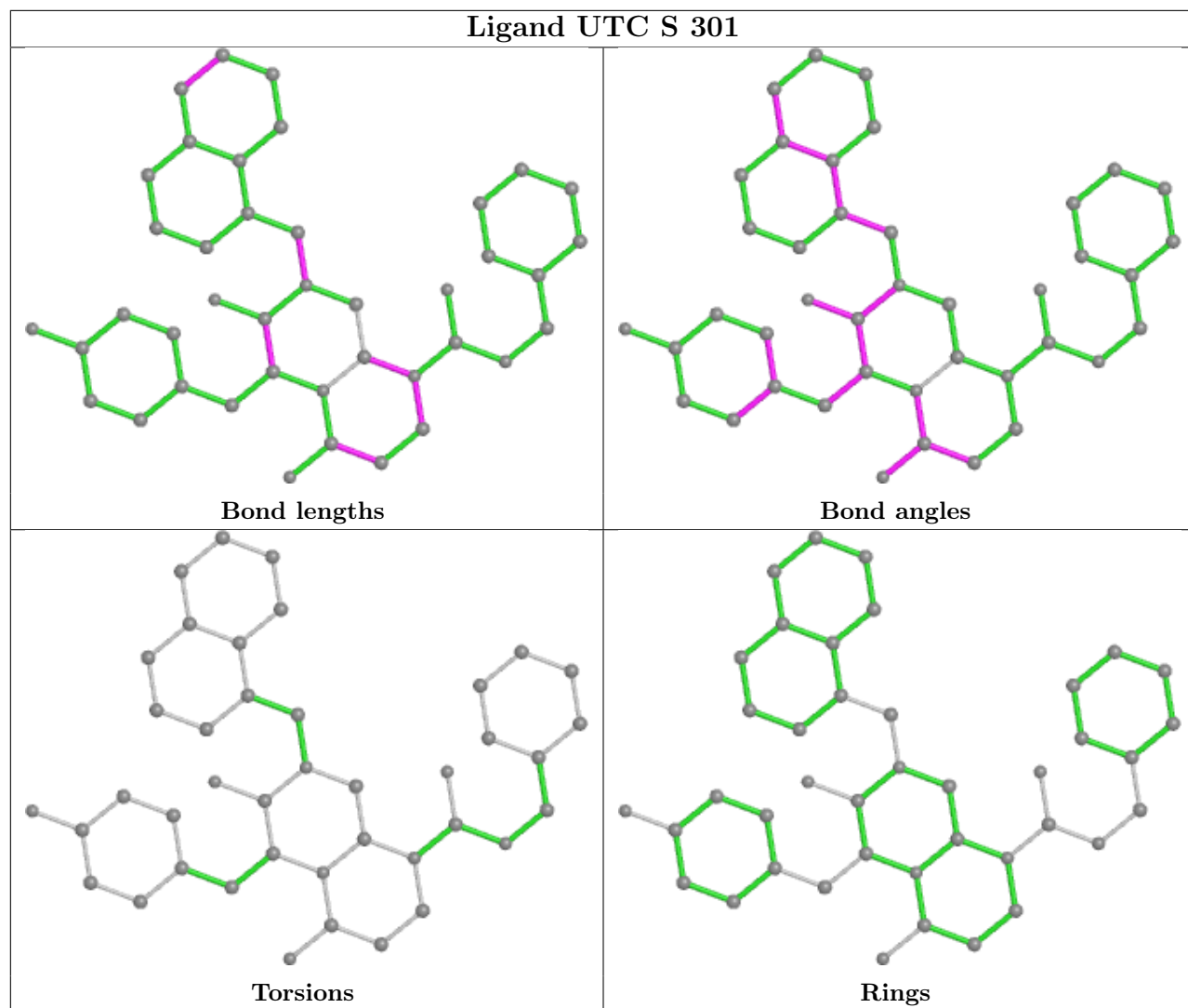
26 monomers are involved in 150 short contacts:

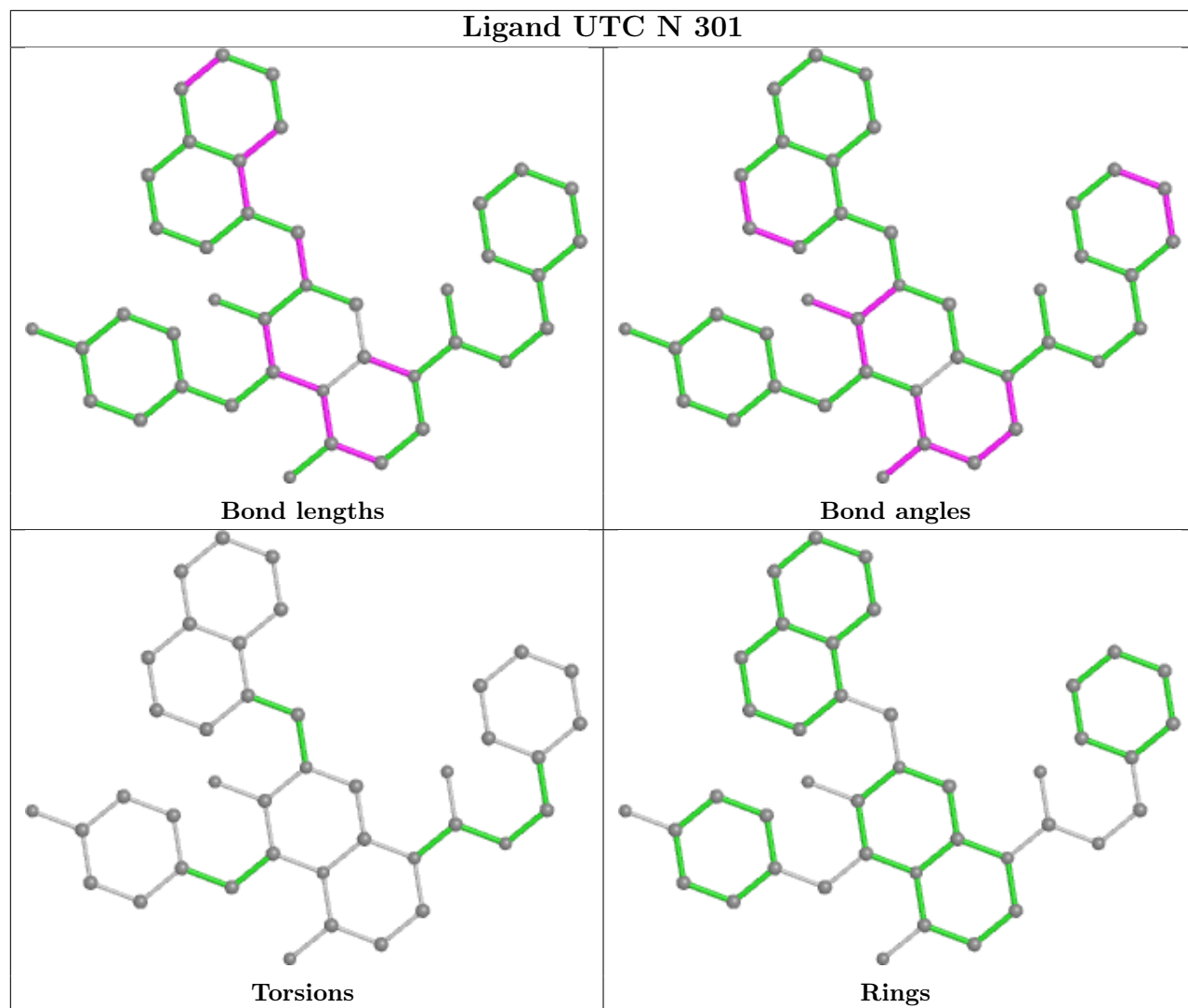
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	MPD	5	0
2	G	302	MPD	6	0
2	S	302	MPD	6	0
2	T	301	MPD	5	0
2	M	302	MPD	4	0
2	A	301	MPD	5	0
2	N	302	MPD	5	0
3	K	301	UTC	7	0
3	S	301	UTC	7	0
3	N	301	UTC	8	0
3	L	301	UTC	9	0
2	I	301	MPD	6	0
2	F	302	MPD	4	0
2	E	301	MPD	7	0
3	F	301	UTC	5	0
2	L	302	MPD	5	0
2	K	302	MPD	4	0
2	C	302	MPD	6	0
3	C	301	UTC	6	0
3	G	301	UTC	6	0
3	M	301	UTC	6	0
3	A	302	UTC	6	0
3	B	301	UTC	6	0
3	I	302	UTC	4	0
3	S	303	UTC	8	0
2	B	302	MPD	4	0

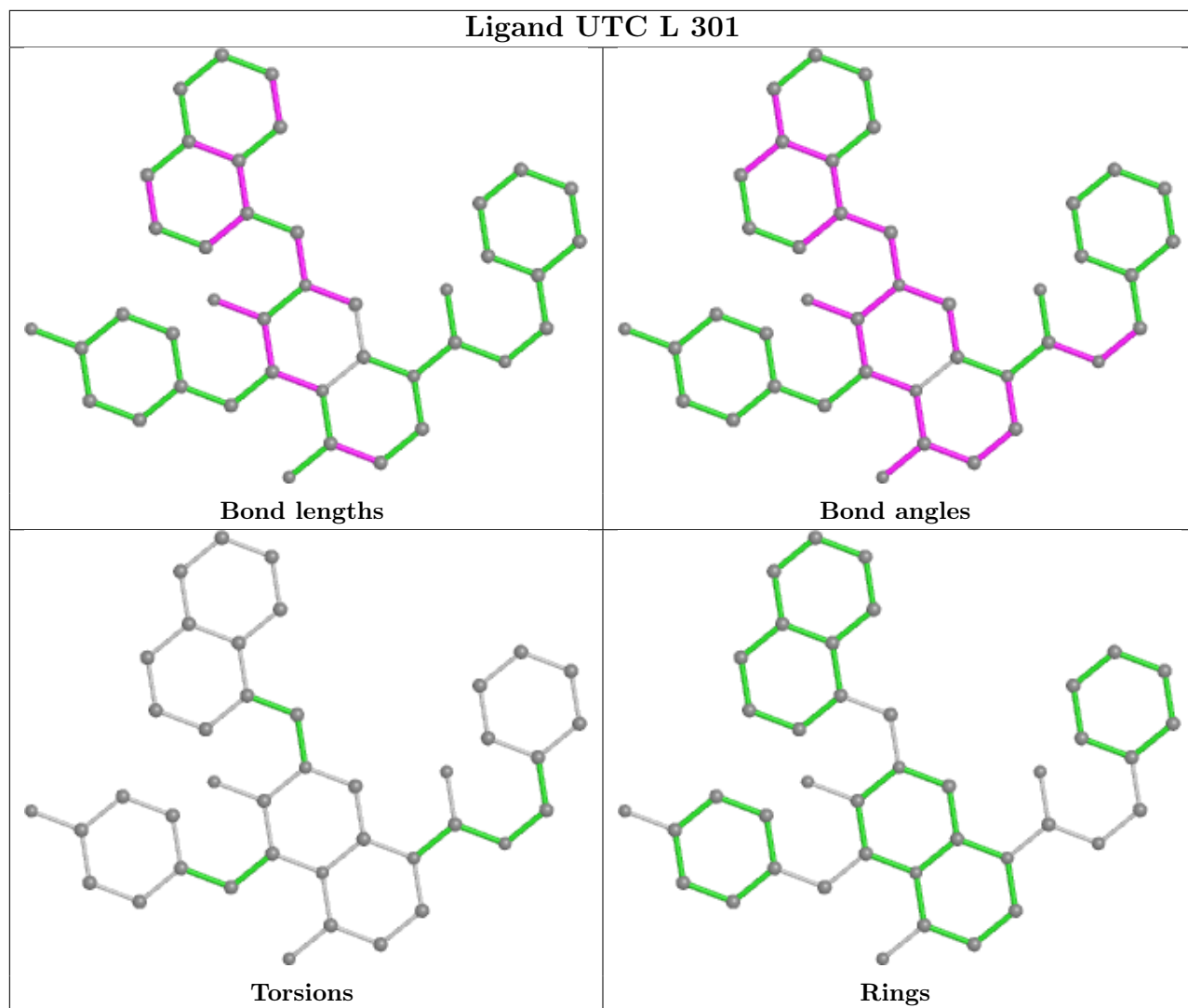
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

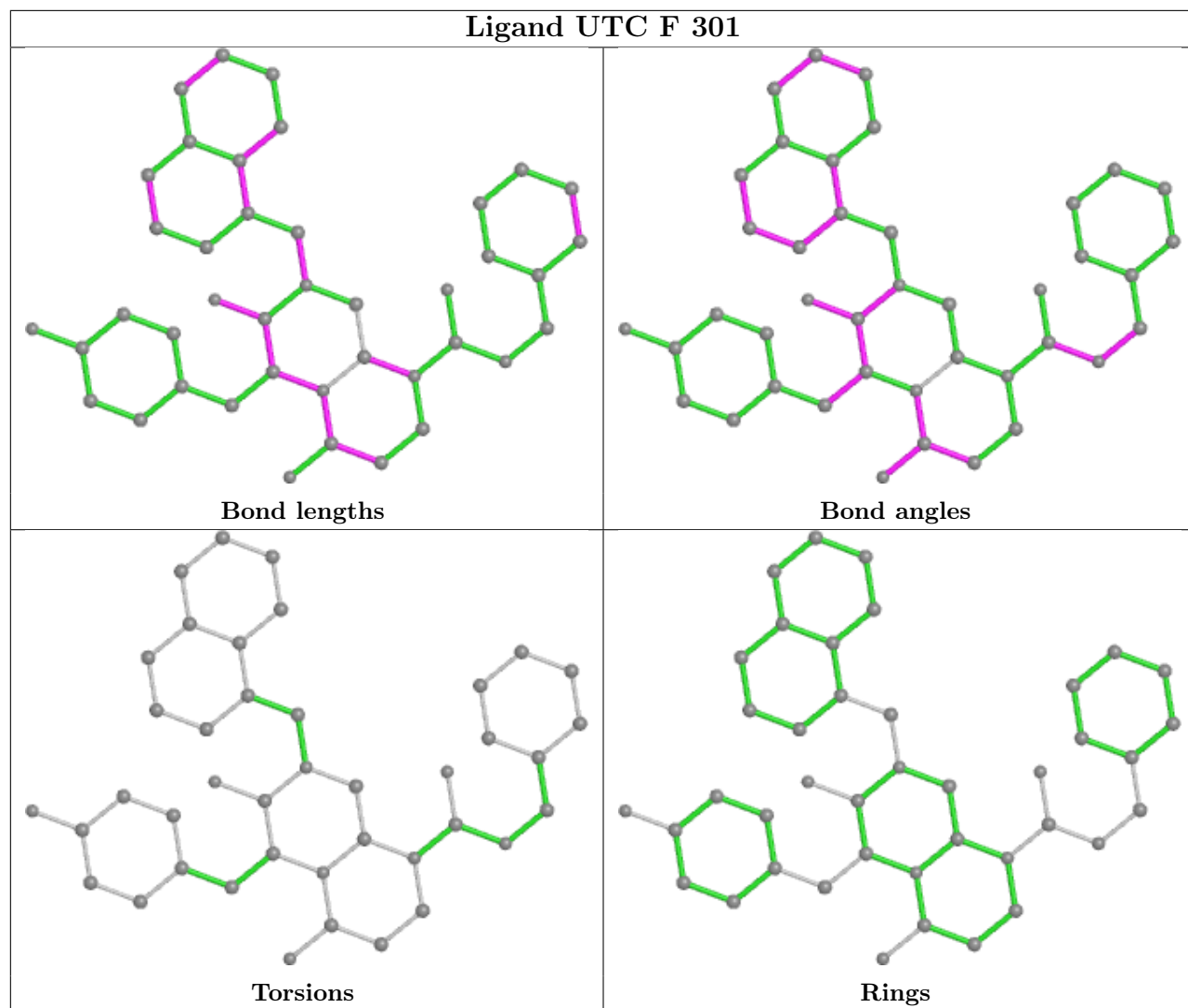


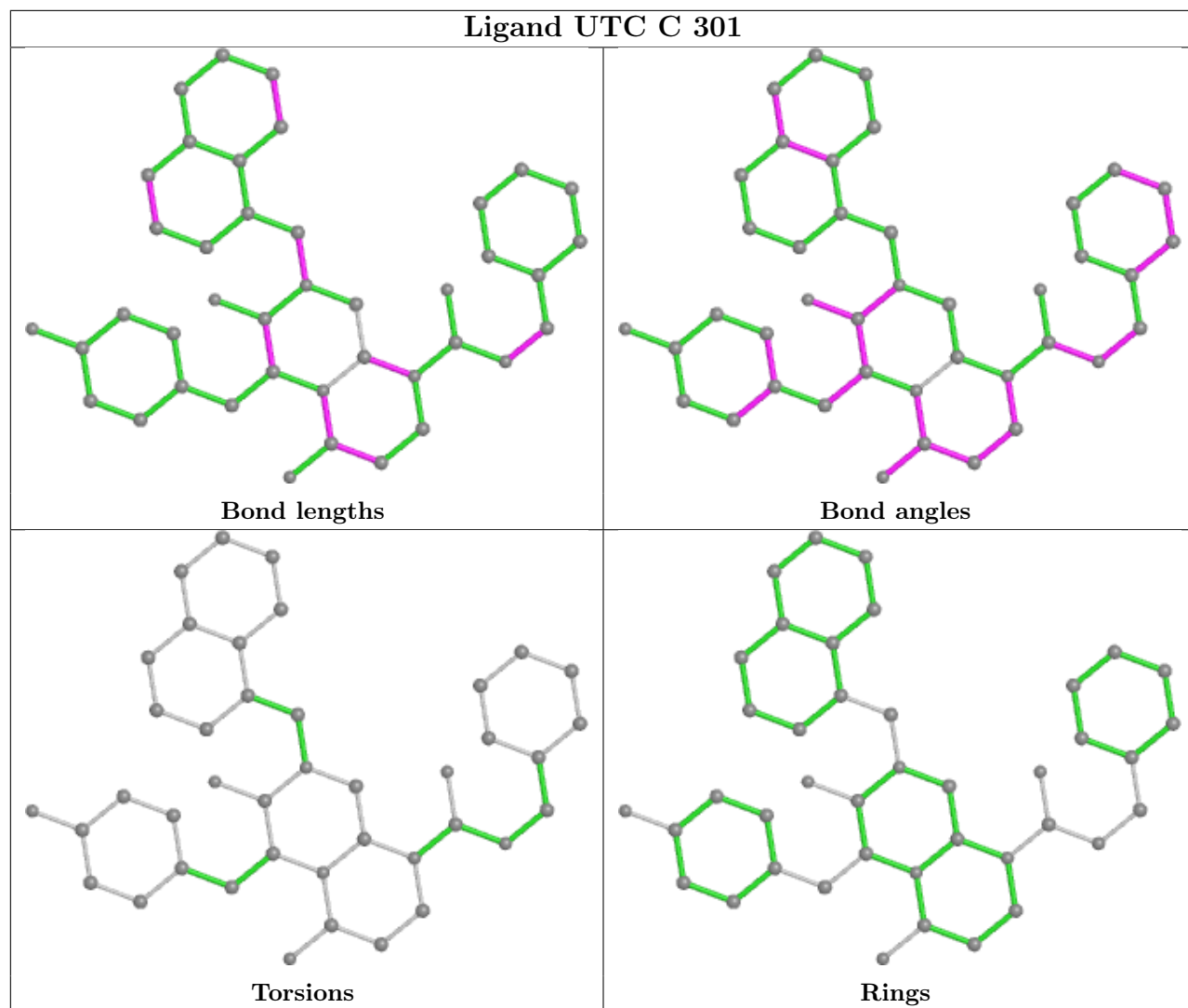


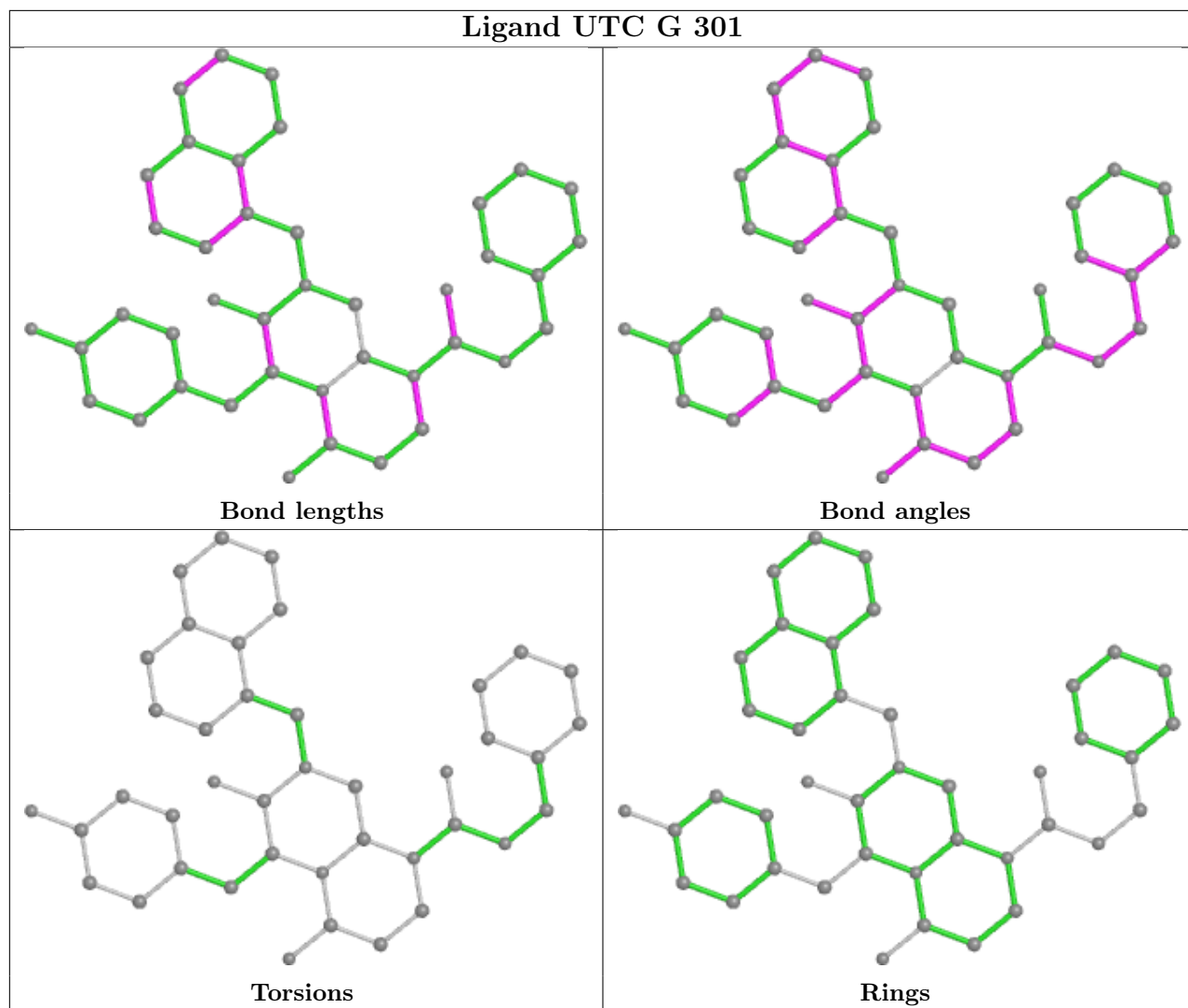


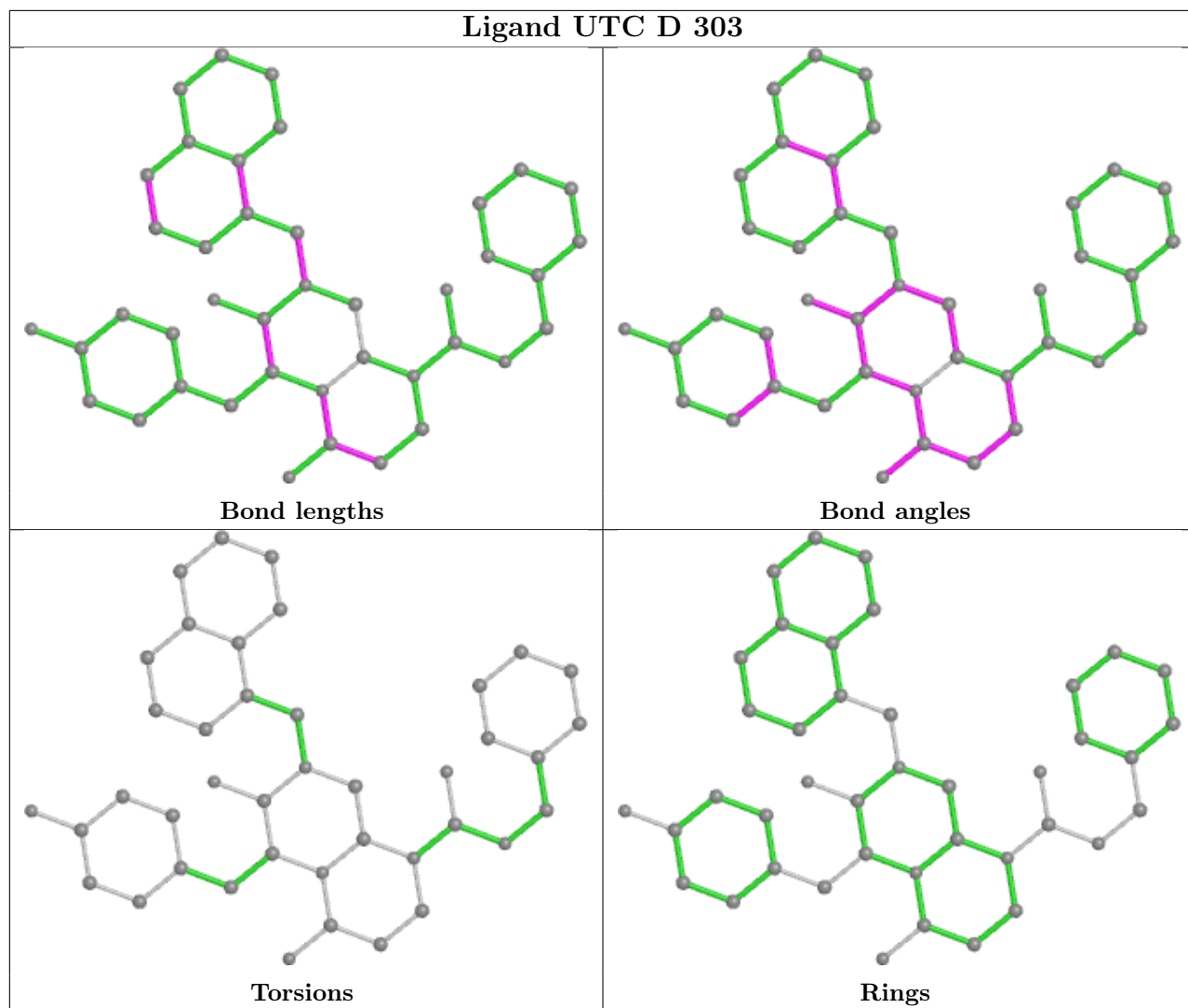


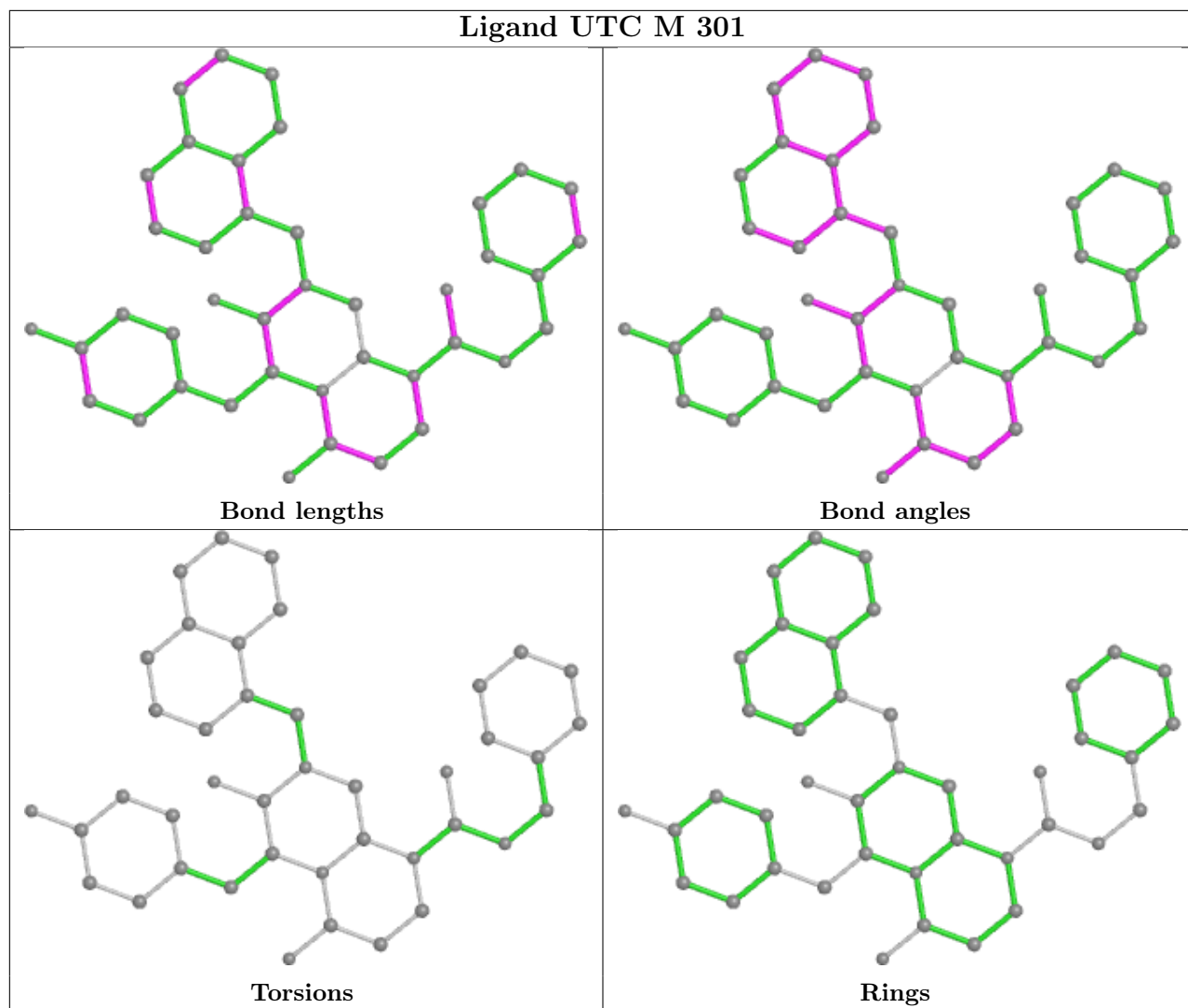


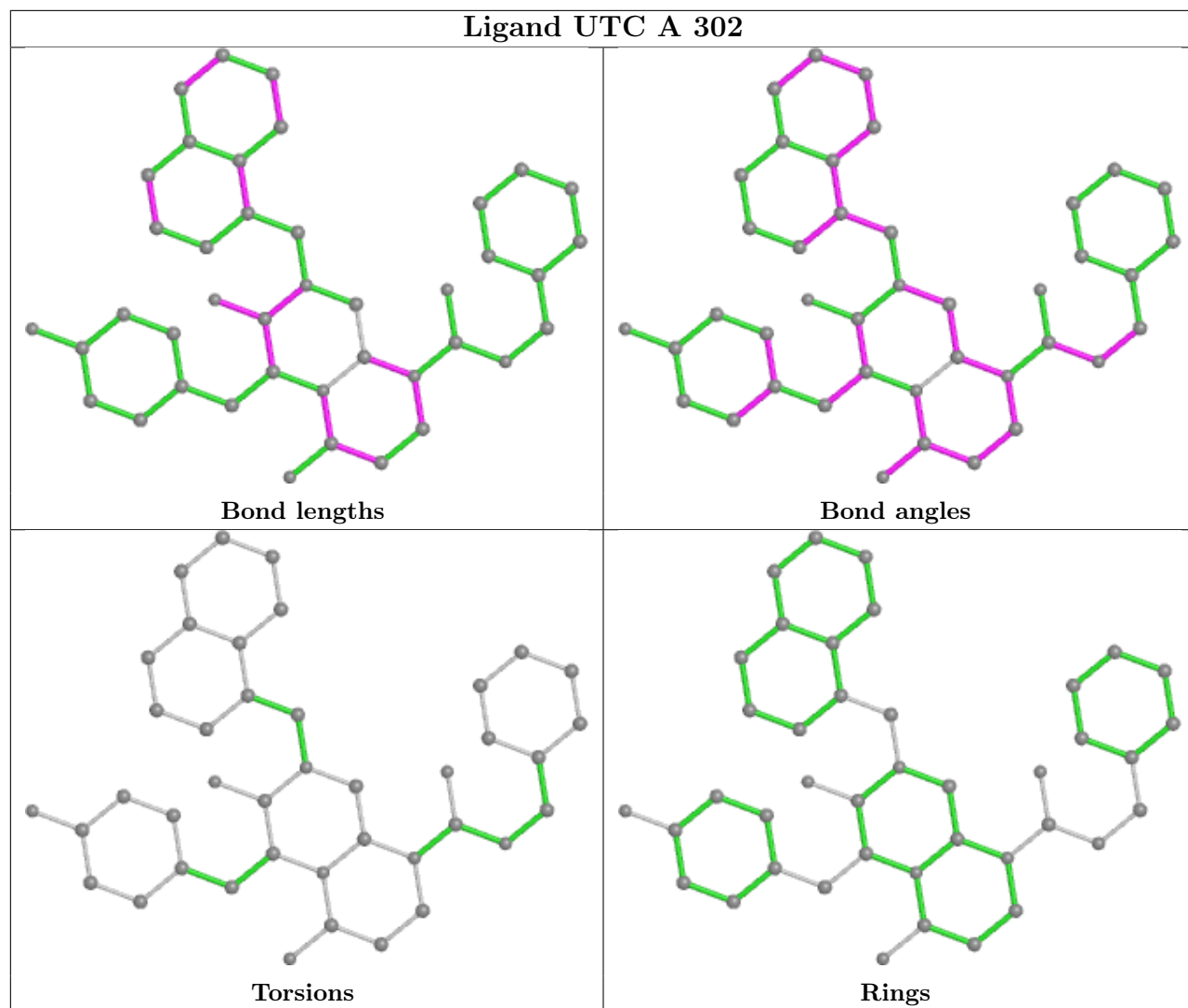


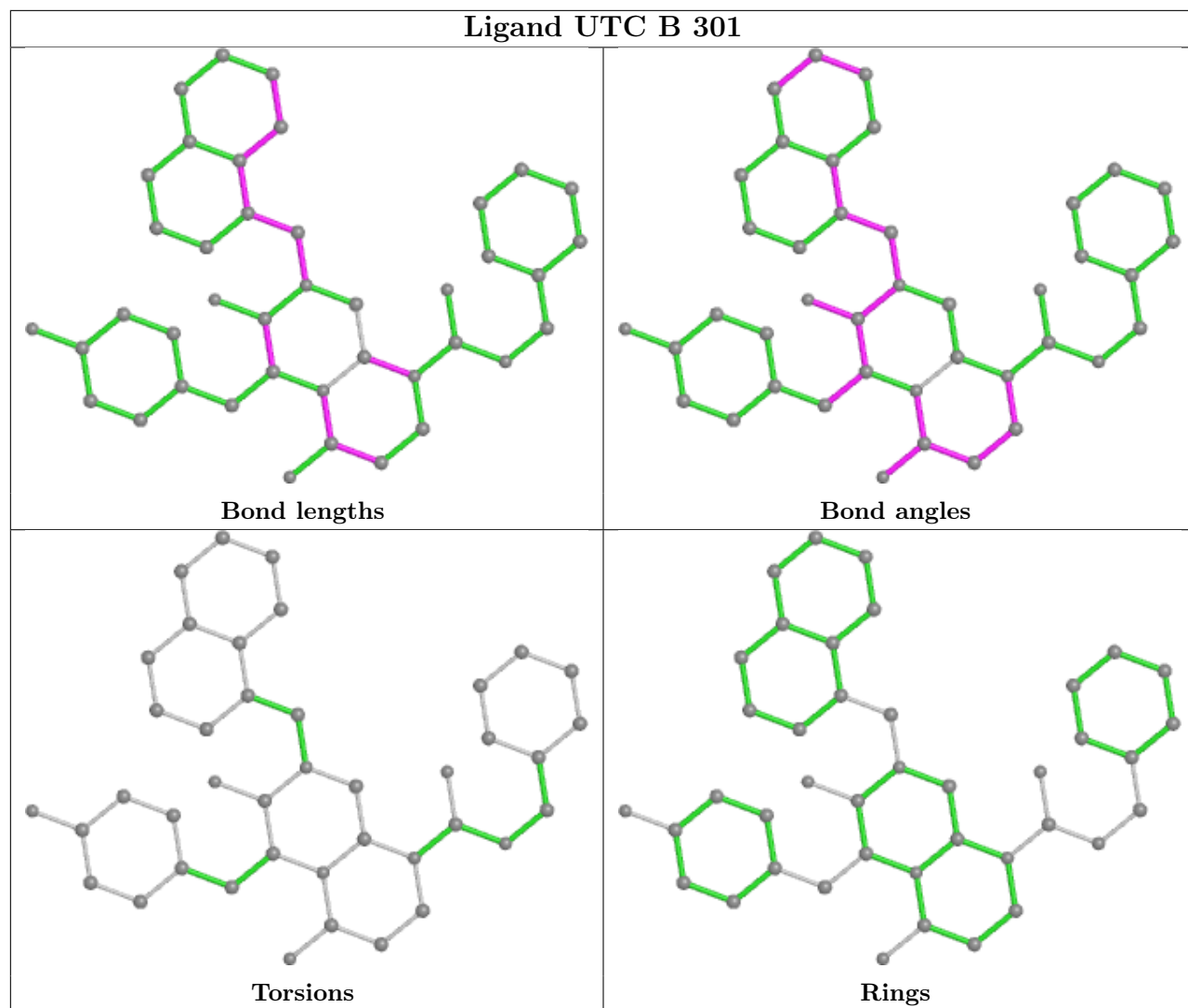


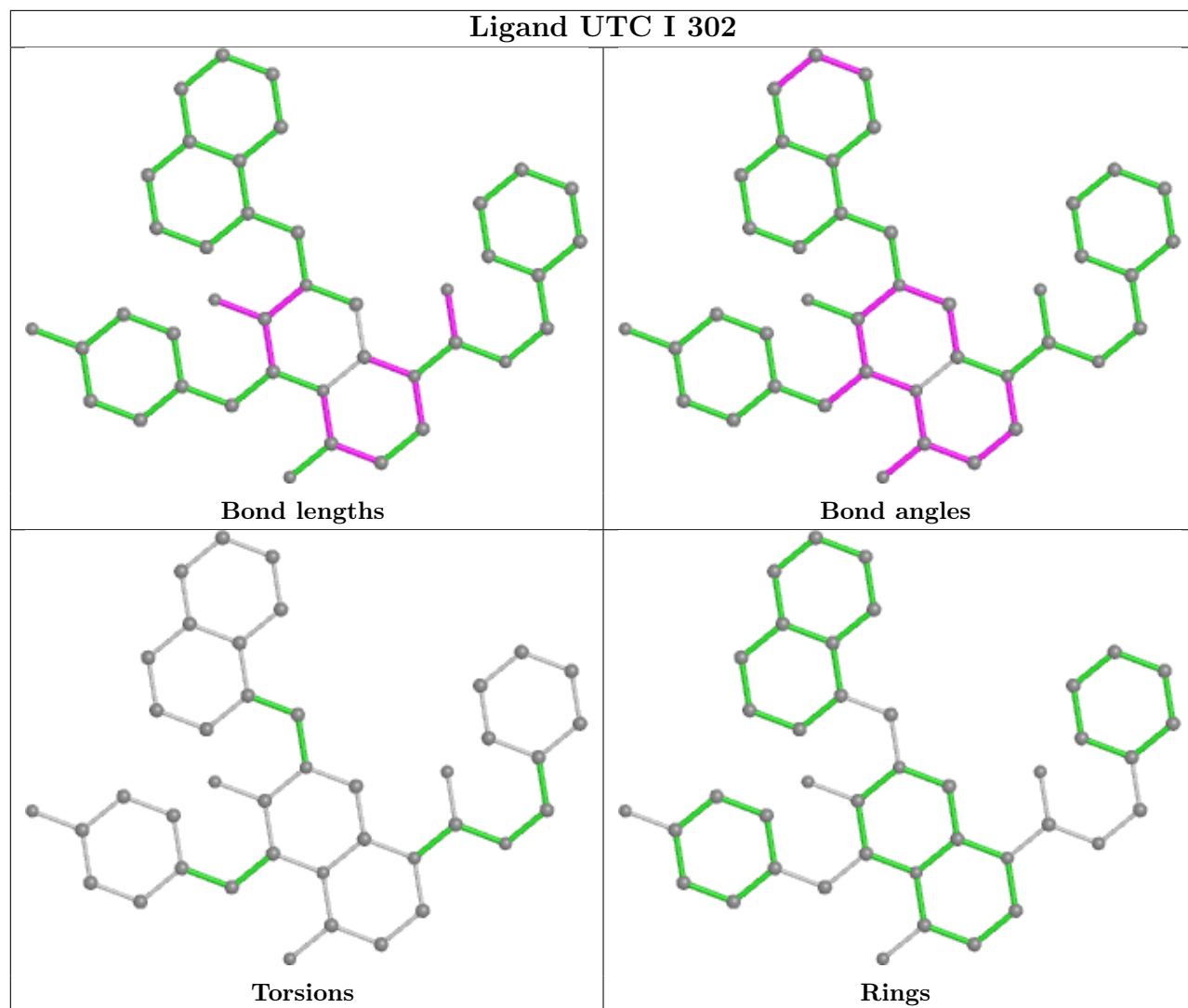




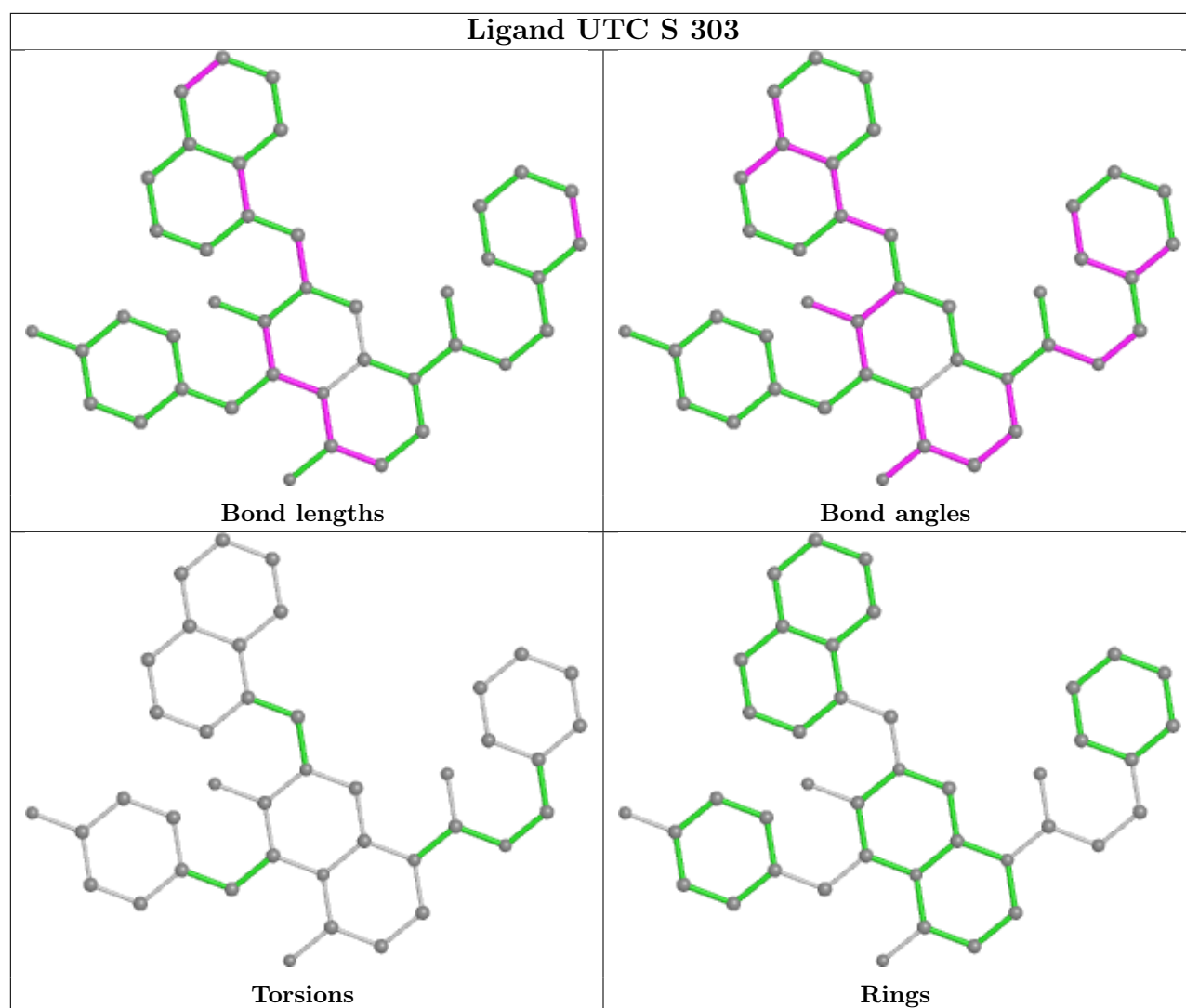












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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	180/203 (88%)	-0.26	2 (1%) 80 83	20, 26, 44, 65	0
1	B	180/203 (88%)	-0.24	3 (1%) 70 74	21, 27, 43, 65	0
1	C	184/203 (90%)	-0.27	0 100 100	16, 21, 38, 64	0
1	D	186/203 (91%)	-0.38	0 100 100	13, 19, 34, 58	0
1	E	183/203 (90%)	-0.20	4 (2%) 62 65	14, 19, 38, 59	0
1	F	178/203 (87%)	-0.34	3 (1%) 70 74	15, 20, 40, 55	0
1	G	181/203 (89%)	-0.28	4 (2%) 62 65	18, 26, 43, 64	0
1	I	181/203 (89%)	-0.30	2 (1%) 80 83	20, 27, 44, 61	0
1	K	180/203 (88%)	-0.27	0 100 100	16, 22, 36, 52	0
1	L	183/203 (90%)	-0.35	2 (1%) 80 83	14, 19, 35, 50	0
1	M	184/203 (90%)	-0.29	2 (1%) 80 83	14, 19, 36, 61	0
1	N	179/203 (88%)	-0.37	1 (0%) 89 91	16, 21, 39, 50	0
1	S	179/203 (88%)	-0.28	4 (2%) 62 65	18, 26, 42, 60	0
1	T	179/203 (88%)	-0.15	1 (0%) 89 91	20, 26, 44, 60	0
All	All	2537/2842 (89%)	-0.29	28 (1%) 80 83	13, 23, 42, 65	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	18	TYR	4.9
1	B	18	TYR	4.6
1	F	18	TYR	4.5
1	N	18	TYR	3.5
1	M	17	ALA	3.5
1	S	191	VAL	3.4
1	T	18	TYR	3.4
1	G	18	TYR	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	191	VAL	3.2
1	G	63	TYR	3.1
1	E	17	ALA	3.1
1	E	8	ILE	3.1
1	F	6	THR	3.0
1	F	63	TYR	3.0
1	G	8	ILE	2.9
1	L	17	ALA	2.6
1	S	7	VAL	2.6
1	A	18	TYR	2.6
1	B	8	ILE	2.5
1	I	18	TYR	2.5
1	G	191	VAL	2.5
1	B	7	VAL	2.3
1	A	17	ALA	2.2
1	S	6	THR	2.2
1	E	191	VAL	2.2
1	E	193	GLU	2.1
1	L	63	TYR	2.1
1	I	8	ILE	2.0

## 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 monosaccharides 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	F	302	8/8	0.78	0.14	22,33,36,38	0
3	UTC	A	302	41/41	0.81	0.32	35,41,87,100	0
3	UTC	G	301	41/41	0.83	0.20	25,36,72,81	0

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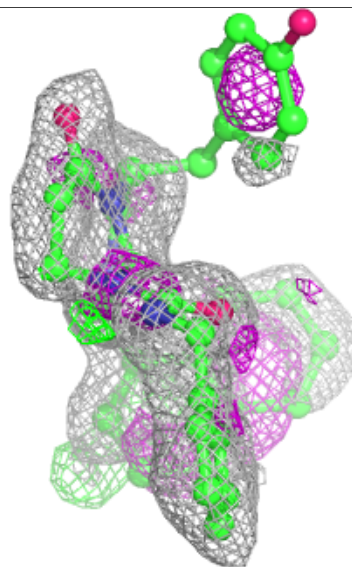
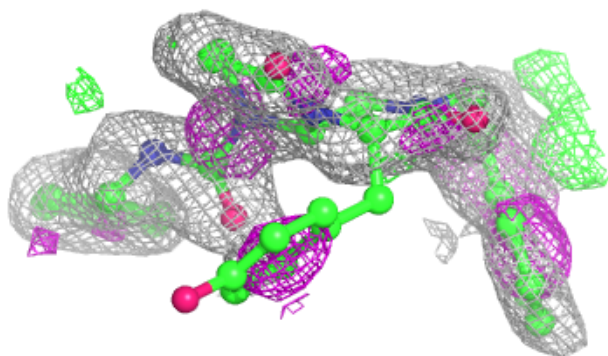
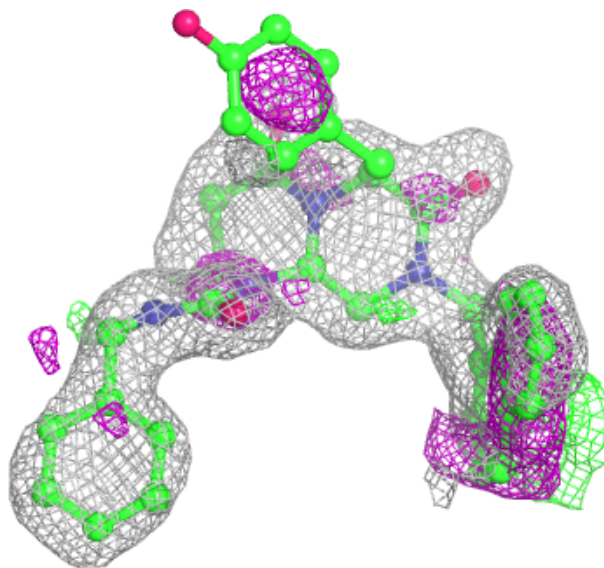
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UTC	I	302	41/41	0.84	0.23	29,38,69,77	0
3	UTC	M	301	41/41	0.84	0.20	22,32,74,91	0
2	MPD	B	302	8/8	0.85	0.13	26,34,41,42	0
2	MPD	M	302	8/8	0.85	0.14	19,28,35,35	0
3	UTC	K	301	41/41	0.86	0.20	28,35,72,84	0
3	UTC	L	301	41/41	0.86	0.19	25,33,75,90	0
2	MPD	C	302	8/8	0.86	0.11	22,32,36,42	0
3	UTC	C	301	41/41	0.87	0.24	28,36,67,81	0
2	MPD	I	301	8/8	0.88	0.15	27,38,41,43	0
2	MPD	L	302	8/8	0.88	0.12	21,32,36,39	0
3	UTC	S	303	41/41	0.88	0.29	29,37,75,83	0
2	MPD	D	301	8/8	0.89	0.16	20,28,33,34	0
2	MPD	K	302	8/8	0.89	0.12	22,32,38,41	0
2	MPD	A	301	8/8	0.89	0.12	28,36,42,49	0
2	MPD	G	302	8/8	0.89	0.15	26,38,47,50	0
2	MPD	S	302	8/8	0.90	0.14	26,35,42,46	0
2	MPD	T	301	8/8	0.90	0.14	26,41,43,46	0
3	UTC	S	301	41/41	0.90	0.14	25,35,73,77	0
3	UTC	F	301	41/41	0.90	0.14	18,25,49,59	41
2	MPD	E	301	8/8	0.91	0.13	24,31,36,40	0
3	UTC	B	301	41/41	0.92	0.15	29,35,70,80	0
3	UTC	N	301	41/41	0.92	0.15	22,30,65,71	0
2	MPD	N	302	8/8	0.93	0.08	22,32,36,37	0
3	UTC	D	303	41/41	0.94	0.08	21,25,55,70	0
2	MPD	D	302	8/8	0.94	0.11	34,37,40,45	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.

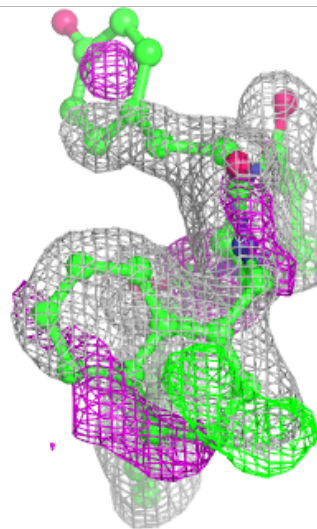
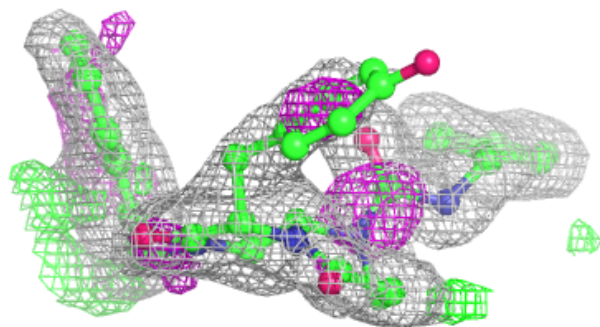
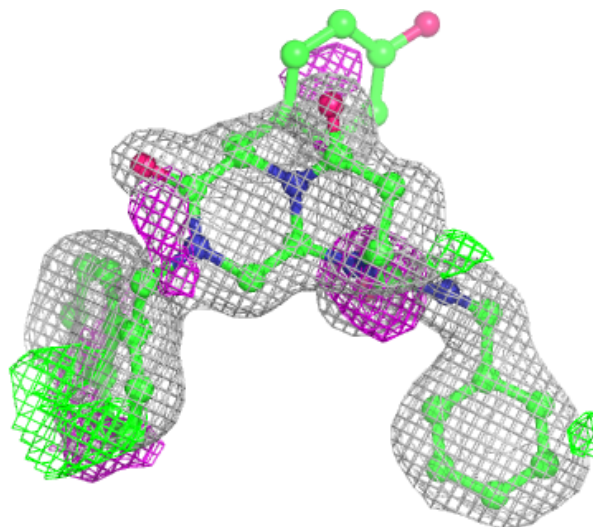
**Electron density around UTC A 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



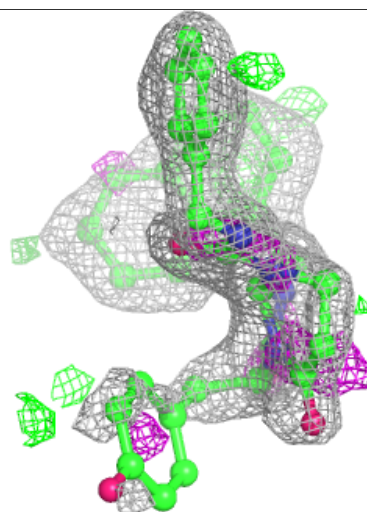
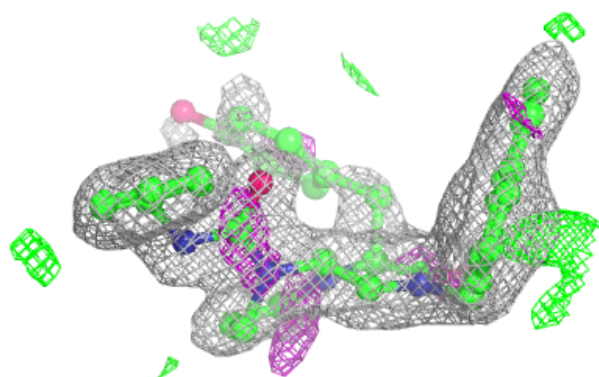
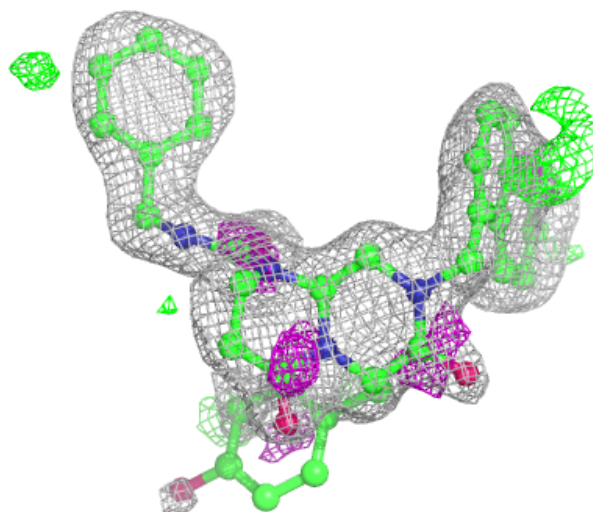
**Electron density around UTC G 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



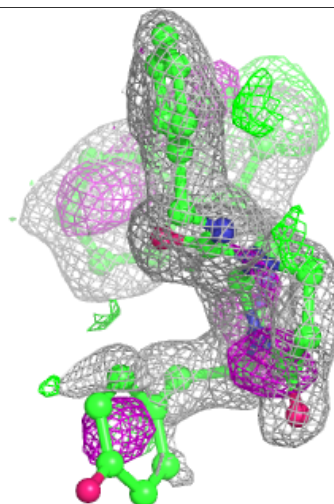
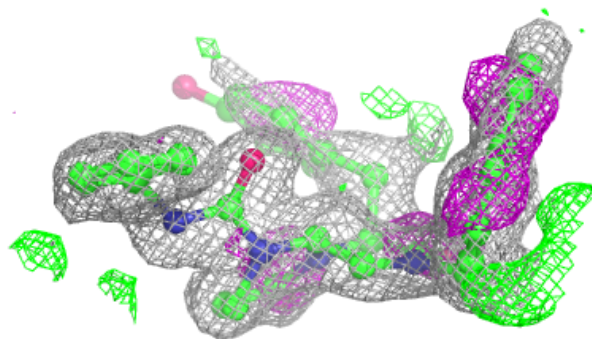
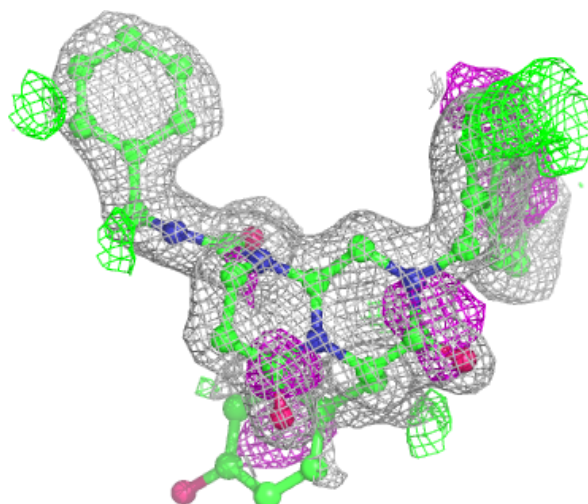
**Electron density around UTC I 302:**

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



**Electron density around UTC M 301:**

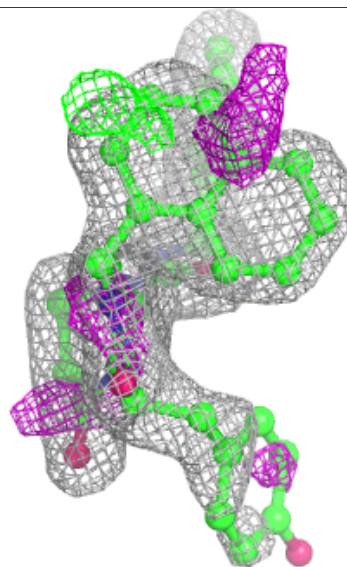
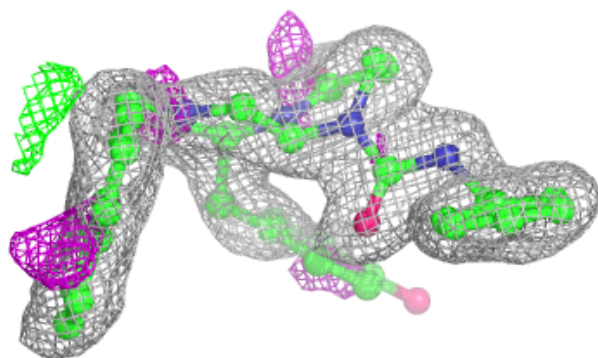
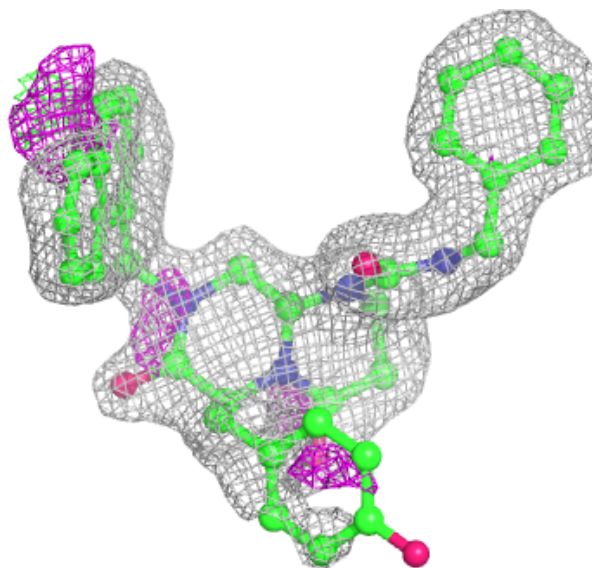
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





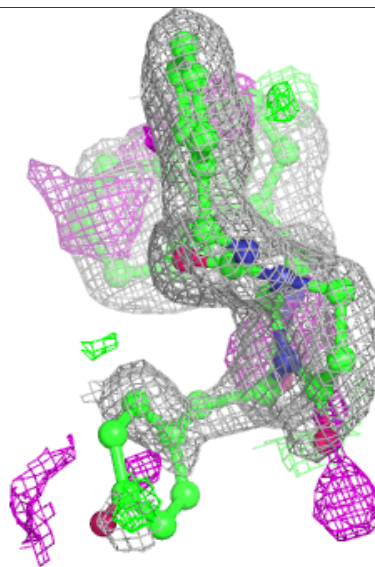
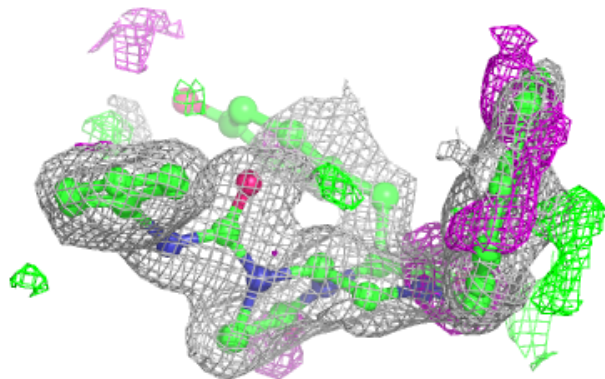
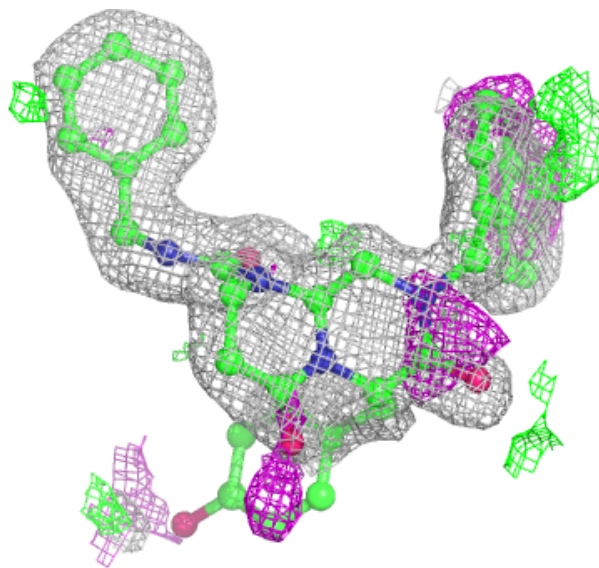
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



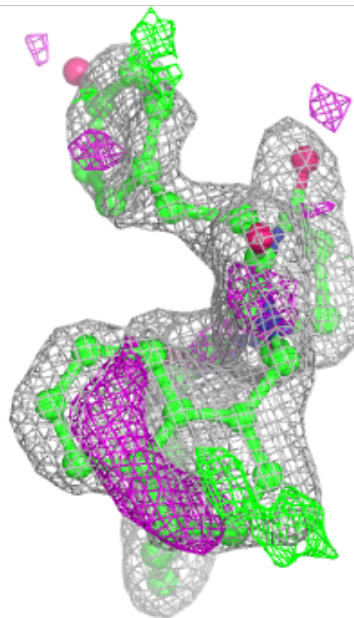
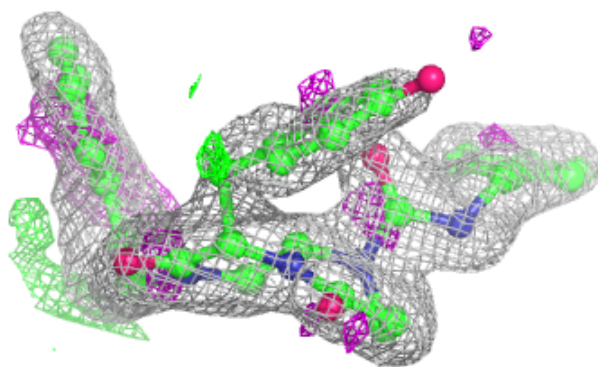
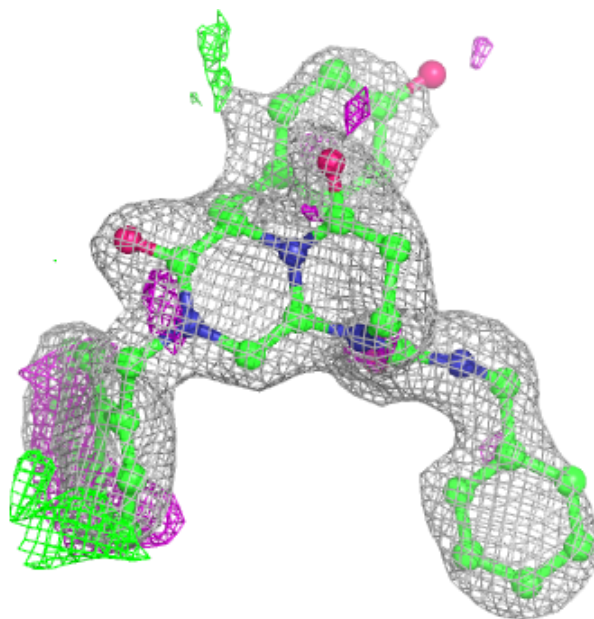
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and green (positive)



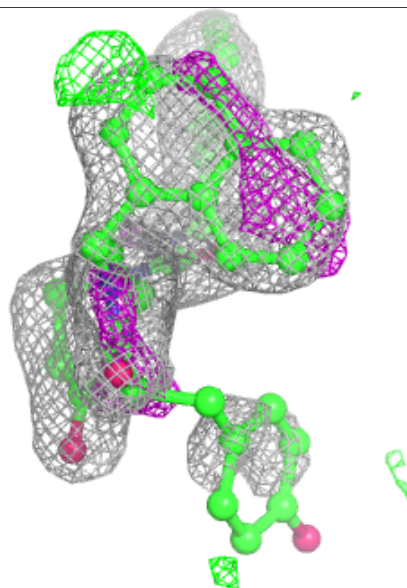
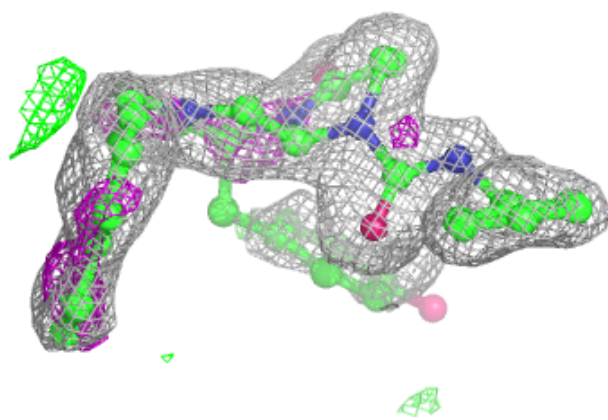
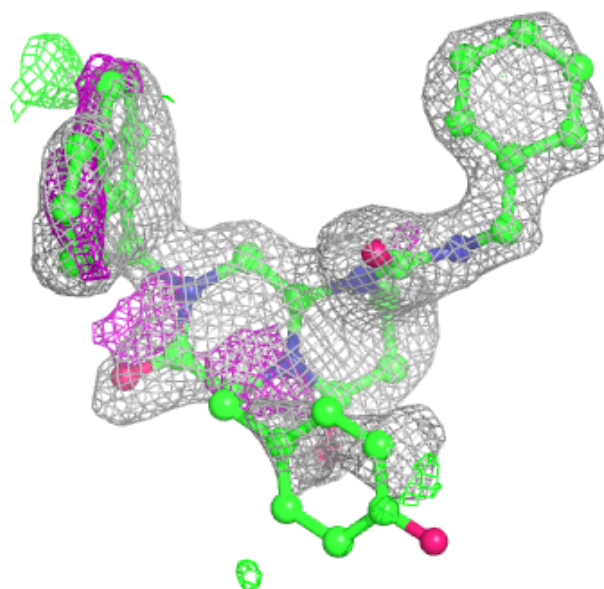
**Electron density around UTC C 301:**

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and green (positive)



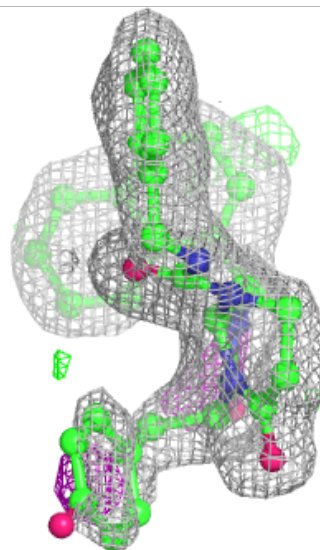
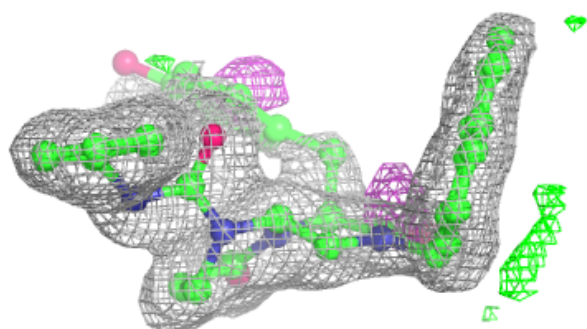
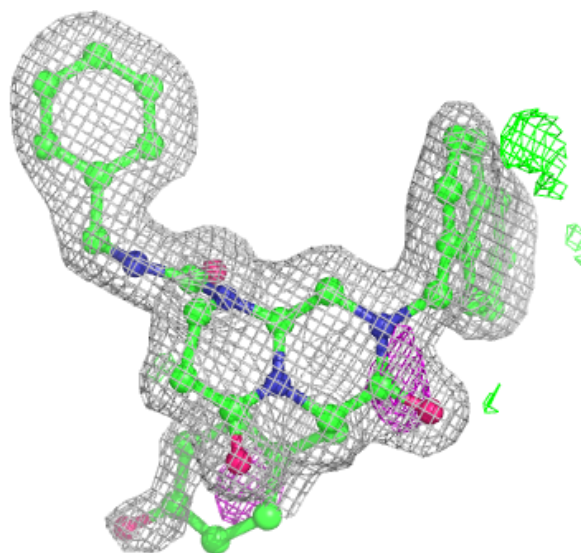
**Electron density around UTC S 303:**

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and green (positive)



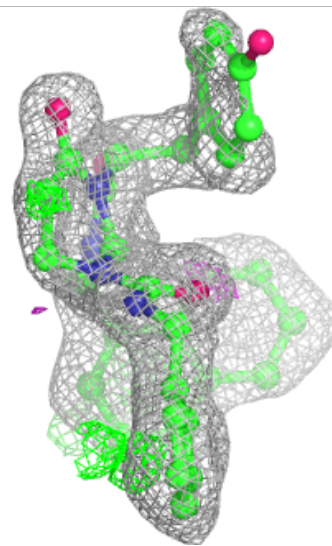
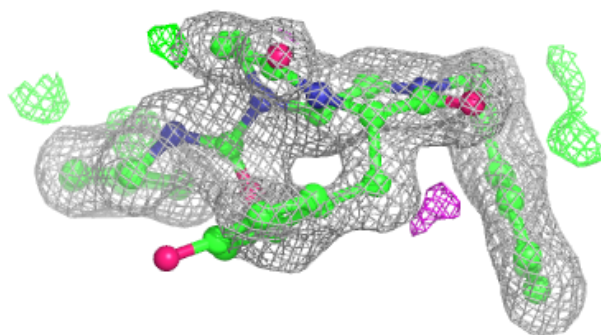
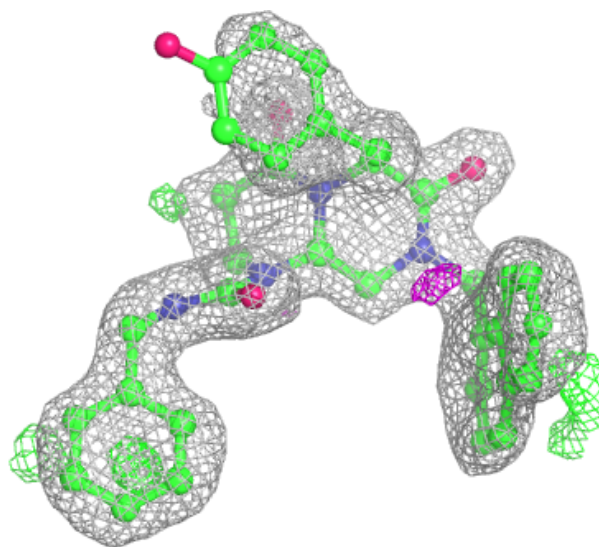
**Electron density around UTC S 301:**

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



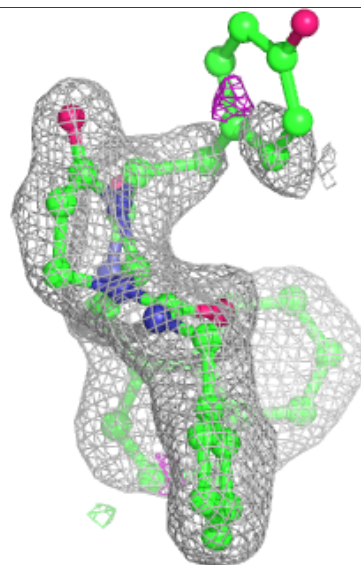
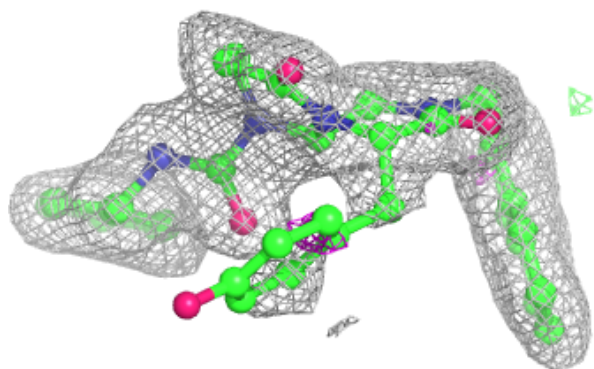
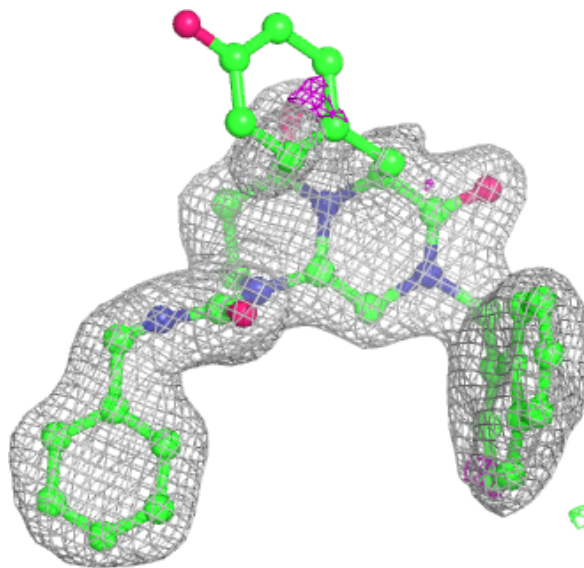
**Electron density around UTC F 301:**

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



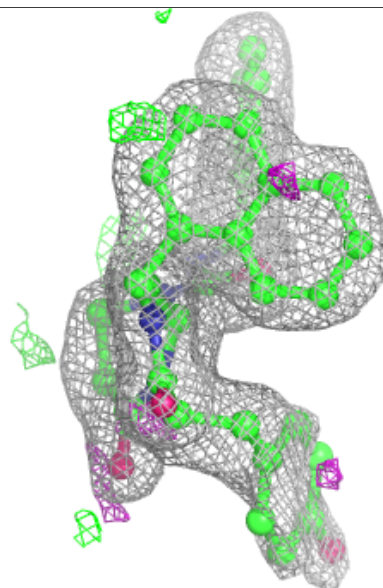
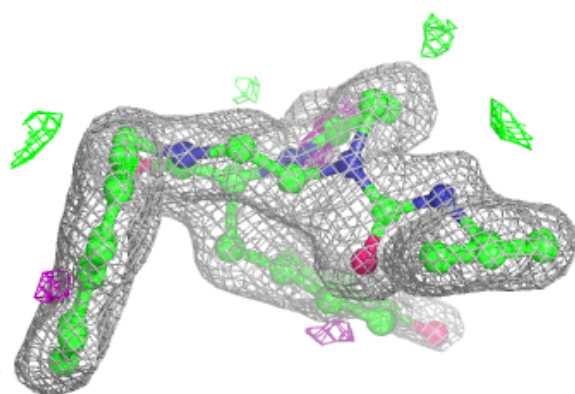
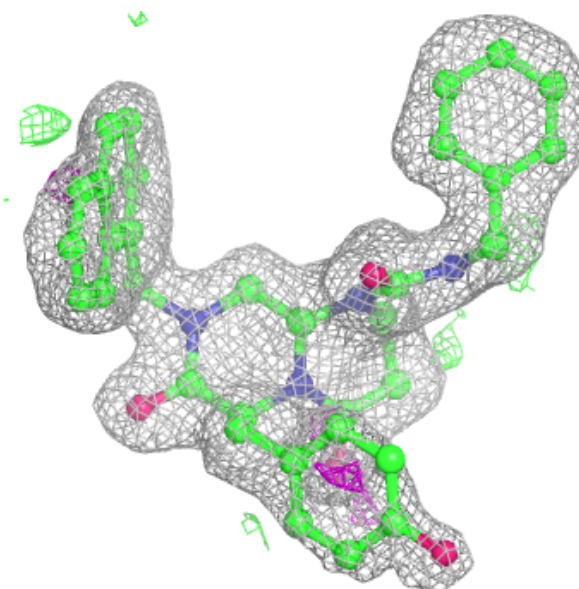
**Electron density around UTC B 301:**

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

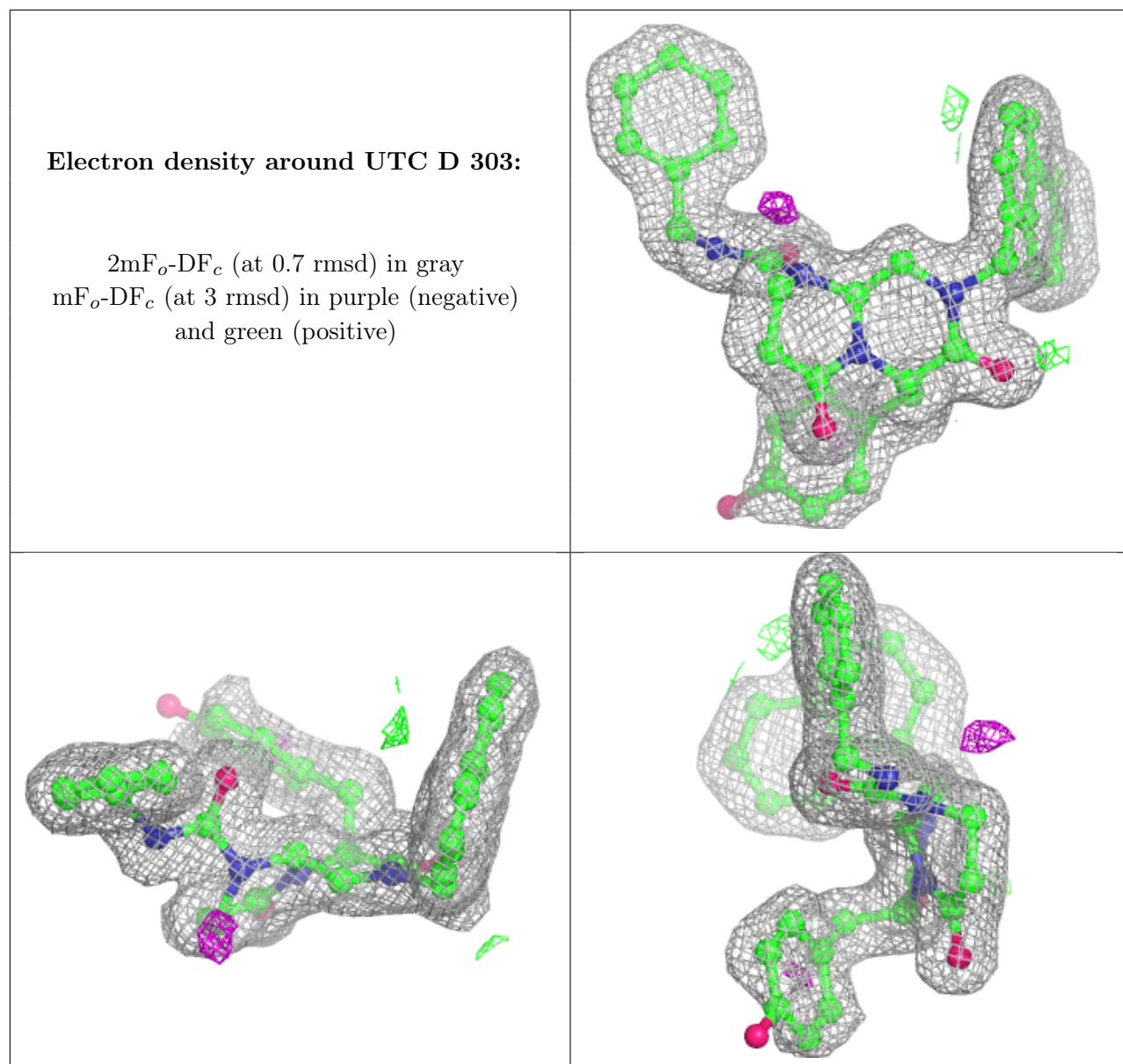


**Electron density around UTC N 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







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

There are no such residues in this entry.