



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2021 – 12:06 PM EDT

PDB ID : 3PEO  
Title : Crystal structure of acetylcholine binding protein complexed with metocurine  
Authors : Talley, T.T.; Harel, M.; Yamauchi, G.J.; Radic, Z.; Hansen, S.; Huxford, T.; Taylor, P.W.  
Deposited on : 2010-10-27  
Resolution : 2.10 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.

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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 : 2.17.1  
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) : 2.17.1

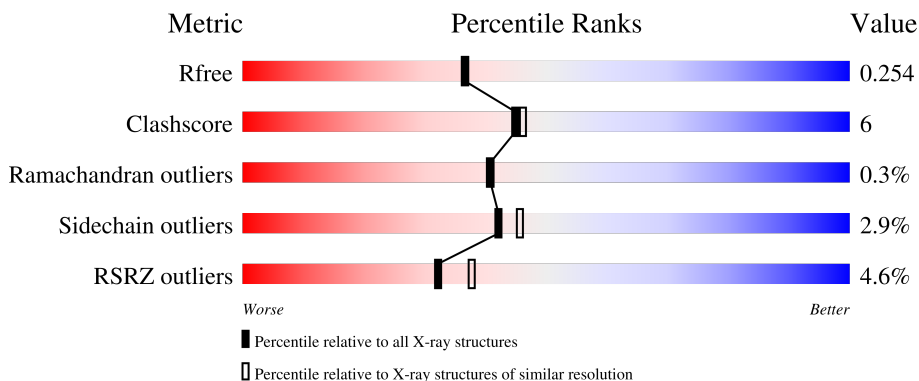
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	228	 3% 71% 17% 11%
1	B	228	 2% 77% 13% 9%
1	C	228	 4% 82% 11% 7%
1	D	228	 8% 71% 15% 11%
1	E	228	 5% 75% 14% 10%

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Mol	Chain	Length	Quality of chain
1	F	228	<div><div></div><div>5%</div><div>75%</div><div>13%</div><div>11%</div></div>
1	G	228	<div><div></div><div>2%</div><div>76%</div><div>12%</div><div>9%</div></div>
1	H	228	<div><div></div><div>3%</div><div>80%</div><div>11%</div><div>7%</div></div>
1	I	228	<div><div></div><div>5%</div><div>78%</div><div>10%</div><div>11%</div></div>
1	J	228	<div><div></div><div>5%</div><div>78%</div><div>12%</div><div>9%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18224 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1617	1022	264	323	8			
1	B	208	Total	C	N	O	S	0	2	0
			1673	1058	278	329	8			
1	C	211	Total	C	N	O	S	0	1	0
			1689	1065	278	338	8			
1	D	204	Total	C	N	O	S	0	3	0
			1639	1037	268	326	8			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1033	269	325	9			
1	F	202	Total	C	N	O	S	0	2	0
			1621	1027	265	321	8			
1	G	207	Total	C	N	O	S	0	4	0
			1678	1062	280	328	8			
1	H	211	Total	C	N	O	S	0	1	0
			1689	1065	278	338	8			
1	I	204	Total	C	N	O	S	0	3	0
			1639	1037	268	326	8			
1	J	207	Total	C	N	O	S	0	0	0
			1649	1041	271	328	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8

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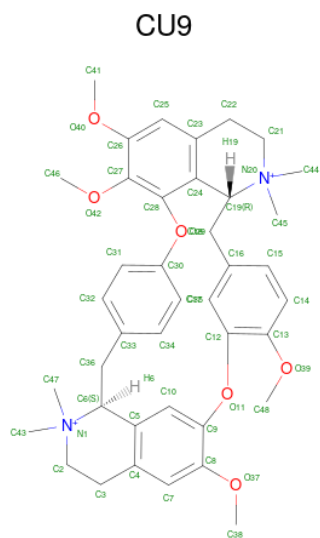
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is 6,6',7',12'-tetramethoxy-2,2,2',2'-tetramethyltubocuraran-2,2'-diium (three-letter code: CU9) (formula: C<sub>40</sub>H<sub>48</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 48	C 40	N 2	O 6	0	0
2	B	1	Total 48	C 40	N 2	O 6	0	0
2	C	1	Total 48	C 40	N 2	O 6	0	0
2	D	1	Total 48	C 40	N 2	O 6	0	0
2	F	1	Total 48	C 40	N 2	O 6	0	0
2	F	1	Total 48	C 40	N 2	O 6	0	0
2	H	1	Total 48	C 40	N 2	O 6	0	0
2	J	1	Total 48	C 40	N 2	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	148	Total O 148 148	0	0
3	B	155	Total O 155 155	0	0
3	C	125	Total O 125 125	0	0
3	D	117	Total O 117 117	0	0

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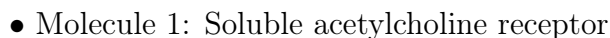
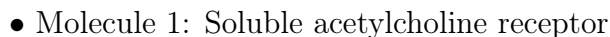
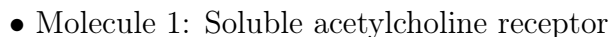
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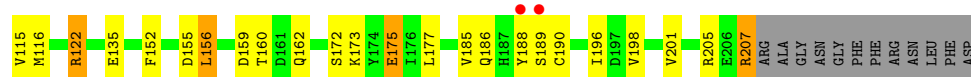
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	112	Total 112	O 112	0	0
3	F	138	Total 138	O 138	0	0
3	G	166	Total 166	O 166	0	0
3	H	133	Total 133	O 133	0	0
3	I	110	Total 110	O 110	0	0
3	J	106	Total 106	O 106	0	0



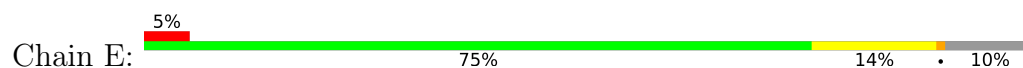


- Molecule 1: Soluble acetylcholine receptor

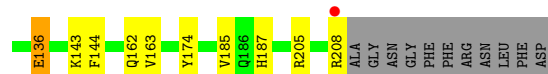
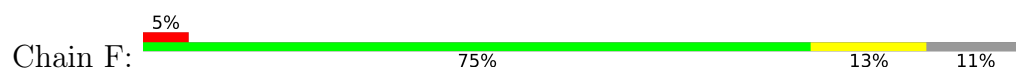




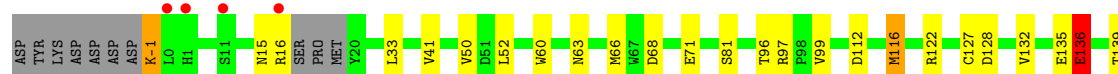
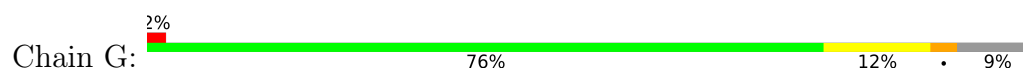
- Molecule 1: Soluble acetylcholine receptor



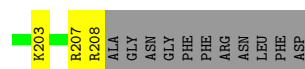
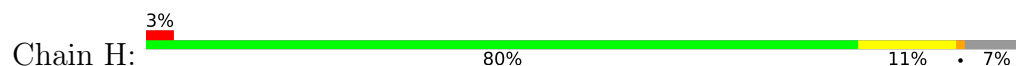
- Molecule 1: Soluble acetylcholine receptor



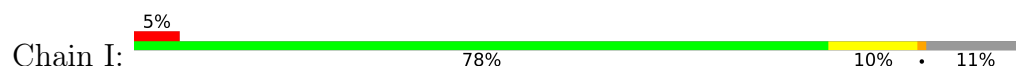
- Molecule 1: Soluble acetylcholine receptor

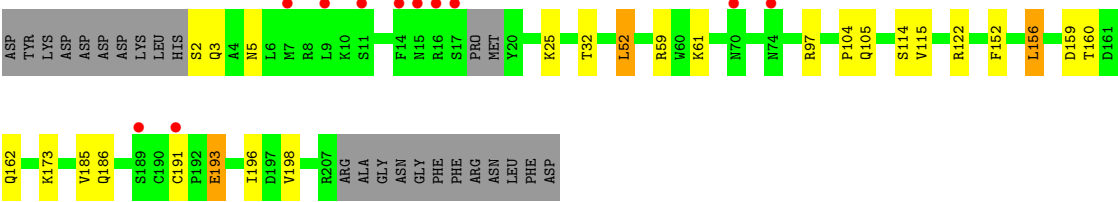


- Molecule 1: Soluble acetylcholine receptor

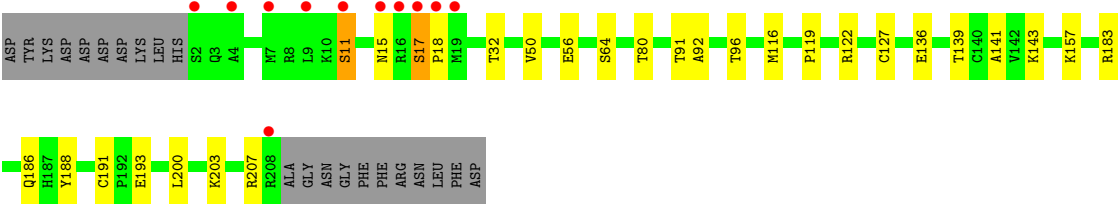
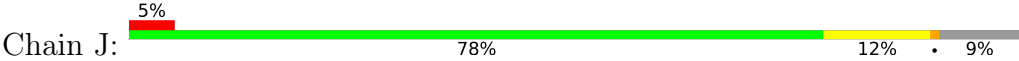


- Molecule 1: Soluble acetylcholine receptor





● Molecule 1: Soluble acetylcholine receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.70Å 147.57Å 148.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.83 – 2.10 43.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (104.83-2.10) 99.3 (43.74-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.255 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	1593 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU9

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	1.19	1/1655 (0.1%)	1.03	4/2256 (0.2%)
1	B	1.24	6/1718 (0.3%)	1.02	1/2340 (0.0%)
1	C	1.17	2/1731 (0.1%)	0.98	4/2358 (0.2%)
1	D	1.13	4/1686 (0.2%)	1.07	8/2299 (0.3%)
1	E	1.14	1/1674 (0.1%)	0.98	5/2280 (0.2%)
1	F	1.17	4/1665 (0.2%)	1.01	4/2270 (0.2%)
1	G	1.16	4/1729 (0.2%)	1.06	7/2354 (0.3%)
1	H	1.18	4/1731 (0.2%)	1.01	3/2358 (0.1%)
1	I	1.12	1/1686 (0.1%)	1.01	2/2299 (0.1%)
1	J	1.08	0/1689	0.98	3/2303 (0.1%)
All	All	1.16	27/16964 (0.2%)	1.01	41/23117 (0.2%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	191	CYS	CB-SG	6.98	1.94	1.82
1	H	140	CYS	CB-SG	6.93	1.94	1.82
1	H	53	VAL	CB-CG1	6.75	1.67	1.52
1	F	185	VAL	CB-CG1	6.71	1.67	1.52
1	B	56	GLU	CD-OE2	-6.64	1.18	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	F	208	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	I	52	LEU	CB-CG-CD2	7.32	123.44	111.00
1	A	97	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	E	122	ARG	NE-CZ-NH2	-6.96	116.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1617	0	1544	33	0
1	B	1673	0	1618	17	0
1	C	1689	0	1617	15	0
1	D	1639	0	1578	32	0
1	E	1636	0	1566	19	0
1	F	1621	0	1560	24	0
1	G	1678	0	1631	19	0
1	H	1689	0	1617	14	0
1	I	1639	0	1578	21	0
1	J	1649	0	1579	12	0
2	A	48	0	48	2	0
2	B	48	0	48	2	0
2	C	48	0	48	2	0
2	D	48	0	48	8	0
2	F	96	0	96	6	0
2	H	48	0	48	0	0
2	J	48	0	48	12	0
3	A	148	0	0	11	0
3	B	155	0	0	1	0
3	C	125	0	0	4	0
3	D	117	0	0	5	0
3	E	112	0	0	1	0
3	F	138	0	0	12	0
3	G	166	0	0	4	0
3	H	133	0	0	2	0
3	I	110	0	0	6	0
3	J	106	0	0	1	0
All	All	18224	0	16272	215	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 6.

The worst 5 of 215 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)
2:F:220:CU9:H47	3:F:822:HOH:O	1.41	1.19
1:D:97[A]:ARG:HH11	1:D:97[A]:ARG:CG	1.57	1.18
1:D:97[A]:ARG:HG2	1:D:97[A]:ARG:NH1	1.41	1.02
2:J:301:CU9:H46B	2:J:301:CU9:C30	1.99	0.93
1:F:143:LYS:HE3	3:F:280:HOH:O	1.67	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	199/228 (87%)	187 (94%)	11 (6%)	1 (0%)	29	26
1	B	206/228 (90%)	199 (97%)	7 (3%)	0	100	100
1	C	208/228 (91%)	204 (98%)	4 (2%)	0	100	100
1	D	203/228 (89%)	198 (98%)	3 (2%)	2 (1%)	15	11
1	E	201/228 (88%)	191 (95%)	9 (4%)	1 (0%)	29	26
1	F	200/228 (88%)	192 (96%)	8 (4%)	0	100	100
1	G	207/228 (91%)	201 (97%)	6 (3%)	0	100	100
1	H	208/228 (91%)	204 (98%)	4 (2%)	0	100	100
1	I	203/228 (89%)	195 (96%)	8 (4%)	0	100	100
1	J	205/228 (90%)	195 (95%)	7 (3%)	3 (2%)	10	5
All	All	2040/2280 (90%)	1966 (96%)	67 (3%)	7 (0%)	41	41

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	15	ASN
1	A	64	SER
1	J	64	SER

*Continued on next page...*

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Mol	Chain	Res	Type
1	E	64	SER
1	J	18	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	184/206 (89%)	180 (98%)	4 (2%)	52	57
1	B	191/206 (93%)	183 (96%)	8 (4%)	30	30
1	C	193/206 (94%)	191 (99%)	2 (1%)	76	82
1	D	188/206 (91%)	180 (96%)	8 (4%)	29	29
1	E	186/206 (90%)	181 (97%)	5 (3%)	44	48
1	F	185/206 (90%)	182 (98%)	3 (2%)	62	69
1	G	192/206 (93%)	182 (95%)	10 (5%)	23	21
1	H	193/206 (94%)	188 (97%)	5 (3%)	46	50
1	I	188/206 (91%)	182 (97%)	6 (3%)	39	41
1	J	188/206 (91%)	183 (97%)	5 (3%)	44	48
All	All	1888/2060 (92%)	1832 (97%)	56 (3%)	42	44

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	59	ARG
1	J	207	ARG
1	G	157	LYS
1	J	116	MET
1	I	186	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	J	186	GLN
1	G	5	ASN
1	I	162	GLN
1	F	187	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 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	CU9	H	301	-	53,54,54	1.03	3 (5%)	78,82,82	1.89	12 (15%)
2	CU9	D	301	-	53,54,54	1.01	4 (7%)	78,82,82	1.95	16 (20%)
2	CU9	A	301	-	53,54,54	1.05	2 (3%)	78,82,82	1.58	12 (15%)
2	CU9	J	301	-	53,54,54	0.94	2 (3%)	78,82,82	2.05	16 (20%)
2	CU9	C	301	-	53,54,54	1.30	5 (9%)	78,82,82	1.89	7 (8%)
2	CU9	F	220	-	53,54,54	1.09	3 (5%)	78,82,82	1.73	13 (16%)
2	CU9	F	301	-	53,54,54	1.12	2 (3%)	78,82,82	1.39	7 (8%)
2	CU9	B	301	-	53,54,54	1.08	4 (7%)	78,82,82	1.62	11 (14%)

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	CU9	H	301	-	-	2/24/56/56	-
2	CU9	D	301	-	-	8/24/56/56	-
2	CU9	A	301	-	-	0/24/56/56	-
2	CU9	J	301	-	-	7/24/56/56	-
2	CU9	C	301	-	-	2/24/56/56	-
2	CU9	F	220	-	-	3/24/56/56	-
2	CU9	F	301	-	-	1/24/56/56	-
2	CU9	B	301	-	-	3/24/56/56	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CU9	C25-C23	3.03	1.44	1.39
2	F	220	CU9	C22-C23	2.81	1.56	1.51
2	C	301	CU9	C15-C14	2.76	1.43	1.38
2	C	301	CU9	C6-N1	-2.75	1.45	1.54
2	A	301	CU9	O37-C8	2.73	1.41	1.37

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	CU9	C48-O39-C13	8.75	130.74	117.53
2	C	301	CU9	C30-O29-C28	8.40	131.99	118.48
2	F	220	CU9	C30-O29-C28	7.91	131.20	118.48
2	D	301	CU9	C48-O39-C13	7.42	128.73	117.53
2	H	301	CU9	C38-O37-C8	6.92	127.97	117.53

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	301	CU9	C27-C26-O40-C41
2	J	301	CU9	C12-C13-O39-C48
2	J	301	CU9	C26-C27-O42-C46
2	D	301	CU9	C25-C26-O40-C41
2	D	301	CU9	C26-C27-O42-C46

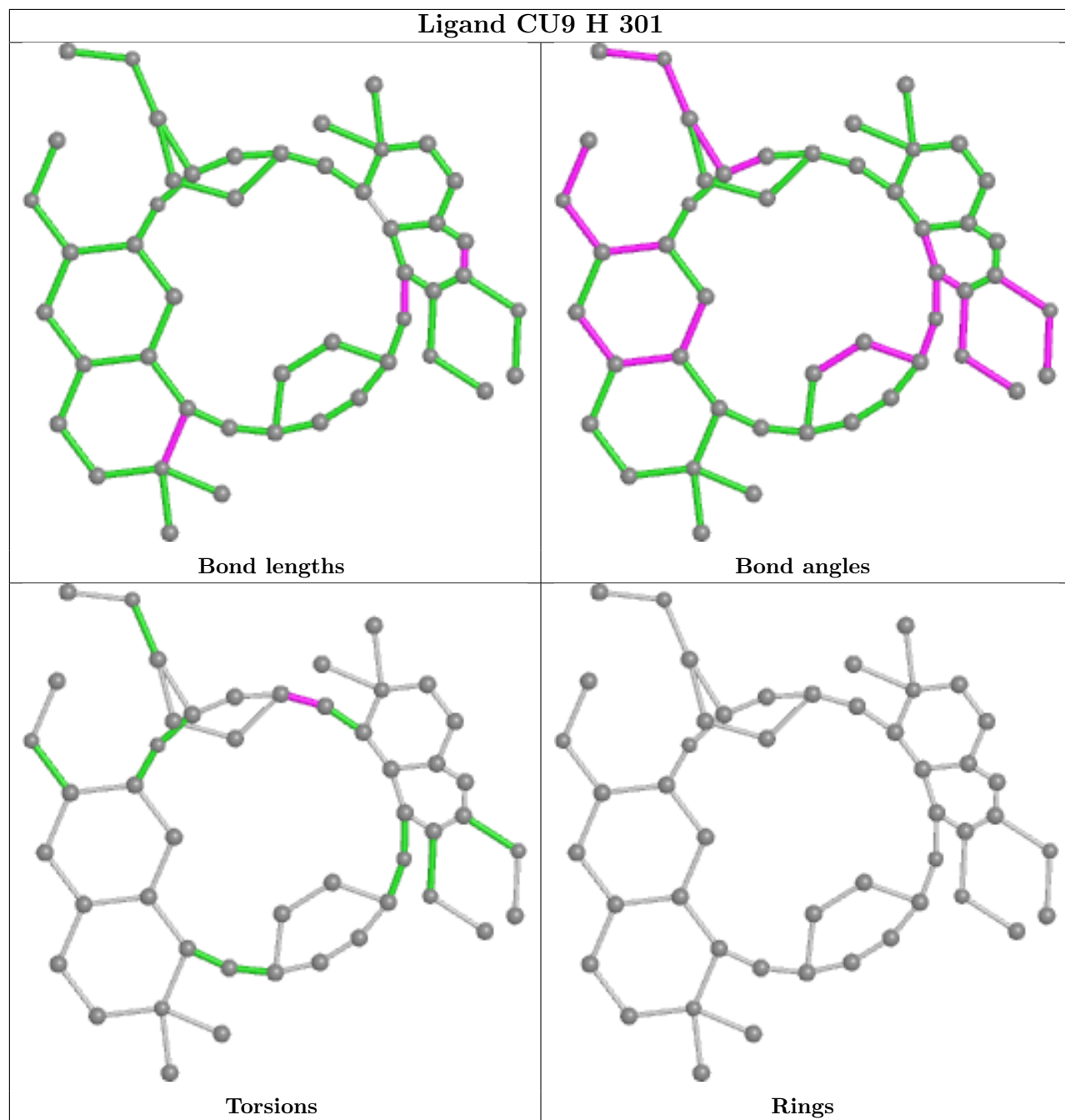
There are no ring outliers.

6 monomers are involved in 32 short contacts:

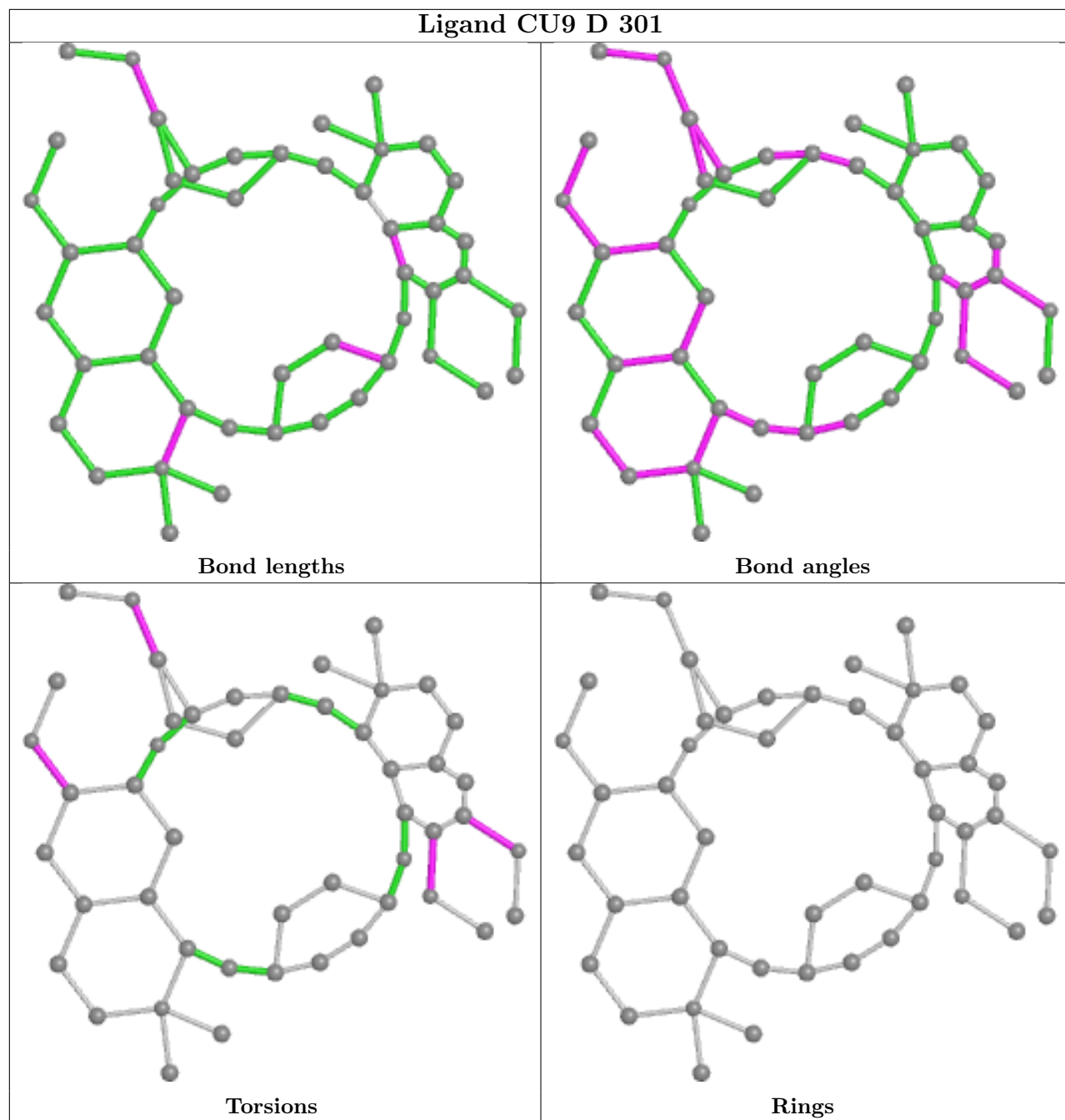
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	CU9	8	0
2	A	301	CU9	2	0
2	J	301	CU9	12	0
2	C	301	CU9	2	0
2	F	220	CU9	6	0
2	B	301	CU9	2	0

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

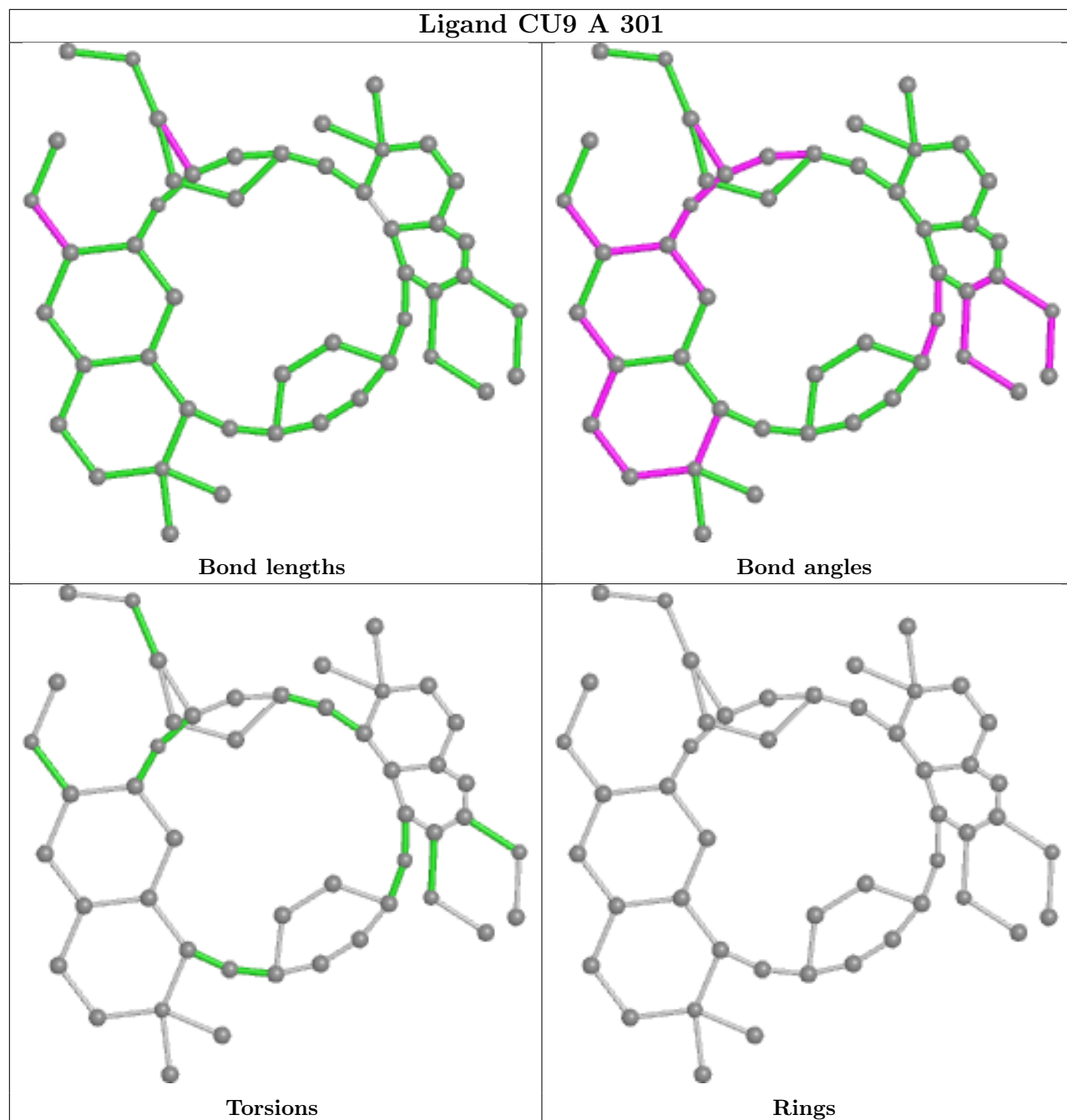
## Ligand CU9 H 301



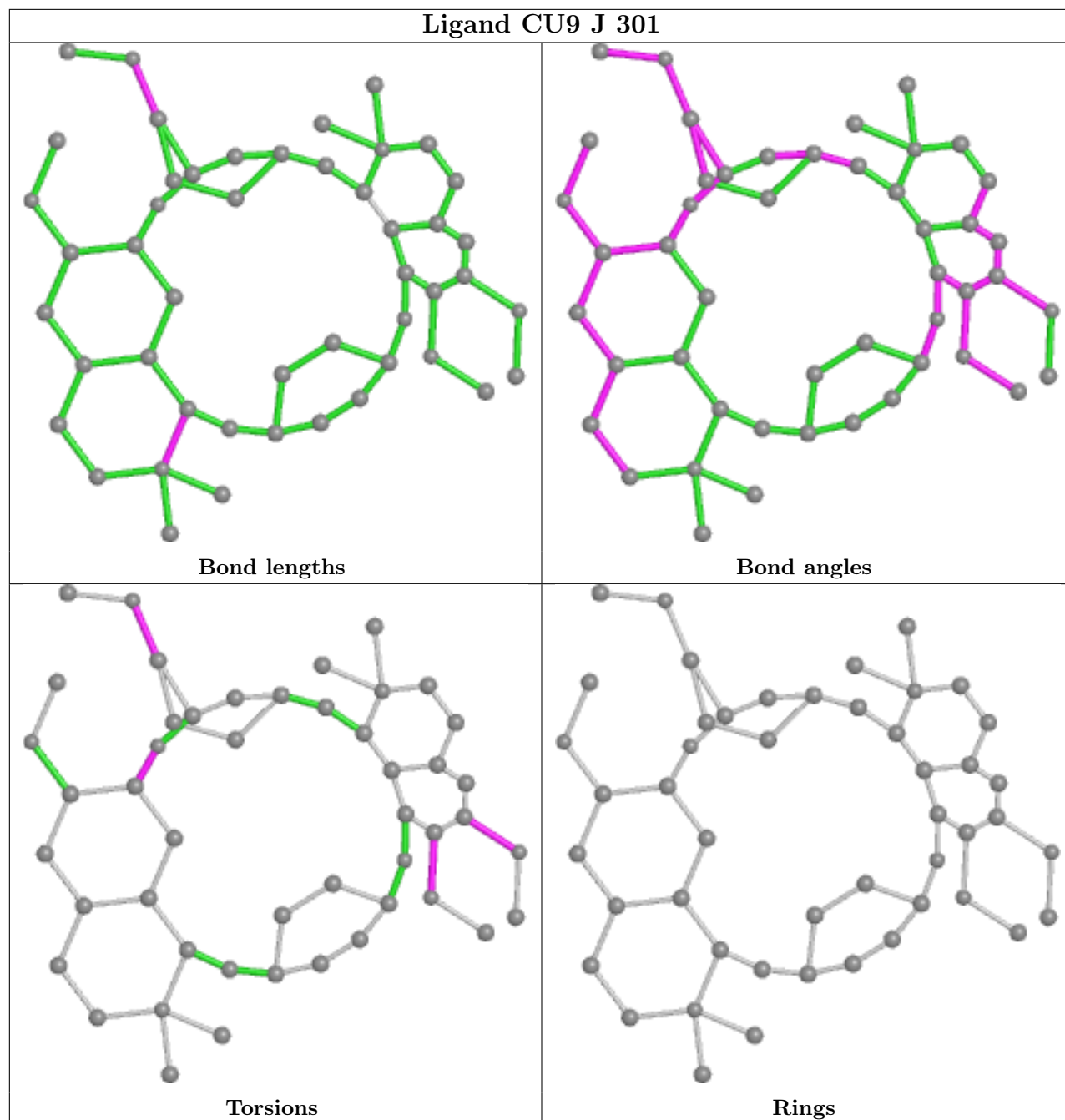
## Ligand CU9 D 301



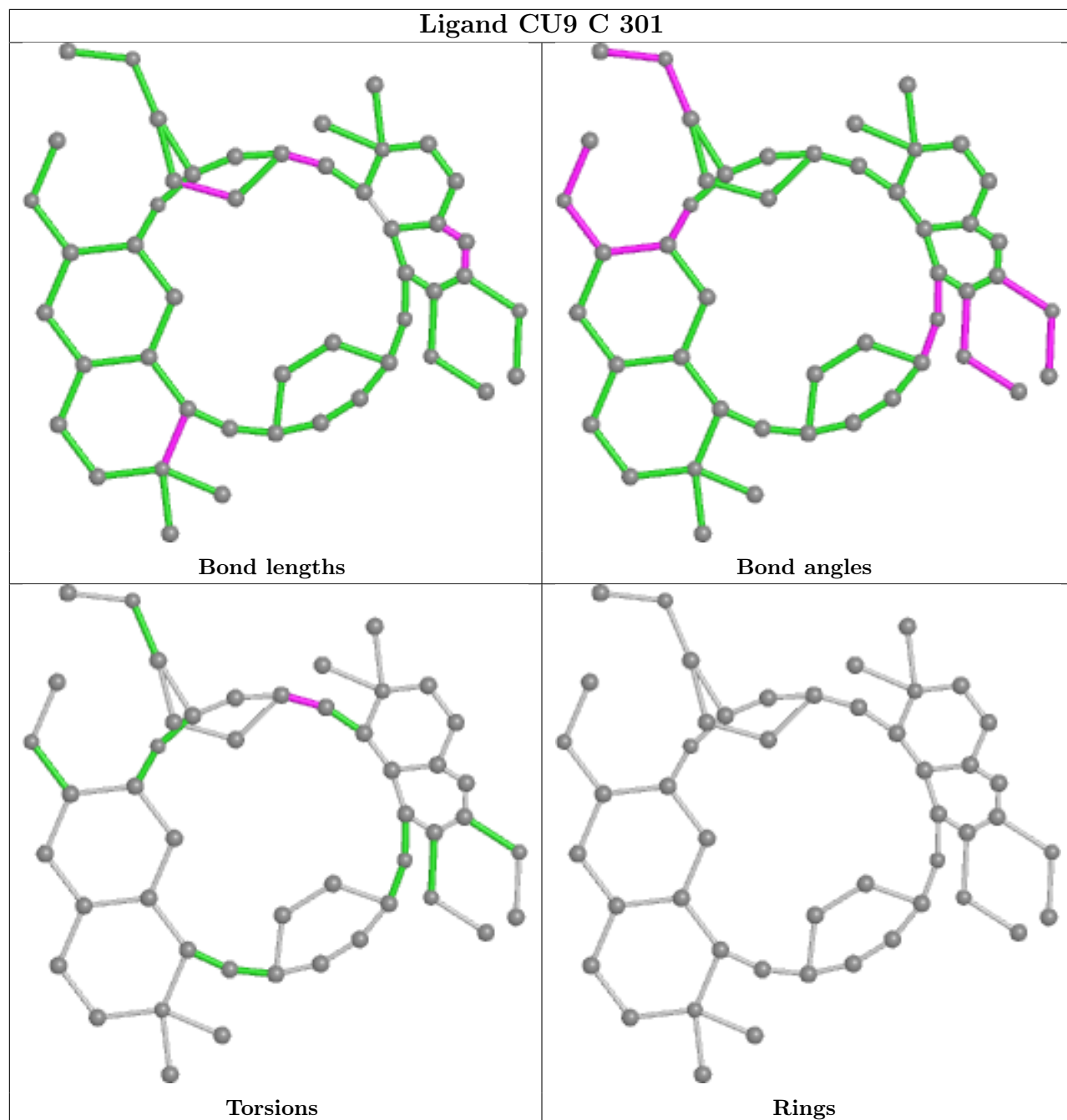
## Ligand CU9 A 301



## Ligand CU9 J 301

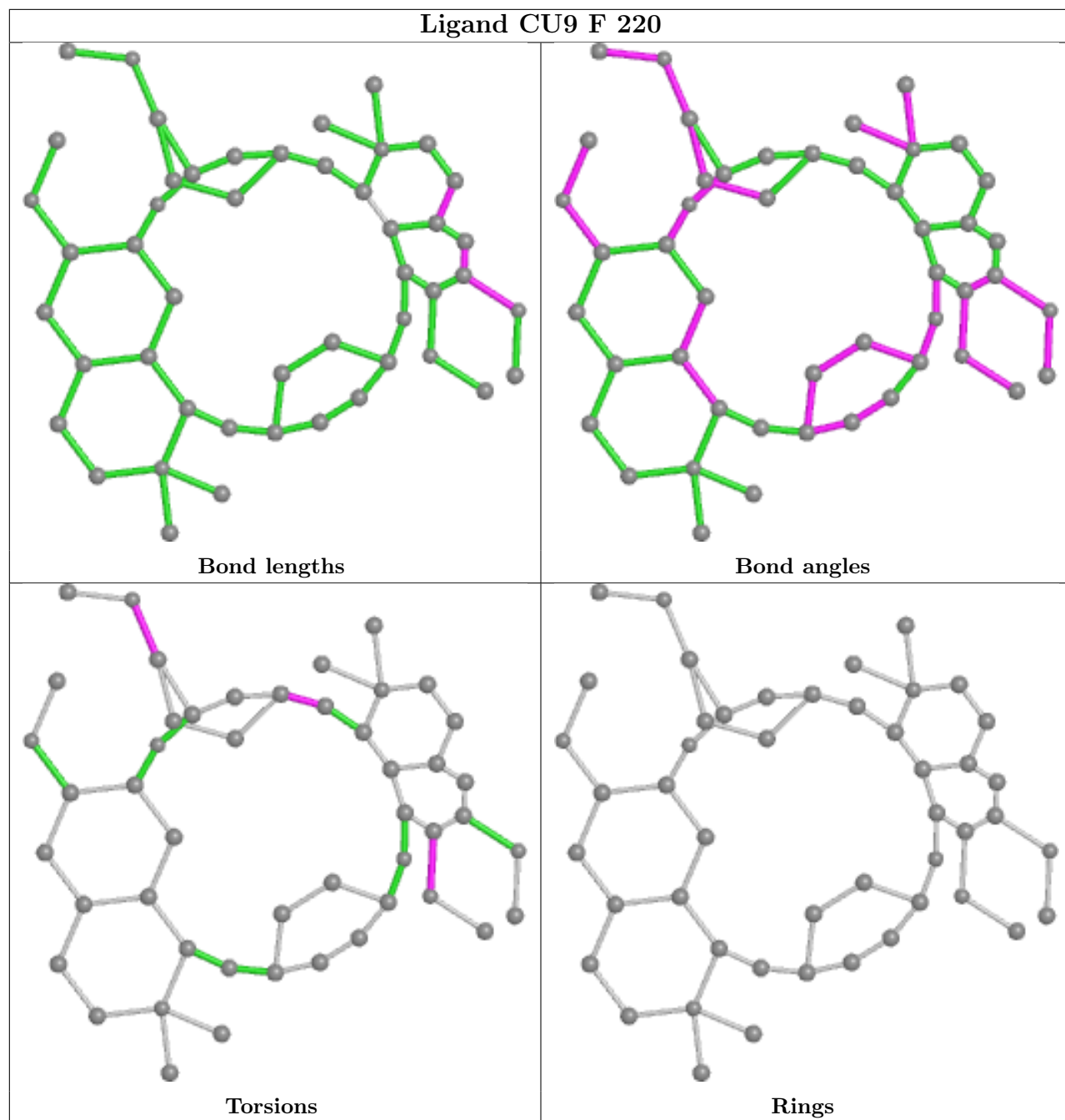


## Ligand CU9 C 301

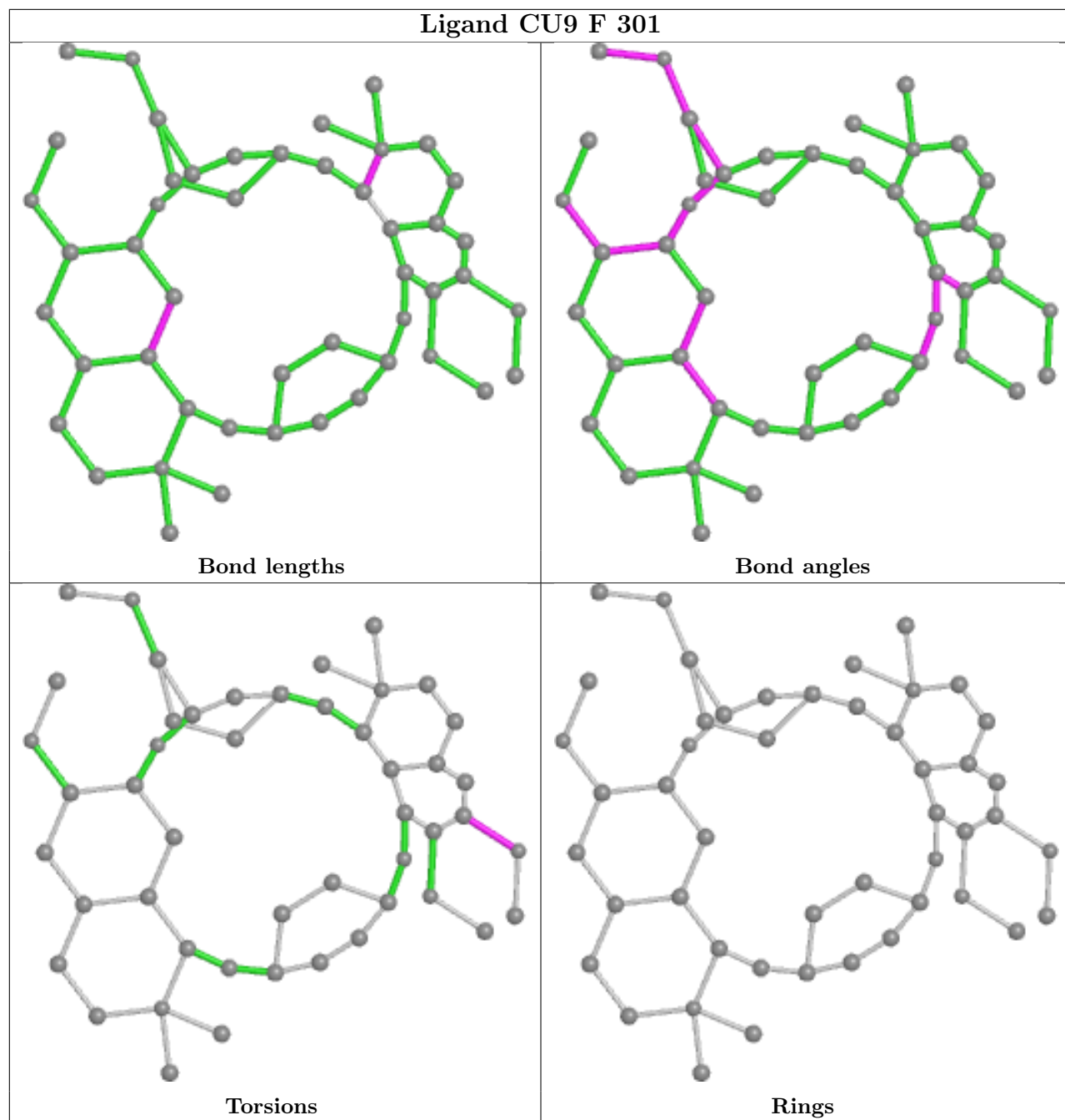


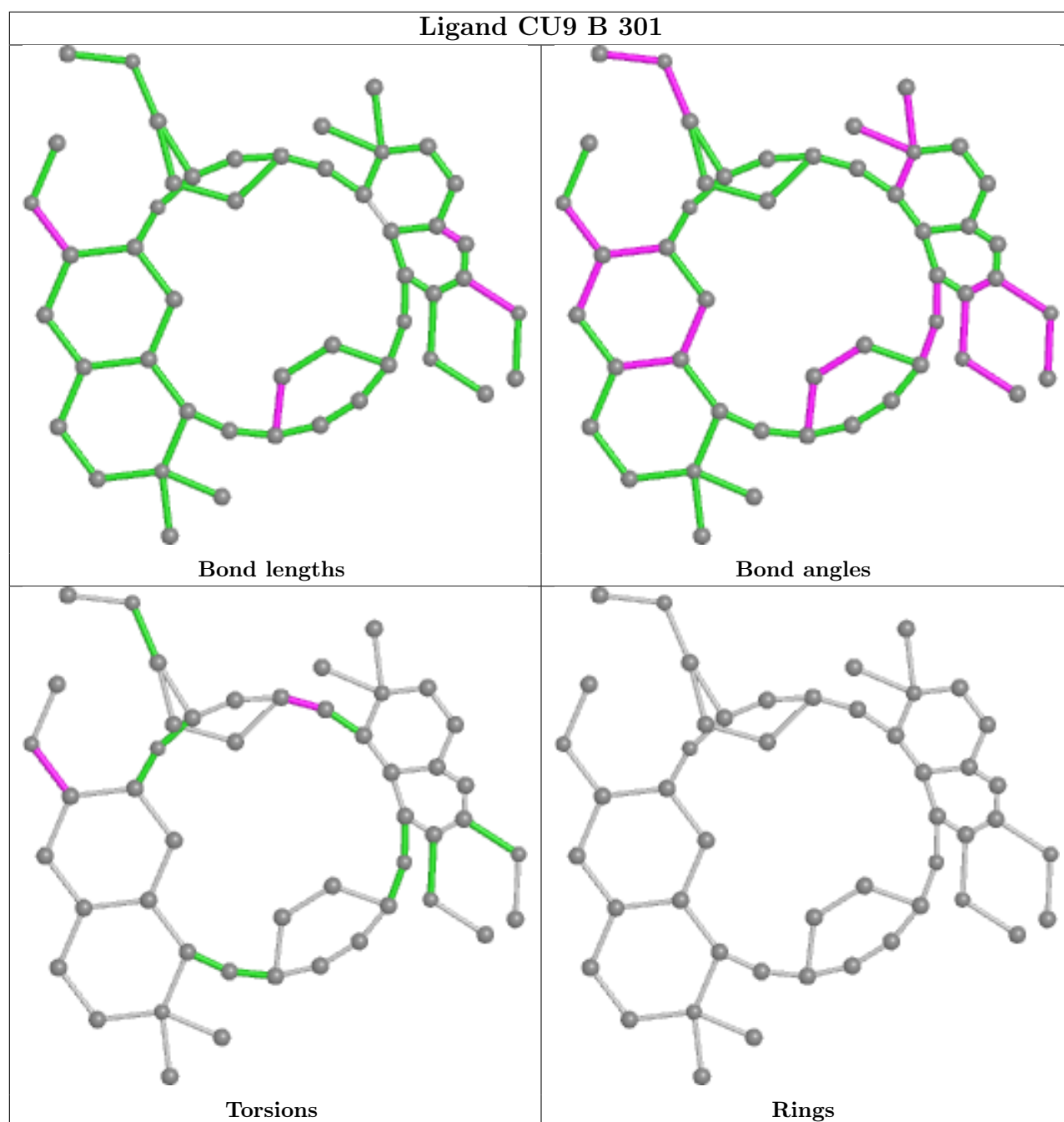


## Ligand CU9 F 220



## Ligand CU9 F 301





## 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	203/228 (89%)	-0.13	6 (2%)	50	56	9, 20, 60, 79	0
1	B	208/228 (91%)	-0.28	5 (2%)	59	64	9, 19, 43, 70	0
1	C	211/228 (92%)	-0.18	9 (4%)	35	41	9, 21, 50, 84	0
1	D	204/228 (89%)	0.01	18 (8%)	10	12	9, 23, 68, 93	0
1	E	205/228 (89%)	-0.14	11 (5%)	25	31	11, 22, 56, 72	0
1	F	202/228 (88%)	-0.11	12 (5%)	22	27	9, 20, 66, 75	0
1	G	207/228 (90%)	-0.21	4 (1%)	66	71	9, 19, 49, 75	0
1	H	211/228 (92%)	-0.29	7 (3%)	46	53	10, 21, 45, 71	0
1	I	204/228 (89%)	-0.01	11 (5%)	25	31	9, 23, 64, 91	0
1	J	207/228 (90%)	-0.05	11 (5%)	26	32	10, 23, 58, 78	0
All	All	2062/2280 (90%)	-0.14	94 (4%)	32	38	9, 21, 60, 93	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	17	SER	6.9
1	J	18	PRO	6.1
1	D	16	ARG	5.8
1	I	15	ASN	5.6
1	J	19	MET	5.6

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

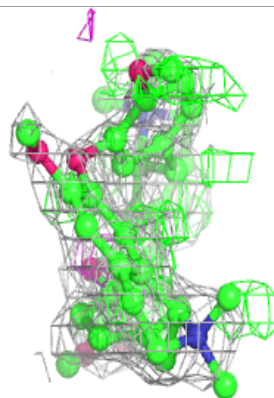
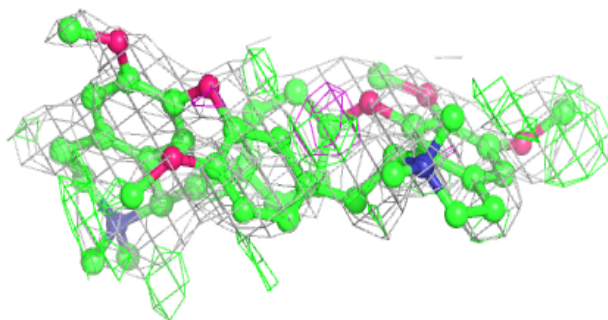
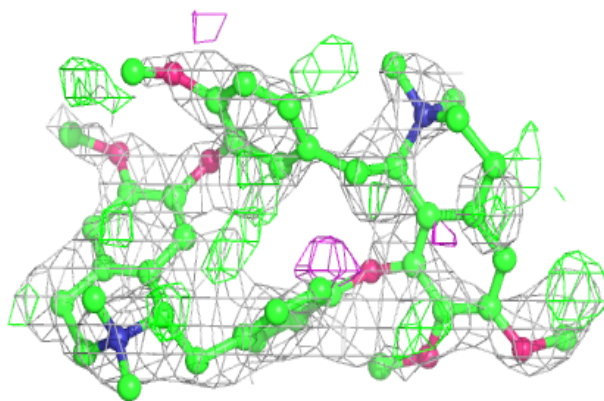
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CU9	J	301	48/48	0.64	0.27	30,39,45,49	48
2	CU9	D	301	48/48	0.69	0.26	31,42,46,47	48
2	CU9	F	220	48/48	0.91	0.15	6,23,28,31	48
2	CU9	C	301	48/48	0.91	0.13	17,28,32,34	0
2	CU9	A	301	48/48	0.92	0.14	8,22,27,29	48
2	CU9	H	301	48/48	0.94	0.13	14,19,25,30	48
2	CU9	F	301	48/48	0.97	0.08	4,13,17,19	0
2	CU9	B	301	48/48	0.97	0.09	5,12,15,18	0

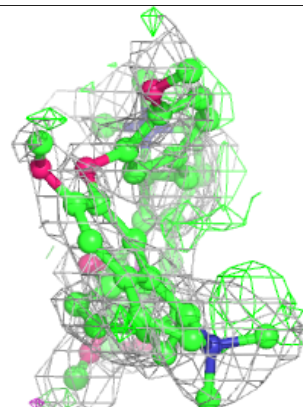
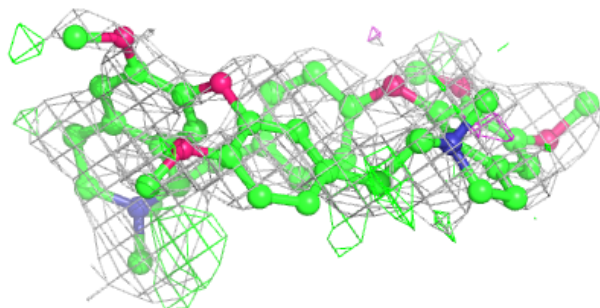
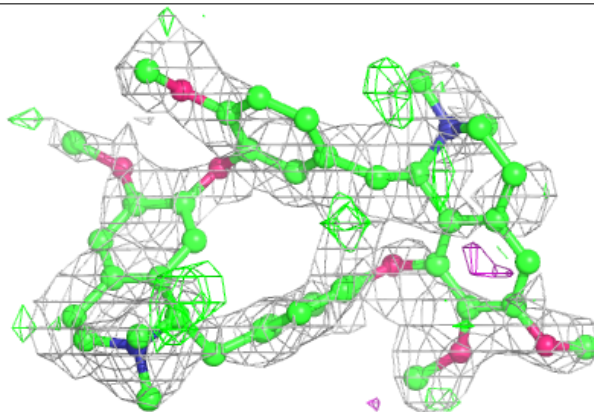
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CU9 J 301:**

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

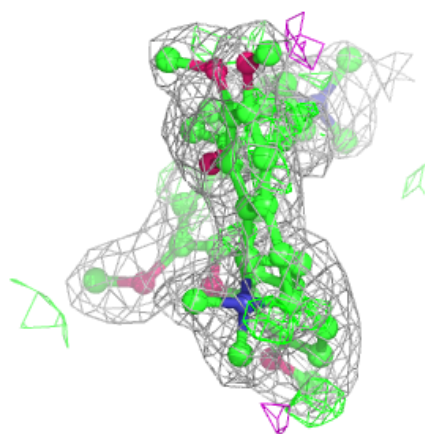
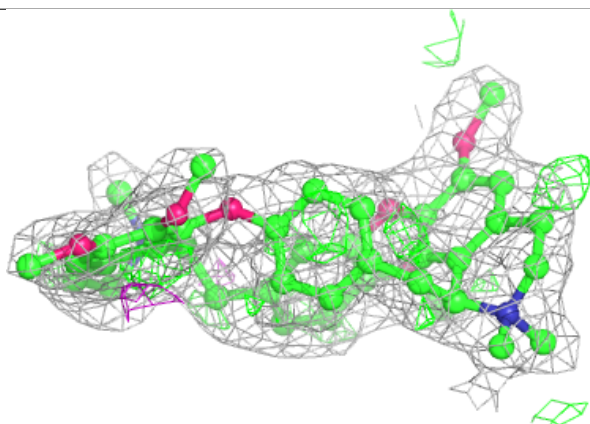
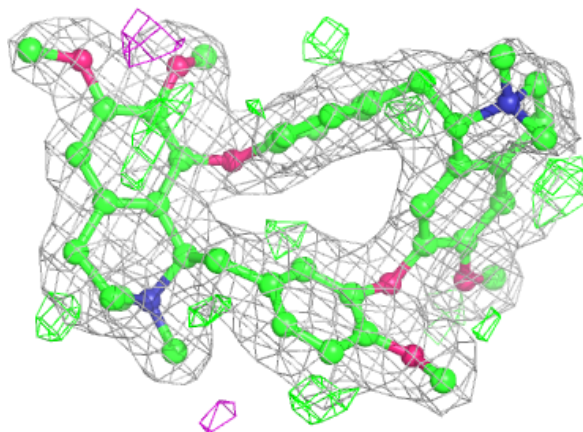
**Electron density around CU9 D 301:**

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



**Electron density around CU9 F 220:**

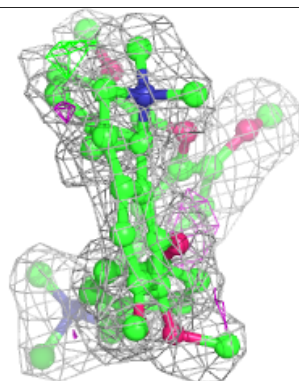
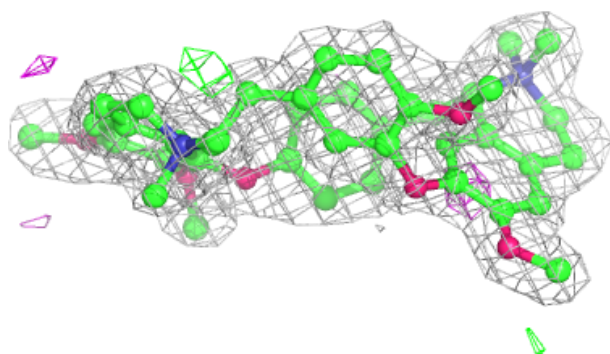
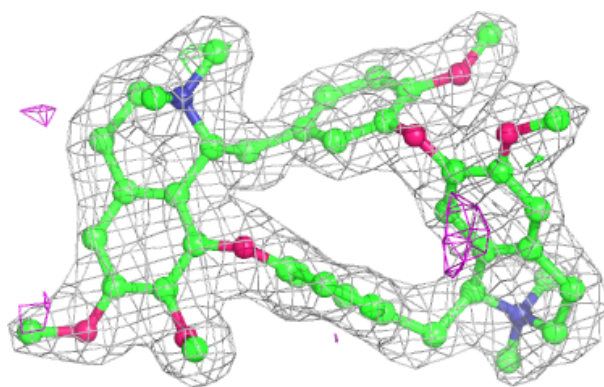
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CU9 C 301:**

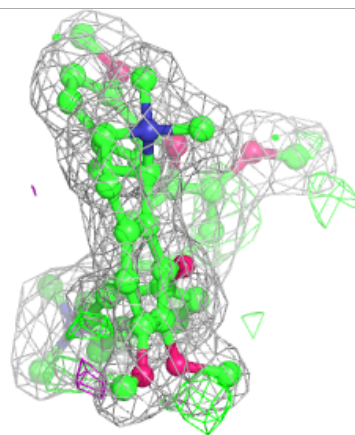
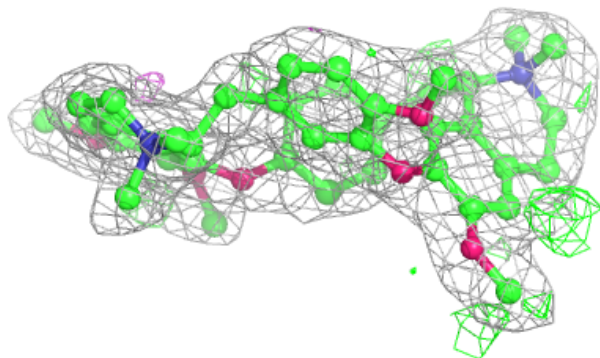
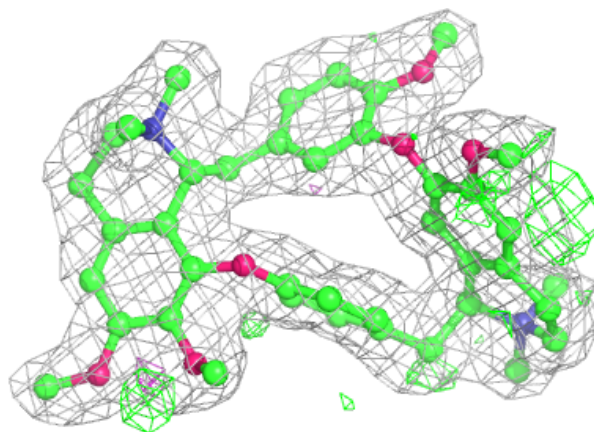
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





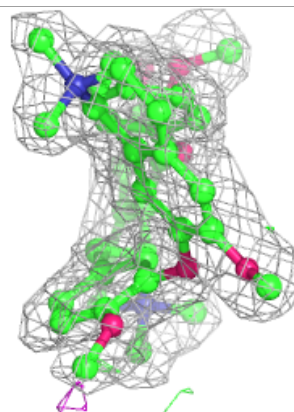
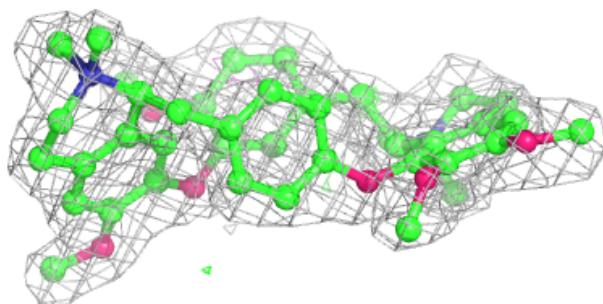
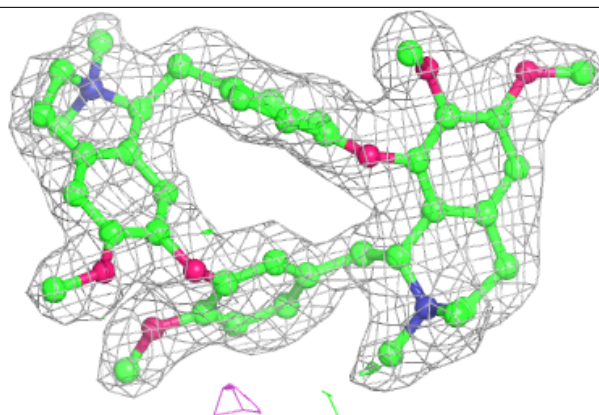
**Electron density around CU9 A 301:**

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

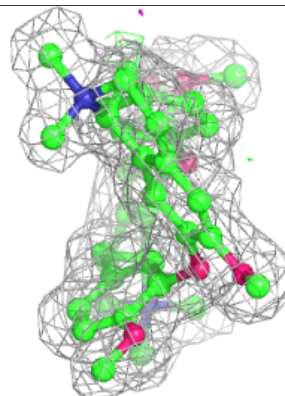
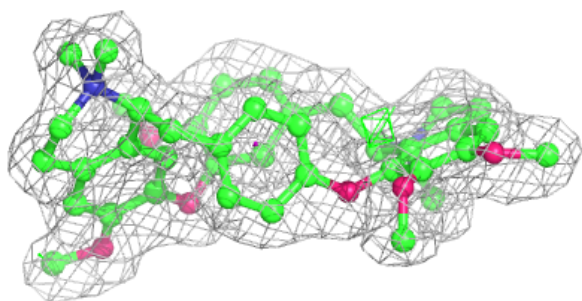
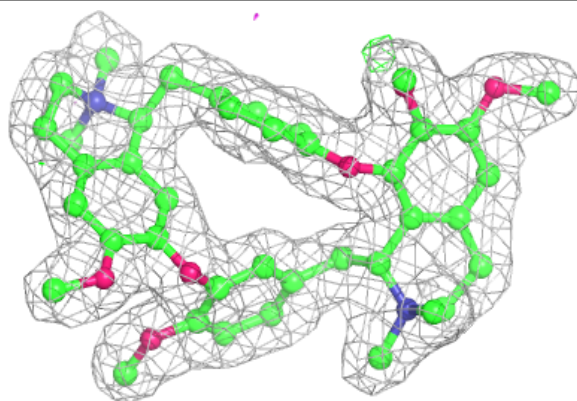


**Electron density around CU9 H 301:**

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

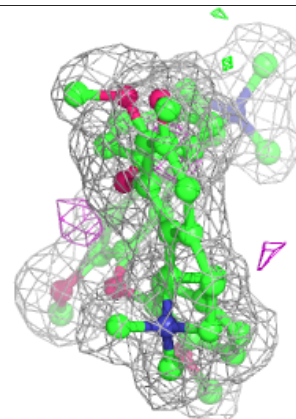
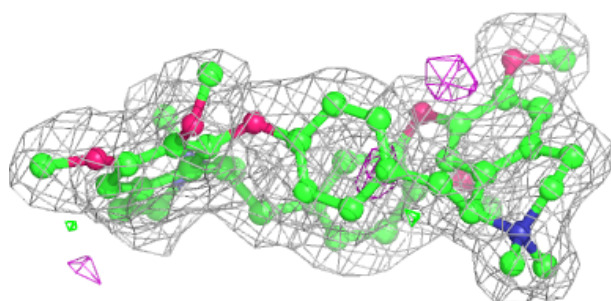
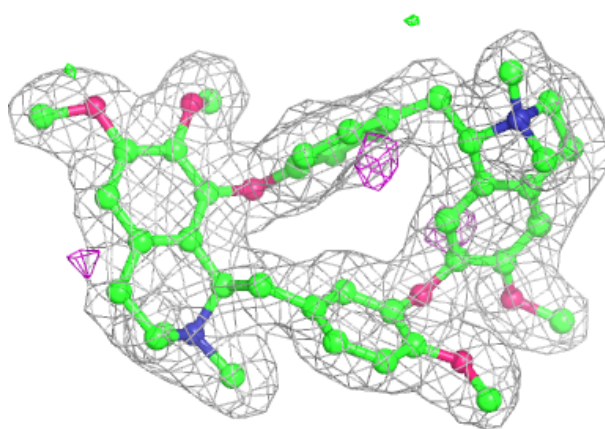
**Electron density around CU9 F 301:**

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



**Electron density around CU9 B 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.