



# Full wwPDB X-ray Structure Validation Report i

Nov 16, 2023 – 06:09 AM JST

PDB ID : 6L37  
Title : X-ray structure of human PPARalpha ligand binding domain-GW9662-ciprofibrate co-crystals obtained by delipidation and co-crystallization  
Authors : Kamata, S.; Saito, K.; Honda, A.; Ishikawa, R.; Oyama, T.; Ishii, I.  
Deposited on : 2019-10-09  
Resolution : 2.91 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 i 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](#) i) 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

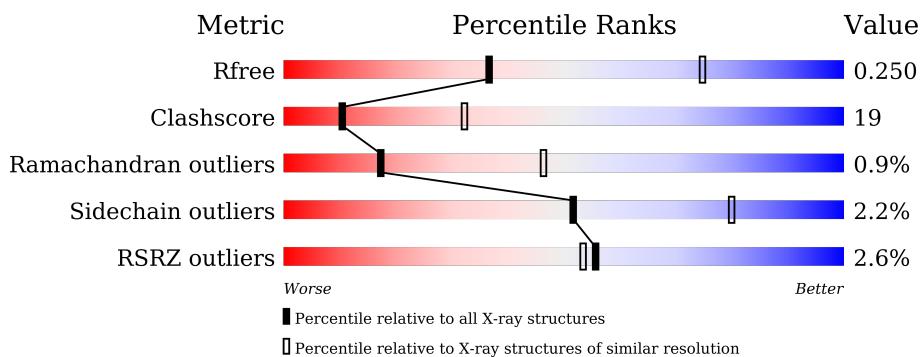
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 >=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 <=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	273	4%	61%	36%	..
1	B	273	.%	70%	26%	..

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4471 atoms, of which 80 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.

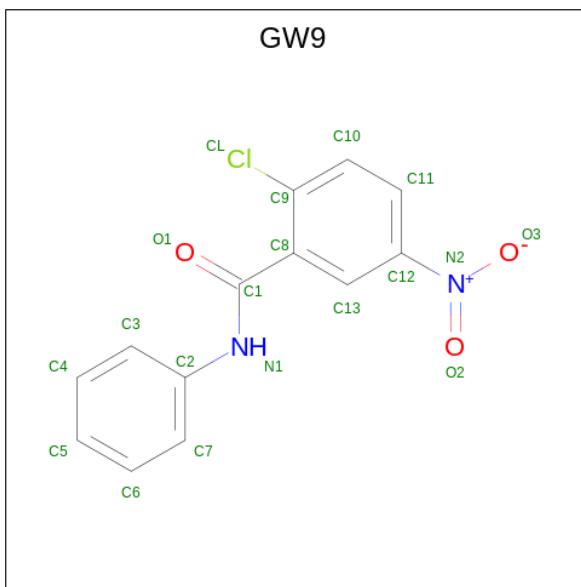
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C 2125	N 1364	O 357	S 386	18	0	0
1	B	269	Total	C 2122	N 1360	O 355	S 389	18	0	0

There are 8 discrepancies between the modelled and reference sequences:

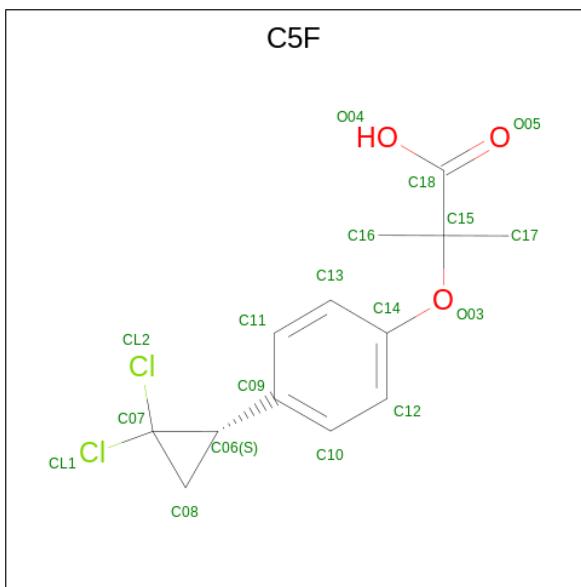
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLY	-	expression tag	UNP Q07869
A	197	SER	-	expression tag	UNP Q07869
A	198	HIS	-	expression tag	UNP Q07869
A	199	MET	-	expression tag	UNP Q07869
B	196	GLY	-	expression tag	UNP Q07869
B	197	SER	-	expression tag	UNP Q07869
B	198	HIS	-	expression tag	UNP Q07869
B	199	MET	-	expression tag	UNP Q07869

- Molecule 2 is 2-chloro-5-nitro-N-phenylbenzamide (three-letter code: GW9) (formula: C<sub>13</sub>H<sub>9</sub>ClN<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total		C	H	N	O	
			27	13	9	2	3		
2	A	1	Total		C	H	N	O	
			27	13	9	2	3		
2	A	1	Total		C	H	N	O	
			27	13	9	2	3		
2	B	1	Total		C	H	N	O	
			27	13	9	2	3		
2	B	1	Total		C	H	N	O	
			27	13	9	2	3		
2	B	1	Total		C	H	N	O	
			27	13	9	2	3		

- Molecule 3 is 2-{(1S)-2,2-dichlorocyclopropylphenoxy}-2-methylpropanoic acid (three-letter code: C5F) (formula:  $\text{C}_{13}\text{H}_{14}\text{Cl}_2\text{O}_3$ ) (labeled as "Ligand of Interest" by depositor).

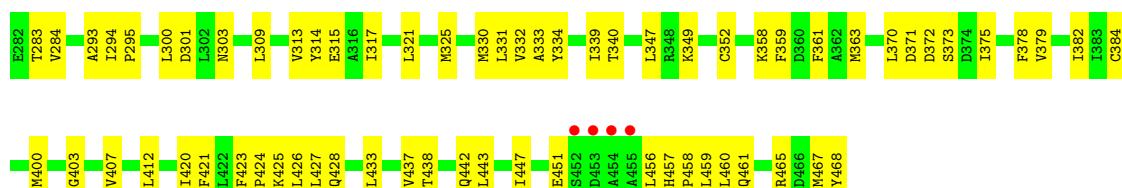
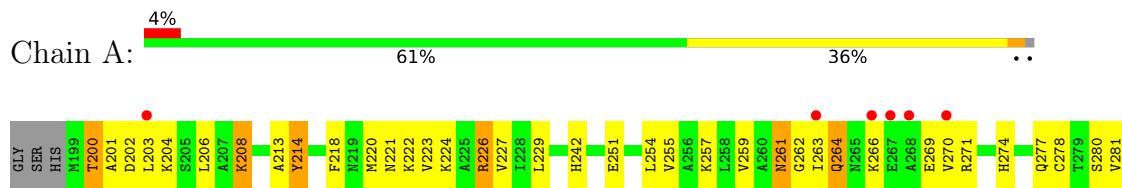


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total		C	Cl	H	O	
			31		13	2	13	3	
3	B	1	Total		C	Cl	H	O	
			31		13	2	13	3	

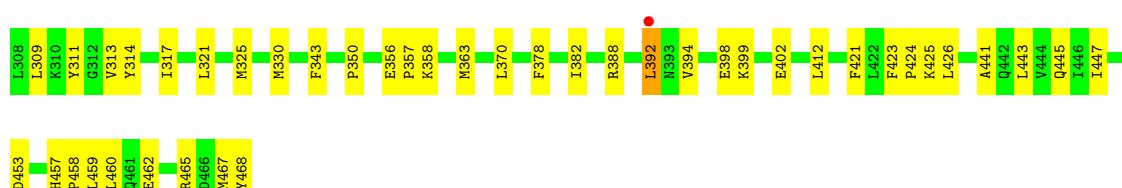
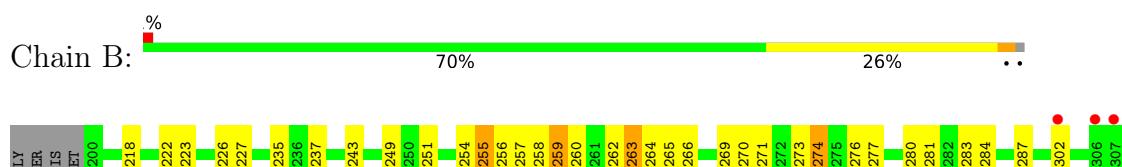
### 3 Residue-property plots

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: Peroxisome proliferator-activated receptor alpha



- Molecule 1: Peroxisome proliferator-activated receptor alpha



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.01Å 103.26Å 61.13Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	36.48 – 2.91 39.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.48-2.91) 99.0 (39.16-2.91)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	3.52 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575-000	Depositor
$R$ , $R_{free}$	0.189 , 0.248 0.191 , 0.250	Depositor DCC
$R_{free}$ test set	824 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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.













*Continued from previous page...*

Mol	Chain	Res	Type
1	A	208	LYS
1	A	226	ARG
1	A	261	ASN
1	A	264	GLN
1	A	278	CYS
1	B	274	HIS
1	B	302	LEU
1	B	392	LEU
1	B	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN

### 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.

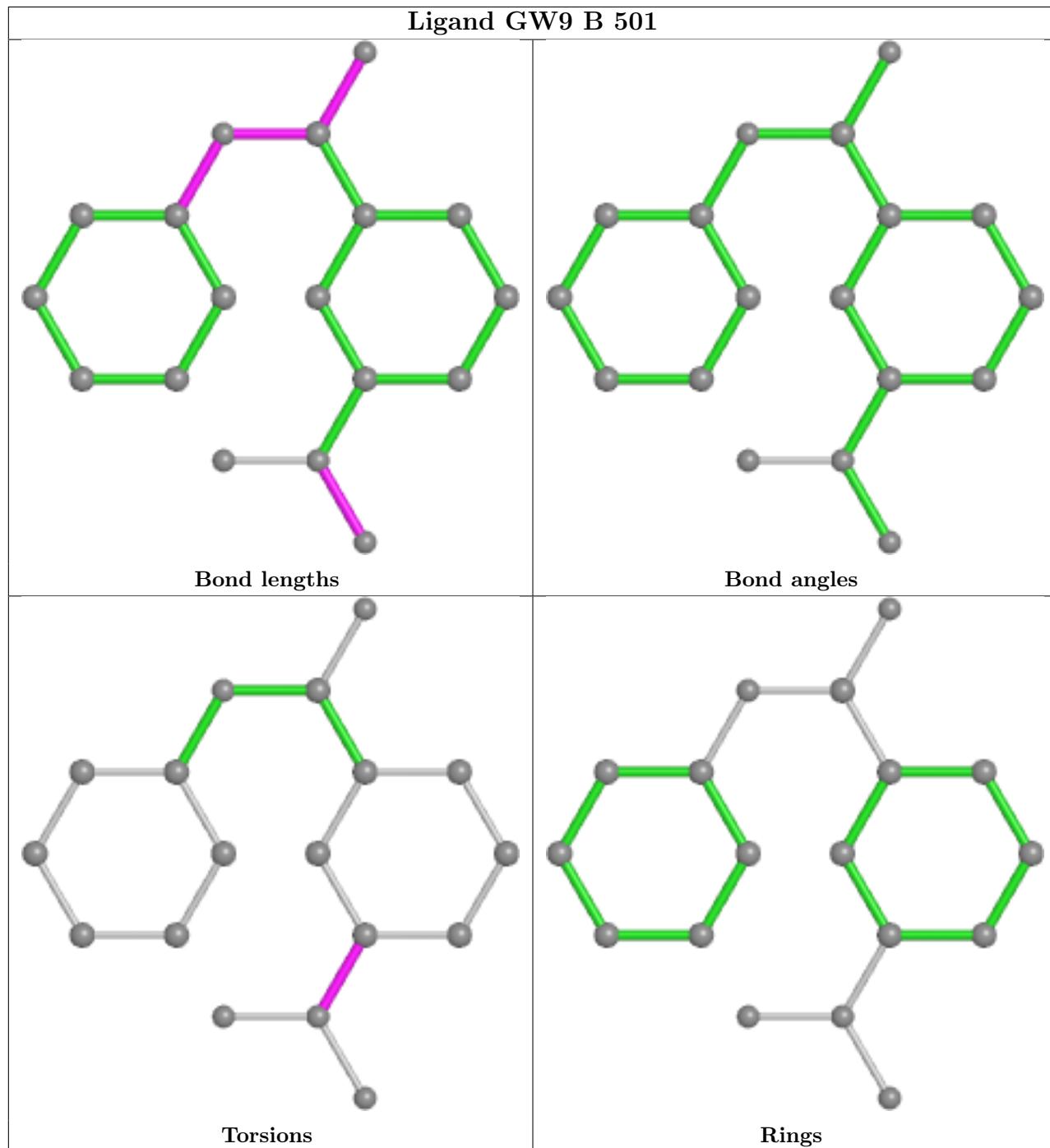
In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists 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).

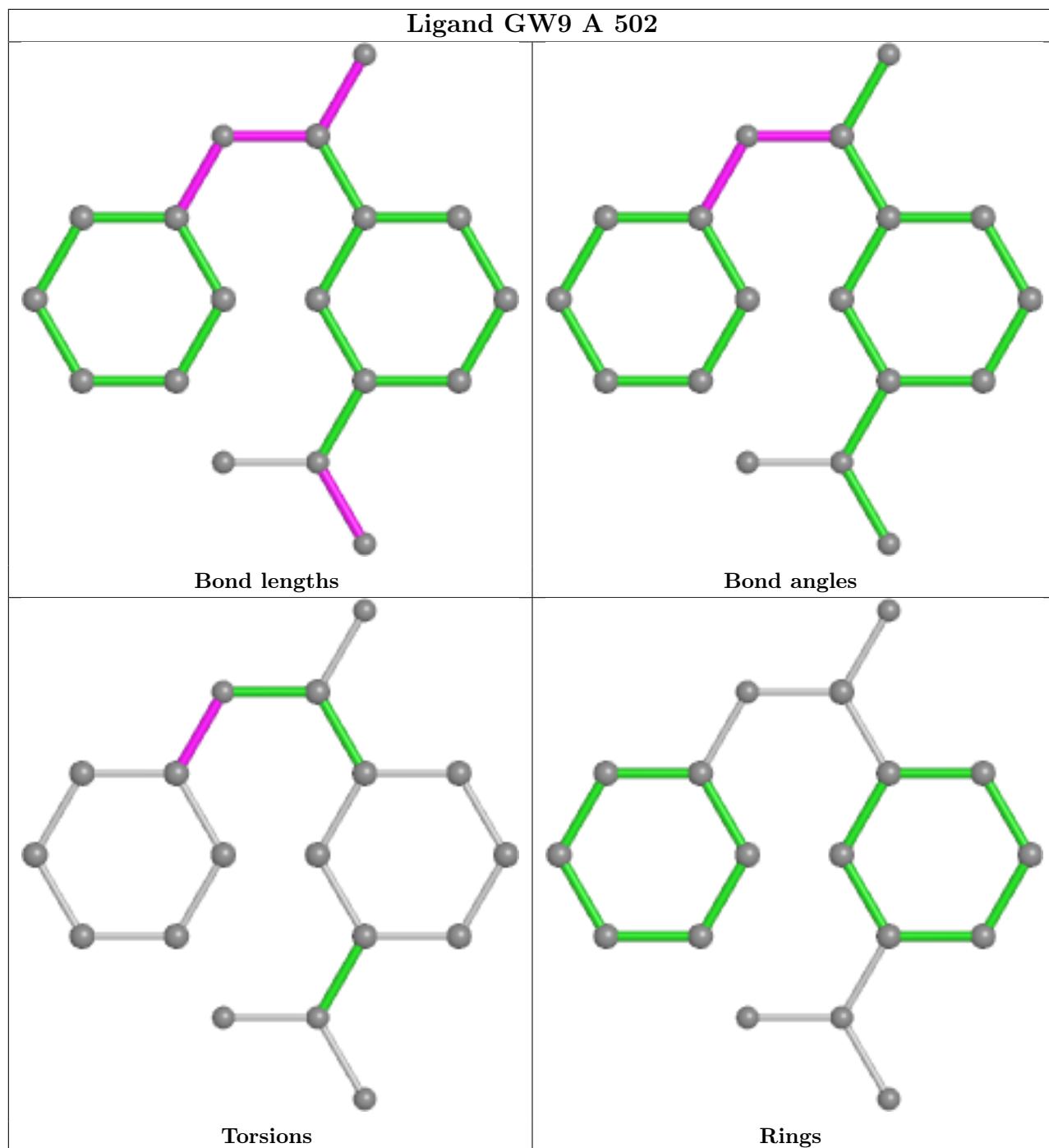


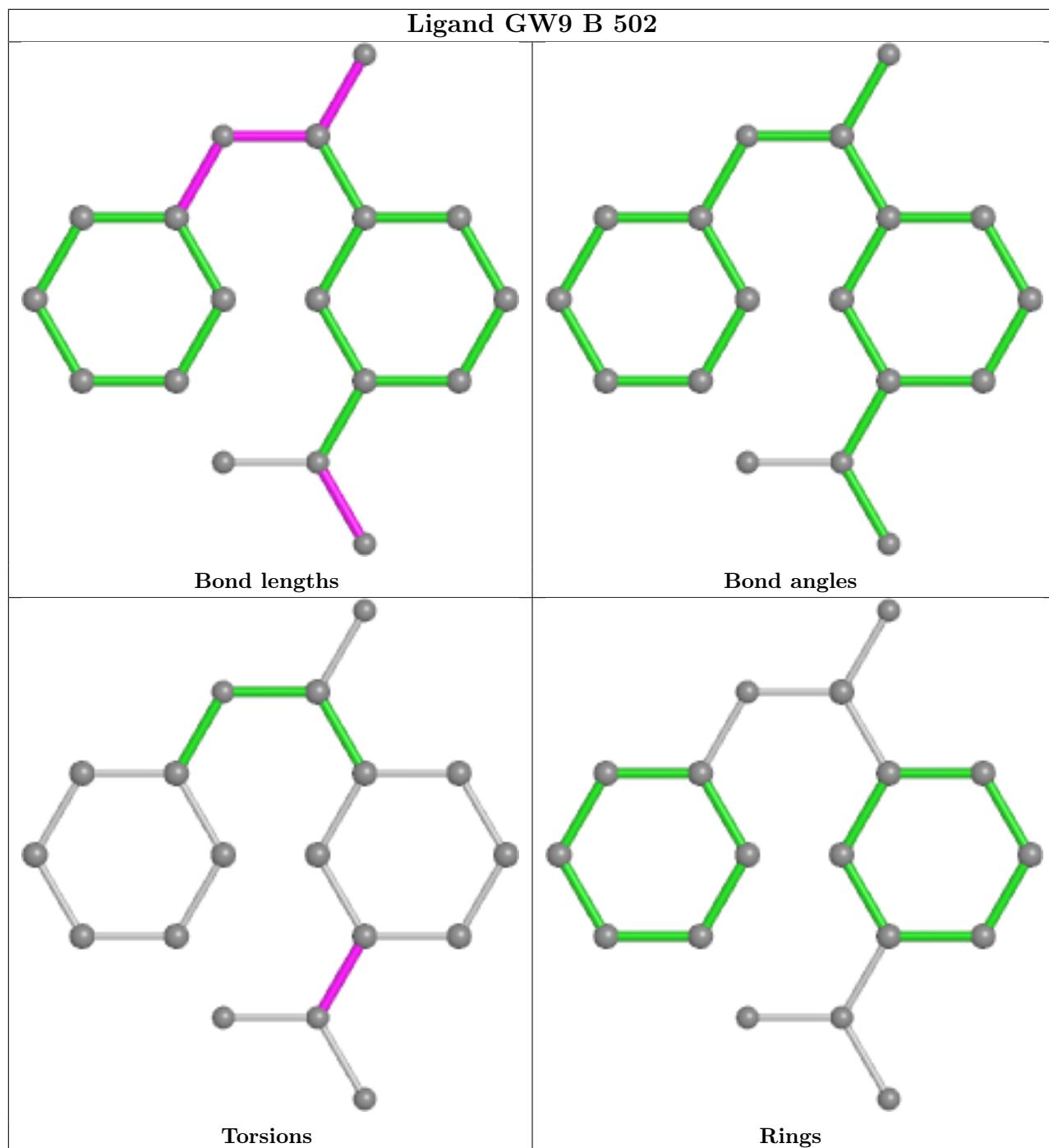


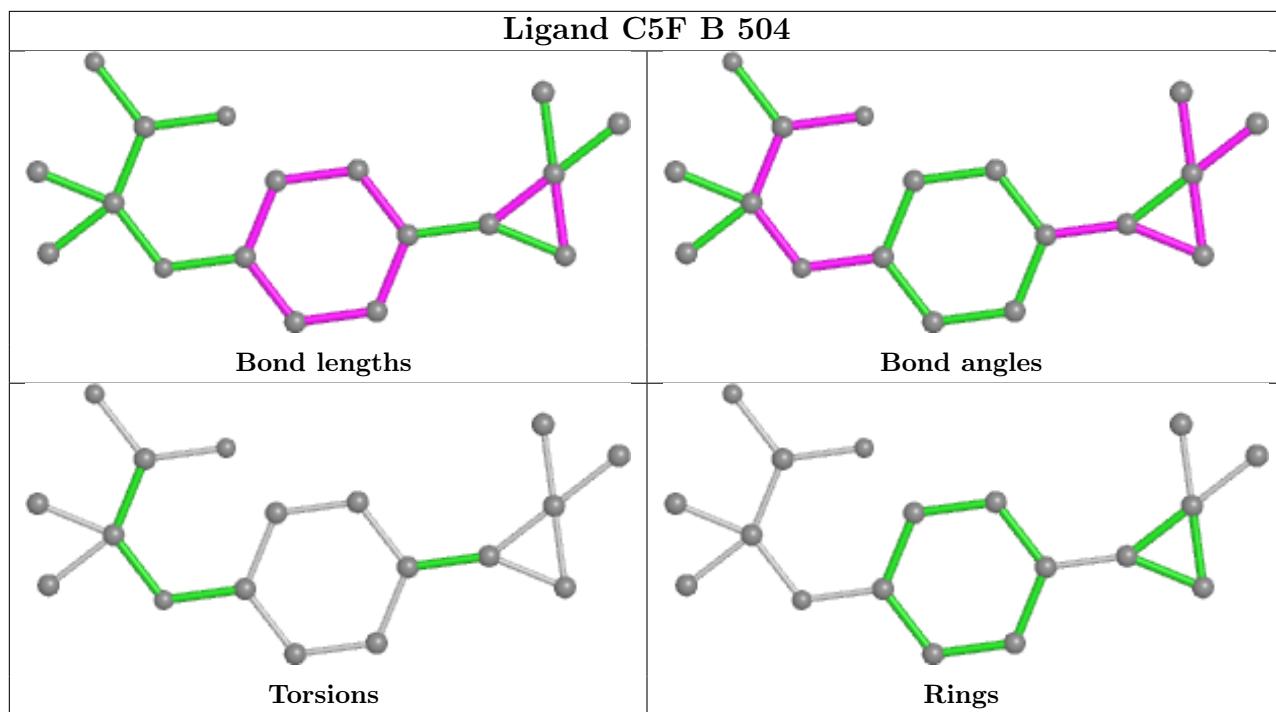


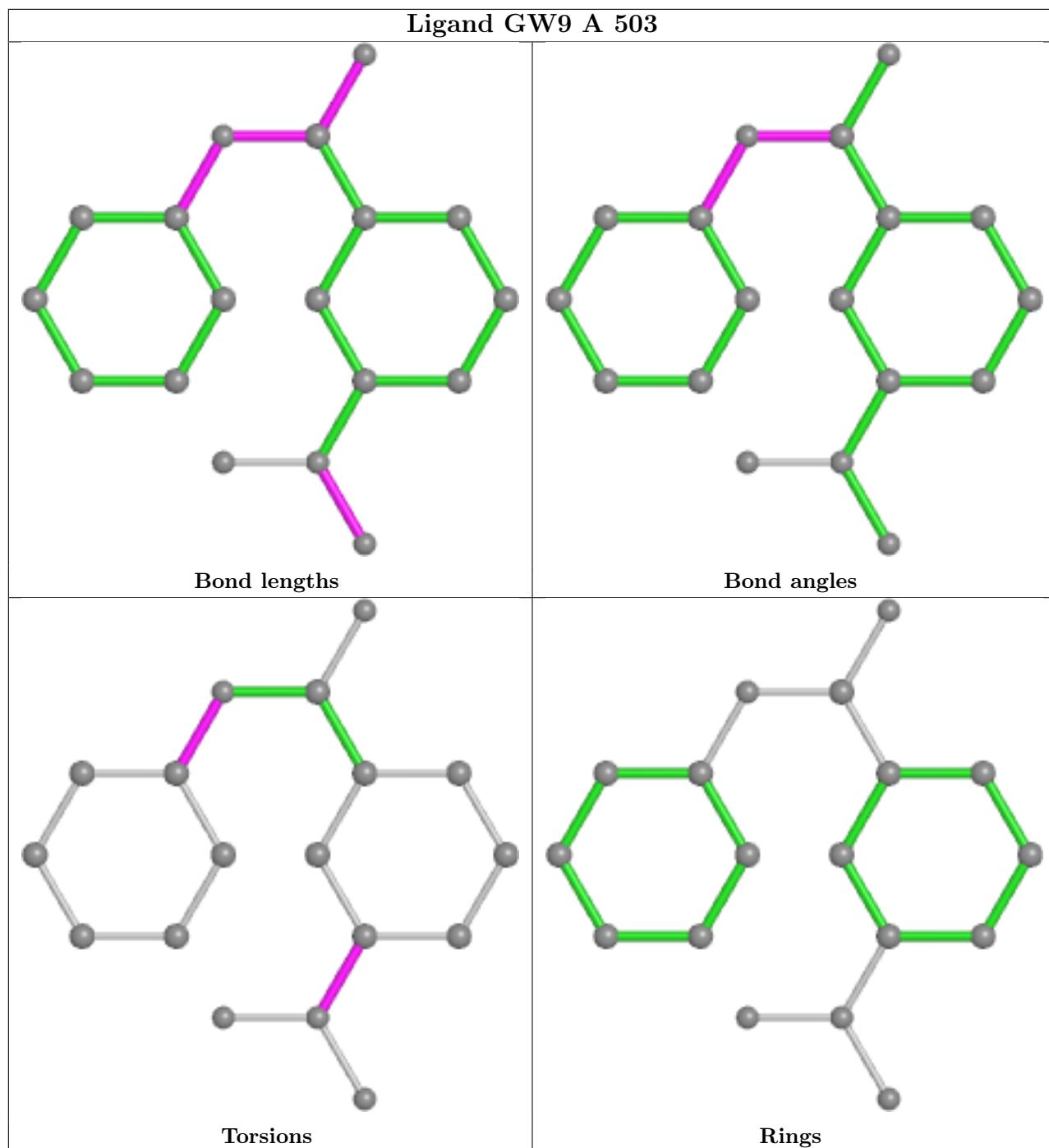
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

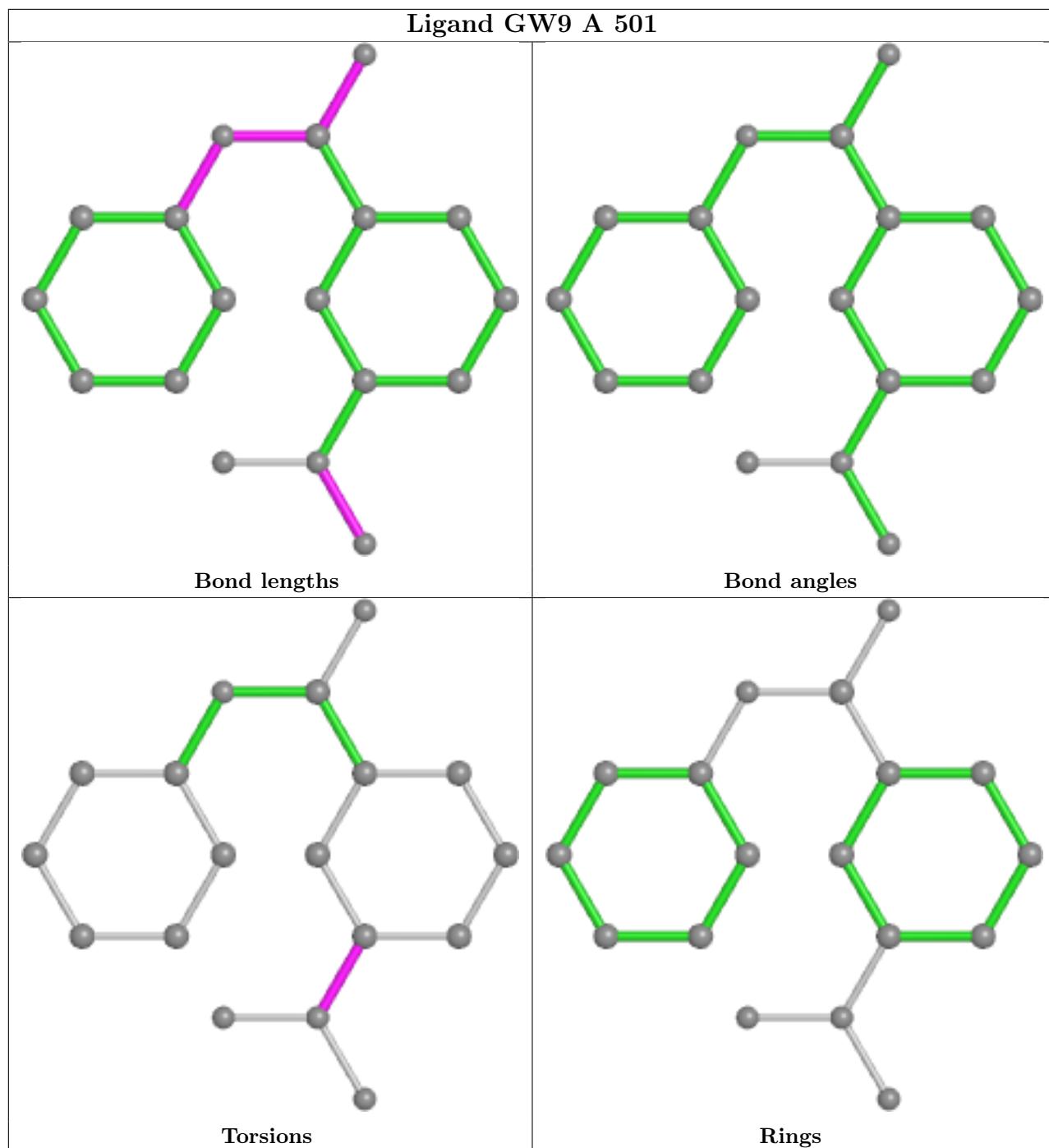


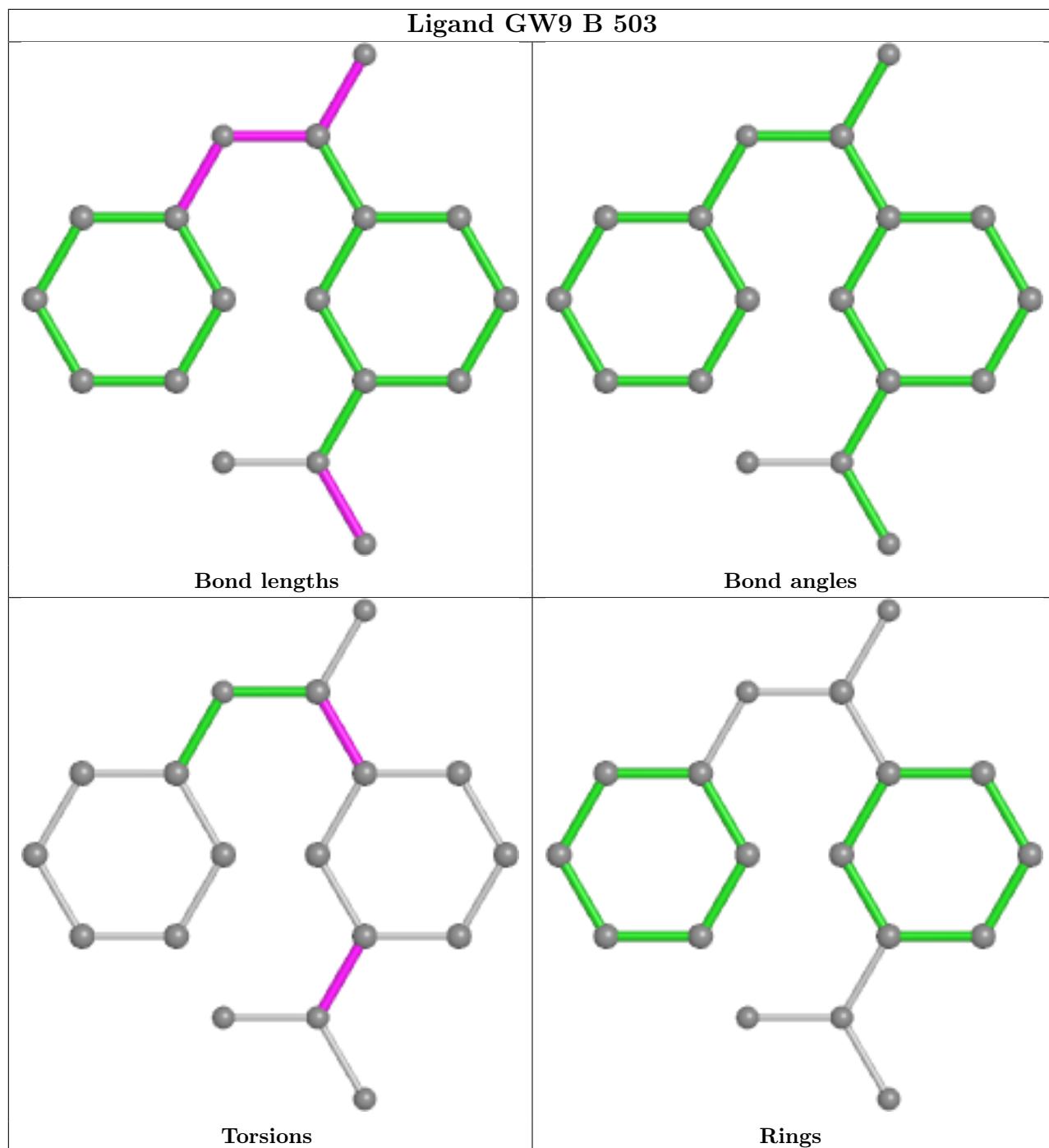


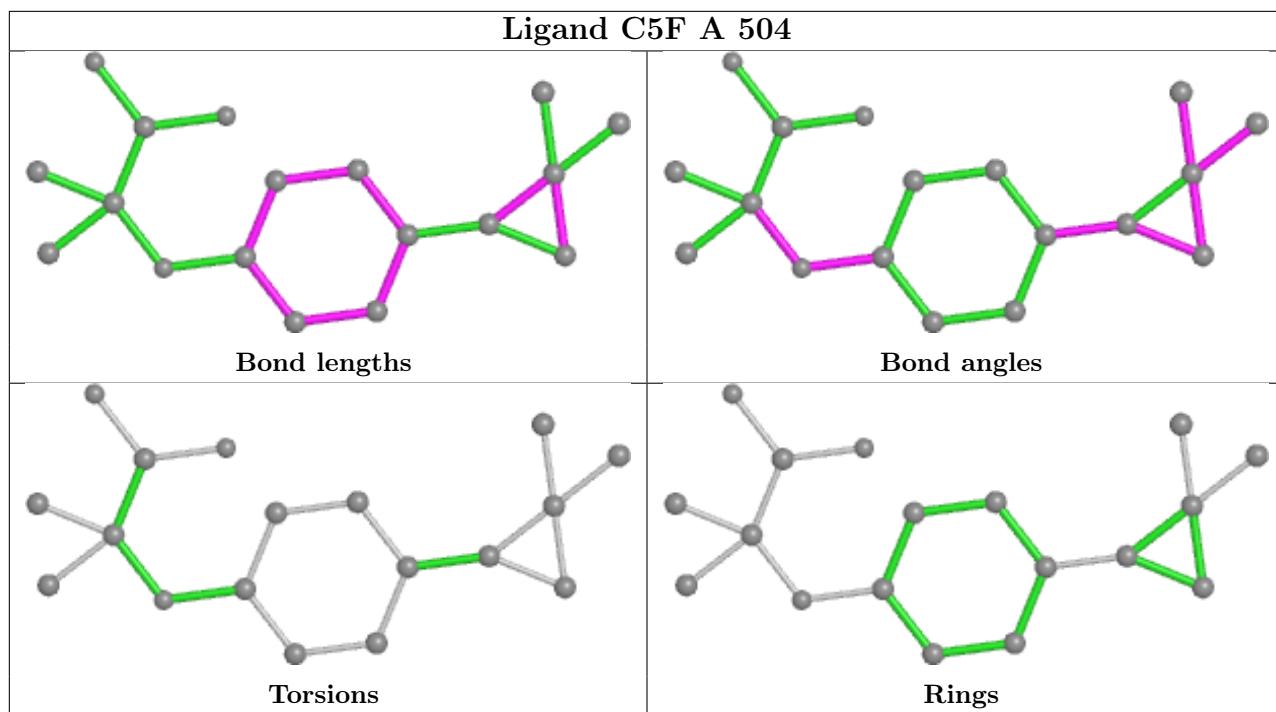












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	270/273 (98%)	0.19	10 (3%) 41 38	54, 80, 116, 150	0
1	B	269/273 (98%)	0.05	4 (1%) 73 73	55, 80, 116, 132	0
All	All	539/546 (98%)	0.12	14 (2%) 56 53	54, 80, 117, 150	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	ALA	4.3
1	A	454	ALA	4.0
1	A	203	LEU	3.4
1	A	453	ASP	3.2
1	B	302	LEU	3.0
1	B	306	VAL	2.8
1	A	263	ILE	2.7
1	A	270	VAL	2.6
1	A	266	LYS	2.3
1	A	452	SER	2.1
1	A	267	GLU	2.0
1	B	307	THR	2.0
1	A	268	ALA	2.0
1	B	392	LEU	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

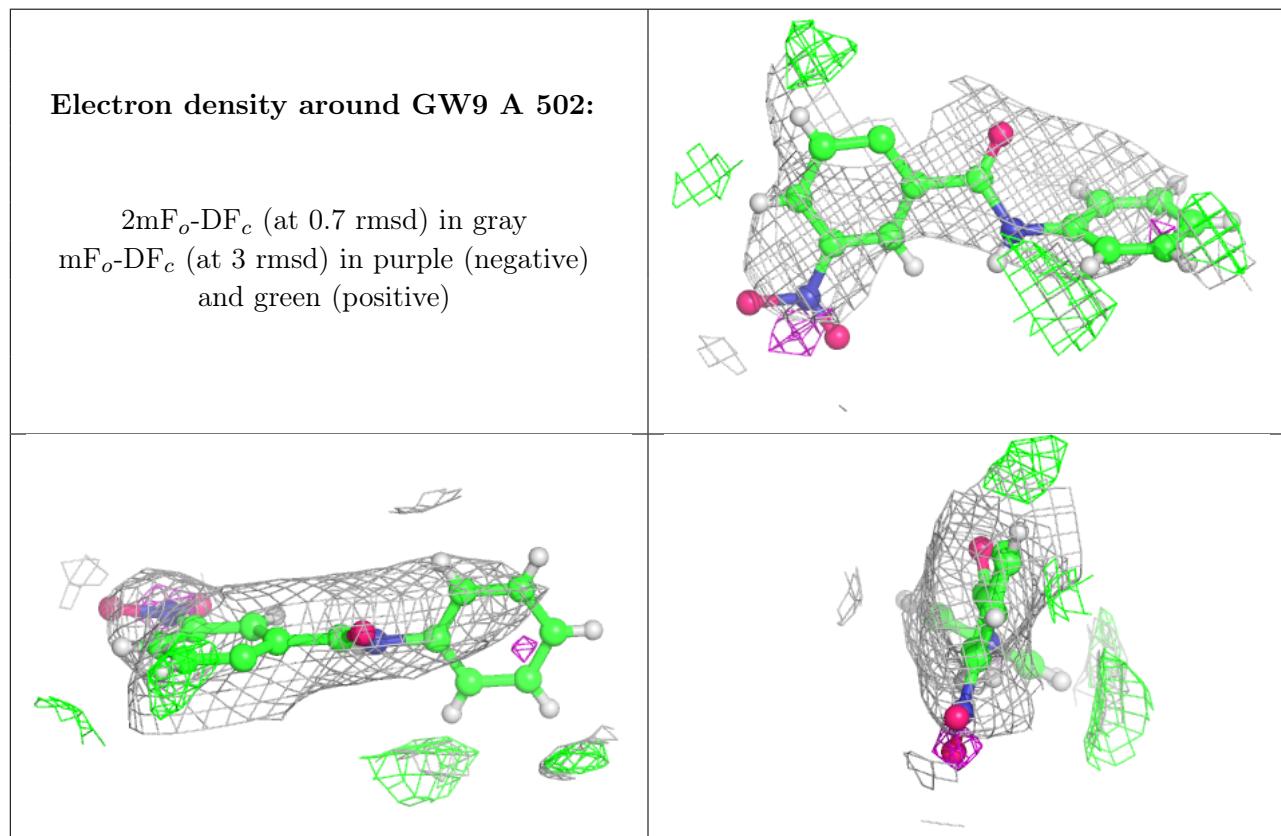
There are no monosaccharides in this entry.

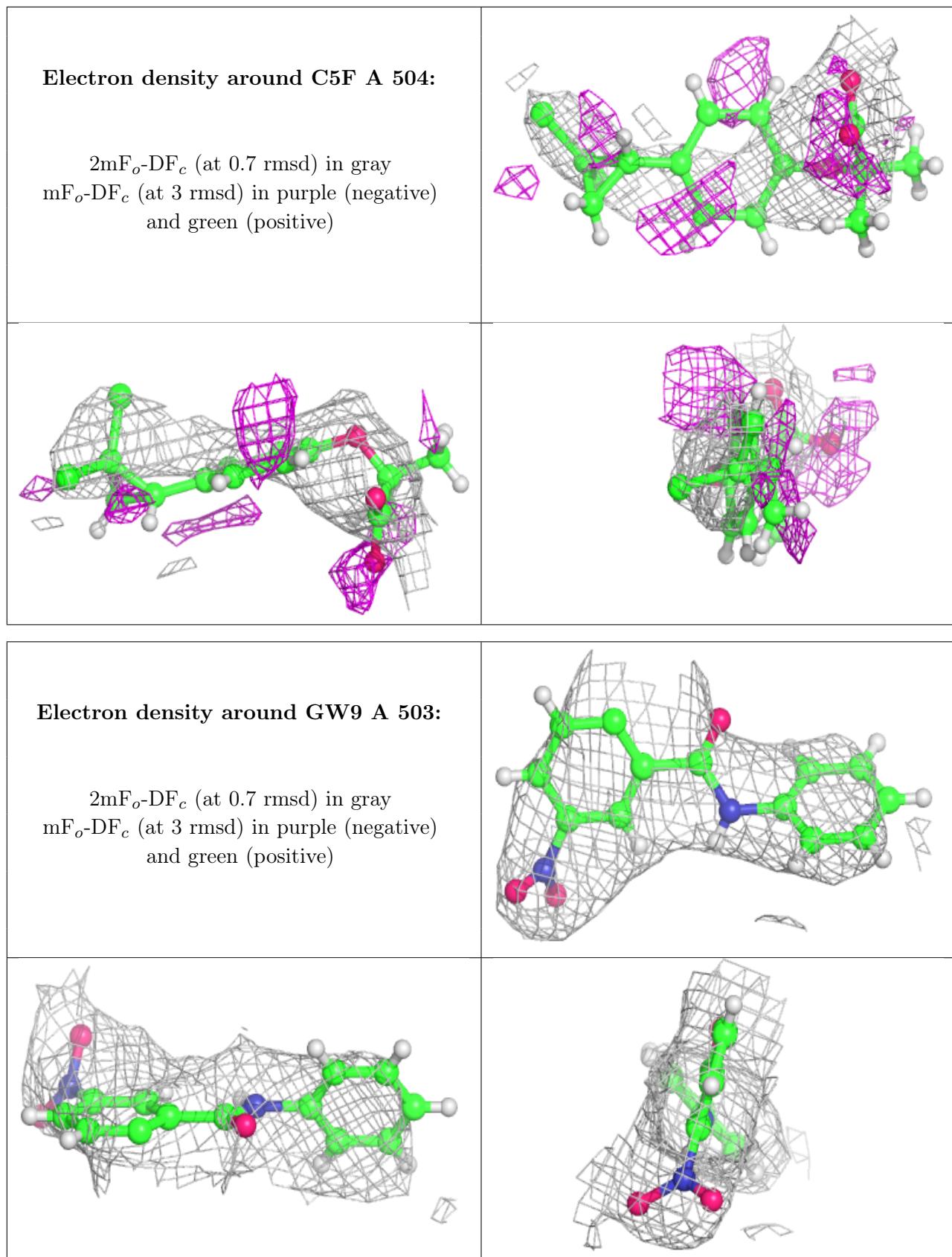
## 6.4 Ligands (i)

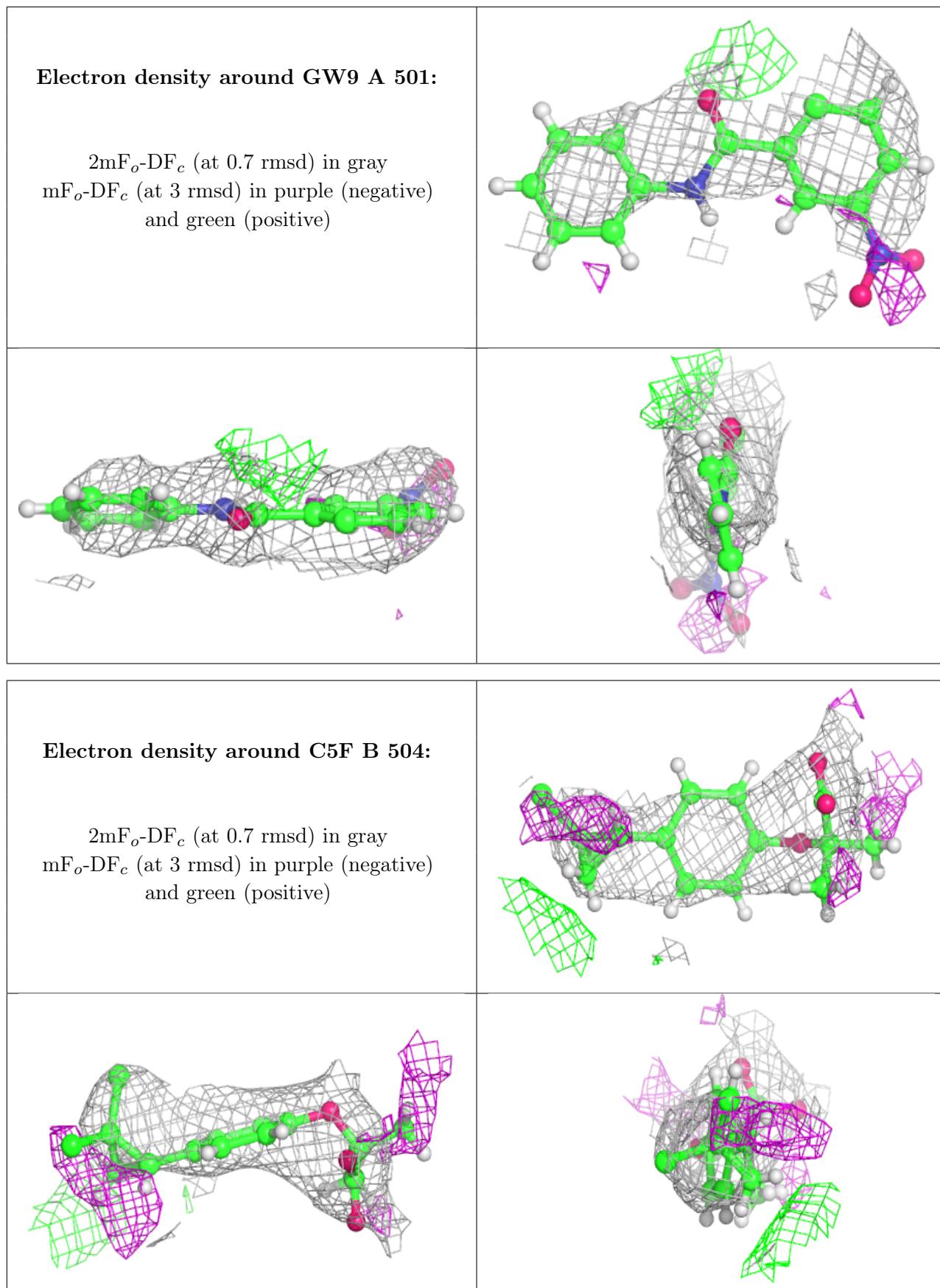
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

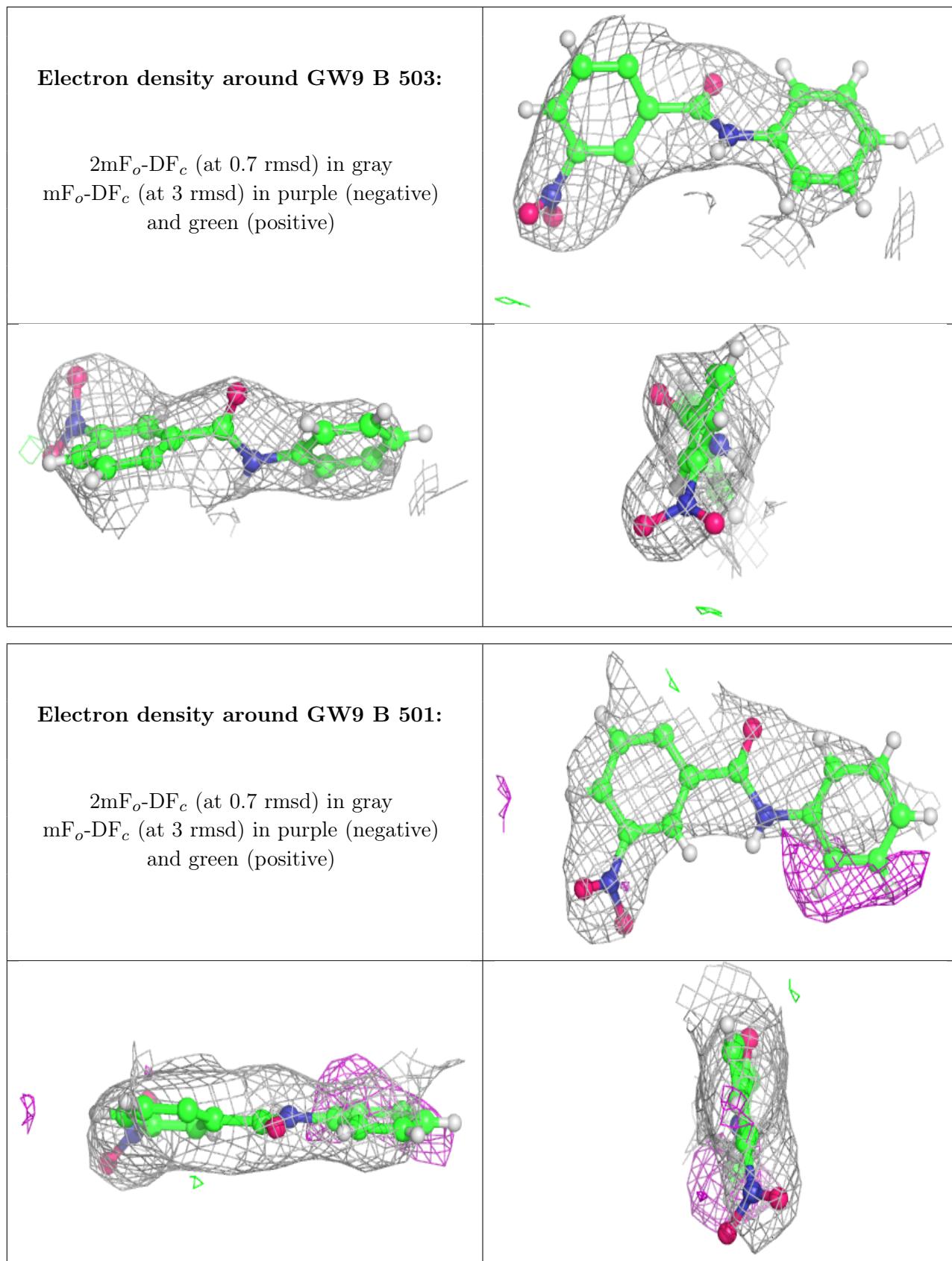
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GW9	A	502	18/19	0.82	0.32	97,116,162,183	0
3	C5F	A	504	18/18	0.83	0.66	97,124,161,175	0
2	GW9	A	503	18/19	0.85	0.32	111,121,145,146	0
2	GW9	A	501	18/19	0.87	0.40	70,111,137,139	0
3	C5F	B	504	18/18	0.88	0.45	83,104,135,160	0
2	GW9	B	503	18/19	0.91	0.29	95,108,125,133	0
2	GW9	B	501	18/19	0.92	0.33	64,91,111,130	0
2	GW9	B	502	18/19	0.93	0.25	78,105,142,150	0

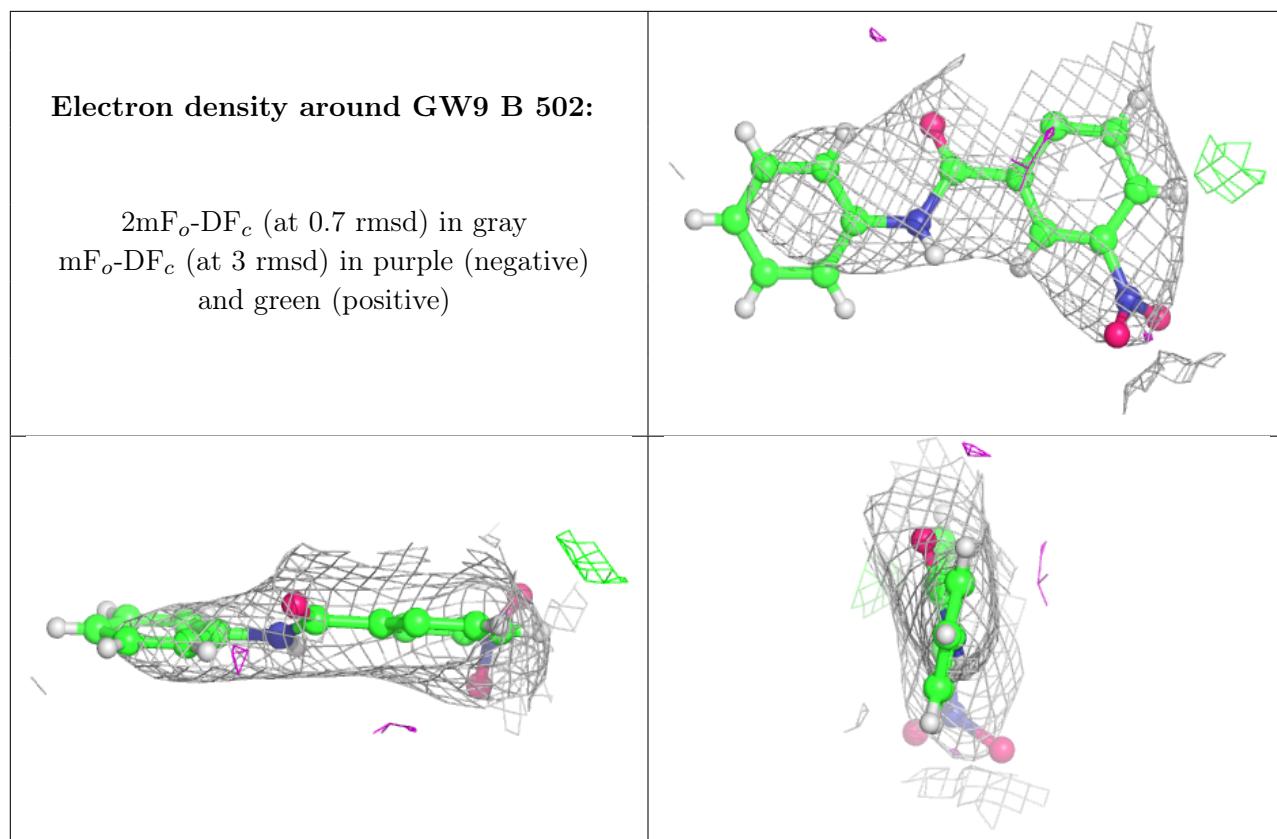
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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











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

There are no such residues in this entry.