



# Full wwPDB X-ray Structure Validation Report i

Feb 23, 2022 – 12:30 pm GMT

PDB ID : 6QKK  
Title : Aplysia californica AChBP in complex with 2-Fluoro-(carbamoylpyridinyl)deschloroepibatidine analogue (1)  
Authors : Davis, S.; Bueno, R.V.; Dawson, A.; Hunter, W.N.  
Deposited on : 2019-01-29  
Resolution : 2.20 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.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

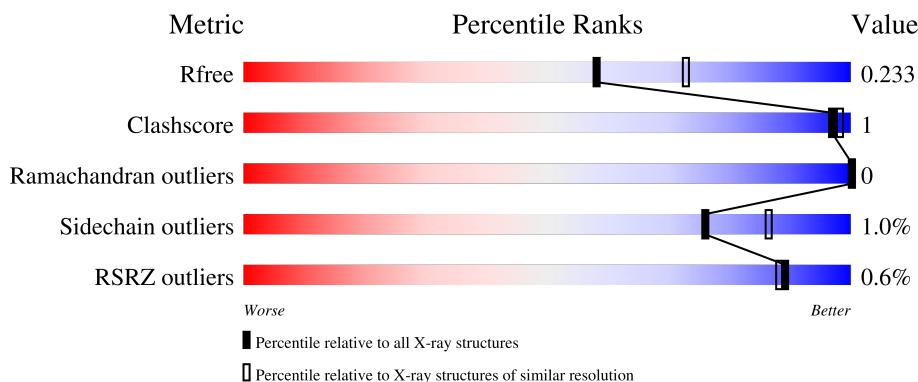
## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

### X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 <sub>free</sub>	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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.



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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
5	NAG	A	406	-	-	-	X







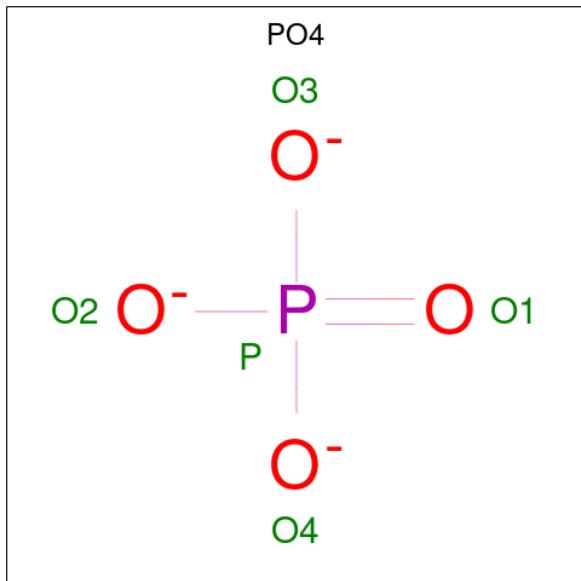




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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C F N O 23 18 1 3 1	0	0
2	E	1	Total C F N O 23 18 1 3 1	0	0
2	F	1	Total C F N O 23 18 1 3 1	0	0
2	G	1	Total C F N O 23 18 1 3 1	0	0
2	H	1	Total C F N O 23 18 1 3 1	0	0
2	I	1	Total C F N O 23 18 1 3 1	0	0
2	J	1	Total C F N O 23 18 1 3 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



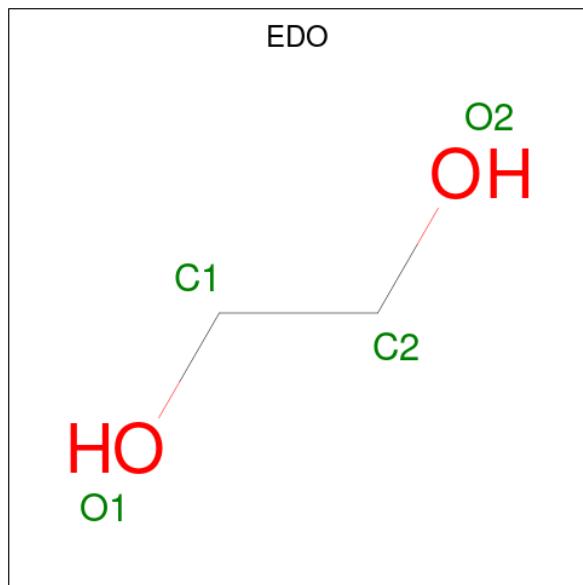
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	J	1	Total O P 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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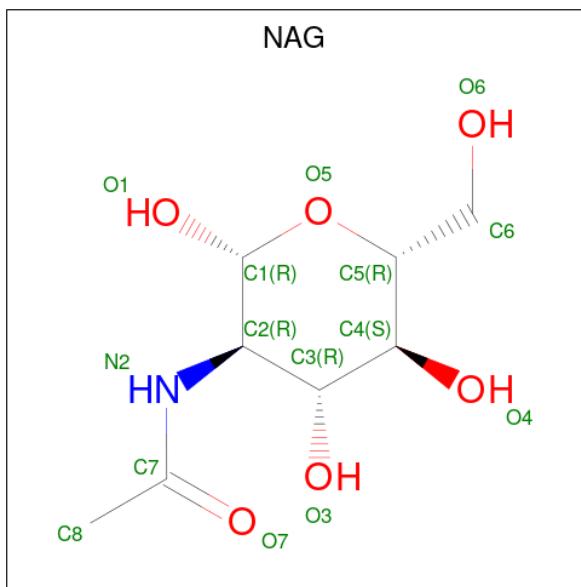
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

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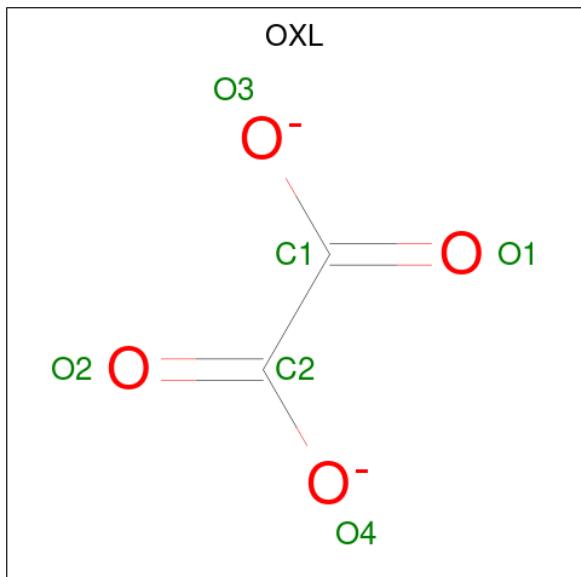
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total    C    N    O 14    8    1    5	0	0
5	D	1	Total    C    N    O 14    8    1    5	0	0
5	I	1	Total    C    N    O 14    8    1    5	0	0
5	J	1	Total    C    N    O 14    8    1    5	0	0

- Molecule 6 is OXALATE ION (three-letter code: OXL) (formula:  $C_2O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 2 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	115	Total O 115 115	0	0
7	B	135	Total O 135 135	0	0
7	C	127	Total O 127 127	0	0
7	D	104	Total O 104 104	0	0
7	E	124	Total O 124 124	0	0
7	F	112	Total O 112 112	0	0
7	G	113	Total O 113 113	0	0
7	H	104	Total O 104 104	0	0
7	I	92	Total O 92 92	0	0
7	J	112	Total O 112 112	0	0





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.00Å    131.58Å    131.82Å 90.00°    102.77°    90.00°	Depositor
Resolution (Å)	48.88 – 2.20 48.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.88-2.20) 99.9 (48.83-2.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.16 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
$R$ , $R_{free}$	0.199 , 0.228 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	8867 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	1.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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.











Mol	Chain	Res	Type
1	A	20	GLN
1	A	152	GLU
1	B	20	GLN
1	B	34	SER
1	C	20	GLN
1	D	20	GLN
1	D	225	ARG
1	E	20	GLN
1	E	201	GLN
1	F	20	GLN
1	F	201	GLN
1	G	20	GLN
1	H	20	GLN
1	I	20	GLN
1	J	20	GLN
1	J	133	MET
1	J	201	GLN
1	J	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	216	ASN
1	B	20	GLN
1	B	32	ASN
1	B	87	ASN
1	B	91	ASN
1	B	138	GLN
1	C	20	GLN
1	C	138	GLN
1	C	216	ASN
1	D	32	ASN
1	D	138	GLN
1	E	32	ASN
1	E	138	GLN
1	E	216	ASN
1	F	32	ASN
1	F	87	ASN
1	F	138	GLN
1	F	216	ASN
1	G	20	GLN
1	G	32	ASN

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Mol	Chain	Res	Type
1	G	74	GLN
1	G	87	ASN
1	G	138	GLN
1	G	216	ASN
1	H	32	ASN
1	H	87	ASN
1	H	138	GLN
1	H	216	ASN
1	I	32	ASN
1	I	55	GLN
1	I	87	ASN
1	I	138	GLN
1	I	216	ASN
1	J	32	ASN
1	J	87	ASN
1	J	138	GLN
1	J	216	ASN

### 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)

65 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).









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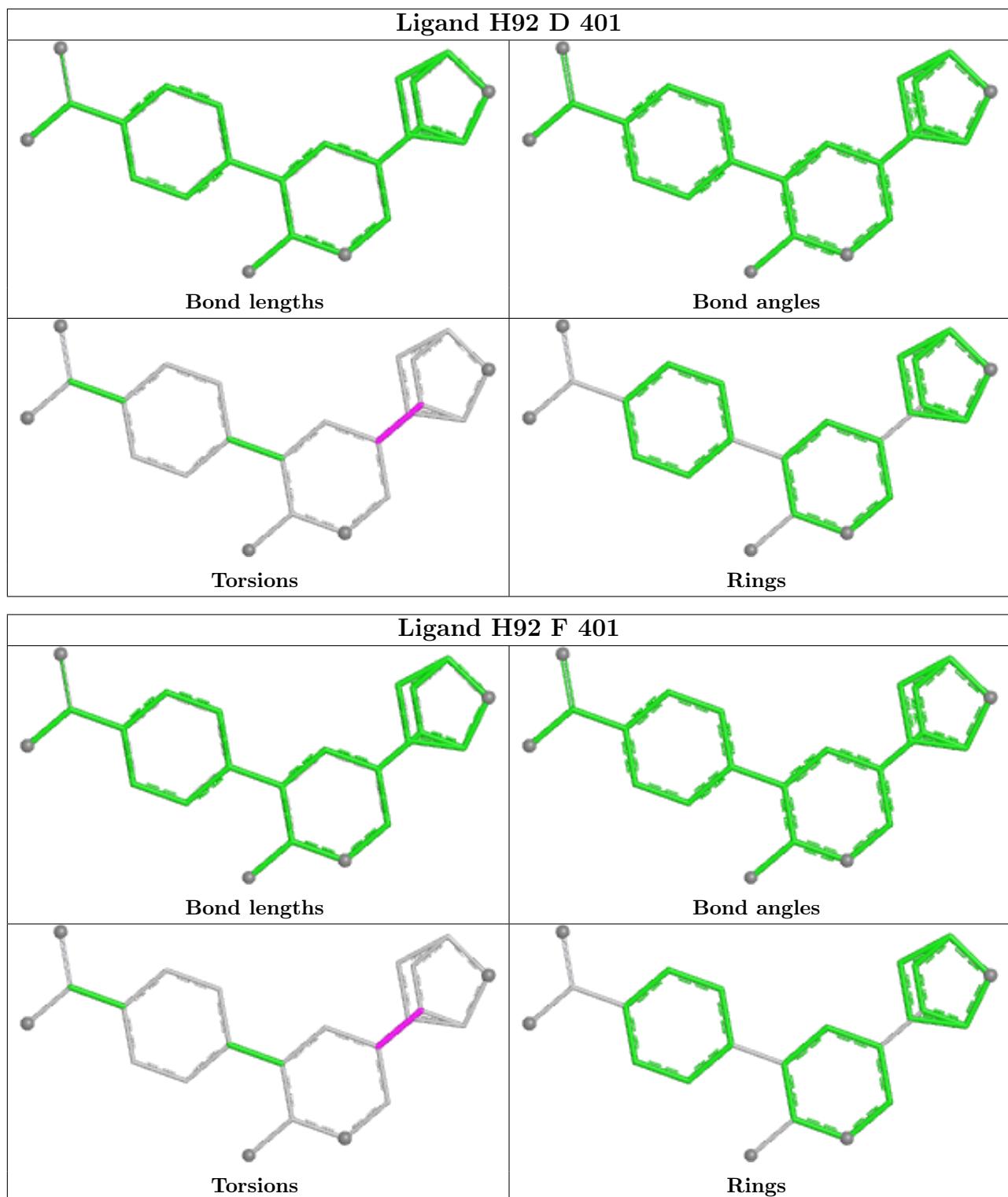
Mol	Chain	Res	Type	Atoms
2	I	401	H92	C2-C3-C6-C10
2	J	302	H92	C2-C3-C6-C10
4	A	404	EDO	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
4	G	406	EDO	O1-C1-C2-O2
4	I	405	EDO	O1-C1-C2-O2
5	J	307	NAG	C1-C2-N2-C7
4	C	403	EDO	O1-C1-C2-O2
4	I	404	EDO	O1-C1-C2-O2
4	I	403	EDO	O1-C1-C2-O2
4	I	406	EDO	O1-C1-C2-O2
5	D	406	NAG	C3-C2-N2-C7
5	J	307	NAG	C3-C2-N2-C7
4	B	402	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	F	403	EDO	O1-C1-C2-O2
4	F	406	EDO	O1-C1-C2-O2
4	G	403	EDO	O1-C1-C2-O2
4	H	403	EDO	O1-C1-C2-O2
4	J	306	EDO	O1-C1-C2-O2

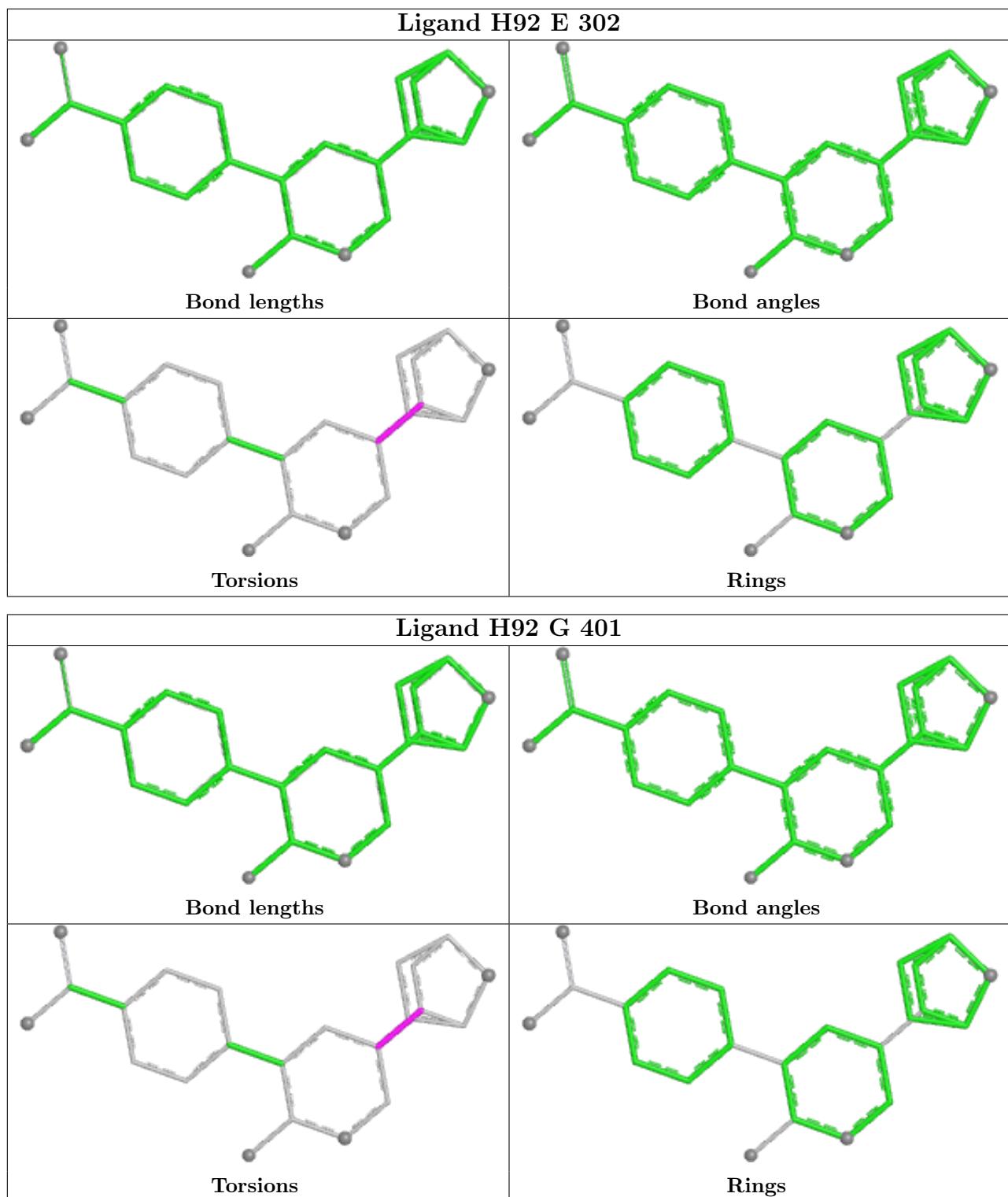
There are no ring outliers.

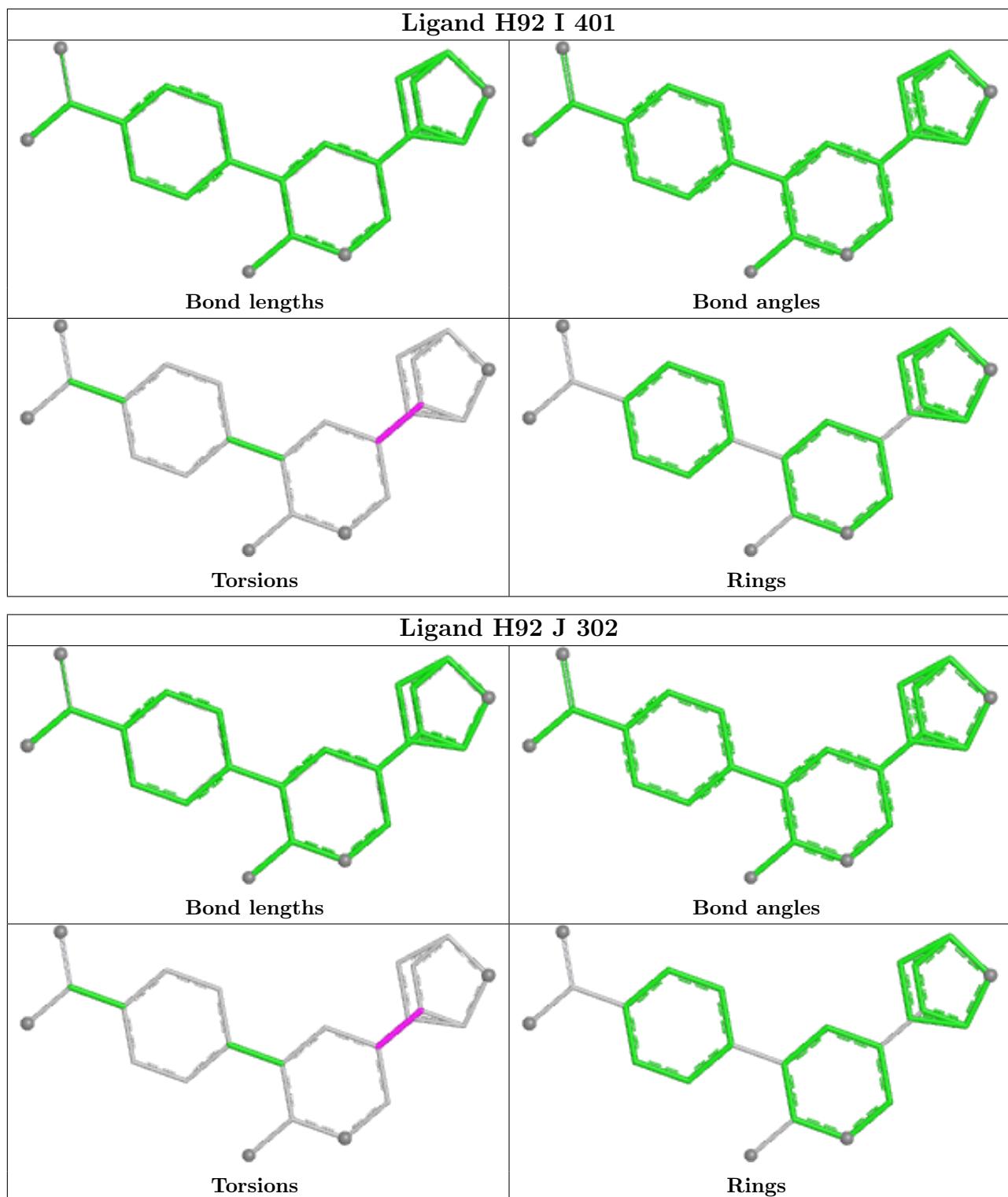
1 monomer is involved in 1 short contact:

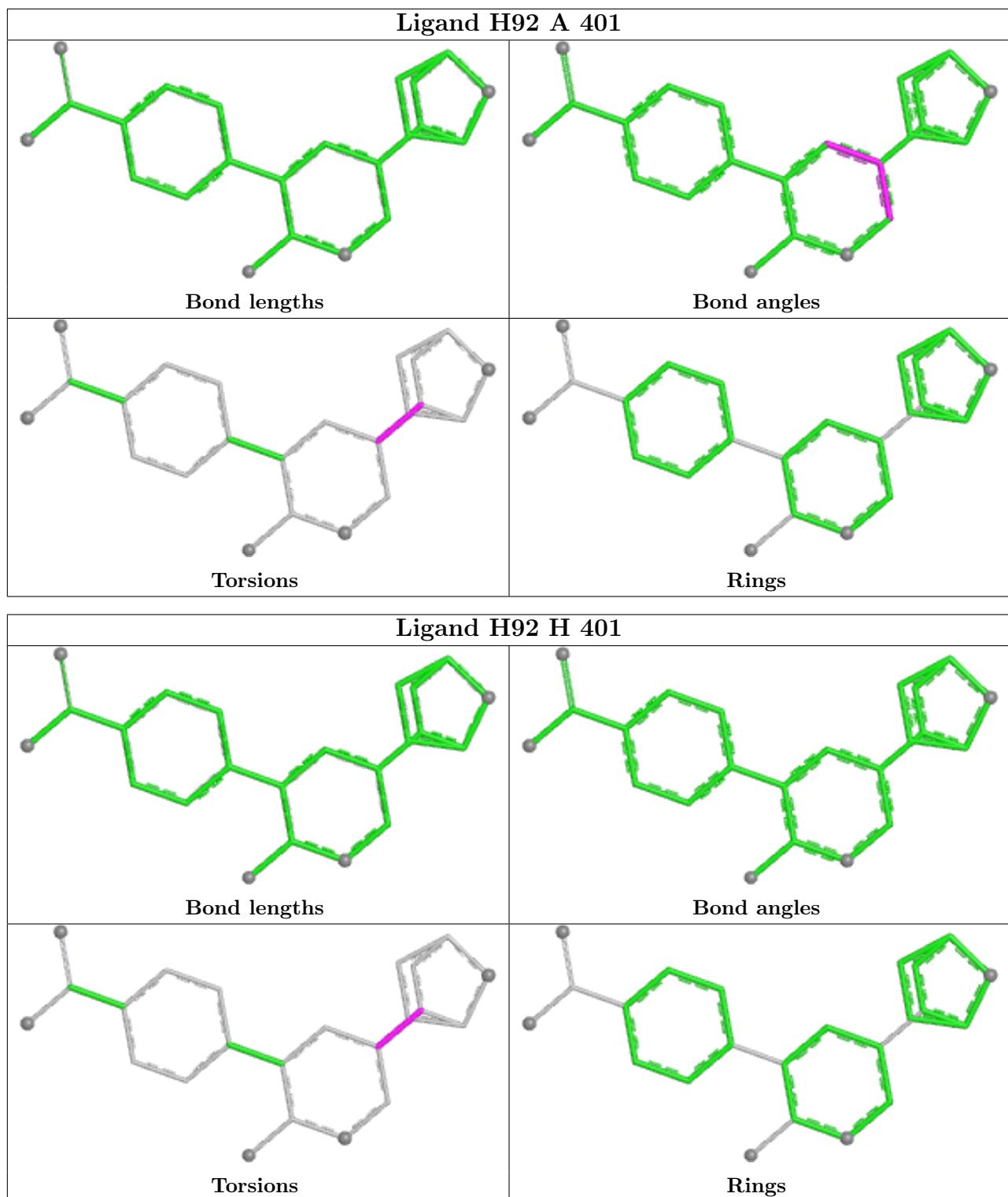
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	EDO	1	0

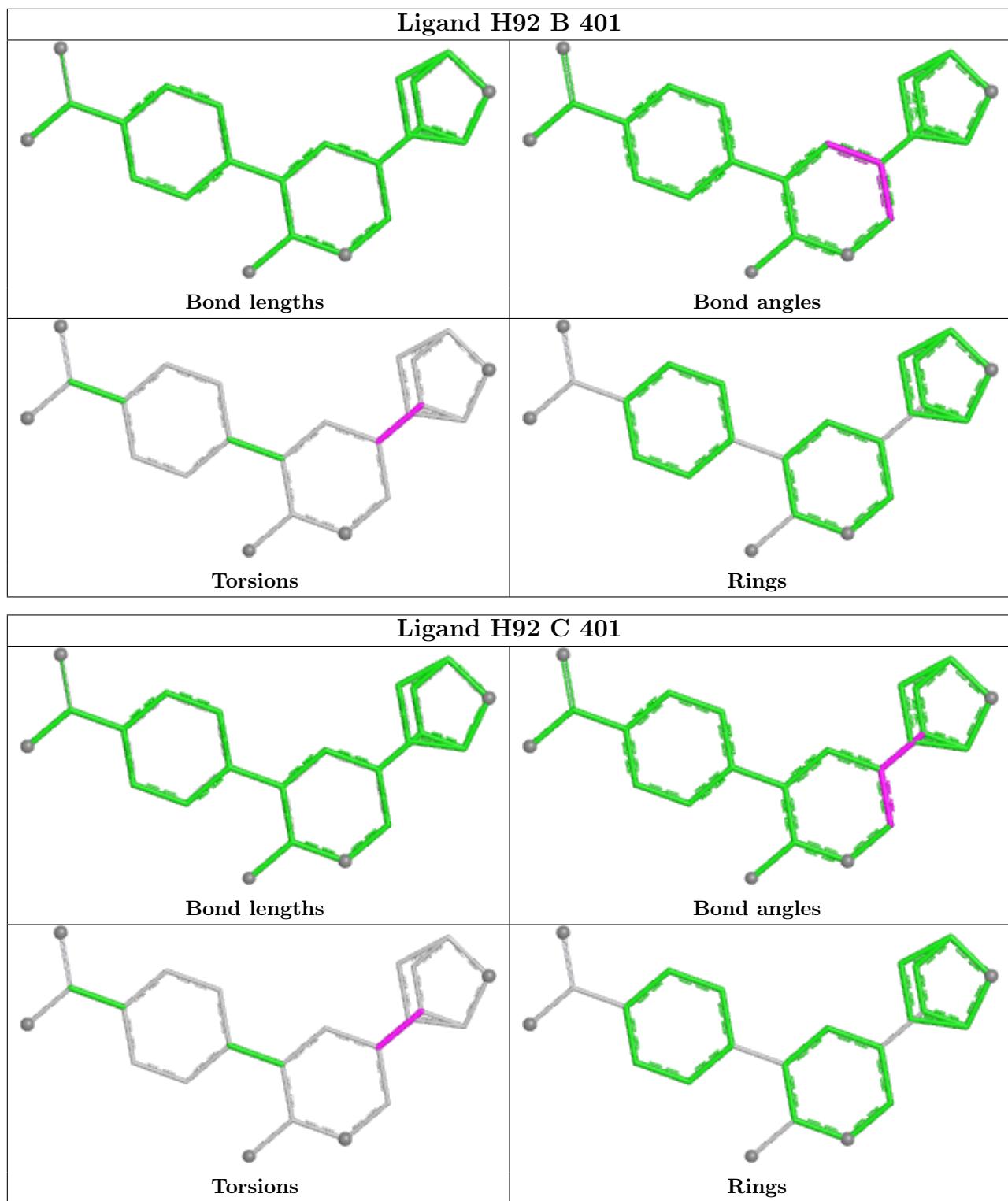
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

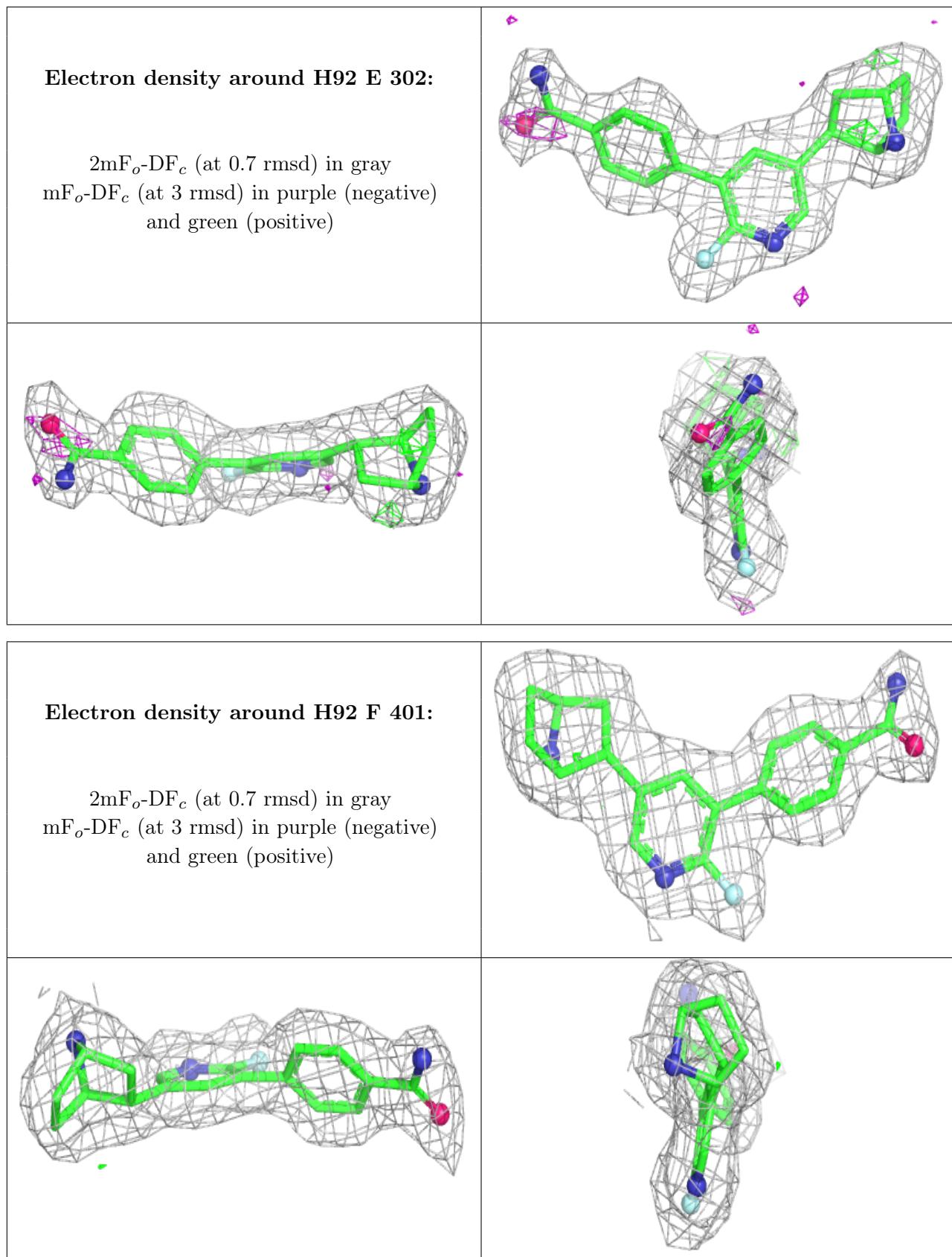
## 5.8 Polymer linkage issues

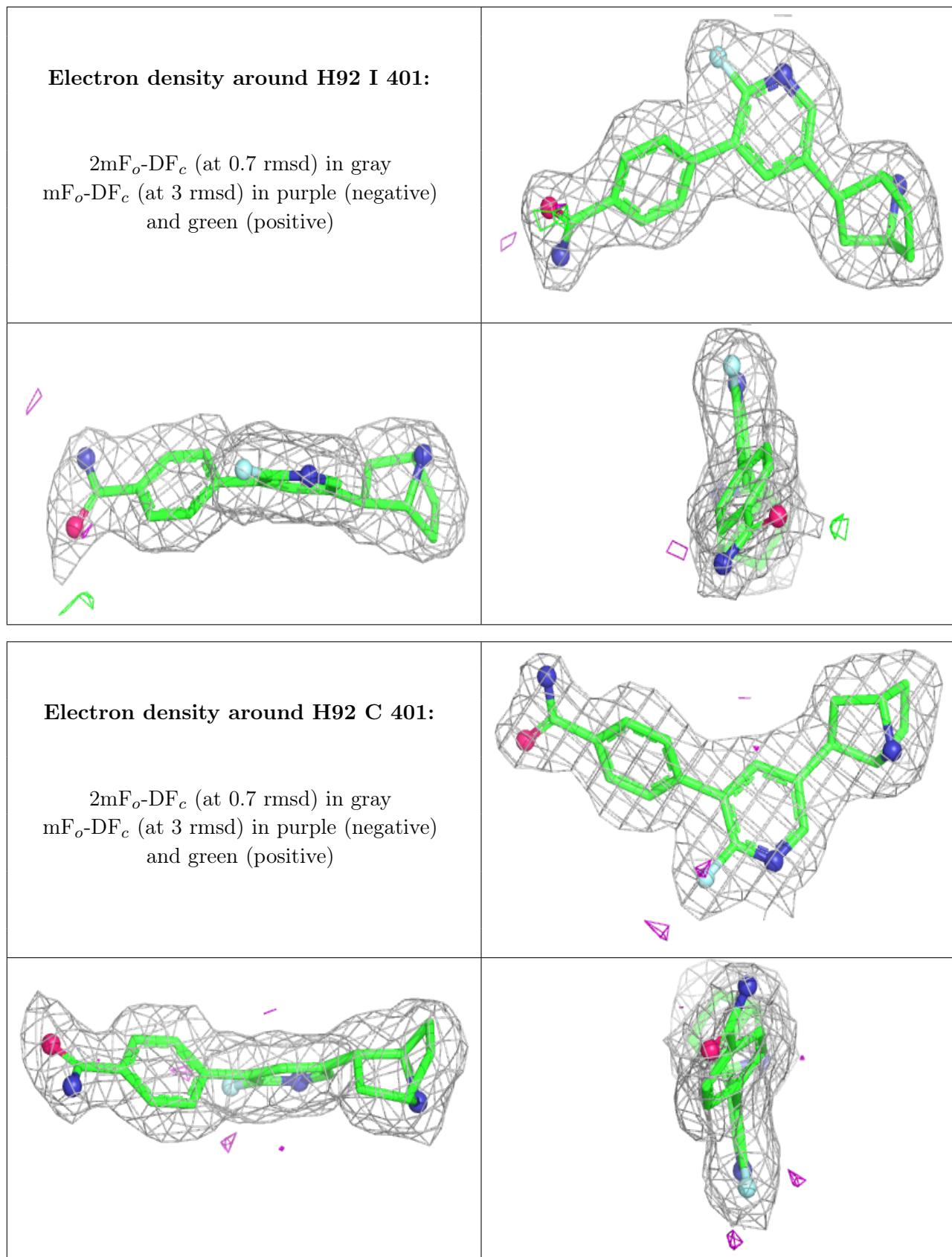
There are no chain breaks in this entry.

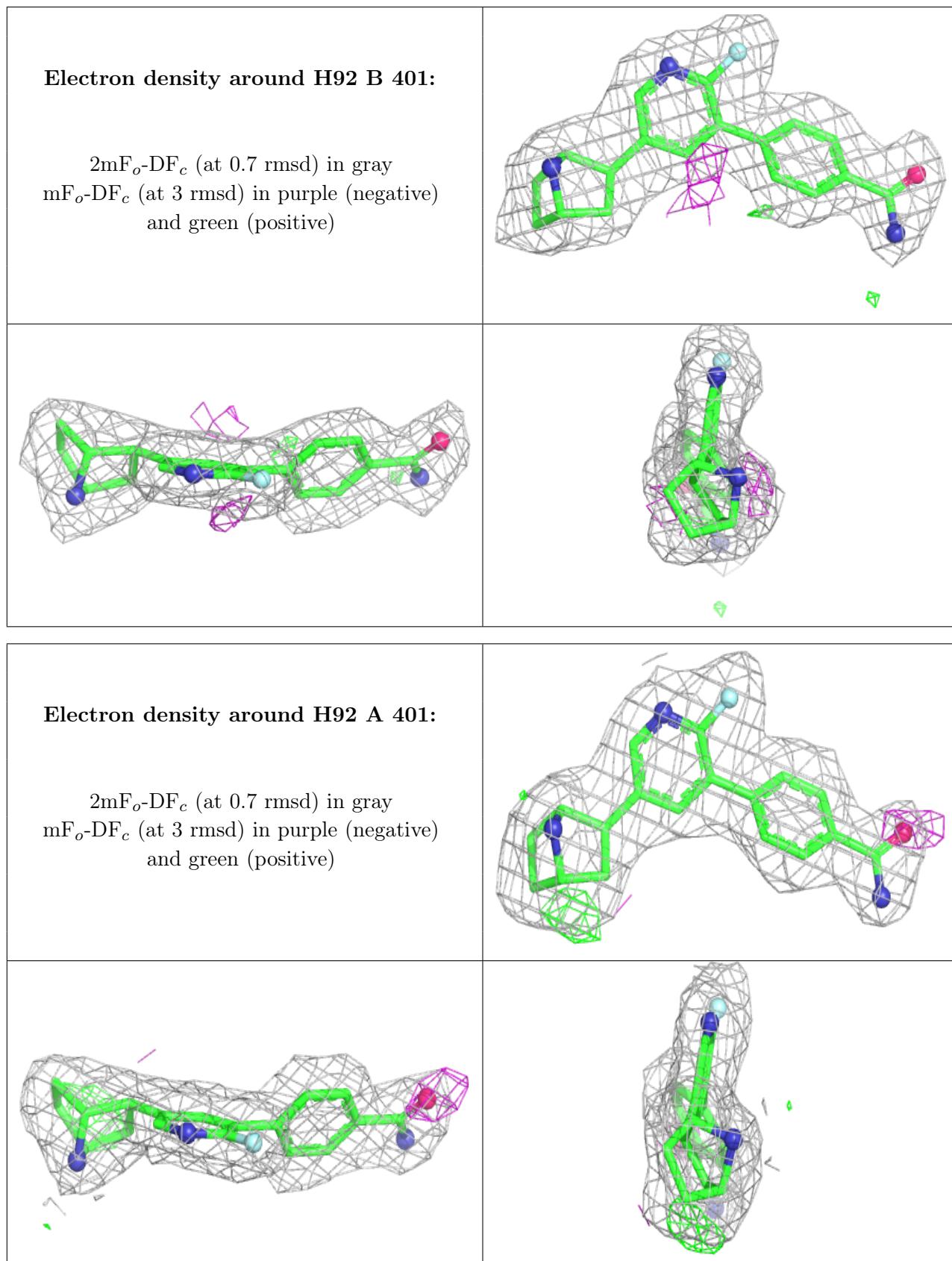


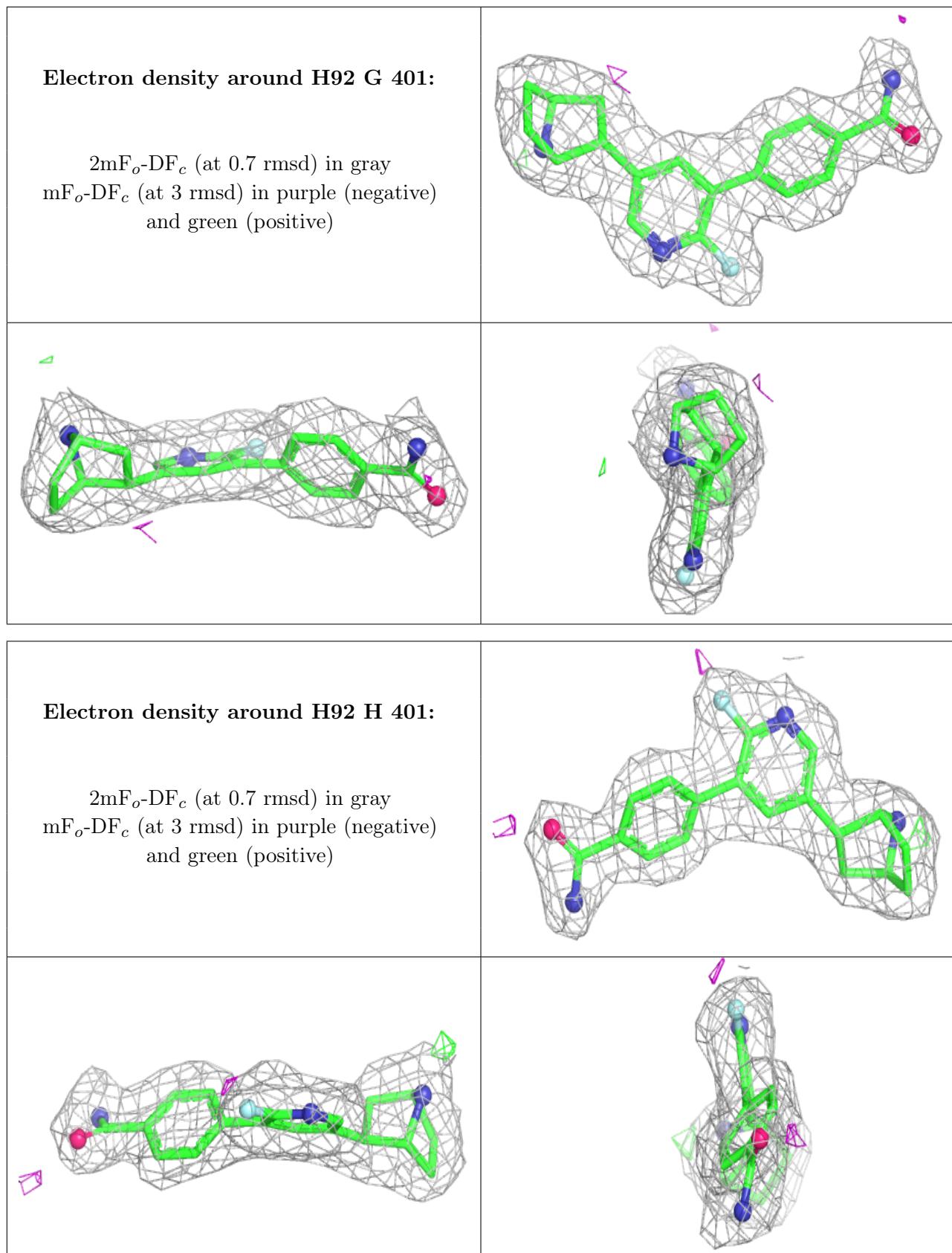


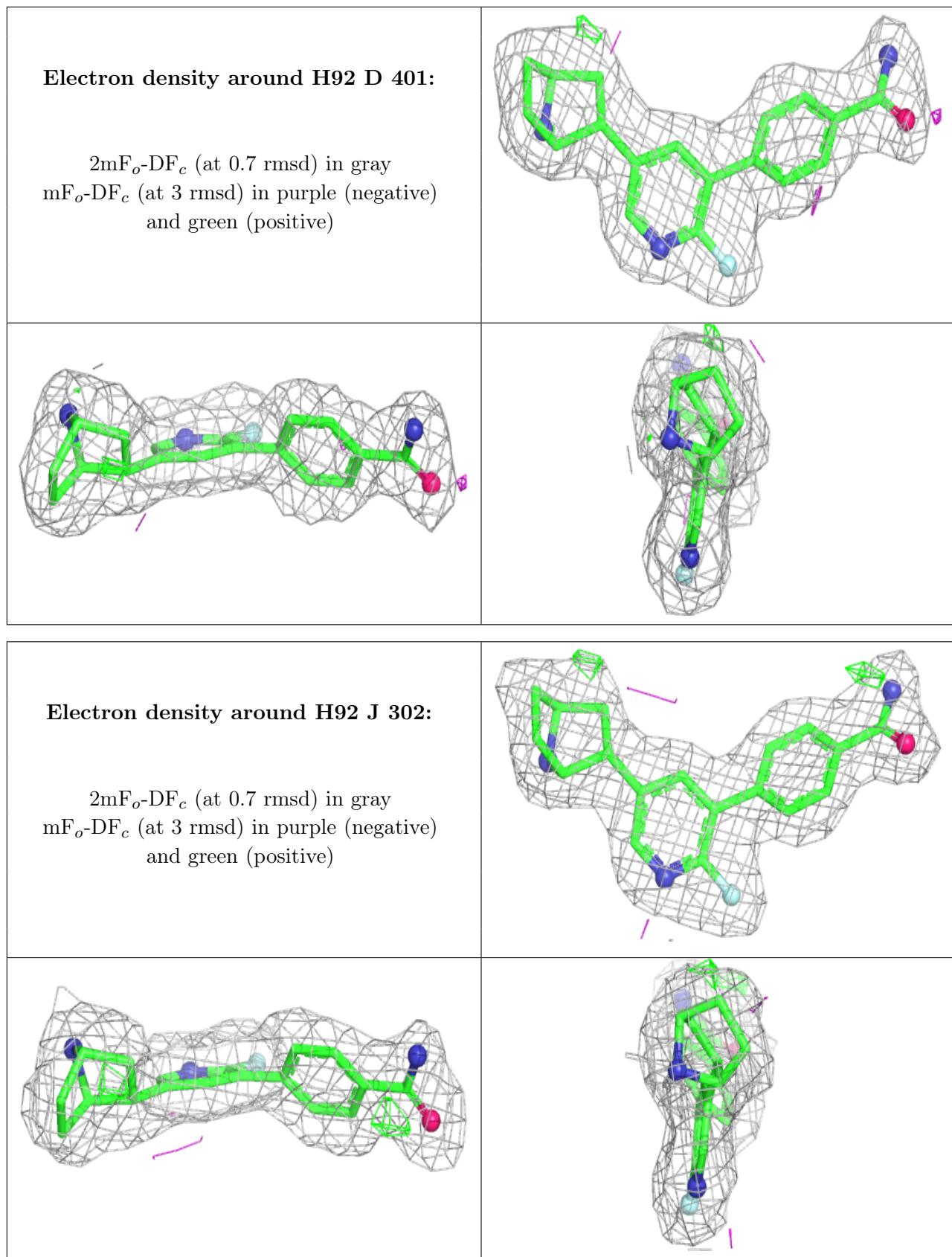












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.