



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 03:27 pm GMT

PDB ID : 8AMG  
Title : Crystal structure of AUGUGGCAU duplex with barium ions (model 1)  
Authors : Kiliszek, A.; Rypniewski, W.  
Deposited on : 2022-08-03  
Resolution : 2.26 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  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

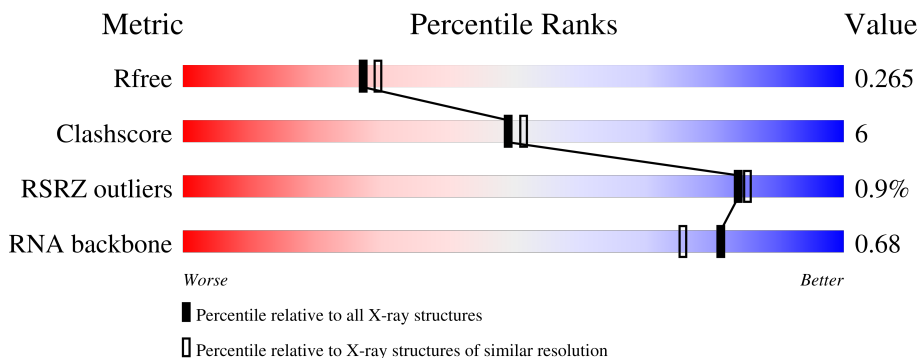
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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.





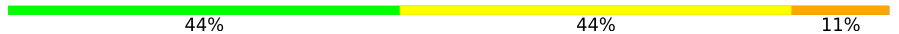
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)
RNA backbone	3102	1016 (2.66-1.86)

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	9	56% (Green), 44% (Yellow)
1	B	9	67% (Green), 33% (Yellow)
1	C	9	78% (Green), 22% (Yellow)
1	D	9	78% (Green), 11% (Yellow), 11% (Orange)
1	E	9	100% (Green)
1	F	9	89% (Green), 11% (Orange)

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Mol	Chain	Length	Quality of chain
1	G	9	 78% 22%
1	H	9	 56% 44%
1	I	9	 67% 22% 11%
1	J	9	 78% 22%
1	K	9	 11% 44% 44% 11%
1	L	9	 44% 44% 11%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2404 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 RNA chain called RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	B	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	C	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	D	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	E	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	F	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	G	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	H	9	Total	C	N	O	P	0	1	0
			213	96	39	69	9			
1	I	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	J	9	Total	C	N	O	P	0	1	0
			213	96	39	69	9			
1	K	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	L	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ba	0	0
			1	1		
2	B	1	Total	Ba	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Ba 2 2	0	0
2	E	2	Total Ba 2 2	0	0
2	H	2	Total Ba 2 2	0	0
2	I	1	Total Ba 1 1	0	0
2	J	1	Total Ba 1 1	0	0
2	K	2	Total Ba 2 2	0	0

- Molecule 3 is water.

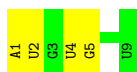
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	7	Total O 7 7	0	0
3	C	5	Total O 5 5	0	0
3	D	6	Total O 6 6	0	0
3	E	7	Total O 7 7	0	0
3	F	6	Total O 6 6	0	0
3	G	6	Total O 6 6	0	0
3	H	5	Total O 5 5	0	0
3	I	3	Total O 3 3	0	0
3	J	6	Total O 6 6	0	0
3	K	5	Total O 5 5	0	0
3	L	4	Total O 4 4	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: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain A:  56% 44%




- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain B:  67% 33%




- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain C:  78% 22%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain D:  78% 11% 11%




- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain E:  100%

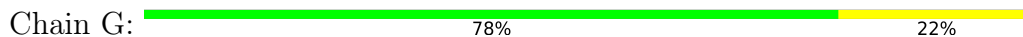
There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

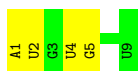
Chain F:  89% 11%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



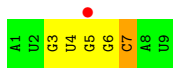
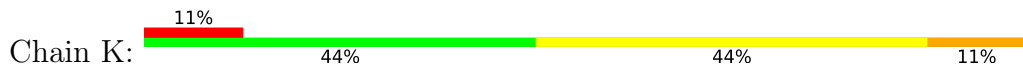
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.01Å 84.01Å 138.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.01 – 2.26 42.01 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.01-2.26) 95.6 (42.01-2.26)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.191 , 0.240 0.210 , 0.265	Depositor DCC
$R_{free}$ test set	708 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.115	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>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.24% 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: BA

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	0.63	0/212	1.19	1/329 (0.3%)
1	B	0.66	0/212	1.03	0/329
1	C	0.69	0/212	1.01	0/329
1	D	0.60	0/212	0.91	0/329
1	E	0.58	0/212	1.02	0/329
1	F	0.64	0/212	1.11	1/329 (0.3%)
1	G	0.65	0/212	1.28	3/329 (0.9%)
1	H	0.52	0/238	1.02	0/370
1	I	0.60	0/212	1.17	1/329 (0.3%)
1	J	0.48	0/238	1.07	0/370
1	K	0.58	0/212	0.93	0/329
1	L	0.54	0/212	1.15	1/329 (0.3%)
All	All	0.60	0/2596	1.08	7/4030 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	5	G	O4'-C1'-N9	5.96	112.97	108.20
1	G	5	G	C4-C5-N7	5.88	113.15	110.80
1	F	5	G	O4'-C1'-N9	5.86	112.89	108.20
1	G	5	G	N1-C6-O6	5.71	123.33	119.90
1	I	3	G	N1-C6-O6	5.69	123.31	119.90
1	G	5	G	C6-C5-N7	-5.28	127.23	130.40
1	A	4	U	C6-N1-C2	-5.04	117.98	121.00

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	190	0	98	1	0
1	B	190	0	98	3	0
1	C	190	0	98	1	0
1	D	190	0	98	1	0
1	E	190	0	98	0	0
1	F	190	0	98	1	0
1	G	190	0	98	1	0
1	H	213	0	109	2	1
1	I	190	0	98	1	0
1	J	213	0	109	1	0
1	K	190	0	98	5	0
1	L	190	0	98	3	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
3	A	6	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	0	0
3	E	7	0	0	0	0
3	F	6	0	0	1	0
3	G	6	0	0	0	0
3	H	5	0	0	0	0
3	I	3	0	0	0	0
3	J	6	0	0	0	0
3	K	5	0	0	0	0
3	L	4	0	0	0	0
All	All	2404	0	1198	18	1

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.

All (18) 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:K:4:U:H2'	1:K:5:G:C8	2.21	0.76
1:L:7:C:H2'	1:L:8:A:H8	1.62	0.63
1:K:4:U:H2'	1:K:5:G:H8	1.71	0.56
1:B:1:A:H4'	1:L:9:U:H3'	1.92	0.50
1:B:9:U:H4'	1:G:3:G:H4'	1.92	0.49
1:F:5:G:N1	3:F:101:HOH:O	2.27	0.47
1:C:4:U:H2'	1:C:5:G:C8	2.50	0.46
1:J:4:U:H2'	1:J:5[B]:G:C8	2.51	0.46
1:B:1:A:H2'	1:B:2:U:C6	2.50	0.46
1:K:6:G:H2'	1:K:7:C:C6	2.51	0.44
1:K:5:G:O2'	1:K:6:G:H5'	2.17	0.44
1:L:7:C:H2'	1:L:8:A:C8	2.50	0.43
1:H:4:U:H2'	1:H:5[B]:G:C8	2.53	0.42
1:K:3:G:C6	1:K:4:U:N3	2.87	0.42
1:H:1:A:H2'	1:H:2:U:C6	2.54	0.41
1:I:3:G:C6	1:I:4:U:C4	3.08	0.41
1:D:5:G:H5''	1:D:5:G:N3	2.36	0.41
1:A:1:A:H2'	1:A:2:U:C6	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5[A]:G:O2'	1:L:9:U:O2'[12_554]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	8/9 (88%)	1 (12%)	0
1	B	8/9 (88%)	0	0
1	C	8/9 (88%)	0	0
1	D	8/9 (88%)	2 (25%)	0
1	E	8/9 (88%)	0	0
1	F	8/9 (88%)	0	0
1	G	8/9 (88%)	0	0
1	H	7/9 (77%)	0	0
1	I	8/9 (88%)	1 (12%)	0
1	J	7/9 (77%)	0	0
1	K	8/9 (88%)	1 (12%)	0
1	L	8/9 (88%)	2 (25%)	0
All	All	94/108 (87%)	7 (7%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	D	5	G
1	D	6	G
1	I	6	G
1	K	7	C
1	L	6	G
1	L	9	U

There are no RNA pucker outliers to report.

## 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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	9/9 (100%)	-0.17	0 <a href="#">100</a> <a href="#">100</a>	36, 39, 51, 56	0
1	B	9/9 (100%)	-0.03	0 <a href="#">100</a> <a href="#">100</a>	40, 42, 61, 61	0
1	C	9/9 (100%)	-0.23	0 <a href="#">100</a> <a href="#">100</a>	37, 40, 46, 47	0
1	D	9/9 (100%)	-0.05	0 <a href="#">100</a> <a href="#">100</a>	38, 48, 52, 54	0
1	E	9/9 (100%)	-0.15	0 <a href="#">100</a> <a href="#">100</a>	37, 41, 44, 45	0
1	F	9/9 (100%)	-0.22	0 <a href="#">100</a> <a href="#">100</a>	34, 41, 48, 48	0
1	G	9/9 (100%)	-0.28	0 <a href="#">100</a> <a href="#">100</a>	41, 44, 46, 47	0
1	H	9/9 (100%)	-0.32	0 <a href="#">100</a> <a href="#">100</a>	42, 44, 47, 47	0
1	I	9/9 (100%)	0.27	0 <a href="#">100</a> <a href="#">100</a>	48, 54, 59, 60	0
1	J	9/9 (100%)	0.13	0 <a href="#">100</a> <a href="#">100</a>	44, 52, 54, 54	0
1	K	9/9 (100%)	0.62	1 (11%) <a href="#">5</a> <a href="#">5</a>	53, 62, 65, 67	0
1	L	9/9 (100%)	0.22	0 <a href="#">100</a> <a href="#">100</a>	41, 46, 61, 64	0
All	All	108/108 (100%)	-0.02	1 (0%) <a href="#">84</a> <a href="#">85</a>	34, 46, 62, 67	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	5	G	2.1

### 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](#)

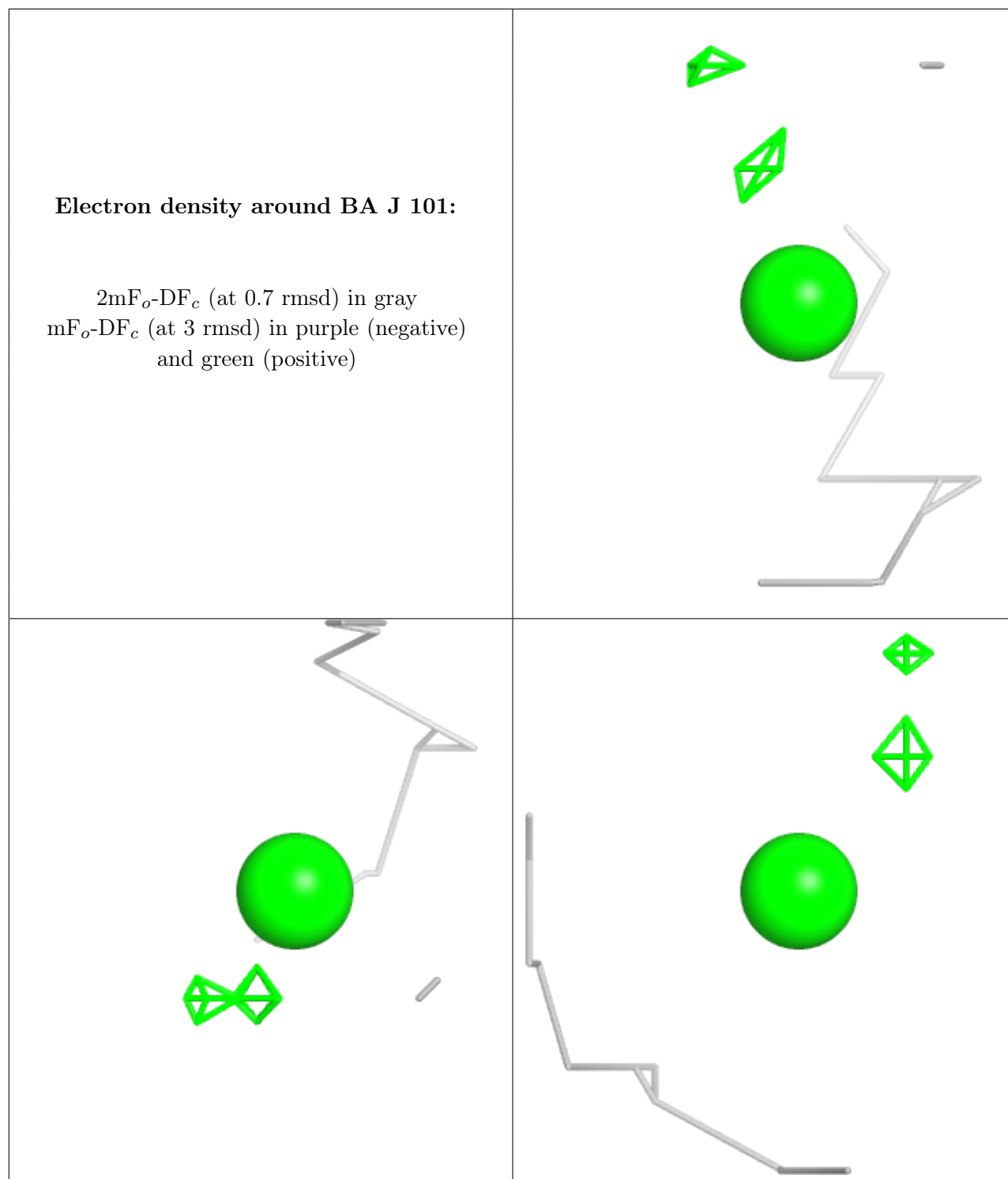
There are no monosaccharides in this entry.

## 6.4 Ligands

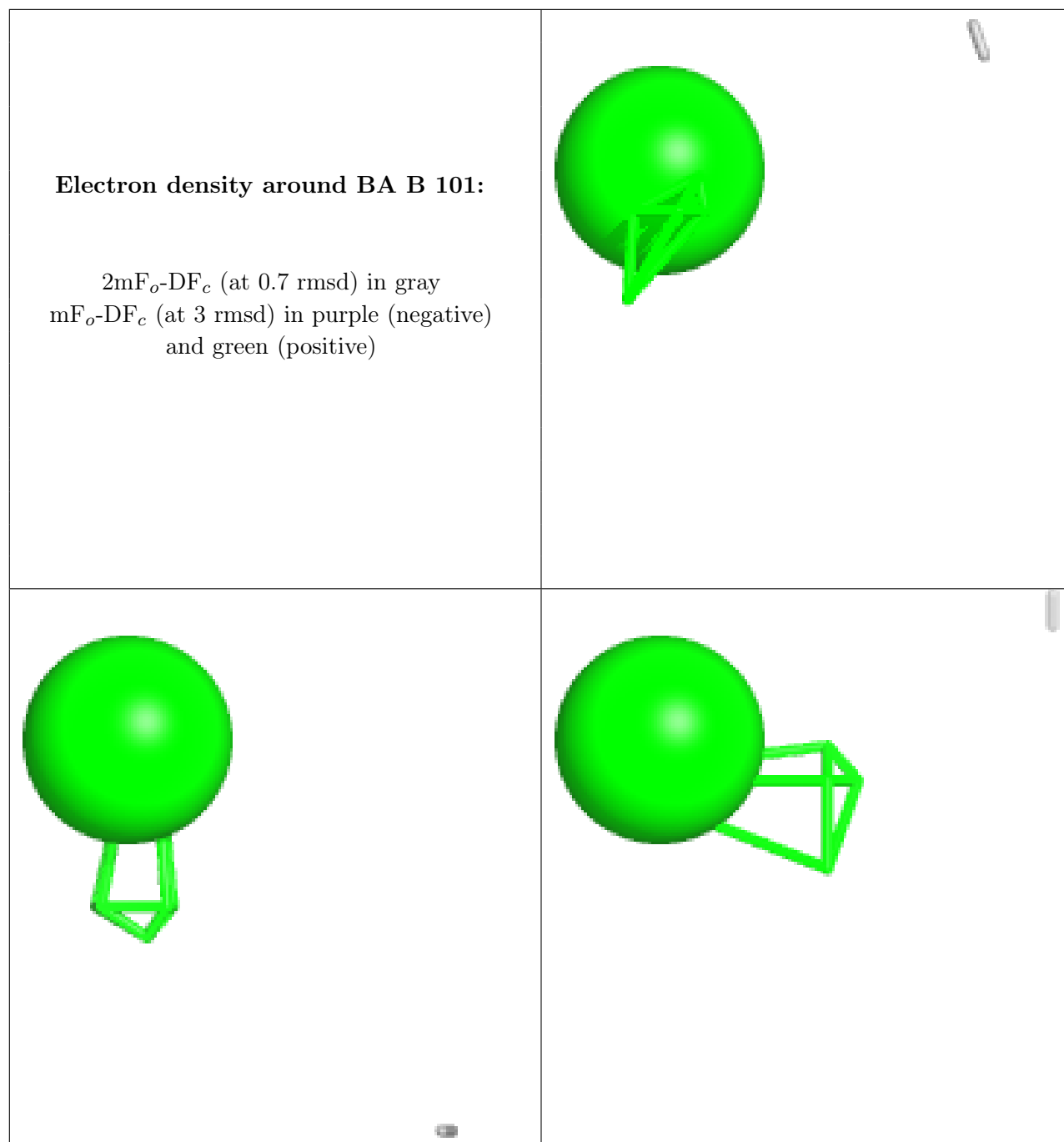
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

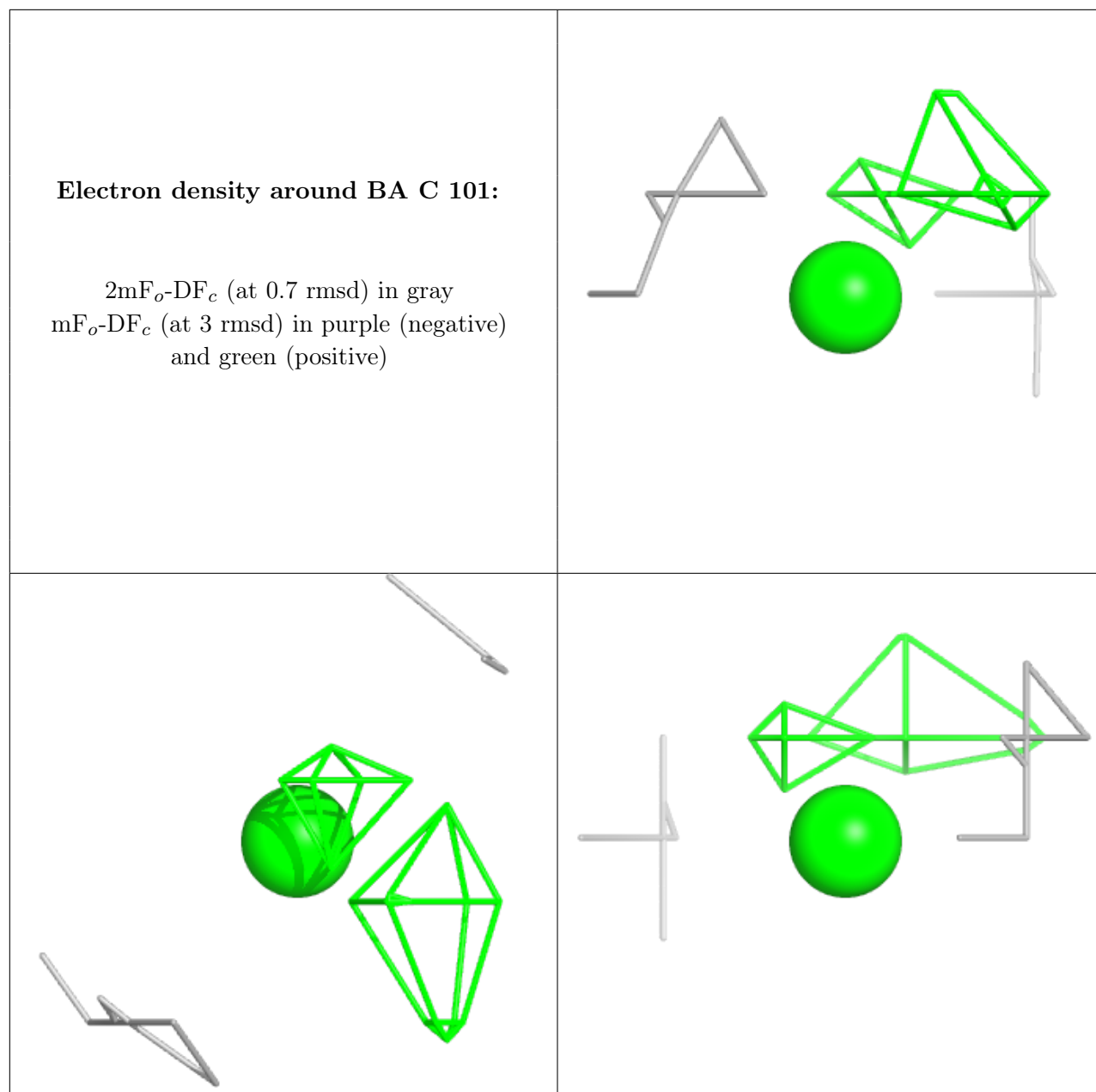
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BA	J	101	1/1	0.99	0.18	55,55,55,55	0
2	BA	B	101	1/1	1.00	0.20	46,46,46,46	0
2	BA	C	101	1/1	1.00	0.19	60,60,60,60	0
2	BA	C	102	1/1	1.00	0.16	56,56,56,56	0
2	BA	E	101	1/1	1.00	0.18	46,46,46,46	0
2	BA	E	102	1/1	1.00	0.20	45,45,45,45	0
2	BA	H	101	1/1	1.00	0.18	47,47,47,47	0
2	BA	H	102	1/1	1.00	0.18	51,51,51,51	0
2	BA	I	101	1/1	1.00	0.16	52,52,52,52	0
2	BA	A	101	1/1	1.00	0.18	44,44,44,44	0
2	BA	K	101	1/1	1.00	0.18	55,55,55,55	0
2	BA	K	102	1/1	1.00	0.17	55,55,55,55	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.





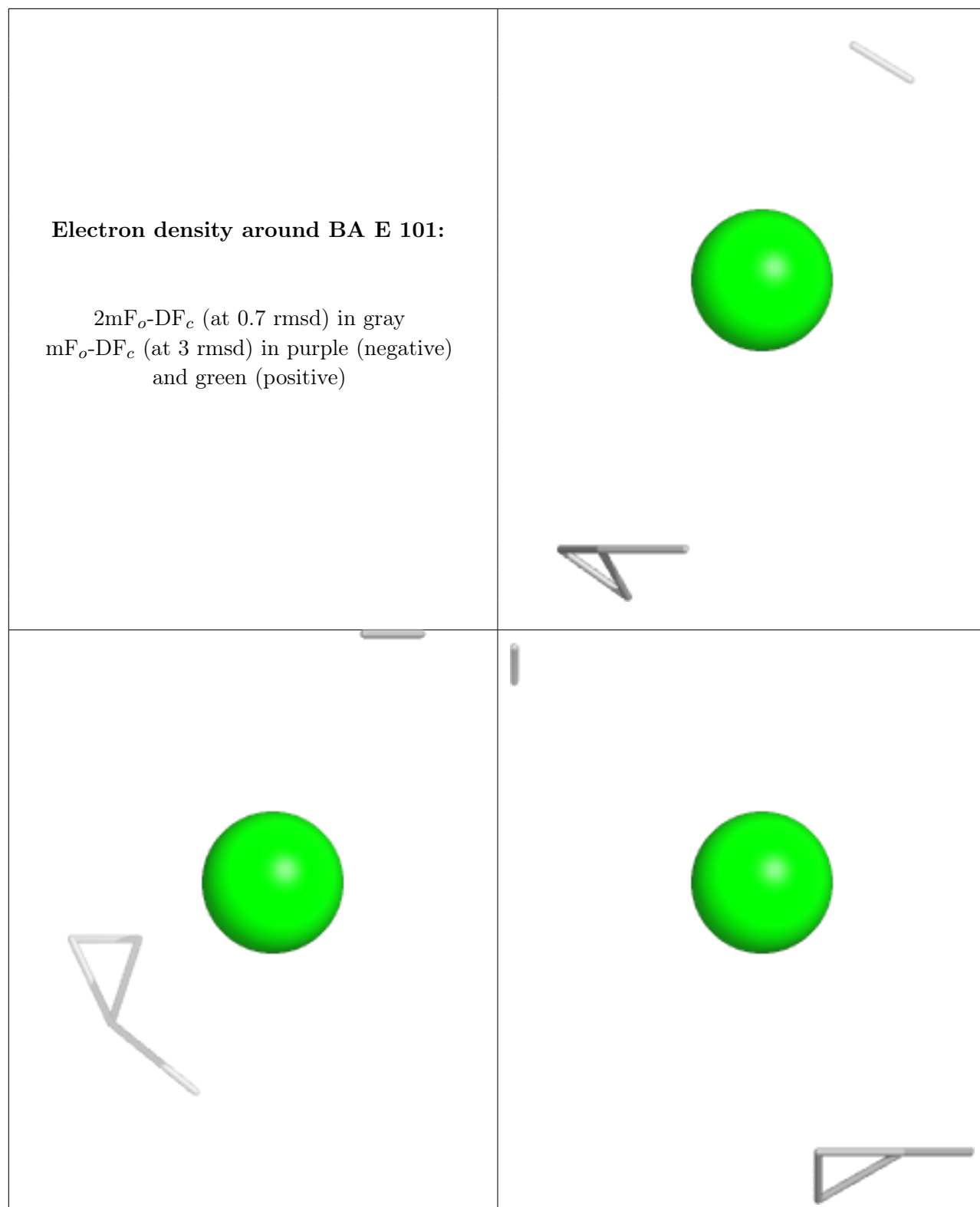


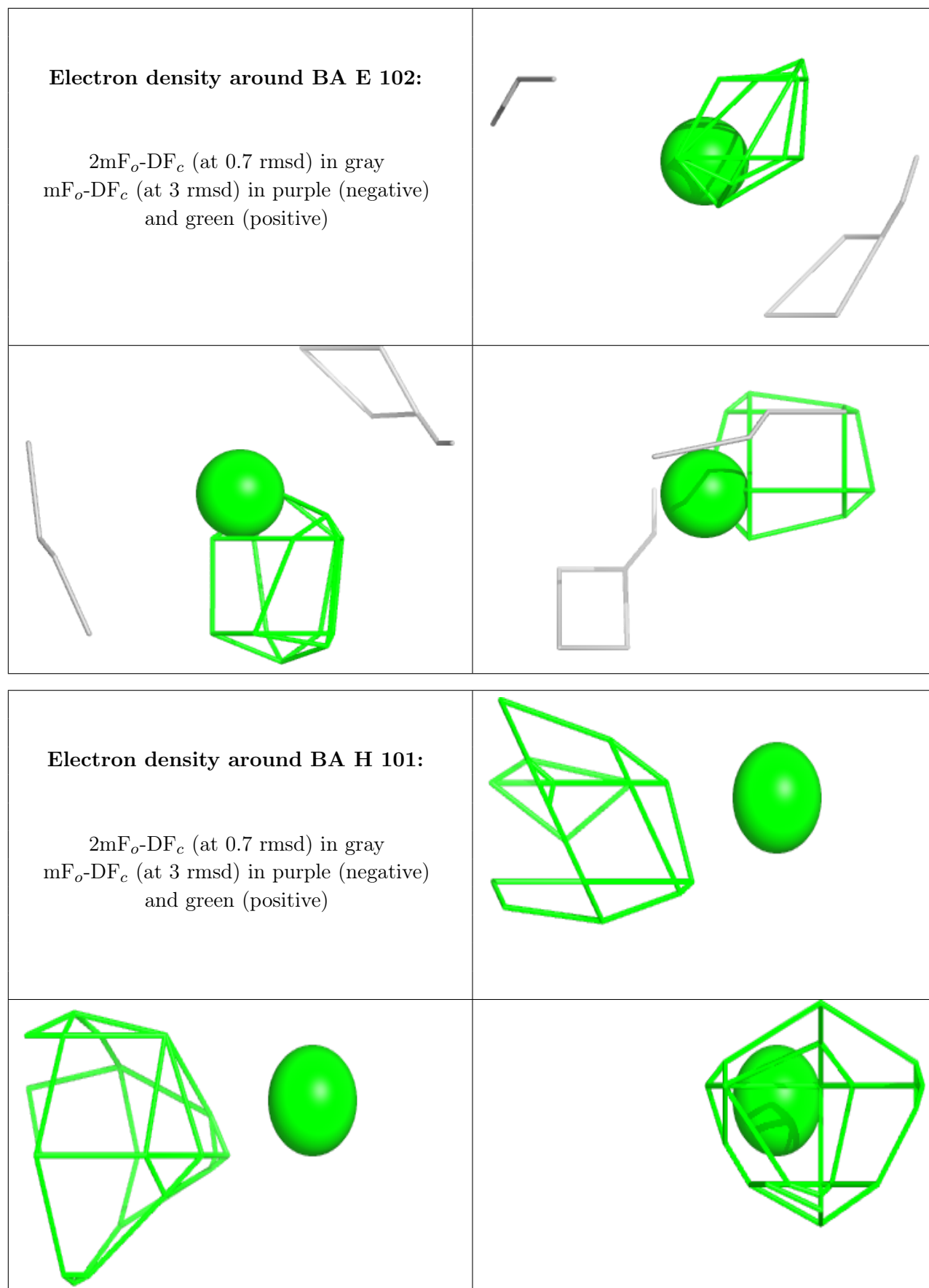


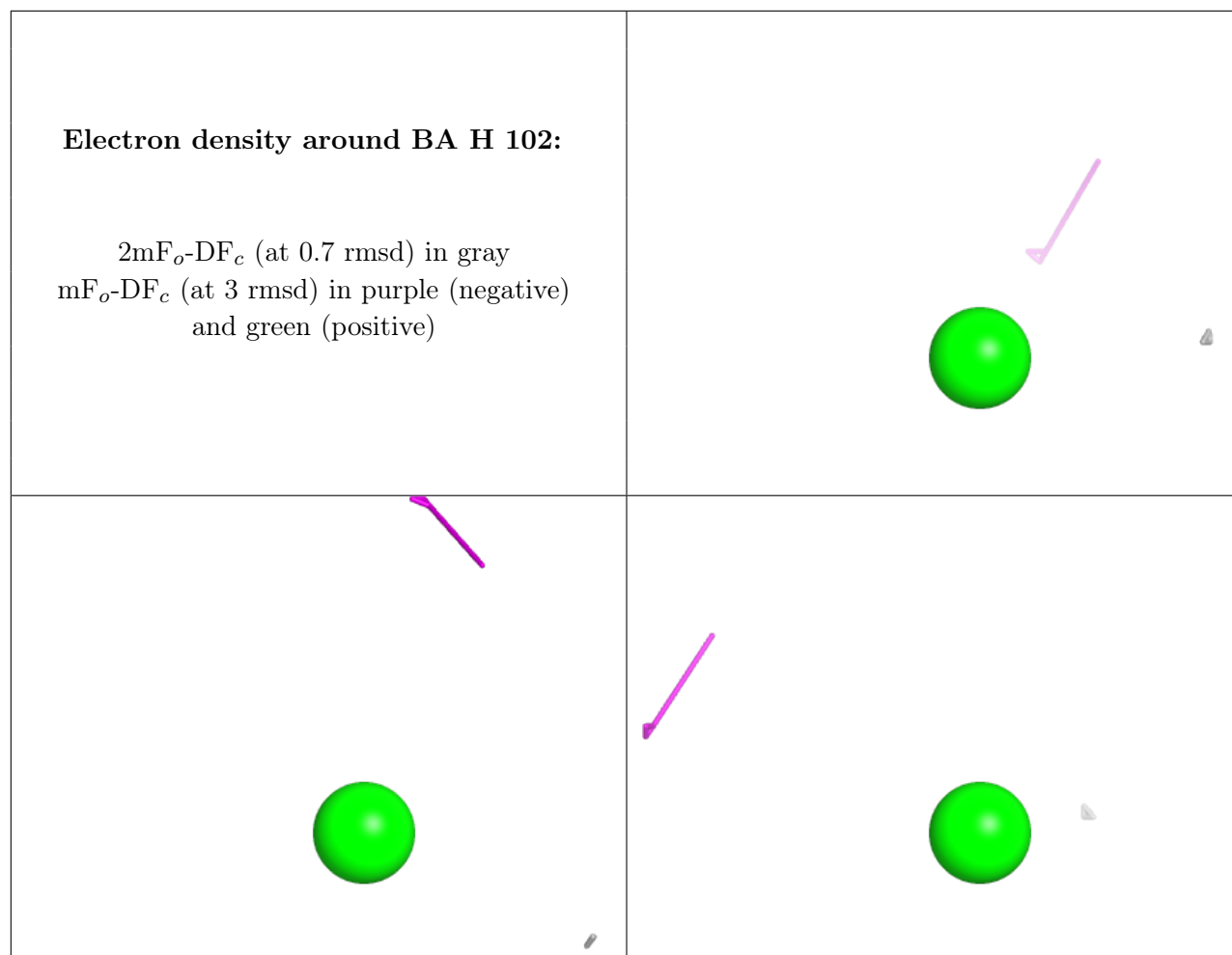
**Electron density around BA C 102:**

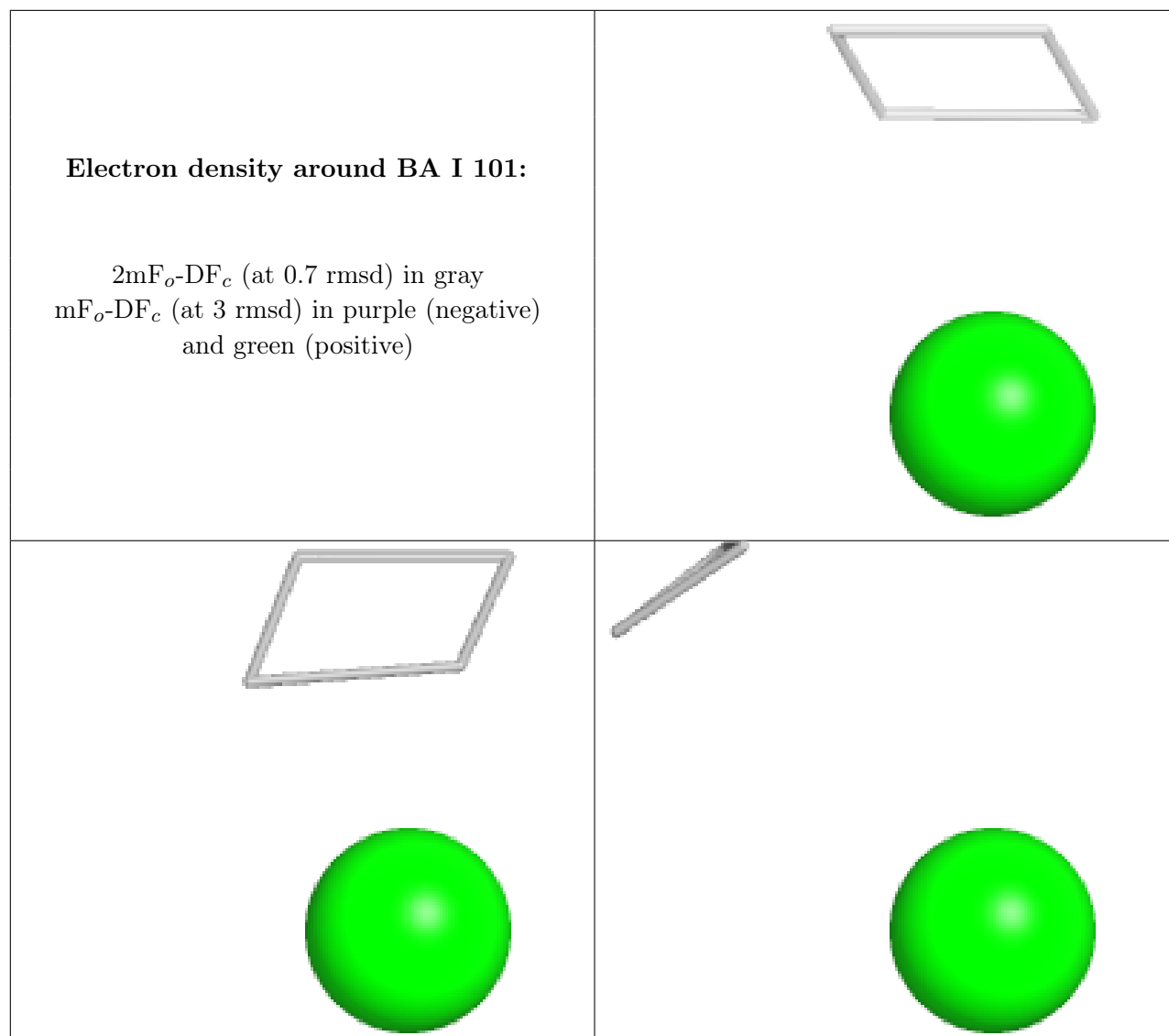
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

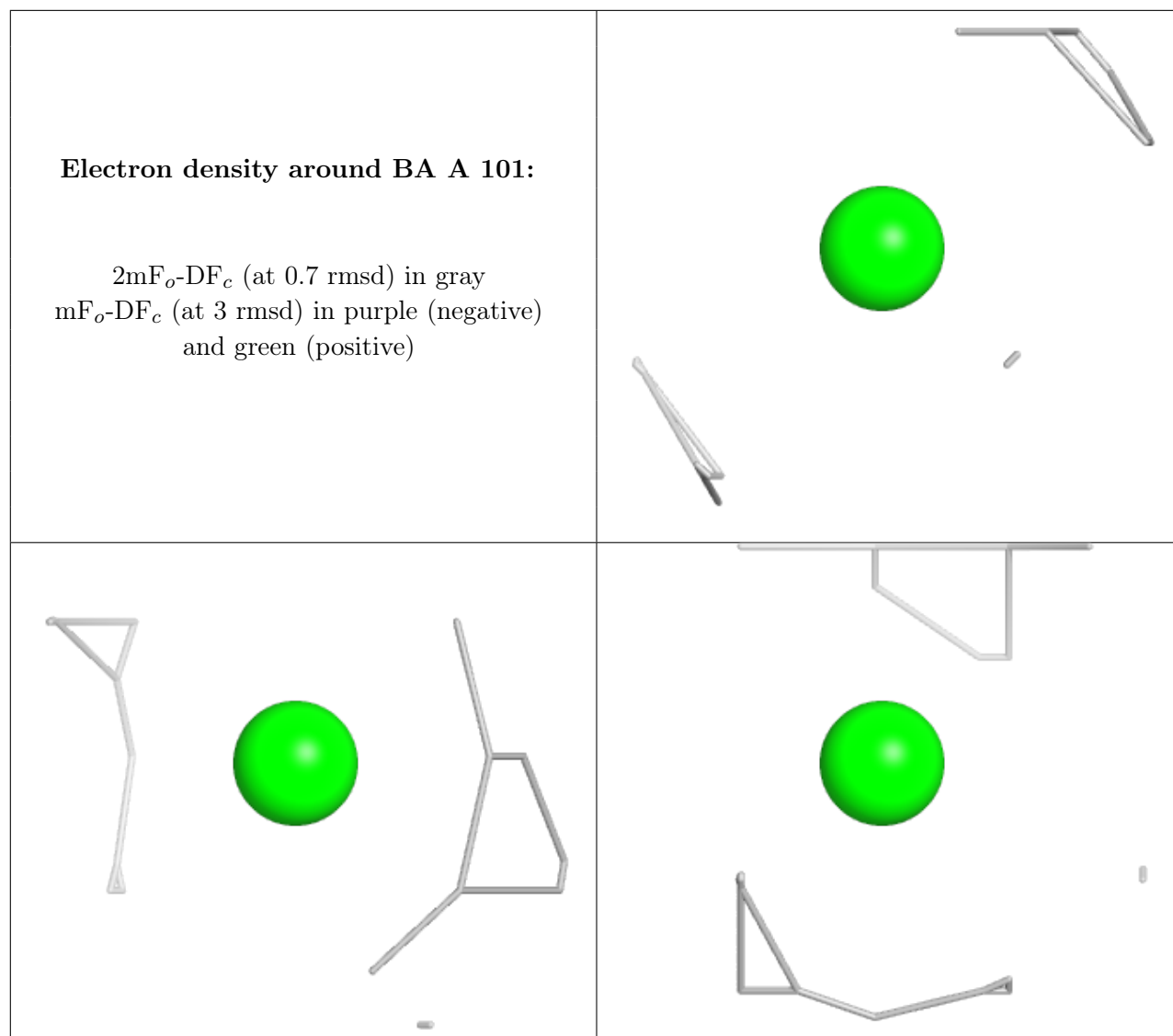




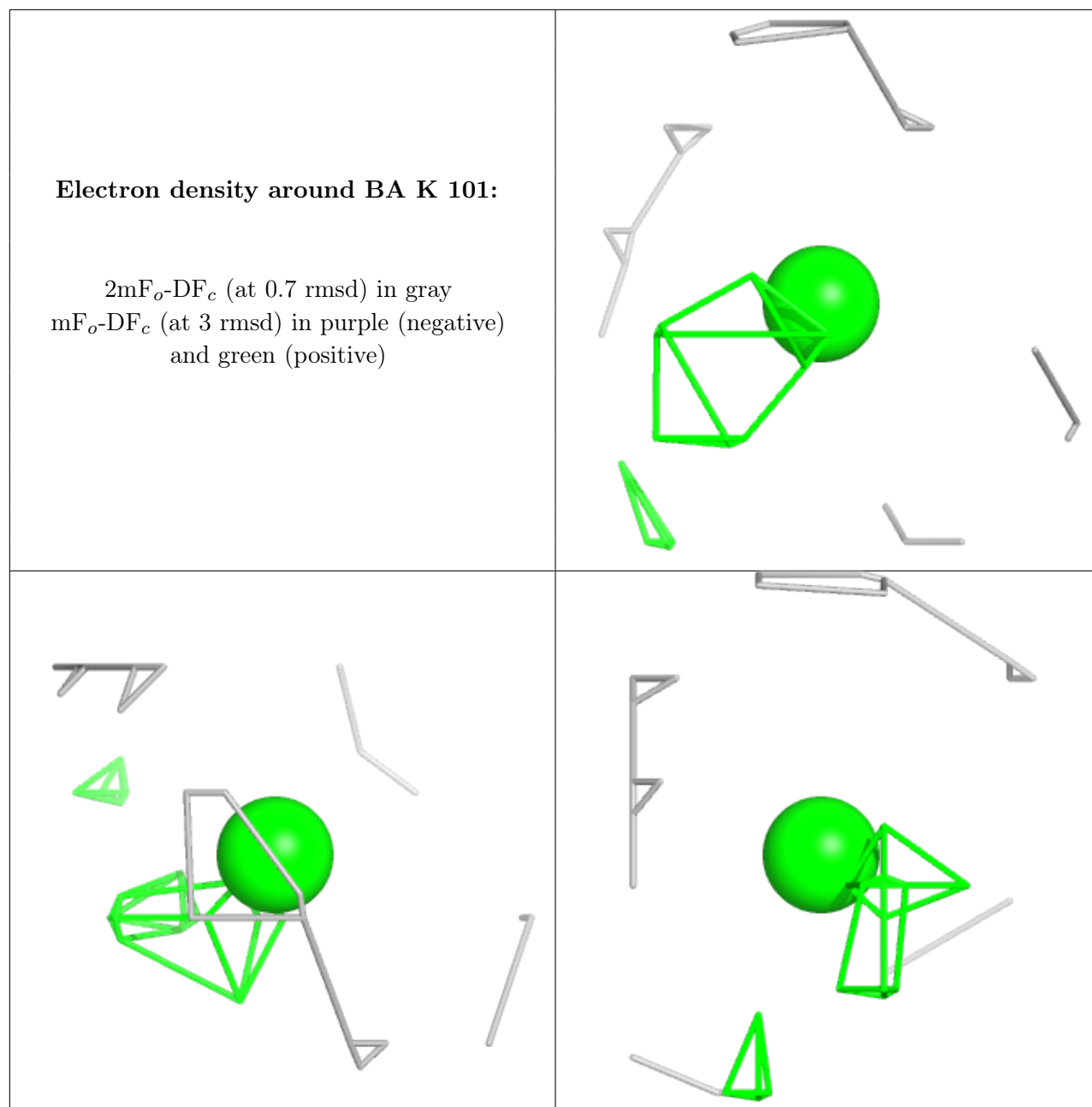


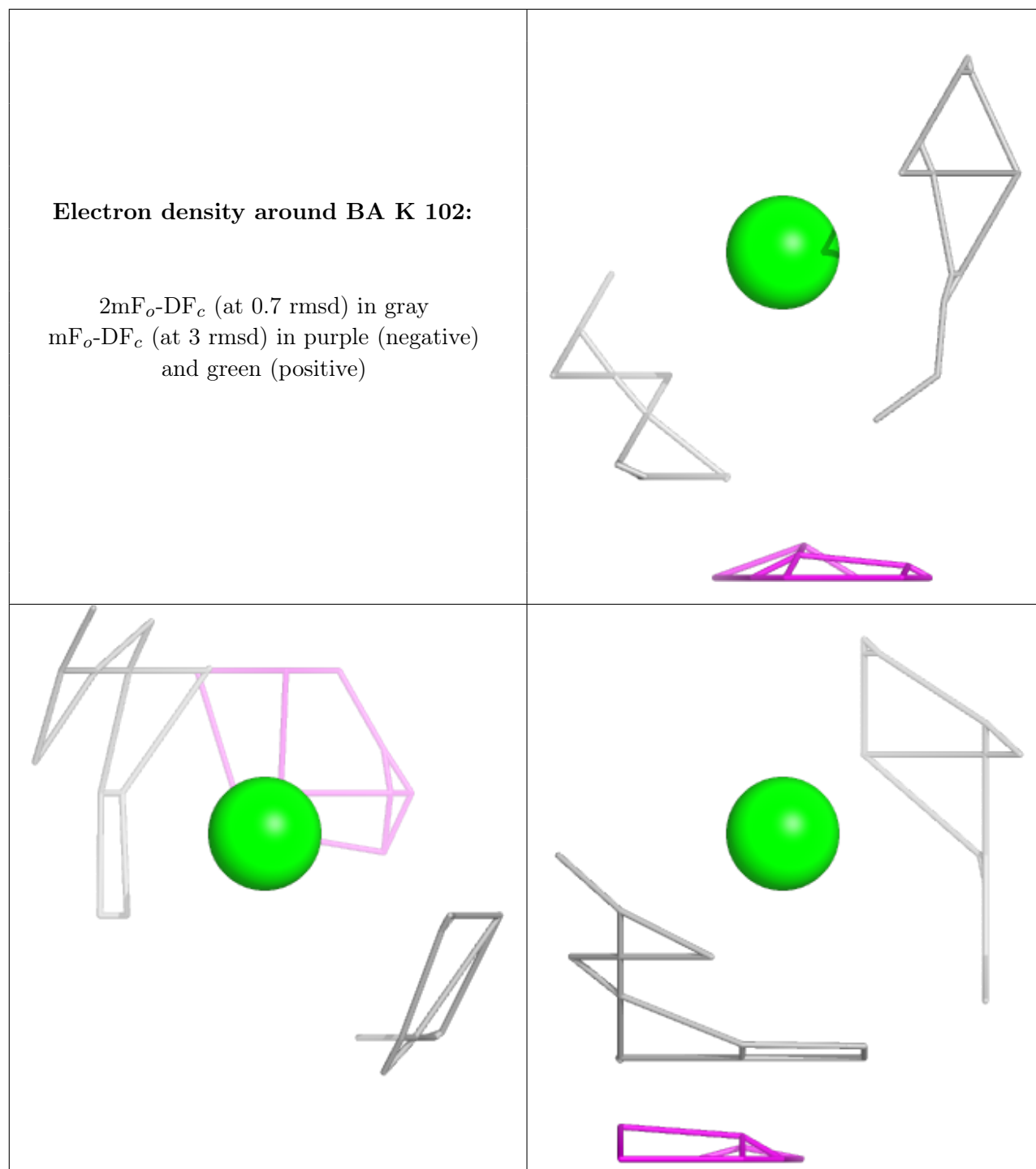












## 6.5 Other polymers [i](#)

There are no such residues in this entry.