Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 03:27 pm GMT

PDB ID	:	8AMM
Title	:	Crystal structure of AUGUGGCAU duplex with cesium ions
Authors	:	Kiliszek, A.; Rypniewski, W.
Deposited on	:	2022-08-03
Resolution	:	2.86 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

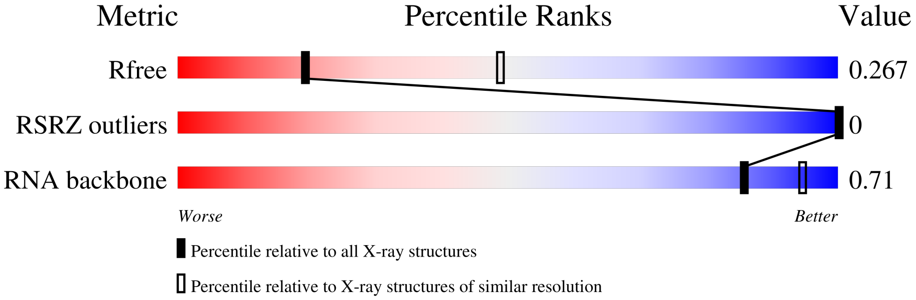
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

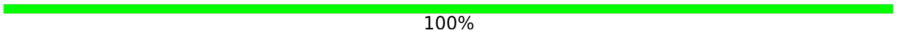
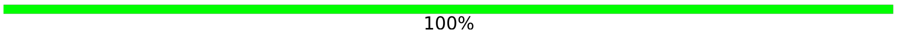
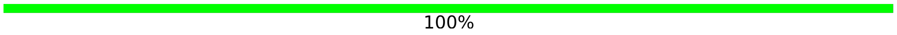
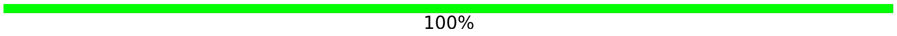
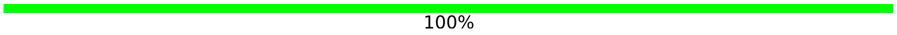
The reported resolution of this entry is 2.86 Å.

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	3168 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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	9	
1	B	9	
1	C	9	
1	D	9	
1	E	9	
1	F	9	
1	G	9	
1	H	9	

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Mol	Chain	Length	Quality of chain
1	I	9	89% 11%
1	J	9	100%
1	K	9	100%
1	L	9	89% 11%
1	M	9	89% 11%
1	N	9	89% 11%
1	O	9	89% 11%
1	P	9	89% 11%
1	Q	9	89% 11%
1	R	9	100%
1	S	9	78% 22%
1	T	9	89% 11%
1	U	9	89% 11%
1	V	9	100%
1	Y	9	89% 11%
1	Z	9	100%
1	a	9	100%
1	b	9	89% 11%
1	c	9	100%
1	d	9	100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5371 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 190 86 34 62 8	0	0	0
1	B	9	Total C N O P 190 86 34 62 8	0	0	0
1	C	9	Total C N O P 190 86 34 62 8	0	0	0
1	D	9	Total C N O P 190 86 34 62 8	0	0	0
1	E	9	Total C N O P 190 86 34 62 8	0	0	0
1	F	9	Total C N O P 190 86 34 62 8	0	0	0
1	G	9	Total C N O P 190 86 34 62 8	0	0	0
1	H	9	Total C N O P 190 86 34 62 8	0	0	0
1	I	9	Total C N O P 190 86 34 62 8	0	0	0
1	J	9	Total C N O P 190 86 34 62 8	0	0	0
1	K	9	Total C N O P 190 86 34 62 8	0	0	0
1	L	9	Total C N O P 190 86 34 62 8	0	0	0
1	M	9	Total C N O P 190 86 34 62 8	0	0	0
1	N	9	Total C N O P 190 86 34 62 8	0	0	0
1	O	9	Total C N O P 190 86 34 62 8	0	0	0
1	P	9	Total C N O P 190 86 34 62 8	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Q	9	Total C N O P 190 86 34 62 8	0	0	0
1	R	9	Total C N O P 190 86 34 62 8	0	0	0
1	S	9	Total C N O P 190 86 34 62 8	0	0	0
1	T	9	Total C N O P 190 86 34 62 8	0	0	0
1	U	9	Total C N O P 190 86 34 62 8	0	0	0
1	V	9	Total C N O P 190 86 34 62 8	0	0	0
1	Y	9	Total C N O P 190 86 34 62 8	0	0	0
1	Z	9	Total C N O P 213 96 39 69 9	0	1	0
1	a	9	Total C N O P 190 86 34 62 8	0	0	0
1	b	9	Total C N O P 190 86 34 62 8	0	0	0
1	c	9	Total C N O P 190 86 34 62 8	0	0	0
1	d	9	Total C N O P 190 86 34 62 8	0	0	0

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cs 2 2	0	0
2	C	2	Total Cs 2 2	0	0
2	E	2	Total Cs 2 2	0	0
2	G	2	Total Cs 2 2	0	0
2	I	2	Total Cs 2 2	0	0
2	K	2	Total Cs 2 2	0	0
2	M	1	Total Cs 1 1	0	0

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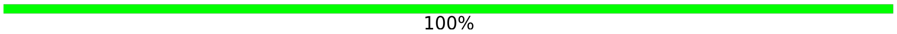
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	1	Total Cs 1 1	0	0
2	O	2	Total Cs 2 2	0	0
2	Q	2	Total Cs 2 2	0	0
2	S	1	Total Cs 1 1	0	0
2	T	1	Total Cs 1 1	0	0
2	U	2	Total Cs 2 2	0	0
2	Y	2	Total Cs 2 2	0	0
2	a	1	Total Cs 1 1	0	0
2	b	1	Total Cs 1 1	0	0
2	c	2	Total Cs 2 2	0	0

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

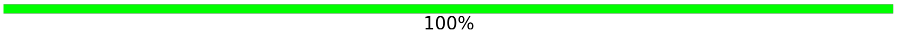
Chain A:



There are no outlier residues recorded for this chain.

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

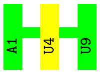
Chain B:



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 C:



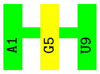
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain D:

There are no outlier residues recorded for this chain.

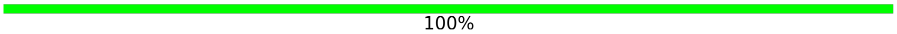
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain E:



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

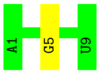
Chain F:



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 G:



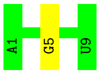
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain H:

There are no outlier residues recorded for this chain.

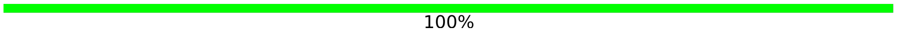
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain I:



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

Chain J:



There are no outlier residues recorded for this chain.

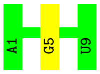
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain K:

There are no outlier residues recorded for this chain.

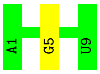
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain L:



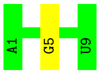
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain M:



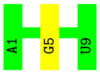
- Molecule 1: RNA (5’-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3’)

Chain N:



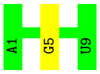
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain O:



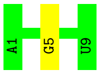
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain P:



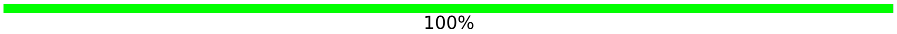
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain Q:



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

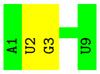
Chain R:



There are no outlier residues recorded for this chain.

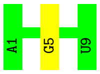
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain S:



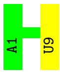
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain T:



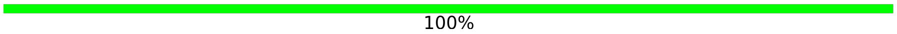
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain U:



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

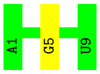
Chain V:



There are no outlier residues recorded for this chain.

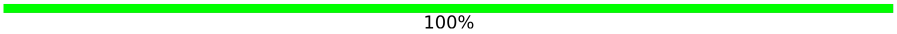
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain Y:



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

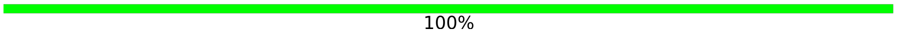
Chain Z:



There are no outlier residues recorded for this chain.

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

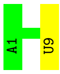
Chain a:



There are no outlier residues recorded for this chain.

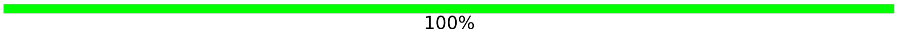
- Molecule 1: RNA (5'-R(*AP*UP*GP*UP*GP*GP*CP*AP*U)-3')

Chain b:



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

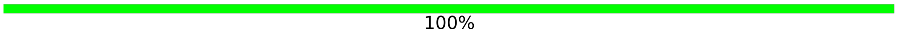
Chain c:



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 d:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	28.23Å 90.61Å 139.93Å 90.00° 91.43° 90.00°	Depositor
Resolution (Å)	45.31 – 2.86 45.31 – 2.86	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.31-2.86) 96.9 (45.31-2.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.221 , 0.269 0.216 , 0.267	Depositor DCC
R_{free} test set	954 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å^2)	85.8	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CS

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	0.27	0/212	1.01	0/329
1	B	0.24	0/212	0.74	0/329
1	C	0.20	0/212	0.72	0/329
1	D	0.18	0/212	0.69	0/329
1	E	0.17	0/212	0.74	0/329
1	F	0.21	0/212	0.78	0/329
1	G	0.19	0/212	0.74	0/329
1	H	0.17	0/212	0.72	0/329
1	I	0.29	0/212	1.00	2/329 (0.6%)
1	J	0.21	0/212	0.72	0/329
1	K	0.19	0/212	0.70	0/329
1	L	0.19	0/212	0.74	0/329
1	M	0.19	0/212	0.73	0/329
1	N	0.19	0/212	0.72	0/329
1	O	0.18	0/212	0.75	0/329
1	P	0.17	0/212	0.72	0/329
1	Q	0.18	0/212	0.77	0/329
1	R	0.17	0/212	0.73	0/329
1	S	0.19	0/212	0.77	0/329
1	T	0.17	0/212	0.72	0/329
1	U	0.19	0/212	0.74	0/329
1	V	0.21	0/212	0.88	0/329
1	Y	0.16	0/212	0.72	0/329
1	Z	0.20	0/238	0.77	0/370
1	a	0.21	0/212	0.77	0/329
1	b	0.26	0/212	0.92	0/329
1	c	0.16	0/212	0.73	0/329
1	d	0.18	0/212	0.77	0/329
All	All	0.20	0/5962	0.77	2/9253 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	5	G	O4'-C1'-N9	5.29	112.43	108.20
1	I	5	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	8/9 (88%)	0	0
1	B	8/9 (88%)	0	0
1	C	8/9 (88%)	1 (12%)	0
1	D	8/9 (88%)	0	0
1	E	8/9 (88%)	1 (12%)	0
1	F	8/9 (88%)	0	0
1	G	8/9 (88%)	1 (12%)	0
1	H	8/9 (88%)	0	0
1	I	8/9 (88%)	0	0
1	J	8/9 (88%)	0	0
1	K	8/9 (88%)	0	0
1	L	8/9 (88%)	1 (12%)	0
1	M	8/9 (88%)	1 (12%)	0
1	N	8/9 (88%)	1 (12%)	0
1	O	8/9 (88%)	1 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	8/9 (88%)	1 (12%)	0
1	Q	8/9 (88%)	1 (12%)	0
1	R	8/9 (88%)	0	0
1	S	8/9 (88%)	2 (25%)	0
1	T	8/9 (88%)	1 (12%)	0
1	U	8/9 (88%)	1 (12%)	0
1	V	8/9 (88%)	0	0
1	Y	8/9 (88%)	1 (12%)	0
1	Z	7/9 (77%)	0	0
1	a	8/9 (88%)	0	0
1	b	8/9 (88%)	1 (12%)	0
1	c	8/9 (88%)	0	0
1	d	8/9 (88%)	0	0
All	All	223/252 (88%)	15 (6%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	4	U
1	E	5	G
1	G	5	G
1	L	5	G
1	M	5	G
1	N	5	G
1	O	5	G
1	P	5	G
1	Q	5	G
1	S	2	U
1	S	3	G
1	T	5	G
1	U	9	U
1	Y	5	G
1	b	9	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 28 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

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^{th} 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^2)	Q<0.9
1	A	9/9 (100%)	-0.51	0 100 100	53, 63, 70, 75	0
1	B	9/9 (100%)	-0.24	0 100 100	61, 64, 67, 68	0
1	C	9/9 (100%)	-0.32	0 100 100	72, 75, 80, 89	0
1	D	9/9 (100%)	-0.49	0 100 100	64, 72, 82, 87	0
1	E	9/9 (100%)	-0.55	0 100 100	64, 86, 90, 91	0
1	F	9/9 (100%)	-0.52	0 100 100	59, 72, 86, 86	0
1	G	9/9 (100%)	-0.62	0 100 100	62, 67, 90, 93	0
1	H	9/9 (100%)	-0.56	0 100 100	57, 63, 84, 87	0
1	I	9/9 (100%)	-0.61	0 100 100	65, 72, 78, 81	0
1	J	9/9 (100%)	-0.62	0 100 100	62, 66, 73, 76	0
1	K	9/9 (100%)	-0.57	0 100 100	54, 74, 89, 92	0
1	L	9/9 (100%)	-0.43	0 100 100	55, 68, 88, 91	0
1	M	9/9 (100%)	-0.31	0 100 100	62, 67, 73, 81	0
1	N	9/9 (100%)	-0.41	0 100 100	59, 67, 94, 99	0
1	O	9/9 (100%)	-0.62	0 100 100	104, 112, 121, 123	0
1	P	9/9 (100%)	-0.54	0 100 100	94, 104, 115, 116	0
1	Q	9/9 (100%)	-0.22	0 100 100	66, 94, 117, 118	0
1	R	9/9 (100%)	-0.19	0 100 100	61, 87, 120, 120	0
1	S	9/9 (100%)	-0.06	0 100 100	90, 102, 114, 118	0
1	T	9/9 (100%)	-0.35	0 100 100	65, 97, 122, 127	0
1	U	9/9 (100%)	-0.39	0 100 100	95, 128, 136, 137	0
1	V	9/9 (100%)	-0.36	0 100 100	80, 117, 135, 135	0
1	Y	9/9 (100%)	-0.49	0 100 100	66, 109, 126, 127	0
1	Z	9/9 (100%)	-0.50	0 100 100	62, 94, 136, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	a	9/9 (100%)	-0.36	0 100 100	110, 119, 121, 122	0
1	b	9/9 (100%)	-0.21	0 100 100	110, 116, 132, 135	0
1	c	9/9 (100%)	-0.46	0 100 100	115, 125, 131, 132	0
1	d	9/9 (100%)	-0.39	0 100 100	123, 131, 139, 139	0
All	All	252/252 (100%)	-0.43	0 100 100	53, 87, 134, 140	0

There are no RSRZ outliers to report.

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 ⓘ

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, 95th 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^2)	Q<0.9
2	CS	O	101	1/1	0.50	0.10	185,185,185,185	0
2	CS	b	101	1/1	0.62	0.10	165,165,165,165	0
2	CS	Q	102	1/1	0.72	0.10	149,149,149,149	0
2	CS	Y	102	1/1	0.74	0.07	164,164,164,164	0
2	CS	O	102	1/1	0.75	0.07	174,174,174,174	0
2	CS	C	102	1/1	0.82	0.09	155,155,155,155	0
2	CS	a	101	1/1	0.85	0.07	177,177,177,177	0
2	CS	c	102	1/1	0.85	0.05	189,189,189,189	0
2	CS	N	101	1/1	0.87	0.11	175,175,175,175	0
2	CS	K	101	1/1	0.90	0.09	131,131,131,131	0
2	CS	S	101	1/1	0.91	0.05	171,171,171,171	0
2	CS	G	101	1/1	0.93	0.09	128,128,128,128	0
2	CS	I	102	1/1	0.93	0.08	139,139,139,139	0
2	CS	U	101	1/1	0.93	0.09	197,197,197,197	0

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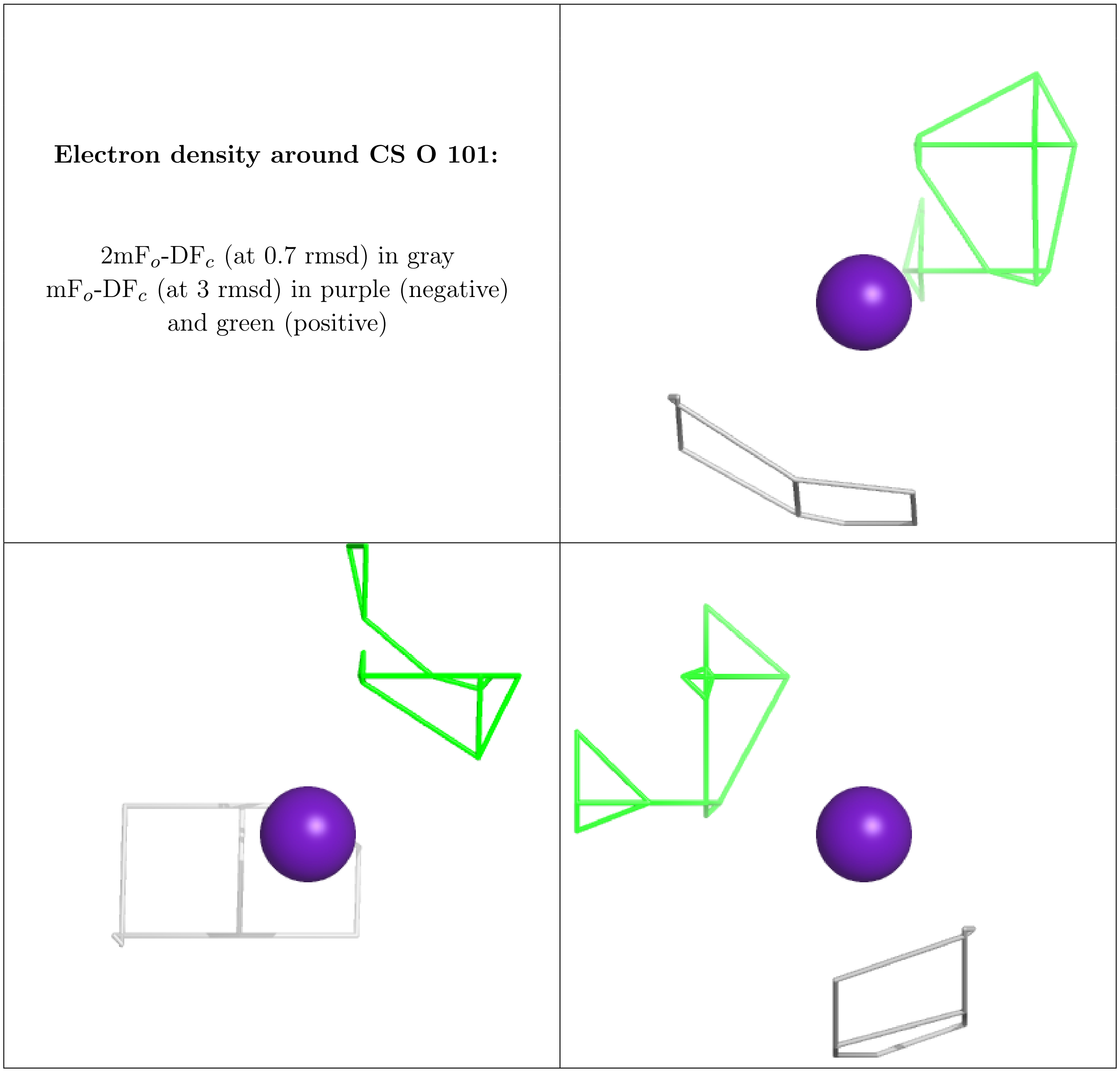
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CS	U	102	1/1	0.93	0.05	201,201,201,201	0
2	CS	G	102	1/1	0.94	0.08	127,127,127,127	0
2	CS	c	101	1/1	0.94	0.06	183,183,183,183	0
2	CS	T	101	1/1	0.94	0.07	154,154,154,154	0
2	CS	M	101	1/1	0.95	0.07	120,120,120,120	0
2	CS	Y	101	1/1	0.96	0.03	162,162,162,162	0
2	CS	E	102	1/1	0.96	0.06	140,140,140,140	0
2	CS	I	101	1/1	0.97	0.09	109,109,109,109	0
2	CS	E	101	1/1	0.97	0.10	123,123,123,123	0
2	CS	C	101	1/1	0.97	0.06	153,153,153,153	0
2	CS	Q	101	1/1	0.98	0.05	150,150,150,150	0
2	CS	A	102	1/1	0.98	0.09	110,110,110,110	0
2	CS	A	101	1/1	0.98	0.09	117,117,117,117	0
2	CS	K	102	1/1	0.99	0.06	124,124,124,124	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.

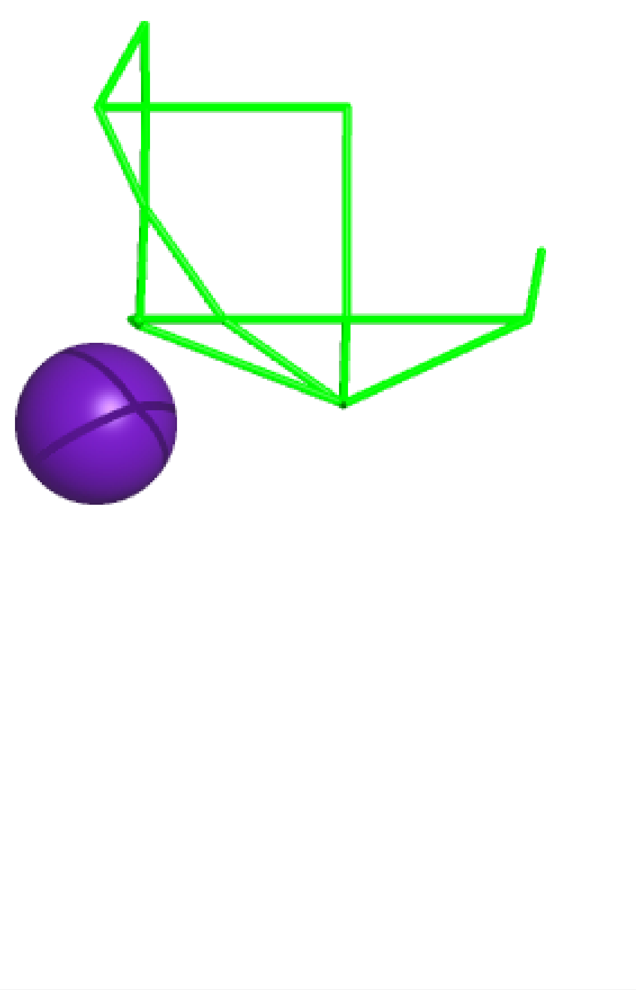


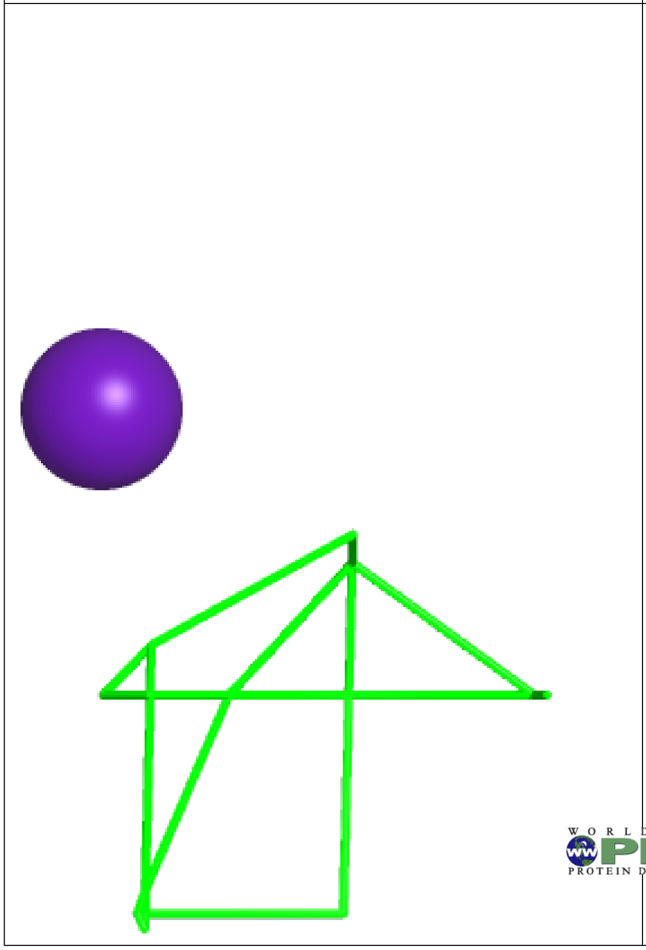
Electron density around CS O 101:

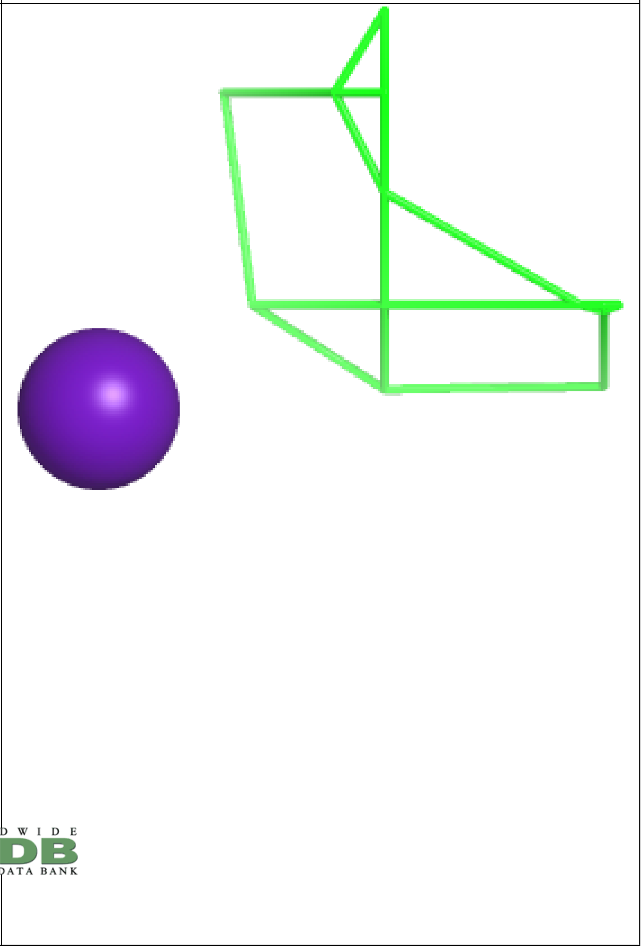
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CS b 101:

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







Electron density around CS Q 102:

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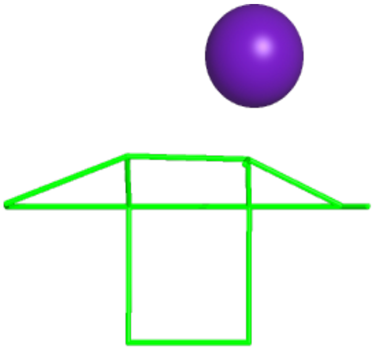
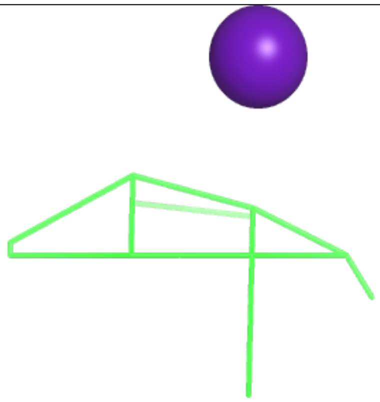
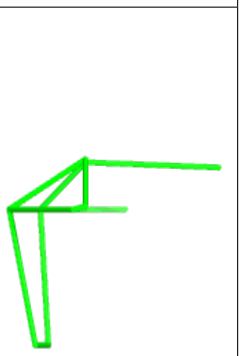
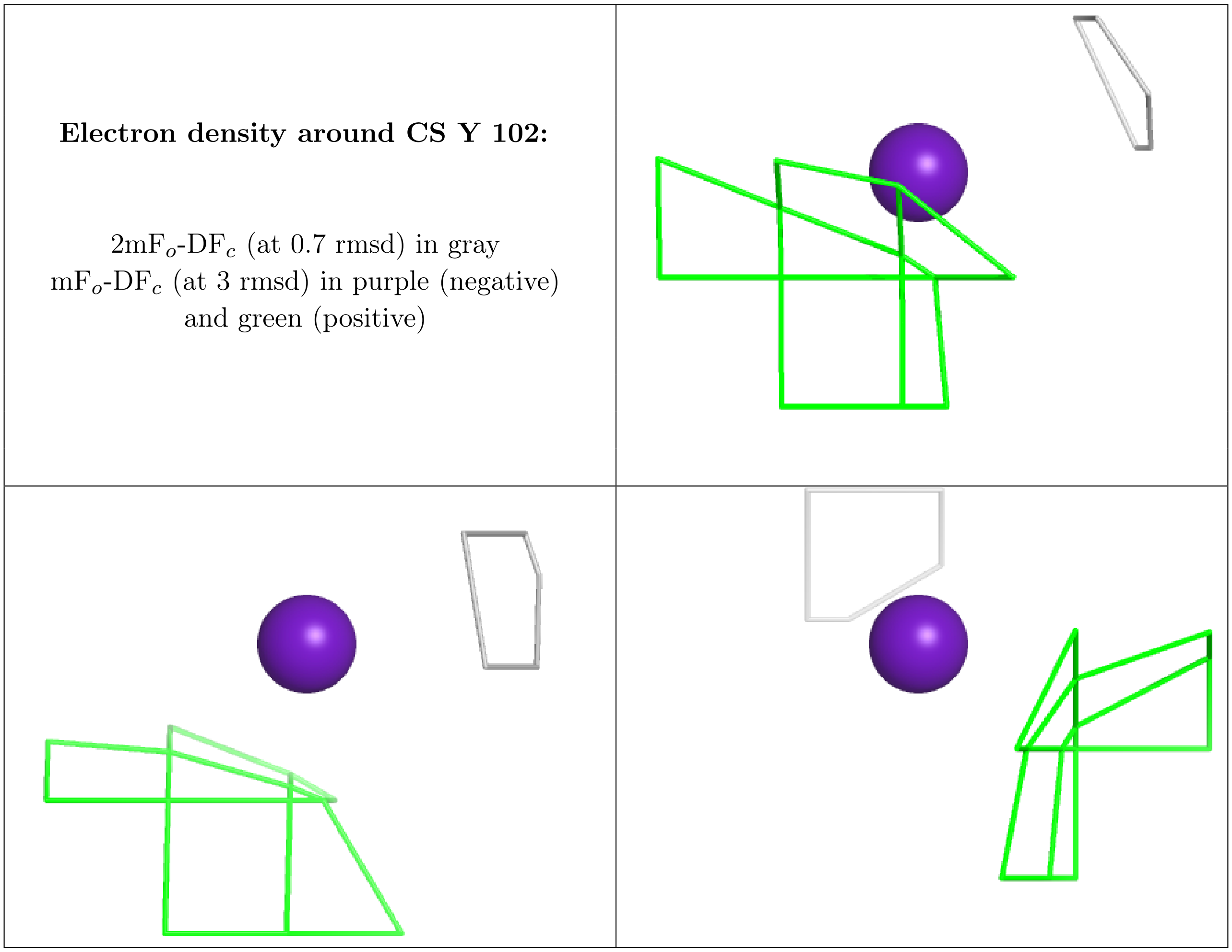
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





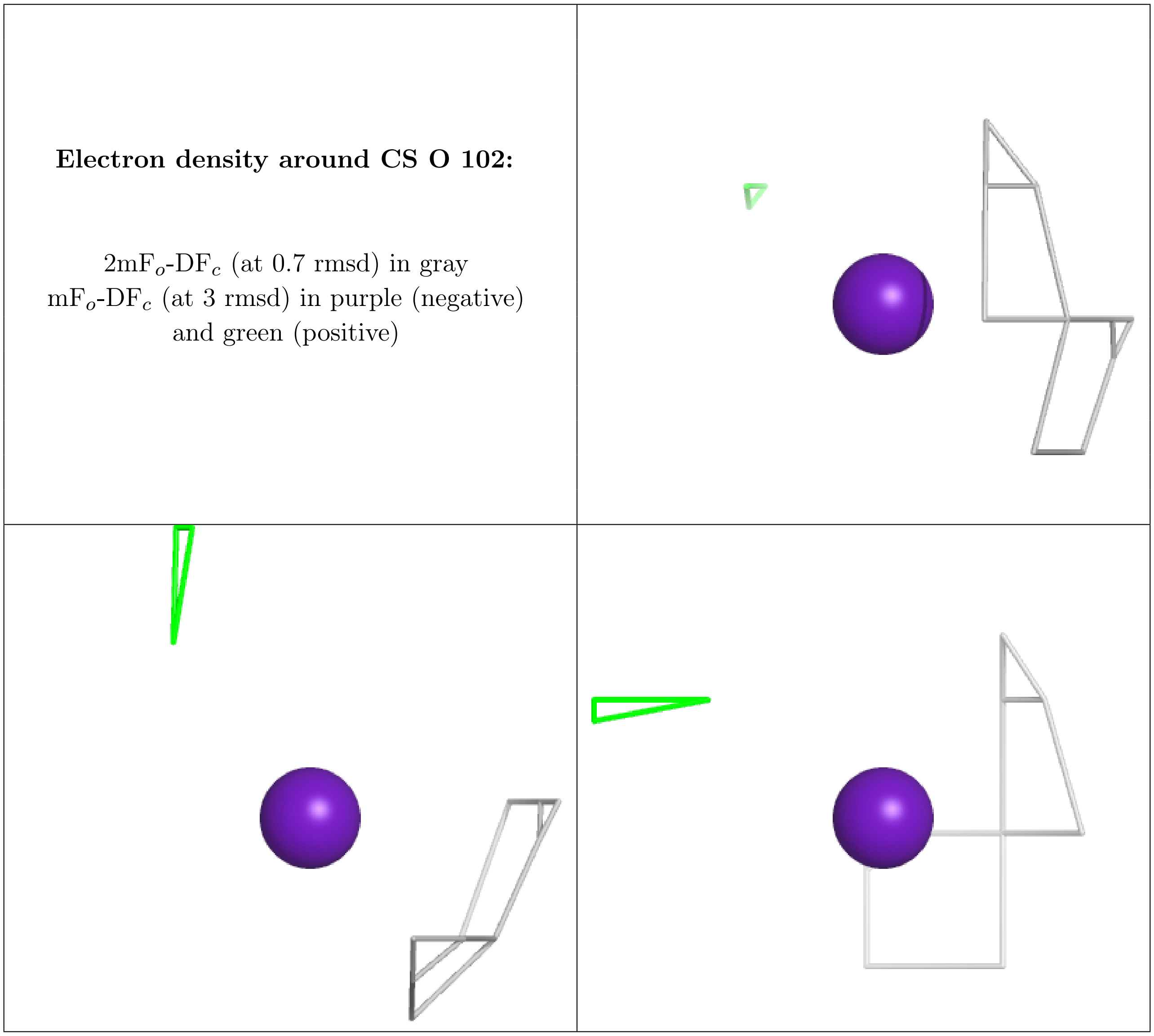




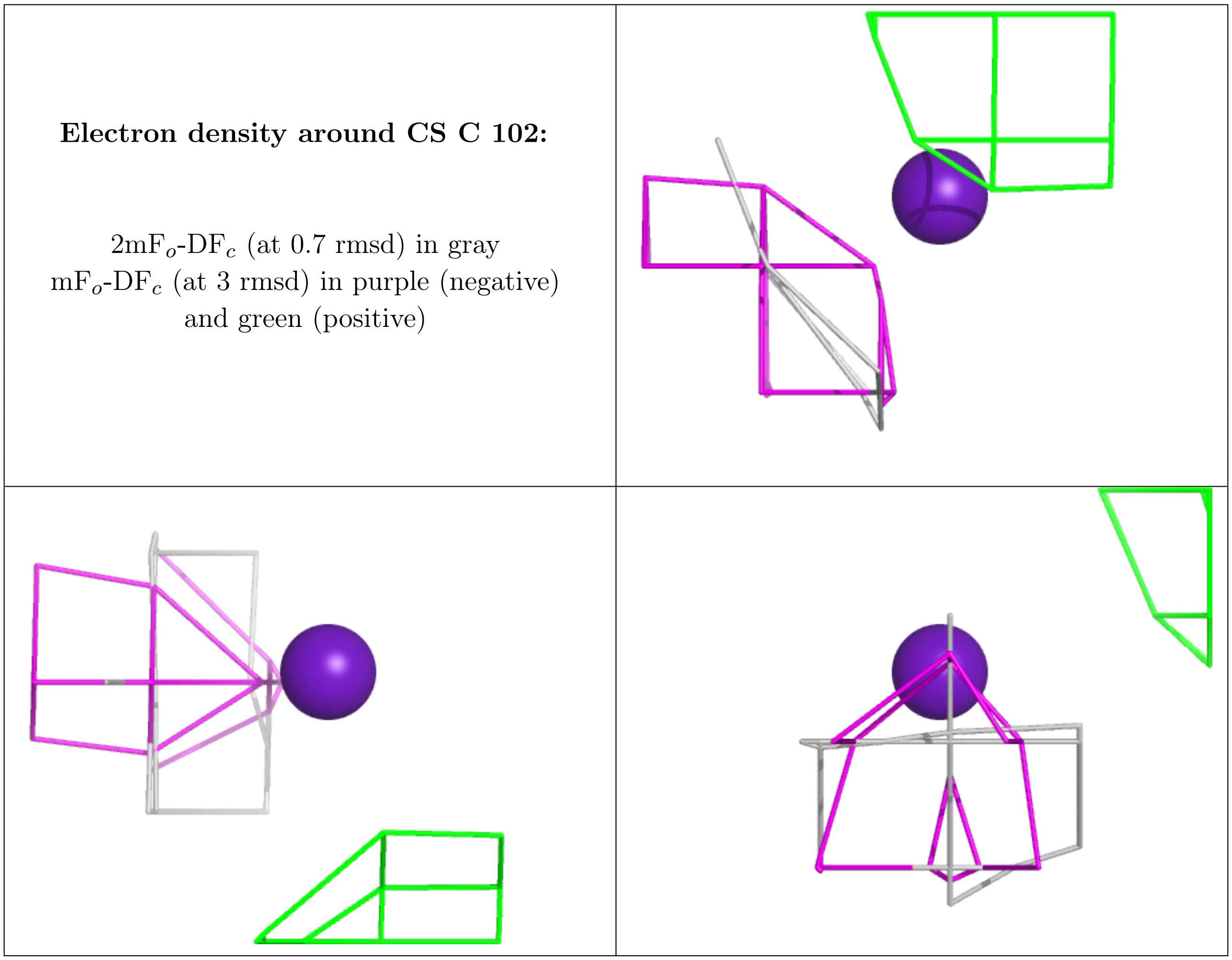
Electron density around CS Y 102:

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 CS O 102:



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

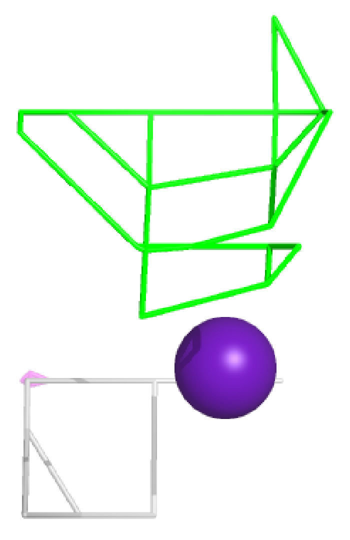


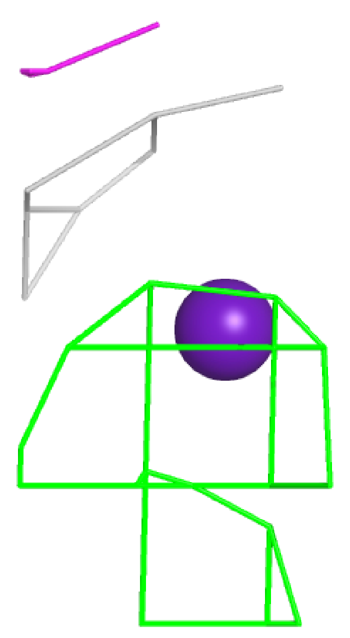
Electron density around CS C 102:

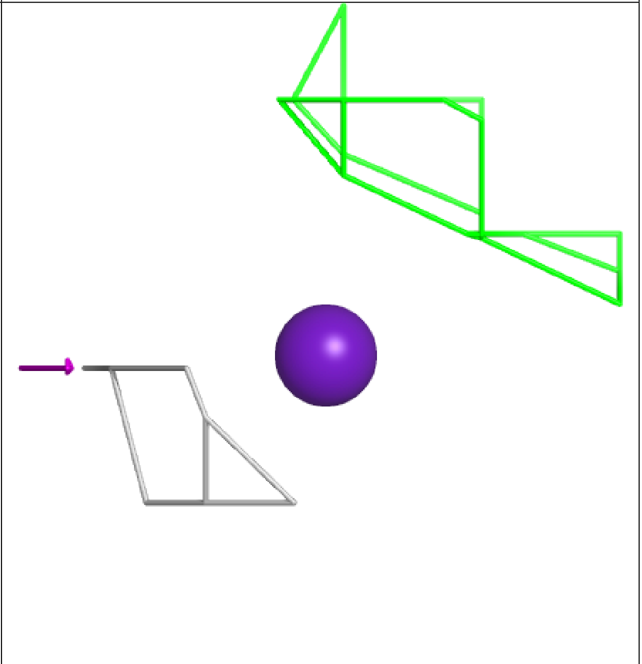
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CS a 101:

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







Electron density around CS c 102:

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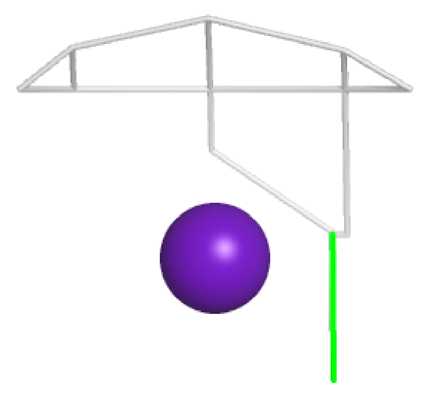
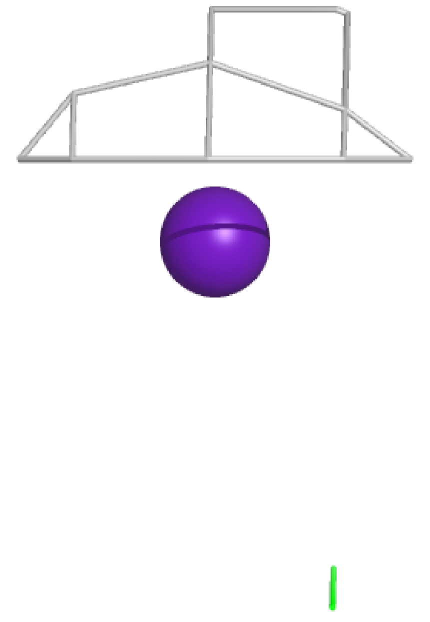
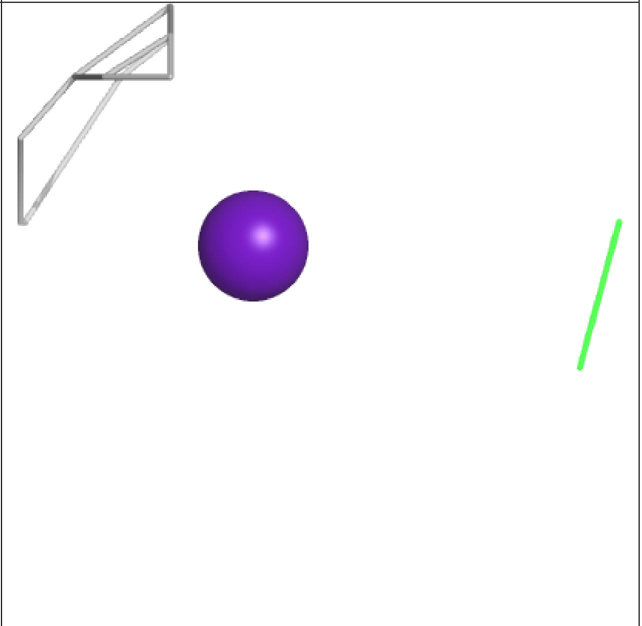
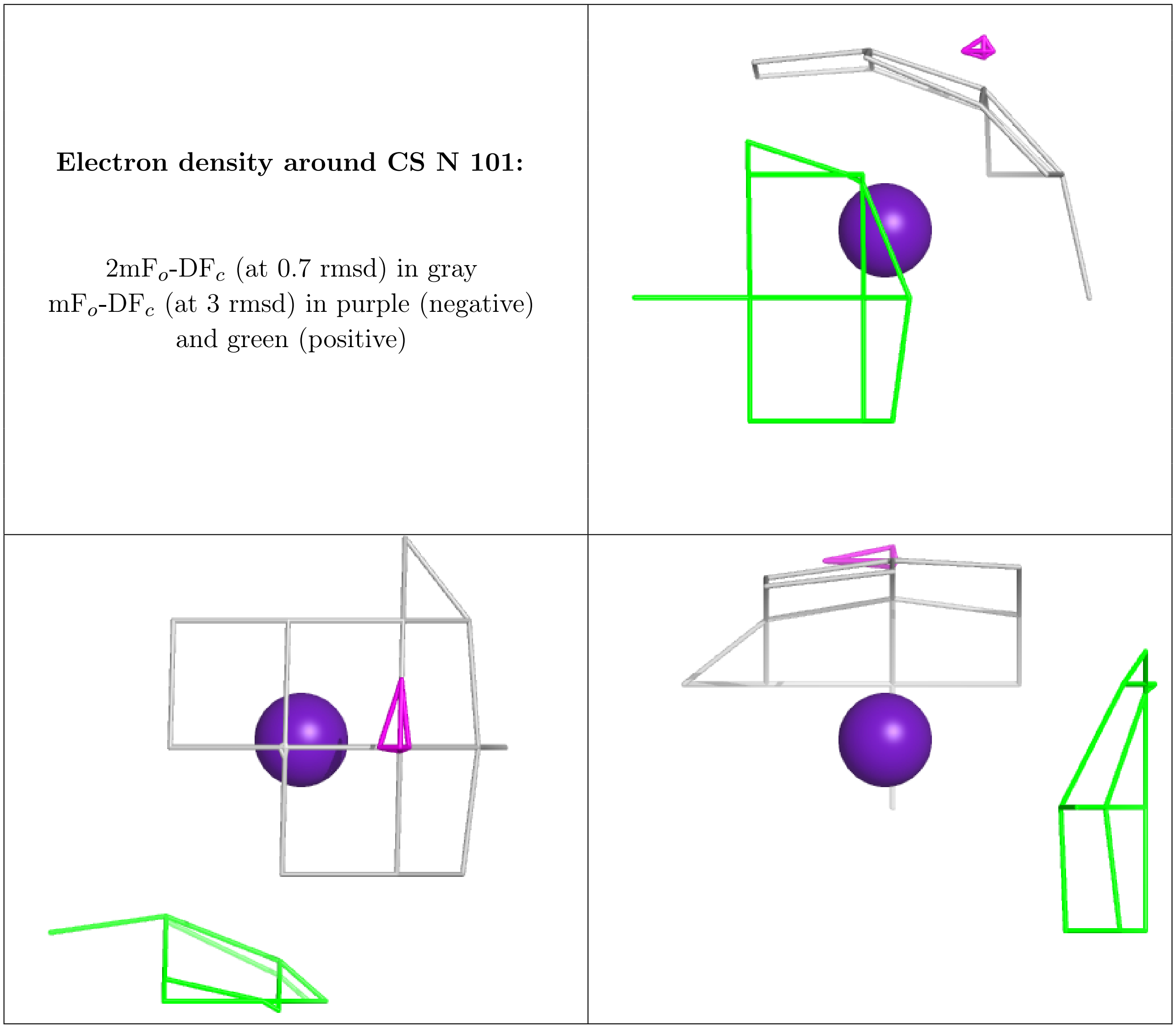
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)









Electron density around CS N 101:

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

Electron density around CS K 101:

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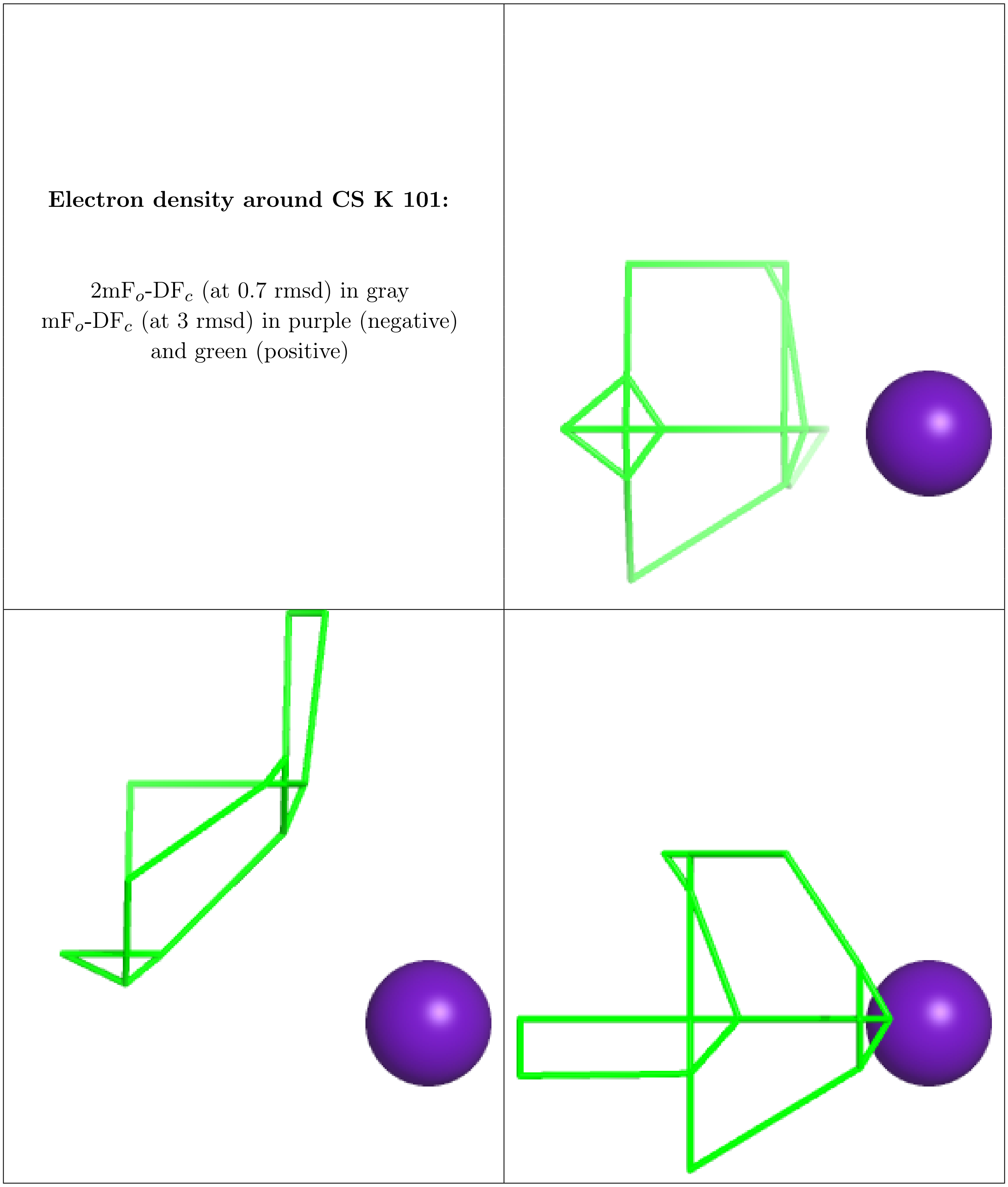
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CS S 101:

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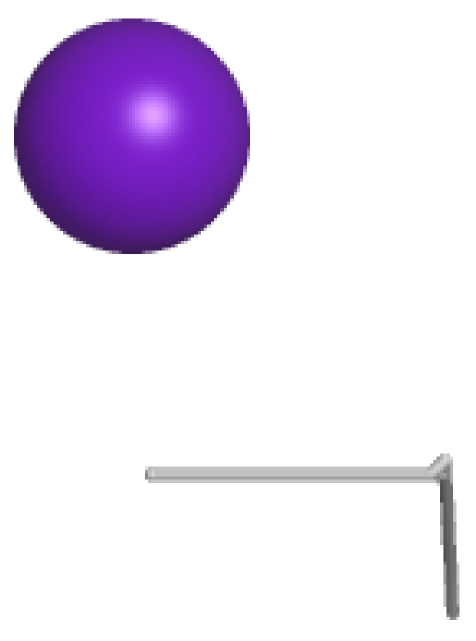
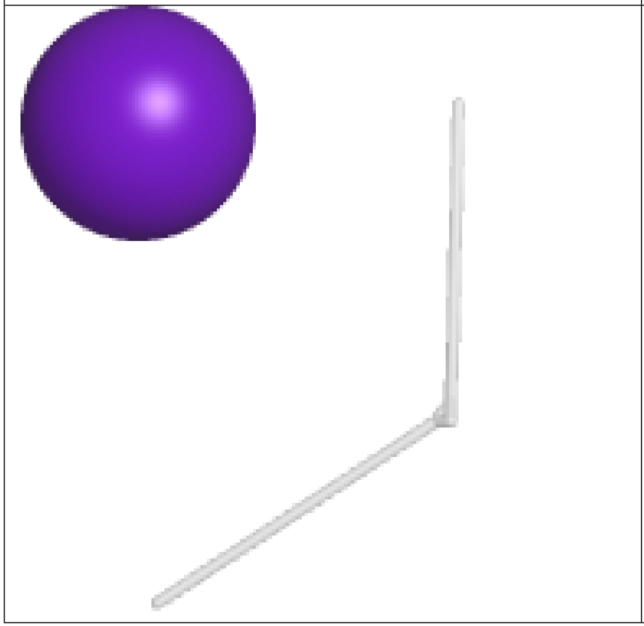
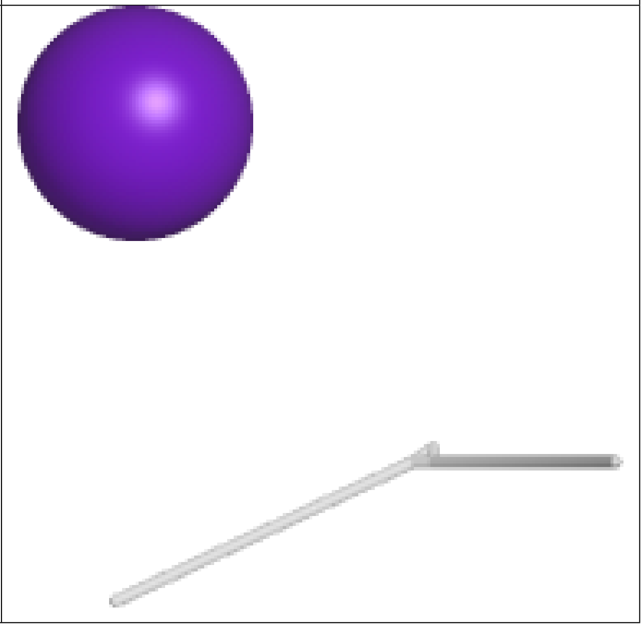
and green (positive)







Electron density around CS G 101:

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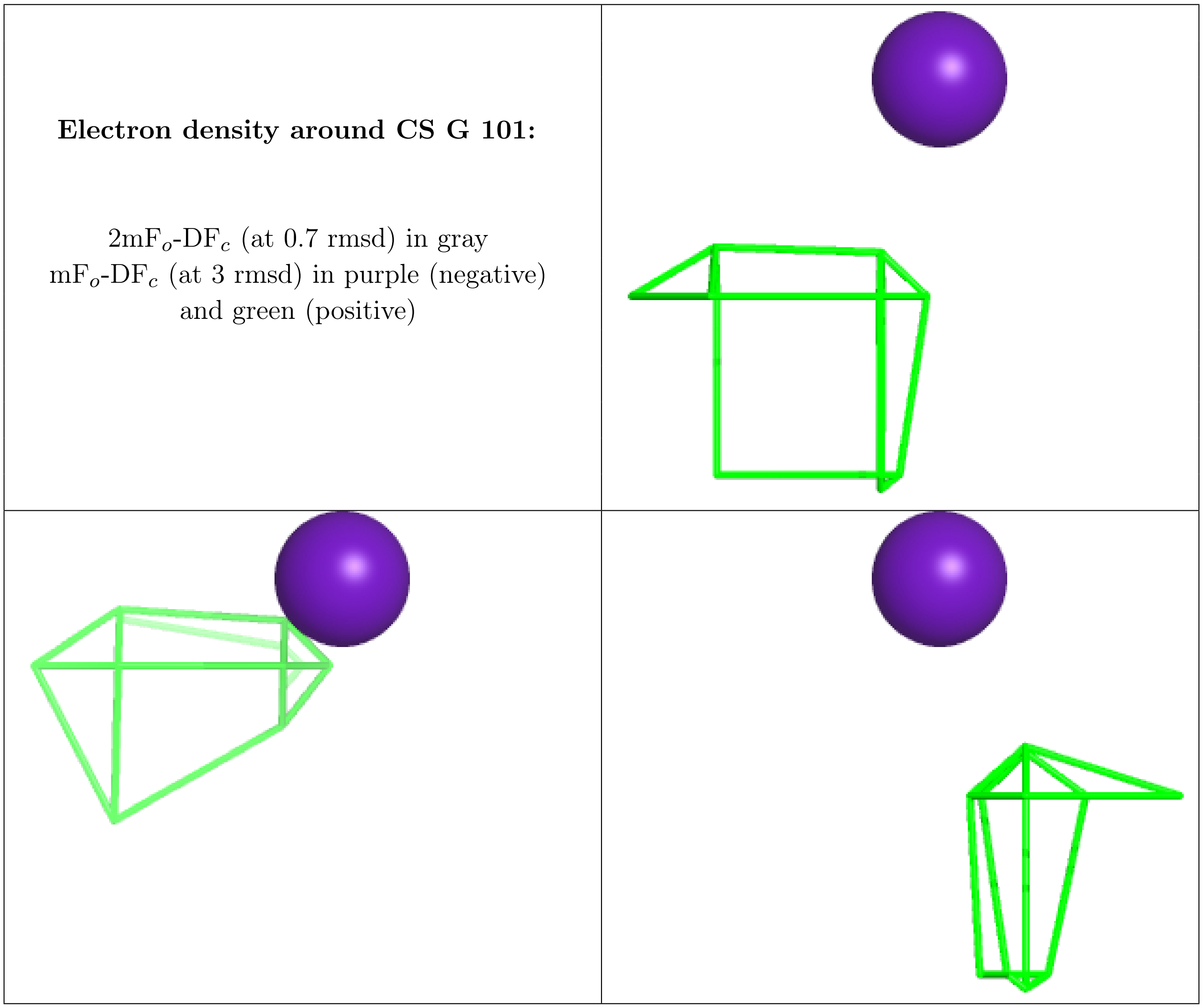
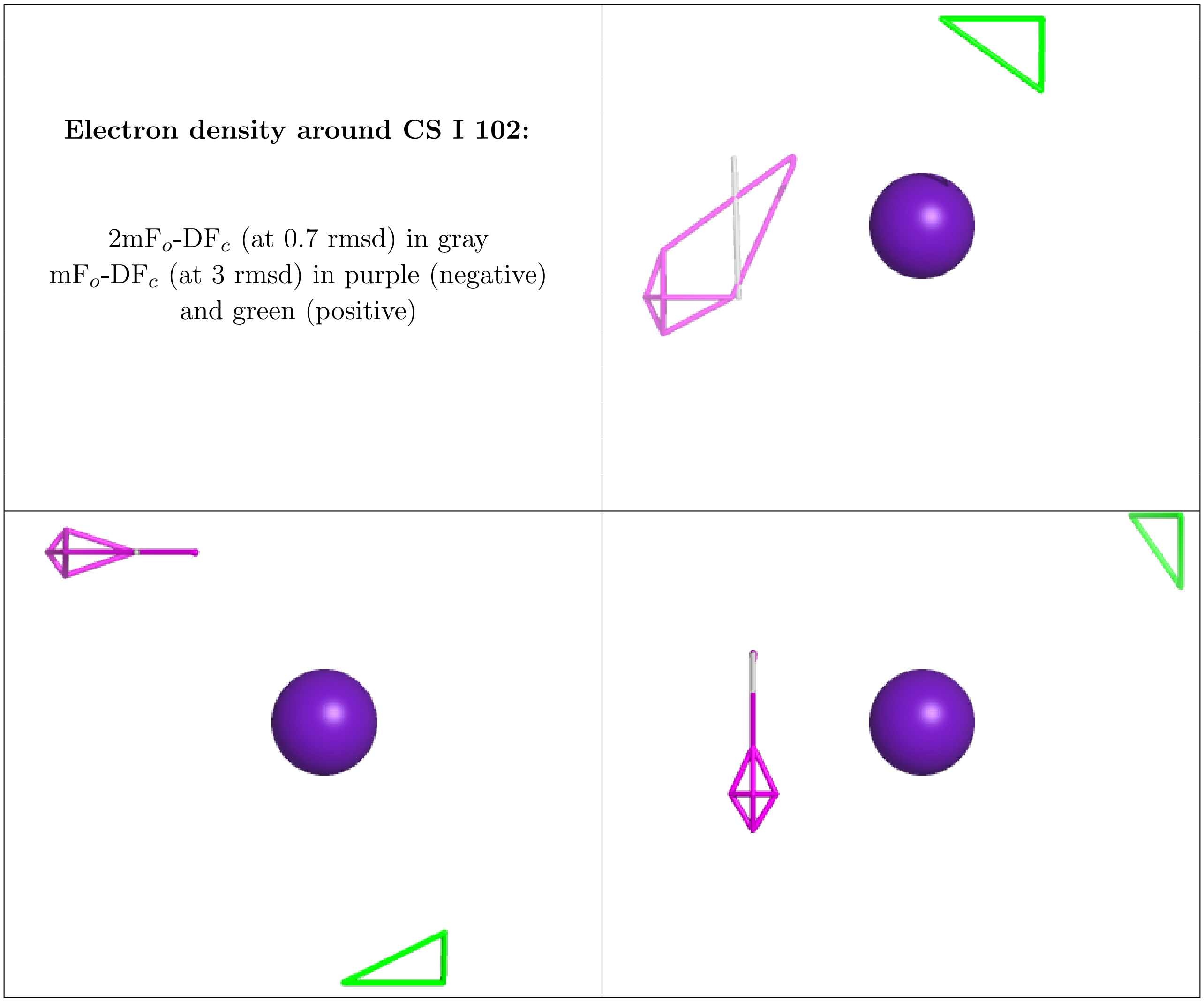
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



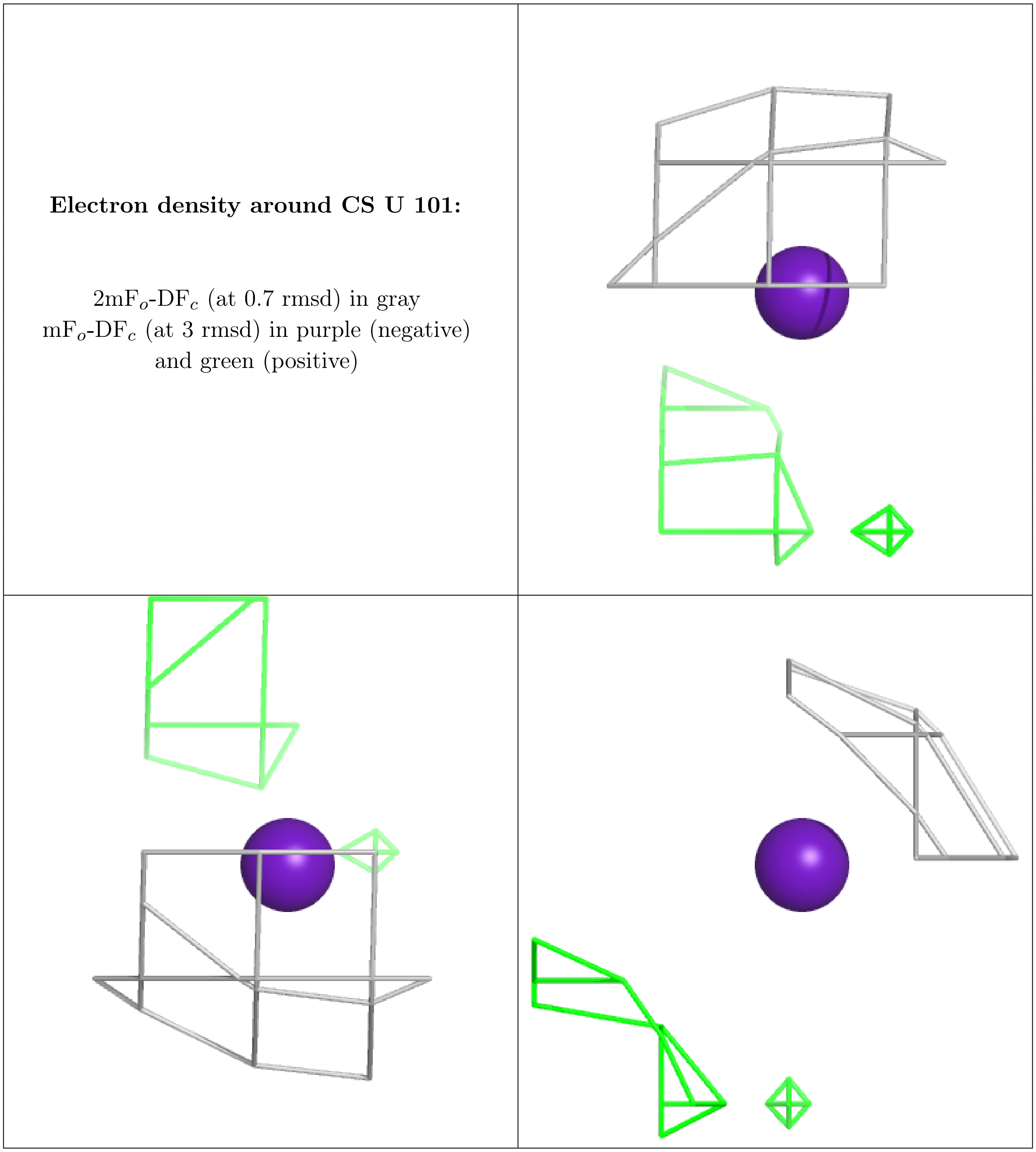


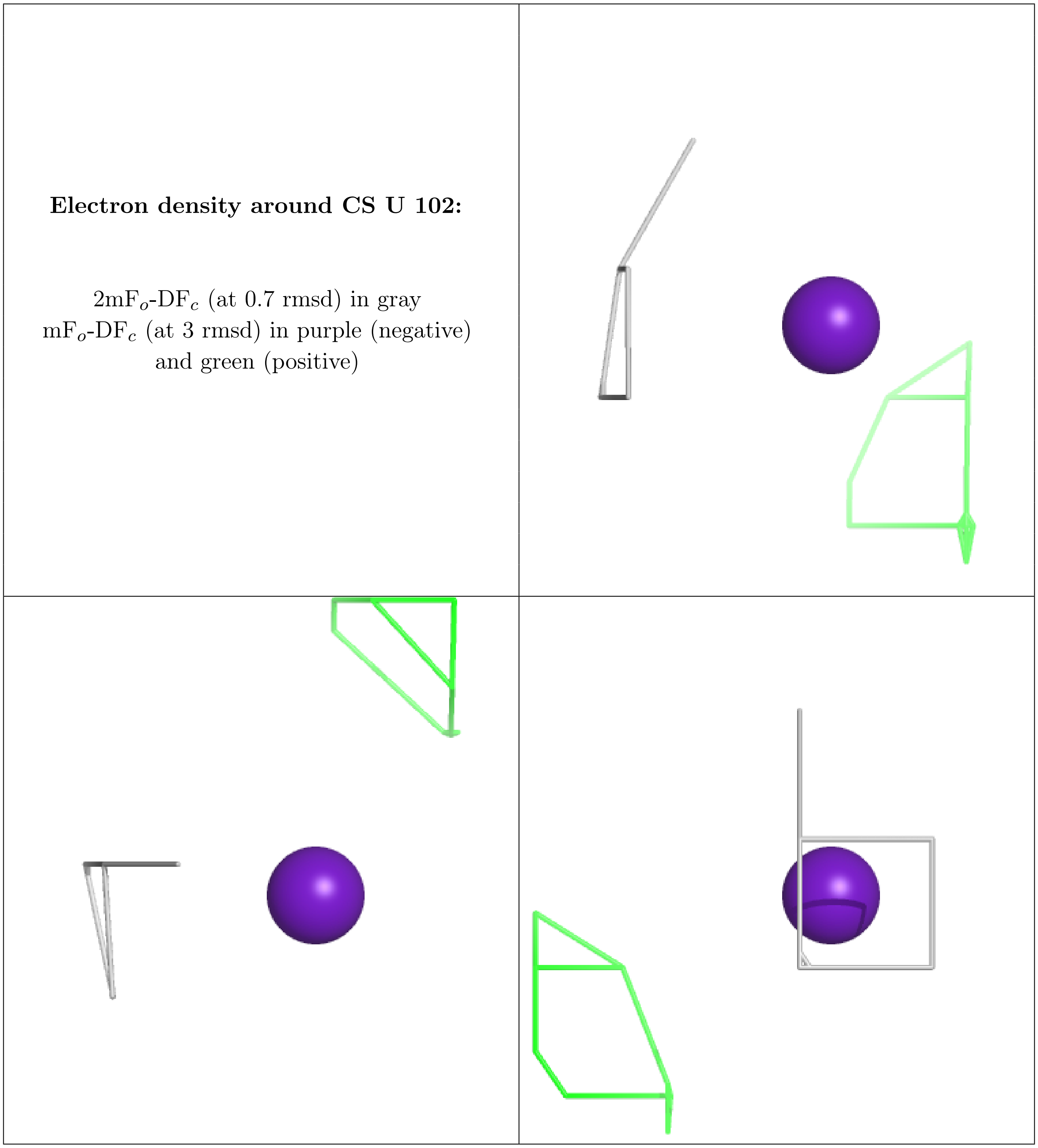
Electron density around CS I 102:

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 CS U 101:

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



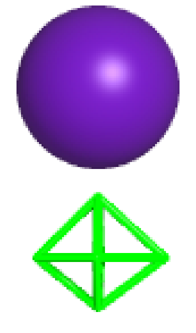


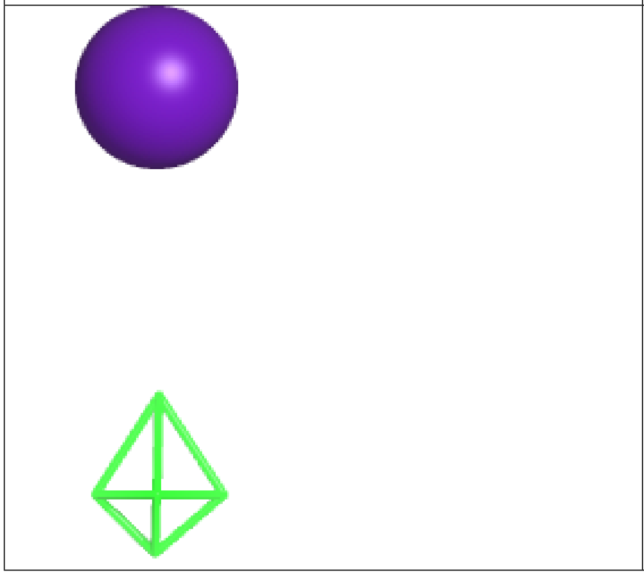
Electron density around CS U 102:

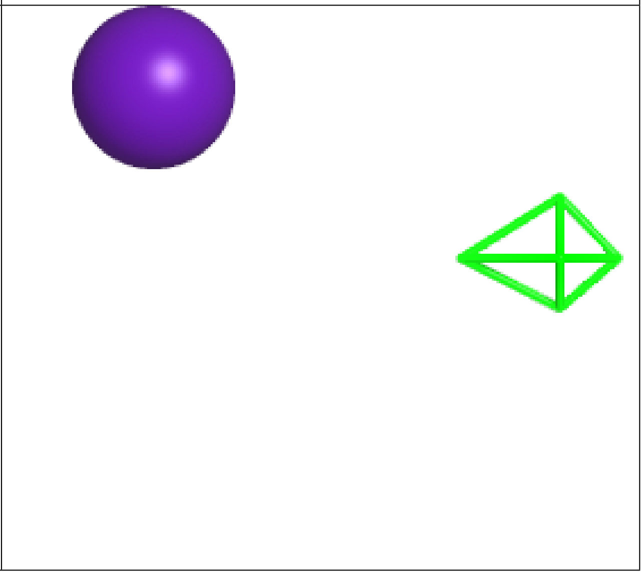
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CS G 102:

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 CS c 101:

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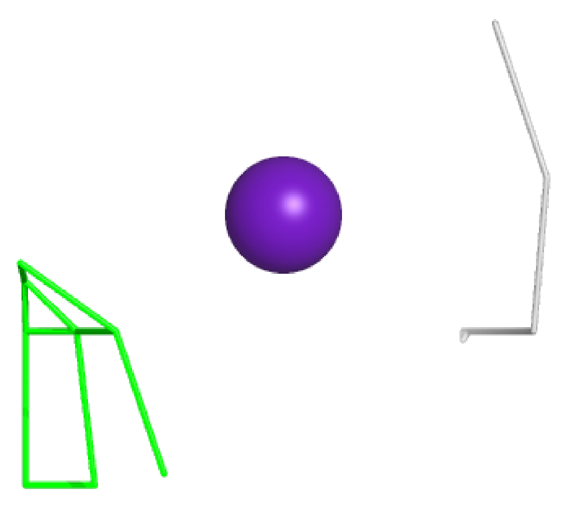
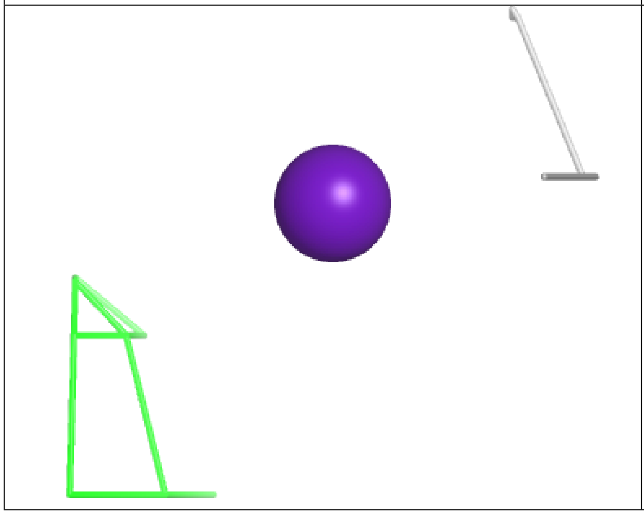
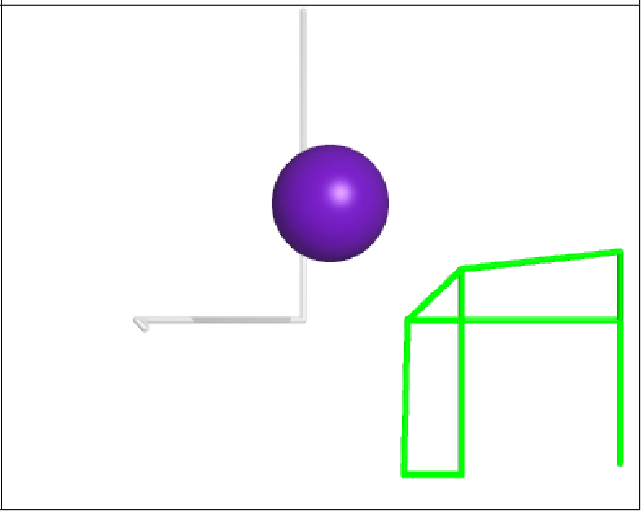
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

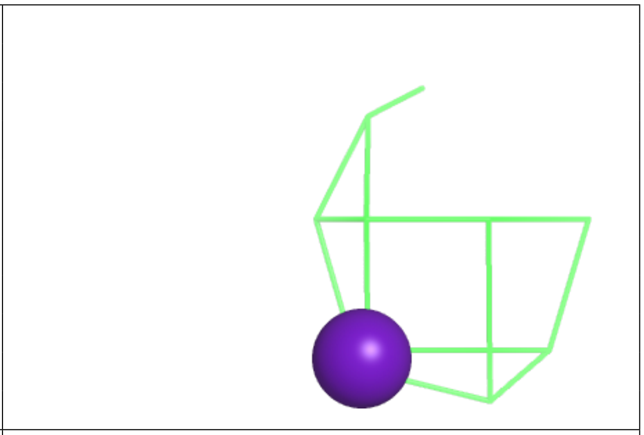


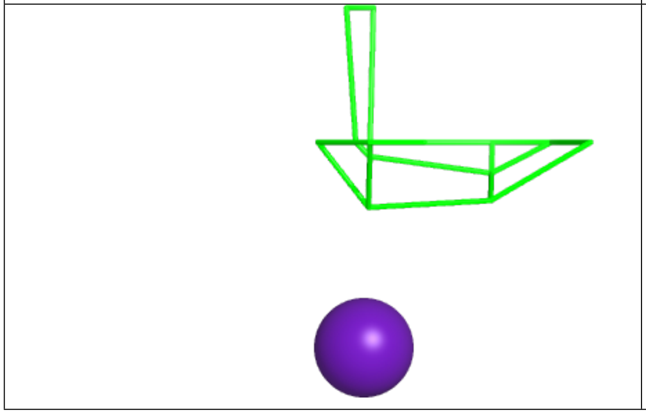


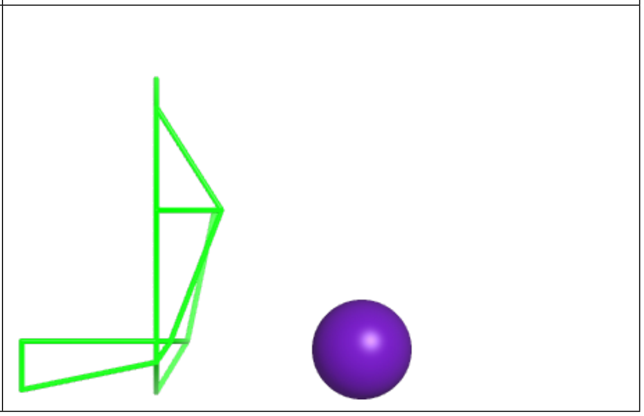


Electron density around CS T 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

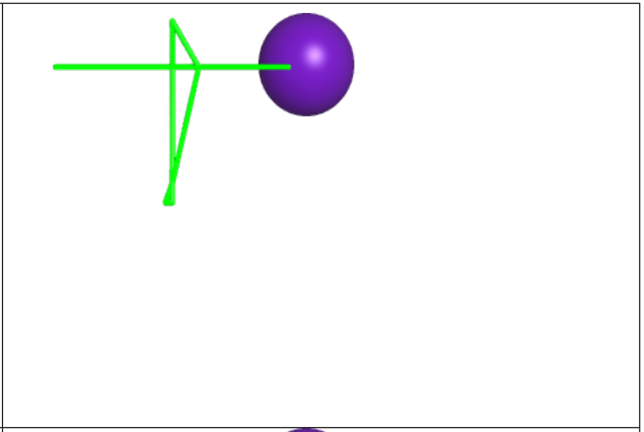


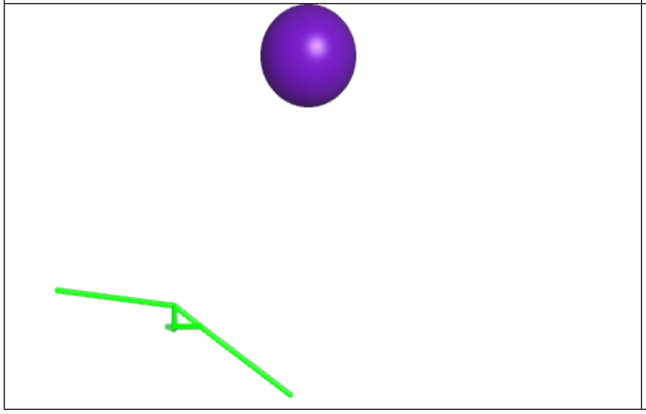


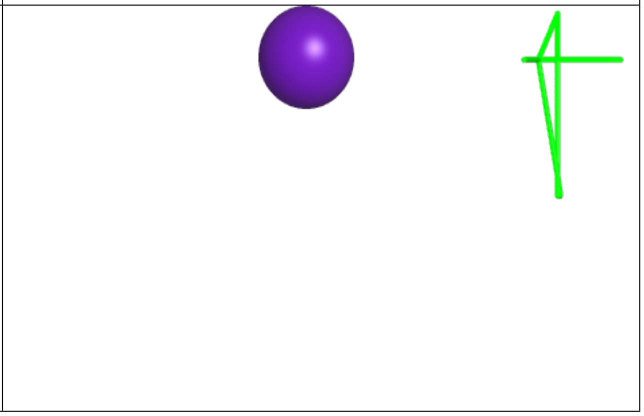


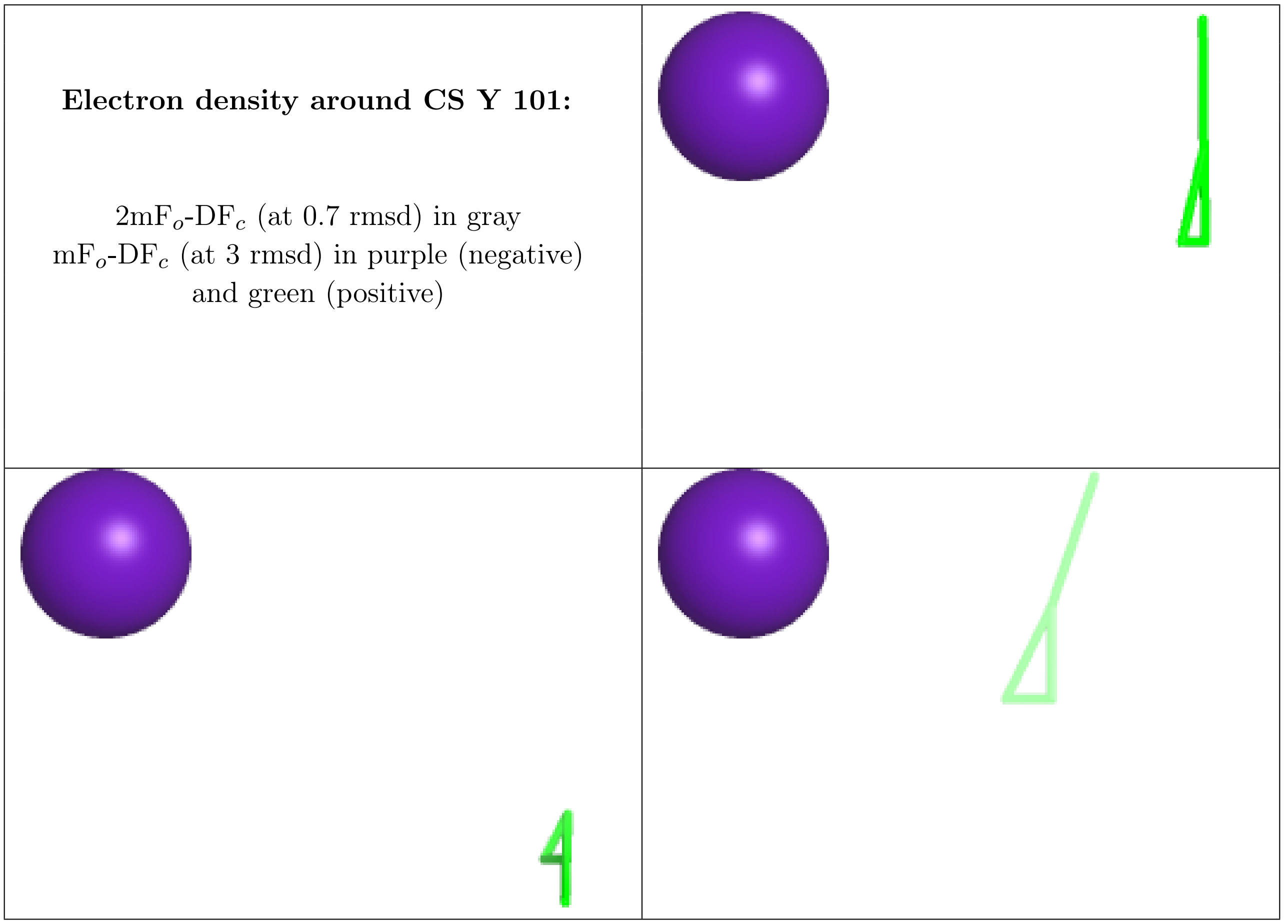
Electron density around CS M 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







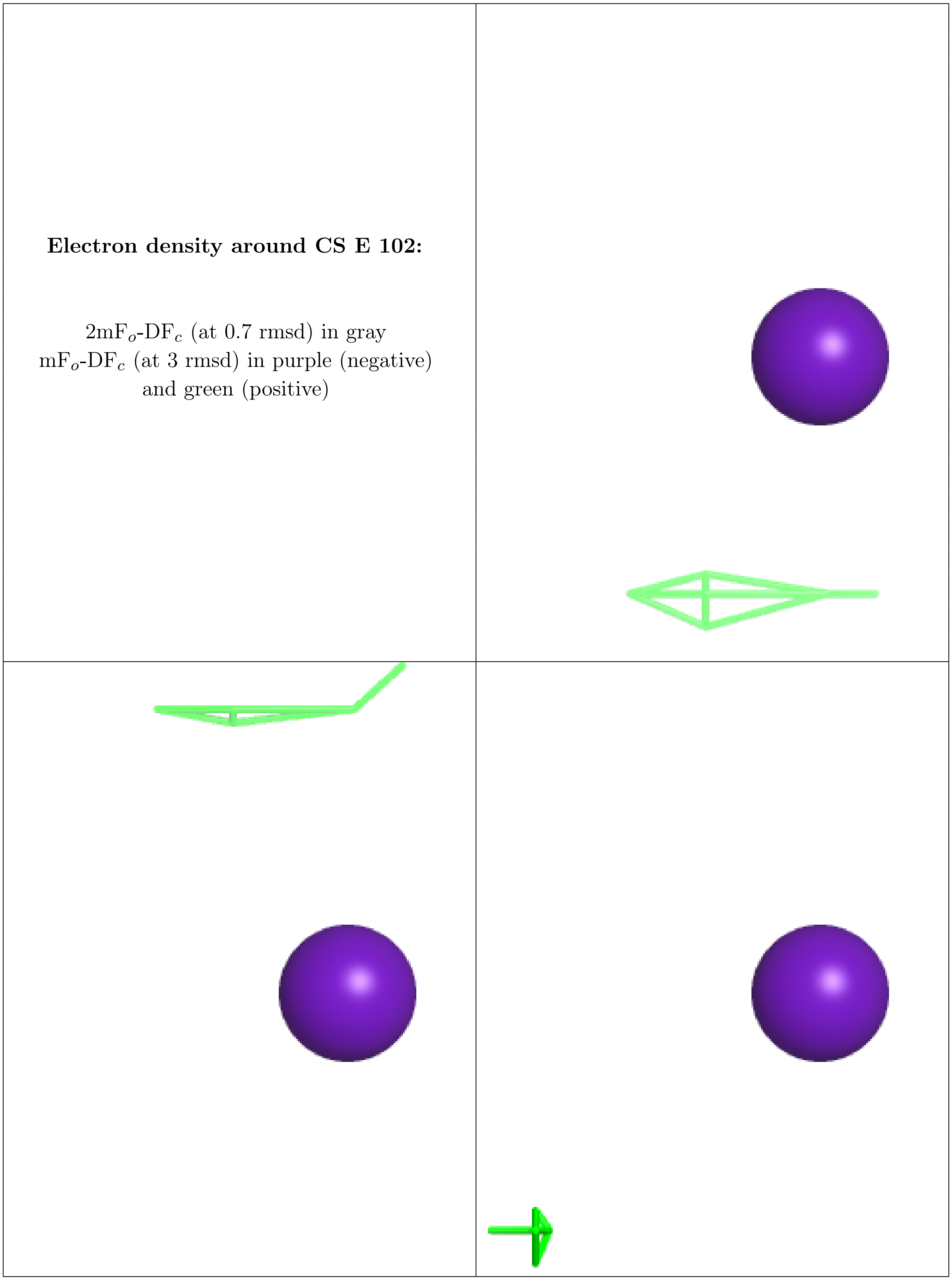


Electron density around CS Y 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

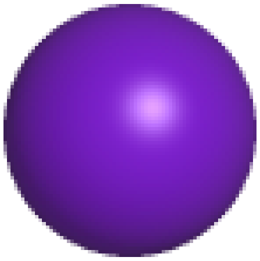
Electron density around CS E 102:

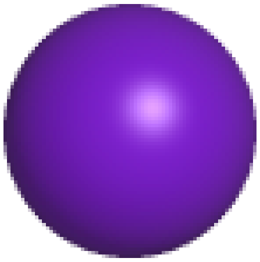
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

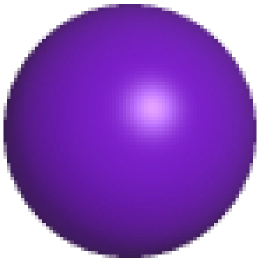


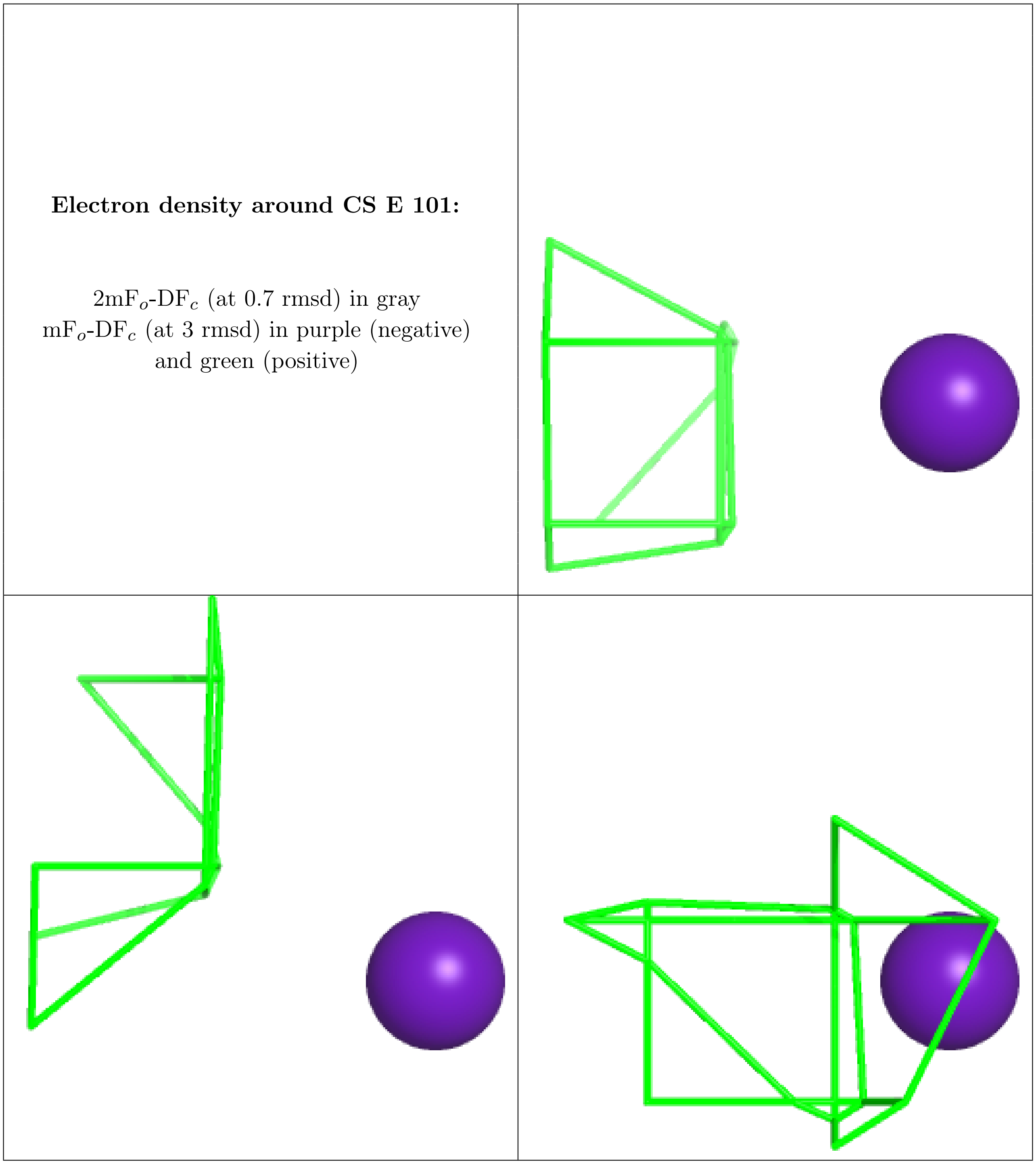
Electron density around CS I 101:

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







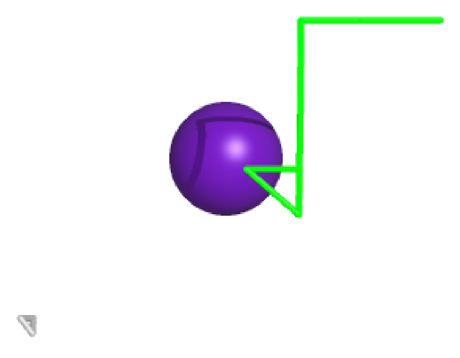


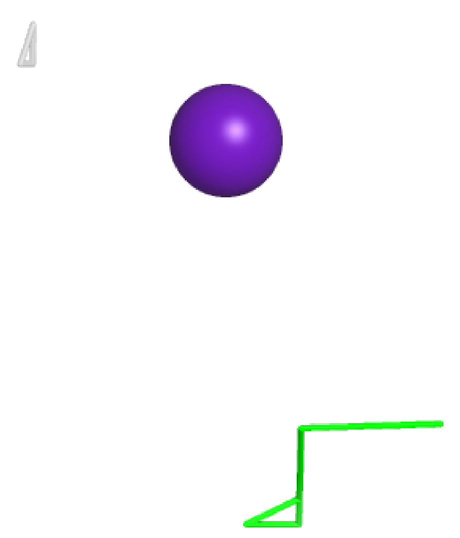
Electron density around CS E 101:

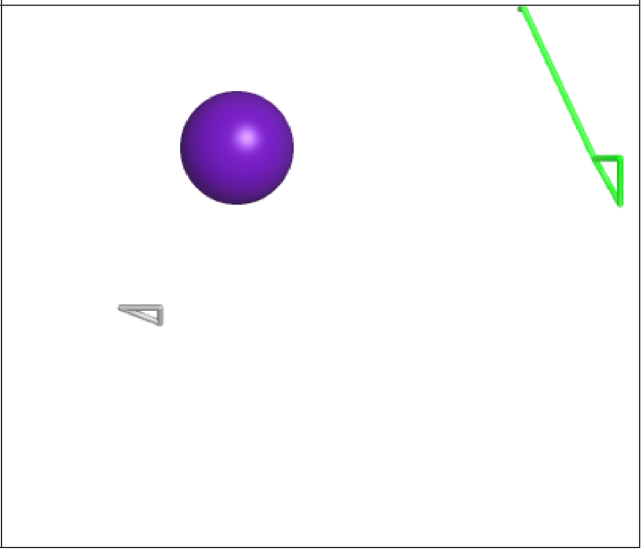
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CS C 101:

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

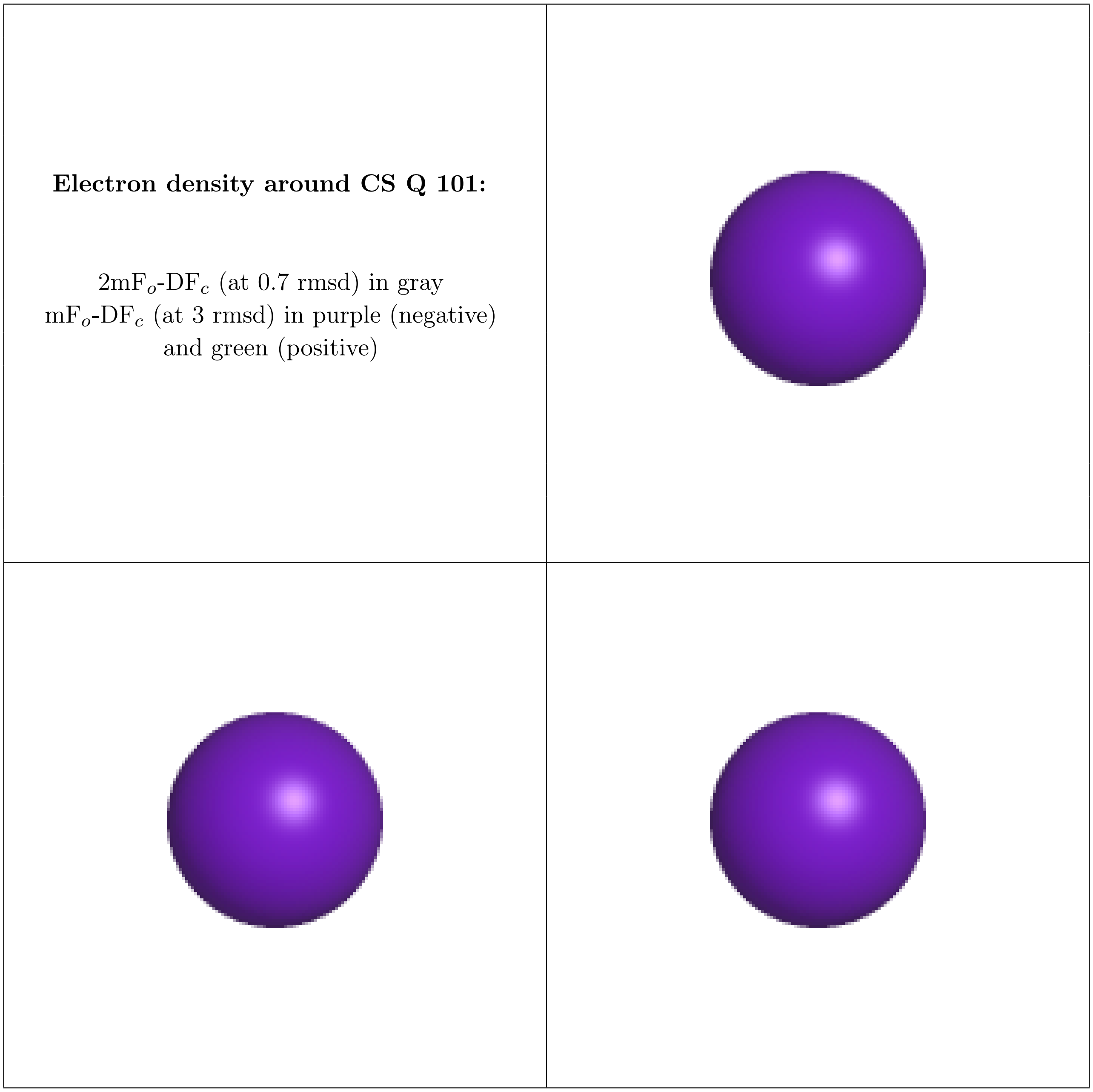






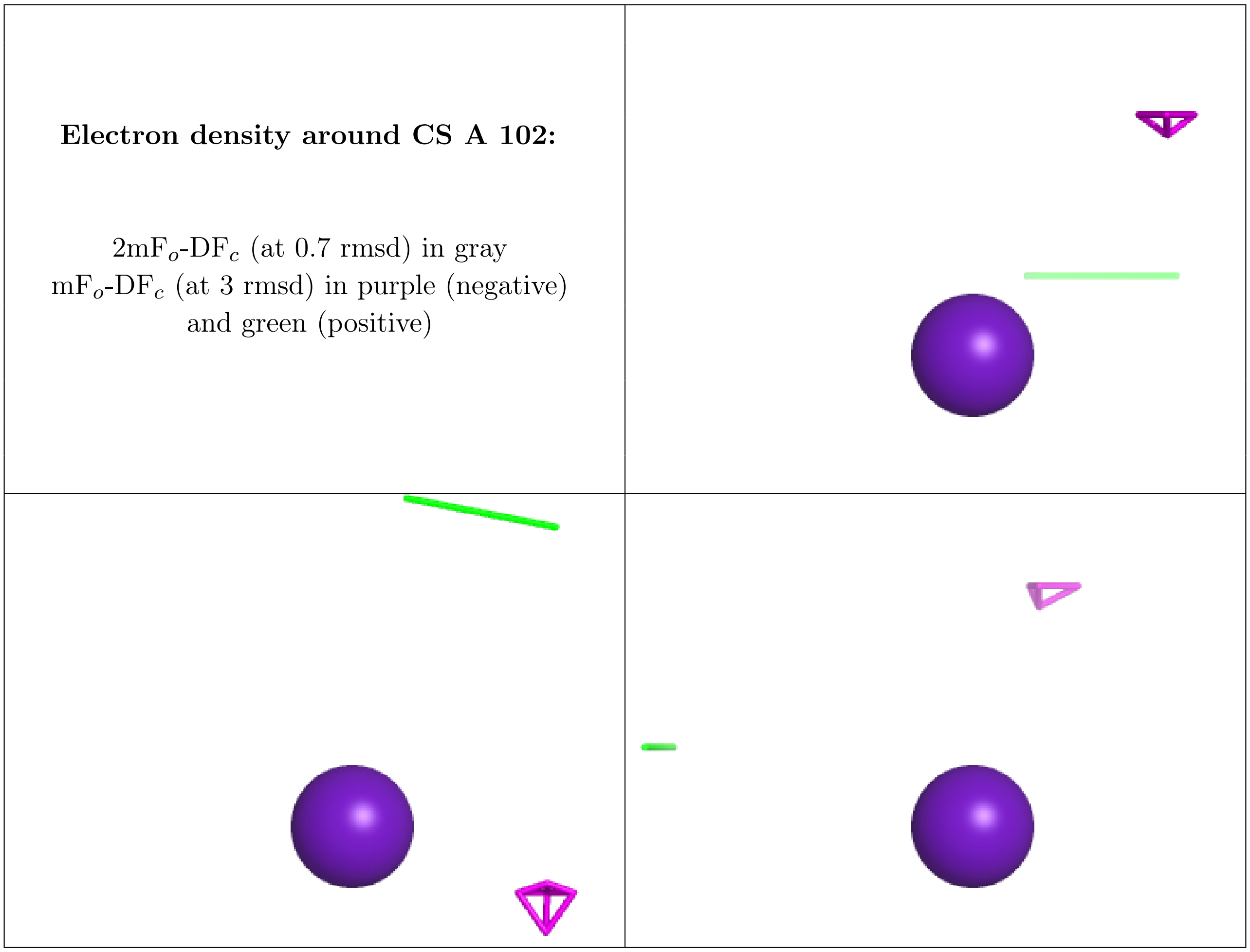
Electron density around CS Q 101:

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



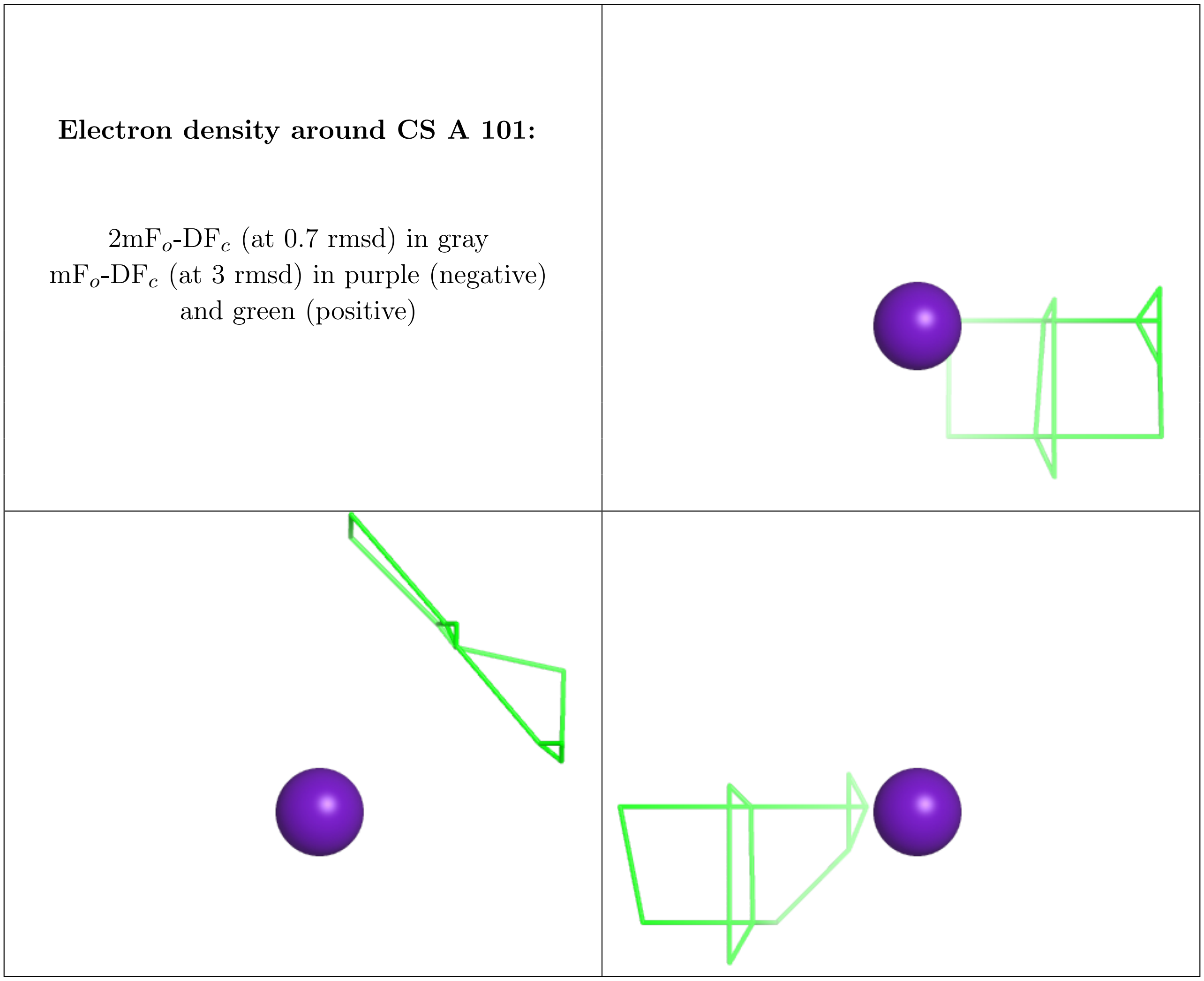
Electron density around CS A 102:

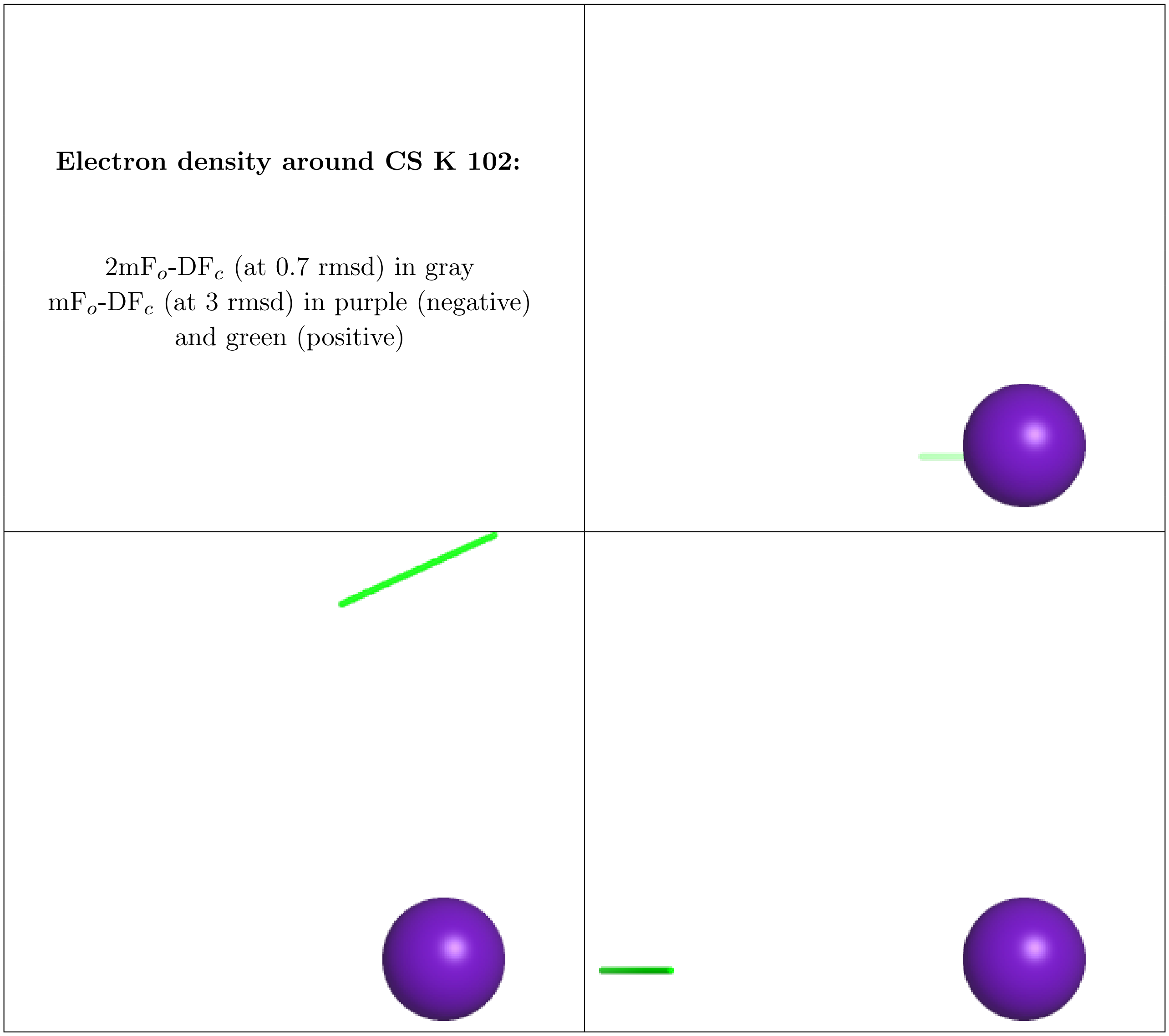
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CS A 101:

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 CS K 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 ⓘ

There are no such residues in this entry.