Full wwPDB X-ray Structure Validation Report (i)

May 10, 2024 – 02:40 PM JST

PDB ID	:	8ZGA
Title	:	F-degron fused ZZ-domain of the Arabidopsis thaliana E3 ubiquitin-protein ligase PRT1
Deposited on	:	2024-05-09
Resolution	:	2.10 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *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.

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

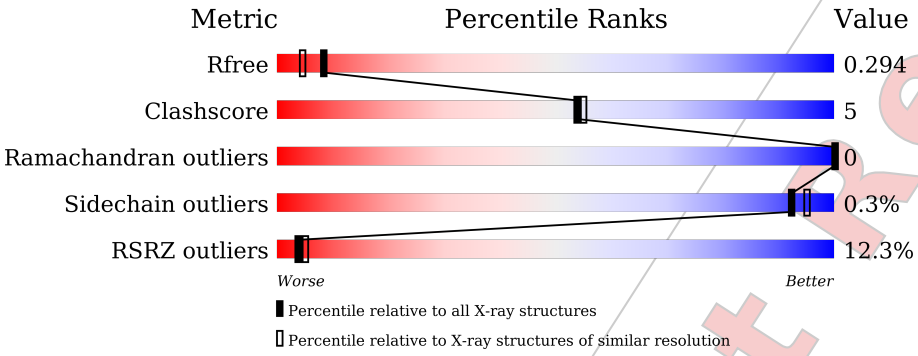
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.10 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 >=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	69	13% 84% 14%
1	B	69	14% 88% 10%
1	C	69	6% 80% 14%
1	D	69	4% 84% 16%

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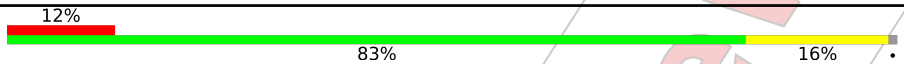
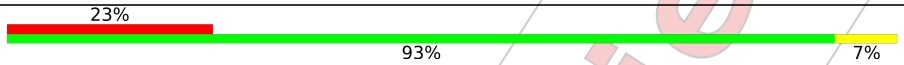
Mol	Chain	Length	Quality of chain
1	E	69	
1	F	69	

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
3	MG	B	403	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6235 atoms, of which 2980 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 F-degron,E3 ubiquitin-protein ligase PRT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	68	Total	C	H	N	O	S	0	0	0
			1030	334	494	95	101	6			
1	B	68	Total	C	H	N	O	S	0	0	0
			1030	334	494	95	101	6			
1	C	66	Total	C	H	N	O	S	0	0	0
			997	325	476	92	98	6			
1	D	69	Total	C	H	N	O	S	0	0	0
			1054	340	507	99	102	6			
1	E	68	Total	C	H	N	O	S	0	0	0
			1043	337	502	98	100	6			
1	F	69	Total	C	H	N	O	S	0	0	0
			1054	340	507	99	102	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

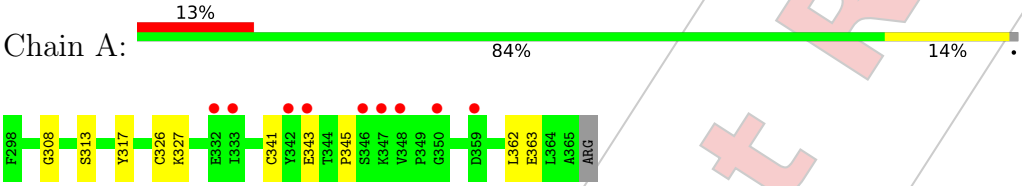
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	3	Total O 3 3	0	0
4	E	4	Total O 4 4	0	0
4	F	1	Total O 1 1	0	0

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.

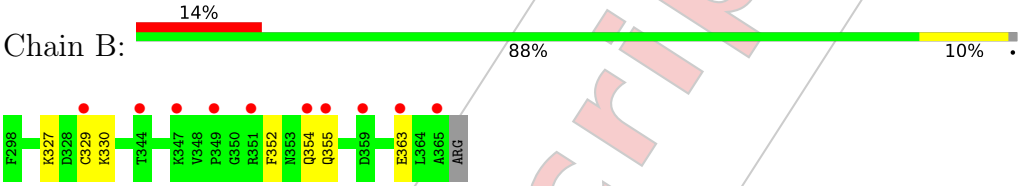
• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain A:



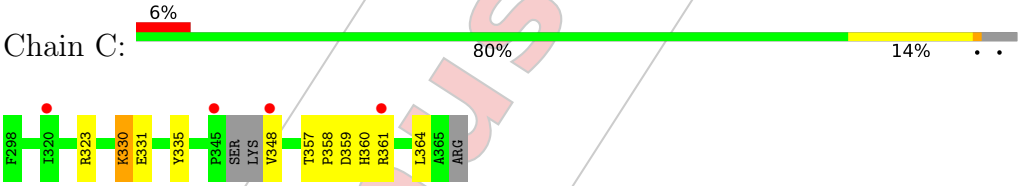
• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain B:



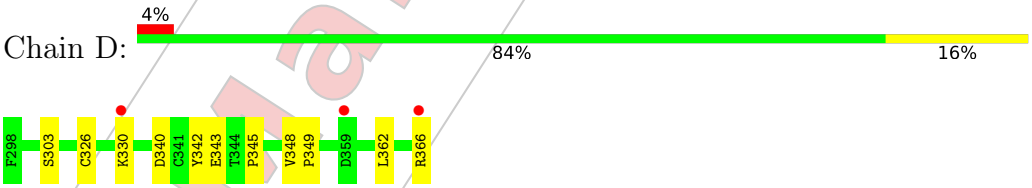
• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain C:



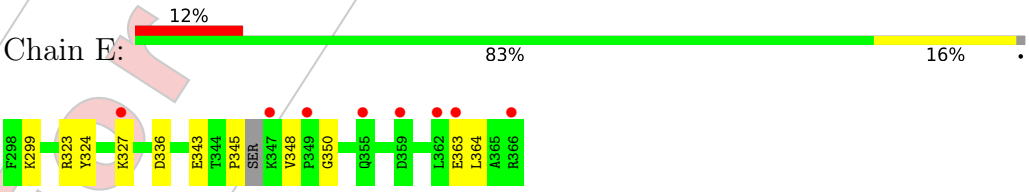
• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain D:



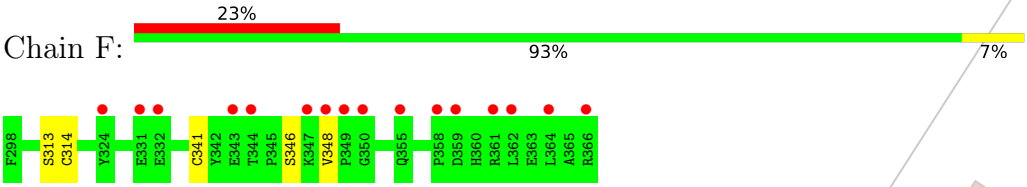
• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain E:



• Molecule 1: F-degron,E3 ubiquitin-protein ligase PRT1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.73Å 86.44Å 89.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 2.10 44.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.83-2.10) 90.4 (44.88-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.67 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18rc7_3834	Depositor
R, R_{free}	0.257 , 0.294 0.257 , 0.294	Depositor DCC
R_{free} test set	1990 reflections (8.74%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, ZN

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	0.32	0/550	0.49	0/739
1	B	0.33	0/550	0.48	0/739
1	C	0.32	0/534	0.45	0/717
1	D	0.30	0/561	0.47	0/753
1	E	0.32	0/554	0.48	0/742
1	F	0.31	0/561	0.47	0/753
All	All	0.32	0/3310	0.47	0/4443

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	536	494	493	7	0
1	B	536	494	493	4	0
1	C	521	476	474	8	0
1	D	547	507	506	7	0
1	E	541	502	500	6	0
1	F	547	507	506	3	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	4	0	0	0	0
4	F	1	0	0	0	0
All	All	3255	2980	2972	33	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 5.

All (33) 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:A:326:CYS:HA	1:A:362:LEU:HD23	1.77	0.66
1:B:352:PHE:O	1:B:354:GLN:NE2	2.39	0.55
1:C:357:THR:HG23	1:C:359:ASP:H	1.73	0.54
1:C:335:TYR:OH	1:C:348:VAL:HG11	2.09	0.52
1:A:313:SER:OG	1:A:341:CYS:SG	2.67	0.52
1:A:341:CYS:HA	1:B:330:LYS:HE2	1.91	0.51
1:C:357:THR:HG22	1:C:360:HIS:CD2	2.46	0.51
1:A:343:GLU:O	1:A:345:PRO:HD3	2.11	0.50
1:E:324:TYR:CE2	1:E:364:LEU:HD13	2.47	0.50
1:B:329:CYS:SG	1:B:355:GLN:O	2.71	0.49
1:D:326:CYS:HA	1:D:362:LEU:HD23	1.94	0.49
1:F:314:CYS:HB3	1:F:341:CYS:SG	2.53	0.48
1:E:343:GLU:O	1:E:345:PRO:HD3	2.15	0.47
1:E:348:VAL:HG12	1:E:350:GLY:N	2.30	0.47
1:D:343:GLU:O	1:D:345:PRO:HD3	2.16	0.45
1:A:308:GLY:O	1:E:299:LYS:HA	2.17	0.45
1:C:323:ARG:O	1:C:364:LEU:HD12	2.16	0.45
1:F:313:SER:OG	1:F:341:CYS:HB3	2.17	0.44
1:C:358:PRO:O	1:C:361:ARG:NH2	2.51	0.43
1:F:346:SER:O	1:F:348:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:SER:OG	1:D:366:ARG:CD	2.67	0.43
1:A:327:LYS:HE3	1:A:363:GLU:HB3	2.00	0.43
1:B:327:LYS:HE2	1:B:363:GLU:HB2	2.01	0.43
1:D:340:ASP:HA	1:D:343:GLU:HG2	2.00	0.42
1:E:323:ARG:NE	1:E:336:ASP:OD2	2.47	0.42
1:C:330:LYS:HG2	1:C:331:GLU:N	2.35	0.41
1:D:342:TYR:HE1	1:D:362:LEU:HD12	1.84	0.41
1:E:327:LYS:HD2	1:E:363:GLU:HB2	2.01	0.41
1:A:308:GLY:HA2	1:A:317:TYR:OH	2.21	0.41
1:C:357:THR:HG23	1:C:359:ASP:N	2.35	0.41
1:D:348:VAL:HG13	1:D:349:PRO:HD2	2.02	0.41
1:D:330:LYS:HE3	1:D:330:LYS:HB2	1.87	0.41
1:C:348:VAL:O	1:C:348:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
1	B	66/69 (96%)	66 (100%)	0	0	100	100
1	C	62/69 (90%)	62 (100%)	0	0	100	100
1	D	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
1	E	64/69 (93%)	63 (98%)	1 (2%)	0	100	100
1	F	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
All	All	392/414 (95%)	386 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	58/59 (98%)	58 (100%)	0	100	100
1	B	58/59 (98%)	58 (100%)	0	100	100
1	C	56/59 (95%)	55 (98%)	1 (2%)	59	65
1	D	59/59 (100%)	59 (100%)	0	100	100
1	E	58/59 (98%)	58 (100%)	0	100	100
1	F	59/59 (100%)	59 (100%)	0	100	100
All	All	348/354 (98%)	347 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	330	LYS

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

Mol	Chain	Res	Type
1	B	354	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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 14 ligands modelled in this entry, 14 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	68/69 (98%)	0.83	9 (13%) 3 4	43, 65, 92, 106	0
1	B	68/69 (98%)	1.01	10 (14%) 2 3	43, 67, 91, 99	0
1	C	66/69 (95%)	0.63	4 (6%) 21 26	42, 63, 89, 98	0
1	D	69/69 (100%)	0.61	3 (4%) 35 41	39, 63, 91, 100	0
1	E	68/69 (98%)	0.81	8 (11%) 4 5	47, 65, 93, 98	0
1	F	69/69 (100%)	1.18	16 (23%) 0 0	49, 75, 99, 115	0
All	All	408/414 (98%)	0.85	50 (12%) 4 5	39, 67, 96, 115	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	GLN	4.0
1	A	359	ASP	4.0
1	F	343	GLU	4.0
1	B	363	GLU	3.9
1	F	331	GLU	3.7
1	F	358	PRO	3.7
1	D	359	ASP	3.7
1	F	362	LEU	3.7
1	E	347	LYS	3.5
1	F	359	ASP	3.4
1	F	347	LYS	3.3
1	E	366	ARG	3.3
1	D	330	LYS	3.3
1	B	344	THR	3.3
1	B	347	LYS	3.2
1	A	348	VAL	3.1
1	A	350	GLY	3.0
1	B	349	PRO	3.0
1	C	348	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLU	2.9
1	F	350	GLY	2.8
1	F	332	GLU	2.8
1	E	355	GLN	2.8
1	F	366	ARG	2.8
1	B	351	ARG	2.8
1	F	355	GLN	2.7
1	A	333	ILE	2.7
1	B	359	ASP	2.7
1	A	332	GLU	2.6
1	E	362	LEU	2.5
1	A	347	LYS	2.5
1	B	329	CYS	2.5
1	F	344	THR	2.4
1	B	365	ALA	2.4
1	F	324	TYR	2.4
1	F	364	LEU	2.3
1	E	359	ASP	2.3
1	E	327	LYS	2.3
1	A	346	SER	2.3
1	F	348	VAL	2.2
1	C	345	PRO	2.2
1	A	342	TYR	2.2
1	D	366	ARG	2.2
1	C	361	ARG	2.2
1	F	361	ARG	2.2
1	F	349	PRO	2.1
1	B	355	GLN	2.1
1	E	349	PRO	2.1
1	E	363	GLU	2.0
1	C	320	ILE	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

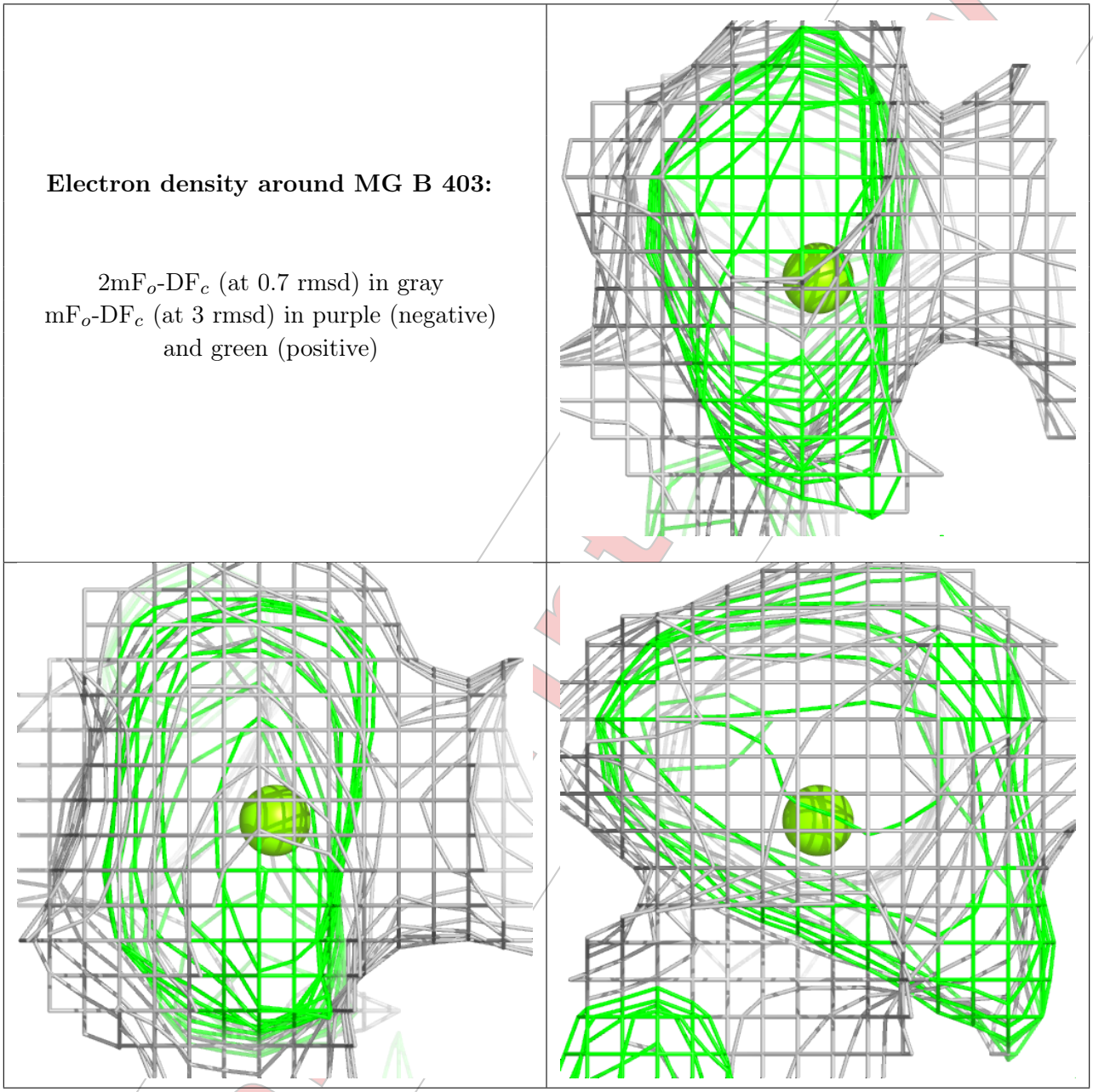
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	B	403	1/1	-0.29	0.78	128,128,128,128	0
2	ZN	A	402	1/1	0.74	0.10	77,77,77,77	0
2	ZN	B	402	1/1	0.78	0.08	81,81,81,81	0
2	ZN	D	402	1/1	0.80	0.10	81,81,81,81	0
3	MG	A	403	1/1	0.86	0.25	23,23,23,23	0
2	ZN	F	402	1/1	0.88	0.14	96,96,96,96	0
2	ZN	E	401	1/1	0.88	0.08	69,69,69,69	0
2	ZN	E	402	1/1	0.88	0.12	82,82,82,82	0
2	ZN	A	401	1/1	0.91	0.07	67,67,67,67	0
2	ZN	C	402	1/1	0.92	0.08	64,64,64,64	0
2	ZN	C	401	1/1	0.92	0.07	59,59,59,59	0
2	ZN	F	401	1/1	0.92	0.04	75,75,75,75	0
2	ZN	B	401	1/1	0.94	0.14	70,70,70,70	0
2	ZN	D	401	1/1	0.96	0.08	57,57,57,57	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.

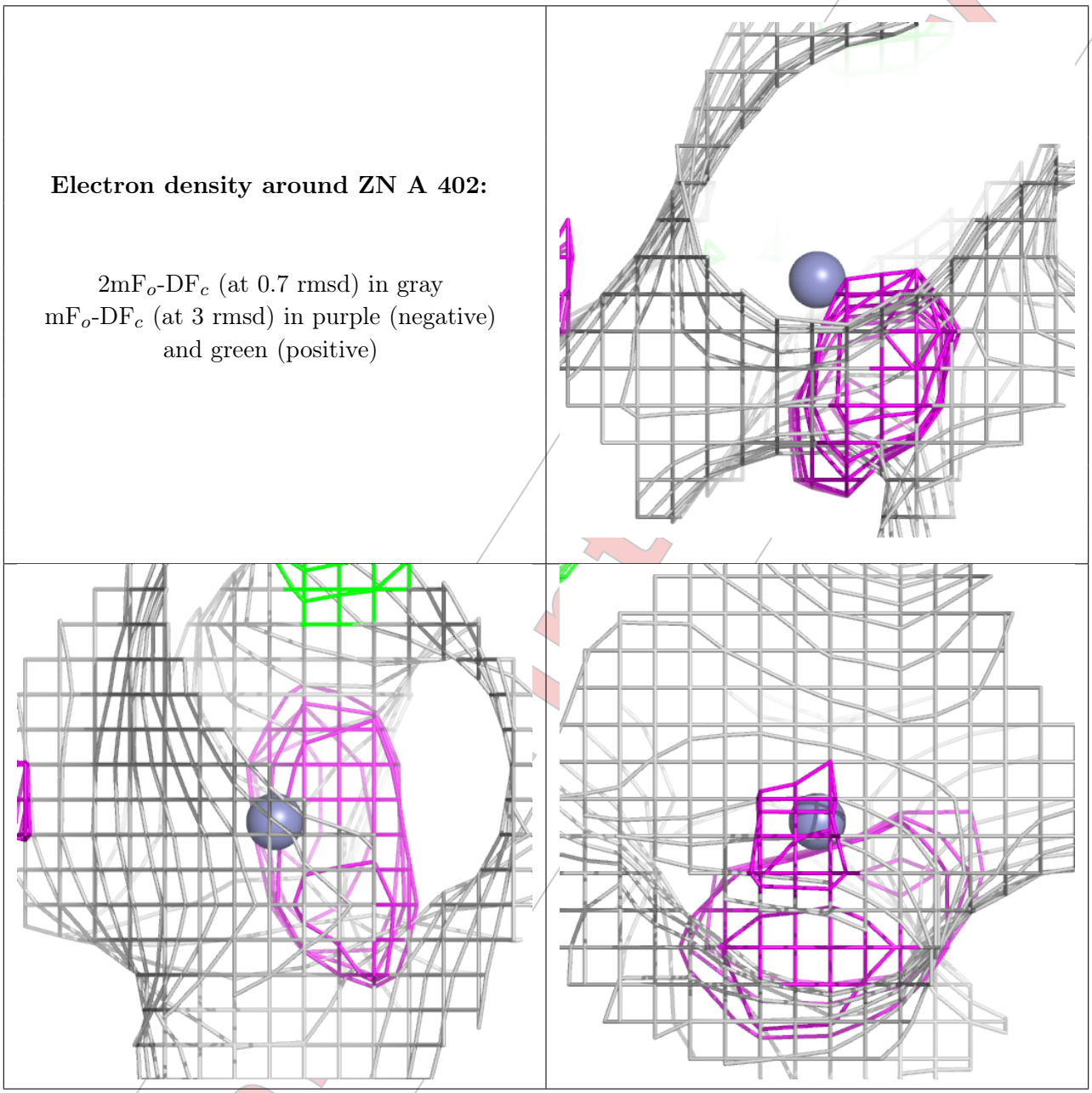
Electron density around MG B 403:

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



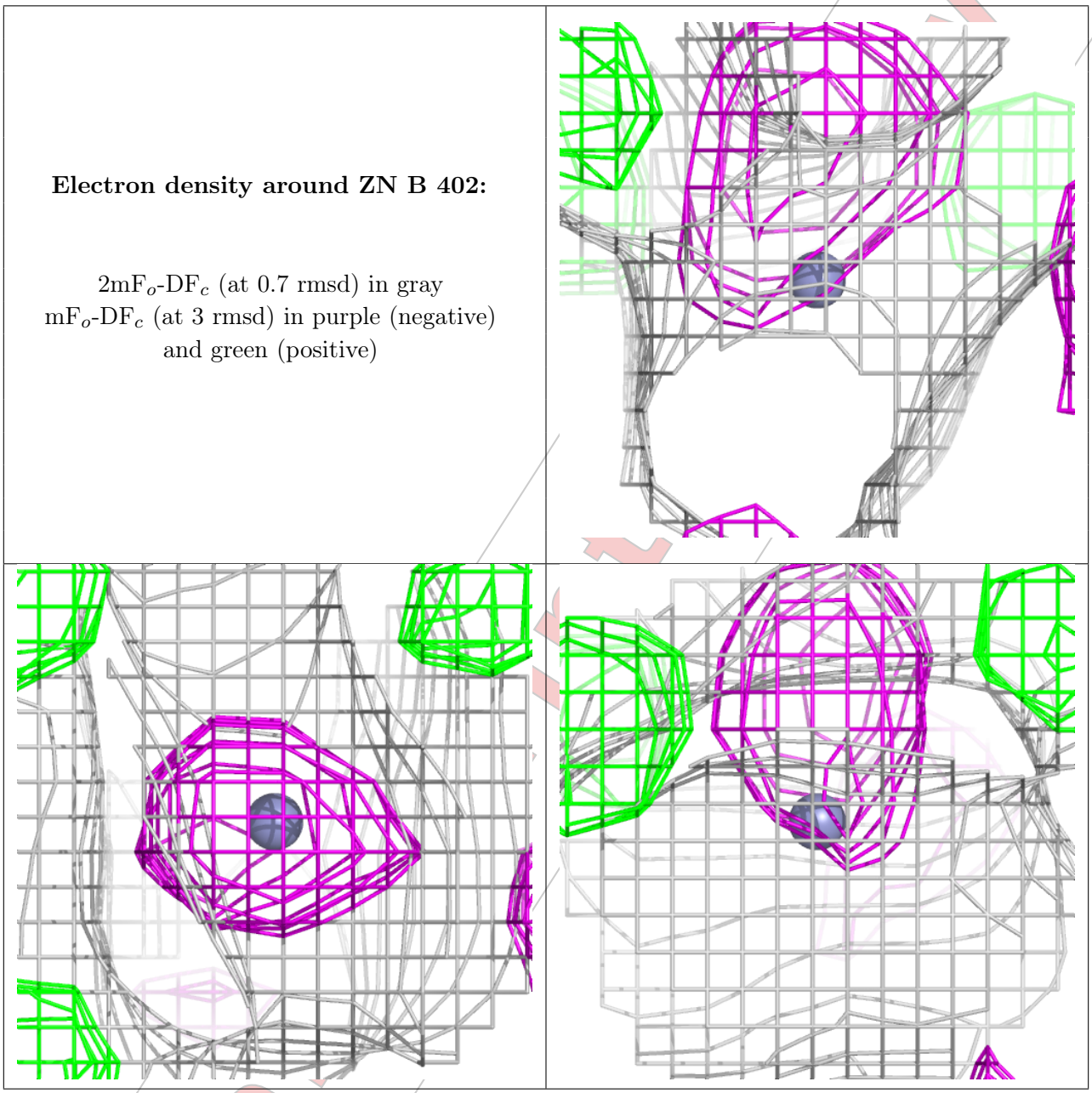
Electron density around ZN A 402:

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



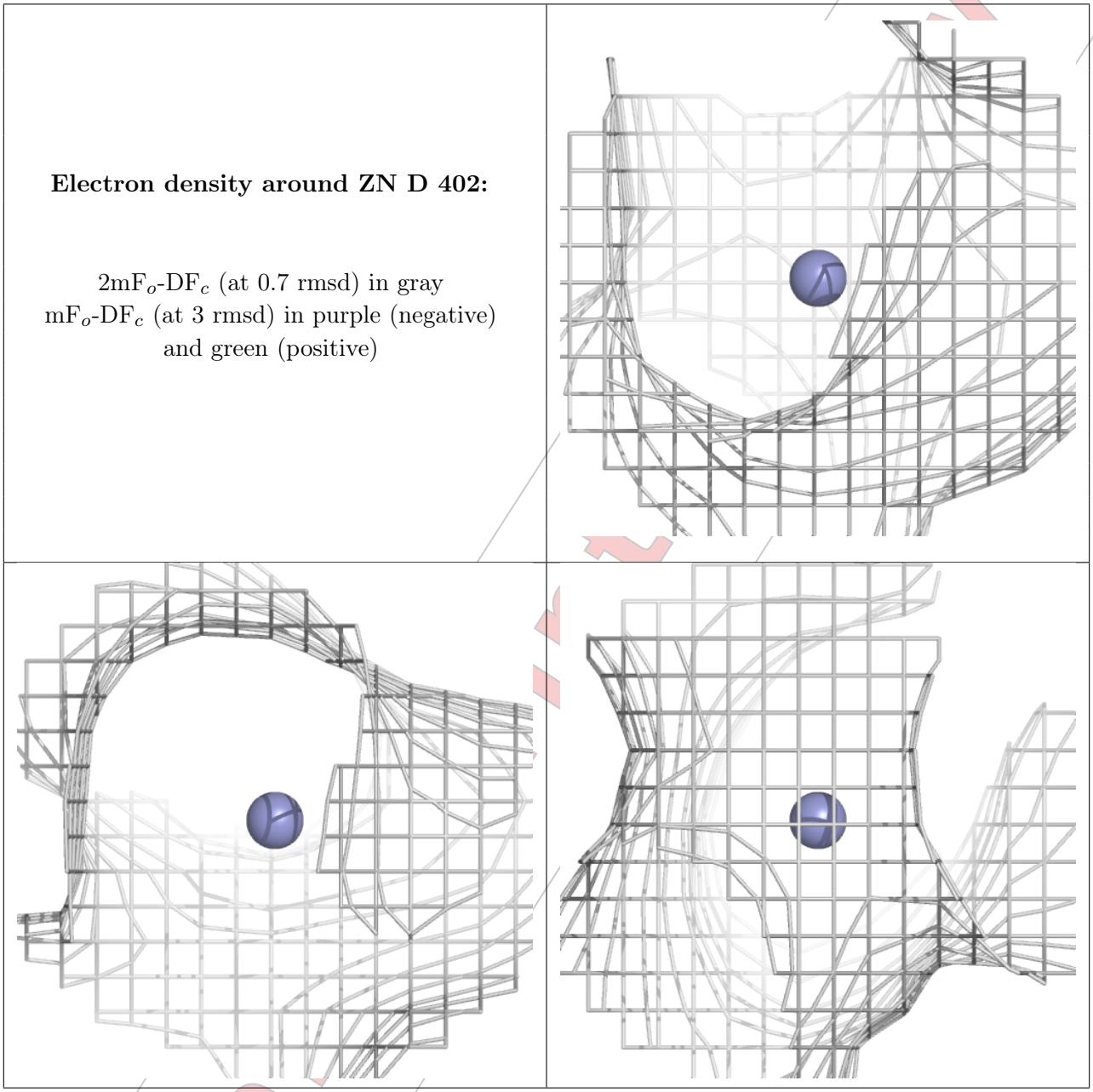
Electron density around ZN B 402:

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



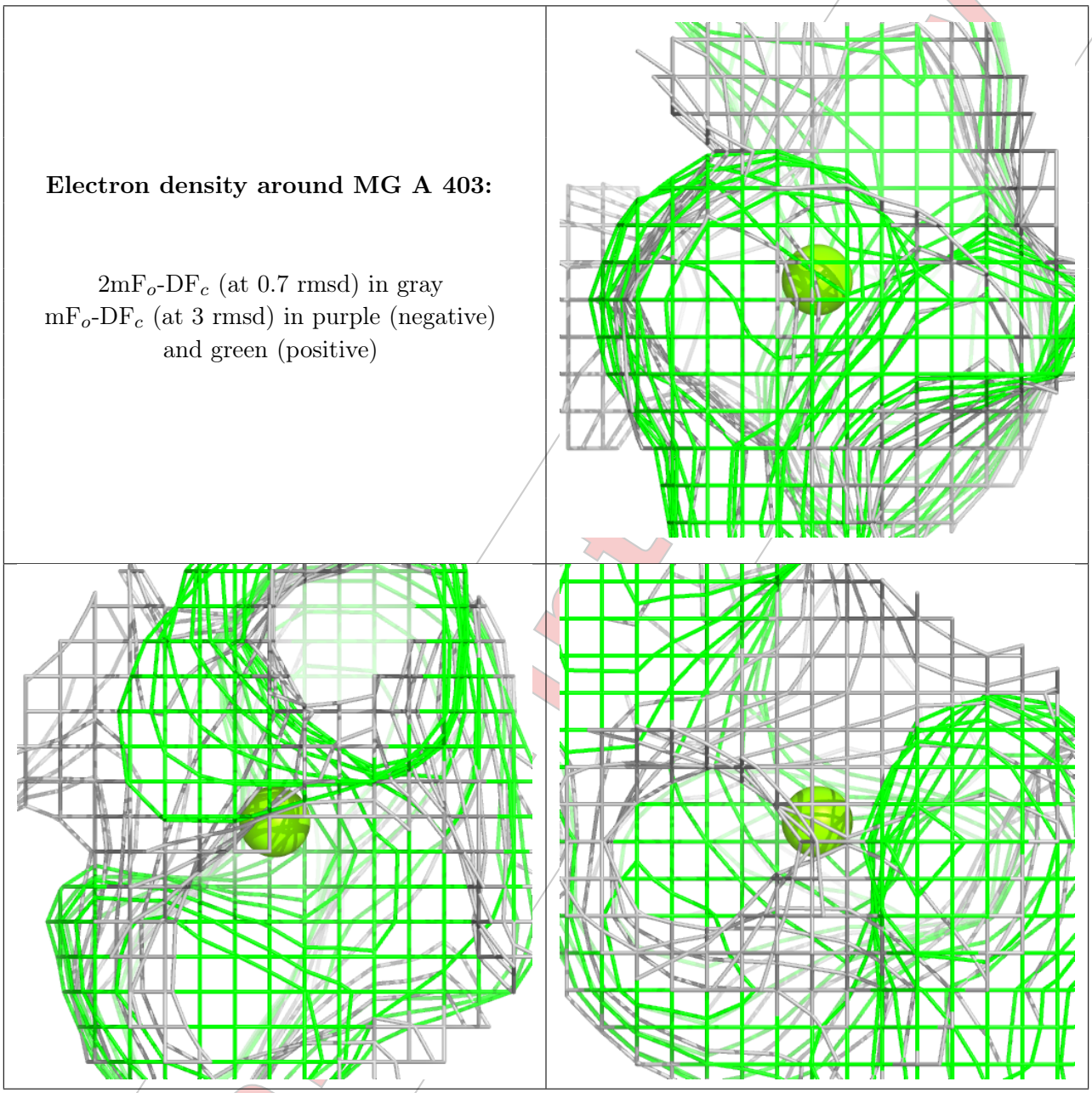
Electron density around ZN D 402:

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



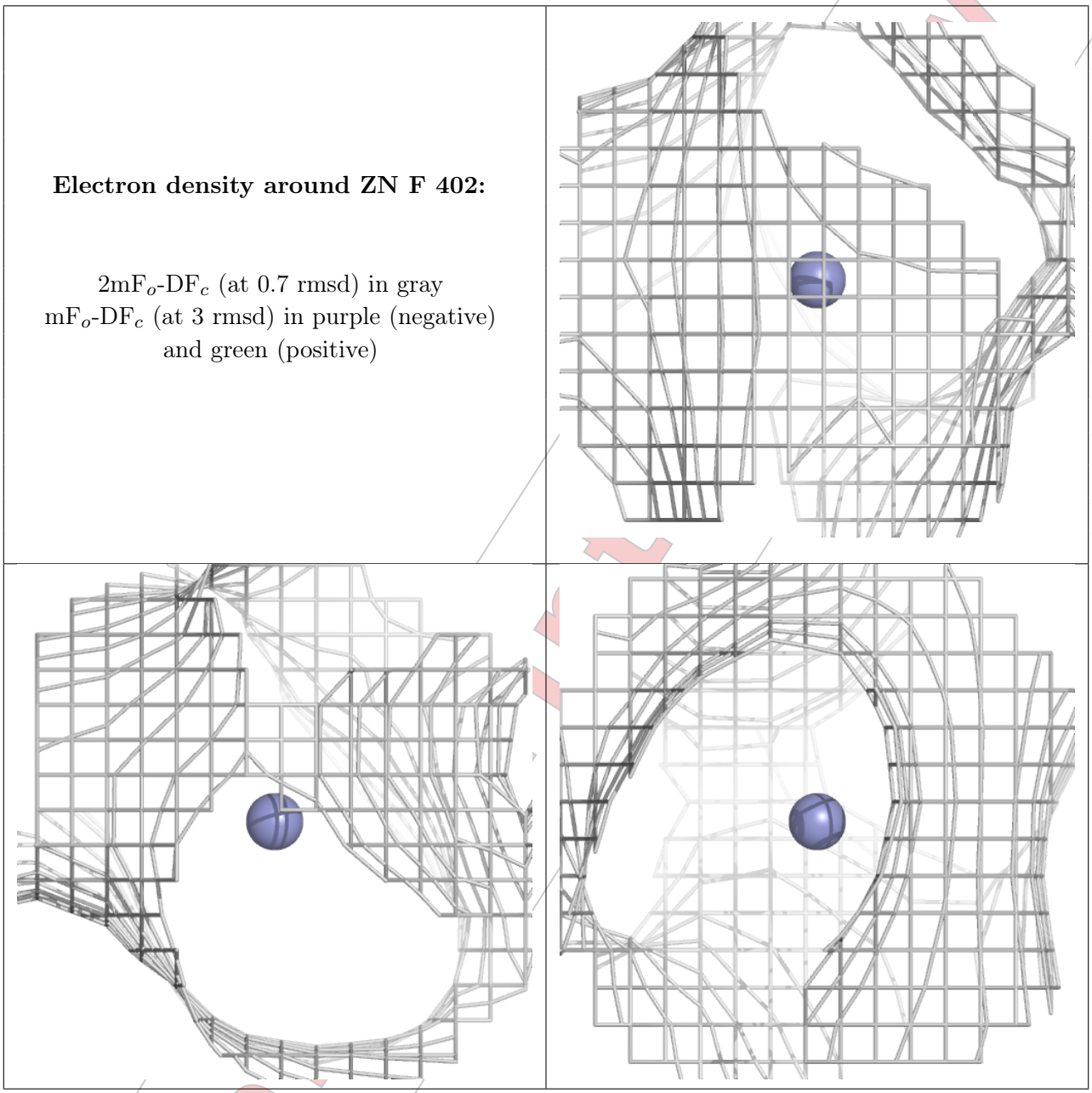
Electron density around MG A 403:

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



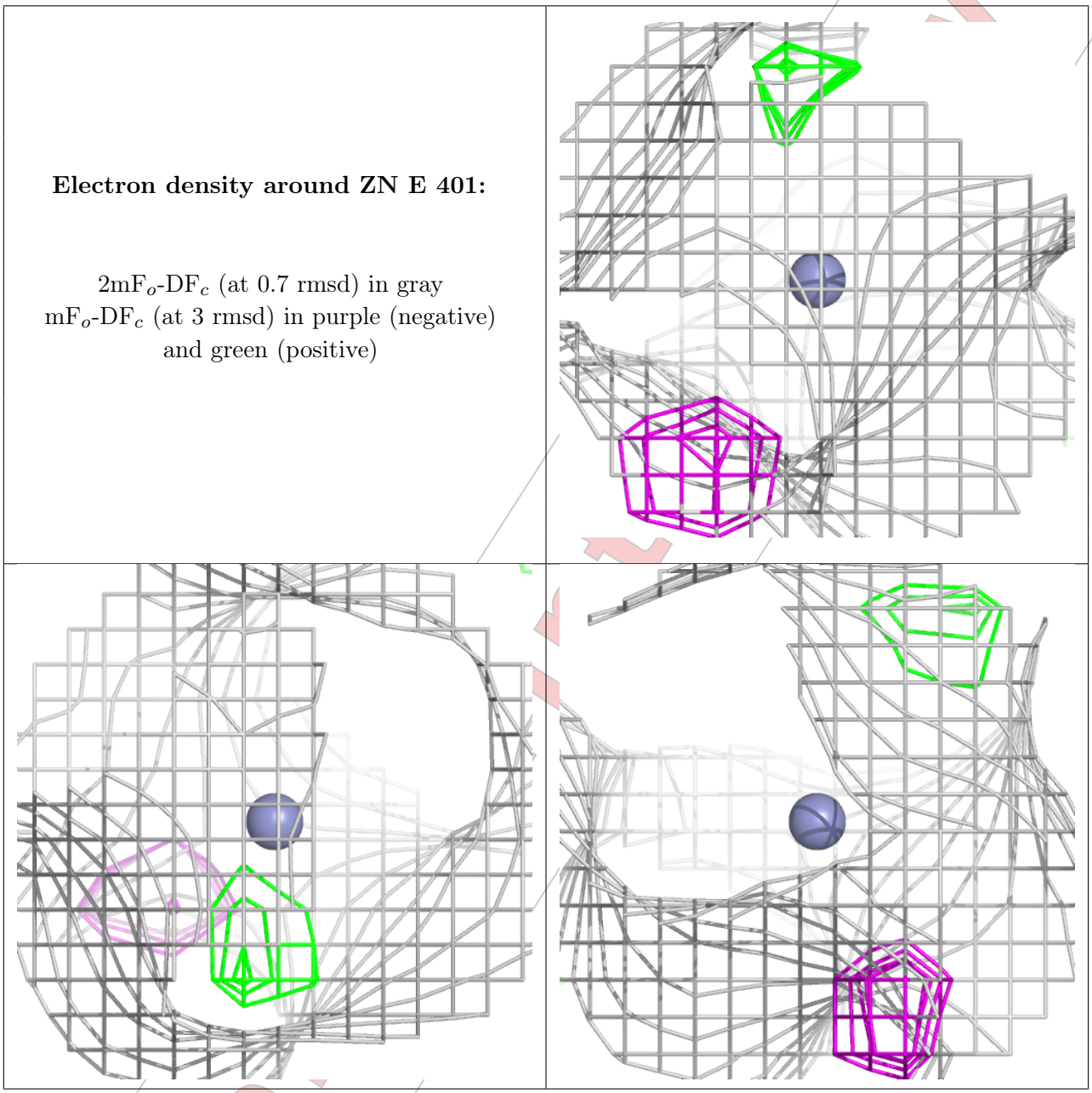
Electron density around ZN F 402:

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



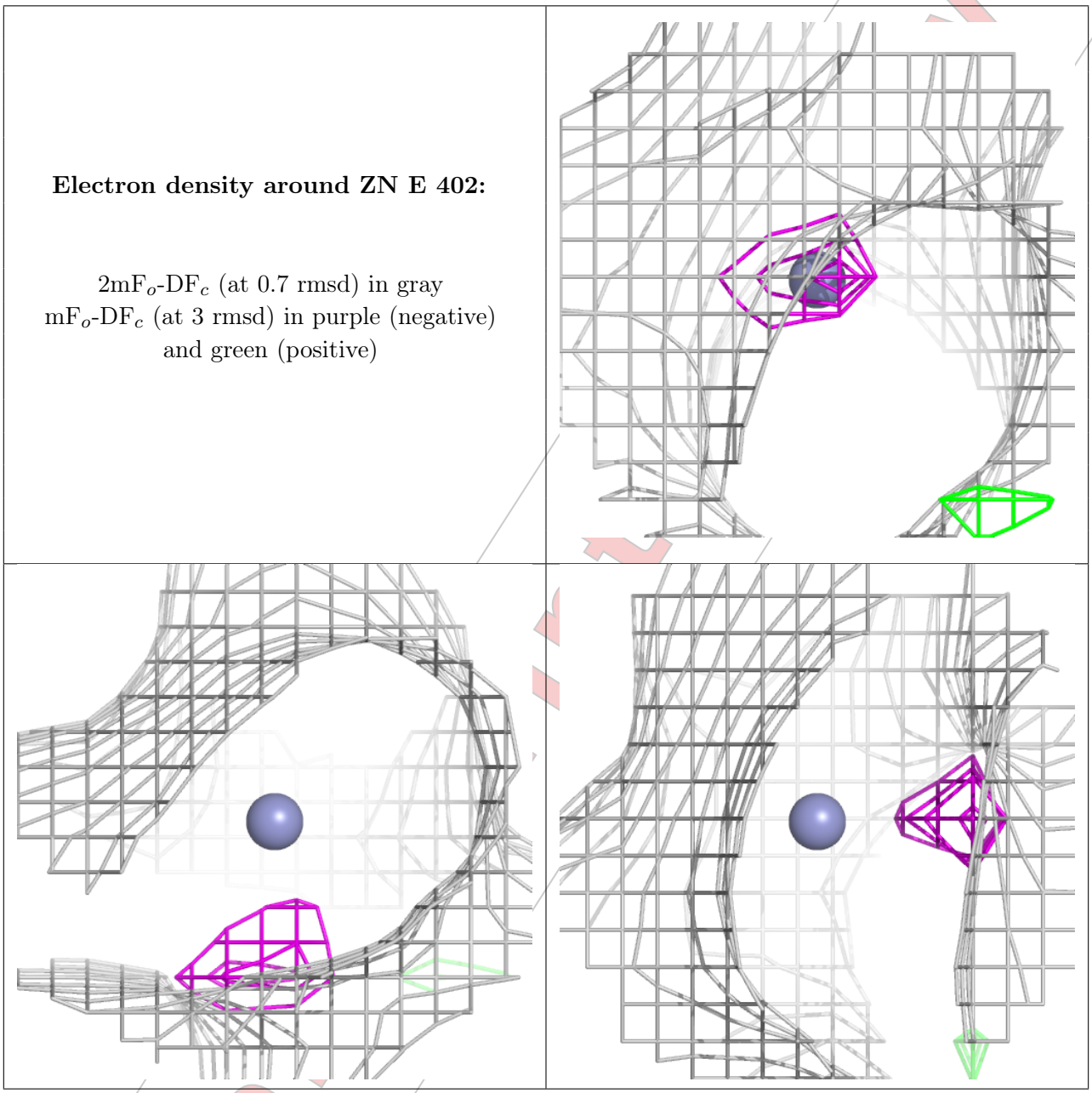
Electron density around ZN E 401:

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



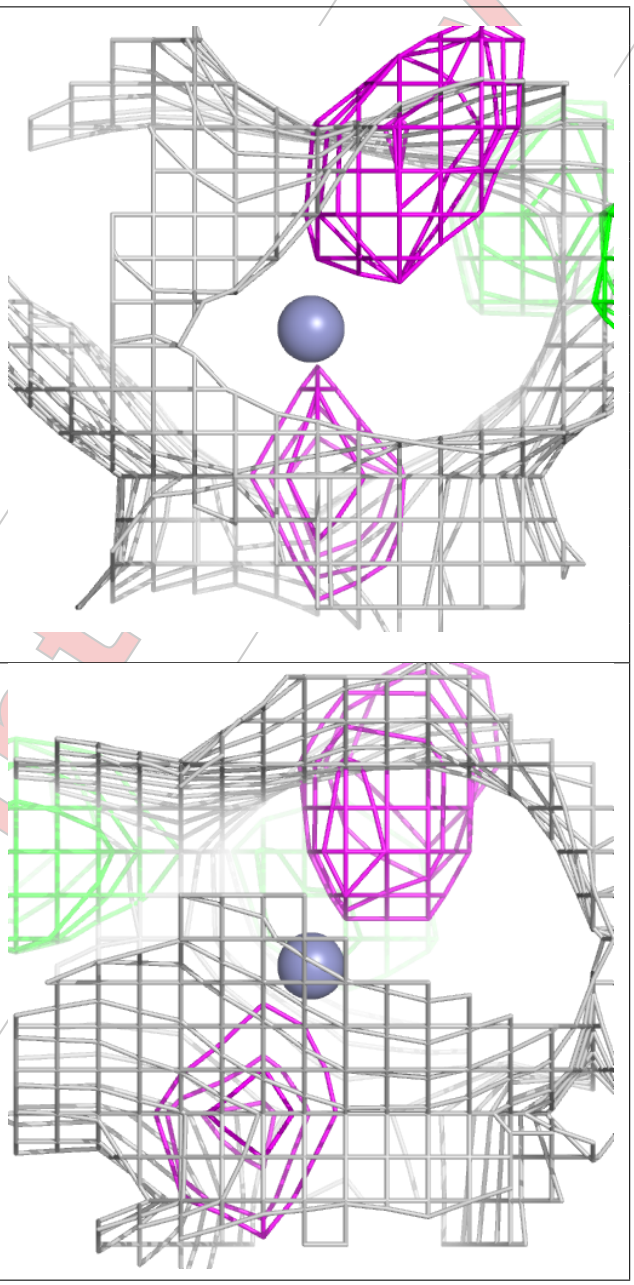
Electron density around ZN E 402:

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



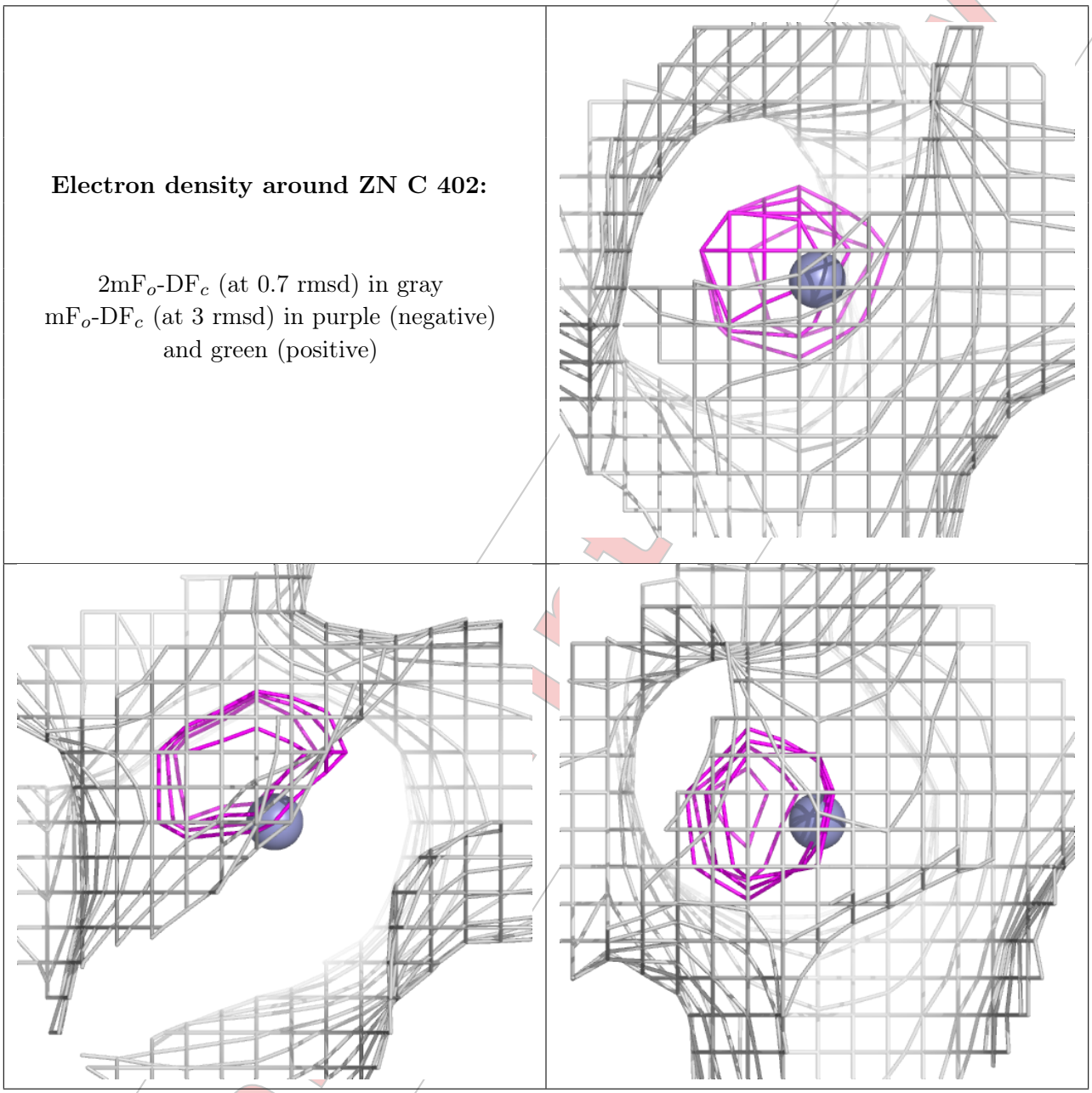
Electron density around ZN A 401:

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



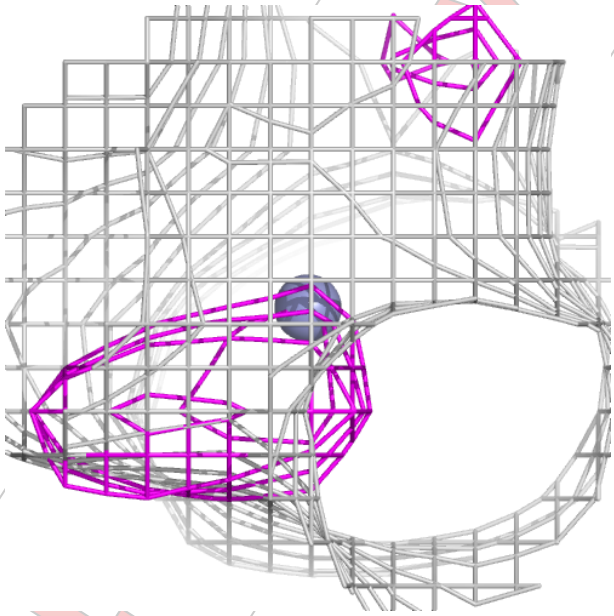
Electron density around ZN C 402:

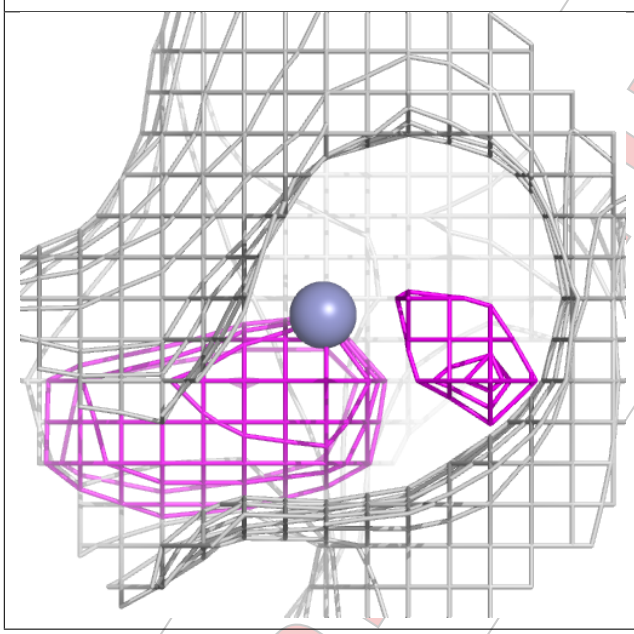
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

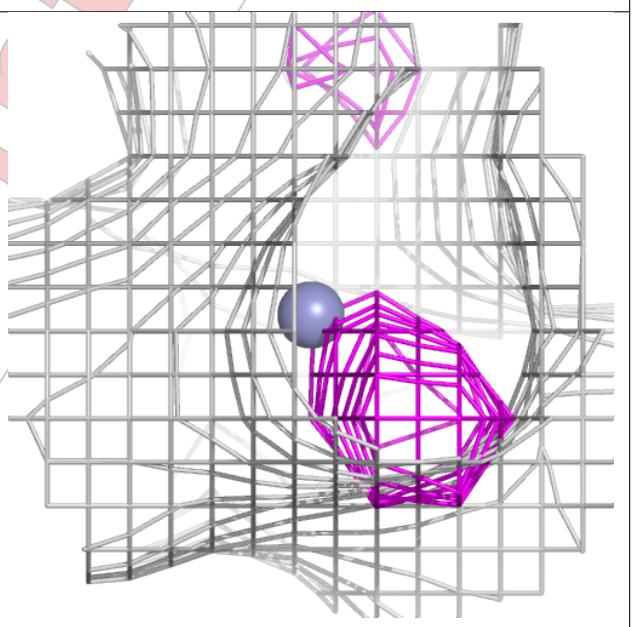


Electron density around ZN C 401:

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

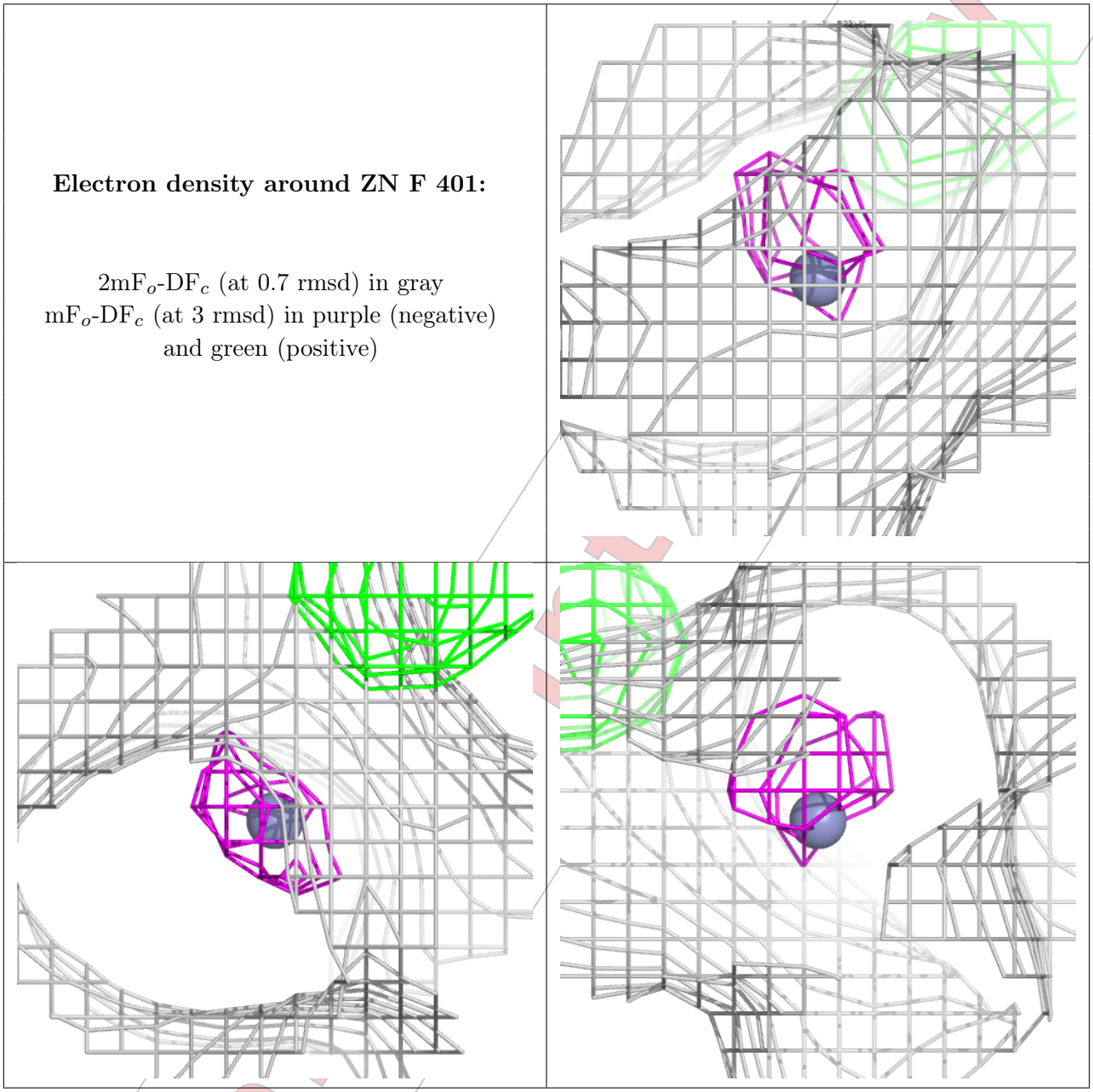






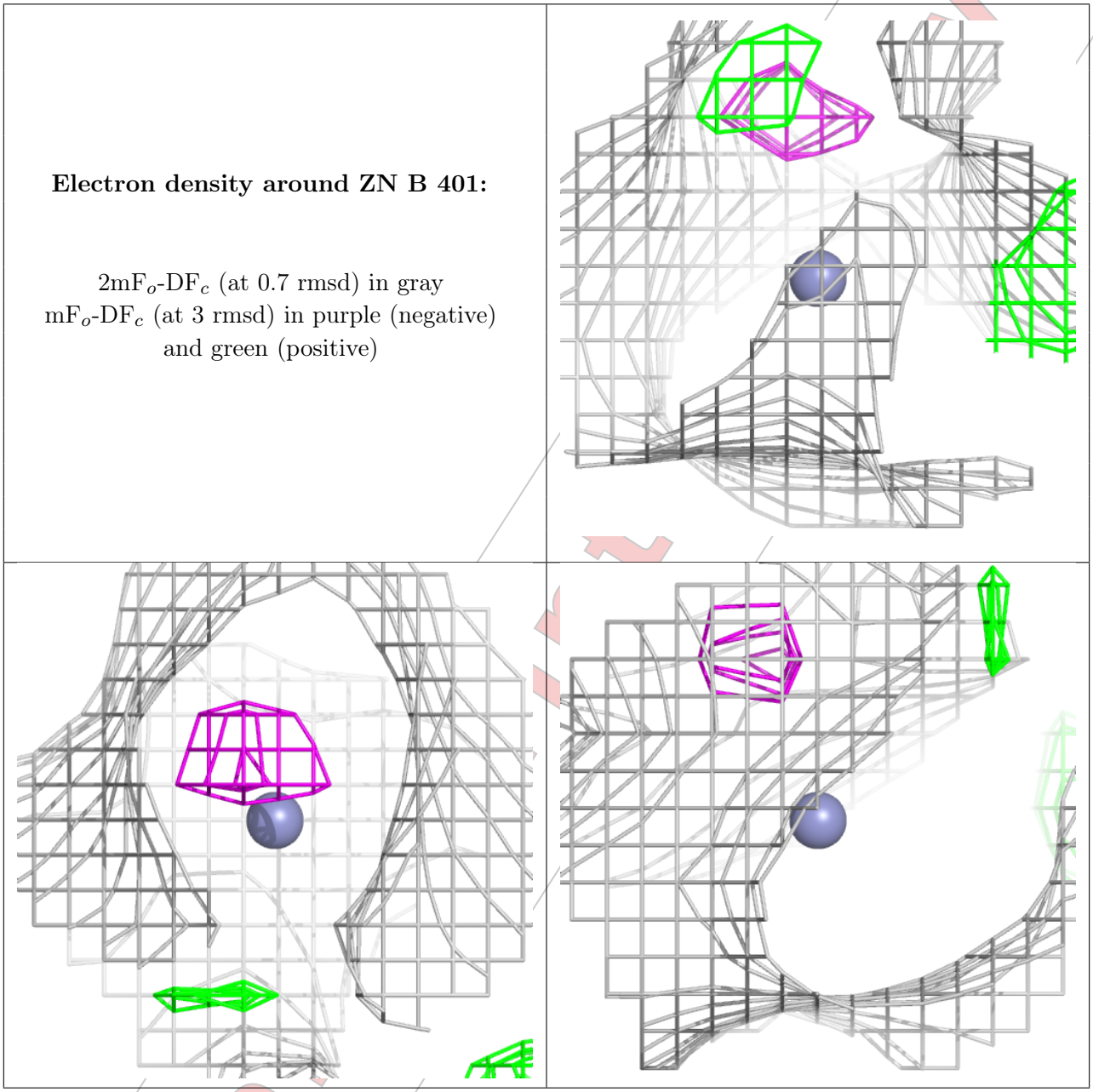
Electron density around ZN F 401:

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



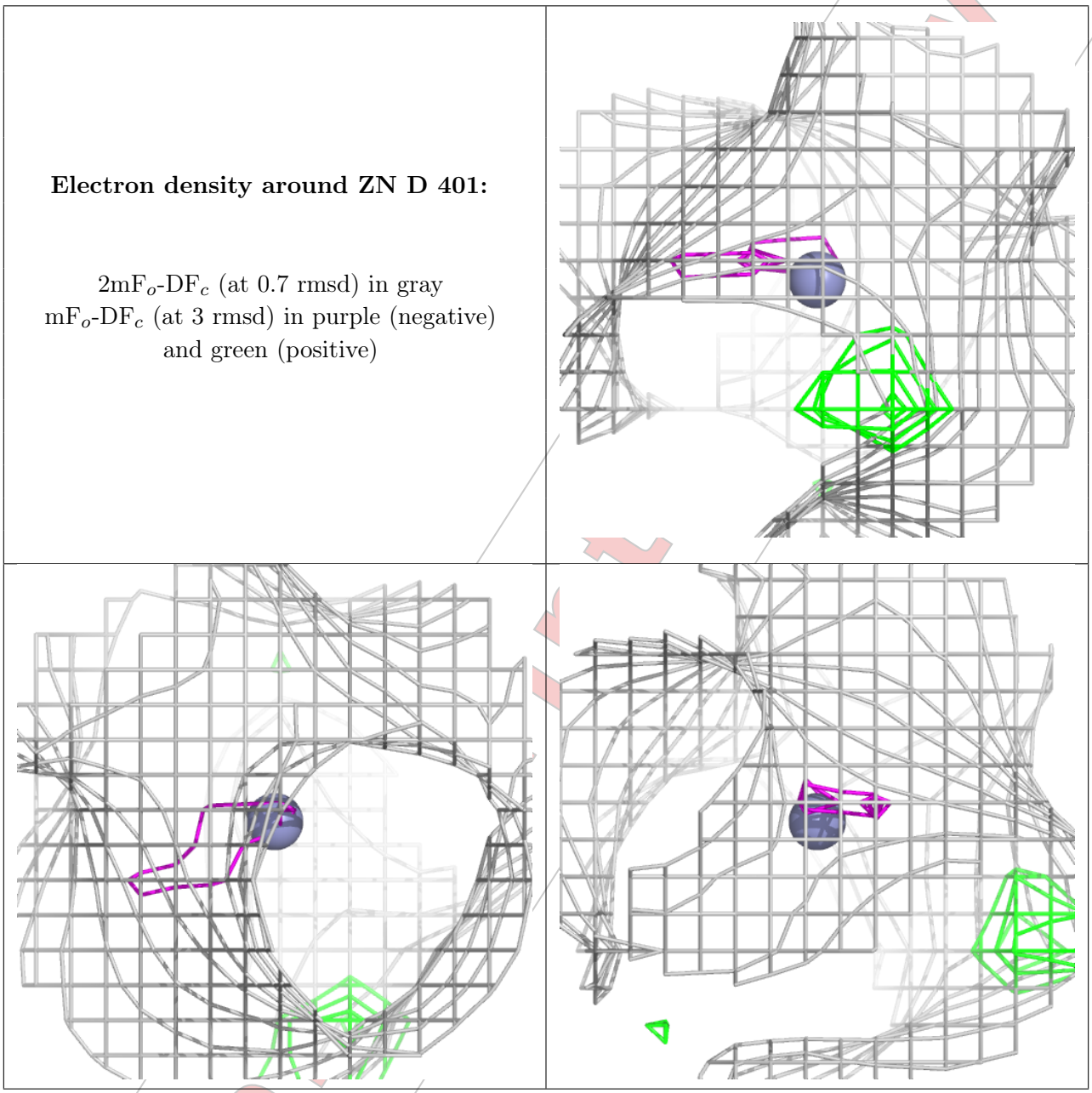
Electron density around ZN B 401:

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



Electron density around ZN D 401:

$2mF_o$-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.