wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2023 – 10:26 PM JST

PDB ID	:	7C06
Title	:	Crystal structure of yeast U2AF1 complex bound to 3' splice site RNA, 5'-UAGGU.
Authors	:	Yoshida, H.; Park, S.Y.; Urano, T.; Obayashi, E.
Deposited on	:	2020-04-30
Resolution	:	3.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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 (1)) were used in the production of this report:

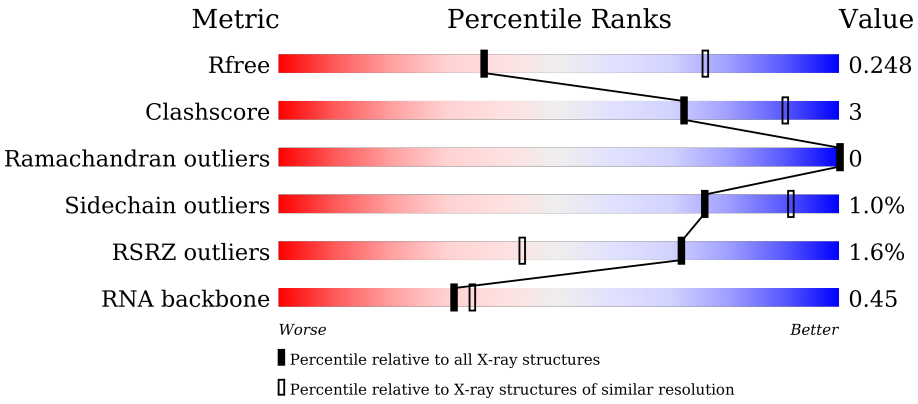
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)
RNA backbone	3102	1066 (3.30-2.74)

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	216	78% 11% 11%
1	D	216	80% 6% 13%
1	G	216	81% 8% 11%
1	J	216	83% 6% 11%

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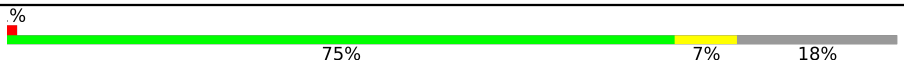
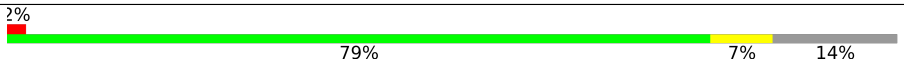
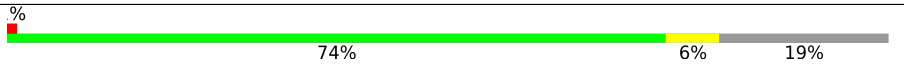
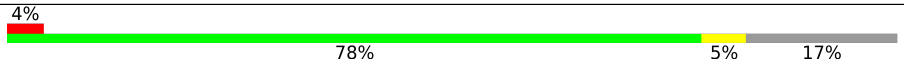
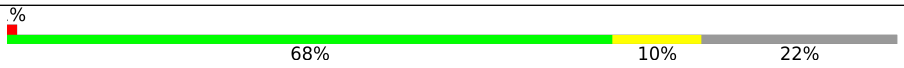
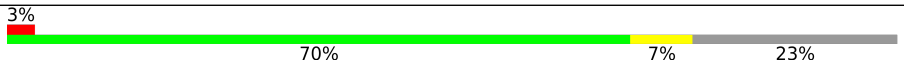
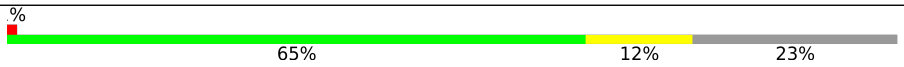
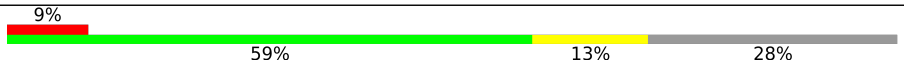
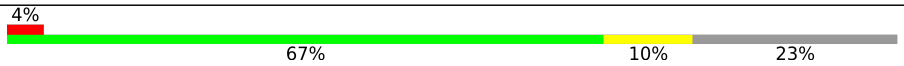
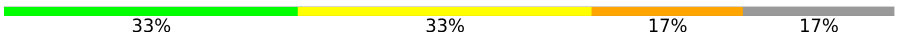
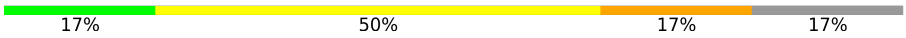
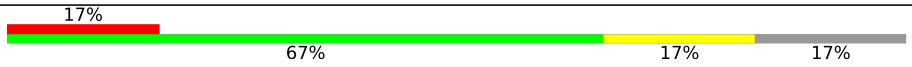
Mol	Chain	Length	Quality of chain
1	M	216	
1	P	216	
1	S	216	
1	V	216	
1	Y	216	
2	B	69	
2	E	69	
2	H	69	
2	K	69	
2	N	69	
2	Q	69	
2	T	69	
2	W	69	
2	Z	69	
3	1	6	
3	C	6	
3	F	6	
3	I	6	
3	L	6	
3	O	6	
3	R	6	
3	U	6	
3	X	6	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18418 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 protein called Splicing factor U2AF 23 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1567	981	278	295	13			
1	D	187	Total	C	N	O	S	0	0	0
			1524	955	270	286	13			
1	G	192	Total	C	N	O	S	0	0	0
			1558	976	277	292	13			
1	J	193	Total	C	N	O	S	0	0	0
			1567	981	278	295	13			
1	M	178	Total	C	N	O	S	0	0	0
			1452	911	259	269	13			
1	P	192	Total	C	N	O	S	0	0	0
			1558	976	277	292	13			
1	S	186	Total	C	N	O	S	0	1	0
			1524	955	271	285	13			
1	V	174	Total	C	N	O	S	0	0	0
			1419	892	254	260	13			
1	Y	179	Total	C	N	O	S	0	0	0
			1461	916	260	272	13			

- Molecule 2 is a protein called Splicing factor U2AF 59 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			455	288	82	84	1			
2	E	51	Total	C	N	O	S	0	0	0
			417	266	74	76	1			
2	H	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	K	54	Total	C	N	O	S	0	0	0
			435	277	77	80	1			
2	N	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	T	50	Total	C	N	O	S	0	0	0
			406	260	70	75	1			
2	W	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	Z	48	Total	C	N	O	S	0	0	0
			392	251	68	72	1			

- Molecule 3 is a RNA chain called RNA (5'-R(*U*UP*AP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	F	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	I	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	L	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	O	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	R	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	U	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	X	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			
3	1	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	J	2	Total	Zn	0	0
			2	2		

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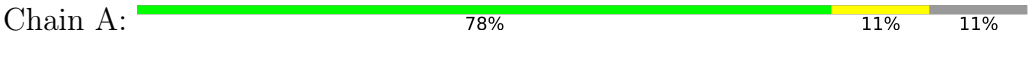
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	2	Total Zn 2 2	0	0
4	P	2	Total Zn 2 2	0	0
4	S	2	Total Zn 2 2	0	0
4	V	2	Total Zn 2 2	0	0
4	Y	2	Total Zn 2 2	0	0

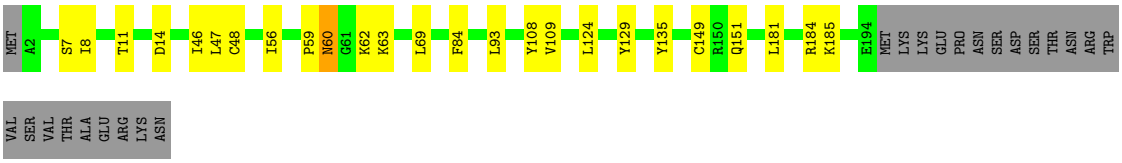
3 Residue-property plots (i)

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: Splicing factor U2AF 23 kDa subunit

Chain A:





• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain D:

• Molecule 1: Splicing factor U2AF 23 kDa subunit

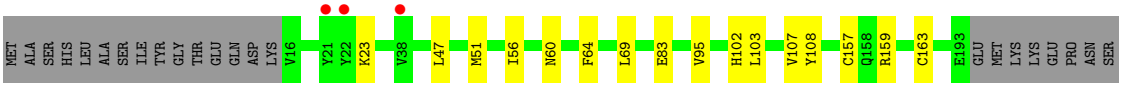
Chain G:

• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain J:

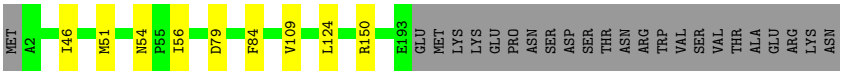
• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain M:



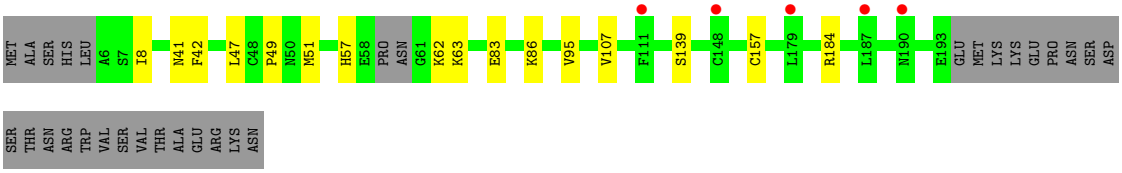
• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain P:



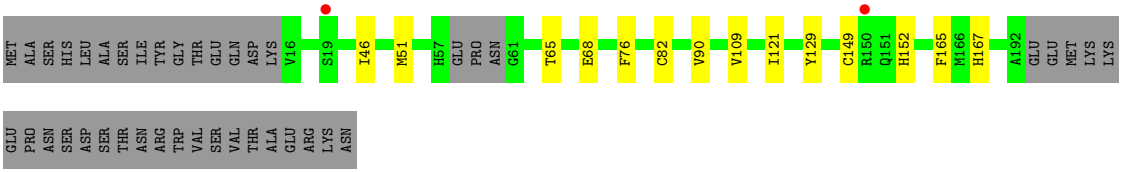
• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain S:



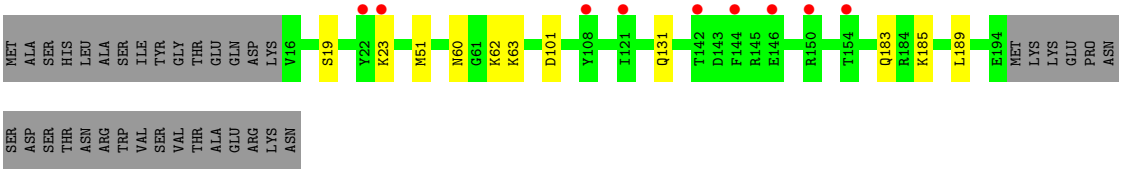
• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain V:



• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain Y:

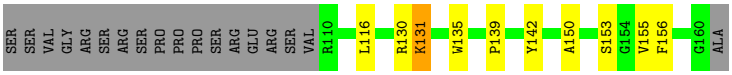


• Molecule 2: Splicing factor U2AF 59 kDa subunit

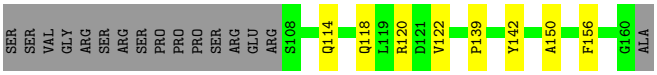
Chain B:

• Molecule 2: Splicing factor U2AF 59 kDa subunit

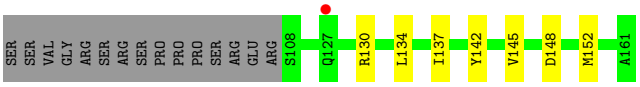
Chain E:



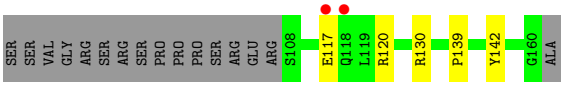
• Molecule 2: Splicing factor U2AF 59 kDa subunit



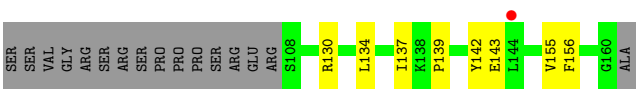
• Molecule 2: Splicing factor U2AF 59 kDa subunit



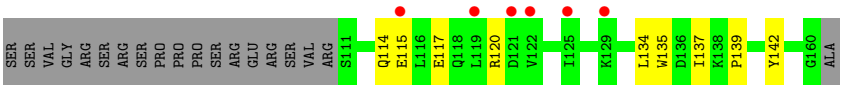
• Molecule 2: Splicing factor U2AF 59 kDa subunit



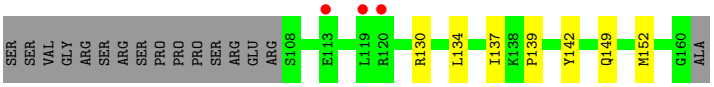
• Molecule 2: Splicing factor U2AF 59 kDa subunit



• Molecule 2: Splicing factor U2AF 59 kDa subunit



• Molecule 2: Splicing factor U2AF 59 kDa subunit

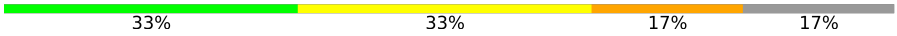


• Molecule 2: Splicing factor U2AF 59 kDa subunit

Chain Z:

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

Chain C:



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

Chain F:

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

Chain I:

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

Chain L:

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

Chain O:

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

Chain R:

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

Chain U:

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

Chain X:

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

Chain 1:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.82Å 255.10Å 94.11Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	38.41 – 3.02 48.86 – 3.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.41-3.02) 100.0 (48.86-3.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.215 , 0.249 0.214 , 0.248	Depositor DCC
R_{free} test set	4117 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18418	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/1604	0.41	0/2163
1	D	0.25	0/1560	0.42	0/2103
1	G	0.25	0/1595	0.42	0/2151
1	J	0.25	0/1604	0.41	0/2163
1	M	0.24	0/1487	0.41	0/2005
1	P	0.24	0/1595	0.41	0/2151
1	S	0.24	0/1559	0.42	0/2099
1	V	0.25	0/1452	0.40	0/1955
1	Y	0.25	0/1496	0.41	0/2017
2	B	0.23	0/465	0.40	0/629
2	E	0.24	0/427	0.41	0/578
2	H	0.24	0/440	0.43	0/596
2	K	0.24	0/445	0.43	0/603
2	N	0.23	0/440	0.40	0/596
2	Q	0.23	0/440	0.39	0/596
2	T	0.23	0/416	0.40	0/564
2	W	0.24	0/440	0.42	0/596
2	Z	0.24	0/402	0.47	0/545
3	1	0.10	0/117	0.56	0/181
3	C	0.17	0/117	0.66	0/181
3	F	0.12	0/117	0.58	0/181
3	I	0.16	0/117	0.61	0/181
3	L	0.14	0/117	0.65	0/181
3	O	0.13	0/117	0.70	0/181
3	R	0.14	0/117	0.58	0/181
3	U	0.12	0/117	0.61	0/181
3	X	0.14	0/117	0.73	0/181
All	All	0.24	0/18920	0.43	0/25739

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	1567	0	1487	16	0
1	D	1524	0	1448	11	0
1	G	1558	0	1481	11	0
1	J	1567	0	1487	9	0
1	M	1452	0	1382	8	0
1	P	1558	0	1481	5	0
1	S	1524	0	1445	12	0
1	V	1419	0	1356	9	0
1	Y	1461	0	1388	8	0
2	B	455	0	460	5	0
2	E	417	0	422	9	0
2	H	430	0	436	6	0
2	K	435	0	441	6	0
2	N	430	0	436	3	0
2	Q	430	0	436	5	0
2	T	406	0	409	6	0
2	W	430	0	436	4	0
2	Z	392	0	393	9	0
3	1	105	0	55	2	0
3	C	105	0	55	2	0
3	F	105	0	55	0	0
3	I	105	0	55	4	0
3	L	105	0	55	0	0
3	O	105	0	55	1	0
3	R	105	0	55	1	0
3	U	105	0	55	0	0
3	X	105	0	55	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	2	0	0	0	0
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
All	All	18418	0	17319	121	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 3.

The worst 5 of 121 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:J:59:PRO:O	1:J:60:ASN:ND2	2.26	0.69
1:A:59:PRO:O	1:A:60:ASN:ND2	2.27	0.67
1:D:155:SER:HA	1:J:59:PRO:HB3	1.78	0.66
1:A:11:THR:HB	3:C:5:U:H5'	1.81	0.62
1:Y:185:LYS:NZ	2:Z:122:VAL:O	2.35	0.60

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	191/216 (88%)	183 (96%)	8 (4%)	0	100	100
1	D	185/216 (86%)	180 (97%)	5 (3%)	0	100	100
1	G	190/216 (88%)	184 (97%)	6 (3%)	0	100	100
1	J	191/216 (88%)	185 (97%)	6 (3%)	0	100	100
1	M	176/216 (82%)	172 (98%)	4 (2%)	0	100	100
1	P	190/216 (88%)	185 (97%)	5 (3%)	0	100	100
1	S	183/216 (85%)	177 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	170/216 (79%)	167 (98%)	3 (2%)	0	100	100
1	Y	177/216 (82%)	172 (97%)	5 (3%)	0	100	100
2	B	54/69 (78%)	51 (94%)	3 (6%)	0	100	100
2	E	49/69 (71%)	45 (92%)	4 (8%)	0	100	100
2	H	51/69 (74%)	49 (96%)	2 (4%)	0	100	100
2	K	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
2	N	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	Q	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	T	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
2	W	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	Z	46/69 (67%)	40 (87%)	6 (13%)	0	100	100
All	All	2106/2565 (82%)	2031 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	170/192 (88%)	169 (99%)	1 (1%)	86	95
1	D	166/192 (86%)	165 (99%)	1 (1%)	86	95
1	G	169/192 (88%)	166 (98%)	3 (2%)	59	84
1	J	170/192 (88%)	169 (99%)	1 (1%)	86	95
1	M	158/192 (82%)	156 (99%)	2 (1%)	69	88
1	P	169/192 (88%)	168 (99%)	1 (1%)	86	95
1	S	165/192 (86%)	162 (98%)	3 (2%)	59	84
1	V	154/192 (80%)	153 (99%)	1 (1%)	86	95
1	Y	159/192 (83%)	156 (98%)	3 (2%)	57	83
2	B	50/62 (81%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	46/62 (74%)	45 (98%)	1 (2%)	52 80
2	H	48/62 (77%)	48 (100%)	0	100 100
2	K	48/62 (77%)	48 (100%)	0	100 100
2	N	48/62 (77%)	48 (100%)	0	100 100
2	Q	48/62 (77%)	48 (100%)	0	100 100
2	T	45/62 (73%)	45 (100%)	0	100 100
2	W	48/62 (77%)	48 (100%)	0	100 100
2	Z	43/62 (69%)	41 (95%)	2 (5%)	26 61
All	All	1904/2286 (83%)	1885 (99%)	19 (1%)	76 91

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	51	MET
2	Z	128	TRP
2	Z	131	LYS
1	Y	183	GLN
1	M	157	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	1	4/6 (66%)	1 (25%)	0
3	C	4/6 (66%)	1 (25%)	0
3	F	4/6 (66%)	0	0
3	I	4/6 (66%)	1 (25%)	0
3	L	4/6 (66%)	1 (25%)	0
3	O	4/6 (66%)	1 (25%)	0
3	R	4/6 (66%)	1 (25%)	0
3	U	4/6 (66%)	1 (25%)	0
3	X	4/6 (66%)	1 (25%)	0
All	All	36/54 (66%)	8 (22%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	5	U
3	I	5	U
3	L	5	U
3	O	5	U
3	R	5	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 18 ligands modelled in this entry, 18 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	193/216 (89%)	-0.15	0 100 100	38, 57, 99, 115	0
1	D	187/216 (86%)	-0.15	0 100 100	36, 53, 96, 114	0
1	G	192/216 (88%)	-0.24	0 100 100	31, 50, 89, 107	0
1	J	193/216 (89%)	-0.08	1 (0%) 91 75	45, 68, 104, 118	0
1	M	178/216 (82%)	0.14	3 (1%) 70 41	38, 67, 108, 121	0
1	P	192/216 (88%)	-0.16	0 100 100	41, 64, 93, 112	0
1	S	186/216 (86%)	0.22	5 (2%) 54 26	53, 74, 118, 136	0
1	V	174/216 (80%)	0.13	2 (1%) 80 55	57, 82, 107, 119	0
1	Y	179/216 (82%)	0.40	9 (5%) 28 10	44, 83, 118, 132	0
2	B	56/69 (81%)	-0.08	0 100 100	44, 65, 107, 126	0
2	E	51/69 (73%)	0.13	0 100 100	40, 66, 135, 138	0
2	H	53/69 (76%)	-0.22	0 100 100	30, 52, 100, 123	0
2	K	54/69 (78%)	0.14	1 (1%) 66 37	40, 68, 112, 143	0
2	N	53/69 (76%)	0.13	2 (3%) 40 16	42, 71, 133, 143	0
2	Q	53/69 (76%)	0.13	1 (1%) 66 37	56, 72, 118, 146	0
2	T	50/69 (72%)	0.50	6 (12%) 4 1	63, 84, 153, 164	0
2	W	53/69 (76%)	0.36	3 (5%) 23 8	66, 86, 135, 140	0
2	Z	48/69 (69%)	0.16	0 100 100	44, 72, 146, 152	0
3	1	5/6 (83%)	0.28	0 100 100	96, 105, 109, 128	0
3	C	5/6 (83%)	0.18	0 100 100	51, 52, 68, 84	0
3	F	5/6 (83%)	0.39	0 100 100	51, 52, 89, 115	0
3	I	5/6 (83%)	0.23	0 100 100	49, 59, 89, 89	0
3	L	5/6 (83%)	0.66	1 (20%) 1 0	66, 71, 80, 113	0
3	O	5/6 (83%)	0.04	0 100 100	90, 94, 103, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	R	5/6 (83%)	0.08	0 100 100	55, 56, 72, 90	0
3	U	5/6 (83%)	0.51	0 100 100	65, 65, 92, 130	0
3	X	5/6 (83%)	-0.05	0 100 100	89, 90, 100, 112	0
All	All	2190/2619 (83%)	0.04	34 (1%) 72 43	30, 68, 117, 164	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	120	ARG	3.5
2	T	129	LYS	3.3
2	T	119	LEU	3.3
1	Y	144	PHE	3.3
1	S	187	LEU	3.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	ZN	Y	302	1/1	0.97	0.12	73,73,73,73	0
4	ZN	V	302	1/1	0.98	0.14	67,67,67,67	0
4	ZN	J	302	1/1	0.98	0.18	62,62,62,62	0
4	ZN	G	301	1/1	0.99	0.18	44,44,44,44	0
4	ZN	G	302	1/1	0.99	0.18	41,41,41,41	0
4	ZN	J	301	1/1	0.99	0.18	55,55,55,55	0
4	ZN	A	301	1/1	0.99	0.20	51,51,51,51	0
4	ZN	M	301	1/1	0.99	0.17	78,78,78,78	0
4	ZN	M	302	1/1	0.99	0.15	54,54,54,54	0

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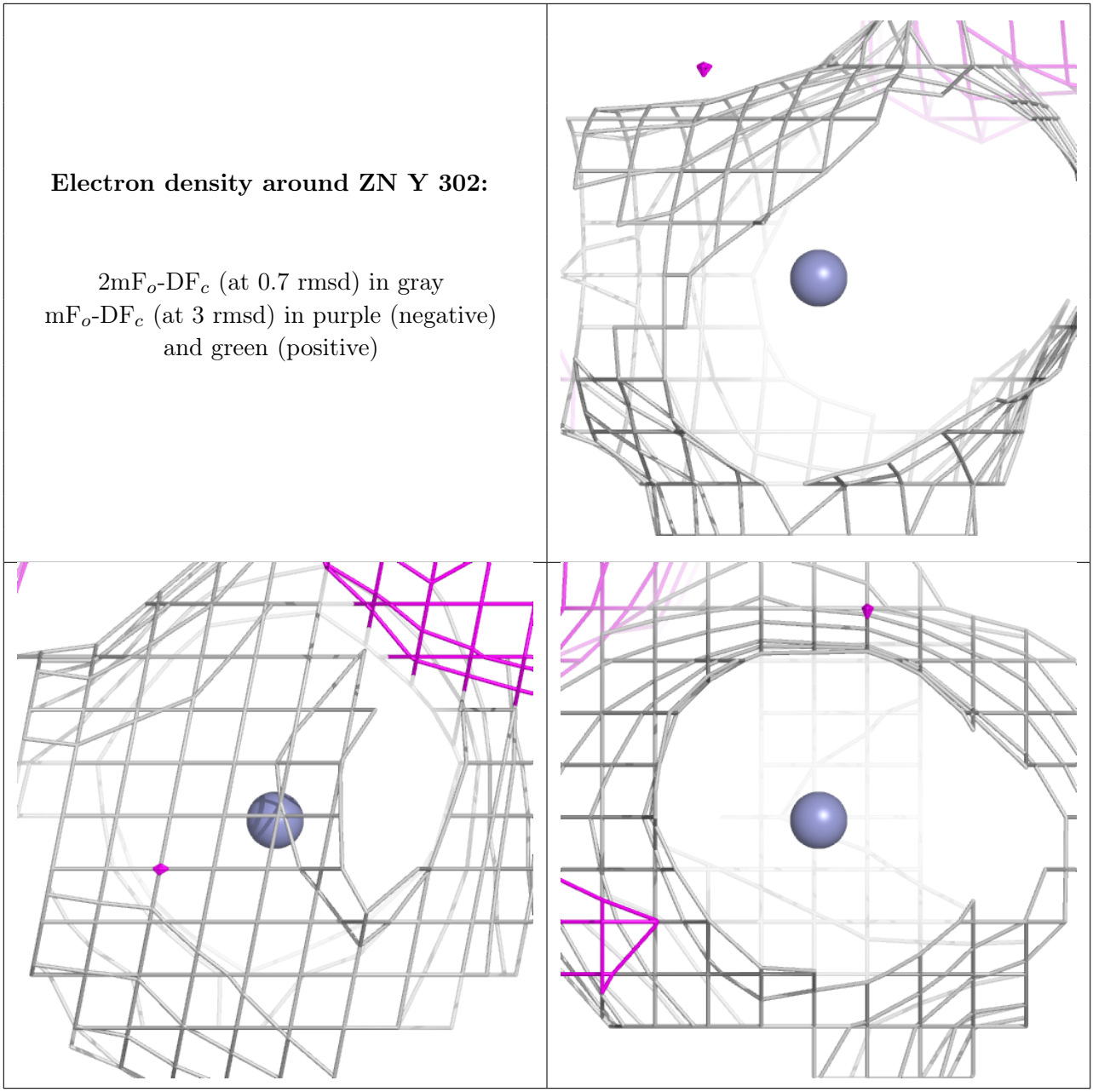
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	P	301	1/1	0.99	0.21	51,51,51,51	0
4	ZN	S	301	1/1	0.99	0.21	51,51,51,51	0
4	ZN	S	302	1/1	0.99	0.14	67,67,67,67	0
4	ZN	A	302	1/1	0.99	0.19	50,50,50,50	0
4	ZN	Y	301	1/1	0.99	0.14	83,83,83,83	0
4	ZN	D	302	1/1	0.99	0.19	46,46,46,46	0
4	ZN	D	301	1/1	1.00	0.18	44,44,44,44	0
4	ZN	P	302	1/1	1.00	0.18	49,49,49,49	0
4	ZN	V	301	1/1	1.00	0.18	65,65,65,65	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.

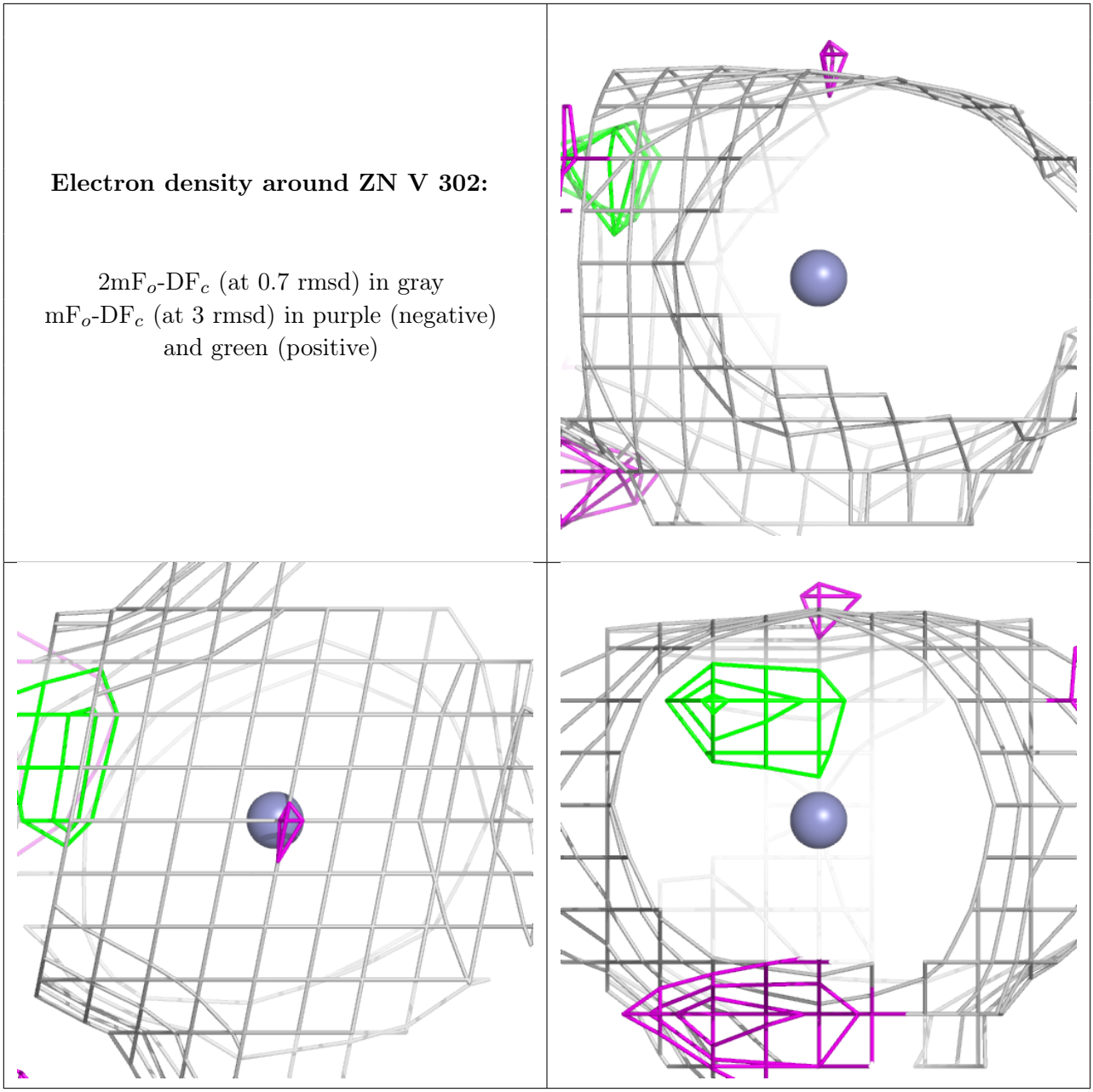
Electron density around ZN Y 302:

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



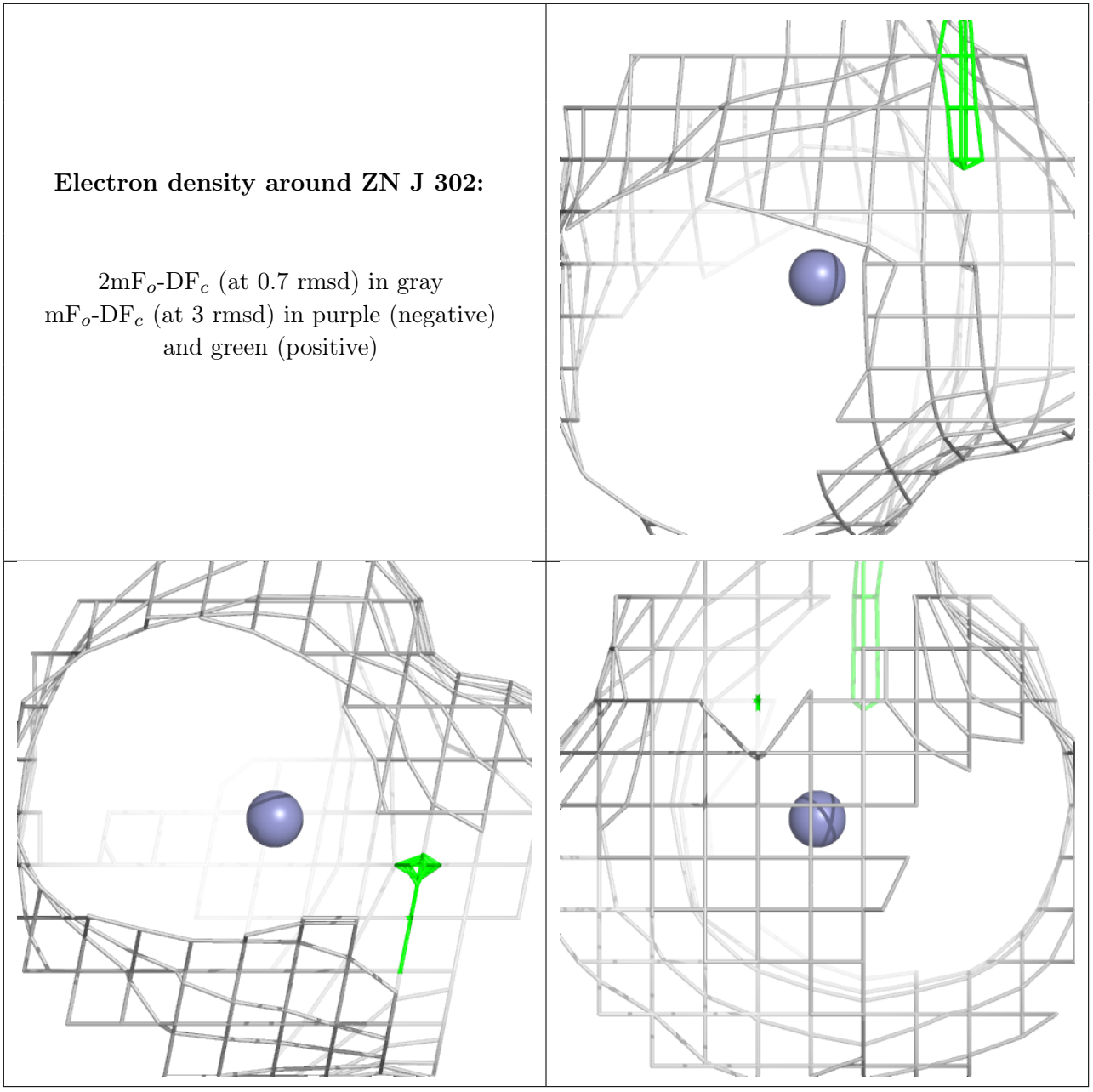
Electron density around ZN V 302:

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



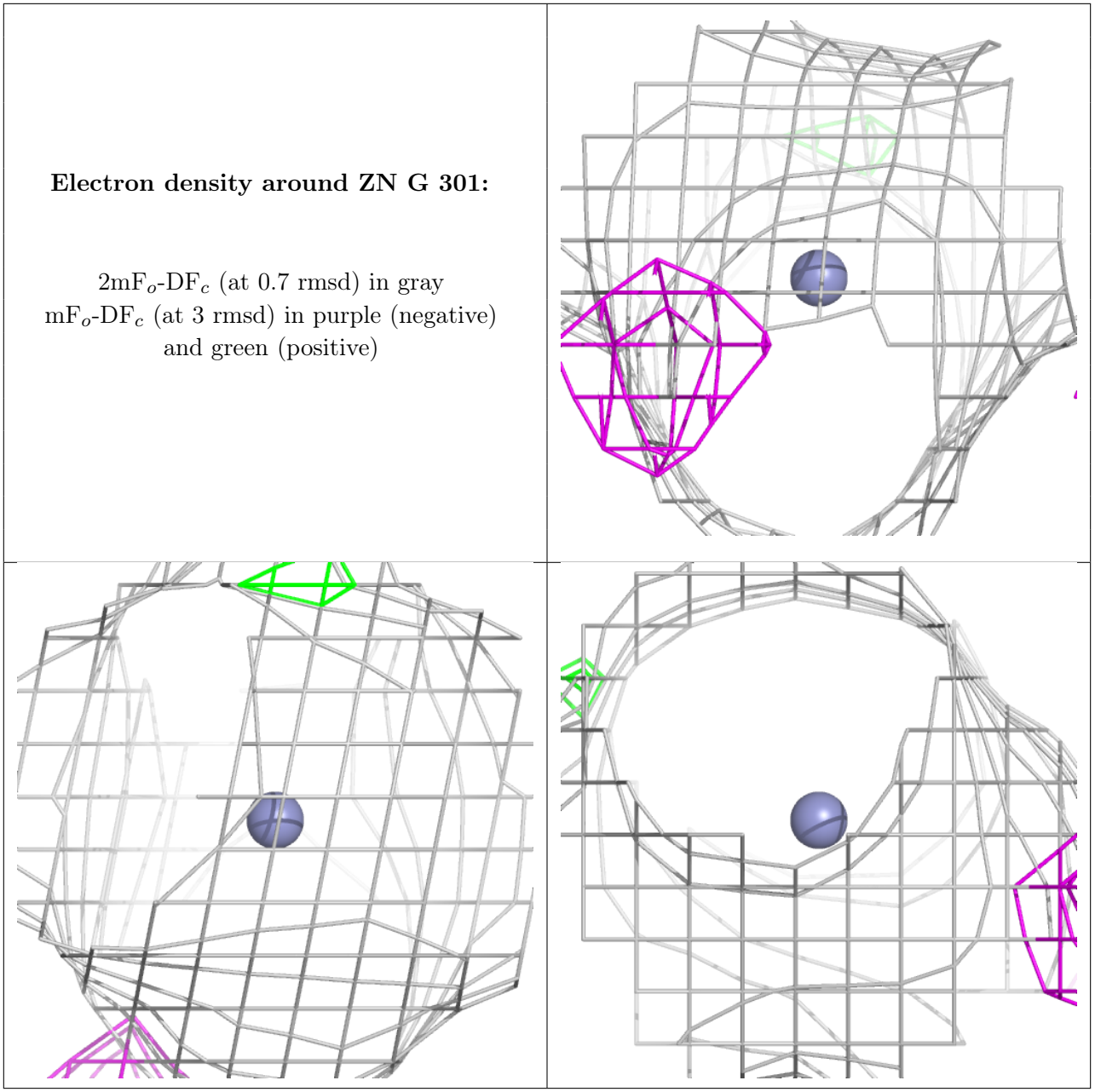
Electron density around ZN J 302:

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



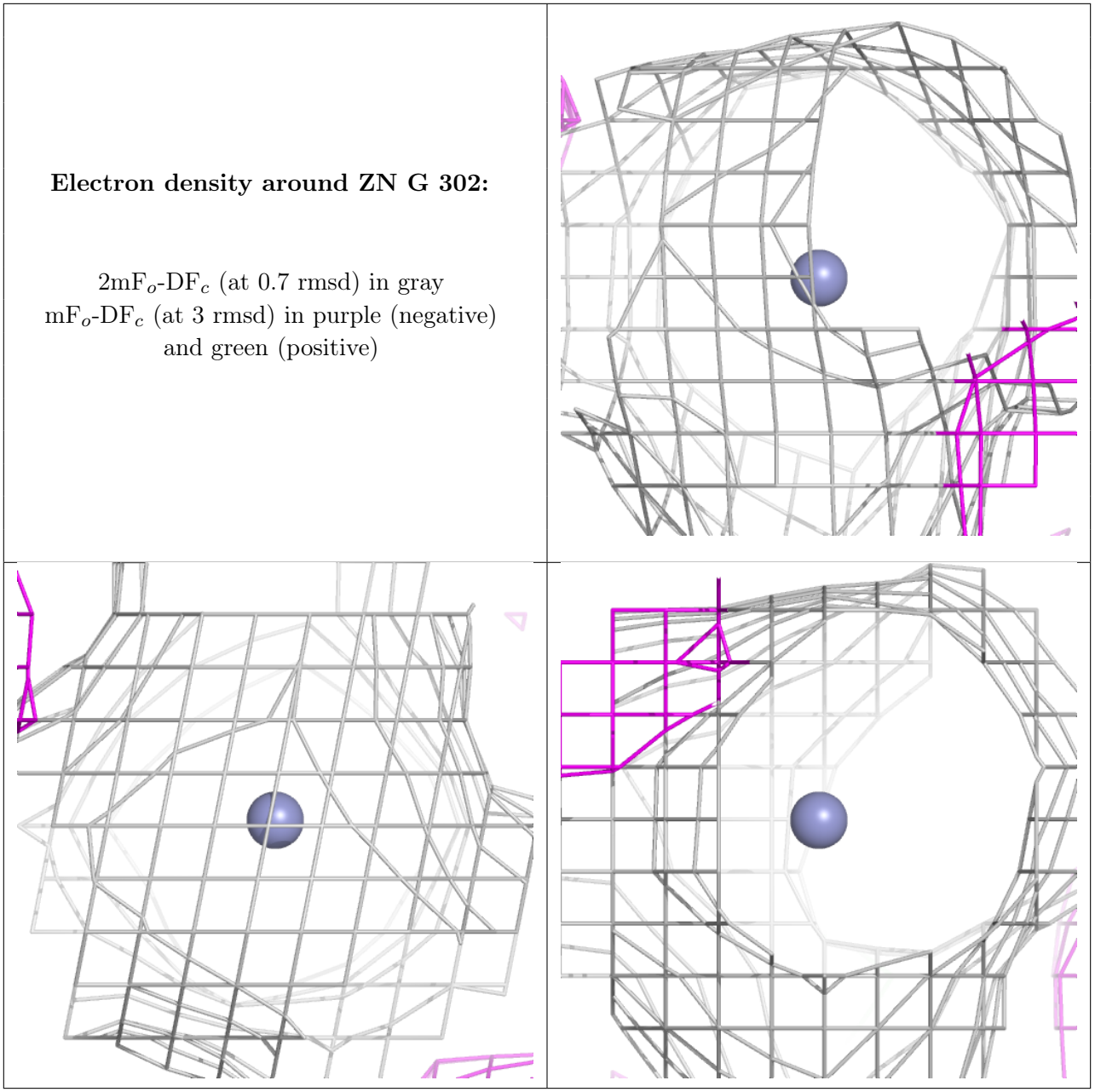
Electron density around ZN G 301:

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



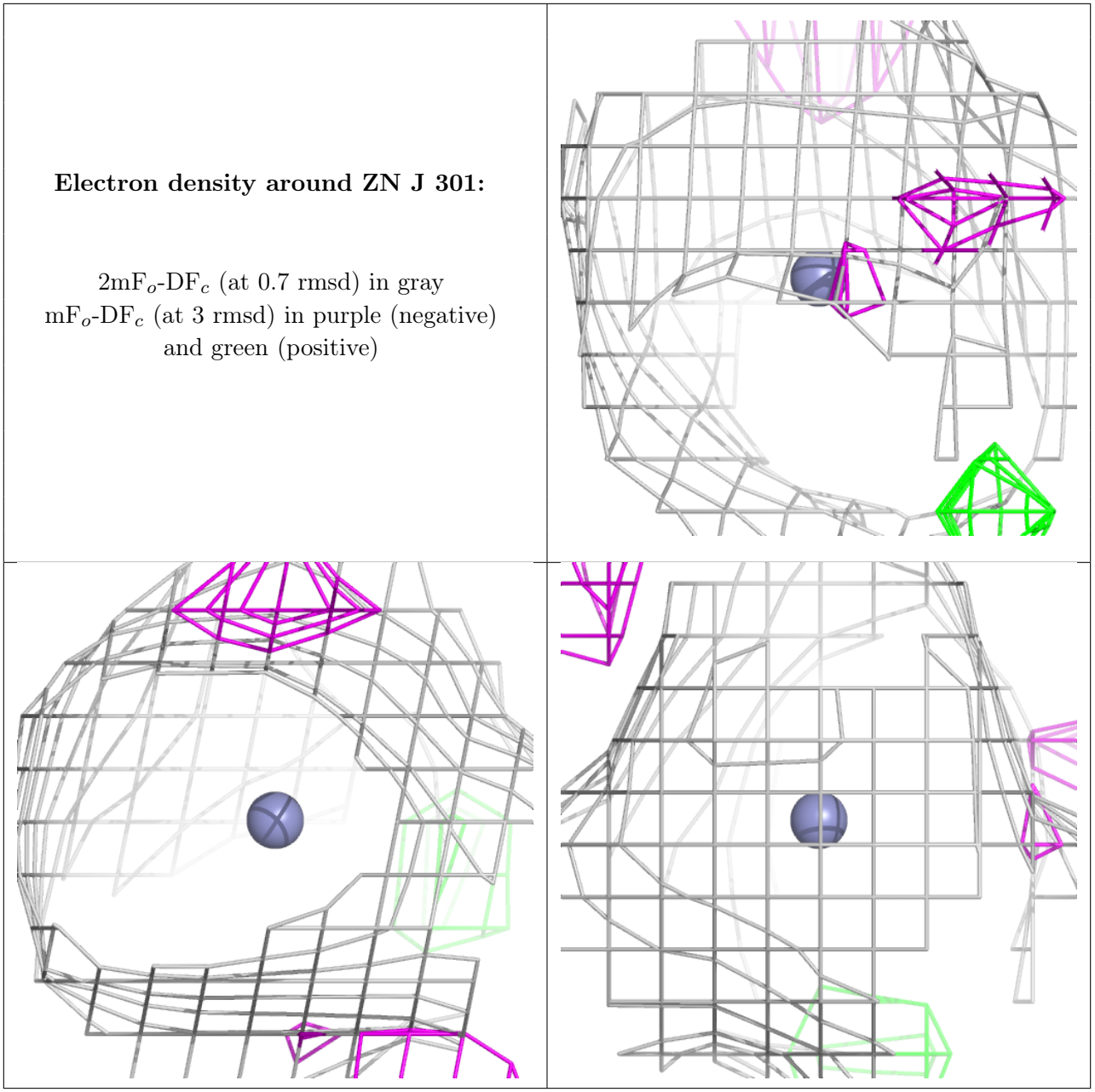
Electron density around ZN G 302:

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



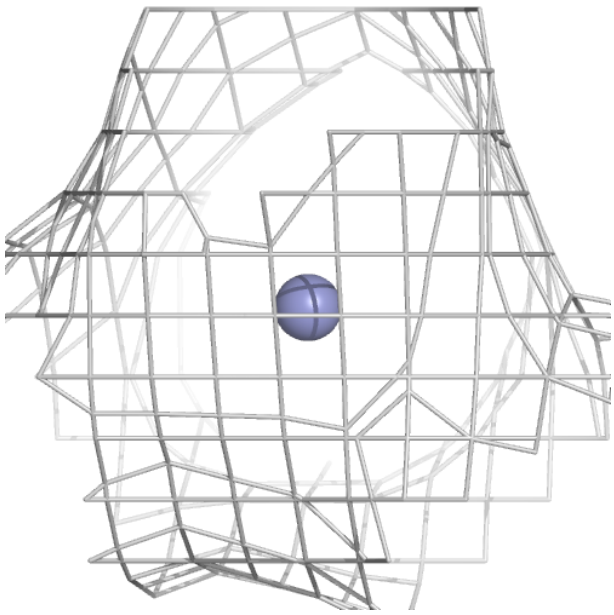
Electron density around ZN J 301:

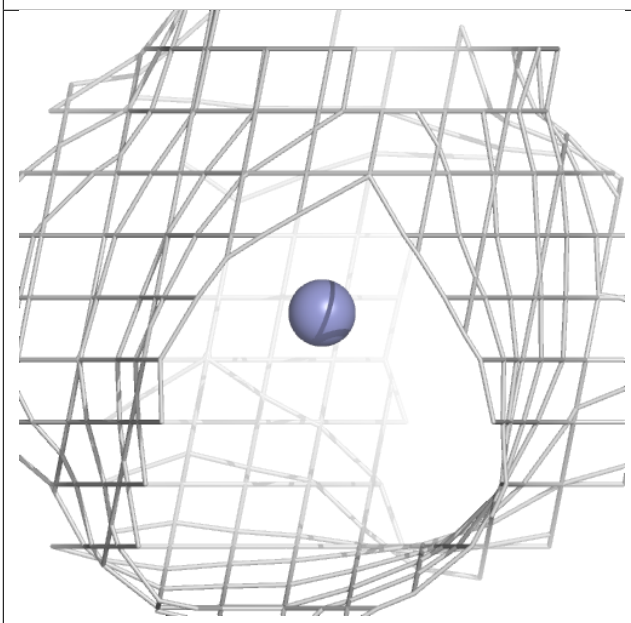
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

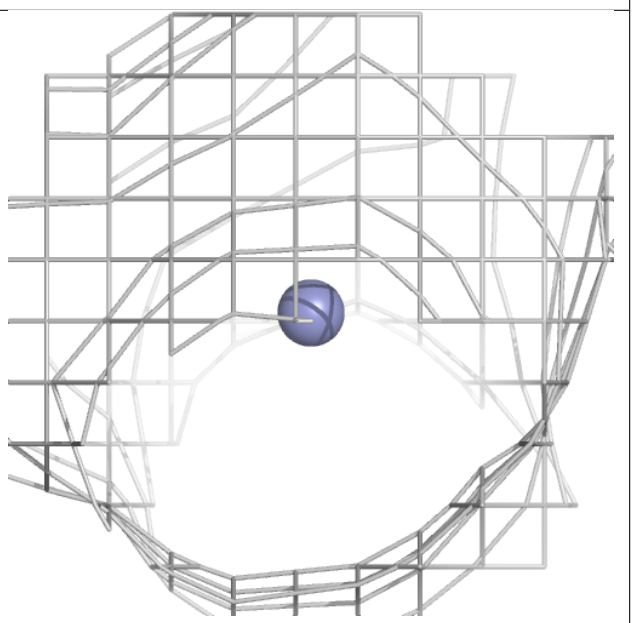


Electron density around ZN A 301:

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

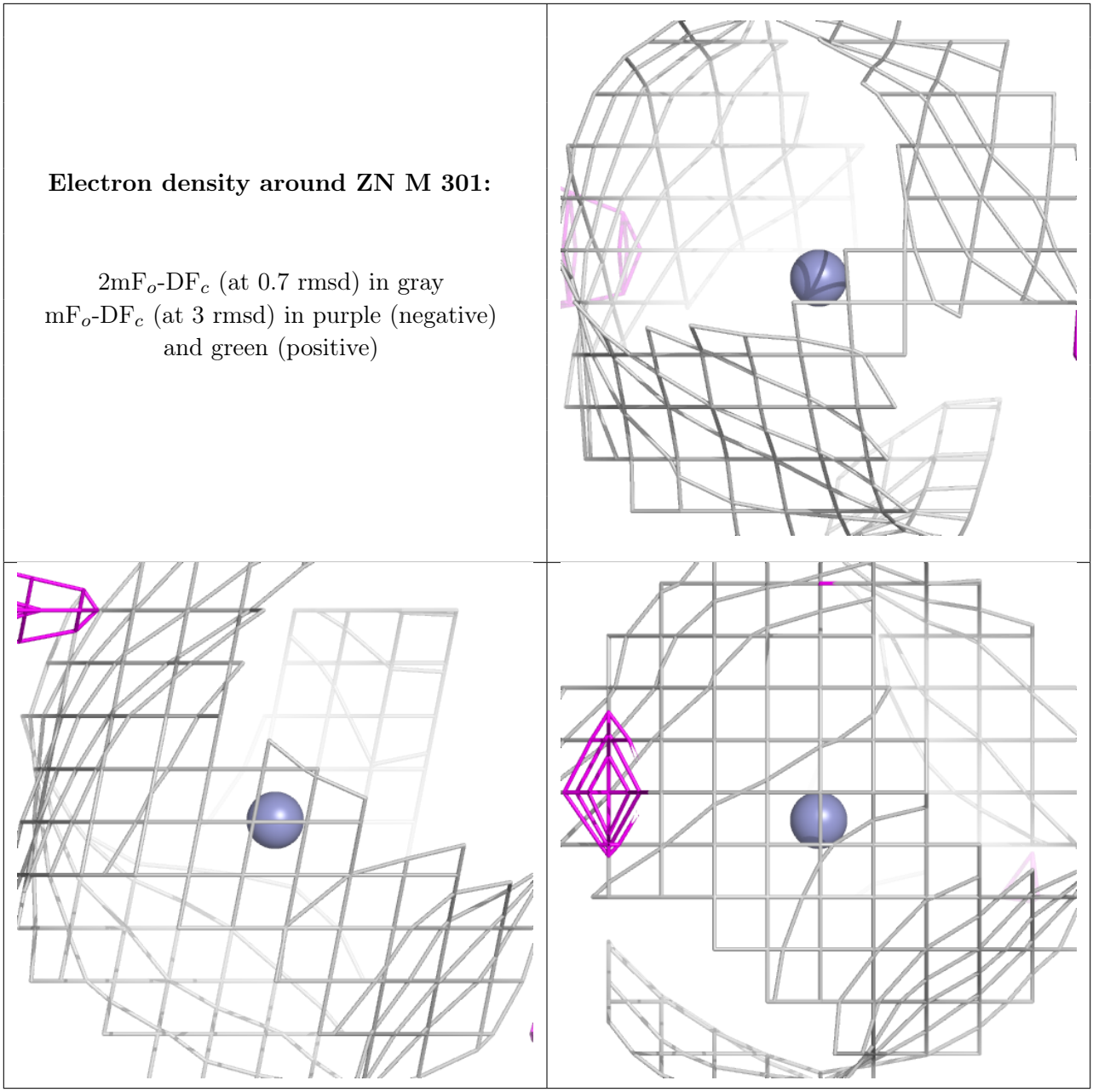






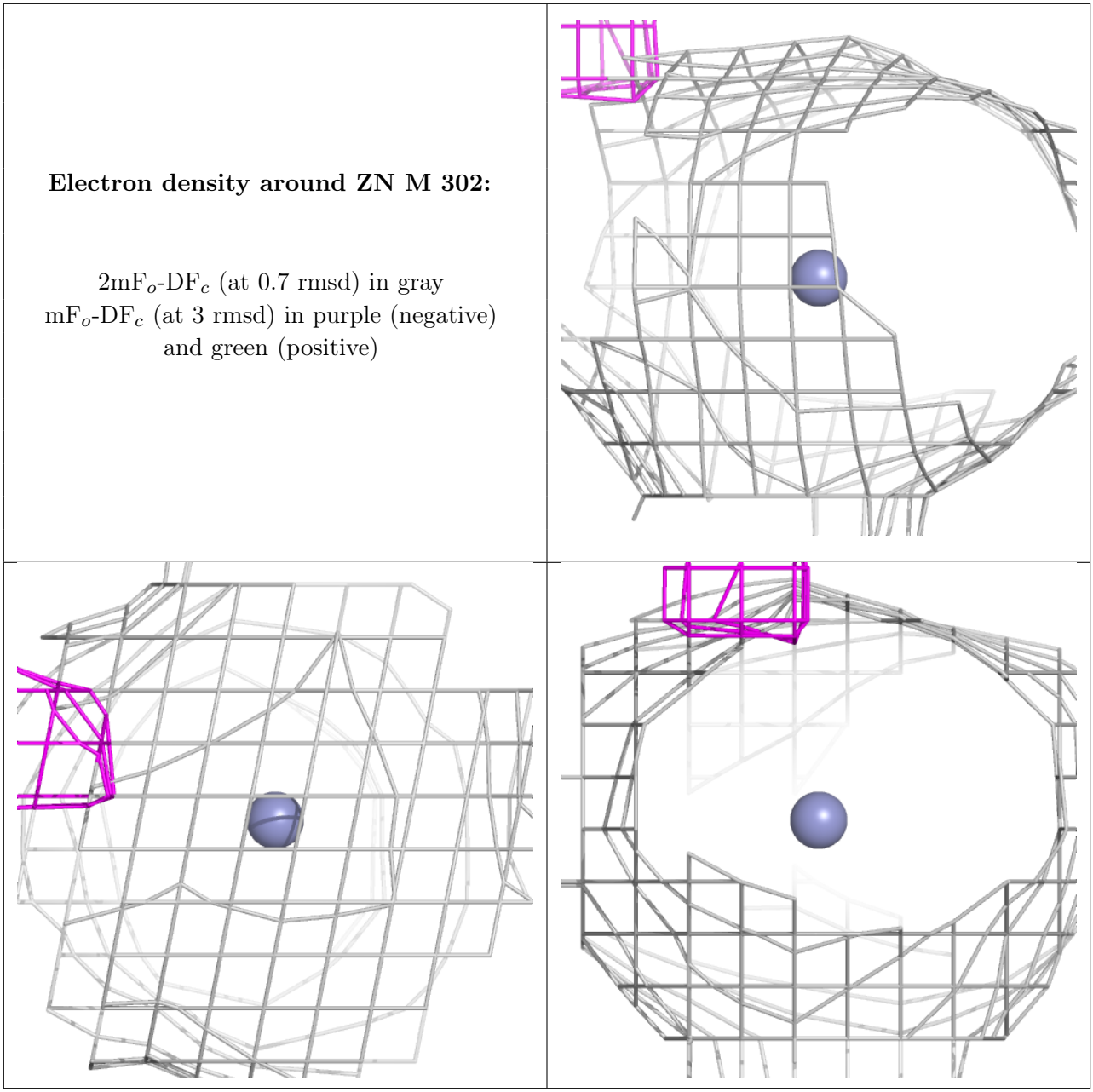
Electron density around ZN M 301:

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



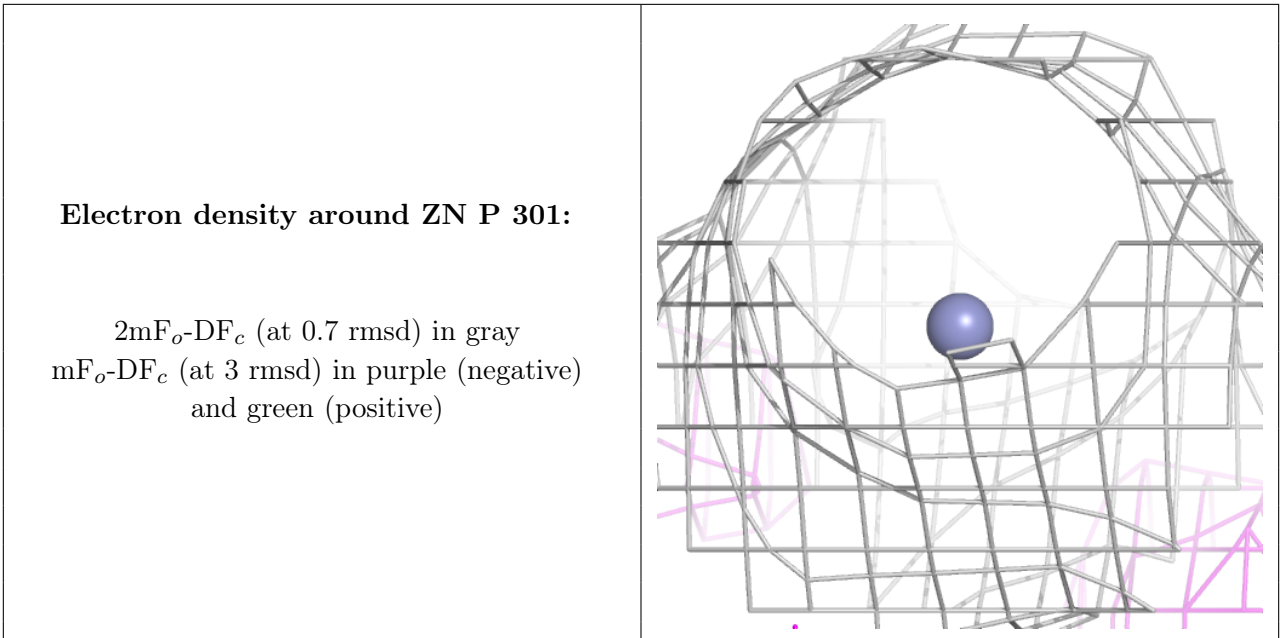
Electron density around ZN M 302:

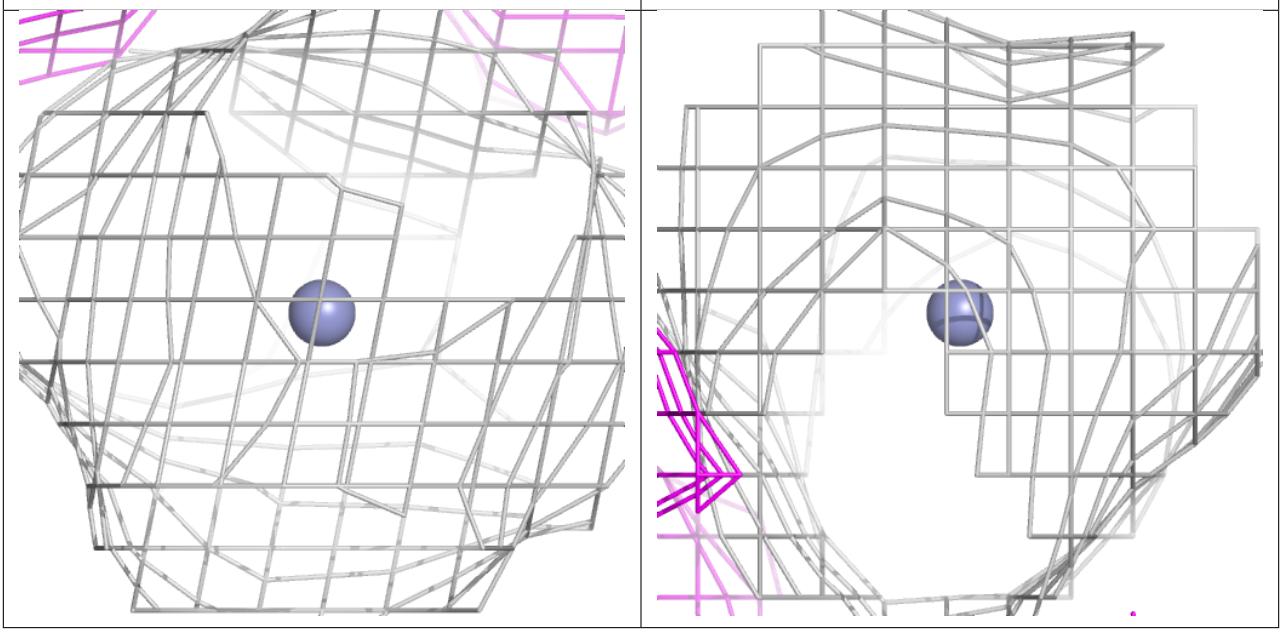
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZN P 301:

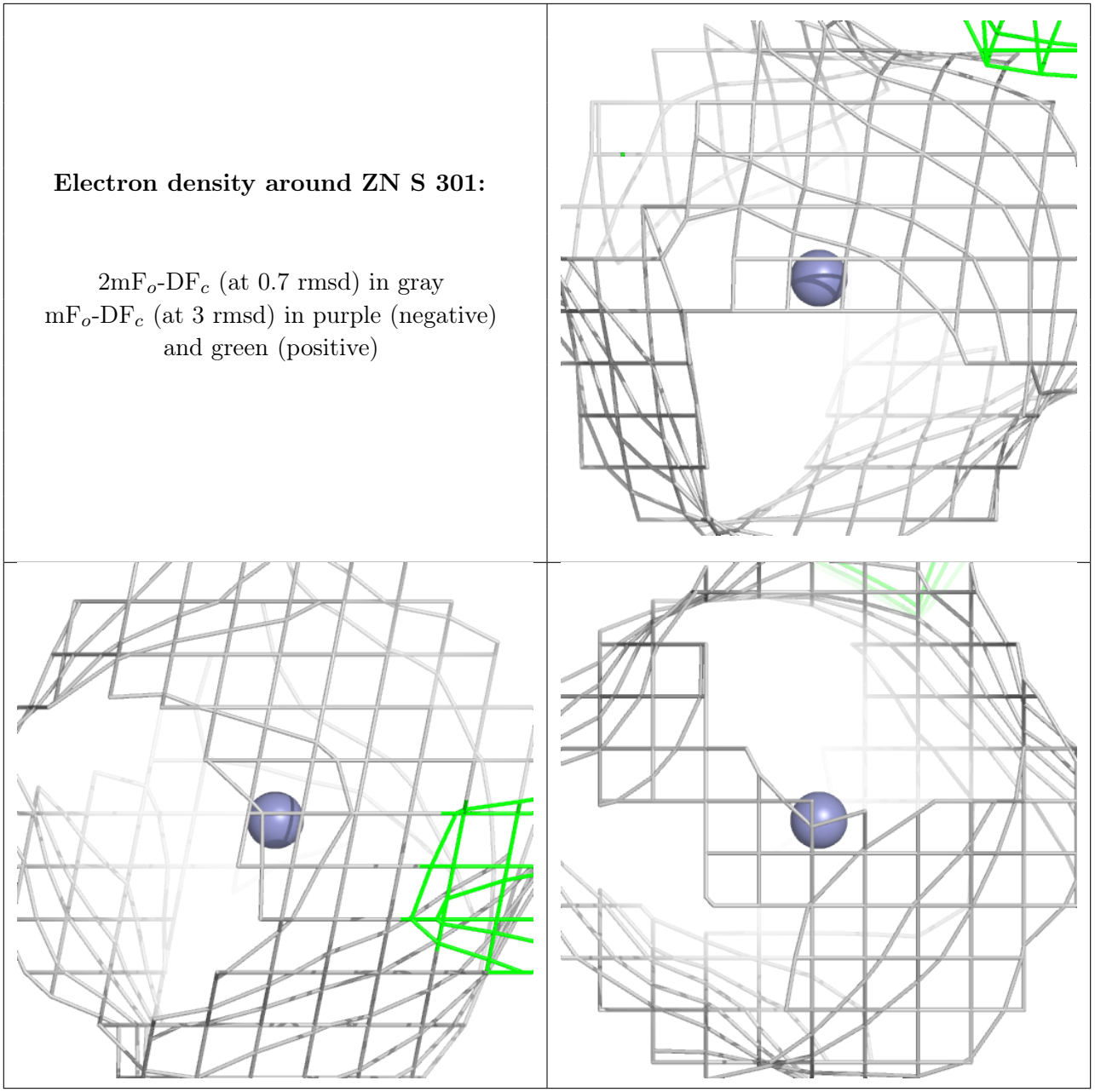
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





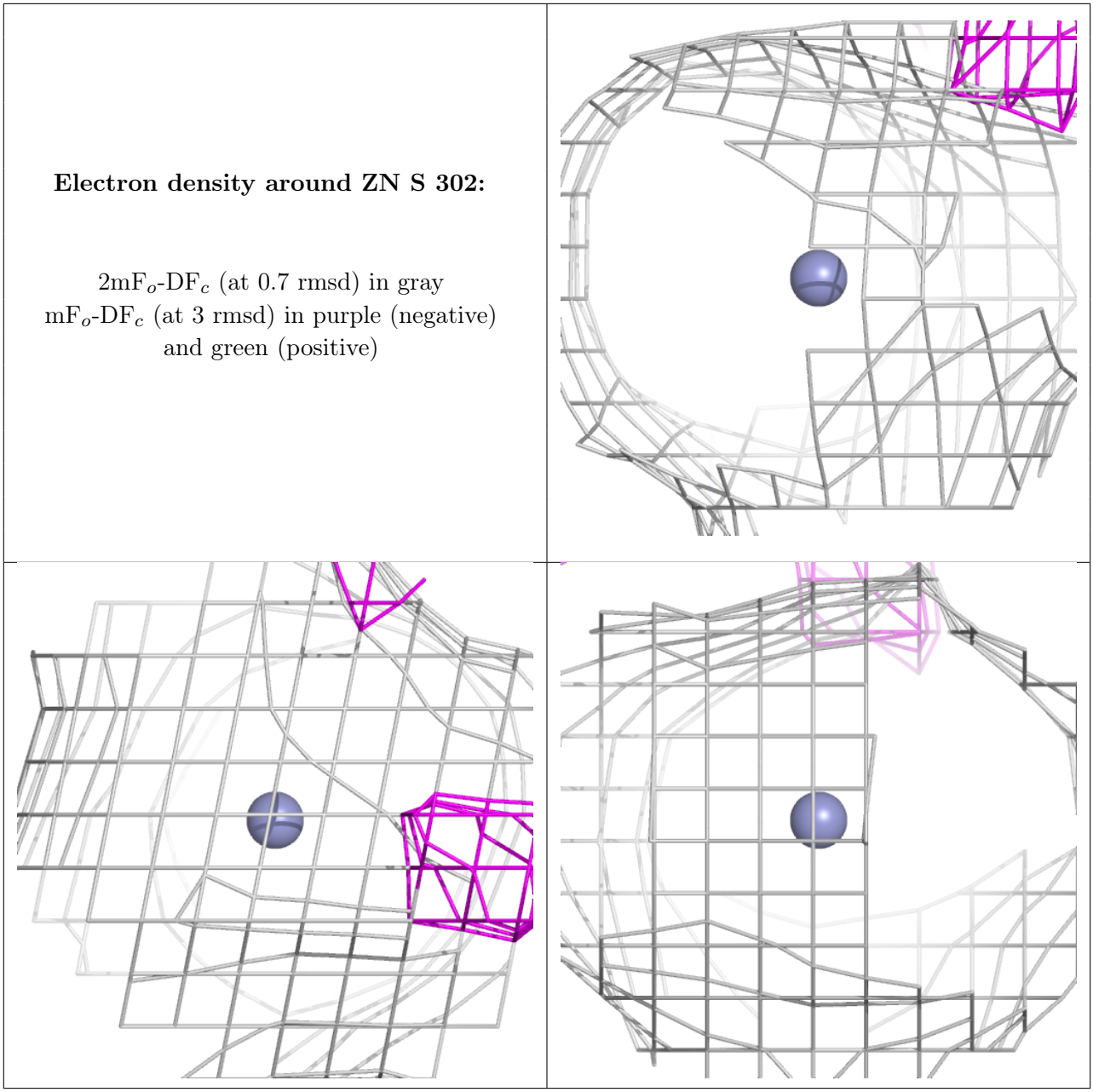
Electron density around ZN S 301:

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



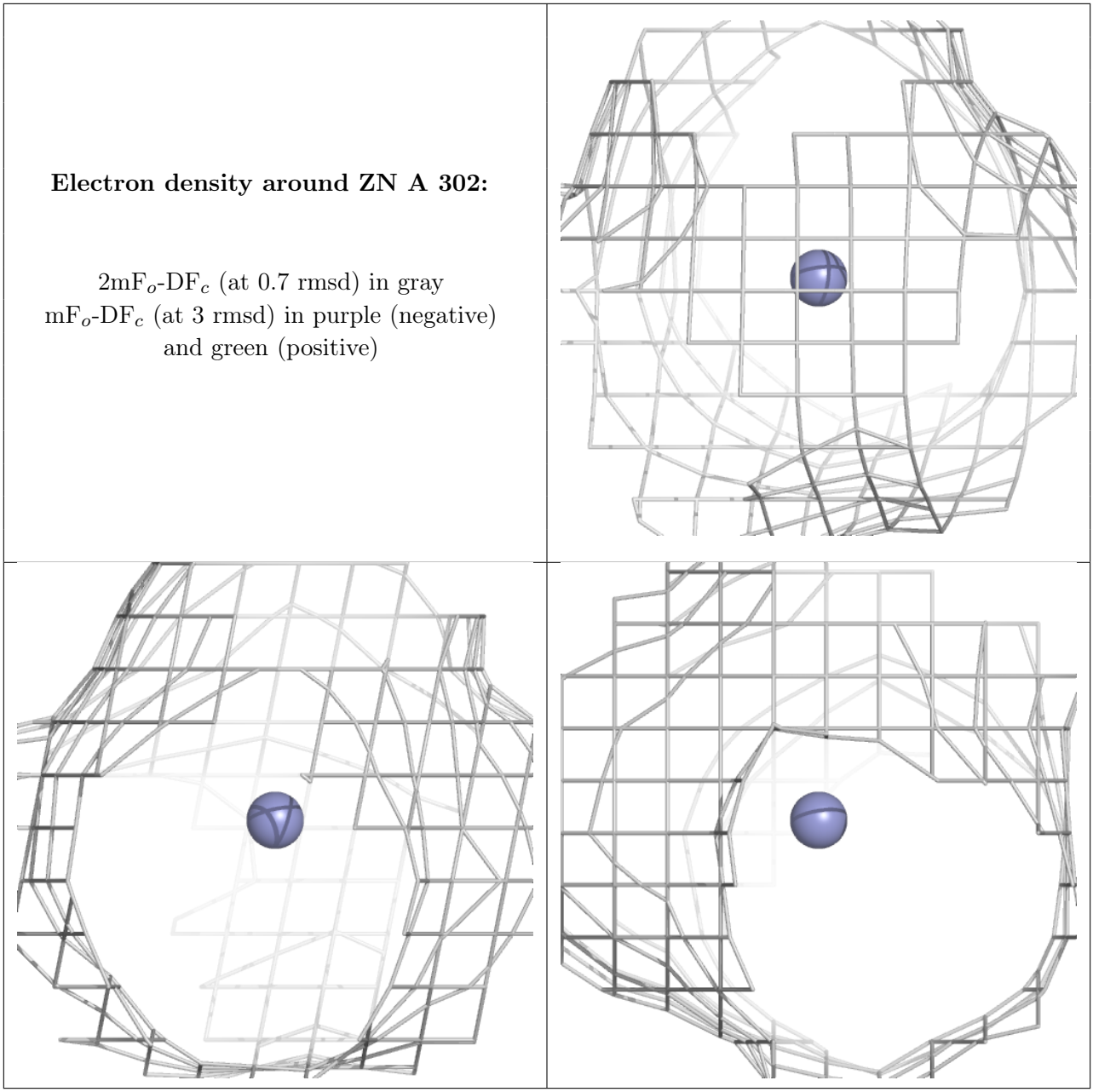
Electron density around ZN S 302:

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



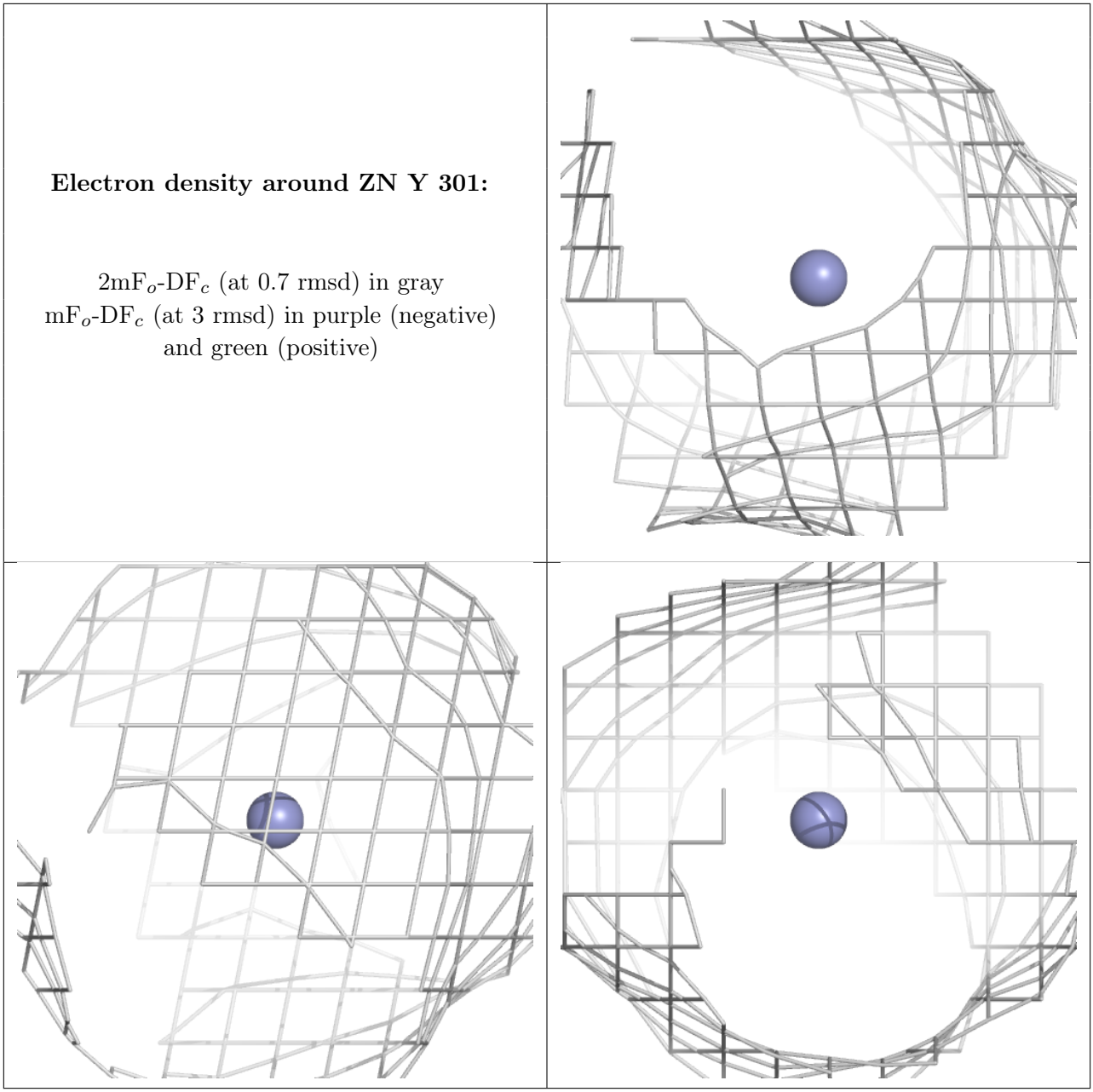
Electron density around ZN A 302:

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



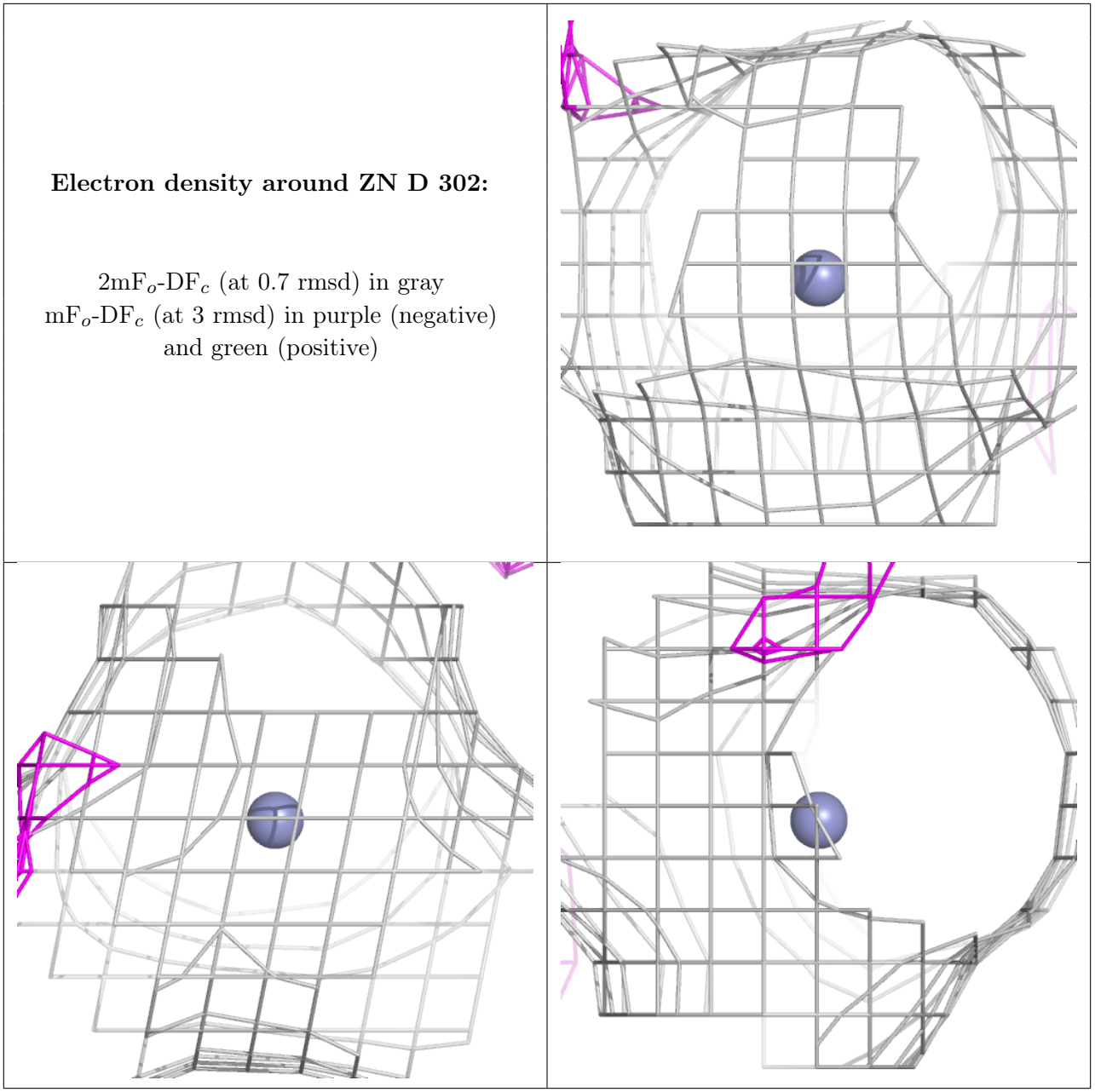
Electron density around ZN Y 301:

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



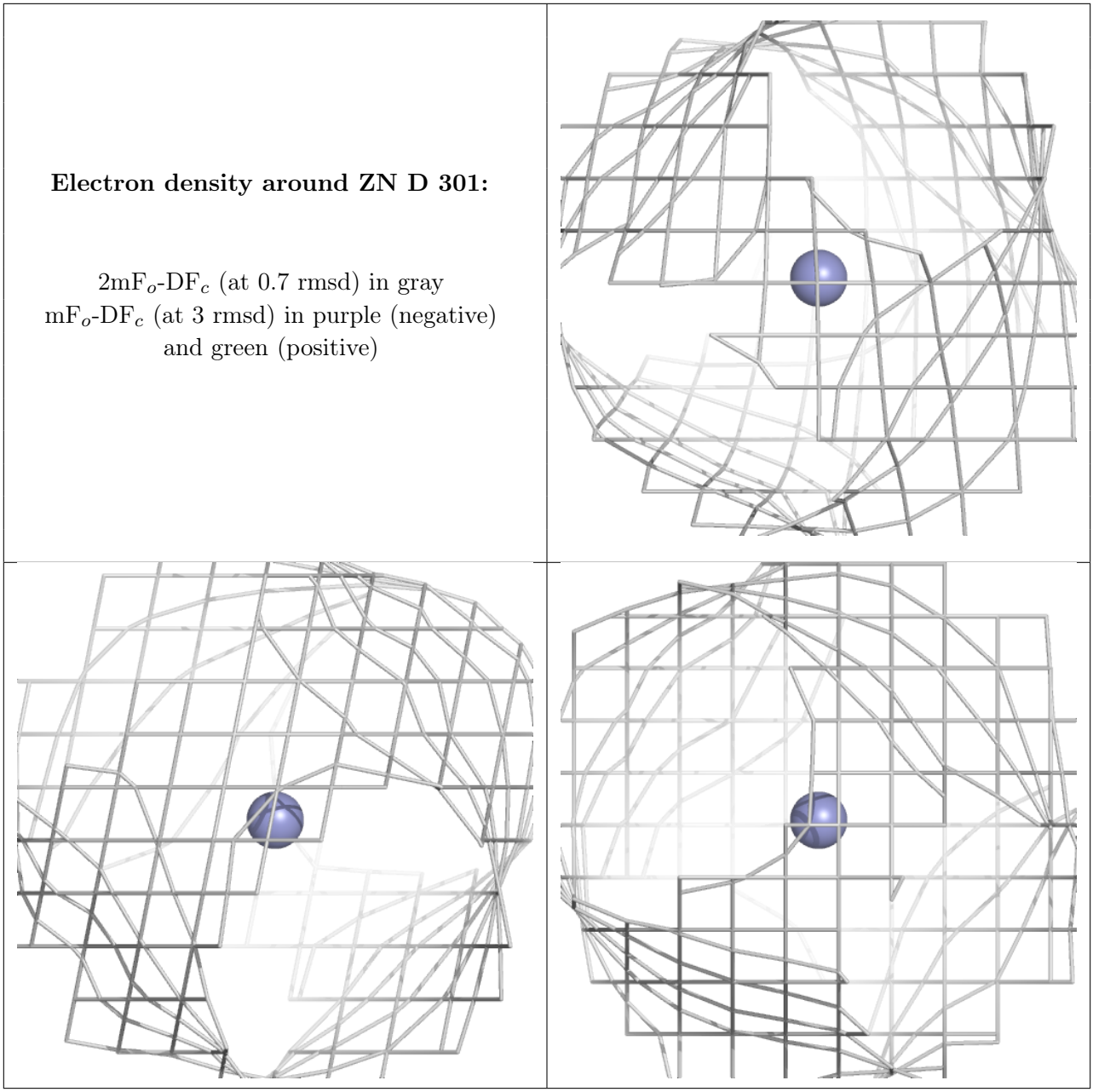
Electron density around ZN D 302:

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



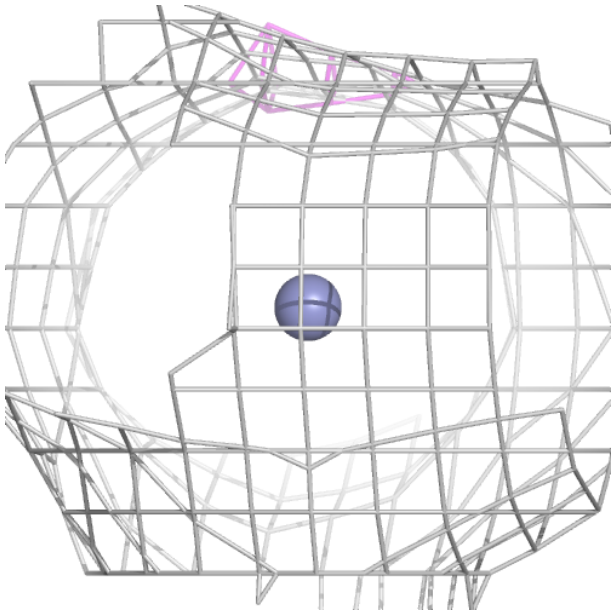
Electron density around ZN D 301:

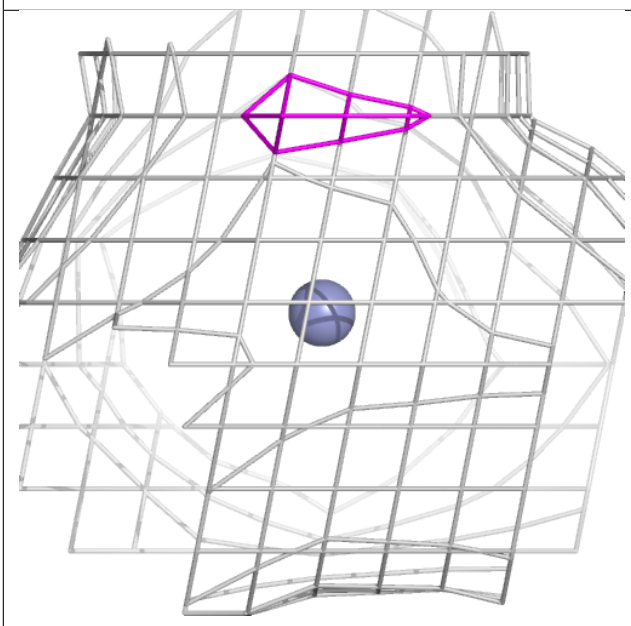
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

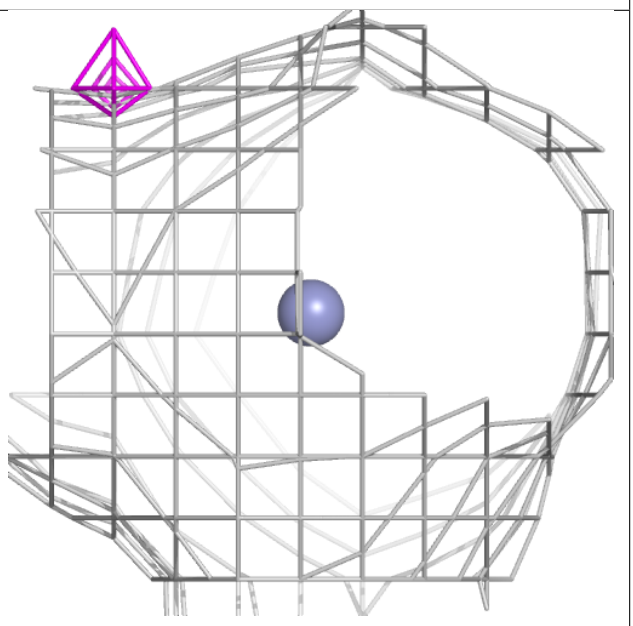


Electron density around ZN P 302:

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

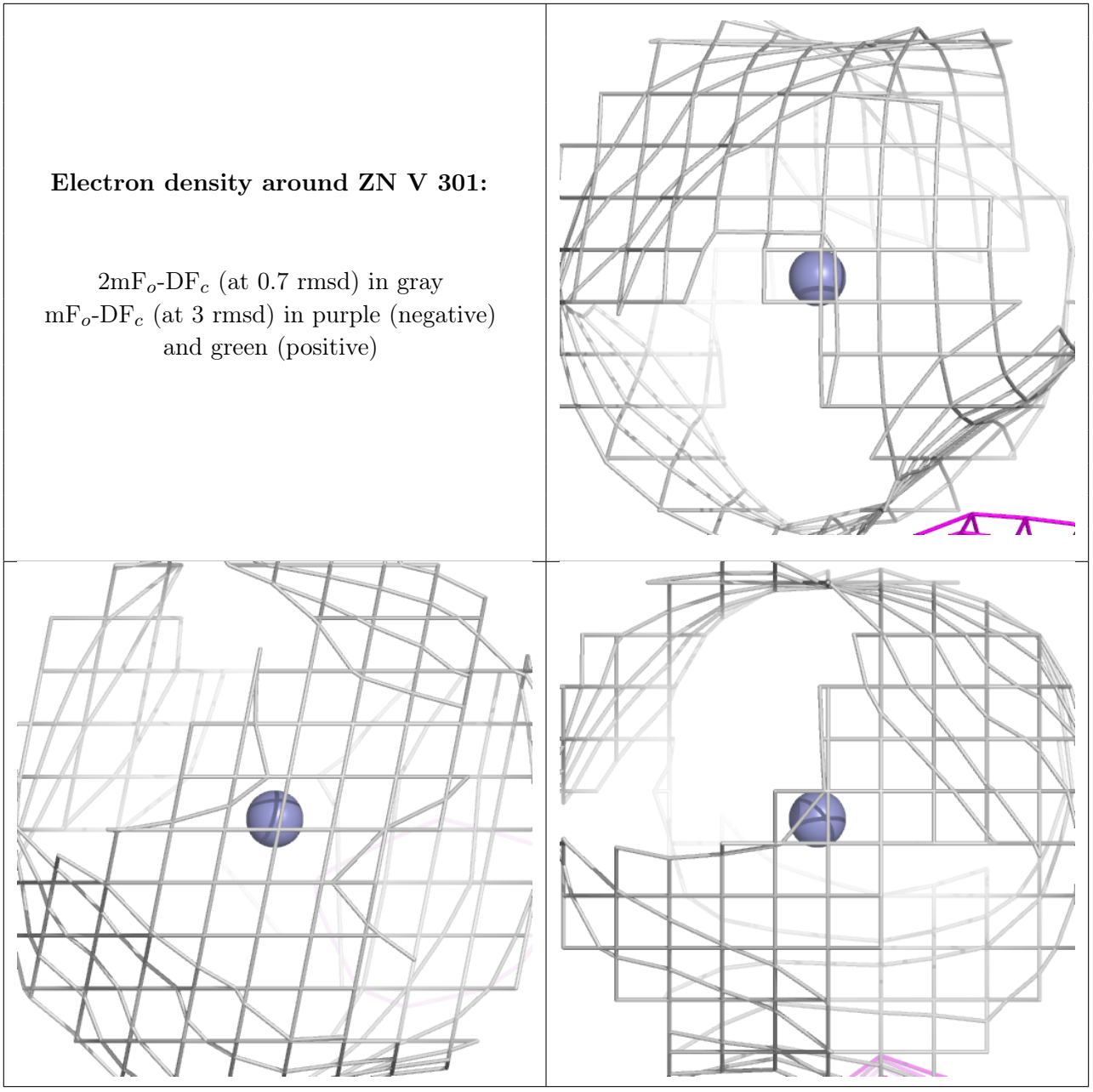






Electron density around ZN V 301:

$2mF_o$-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.