wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 – 02:13 AM JST

PDB ID	:	7Y6X
Title	:	RRGSGG-AtPRT6 UBR box (P32)
Authors	:	Kim, L.; Song, H.K.
Deposited on	:	2022-06-21
Resolution	:	2.20 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 (i)) were used in the production of this report:

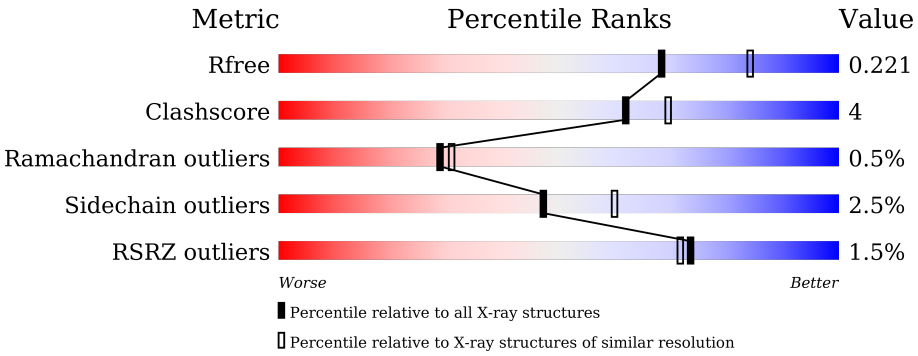
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	76	3% 89% 11%
1	B	76	% 86% 12%
1	C	76	% 89% 11%
1	D	76	92% 7%
1	E	76	4% 87% 12%
1	F	76	84% 14%

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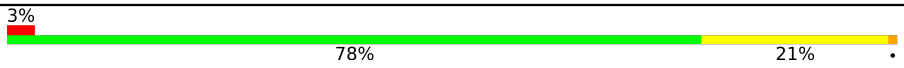
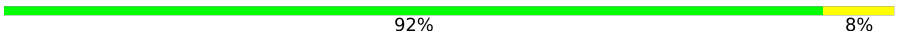
Mol	Chain	Length	Quality of chain
1	G	76	
1	H	76	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8354 atoms, of which 3760 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 E3 ubiquitin-protein ligase PRT6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	76	Total	C	H	N	O	S	0	0	0
			1023	337	458	105	113	10			
1	B	74	Total	C	H	N	O	S	0	0	0
			1034	333	477	103	111	10			
1	D	76	Total	C	H	N	O	S	0	0	0
			1038	336	475	105	112	10			
1	E	76	Total	C	H	N	O	S	0	0	0
			1025	337	460	105	113	10			
1	F	75	Total	C	H	N	O	S	0	0	0
			1034	335	473	104	112	10			
1	G	76	Total	C	H	N	O	S	0	0	0
			1035	337	470	105	113	10			
1	H	76	Total	C	H	N	O	S	0	0	0
			1046	337	481	105	113	10			
1	C	76	Total	C	H	N	O	S	0	0	0
			1031	337	466	105	113	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ARG	-	expression tag	UNP F4KCC2
A	114	ARG	-	expression tag	UNP F4KCC2
A	115	GLY	-	expression tag	UNP F4KCC2
A	116	SER	-	expression tag	UNP F4KCC2
A	117	GLY	-	expression tag	UNP F4KCC2
A	118	GLY	-	expression tag	UNP F4KCC2
B	113	ARG	-	expression tag	UNP F4KCC2
B	114	ARG	-	expression tag	UNP F4KCC2
B	115	GLY	-	expression tag	UNP F4KCC2
B	116	SER	-	expression tag	UNP F4KCC2
B	117	GLY	-	expression tag	UNP F4KCC2
B	118	GLY	-	expression tag	UNP F4KCC2
D	113	ARG	-	expression tag	UNP F4KCC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	114	ARG	-	expression tag	UNP F4KCC2
D	115	GLY	-	expression tag	UNP F4KCC2
D	116	SER	-	expression tag	UNP F4KCC2
D	117	GLY	-	expression tag	UNP F4KCC2
D	118	GLY	-	expression tag	UNP F4KCC2
E	113	ARG	-	expression tag	UNP F4KCC2
E	114	ARG	-	expression tag	UNP F4KCC2
E	115	GLY	-	expression tag	UNP F4KCC2
E	116	SER	-	expression tag	UNP F4KCC2
E	117	GLY	-	expression tag	UNP F4KCC2
E	118	GLY	-	expression tag	UNP F4KCC2
F	113	ARG	-	expression tag	UNP F4KCC2
F	114	ARG	-	expression tag	UNP F4KCC2
F	115	GLY	-	expression tag	UNP F4KCC2
F	116	SER	-	expression tag	UNP F4KCC2
F	117	GLY	-	expression tag	UNP F4KCC2
F	118	GLY	-	expression tag	UNP F4KCC2
G	113	ARG	-	expression tag	UNP F4KCC2
G	114	ARG	-	expression tag	UNP F4KCC2
G	115	GLY	-	expression tag	UNP F4KCC2
G	116	SER	-	expression tag	UNP F4KCC2
G	117	GLY	-	expression tag	UNP F4KCC2
G	118	GLY	-	expression tag	UNP F4KCC2
H	113	ARG	-	expression tag	UNP F4KCC2
H	114	ARG	-	expression tag	UNP F4KCC2
H	115	GLY	-	expression tag	UNP F4KCC2
H	116	SER	-	expression tag	UNP F4KCC2
H	117	GLY	-	expression tag	UNP F4KCC2
H	118	GLY	-	expression tag	UNP F4KCC2
C	113	ARG	-	expression tag	UNP F4KCC2
C	114	ARG	-	expression tag	UNP F4KCC2
C	115	GLY	-	expression tag	UNP F4KCC2
C	116	SER	-	expression tag	UNP F4KCC2
C	117	GLY	-	expression tag	UNP F4KCC2
C	118	GLY	-	expression tag	UNP F4KCC2

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	3	3	3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Zn 3 3	0	0
2	D	3	Total Zn 3 3	0	0
2	E	3	Total Zn 3 3	0	0
2	F	3	Total Zn 3 3	0	0
2	G	3	Total Zn 3 3	0	0
2	H	3	Total Zn 3 3	0	0
2	C	3	Total Zn 3 3	0	0

- Molecule 3 is water.

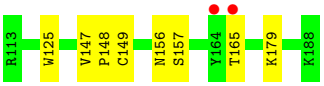
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	8	Total O 8 8	0	0
3	D	7	Total O 7 7	0	0
3	E	9	Total O 9 9	0	0
3	F	6	Total O 6 6	0	0
3	G	11	Total O 11 11	0	0
3	H	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0

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: E3 ubiquitin-protein ligase PRT6

Chain A:

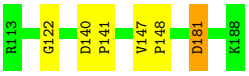


• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain B:

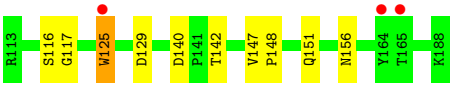
• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain D:



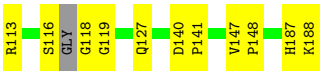
• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain E:



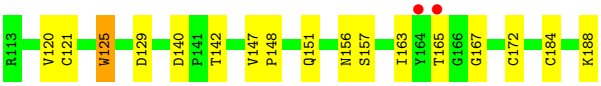
• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain F:



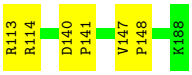
• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain G:



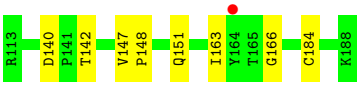
• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain H:



• Molecule 1: E3 ubiquitin-protein ligase PRT6

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	93.67Å 93.67Å 106.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 2.20 44.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.65-2.20) 97.1 (44.65-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.201 , 0.220 0.203 , 0.221	Depositor DCC
R_{free} test set	1996 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 16.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.466 for -h,-k,l 0.468 for h,-h-k,-l 0.467 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8354	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	0.77	1/579 (0.2%)	0.82	0/783
1	B	0.58	0/570	0.73	0/770
1	C	0.64	0/579	0.78	0/783
1	D	0.59	0/577	0.74	0/780
1	E	0.69	0/579	0.72	0/783
1	F	0.58	0/574	0.75	0/775
1	G	0.75	1/579 (0.2%)	0.77	0/783
1	H	0.63	0/579	0.74	0/783
All	All	0.66	2/4616 (0.0%)	0.76	0/6240

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	CYS	CB-SG	5.74	1.92	1.82
1	G	184	CYS	CB-SG	5.72	1.92	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	565	458	487	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	557	477	480	4	0
1	C	565	466	487	3	0
1	D	563	475	483	3	0
1	E	565	460	487	6	0
1	F	561	473	483	9	0
1	G	565	470	487	8	0
1	H	565	481	487	4	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
3	D	7	0	0	0	0
3	E	9	0	0	0	0
3	F	6	0	0	0	0
3	G	11	0	0	0	0
3	H	7	0	0	0	0
All	All	4594	3760	3881	37	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 4.

The worst 5 of 37 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:E:140:ASP:OD2	1:E:142:THR:HB	1.94	0.68
1:D:181:ASP:N	1:D:181:ASP:OD1	2.37	0.58
1:C:140:ASP:OD2	1:C:142:THR:HG23	2.03	0.58
1:A:147:VAL:HB	1:A:148:PRO:HD3	1.84	0.58
1:E:117:GLY:O	1:F:127:GLN:OE1	2.21	0.58

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	74/76 (97%)	71 (96%)	3 (4%)	0	100 100
1	B	70/76 (92%)	65 (93%)	4 (6%)	1 (1%)	11 8
1	C	74/76 (97%)	69 (93%)	4 (5%)	1 (1%)	11 8
1	D	74/76 (97%)	71 (96%)	2 (3%)	1 (1%)	11 8
1	E	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
1	F	71/76 (93%)	67 (94%)	4 (6%)	0	100 100
1	G	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
1	H	74/76 (97%)	70 (95%)	4 (5%)	0	100 100
All	All	585/608 (96%)	557 (95%)	25 (4%)	3 (0%)	29 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	GLY
1	C	166	GLY
1	D	122	GLY

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	61/61 (100%)	59 (97%)	2 (3%)	38 49
1	B	61/61 (100%)	61 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	61/61 (100%)	59 (97%)	2 (3%)	38 49
1	D	60/61 (98%)	59 (98%)	1 (2%)	60 74
1	E	61/61 (100%)	58 (95%)	3 (5%)	25 31
1	F	61/61 (100%)	61 (100%)	0	100 100
1	G	61/61 (100%)	57 (93%)	4 (7%)	16 19
1	H	61/61 (100%)	61 (100%)	0	100 100
All	All	487/488 (100%)	475 (98%)	12 (2%)	47 60

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	163	ILE
1	G	165	THR
1	C	184	CYS
1	G	188	LYS
1	E	116	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	156	ASN
1	E	156	ASN
1	G	156	ASN
1	C	156	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 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	76/76 (100%)	0.36	2 (2%) 56 53	30, 40, 53, 72	0
1	B	74/76 (97%)	0.25	1 (1%) 75 73	30, 41, 57, 62	0
1	C	76/76 (100%)	0.32	1 (1%) 77 75	30, 40, 54, 62	0
1	D	76/76 (100%)	0.29	0 100 100	30, 40, 64, 69	0
1	E	76/76 (100%)	0.37	3 (3%) 39 37	29, 40, 56, 62	0
1	F	75/76 (98%)	0.30	0 100 100	30, 41, 58, 63	0
1	G	76/76 (100%)	0.32	2 (2%) 56 53	31, 39, 57, 62	0
1	H	76/76 (100%)	0.24	0 100 100	30, 41, 58, 66	0
All	All	605/608 (99%)	0.31	9 (1%) 73 72	29, 40, 58, 72	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	164	TYR	3.5
1	E	164	TYR	3.4
1	C	164	TYR	3.3
1	E	125	TRP	2.8
1	A	165	THR	2.7

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 (i)

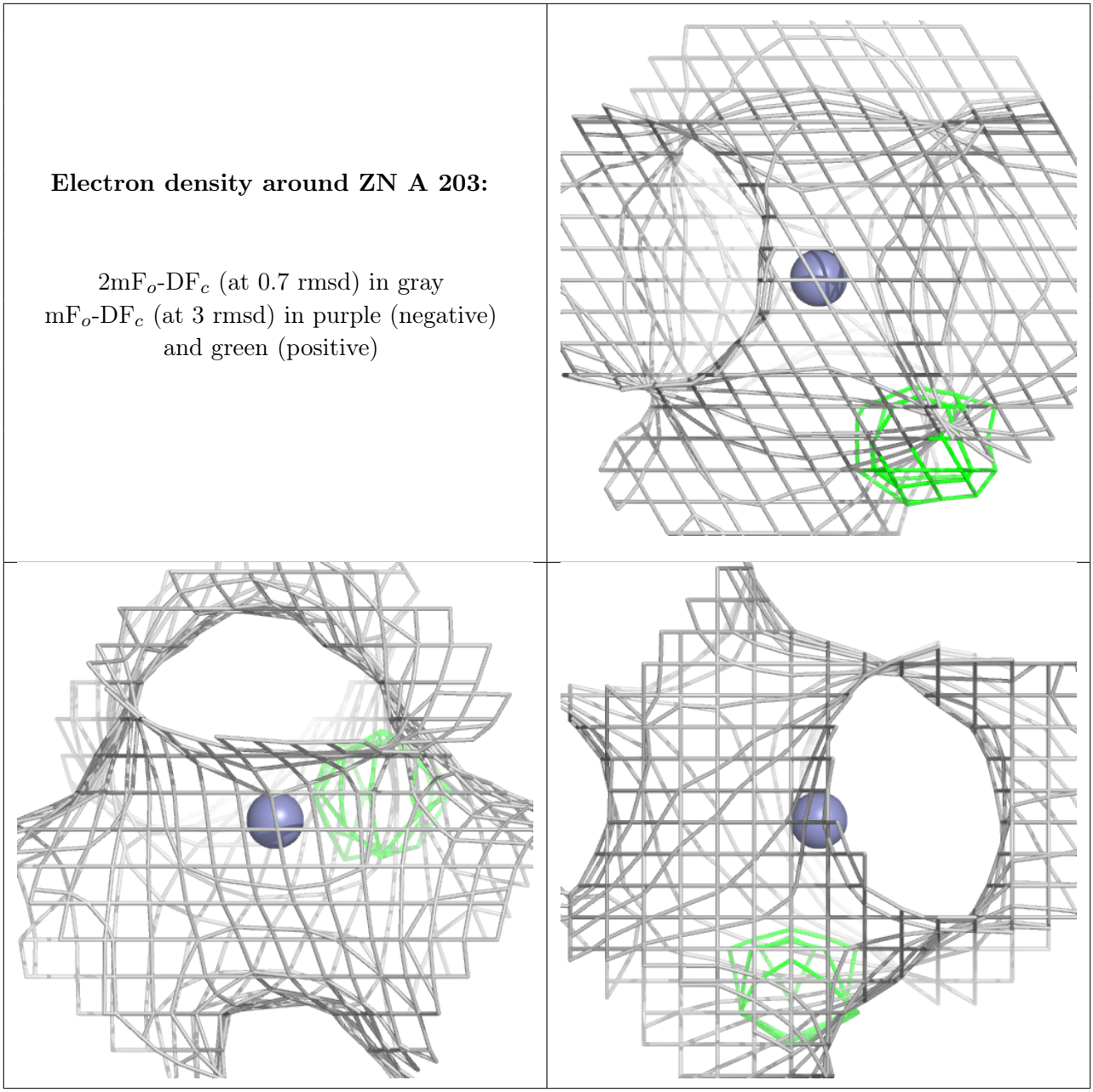
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ZN	A	203	1/1	0.99	0.17	34,34,34,34	0
2	ZN	E	203	1/1	0.99	0.16	33,33,33,33	0
2	ZN	G	201	1/1	0.99	0.18	34,34,34,34	0
2	ZN	G	202	1/1	0.99	0.20	32,32,32,32	0
2	ZN	B	202	1/1	1.00	0.18	35,35,35,35	0
2	ZN	B	203	1/1	1.00	0.18	34,34,34,34	0
2	ZN	D	201	1/1	1.00	0.16	42,42,42,42	0
2	ZN	D	202	1/1	1.00	0.18	36,36,36,36	0
2	ZN	D	203	1/1	1.00	0.18	34,34,34,34	0
2	ZN	E	201	1/1	1.00	0.17	35,35,35,35	0
2	ZN	E	202	1/1	1.00	0.20	30,30,30,30	0
2	ZN	A	202	1/1	1.00	0.19	34,34,34,34	0
2	ZN	F	201	1/1	1.00	0.19	40,40,40,40	0
2	ZN	F	202	1/1	1.00	0.18	35,35,35,35	0
2	ZN	F	203	1/1	1.00	0.17	34,34,34,34	0
2	ZN	A	201	1/1	1.00	0.19	32,32,32,32	0
2	ZN	B	201	1/1	1.00	0.18	41,41,41,41	0
2	ZN	G	203	1/1	1.00	0.17	35,35,35,35	0
2	ZN	H	201	1/1	1.00	0.17	41,41,41,41	0
2	ZN	H	202	1/1	1.00	0.16	36,36,36,36	0
2	ZN	H	203	1/1	1.00	0.18	34,34,34,34	0
2	ZN	C	201	1/1	1.00	0.18	35,35,35,35	0
2	ZN	C	202	1/1	1.00	0.20	29,29,29,29	0
2	ZN	C	203	1/1	1.00	0.19	35,35,35,35	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.

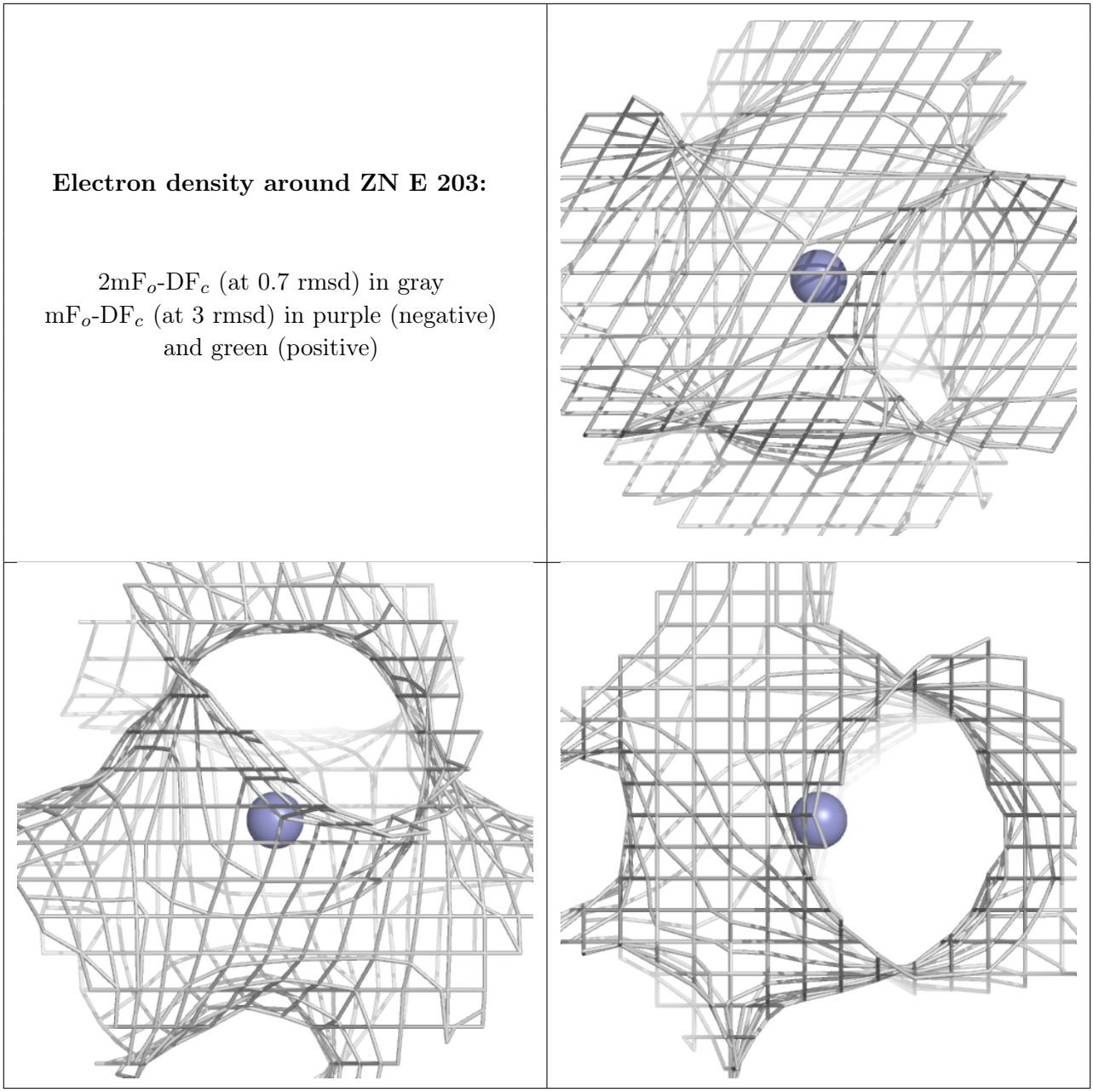
Electron density around ZN A 203:

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



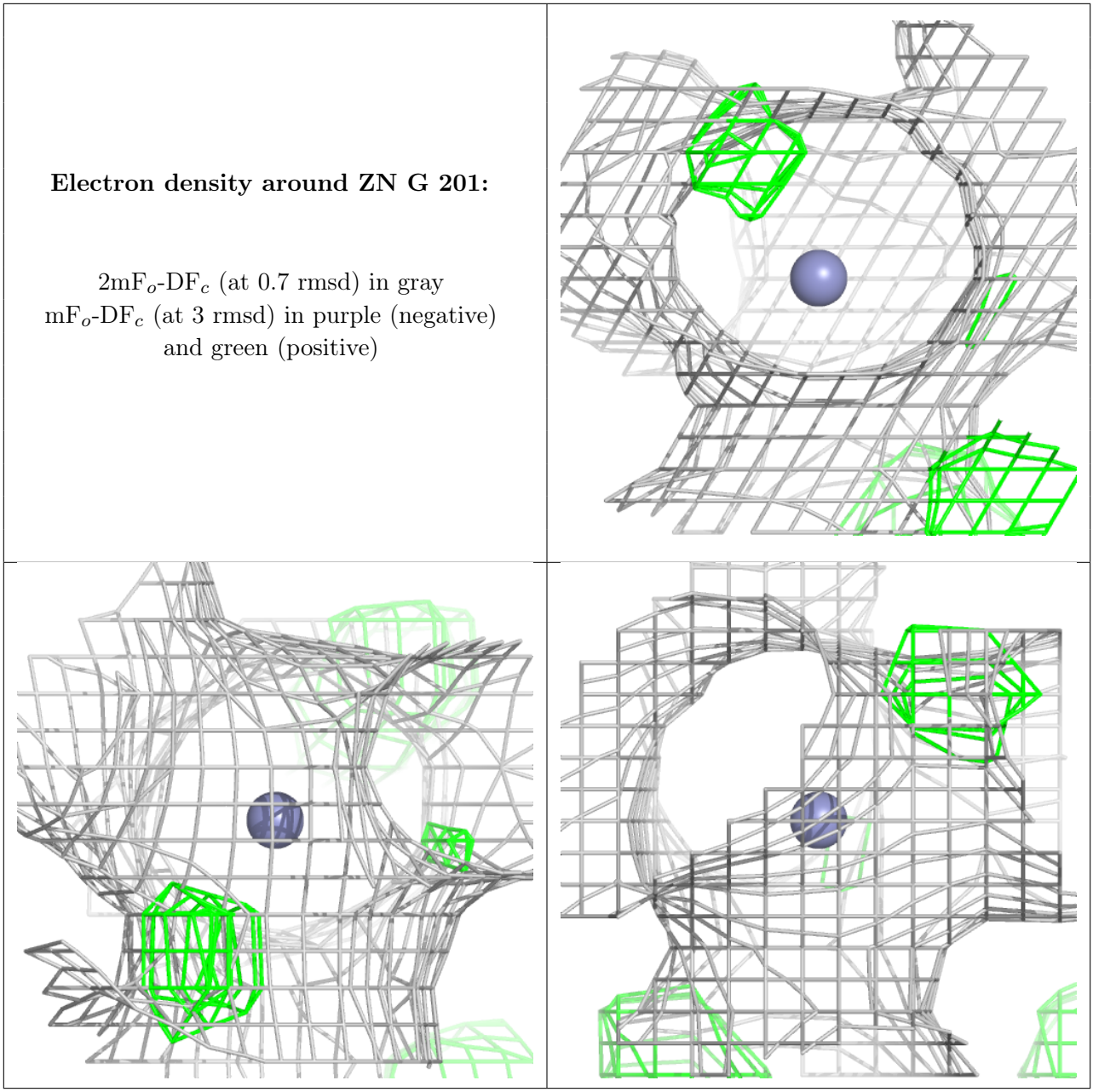
Electron density around ZN E 203:

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



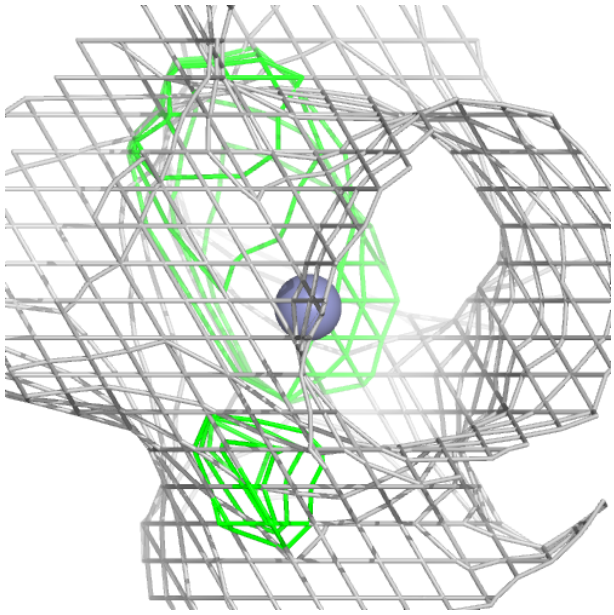
Electron density around ZN G 201:

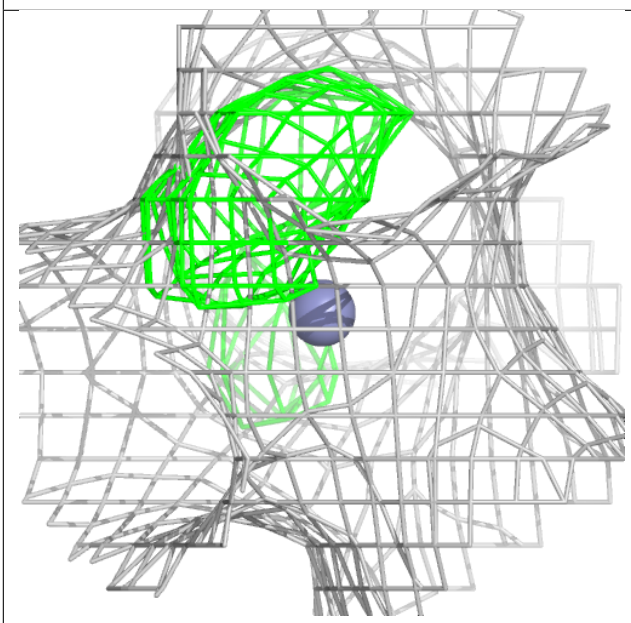
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

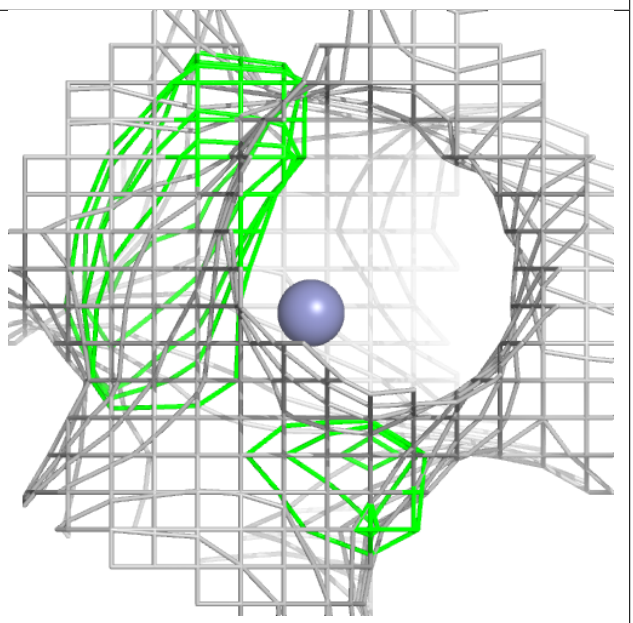


Electron density around ZN G 202:

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

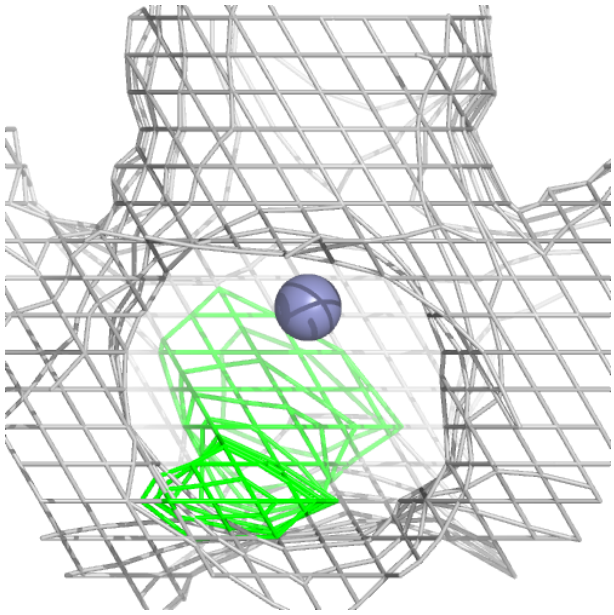


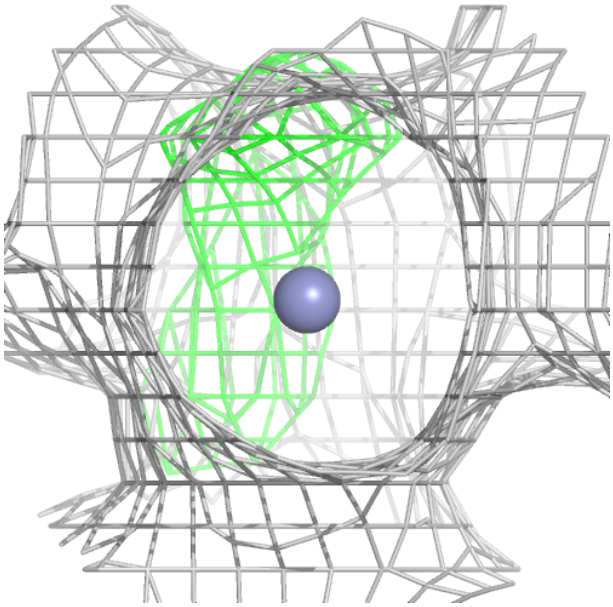


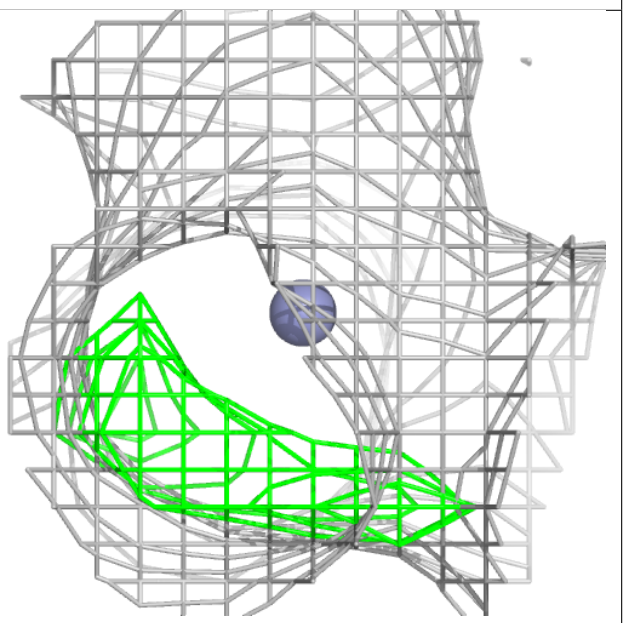


Electron density around ZN B 202:

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

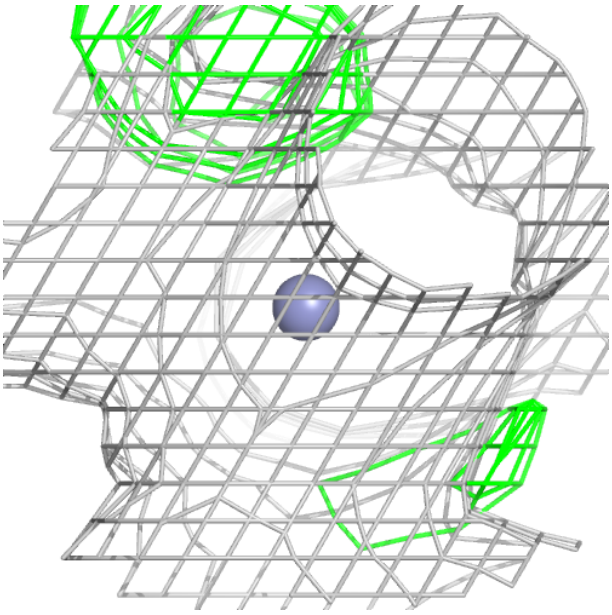


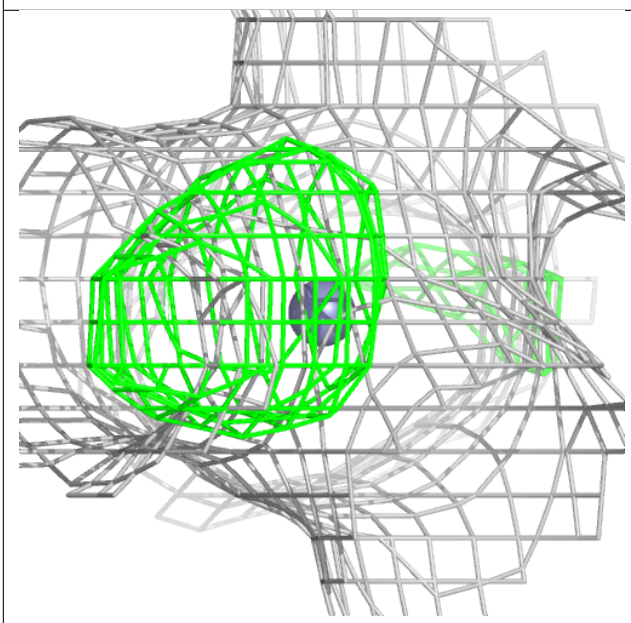


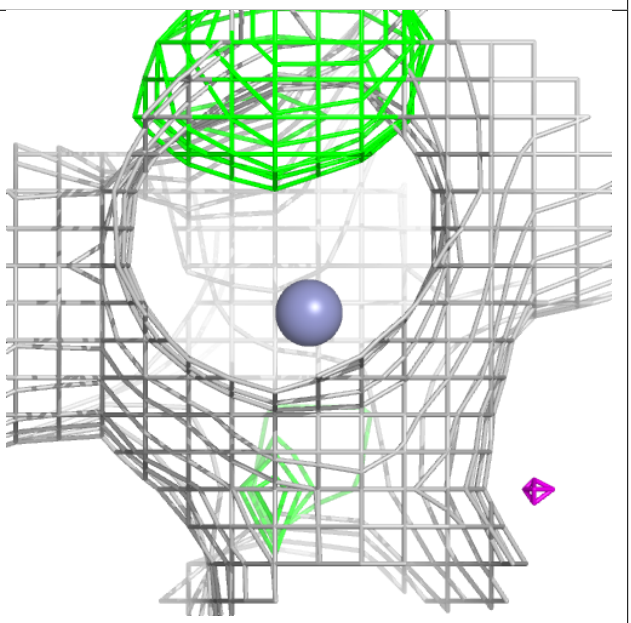


Electron density around ZN B 203:

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

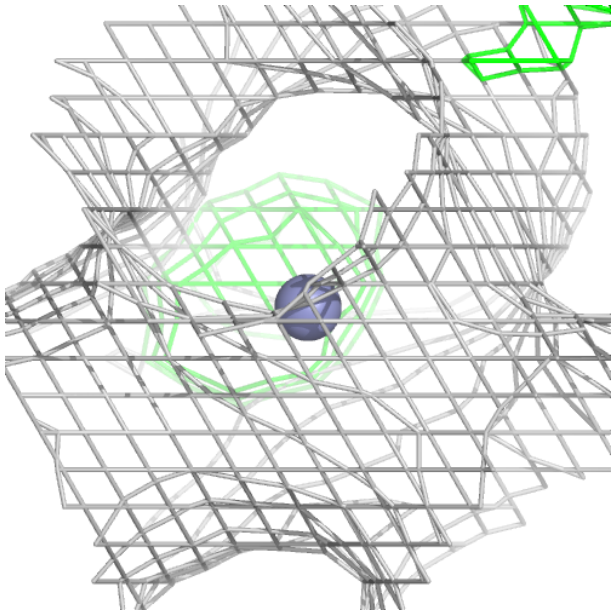


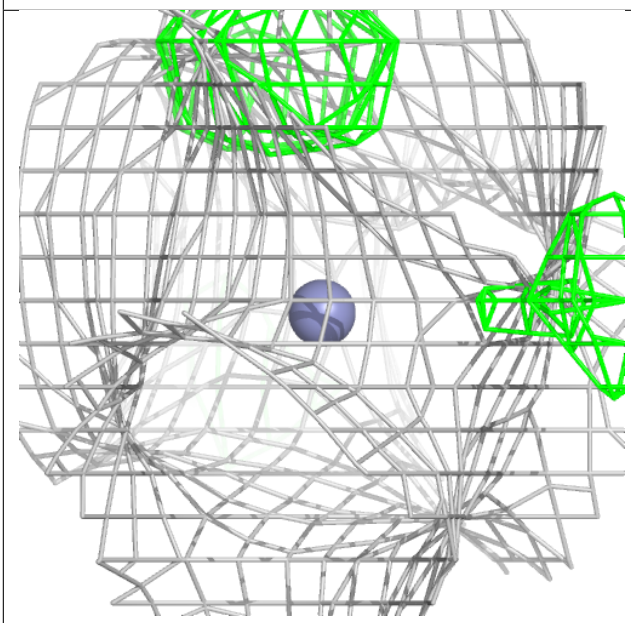


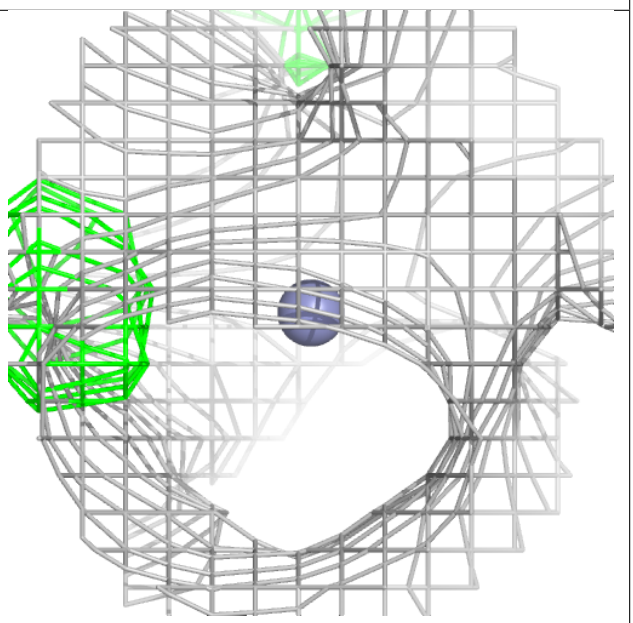


Electron density around ZN D 201:

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

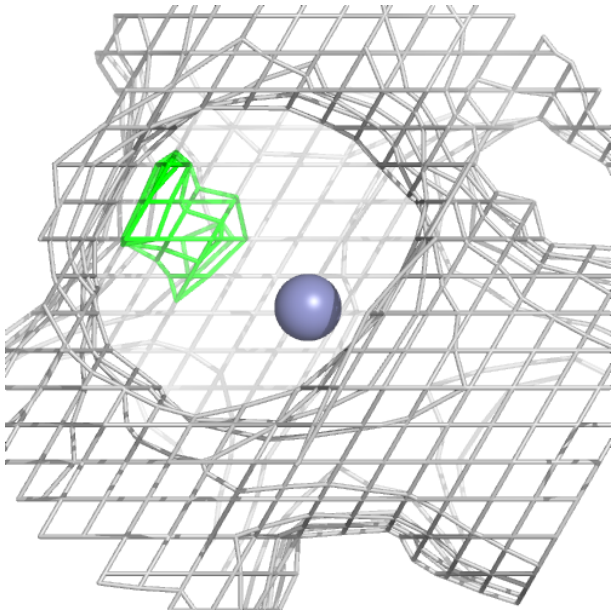


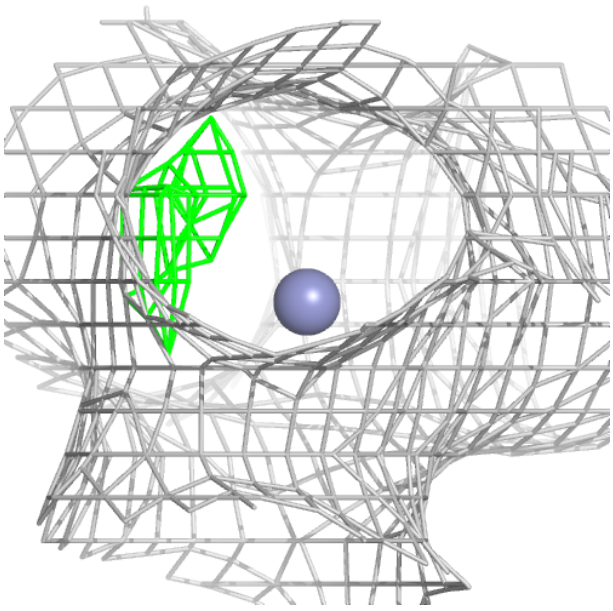


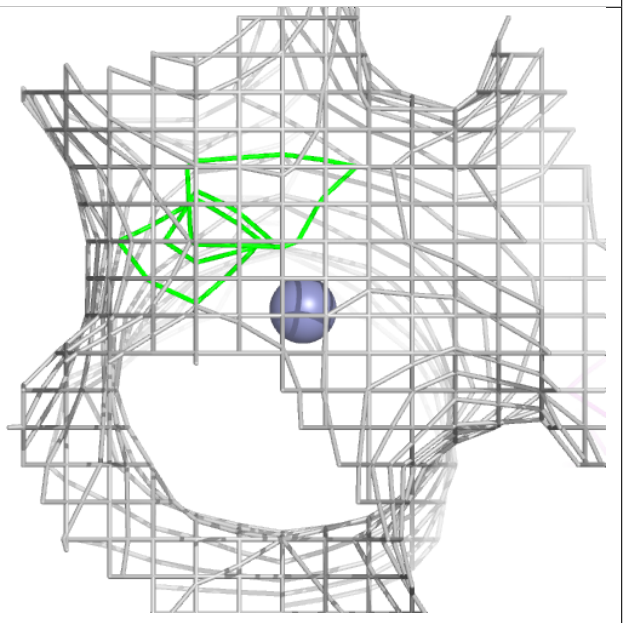


Electron density around ZN D 202:

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

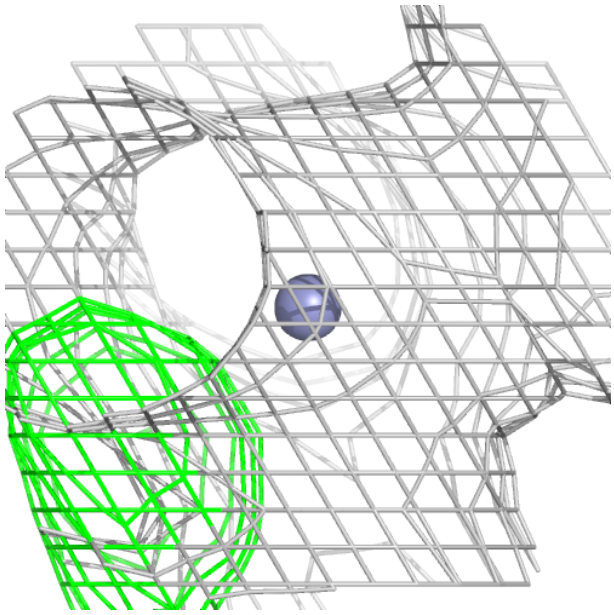


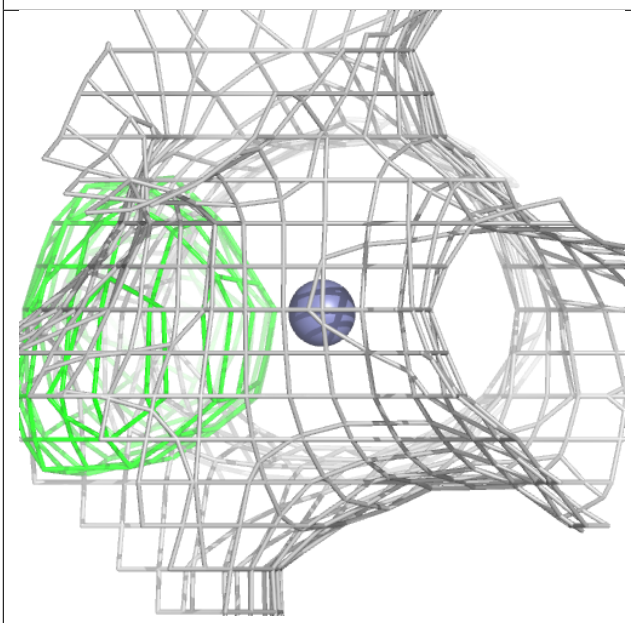


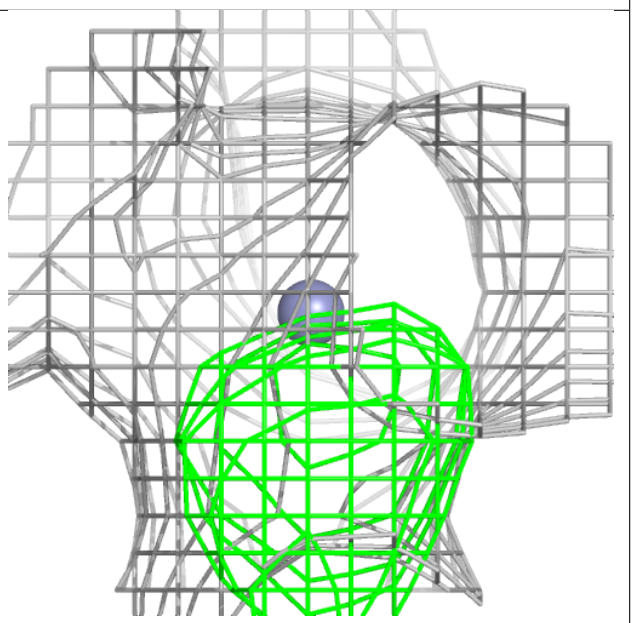


Electron density around ZN D 203:

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

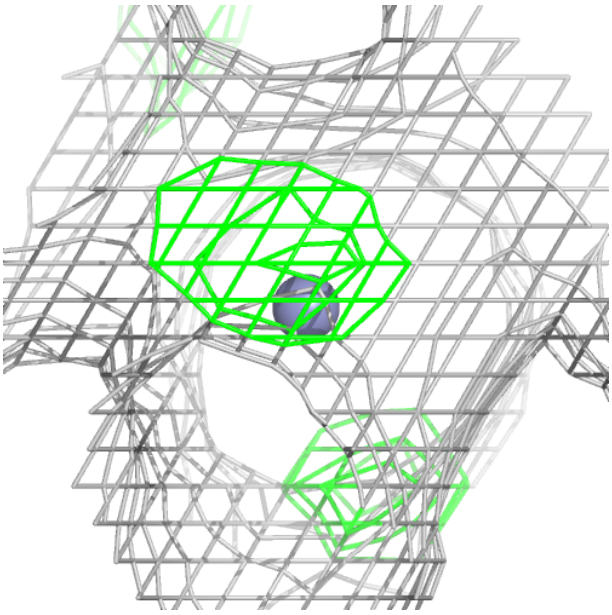


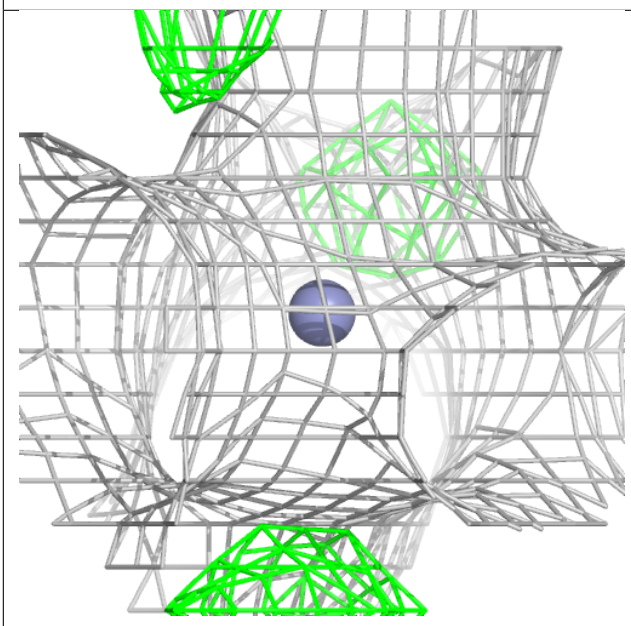


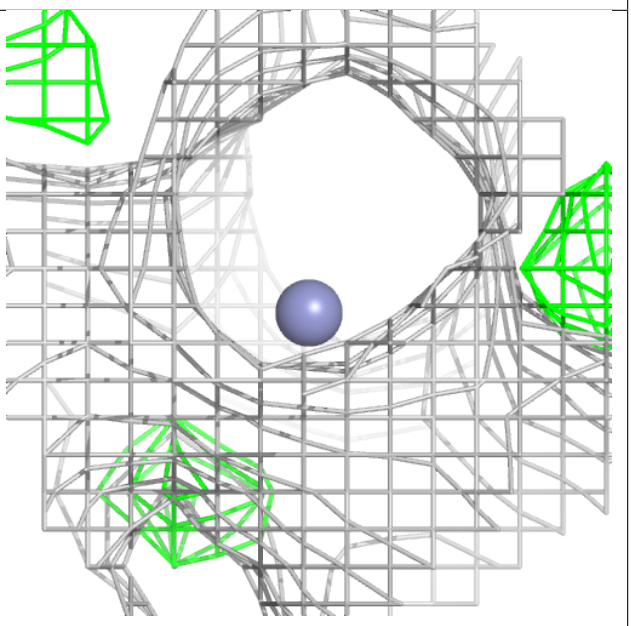


Electron density around ZN E 201:

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

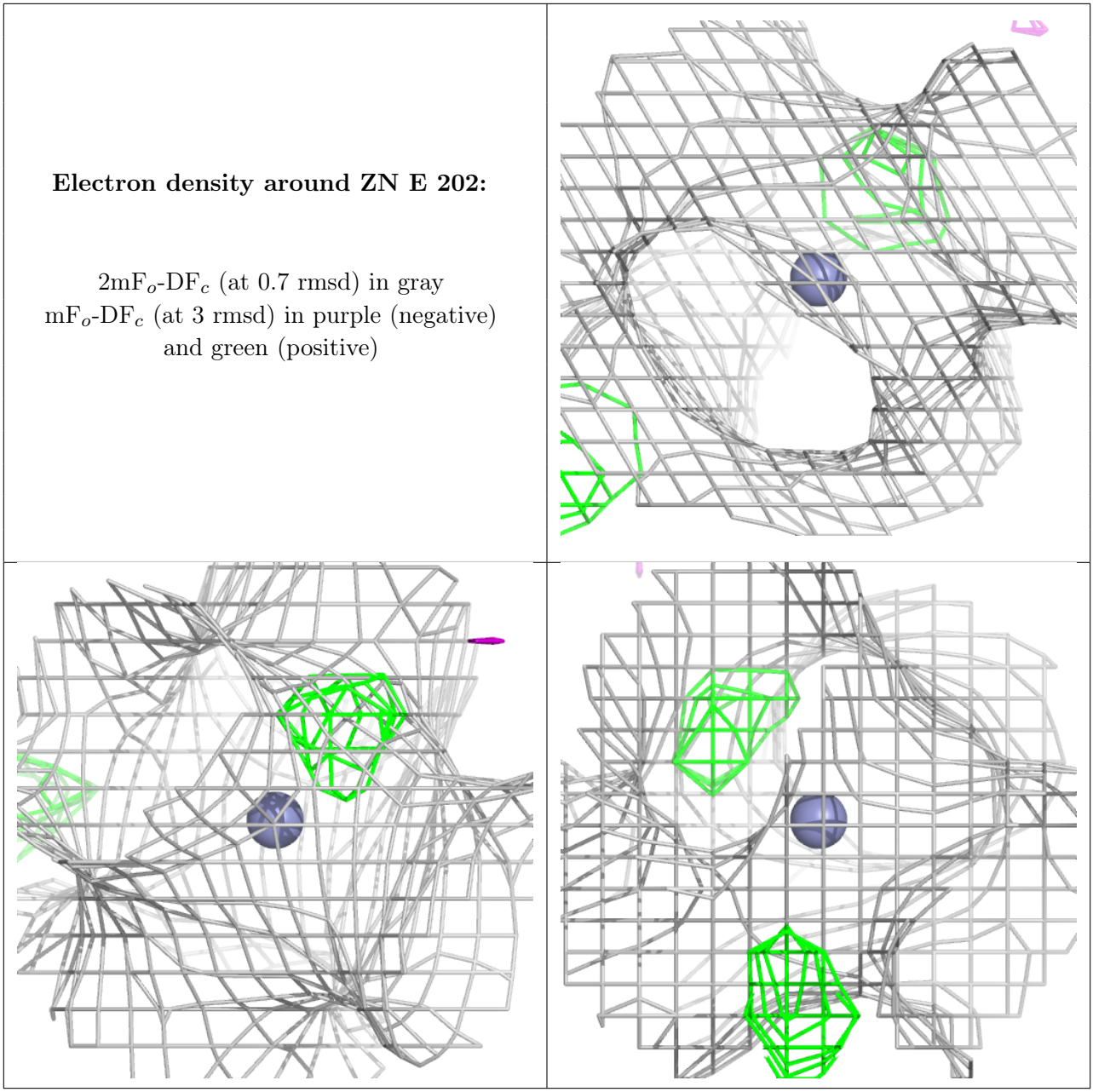






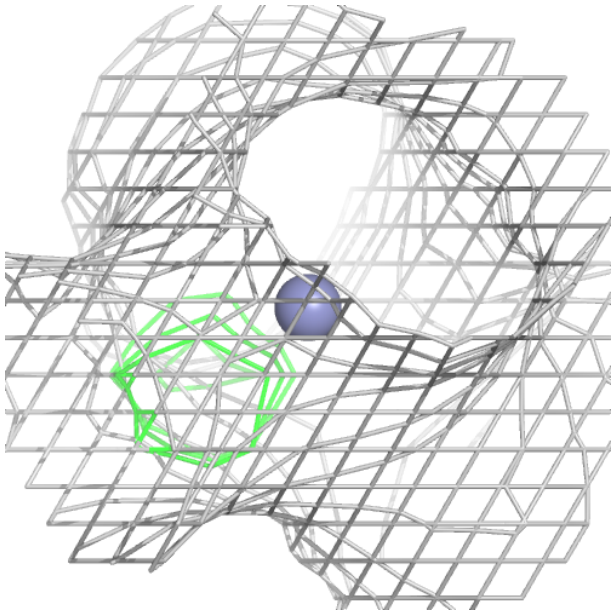
Electron density around ZN E 202:

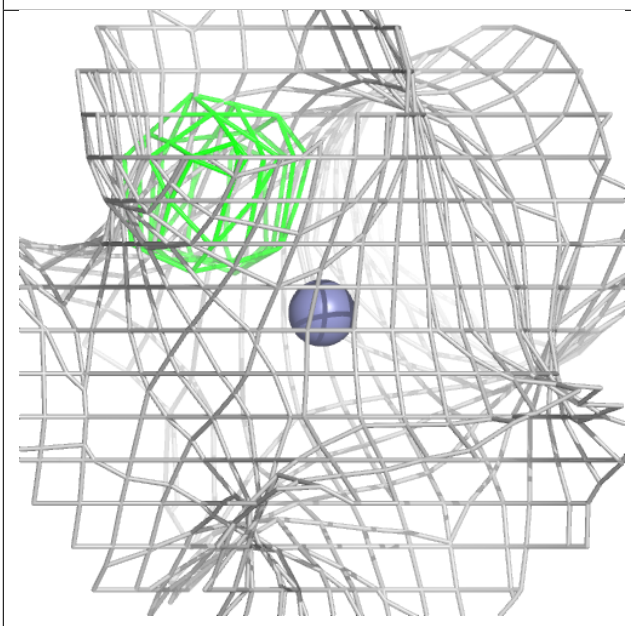
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

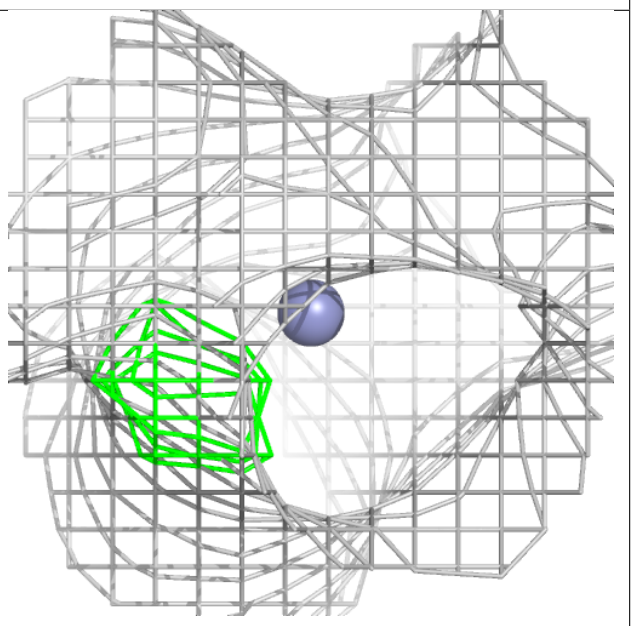


Electron density around ZN A 202:

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

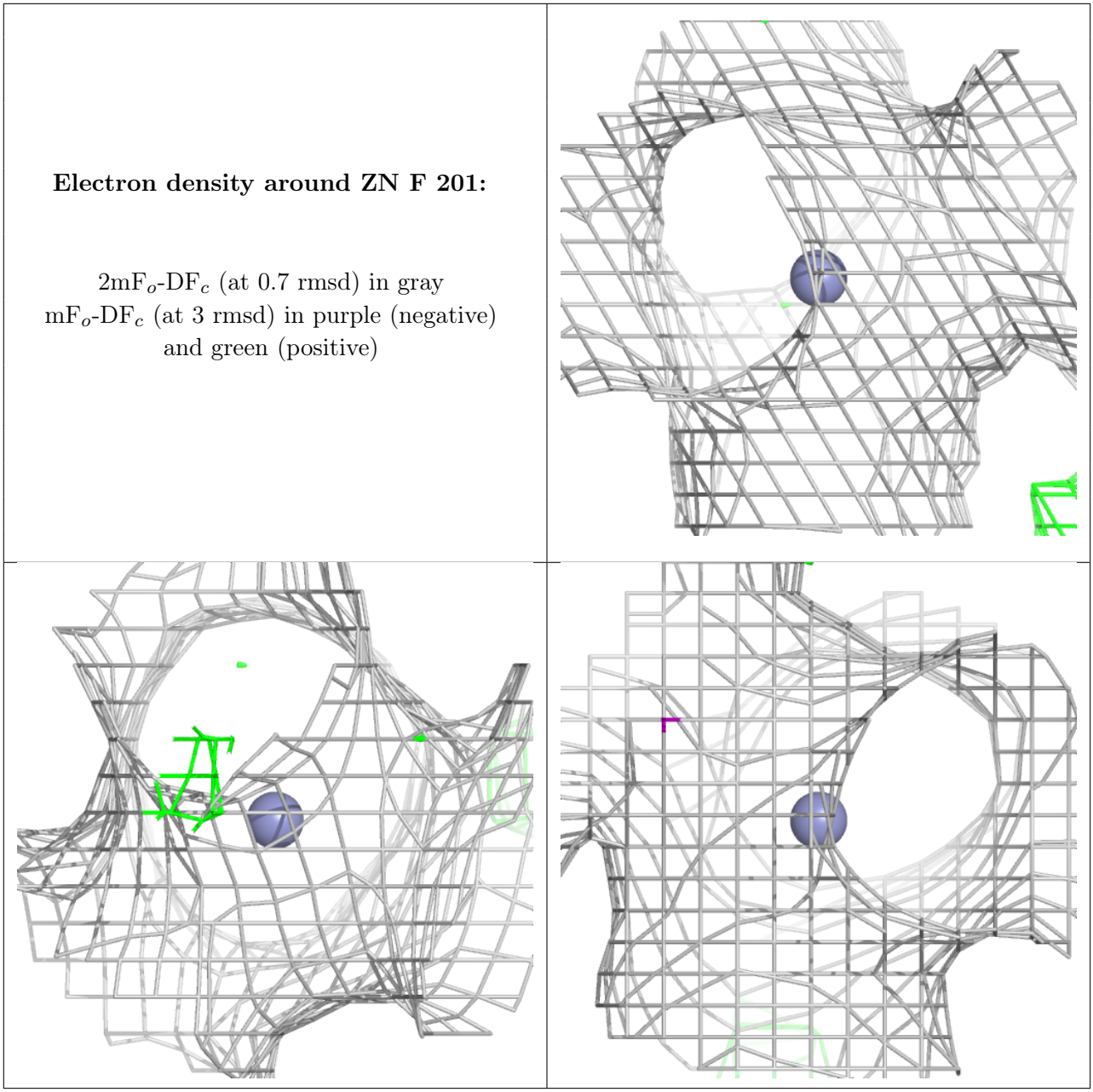






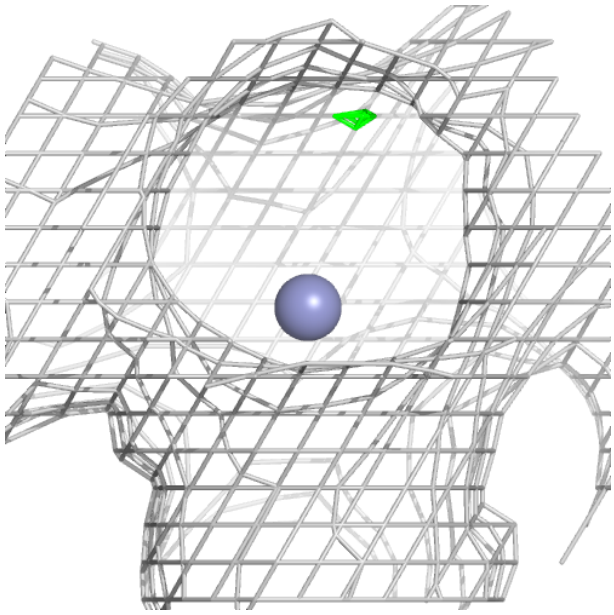
Electron density around ZN F 201:

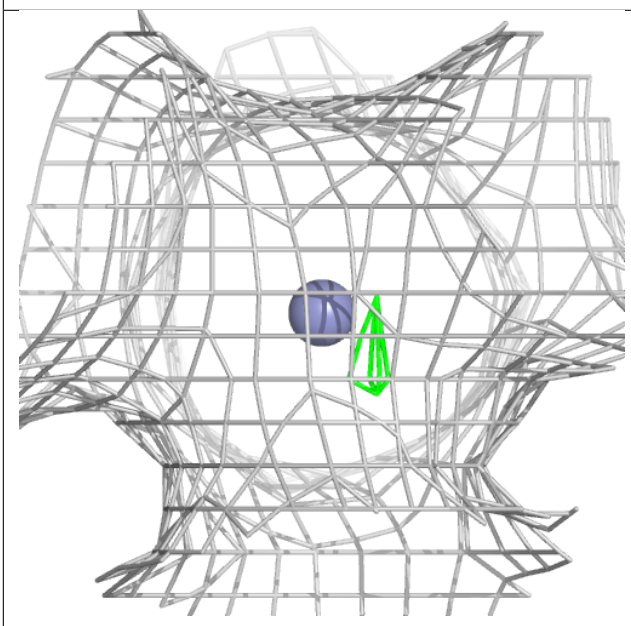
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

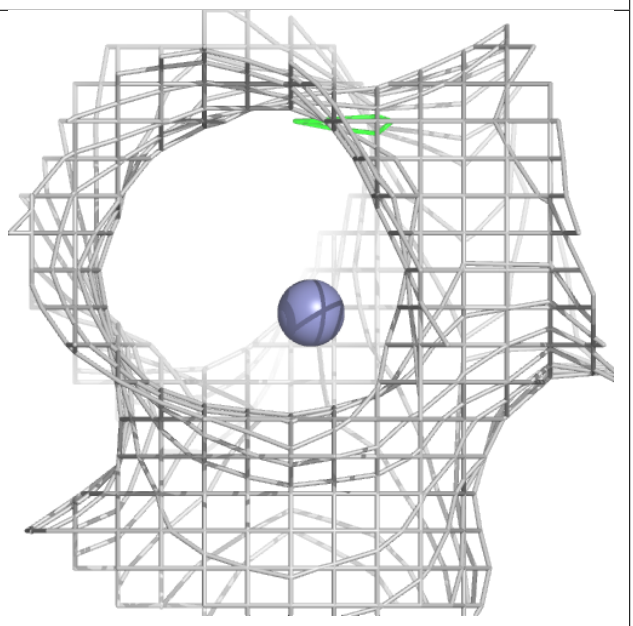


Electron density around ZN F 202:

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

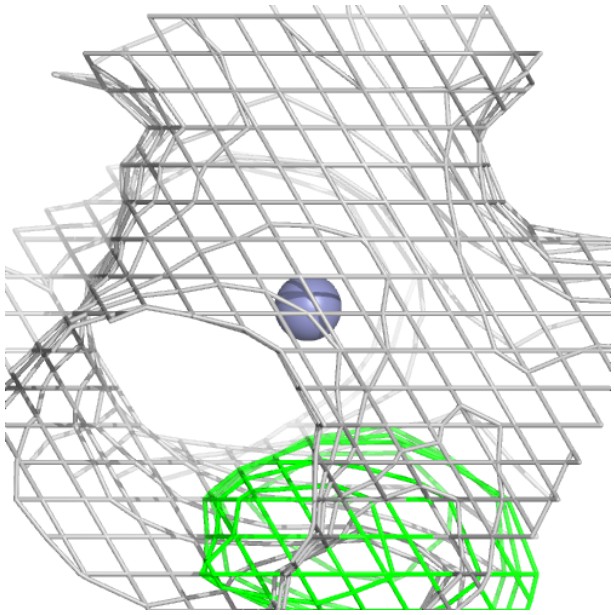


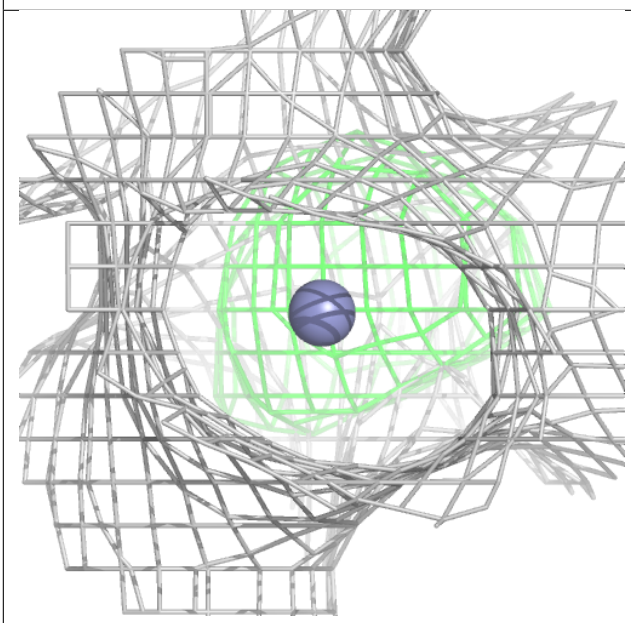


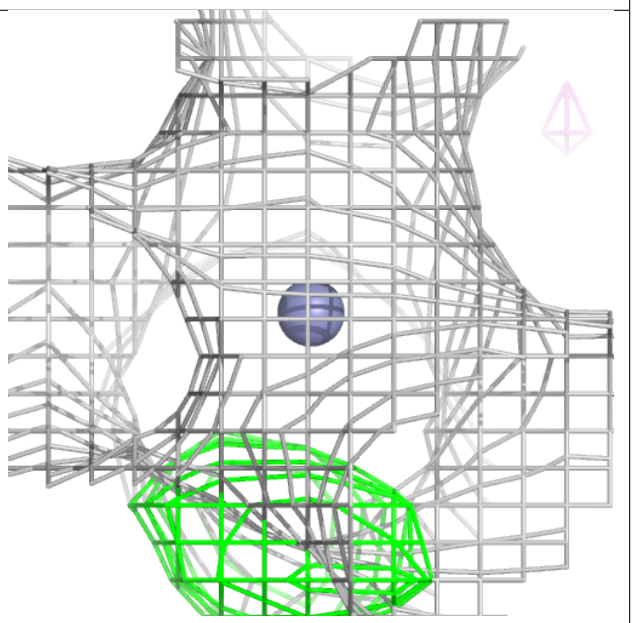


Electron density around ZN F 203:

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

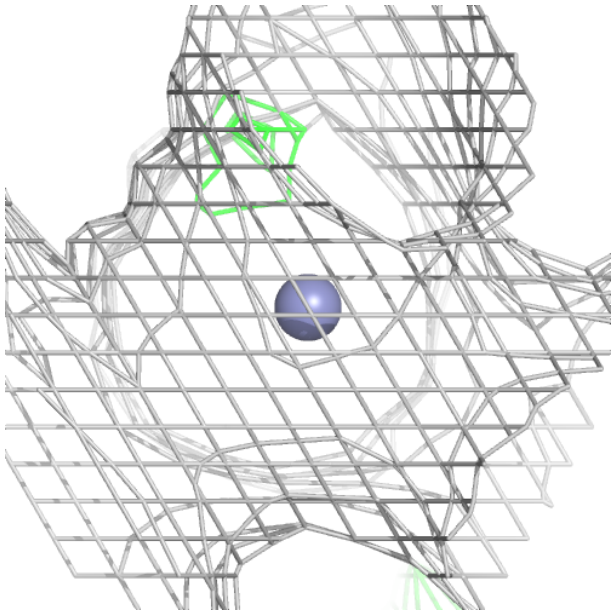


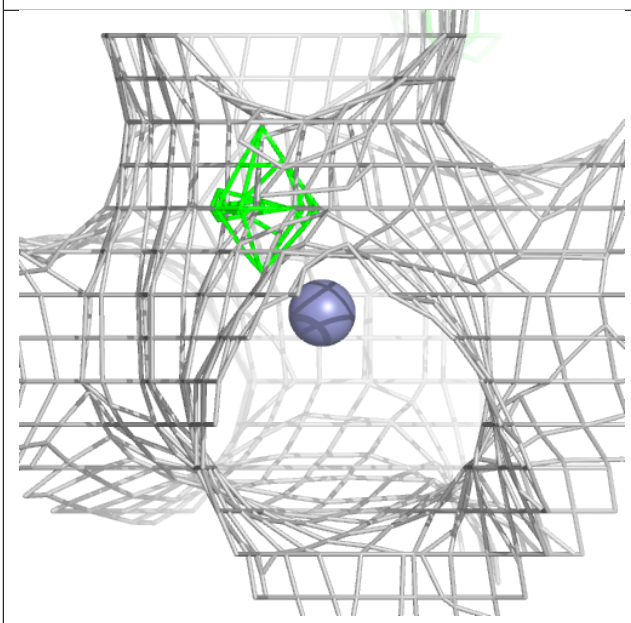


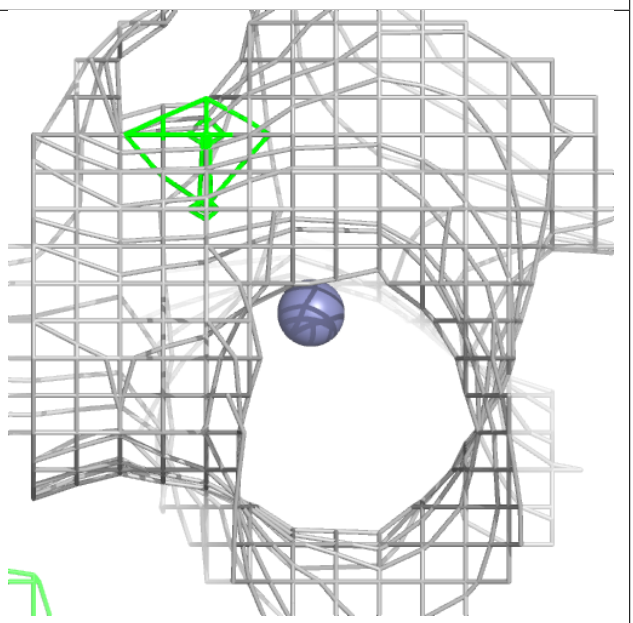


Electron density around ZN A 201:

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

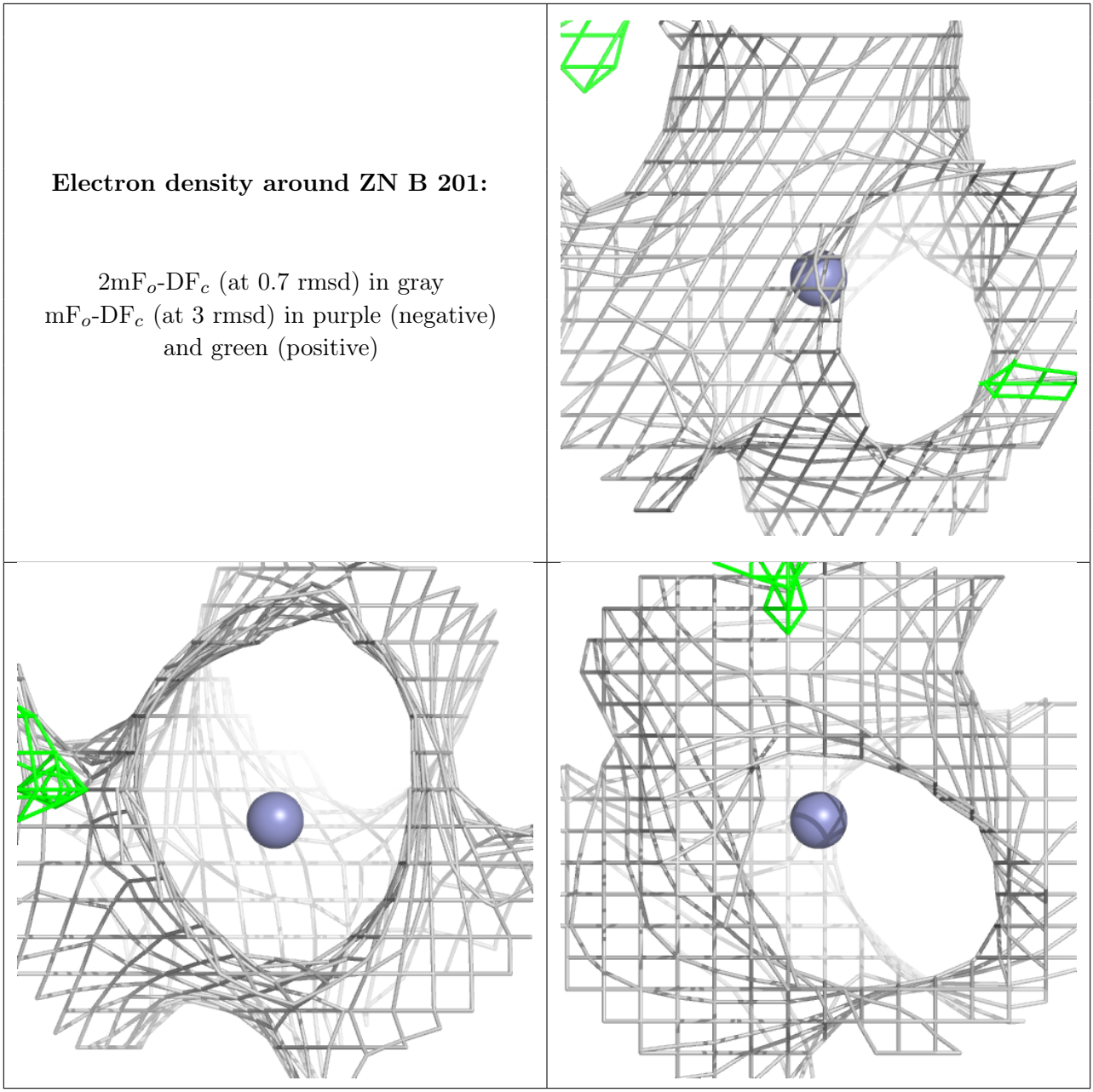






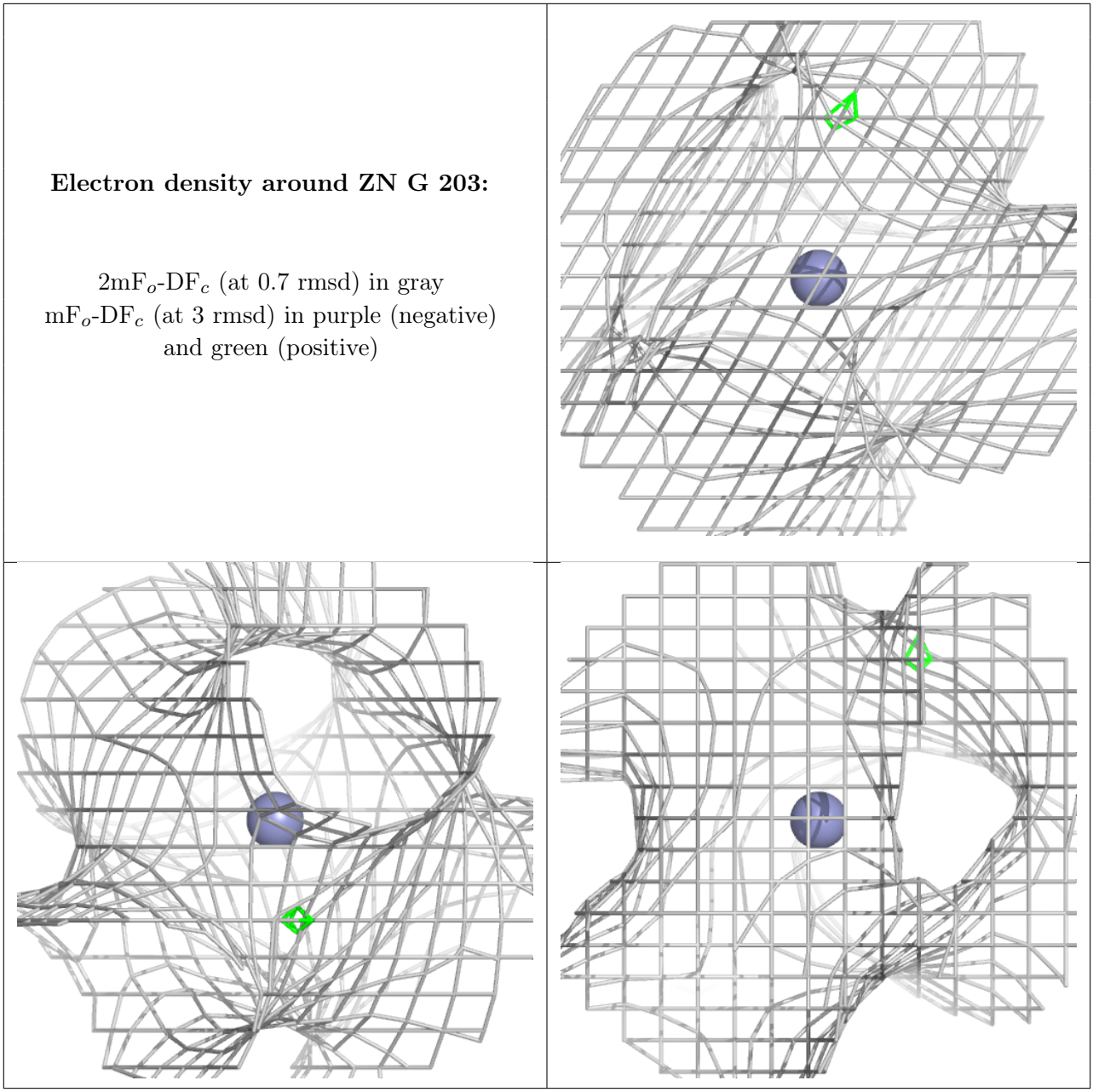
Electron density around ZN B 201:

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



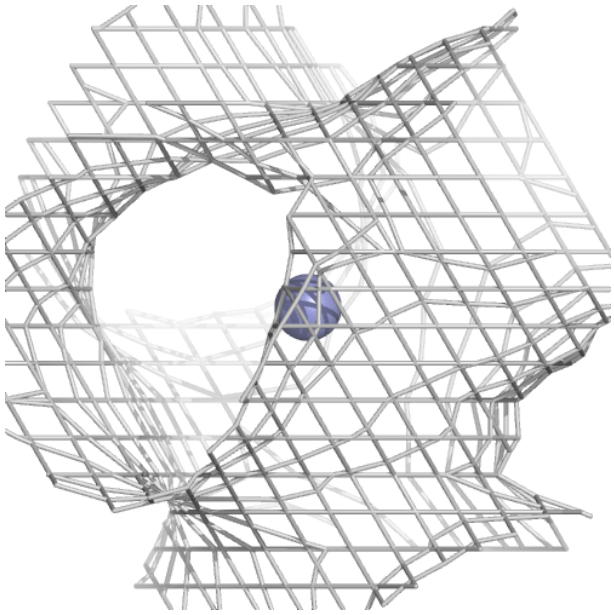
Electron density around ZN G 203:

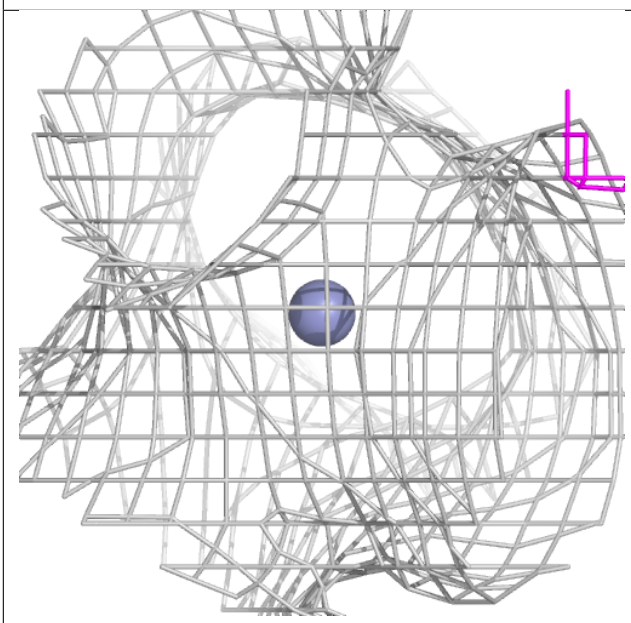
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

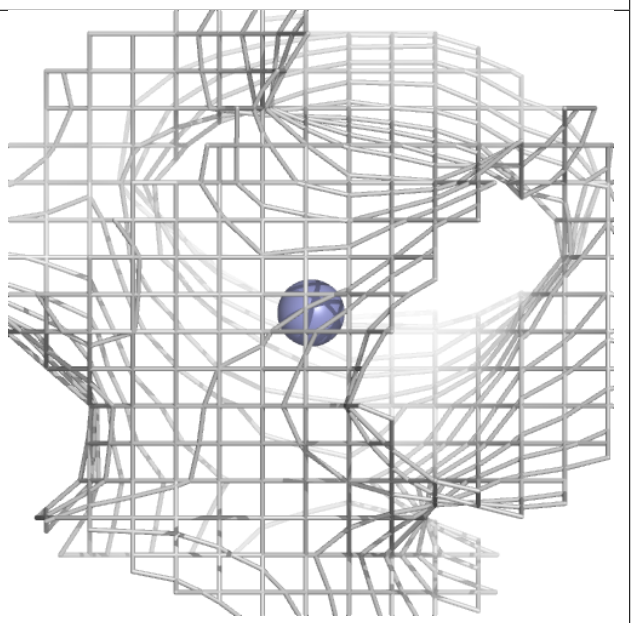


Electron density around ZN H 201:

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

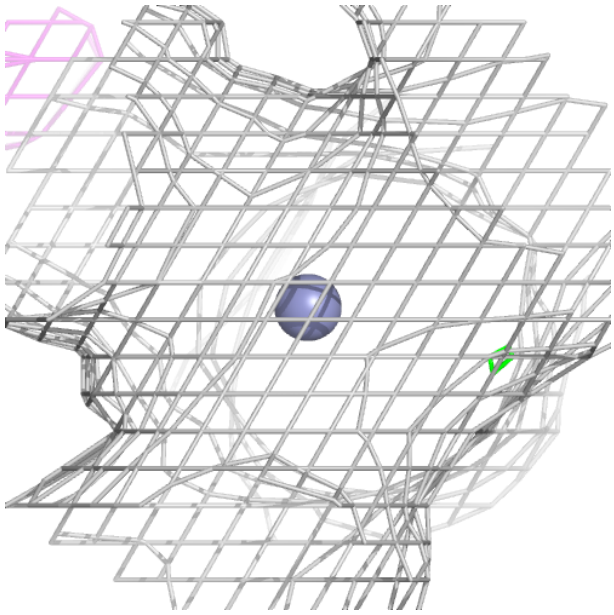


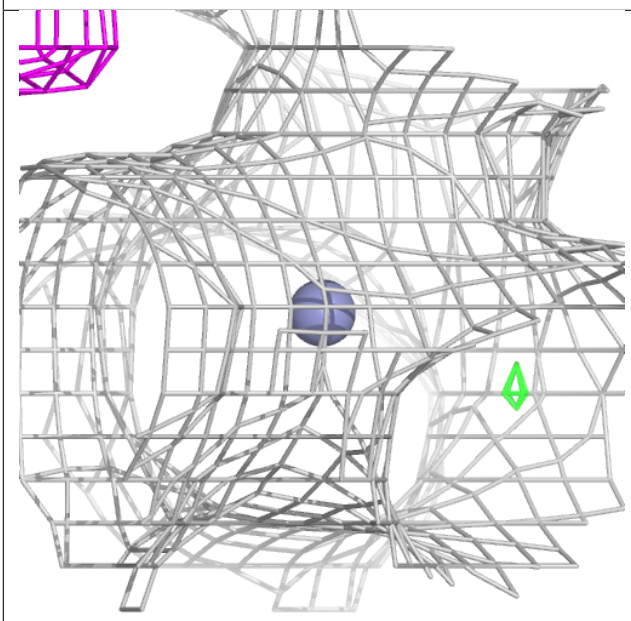


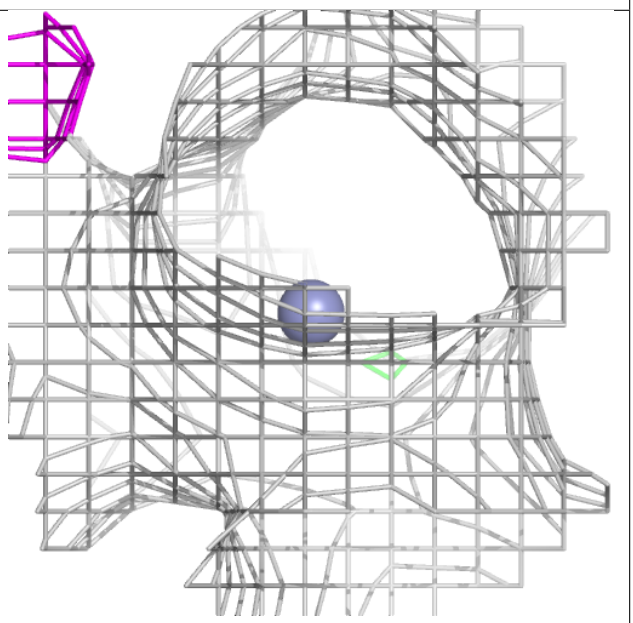


Electron density around ZN H 202:

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

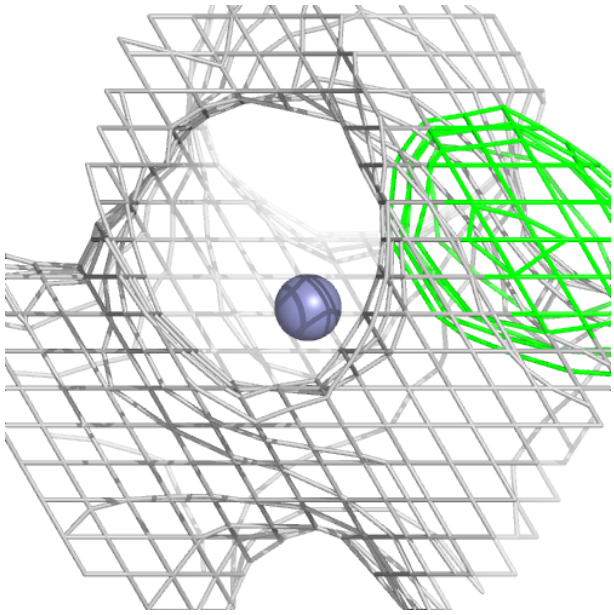


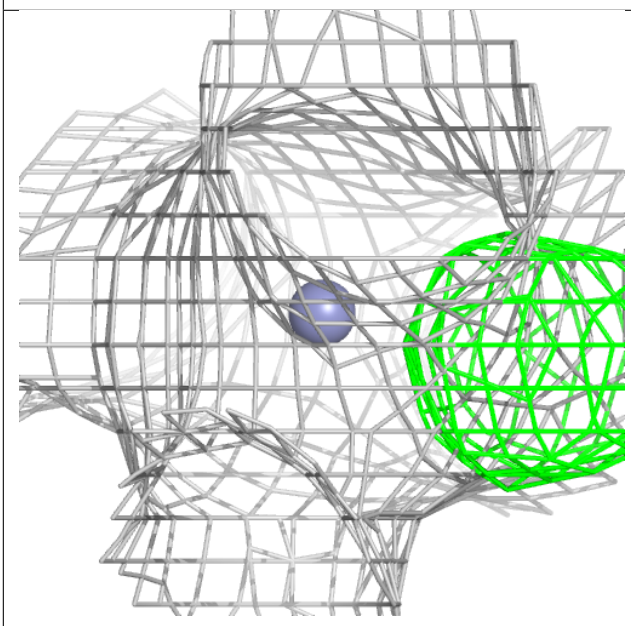


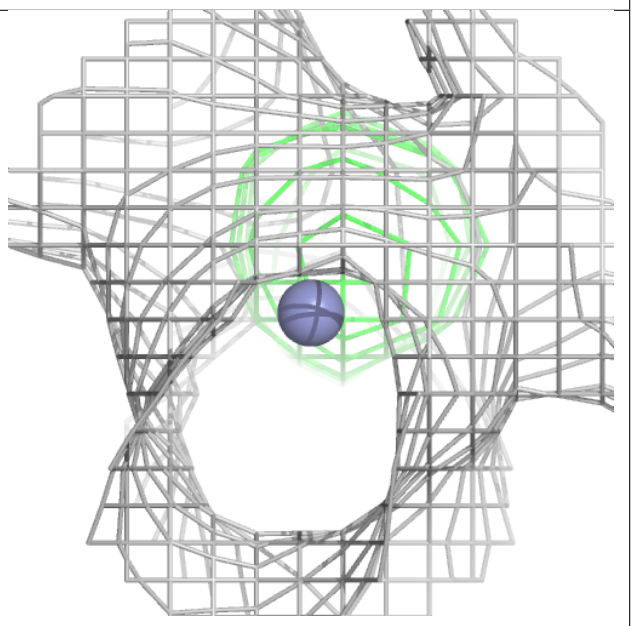


Electron density around ZN H 203:

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

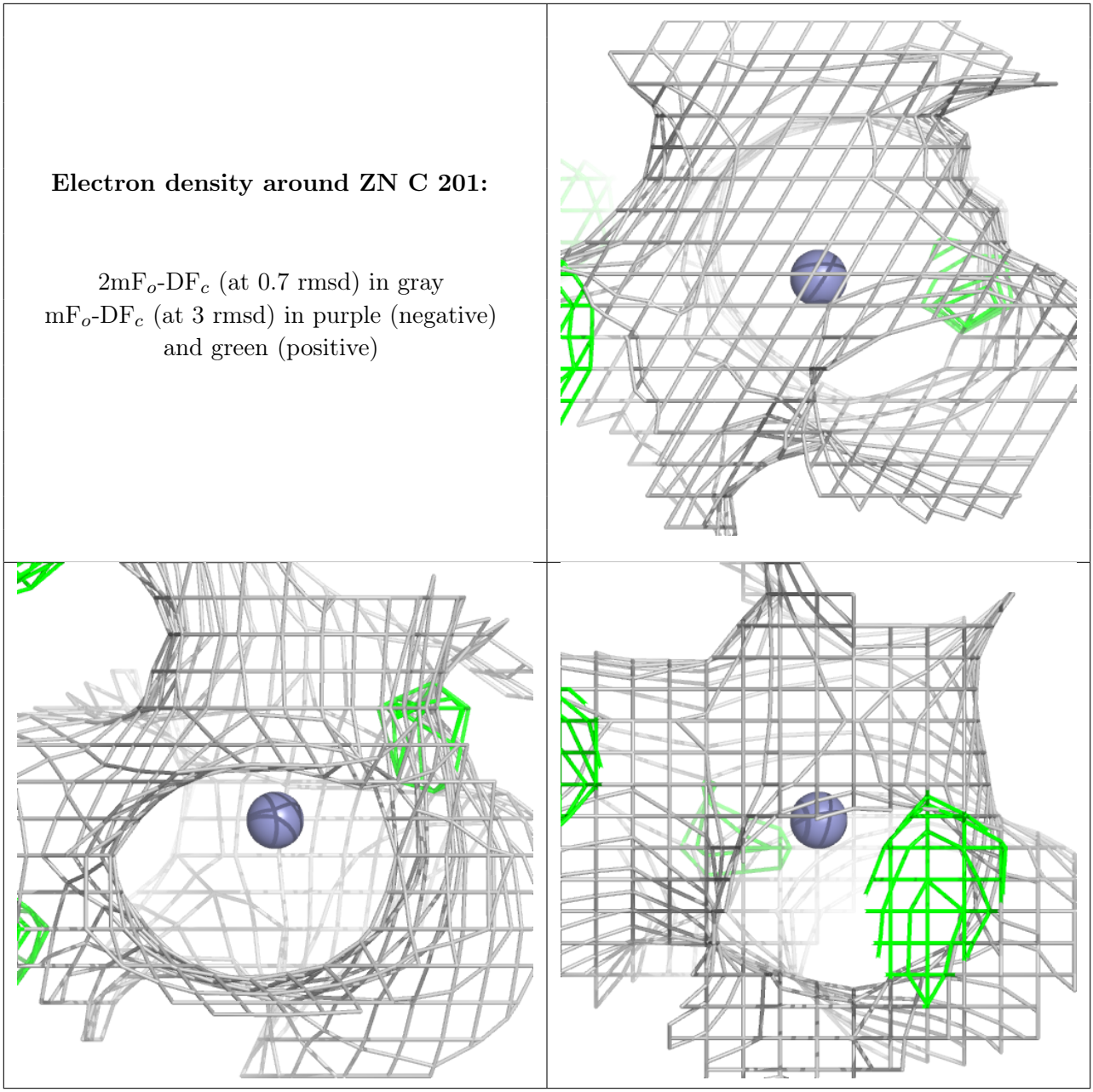






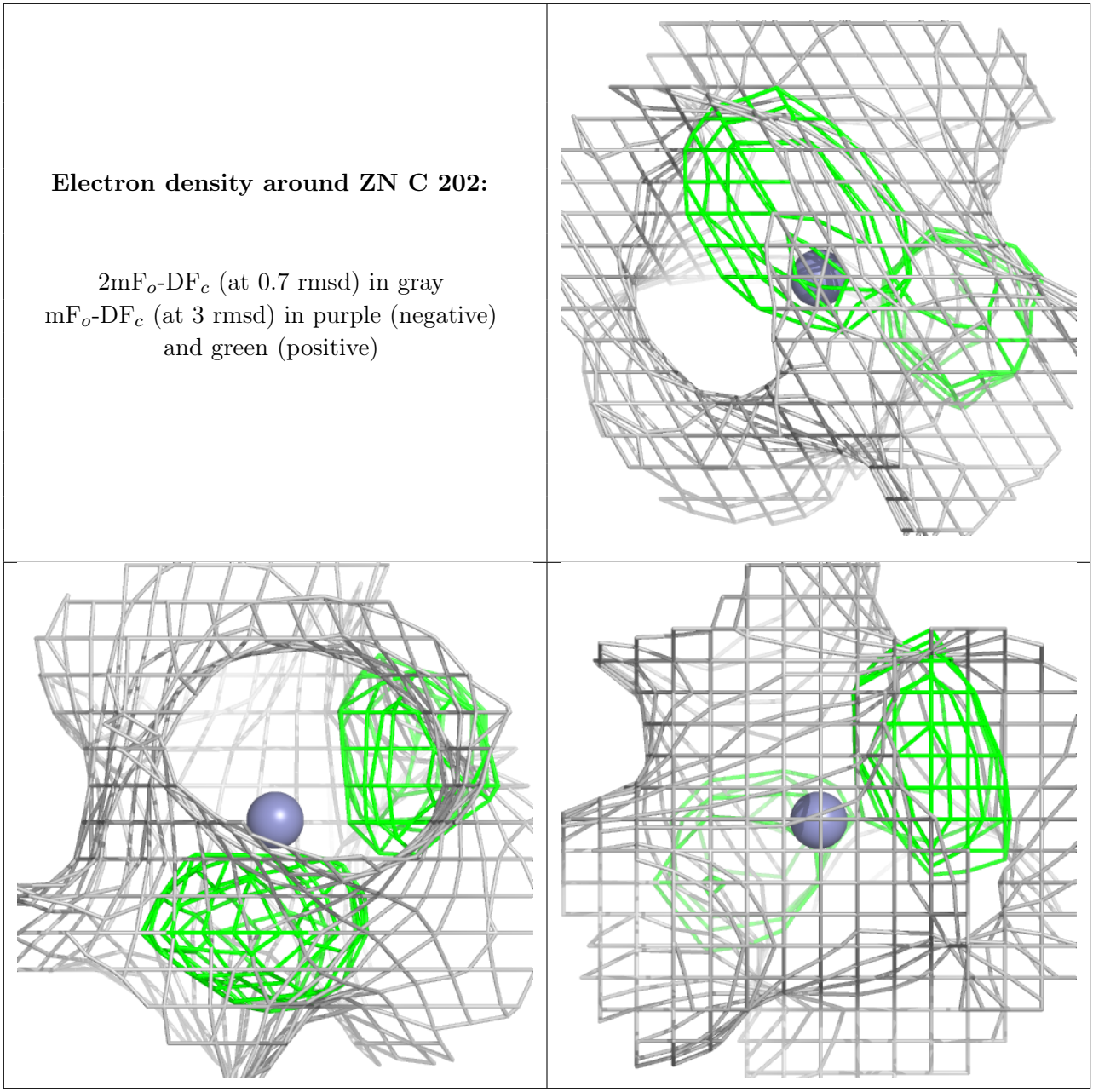
Electron density around ZN C 201:

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



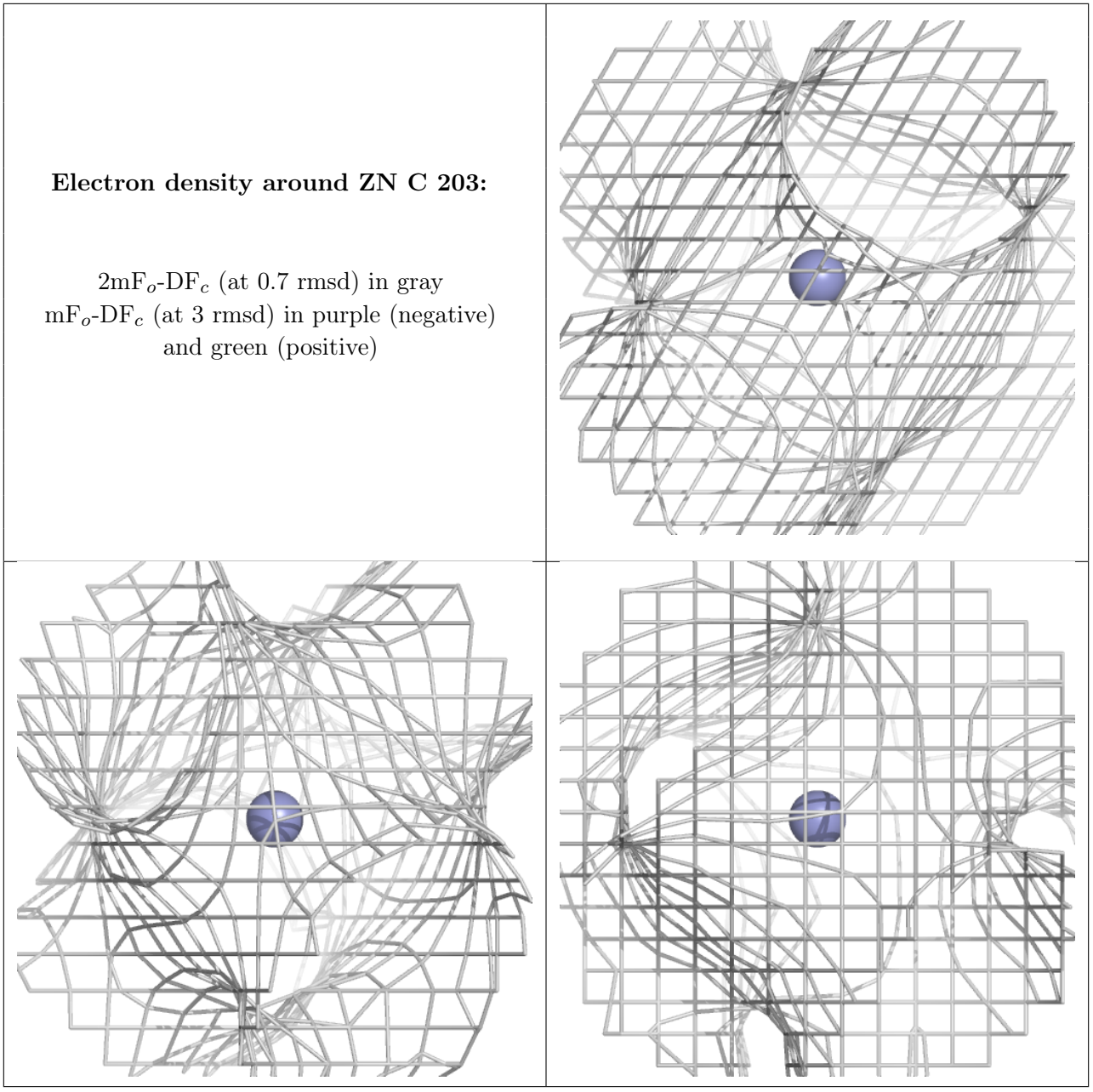
Electron density around ZN C 202:

$2mF_o$-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 203:

$2mF_o$-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.