Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 07:21 AM JST

PDB ID	:	6L56
Title	:	Fe(II) loaded Tegillarca granosa ferritin
Authors	:	Jiang, Q.Q.; Su, X.R.; Ming, T.H.; Huan, H.S.
Deposited on	:	2019-10-22
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

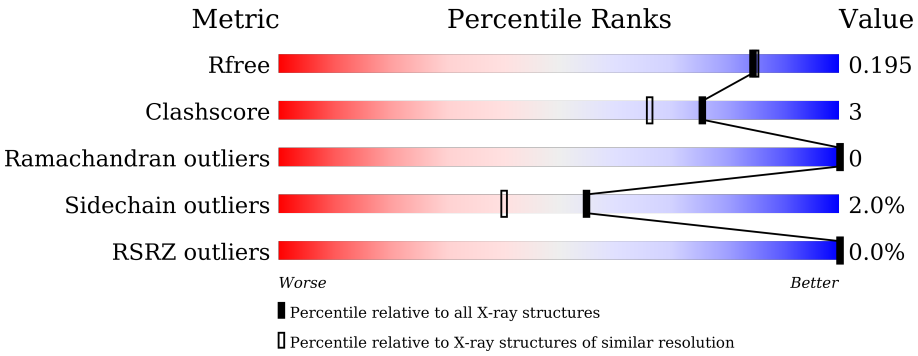
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	172	90% 8% .
1	B	172	92% 6% .
1	C	172	90% 9% .
1	D	172	89% 9% .
1	E	172	91% 8% .
1	F	172	89% 9% .

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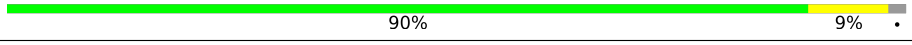
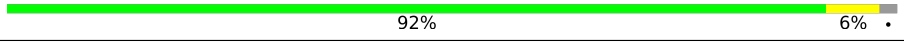
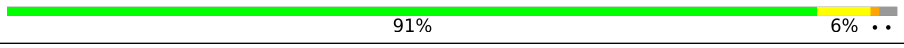
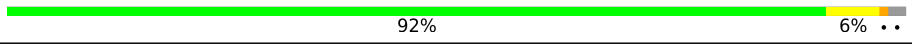
Mol	Chain	Length	Quality of chain
1	G	172	
1	H	172	
1	I	172	
1	J	172	
1	K	172	
1	L	172	
1	M	172	
1	N	172	
1	O	172	
1	P	172	
1	Q	172	
1	R	172	
1	S	172	
1	T	172	
1	U	172	
1	V	172	
1	W	172	
1	X	172	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 35724 atoms, of which 73 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 Ferritin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	169	Total C H N O S 1445 862 73 232 269 9	0	0	0
1	B	169	Total C N O S 1370 861 230 270 9	0	0	0
1	C	169	Total C N O S 1362 853 227 273 9	0	0	0
1	D	169	Total C N O S 1363 859 228 267 9	0	0	0
1	E	169	Total C N O S 1370 862 232 267 9	0	0	0
1	F	169	Total C N O S 1365 858 229 269 9	0	0	0
1	G	169	Total C N O S 1367 860 229 269 9	0	0	0
1	H	169	Total C N O S 1360 854 227 270 9	0	0	0
1	I	169	Total C N O S 1366 858 228 271 9	0	0	0
1	J	169	Total C N O S 1366 860 228 269 9	0	0	0
1	K	169	Total C N O S 1372 862 232 269 9	0	0	0
1	L	169	Total C N O S 1376 864 232 271 9	0	0	0
1	M	169	Total C N O S 1358 854 228 267 9	0	0	0
1	N	169	Total C N O S 1370 860 231 270 9	0	0	0
1	O	169	Total C N O S 1364 856 228 271 9	0	0	0
1	P	169	Total C N O S 1371 860 229 273 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	169	Total	C	N	O	S	0	0	0
			1373	862	230	272	9			
1	R	169	Total	C	N	O	S	0	0	0
			1369	860	229	271	9			
1	S	169	Total	C	N	O	S	0	0	0
			1365	858	228	270	9			
1	T	169	Total	C	N	O	S	0	0	0
			1362	857	227	269	9			
1	U	169	Total	C	N	O	S	0	0	0
			1375	863	232	271	9			
1	V	169	Total	C	N	O	S	0	0	0
			1371	860	231	271	9			
1	W	169	Total	C	N	O	S	0	0	0
			1365	858	229	269	9			
1	X	169	Total	C	N	O	S	0	0	0
			1372	862	230	271	9			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	2	Total	Fe	0	0
			2	2		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	P	1	Total Fe 1 1	0	0
2	Q	1	Total Fe 1 1	0	0
2	R	1	Total Fe 1 1	0	0
2	S	1	Total Fe 1 1	0	0
2	T	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	V	1	Total Fe 1 1	0	0
2	W	1	Total Fe 1 1	0	0
2	X	1	Total Fe 1 1	0	0

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	4	Total Fe 4 4	0	0
3	I	4	Total Fe 4 4	0	0
3	J	1	Total Fe 1 1	0	0
3	K	4	Total Fe 4 4	0	0
3	L	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	4	Total Fe 4 4	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	S	1	Total Fe 1 1	0	0
3	T	1	Total Fe 1 1	0	0
3	U	1	Total Fe 1 1	0	0
3	V	1	Total Fe 1 1	0	0
3	W	1	Total Fe 1 1	0	0
3	X	1	Total Fe 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0
4	D	2	Total Na 2 2	0	0
4	E	1	Total Na 1 1	0	0
4	F	2	Total Na 2 2	0	0
4	G	2	Total Na 2 2	0	0
4	H	1	Total Na 1 1	0	0
4	I	1	Total Na 1 1	0	0
4	J	2	Total Na 2 2	0	0
4	K	1	Total Na 1 1	0	0
4	L	2	Total Na 2 2	0	0
4	M	2	Total Na 2 2	0	0
4	N	1	Total Na 1 1	0	0
4	O	2	Total Na 2 2	0	0
4	P	1	Total Na 1 1	0	0
4	Q	1	Total Na 1 1	0	0
4	R	2	Total Na 2 2	0	0
4	S	2	Total Na 2 2	0	0
4	T	1	Total Na 1 1	0	0
4	U	1	Total Na 1 1	0	0
4	V	2	Total Na 2 2	0	0
4	W	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	2	Total Na 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	113	Total O 113 113	0	0
5	B	113	Total O 113 113	0	0
5	C	111	Total O 111 111	0	0
5	D	112	Total O 112 112	0	0
5	E	111	Total O 111 111	0	0
5	F	111	Total O 111 111	0	0
5	G	111	Total O 111 111	0	0
5	H	113	Total O 113 113	0	0
5	I	118	Total O 118 118	0	0
5	J	115	Total O 115 115	0	0
5	K	114	Total O 114 114	0	0
5	L	117	Total O 117 117	0	0
5	M	109	Total O 109 109	0	0
5	N	120	Total O 120 120	0	0
5	O	110	Total O 110 110	0	0
5	P	112	Total O 112 112	0	0
5	Q	113	Total O 113 113	0	0
5	R	111	Total O 111 111	0	0

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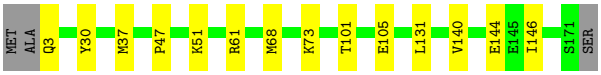
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	114	Total O 114 114	0	0
5	T	121	Total O 121 121	0	0
5	U	112	Total O 112 112	0	0
5	V	115	Total O 115 115	0	0
5	W	111	Total O 111 111	0	0
5	X	112	Total O 112 112	0	0

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: Ferritin

Chain A:

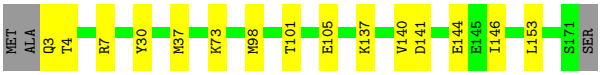


- Molecule 1: Ferritin

Chain B:

- Molecule 1: Ferritin

Chain C:

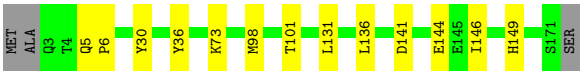


- Molecule 1: Ferritin

Chain D:

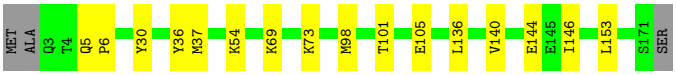
- Molecule 1: Ferritin

Chain E:



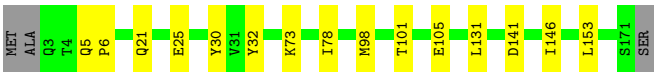
- Molecule 1: Ferritin

Chain F:



• Molecule 1: Ferritin

Chain G:



• Molecule 1: Ferritin

Chain H:

• Molecule 1: Ferritin

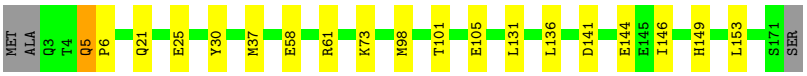
Chain I:

• Molecule 1: Ferritin

Chain J:

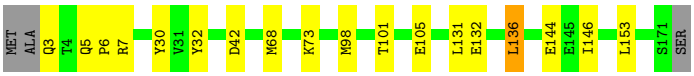
• Molecule 1: Ferritin

Chain K:



• Molecule 1: Ferritin

Chain L:



• Molecule 1: Ferritin

Chain M:

• Molecule 1: Ferritin

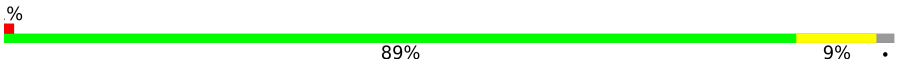
Chain N:

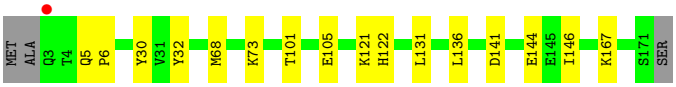
• Molecule 1: Ferritin

Chain O:

• Molecule 1: Ferritin

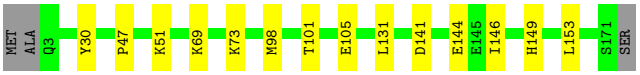
Chain P:





• Molecule 1: Ferritin

Chain Q:



• Molecule 1: Ferritin

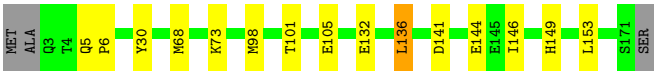
Chain R:

• Molecule 1: Ferritin

Chain S:

• Molecule 1: Ferritin

Chain T:

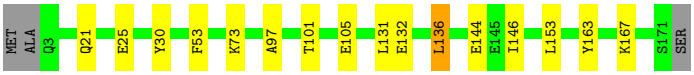


• Molecule 1: Ferritin

Chain U:

• Molecule 1: Ferritin

Chain V:

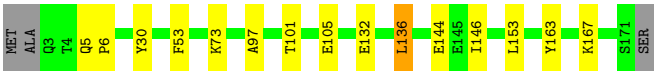


• Molecule 1: Ferritin

Chain W:

• Molecule 1: Ferritin

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.90Å 182.00Å 182.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.12 – 1.85 48.64 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.12-1.85) 99.5 (48.64-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.165 , 0.196 0.165 , 0.195	Depositor DCC
R_{free} test set	25642 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.146 for -h,l,k 0.146 for -l,-k,-h 0.146 for k,h,-l 0.469 for k,l,h 0.469 for l,h,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	35724	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9381e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FE, NA, FE2

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	0.36	0/1398	0.52	0/1879
1	B	0.33	0/1396	0.48	0/1876
1	C	0.35	0/1388	0.49	0/1869
1	D	0.34	0/1389	0.50	0/1868
1	E	0.35	0/1396	0.50	0/1876
1	F	0.34	0/1391	0.49	0/1871
1	G	0.34	0/1393	0.49	0/1873
1	H	0.35	0/1386	0.50	0/1866
1	I	0.34	0/1392	0.49	0/1873
1	J	0.34	0/1392	0.49	0/1872
1	K	0.36	0/1398	0.51	0/1879
1	L	0.34	0/1402	0.50	0/1884
1	M	0.34	0/1384	0.50	0/1862
1	N	0.35	0/1396	0.49	0/1877
1	O	0.35	0/1390	0.51	0/1871
1	P	0.34	0/1397	0.50	0/1879
1	Q	0.35	0/1399	0.50	0/1880
1	R	0.35	0/1395	0.49	0/1876
1	S	0.34	0/1391	0.49	0/1871
1	T	0.35	0/1388	0.50	0/1867
1	U	0.35	0/1401	0.50	0/1883
1	V	0.35	0/1397	0.52	0/1879
1	W	0.35	0/1391	0.48	0/1871
1	X	0.35	0/1398	0.50	0/1879
All	All	0.35	0/33448	0.50	0/44981

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	1372	73	1317	9	0
1	B	1370	0	1310	8	0
1	C	1362	0	1281	11	0
1	D	1363	0	1301	11	0
1	E	1370	0	1317	9	0
1	F	1365	0	1301	11	0
1	G	1367	0	1308	10	0
1	H	1360	0	1284	7	0
1	I	1366	0	1299	10	0
1	J	1366	0	1303	8	0
1	K	1372	0	1316	15	0
1	L	1376	0	1321	14	0
1	M	1358	0	1292	10	0
1	N	1370	0	1311	11	0
1	O	1364	0	1292	9	0
1	P	1371	0	1305	11	0
1	Q	1373	0	1313	11	0
1	R	1369	0	1308	8	0
1	S	1365	0	1302	11	0
1	T	1362	0	1295	11	0
1	U	1375	0	1319	11	0
1	V	1371	0	1308	8	0
1	W	1365	0	1301	11	0
1	X	1372	0	1313	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
3	E	4	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	1	0	0	0	0
3	K	4	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	4	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	O	2	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	2	0	0	0	0
4	W	1	0	0	0	0
4	X	2	0	0	0	0
5	A	113	0	0	1	0
5	B	113	0	0	0	0
5	C	111	0	0	0	0
5	D	112	0	0	0	0
5	E	111	0	0	0	0
5	F	111	0	0	1	0
5	G	111	0	0	0	0
5	H	113	0	0	0	0
5	I	118	0	0	1	0
5	J	115	0	0	0	0
5	K	114	0	0	0	0
5	L	117	0	0	0	0
5	M	109	0	0	0	0
5	N	120	0	0	2	0
5	O	110	0	0	0	0
5	P	112	0	0	0	0
5	Q	113	0	0	1	0
5	R	111	0	0	0	0
5	S	114	0	0	1	0
5	T	121	0	0	0	0
5	U	112	0	0	0	0
5	V	115	0	0	0	0
5	W	111	0	0	0	0
5	X	112	0	0	0	0
All	All	35651	73	31317	202	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.

All (202) 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:T:98:MET:HE3	1:T:146:ILE:HG23	1.53	0.90
1:K:98:MET:HE3	1:K:146:ILE:HG23	1.52	0.89
1:I:98:MET:HE3	1:I:146:ILE:HG23	1.54	0.87
1:I:101:THR:HG22	1:I:146:ILE:HD13	1.53	0.87
1:F:98:MET:HE3	1:F:146:ILE:HG23	1.57	0.87
1:Q:98:MET:HE3	1:Q:146:ILE:HG23	1.58	0.86
1:N:101:THR:HG22	1:N:146:ILE:HD13	1.57	0.84
1:E:98:MET:HE3	1:E:146:ILE:HG23	1.59	0.83
1:N:51:LYS:HE2	5:N:394:HOH:O	1.77	0.83
1:H:98:MET:HE3	1:H:146:ILE:HG23	1.63	0.81
1:N:98:MET:HE3	1:N:146:ILE:HG23	1.64	0.79
1:Q:101:THR:HG22	1:Q:146:ILE:HD13	1.66	0.76
1:N:98:MET:CE	1:N:146:ILE:HG23	2.15	0.75
1:D:98:MET:HE3	1:D:146:ILE:HG23	1.67	0.74
1:G:98:MET:HE3	1:G:146:ILE:HG23	1.69	0.74
1:U:98:MET:HE3	1:U:146:ILE:HG23	1.71	0.73
1:J:101:THR:HG22	1:J:146:ILE:HD13	1.70	0.73
1:C:98:MET:HE3	1:C:146:ILE:HG23	1.69	0.72
1:M:101:THR:HG22	1:M:146:ILE:HD13	1.71	0.72
1:R:98:MET:HE3	1:R:146:ILE:HG23	1.72	0.72
1:T:101:THR:HG22	1:T:146:ILE:HD13	1.72	0.71
1:A:47:PRO:O	1:A:51:LYS:HG2	1.92	0.70
1:R:101:THR:HG22	1:R:146:ILE:HD13	1.74	0.69
1:K:101:THR:HG22	1:K:146:ILE:HD13	1.75	0.68
1:E:101:THR:HG22	1:E:146:ILE:HD13	1.77	0.67
1:X:97:ALA:O	1:X:101:THR:HG23	1.95	0.66
1:B:97:ALA:O	1:B:101:THR:HG23	1.95	0.66
1:H:101:THR:HG22	1:H:146:ILE:HD13	1.78	0.66
1:L:101:THR:HG22	1:L:146:ILE:HD13	1.78	0.65
1:E:98:MET:CE	1:E:146:ILE:HG23	2.25	0.65
1:O:98:MET:HE3	1:O:146:ILE:HG23	1.78	0.65
1:A:3:GLN:N	5:A:301:HOH:O	2.29	0.64
1:V:97:ALA:O	1:V:101:THR:HG23	1.98	0.64
1:K:98:MET:HE2	1:K:149:HIS:HB2	1.80	0.63
1:M:98:MET:HE3	1:M:146:ILE:HG23	1.79	0.63
1:O:97:ALA:O	1:O:101:THR:HG23	1.99	0.62
1:F:101:THR:HG22	1:F:146:ILE:HD13	1.81	0.61
1:Q:98:MET:CE	1:Q:146:ILE:HG23	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:MET:CE	1:I:146:ILE:HG23	2.27	0.61
1:C:101:THR:HG22	1:C:146:ILE:HD13	1.83	0.61
1:W:121:LYS:HE3	1:W:122:HIS:NE2	2.16	0.60
1:K:58:GLU:HG2	1:K:61:ARG:HH22	1.67	0.60
1:N:168:GLU:HB3	1:P:167:LYS:HE2	1.84	0.59
1:R:98:MET:CE	1:R:146:ILE:HG23	2.33	0.59
1:T:98:MET:CE	1:T:146:ILE:HG23	2.30	0.59
1:P:101:THR:HG22	1:P:146:ILE:HD13	1.83	0.58
1:K:5:GLN:HG3	1:L:42:ASP:OD2	2.04	0.58
1:F:98:MET:CE	1:F:146:ILE:HG23	2.31	0.58
1:E:36:TYR:OH	1:F:69:LYS:NZ	2.37	0.57
1:S:48:SER:HA	1:S:51:LYS:HE2	1.86	0.57
1:L:3:GLN:CD	1:L:7:ARG:HD2	2.25	0.56
1:G:98:MET:CE	1:G:146:ILE:HG23	2.35	0.56
1:L:98:MET:HE3	1:L:146:ILE:HG23	1.88	0.55
1:U:101:THR:HG22	1:U:146:ILE:HD13	1.87	0.55
1:K:98:MET:HE2	1:K:149:HIS:CB	2.37	0.54
1:P:121:LYS:HE3	1:P:122:HIS:NE2	2.23	0.54
1:Q:69:LYS:NZ	5:Q:301:HOH:O	2.39	0.54
1:K:98:MET:CE	1:K:146:ILE:HG23	2.34	0.54
1:A:105:GLU:HG3	1:A:146:ILE:CD1	2.37	0.53
1:W:101:THR:HG22	1:W:146:ILE:HD13	1.89	0.53
1:A:101:THR:HG22	1:A:146:ILE:HD13	1.91	0.53
1:S:140:VAL:HG23	5:S:335:HOH:O	2.08	0.53
1:C:105:GLU:HG3	1:C:146:ILE:CD1	2.39	0.53
1:U:98:MET:HE2	1:U:149:HIS:HB2	1.91	0.53
1:P:32:TYR:OH	1:P:101:THR:HG23	2.09	0.53
1:G:32:TYR:OH	1:G:101:THR:HG23	2.09	0.52
1:V:105:GLU:HG3	1:V:146:ILE:CD1	2.40	0.52
1:H:105:GLU:HG3	1:H:146:ILE:CD1	2.40	0.52
1:I:47:PRO:O	1:I:51:LYS:HG2	2.10	0.52
1:T:98:MET:HE2	1:T:149:HIS:HB2	1.92	0.52
1:W:98:MET:HE3	1:W:146:ILE:HG23	1.91	0.52
1:L:105:GLU:HG3	1:L:146:ILE:CD1	2.40	0.51
1:R:105:GLU:HG3	1:R:146:ILE:CD1	2.40	0.51
1:I:105:GLU:HG3	1:I:146:ILE:CD1	2.41	0.50
1:F:105:GLU:HG3	1:F:146:ILE:CD1	2.41	0.50
1:P:105:GLU:HG3	1:P:146:ILE:CD1	2.42	0.50
1:S:101:THR:HG22	1:S:146:ILE:HD13	1.92	0.50
1:Q:105:GLU:HG3	1:Q:146:ILE:CD1	2.42	0.50
1:G:78:ILE:HD11	1:H:37:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:MET:HE2	1:H:149:HIS:HB2	1.94	0.50
1:H:98:MET:CE	1:H:146:ILE:HG23	2.40	0.50
1:D:98:MET:HE2	1:D:149:HIS:HB2	1.93	0.49
1:K:37:MET:HE2	1:L:68:MET:C	2.32	0.49
1:O:105:GLU:HG3	1:O:146:ILE:CD1	2.42	0.49
1:A:61:ARG:CZ	1:B:61:ARG:HD2	2.42	0.49
1:S:36:TYR:CZ	1:S:54:LYS:HD2	2.47	0.49
1:O:53:PHE:HE1	1:O:101:THR:HG21	1.78	0.48
1:I:73:LYS:HD3	1:T:141:ASP:OD1	2.13	0.48
1:L:98:MET:CE	1:L:146:ILE:HG23	2.42	0.48
1:F:36:TYR:CZ	1:F:54:LYS:HD2	2.48	0.48
1:S:105:GLU:HG3	1:S:146:ILE:CD1	2.43	0.48
1:N:105:GLU:HG3	1:N:146:ILE:CD1	2.43	0.48
1:D:137:LYS:O	1:D:140:VAL:HG22	2.14	0.48
1:M:105:GLU:HG3	1:M:146:ILE:CD1	2.44	0.48
1:X:105:GLU:HG3	1:X:146:ILE:CD1	2.44	0.48
1:U:105:GLU:HG3	1:U:146:ILE:CD1	2.44	0.48
1:J:105:GLU:HG3	1:J:146:ILE:CD1	2.43	0.48
1:D:105:GLU:HG3	1:D:146:ILE:CD1	2.44	0.48
1:A:144:GLU:HG3	1:F:73:LYS:HA	1.96	0.47
1:M:98:MET:CE	1:M:146:ILE:HG23	2.42	0.47
1:C:37:MET:HE2	1:D:78:ILE:HD11	1.96	0.47
1:C:98:MET:CE	1:C:146:ILE:HG23	2.39	0.47
1:W:105:GLU:HG3	1:W:146:ILE:CD1	2.45	0.47
1:K:105:GLU:HG3	1:K:146:ILE:CD1	2.45	0.47
1:N:132:GLU:HA	1:N:136:LEU:HB2	1.96	0.46
1:X:53:PHE:HE1	1:X:101:THR:HG21	1.80	0.46
1:D:5:GLN:HB2	1:D:6:PRO:HD3	1.98	0.46
1:G:5:GLN:HB2	1:G:6:PRO:HD3	1.97	0.46
1:K:73:LYS:HA	1:X:144:GLU:HG3	1.97	0.46
1:R:73:LYS:HA	1:S:144:GLU:HG3	1.98	0.45
1:K:141:ASP:OD1	1:Q:73:LYS:HD3	2.16	0.45
1:T:105:GLU:HG3	1:T:146:ILE:CD1	2.47	0.45
1:S:32:TYR:OH	1:S:101:THR:HG23	2.16	0.45
1:D:101:THR:HG22	1:D:146:ILE:HD13	1.97	0.45
1:B:53:PHE:HE1	1:B:101:THR:HG21	1.82	0.45
1:E:73:LYS:HA	1:O:144:GLU:HG3	1.98	0.45
1:I:73:LYS:HA	1:T:144:GLU:HG3	1.99	0.45
1:B:141:ASP:OD1	1:G:73:LYS:HD3	2.17	0.44
1:X:132:GLU:HA	1:X:136:LEU:HB2	1.99	0.44
1:A:73:LYS:HA	1:J:144:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:GLU:HG3	1:Q:73:LYS:HA	2.00	0.44
1:U:32:TYR:OH	1:U:101:THR:HG23	2.17	0.44
1:W:32:TYR:OH	1:W:101:THR:HG23	2.18	0.44
1:F:144:GLU:HG3	1:J:73:LYS:HA	2.00	0.44
1:O:98:MET:CE	1:O:146:ILE:HG23	2.45	0.44
1:P:5:GLN:HB2	1:P:6:PRO:HD3	1.99	0.44
1:U:73:LYS:HA	1:W:144:GLU:HG3	1.99	0.44
1:D:32:TYR:OH	1:D:101:THR:HG23	2.17	0.44
1:O:132:GLU:HA	1:O:136:LEU:HB2	2.00	0.44
1:V:132:GLU:HA	1:V:136:LEU:HB2	1.99	0.44
1:L:144:GLU:HG3	1:M:73:LYS:HA	1.99	0.44
1:U:5:GLN:HB2	1:U:6:PRO:HD3	2.00	0.44
1:F:140:VAL:HG23	5:F:362:HOH:O	2.18	0.44
1:B:5:GLN:HB2	1:B:6:PRO:HD3	1.99	0.44
1:C:144:GLU:HG3	1:L:73:LYS:HA	1.99	0.44
1:Q:144:GLU:HG3	1:X:73:LYS:HA	2.00	0.44
1:S:37:MET:HB3	1:S:37:MET:HE3	1.93	0.44
1:P:121:LYS:HE3	1:P:122:HIS:CE1	2.53	0.43
1:T:73:LYS:HA	1:V:144:GLU:HG3	2.00	0.43
1:C:73:LYS:HA	1:M:144:GLU:HG3	2.00	0.43
1:C:141:ASP:OD1	1:L:73:LYS:HD3	2.18	0.43
1:J:25:GLU:HB2	1:J:64:ALA:HB2	1.99	0.43
1:E:98:MET:HE2	1:E:149:HIS:HB2	2.00	0.43
1:P:73:LYS:HA	1:U:144:GLU:HG3	2.00	0.43
1:H:144:GLU:HG3	1:S:73:LYS:HA	1.98	0.43
1:M:163:TYR:CE1	1:M:167:LYS:HE2	2.54	0.43
1:E:141:ASP:OD1	1:N:73:LYS:HD3	2.19	0.43
1:J:5:GLN:HB2	1:J:6:PRO:HD3	2.00	0.43
1:R:25:GLU:HB2	1:R:64:ALA:HB2	2.00	0.43
1:M:5:GLN:HB2	1:M:6:PRO:HD3	2.00	0.43
1:P:141:ASP:OD1	1:W:73:LYS:HD3	2.18	0.43
1:I:144:GLU:HG3	1:V:73:LYS:HA	1.99	0.43
1:M:25:GLU:HB2	1:M:64:ALA:HB2	2.00	0.43
1:C:3:GLN:HE21	1:C:4:THR:H	1.66	0.43
1:E:144:GLU:HG3	1:N:73:LYS:HA	2.00	0.42
1:N:101:THR:HG22	1:N:146:ILE:CD1	2.41	0.42
1:S:55:HIS:NE2	1:S:59:GLU:OE1	2.52	0.42
1:W:98:MET:HE2	1:W:149:HIS:HB2	2.01	0.42
1:R:132:GLU:HA	1:R:136:LEU:HB2	2.01	0.42
1:M:69:LYS:HE3	5:N:355:HOH:O	2.18	0.42
1:I:98:MET:HE2	1:I:149:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:TYR:OH	1:L:101:THR:HG23	2.20	0.42
1:P:144:GLU:HG3	1:W:73:LYS:HA	2.02	0.42
1:G:21:GLN:O	1:G:25:GLU:HG2	2.20	0.42
1:Q:47:PRO:O	1:Q:51:LYS:HG2	2.19	0.42
1:Q:141:ASP:OD1	1:X:73:LYS:HD3	2.19	0.42
1:W:121:LYS:HE3	1:W:122:HIS:CE1	2.55	0.42
1:B:73:LYS:HD3	1:D:141:ASP:OD1	2.19	0.42
1:K:37:MET:HE2	1:L:68:MET:HB3	2.00	0.42
1:N:144:GLU:HG3	1:O:73:LYS:HA	2.01	0.42
5:I:368:HOH:O	1:J:69:LYS:HE3	2.20	0.42
1:O:37:MET:HE1	1:P:68:MET:C	2.40	0.42
1:J:132:GLU:HA	1:J:136:LEU:HB2	2.02	0.41
1:B:144:GLU:HG3	1:G:73:LYS:HA	2.03	0.41
1:E:5:GLN:HB2	1:E:6:PRO:HD3	2.03	0.41
1:W:21:GLN:O	1:W:25:GLU:HG2	2.20	0.41
1:A:37:MET:HB3	1:A:37:MET:HE3	1.94	0.41
1:A:68:MET:C	1:B:37:MET:HE2	2.41	0.41
1:K:21:GLN:O	1:K:25:GLU:HG2	2.20	0.41
1:L:132:GLU:HA	1:L:136:LEU:HB2	2.02	0.41
1:R:32:TYR:OH	1:R:101:THR:HG23	2.21	0.41
1:U:41:ARG:NH1	1:U:90:GLU:HG2	2.36	0.41
1:F:37:MET:HB3	1:F:37:MET:HE3	1.80	0.41
1:K:5:GLN:N	1:K:6:PRO:CD	2.84	0.41
1:L:5:GLN:HB2	1:L:6:PRO:HD3	2.02	0.41
1:X:163:TYR:O	1:X:167:LYS:HG2	2.20	0.41
1:T:5:GLN:HB2	1:T:6:PRO:HD3	2.03	0.41
1:U:132:GLU:HA	1:U:136:LEU:HB2	2.01	0.41
1:V:21:GLN:O	1:V:25:GLU:HG2	2.21	0.41
1:G:105:GLU:HG3	1:G:146:ILE:CD1	2.50	0.41
1:V:53:PHE:HE1	1:V:101:THR:HG21	1.84	0.41
1:Q:98:MET:HE2	1:Q:149:HIS:HB2	2.02	0.41
1:C:137:LYS:O	1:C:140:VAL:HG22	2.21	0.41
1:D:73:LYS:HD3	1:G:141:ASP:OD1	2.21	0.41
1:I:168:GLU:HB3	1:U:167:LYS:HE2	2.03	0.41
1:S:37:MET:HE2	1:T:68:MET:C	2.41	0.41
1:D:98:MET:CE	1:D:146:ILE:HG23	2.42	0.40
1:F:5:GLN:HB2	1:F:6:PRO:HD3	2.03	0.40
1:V:163:TYR:O	1:V:167:LYS:HG2	2.20	0.40
1:X:5:GLN:HB2	1:X:6:PRO:HD3	2.02	0.40
1:C:3:GLN:NE2	1:C:7:ARG:HD2	2.36	0.40
1:T:132:GLU:HA	1:T:136:LEU:HB2	2.03	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	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	B	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	C	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	D	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	E	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	F	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	G	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	H	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	I	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	J	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	K	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	L	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	M	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	N	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	O	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	P	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	Q	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	R	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	S	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
1	T	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	U	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	V	167/172 (97%)	166 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	X	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
All	All	4008/4128 (97%)	3968 (99%)	40 (1%)	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	146/151 (97%)	143 (98%)	3 (2%)	53	38
1	B	145/151 (96%)	144 (99%)	1 (1%)	84	79
1	C	144/151 (95%)	142 (99%)	2 (1%)	67	55
1	D	143/151 (95%)	140 (98%)	3 (2%)	53	38
1	E	145/151 (96%)	142 (98%)	3 (2%)	53	38
1	F	144/151 (95%)	141 (98%)	3 (2%)	53	38
1	G	145/151 (96%)	142 (98%)	3 (2%)	53	38
1	H	143/151 (95%)	140 (98%)	3 (2%)	53	38
1	I	145/151 (96%)	142 (98%)	3 (2%)	53	38
1	J	144/151 (95%)	142 (99%)	2 (1%)	67	55
1	K	145/151 (96%)	140 (97%)	5 (3%)	37	19
1	L	147/151 (97%)	143 (97%)	4 (3%)	44	29
1	M	143/151 (95%)	140 (98%)	3 (2%)	53	38
1	N	146/151 (97%)	143 (98%)	3 (2%)	53	38
1	O	144/151 (95%)	141 (98%)	3 (2%)	53	38
1	P	146/151 (97%)	143 (98%)	3 (2%)	53	38
1	Q	147/151 (97%)	144 (98%)	3 (2%)	55	40
1	R	146/151 (97%)	144 (99%)	2 (1%)	67	55
1	S	145/151 (96%)	143 (99%)	2 (1%)	67	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	T	144/151 (95%)	141 (98%)	3 (2%)	53 38
1	U	147/151 (97%)	144 (98%)	3 (2%)	55 40
1	V	146/151 (97%)	142 (97%)	4 (3%)	44 29
1	W	144/151 (95%)	141 (98%)	3 (2%)	53 38
1	X	147/151 (97%)	144 (98%)	3 (2%)	55 40
All	All	3481/3624 (96%)	3411 (98%)	70 (2%)	55 40

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	131	LEU
1	A	140	VAL
1	B	30	TYR
1	C	30	TYR
1	C	153	LEU
1	D	30	TYR
1	D	131	LEU
1	D	153	LEU
1	E	30	TYR
1	E	131	LEU
1	E	136	LEU
1	F	30	TYR
1	F	136	LEU
1	F	153	LEU
1	G	30	TYR
1	G	131	LEU
1	G	153	LEU
1	H	30	TYR
1	H	137	LYS
1	H	153	LEU
1	I	30	TYR
1	I	131	LEU
1	I	153	LEU
1	J	30	TYR
1	J	136	LEU
1	K	5	GLN
1	K	30	TYR
1	K	131	LEU
1	K	136	LEU

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Mol	Chain	Res	Type
1	K	153	LEU
1	L	30	TYR
1	L	131	LEU
1	L	136	LEU
1	L	153	LEU
1	M	30	TYR
1	M	131	LEU
1	M	136	LEU
1	N	30	TYR
1	N	136	LEU
1	N	153	LEU
1	O	30	TYR
1	O	131	LEU
1	O	136	LEU
1	P	30	TYR
1	P	131	LEU
1	P	136	LEU
1	Q	30	TYR
1	Q	131	LEU
1	Q	153	LEU
1	R	30	TYR
1	R	136	LEU
1	S	30	TYR
1	S	136	LEU
1	T	30	TYR
1	T	136	LEU
1	T	153	LEU
1	U	30	TYR
1	U	131	LEU
1	U	136	LEU
1	V	30	TYR
1	V	131	LEU
1	V	136	LEU
1	V	153	LEU
1	W	30	TYR
1	W	131	LEU
1	W	153	LEU
1	X	30	TYR
1	X	136	LEU
1	X	153	LEU

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

Mol	Chain	Res	Type
1	C	3	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 108 ligands modelled in this entry, 108 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	169/172 (98%)	-0.40	0	100	100	6, 10, 20, 39	0
1	B	169/172 (98%)	-0.39	0	100	100	6, 11, 19, 31	0
1	C	169/172 (98%)	-0.43	0	100	100	6, 10, 20, 28	0
1	D	169/172 (98%)	-0.40	0	100	100	6, 10, 19, 29	0
1	E	169/172 (98%)	-0.42	0	100	100	6, 10, 20, 32	0
1	F	169/172 (98%)	-0.42	0	100	100	6, 10, 18, 32	0
1	G	169/172 (98%)	-0.41	0	100	100	6, 11, 20, 30	0
1	H	169/172 (98%)	-0.42	0	100	100	6, 10, 20, 31	0
1	I	169/172 (98%)	-0.40	0	100	100	6, 11, 20, 30	0
1	J	169/172 (98%)	-0.43	0	100	100	6, 11, 19, 33	0
1	K	169/172 (98%)	-0.42	0	100	100	6, 10, 20, 32	0
1	L	169/172 (98%)	-0.39	0	100	100	6, 10, 21, 30	0
1	M	169/172 (98%)	-0.40	0	100	100	6, 11, 20, 26	0
1	N	169/172 (98%)	-0.40	0	100	100	6, 11, 20, 25	0
1	O	169/172 (98%)	-0.39	0	100	100	6, 11, 21, 30	0
1	P	169/172 (98%)	-0.39	1 (0%)	89	89	6, 10, 21, 31	0
1	Q	169/172 (98%)	-0.38	0	100	100	5, 11, 21, 26	0
1	R	169/172 (98%)	-0.42	0	100	100	6, 11, 20, 32	0
1	S	169/172 (98%)	-0.37	0	100	100	6, 10, 20, 28	0
1	T	169/172 (98%)	-0.42	0	100	100	6, 11, 20, 33	0
1	U	169/172 (98%)	-0.41	0	100	100	6, 11, 21, 30	0
1	V	169/172 (98%)	-0.38	0	100	100	6, 11, 21, 31	0
1	W	169/172 (98%)	-0.39	0	100	100	6, 10, 19, 31	0
1	X	169/172 (98%)	-0.35	0	100	100	6, 11, 20, 29	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4056/4128 (98%)	-0.40	1 (0%)	100	100	5, 11, 21, 39	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	3	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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
2	FE	M	201	1/1	0.71	0.11	72,72,72,72	0
3	FE2	P	205	1/1	0.72	0.40	84,84,84,84	0
2	FE	R	201	1/1	0.77	0.10	74,74,74,74	0
2	FE	C	207	1/1	0.77	0.09	76,76,76,76	0
2	FE	N	201	1/1	0.80	0.14	72,72,72,72	0
2	FE	B	201	1/1	0.80	0.12	71,71,71,71	0
2	FE	C	201	1/1	0.80	0.11	68,68,68,68	0
2	FE	Q	201	1/1	0.81	0.15	75,75,75,75	0
2	FE	J	201	1/1	0.82	0.11	75,75,75,75	0
2	FE	D	201	1/1	0.82	0.15	77,77,77,77	0
2	FE	H	201	1/1	0.82	0.15	69,69,69,69	0
2	FE	F	201	1/1	0.85	0.09	64,64,64,64	0
2	FE	K	201	1/1	0.85	0.06	70,70,70,70	0
2	FE	S	201	1/1	0.85	0.10	64,64,64,64	0
2	FE	V	201	1/1	0.85	0.15	74,74,74,74	0
3	FE2	E	205	1/1	0.85	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	O	201	1/1	0.85	0.06	72,72,72,72	0
2	FE	L	201	1/1	0.86	0.09	67,67,67,67	0
2	FE	A	201	1/1	0.86	0.09	66,66,66,66	0
2	FE	P	201	1/1	0.86	0.13	74,74,74,74	0
3	FE2	A	205	1/1	0.88	0.10	53,53,53,53	0
3	FE2	A	204	1/1	0.89	0.14	61,61,61,61	0
3	FE2	P	203	1/1	0.89	0.13	59,59,59,59	0
2	FE	E	201	1/1	0.89	0.12	69,69,69,69	0
2	FE	U	201	1/1	0.90	0.06	71,71,71,71	0
3	FE2	C	205	1/1	0.91	0.12	55,55,55,55	0
2	FE	X	201	1/1	0.91	0.16	72,72,72,72	0
2	FE	T	201	1/1	0.92	0.14	70,70,70,70	0
3	FE2	H	205	1/1	0.92	0.11	54,54,54,54	0
3	FE2	B	207	1/1	0.92	0.06	54,54,54,54	0
2	FE	W	201	1/1	0.92	0.15	72,72,72,72	0
3	FE2	H	204	1/1	0.93	0.10	60,60,60,60	0
2	FE	I	201	1/1	0.93	0.07	69,69,69,69	0
3	FE2	K	205	1/1	0.94	0.09	52,52,52,52	0
3	FE2	C	204	1/1	0.94	0.13	57,57,57,57	0
3	FE2	P	204	1/1	0.94	0.09	50,50,50,50	0
3	FE2	I	203	1/1	0.94	0.06	51,51,51,51	0
3	FE2	E	204	1/1	0.95	0.17	51,51,51,51	0
3	FE2	A	203	1/1	0.96	0.25	55,55,55,55	0
3	FE2	I	204	1/1	0.96	0.12	54,54,54,54	0
3	FE2	E	203	1/1	0.96	0.15	55,55,55,55	0
3	FE2	B	204	1/1	0.97	0.17	52,52,52,52	0
3	FE2	H	203	1/1	0.97	0.12	51,51,51,51	0
3	FE2	B	203	1/1	0.97	0.15	54,54,54,54	0
3	FE2	K	204	1/1	0.97	0.09	56,56,56,56	0
4	NA	A	206	1/1	0.97	0.08	18,18,18,18	0
4	NA	B	205	1/1	0.97	0.07	10,10,10,10	1
4	NA	B	206	1/1	0.97	0.13	18,18,18,18	0
4	NA	F	204	1/1	0.97	0.05	19,19,19,19	0
3	FE2	C	203	1/1	0.98	0.10	50,50,50,50	0
3	FE2	I	202	1/1	0.98	0.14	49,49,49,49	0
4	NA	D	204	1/1	0.98	0.04	19,19,19,19	0
3	FE2	K	202	1/1	0.98	0.21	50,50,50,50	0
4	NA	G	203	1/1	0.98	0.06	17,17,17,17	0
4	NA	S	204	1/1	0.98	0.07	17,17,17,17	0
4	NA	T	203	1/1	0.98	0.10	17,17,17,17	0
4	NA	U	203	1/1	0.98	0.06	18,18,18,18	0
3	FE2	A	202	1/1	0.99	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE2	N	202	1/1	0.99	0.04	17,17,17,17	0
3	FE2	P	202	1/1	0.99	0.04	17,17,17,17	0
4	NA	C	206	1/1	0.99	0.07	18,18,18,18	0
4	NA	D	203	1/1	0.99	0.06	10,10,10,10	1
3	FE2	C	202	1/1	0.99	0.04	17,17,17,17	0
4	NA	E	206	1/1	0.99	0.04	18,18,18,18	0
4	NA	F	203	1/1	0.99	0.06	10,10,10,10	1
3	FE2	F	202	1/1	0.99	0.04	18,18,18,18	0
4	NA	G	202	1/1	0.99	0.07	9,9,9,9	1
3	FE2	H	202	1/1	0.99	0.04	17,17,17,17	0
4	NA	J	203	1/1	0.99	0.05	14,14,14,14	1
4	NA	J	204	1/1	0.99	0.05	18,18,18,18	0
4	NA	K	206	1/1	0.99	0.05	17,17,17,17	0
4	NA	L	203	1/1	0.99	0.07	10,10,10,10	1
4	NA	L	204	1/1	0.99	0.07	17,17,17,17	0
4	NA	M	203	1/1	0.99	0.06	13,13,13,13	1
4	NA	M	204	1/1	0.99	0.05	17,17,17,17	0
4	NA	N	203	1/1	0.99	0.11	17,17,17,17	0
4	NA	O	204	1/1	0.99	0.07	18,18,18,18	0
4	NA	P	206	1/1	0.99	0.07	18,18,18,18	0
4	NA	Q	203	1/1	0.99	0.07	16,16,16,16	0
4	NA	R	203	1/1	0.99	0.08	14,14,14,14	1
4	NA	R	204	1/1	0.99	0.08	18,18,18,18	0
3	FE2	S	202	1/1	0.99	0.05	17,17,17,17	0
3	FE2	V	202	1/1	0.99	0.05	18,18,18,18	0
3	FE2	X	202	1/1	0.99	0.06	17,17,17,17	0
4	NA	V	204	1/1	0.99	0.05	16,16,16,16	0
4	NA	W	203	1/1	0.99	0.10	18,18,18,18	0
4	NA	X	203	1/1	0.99	0.06	12,12,12,12	1
4	NA	X	204	1/1	0.99	0.07	17,17,17,17	0
3	FE2	L	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	M	202	1/1	1.00	0.04	18,18,18,18	0
3	FE2	B	202	1/1	1.00	0.04	13,13,13,13	0
3	FE2	O	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	I	205	1/1	1.00	0.04	16,16,16,16	0
4	NA	O	203	1/1	1.00	0.05	12,12,12,12	1
3	FE2	J	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	G	201	1/1	1.00	0.04	17,17,17,17	0
3	FE2	K	203	1/1	1.00	0.04	16,16,16,16	0
3	FE2	Q	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	R	202	1/1	1.00	0.04	18,18,18,18	0
4	NA	S	203	1/1	1.00	0.09	9,9,9,9	1

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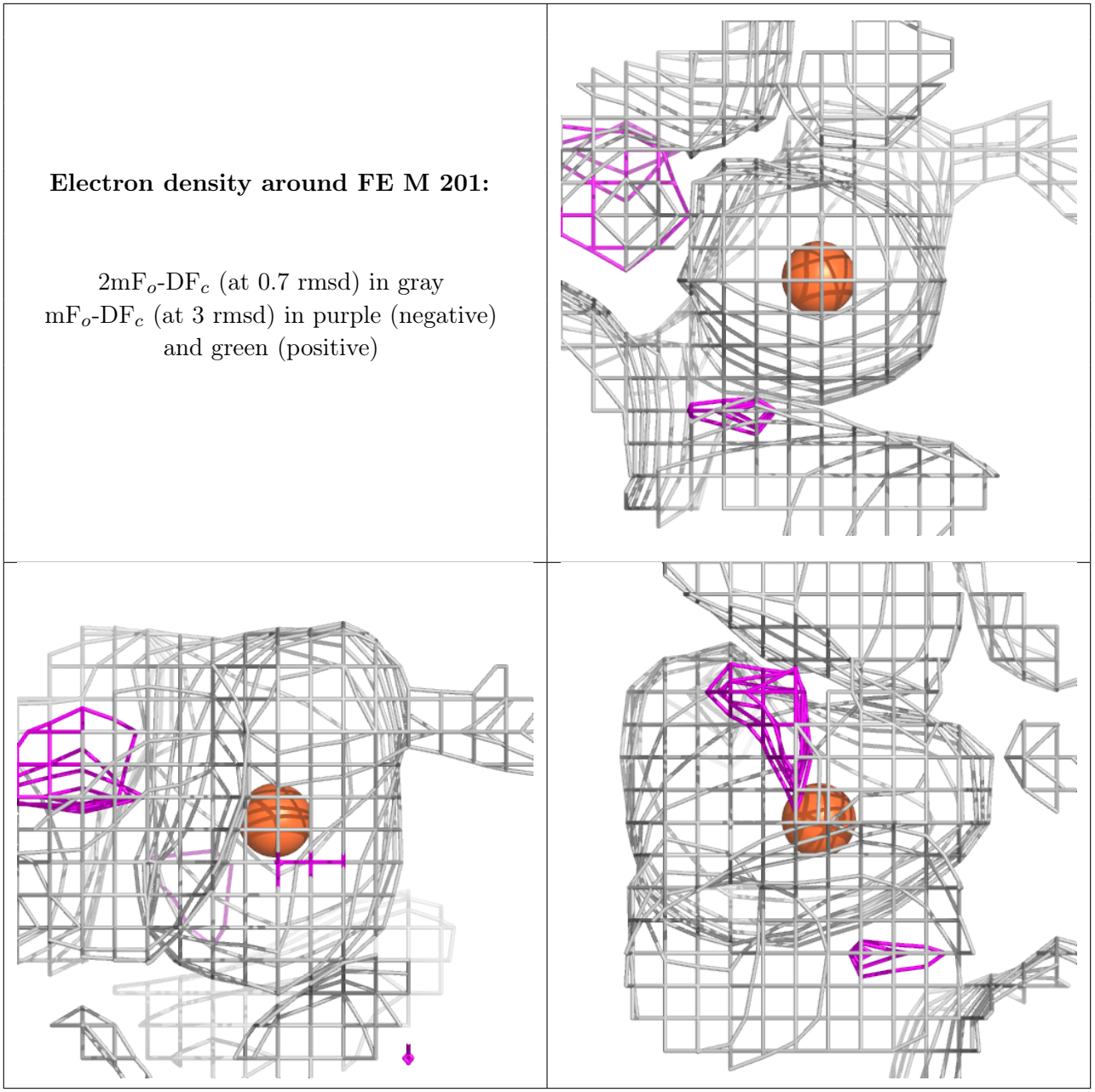
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE2	D	202	1/1	1.00	0.05	16,16,16,16	0
3	FE2	T	202	1/1	1.00	0.04	18,18,18,18	0
4	NA	H	206	1/1	1.00	0.04	18,18,18,18	0
4	NA	V	203	1/1	1.00	0.08	12,12,12,12	1
4	NA	I	206	1/1	1.00	0.06	16,16,16,16	0
3	FE2	U	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	E	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	W	202	1/1	1.00	0.05	17,17,17,17	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.

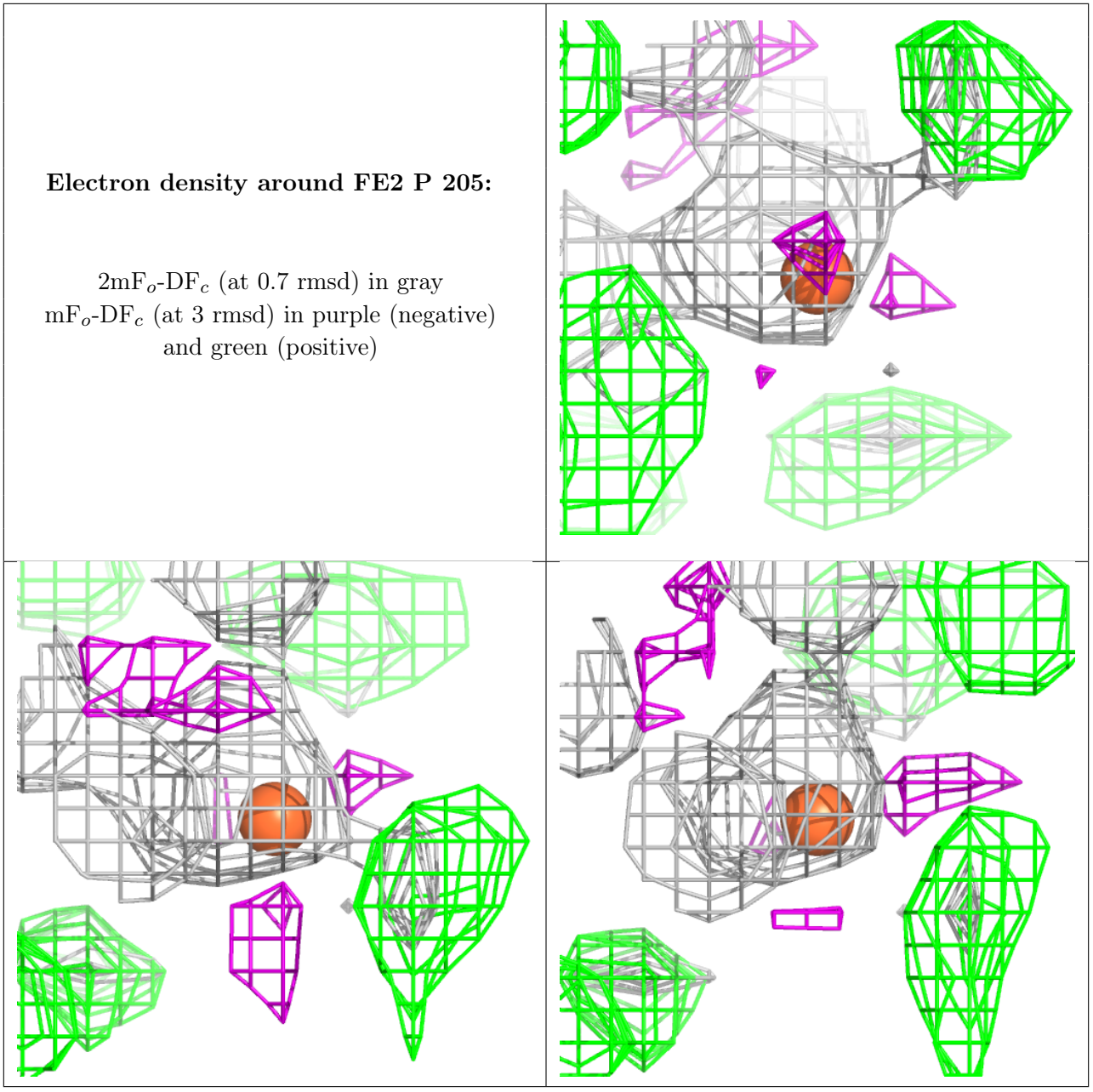
Electron density around FE M 201:

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



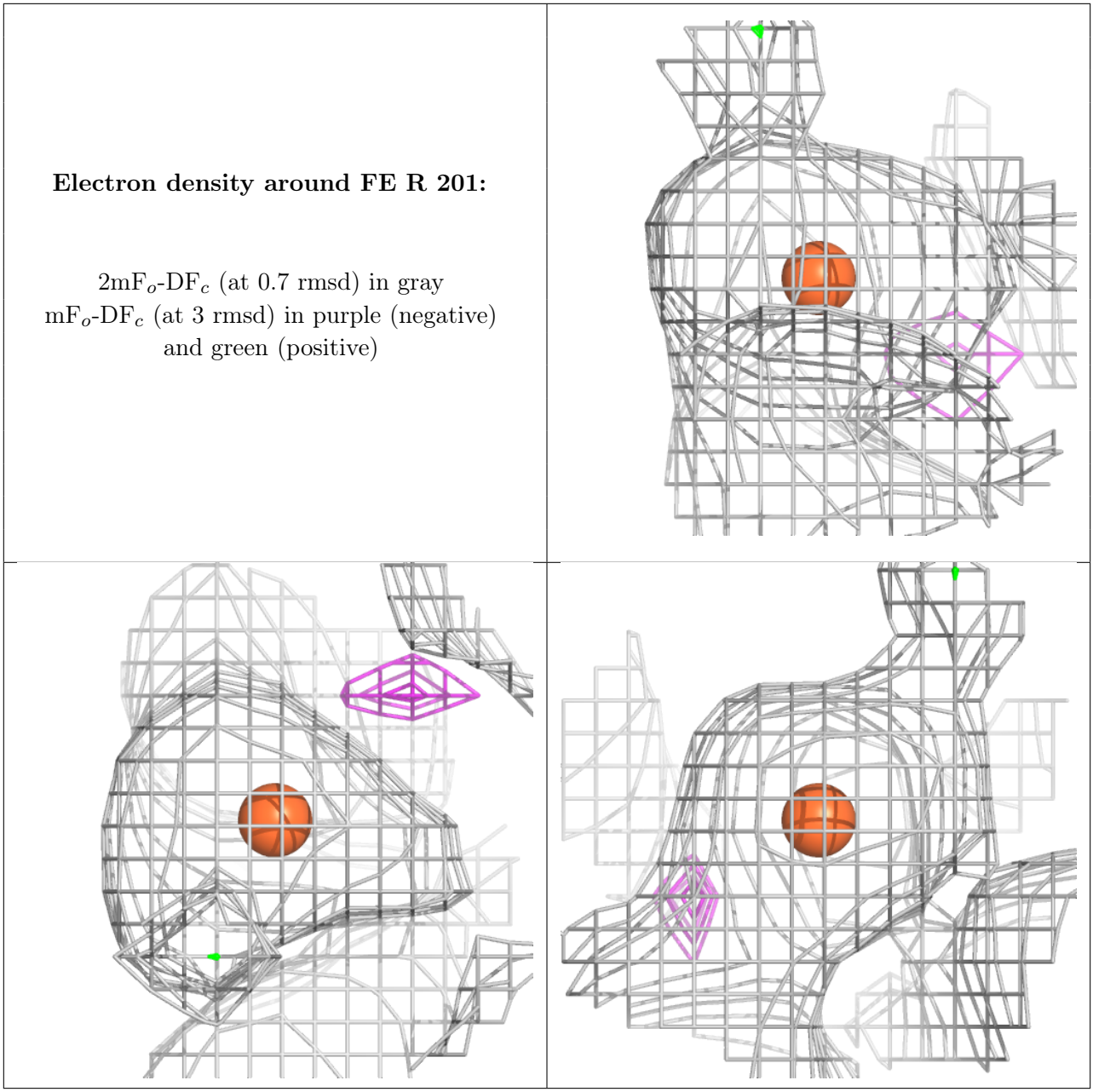
Electron density around FE2 P 205:

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



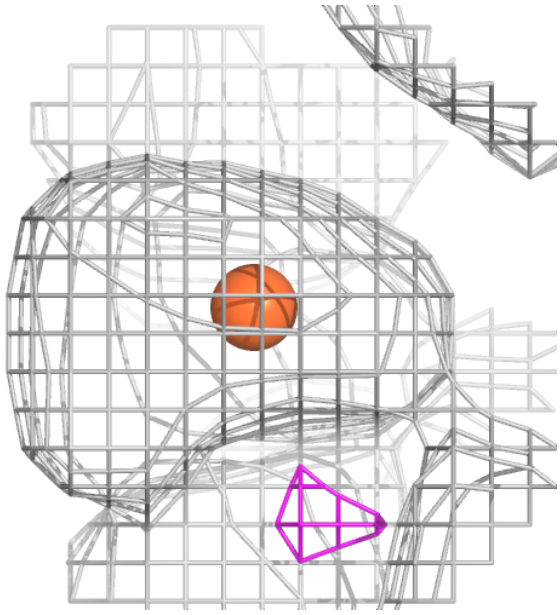
Electron density around FE R 201:

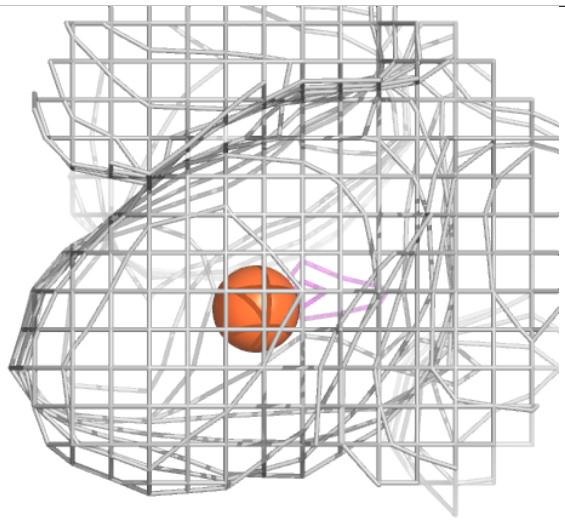
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

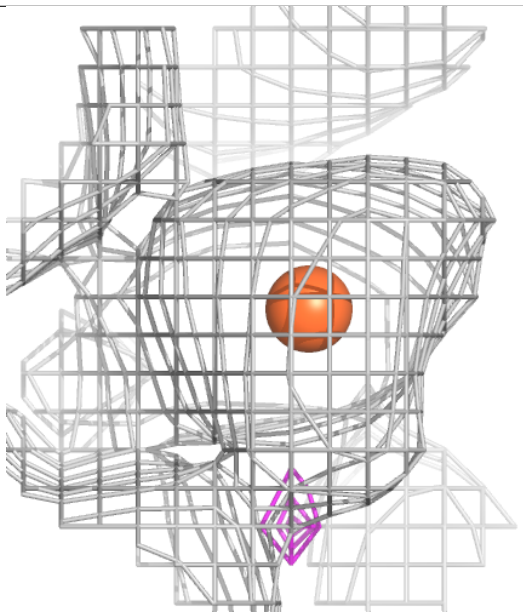


Electron density around FE C 207:

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

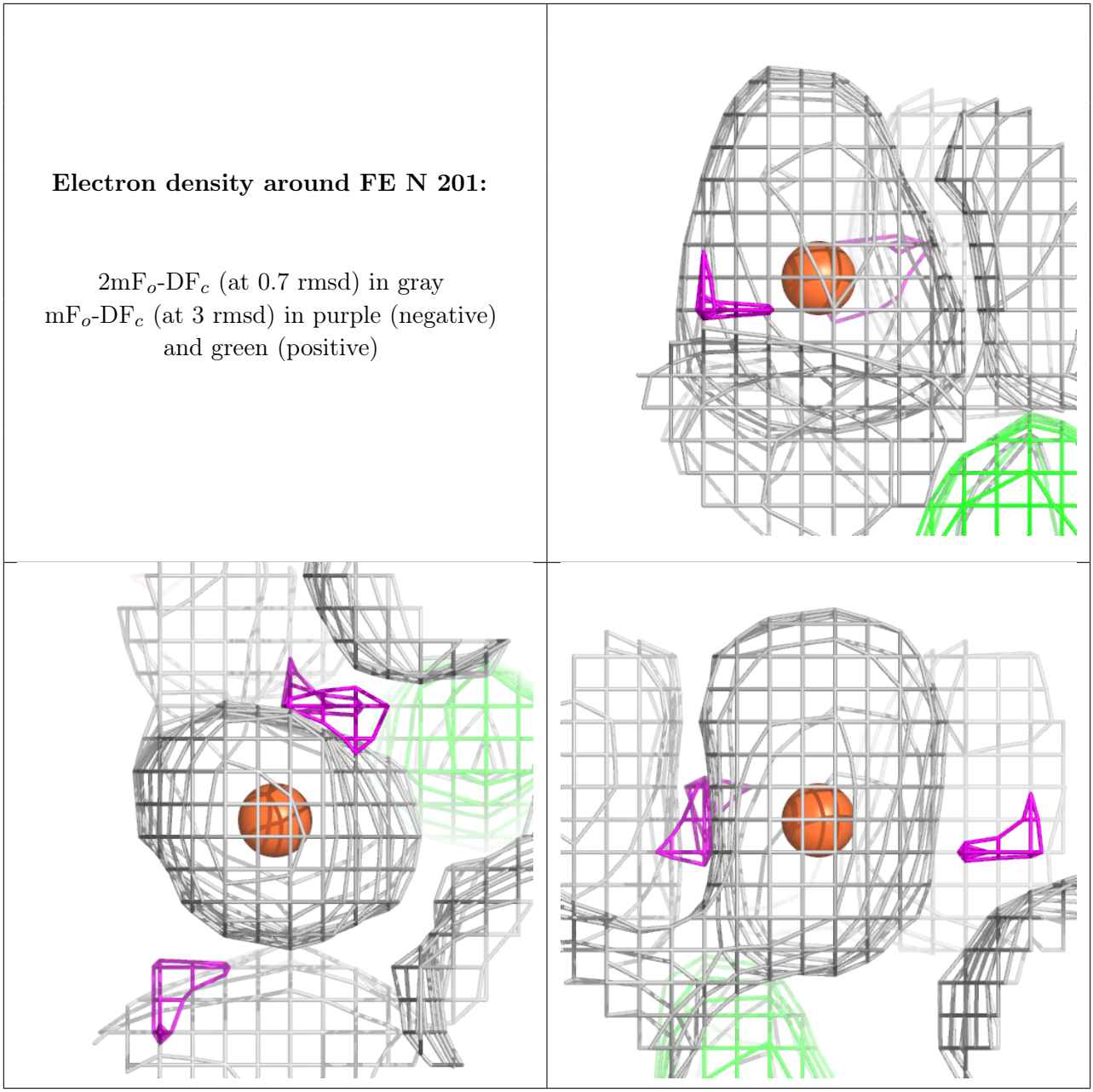






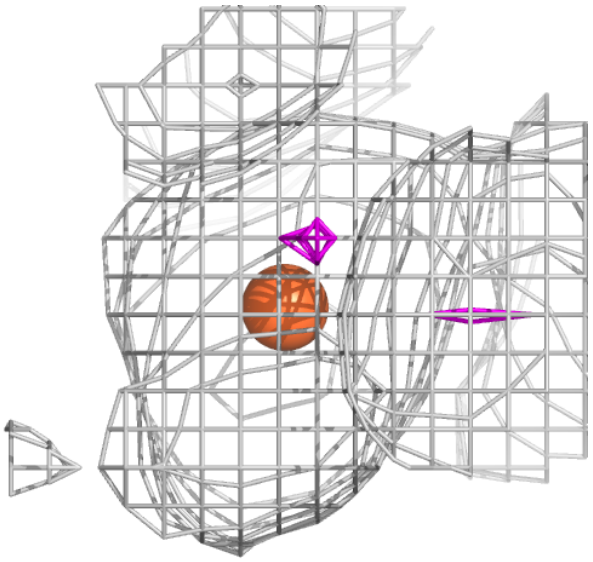
Electron density around FE N 201:

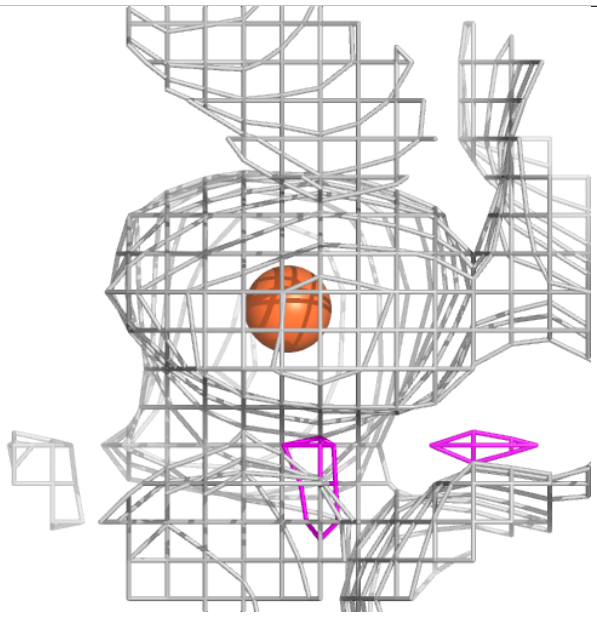
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

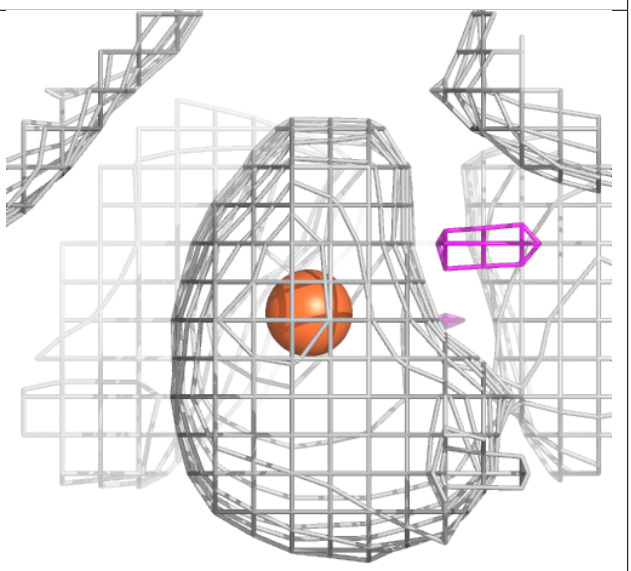


Electron density around FE B 201:

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

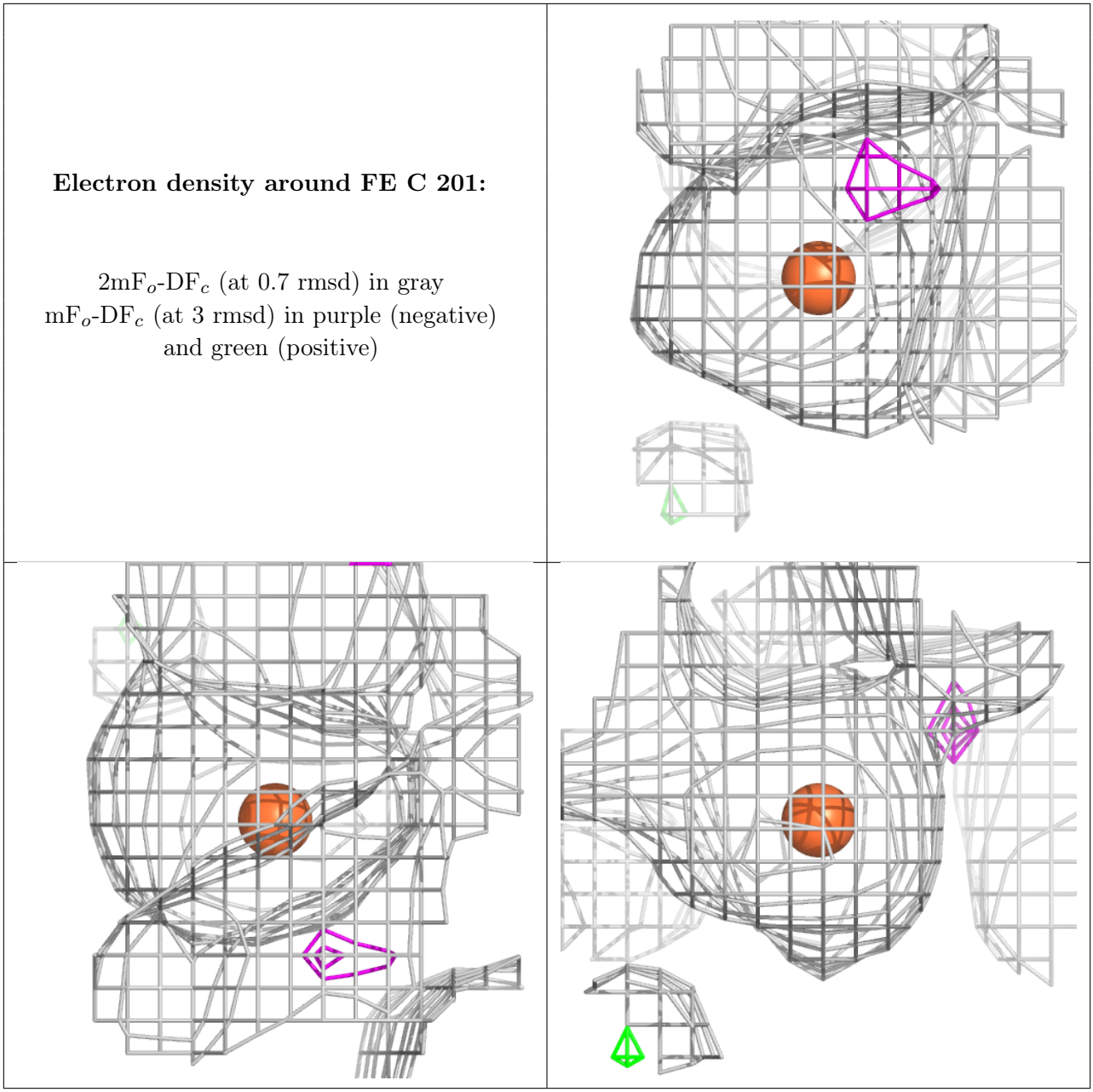






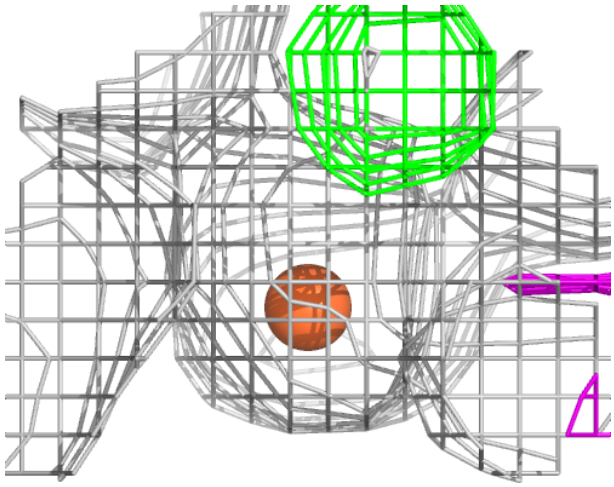
Electron density around FE C 201:

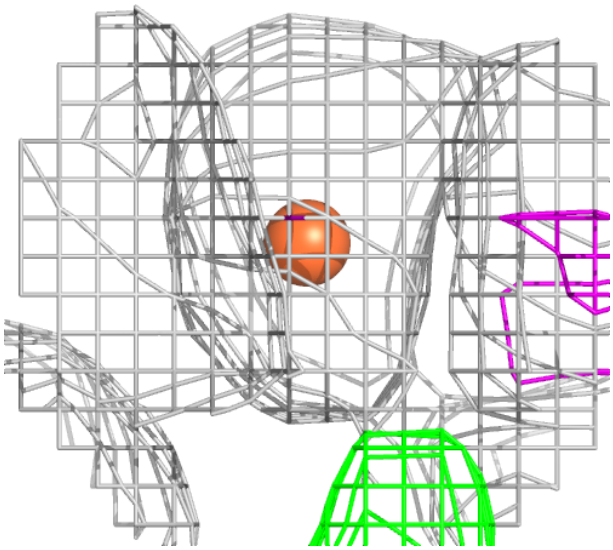
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

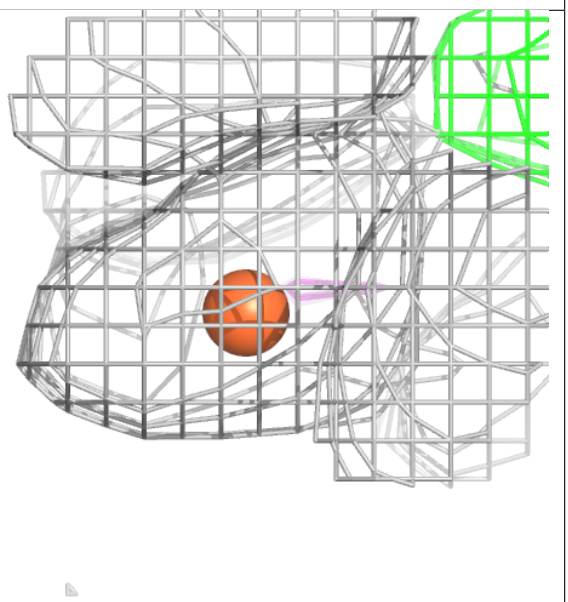


Electron density around FE Q 201:

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

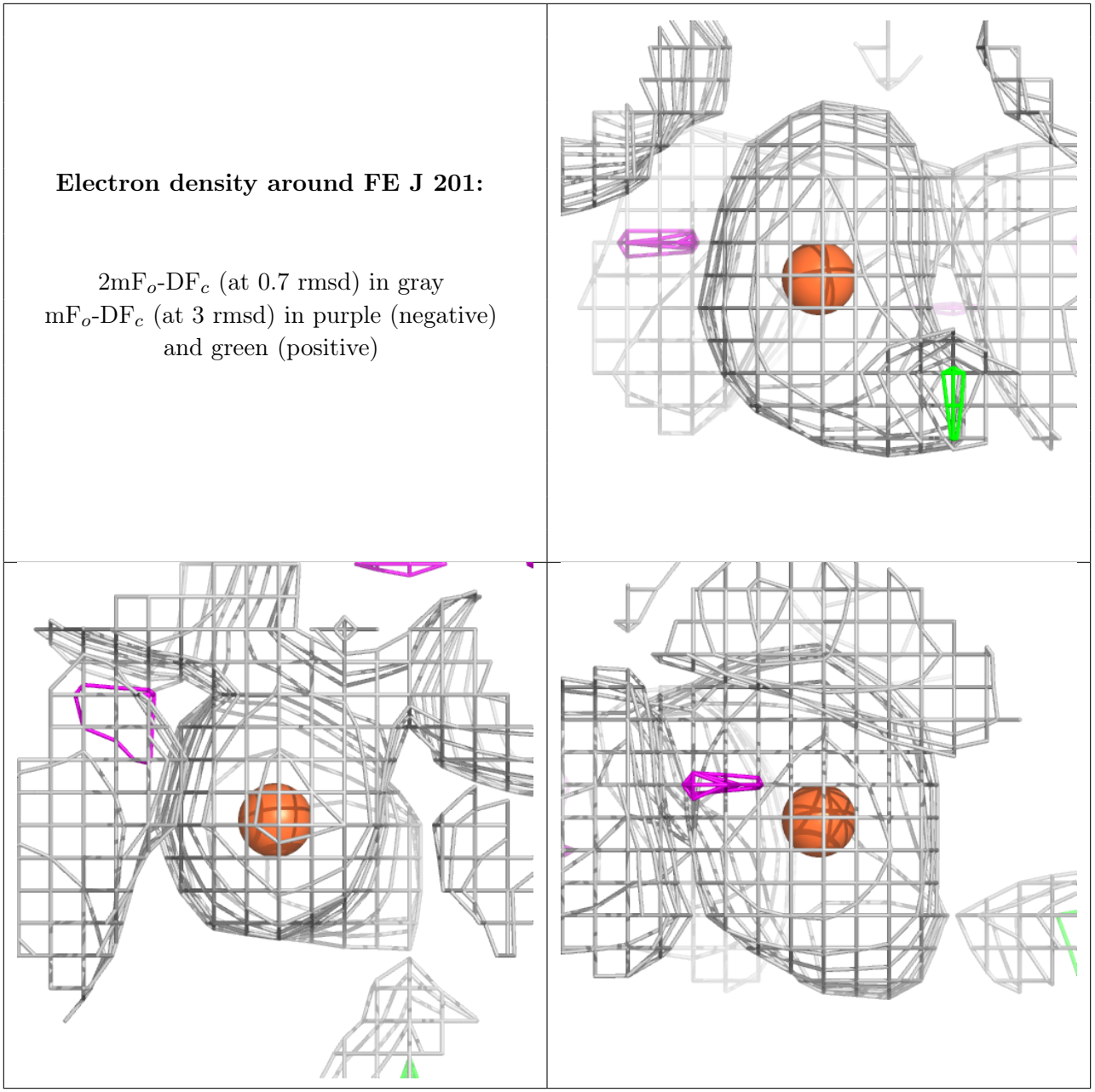






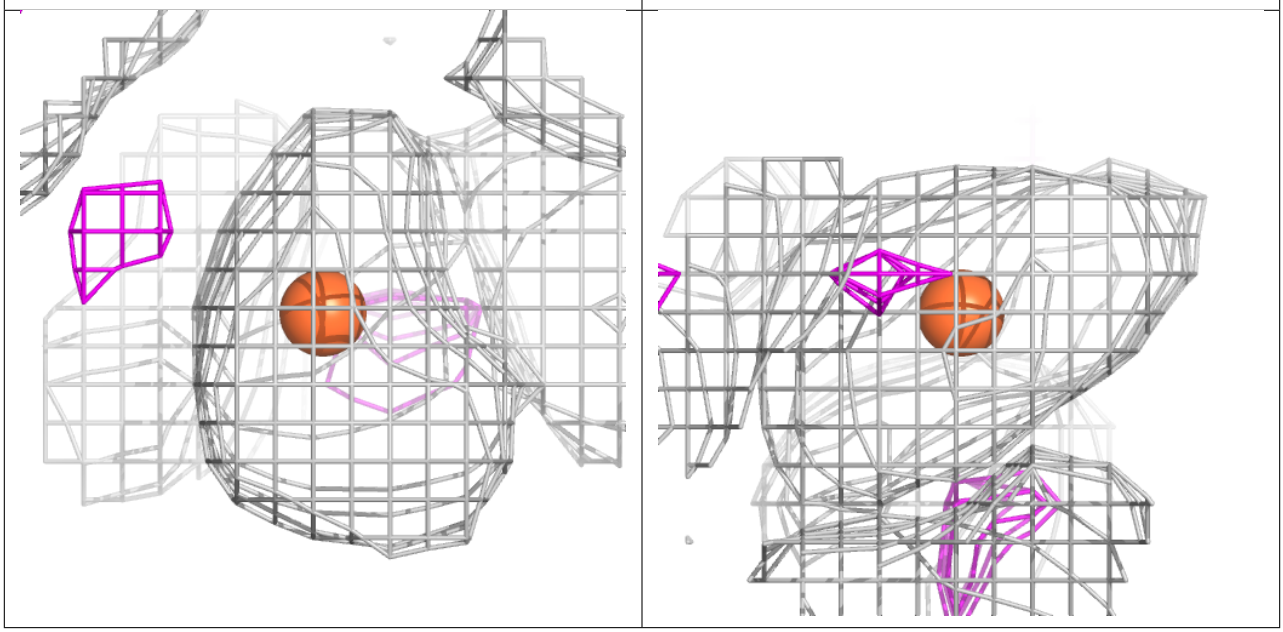
Electron density around FE J 201:

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



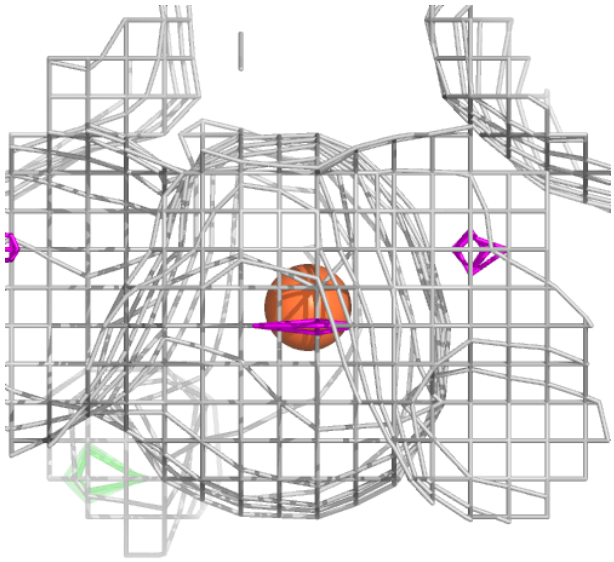
Electron density around FE D 201:

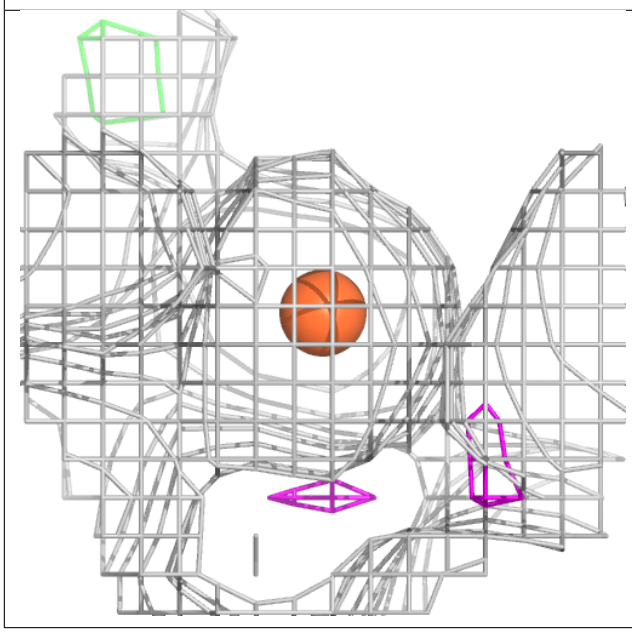
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

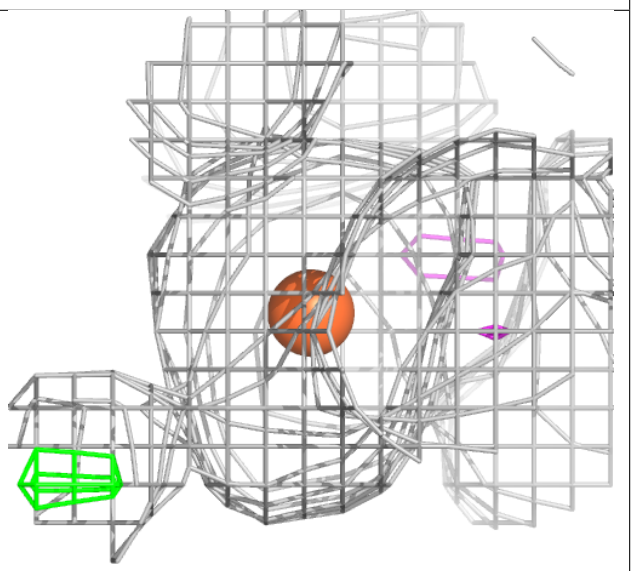


Electron density around FE H 201:

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

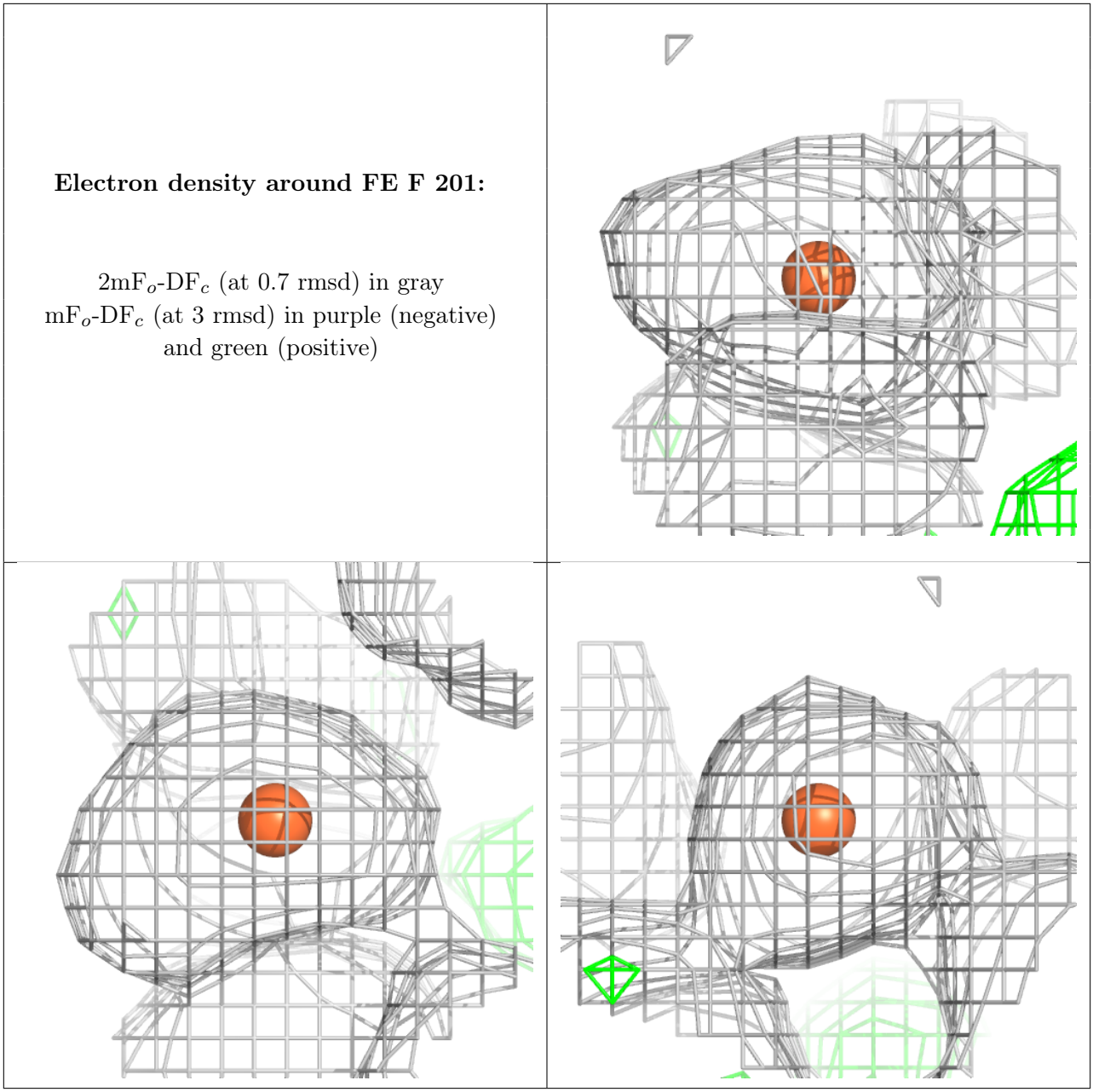






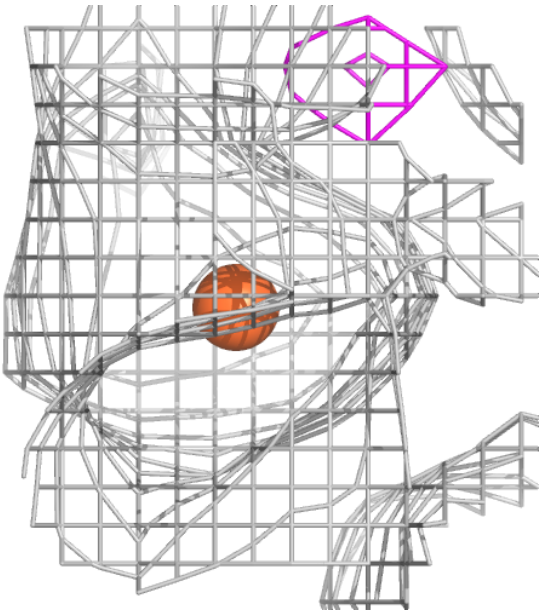
Electron density around FE F 201:

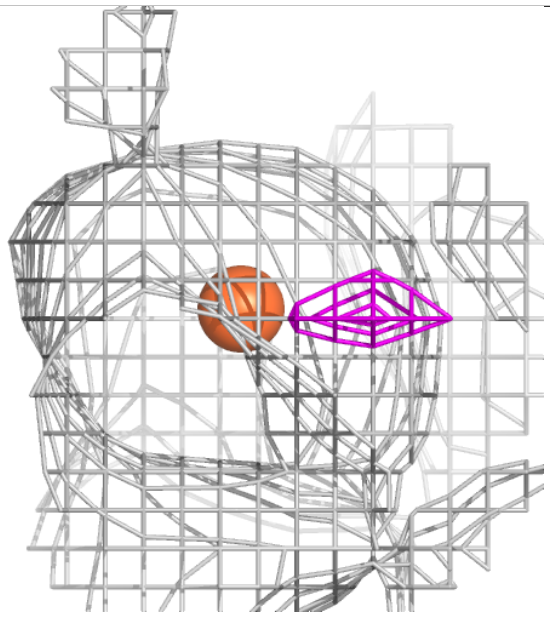
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

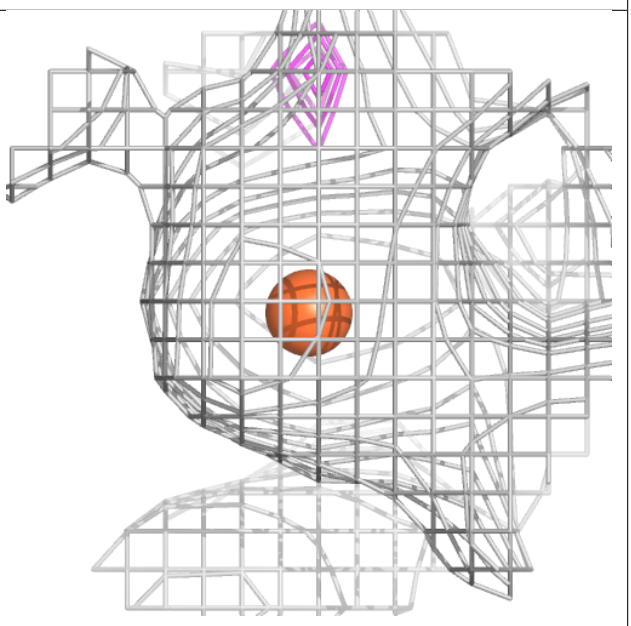


Electron density around FE K 201:

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

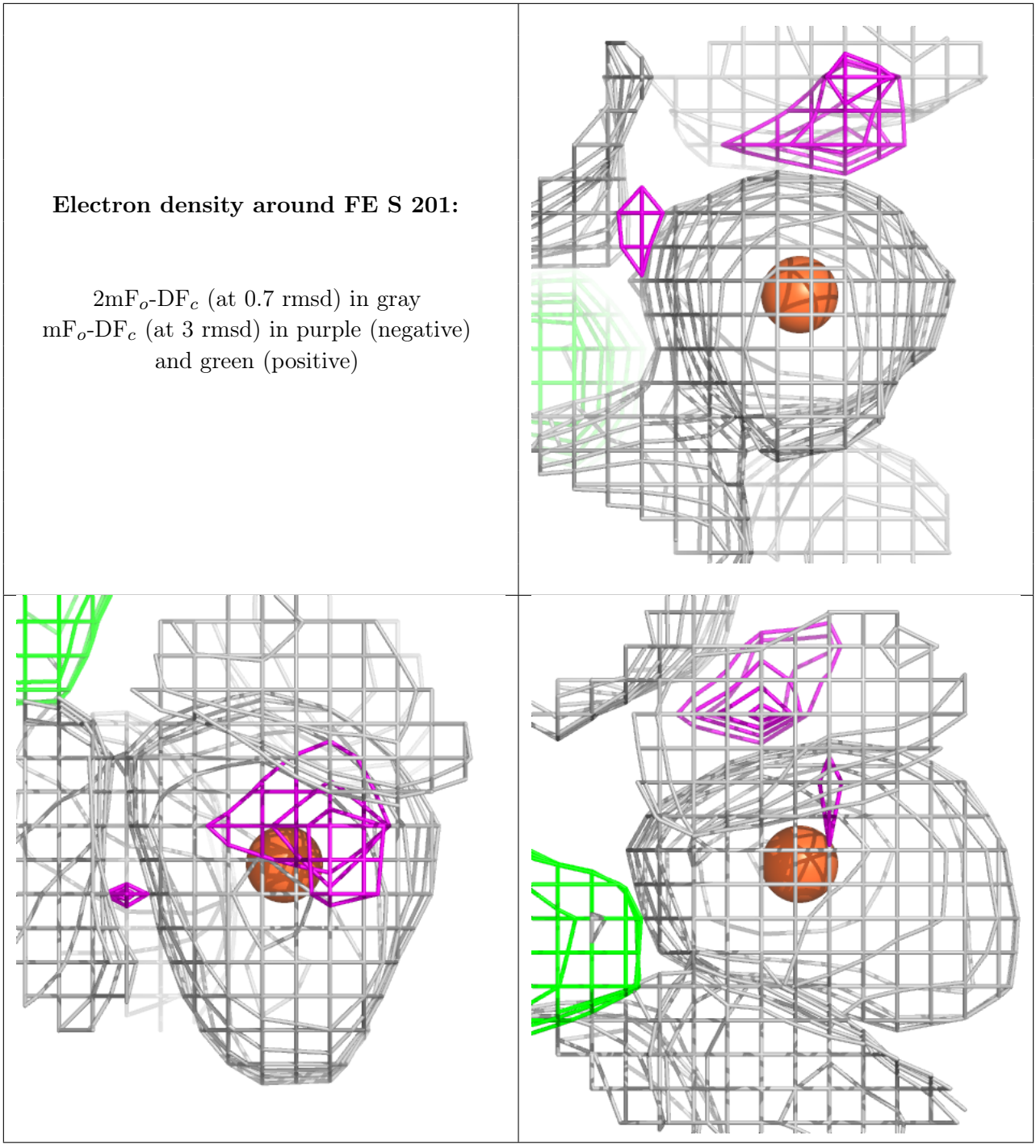






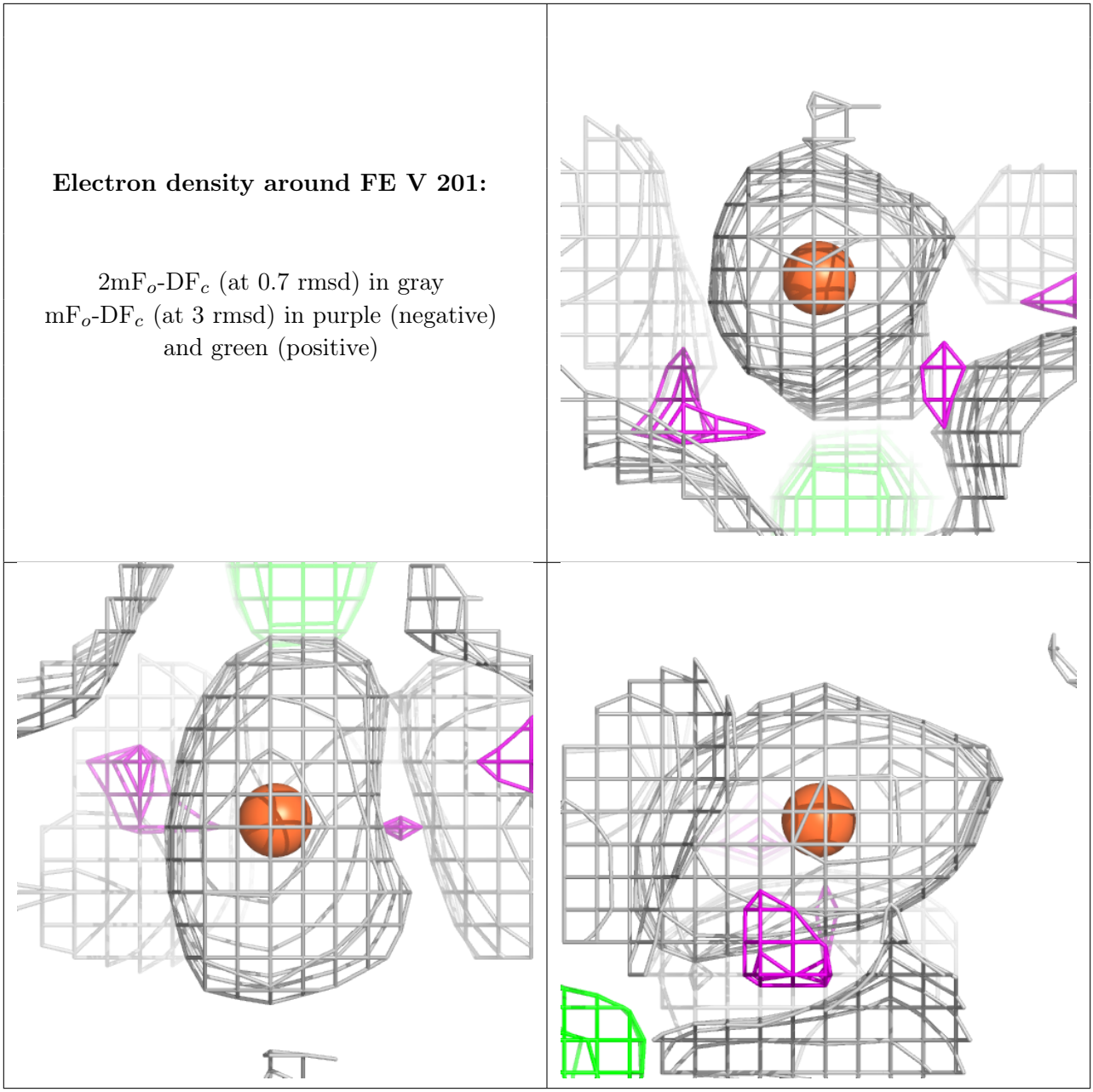
Electron density around FE S 201:

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



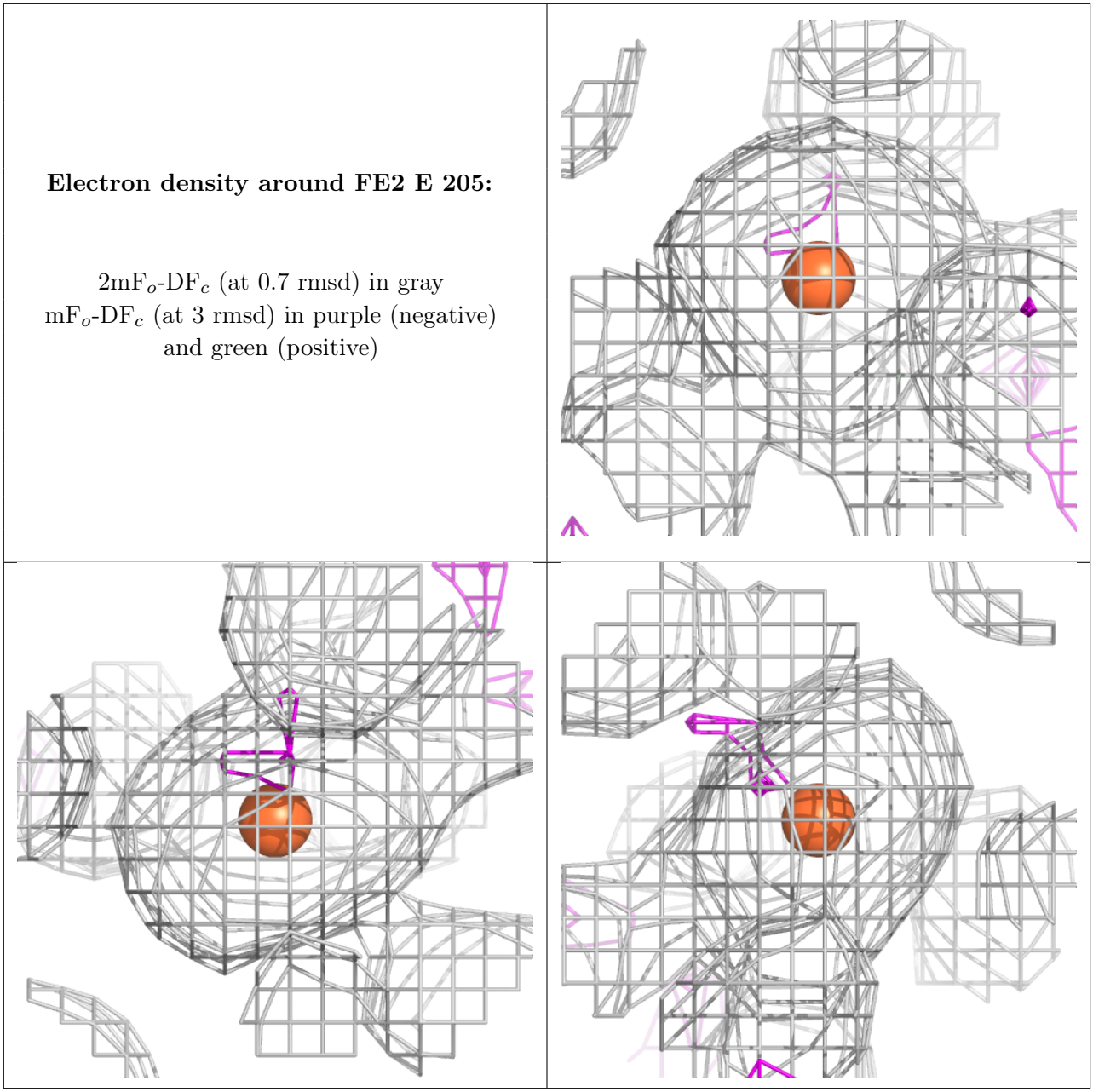
Electron density around FE V 201:

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



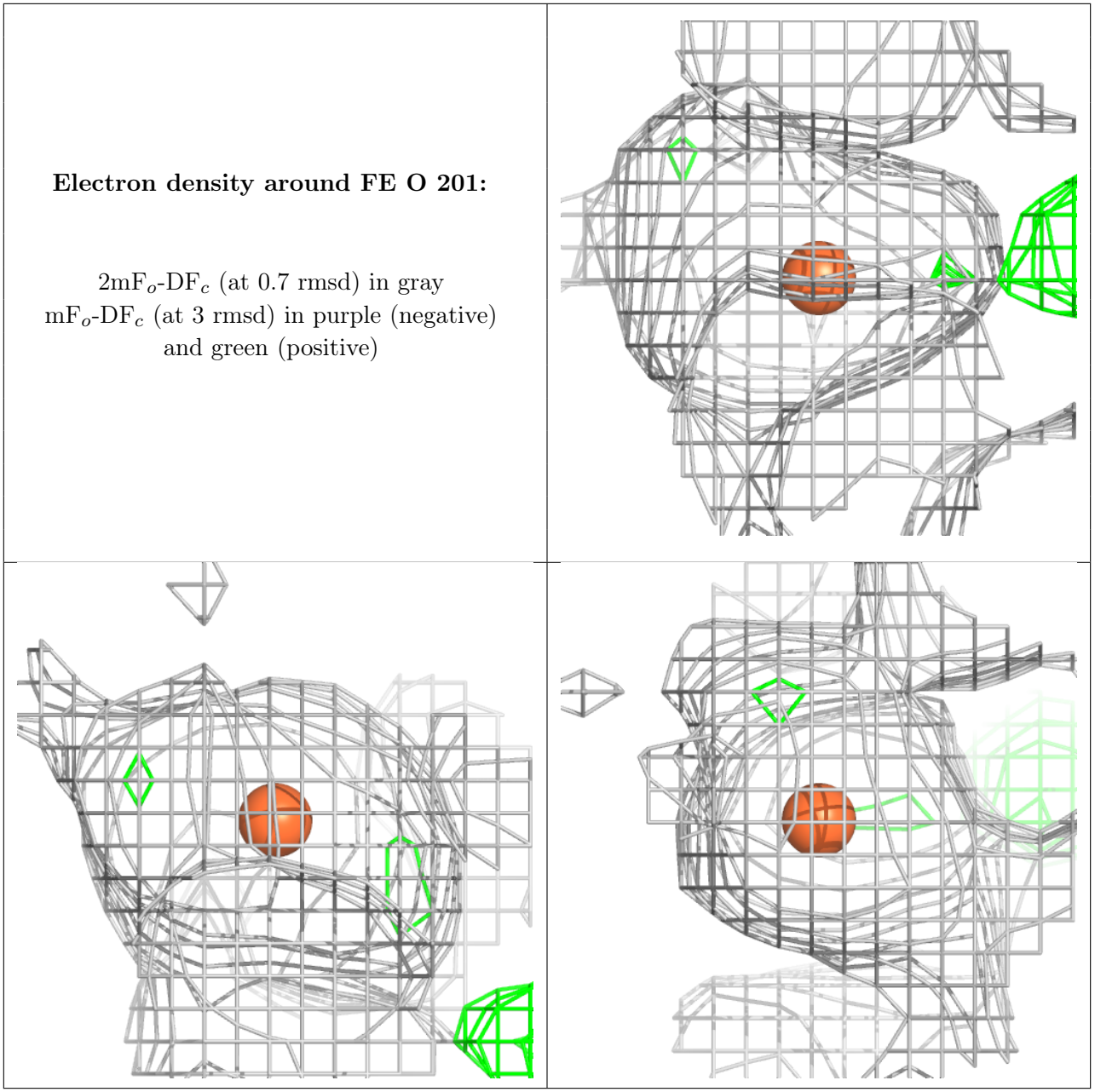
Electron density around FE2 E 205:

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



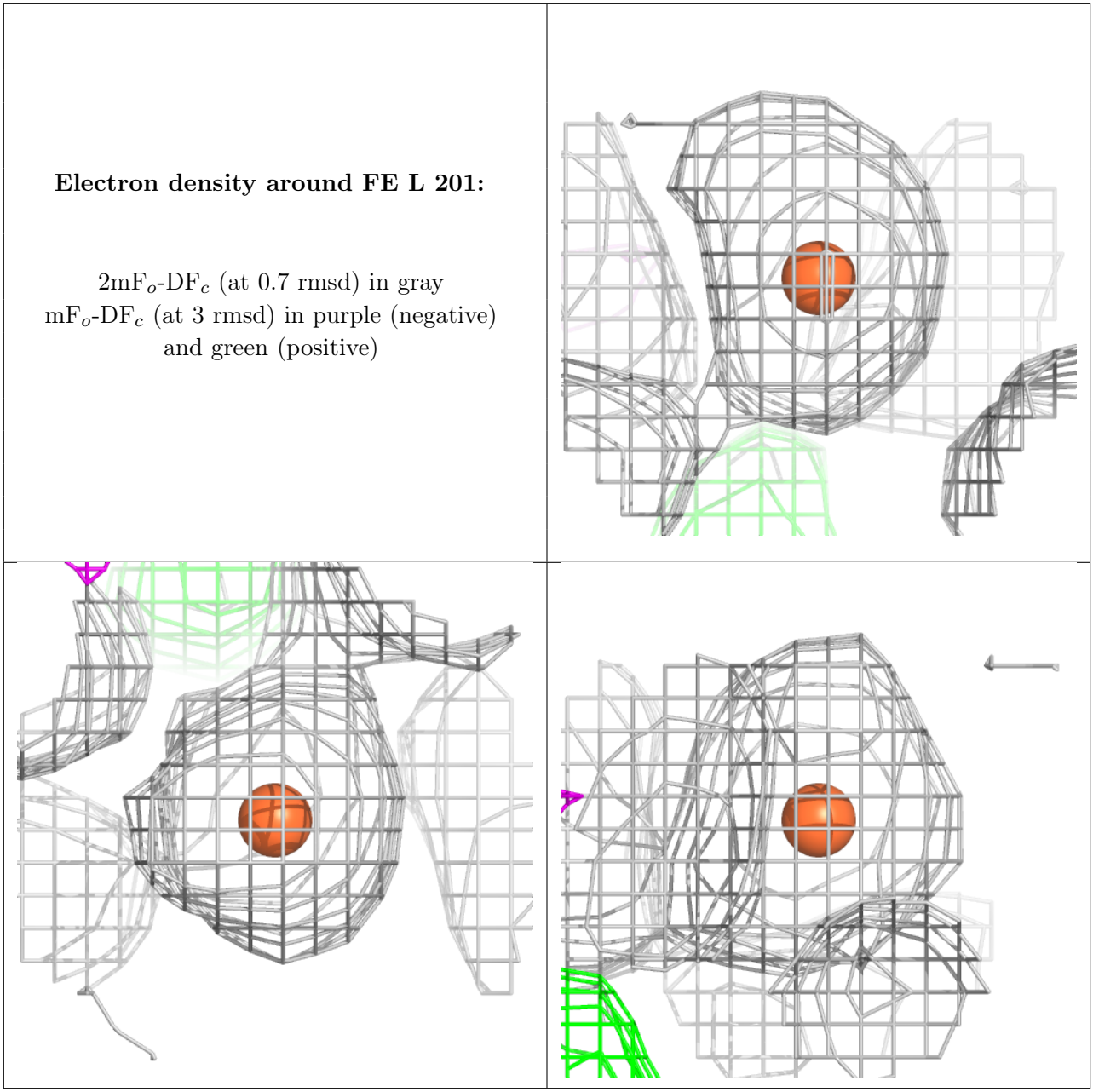
Electron density around FE O 201:

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



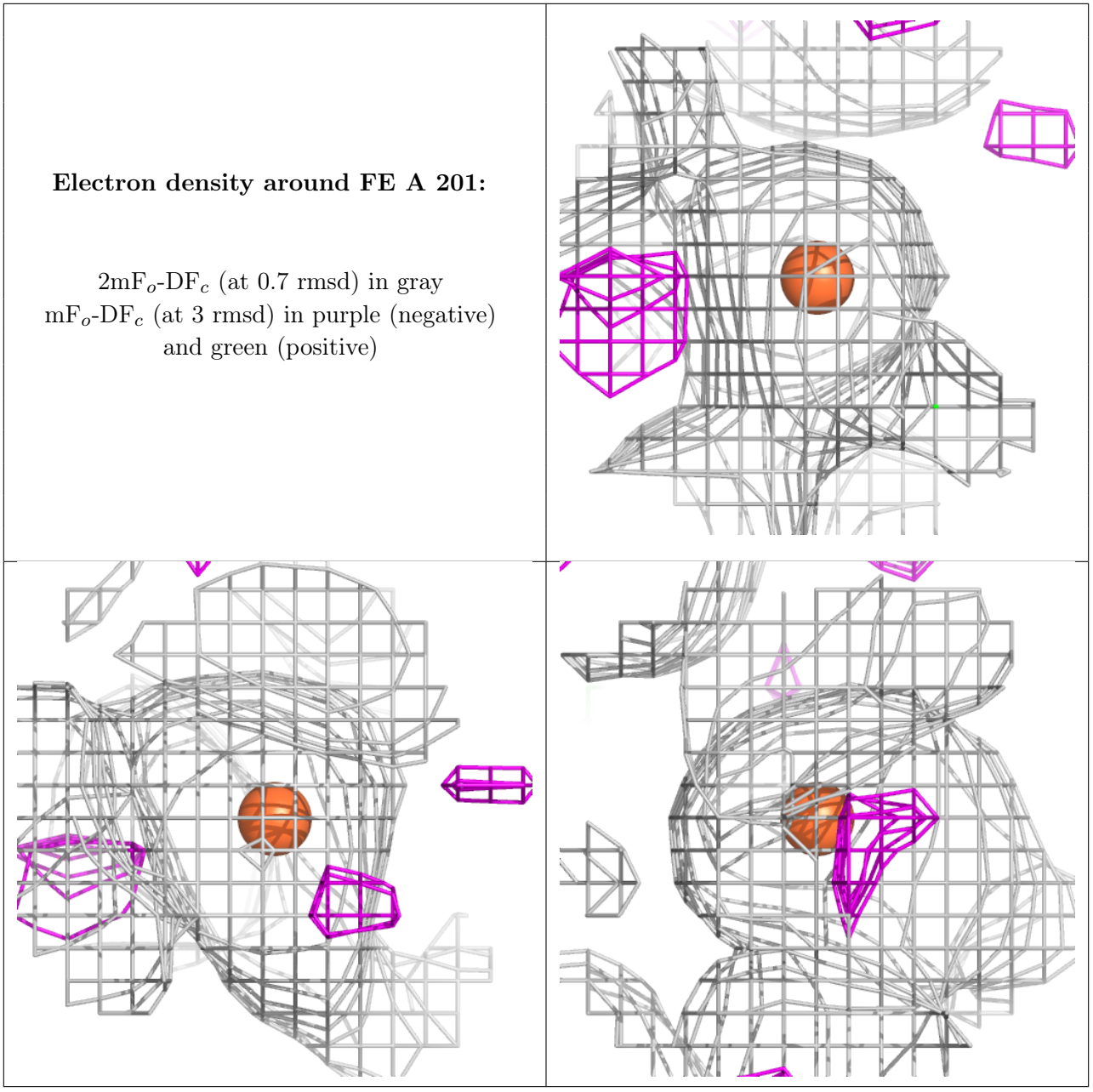
Electron density around FE L 201:

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



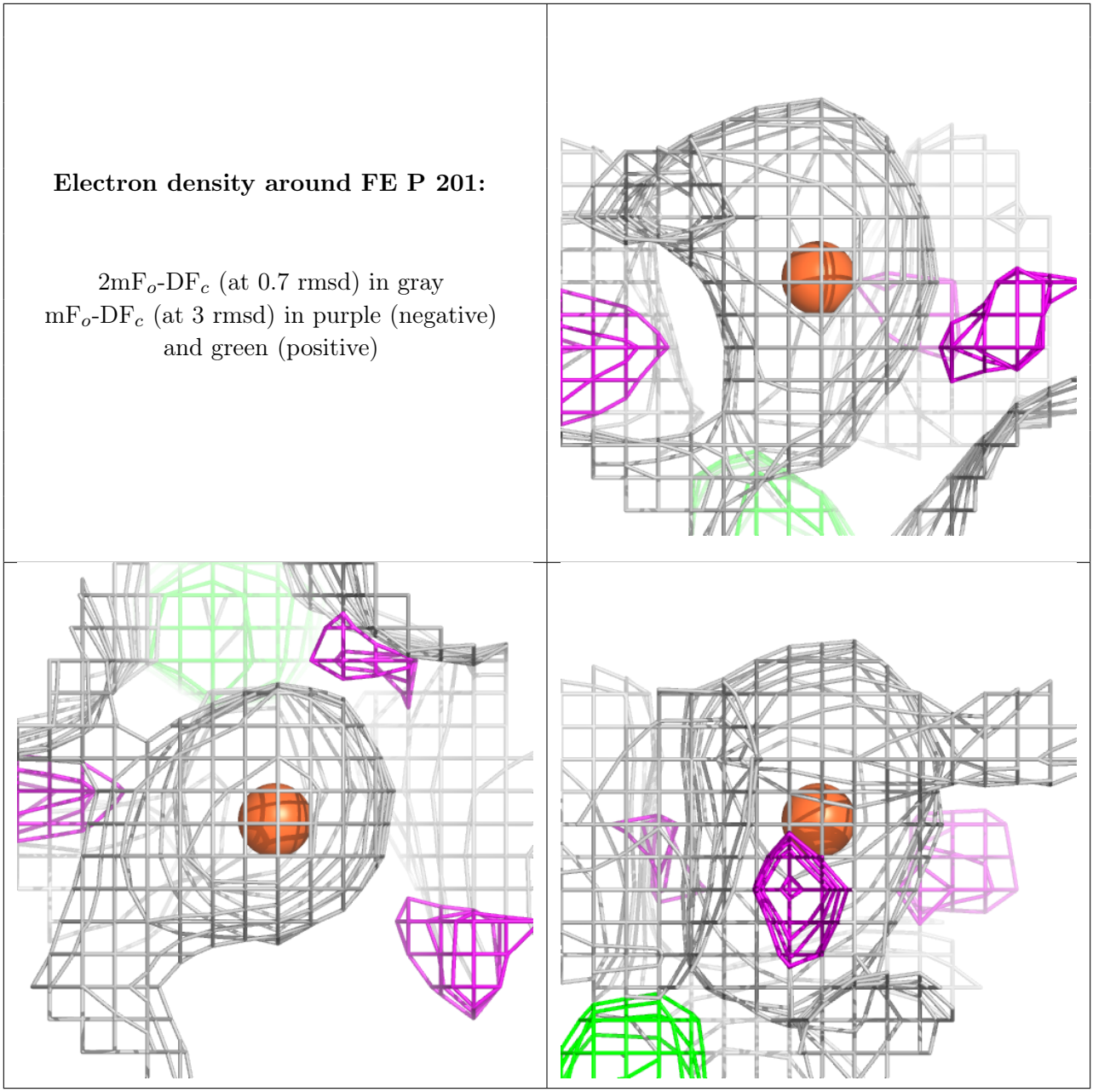
Electron density around FE A 201:

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



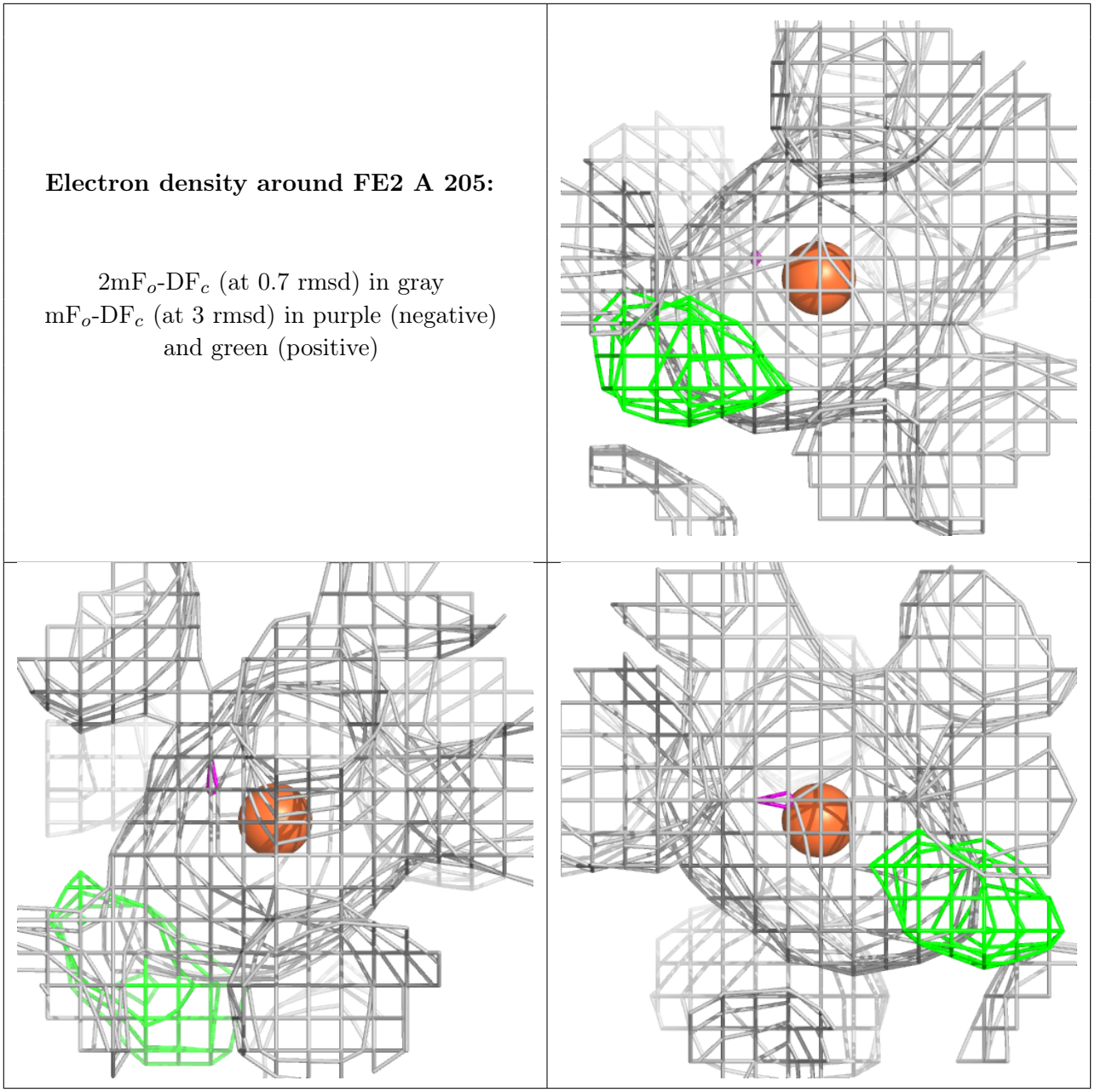
Electron density around FE P 201:

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



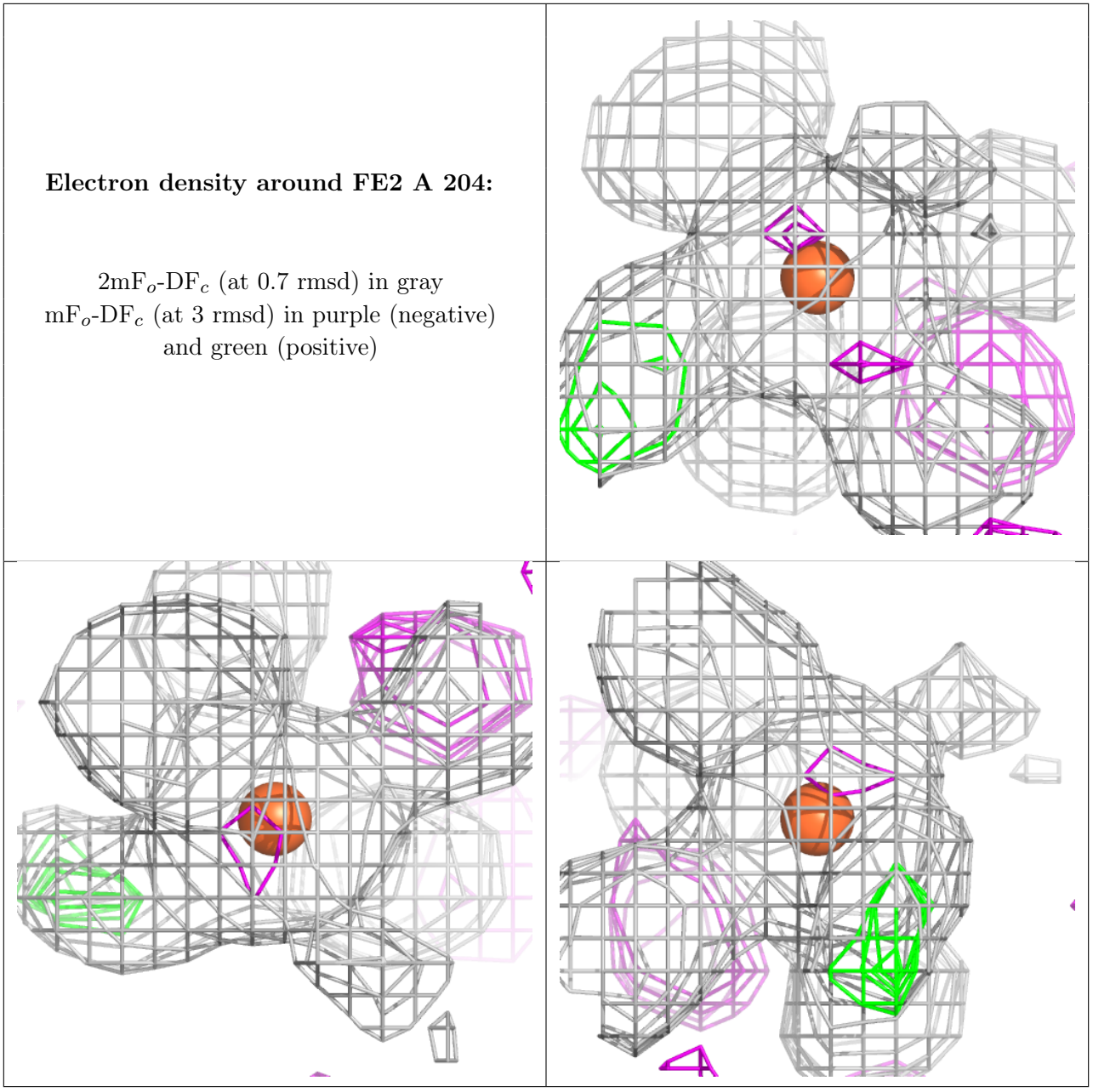
Electron density around FE2 A 205:

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



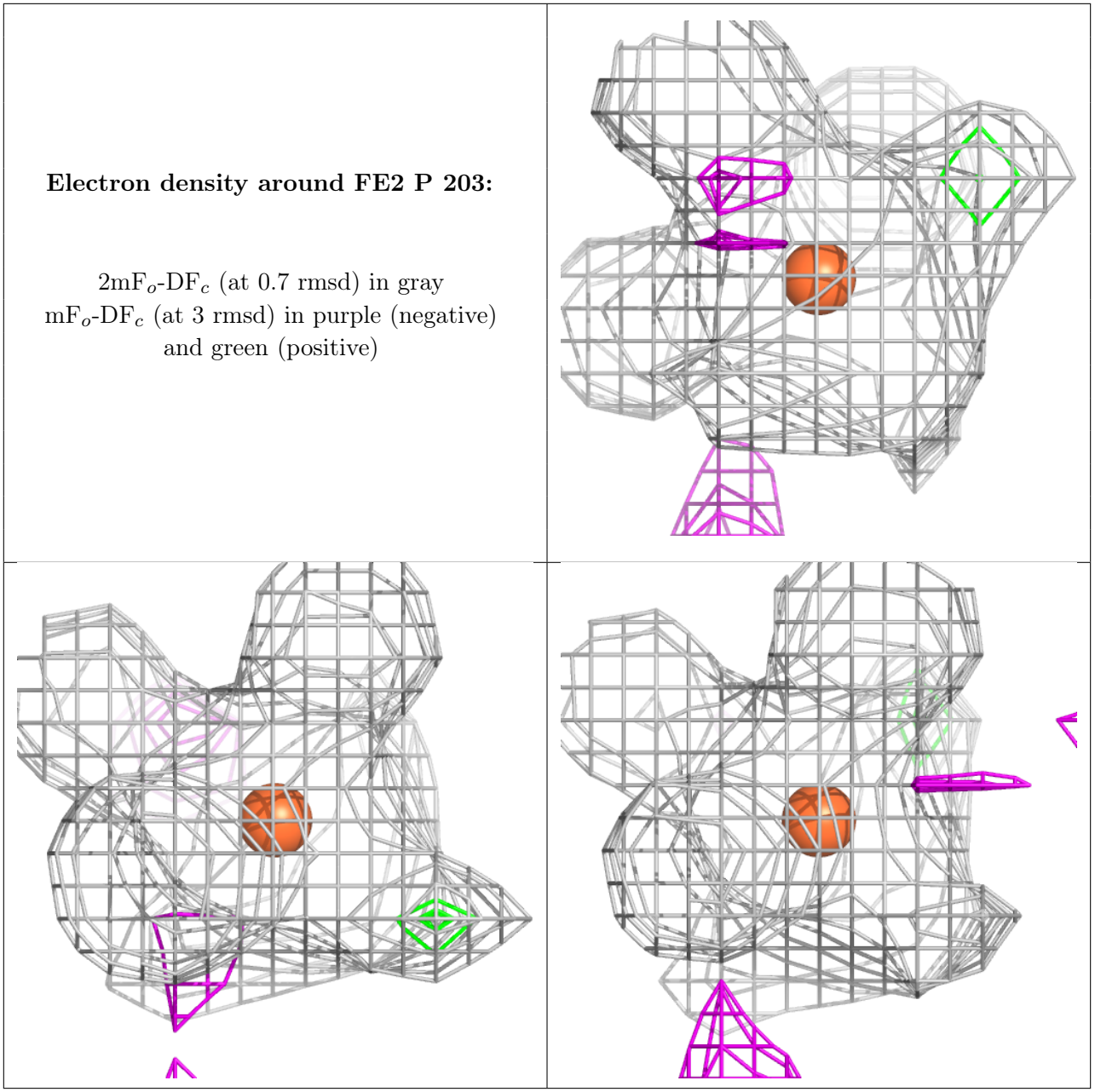
Electron density around FE2 A 204:

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



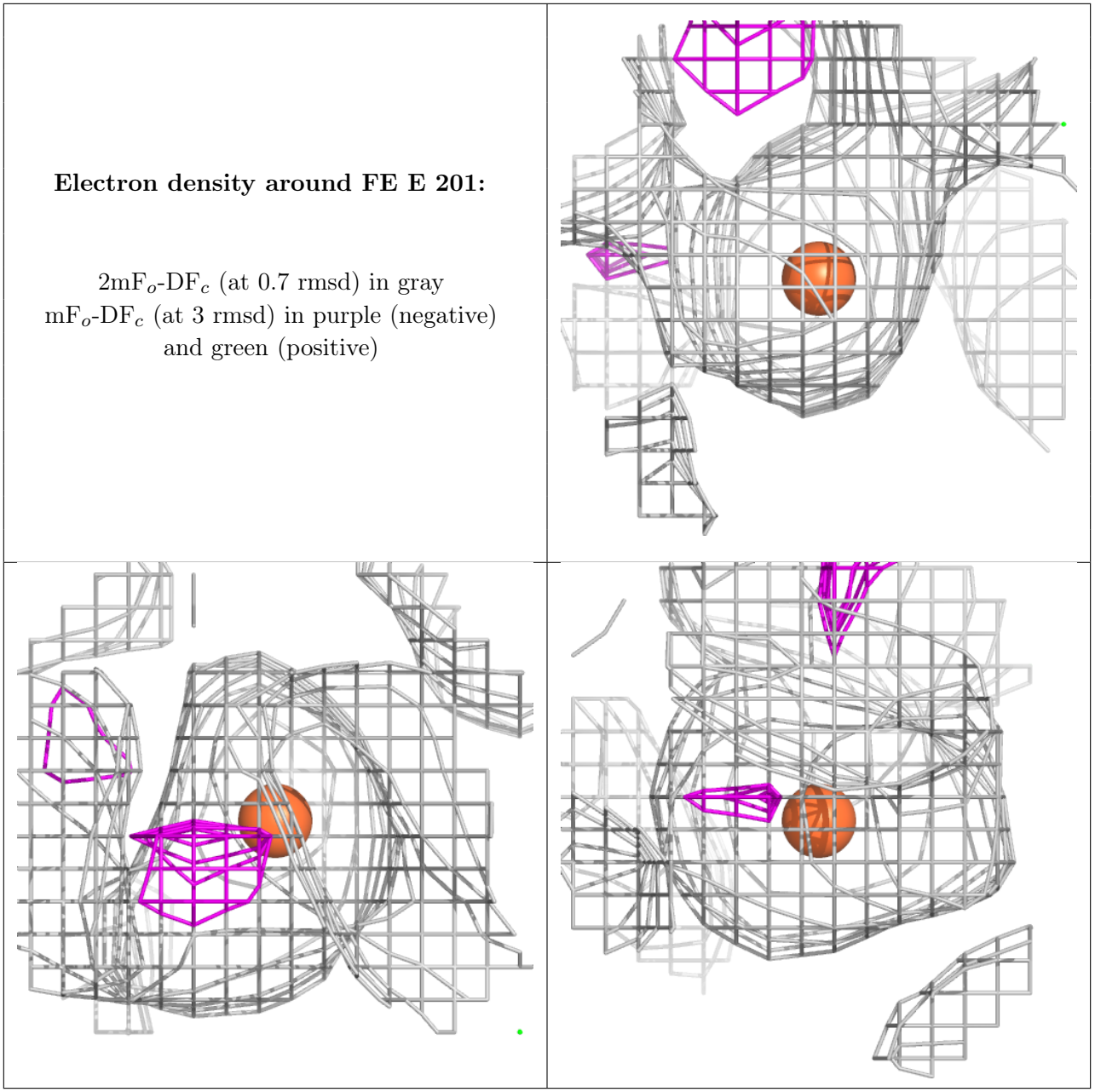
Electron density around FE2 P 203:

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



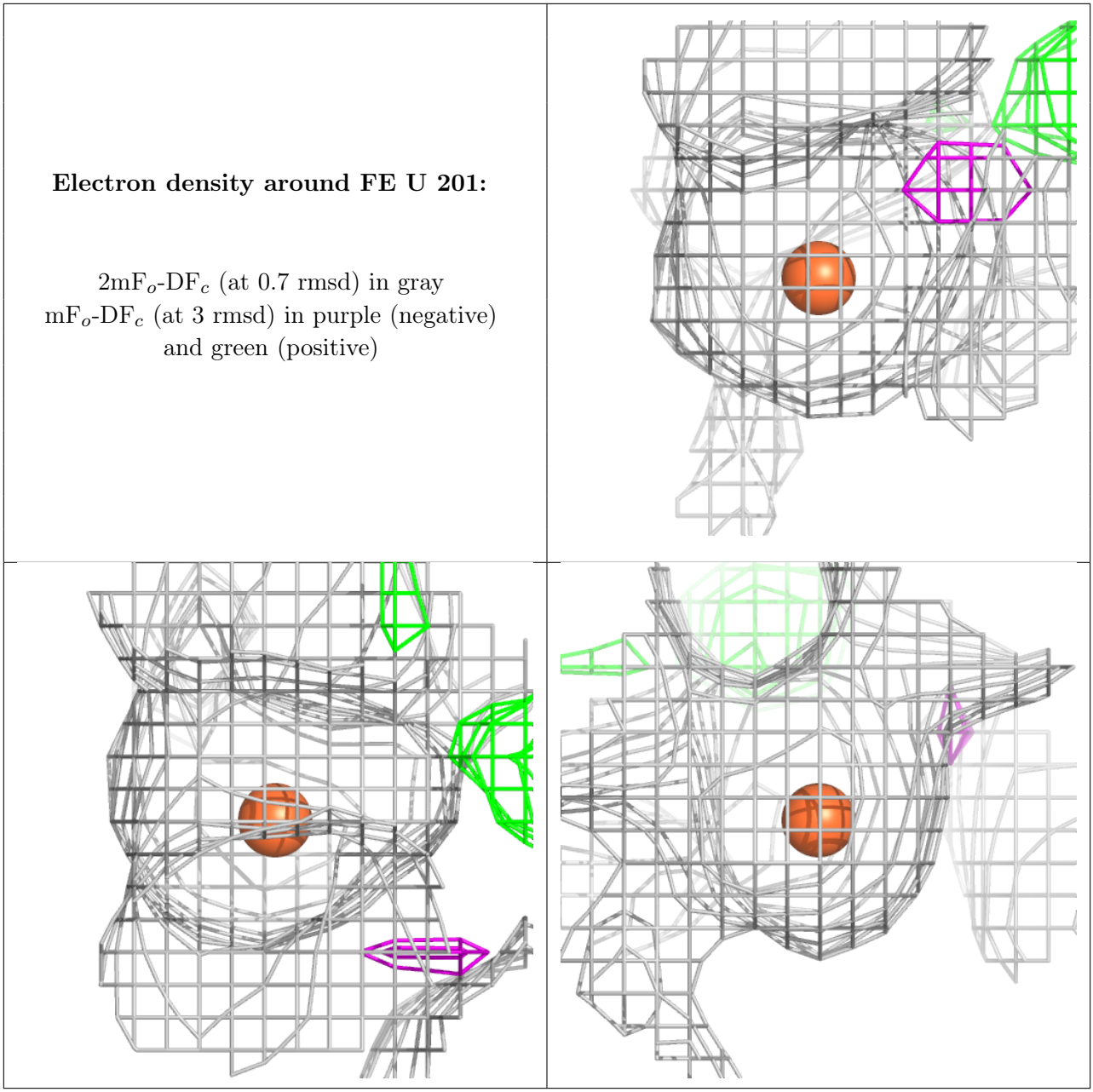
Electron density around FE E 201:

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



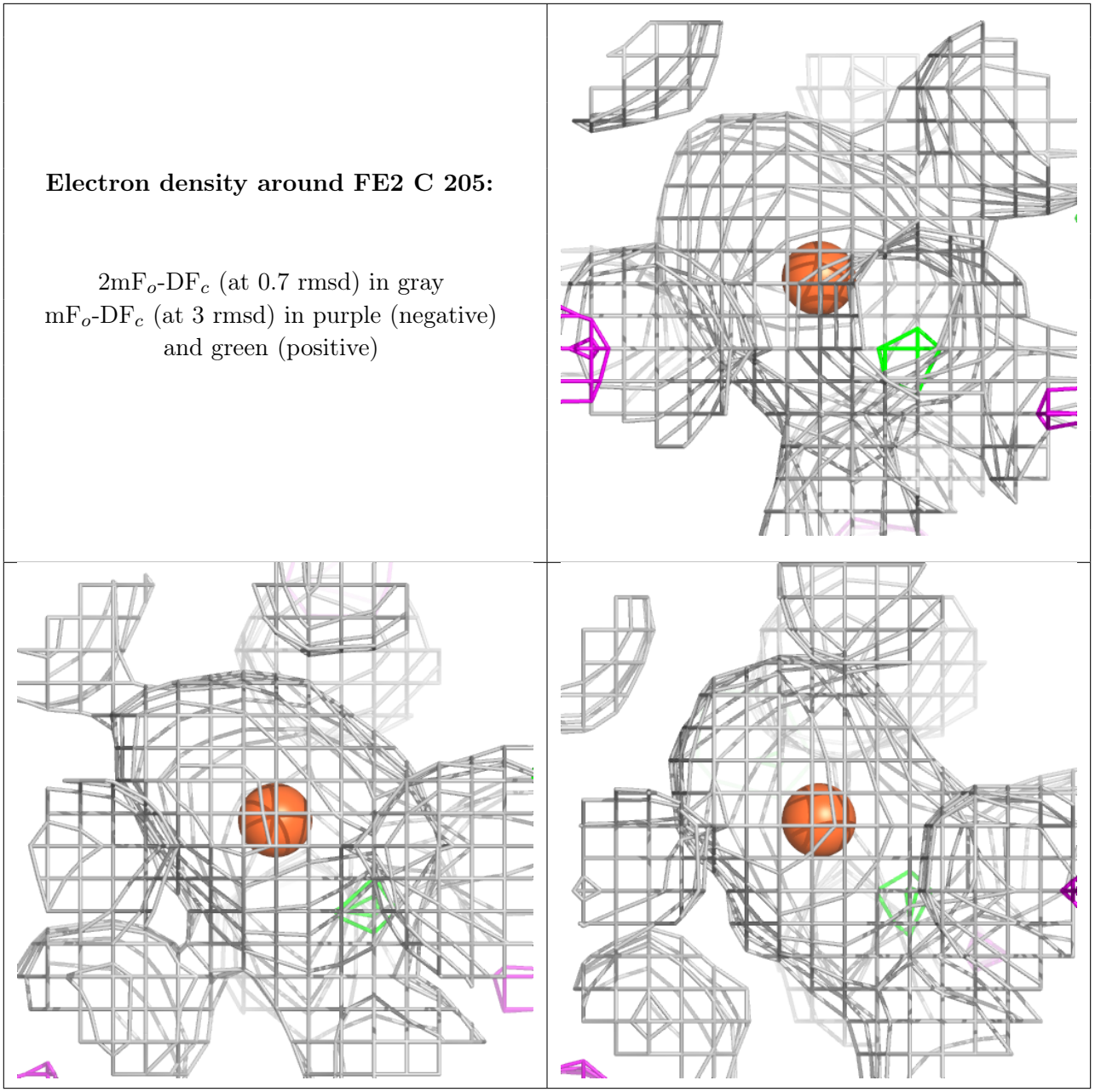
Electron density around FE U 201:

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



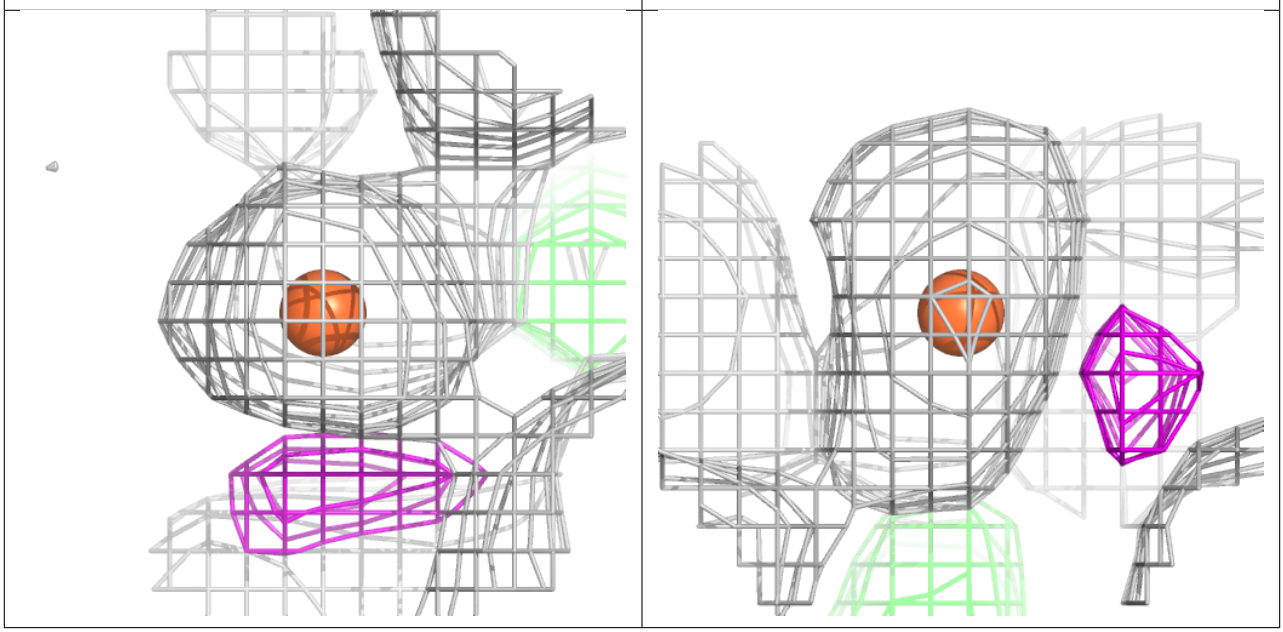
Electron density around FE2 C 205:

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



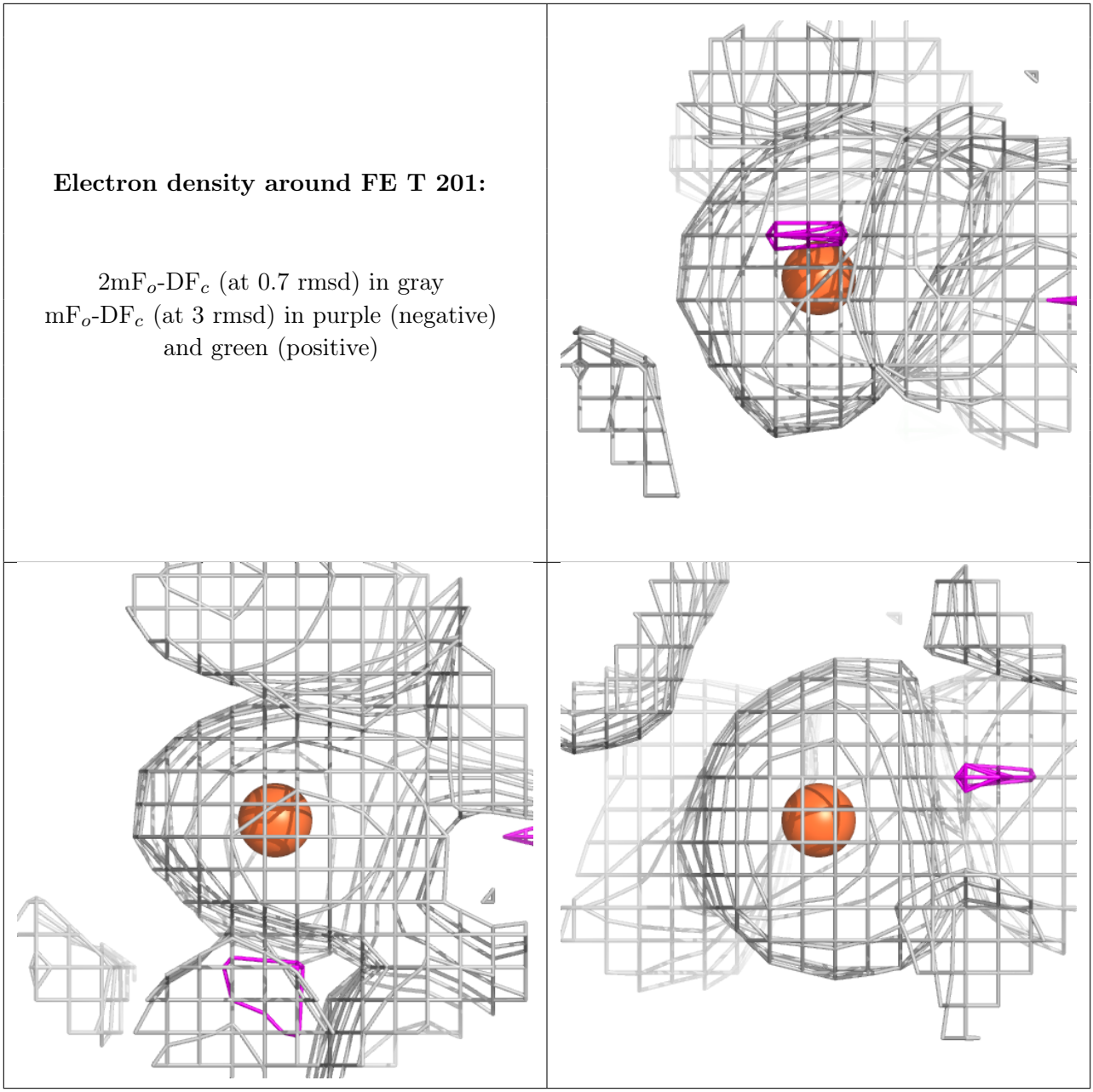
Electron density around FE X 201:

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



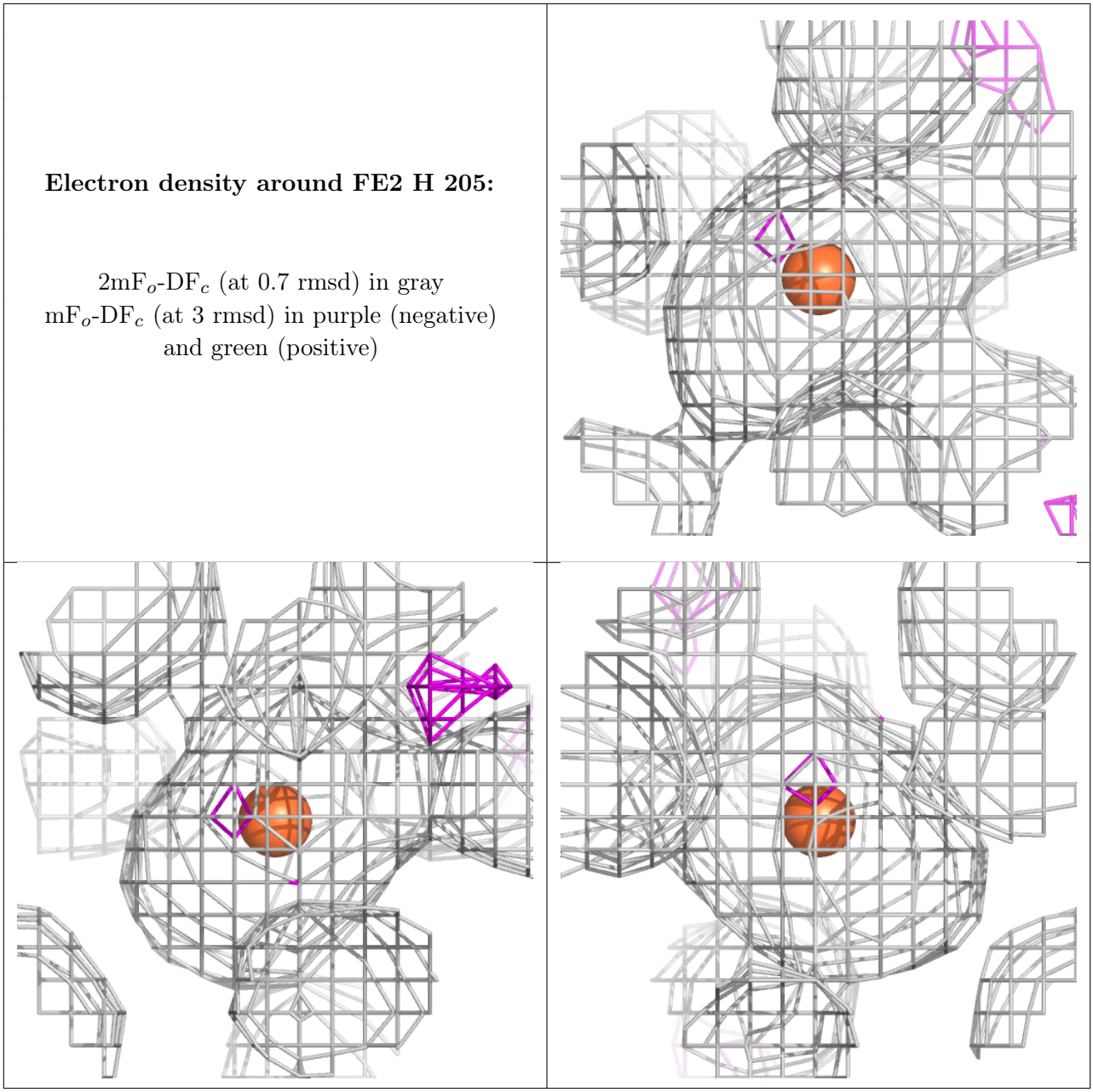
Electron density around FE T 201:

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



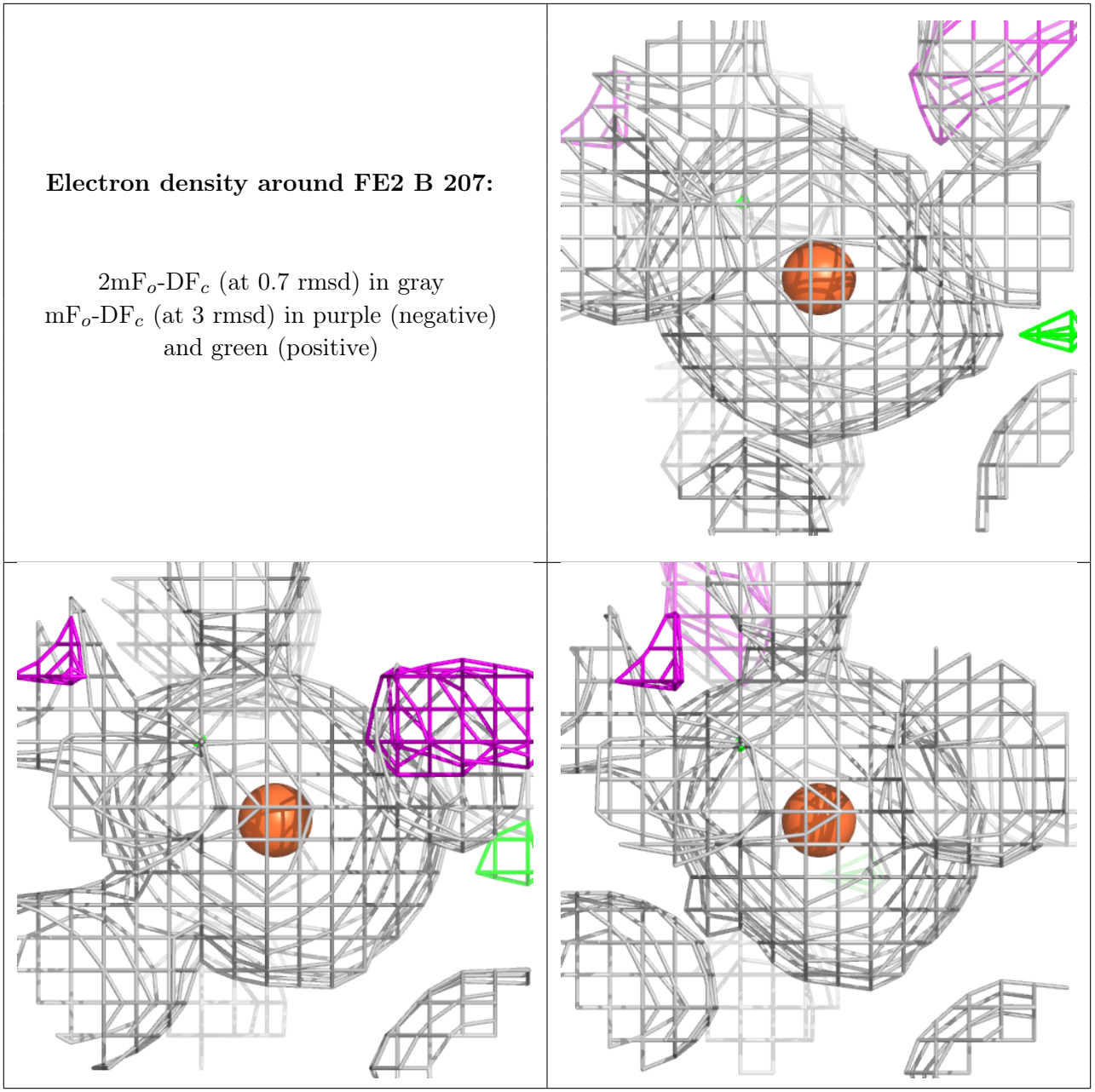
Electron density around FE2 H 205:

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



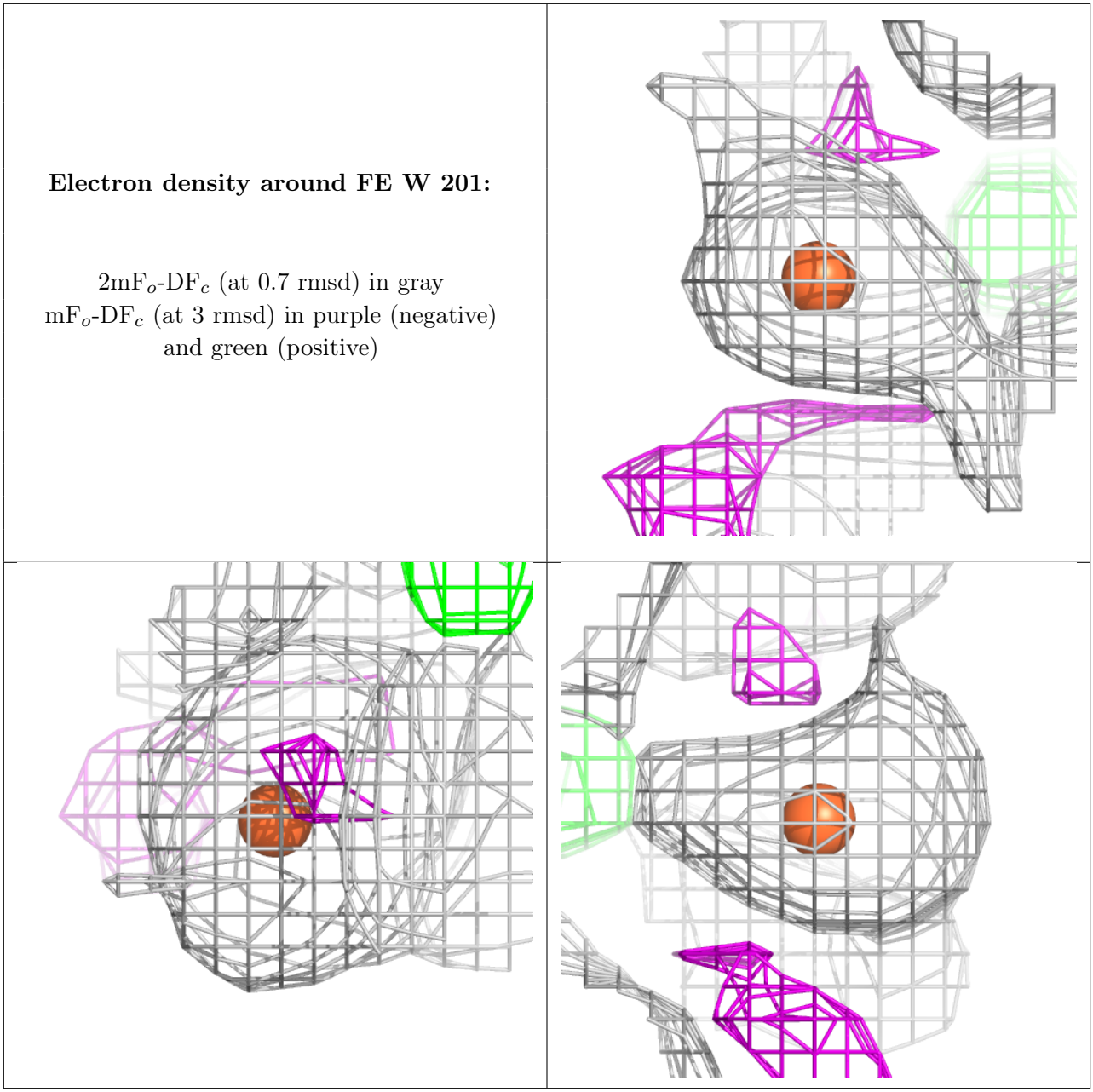
Electron density around FE2 B 207:

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



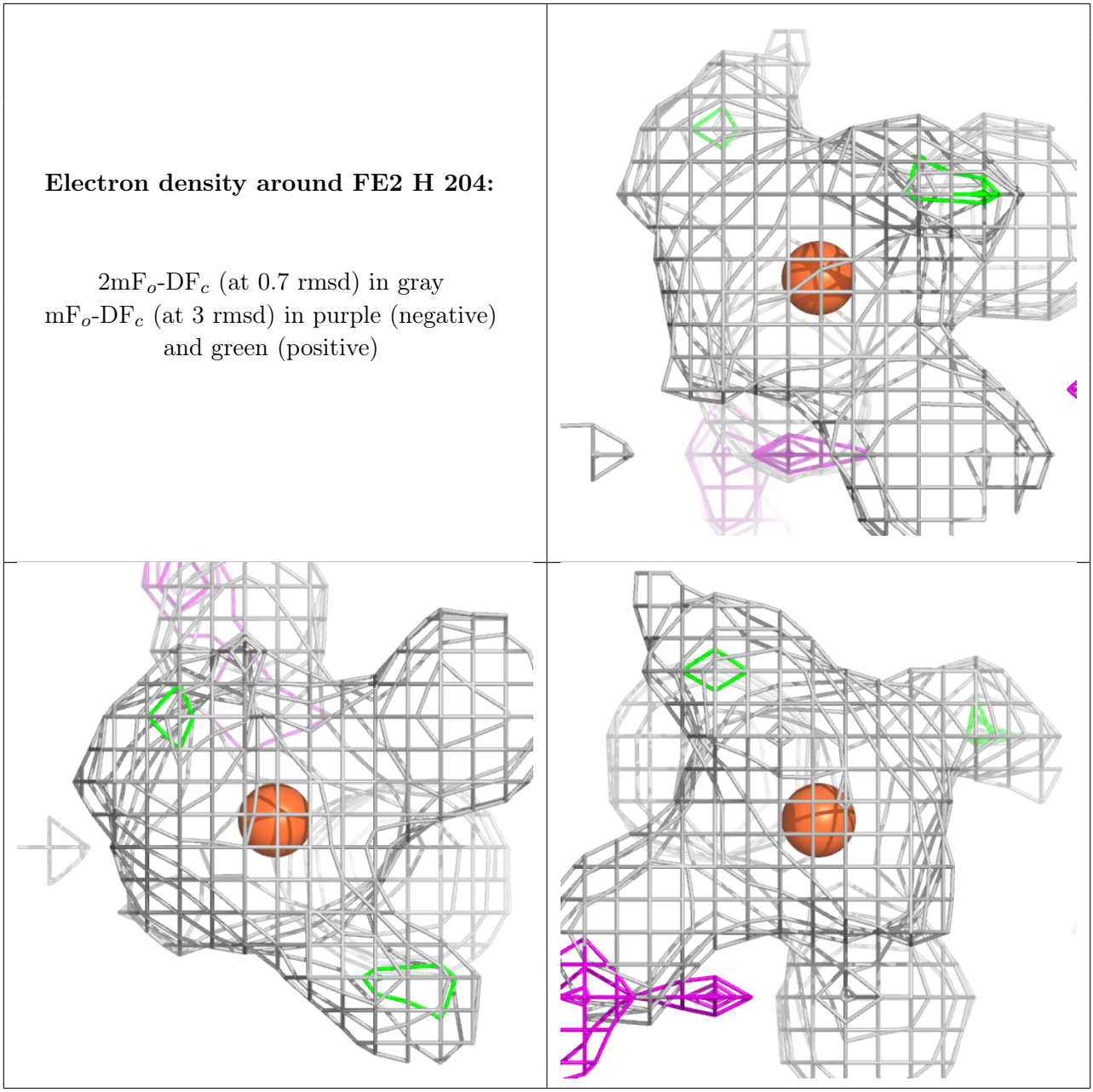
Electron density around FE W 201:

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



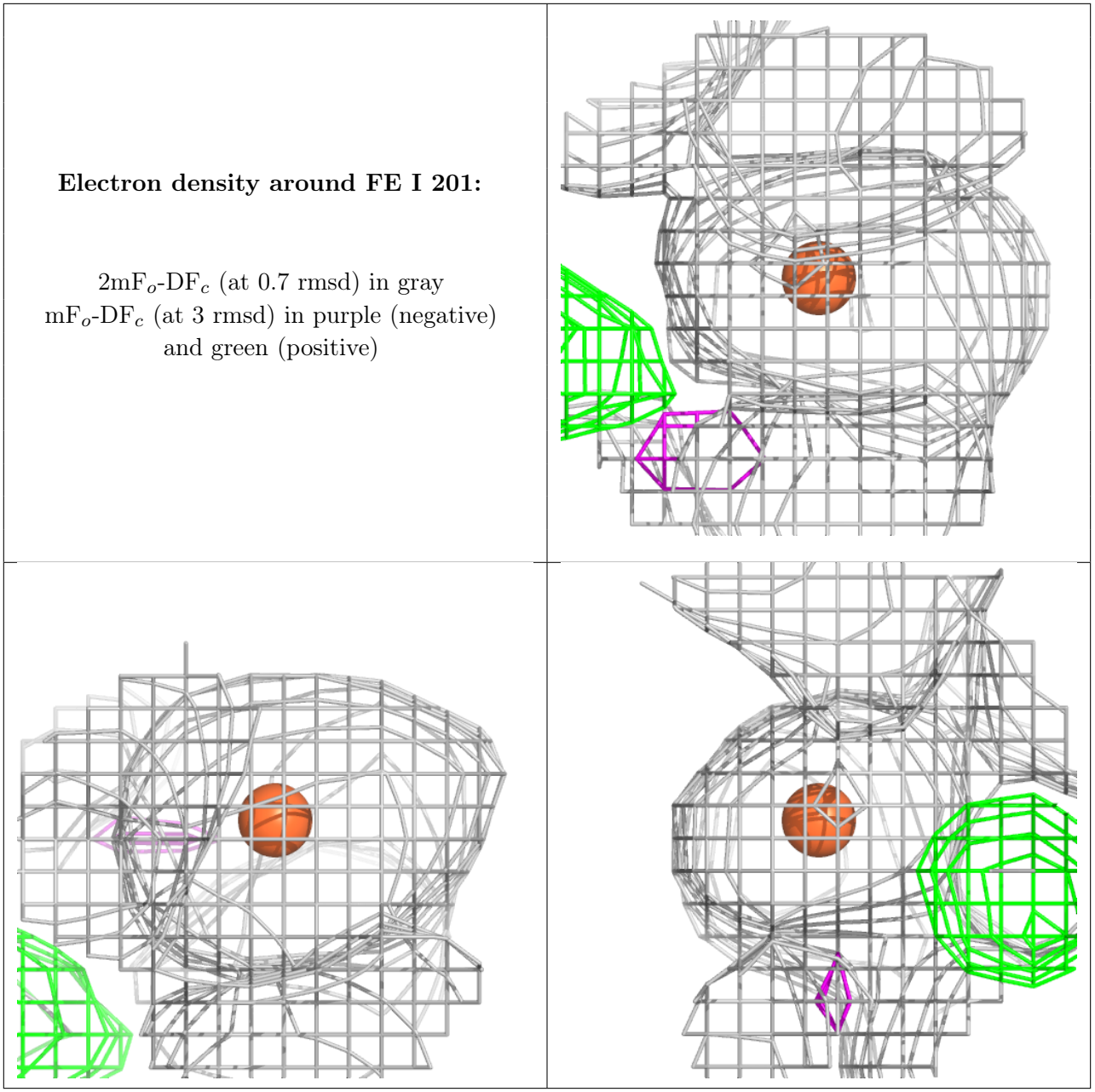
Electron density around FE2 H 204:

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



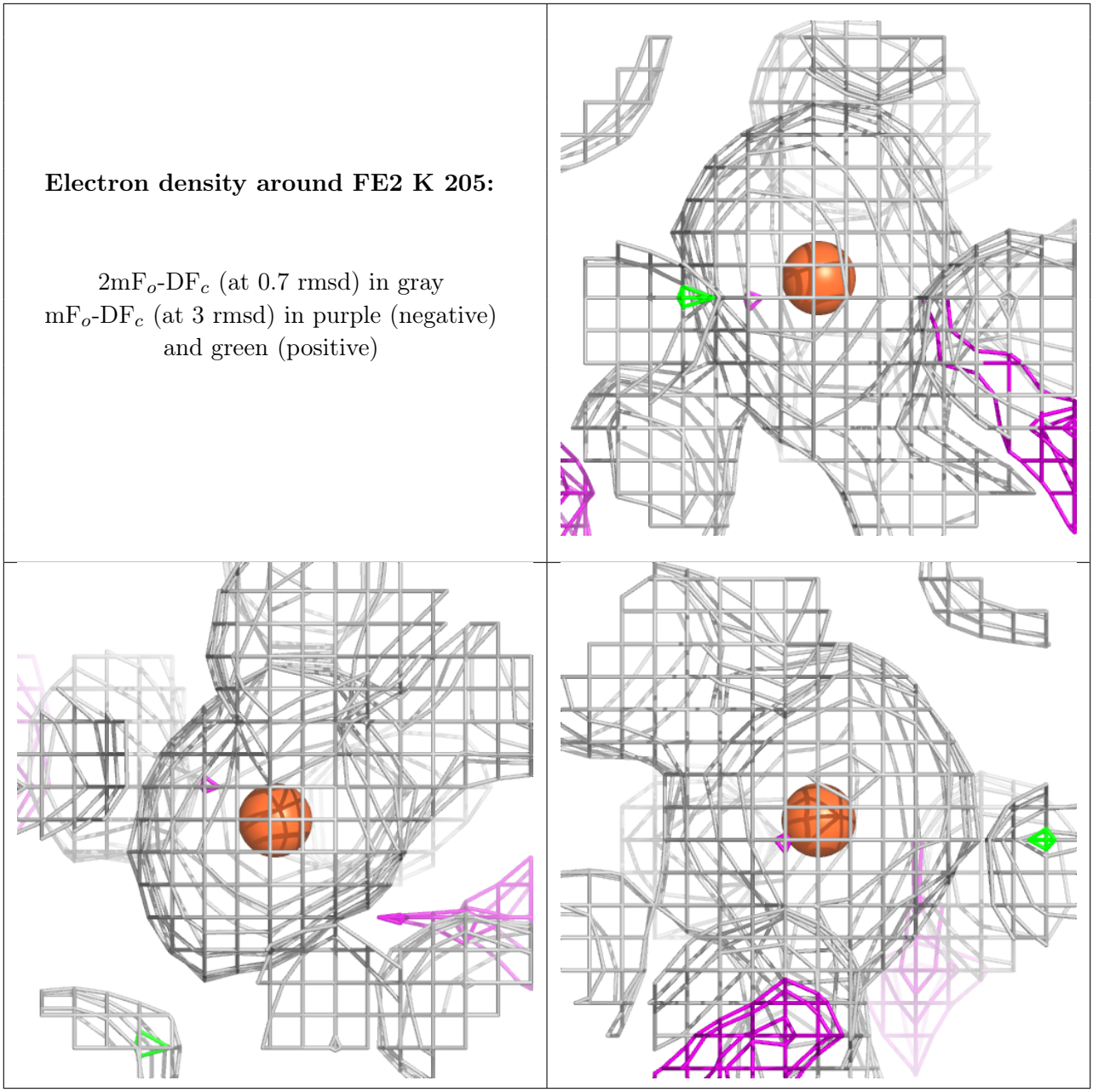
Electron density around FE I 201:

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



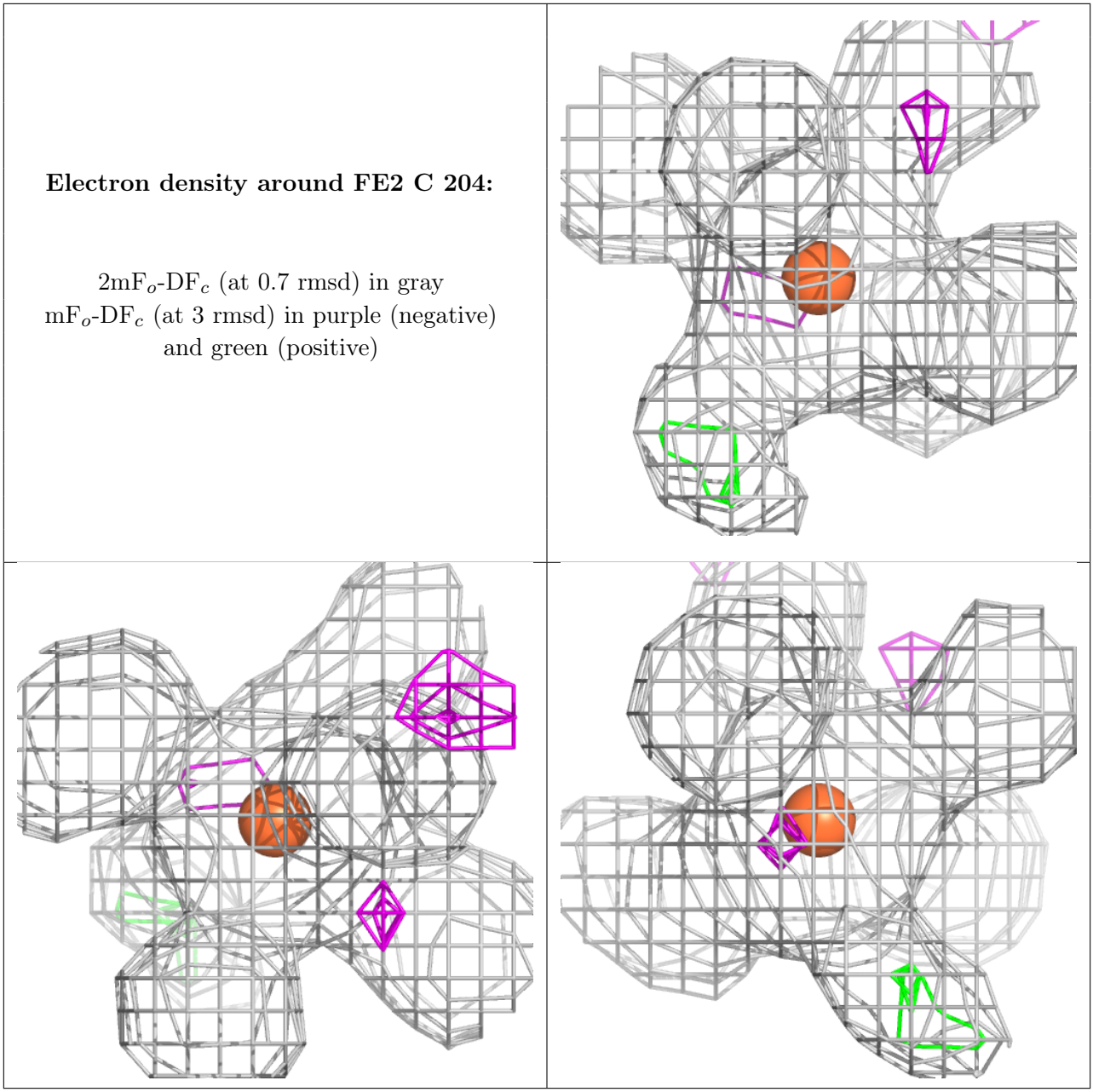
Electron density around FE2 K 205:

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



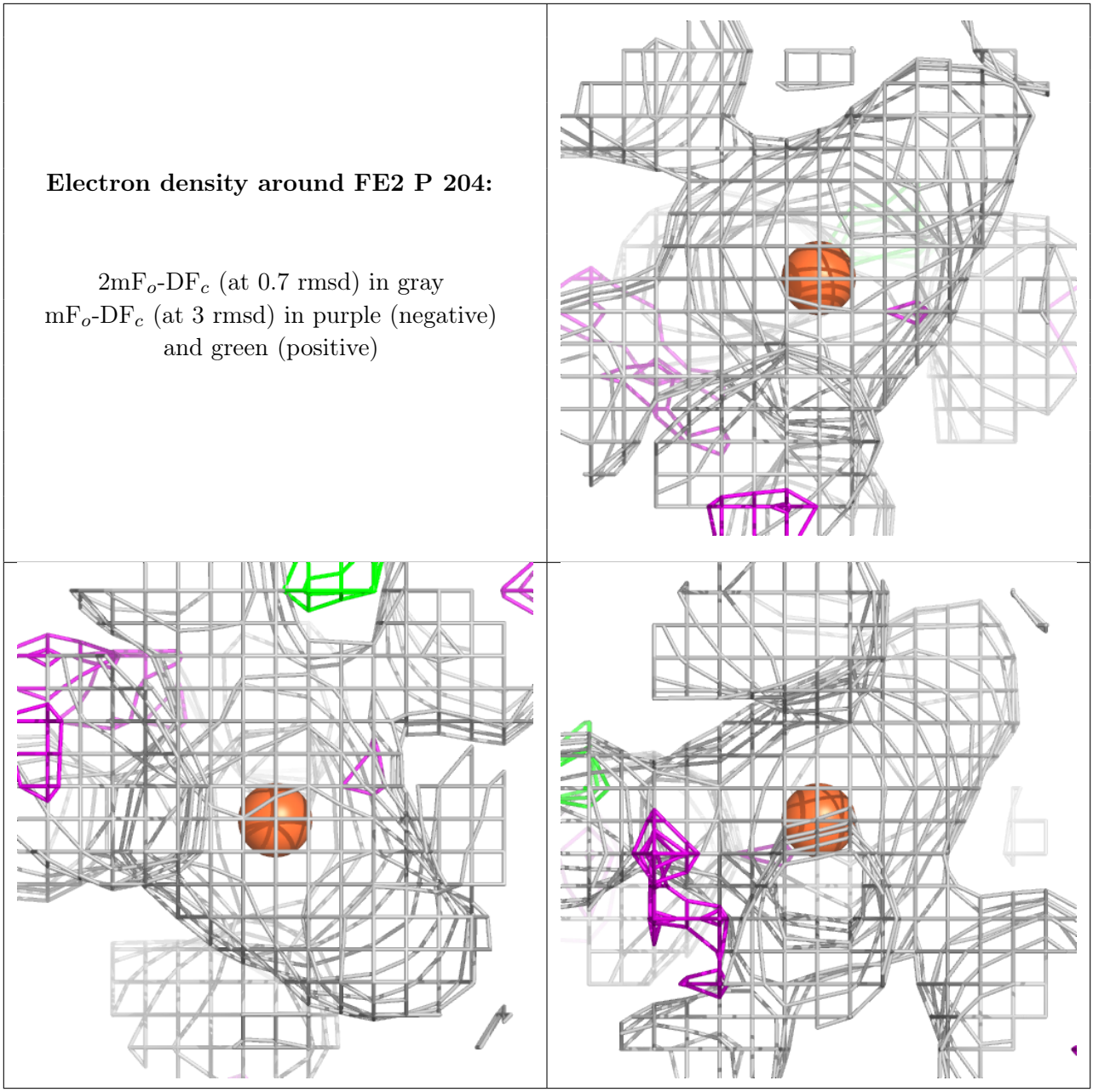
Electron density around FE2 C 204:

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



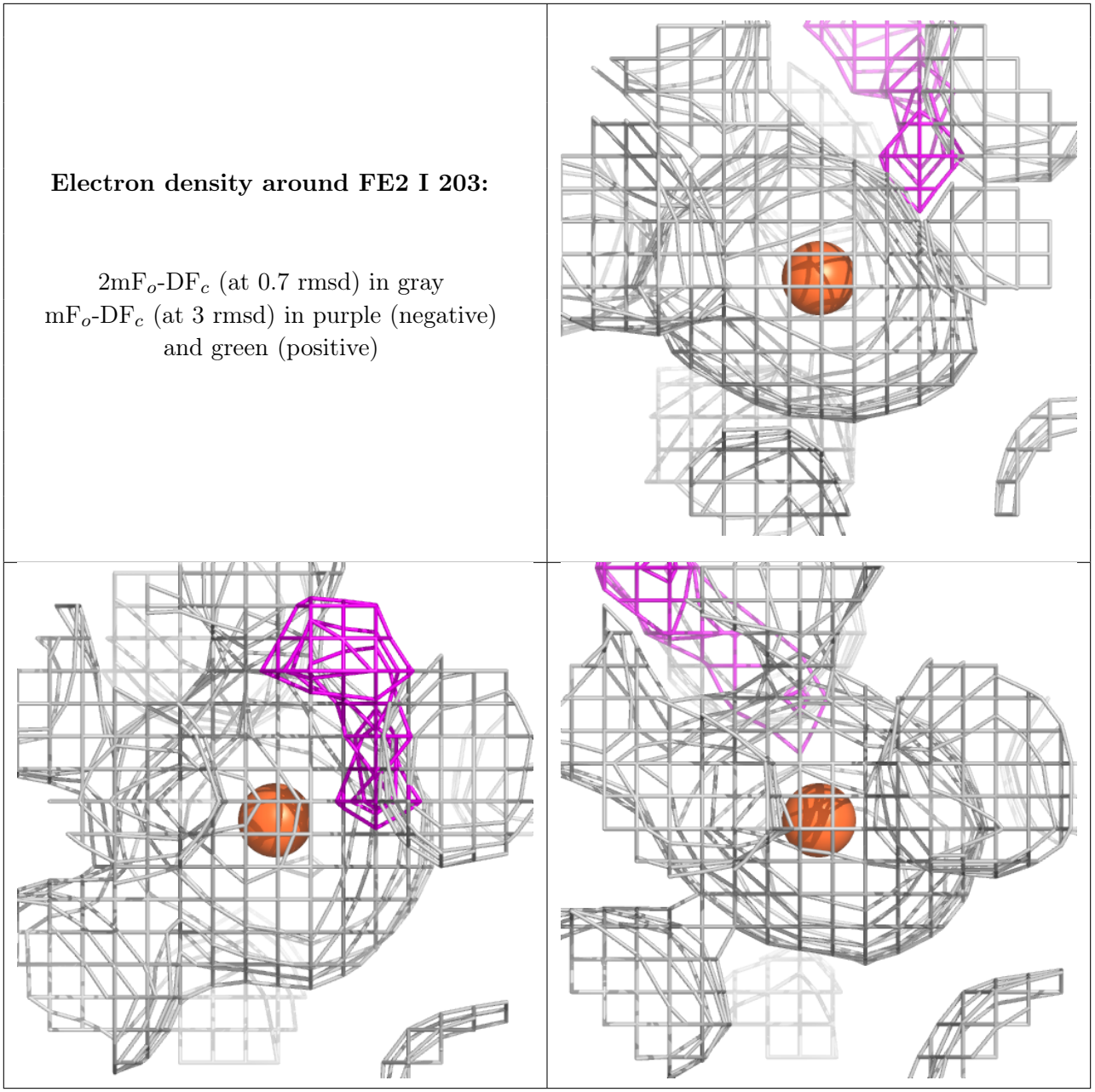
Electron density around FE2 P 204:

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



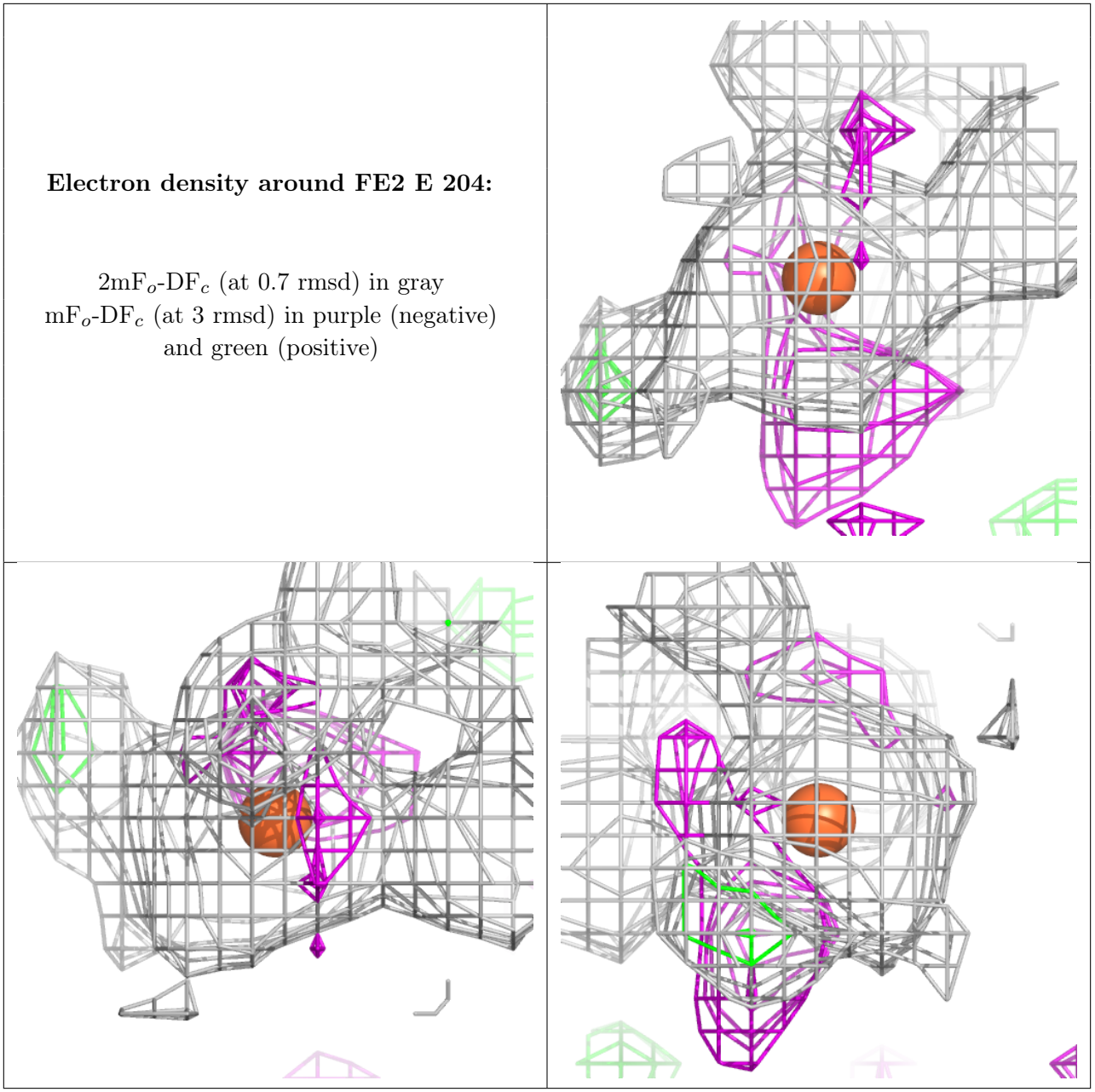
Electron density around FE2 I 203:

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



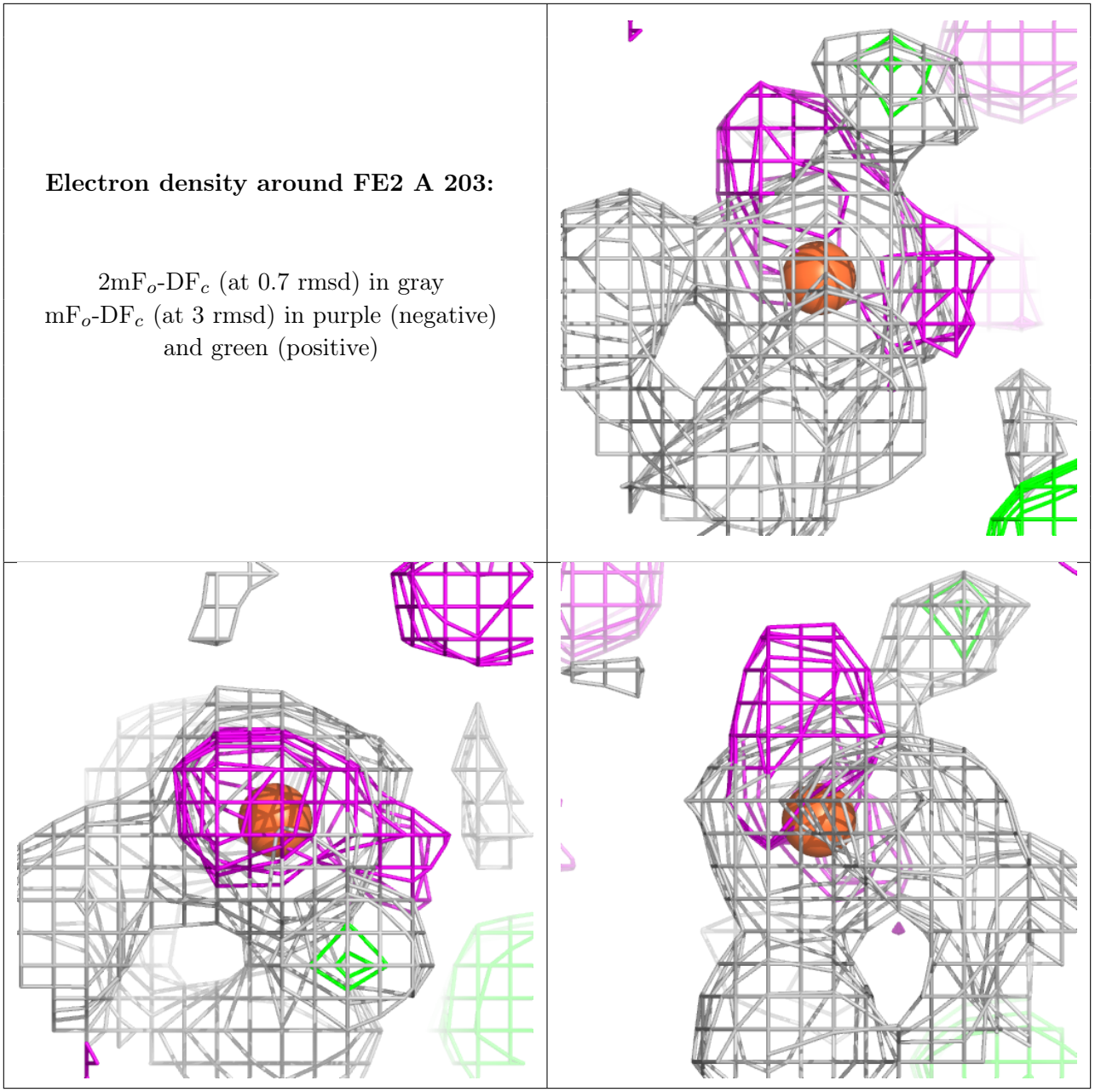
Electron density around FE2 E 204:

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



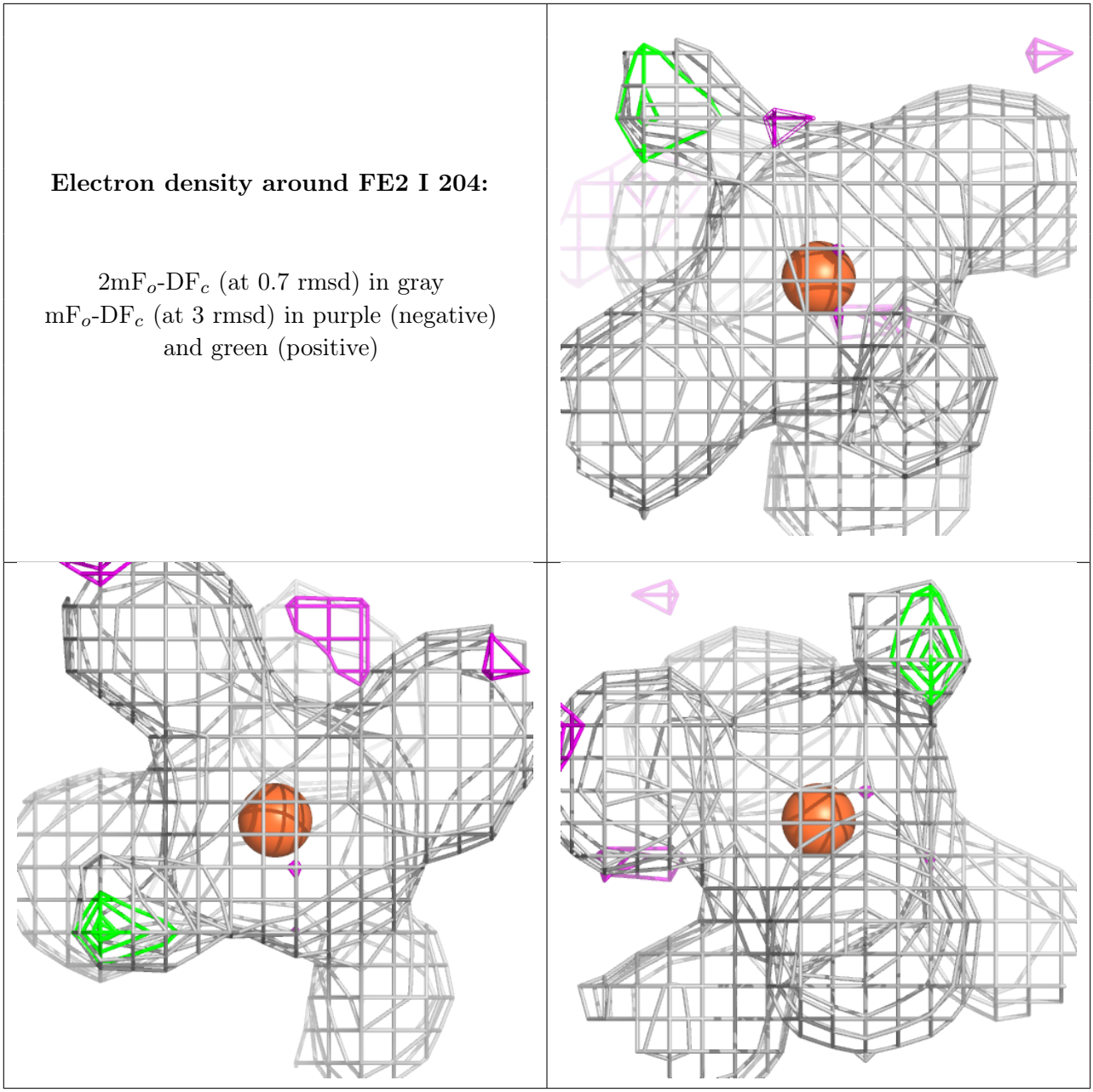
Electron density around FE2 A 203:

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



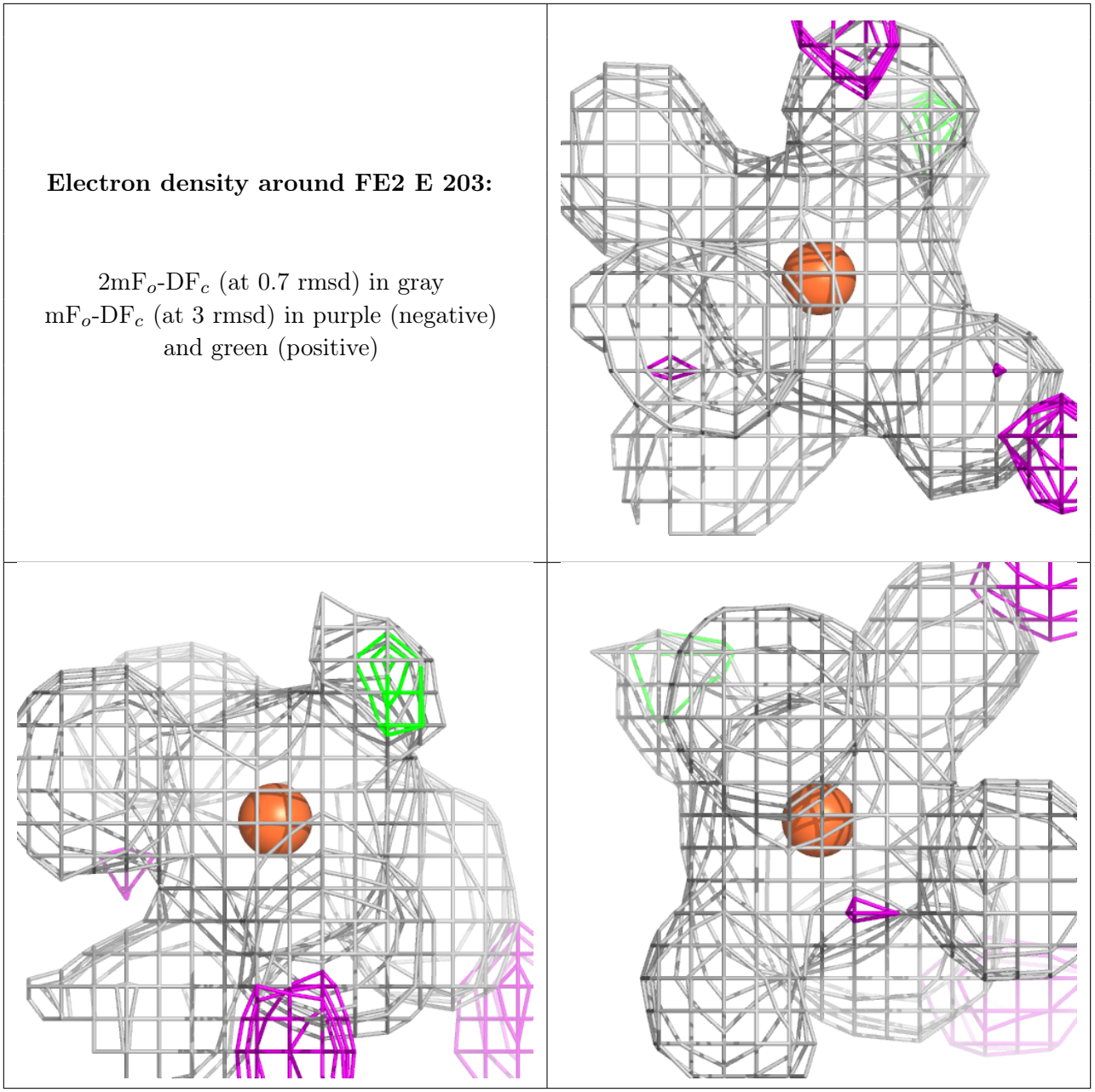
Electron density around FE2 I 204:

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



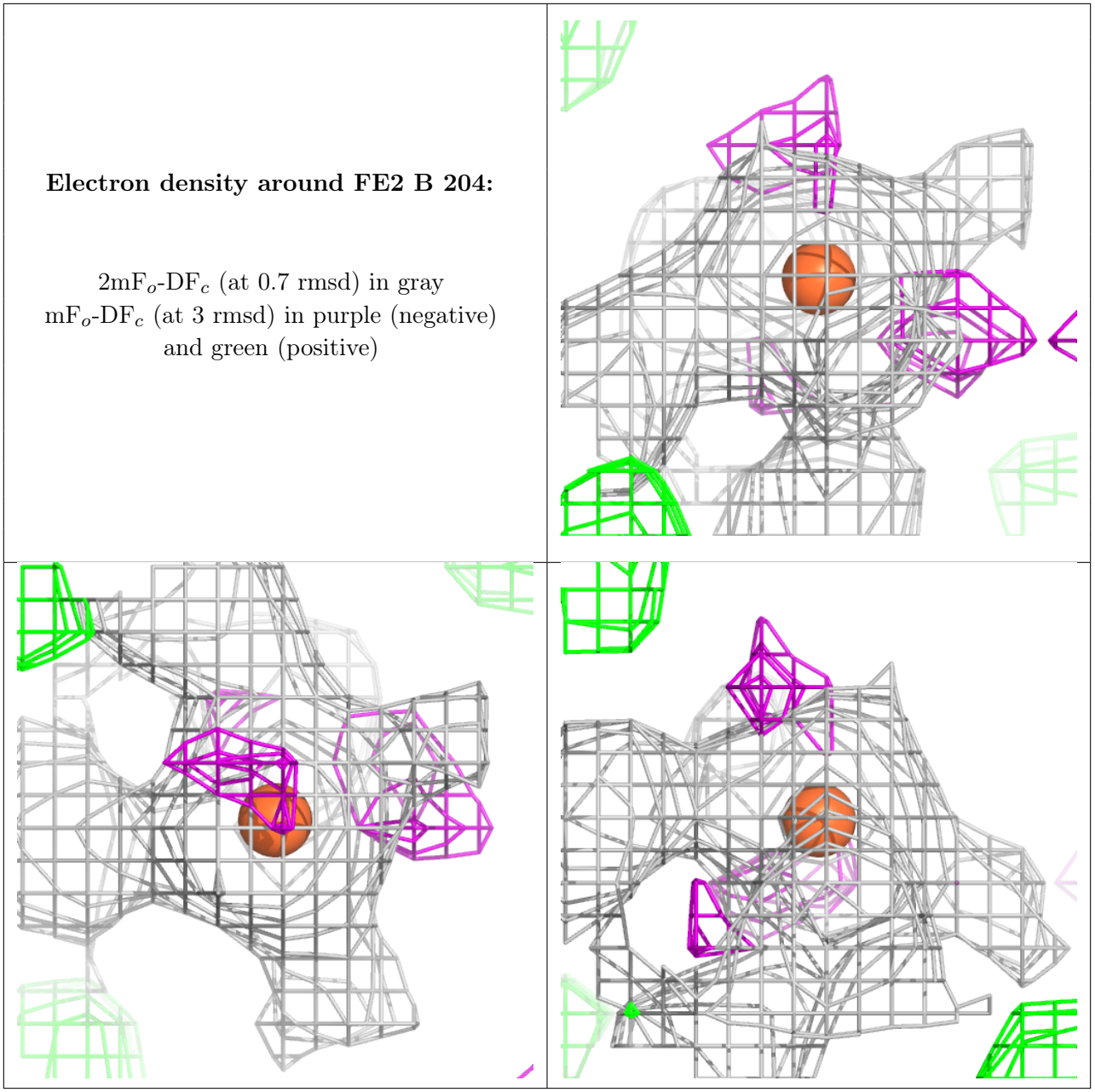
Electron density around FE2 E 203:

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



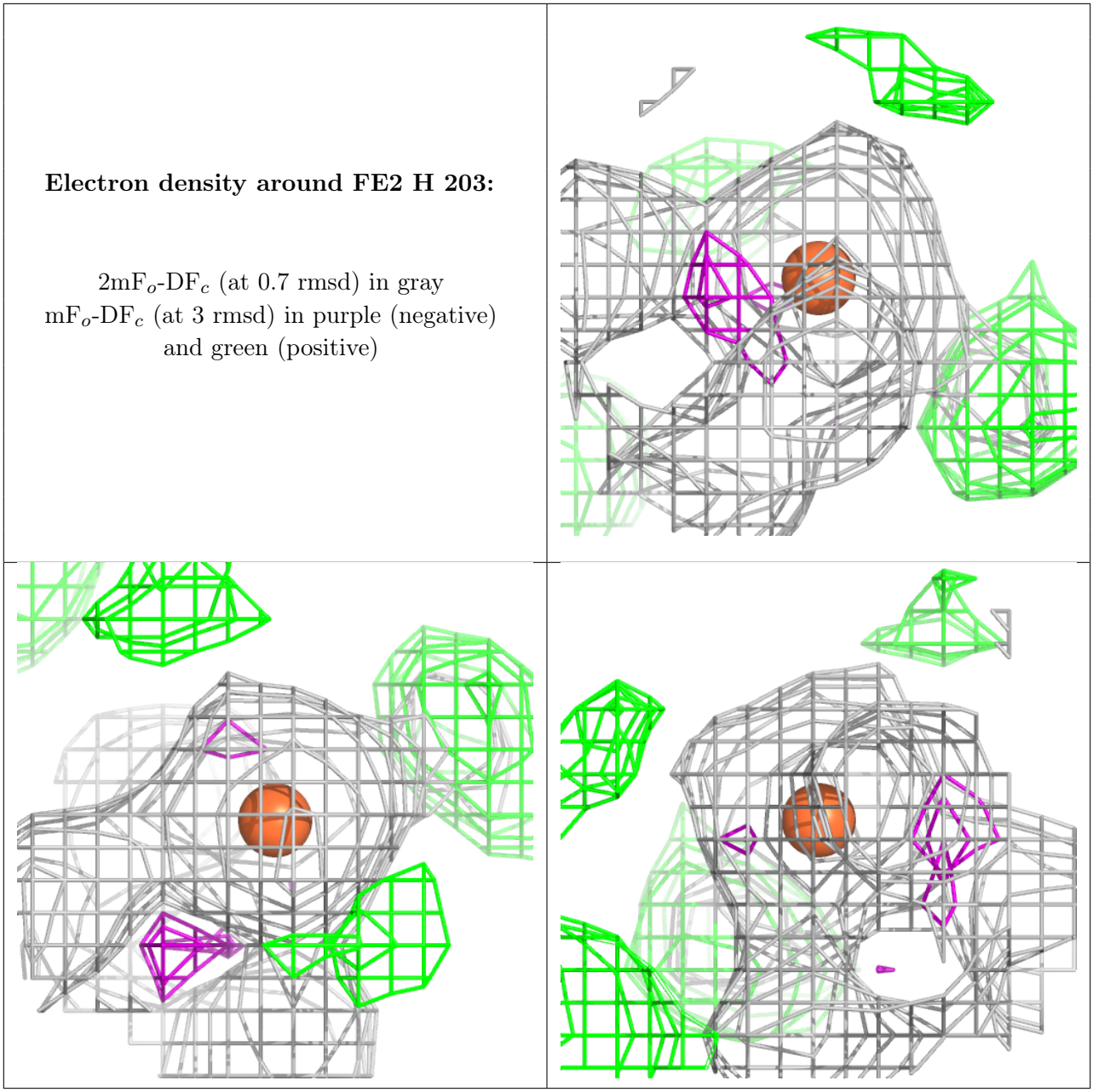
Electron density around FE2 B 204:

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



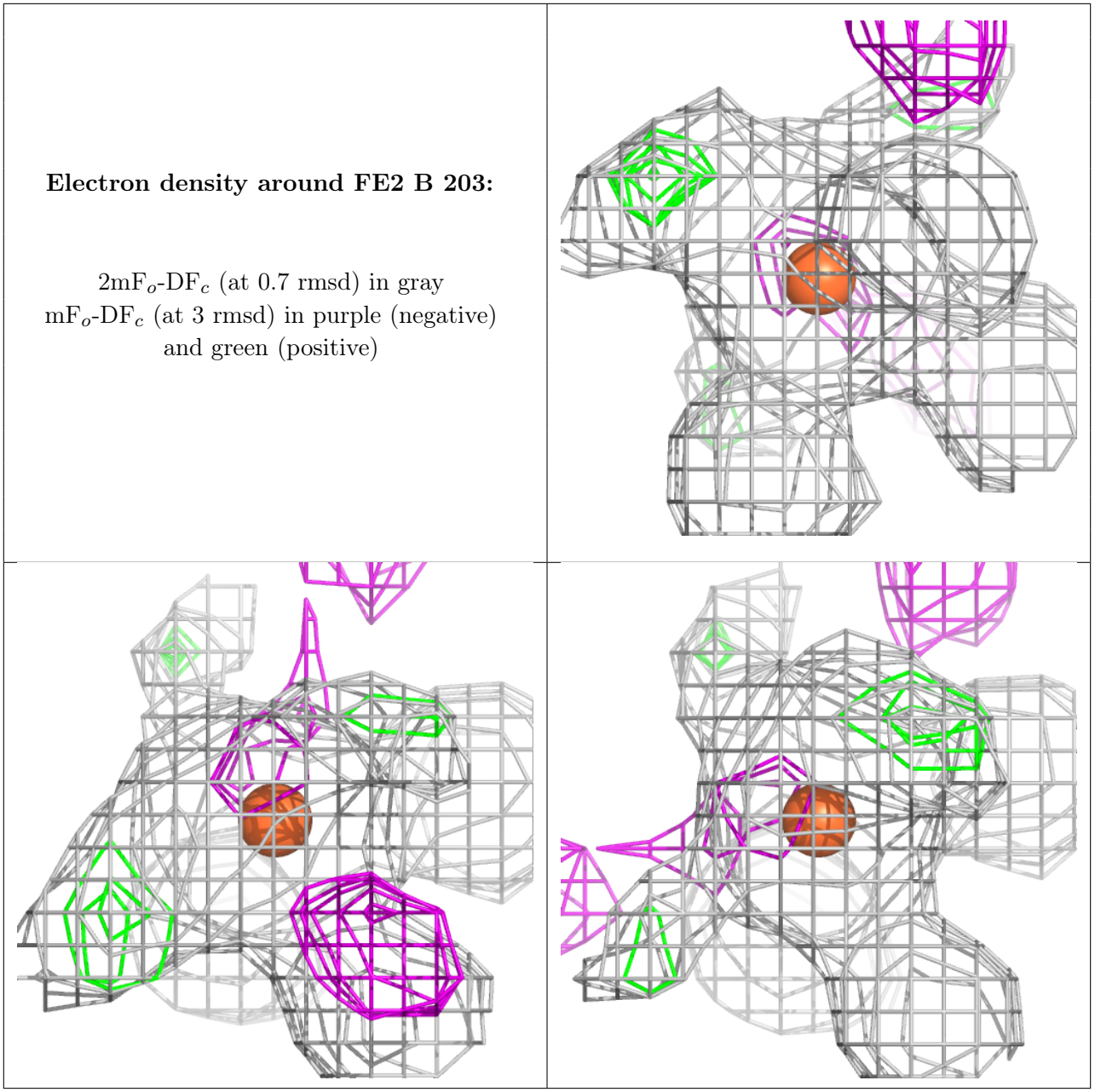
Electron density around FE2 H 203:

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



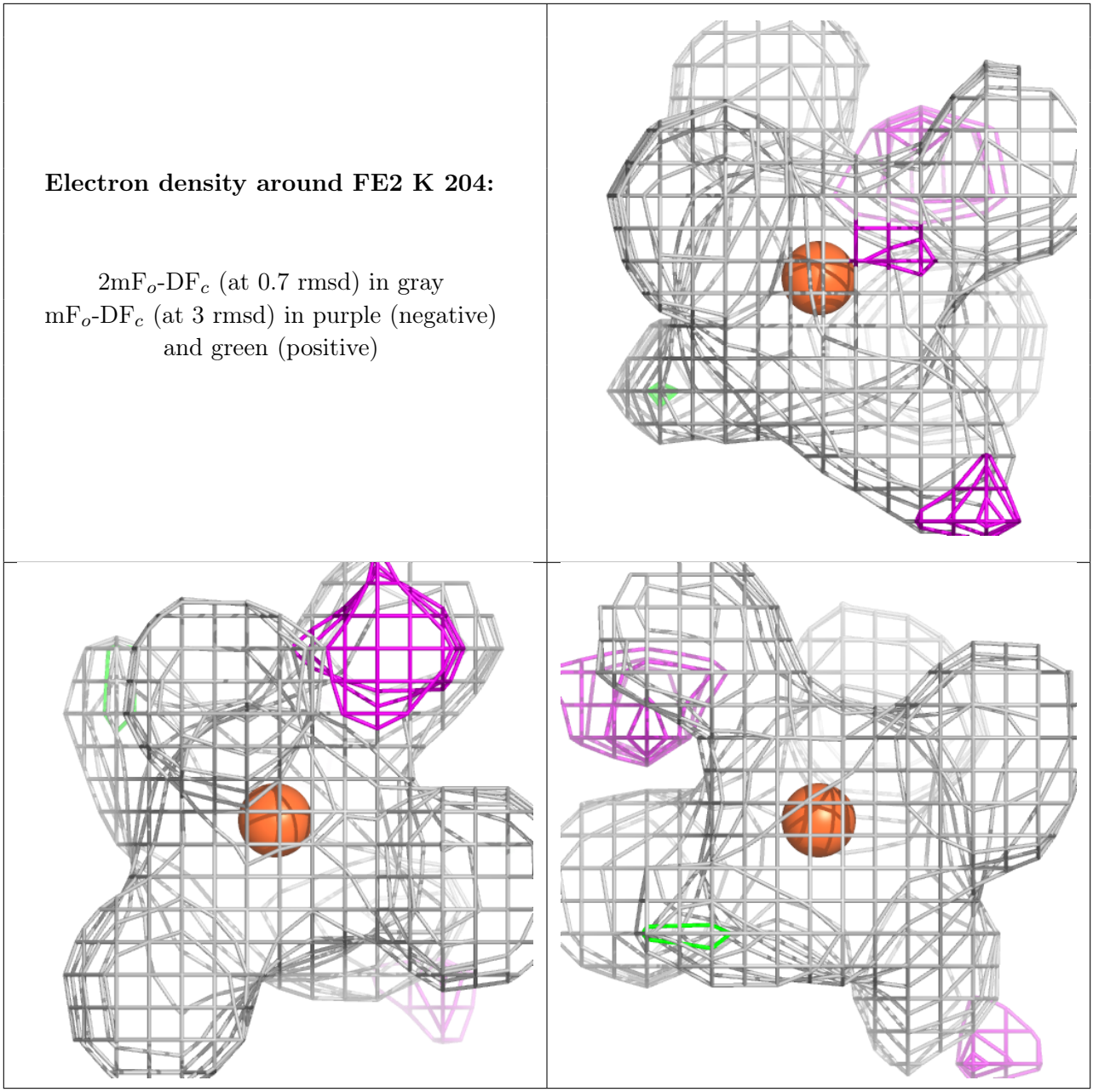
Electron density around FE2 B 203:

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



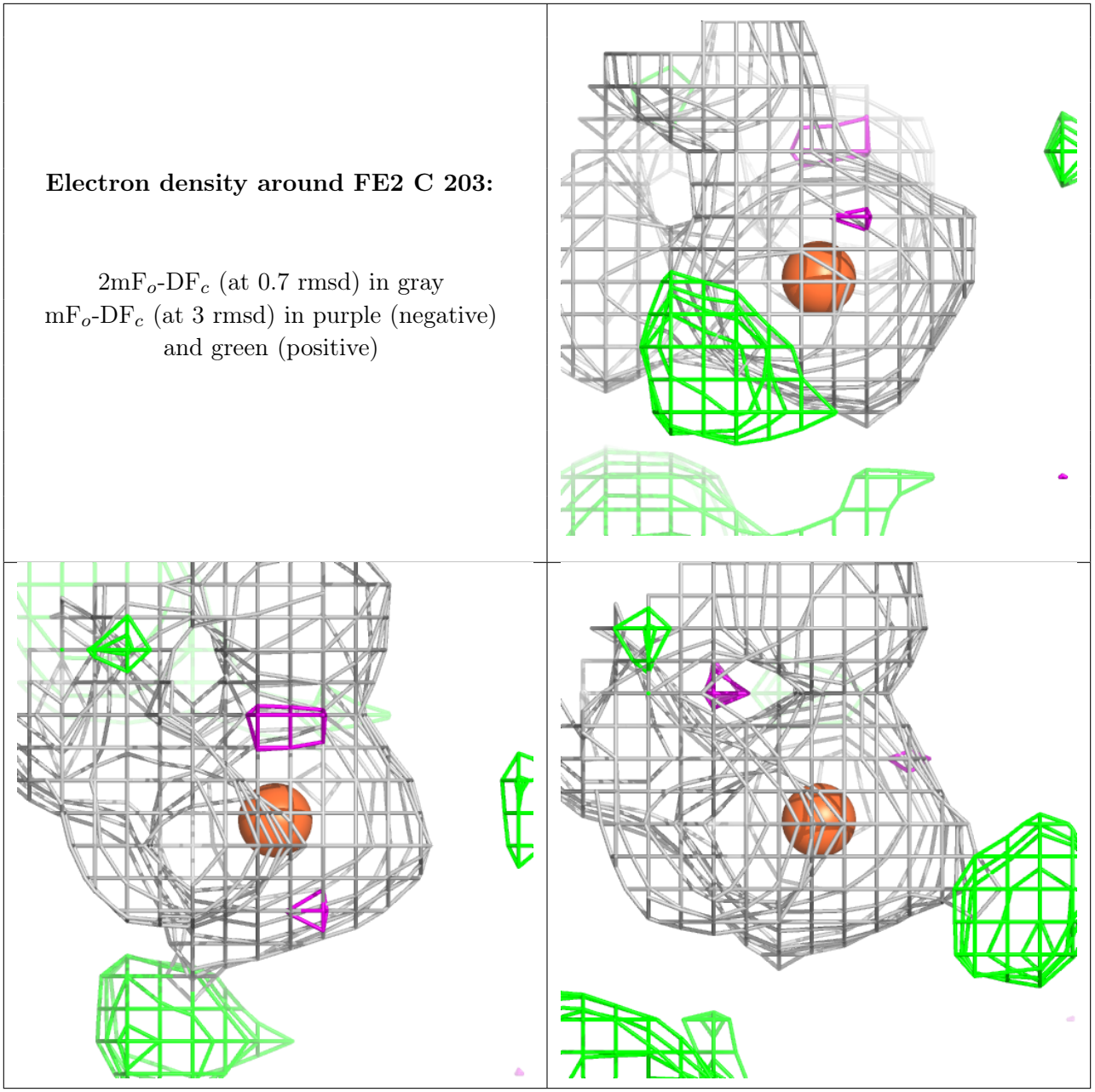
Electron density around FE2 K 204:

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



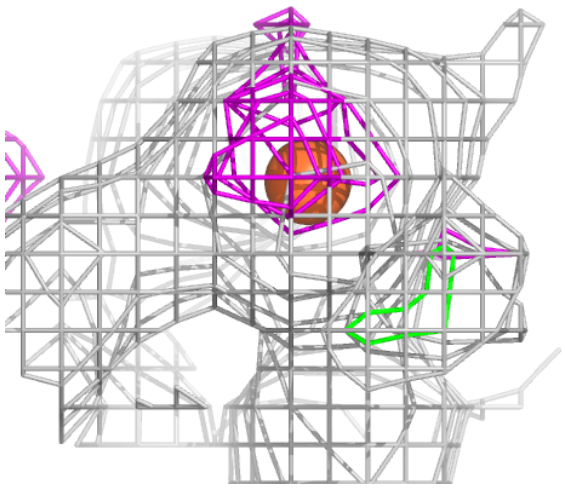
Electron density around FE2 C 203:

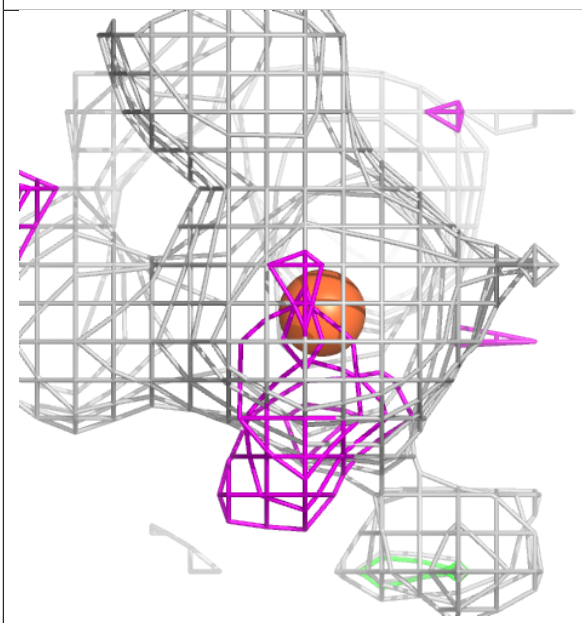
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

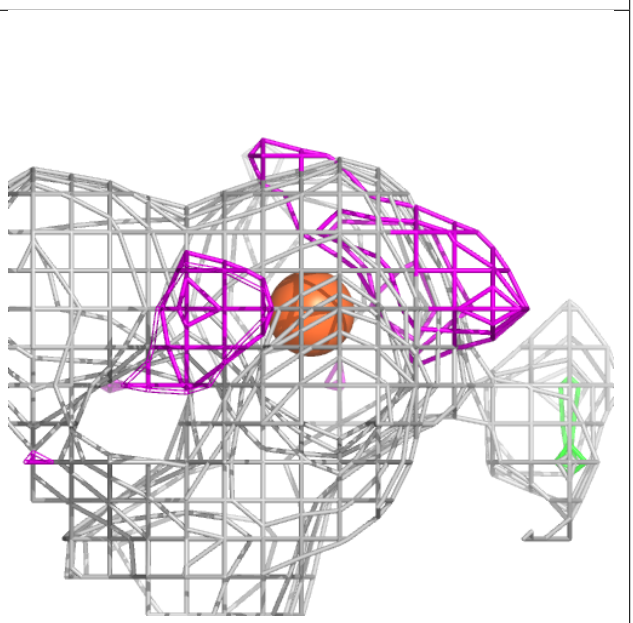


Electron density around FE2 I 202:

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

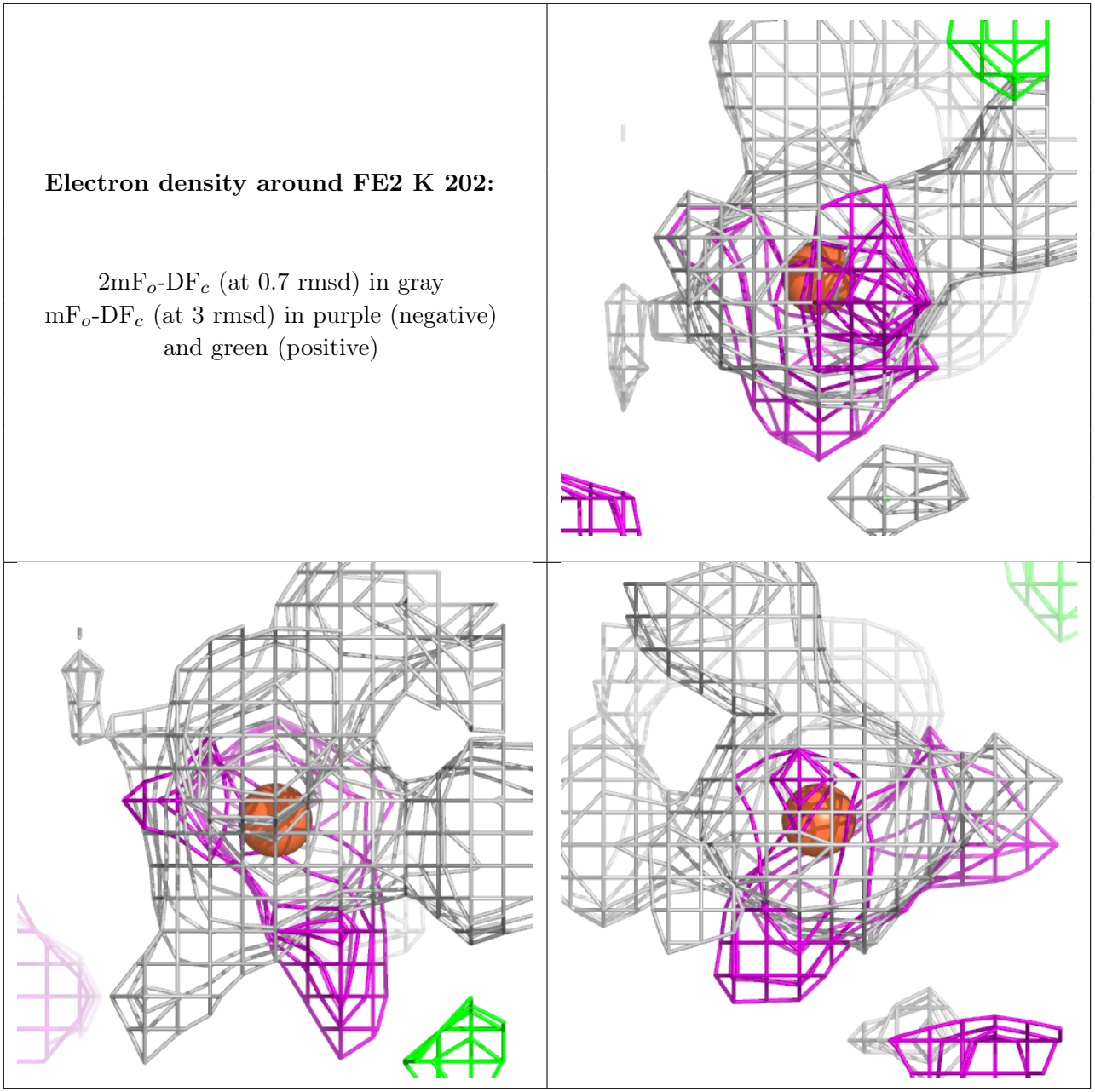






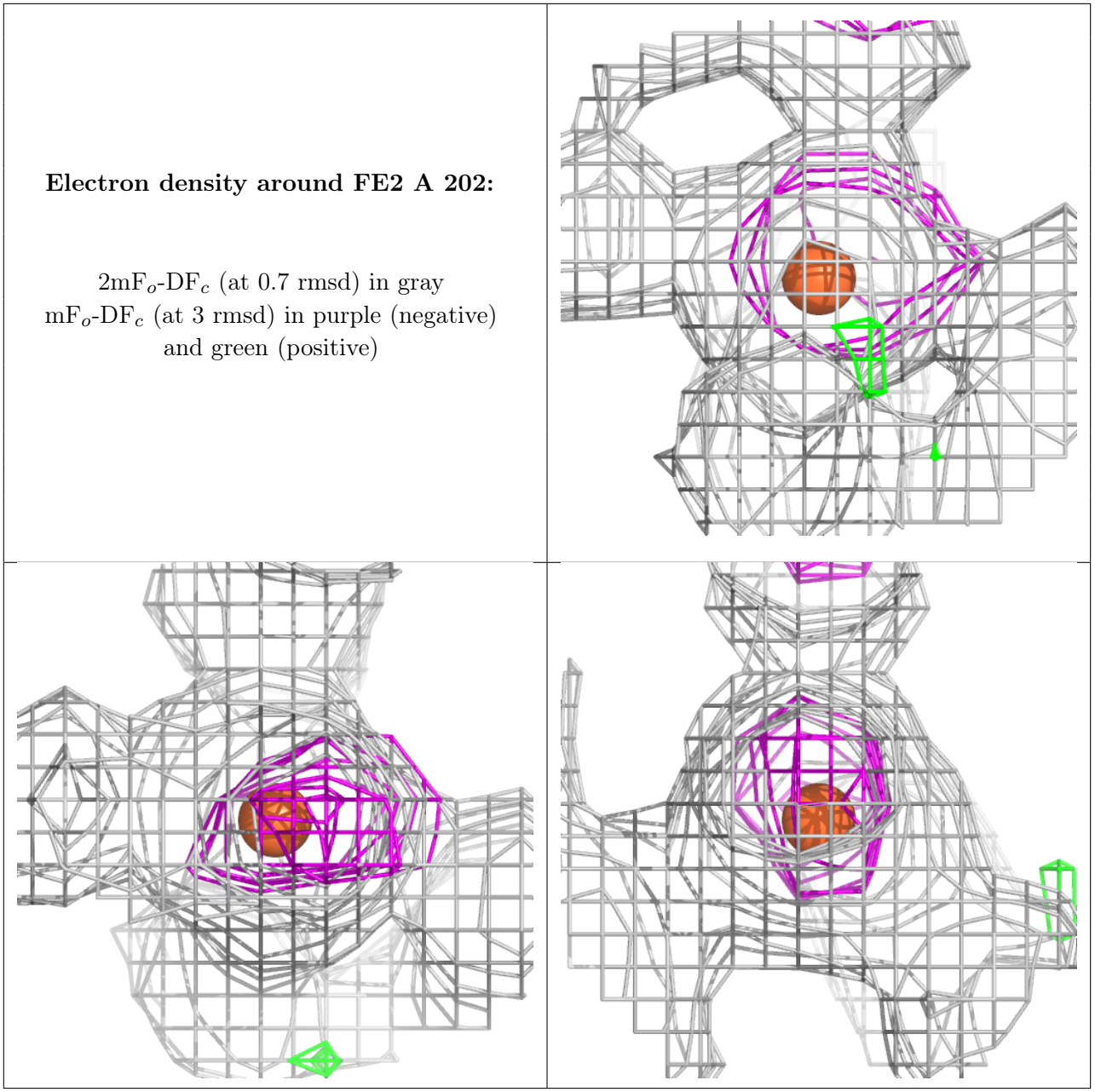
Electron density around FE2 K 202:

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



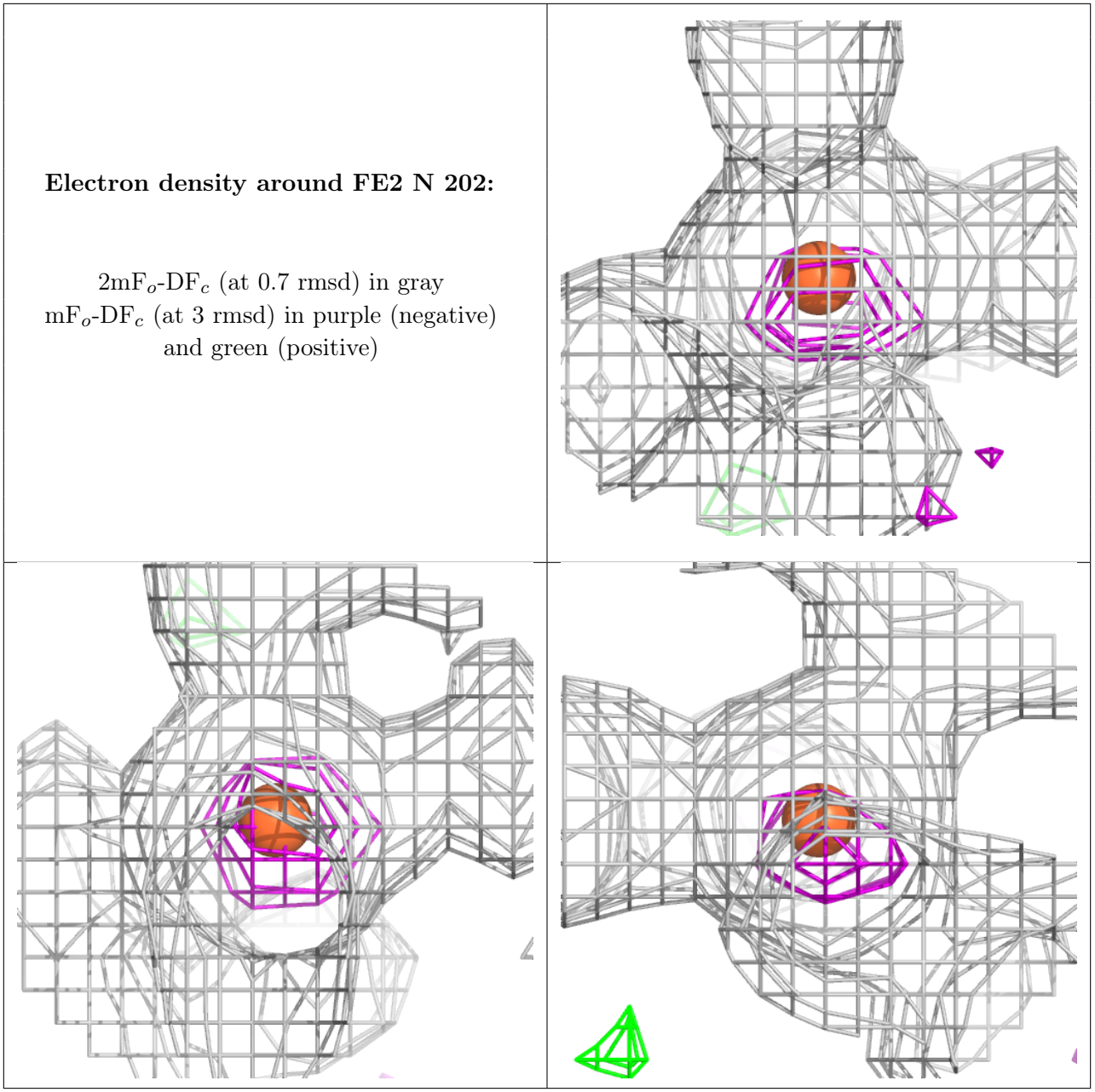
Electron density around FE2 A 202:

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



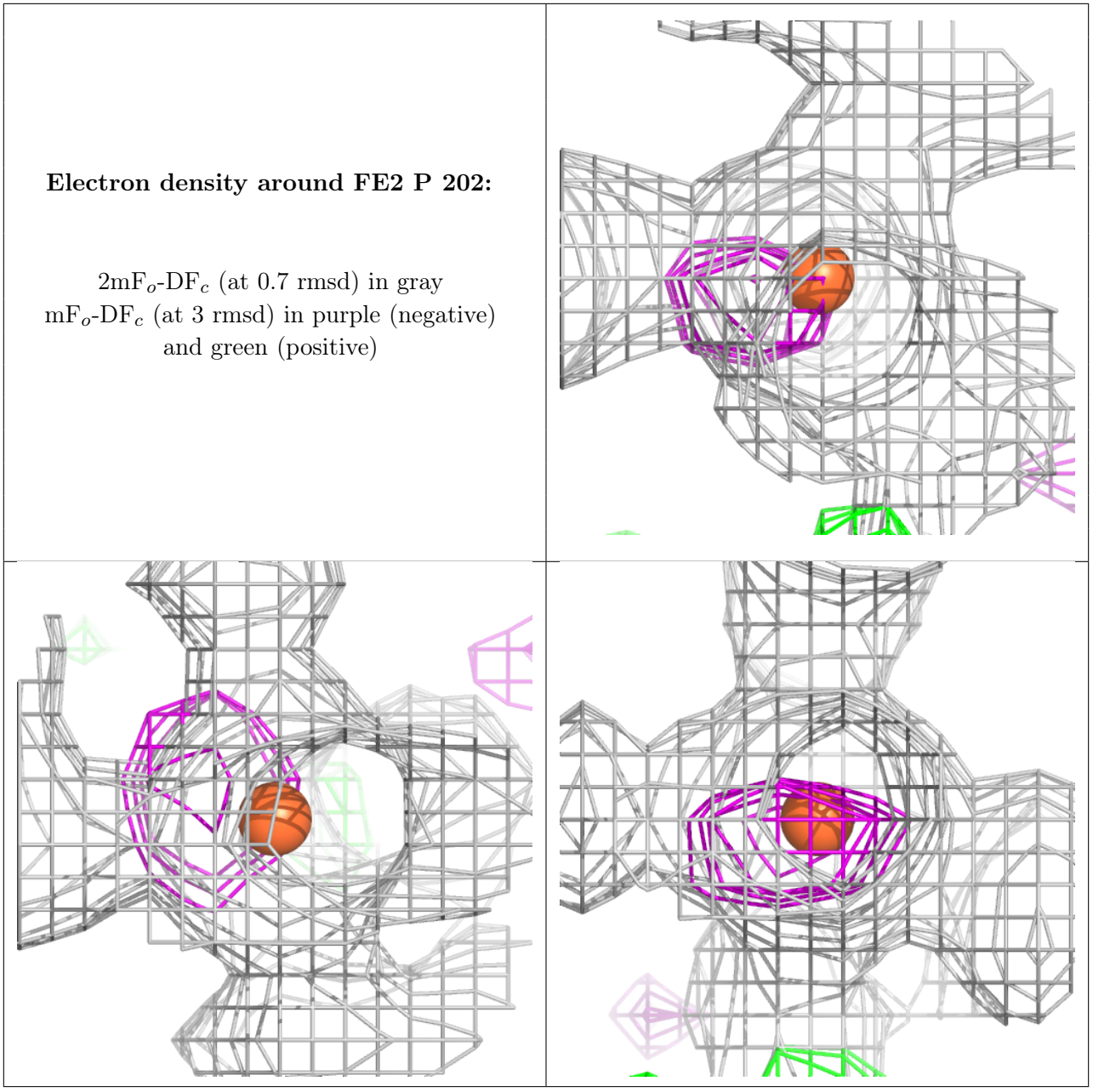
Electron density around FE2 N 202:

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



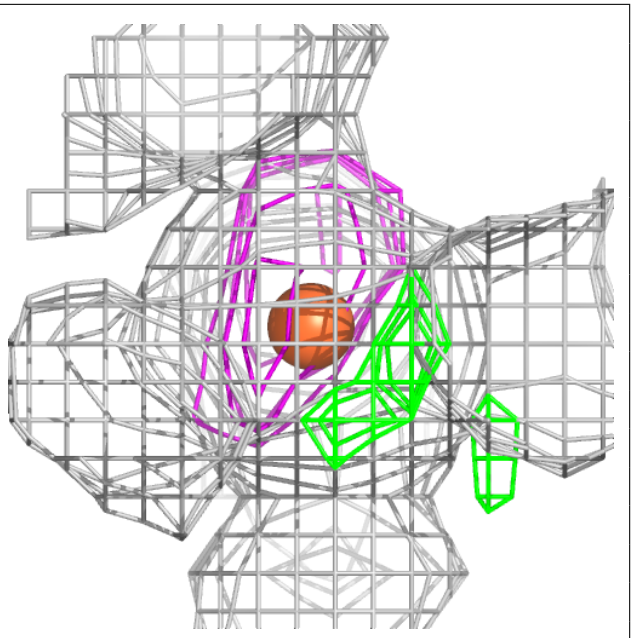
Electron density around FE2 P 202:

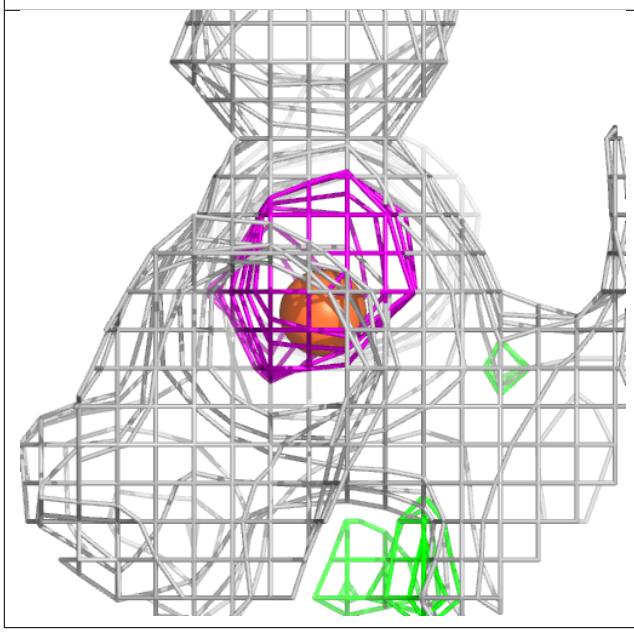
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

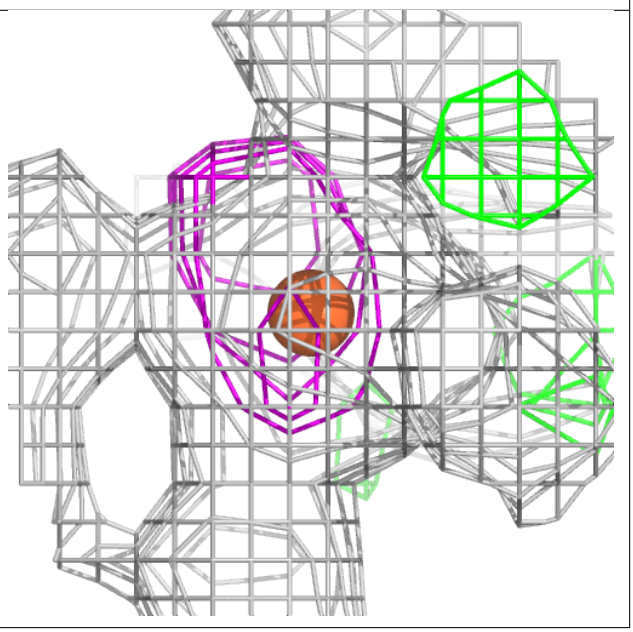


Electron density around FE2 C 202:

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

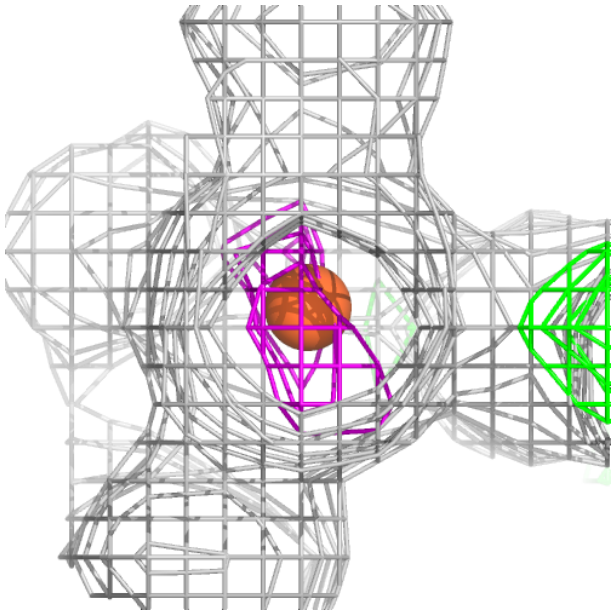


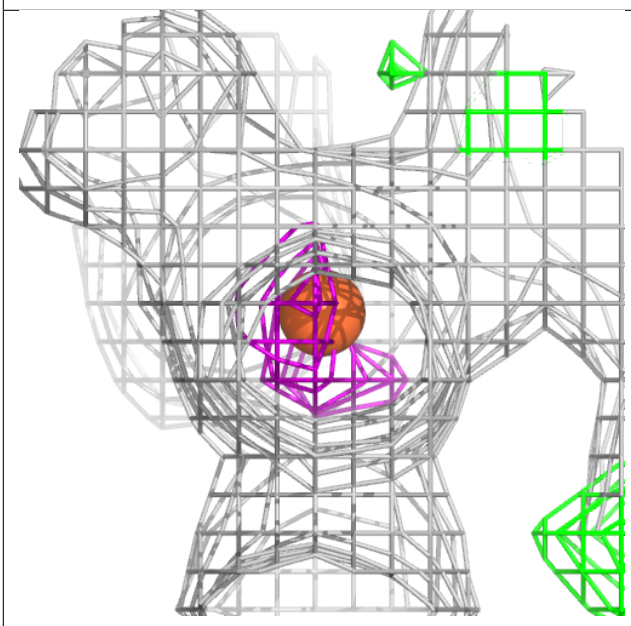


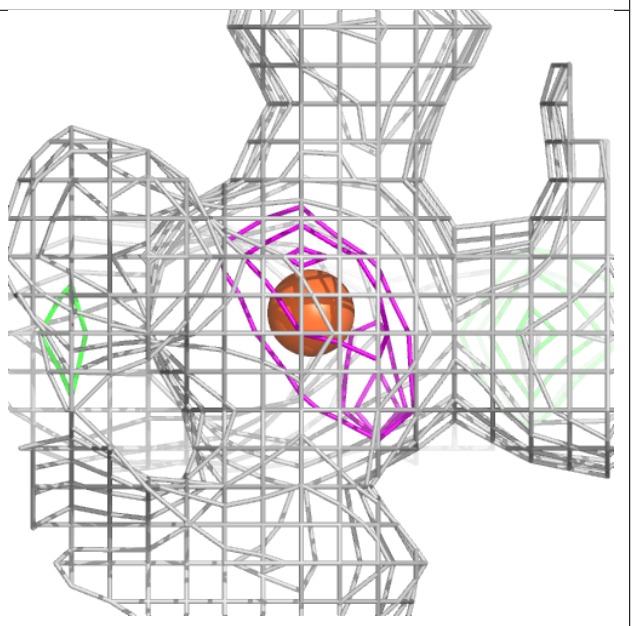


Electron density around FE2 F 202:

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

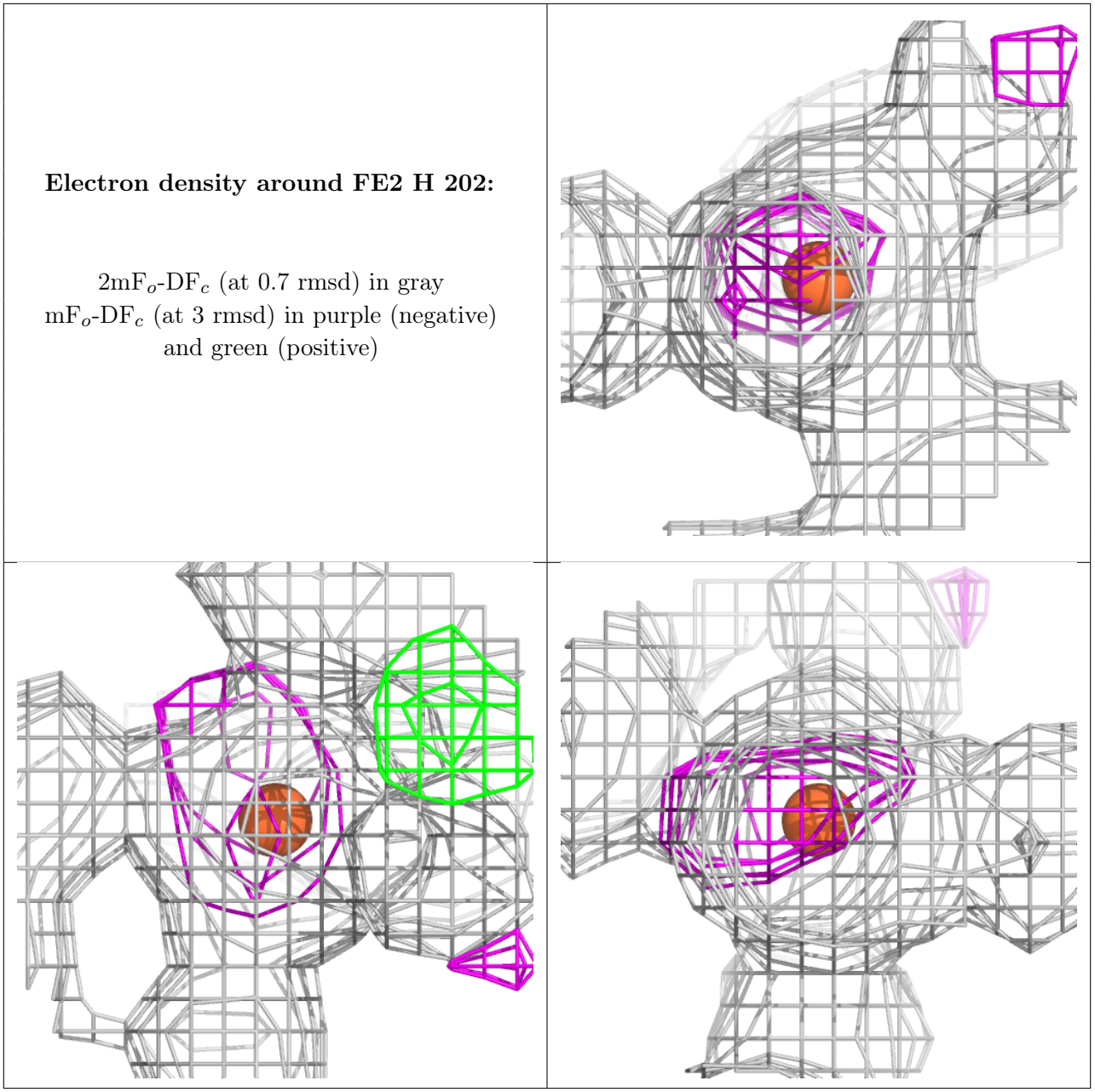






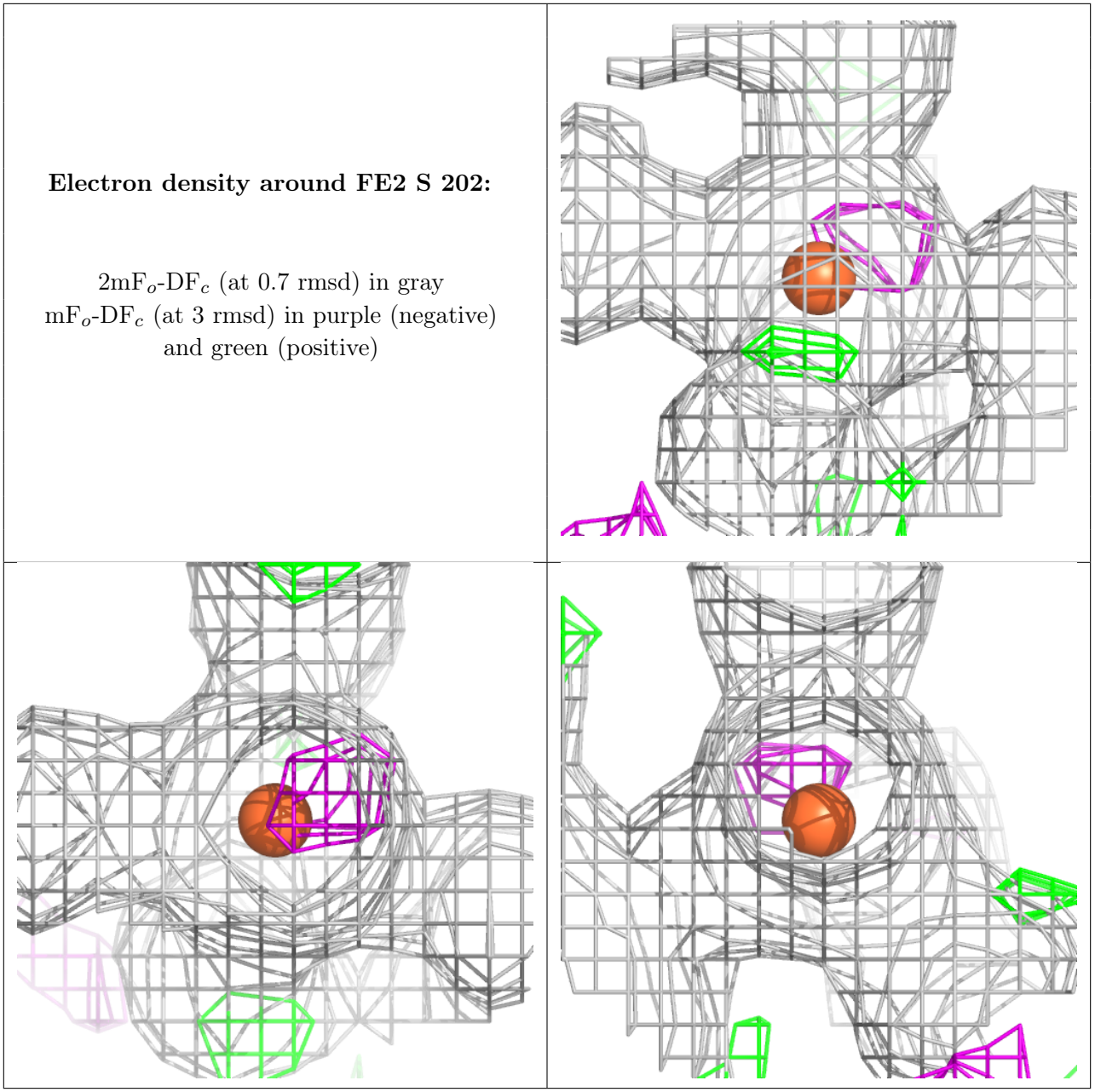
Electron density around FE2 H 202:

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



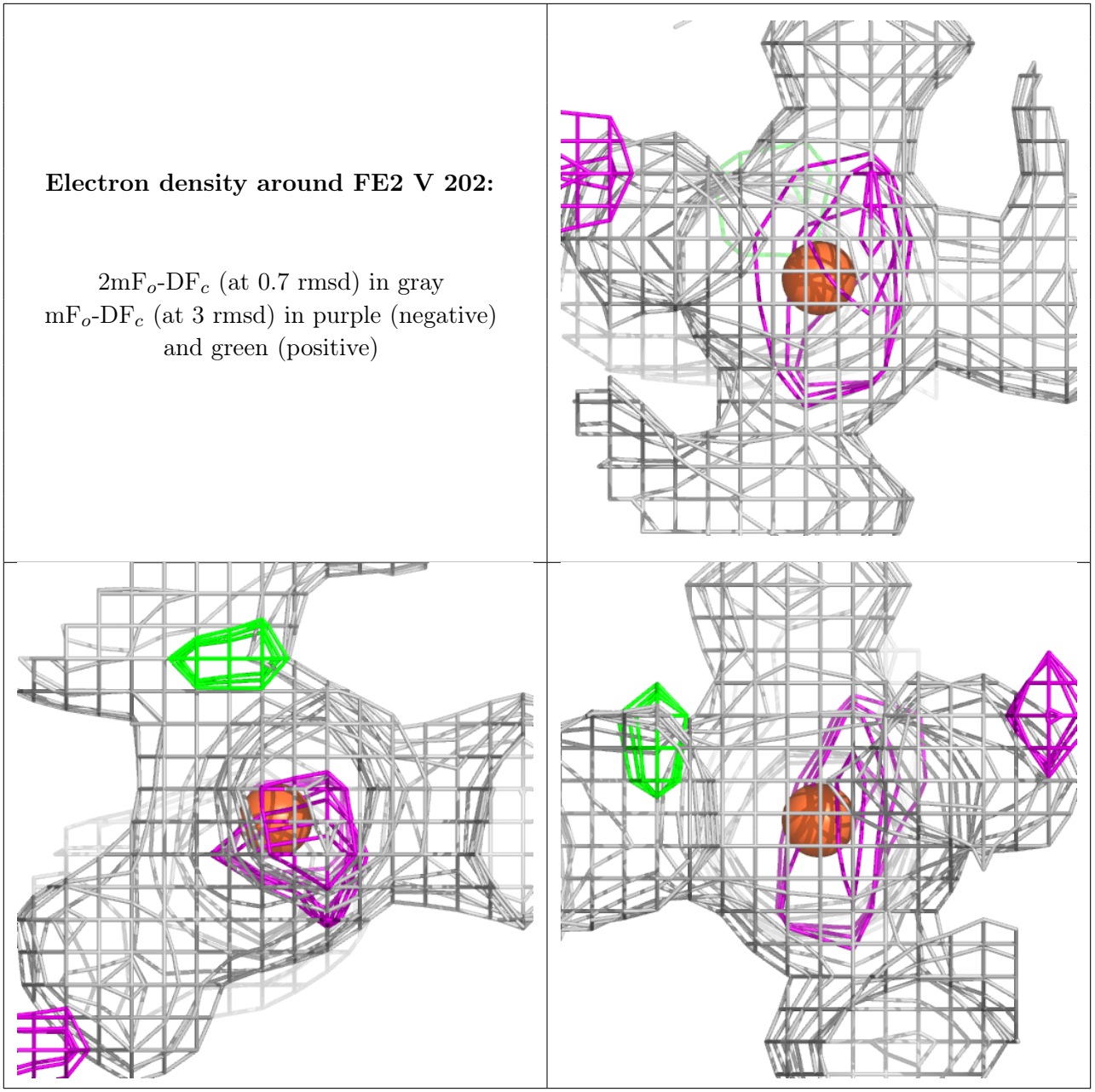
Electron density around FE2 S 202:

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



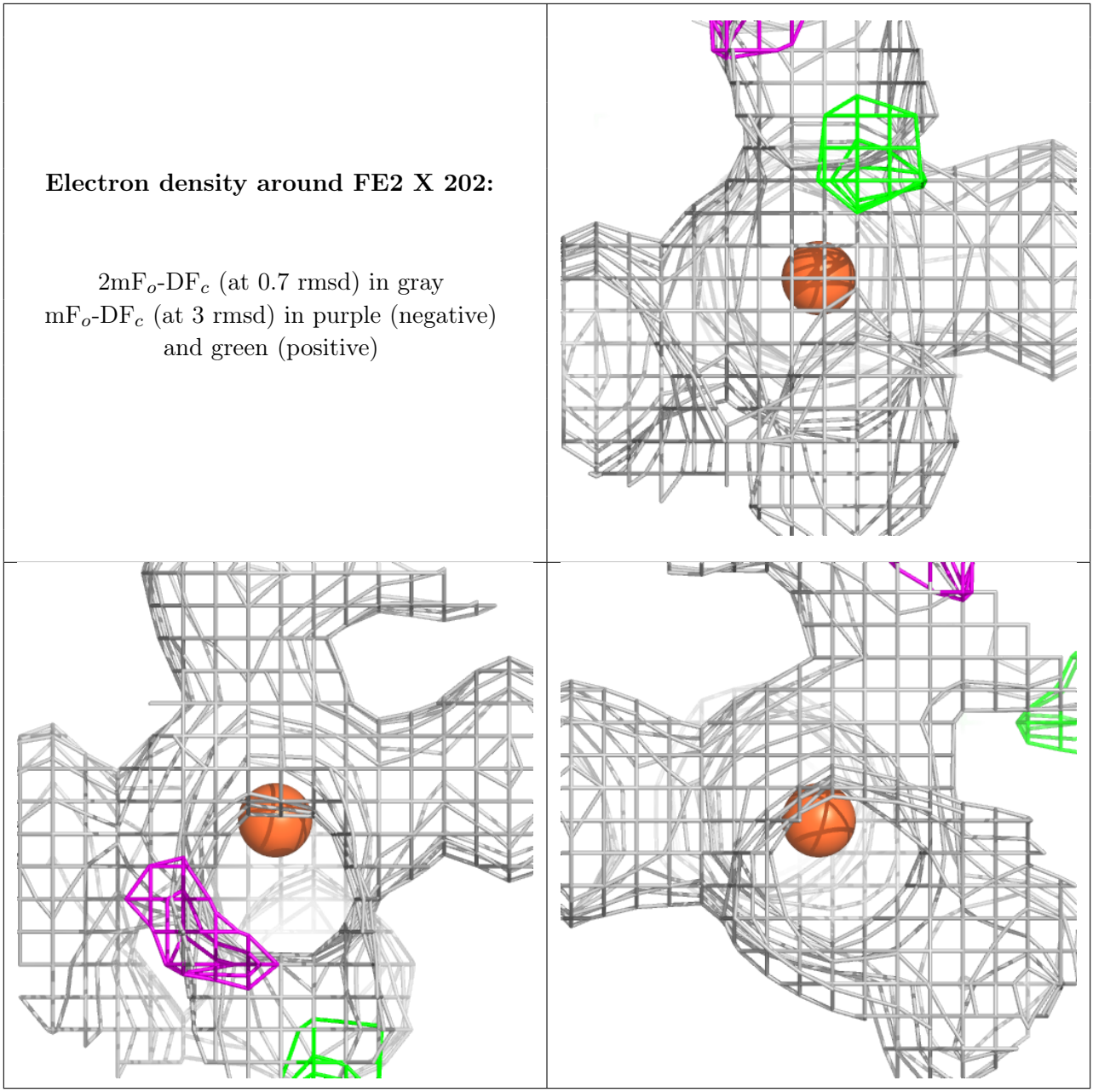
Electron density around FE2 V 202:

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



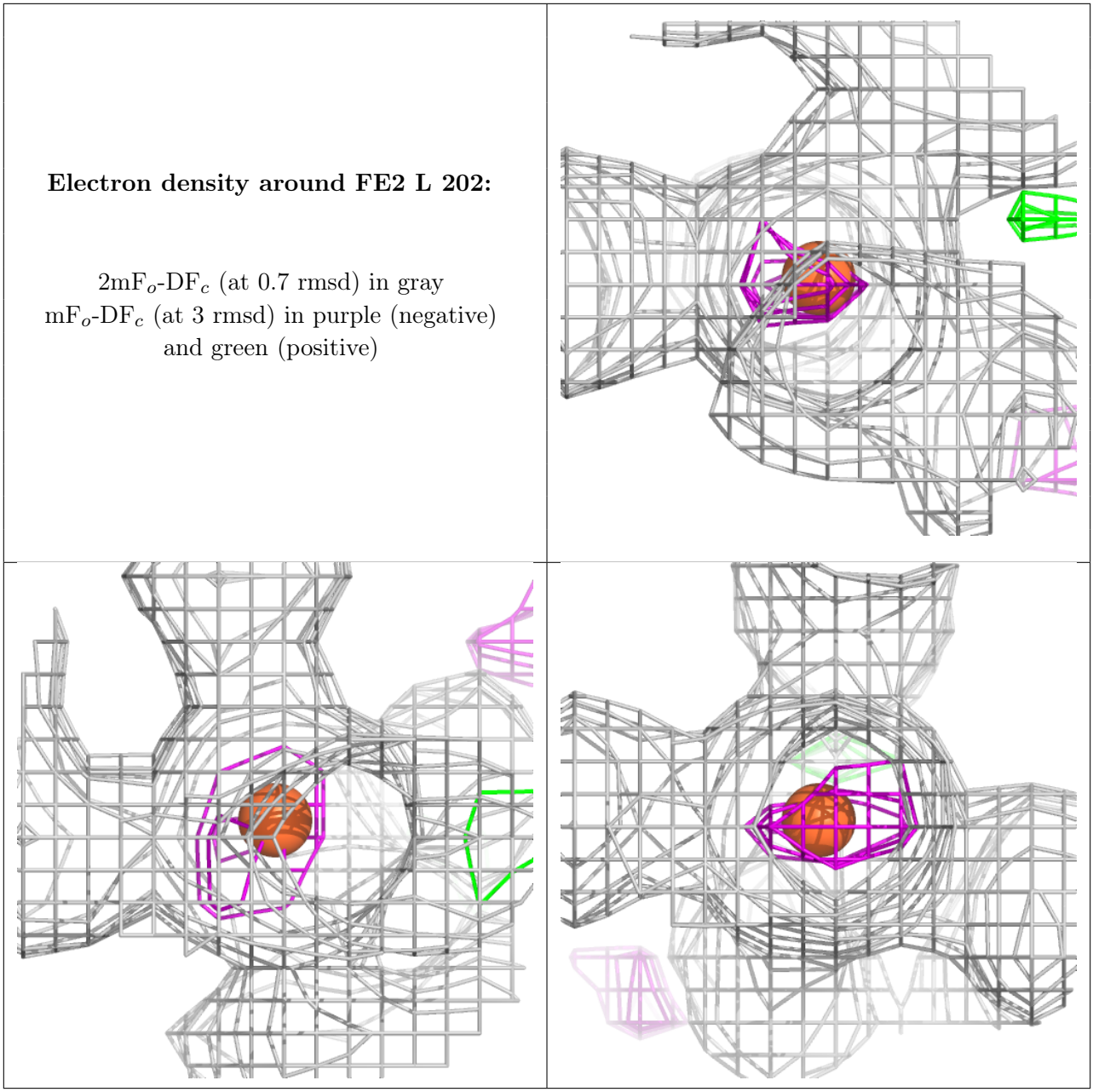
Electron density around FE2 X 202:

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



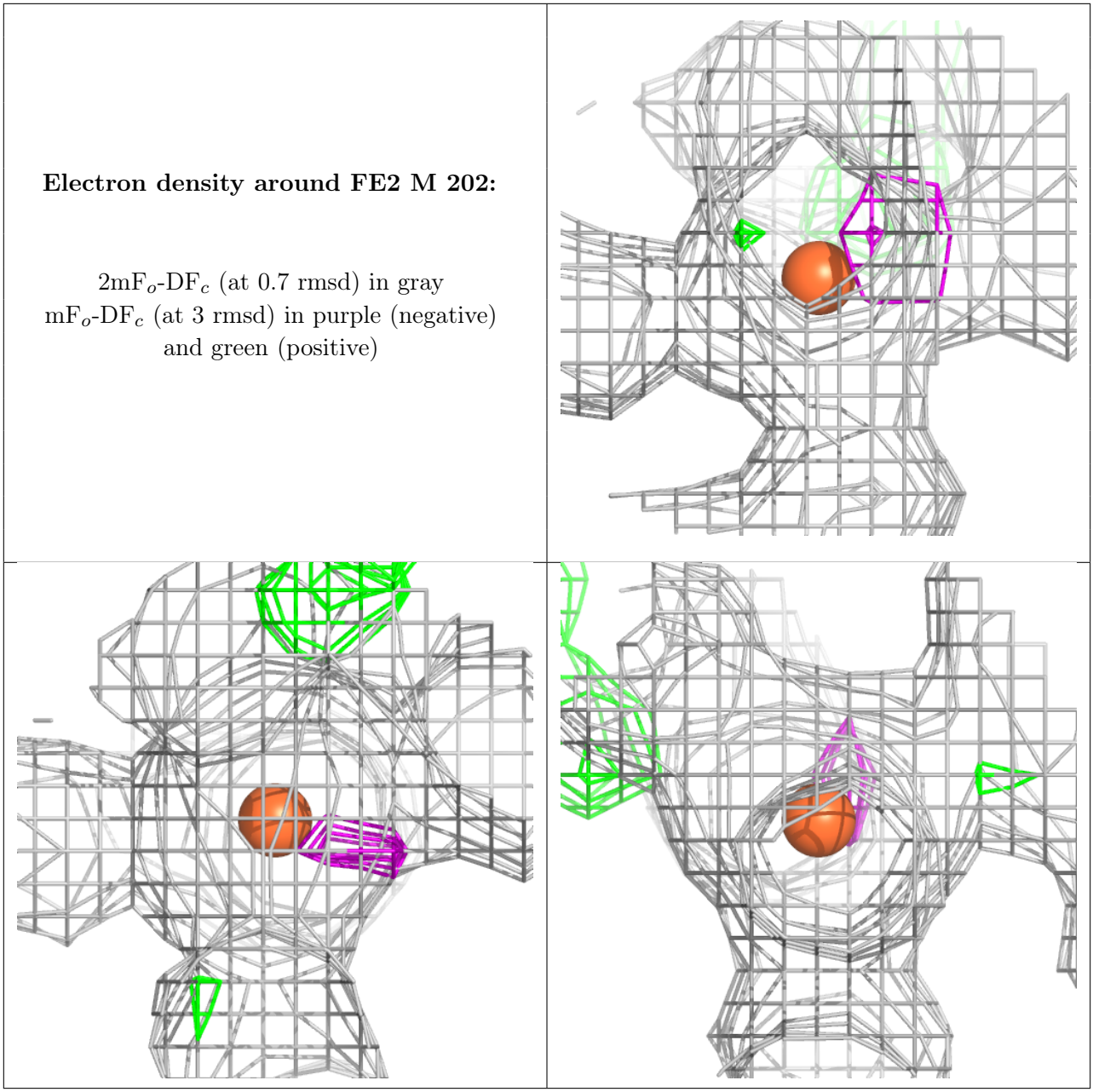
Electron density around FE2 L 202:

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



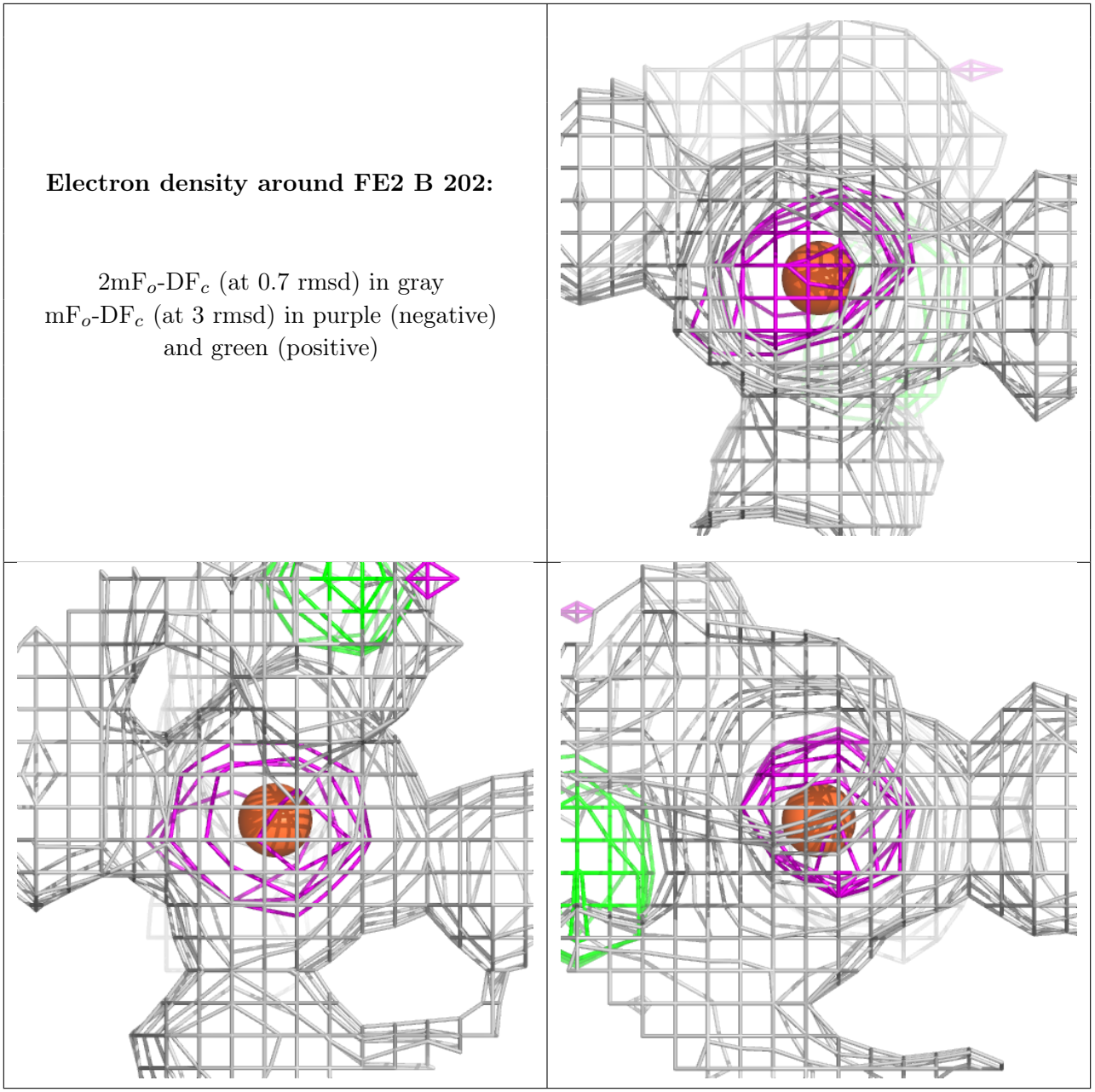
Electron density around FE2 M 202:

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



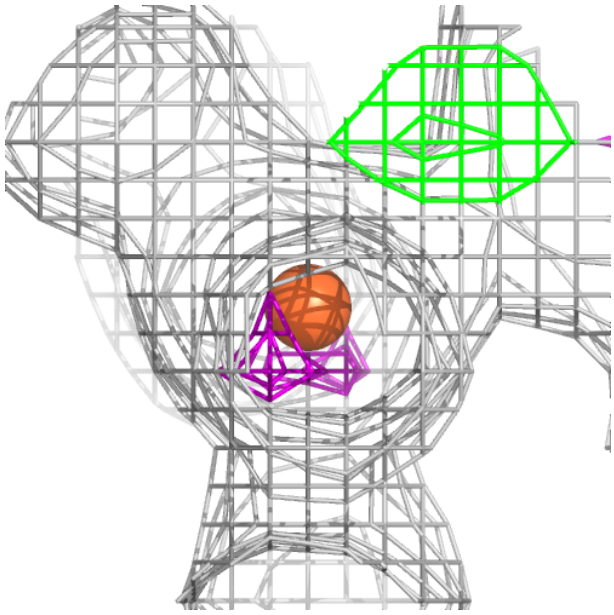
Electron density around FE2 B 202:

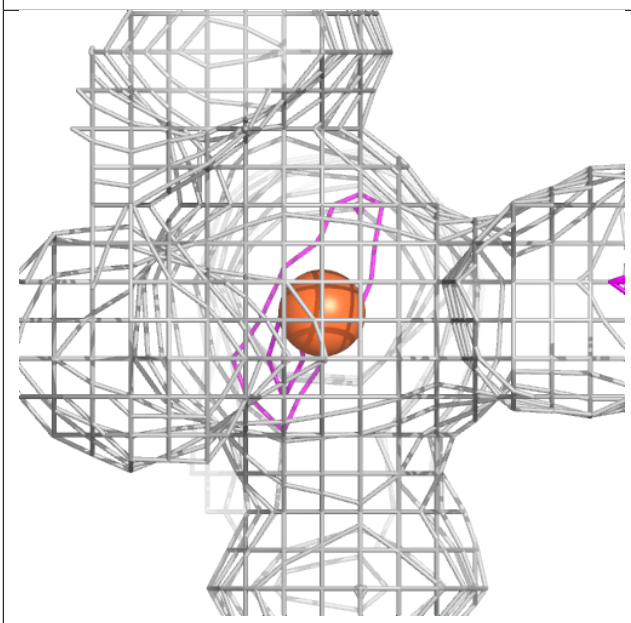
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

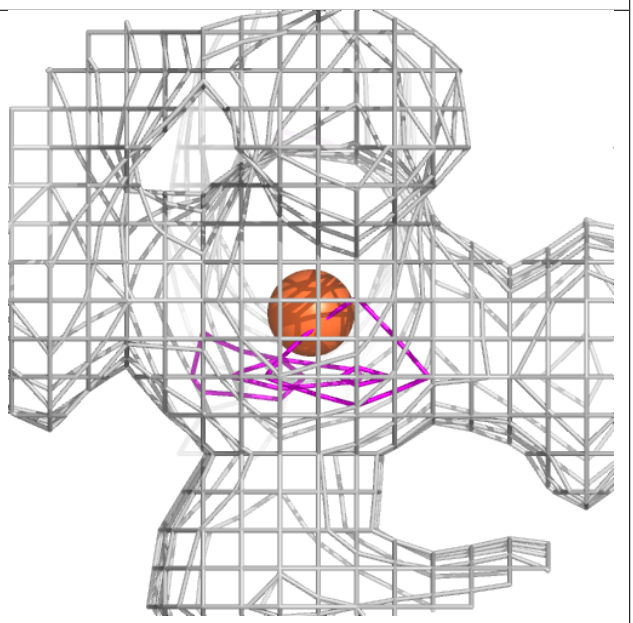


Electron density around FE2 O 202:

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

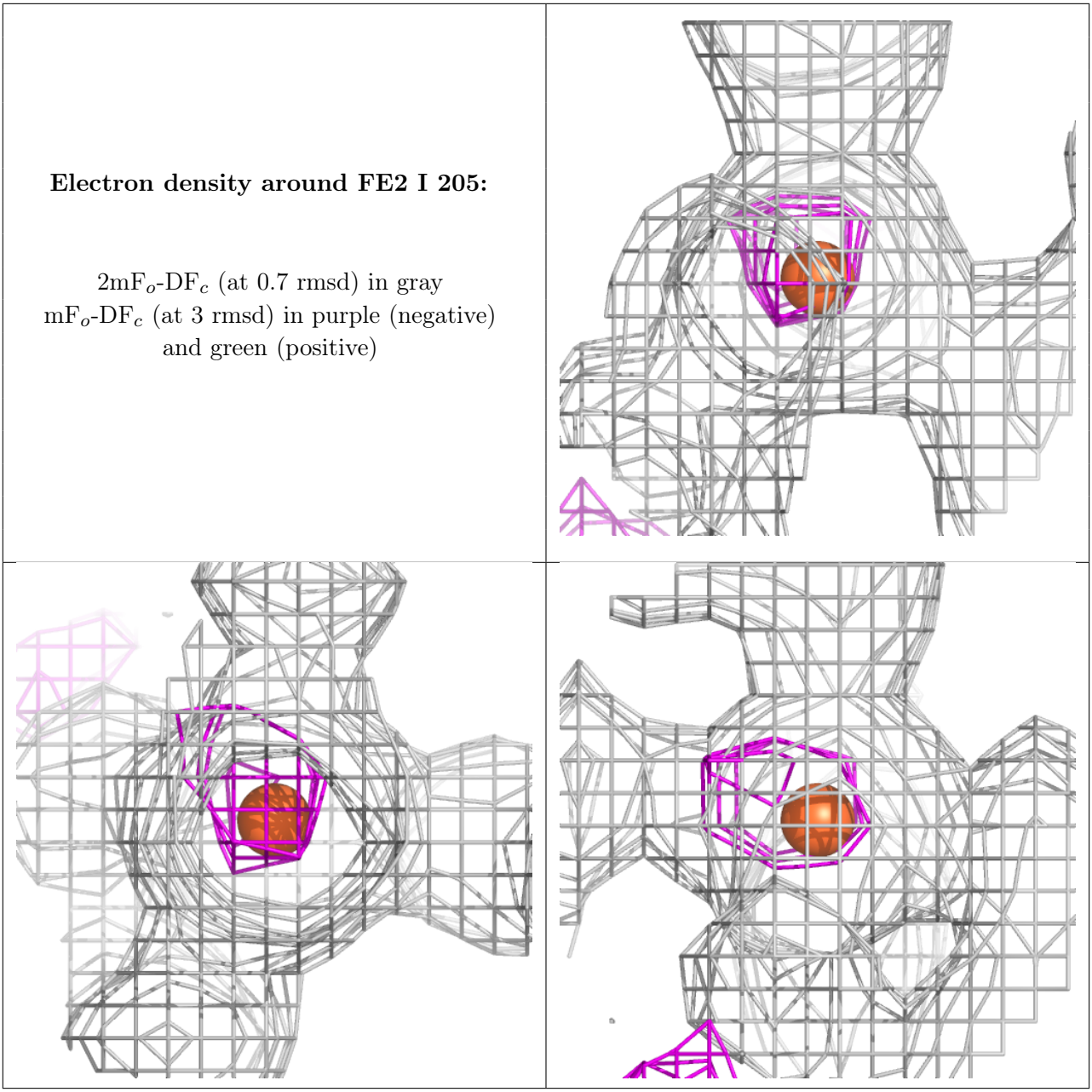






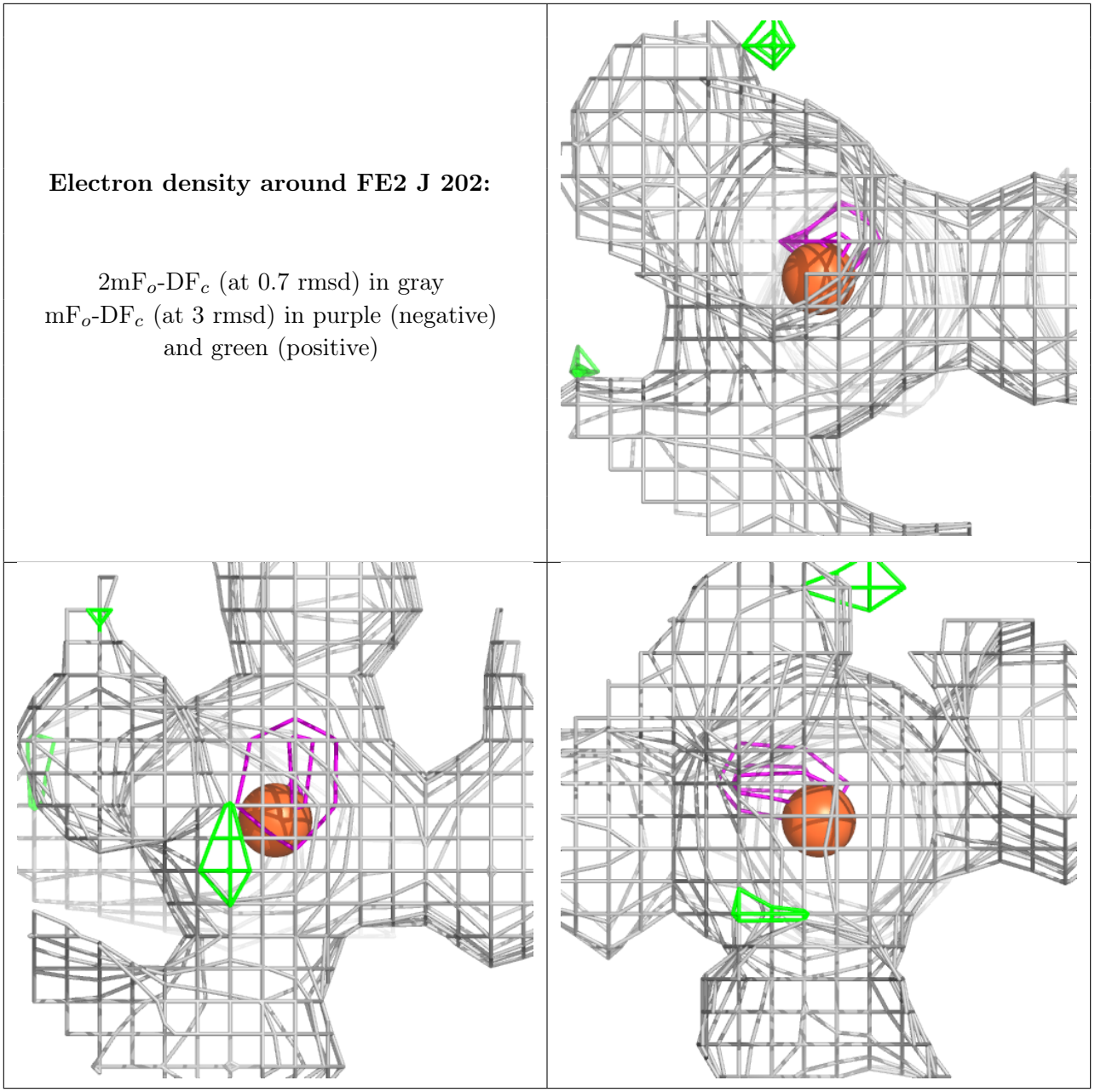
Electron density around FE2 I 205:

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



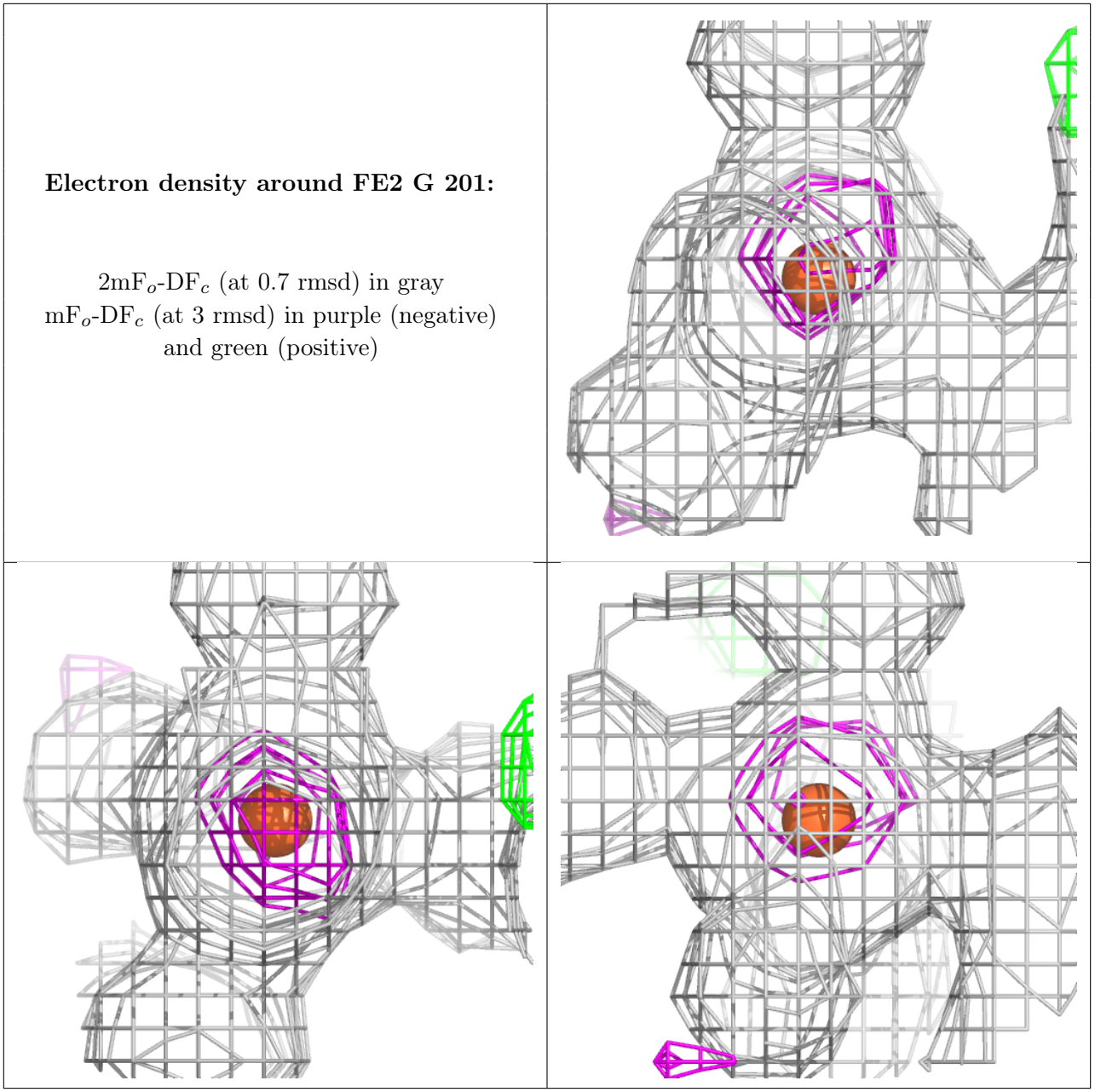
Electron density around FE2 J 202:

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



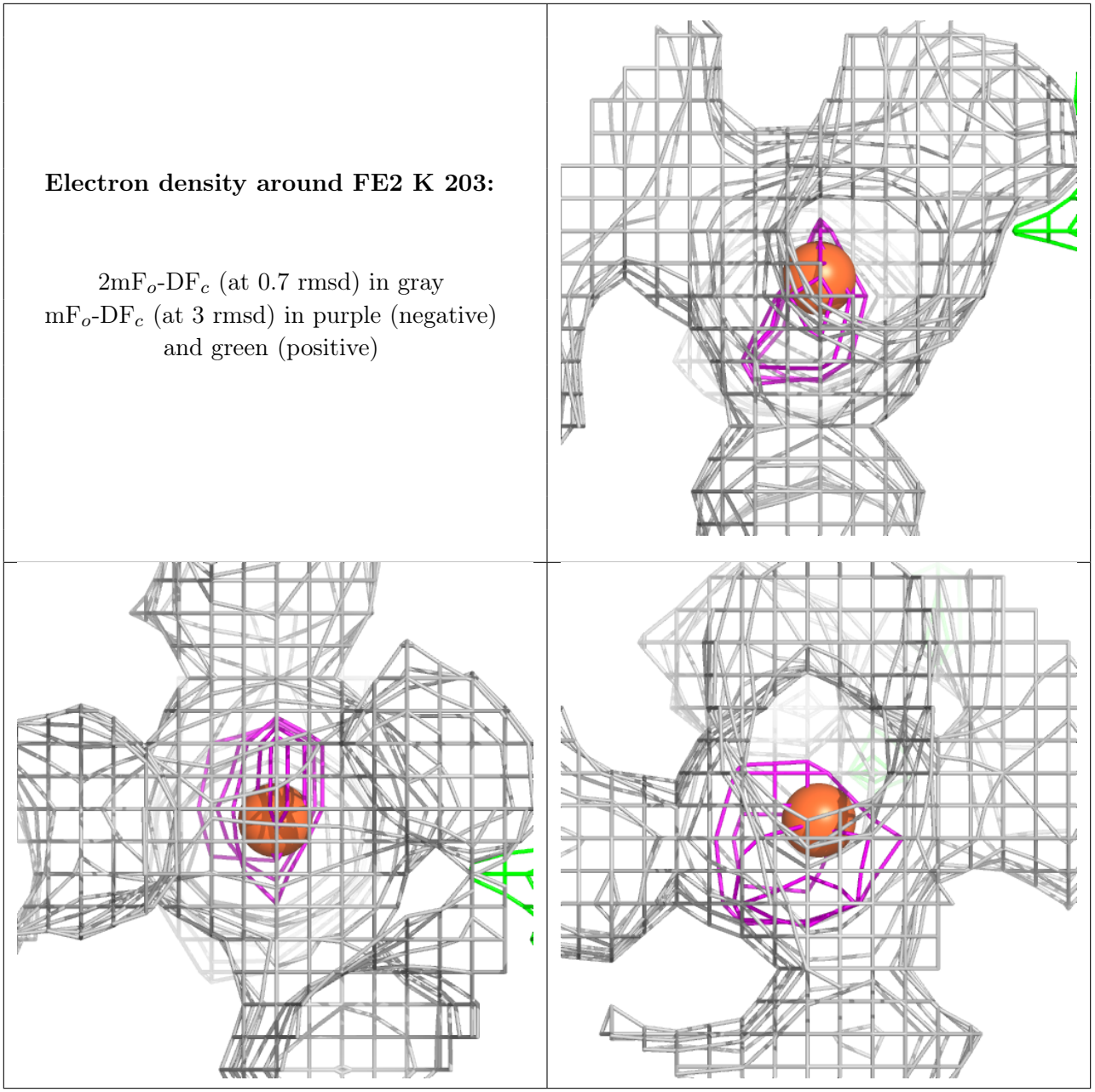
Electron density around FE2 G 201:

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



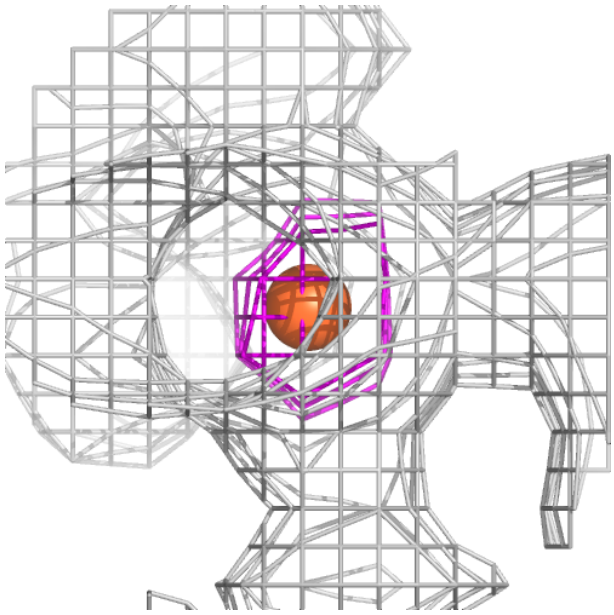
Electron density around FE2 K 203:

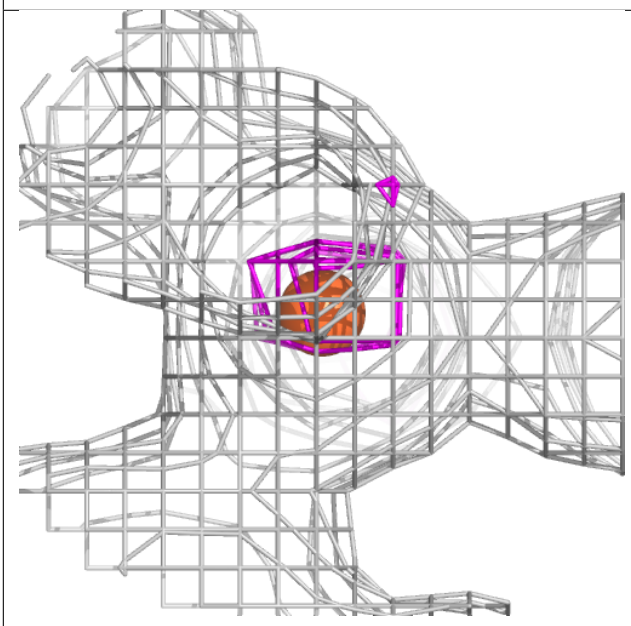
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

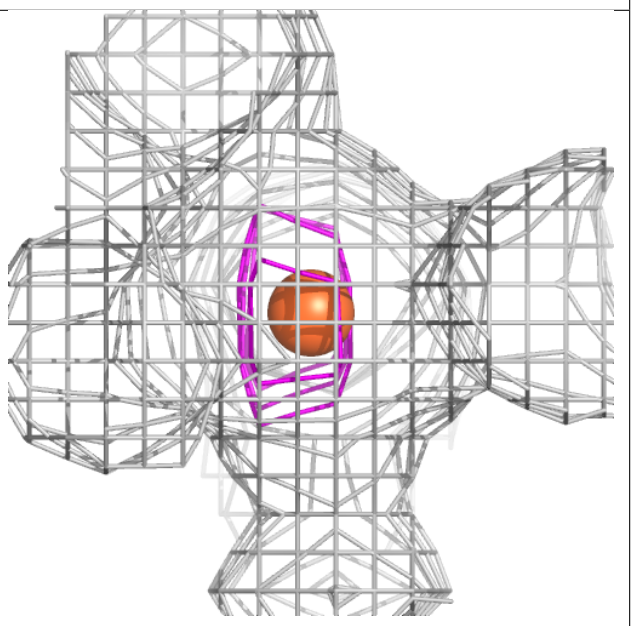


Electron density around FE2 Q 202:

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

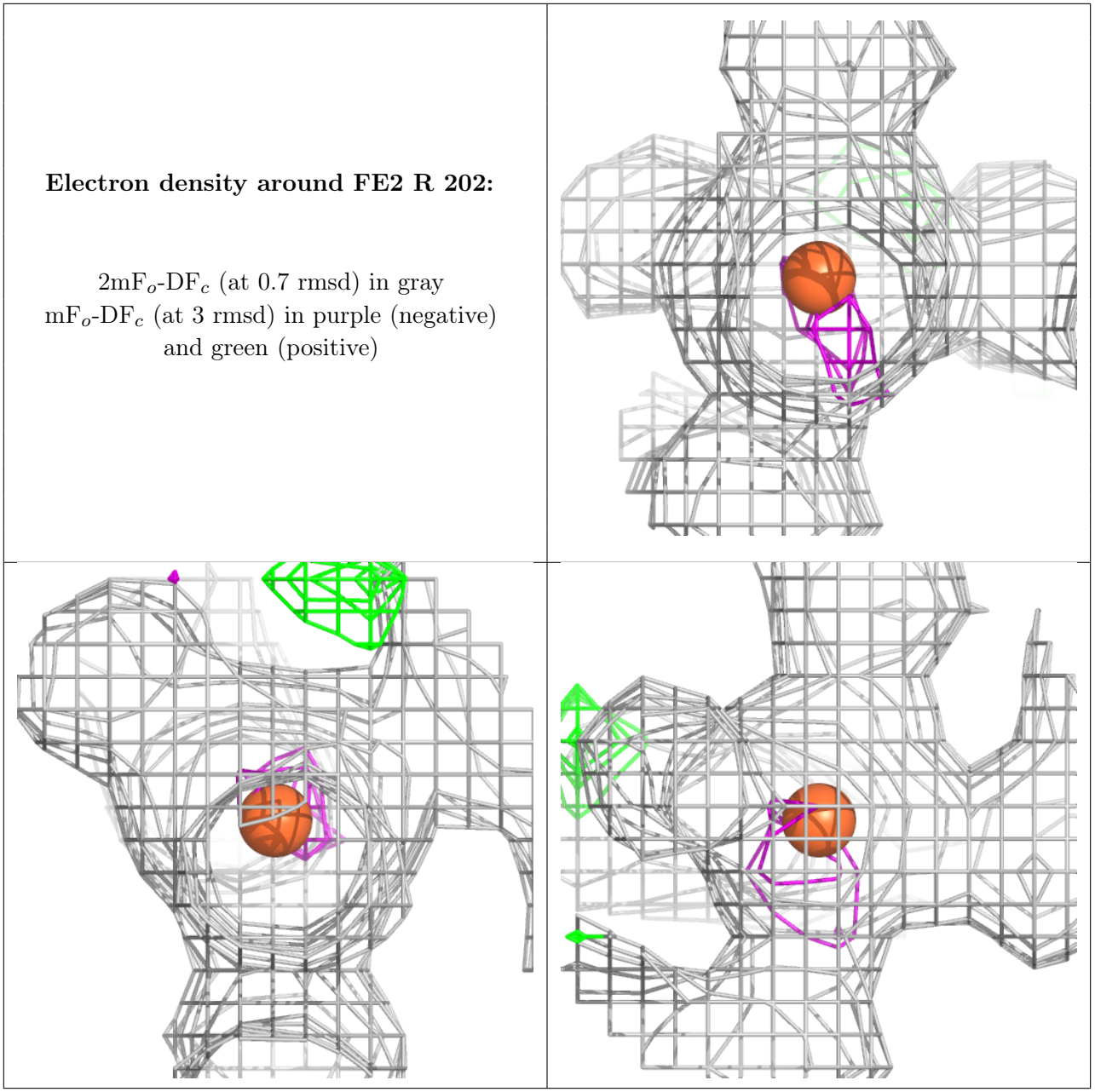






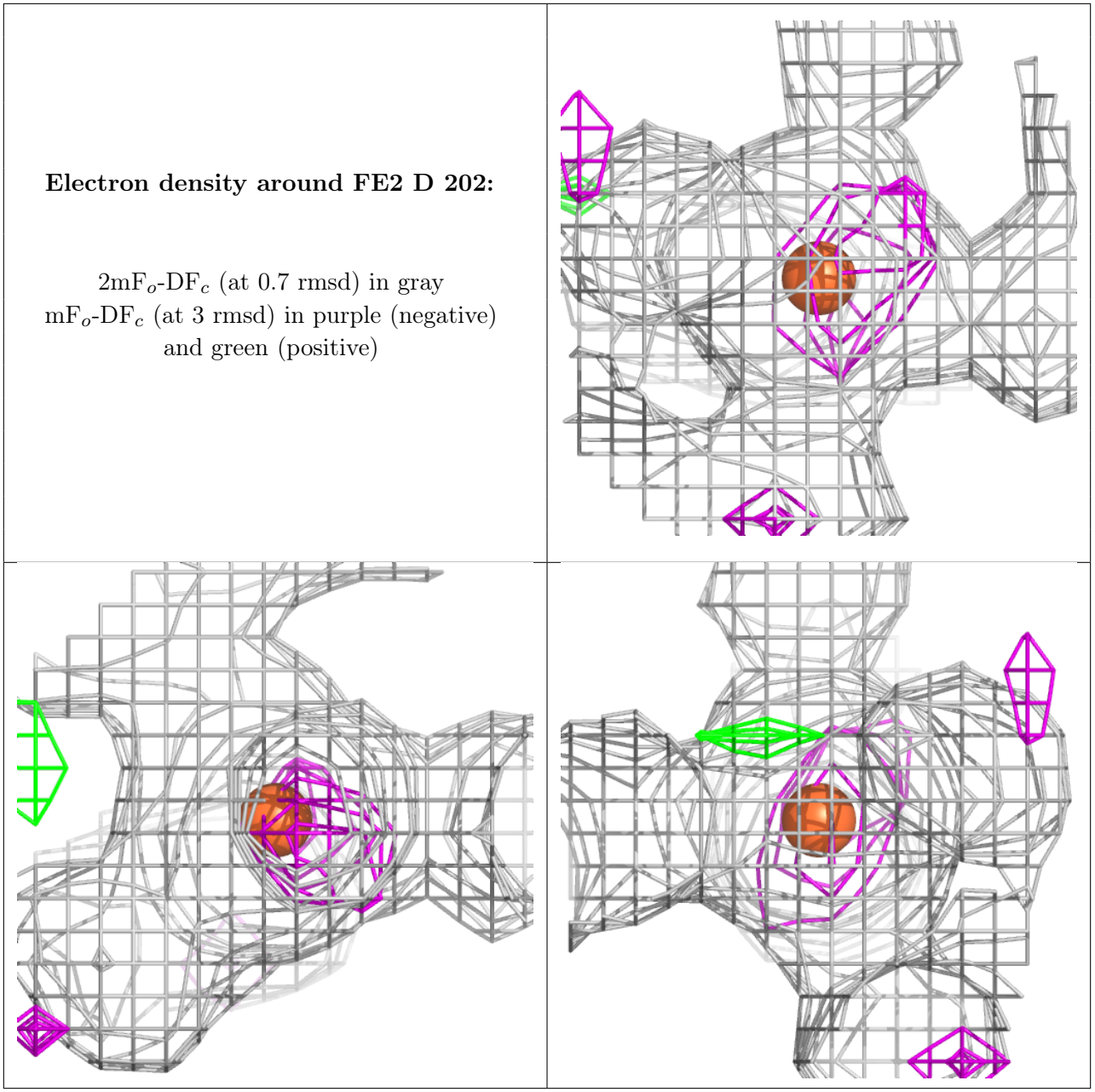
Electron density around FE2 R 202:

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



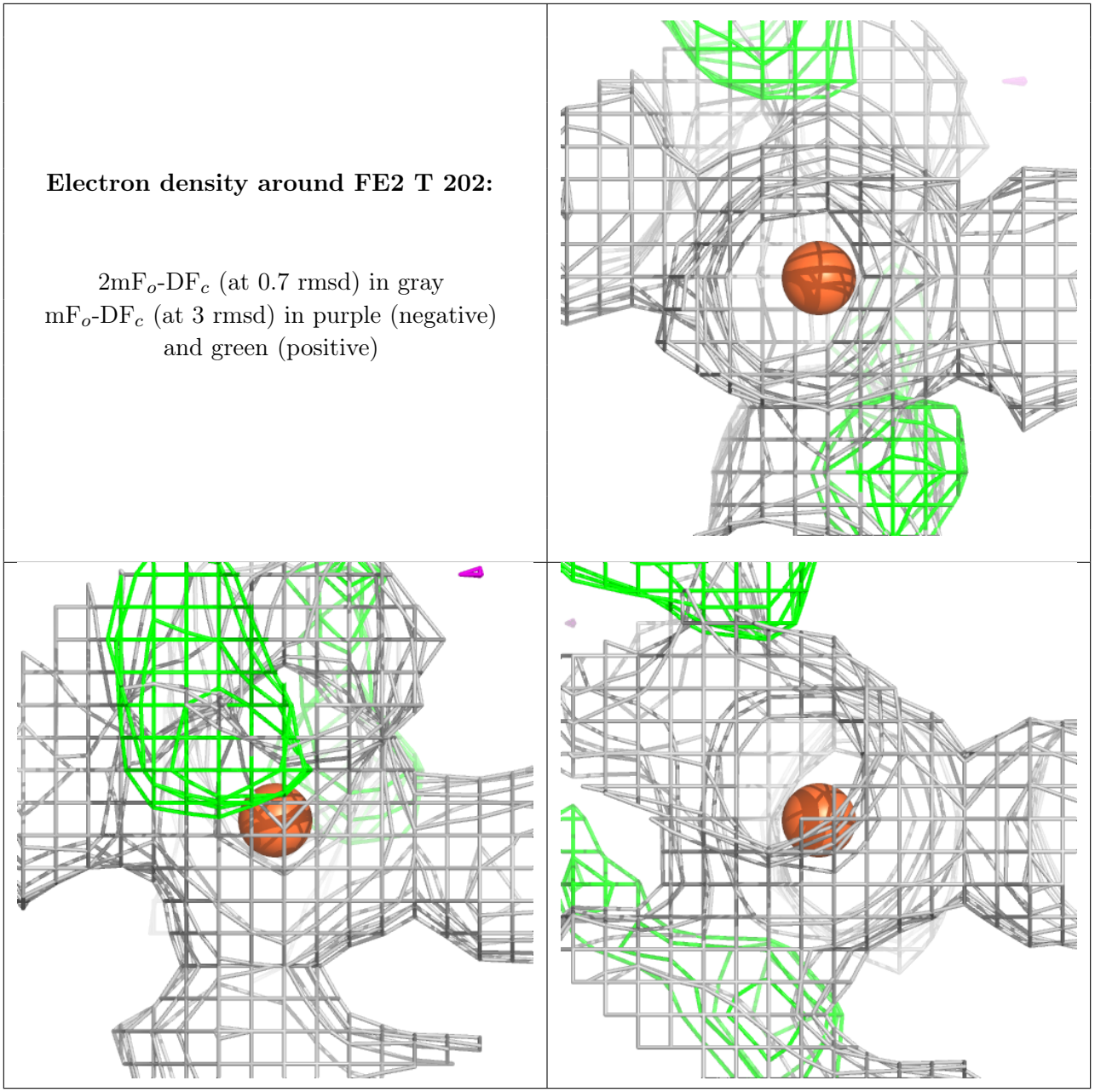
Electron density around FE2 D 202:

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



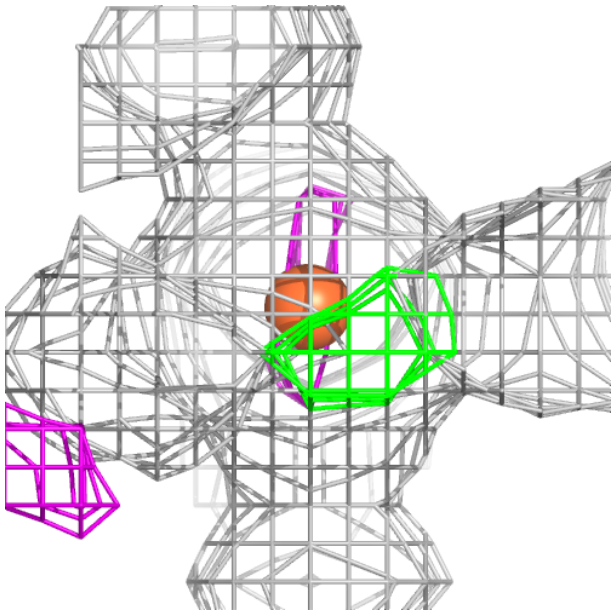
Electron density around FE2 T 202:

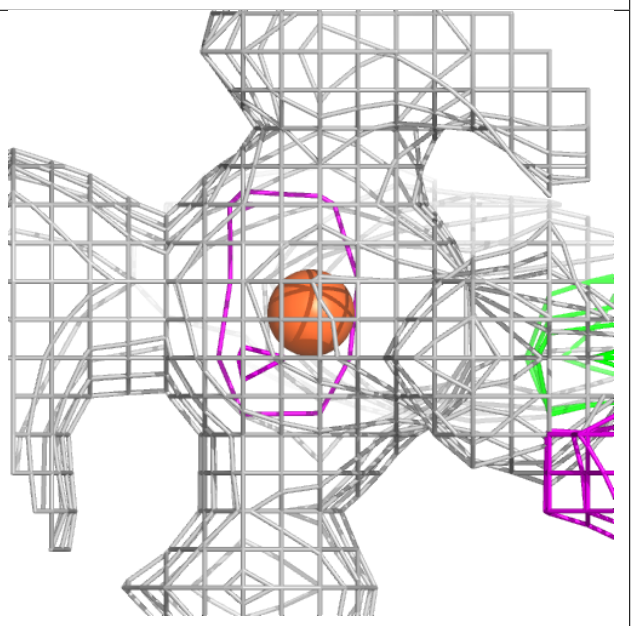
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FE2 U 202:

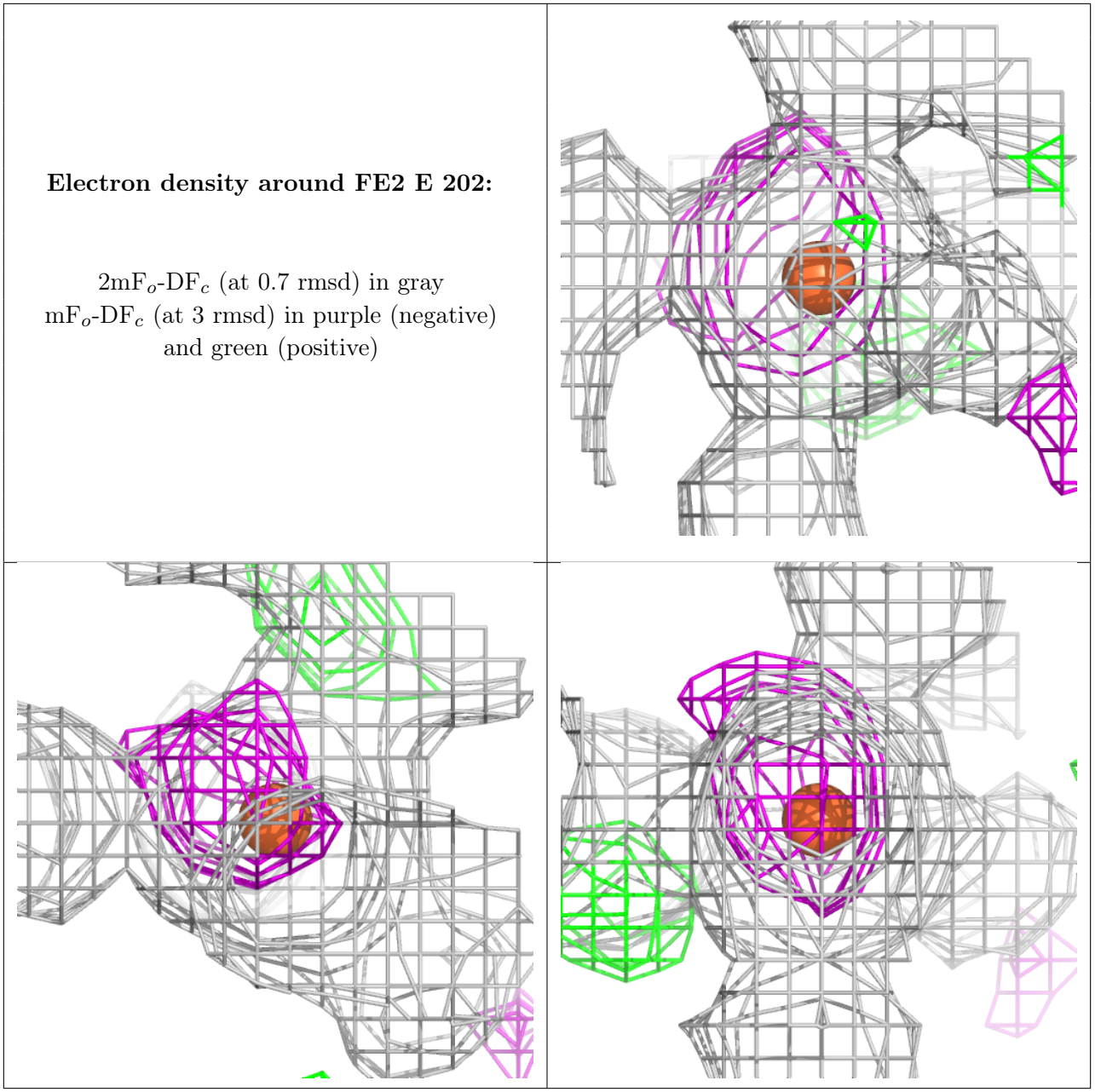
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





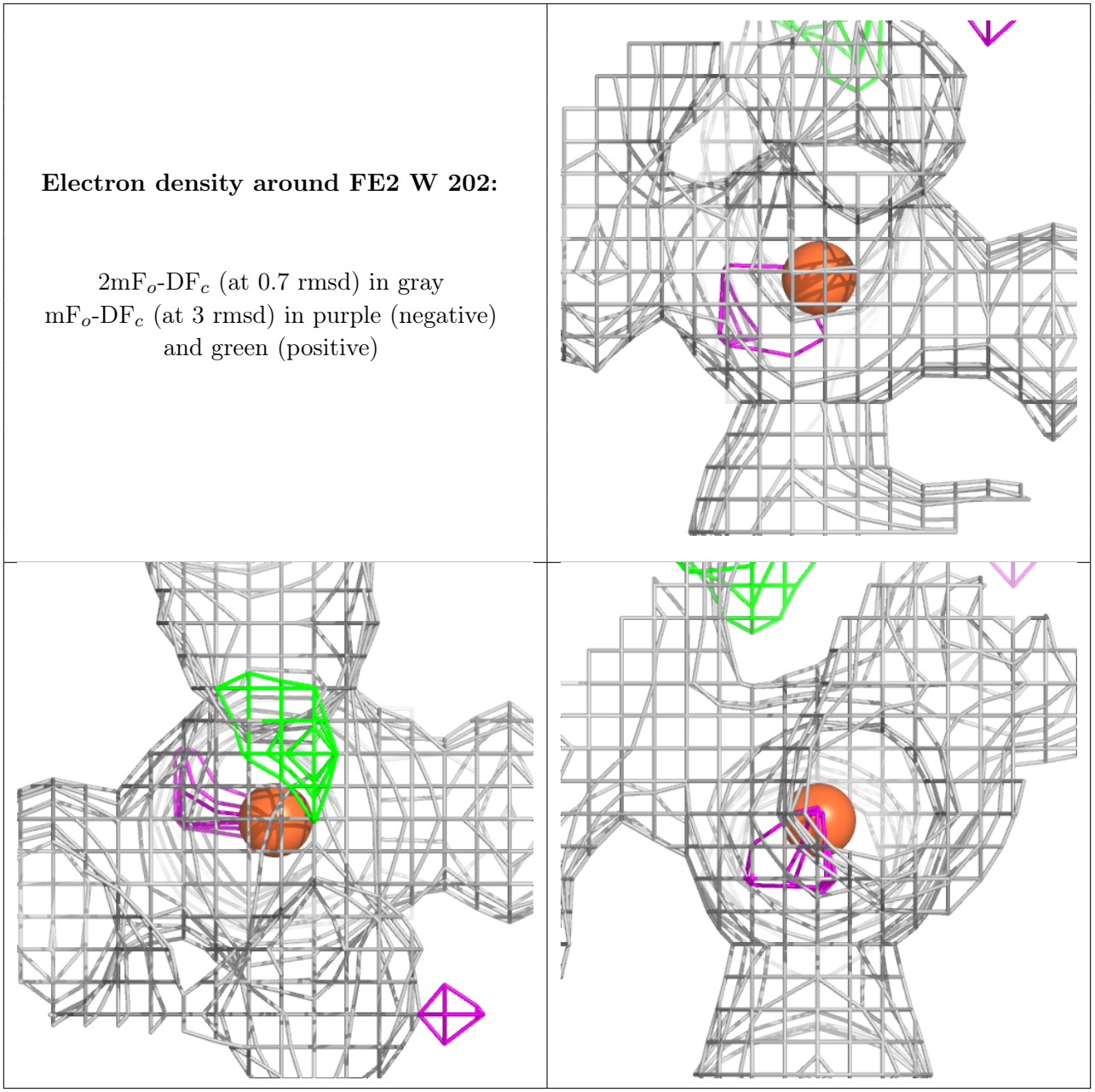
Electron density around FE2 E 202:

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



Electron density around FE2 W 202:

$2mF_o$-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.