



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2023 – 04:16 PM JST

PDB ID : 7Y74
Title : Apostichopus japonicus ferritin mutant-D129A/E132A
Authors : Wu, Y.; Ming, T.H.; Su, X.R.
Deposited on : 2022-06-21
Resolution : 1.98 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

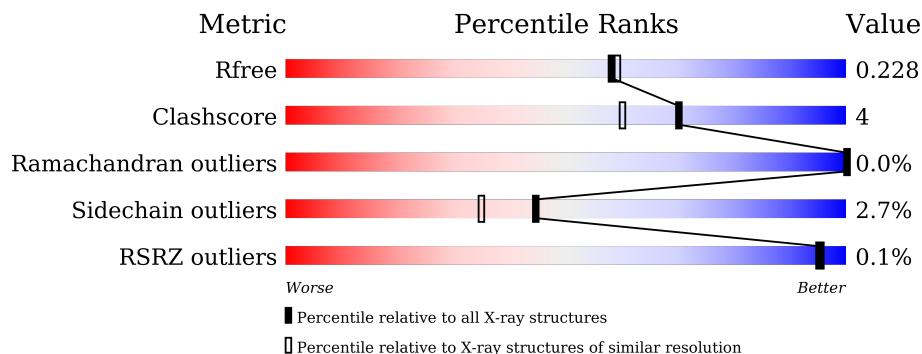
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 $\leq 5\%$. 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	173	 87% 11% ..
1	B	173	 87% 10% ..
1	C	173	 88% 8% ..
1	D	173	 89% 8% ..
1	E	173	 87% 10% ..
1	F	173	 90% 8% ..

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Mol	Chain	Length	Quality of chain
1	G	173	 88% 10% ..
1	H	173	 91% 7% .
1	I	173	 % 90% 9% .
1	J	173	 88% 10% ..
1	K	173	 89% 8% ..
1	L	173	 89% 9% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17989 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	170	Total 1342	C 853	N 229	O 256	S 4	0	0	0
1	B	172	Total 1365	C 866	N 233	O 261	S 5	0	0	0
1	C	169	Total 1347	C 856	N 230	O 257	S 4	0	0	0
1	D	169	Total 1356	C 863	N 230	O 259	S 4	0	0	0
1	E	171	Total 1372	C 870	N 236	O 262	S 4	0	0	0
1	F	170	Total 1356	C 862	N 234	O 256	S 4	0	0	0
1	G	170	Total 1356	C 862	N 230	O 260	S 4	0	0	0
1	H	170	Total 1364	C 866	N 234	O 260	S 4	0	0	0
1	I	173	Total 1373	C 871	N 235	O 263	S 4	0	0	0
1	J	171	Total 1362	C 867	N 231	O 260	S 4	0	0	0
1	K	170	Total 1355	C 859	N 234	O 258	S 4	0	0	0
1	L	170	Total 1357	C 863	N 232	O 258	S 4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ALA	ASP	engineered mutation	UNP Q2QJV4
A	132	ALA	GLU	engineered mutation	UNP Q2QJV4
B	129	ALA	ASP	engineered mutation	UNP Q2QJV4
B	132	ALA	GLU	engineered mutation	UNP Q2QJV4
C	129	ALA	ASP	engineered mutation	UNP Q2QJV4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	GLU	engineered mutation	UNP Q2QJV4
D	129	ALA	ASP	engineered mutation	UNP Q2QJV4
D	132	ALA	GLU	engineered mutation	UNP Q2QJV4
E	129	ALA	ASP	engineered mutation	UNP Q2QJV4
E	132	ALA	GLU	engineered mutation	UNP Q2QJV4
F	129	ALA	ASP	engineered mutation	UNP Q2QJV4
F	132	ALA	GLU	engineered mutation	UNP Q2QJV4
G	129	ALA	ASP	engineered mutation	UNP Q2QJV4
G	132	ALA	GLU	engineered mutation	UNP Q2QJV4
H	129	ALA	ASP	engineered mutation	UNP Q2QJV4
H	132	ALA	GLU	engineered mutation	UNP Q2QJV4
I	129	ALA	ASP	engineered mutation	UNP Q2QJV4
I	132	ALA	GLU	engineered mutation	UNP Q2QJV4
J	129	ALA	ASP	engineered mutation	UNP Q2QJV4
J	132	ALA	GLU	engineered mutation	UNP Q2QJV4
K	129	ALA	ASP	engineered mutation	UNP Q2QJV4
K	132	ALA	GLU	engineered mutation	UNP Q2QJV4
L	129	ALA	ASP	engineered mutation	UNP Q2QJV4
L	132	ALA	GLU	engineered mutation	UNP Q2QJV4

- 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	3	Total Fe 3 3	0	0
2	B	3	Total Fe 3 3	0	0
2	C	3	Total Fe 3 3	0	0
2	D	3	Total Fe 3 3	0	0
2	E	3	Total Fe 3 3	0	0
2	F	3	Total Fe 3 3	0	0
2	G	3	Total Fe 3 3	0	0
2	H	3	Total Fe 3 3	0	0
2	I	3	Total Fe 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	3	Total 3	Fe 3	0	0
2	K	3	Total 3	Fe 3	0	0
2	L	3	Total 3	Fe 3	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0
4	B	148	Total 148	O 148	0	0

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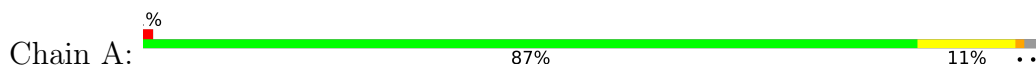
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	144	Total 144	O 144	0	0
4	D	144	Total 144	O 144	0	0
4	E	151	Total 151	O 151	0	0
4	F	126	Total 126	O 126	0	0
4	G	138	Total 138	O 138	0	0
4	H	129	Total 129	O 129	0	0
4	I	142	Total 142	O 142	0	0
4	J	112	Total 112	O 112	0	0
4	K	123	Total 123	O 123	0	0
4	L	139	Total 139	O 139	0	0

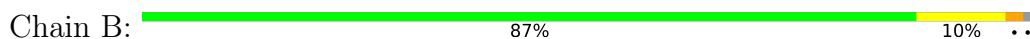
3 Residue-property plots [i](#)

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.

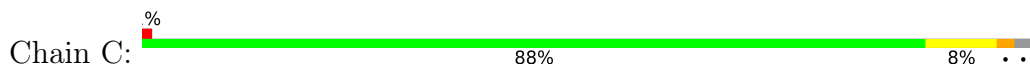
- Molecule 1: Ferritin



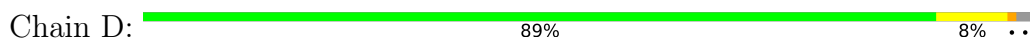
- Molecule 1: Ferritin



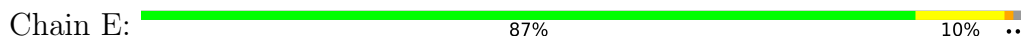
- Molecule 1: Ferritin



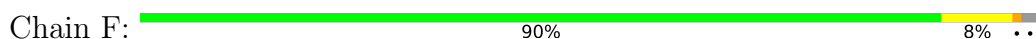
- Molecule 1: Ferritin



- Molecule 1: Ferritin

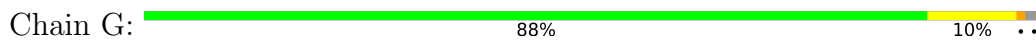


- Molecule 1: Ferritin

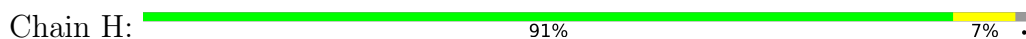




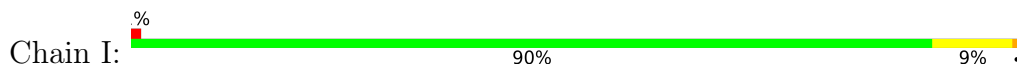
- Molecule 1: Ferritin



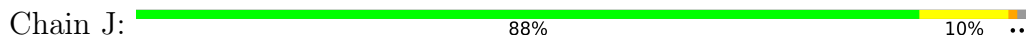
- Molecule 1: Ferritin



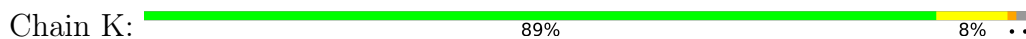
- Molecule 1: Ferritin



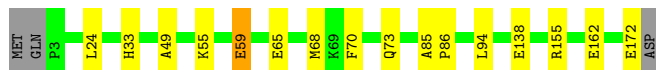
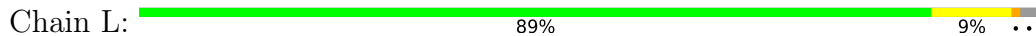
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.83Å 130.95Å 122.62Å 90.00° 119.40° 90.00°	Depositor
Resolution (Å)	47.91 – 1.98 47.91 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.91-1.98) 98.4 (47.91-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.176 , 0.220 0.189 , 0.228	Depositor DCC
R_{free} test set	8970 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17989	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CD

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	0.84	3/1368 (0.2%)	0.79	2/1845 (0.1%)
1	B	0.80	4/1391 (0.3%)	0.81	3/1873 (0.2%)
1	C	0.94	5/1370 (0.4%)	0.86	3/1845 (0.2%)
1	D	0.92	4/1382 (0.3%)	0.74	2/1857 (0.1%)
1	E	0.89	2/1397 (0.1%)	0.77	2/1879 (0.1%)
1	F	0.85	3/1382 (0.2%)	0.77	1/1857 (0.1%)
1	G	0.68	0/1381	0.72	1/1857 (0.1%)
1	H	0.82	1/1390 (0.1%)	0.80	3/1867 (0.2%)
1	I	0.94	4/1399 (0.3%)	0.78	2/1882 (0.1%)
1	J	0.87	2/1388 (0.1%)	0.81	2/1867 (0.1%)
1	K	0.83	3/1378 (0.2%)	0.76	2/1856 (0.1%)
1	L	0.73	2/1382 (0.1%)	0.72	1/1857 (0.1%)
All	All	0.85	33/16608 (0.2%)	0.78	24/22342 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
1	I	0	1
All	All	0	3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	GLU	CD-OE2	19.05	1.46	1.25
1	I	138	GLU	CD-OE2	18.58	1.46	1.25
1	D	138	GLU	CD-OE2	18.32	1.45	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	138	GLU	CD-OE2	17.45	1.44	1.25
1	E	138	GLU	CD-OE2	17.17	1.44	1.25
1	F	138	GLU	CD-OE2	16.79	1.44	1.25
1	H	138	GLU	CD-OE2	15.78	1.43	1.25
1	K	138	GLU	CD-OE2	15.73	1.43	1.25
1	A	138	GLU	CD-OE2	14.13	1.41	1.25
1	L	138	GLU	CD-OE2	9.65	1.36	1.25
1	I	25	GLU	CD-OE1	-7.41	1.17	1.25
1	C	157	GLY	N-CA	7.19	1.56	1.46
1	I	138	GLU	CB-CG	7.00	1.65	1.52
1	D	25	GLU	CD-OE1	-6.85	1.18	1.25
1	C	25	GLU	CD-OE1	-6.74	1.18	1.25
1	C	138	GLU	CB-CG	6.55	1.64	1.52
1	B	25	GLU	CD-OE1	-6.48	1.18	1.25
1	A	138	GLU	CB-CG	6.45	1.64	1.52
1	K	138	GLU	CB-CG	6.18	1.63	1.52
1	D	138	GLU	CB-CG	6.06	1.63	1.52
1	E	25	GLU	CD-OE1	-5.93	1.19	1.25
1	B	138	GLU	CD-OE2	5.85	1.32	1.25
1	K	25	GLU	CD-OE1	-5.85	1.19	1.25
1	F	138	GLU	CB-CG	5.84	1.63	1.52
1	J	138	GLU	CB-CG	5.84	1.63	1.52
1	B	159	GLY	N-CA	5.76	1.54	1.46
1	B	157	GLY	N-CA	5.63	1.54	1.46
1	F	25	GLU	CD-OE1	-5.63	1.19	1.25
1	L	59	GLU	C-N	-5.58	1.21	1.34
1	D	60	GLU	C-N	-5.45	1.21	1.34
1	A	138	GLU	N-CA	5.18	1.56	1.46
1	C	138	GLU	CG-CD	5.01	1.59	1.51
1	I	138	GLU	CG-CD	5.01	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	155	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	A	138	GLU	N-CA-CB	8.10	125.18	110.60
1	C	155	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	J	138	GLU	N-CA-CB	7.77	124.59	110.60
1	B	155	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	I	138	GLU	N-CA-CB	7.63	124.34	110.60
1	D	138	GLU	N-CA-CB	7.20	123.56	110.60
1	C	138	GLU	N-CA-CB	7.19	123.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	155	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	K	138	GLU	N-CA-CB	6.60	122.48	110.60
1	J	155	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	H	155	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	126	GLN	CB-CG-CD	-6.37	95.05	111.60
1	H	155	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	F	138	GLU	N-CA-CB	6.13	121.63	110.60
1	E	138	GLU	N-CA-CB	5.96	121.33	110.60
1	C	156	VAL	C-N-CA	-5.69	110.36	122.30
1	D	155	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	I	138	GLU	CB-CG-CD	5.50	129.04	114.20
1	H	138	GLU	N-CA-CB	5.46	120.42	110.60
1	G	155	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	138	GLU	CB-CG-CD	5.30	128.50	114.20
1	E	2	GLN	CB-CA-C	5.19	120.78	110.40
1	B	155	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	77	ARG	Sidechain
1	G	41	ARG	Sidechain
1	I	41	ARG	Sidechain

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	1342	0	1274	16	0
1	B	1365	0	1303	13	0
1	C	1347	0	1288	11	0
1	D	1356	0	1306	8	0
1	E	1372	0	1326	12	0
1	F	1356	0	1316	7	0
1	G	1356	0	1309	10	0
1	H	1364	0	1323	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1373	0	1318	11	0
1	J	1362	0	1302	10	0
1	K	1355	0	1295	10	0
1	L	1357	0	1308	8	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
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	140	0	0	2	0
4	B	148	0	0	2	0
4	C	144	0	0	4	0
4	D	144	0	0	3	0
4	E	151	0	0	2	0
4	F	126	0	0	0	0
4	G	138	0	0	2	0
4	H	129	0	0	0	0
4	I	142	0	0	3	0
4	J	112	0	0	1	0
4	K	123	0	0	1	0
4	L	139	0	0	2	0
All	All	17989	0	15668	114	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.

All (114) 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:I:128:CYS:SG	4:I:435:HOH:O	2.25	0.94
1:B:157:GLY:HA3	4:B:326:HOH:O	1.70	0.92
1:E:167:LYS:CD	1:E:167:LYS:NZ	2.41	0.82
1:A:2:GLN:CB	1:A:3:PRO:HD2	2.11	0.80
1:A:128:CYS:SG	4:A:435:HOH:O	2.38	0.79
1:A:2:GLN:CB	1:A:3:PRO:CD	2.63	0.76
1:B:87:GLU:CG	4:B:441:HOH:O	2.34	0.76
1:J:172:GLU:HG3	4:J:386:HOH:O	1.88	0.74
1:C:157:GLY:HA3	4:C:358:HOH:O	1.90	0.71
1:C:33:HIS:HE1	1:H:65:GLU:OE2	1.74	0.70
1:E:11:HIS:HD2	1:E:13:LEU:H	1.39	0.69
1:A:11:HIS:HD2	1:A:13:LEU:H	1.41	0.67
1:D:11:HIS:HD2	1:D:13:LEU:H	1.43	0.67
1:A:65:GLU:OE2	1:I:33:HIS:HE1	1.77	0.66
1:L:172:GLU:CB	4:L:399:HOH:O	2.44	0.65
1:E:2:GLN:HB3	1:E:3:PRO:HD3	1.78	0.65
1:D:55:LYS:O	1:D:59:GLU:HG3	1.98	0.64
1:G:70:PHE:HA	1:G:73:GLN:HE21	1.63	0.63
1:K:74:ARG:HH11	1:K:126:GLN:HE21	1.48	0.61
1:K:51:LYS:CD	1:K:51:LYS:NZ	2.63	0.61
1:E:11:HIS:CD2	1:E:13:LEU:H	2.19	0.61
1:G:3:PRO:CB	4:G:425:HOH:O	2.48	0.60
1:A:33:HIS:HE1	1:I:65:GLU:OE2	1.85	0.60
1:F:65:GLU:OE2	1:J:33:HIS:HE1	1.85	0.59
1:H:70:PHE:HA	1:H:73:GLN:HE21	1.65	0.59
1:C:59:GLU:OE2	1:C:138:GLU:OE2	2.21	0.59
1:C:36:ALA:O	1:C:50:HIS:HD2	1.86	0.58
1:G:3:PRO:HB2	4:G:425:HOH:O	2.04	0.57
1:A:65:GLU:HA	1:A:68:MET:CE	2.35	0.57
1:F:167:LYS:HE2	1:F:172:GLU:OE2	2.05	0.57
1:I:70:PHE:HA	1:I:73:GLN:HE21	1.68	0.57
1:E:70:PHE:HA	1:E:73:GLN:HE21	1.70	0.56
1:L:65:GLU:HA	1:L:68:MET:HE3	1.87	0.56
1:D:11:HIS:CD2	1:D:13:LEU:H	2.22	0.56
1:I:59:GLU:OE2	1:I:138:GLU:OE2	2.23	0.56
1:I:99:LYS:HE2	4:I:325:HOH:O	2.07	0.55
1:J:52:TYR:O	1:J:56:GLN:HG2	2.05	0.55
1:K:74:ARG:HH11	1:K:126:GLN:NE2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:74:ARG:NH1	1:K:126:GLN:HE21	2.03	0.55
1:J:49:ALA:HB2	1:J:94:LEU:HD11	1.90	0.54
1:J:105:GLU:HG3	1:J:146:ILE:CD1	2.38	0.54
1:E:105:GLU:HG3	1:E:146:ILE:CD1	2.38	0.54
1:J:70:PHE:HA	1:J:73:GLN:HE21	1.73	0.54
1:E:2:GLN:NE2	4:E:302:HOH:O	2.34	0.53
1:C:70:PHE:HA	1:C:73:GLN:HE21	1.72	0.53
1:B:70:PHE:HA	1:B:73:GLN:HE21	1.74	0.53
1:C:138:GLU:HG2	4:C:305:HOH:O	2.07	0.52
1:A:70:PHE:HA	1:A:73:GLN:HE21	1.73	0.52
1:B:126:GLN:CA	1:B:126:GLN:OE1	2.52	0.52
1:H:126:GLN:OE1	1:H:126:GLN:CA	2.55	0.52
1:K:138:GLU:HG2	4:K:317:HOH:O	2.11	0.51
1:K:49:ALA:HB2	1:K:94:LEU:HD21	1.92	0.51
1:A:105:GLU:HG3	1:A:146:ILE:CD1	2.41	0.51
1:A:11:HIS:CD2	1:A:13:LEU:H	2.25	0.50
1:B:74:ARG:HH11	1:B:126:GLN:CG	2.24	0.50
1:A:65:GLU:HA	1:A:68:MET:HE2	1.92	0.50
1:L:55:LYS:O	1:L:59:GLU:HG3	2.11	0.50
1:D:51:LYS:CD	4:D:338:HOH:O	2.59	0.50
1:D:138:GLU:HG2	4:D:303:HOH:O	2.11	0.49
1:G:105:GLU:HG3	1:G:146:ILE:CD1	2.43	0.49
1:B:4:SER:OG	1:B:6:VAL:HG22	2.13	0.48
1:D:138:GLU:CD	4:D:303:HOH:O	2.51	0.48
1:L:65:GLU:HA	1:L:68:MET:CE	2.43	0.48
1:D:105:GLU:HG3	1:D:146:ILE:CD1	2.43	0.48
1:J:55:LYS:O	1:J:59:GLU:HG3	2.13	0.48
1:B:126:GLN:OE1	1:B:126:GLN:HA	2.14	0.48
1:C:138:GLU:CD	4:C:305:HOH:O	2.53	0.47
1:F:167:LYS:NZ	1:F:168:GLU:OE2	2.43	0.47
1:L:49:ALA:HB2	1:L:94:LEU:HD21	1.96	0.47
1:C:157:GLY:CA	4:C:358:HOH:O	2.57	0.47
1:I:105:GLU:HG3	1:I:146:ILE:CD1	2.45	0.47
1:C:50:HIS:CE1	1:C:54:LYS:HE2	2.49	0.46
1:A:65:GLU:OE2	1:I:33:HIS:CE1	2.65	0.46
1:E:2:GLN:CB	1:E:3:PRO:HD3	2.45	0.46
1:F:70:PHE:HA	1:F:73:GLN:HE21	1.80	0.46
1:E:2:GLN:CB	1:E:3:PRO:CD	2.94	0.46
1:A:168:GLU:HB3	1:C:167:LYS:HE3	1.98	0.46
1:B:74:ARG:HD3	1:B:126:GLN:HG2	1.97	0.46
1:H:126:GLN:OE1	1:H:126:GLN:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:PHE:HE1	1:E:126:GLN:HE22	1.64	0.45
1:B:167:LYS:O	1:B:172:GLU:HG2	2.17	0.45
1:K:70:PHE:HE1	1:K:126:GLN:HE22	1.65	0.45
1:K:105:GLU:HG3	1:K:146:ILE:HD12	1.98	0.45
1:A:33:HIS:CE1	1:I:65:GLU:OE2	2.68	0.45
1:J:74:ARG:HD3	1:J:126:GLN:HG2	1.99	0.45
1:B:105:GLU:HG3	1:B:146:ILE:CD1	2.47	0.45
1:C:33:HIS:CE1	1:H:65:GLU:OE2	2.63	0.45
1:B:74:ARG:NH1	1:B:126:GLN:CG	2.80	0.45
1:F:105:GLU:HG3	1:F:146:ILE:CD1	2.46	0.44
1:G:87:GLU:HG3	1:G:88:LYS:HG3	1.99	0.44
1:H:74:ARG:HD3	1:H:126:GLN:HG2	1.99	0.44
1:I:169:ASN:ND2	4:I:307:HOH:O	2.50	0.44
1:F:33:HIS:HE1	1:J:65:GLU:OE2	2.00	0.44
1:A:65:GLU:HA	1:A:68:MET:HE3	2.00	0.43
1:E:110:GLN:NE2	4:E:305:HOH:O	2.44	0.43
1:G:164:ILE:HD13	1:H:164:ILE:HD11	1.99	0.43
1:K:105:GLU:HG3	1:K:146:ILE:CD1	2.49	0.43
1:A:56:GLN:NE2	4:A:311:HOH:O	2.52	0.43
1:G:46:LEU:HD13	1:G:94:LEU:HG	2.01	0.43
1:B:74:ARG:HH11	1:B:126:GLN:HG2	1.83	0.43
1:L:70:PHE:HA	1:L:73:GLN:HE21	1.84	0.42
1:L:162:GLU:OE2	4:L:301:HOH:O	2.21	0.42
1:G:55:LYS:O	1:G:59:GLU:HG3	2.19	0.42
1:E:49:ALA:HB2	1:E:94:LEU:HD21	2.02	0.42
1:F:24:LEU:HD23	1:F:24:LEU:HA	1.92	0.41
1:I:4:SER:OG	1:I:6:VAL:HG22	2.20	0.41
1:H:91:TRP:CZ3	1:H:100:VAL:HG11	2.55	0.41
1:J:105:GLU:HG3	1:J:146:ILE:HD12	2.02	0.41
1:B:116:HIS:CD2	1:B:116:HIS:C	2.94	0.41
1:K:123:LYS:CD	1:K:123:LYS:NZ	2.84	0.41
1:D:70:PHE:HA	1:D:73:GLN:HE21	1.86	0.41
1:G:74:ARG:HH11	1:G:126:GLN:NE2	2.18	0.41
1:G:74:ARG:NH1	1:G:126:GLN:HE21	2.19	0.41
1:L:85:ALA:HA	1:L:86:PRO:HD3	1.96	0.41

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	168/173 (97%)	167 (99%)	1 (1%)	0	100	100
1	B	170/173 (98%)	168 (99%)	2 (1%)	0	100	100
1	C	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
1	D	167/173 (96%)	167 (100%)	0	0	100	100
1	E	169/173 (98%)	168 (99%)	1 (1%)	0	100	100
1	F	168/173 (97%)	166 (99%)	2 (1%)	0	100	100
1	G	168/173 (97%)	167 (99%)	1 (1%)	0	100	100
1	H	168/173 (97%)	166 (99%)	2 (1%)	0	100	100
1	I	171/173 (99%)	168 (98%)	2 (1%)	1 (1%)	25	14
1	J	169/173 (98%)	169 (100%)	0	0	100	100
1	K	168/173 (97%)	167 (99%)	1 (1%)	0	100	100
1	L	168/173 (97%)	168 (100%)	0	0	100	100
All	All	2021/2076 (97%)	2007 (99%)	13 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	2	GLN

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	134/149 (90%)	128 (96%)	6 (4%)	27	15
1	B	138/149 (93%)	133 (96%)	5 (4%)	35	23
1	C	134/149 (90%)	129 (96%)	5 (4%)	34	22
1	D	137/149 (92%)	135 (98%)	2 (2%)	65	59
1	E	141/149 (95%)	135 (96%)	6 (4%)	29	17
1	F	139/149 (93%)	135 (97%)	4 (3%)	42	31
1	G	138/149 (93%)	135 (98%)	3 (2%)	52	46
1	H	139/149 (93%)	137 (99%)	2 (1%)	67	62
1	I	139/149 (93%)	137 (99%)	2 (1%)	67	62
1	J	137/149 (92%)	134 (98%)	3 (2%)	52	46
1	K	136/149 (91%)	131 (96%)	5 (4%)	34	22
1	L	137/149 (92%)	135 (98%)	2 (2%)	65	59
All	All	1649/1788 (92%)	1604 (97%)	45 (3%)	44	35

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	33	HIS
1	A	59	GLU
1	A	80	LEU
1	A	94	LEU
1	A	169	ASN
1	B	24	LEU
1	B	33	HIS
1	B	80	LEU
1	B	169	ASN
1	B	172	GLU
1	C	24	LEU
1	C	30	TYR
1	C	33	HIS
1	C	121	SER
1	C	169	ASN
1	D	24	LEU
1	D	33	HIS
1	E	24	LEU
1	E	30	TYR
1	E	66	LYS
1	E	80	LEU

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Mol	Chain	Res	Type
1	E	126	GLN
1	E	139	GLN
1	F	24	LEU
1	F	33	HIS
1	F	80	LEU
1	F	158	THR
1	G	24	LEU
1	G	33	HIS
1	G	126	GLN
1	H	33	HIS
1	H	167	LYS
1	I	24	LEU
1	I	33	HIS
1	J	24	LEU
1	J	33	HIS
1	J	169	ASN
1	K	24	LEU
1	K	33	HIS
1	K	80	LEU
1	K	126	GLN
1	K	158	THR
1	L	24	LEU
1	L	33	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	33	HIS
1	A	73	GLN
1	A	116	HIS
1	B	73	GLN
1	B	116	HIS
1	B	139	GLN
1	C	33	HIS
1	C	50	HIS
1	C	73	GLN
1	C	116	HIS
1	D	11	HIS
1	D	73	GLN
1	D	116	HIS
1	E	11	HIS

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Mol	Chain	Res	Type
1	E	73	GLN
1	E	116	HIS
1	E	126	GLN
1	F	33	HIS
1	F	73	GLN
1	F	116	HIS
1	G	73	GLN
1	G	116	HIS
1	G	126	GLN
1	H	33	HIS
1	H	73	GLN
1	H	116	HIS
1	I	33	HIS
1	I	73	GLN
1	I	116	HIS
1	I	169	ASN
1	J	33	HIS
1	J	73	GLN
1	J	116	HIS
1	J	139	GLN
1	K	33	HIS
1	K	116	HIS
1	K	126	GLN
1	L	73	GLN
1	L	116	HIS

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 48 ligands modelled in this entry, 48 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	170/173 (98%)	-0.29	1 (0%) 89 90	19, 26, 38, 68	0
1	B	172/173 (99%)	-0.35	0 100 100	20, 25, 37, 67	0
1	C	169/173 (97%)	-0.37	1 (0%) 89 90	21, 27, 38, 49	0
1	D	169/173 (97%)	-0.40	0 100 100	20, 25, 38, 48	0
1	E	171/173 (98%)	-0.34	0 100 100	20, 26, 39, 61	0
1	F	170/173 (98%)	-0.40	0 100 100	23, 29, 40, 64	0
1	G	170/173 (98%)	-0.44	0 100 100	21, 26, 40, 66	0
1	H	170/173 (98%)	-0.45	0 100 100	22, 28, 40, 65	0
1	I	173/173 (100%)	-0.29	1 (0%) 89 90	20, 25, 42, 76	0
1	J	171/173 (98%)	-0.37	0 100 100	22, 28, 40, 65	0
1	K	170/173 (98%)	-0.39	0 100 100	21, 27, 39, 62	0
1	L	170/173 (98%)	-0.44	0 100 100	21, 28, 39, 58	0
All	All	2045/2076 (98%)	-0.38	3 (0%) 95 95	19, 27, 40, 76	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	2.1
1	C	157	GLY	2.1
1	I	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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	H	203	1/1	0.66	0.20	30,30,30,30	0
2	FE	C	202	1/1	0.80	0.36	30,30,30,30	0
2	FE	C	203	1/1	0.82	0.20	30,30,30,30	0
2	FE	E	203	1/1	0.83	0.38	30,30,30,30	0
2	FE	F	203	1/1	0.89	0.14	30,30,30,30	0
2	FE	F	202	1/1	0.94	0.34	30,30,30,30	0
2	FE	H	202	1/1	0.96	0.13	29,29,29,29	0
2	FE	L	202	1/1	0.96	0.12	28,28,28,28	0
2	FE	L	203	1/1	0.96	0.12	30,30,30,30	0
2	FE	J	203	1/1	0.97	0.13	28,28,28,28	0
2	FE	A	203	1/1	0.97	0.36	30,30,30,30	0
2	FE	I	202	1/1	0.97	0.11	25,25,25,25	0
2	FE	C	201	1/1	0.98	0.14	30,30,30,30	0
2	FE	F	201	1/1	0.98	0.14	28,28,28,28	0
2	FE	D	203	1/1	0.98	0.10	26,26,26,26	0
2	FE	I	203	1/1	0.98	0.12	27,27,27,27	0
2	FE	J	202	1/1	0.98	0.13	25,25,25,25	0
2	FE	E	202	1/1	0.98	0.15	26,26,26,26	0
2	FE	K	203	1/1	0.98	0.12	26,26,26,26	0
2	FE	G	202	1/1	0.98	0.13	26,26,26,26	0
2	FE	G	203	1/1	0.98	0.15	24,24,24,24	0
2	FE	B	202	1/1	0.99	0.14	22,22,22,22	0
2	FE	D	201	1/1	0.99	0.20	12,12,12,12	0
2	FE	J	201	1/1	0.99	0.22	15,15,15,15	0
2	FE	D	202	1/1	0.99	0.13	23,23,23,23	0
2	FE	B	203	1/1	0.99	0.15	25,25,25,25	0
2	FE	K	202	1/1	0.99	0.12	25,25,25,25	0
2	FE	E	201	1/1	0.99	0.12	26,26,26,26	0
2	FE	A	202	1/1	0.99	0.12	25,25,25,25	0
2	FE	A	201	1/1	0.99	0.13	23,23,23,23	0
3	CD	A	204	1/1	0.99	0.04	36,36,36,36	1
3	CD	B	204	1/1	0.99	0.07	31,31,31,31	1

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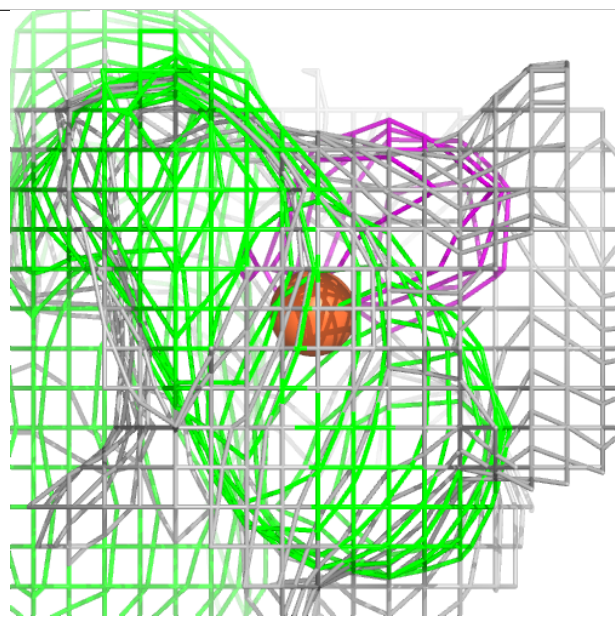
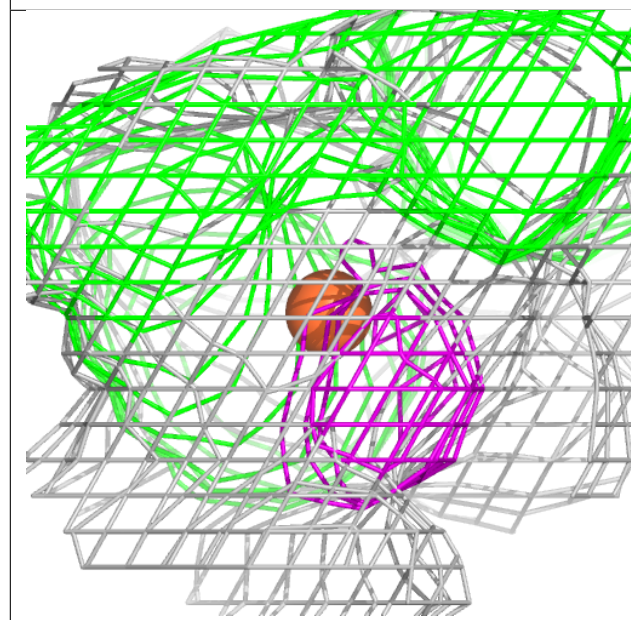
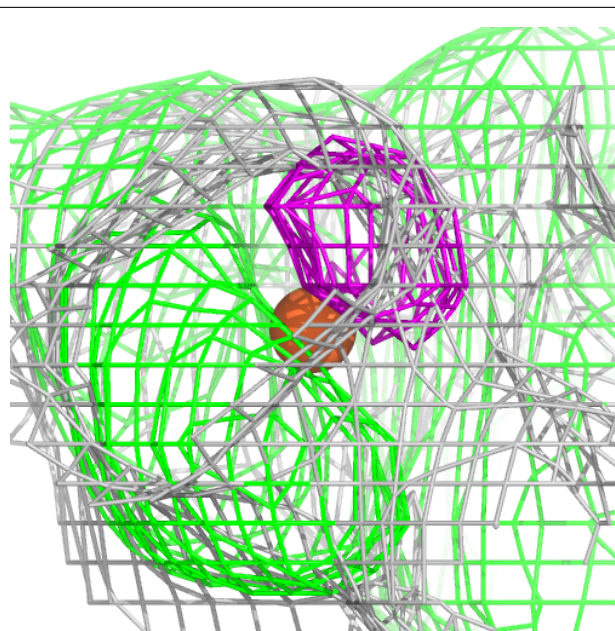
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CD	C	204	1/1	0.99	0.06	29,29,29,29	1
3	CD	D	204	1/1	0.99	0.05	32,32,32,32	1
3	CD	F	204	1/1	0.99	0.08	32,32,32,32	1
3	CD	H	204	1/1	0.99	0.03	37,37,37,37	1
3	CD	I	204	1/1	0.99	0.04	26,26,26,26	1
3	CD	K	204	1/1	0.99	0.05	32,32,32,32	1
3	CD	L	204	1/1	0.99	0.05	35,35,35,35	1
2	FE	L	201	1/1	1.00	0.21	14,14,14,14	0
3	CD	E	204	1/1	1.00	0.07	28,28,28,28	1
2	FE	I	201	1/1	1.00	0.20	12,12,12,12	0
3	CD	G	204	1/1	1.00	0.06	34,34,34,34	1
2	FE	H	201	1/1	1.00	0.22	15,15,15,15	0
2	FE	K	201	1/1	1.00	0.20	14,14,14,14	0
3	CD	J	204	1/1	1.00	0.05	34,34,34,34	1
2	FE	B	201	1/1	1.00	0.21	12,12,12,12	0
2	FE	G	201	1/1	1.00	0.17	13,13,13,13	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.

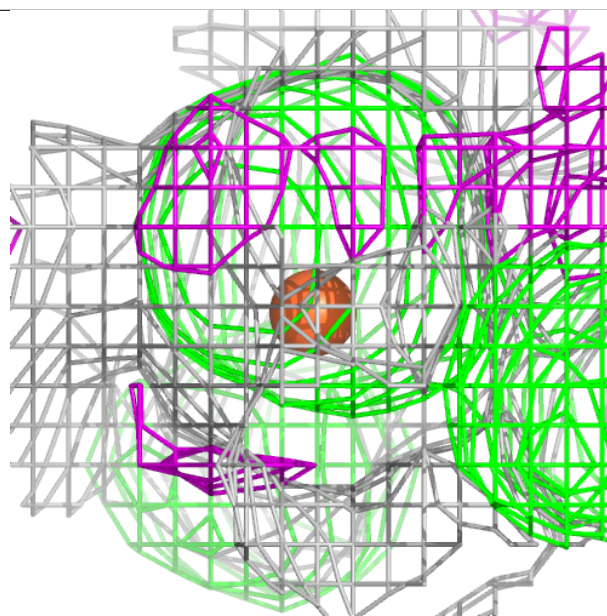
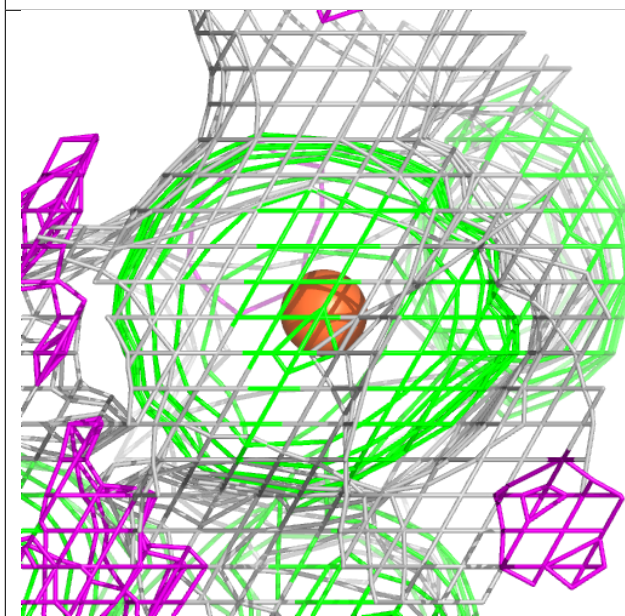
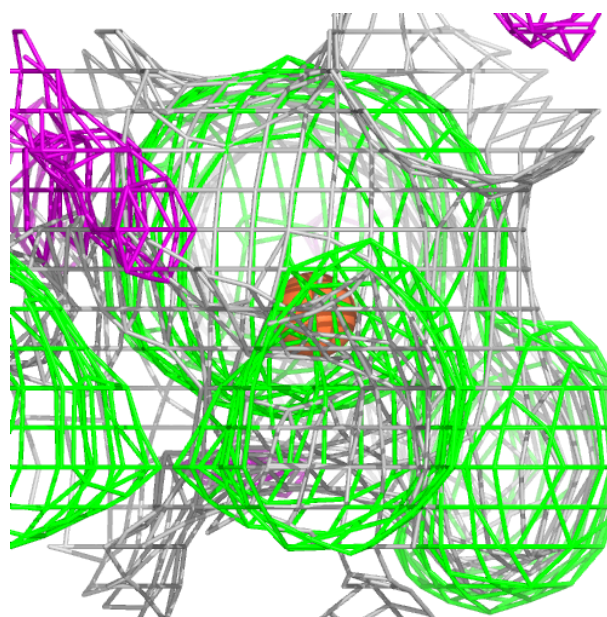
Electron density around FE H 203:

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



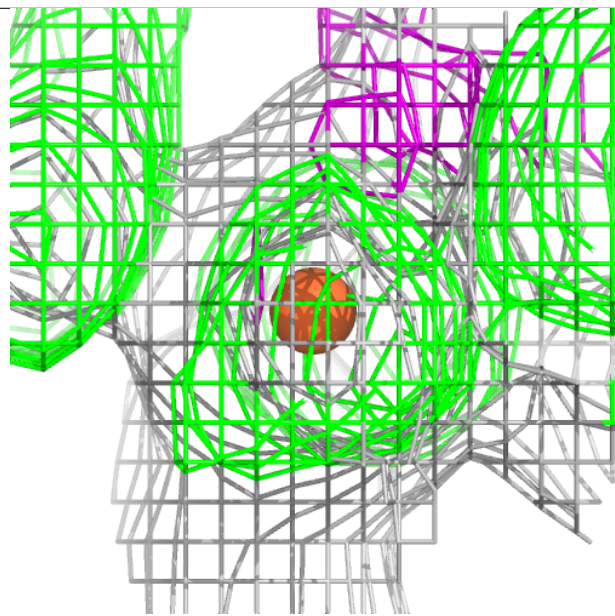
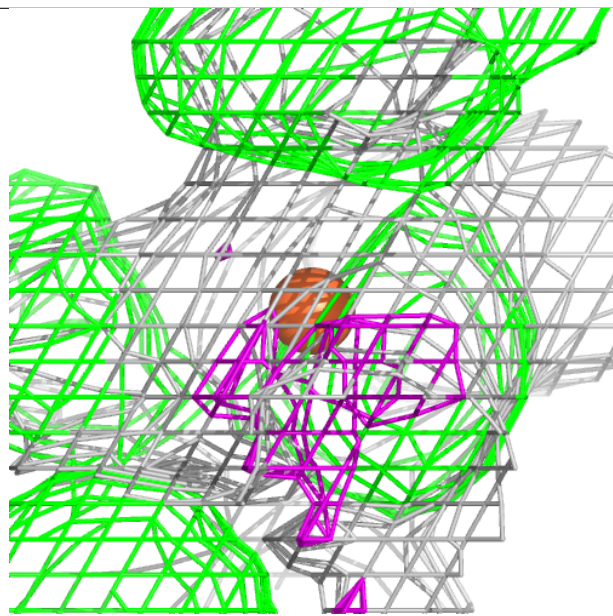
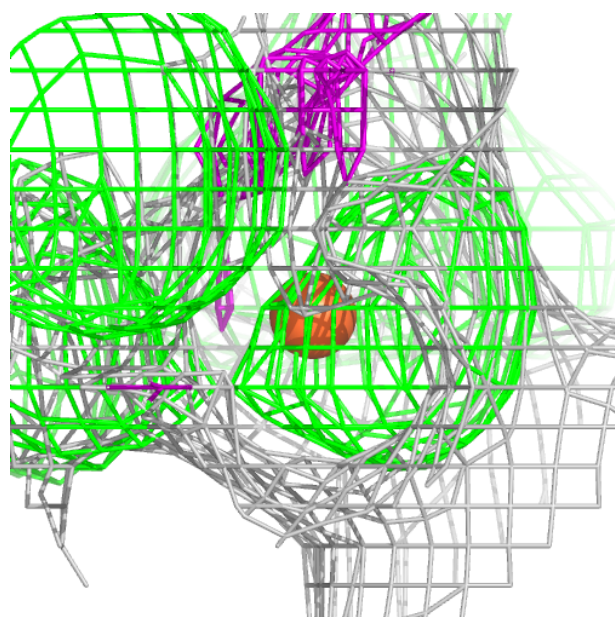
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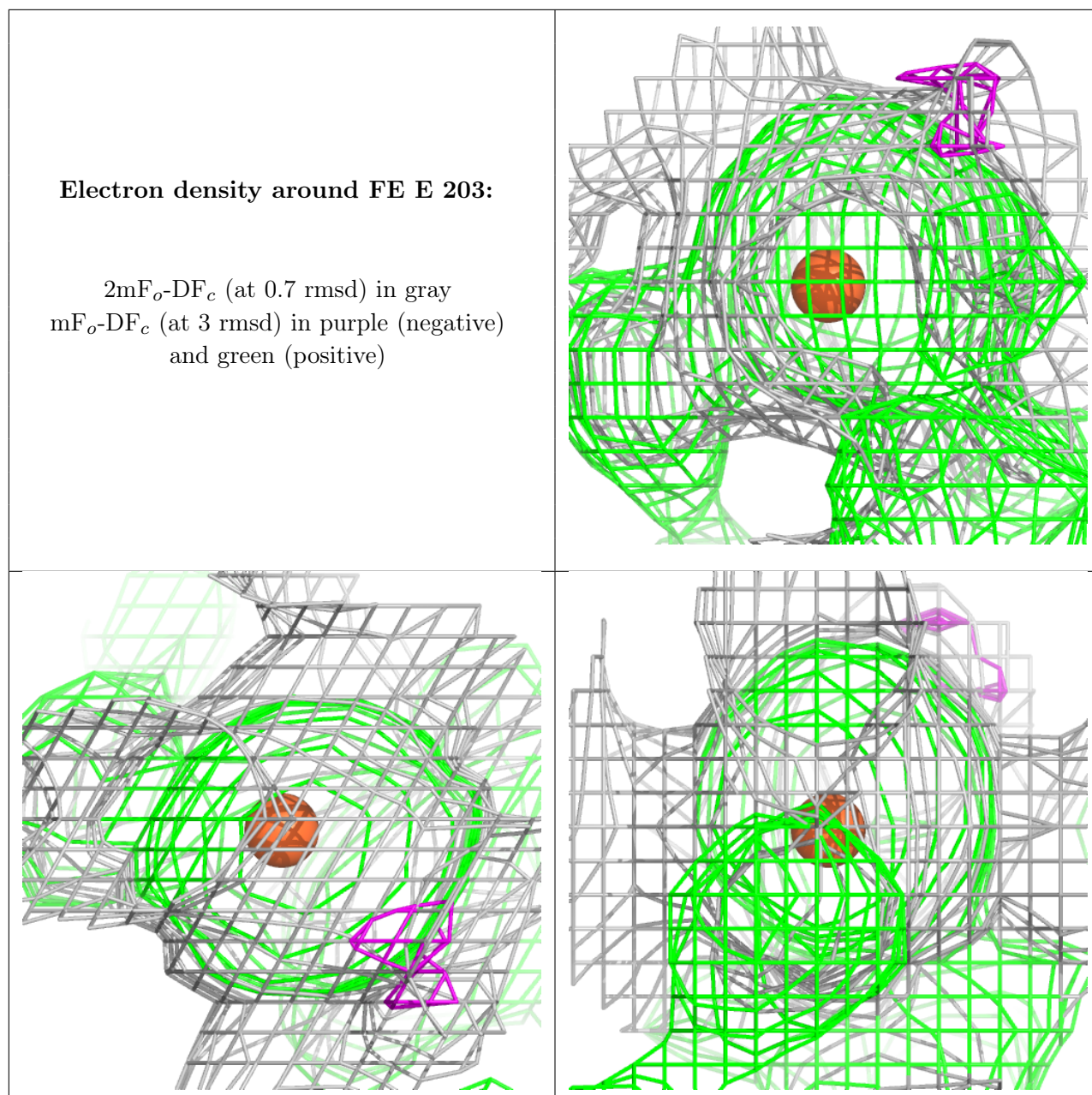
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE C 203:

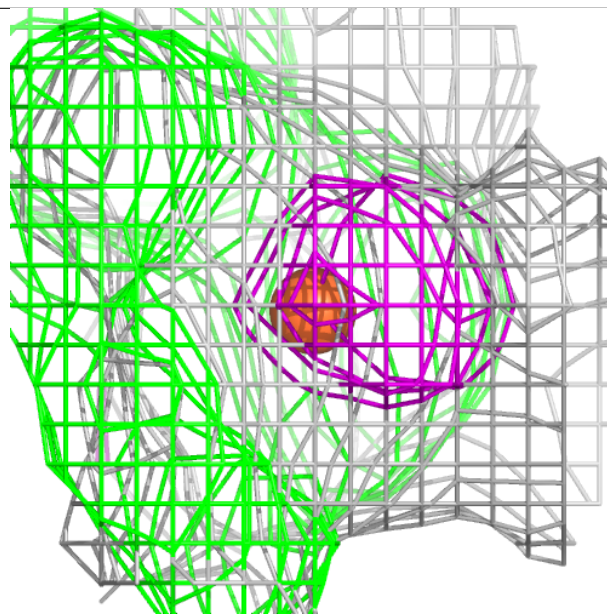
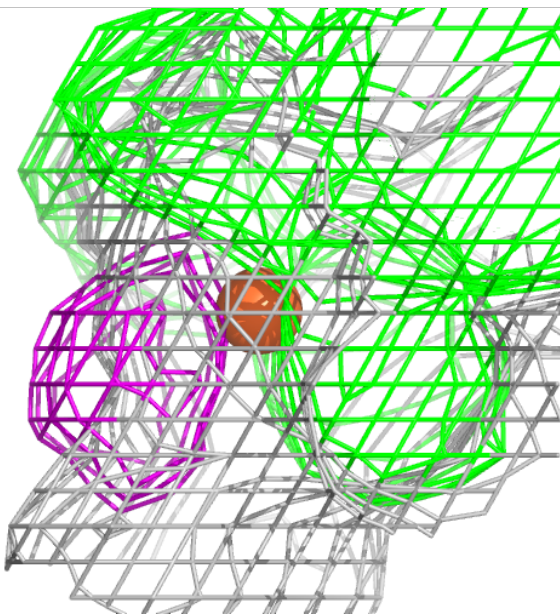
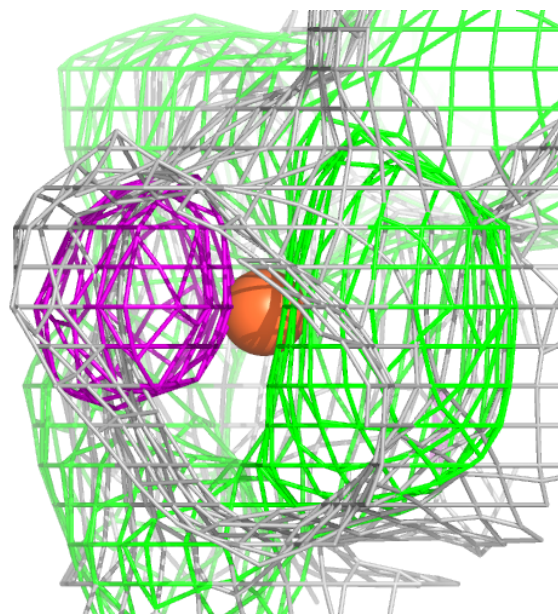
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

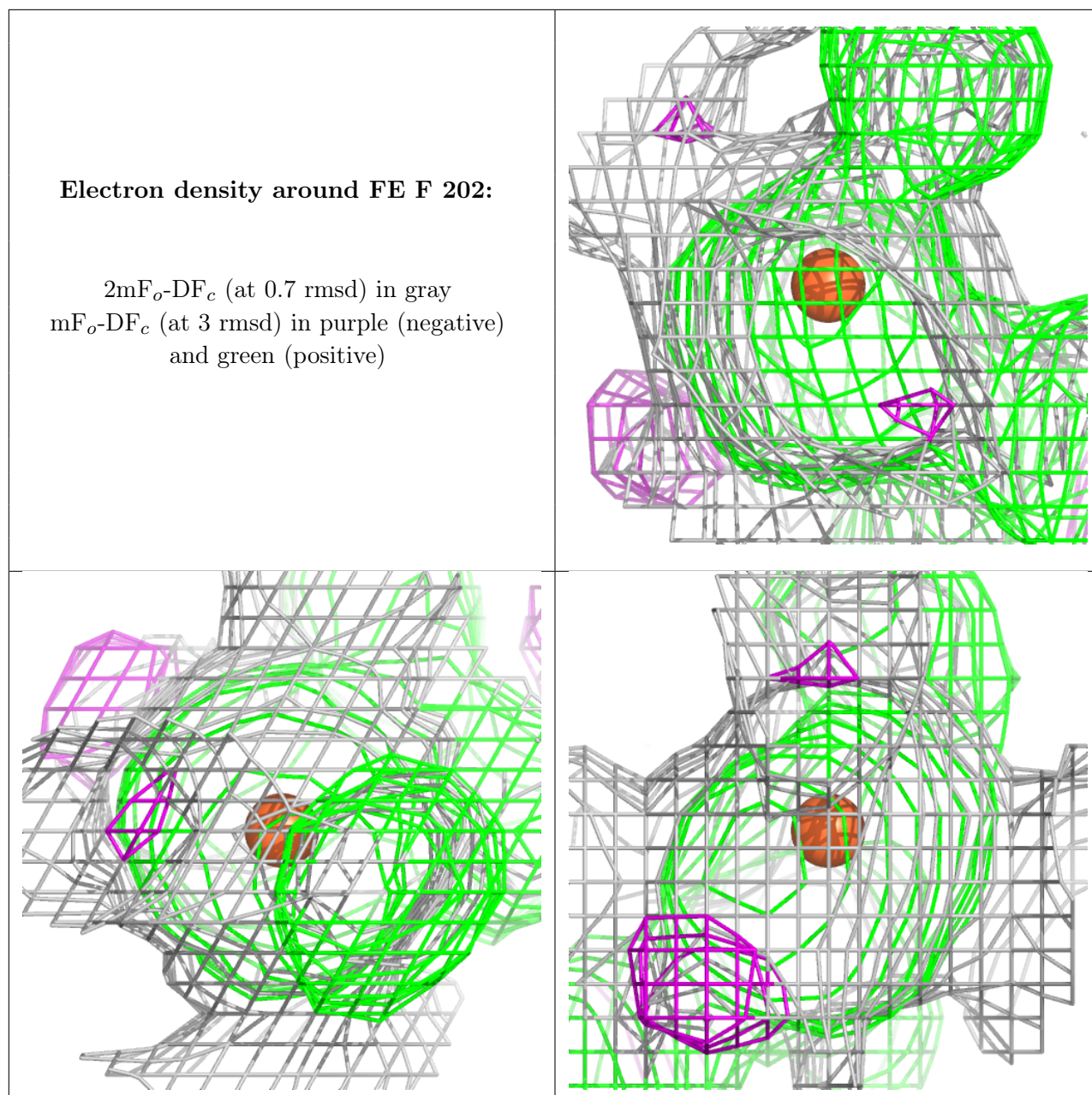




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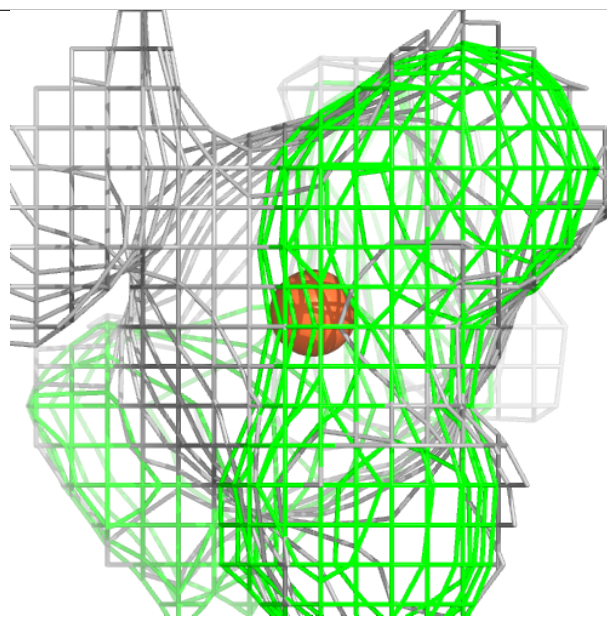
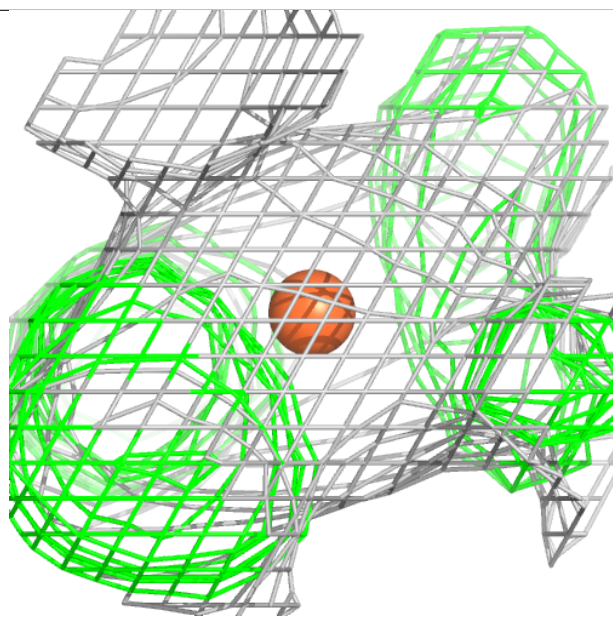
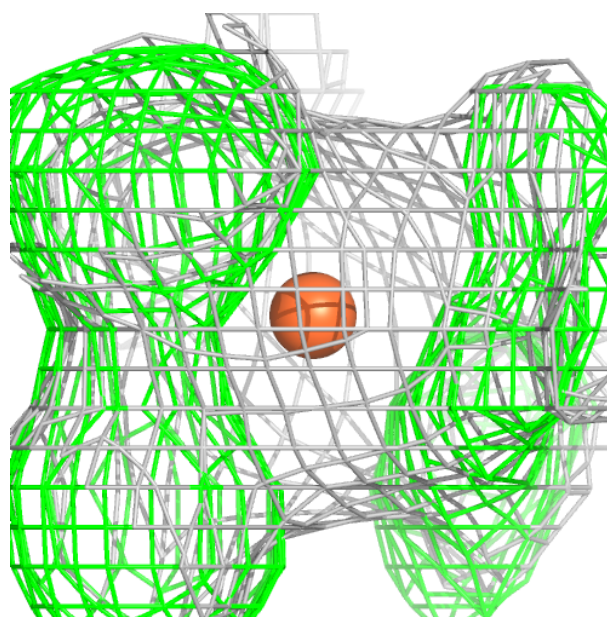
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

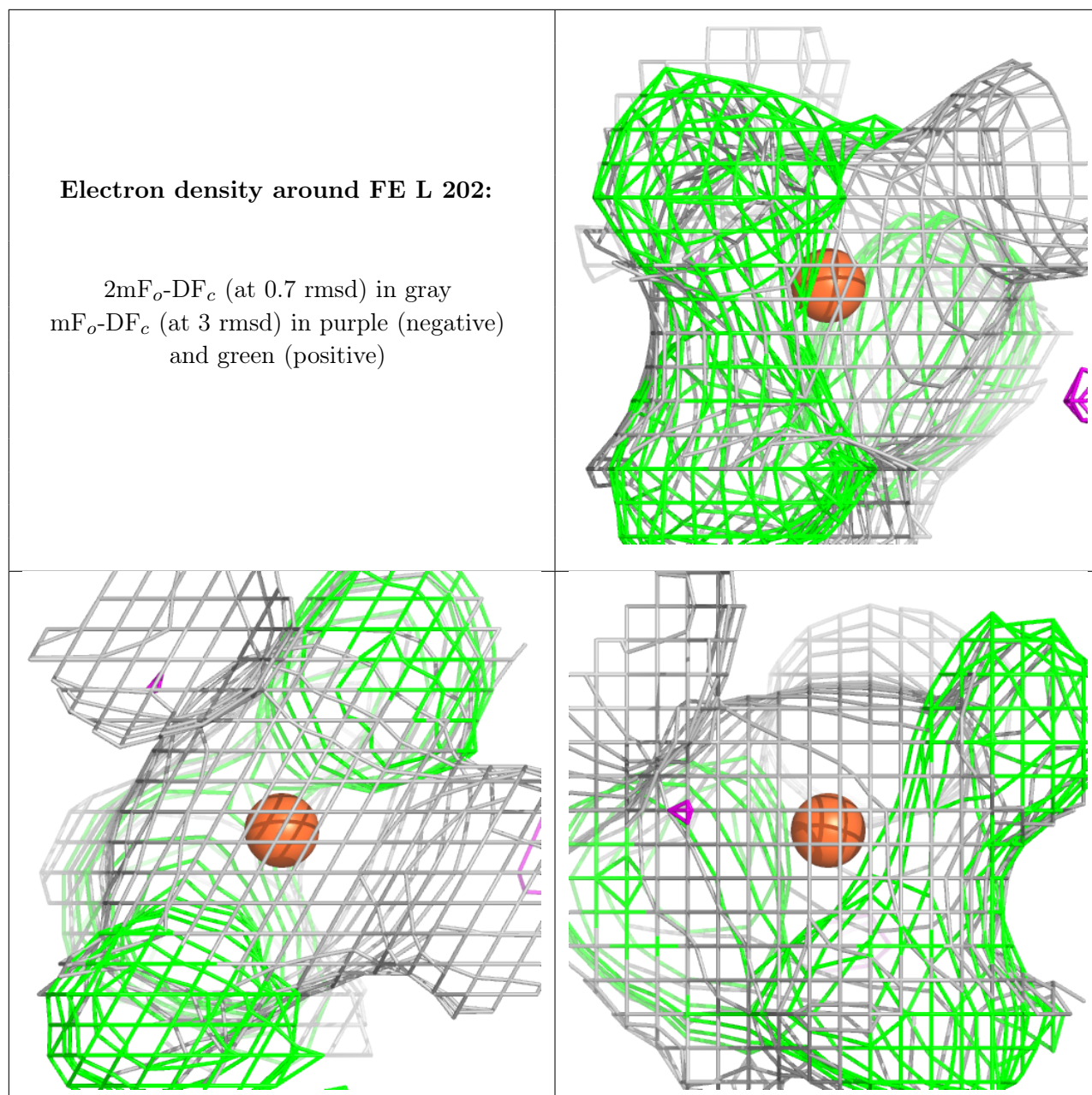


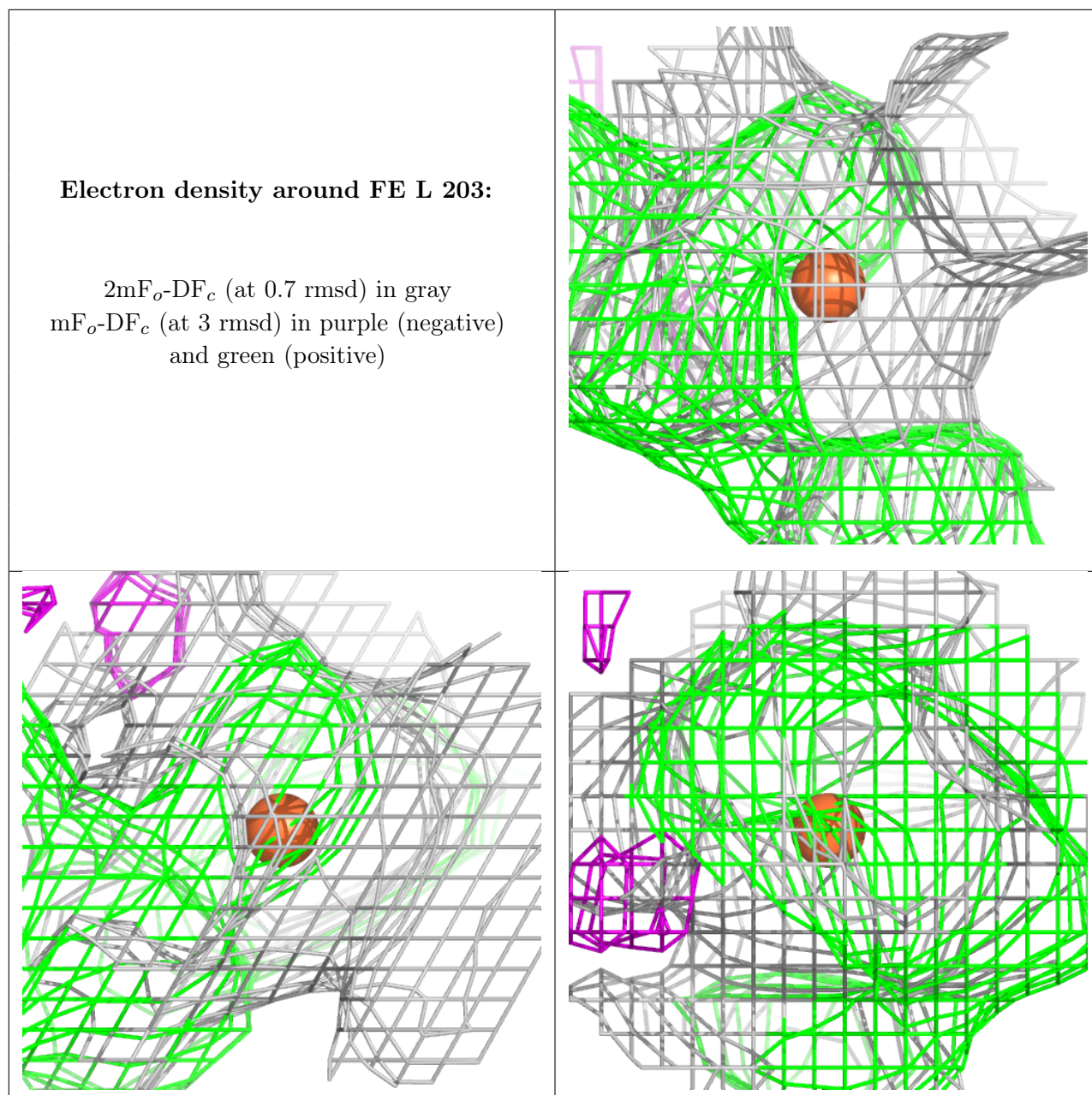


Electron density around FE H 202:

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and green (positive)

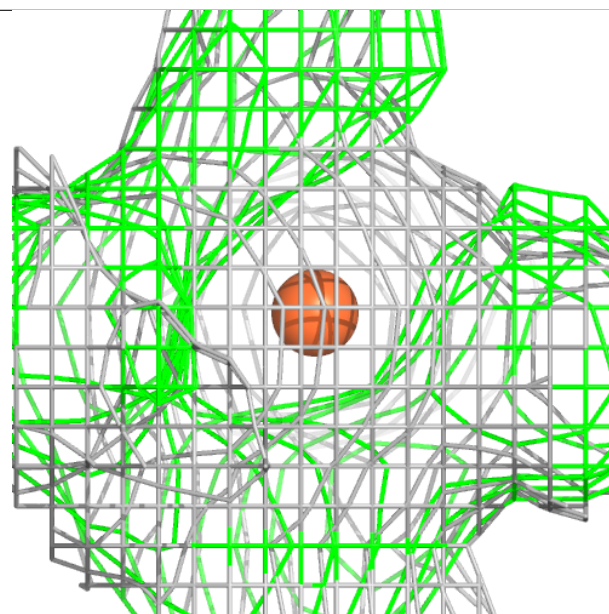
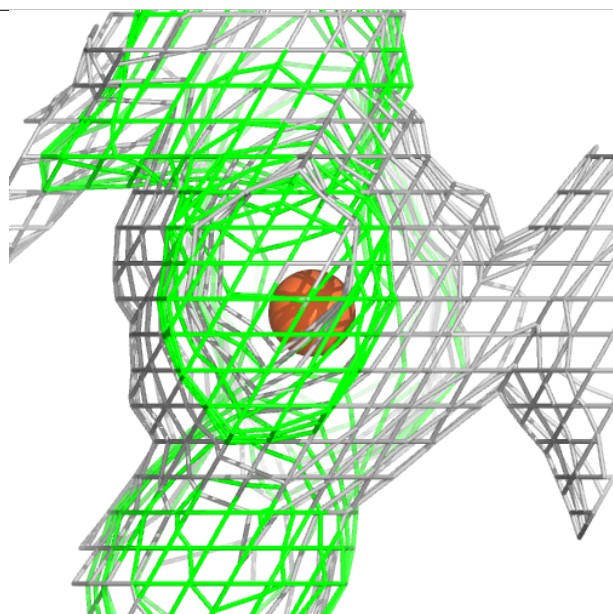
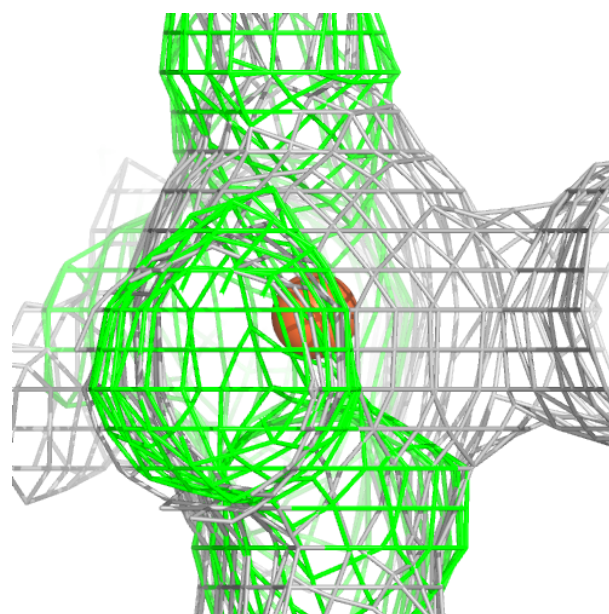






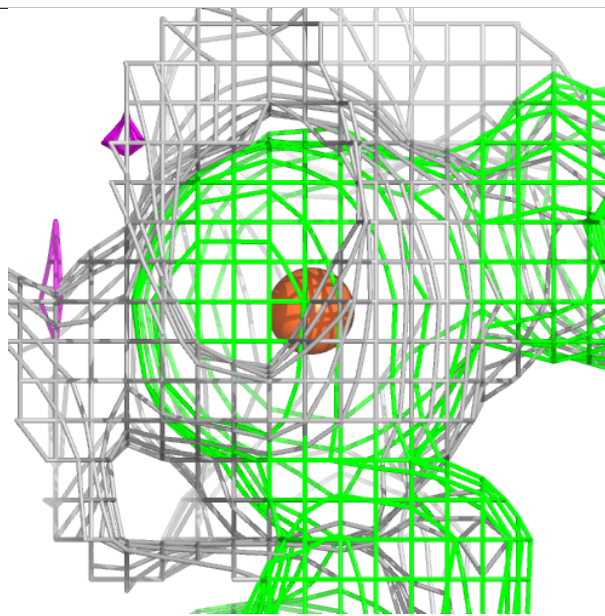
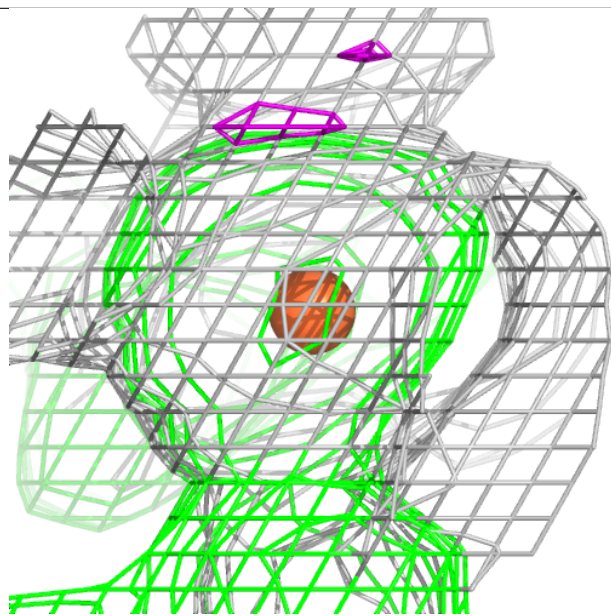
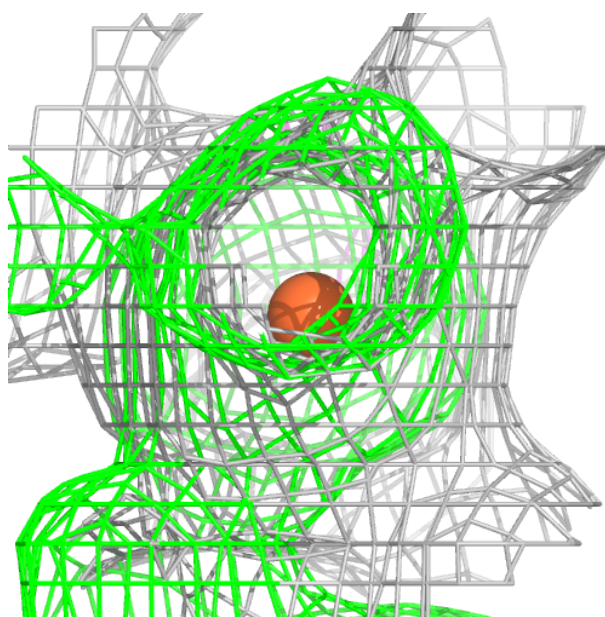
Electron density around FE J 203:

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



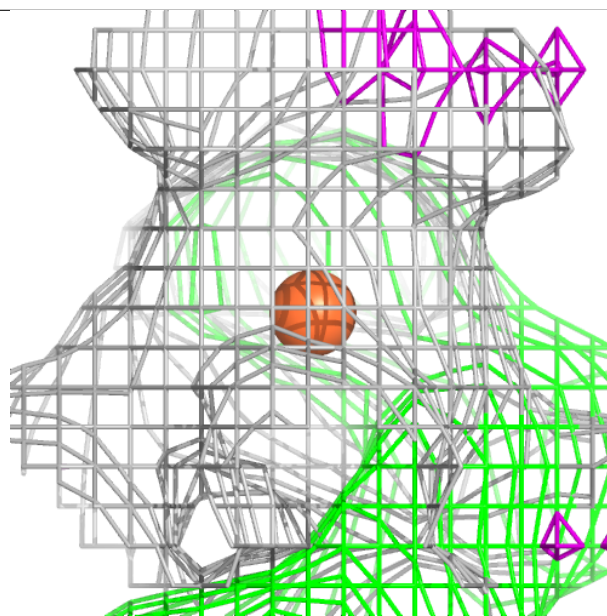
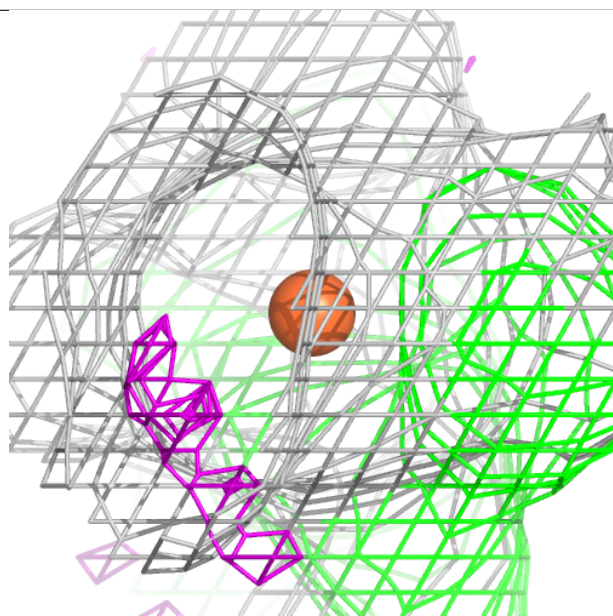
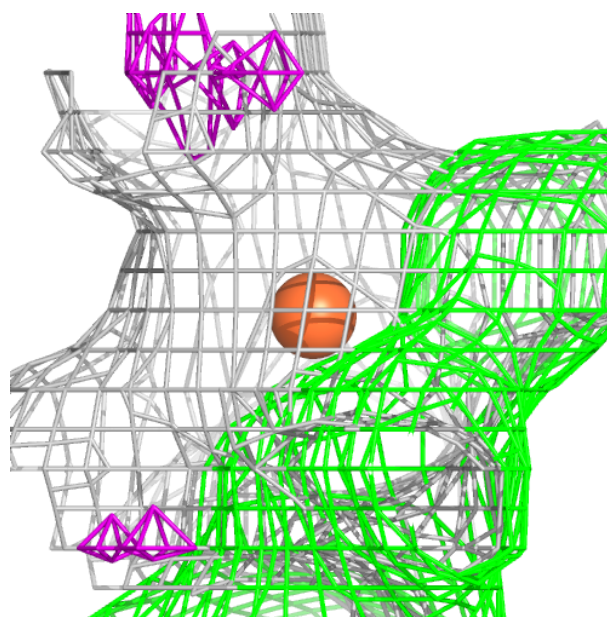
Electron density around FE A 203:

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and green (positive)



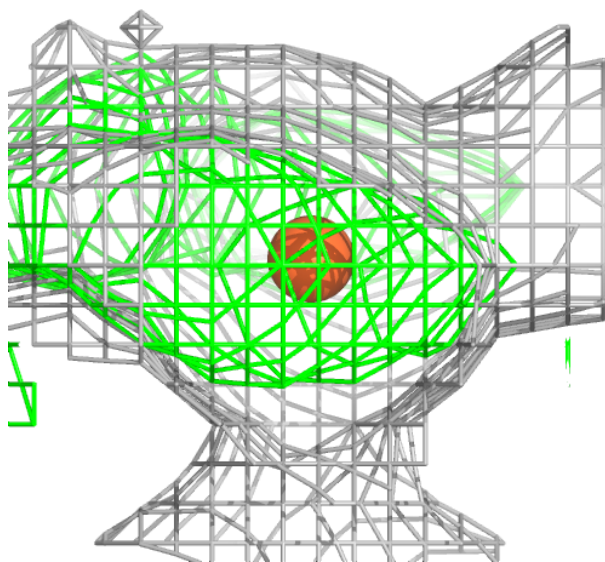
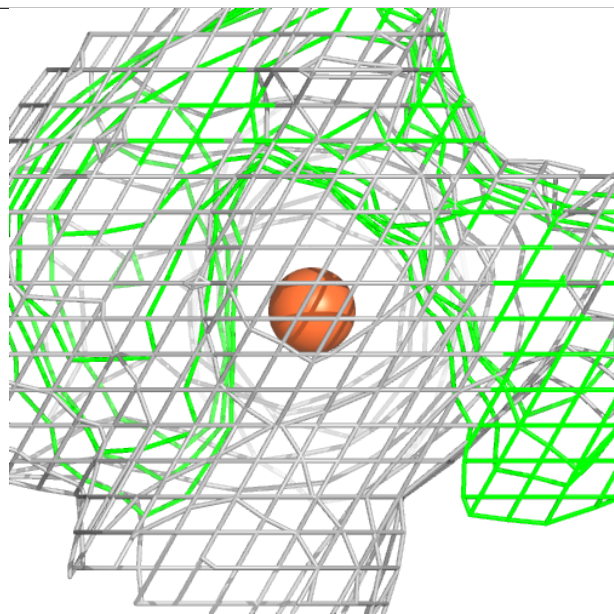
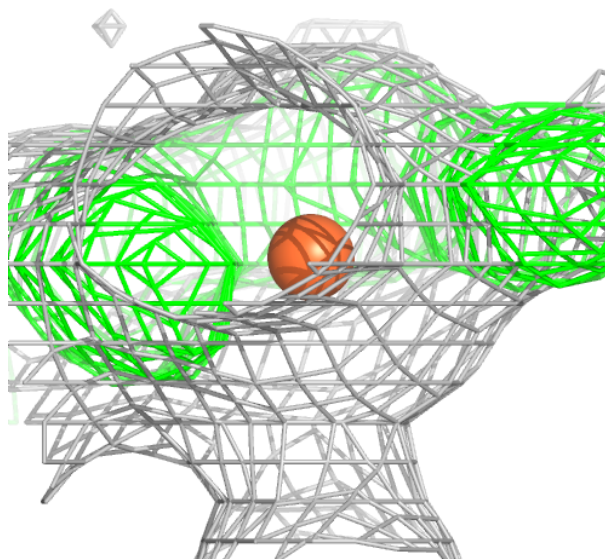
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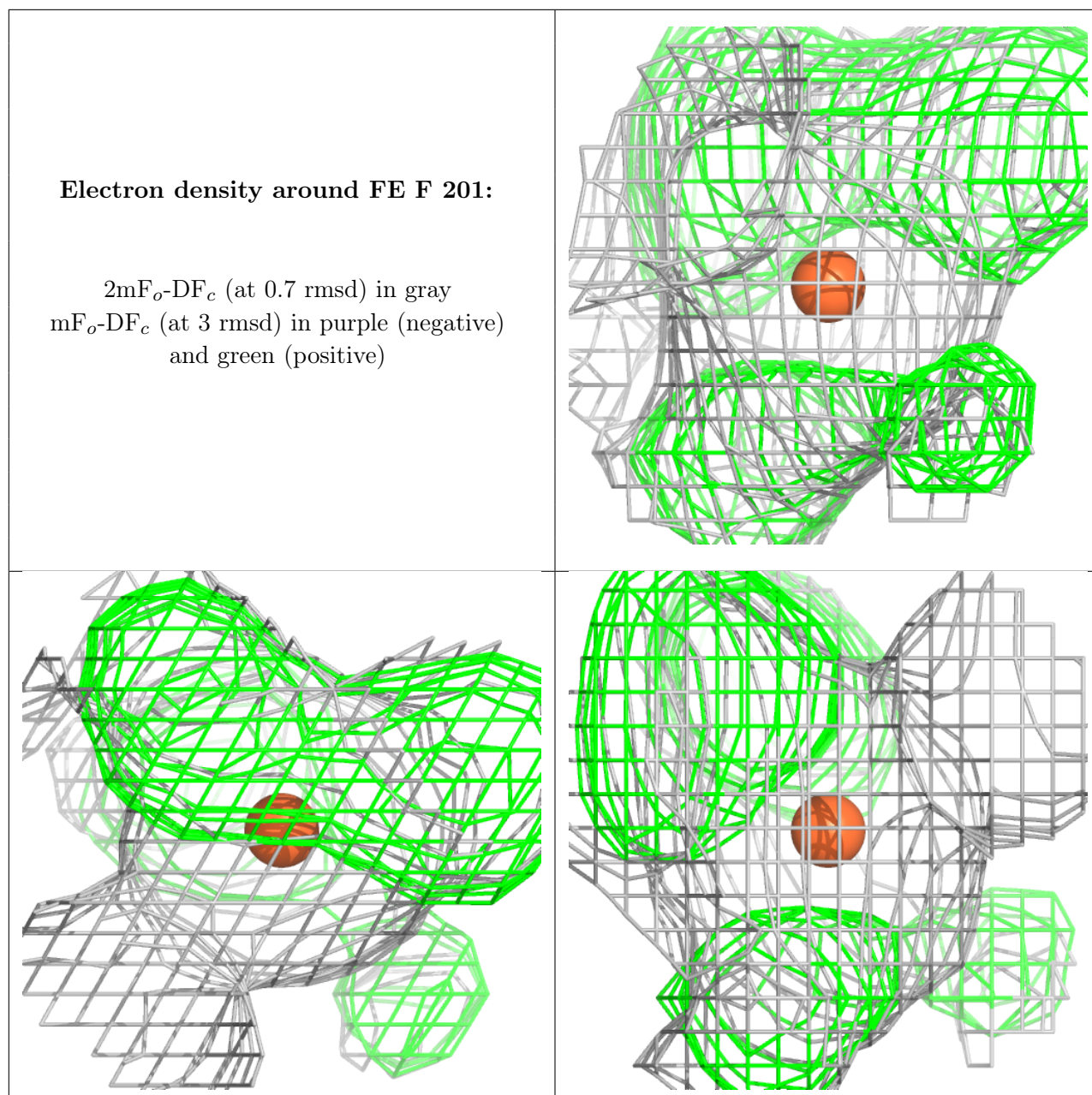
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and green (positive)



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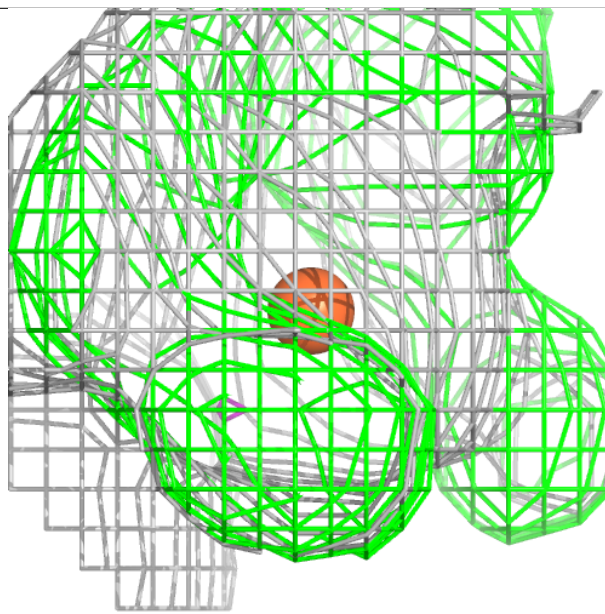
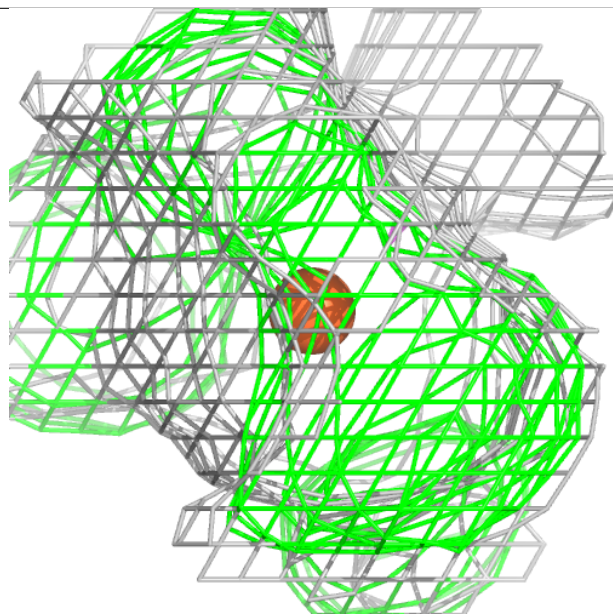
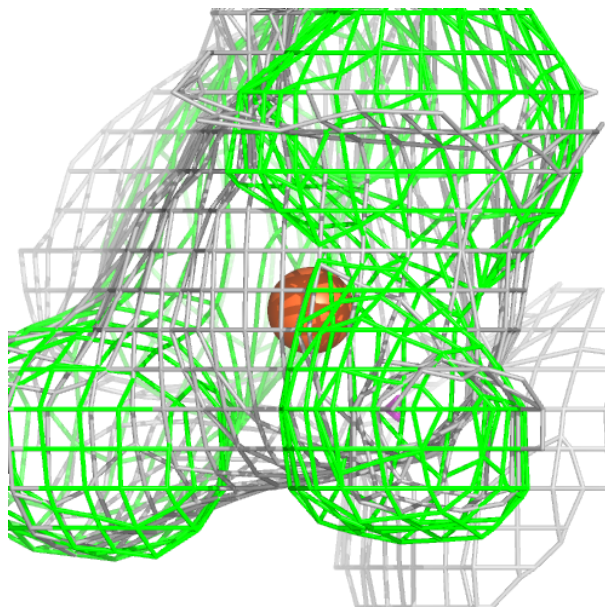
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





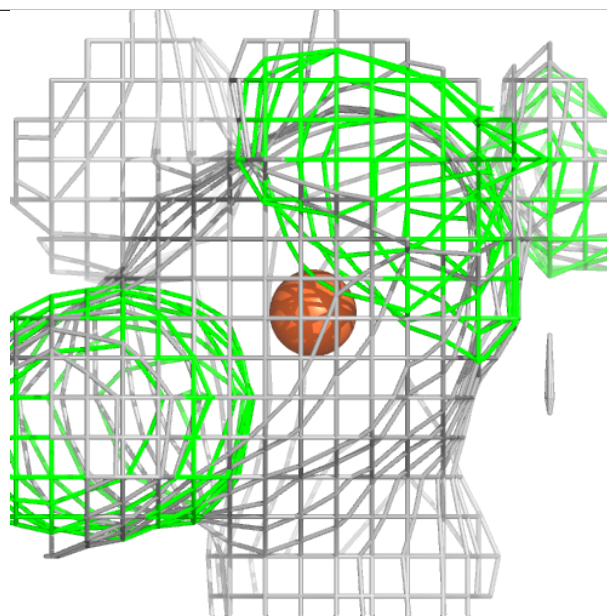
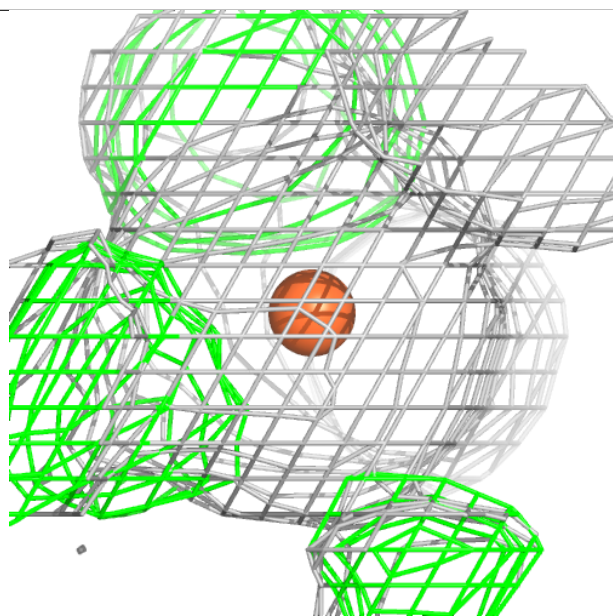
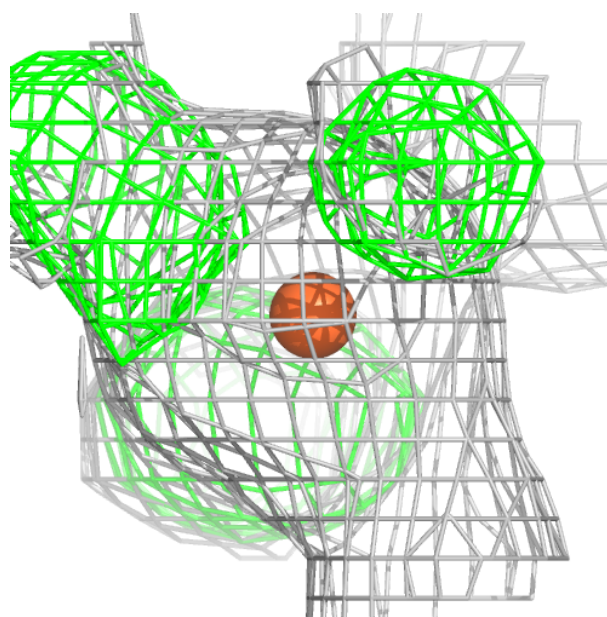
Electron density around FE D 203:

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and green (positive)



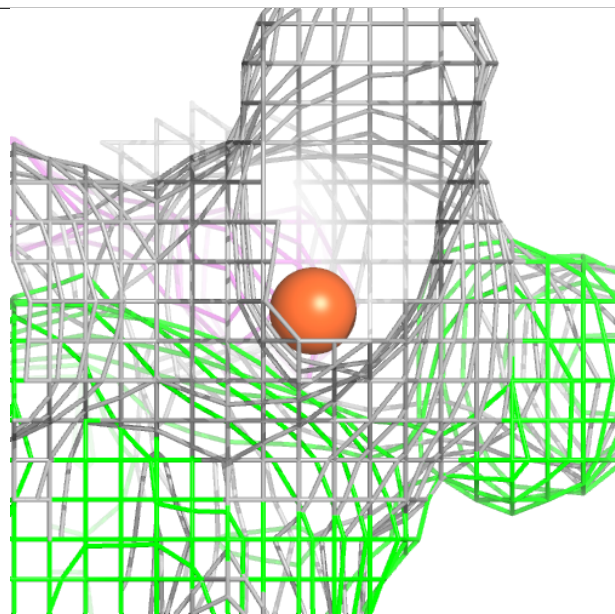
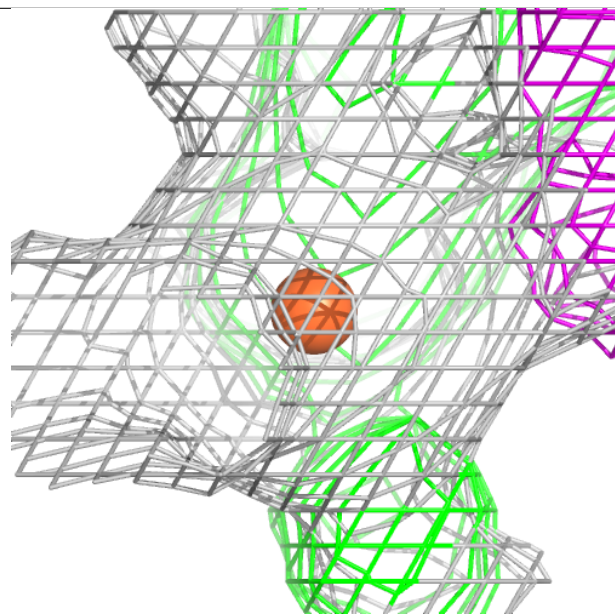
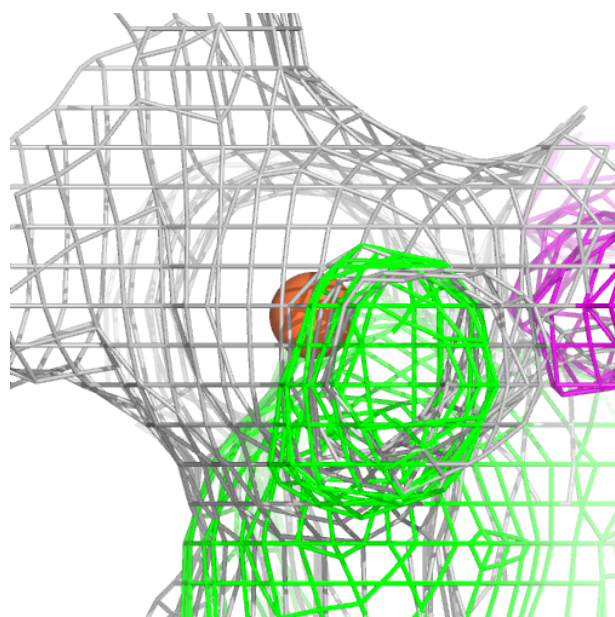
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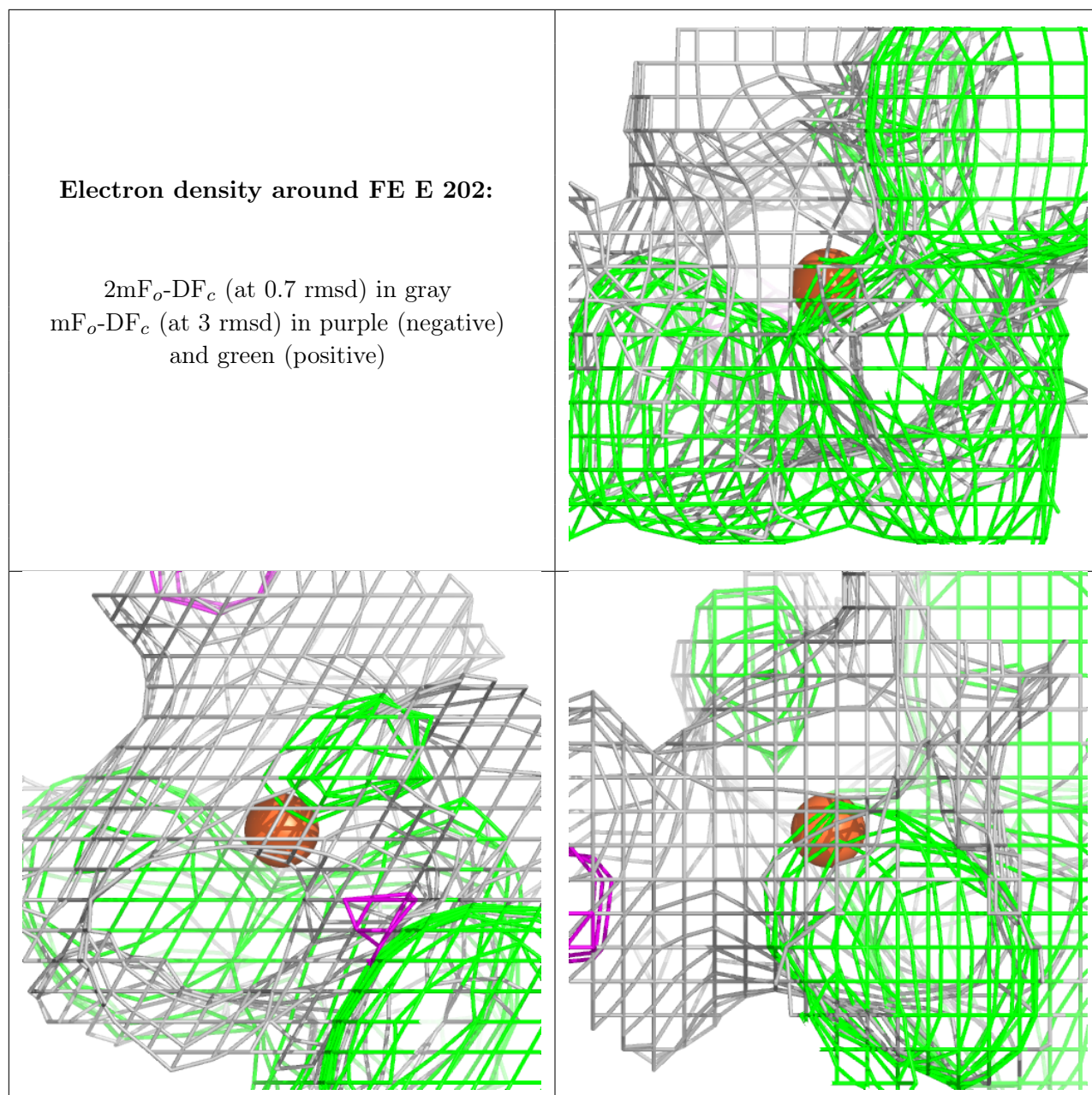
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and green (positive)



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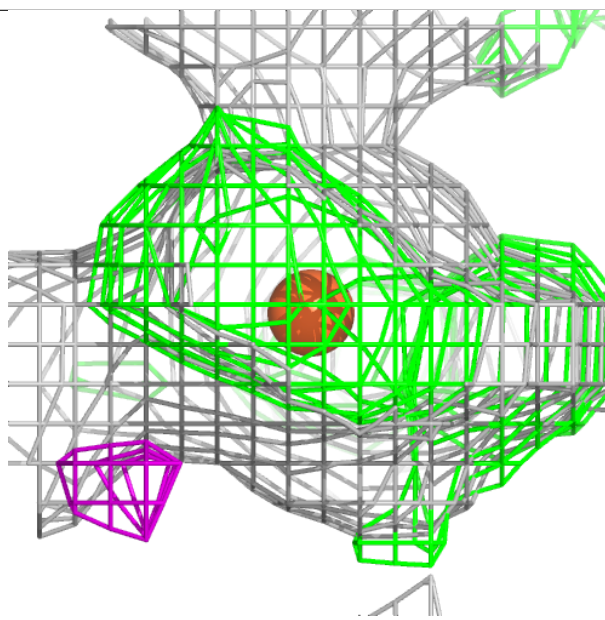
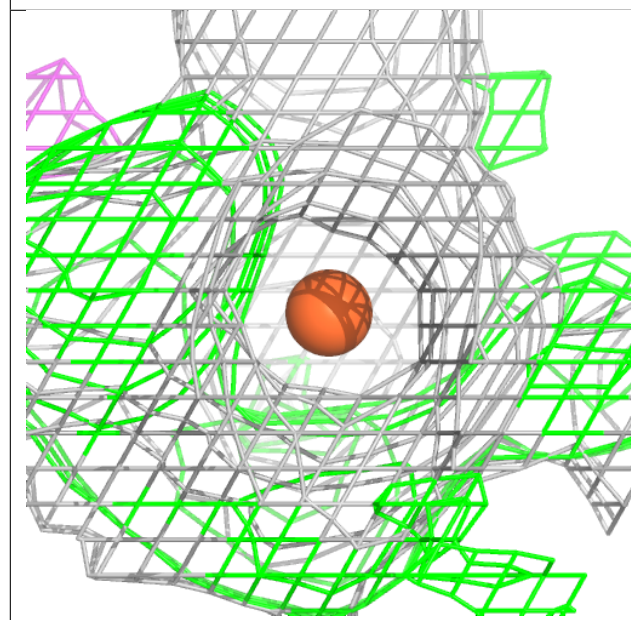
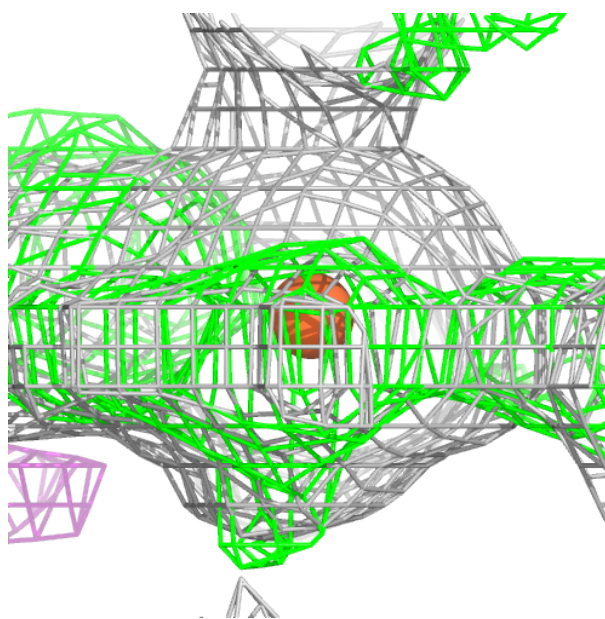
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and green (positive)





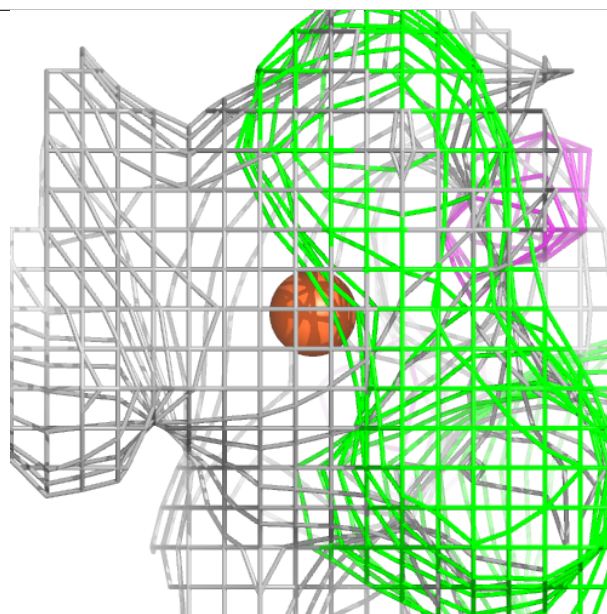
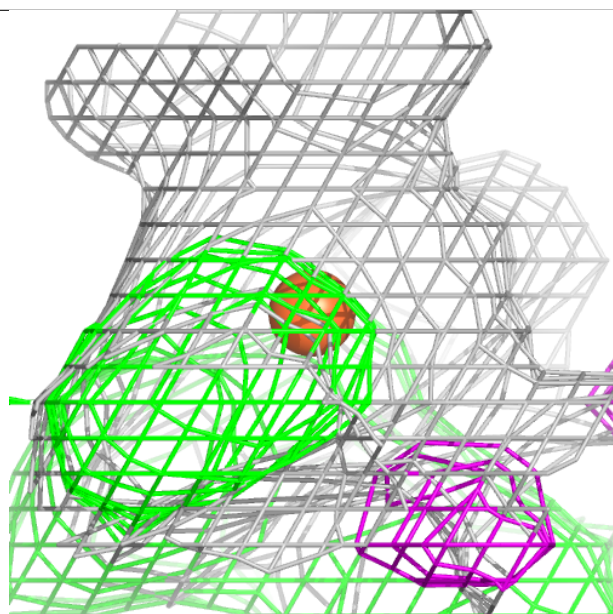
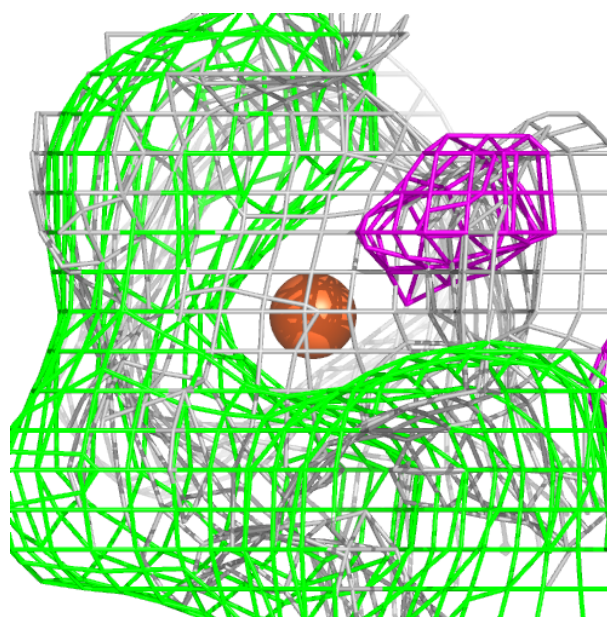
Electron density around FE K 203:

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and green (positive)



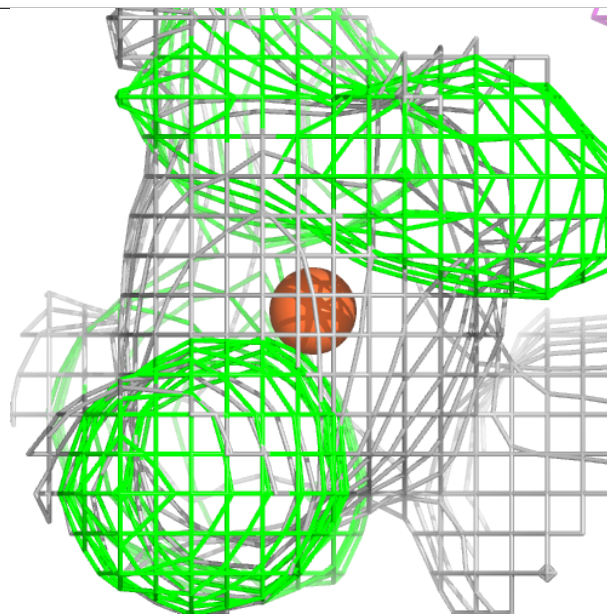
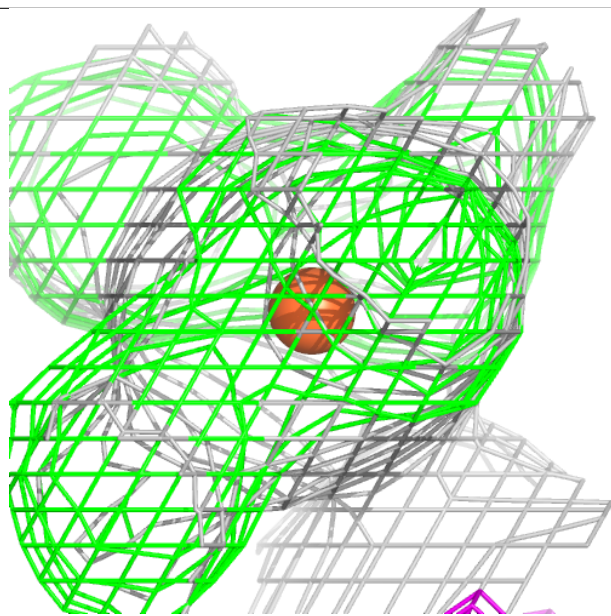
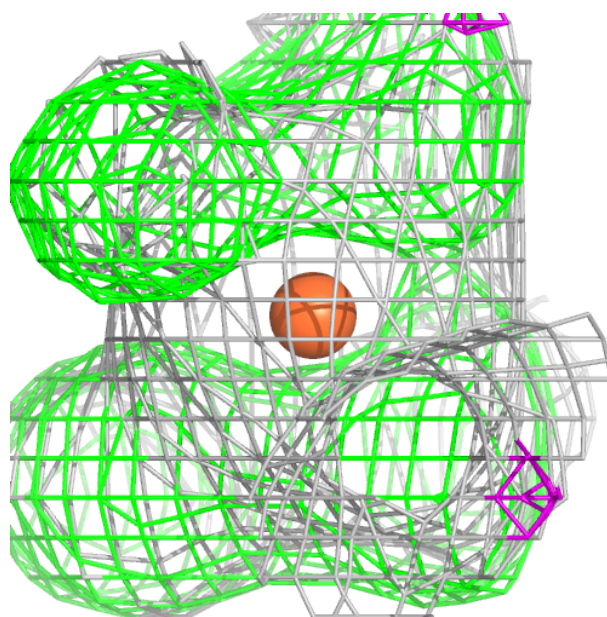
Electron density around FE G 202:

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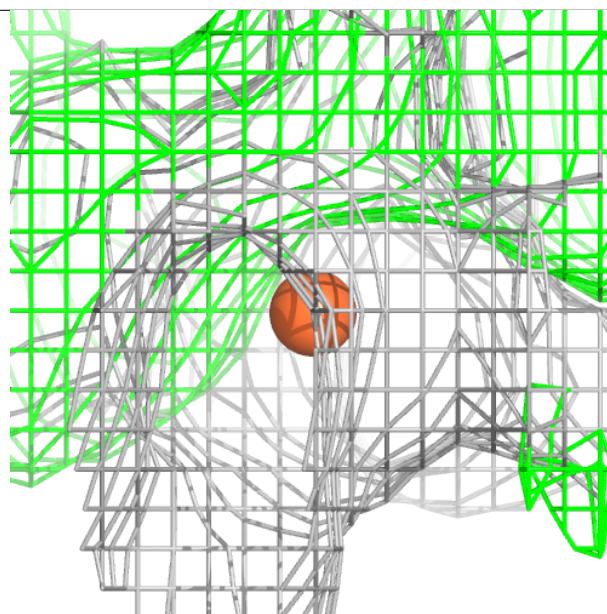
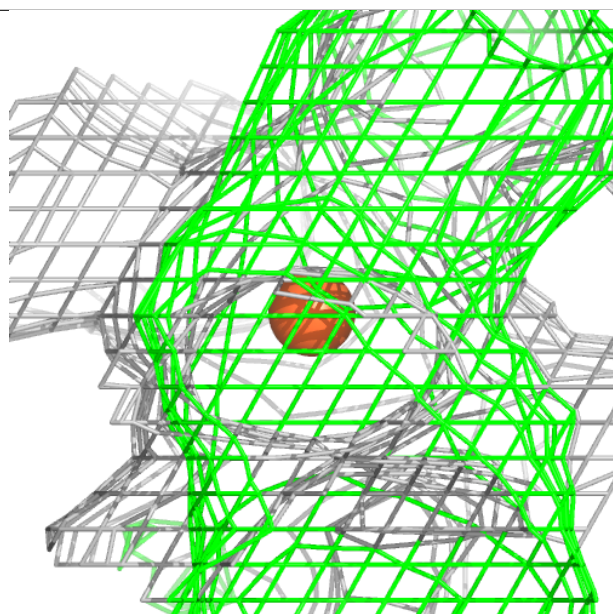
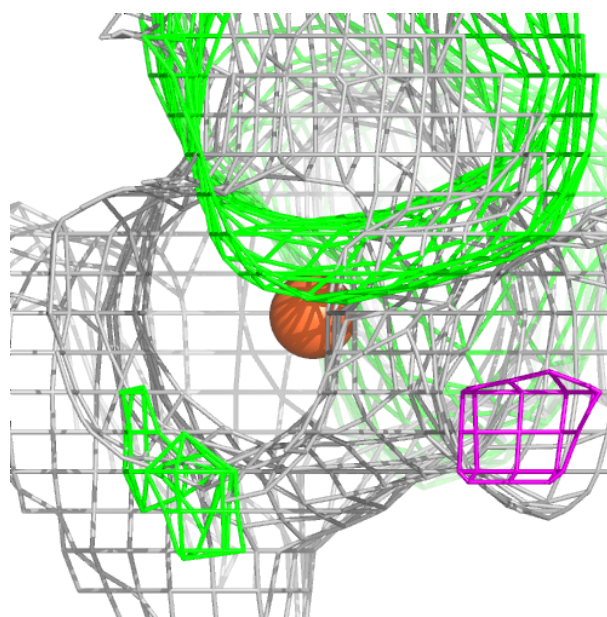
Electron density around FE G 203:

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and green (positive)



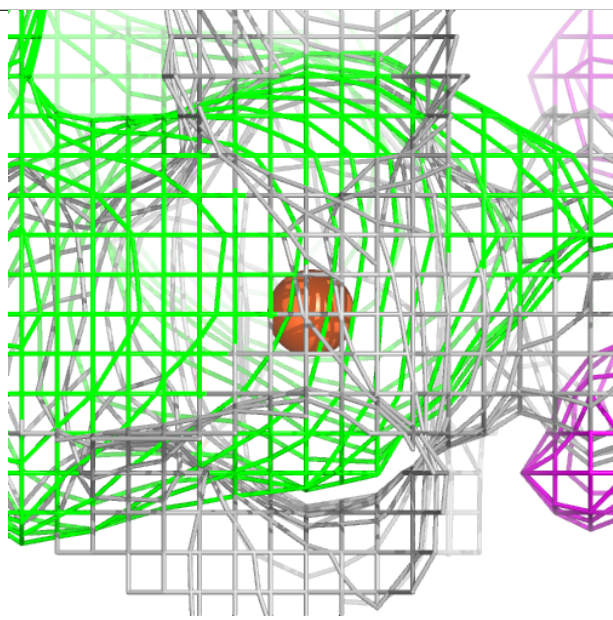
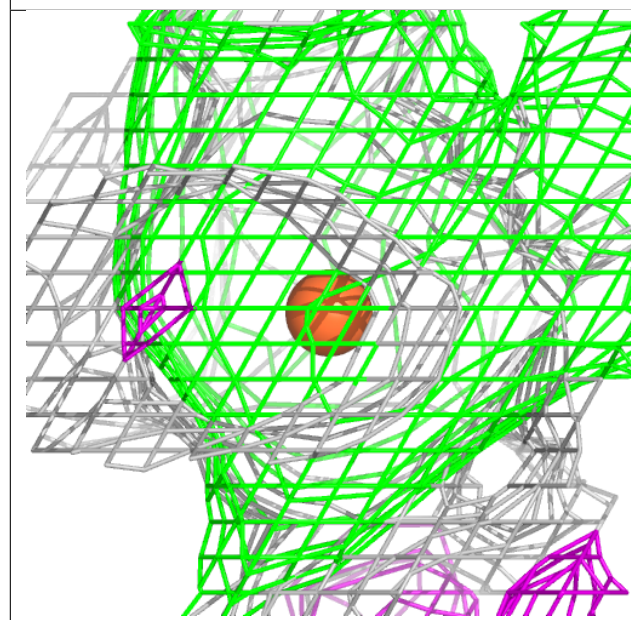
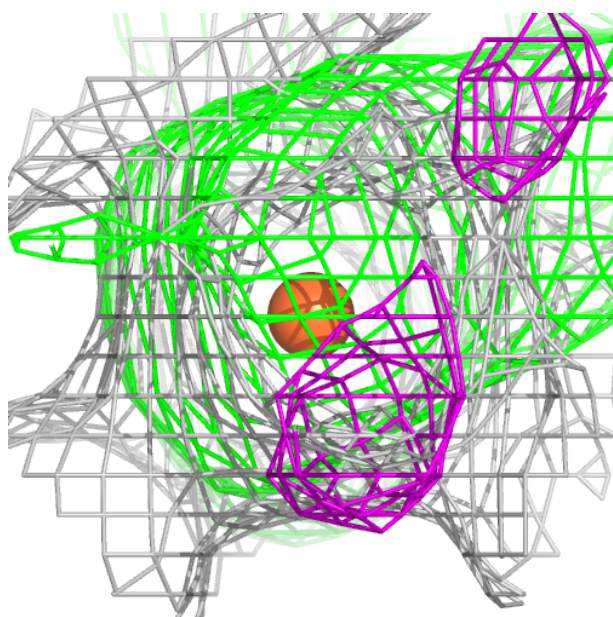
Electron density around FE B 202:

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and green (positive)



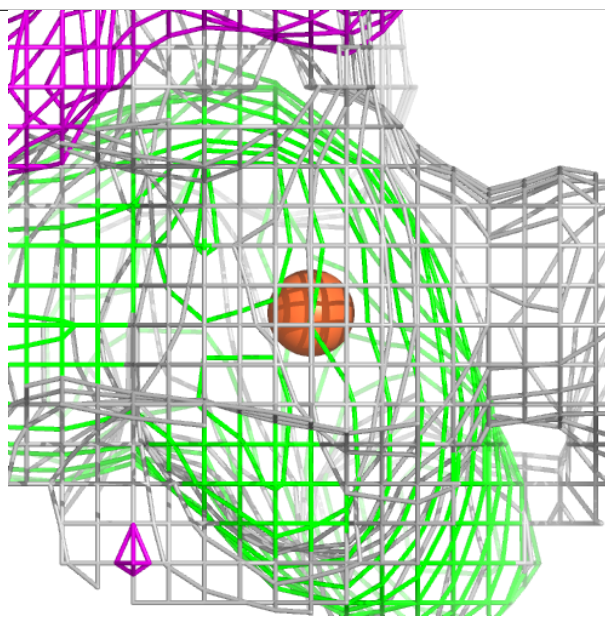
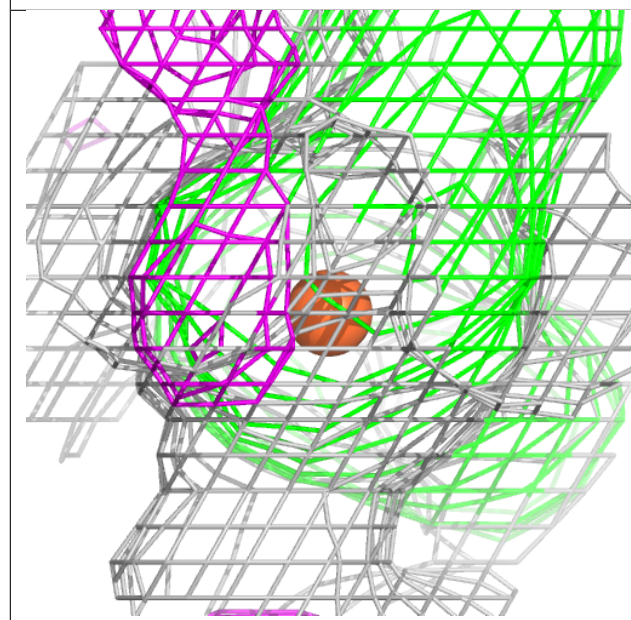
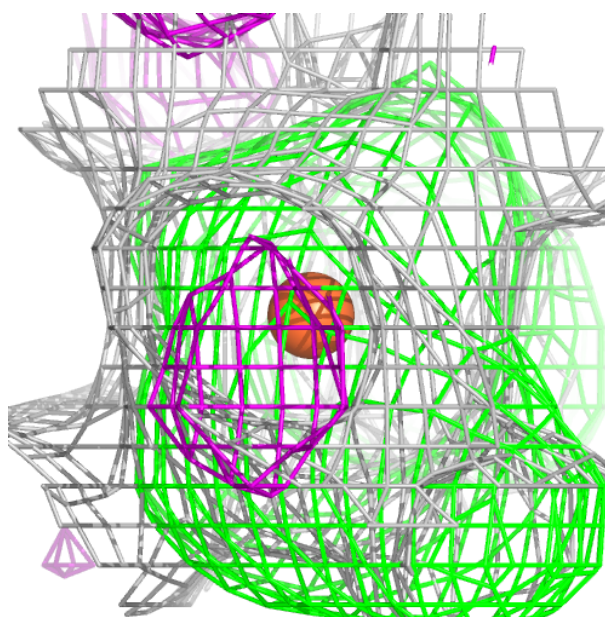
Electron density around FE D 201:

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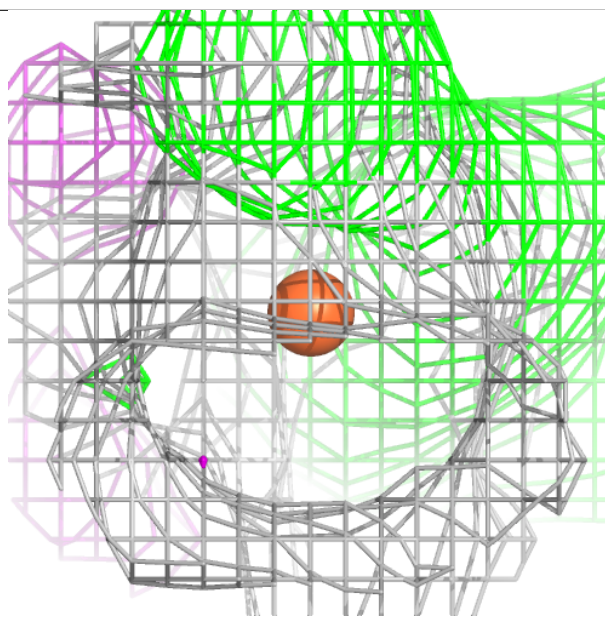
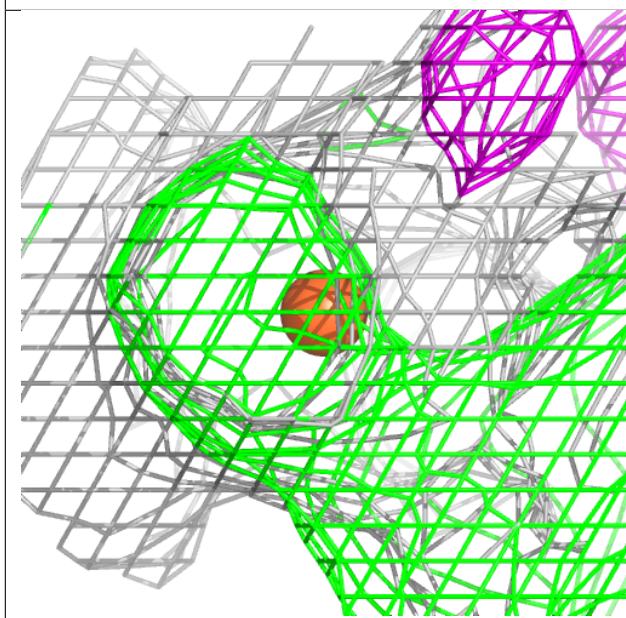
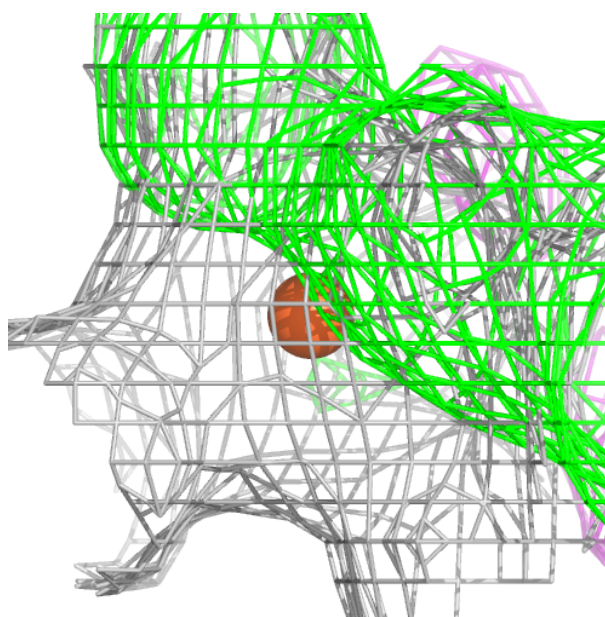
Electron density around FE J 201:

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and green (positive)



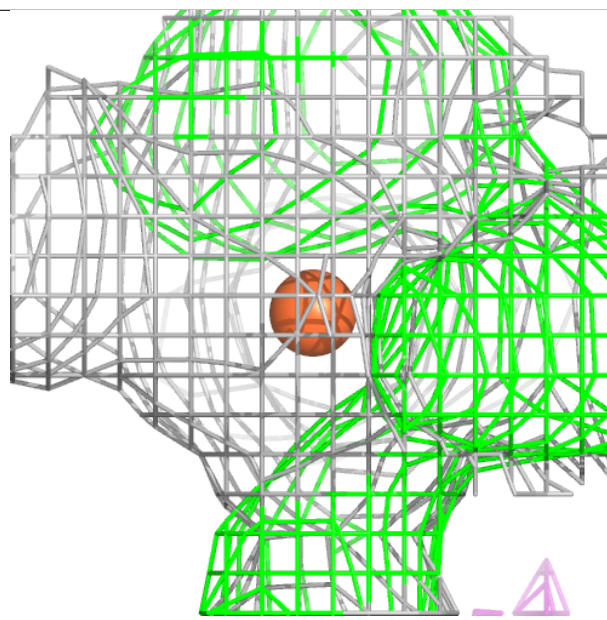
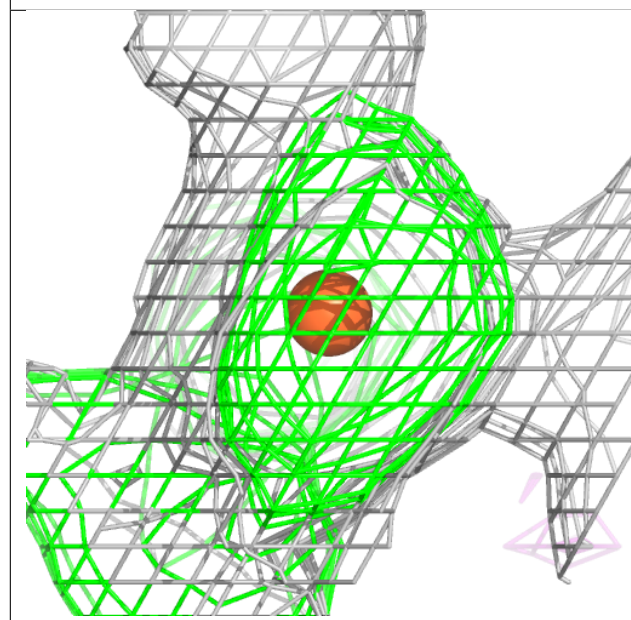
Electron density around FE D 202:

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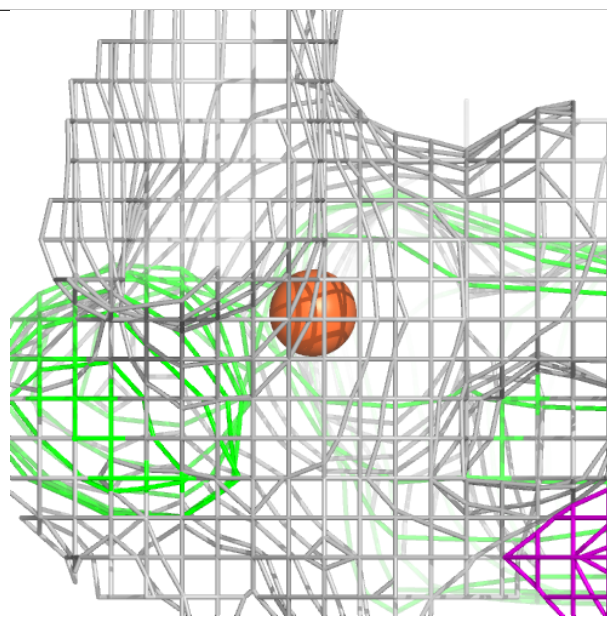
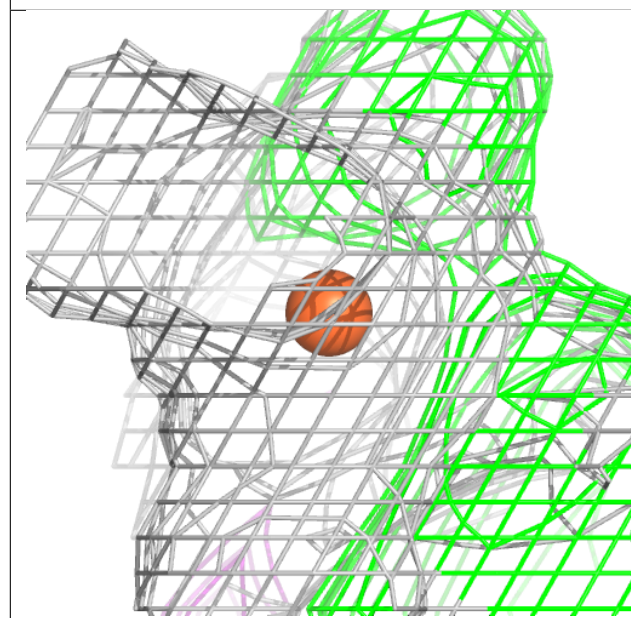
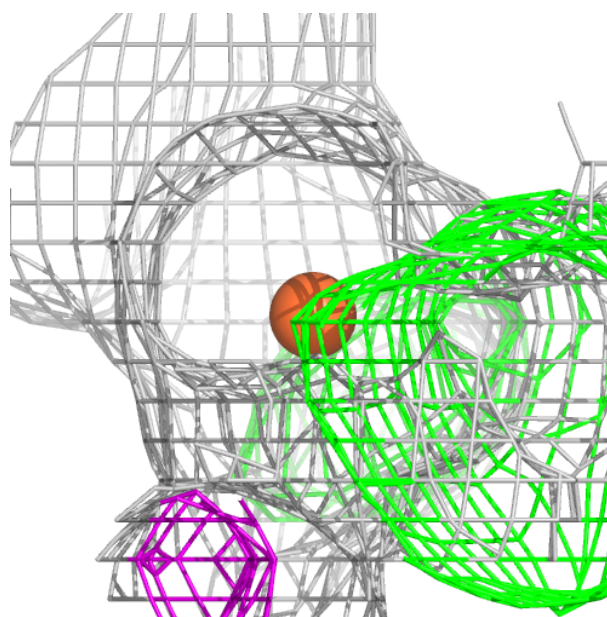
Electron density around FE B 203:

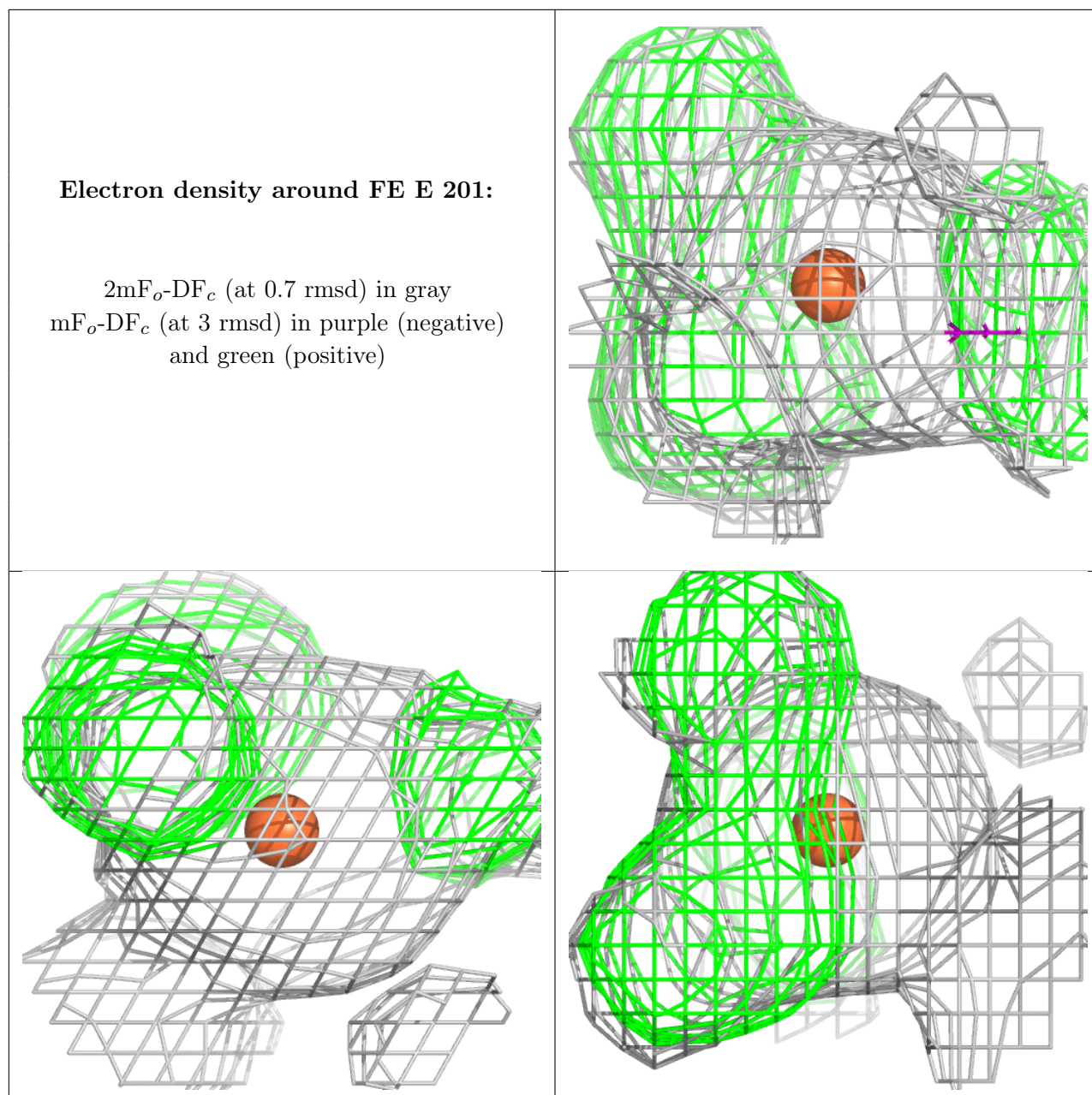
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around FE K 202:

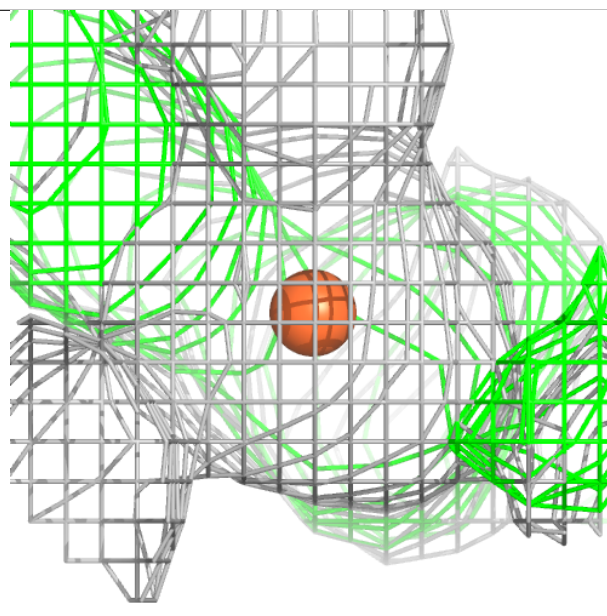
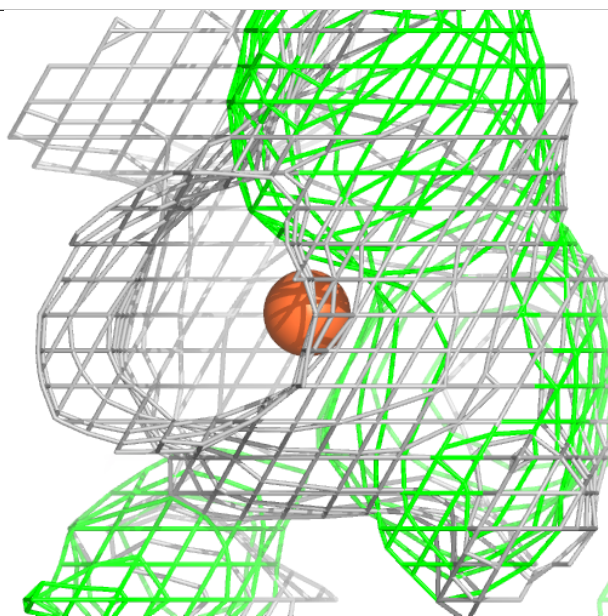
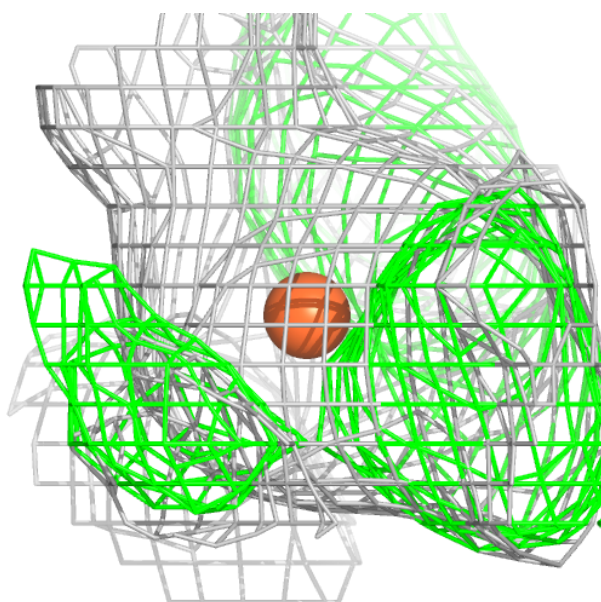
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)





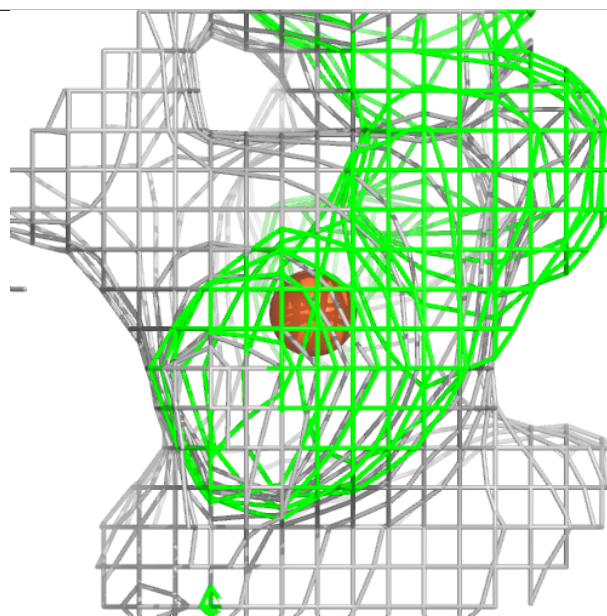
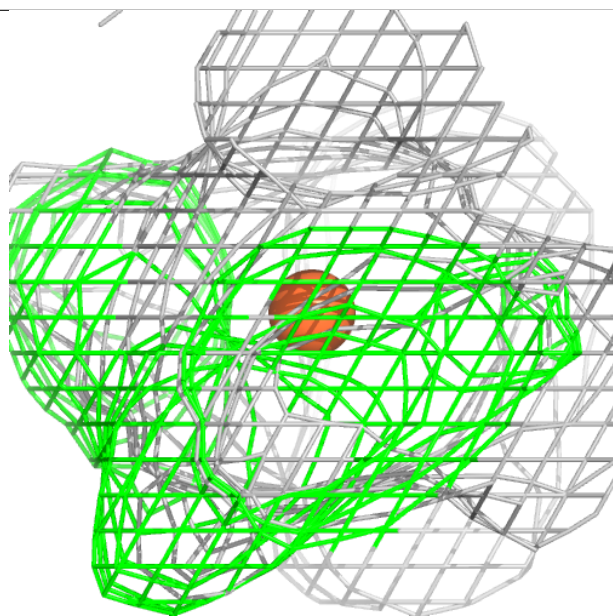
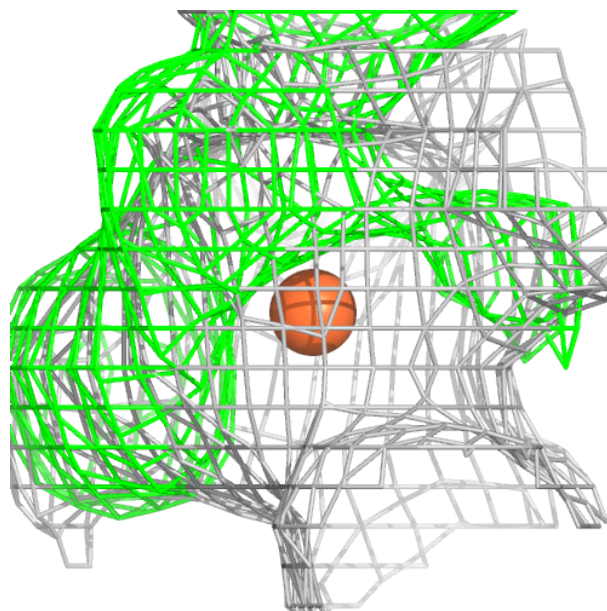
Electron density around FE A 202:

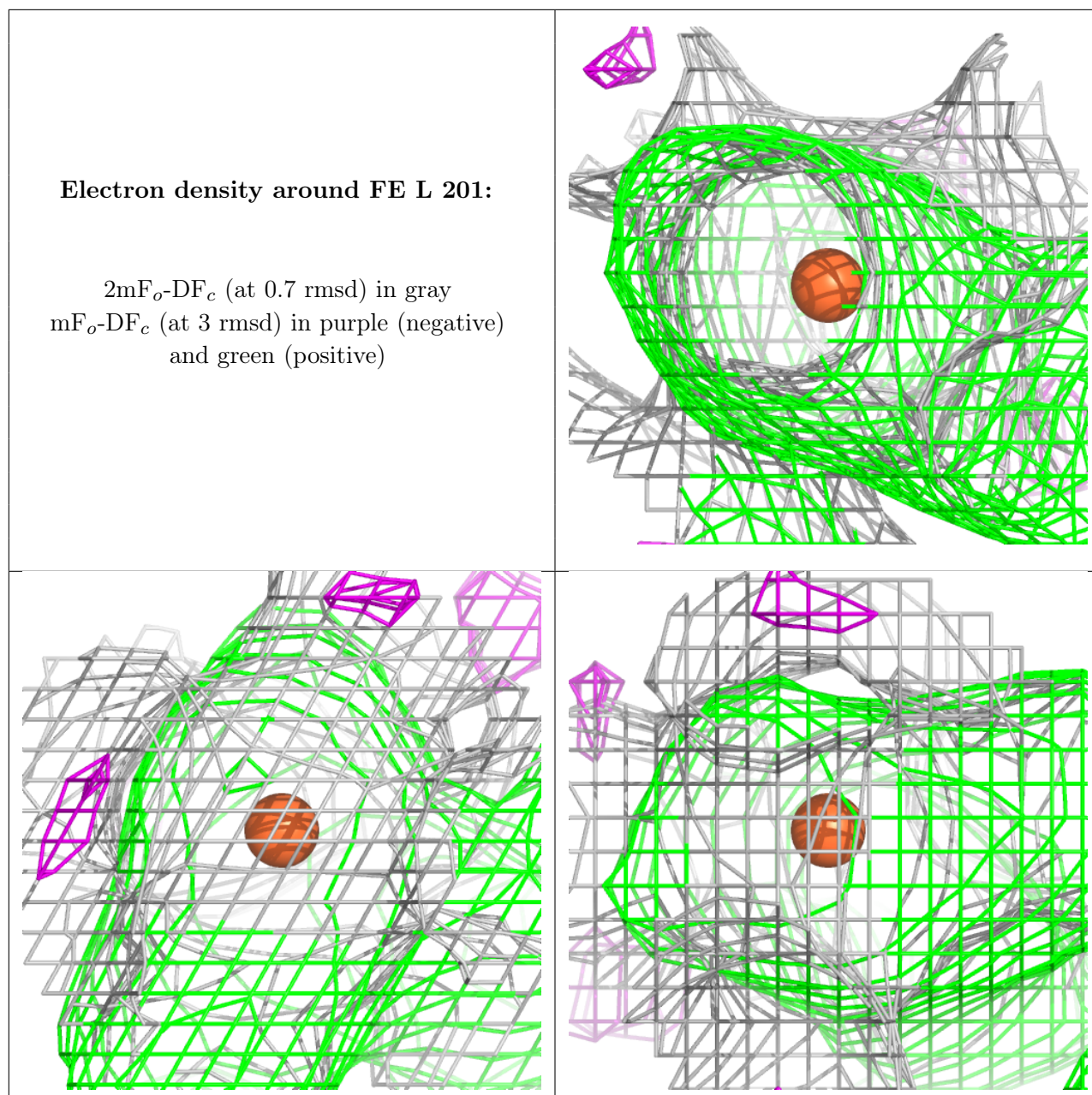
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 201:

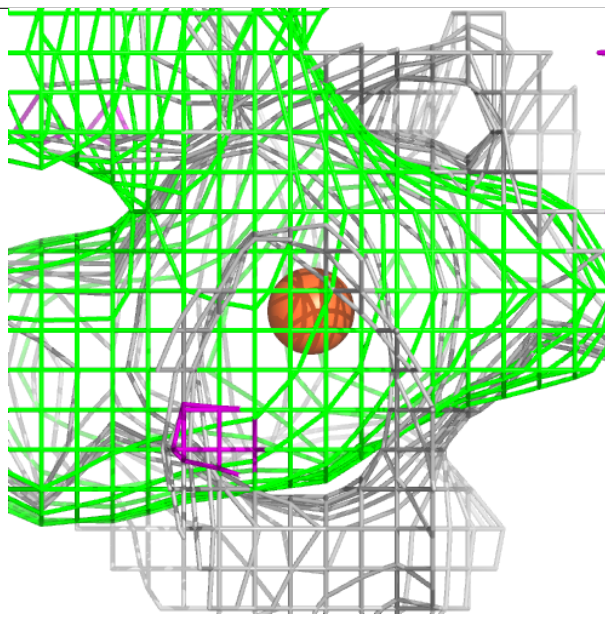
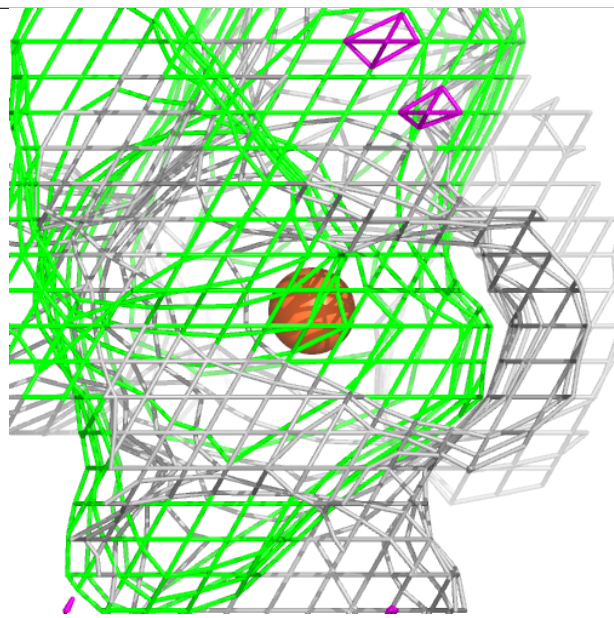
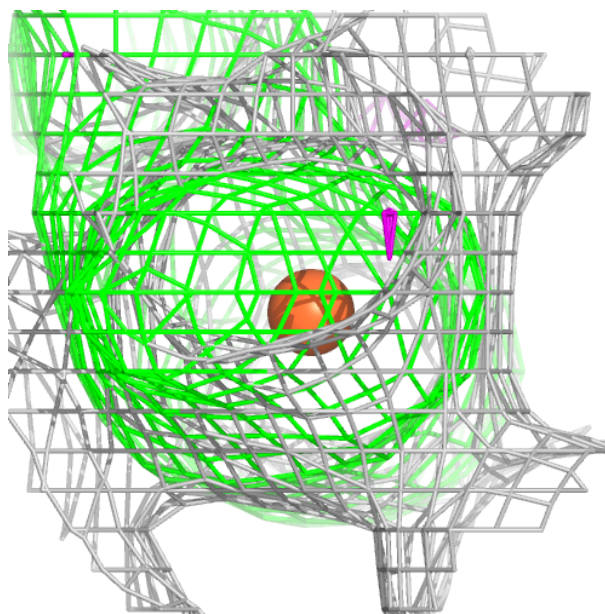
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





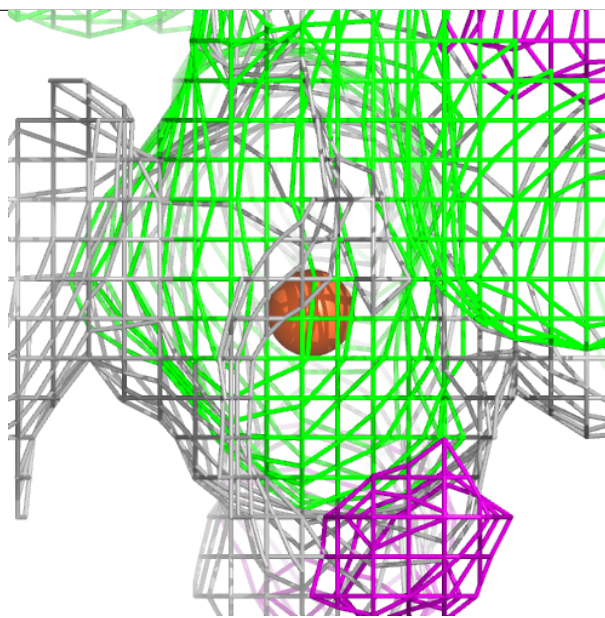
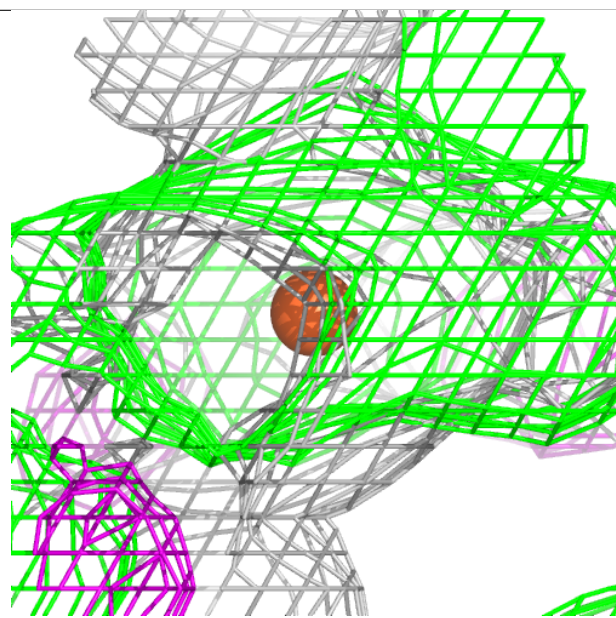
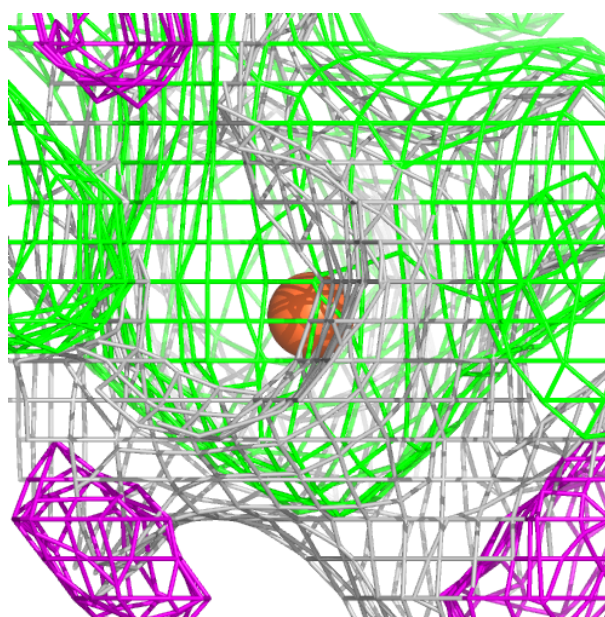
Electron density around FE I 201:

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



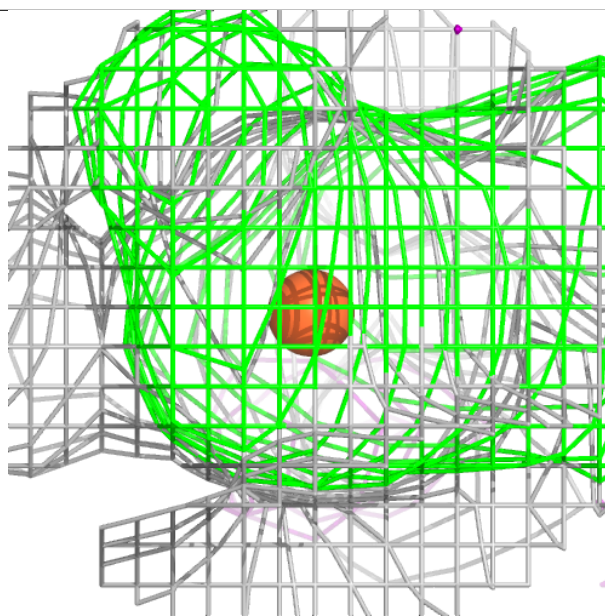
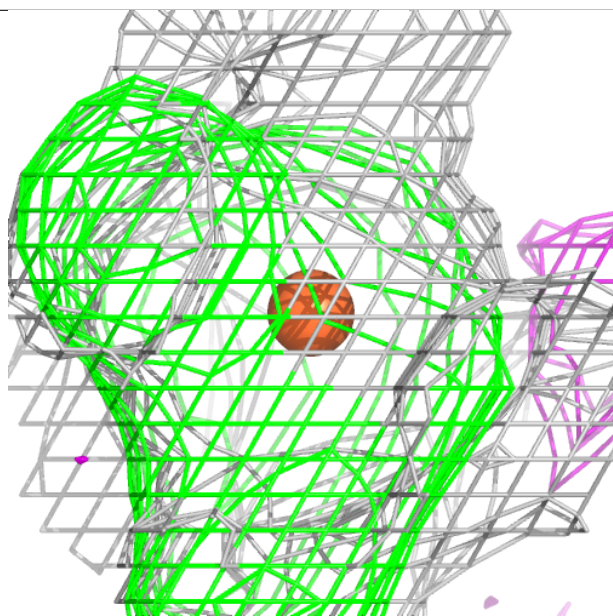
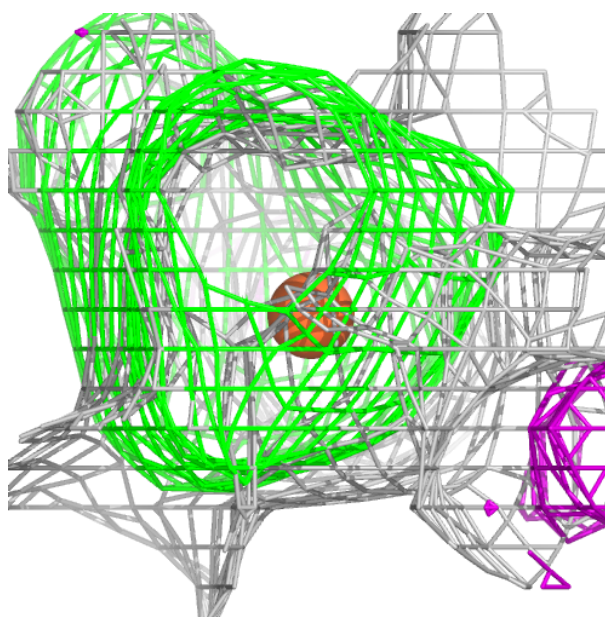
Electron density around FE H 201:

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



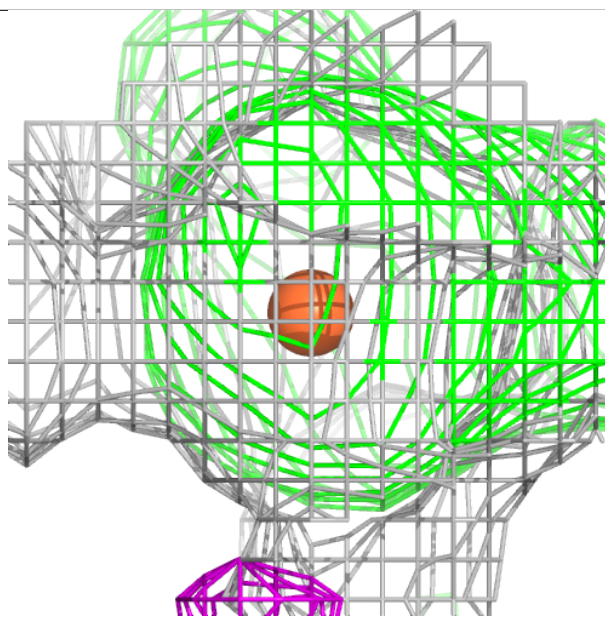
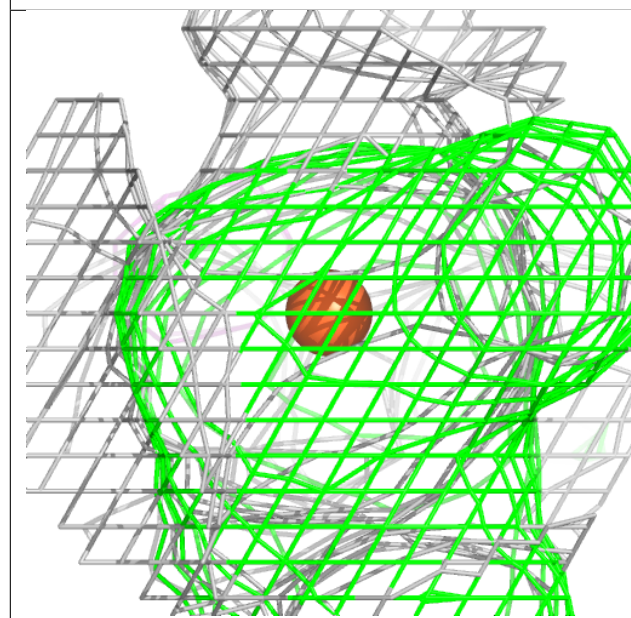
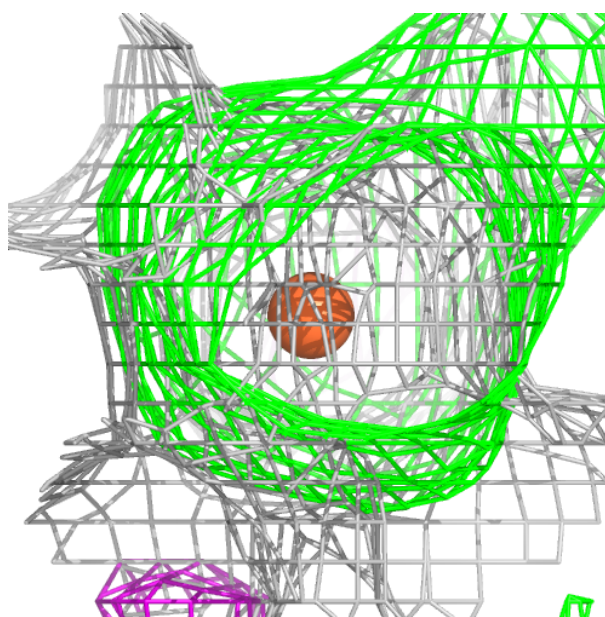
Electron density around FE K 201:

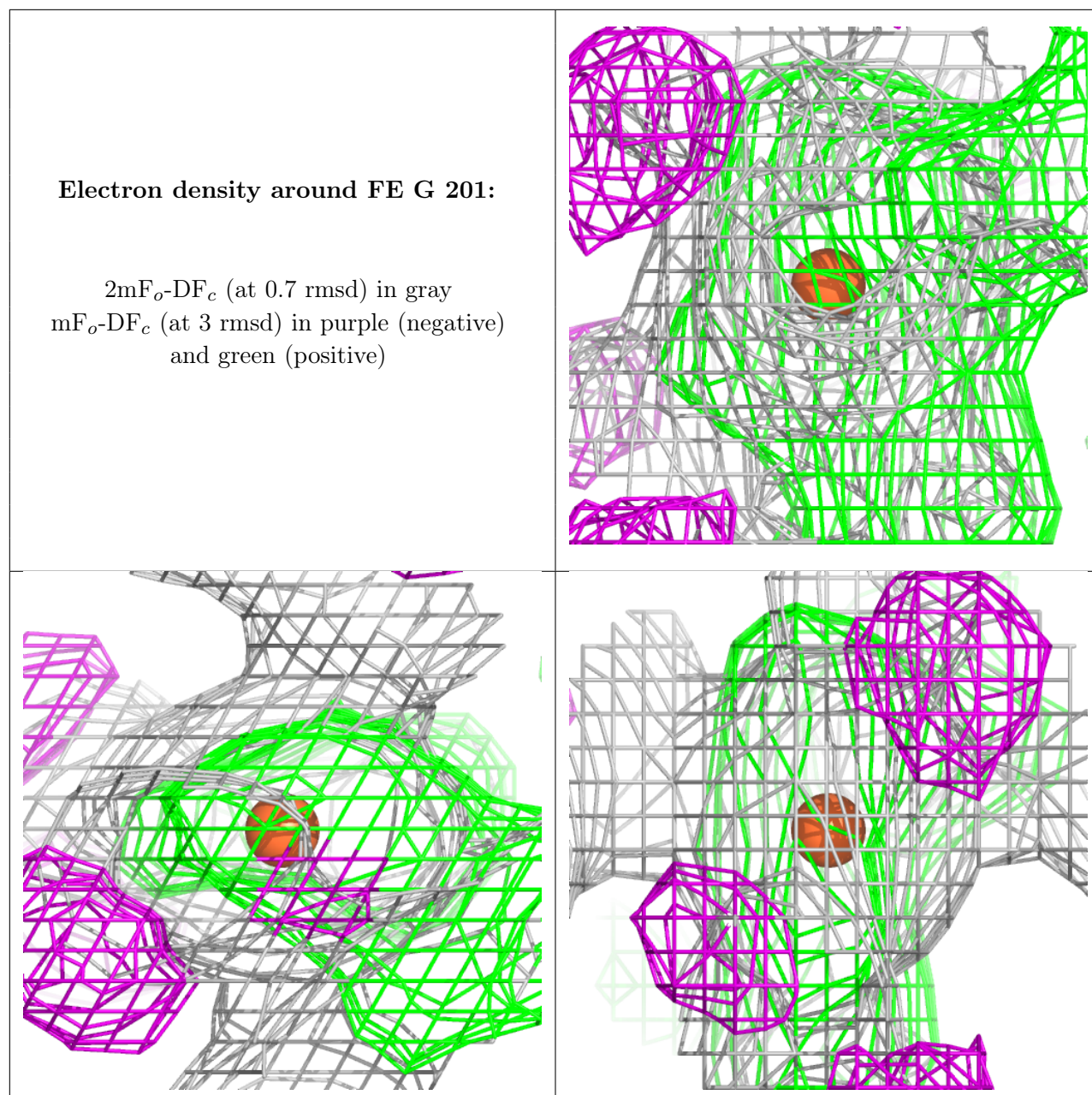
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.