



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:33 AM UTC

PDB ID : 6L56 / pdb_00006l56
Title : Fe(II) loaded Tegillarca granosa ferritin
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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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

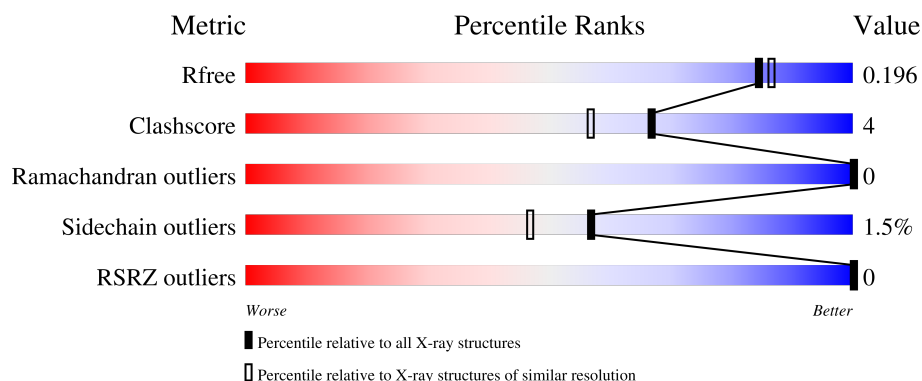
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 $\leq 5\%$. 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	172	 89% 9% .
1	B	172	 91% 8% .
1	C	172	 89% 9% .
1	D	172	 90% 9% .
1	E	172	 91% 8% .

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Mol	Chain	Length	Quality of chain
1	F	172	 89% 9% .
1	G	172	 90% 9% .
1	H	172	 92% 6% .
1	I	172	 91% 7% .
1	J	172	 90% 8% ..
1	K	172	 88% 10% ..
1	L	172	 87% 11% ..
1	M	172	 88% 10% .
1	N	172	 91% 7% ..
1	O	172	 90% 8% ..
1	P	172	 88% 10% .
1	Q	172	 91% 8% .
1	R	172	 92% 6% ..
1	S	172	 89% 9% .
1	T	172	 89% 9% ..
1	U	172	 88% 9% ..
1	V	172	 88% 9% ..
1	W	172	 90% 9% .
1	X	172	 88% 9% ..

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

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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 (CCD ID: 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 1	Fe 1	0	0
2	N	1	Total 1	Fe 1	0	0
2	O	1	Total 1	Fe 1	0	0
2	P	1	Total 1	Fe 1	0	0
2	Q	1	Total 1	Fe 1	0	0
2	R	1	Total 1	Fe 1	0	0
2	S	1	Total 1	Fe 1	0	0
2	T	1	Total 1	Fe 1	0	0
2	U	1	Total 1	Fe 1	0	0
2	V	1	Total 1	Fe 1	0	0
2	W	1	Total 1	Fe 1	0	0
2	X	1	Total 1	Fe 1	0	0

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

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

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

- Molecule 5 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	S	114	Total 114	O 114	0	0
5	T	121	Total 121	O 121	0	0
5	U	112	Total 112	O 112	0	0
5	V	115	Total 115	O 115	0	0
5	W	111	Total 111	O 111	0	0
5	X	112	Total 112	O 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: 90% 9% .



- Molecule 1: Ferritin

Chain H: 92% 6% .



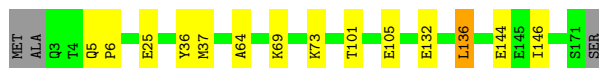
- Molecule 1: Ferritin

Chain I: 91% 7% .



- Molecule 1: Ferritin

Chain J: 90% 8% ..



- Molecule 1: Ferritin

Chain K: 88% 10% ..



- Molecule 1: Ferritin

Chain L: 87% 11% ..



- Molecule 1: Ferritin

Chain M: 88% 10% .



- Molecule 1: Ferritin

Chain N: 91% 7% ..



- Molecule 1: Ferritin

Chain O: 90% 8% ..



- Molecule 1: Ferritin

Chain P: 88% 10% .



- Molecule 1: Ferritin

Chain Q: 91% 8% .



- Molecule 1: Ferritin

Chain R: 92% 6% ..



- Molecule 1: Ferritin

Chain S: 89% 9% .



- Molecule 1: Ferritin

Chain T: 89% 9% ..



- Molecule 1: Ferritin

Chain U: 88% 9% ..



- Molecule 1: Ferritin

Chain V: 88% 9% ..



- Molecule 1: Ferritin

Chain W: 90% 9% .



- Molecule 1: Ferritin

Chain X: 88% 9% ..



4 Data and refinement statistics

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 44.12 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.12-1.85) 99.5 (44.12-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.165 , 0.196 0.165 , 0.196	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)	0.38 , 21.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FE, 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	0.27	0/1398	0.45	0/1879
1	B	0.25	0/1396	0.41	0/1876
1	C	0.26	0/1388	0.42	0/1869
1	D	0.26	0/1389	0.43	0/1868
1	E	0.27	0/1396	0.44	0/1876
1	F	0.26	0/1391	0.43	0/1871
1	G	0.26	0/1393	0.42	0/1873
1	H	0.27	0/1386	0.44	0/1866
1	I	0.26	0/1392	0.42	0/1873
1	J	0.26	0/1392	0.42	0/1872
1	K	0.28	0/1398	0.46	0/1879
1	L	0.27	0/1402	0.43	0/1884
1	M	0.26	0/1384	0.43	0/1862
1	N	0.27	0/1396	0.42	0/1877
1	O	0.27	0/1390	0.45	0/1871
1	P	0.26	0/1397	0.42	0/1879
1	Q	0.27	0/1399	0.42	0/1880
1	R	0.26	0/1395	0.43	0/1876
1	S	0.27	0/1391	0.43	0/1871
1	T	0.27	0/1388	0.44	0/1867
1	U	0.27	0/1401	0.42	0/1883
1	V	0.26	0/1397	0.44	0/1879
1	W	0.27	0/1391	0.40	0/1871
1	X	0.27	0/1398	0.45	0/1879
All	All	0.27	0/33448	0.43	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

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	11	0
1	B	1370	0	1310	11	0
1	C	1362	0	1281	15	0
1	D	1363	0	1301	13	0
1	E	1370	0	1317	11	0
1	F	1365	0	1301	13	0
1	G	1367	0	1308	12	0
1	H	1360	0	1284	8	0
1	I	1366	0	1299	11	0
1	J	1366	0	1303	9	0
1	K	1372	0	1316	15	0
1	L	1376	0	1321	16	0
1	M	1358	0	1292	13	0
1	N	1370	0	1311	13	0
1	O	1364	0	1292	11	0
1	P	1371	0	1305	12	0
1	Q	1373	0	1313	12	0
1	R	1369	0	1308	9	0
1	S	1365	0	1302	11	0
1	T	1362	0	1295	13	0
1	U	1375	0	1319	13	0
1	V	1371	0	1308	9	0
1	W	1365	0	1301	13	0
1	X	1372	0	1313	11	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	236	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 (236) 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:101:THR:HG22	1:I:146:ILE:HD13	1.53	0.87
1:T:98:MET:HE3	1:T:146:ILE:HG23	1.59	0.84
1:N:101:THR:HG22	1:N:146:ILE:HD13	1.57	0.84
1:E:98:MET:HE3	1:E:146:ILE:HG23	1.60	0.83
1:Q:98:MET:HE3	1:Q:146:ILE:HG23	1.60	0.83
1:N:51:LYS:HE2	5:N:394:HOH:O	1.77	0.83
1:I:98:MET:HE3	1:I:146:ILE:HG23	1.58	0.82
1:N:98:MET:HE3	1:N:146:ILE:HG23	1.63	0.79
1:F:98:MET:HE3	1:F:146:ILE:HG23	1.65	0.78
1:H:98:MET:HE2	1:H:149:HIS:HB2	1.65	0.77
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:K:98:MET:HE3	1:K:146:ILE:HG23	1.66	0.75
1:Q:98:MET:HE2	1:Q:149:HIS:HB2	1.70	0.73
1:K:98:MET:HE2	1:K:149:HIS:HB2	1.69	0.73
1:T:98:MET:HE2	1:T:149:HIS:HB2	1.71	0.73
1:J:101:THR:HG22	1:J:146:ILE:HD13	1.70	0.73
1:M:101:THR:HG22	1:M:146:ILE:HD13	1.71	0.72
1:K:98:MET:HE2	1:K:149:HIS:CB	2.20	0.72
1:O:98:MET:HE3	1:O:146:ILE:HG23	1.71	0.71
1:H:98:MET:HE3	1:H:146:ILE:HG23	1.71	0.71
1:T:101:THR:HG22	1:T:146:ILE:HD13	1.72	0.71
1:G:98:MET:HE3	1:G:146:ILE:HG23	1.72	0.70
1:A:47:PRO:O	1:A:51:LYS:HG2	1.92	0.70
1:C:98:MET:HE3	1:C:146:ILE:HG23	1.72	0.69
1:D:98:MET:HE2	1:D:149:HIS:HB2	1.72	0.69
1:R:101:THR:HG22	1:R:146:ILE:HD13	1.74	0.69
1:D:98:MET:HE3	1:D:146:ILE:HG23	1.74	0.69
1:U:98:MET:HE3	1:U:146:ILE:HG23	1.75	0.69
1:R:98:MET:HE3	1:R:146:ILE:HG23	1.74	0.68
1:K:101:THR:HG22	1:K:146:ILE:HD13	1.75	0.68
1:U:98:MET:HE2	1:U:149:HIS:HB2	1.76	0.68
1:O:98:MET:HE2	1:O:149:HIS:HB2	1.74	0.68
1:I:98:MET:HE2	1:I:149:HIS:HB2	1.76	0.68
1:F:98:MET:HE2	1:F:149:HIS:HB2	1.77	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:MET:HE3	1:M:146:ILE:HG23	1.78	0.66
1:H:98:MET:HE2	1:H:149:HIS:CB	2.25	0.66
1:H:101:THR:HG22	1:H:146:ILE:HD13	1.78	0.66
1:E:98:MET:CE	1:E:146:ILE:HG23	2.25	0.65
1:L:101:THR:HG22	1:L:146:ILE:HD13	1.78	0.65
1:O:37:MET:HE2	1:P:68:MET:HB3	1.79	0.65
1:K:37:MET:HE2	1:L:68:MET:HB3	1.79	0.65
1:C:98:MET:HE2	1:C:149:HIS:HB2	1.79	0.64
1:T:98:MET:HE2	1:T:149:HIS:CB	2.28	0.64
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:E:98:MET:HE2	1:E:149:HIS:HB2	1.80	0.63
1:L:98:MET:HE3	1:L:146:ILE:HG23	1.81	0.62
1:O:97:ALA:O	1:O:101:THR:HG23	1.99	0.62
1:W:68:MET:HB3	1:X:37:MET:HE2	1.82	0.62
1:F:101:THR:HG22	1:F:146:ILE:HD13	1.81	0.61
1:I:98:MET:CE	1:I:146:ILE:HG23	2.27	0.61
1:L:3:GLN:CD	1:L:7:ARG:HD2	2.25	0.61
1:O:98:MET:HE2	1:O:149:HIS:CB	2.30	0.61
1:Q:98:MET:CE	1:Q:146:ILE:HG23	2.30	0.61
1:G:98:MET:HE2	1:G:149:HIS:HB2	1.83	0.61
1:T:98:MET:CE	1:T:146:ILE:HG23	2.30	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:D:98:MET:HE2	1:D:149:HIS:CB	2.32	0.60
1:K:58:GLU:HG2	1:K:61:ARG:HH22	1.67	0.60
1:U:98:MET:HE2	1:U:149:HIS:CB	2.32	0.60
1:N:168:GLU:HB3	1:P:167:LYS:HE2	1.84	0.59
1:U:68:MET:HB3	1:V:37:MET:HE2	1.84	0.59
1:R:98:MET:CE	1:R:146:ILE:HG23	2.33	0.59
1:P:101:THR:HG22	1:P:146:ILE:HD13	1.83	0.58
1:F:98:MET:HE2	1:F:149:HIS:CB	2.33	0.58
1:K:5:GLN:HG3	1:L:42:ASP:OD2	2.04	0.58
1:K:98:MET:CE	1:K:146:ILE:HG23	2.34	0.58
1:Q:98:MET:HE2	1:Q:149:HIS:CB	2.32	0.58
1:F:98:MET:CE	1:F:146:ILE:HG23	2.31	0.58
1:G:68:MET:HB3	1:H:37:MET:HE2	1.86	0.57
1:W:98:MET:HE2	1:W:149:HIS:HB2	1.86	0.57
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:G:98:MET:CE	1:G:146:ILE:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:101:THR:HG22	1:U:146:ILE:HD13	1.87	0.55
1:P:52:TYR:CE2	1:P:98:MET:HE1	2.42	0.55
1:P:121:LYS:HE3	1:P:122:HIS:NE2	2.23	0.54
1:R:98:MET:HE2	1:R:149:HIS:HB2	1.89	0.54
1:C:98:MET:HE2	1:C:149:HIS:CB	2.37	0.54
1:Q:69:LYS:NZ	5:Q:301:HOH:O	2.39	0.54
1:A:52:TYR:CE2	1:A:98:MET:HE1	2.43	0.54
1:I:98:MET:HE2	1:I:149:HIS:CB	2.36	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:M:98:MET:HE2	1:M:149:HIS:HB2	1.91	0.53
1:P:32:TYR:OH	1:P:101:THR:HG23	2.09	0.53
1:W:98:MET:HE3	1:W:146:ILE:HG23	1.91	0.53
1:G:32:TYR:OH	1:G:101:THR:HG23	2.09	0.52
1:C:98:MET:CE	1:C:146:ILE:HG23	2.39	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: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:T:36:TYR:CE2	1:T:37:MET:HE2	2.46	0.50
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:H:98:MET:CE	1:H:146:ILE:HG23	2.40	0.50
1:W:98:MET:HE2	1:W:149:HIS:CB	2.42	0.49
1:L:36:TYR:CE2	1:L:37:MET:HE2	2.48	0.49
1:D:98:MET:CE	1:D:146:ILE:HG23	2.42	0.49
1:M:98:MET:CE	1:M:146:ILE:HG23	2.42	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:A:37:MET:HE2	1:B:68:MET:HB3	1.94	0.49
1:N:98:MET:HE2	1:N:149:HIS:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:98:MET:HE2	1:G:149:HIS:CB	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:A:68:MET:HB3	1:B:37:MET:HE2	1.96	0.48
1:E:98:MET:HE2	1:E:149:HIS:CB	2.43	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:L:98:MET:CE	1:L:146:ILE:HG23	2.42	0.47
1:A:144:GLU:HG3	1:F:73:LYS:HA	1.96	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:A:72:ASN:ND2	1:B:37:MET:HE3	2.30	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:E:68:MET:HB3	1:F:37:MET:HE2	1.98	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:C:68:MET:HB3	1:D:37:MET:HE2	1.97	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:37:MET:HE2	1:T:68:MET:HB3	1.97	0.45
1:S:32:TYR:OH	1:S:101:THR:HG23	2.16	0.45
1:M:37:MET:HE3	1:N:72:ASN:ND2	2.31	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:C:72:ASN:ND2	1:D:37:MET:HE3	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:GLU:HG3	1:J:73:LYS:HA	2.00	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:X:98:MET:HE3	1:X:146:ILE:HG23	2.00	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:B:52:TYR:CE2	1:B:98:MET:HE1	2.53	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:M:98:MET:HE2	1:M:149:HIS:CB	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:98:MET:HE3	1:S:146:ILE:HG23	2.01	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:N:144:GLU:HG3	1:O:73:LYS:HA	2.01	0.42
1:O:98:MET:CE	1:O:146:ILE:HG23	2.45	0.42
1:C:3:GLN:CD	1:C:7:ARG:HD2	2.45	0.42
5:I:368:HOH:O	1:J:69:LYS:HE3	2.20	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:L:98:MET:HE2	1:L:149:HIS:HB2	2.03	0.41
1:W:21:GLN:O	1:W:25:GLU:HG2	2.20	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: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:J:36:TYR:CE2	1:J:37:MET:HE2	2.56	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:K:37:MET:HE2	1:L:68:MET:CB	2.50	0.41
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

5.3.1 Protein backbone

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
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 ⓘ

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%)	144 (99%)	2 (1%)	59	49
1	B	145/151 (96%)	145 (100%)	0	100	100
1	C	144/151 (95%)	143 (99%)	1 (1%)	76	70
1	D	143/151 (95%)	141 (99%)	2 (1%)	59	49
1	E	145/151 (96%)	143 (99%)	2 (1%)	59	49
1	F	144/151 (95%)	142 (99%)	2 (1%)	59	49
1	G	145/151 (96%)	143 (99%)	2 (1%)	59	49
1	H	143/151 (95%)	139 (97%)	4 (3%)	38	23
1	I	145/151 (96%)	143 (99%)	2 (1%)	59	49
1	J	144/151 (95%)	143 (99%)	1 (1%)	76	70
1	K	145/151 (96%)	141 (97%)	4 (3%)	38	23
1	L	147/151 (97%)	144 (98%)	3 (2%)	48	36
1	M	143/151 (95%)	141 (99%)	2 (1%)	59	49
1	N	146/151 (97%)	144 (99%)	2 (1%)	59	49
1	O	144/151 (95%)	141 (98%)	3 (2%)	47	33
1	P	146/151 (97%)	144 (99%)	2 (1%)	59	49
1	Q	147/151 (97%)	145 (99%)	2 (1%)	59	49
1	R	146/151 (97%)	145 (99%)	1 (1%)	76	70
1	S	145/151 (96%)	144 (99%)	1 (1%)	76	70
1	T	144/151 (95%)	142 (99%)	2 (1%)	59	49
1	U	147/151 (97%)	145 (99%)	2 (1%)	59	49
1	V	146/151 (97%)	142 (97%)	4 (3%)	39	24
1	W	144/151 (95%)	142 (99%)	2 (1%)	59	49
1	X	147/151 (97%)	144 (98%)	3 (2%)	48	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3481/3624 (96%)	3430 (98%)	51 (2%)	57 47

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	140	VAL
1	C	153	LEU
1	D	131	LEU
1	D	153	LEU
1	E	131	LEU
1	E	136	LEU
1	F	136	LEU
1	F	153	LEU
1	G	131	LEU
1	G	153	LEU
1	H	3	GLN
1	H	30	TYR
1	H	140	VAL
1	H	153	LEU
1	I	131	LEU
1	I	153	LEU
1	J	136	LEU
1	K	5	GLN
1	K	131	LEU
1	K	136	LEU
1	K	153	LEU
1	L	131	LEU
1	L	136	LEU
1	L	153	LEU
1	M	131	LEU
1	M	136	LEU
1	N	136	LEU
1	N	153	LEU
1	O	131	LEU
1	O	136	LEU
1	O	140	VAL
1	P	131	LEU
1	P	136	LEU
1	Q	131	LEU
1	Q	153	LEU
1	R	136	LEU

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Mol	Chain	Res	Type
1	S	136	LEU
1	T	136	LEU
1	T	153	LEU
1	U	131	LEU
1	U	136	LEU
1	V	131	LEU
1	V	136	LEU
1	V	140	VAL
1	V	153	LEU
1	W	131	LEU
1	W	153	LEU
1	X	136	LEU
1	X	140	VAL
1	X	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	109	ASN
1	A	152	ASN
1	B	109	ASN
1	C	3	GLN
1	C	109	ASN
1	D	109	ASN
1	E	33	GLN
1	E	109	ASN
1	E	152	ASN
1	F	109	ASN
1	G	3	GLN
1	G	109	ASN
1	H	81	GLN
1	H	84	GLN
1	H	109	ASN
1	H	152	ASN
1	I	55	HIS
1	I	109	ASN
1	J	81	GLN
1	J	109	ASN
1	K	84	GLN
1	K	109	ASN
1	L	109	ASN

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Mol	Chain	Res	Type
1	L	152	ASN
1	M	81	GLN
1	M	109	ASN
1	M	152	ASN
1	N	56	ASN
1	N	109	ASN
1	N	152	ASN
1	O	33	GLN
1	O	84	GLN
1	O	109	ASN
1	P	109	ASN
1	Q	109	ASN
1	Q	152	ASN
1	R	109	ASN
1	S	109	ASN
1	T	55	HIS
1	T	109	ASN
1	U	33	GLN
1	U	109	ASN
1	V	33	GLN
1	V	109	ASN
1	W	109	ASN
1	X	109	ASN

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 oligosaccharides 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, 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	169/172 (98%)	-1.46	0 100 100	6, 11, 20, 39	0
1	B	169/172 (98%)	-1.44	0 100 100	6, 11, 19, 31	0
1	C	169/172 (98%)	-1.46	0 100 100	6, 10, 20, 28	0
1	D	169/172 (98%)	-1.46	0 100 100	6, 10, 19, 29	0
1	E	169/172 (98%)	-1.46	0 100 100	6, 10, 20, 32	0
1	F	169/172 (98%)	-1.46	0 100 100	6, 10, 18, 32	0
1	G	169/172 (98%)	-1.44	0 100 100	6, 11, 20, 30	0
1	H	169/172 (98%)	-1.45	0 100 100	6, 10, 20, 31	0
1	I	169/172 (98%)	-1.44	0 100 100	6, 11, 20, 30	0
1	J	169/172 (98%)	-1.45	0 100 100	6, 11, 19, 33	0
1	K	169/172 (98%)	-1.46	0 100 100	6, 10, 20, 32	0
1	L	169/172 (98%)	-1.44	0 100 100	6, 10, 21, 30	0
1	M	169/172 (98%)	-1.46	0 100 100	6, 11, 20, 26	0
1	N	169/172 (98%)	-1.44	0 100 100	6, 11, 20, 25	0
1	O	169/172 (98%)	-1.46	0 100 100	6, 11, 21, 30	0
1	P	169/172 (98%)	-1.46	0 100 100	6, 10, 21, 31	0
1	Q	169/172 (98%)	-1.45	0 100 100	5, 11, 21, 26	0
1	R	169/172 (98%)	-1.46	0 100 100	6, 11, 20, 32	0
1	S	169/172 (98%)	-1.44	0 100 100	6, 10, 20, 28	0
1	T	169/172 (98%)	-1.44	0 100 100	6, 11, 20, 33	0
1	U	169/172 (98%)	-1.47	0 100 100	6, 11, 21, 30	0
1	V	169/172 (98%)	-1.44	0 100 100	6, 11, 21, 31	0
1	W	169/172 (98%)	-1.45	0 100 100	6, 10, 19, 31	0
1	X	169/172 (98%)	-1.43	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%)	-1.45	0 100 100	5, 11, 21, 39	0

There are no RSRZ outliers to report.

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 oligosaccharides 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	D	201	1/1	0.95	0.09	77,77,77,77	0
2	FE	W	201	1/1	0.95	0.09	72,72,72,72	0
2	FE	X	201	1/1	0.95	0.10	72,72,72,72	0
2	FE	N	201	1/1	0.96	0.09	72,72,72,72	0
2	FE	Q	201	1/1	0.96	0.08	75,75,75,75	0
2	FE	V	201	1/1	0.96	0.08	74,74,74,74	0
2	FE	J	201	1/1	0.96	0.08	75,75,75,75	0
2	FE	M	201	1/1	0.96	0.08	72,72,72,72	0
3	FE2	B	203	1/1	0.96	0.13	54,54,54,54	0
3	FE2	P	203	1/1	0.96	0.09	59,59,59,59	0
3	FE2	P	205	1/1	0.96	0.12	84,84,84,84	0
2	FE	E	201	1/1	0.97	0.07	69,69,69,69	0
2	FE	R	201	1/1	0.97	0.06	74,74,74,74	0
2	FE	S	201	1/1	0.97	0.08	64,64,64,64	0
2	FE	T	201	1/1	0.97	0.07	70,70,70,70	0
2	FE	H	201	1/1	0.97	0.07	69,69,69,69	0
2	FE	C	201	1/1	0.97	0.06	68,68,68,68	0
2	FE	C	207	1/1	0.97	0.07	76,76,76,76	0
3	FE2	A	204	1/1	0.97	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE2	A	205	1/1	0.97	0.06	53,53,53,53	0
2	FE	B	201	1/1	0.97	0.07	71,71,71,71	0
3	FE2	C	205	1/1	0.97	0.06	55,55,55,55	0
3	FE2	E	203	1/1	0.97	0.12	55,55,55,55	0
3	FE2	E	205	1/1	0.97	0.06	54,54,54,54	0
3	FE2	H	204	1/1	0.97	0.08	60,60,60,60	0
3	FE2	H	205	1/1	0.97	0.07	54,54,54,54	0
2	FE	O	201	1/1	0.97	0.06	72,72,72,72	0
2	FE	P	201	1/1	0.97	0.08	74,74,74,74	0
3	FE2	B	204	1/1	0.98	0.14	52,52,52,52	0
3	FE2	C	204	1/1	0.98	0.12	57,57,57,57	0
2	FE	K	201	1/1	0.98	0.04	70,70,70,70	0
2	FE	L	201	1/1	0.98	0.07	67,67,67,67	0
3	FE2	E	204	1/1	0.98	0.17	51,51,51,51	0
2	FE	A	201	1/1	0.98	0.08	66,66,66,66	0
3	FE2	H	203	1/1	0.98	0.12	51,51,51,51	0
3	FE2	A	203	1/1	0.98	0.20	55,55,55,55	0
2	FE	I	201	1/1	0.98	0.06	69,69,69,69	0
3	FE2	I	204	1/1	0.98	0.11	54,54,54,54	0
3	FE2	K	202	1/1	0.98	0.18	50,50,50,50	0
3	FE2	K	204	1/1	0.98	0.09	56,56,56,56	0
3	FE2	K	205	1/1	0.98	0.05	52,52,52,52	0
2	FE	F	201	1/1	0.98	0.06	64,64,64,64	0
2	FE	U	201	1/1	0.98	0.07	71,71,71,71	0
3	FE2	I	202	1/1	0.99	0.15	49,49,49,49	0
3	FE2	I	203	1/1	0.99	0.05	51,51,51,51	0
3	FE2	B	207	1/1	0.99	0.04	54,54,54,54	0
3	FE2	P	204	1/1	0.99	0.05	50,50,50,50	0
3	FE2	C	203	1/1	0.99	0.10	50,50,50,50	0
4	NA	A	206	1/1	0.99	0.05	18,18,18,18	0
4	NA	B	205	1/1	0.99	0.04	10,10,10,10	1
4	NA	B	206	1/1	0.99	0.07	18,18,18,18	0
4	NA	E	206	1/1	0.99	0.02	18,18,18,18	0
4	NA	F	204	1/1	0.99	0.04	19,19,19,19	0
4	NA	J	204	1/1	0.99	0.02	18,18,18,18	0
4	NA	K	206	1/1	0.99	0.04	17,17,17,17	0
4	NA	M	204	1/1	0.99	0.04	17,17,17,17	0
4	NA	O	204	1/1	0.99	0.03	18,18,18,18	0
4	NA	Q	203	1/1	0.99	0.05	16,16,16,16	0
4	NA	S	204	1/1	0.99	0.05	17,17,17,17	0
4	NA	T	203	1/1	0.99	0.05	17,17,17,17	0
3	FE2	P	202	1/1	1.00	0.04	17,17,17,17	0

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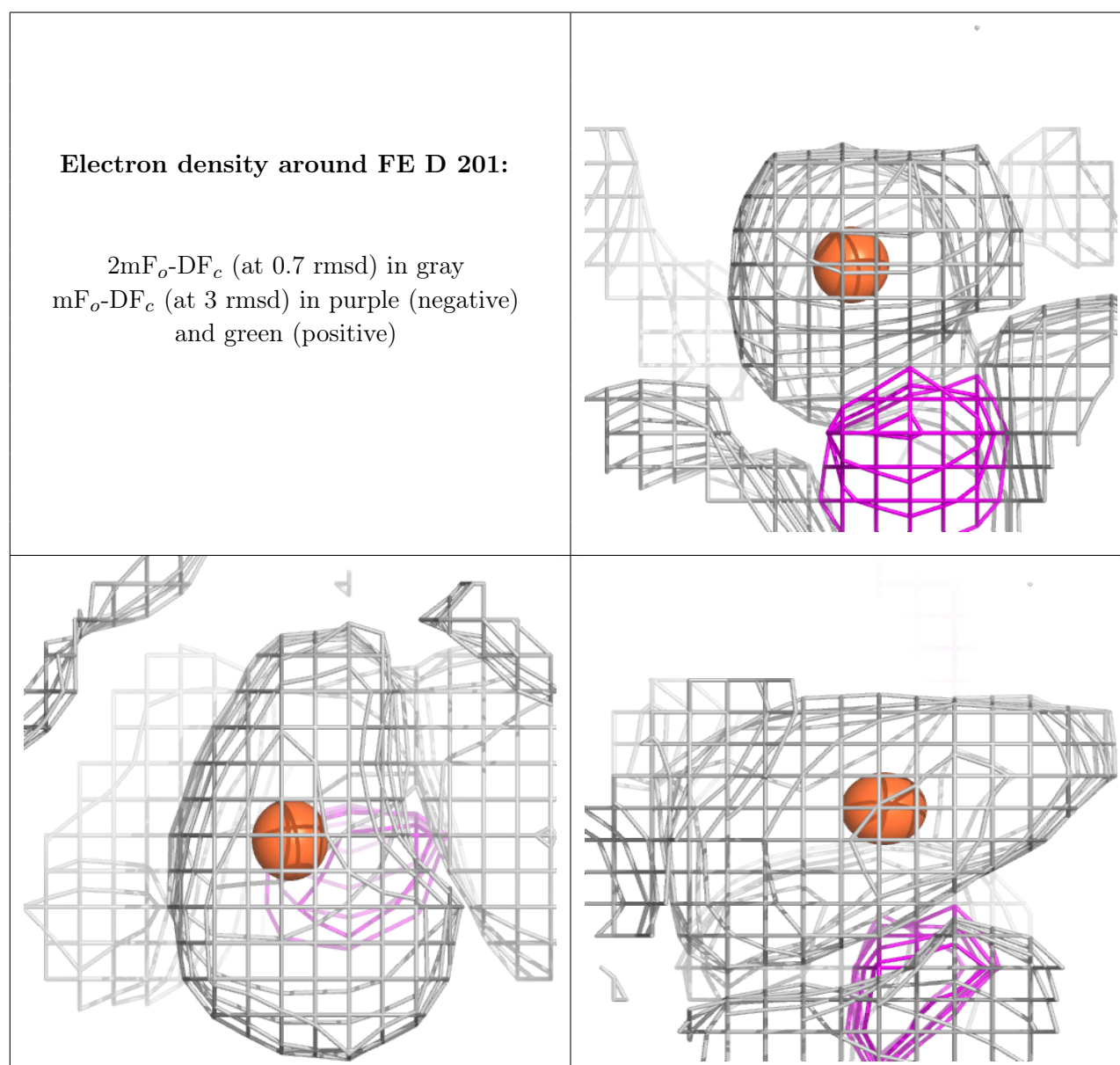
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE2	E	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	B	202	1/1	1.00	0.04	13,13,13,13	0
3	FE2	A	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	Q	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	R	202	1/1	1.00	0.04	18,18,18,18	0
3	FE2	S	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	T	202	1/1	1.00	0.03	18,18,18,18	0
3	FE2	U	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	V	202	1/1	1.00	0.05	18,18,18,18	0
3	FE2	W	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	X	202	1/1	1.00	0.04	17,17,17,17	0
3	FE2	C	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	F	202	1/1	1.00	0.04	18,18,18,18	0
3	FE2	I	205	1/1	1.00	0.05	16,16,16,16	0
4	NA	C	206	1/1	1.00	0.05	18,18,18,18	0
4	NA	D	203	1/1	1.00	0.01	10,10,10,10	1
4	NA	D	204	1/1	1.00	0.02	19,19,19,19	0
3	FE2	J	202	1/1	1.00	0.04	17,17,17,17	0
4	NA	F	203	1/1	1.00	0.03	10,10,10,10	1
3	FE2	G	201	1/1	1.00	0.04	17,17,17,17	0
4	NA	G	202	1/1	1.00	0.01	9,9,9,9	1
4	NA	G	203	1/1	1.00	0.05	17,17,17,17	0
4	NA	H	206	1/1	1.00	0.03	18,18,18,18	0
4	NA	I	206	1/1	1.00	0.06	16,16,16,16	0
4	NA	J	203	1/1	1.00	0.03	14,14,14,14	1
3	FE2	K	203	1/1	1.00	0.04	16,16,16,16	0
3	FE2	H	202	1/1	1.00	0.05	17,17,17,17	0
4	NA	L	203	1/1	1.00	0.01	10,10,10,10	1
4	NA	L	204	1/1	1.00	0.03	17,17,17,17	0
4	NA	M	203	1/1	1.00	0.01	13,13,13,13	1
3	FE2	D	202	1/1	1.00	0.04	16,16,16,16	0
4	NA	N	203	1/1	1.00	0.06	17,17,17,17	0
4	NA	O	203	1/1	1.00	0.03	12,12,12,12	1
3	FE2	L	202	1/1	1.00	0.04	17,17,17,17	0
4	NA	P	206	1/1	1.00	0.05	18,18,18,18	0
3	FE2	M	202	1/1	1.00	0.04	18,18,18,18	0
4	NA	R	203	1/1	1.00	0.06	14,14,14,14	1
4	NA	R	204	1/1	1.00	0.06	18,18,18,18	0
4	NA	S	203	1/1	1.00	0.01	9,9,9,9	1
3	FE2	N	202	1/1	1.00	0.05	17,17,17,17	0
3	FE2	O	202	1/1	1.00	0.04	17,17,17,17	0
4	NA	U	203	1/1	1.00	0.05	18,18,18,18	0

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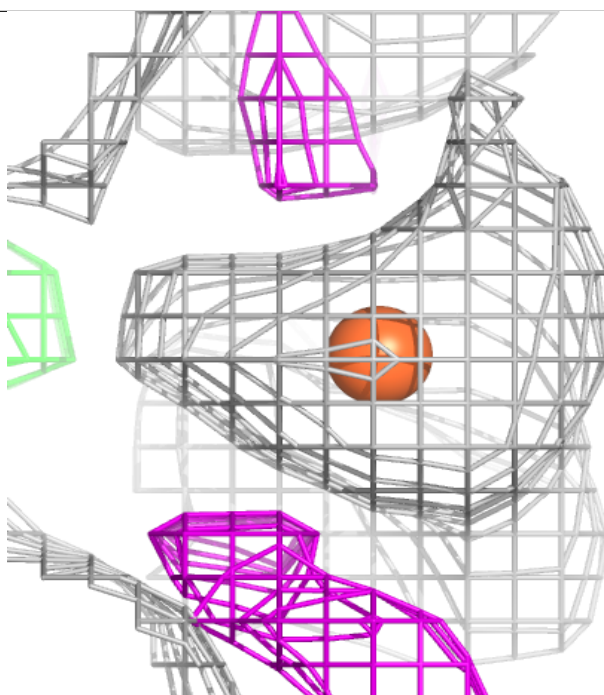
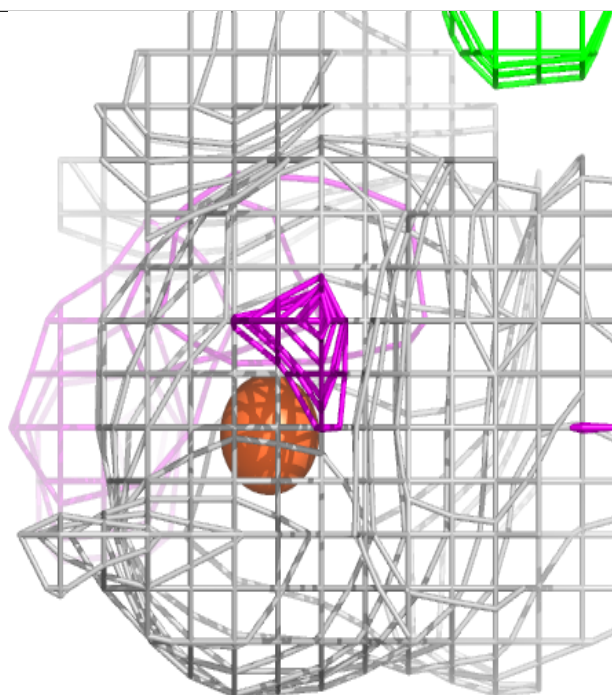
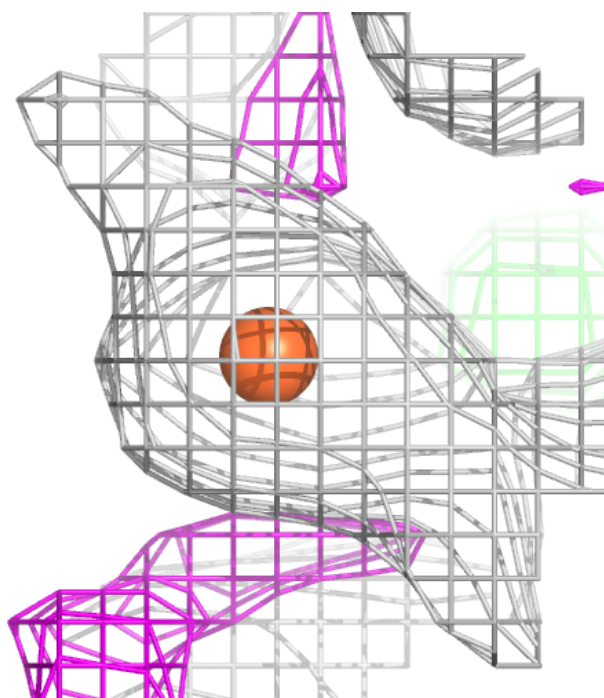
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	V	203	1/1	1.00	0.01	12,12,12,12	1
4	NA	V	204	1/1	1.00	0.02	16,16,16,16	0
4	NA	W	203	1/1	1.00	0.06	18,18,18,18	0
4	NA	X	203	1/1	1.00	0.02	12,12,12,12	1
4	NA	X	204	1/1	1.00	0.04	17,17,17,17	0

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.



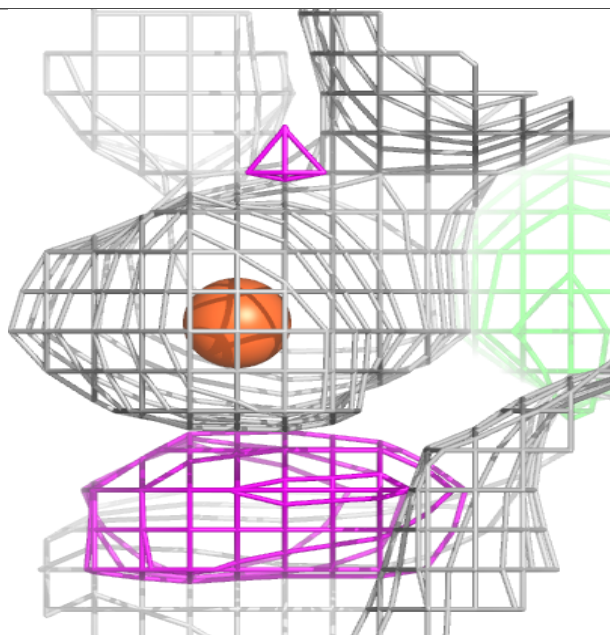
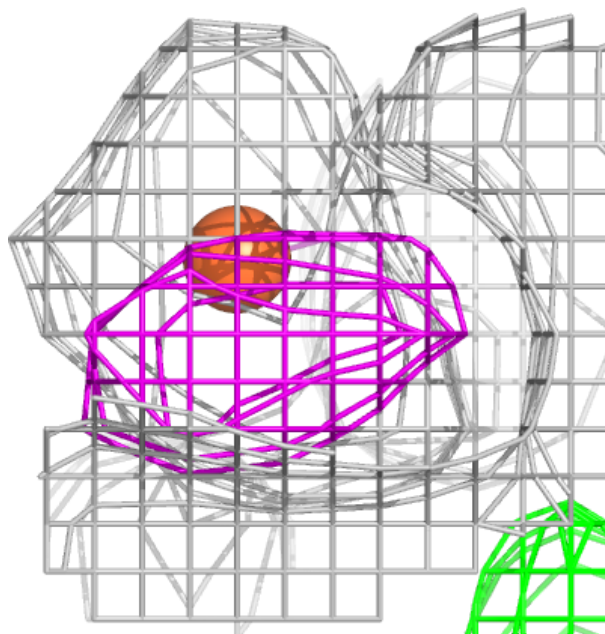
Electron density around FE W 201:

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



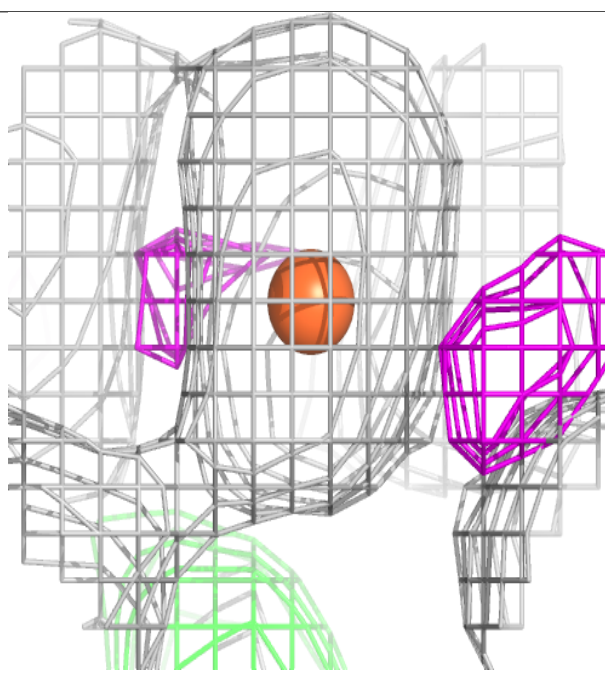
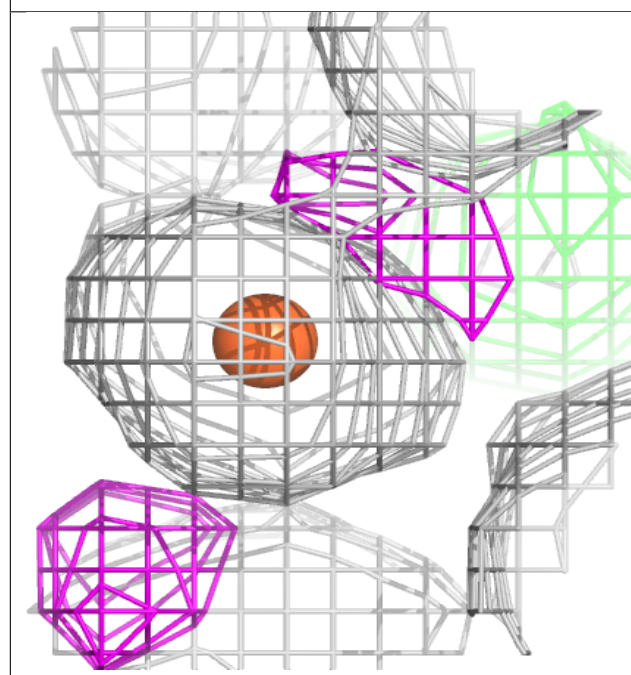
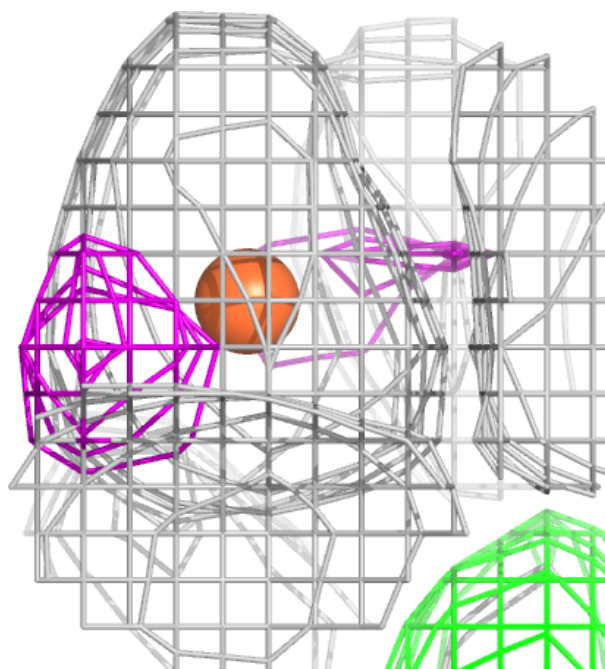
Electron density around FE X 201:

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and green (positive)



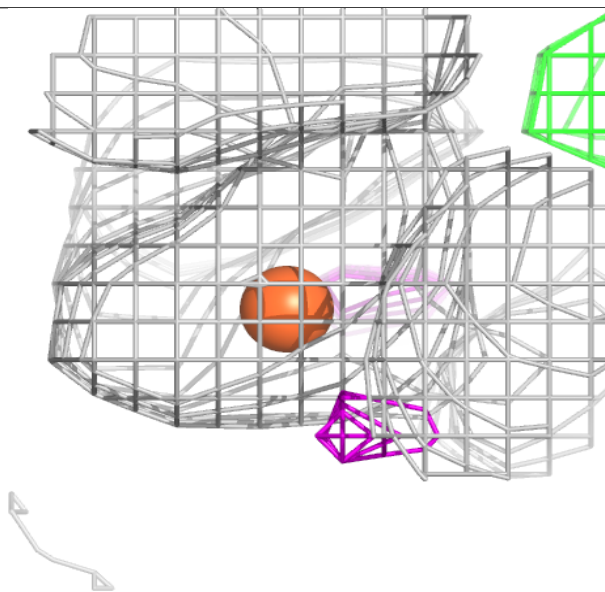
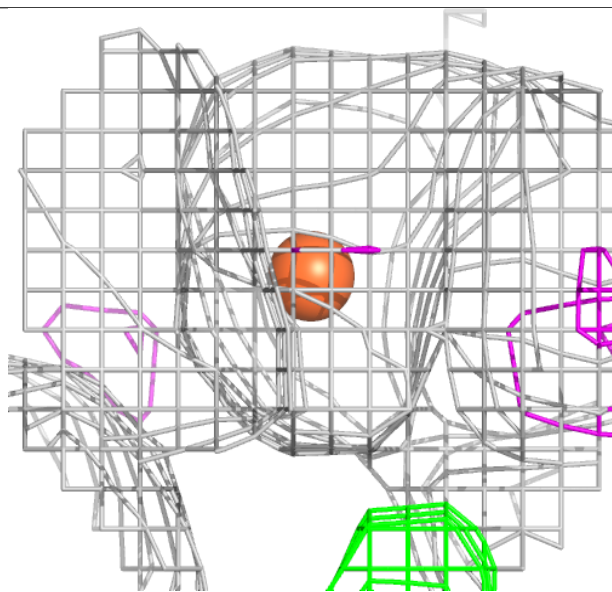
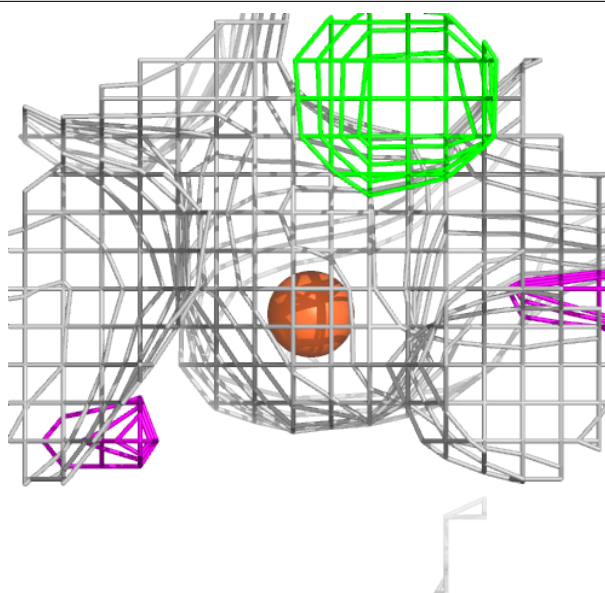
Electron density around FE N 201:

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



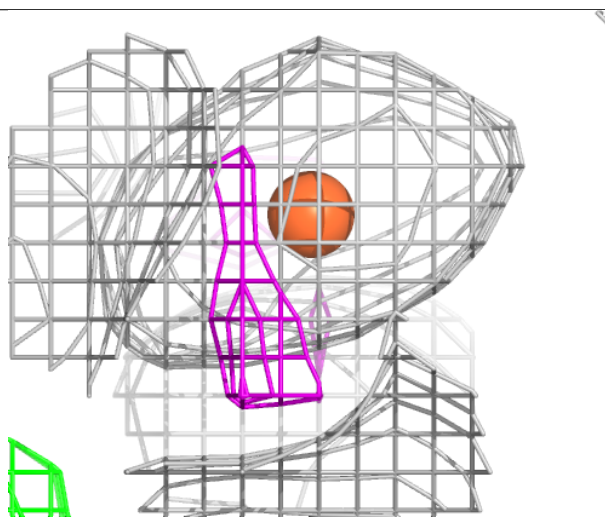
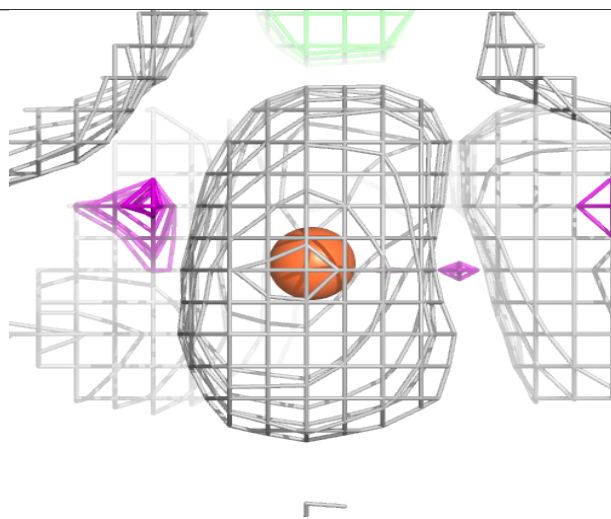
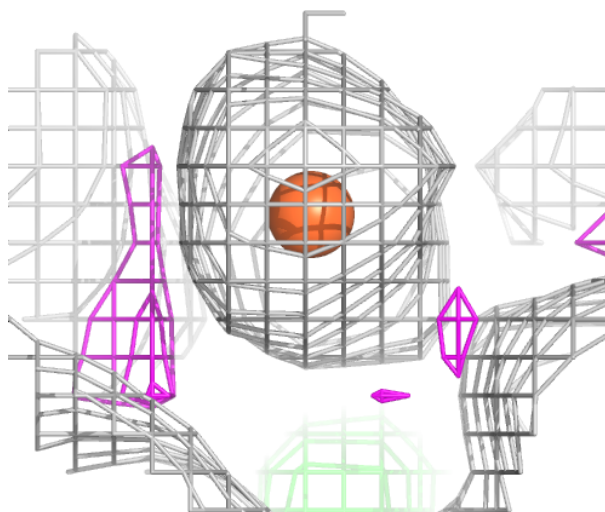
Electron density around FE Q 201:

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



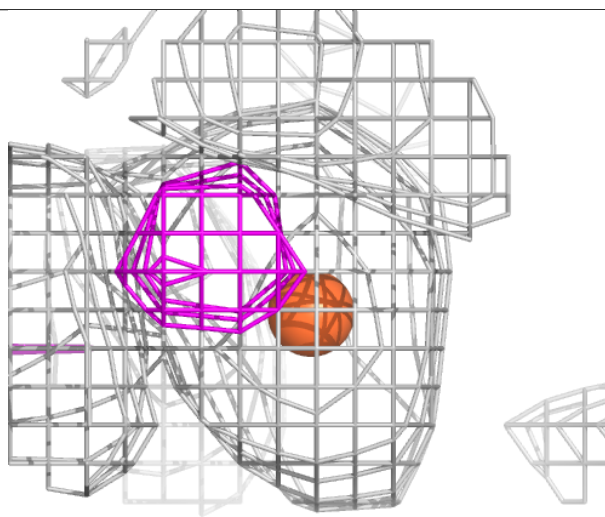
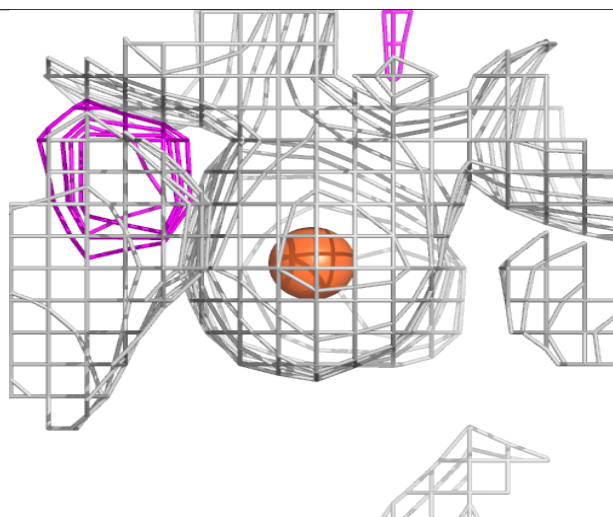
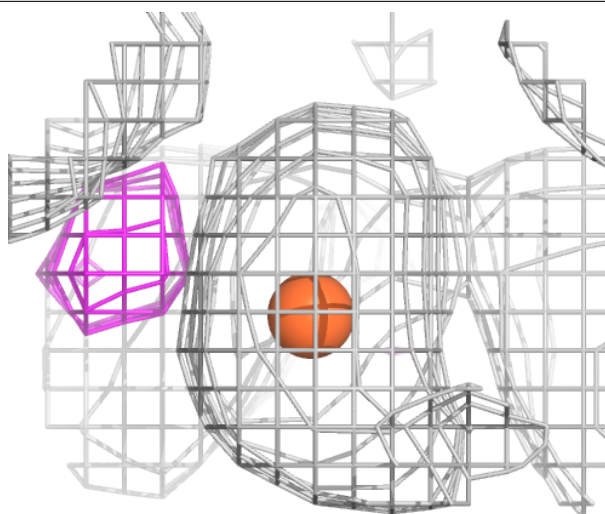
Electron density around FE V 201:

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



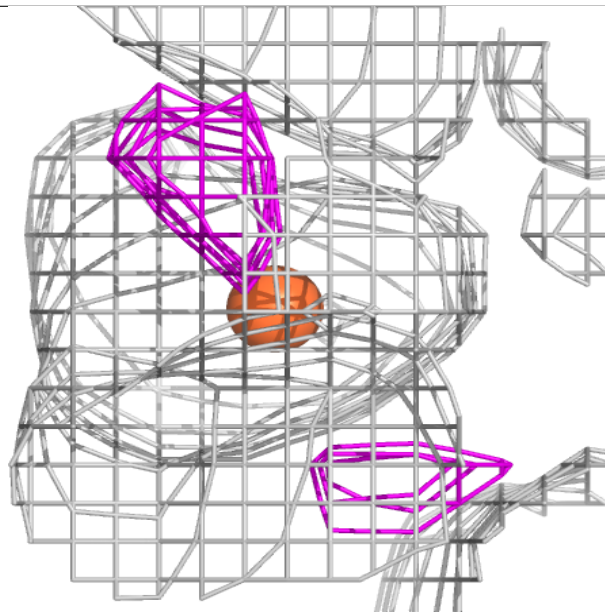
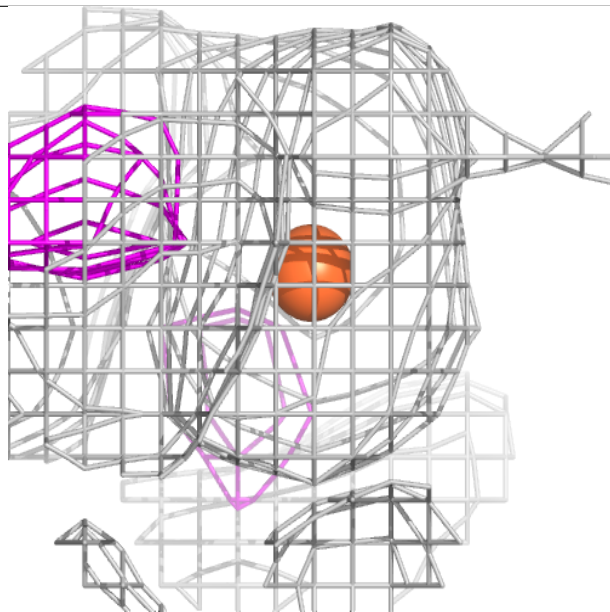
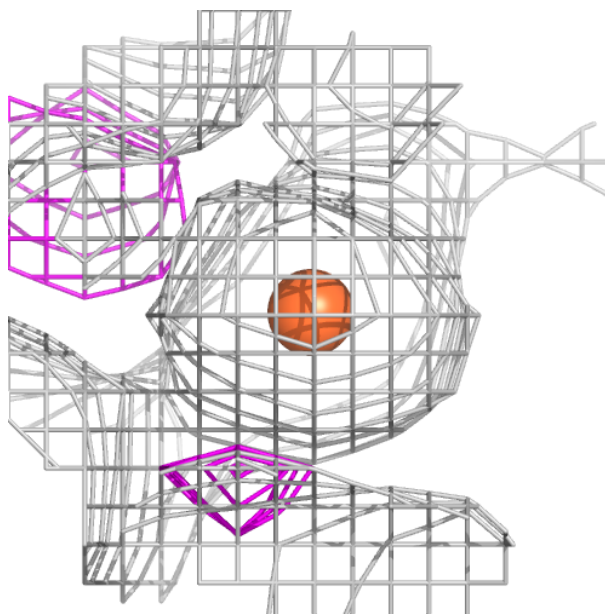
Electron density around FE J 201:

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



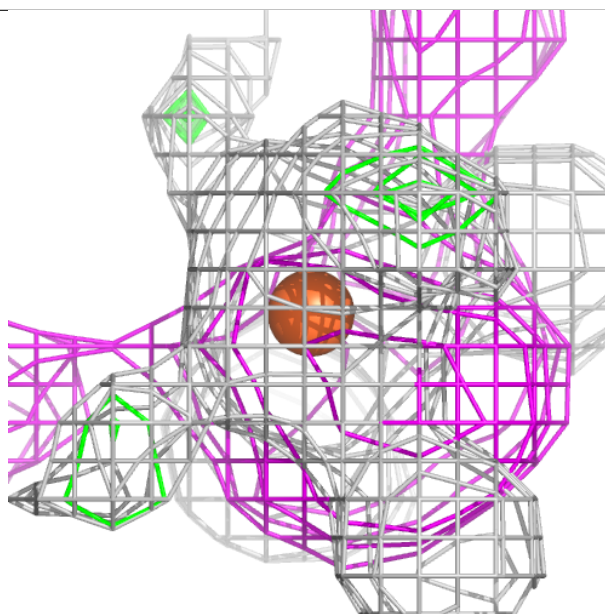
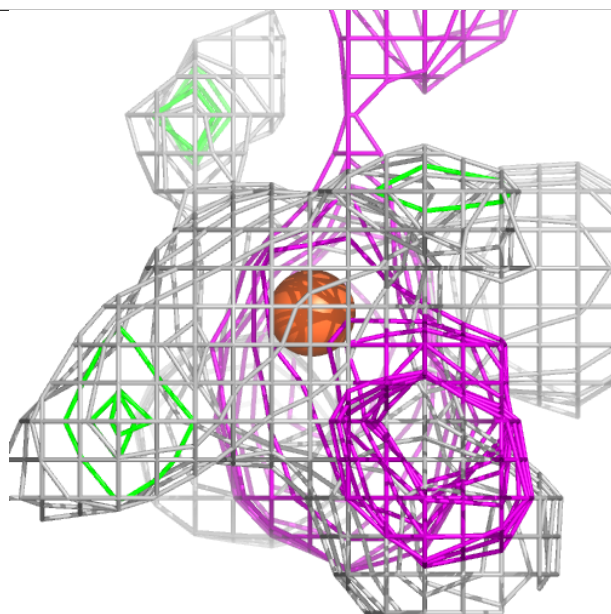
Electron density around FE M 201:

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and green (positive)



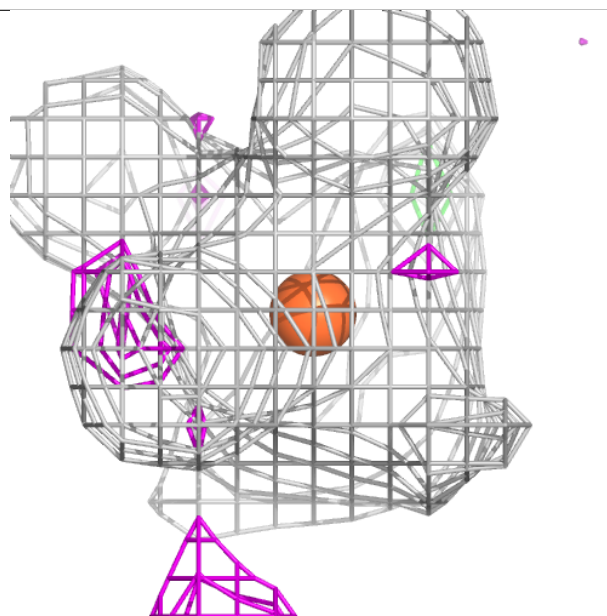
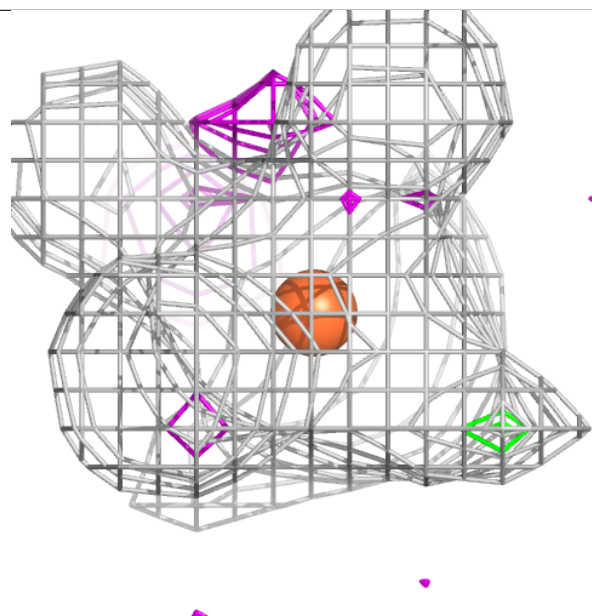
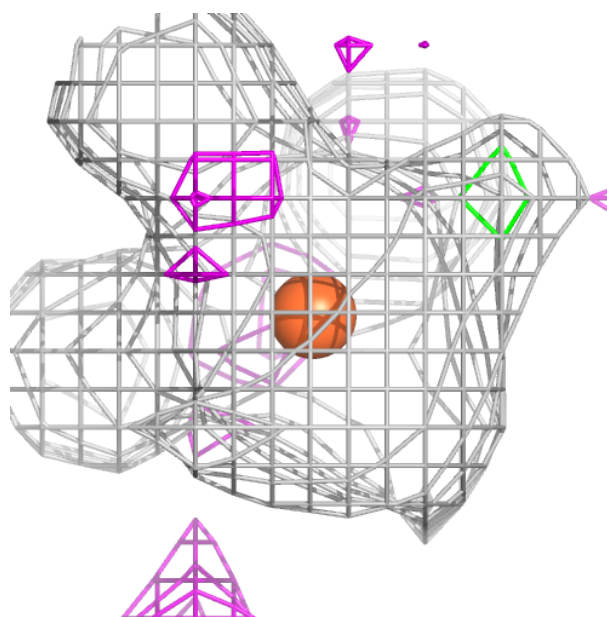
Electron density around FE2 B 203:

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



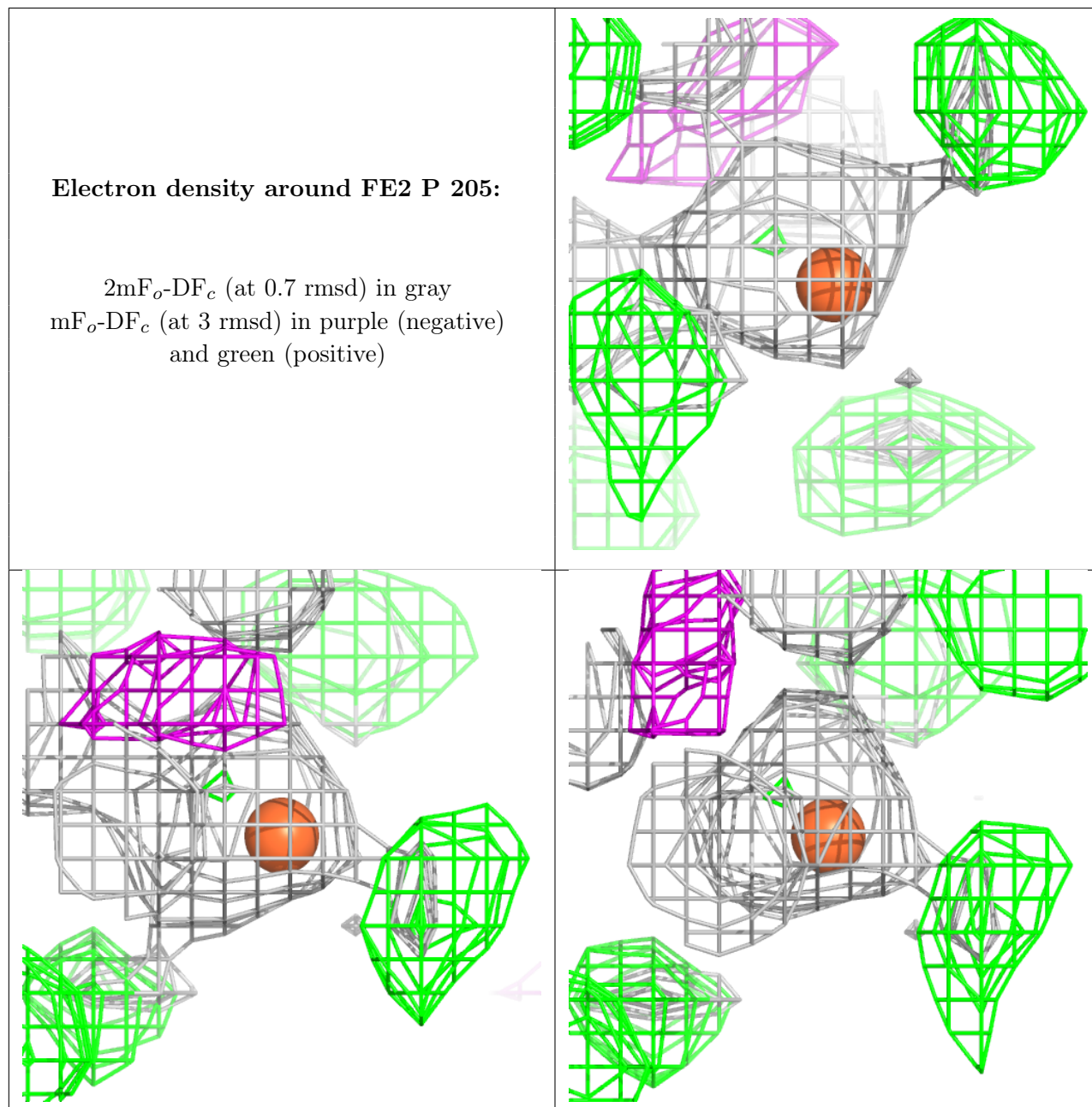
Electron density around FE2 P 203:

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



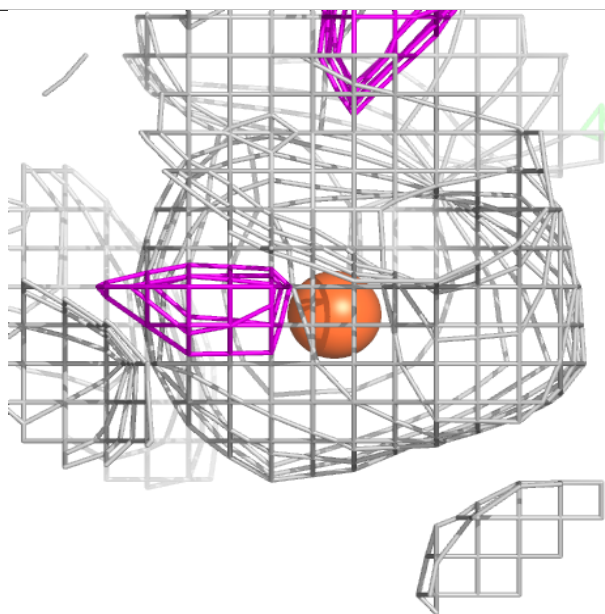
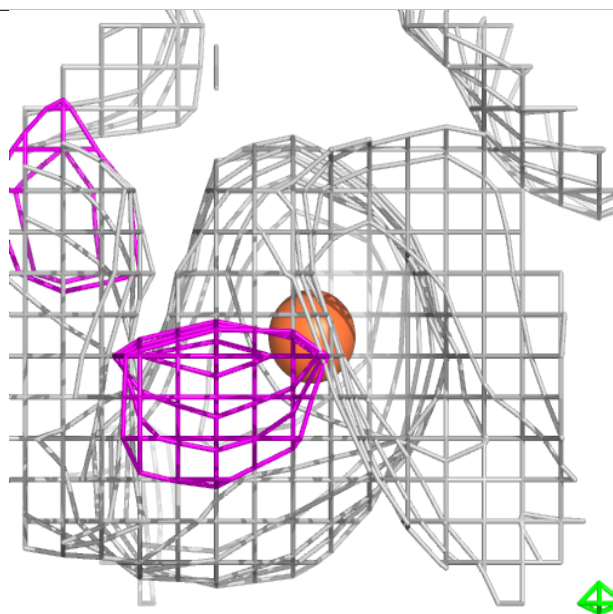
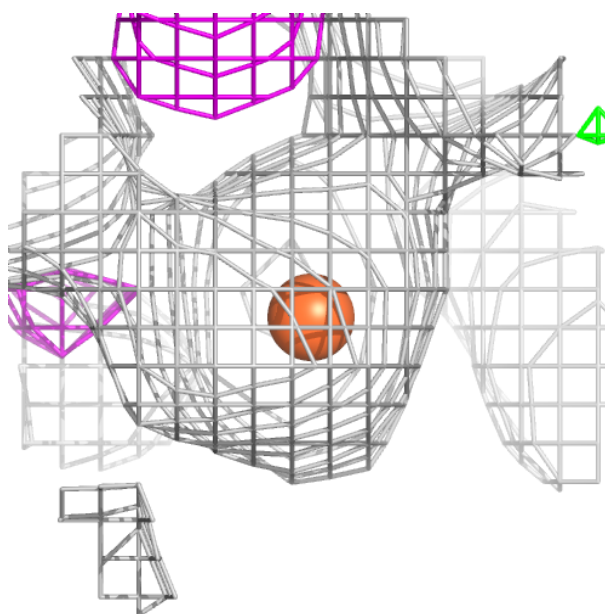
Electron density around FE2 P 205:

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



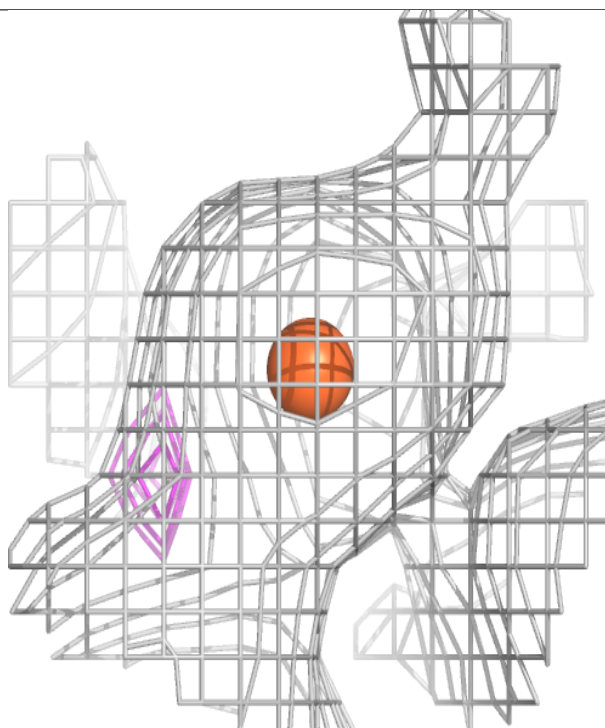
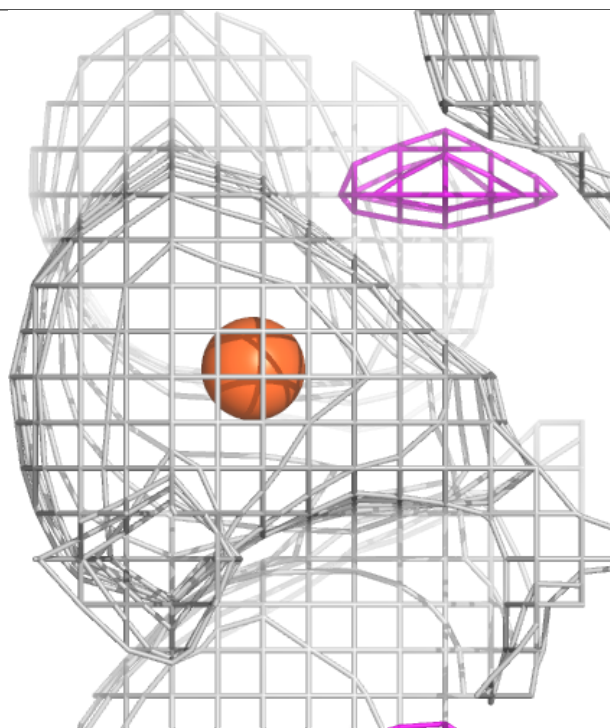
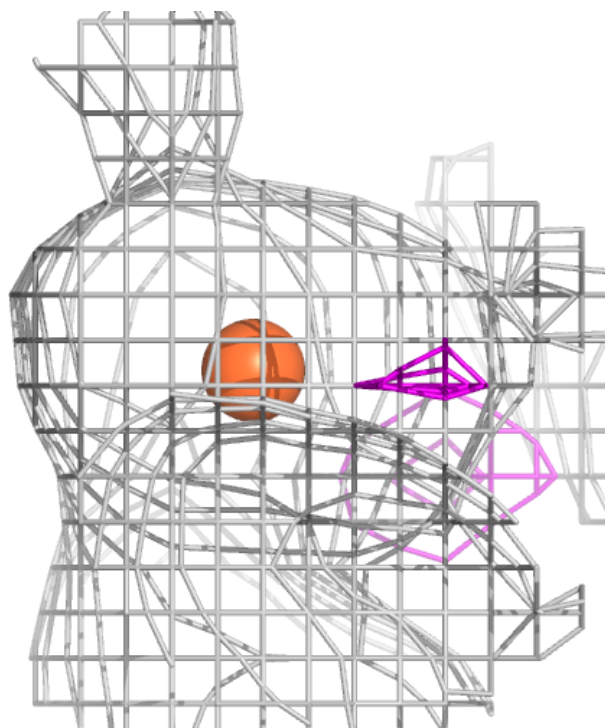
Electron density around FE E 201:

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



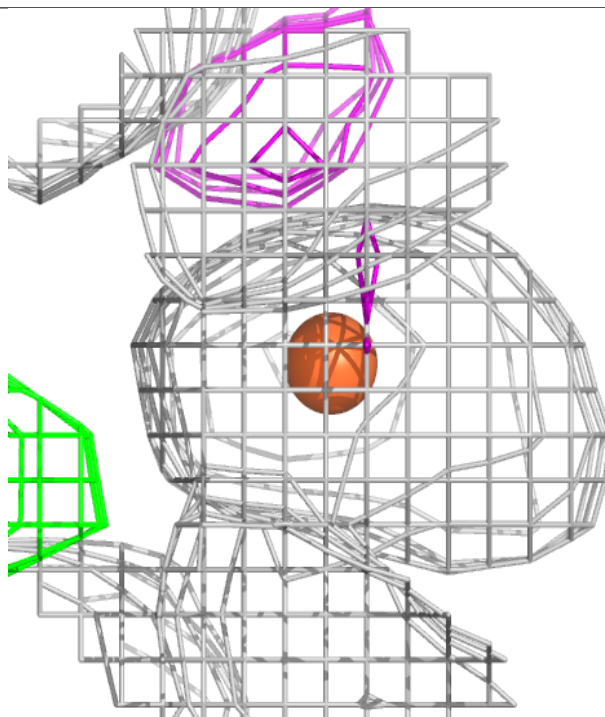
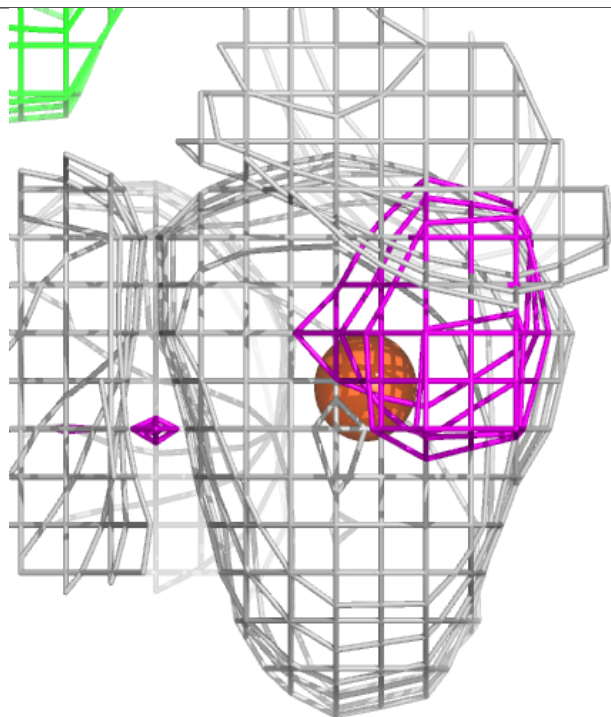
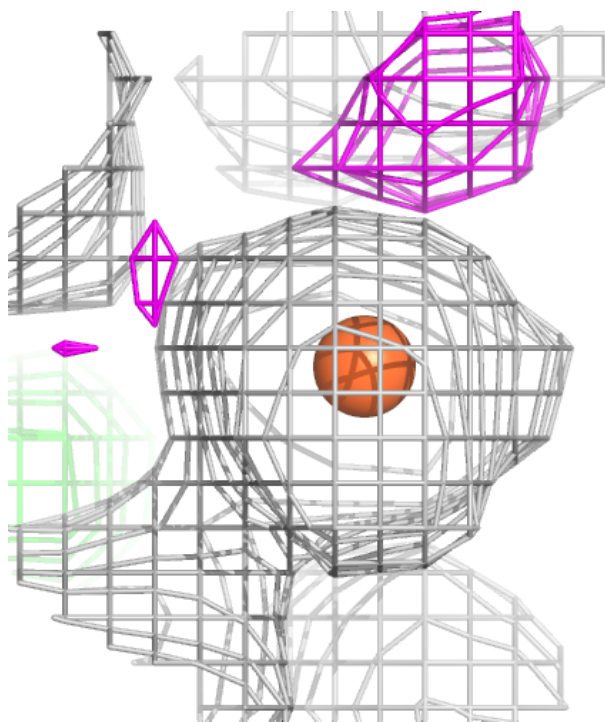
Electron density around FE R 201:

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



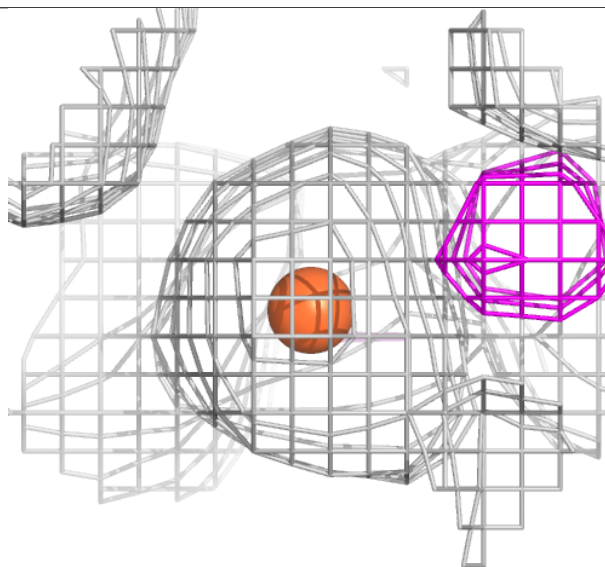
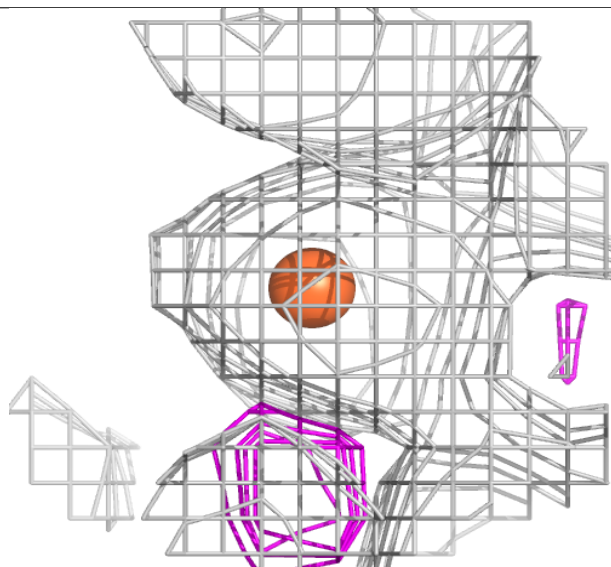
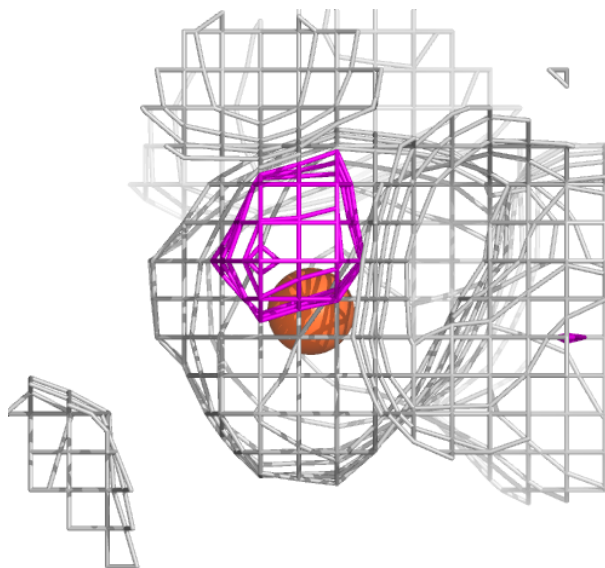
Electron density around FE S 201:

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and green (positive)



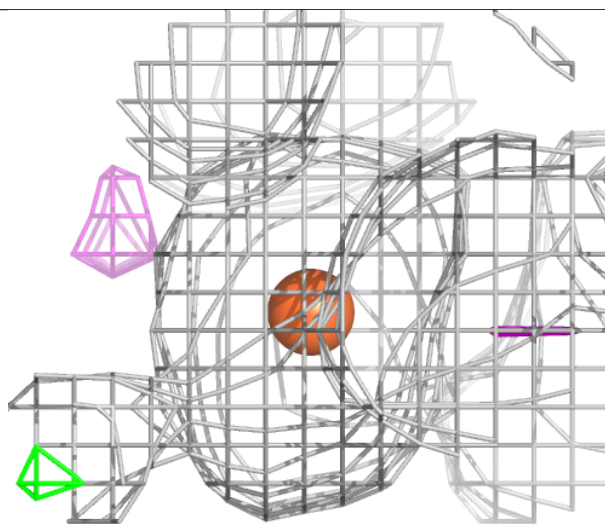
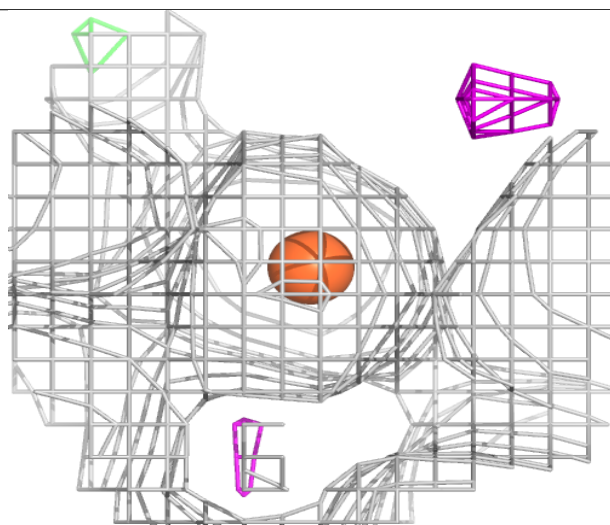
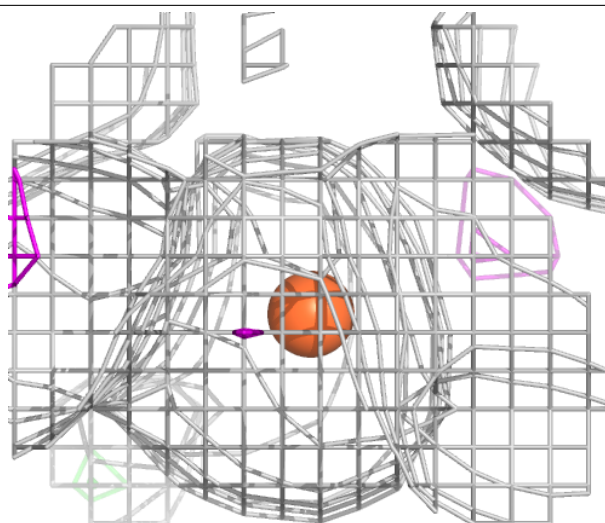
Electron density around FE T 201:

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



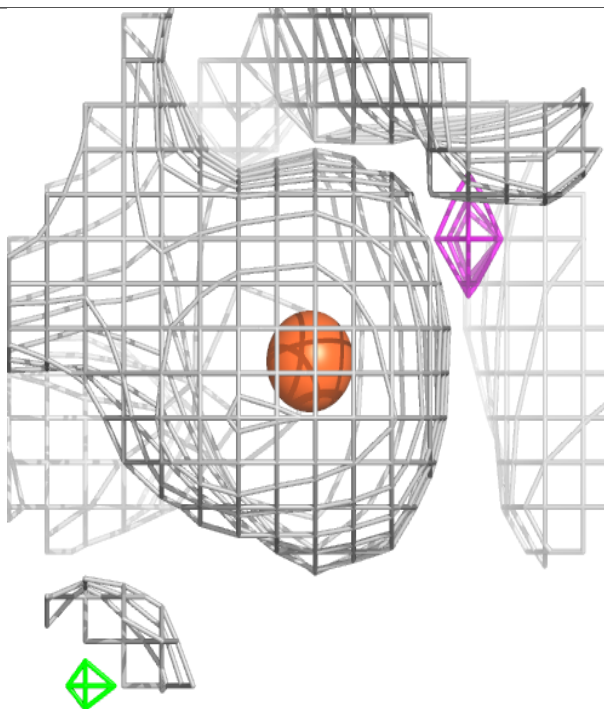
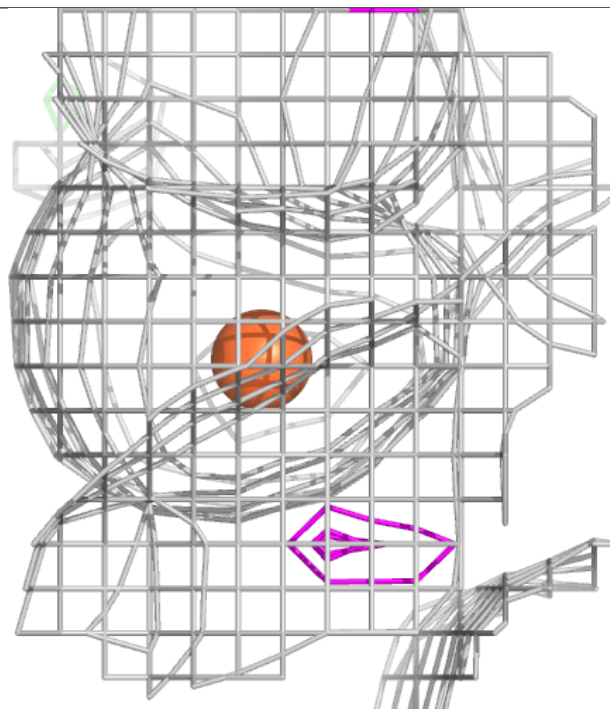
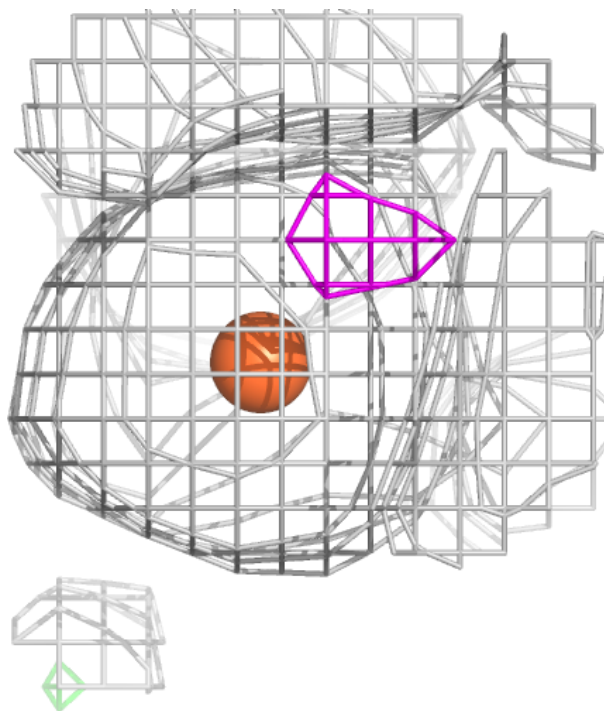
Electron density around FE H 201:

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



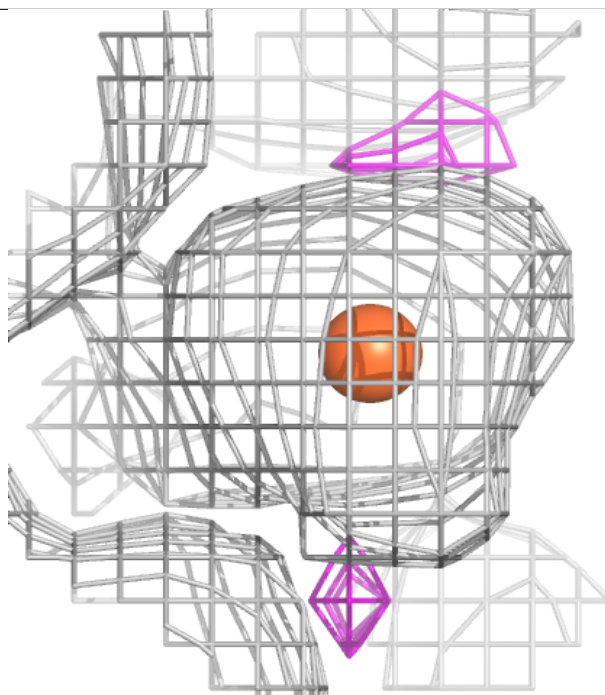
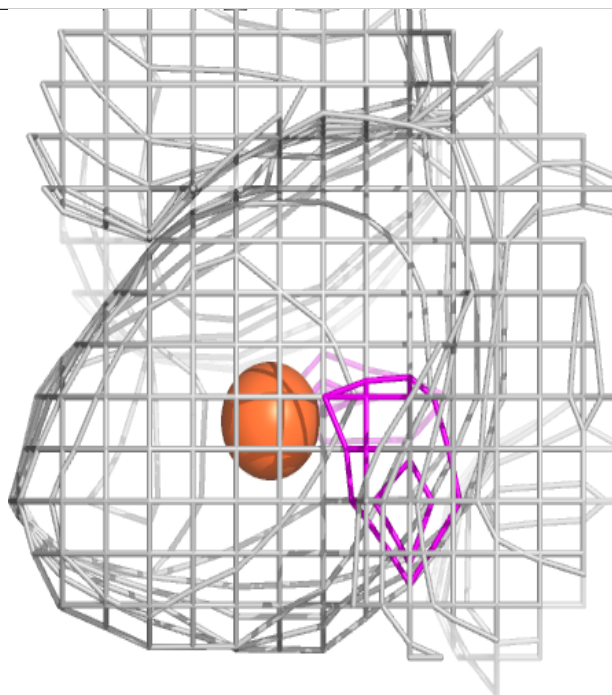
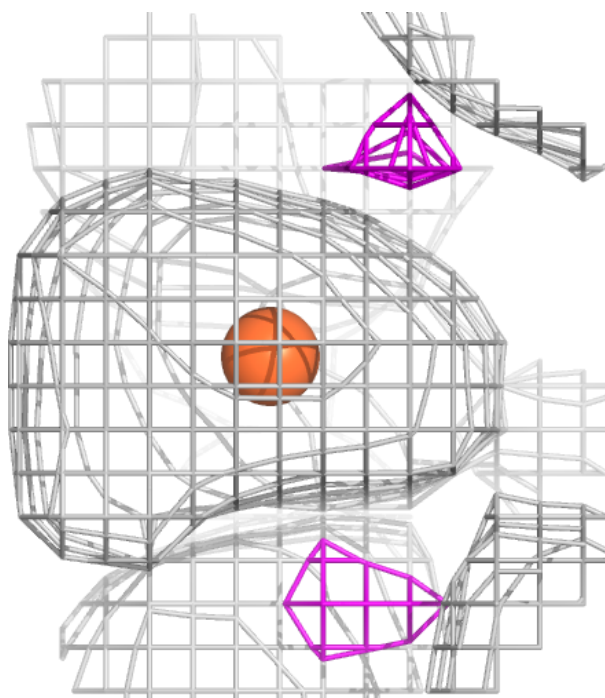
Electron density around FE C 201:

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



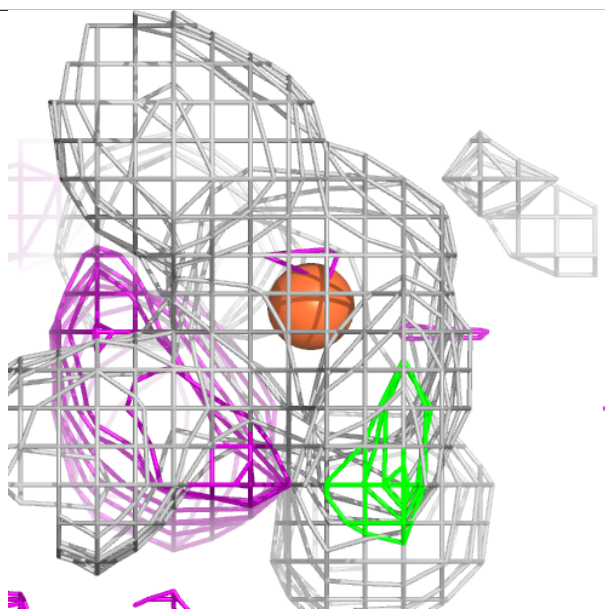
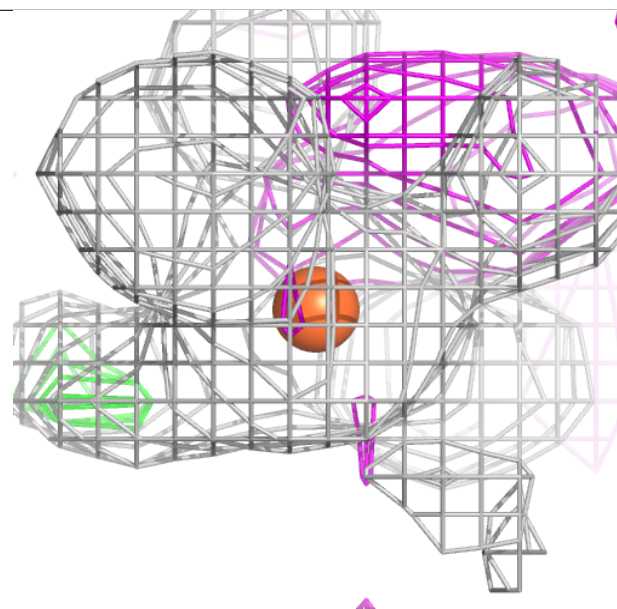
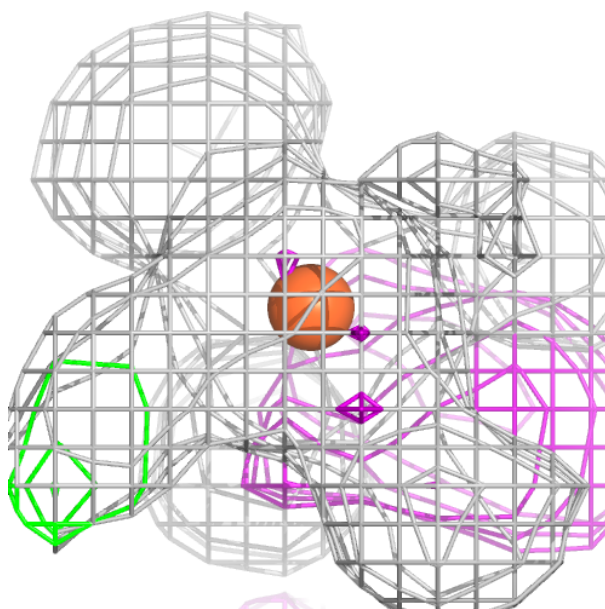
Electron density around FE C 207:

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and green (positive)



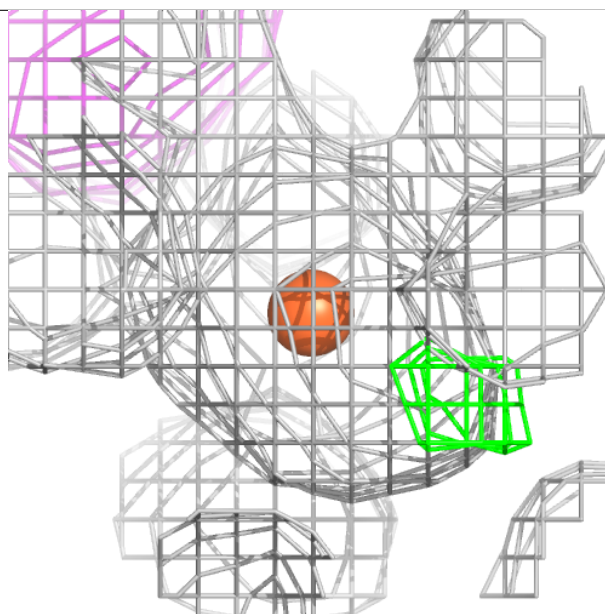
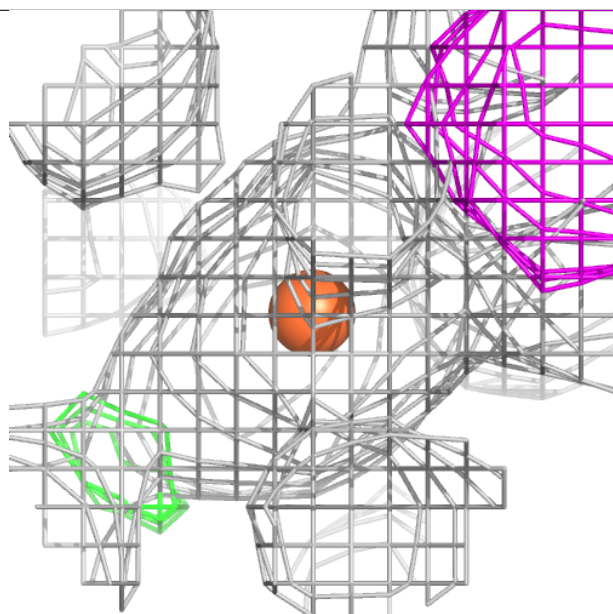
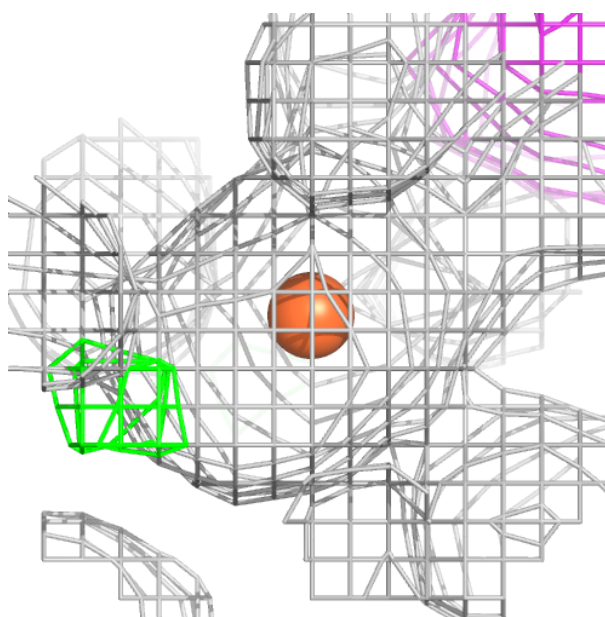
Electron density around FE2 A 204:

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and green (positive)



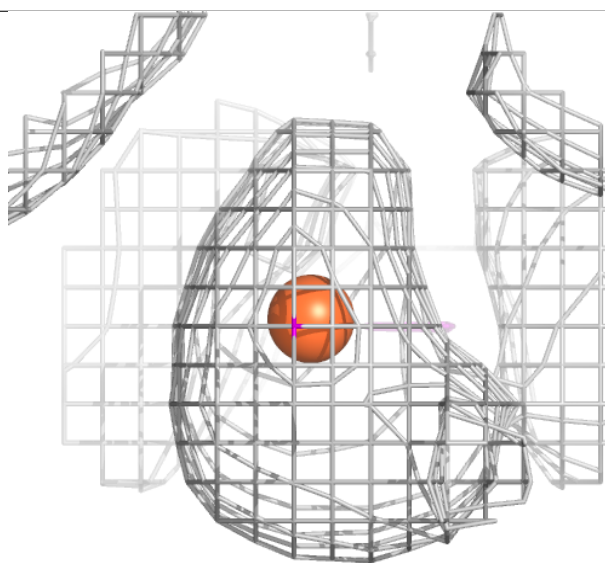
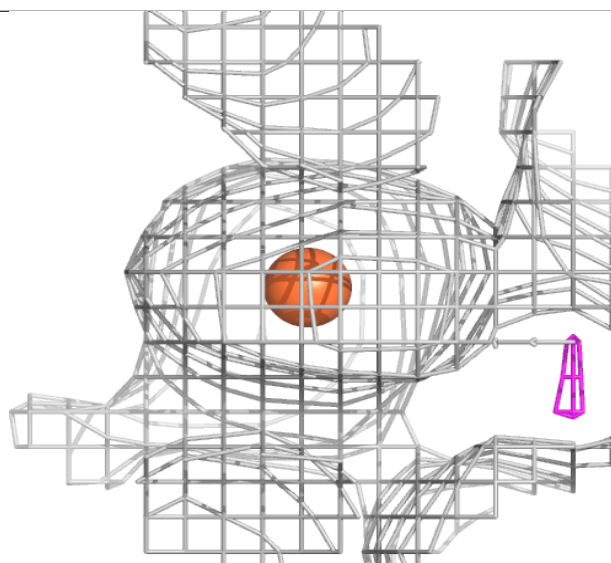
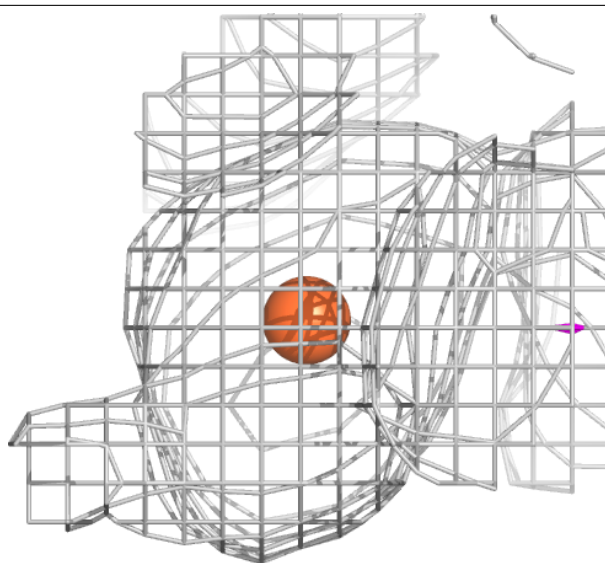
Electron density around FE2 A 205:

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



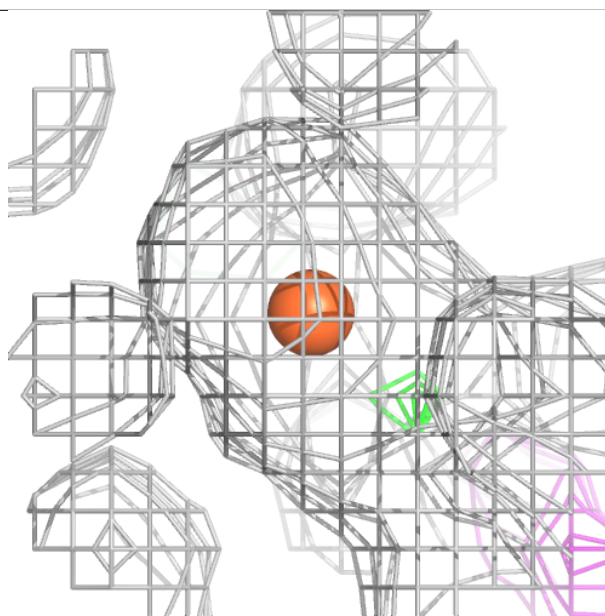
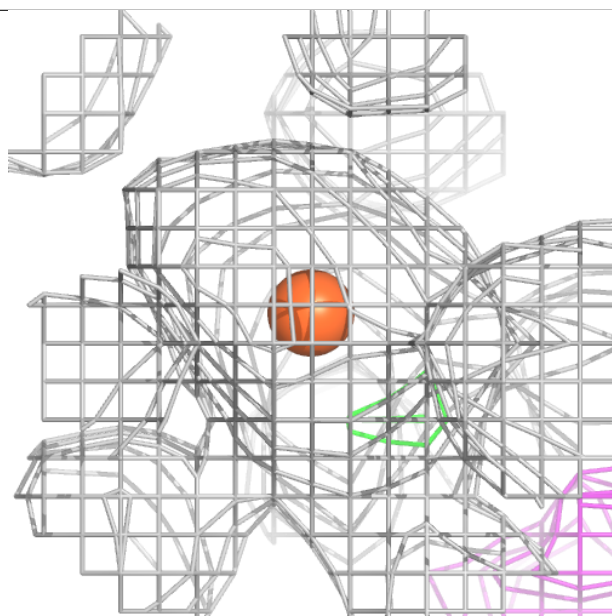
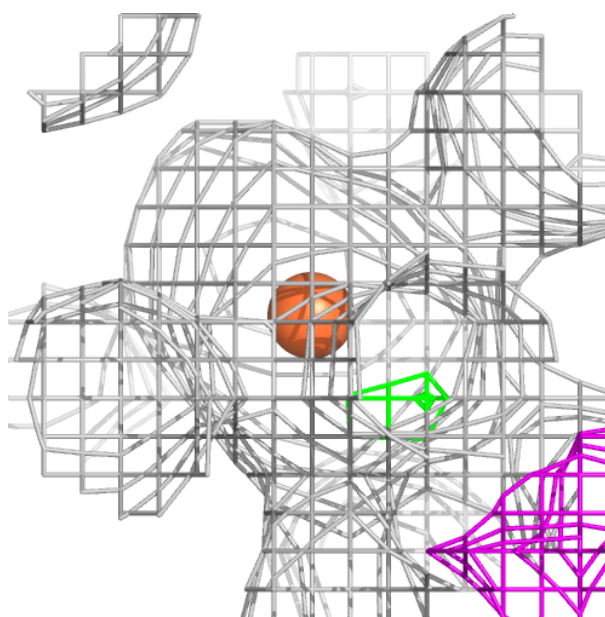
Electron density around FE B 201:

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and green (positive)



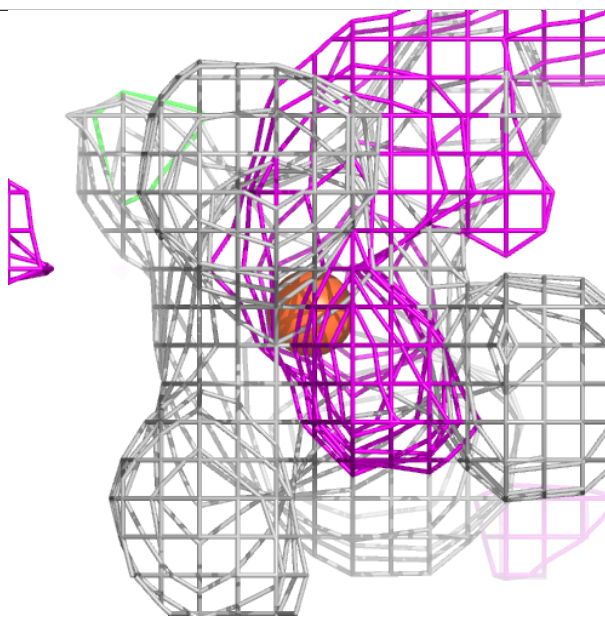
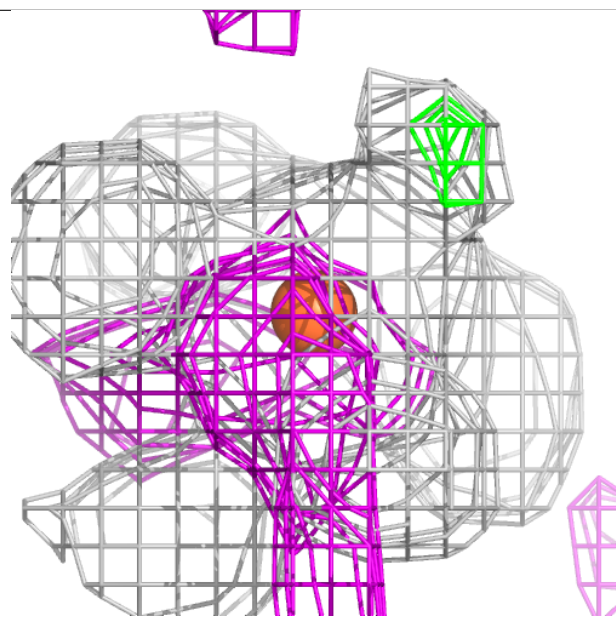
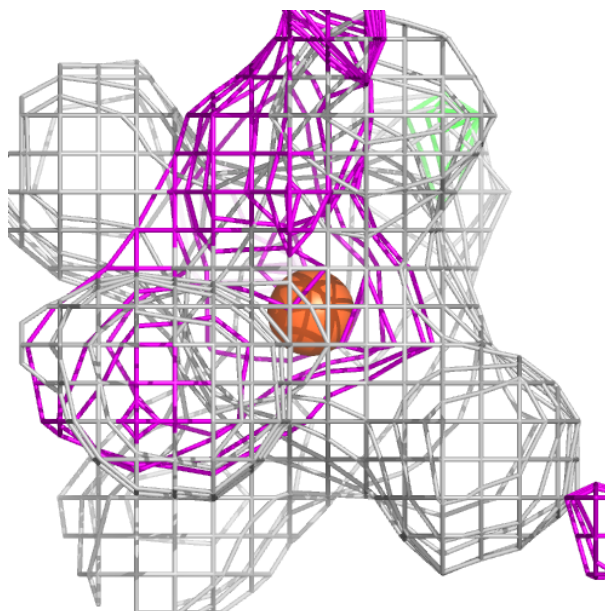
Electron density around FE2 C 205:

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



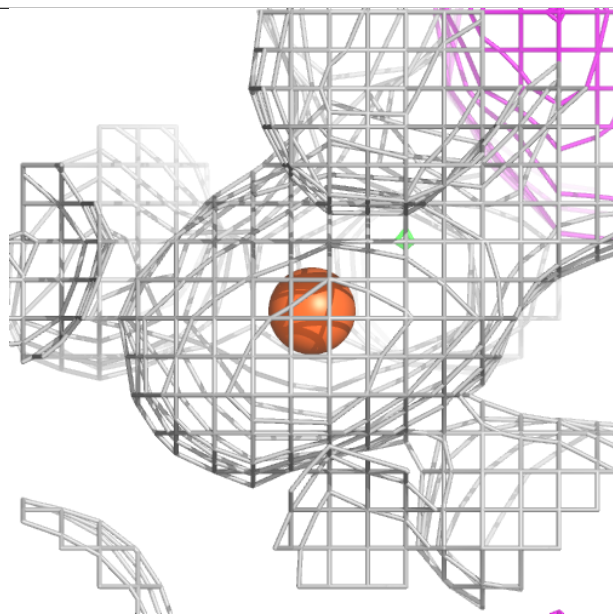
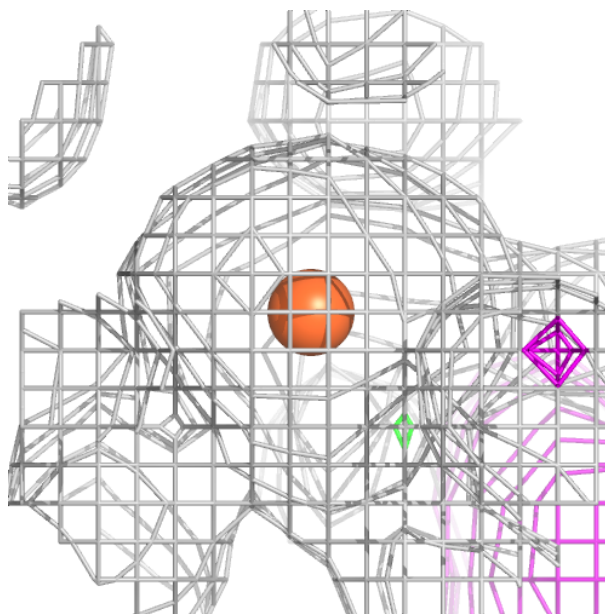
Electron density around FE2 E 203:

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and green (positive)



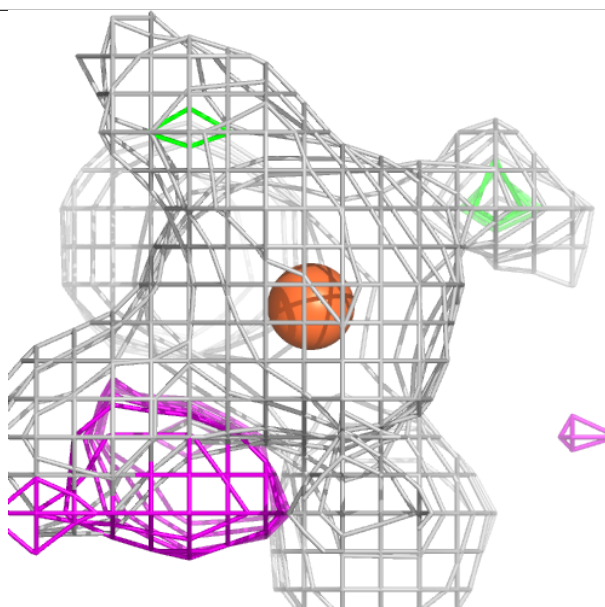
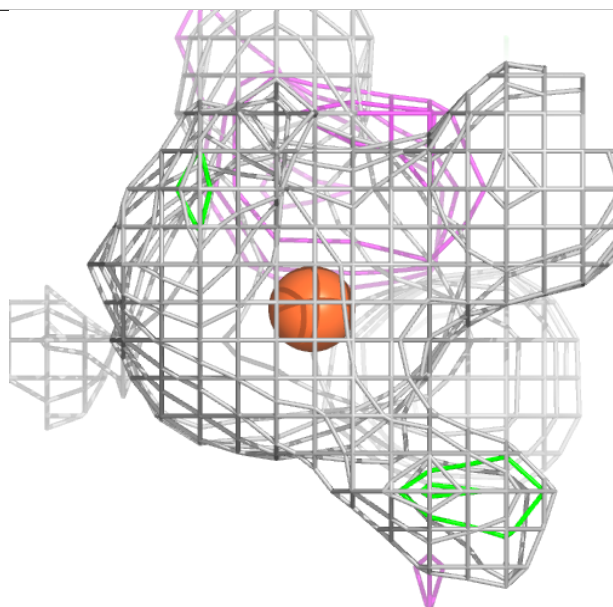
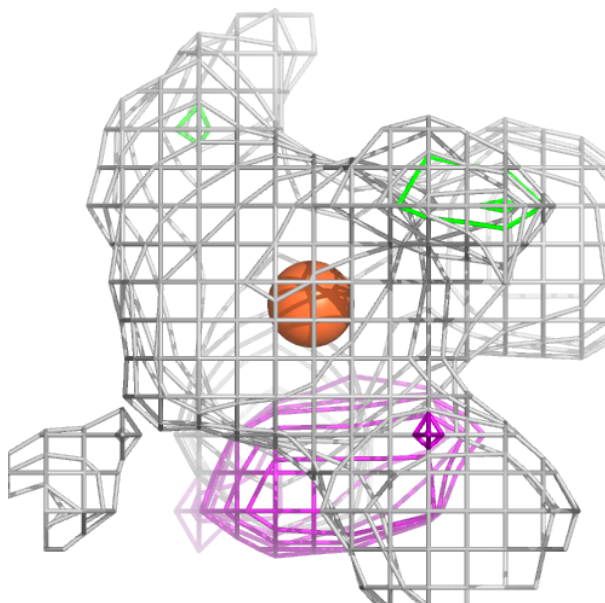
Electron density around FE2 E 205:

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



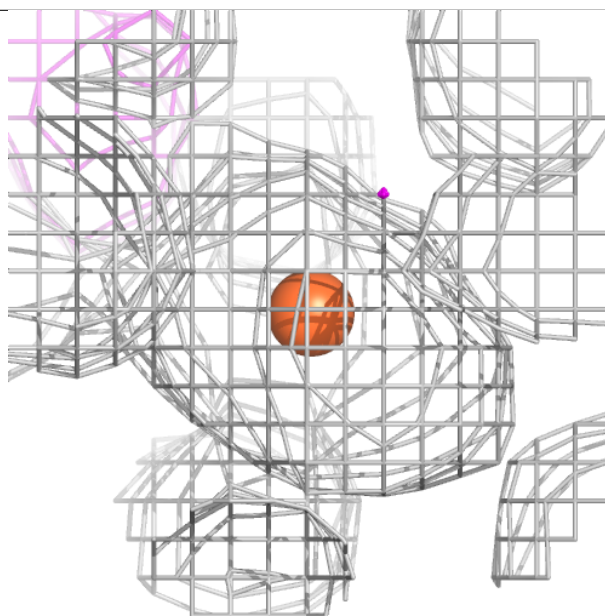
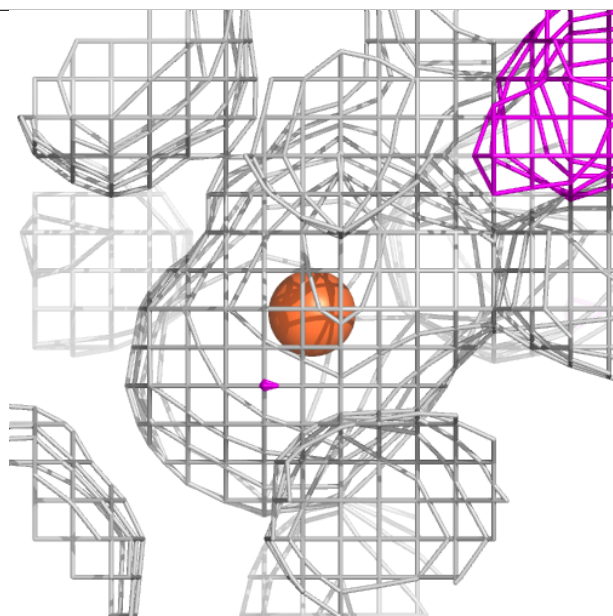
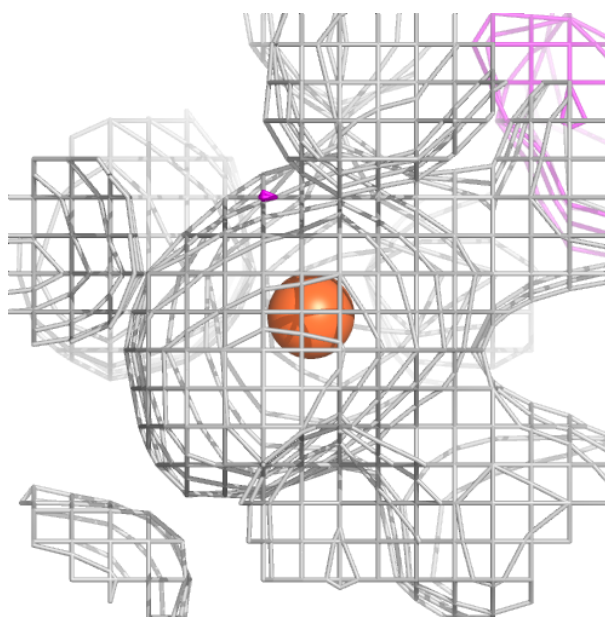
Electron density around FE2 H 204:

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



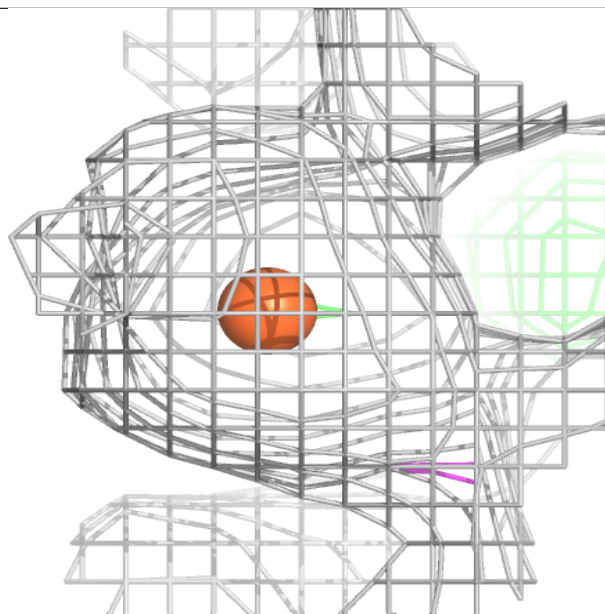
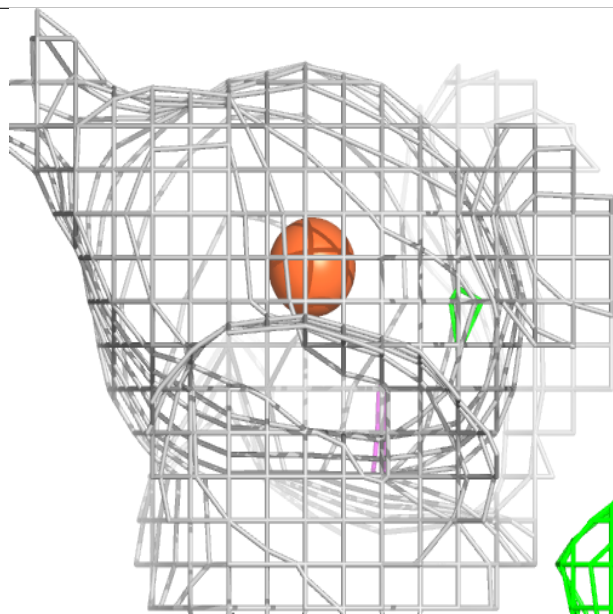
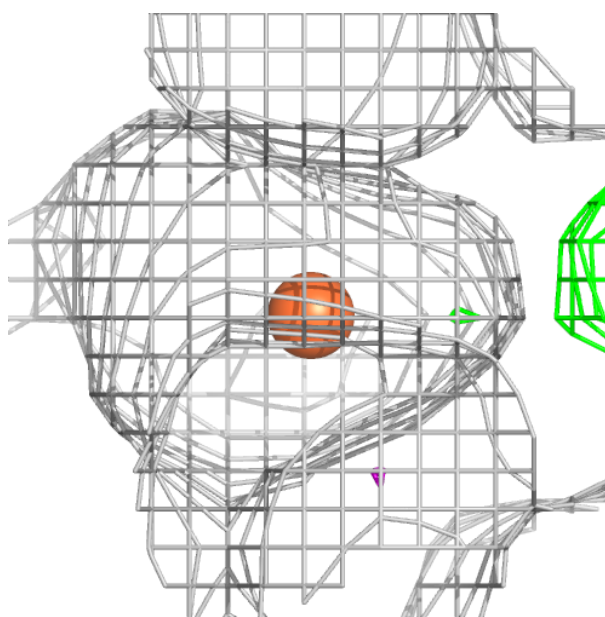
Electron density around FE2 H 205:

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



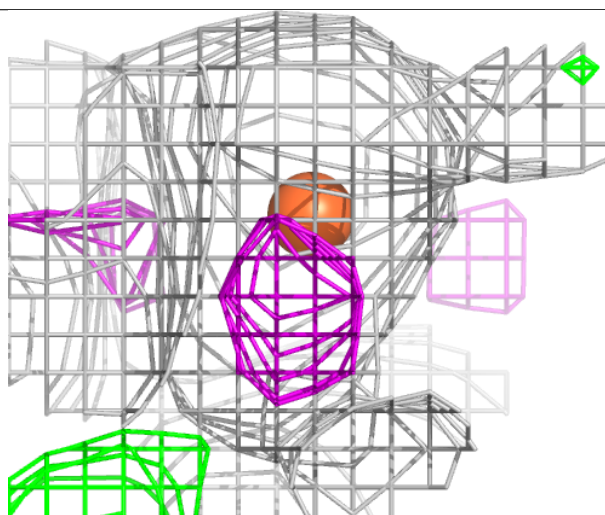
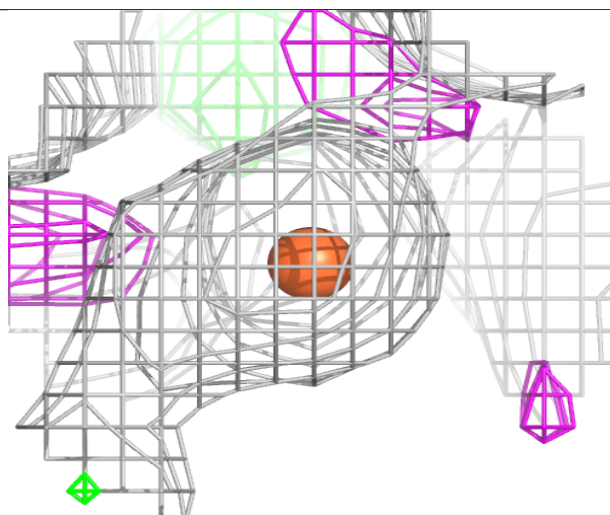
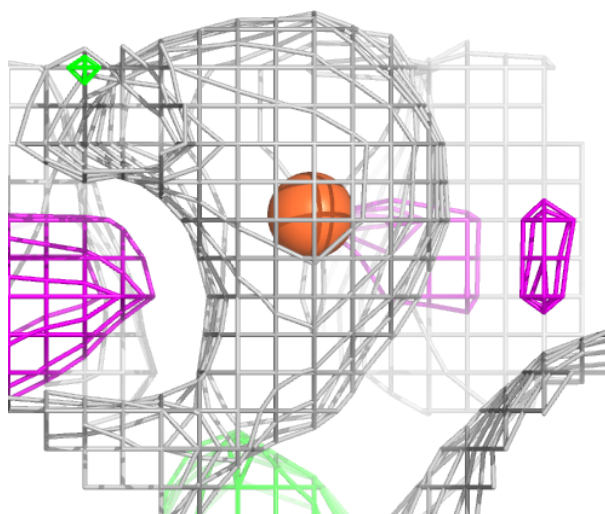
Electron density around FE O 201:

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and green (positive)



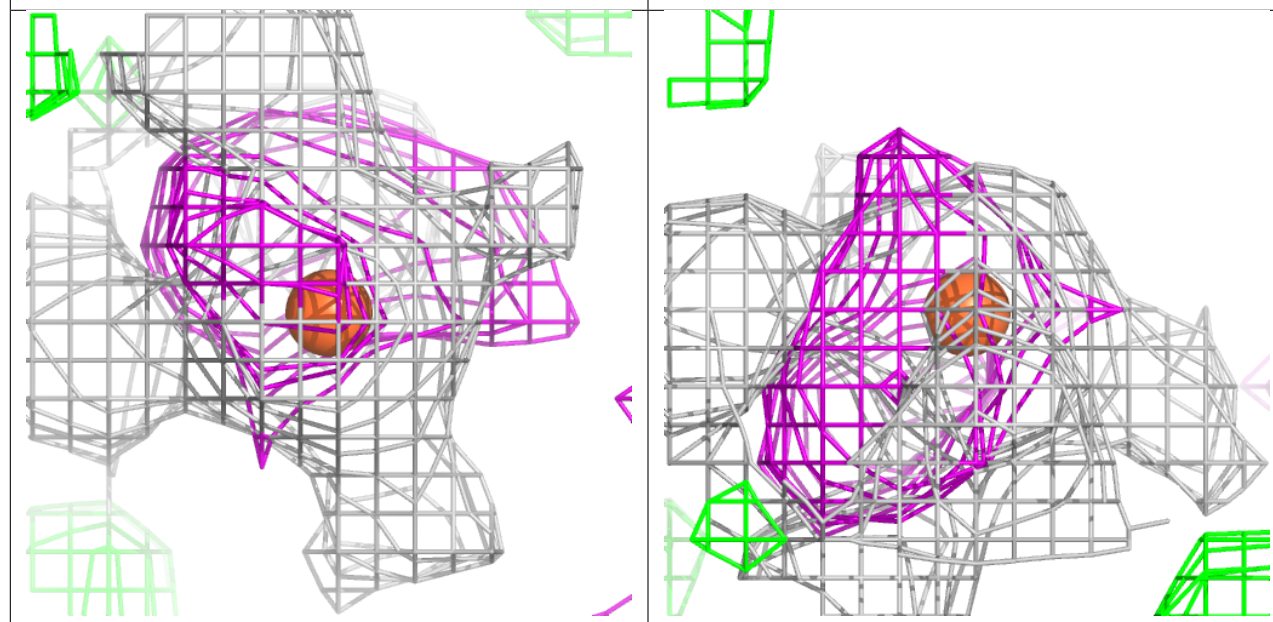
Electron density around FE P 201:

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and green (positive)



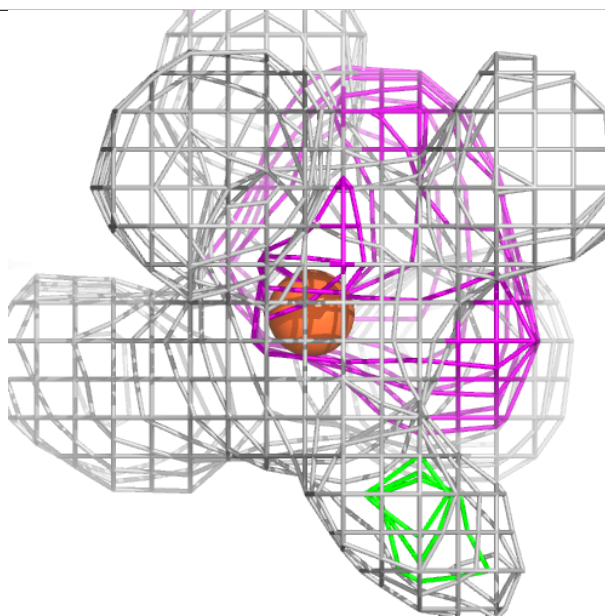
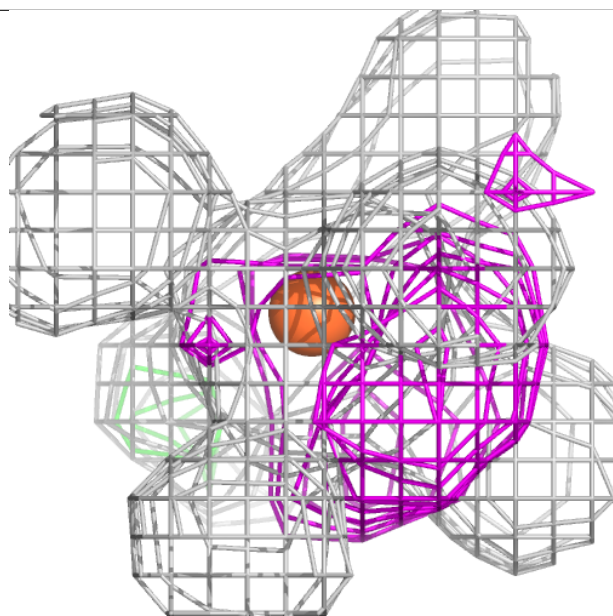
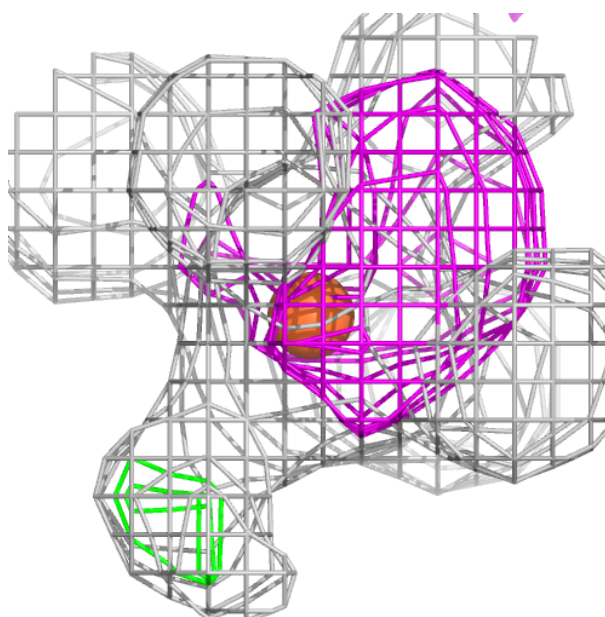
Electron density around FE2 B 204:

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



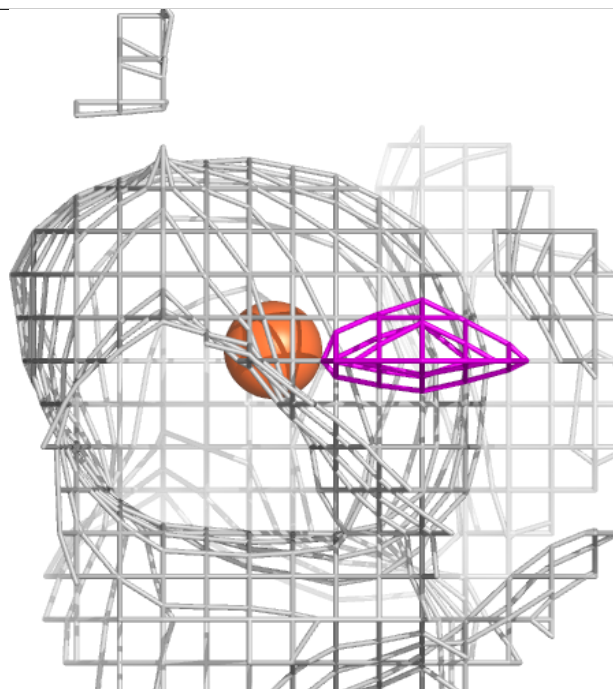
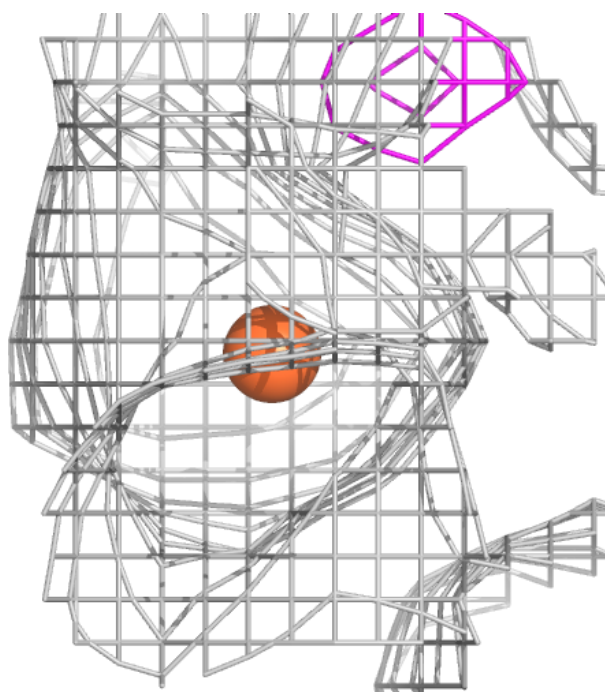
Electron density around FE2 C 204:

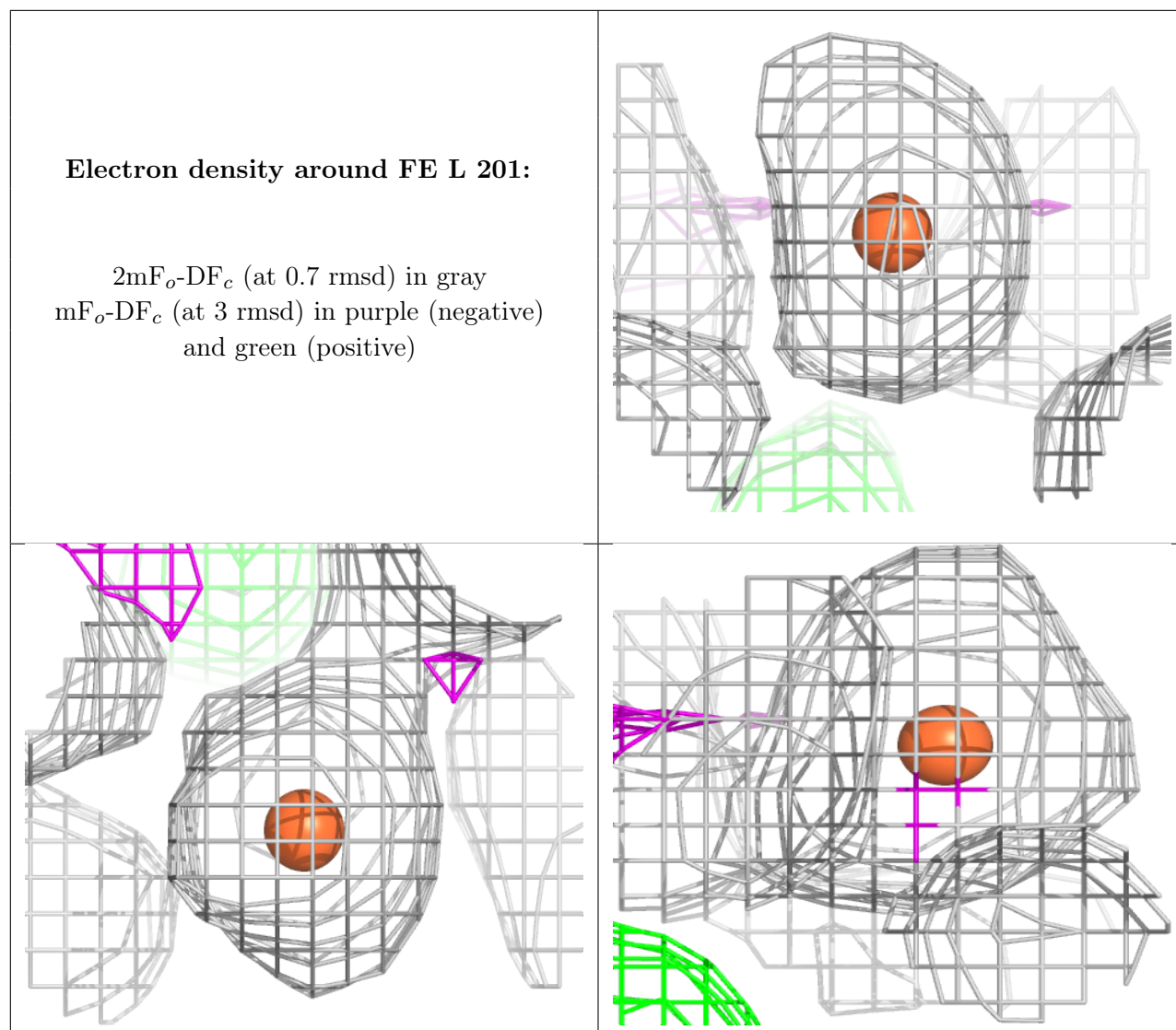
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE K 201:

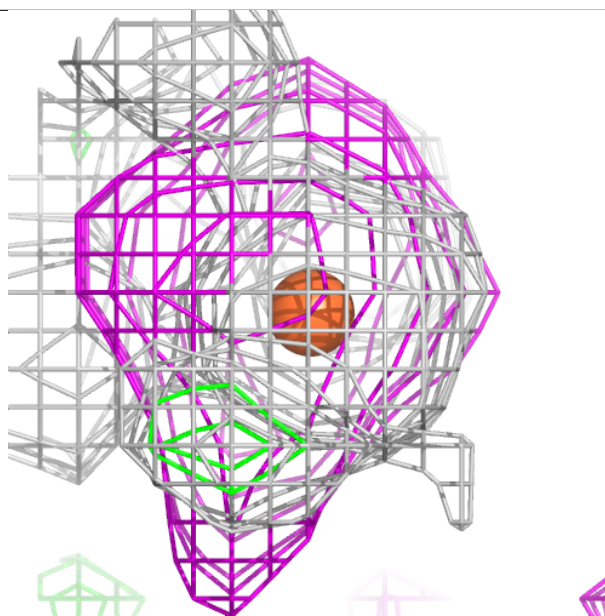
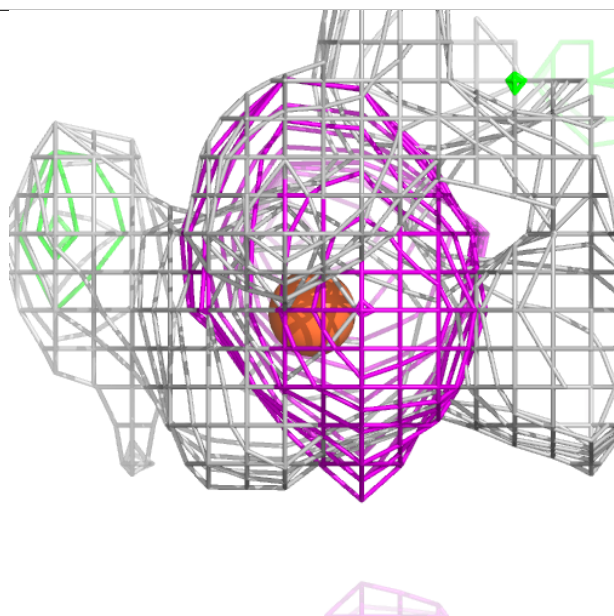
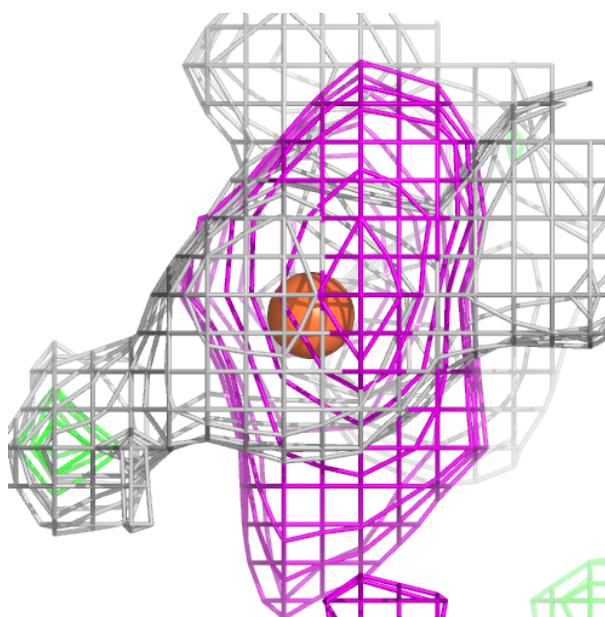
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





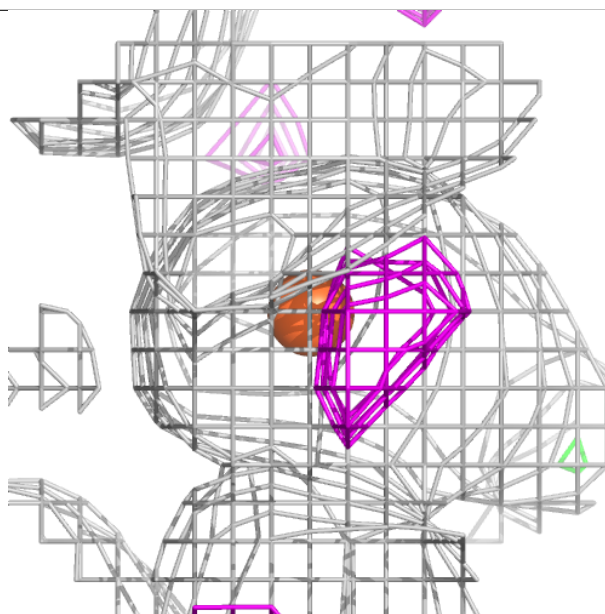
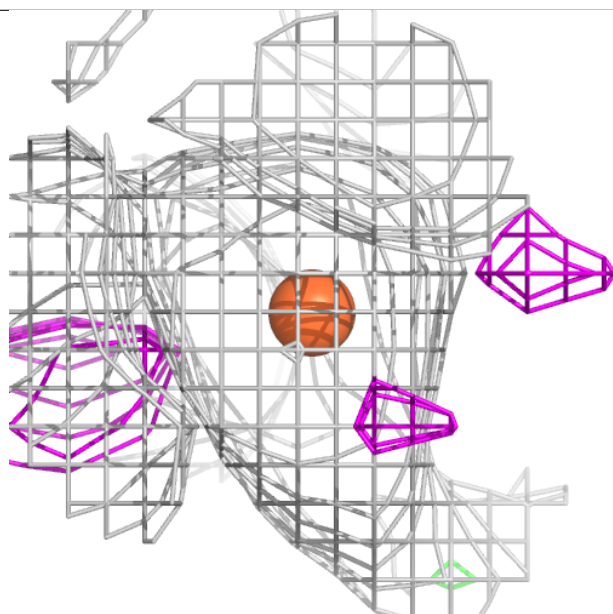
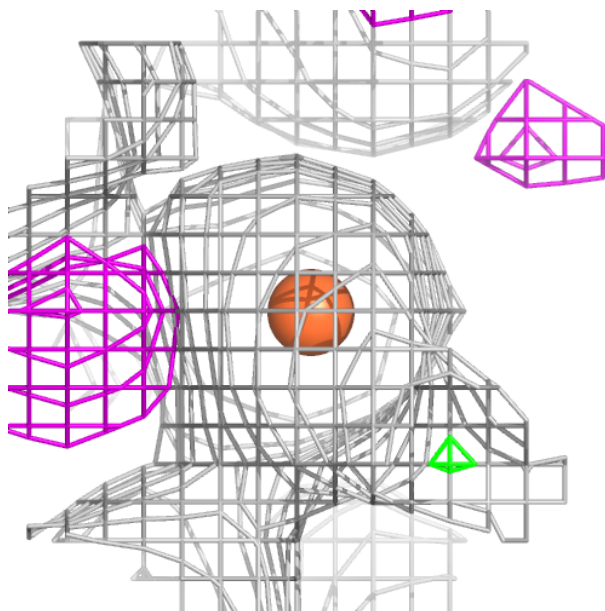
Electron density around FE2 E 204:

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



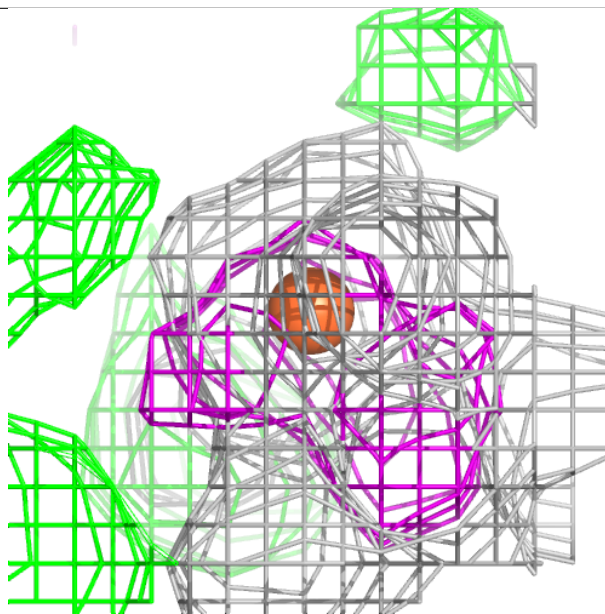
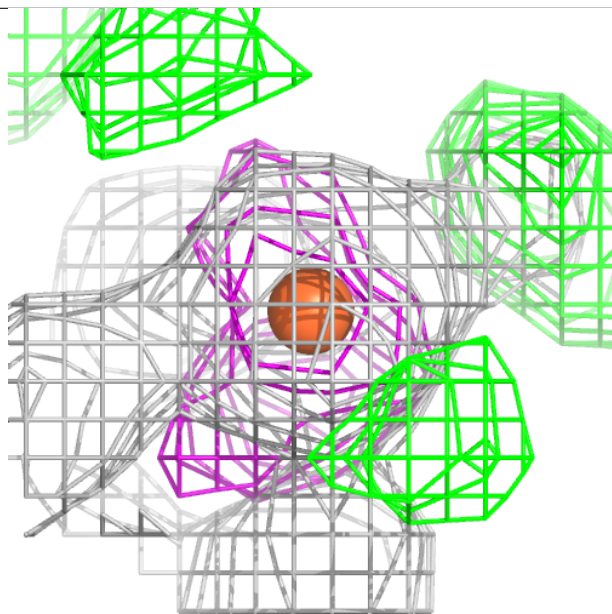
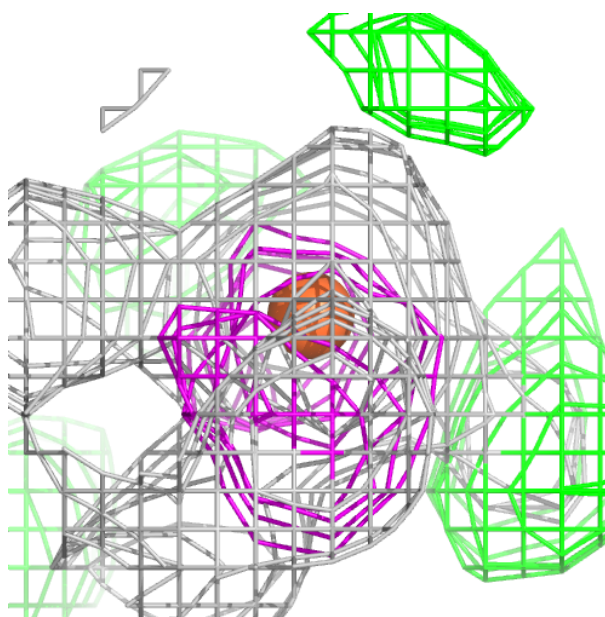
Electron density around FE A 201:

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



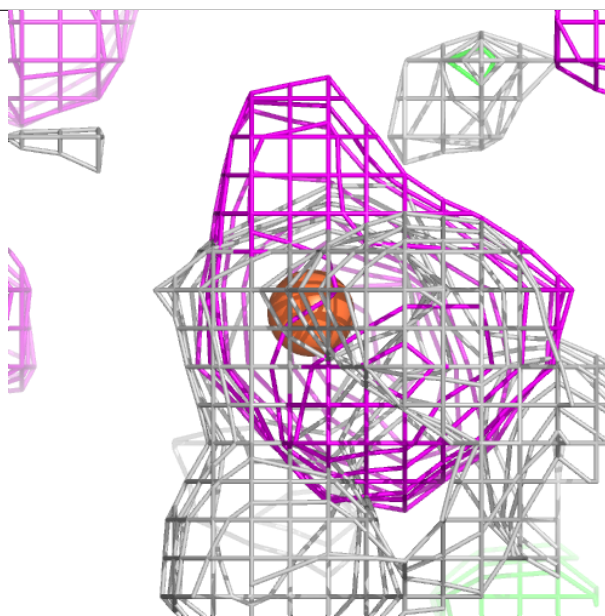
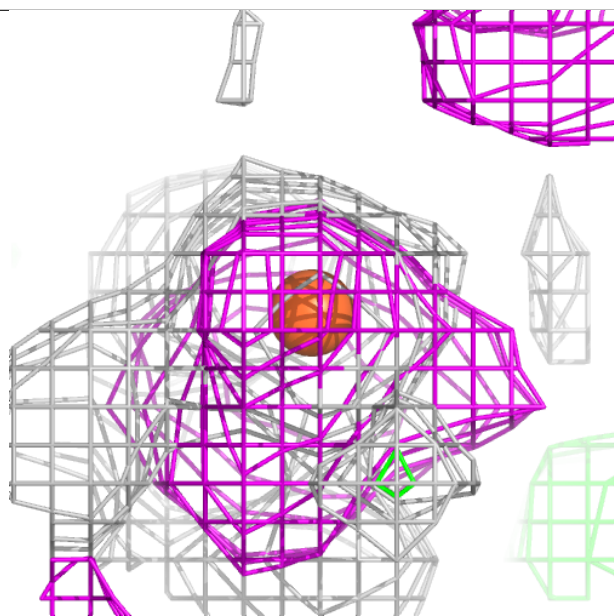
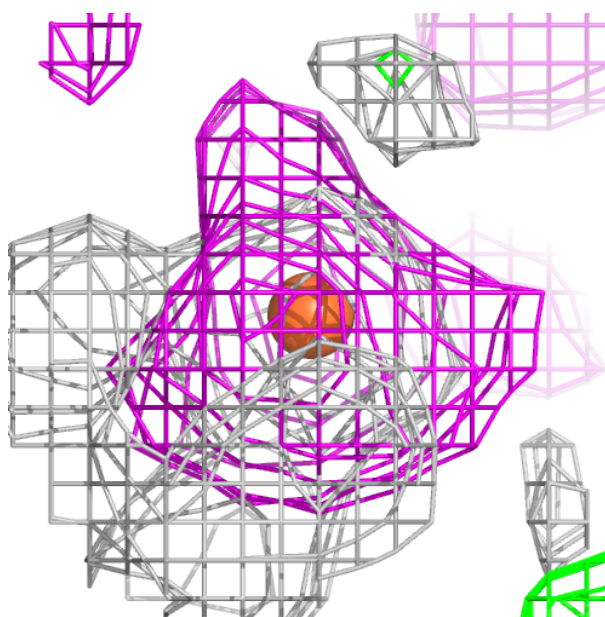
Electron density around FE2 H 203:

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



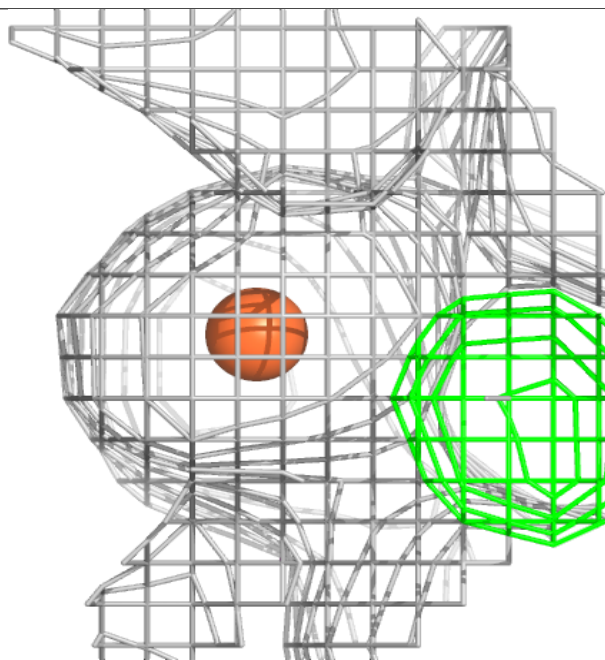
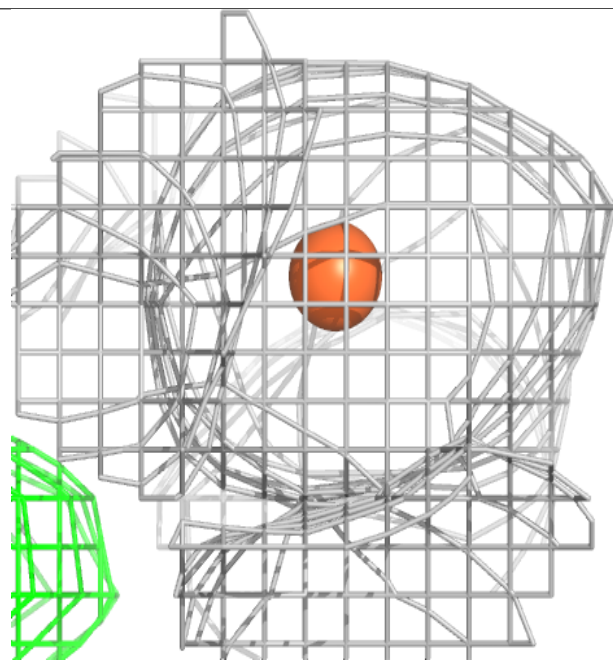
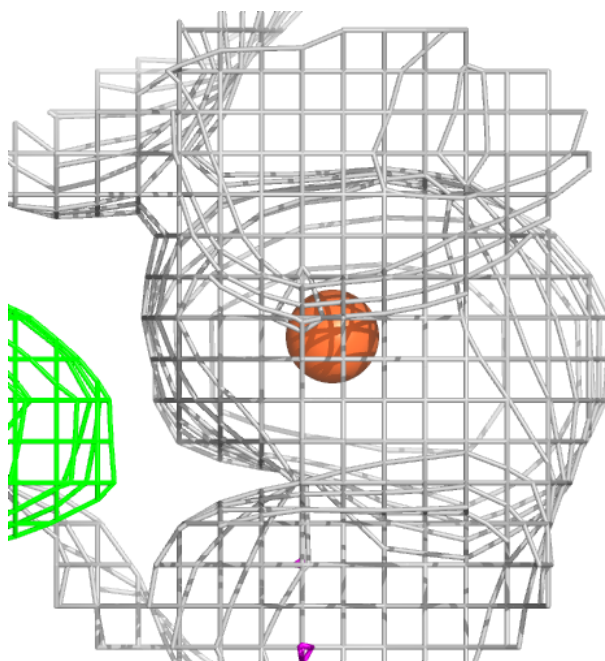
Electron density around FE2 A 203:

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



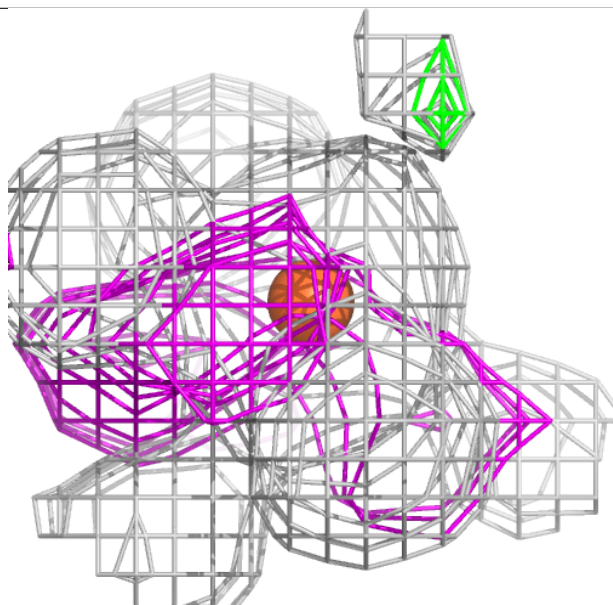
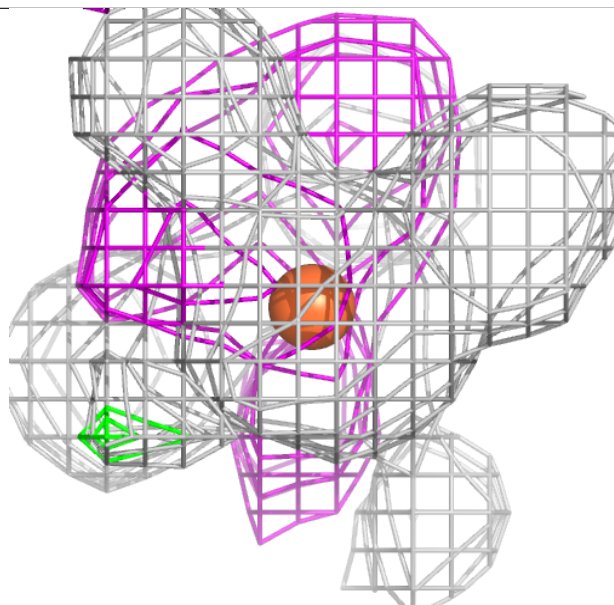
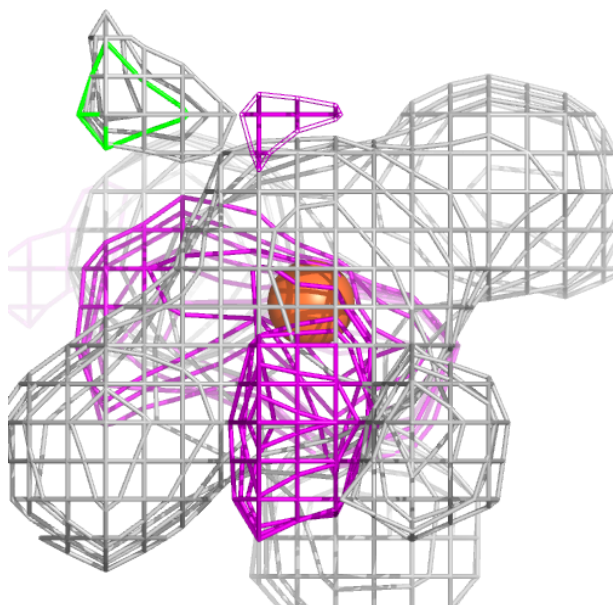
Electron density around FE I 201:

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



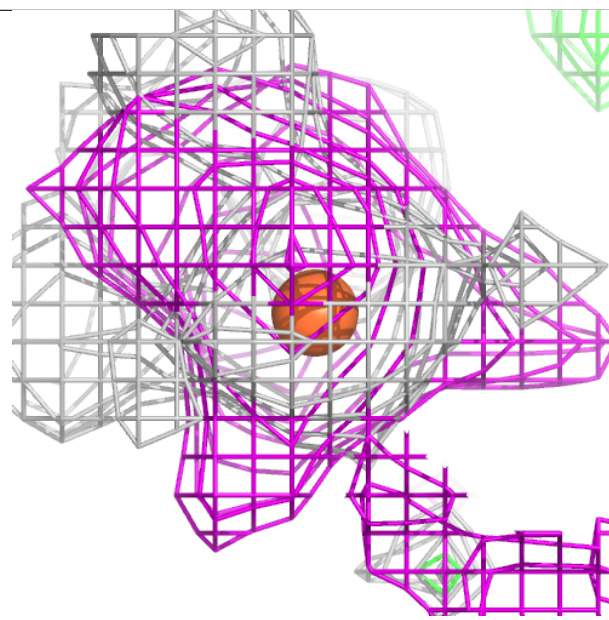
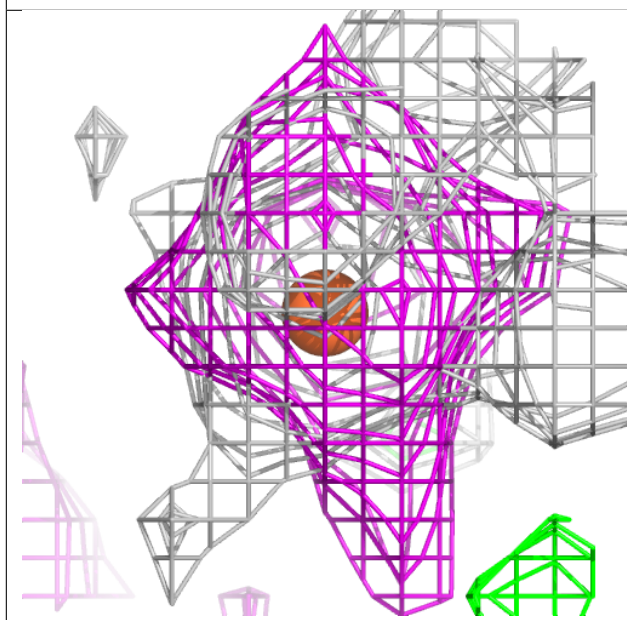
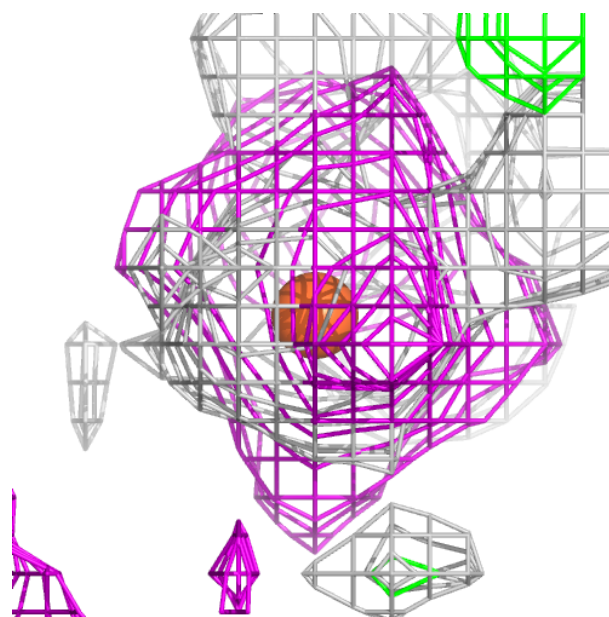
Electron density around FE2 I 204:

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



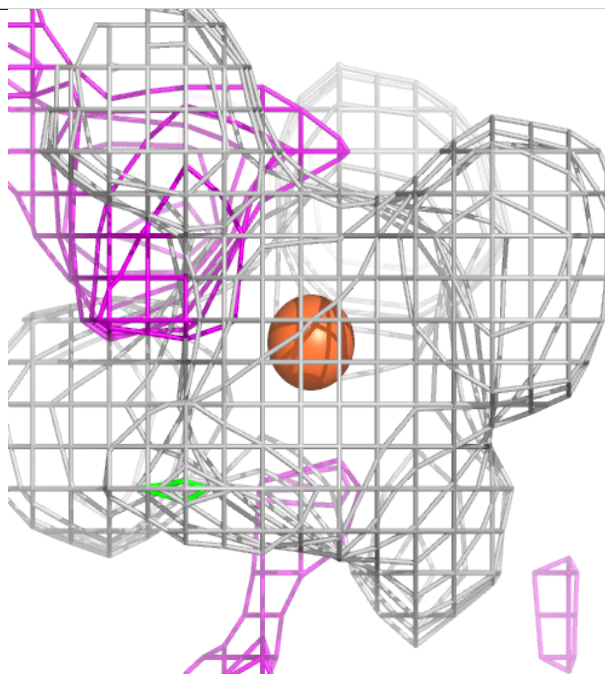
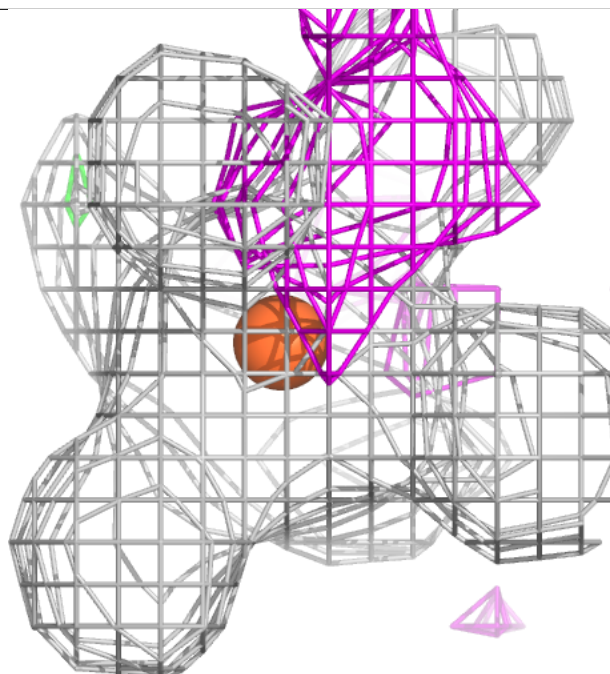
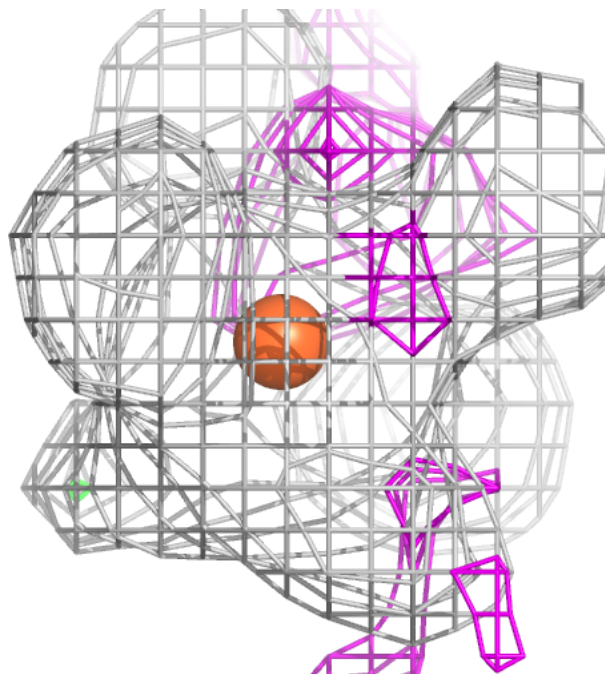
Electron density around FE2 K 202:

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



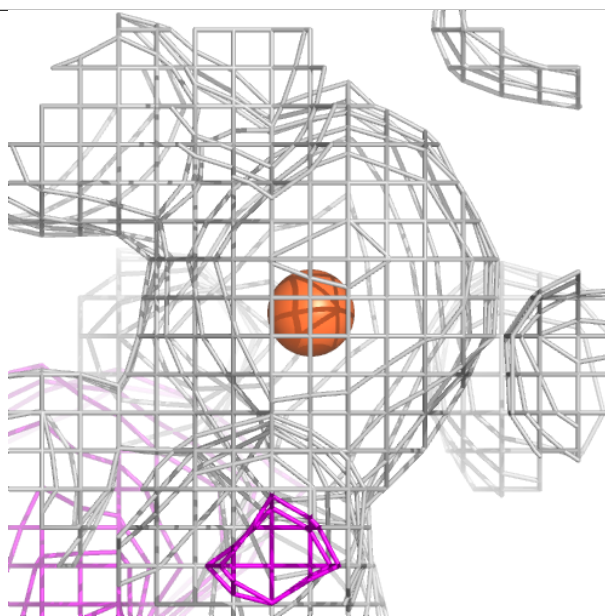
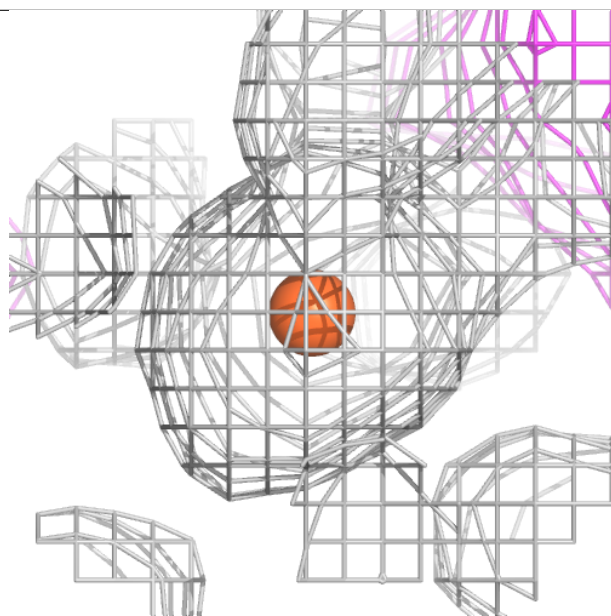
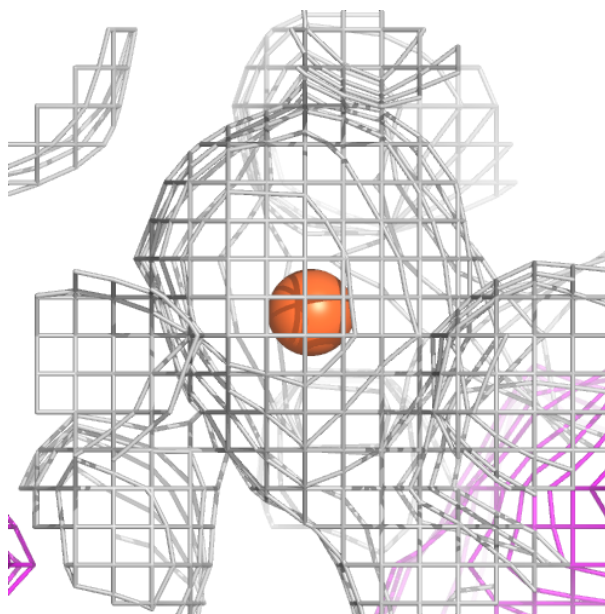
Electron density around FE2 K 204:

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



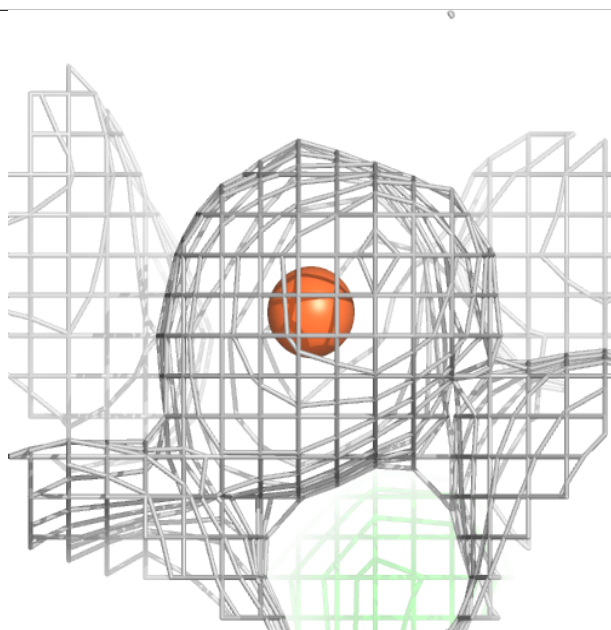
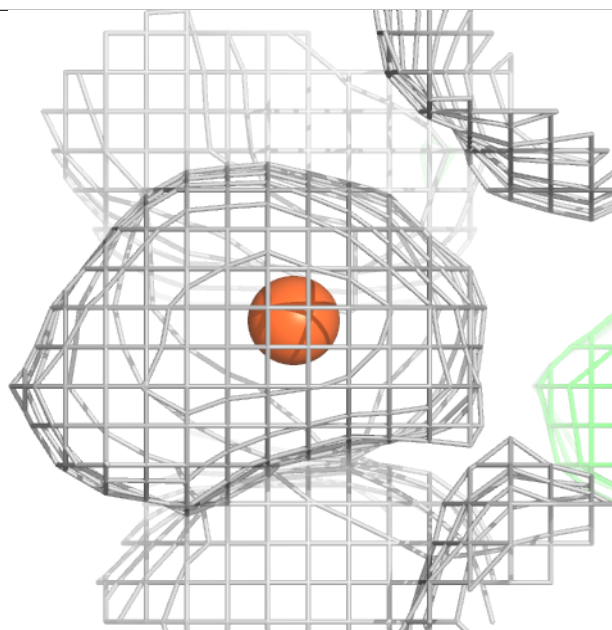
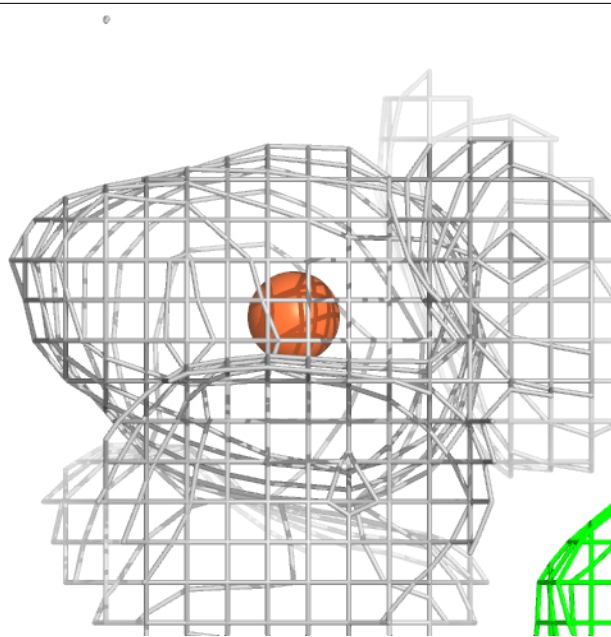
Electron density around FE2 K 205:

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



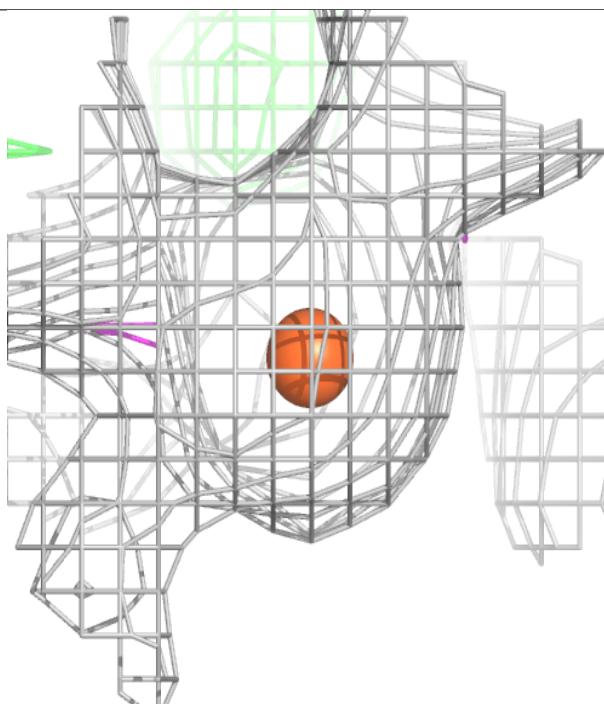
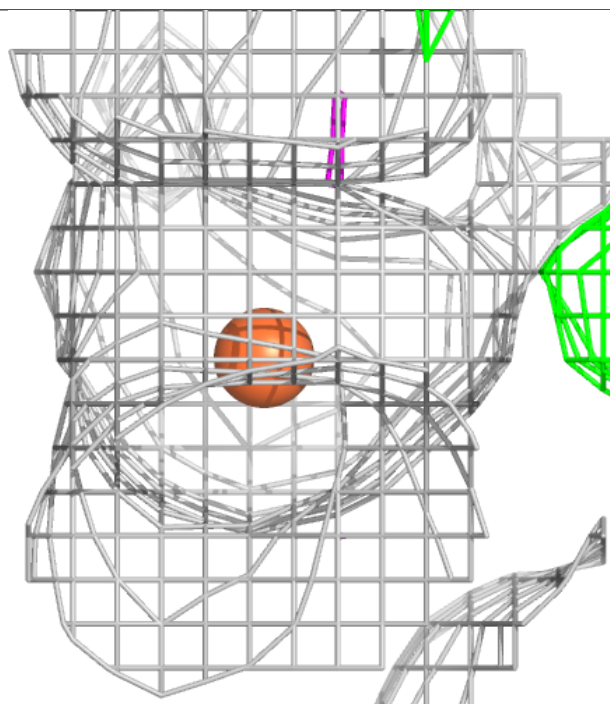
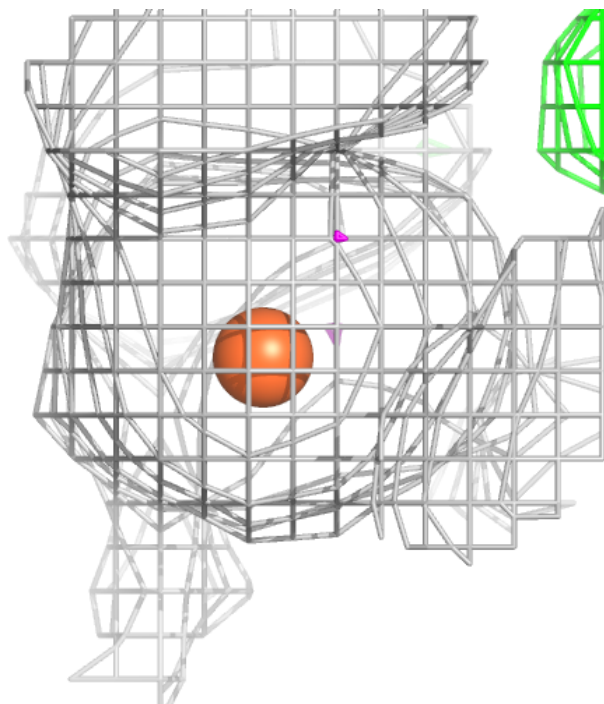
Electron density around FE F 201:

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



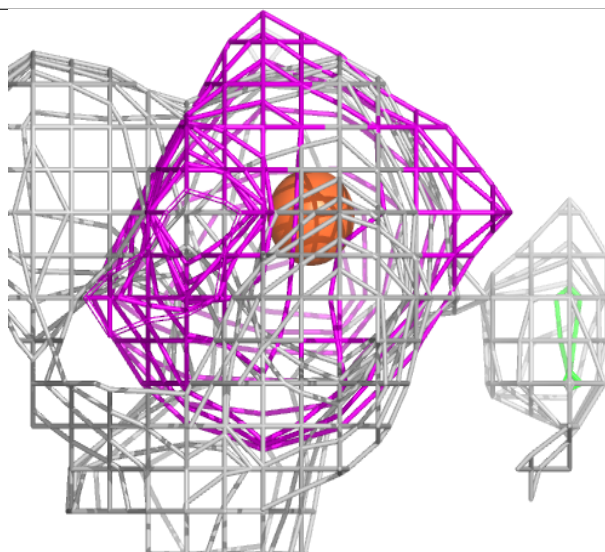
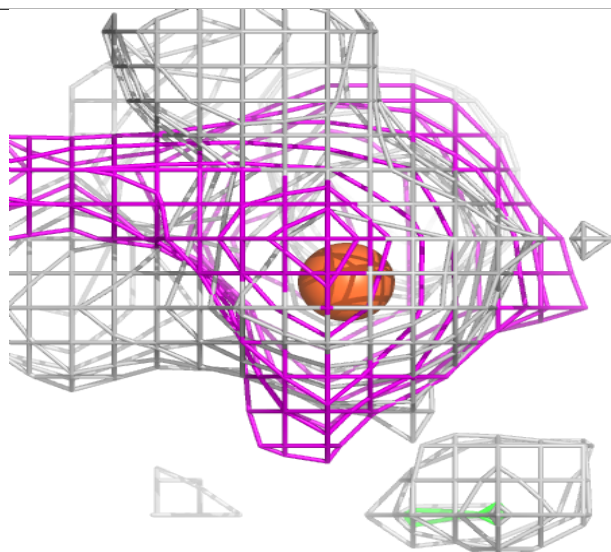
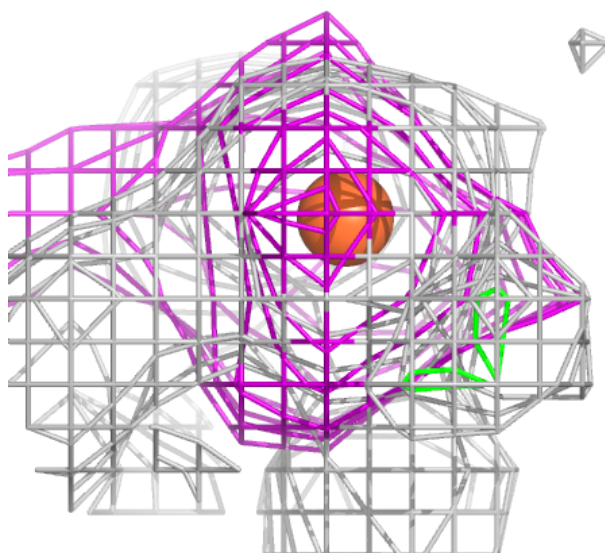
Electron density around FE U 201:

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



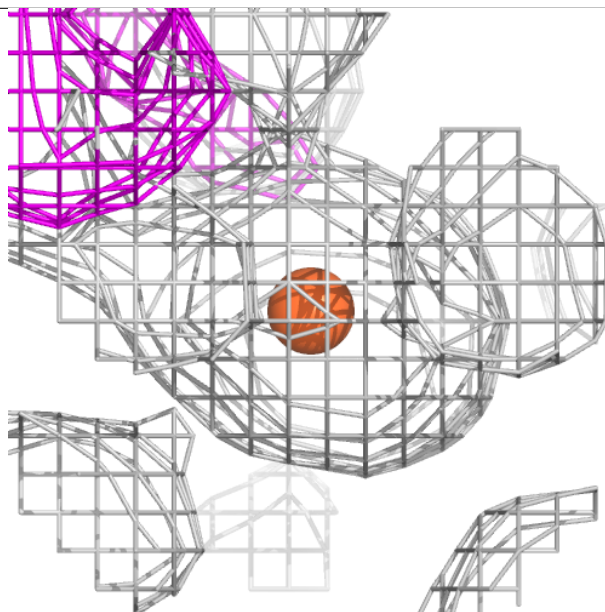
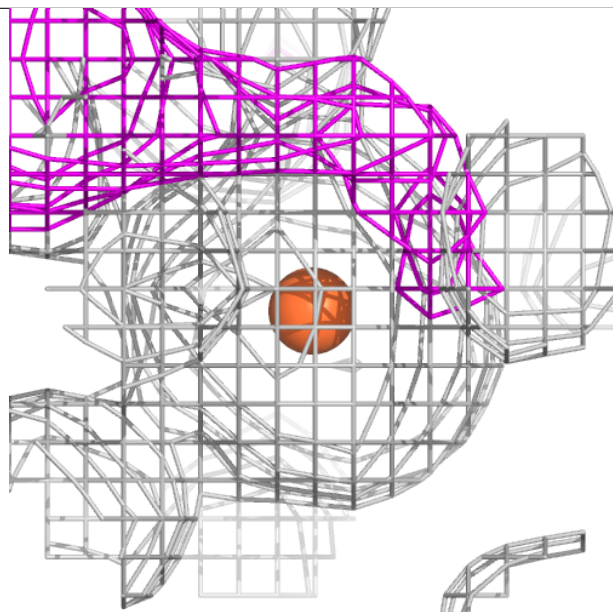
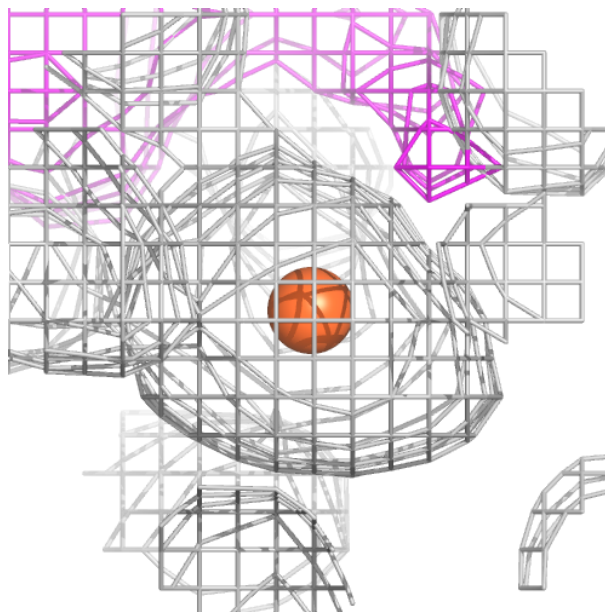
Electron density around FE2 I 202:

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



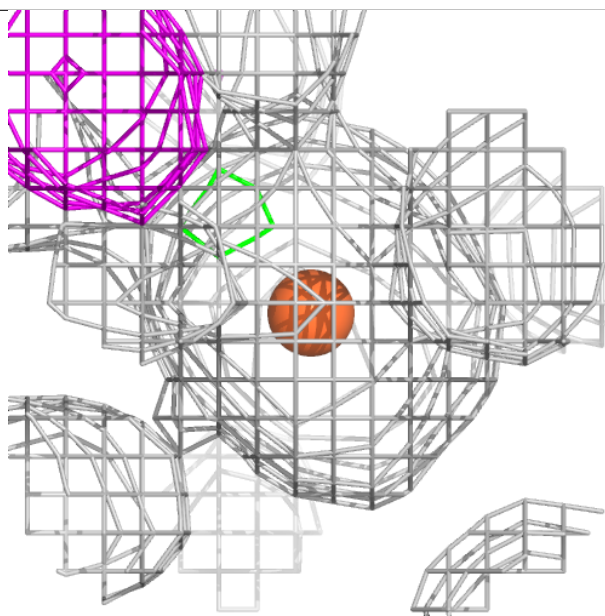
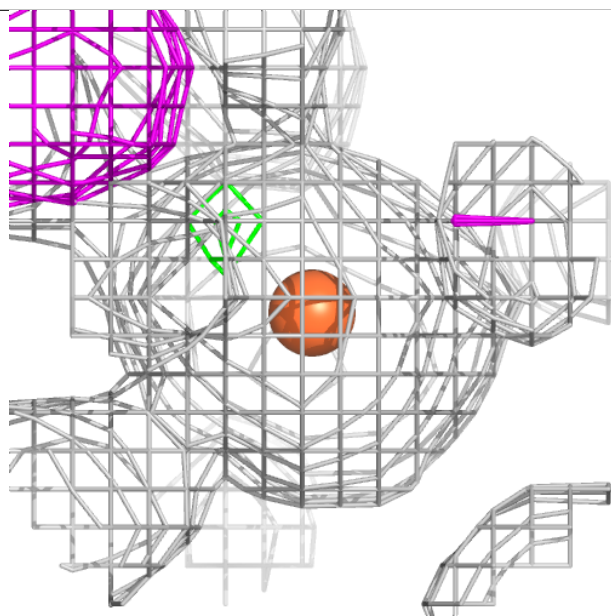
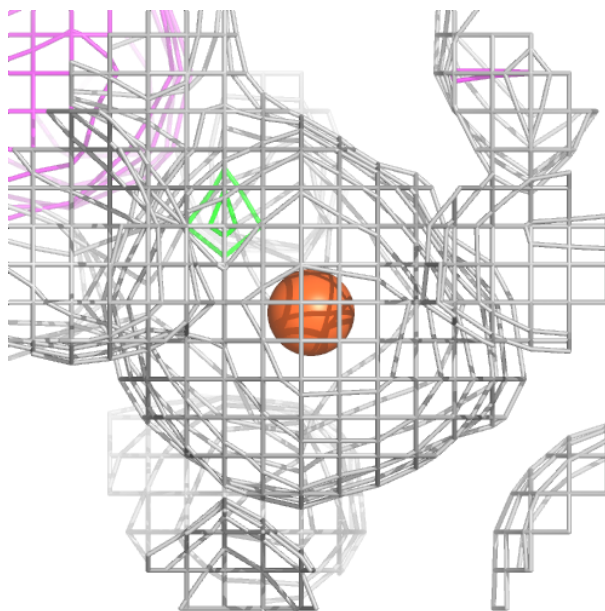
Electron density around FE2 I 203:

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



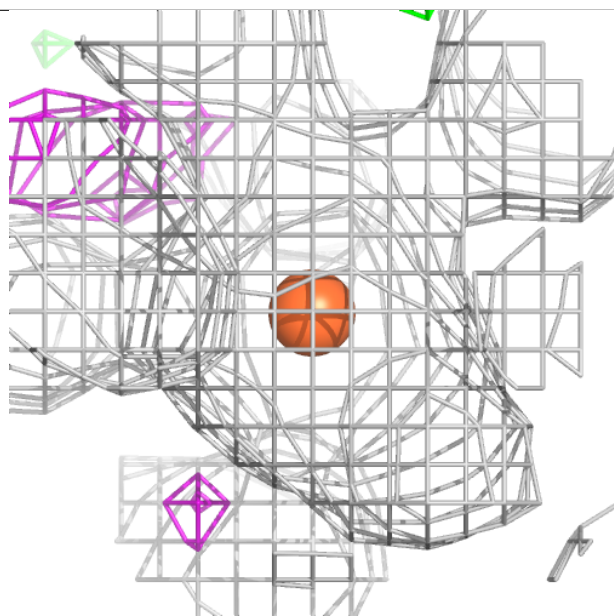
Electron density around FE2 B 207:

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



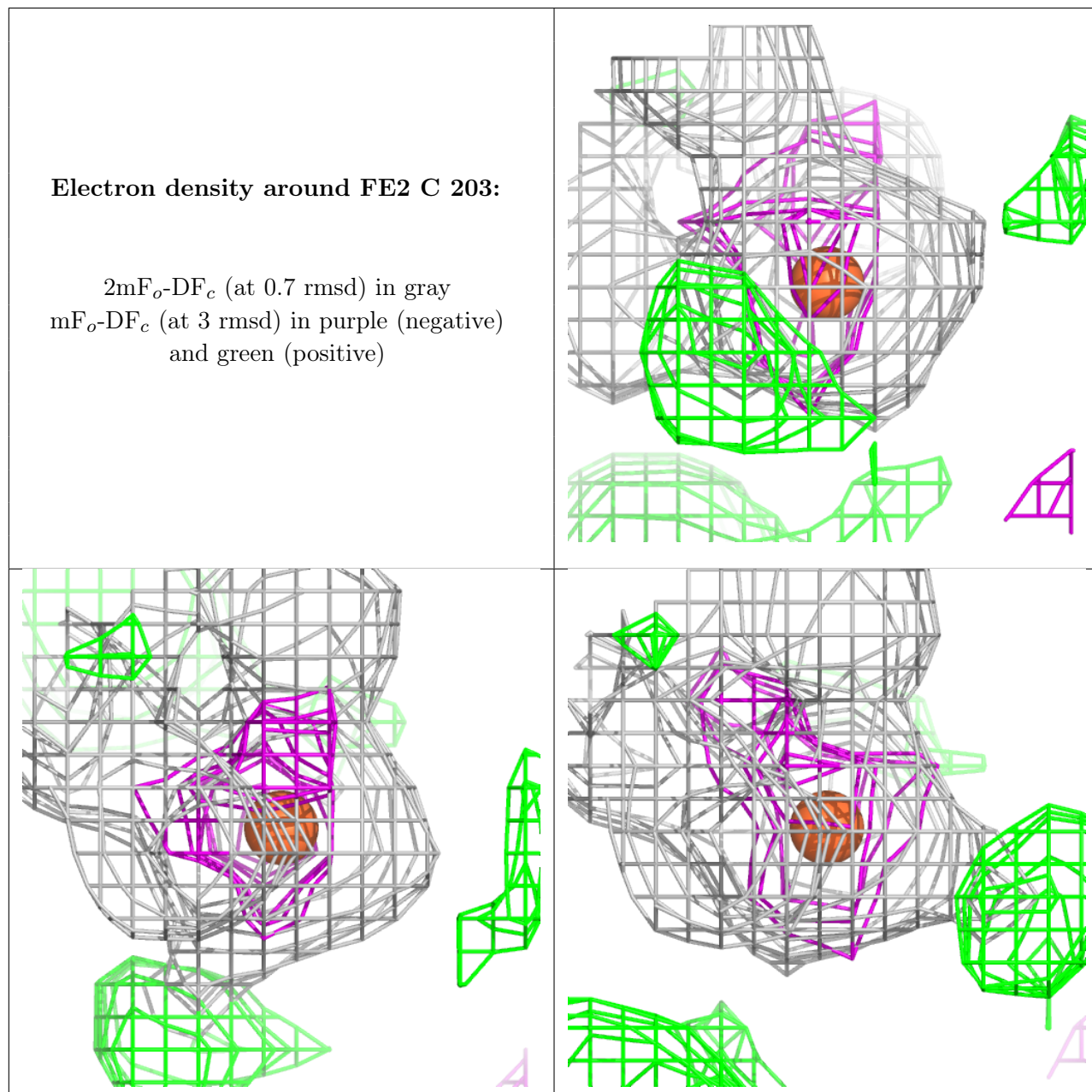
Electron density around FE2 P 204:

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



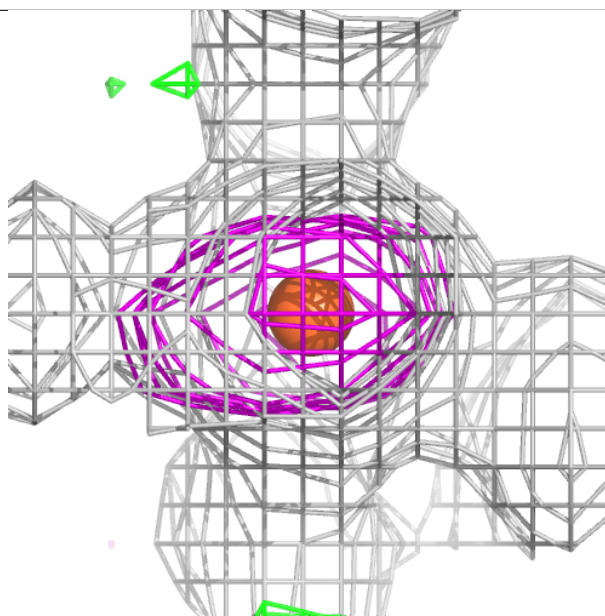
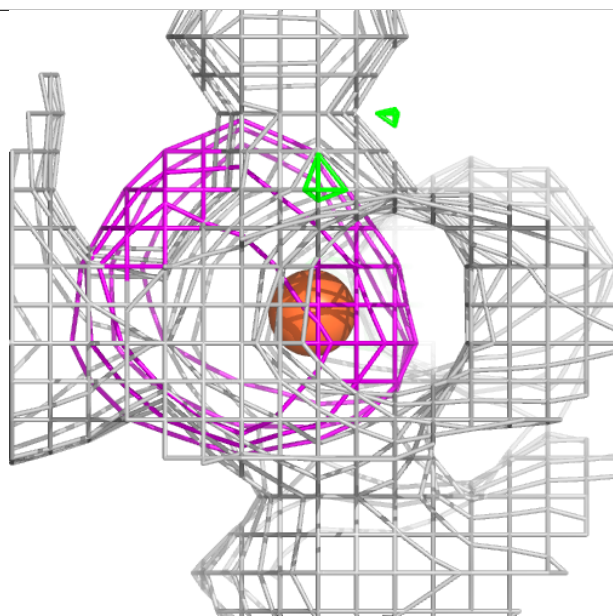
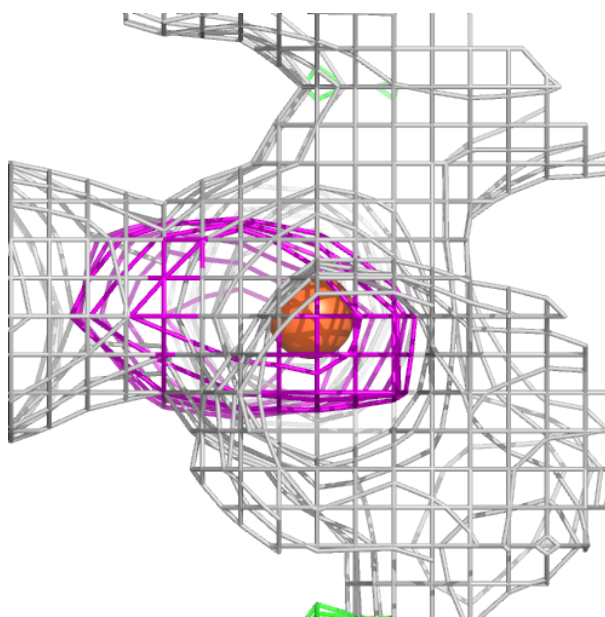
Electron density around FE2 C 203:

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



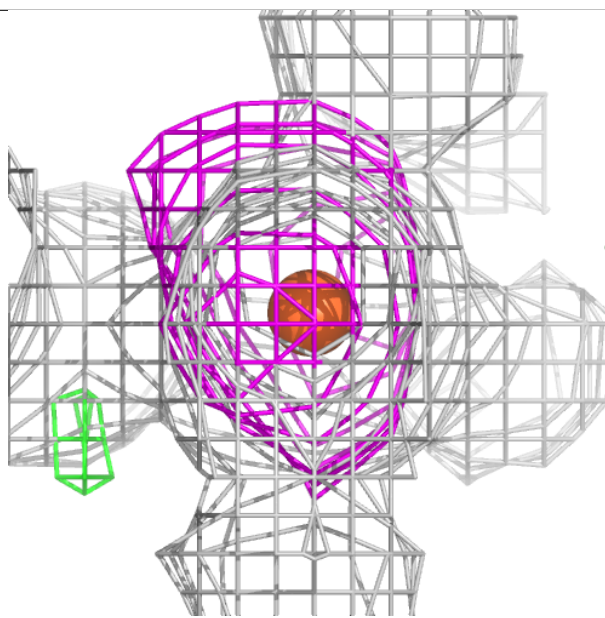
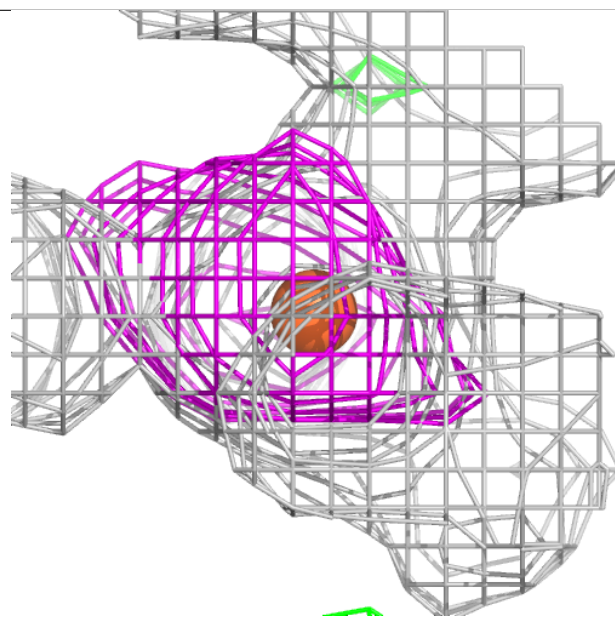
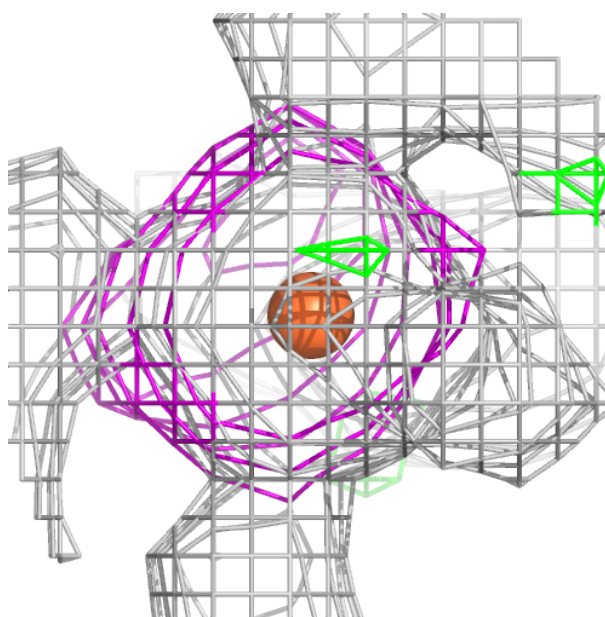
Electron density around FE2 P 202:

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



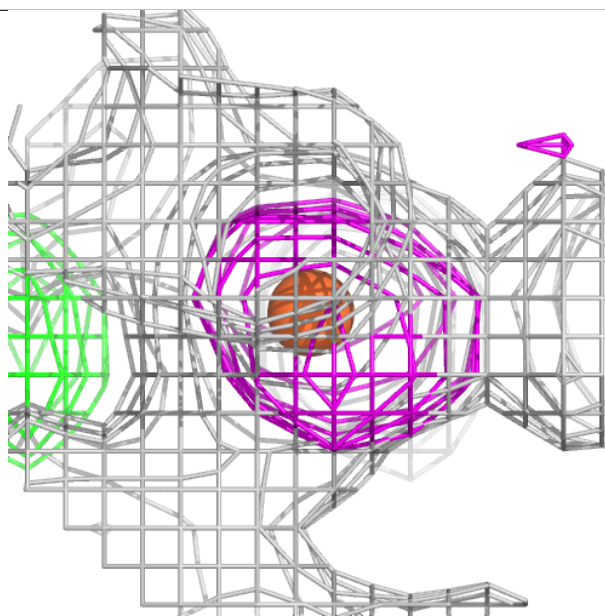
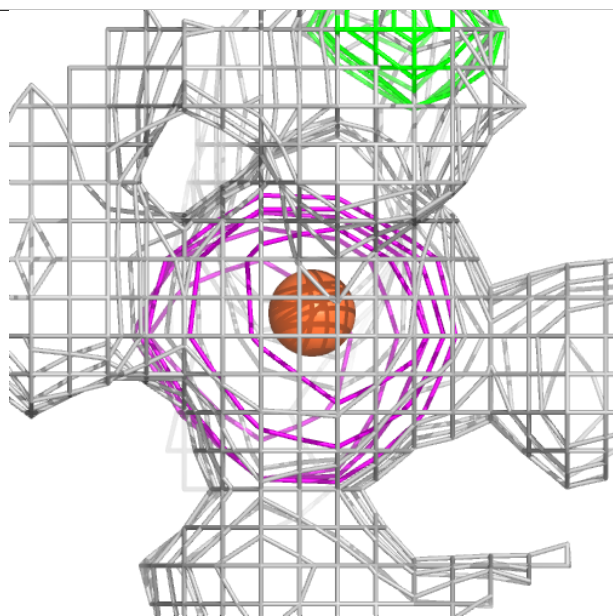
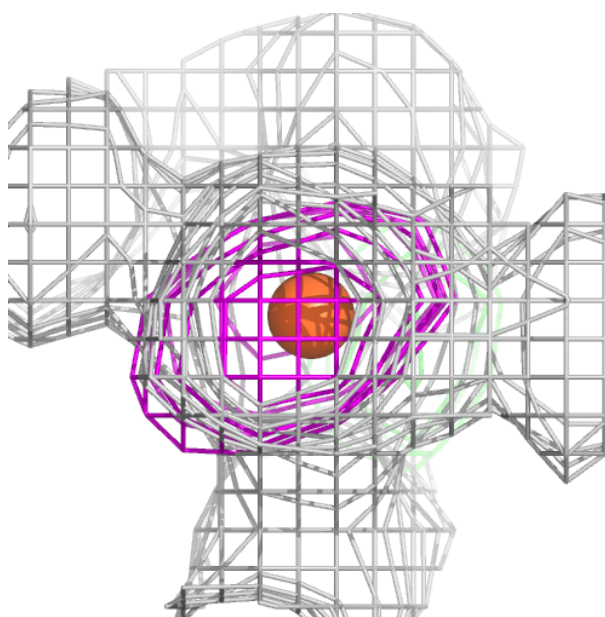
Electron density around FE2 E 202:

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



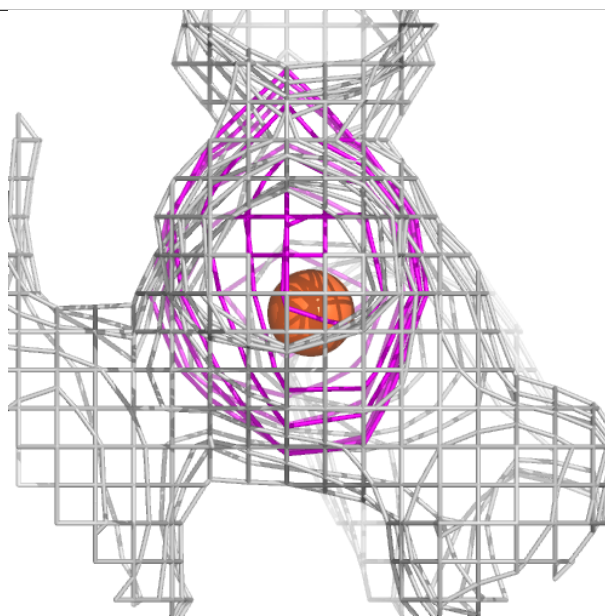
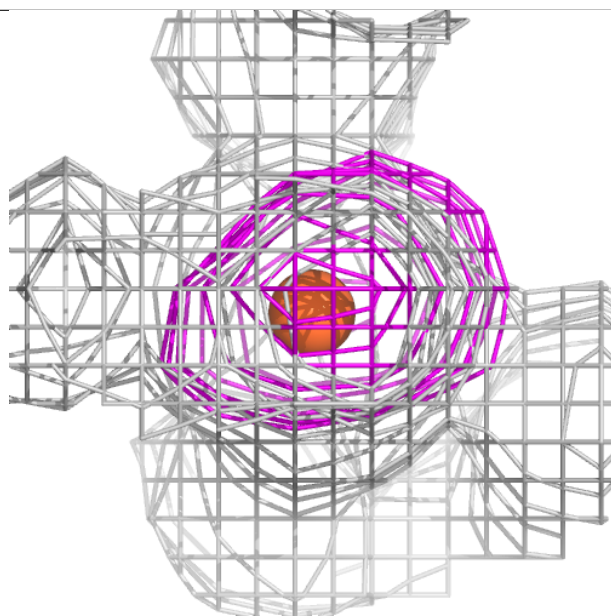
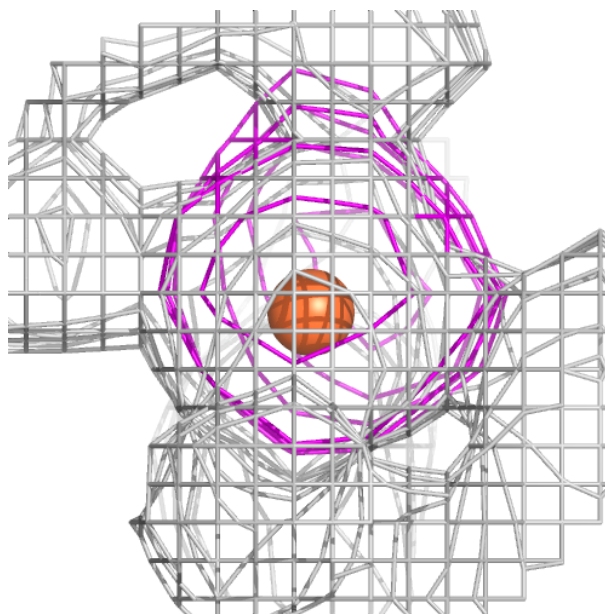
Electron density around FE2 B 202:

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



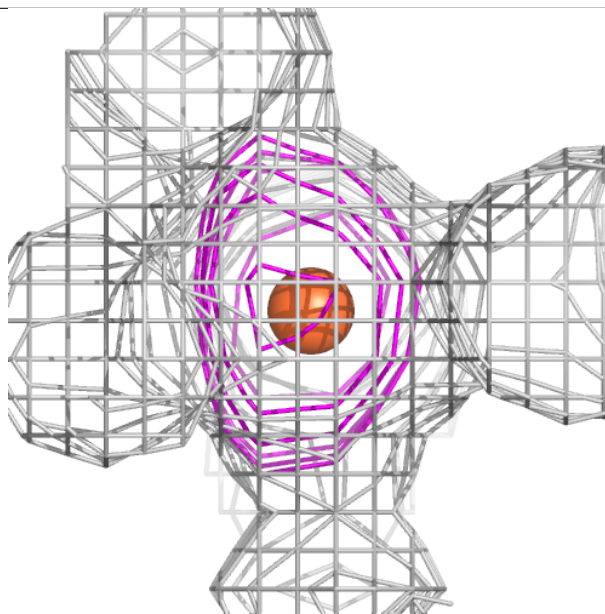
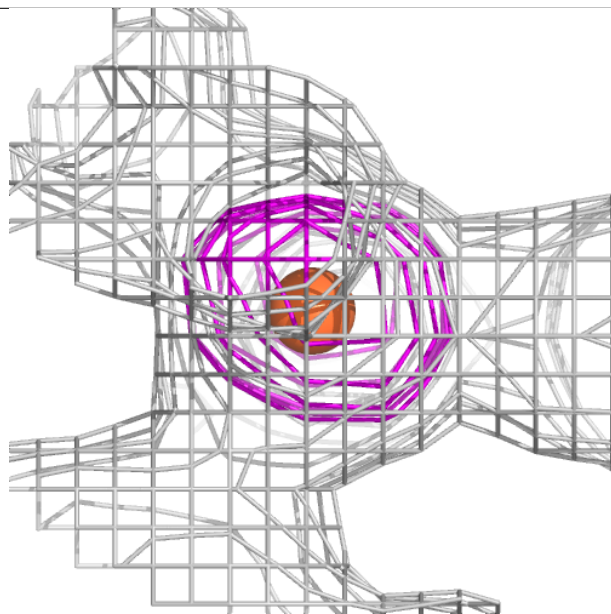
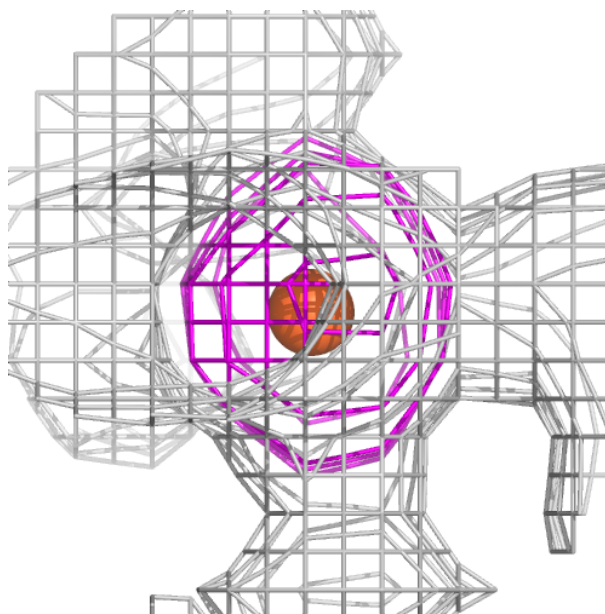
Electron density around FE2 A 202:

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



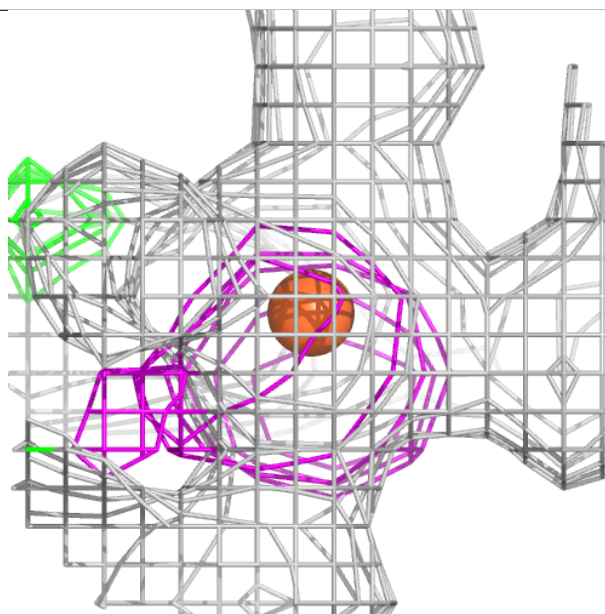
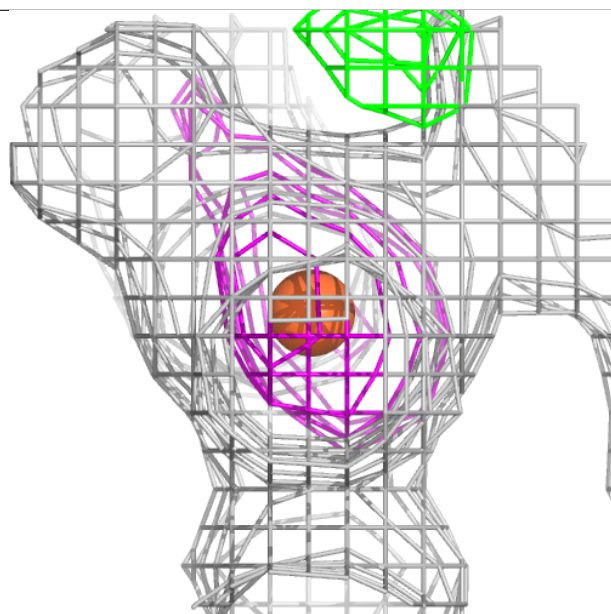
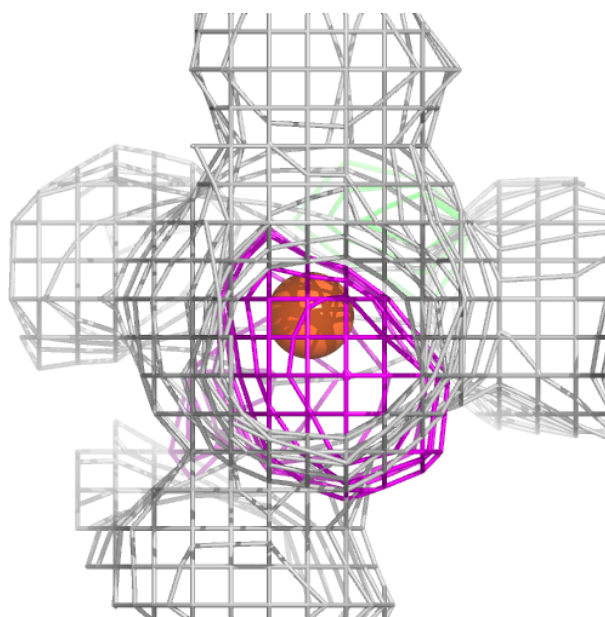
Electron density around FE2 Q 202:

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



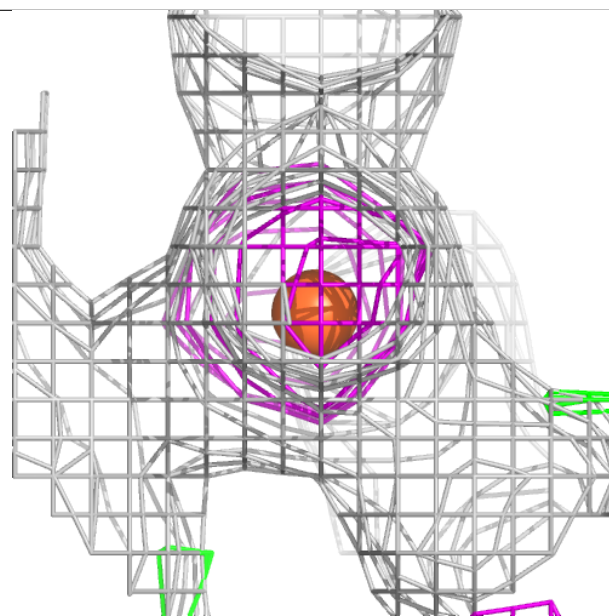
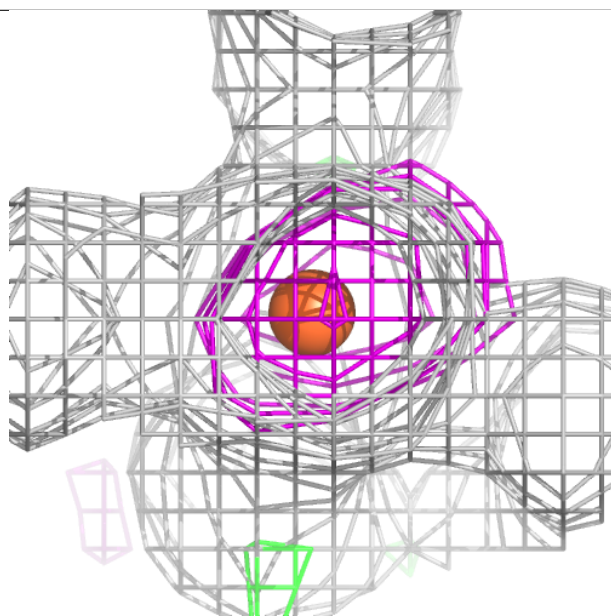
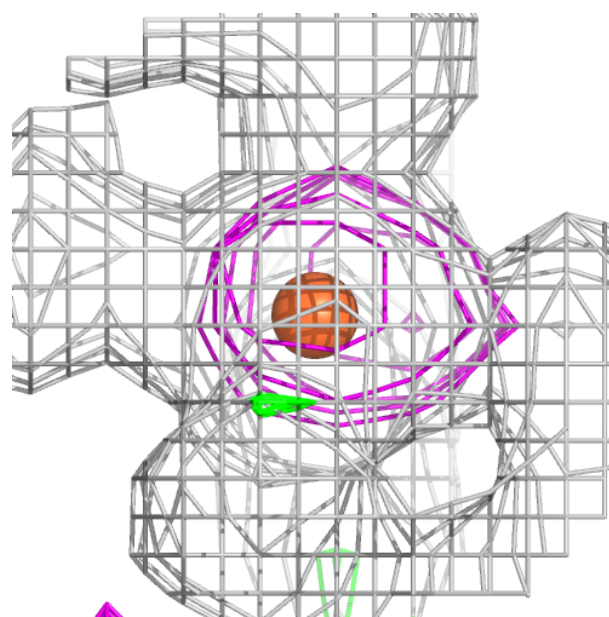
Electron density around FE2 R 202:

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



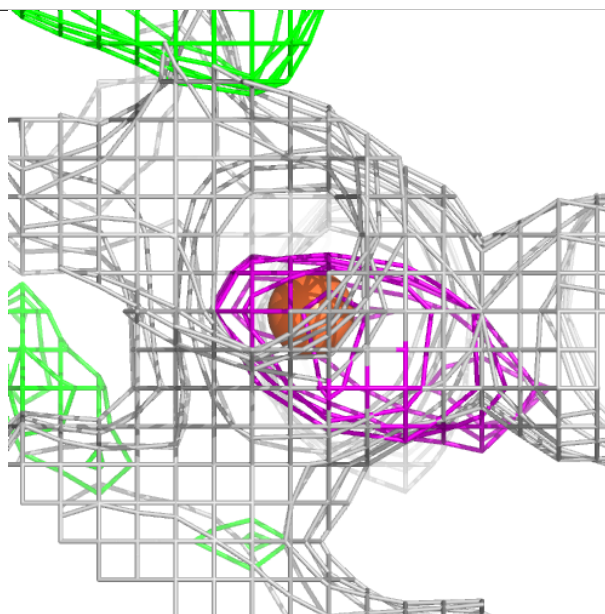
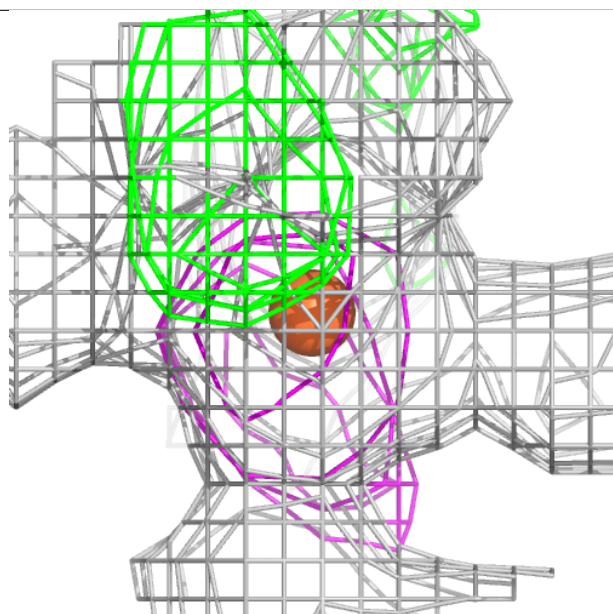
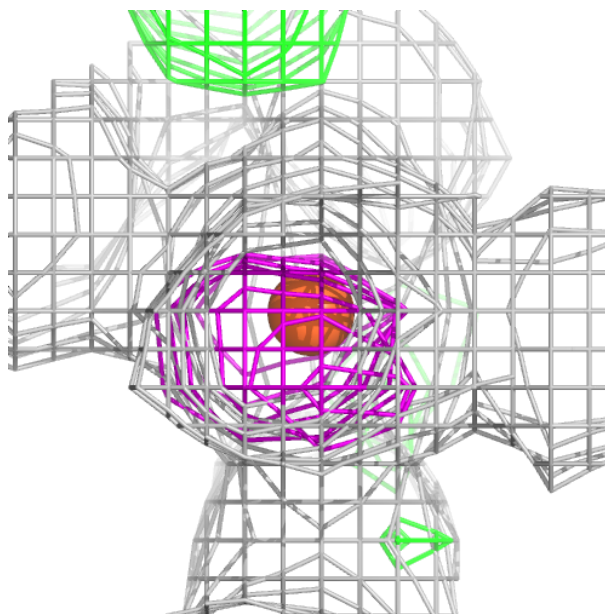
Electron density around FE2 S 202:

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



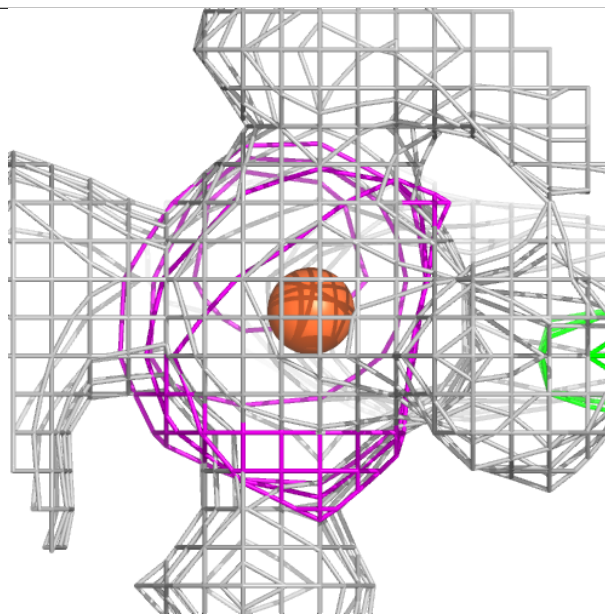
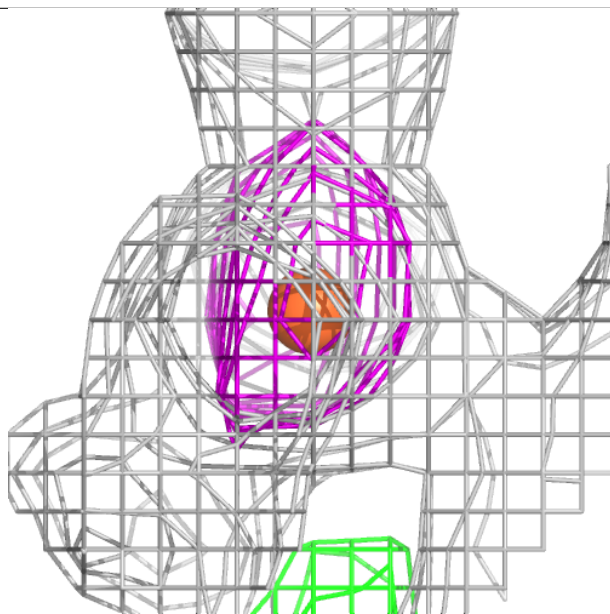
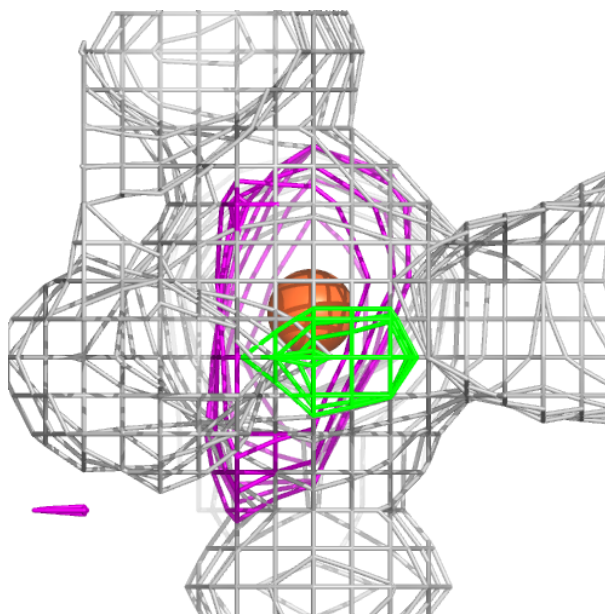
Electron density around FE2 T 202:

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



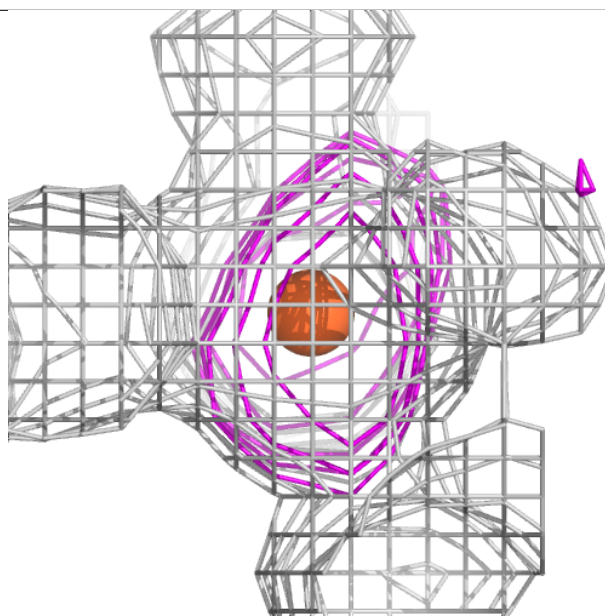
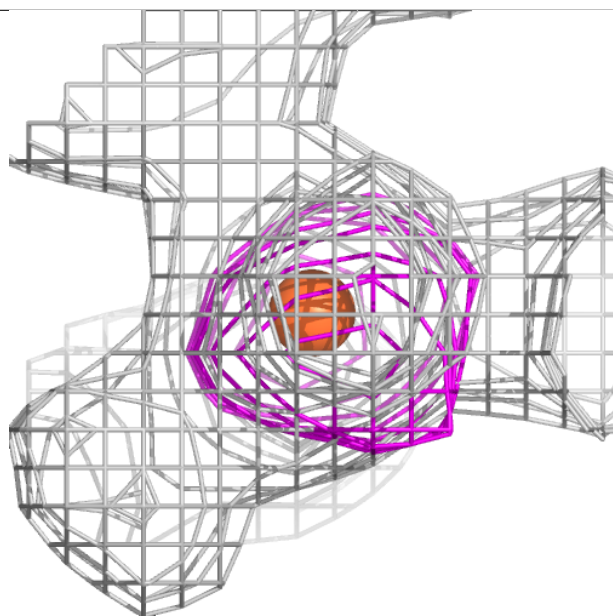
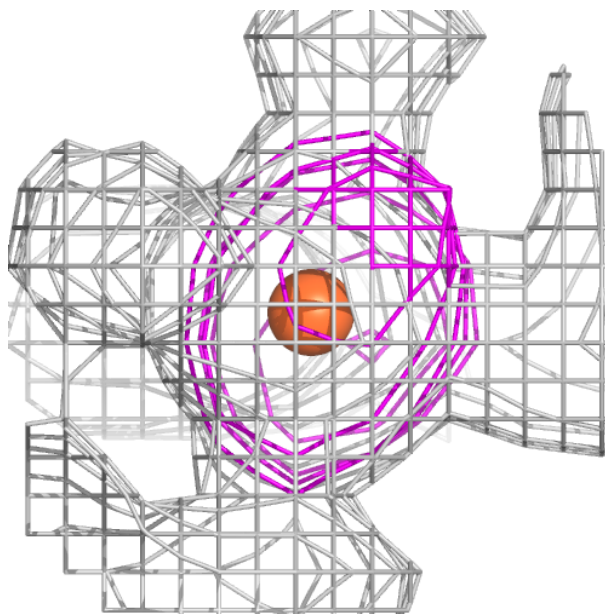
Electron density around FE2 U 202:

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



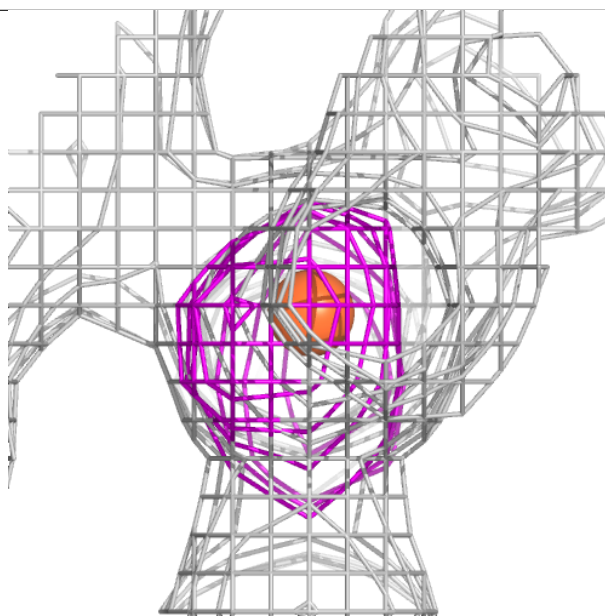
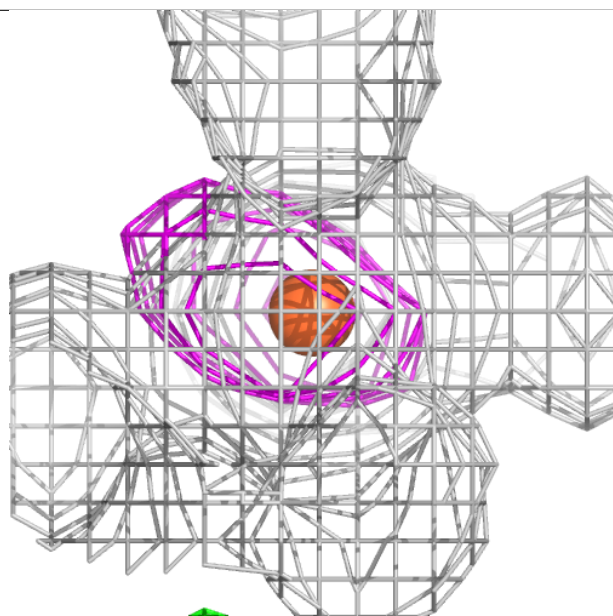
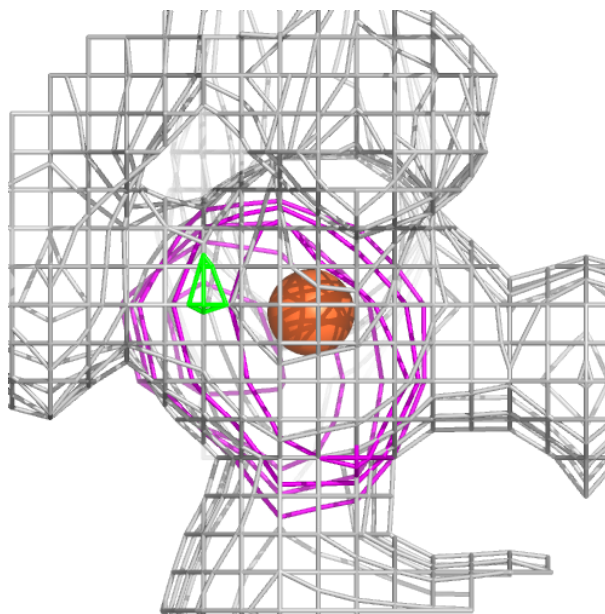
Electron density around FE2 V 202:

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



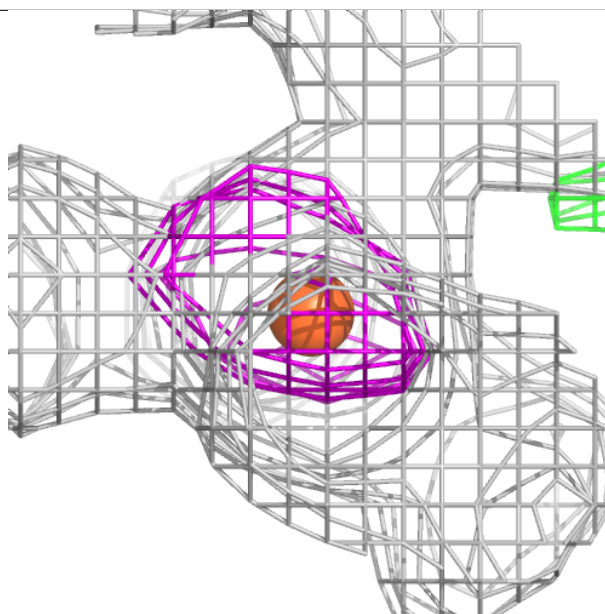
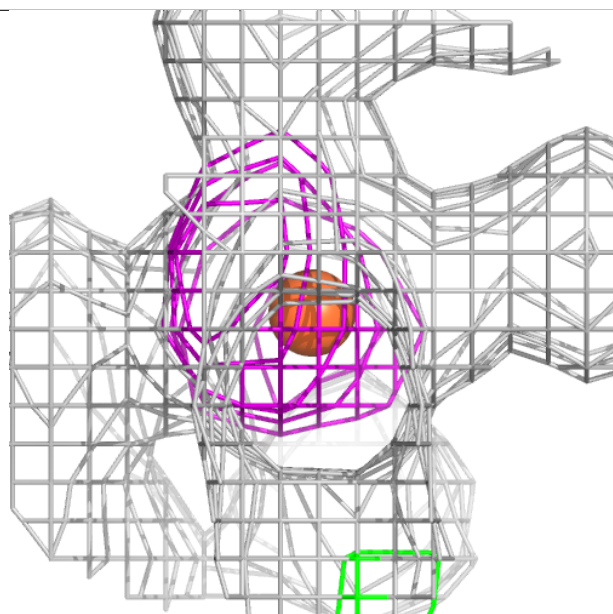
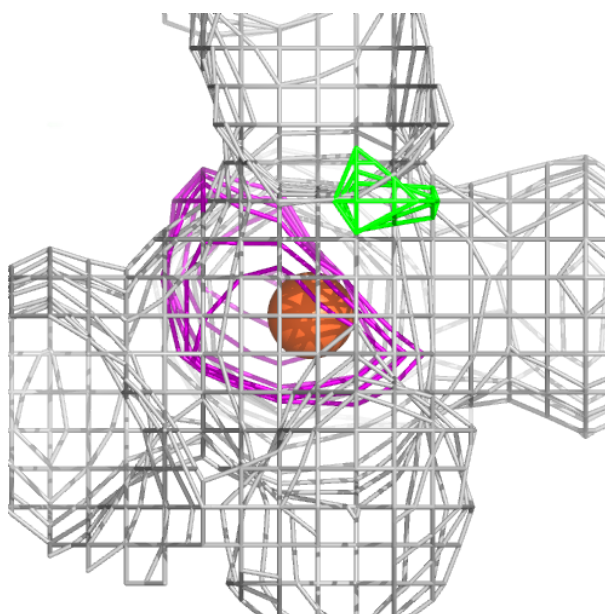
Electron density around FE2 W 202:

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



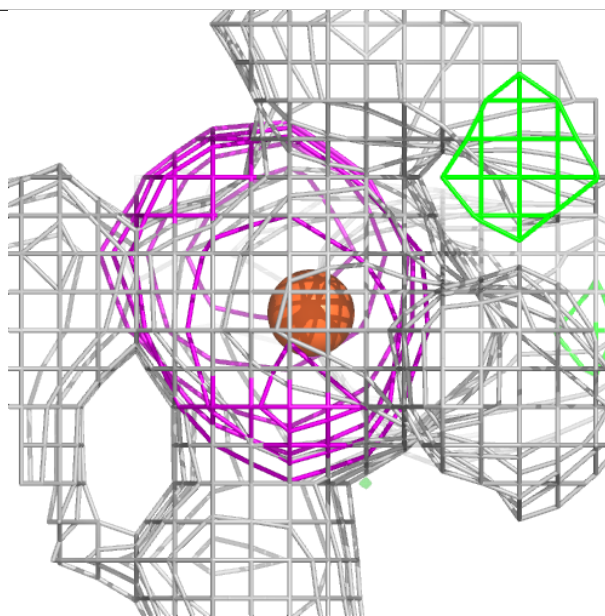
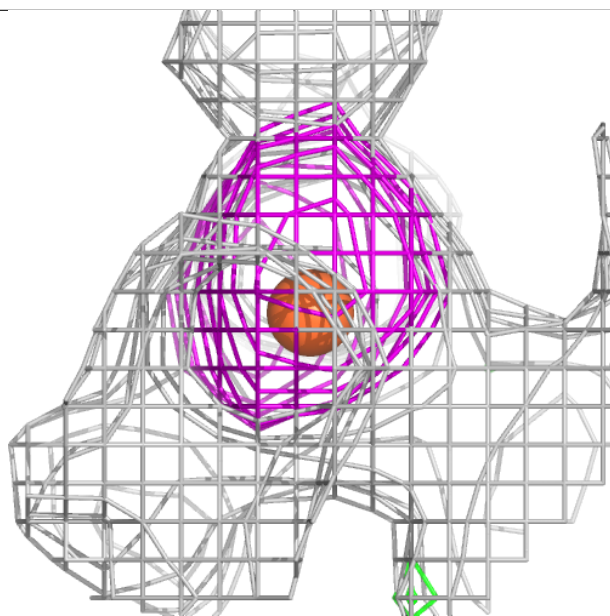
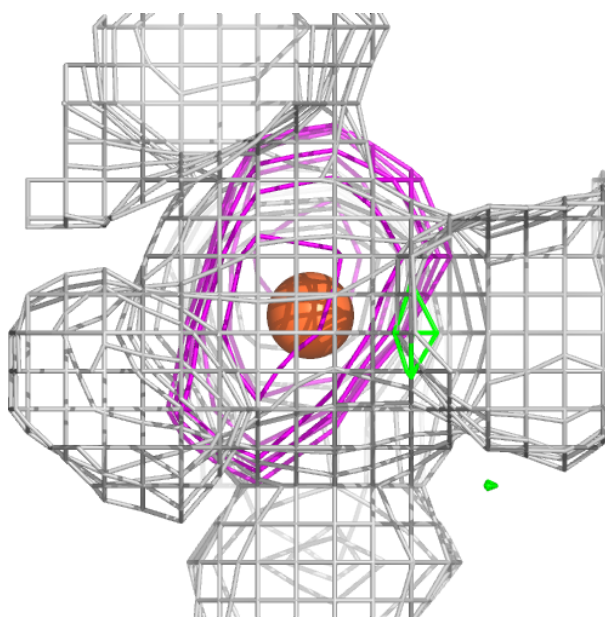
Electron density around FE2 X 202:

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



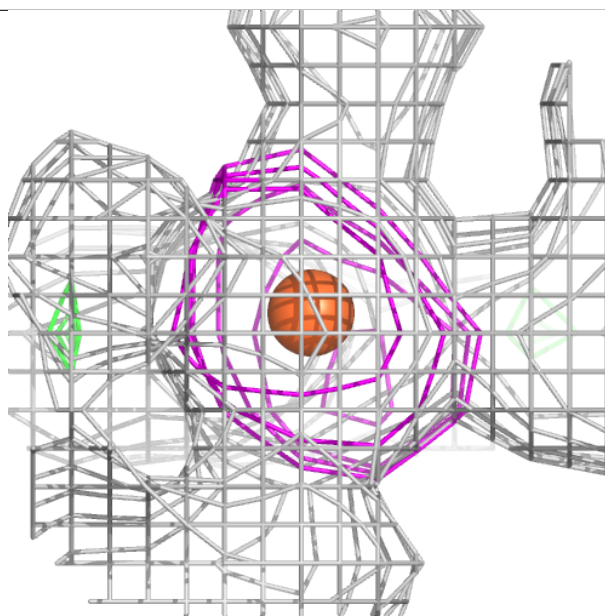
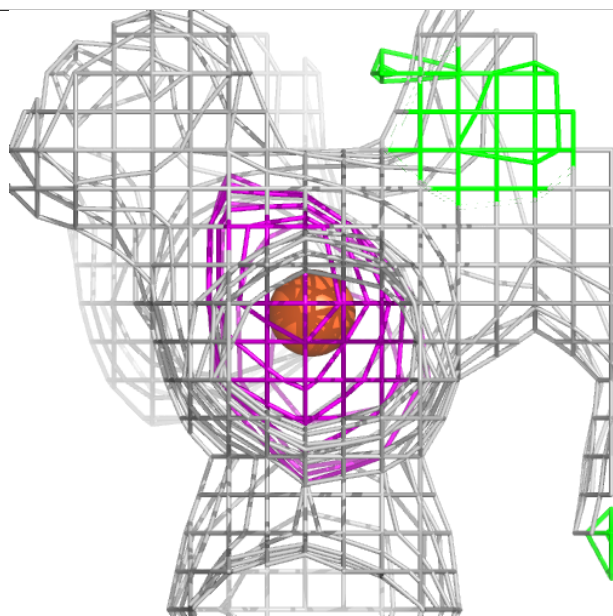
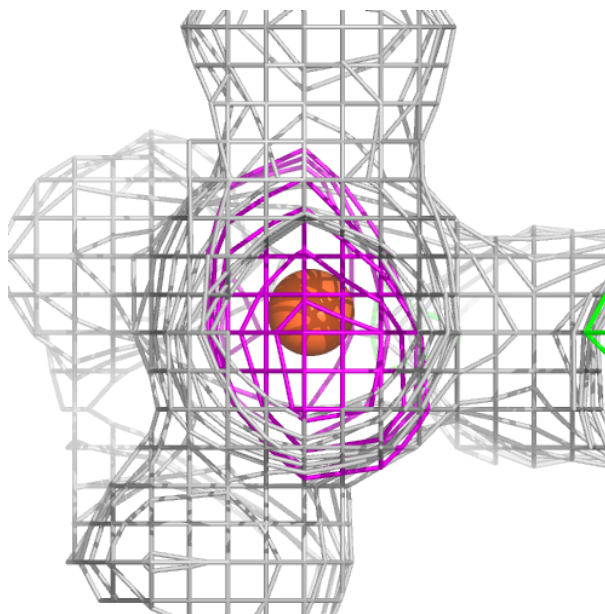
Electron density around FE2 C 202:

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



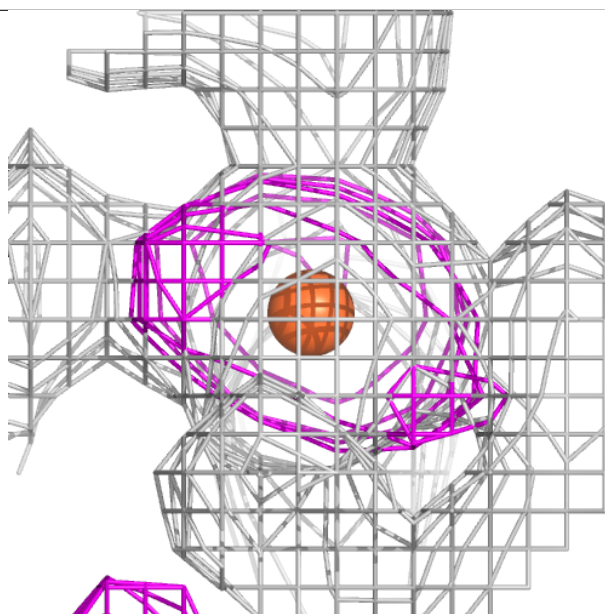
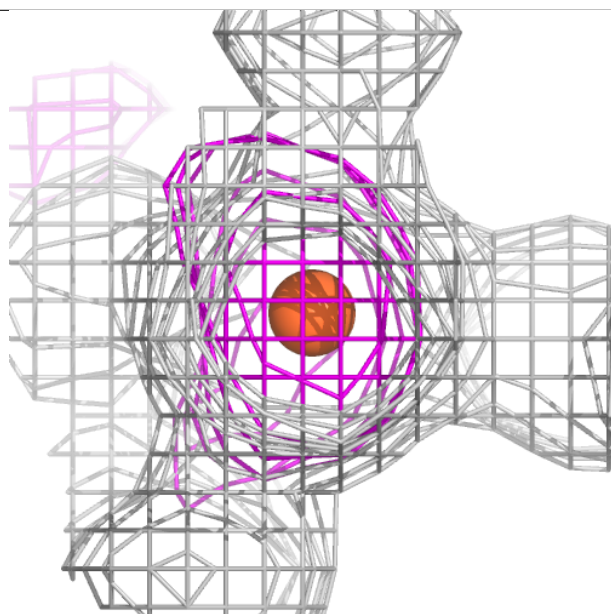
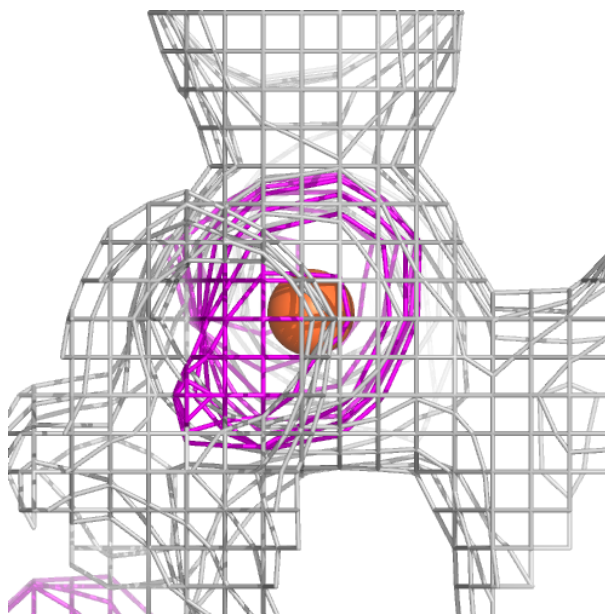
Electron density around FE2 F 202:

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



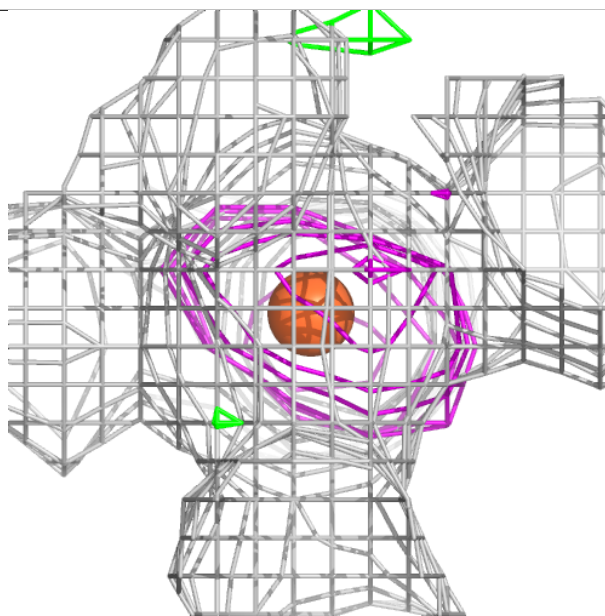
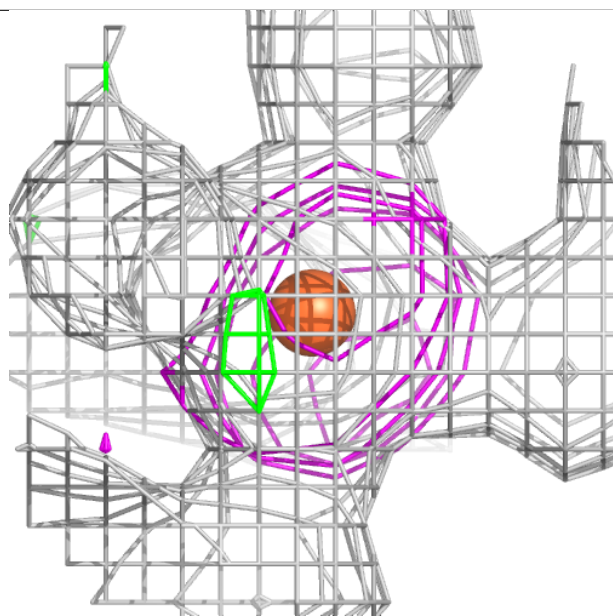
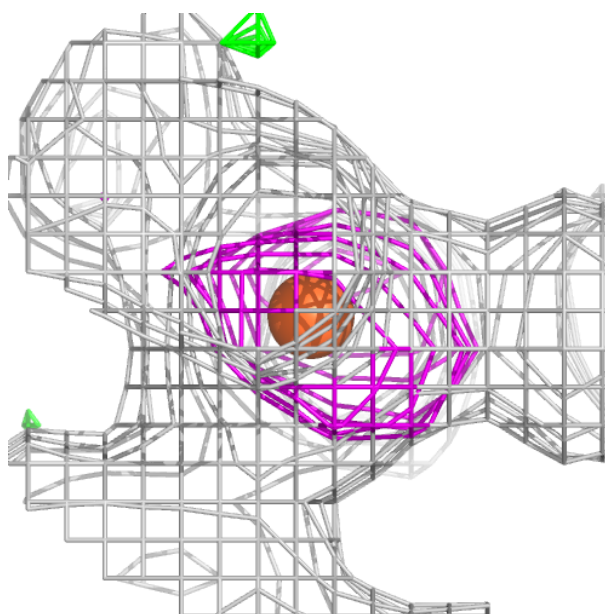
Electron density around FE2 I 205:

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



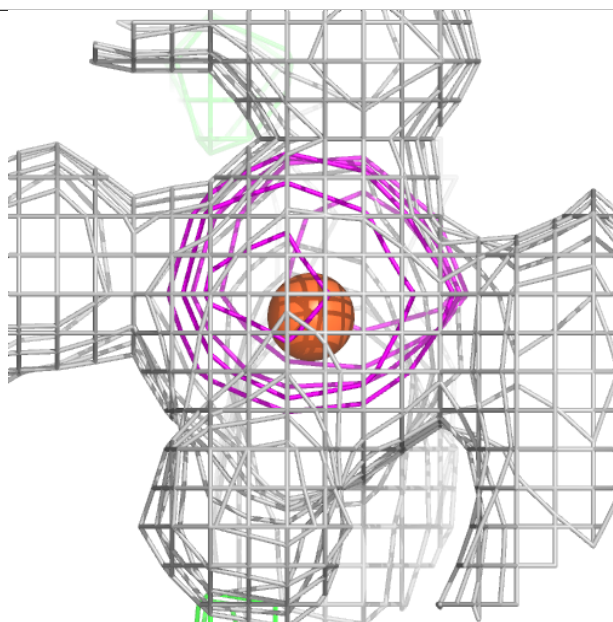
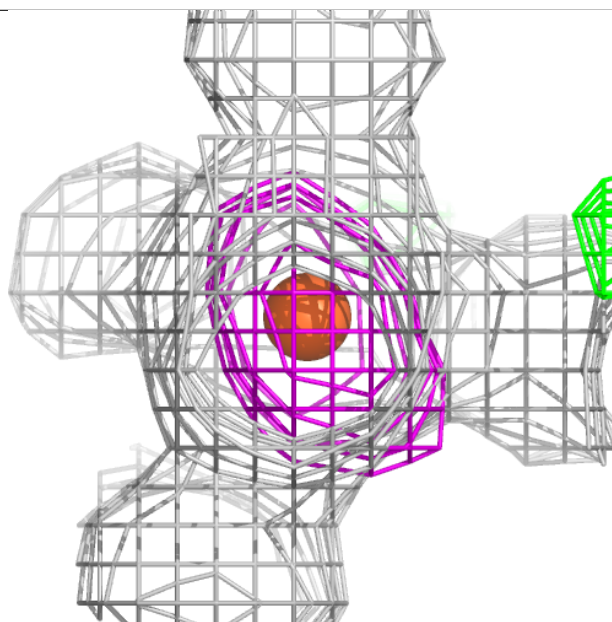
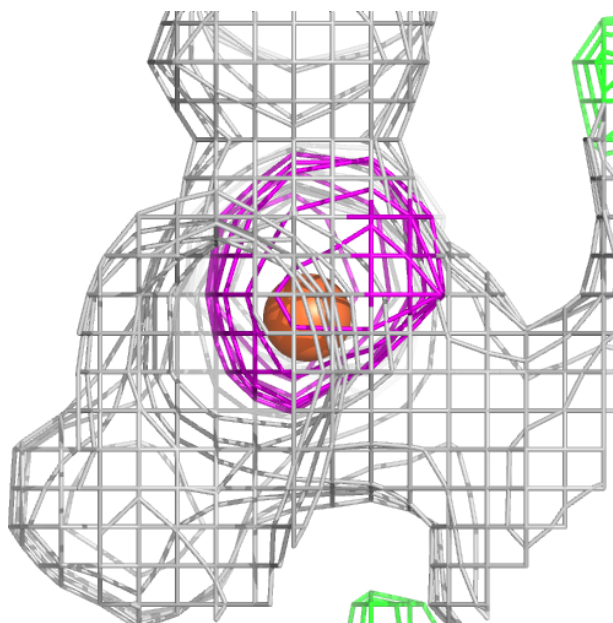
Electron density around FE2 J 202:

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



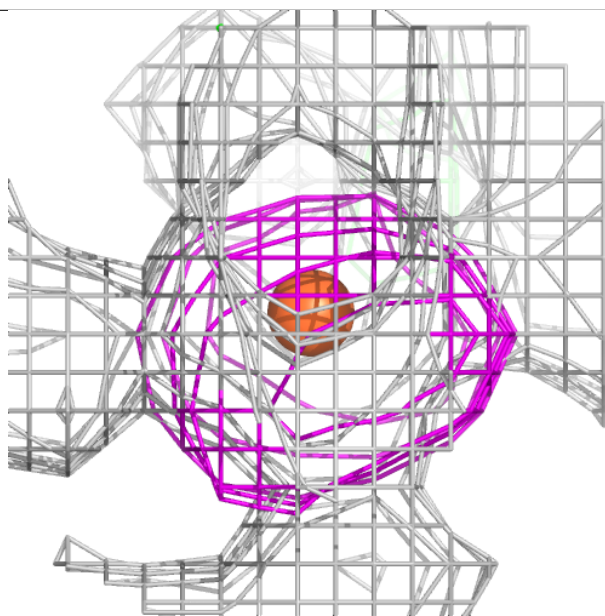
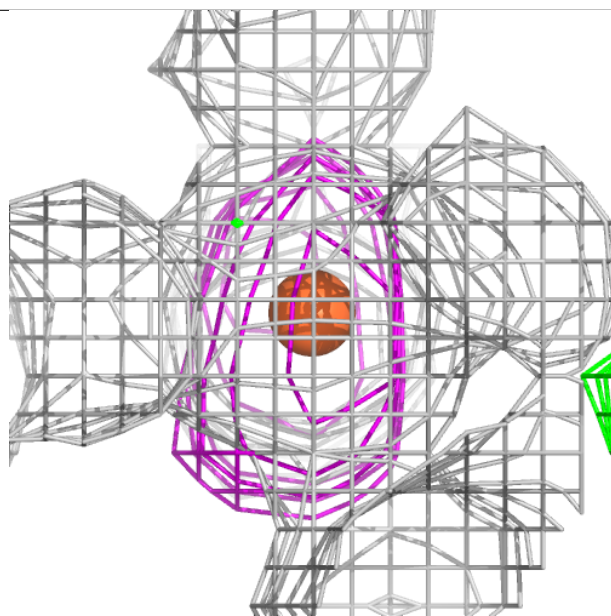
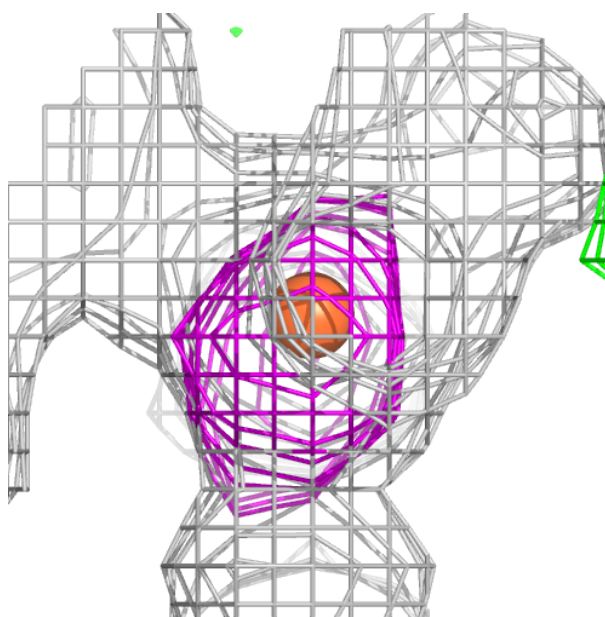
Electron density around FE2 G 201:

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



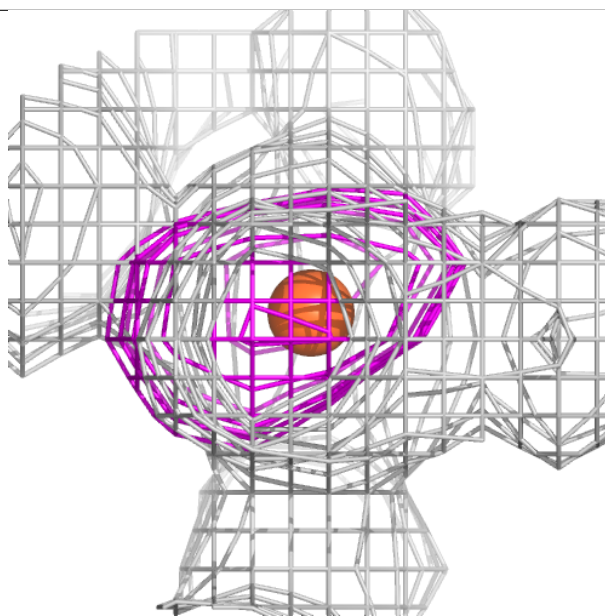
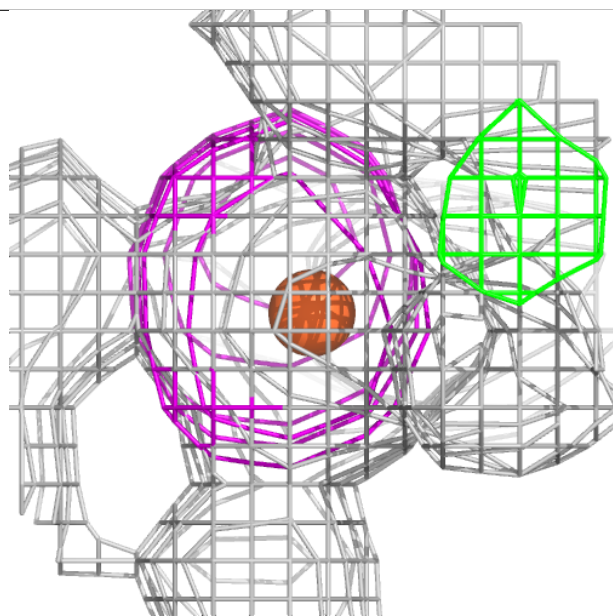
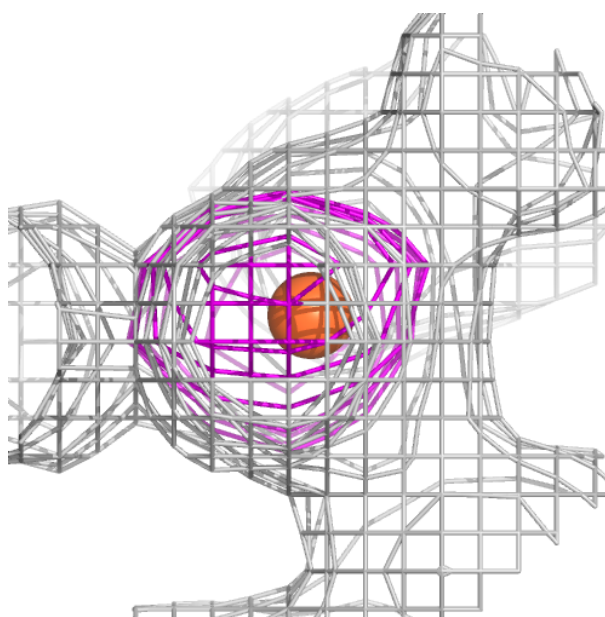
Electron density around FE2 K 203:

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



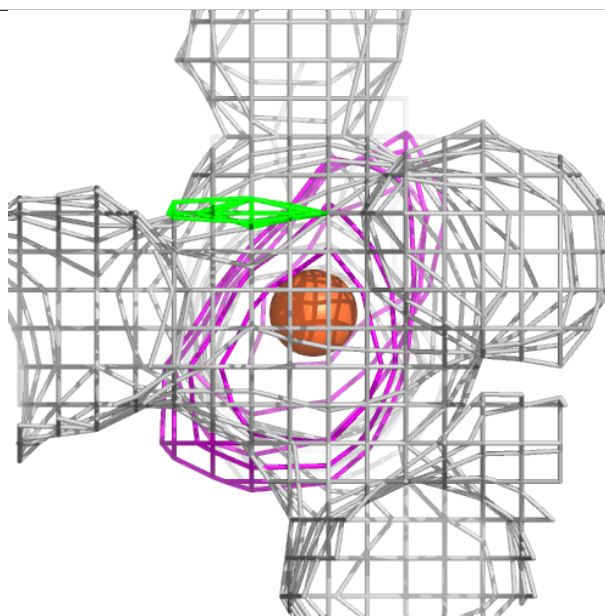
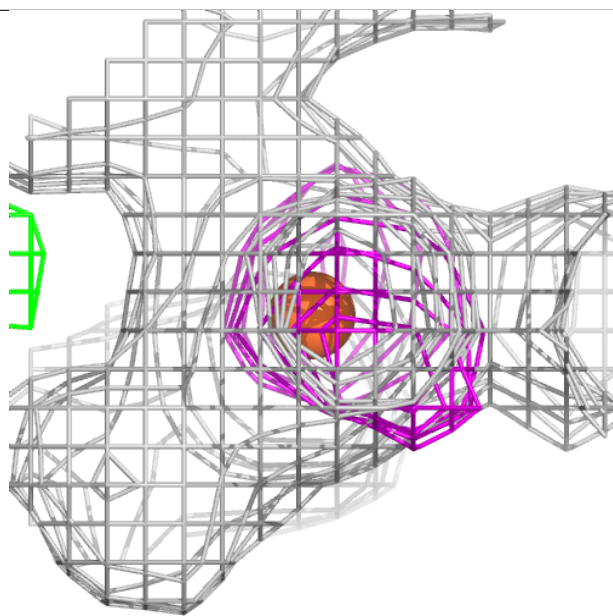
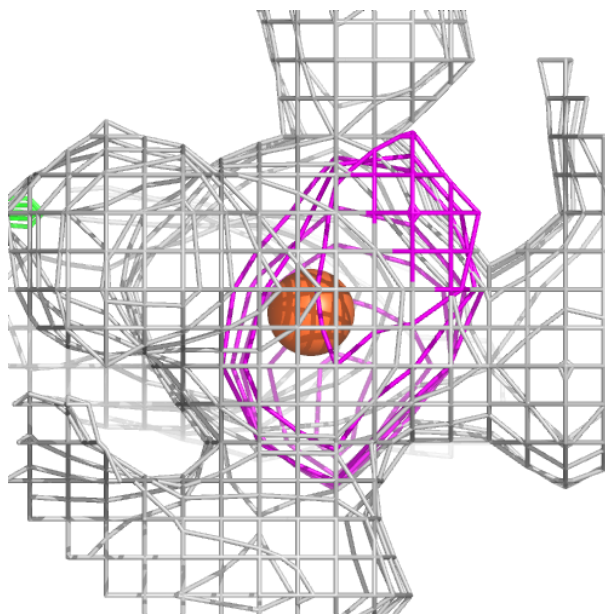
Electron density around FE2 H 202:

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



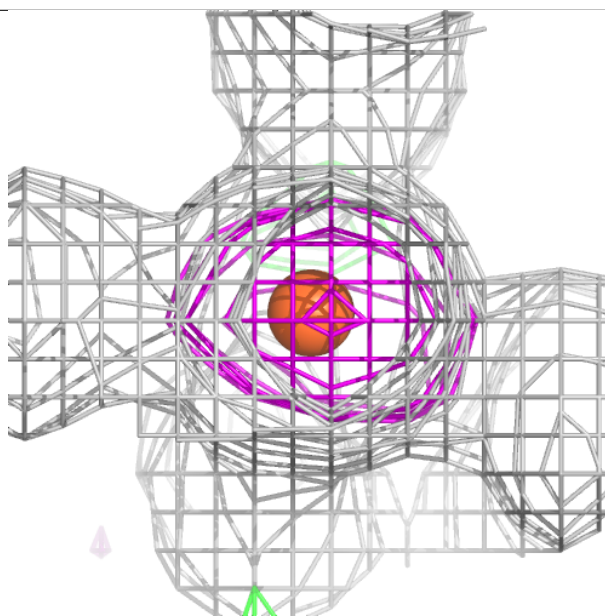
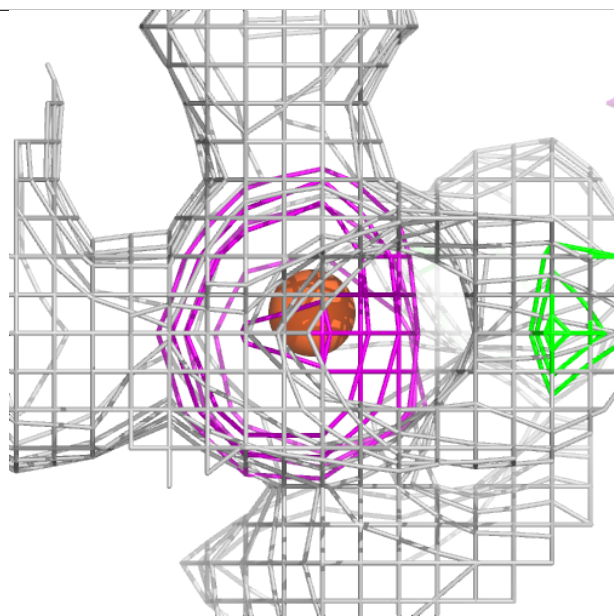
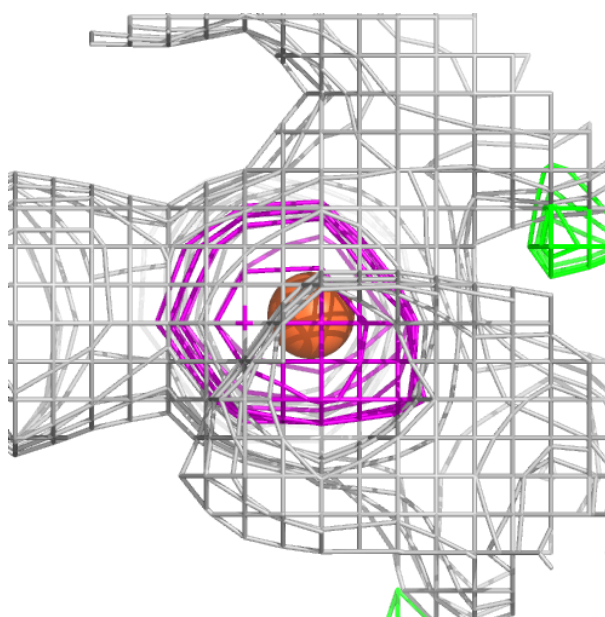
Electron density around FE2 D 202:

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



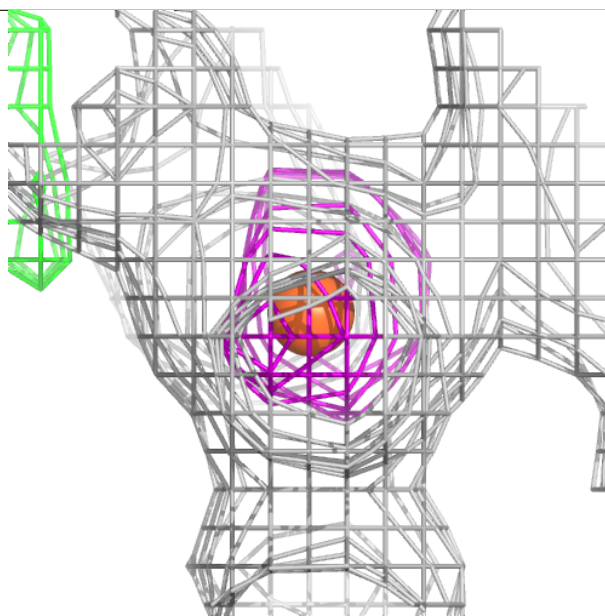
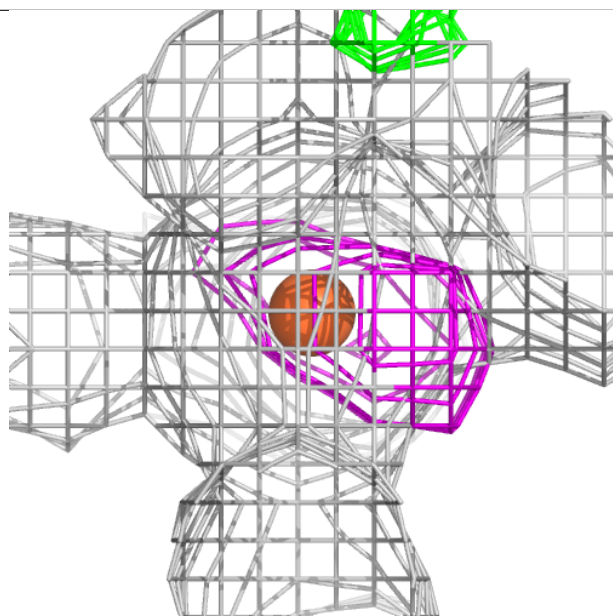
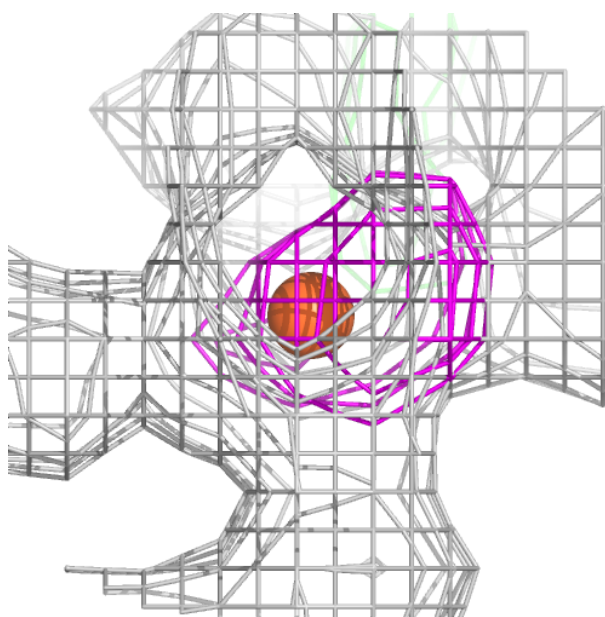
Electron density around FE2 L 202:

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



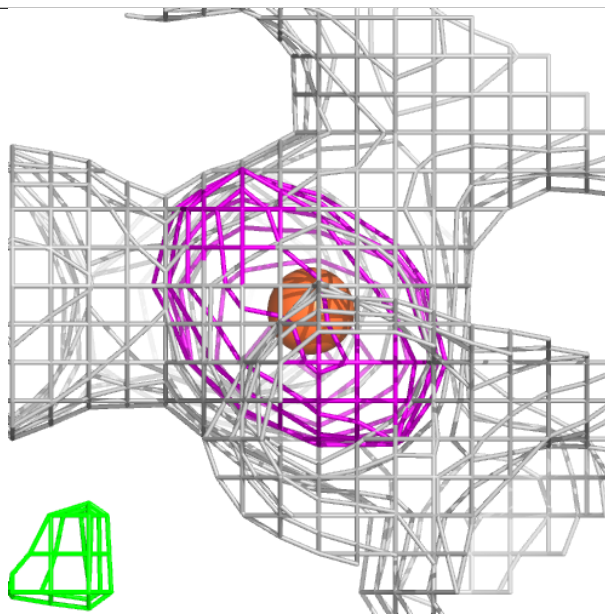
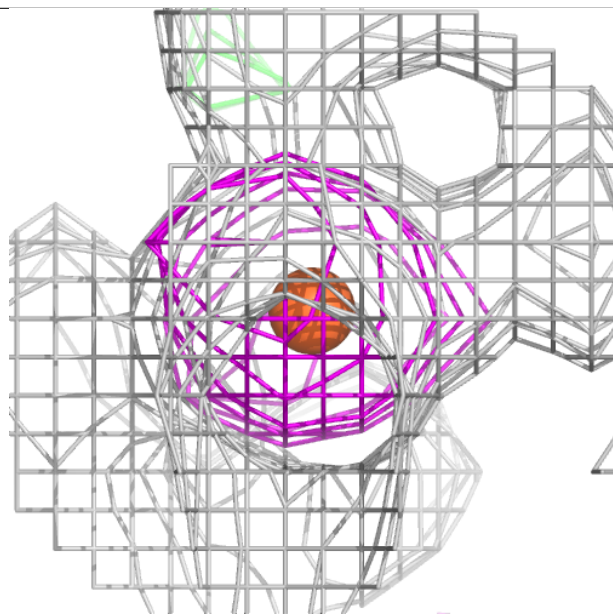
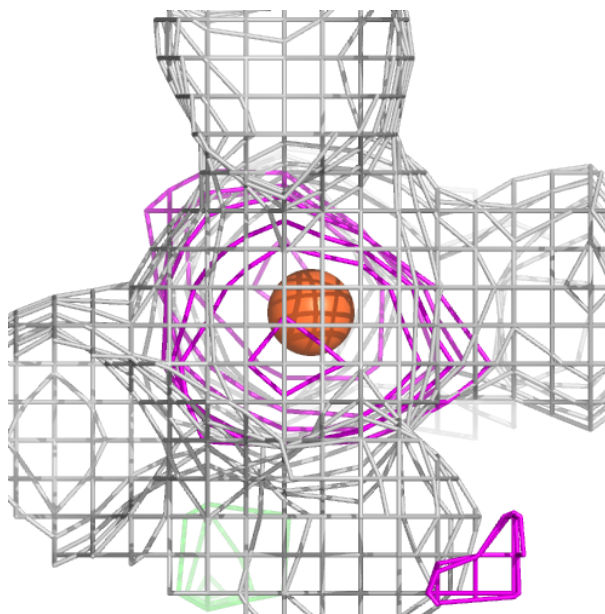
Electron density around FE2 M 202:

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



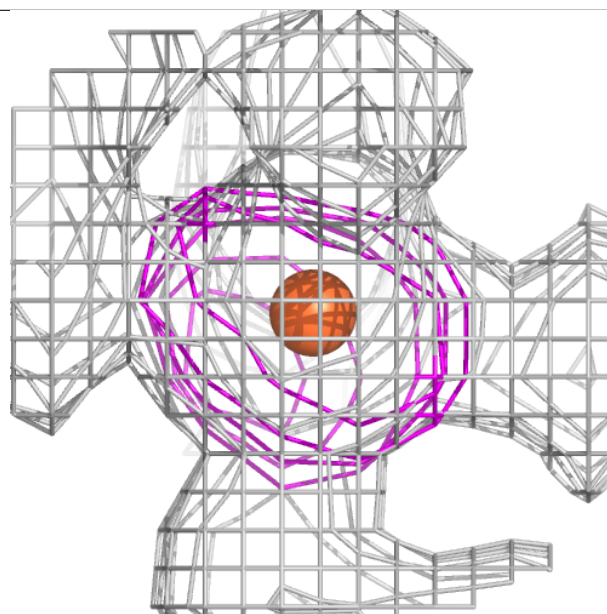
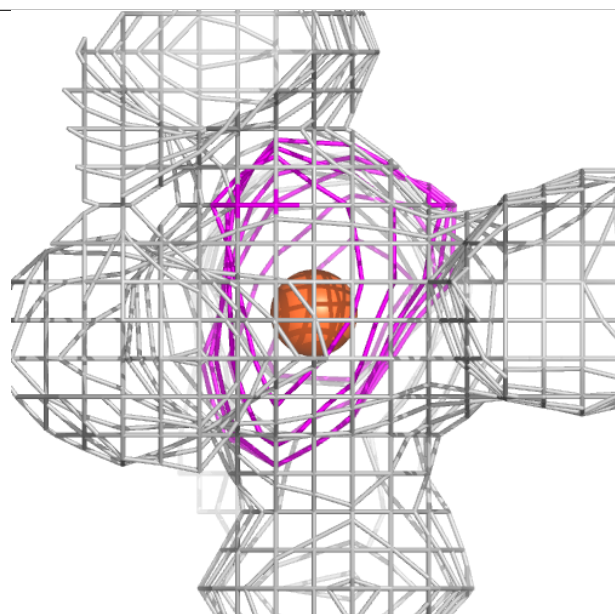
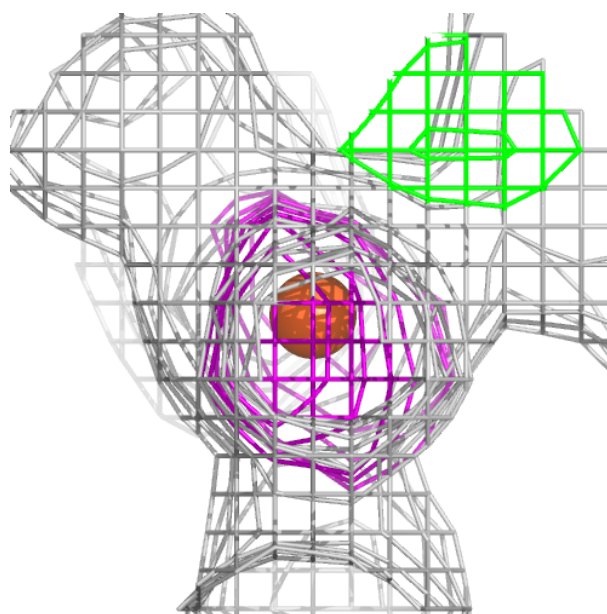
Electron density around FE2 N 202:

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



Electron density around FE2 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.