



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 08:13 PM UTC

PDB ID : 8Y6F / pdb_00008y6f
Title : The crystal structure of MMPs cleavable human heavy chain ferritin
Authors : Yuan, C.; Huang, M.
Deposited on : 2024-02-02
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

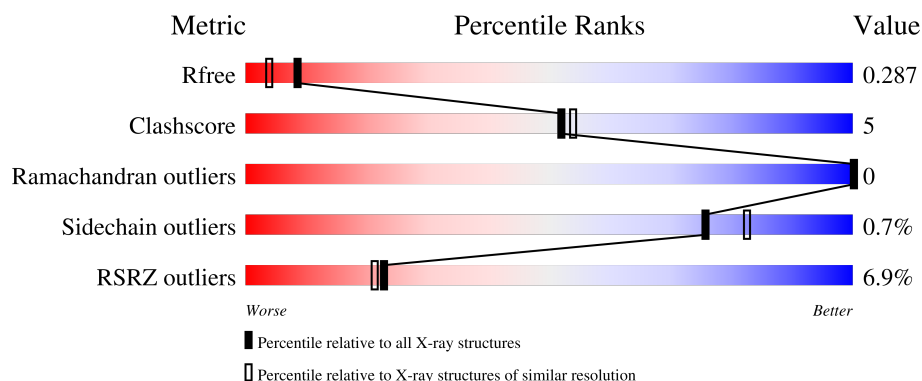
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	196	7% 77% 11% 12%
1	B	196	6% 76% 12% 13%
1	C	196	6% 80% 8% 12%
1	D	196	5% 82% 6% 13%
1	E	196	8% 79% 9% 12%

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Mol	Chain	Length	Quality of chain
1	F	196	
1	G	196	
1	H	196	
1	I	196	
1	J	196	
1	K	196	
1	L	196	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19365 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
1	A	172	Total	C	N	O	S	0	2	0
			1416	887	250	272	7			
1	B	171	Total	C	N	O	S	0	1	0
			1403	879	246	271	7			
1	C	172	Total	C	N	O	S	0	1	0
			1415	885	248	275	7			
1	D	171	Total	C	N	O	S	0	0	0
			1397	875	246	269	7			
1	E	173	Total	C	N	O	S	0	1	0
			1397	874	246	269	8			
1	F	172	Total	C	N	O	S	0	2	0
			1409	883	250	268	8			
1	G	173	Total	C	N	O	S	0	1	0
			1405	879	247	271	8			
1	H	174	Total	C	N	O	S	0	2	0
			1414	884	250	272	8			
1	I	171	Total	C	N	O	S	0	0	0
			1386	869	245	265	7			
1	J	171	Total	C	N	O	S	0	1	0
			1398	876	246	269	7			
1	K	171	Total	C	N	O	S	0	0	0
			1393	872	246	268	7			
1	L	171	Total	C	N	O	S	0	0	0
			1386	869	245	265	7			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q6NZ44
A	-5	HIS	-	expression tag	UNP Q6NZ44
A	-4	HIS	-	expression tag	UNP Q6NZ44
A	-3	HIS	-	expression tag	UNP Q6NZ44
A	-2	HIS	-	expression tag	UNP Q6NZ44

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP Q6NZ44
A	0	HIS	-	expression tag	UNP Q6NZ44
A	163	GLY	-	insertion	UNP Q6NZ44
A	164	PRO	-	insertion	UNP Q6NZ44
A	165	LEU	-	insertion	UNP Q6NZ44
A	166	GLY	-	insertion	UNP Q6NZ44
A	167	LEU	-	insertion	UNP Q6NZ44
A	168	ALA	-	insertion	UNP Q6NZ44
A	169	GLY	-	insertion	UNP Q6NZ44
B	-6	MET	-	initiating methionine	UNP Q6NZ44
B	-5	HIS	-	expression tag	UNP Q6NZ44
B	-4	HIS	-	expression tag	UNP Q6NZ44
B	-3	HIS	-	expression tag	UNP Q6NZ44
B	-2	HIS	-	expression tag	UNP Q6NZ44
B	-1	HIS	-	expression tag	UNP Q6NZ44
B	0	HIS	-	expression tag	UNP Q6NZ44
B	163	GLY	-	insertion	UNP Q6NZ44
B	164	PRO	-	insertion	UNP Q6NZ44
B	165	LEU	-	insertion	UNP Q6NZ44
B	166	GLY	-	insertion	UNP Q6NZ44
B	167	LEU	-	insertion	UNP Q6NZ44
B	168	ALA	-	insertion	UNP Q6NZ44
B	169	GLY	-	insertion	UNP Q6NZ44
C	-6	MET	-	initiating methionine	UNP Q6NZ44
C	-5	HIS	-	expression tag	UNP Q6NZ44
C	-4	HIS	-	expression tag	UNP Q6NZ44
C	-3	HIS	-	expression tag	UNP Q6NZ44
C	-2	HIS	-	expression tag	UNP Q6NZ44
C	-1	HIS	-	expression tag	UNP Q6NZ44
C	0	HIS	-	expression tag	UNP Q6NZ44
C	163	GLY	-	insertion	UNP Q6NZ44
C	164	PRO	-	insertion	UNP Q6NZ44
C	165	LEU	-	insertion	UNP Q6NZ44
C	166	GLY	-	insertion	UNP Q6NZ44
C	167	LEU	-	insertion	UNP Q6NZ44
C	168	ALA	-	insertion	UNP Q6NZ44
C	169	GLY	-	insertion	UNP Q6NZ44
D	-6	MET	-	initiating methionine	UNP Q6NZ44
D	-5	HIS	-	expression tag	UNP Q6NZ44
D	-4	HIS	-	expression tag	UNP Q6NZ44
D	-3	HIS	-	expression tag	UNP Q6NZ44
D	-2	HIS	-	expression tag	UNP Q6NZ44

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	expression tag	UNP Q6NZ44
D	0	HIS	-	expression tag	UNP Q6NZ44
D	163	GLY	-	insertion	UNP Q6NZ44
D	164	PRO	-	insertion	UNP Q6NZ44
D	165	LEU	-	insertion	UNP Q6NZ44
D	166	GLY	-	insertion	UNP Q6NZ44
D	167	LEU	-	insertion	UNP Q6NZ44
D	168	ALA	-	insertion	UNP Q6NZ44
D	169	GLY	-	insertion	UNP Q6NZ44
E	-6	MET	-	initiating methionine	UNP Q6NZ44
E	-5	HIS	-	expression tag	UNP Q6NZ44
E	-4	HIS	-	expression tag	UNP Q6NZ44
E	-3	HIS	-	expression tag	UNP Q6NZ44
E	-2	HIS	-	expression tag	UNP Q6NZ44
E	-1	HIS	-	expression tag	UNP Q6NZ44
E	0	HIS	-	expression tag	UNP Q6NZ44
E	163	GLY	-	insertion	UNP Q6NZ44
E	164	PRO	-	insertion	UNP Q6NZ44
E	165	LEU	-	insertion	UNP Q6NZ44
E	166	GLY	-	insertion	UNP Q6NZ44
E	167	LEU	-	insertion	UNP Q6NZ44
E	168	ALA	-	insertion	UNP Q6NZ44
E	169	GLY	-	insertion	UNP Q6NZ44
F	-6	MET	-	initiating methionine	UNP Q6NZ44
F	-5	HIS	-	expression tag	UNP Q6NZ44
F	-4	HIS	-	expression tag	UNP Q6NZ44
F	-3	HIS	-	expression tag	UNP Q6NZ44
F	-2	HIS	-	expression tag	UNP Q6NZ44
F	-1	HIS	-	expression tag	UNP Q6NZ44
F	0	HIS	-	expression tag	UNP Q6NZ44
F	163	GLY	-	insertion	UNP Q6NZ44
F	164	PRO	-	insertion	UNP Q6NZ44
F	165	LEU	-	insertion	UNP Q6NZ44
F	166	GLY	-	insertion	UNP Q6NZ44
F	167	LEU	-	insertion	UNP Q6NZ44
F	168	ALA	-	insertion	UNP Q6NZ44
F	169	GLY	-	insertion	UNP Q6NZ44
G	-6	MET	-	initiating methionine	UNP Q6NZ44
G	-5	HIS	-	expression tag	UNP Q6NZ44
G	-4	HIS	-	expression tag	UNP Q6NZ44
G	-3	HIS	-	expression tag	UNP Q6NZ44
G	-2	HIS	-	expression tag	UNP Q6NZ44

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	HIS	-	expression tag	UNP Q6NZ44
G	0	HIS	-	expression tag	UNP Q6NZ44
G	163	GLY	-	insertion	UNP Q6NZ44
G	164	PRO	-	insertion	UNP Q6NZ44
G	165	LEU	-	insertion	UNP Q6NZ44
G	166	GLY	-	insertion	UNP Q6NZ44
G	167	LEU	-	insertion	UNP Q6NZ44
G	168	ALA	-	insertion	UNP Q6NZ44
G	169	GLY	-	insertion	UNP Q6NZ44
H	-6	MET	-	initiating methionine	UNP Q6NZ44
H	-5	HIS	-	expression tag	UNP Q6NZ44
H	-4	HIS	-	expression tag	UNP Q6NZ44
H	-3	HIS	-	expression tag	UNP Q6NZ44
H	-2	HIS	-	expression tag	UNP Q6NZ44
H	-1	HIS	-	expression tag	UNP Q6NZ44
H	0	HIS	-	expression tag	UNP Q6NZ44
H	163	GLY	-	insertion	UNP Q6NZ44
H	164	PRO	-	insertion	UNP Q6NZ44
H	165	LEU	-	insertion	UNP Q6NZ44
H	166	GLY	-	insertion	UNP Q6NZ44
H	167	LEU	-	insertion	UNP Q6NZ44
H	168	ALA	-	insertion	UNP Q6NZ44
H	169	GLY	-	insertion	UNP Q6NZ44
I	-6	MET	-	initiating methionine	UNP Q6NZ44
I	-5	HIS	-	expression tag	UNP Q6NZ44
I	-4	HIS	-	expression tag	UNP Q6NZ44
I	-3	HIS	-	expression tag	UNP Q6NZ44
I	-2	HIS	-	expression tag	UNP Q6NZ44
I	-1	HIS	-	expression tag	UNP Q6NZ44
I	0	HIS	-	expression tag	UNP Q6NZ44
I	163	GLY	-	insertion	UNP Q6NZ44
I	164	PRO	-	insertion	UNP Q6NZ44
I	165	LEU	-	insertion	UNP Q6NZ44
I	166	GLY	-	insertion	UNP Q6NZ44
I	167	LEU	-	insertion	UNP Q6NZ44
I	168	ALA	-	insertion	UNP Q6NZ44
I	169	GLY	-	insertion	UNP Q6NZ44
J	-6	MET	-	initiating methionine	UNP Q6NZ44
J	-5	HIS	-	expression tag	UNP Q6NZ44
J	-4	HIS	-	expression tag	UNP Q6NZ44
J	-3	HIS	-	expression tag	UNP Q6NZ44
J	-2	HIS	-	expression tag	UNP Q6NZ44

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	HIS	-	expression tag	UNP Q6NZ44
J	0	HIS	-	expression tag	UNP Q6NZ44
J	163	GLY	-	insertion	UNP Q6NZ44
J	164	PRO	-	insertion	UNP Q6NZ44
J	165	LEU	-	insertion	UNP Q6NZ44
J	166	GLY	-	insertion	UNP Q6NZ44
J	167	LEU	-	insertion	UNP Q6NZ44
J	168	ALA	-	insertion	UNP Q6NZ44
J	169	GLY	-	insertion	UNP Q6NZ44
K	-6	MET	-	initiating methionine	UNP Q6NZ44
K	-5	HIS	-	expression tag	UNP Q6NZ44
K	-4	HIS	-	expression tag	UNP Q6NZ44
K	-3	HIS	-	expression tag	UNP Q6NZ44
K	-2	HIS	-	expression tag	UNP Q6NZ44
K	-1	HIS	-	expression tag	UNP Q6NZ44
K	0	HIS	-	expression tag	UNP Q6NZ44
K	163	GLY	-	insertion	UNP Q6NZ44
K	164	PRO	-	insertion	UNP Q6NZ44
K	165	LEU	-	insertion	UNP Q6NZ44
K	166	GLY	-	insertion	UNP Q6NZ44
K	167	LEU	-	insertion	UNP Q6NZ44
K	168	ALA	-	insertion	UNP Q6NZ44
K	169	GLY	-	insertion	UNP Q6NZ44
L	-6	MET	-	initiating methionine	UNP Q6NZ44
L	-5	HIS	-	expression tag	UNP Q6NZ44
L	-4	HIS	-	expression tag	UNP Q6NZ44
L	-3	HIS	-	expression tag	UNP Q6NZ44
L	-2	HIS	-	expression tag	UNP Q6NZ44
L	-1	HIS	-	expression tag	UNP Q6NZ44
L	0	HIS	-	expression tag	UNP Q6NZ44
L	163	GLY	-	insertion	UNP Q6NZ44
L	164	PRO	-	insertion	UNP Q6NZ44
L	165	LEU	-	insertion	UNP Q6NZ44
L	166	GLY	-	insertion	UNP Q6NZ44
L	167	LEU	-	insertion	UNP Q6NZ44
L	168	ALA	-	insertion	UNP Q6NZ44
L	169	GLY	-	insertion	UNP Q6NZ44

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	E	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total 1	Na 1	0	0
4	L	1	Total 1	Na 1	0	0

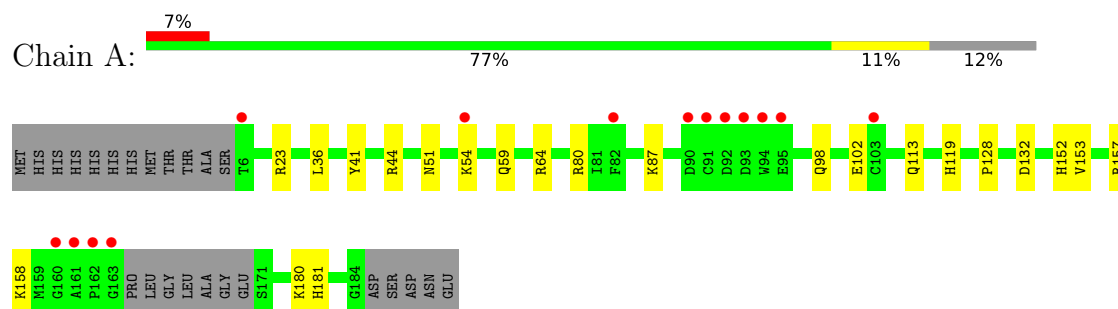
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total 227	O 227	0	0
5	B	195	Total 195	O 195	0	0
5	C	211	Total 211	O 211	0	0
5	D	193	Total 193	O 193	0	0
5	E	200	Total 200	O 200	0	0
5	F	216	Total 216	O 216	0	0
5	G	213	Total 213	O 213	0	0
5	H	208	Total 208	O 208	0	0
5	I	223	Total 223	O 223	0	0
5	J	209	Total 209	O 209	0	0
5	K	220	Total 220	O 220	0	0
5	L	206	Total 206	O 206	0	0

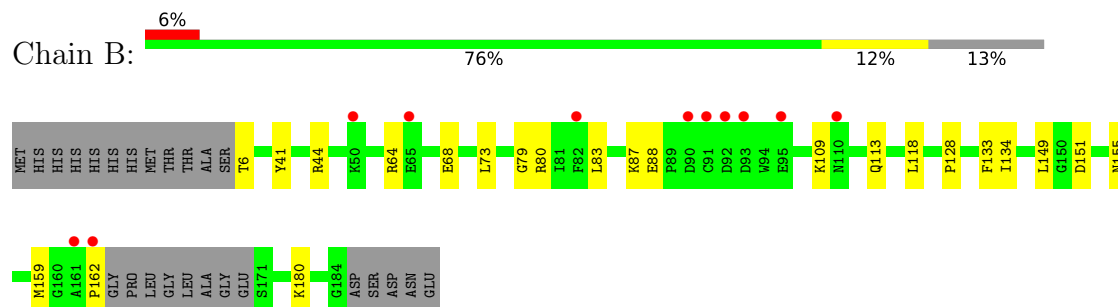
3 Residue-property plots [i](#)

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.

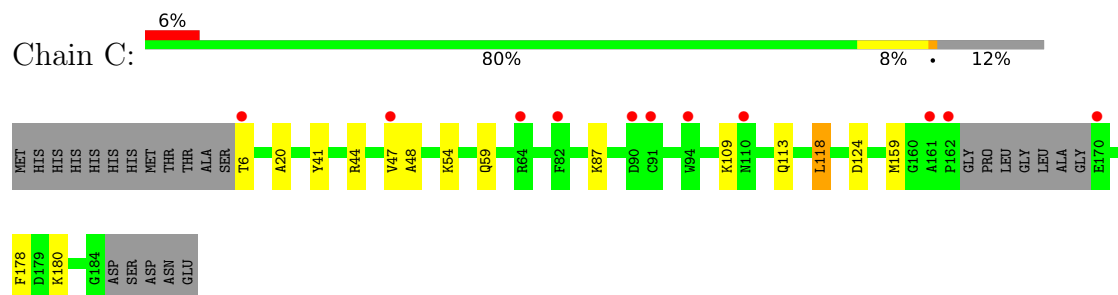
- Molecule 1: Ferritin



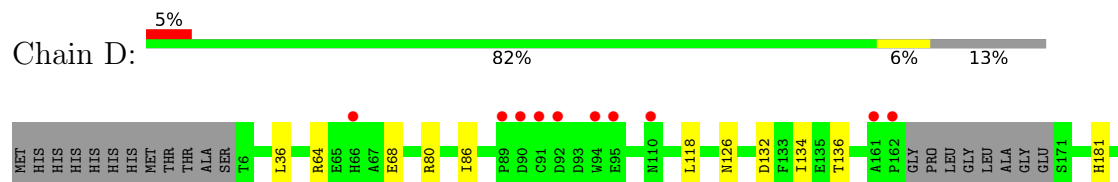
- Molecule 1: Ferritin

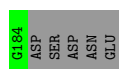


- Molecule 1: Ferritin

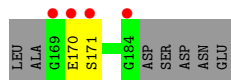
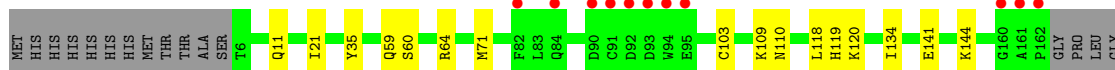
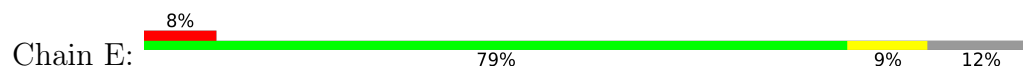


- Molecule 1: Ferritin

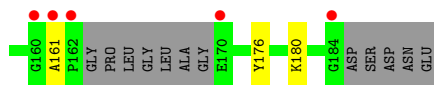
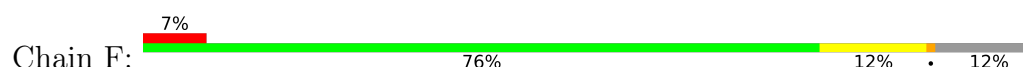




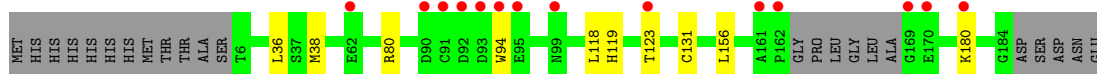
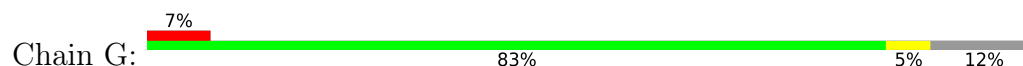
• Molecule 1: Ferritin



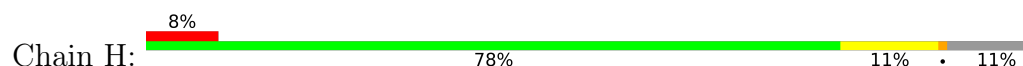
• Molecule 1: Ferritin



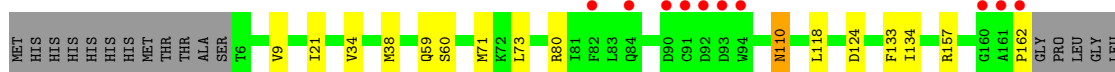
• Molecule 1: Ferritin

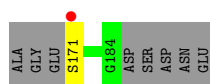


• Molecule 1: Ferritin

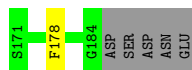
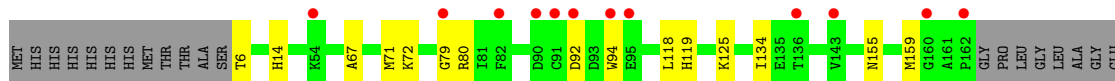
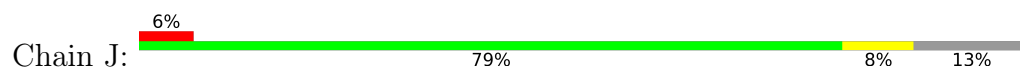


• Molecule 1: Ferritin

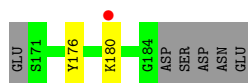
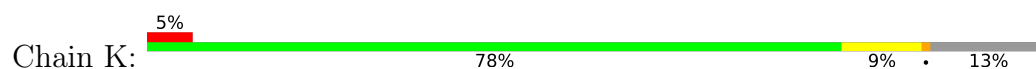




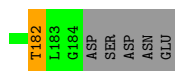
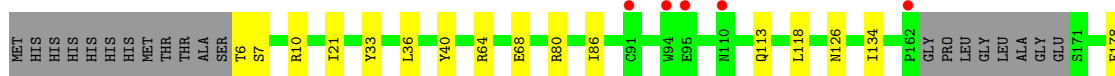
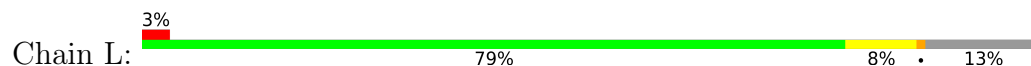
• Molecule 1: Ferritin



• Molecule 1: Ferritin



• Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.66Å 219.66Å 148.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.52 – 2.01 23.52 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.52-2.01) 99.5 (23.52-2.01)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.245 , 0.287 0.245 , 0.287	Depositor DCC
R_{free} test set	11708 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19365	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 50.49 % 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 6.4218e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/1450	0.54	0/1951
1	B	0.34	0/1434	0.56	0/1931
1	C	0.35	0/1446	0.54	0/1947
1	D	0.33	0/1425	0.53	0/1919
1	E	0.33	0/1428	0.51	0/1926
1	F	0.31	0/1443	0.50	0/1943
1	G	0.32	0/1436	0.49	0/1935
1	H	0.32	0/1448	0.51	0/1951
1	I	0.32	0/1414	0.52	0/1906
1	J	0.34	0/1429	0.55	2/1925 (0.1%)
1	K	0.33	0/1421	0.54	0/1915
1	L	0.33	0/1414	0.52	0/1906
All	All	0.33	0/17188	0.53	2/23155 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	94	TRP	CA-C-N	5.27	131.60	121.54
1	J	94	TRP	C-N-CA	5.27	131.60	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1416	0	1358	25	0
1	B	1403	0	1336	19	0
1	C	1415	0	1346	16	0
1	D	1397	0	1330	9	0
1	E	1397	0	1314	18	0
1	F	1409	0	1346	21	0
1	G	1405	0	1329	8	0
1	H	1414	0	1340	19	0
1	I	1386	0	1313	15	0
1	J	1398	0	1330	11	0
1	K	1393	0	1321	15	0
1	L	1386	0	1313	15	0
2	A	2	0	0	0	0
2	E	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	1
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	2	0	0	0	1
3	I	2	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
3	L	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	227	0	0	13	0
5	B	195	0	0	5	0
5	C	211	0	0	8	1
5	D	193	0	0	1	2
5	E	200	0	0	5	0
5	F	216	0	0	6	1
5	G	213	0	0	1	0
5	H	208	0	0	4	3
5	I	223	0	0	7	0
5	J	209	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	220	0	0	5	0
5	L	206	0	0	5	1
All	All	19365	0	15976	168	6

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 5.

The worst 5 of 168 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:C:6:THR:N	5:C:303:HOH:O	2.14	0.81
1:B:155:ASN:O	1:B:159:MET:HG3	1.87	0.75
1:I:171:SER:N	5:I:302:HOH:O	2.21	0.73
1:F:6:THR:N	5:F:302:HOH:O	2.22	0.72
1:A:23:ARG:NH1	5:A:303:HOH:O	2.22	0.71

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:202:FE:FE	3:H:201:FE:FE[7_556]	1.71	0.49
5:C:444:HOH:O	5:F:462:HOH:O[7_556]	2.12	0.08
5:H:457:HOH:O	5:H:457:HOH:O[7_556]	2.15	0.05
5:D:440:HOH:O	5:H:404:HOH:O[7_556]	2.16	0.04
5:D:400:HOH:O	5:J:432:HOH:O[7_556]	2.17	0.03

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	170/196 (87%)	166 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	168/196 (86%)	163 (97%)	5 (3%)	0	100	100
1	C	169/196 (86%)	166 (98%)	3 (2%)	0	100	100
1	D	167/196 (85%)	163 (98%)	4 (2%)	0	100	100
1	E	170/196 (87%)	164 (96%)	6 (4%)	0	100	100
1	F	170/196 (87%)	168 (99%)	2 (1%)	0	100	100
1	G	170/196 (87%)	167 (98%)	3 (2%)	0	100	100
1	H	172/196 (88%)	169 (98%)	3 (2%)	0	100	100
1	I	167/196 (85%)	165 (99%)	2 (1%)	0	100	100
1	J	168/196 (86%)	165 (98%)	3 (2%)	0	100	100
1	K	167/196 (85%)	164 (98%)	3 (2%)	0	100	100
1	L	167/196 (85%)	163 (98%)	4 (2%)	0	100	100
All	All	2025/2352 (86%)	1983 (98%)	42 (2%)	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	153/172 (89%)	153 (100%)	0	100	100
1	B	151/172 (88%)	151 (100%)	0	100	100
1	C	153/172 (89%)	152 (99%)	1 (1%)	76	82
1	D	150/172 (87%)	150 (100%)	0	100	100
1	E	148/172 (86%)	146 (99%)	2 (1%)	59	66
1	F	151/172 (88%)	150 (99%)	1 (1%)	76	82
1	G	150/172 (87%)	149 (99%)	1 (1%)	76	82
1	H	151/172 (88%)	150 (99%)	1 (1%)	76	82
1	I	147/172 (86%)	145 (99%)	2 (1%)	59	66
1	J	150/172 (87%)	149 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	149/172 (87%)	147 (99%)	2 (1%)	61	68
1	L	147/172 (86%)	145 (99%)	2 (1%)	59	66
All	All	1800/2064 (87%)	1787 (99%)	13 (1%)	76	82

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	110	ASN
1	J	92	ASP
1	L	182	THR
1	K	118	LEU
1	L	33	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	15	GLN
1	I	126	ASN
1	H	58	HIS
1	H	155	ASN
1	K	98	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	172/196 (87%)	0.70	14 (8%)	18	17	11, 17, 32, 48	2 (1%)
1	B	171/196 (87%)	0.56	11 (6%)	25	24	11, 17, 30, 45	1 (0%)
1	C	172/196 (87%)	0.54	11 (6%)	25	24	12, 17, 33, 62	1 (0%)
1	D	171/196 (87%)	0.50	10 (5%)	29	27	14, 18, 31, 47	0
1	E	173/196 (88%)	0.55	15 (8%)	16	15	13, 17, 36, 58	1 (0%)
1	F	172/196 (87%)	0.52	14 (8%)	18	17	12, 17, 35, 59	2 (1%)
1	G	173/196 (88%)	0.53	14 (8%)	18	17	14, 18, 37, 67	1 (0%)
1	H	174/196 (88%)	0.49	16 (9%)	14	13	12, 18, 39, 69	2 (1%)
1	I	171/196 (87%)	0.58	11 (6%)	25	24	13, 17, 30, 49	0
1	J	171/196 (87%)	0.56	12 (7%)	22	21	13, 17, 32, 47	1 (0%)
1	K	171/196 (87%)	0.52	10 (5%)	29	27	13, 17, 29, 47	0
1	L	171/196 (87%)	0.40	5 (2%)	53	52	14, 18, 31, 51	0
All	All	2062/2352 (87%)	0.54	143 (6%)	23	21	11, 17, 33, 69	11 (0%)

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	169	GLY	7.2
1	B	91	CYS	6.1
1	A	91	CYS	6.1
1	K	91	CYS	5.9
1	G	170	GLU	5.9

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

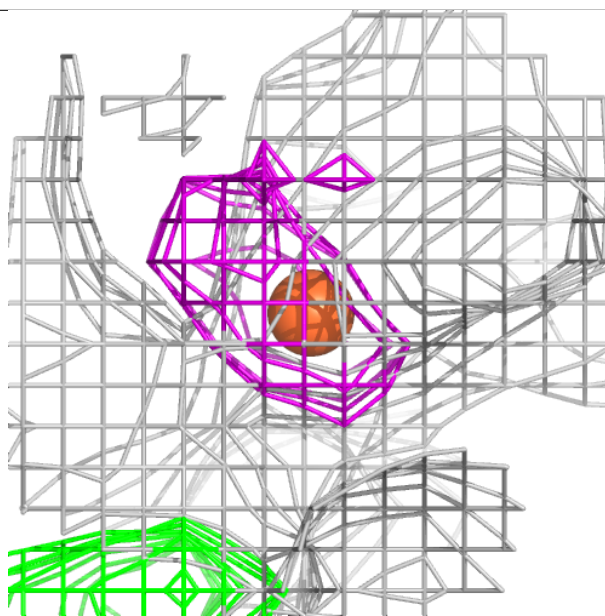
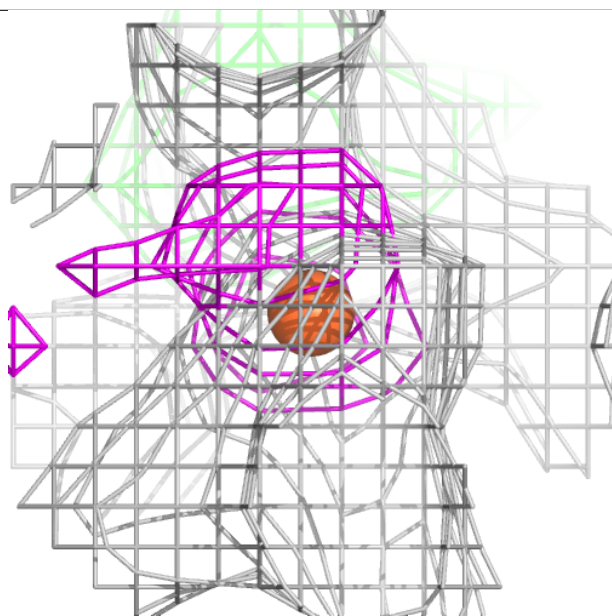
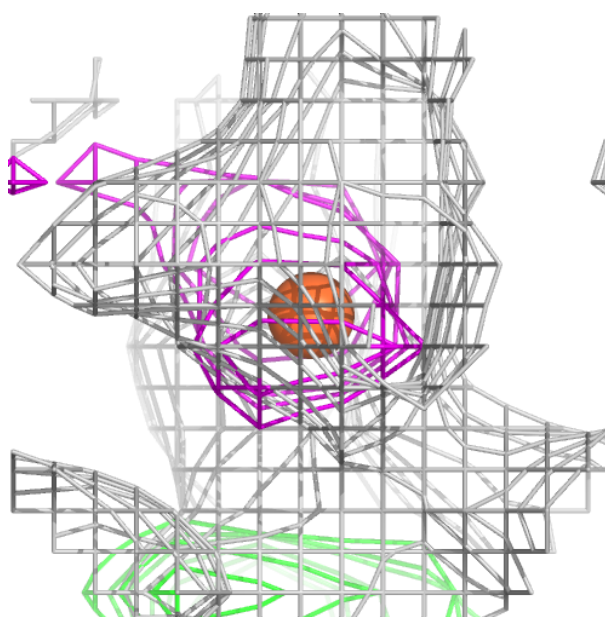
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FE	I	201	1/1	0.59	0.30	65,65,65,65	0
4	NA	L	202	1/1	0.82	0.10	23,23,23,23	0
2	CL	L	201	1/1	0.88	0.18	44,44,44,44	0
4	NA	J	201	1/1	0.91	0.09	22,22,22,22	0
4	NA	D	201	1/1	0.94	0.08	21,21,21,21	0
3	FE	H	201	1/1	0.94	0.28	69,69,69,69	0
2	CL	A	201	1/1	0.94	0.33	30,30,30,30	0
3	FE	D	203	1/1	0.95	0.10	36,36,36,36	0
3	FE	K	202	1/1	0.95	0.08	33,33,33,33	0
4	NA	C	201	1/1	0.95	0.15	12,12,12,12	0
2	CL	E	201	1/1	0.97	0.33	31,31,31,31	1
3	FE	A	203	1/1	0.97	0.09	32,32,32,32	0
3	FE	B	202	1/1	0.97	0.10	37,37,37,37	0
3	FE	D	202	1/1	0.97	0.19	39,39,39,39	0
3	FE	J	202	1/1	0.98	0.10	36,36,36,36	0
2	CL	A	202	1/1	0.98	0.16	29,29,29,29	0
3	FE	L	203	1/1	0.98	0.10	31,31,31,31	0
3	FE	F	201	1/1	0.98	0.14	34,34,34,34	0
3	FE	C	202	1/1	0.98	0.08	30,30,30,30	0
3	FE	H	202	1/1	0.98	0.14	35,35,35,35	0
3	FE	B	201	1/1	0.98	0.04	31,31,31,31	0
3	FE	G	201	1/1	0.99	0.10	33,33,33,33	0
3	FE	K	201	1/1	0.99	0.06	30,30,30,30	0
3	FE	E	202	1/1	0.99	0.11	32,32,32,32	0
3	FE	I	202	1/1	0.99	0.10	34,34,34,34	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.

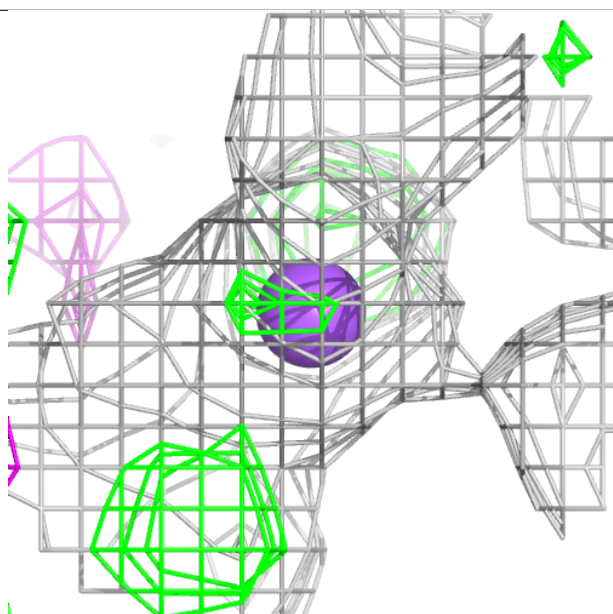
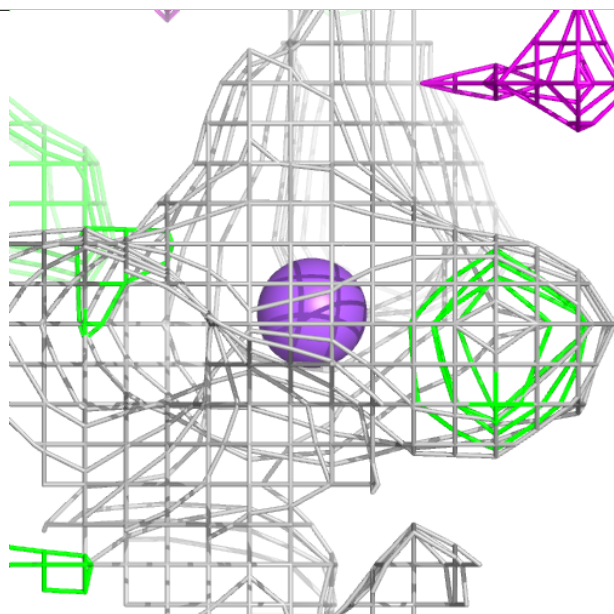
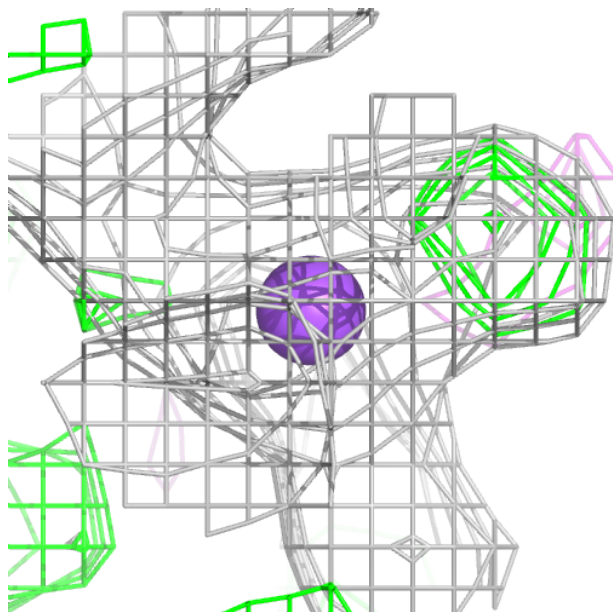
Electron density around FE I 201:

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



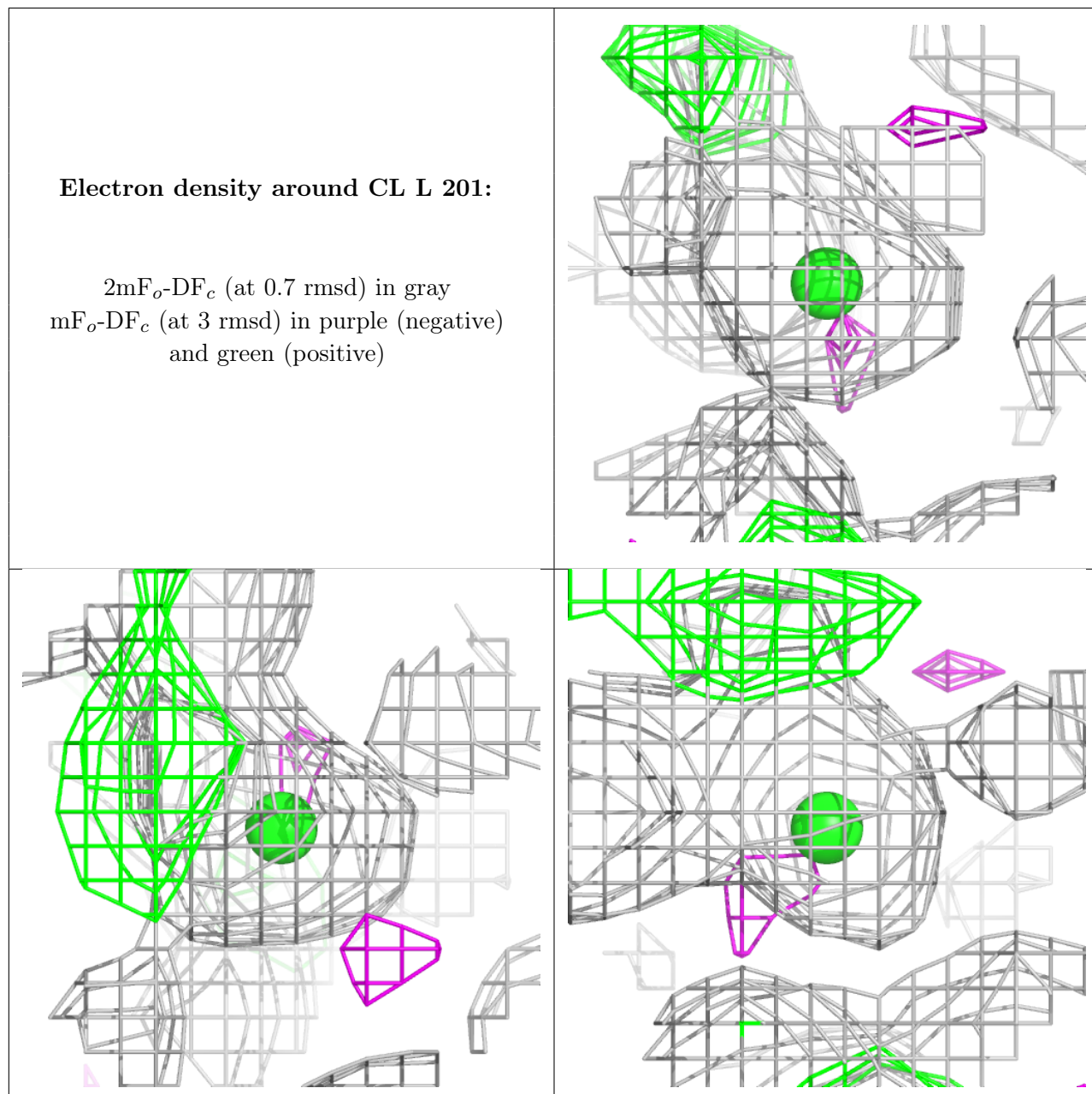
Electron density around NA L 202:

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



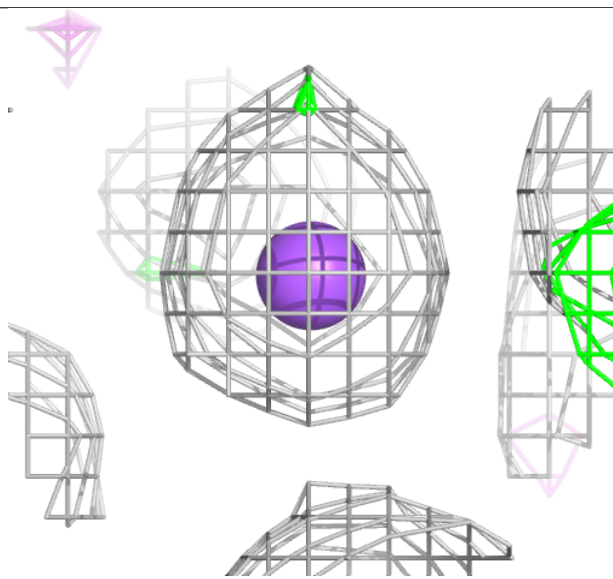
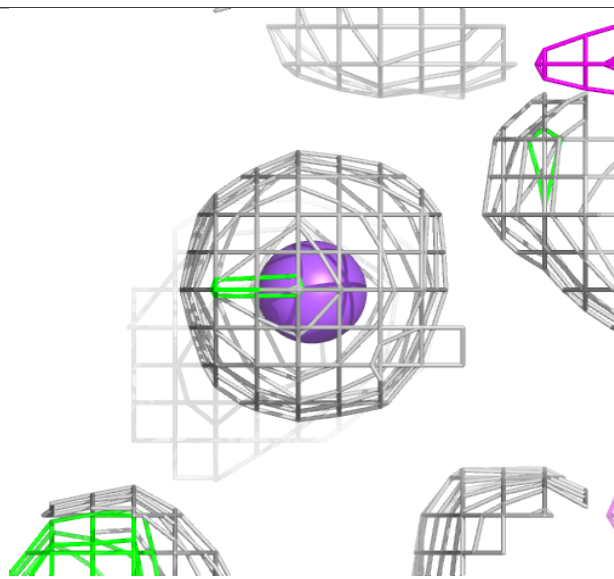
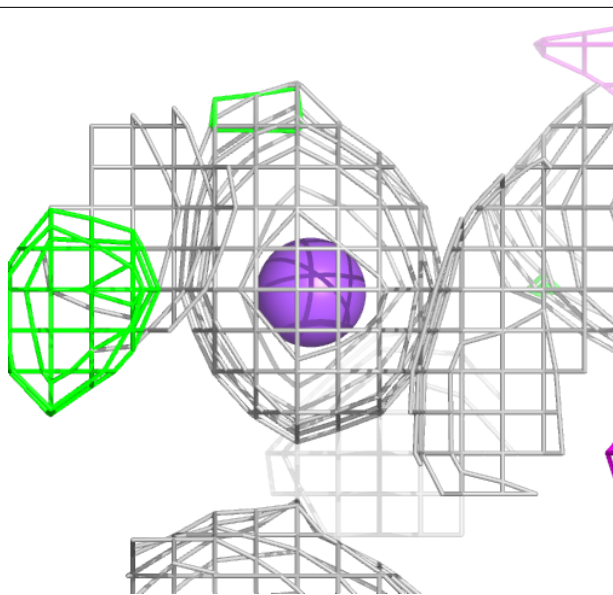
Electron density around CL L 201:

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



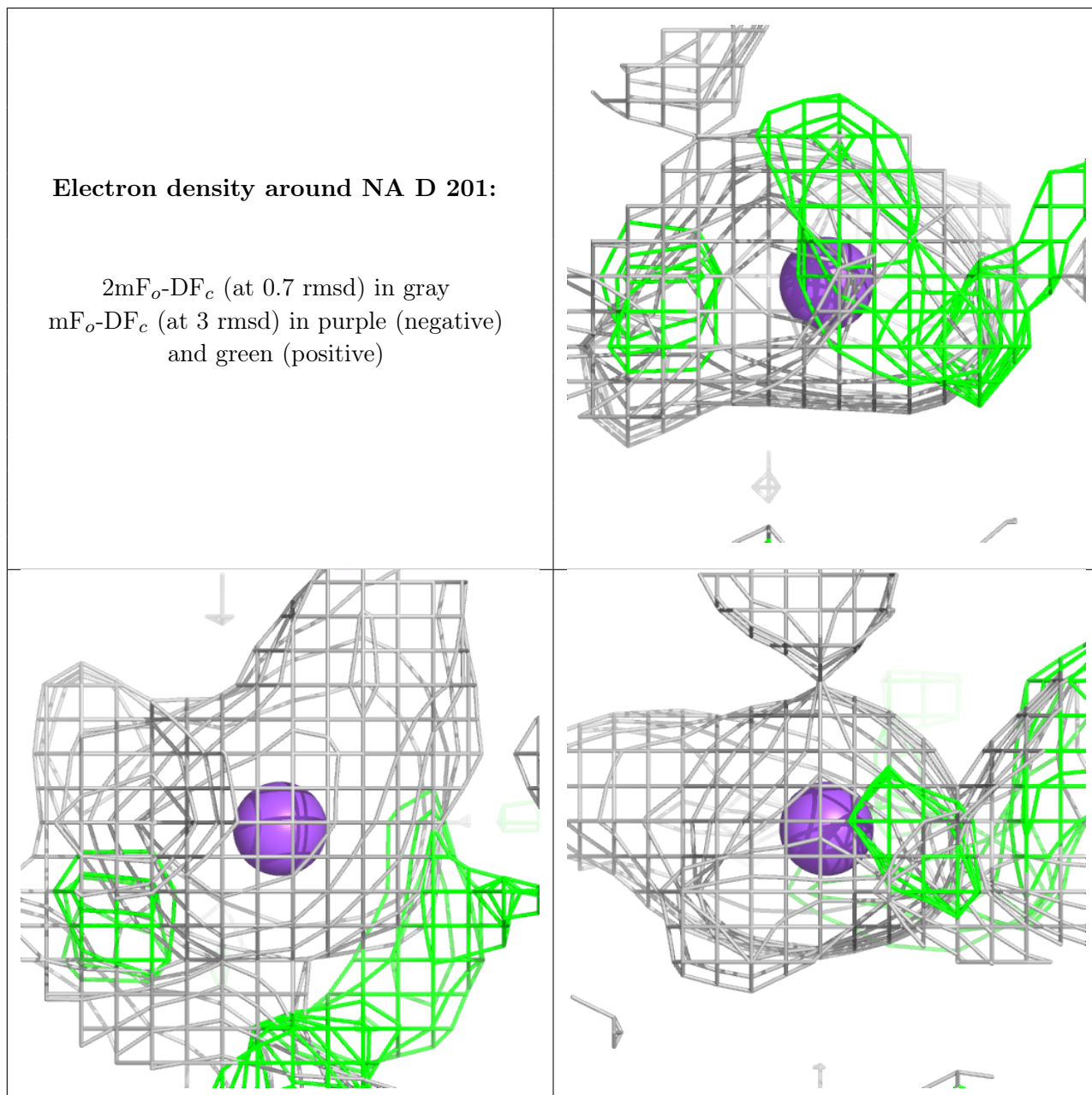
Electron density around NA J 201:

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



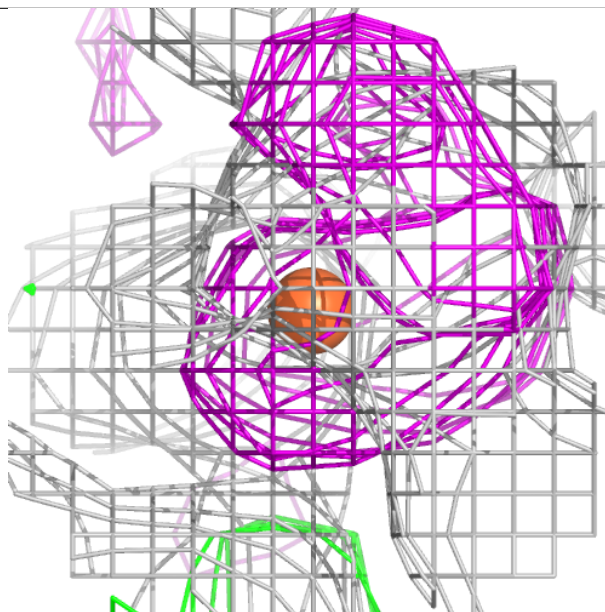
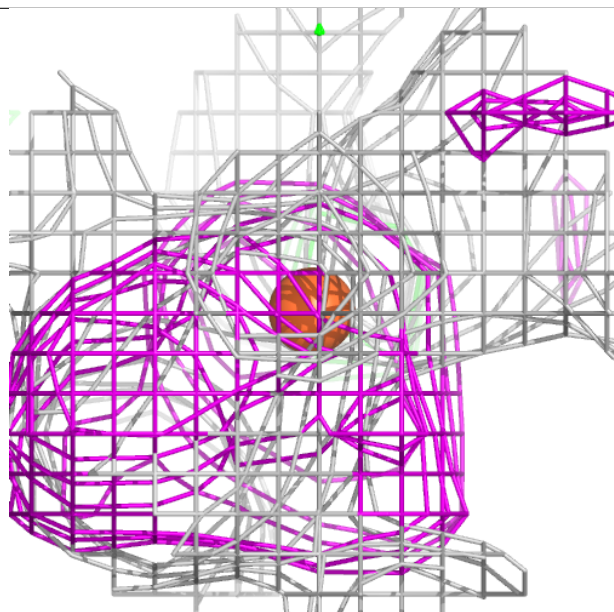
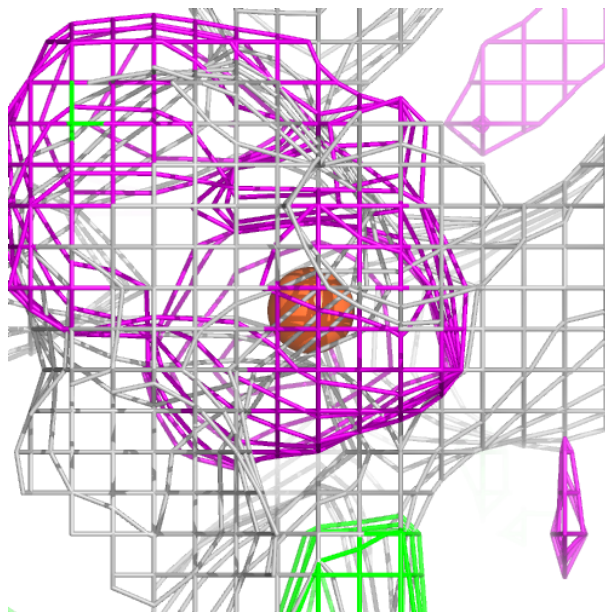
Electron density around NA D 201:

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and green (positive)



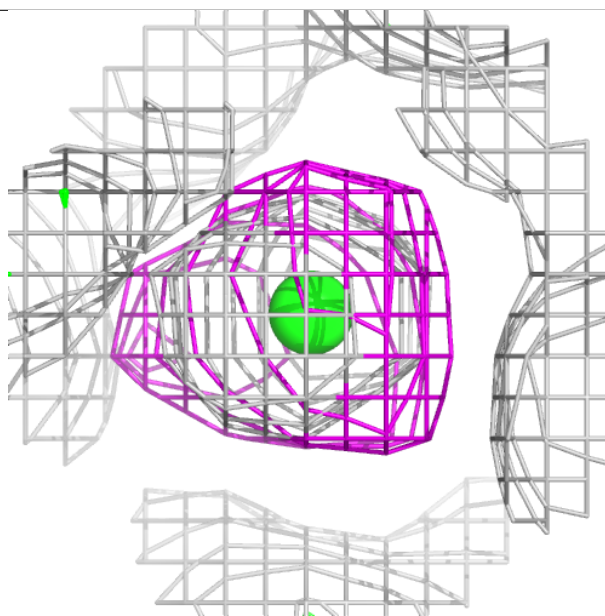
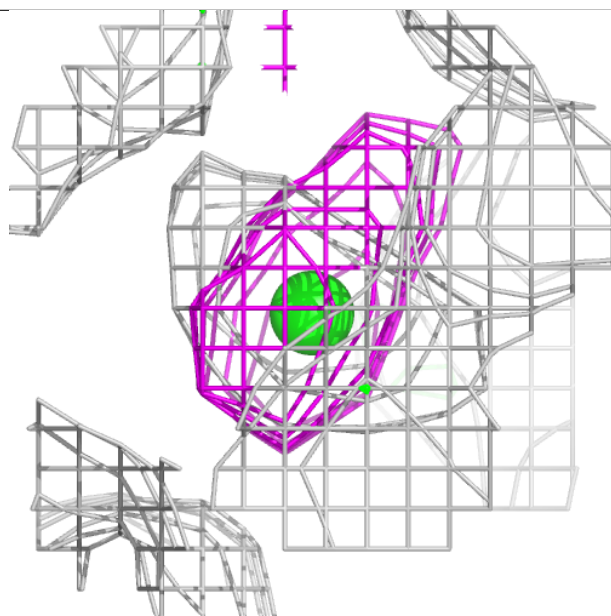
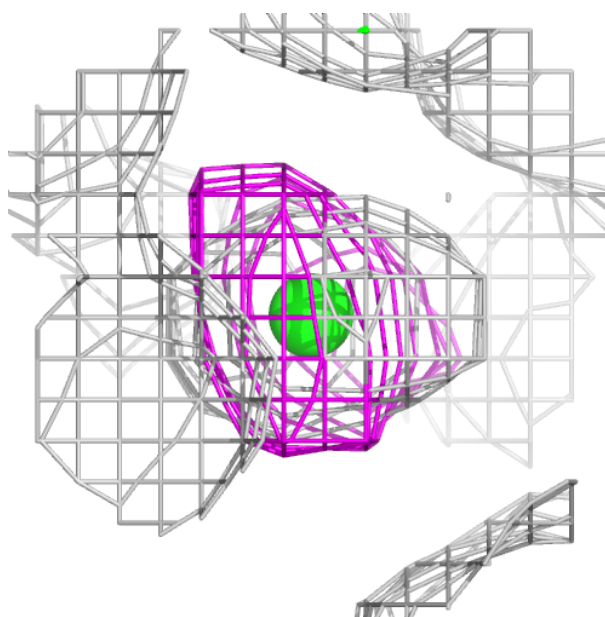
Electron density around FE H 201:

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



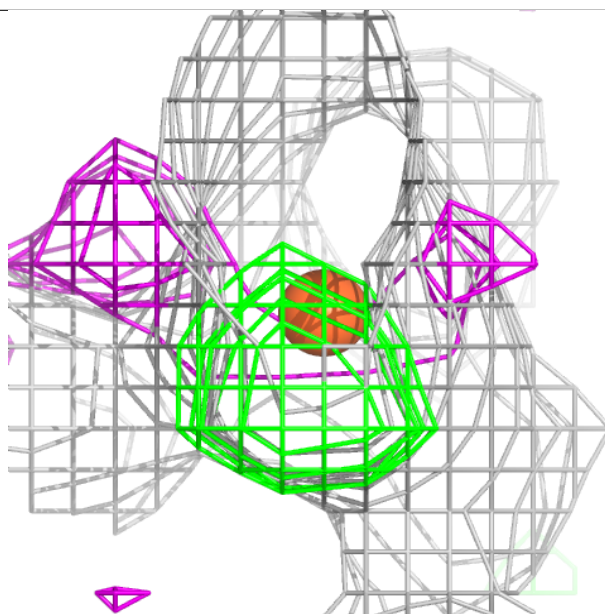
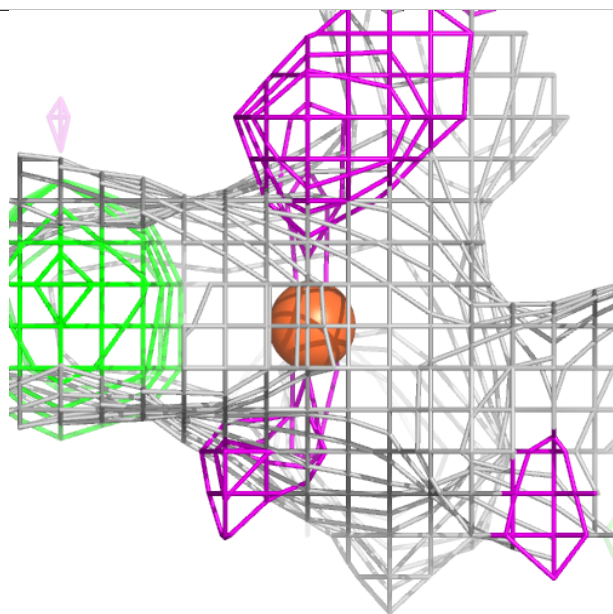
Electron density around CL A 201:

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



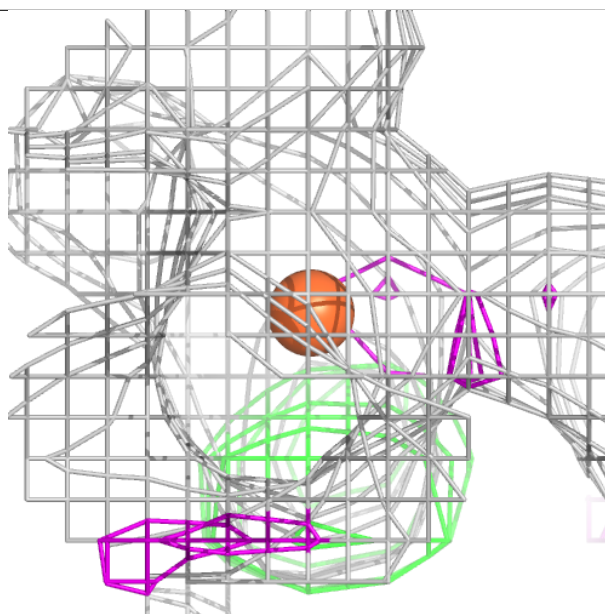
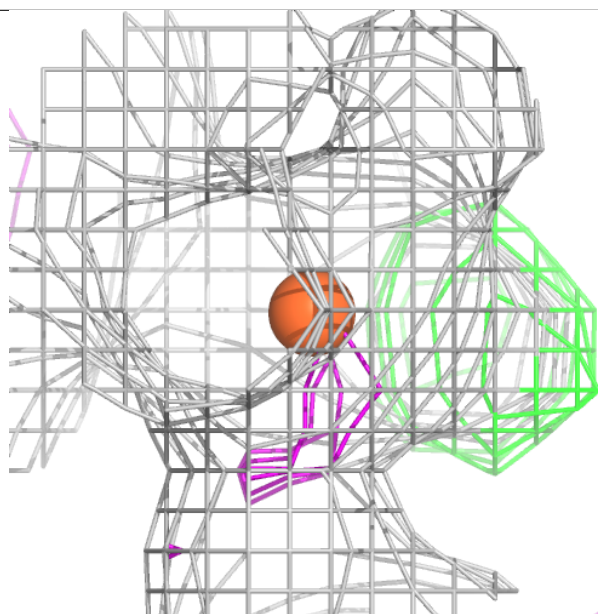
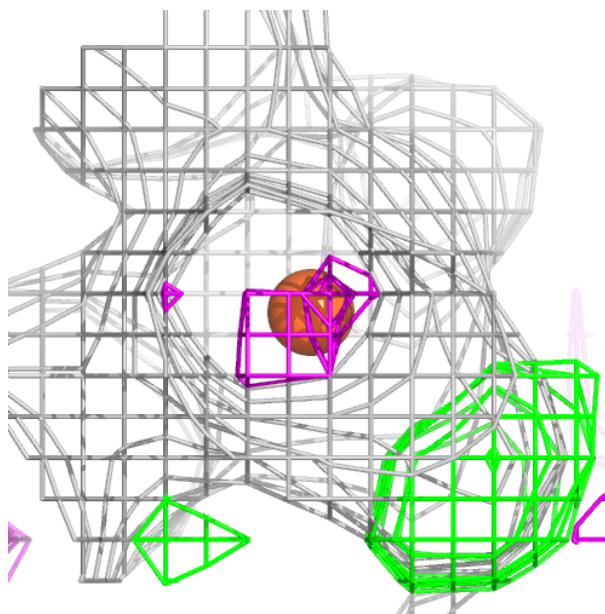
Electron density around FE D 203:

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



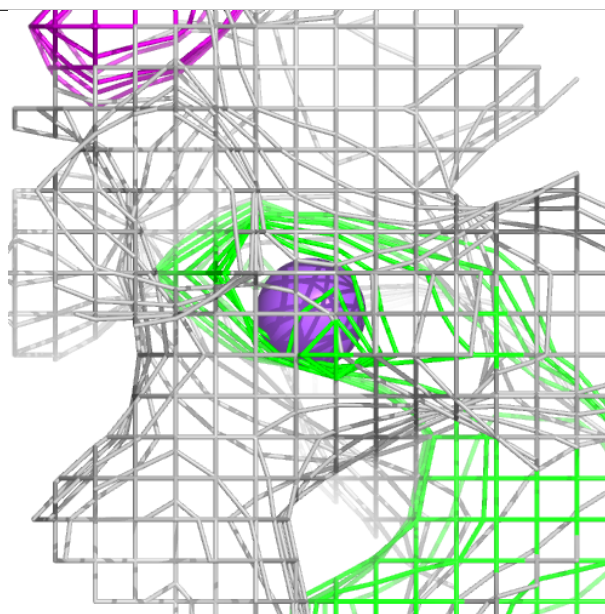
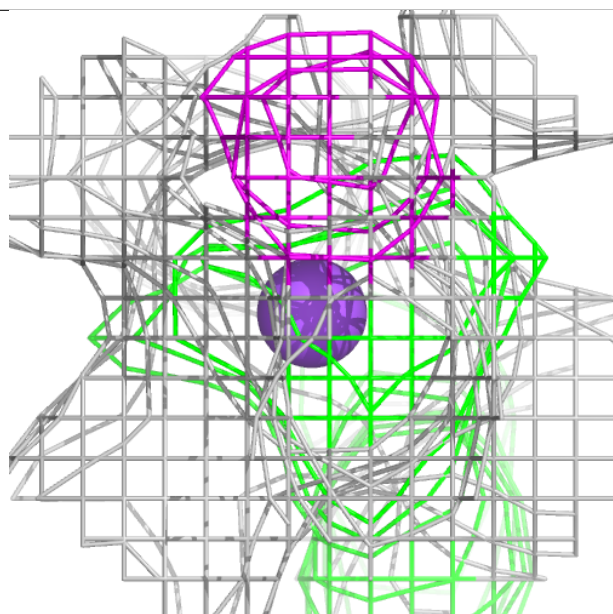
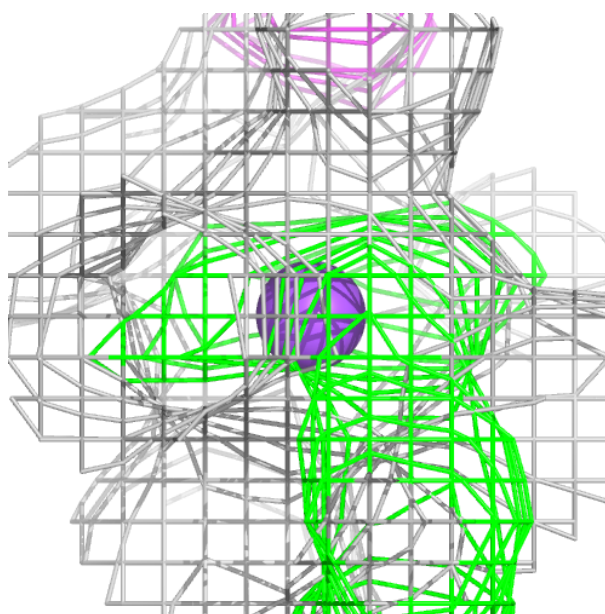
Electron density around FE K 202:

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



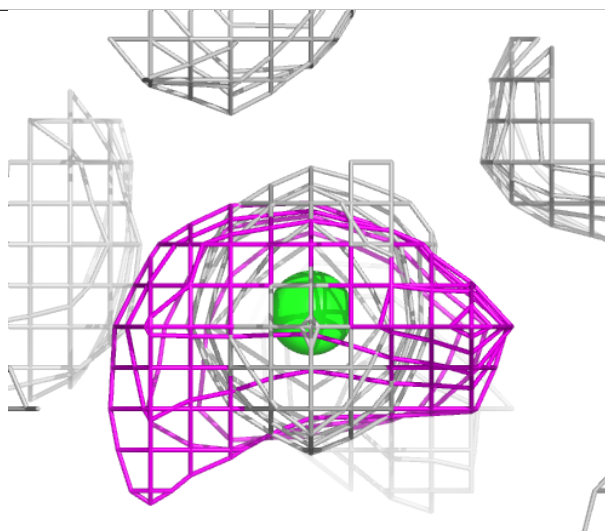
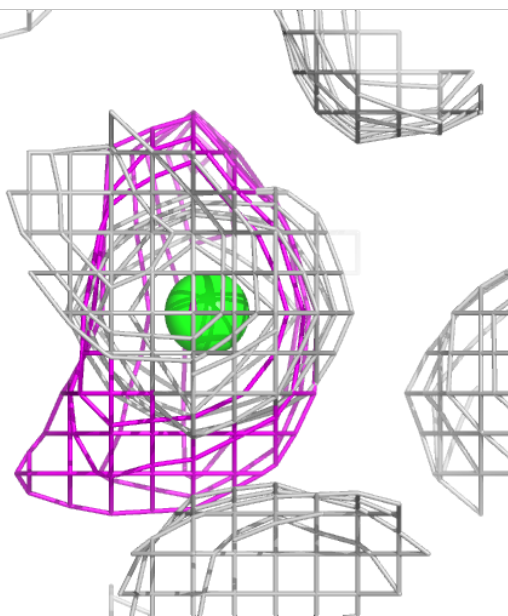
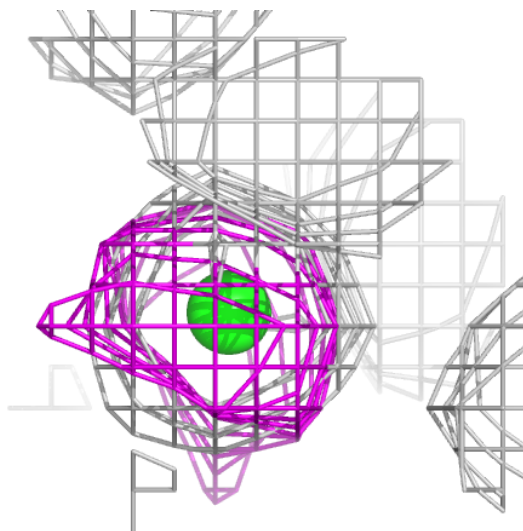
Electron density around NA C 201:

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



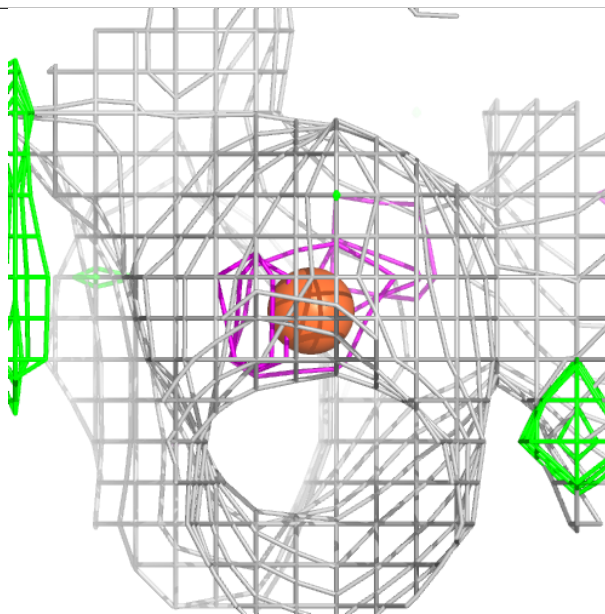
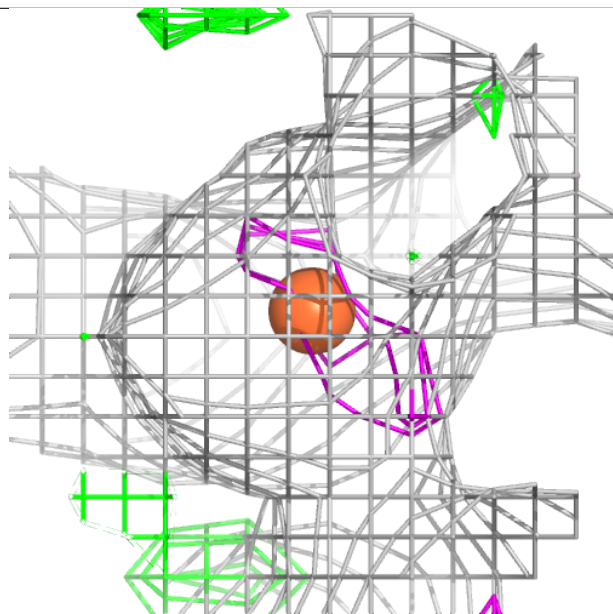
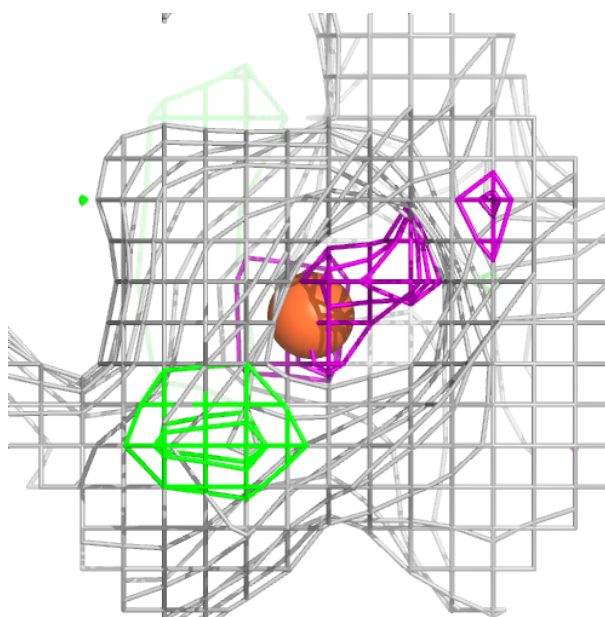
Electron density around CL E 201:

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



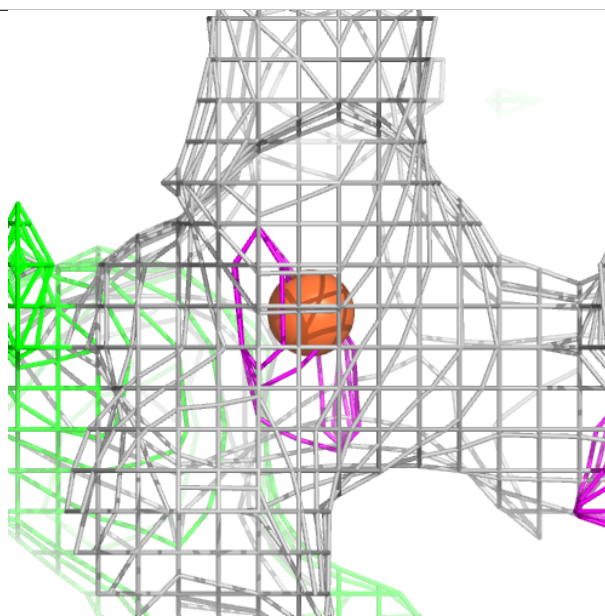
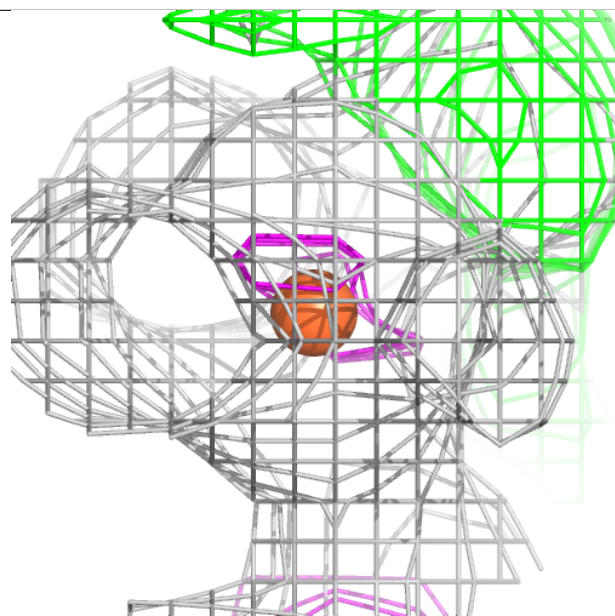
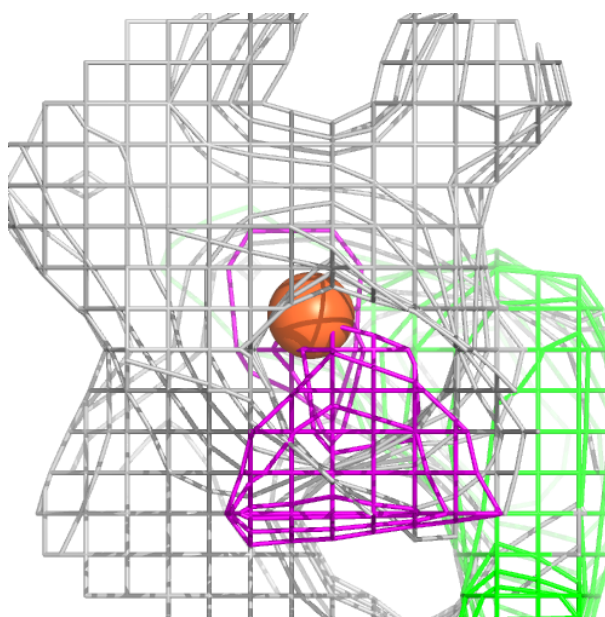
Electron density around FE A 203:

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



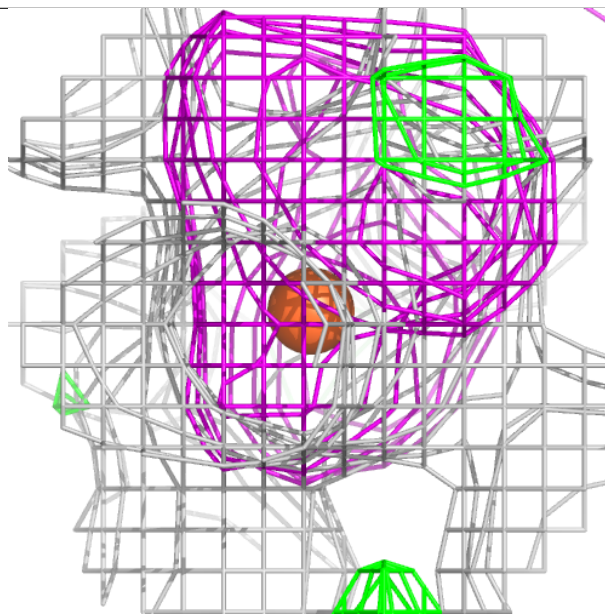
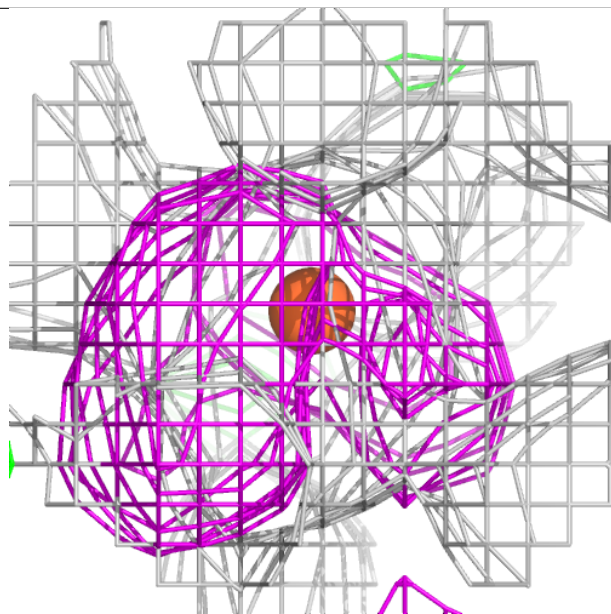
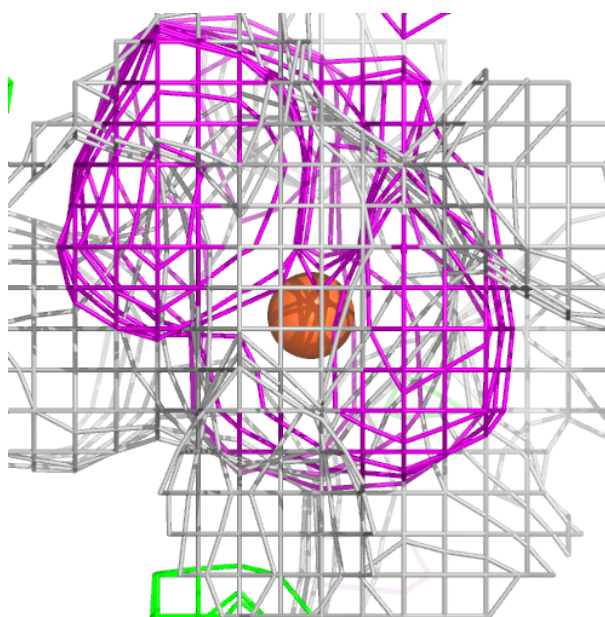
Electron density around FE B 202:

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



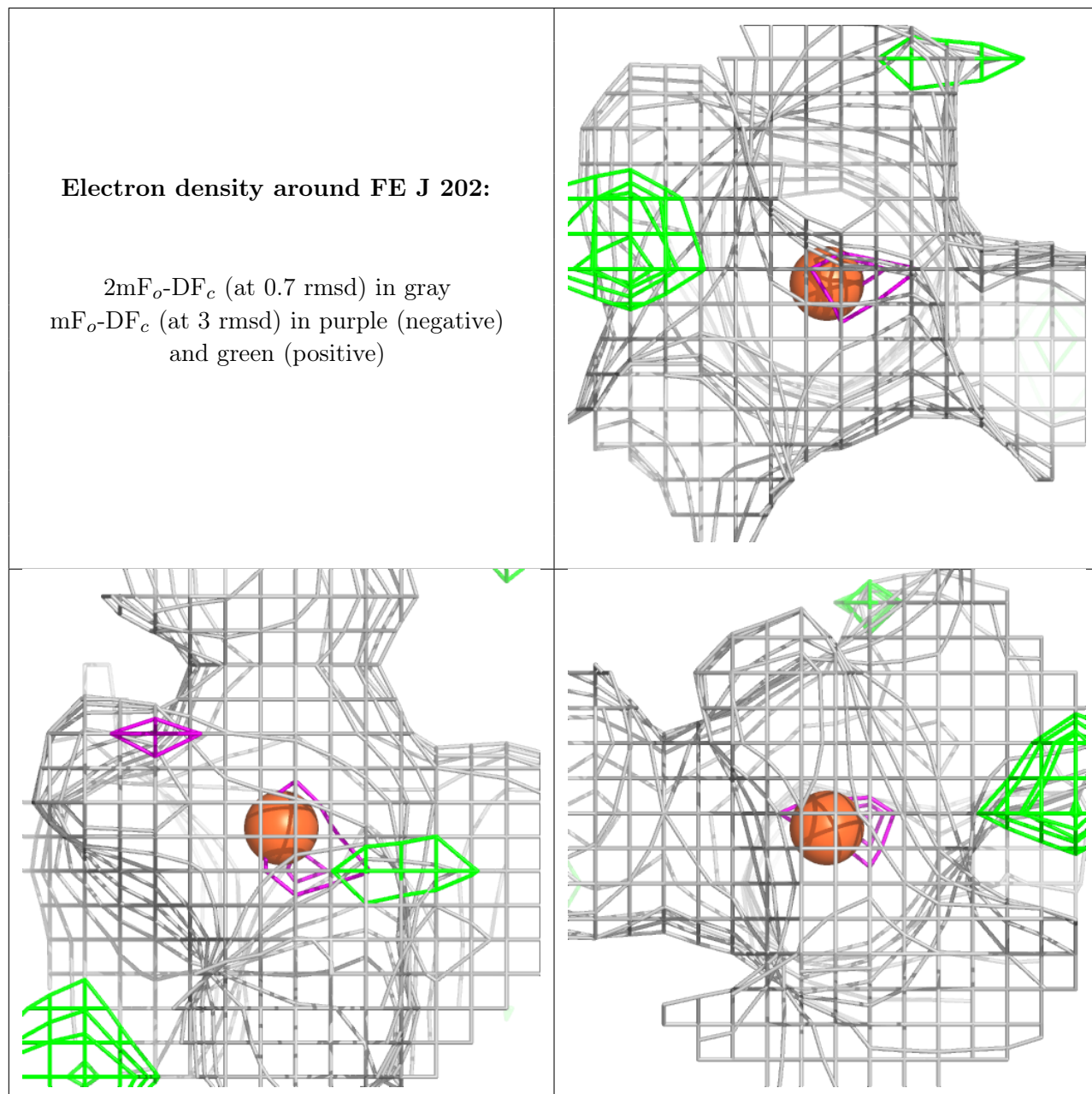
Electron density around FE D 202:

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



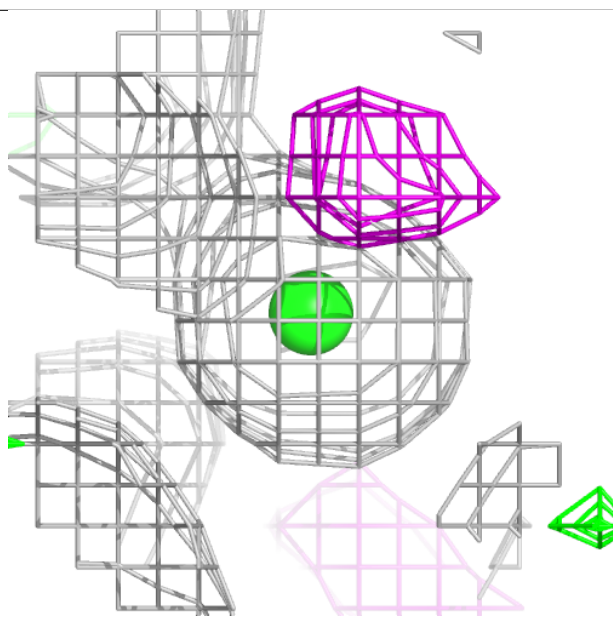
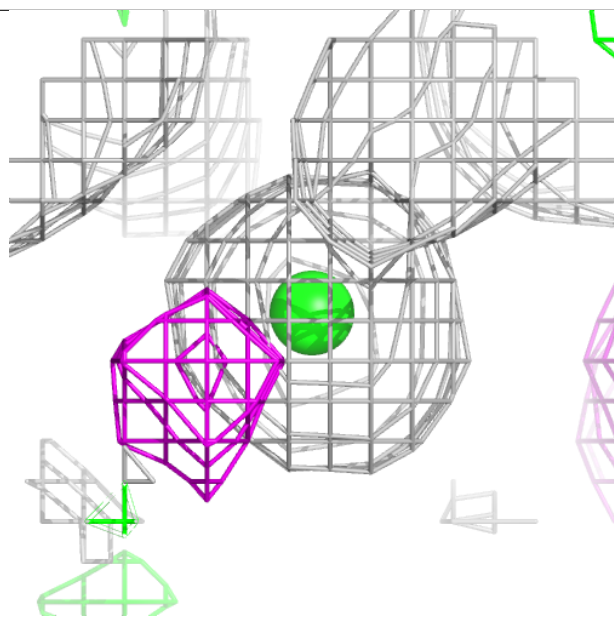
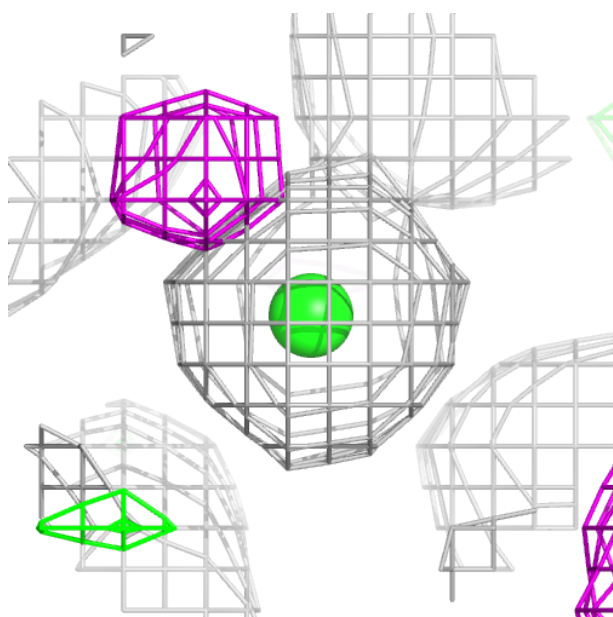
Electron density around FE J 202:

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



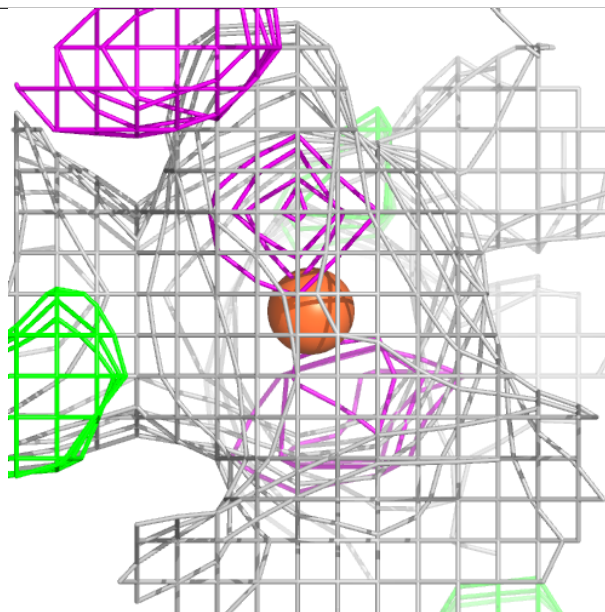
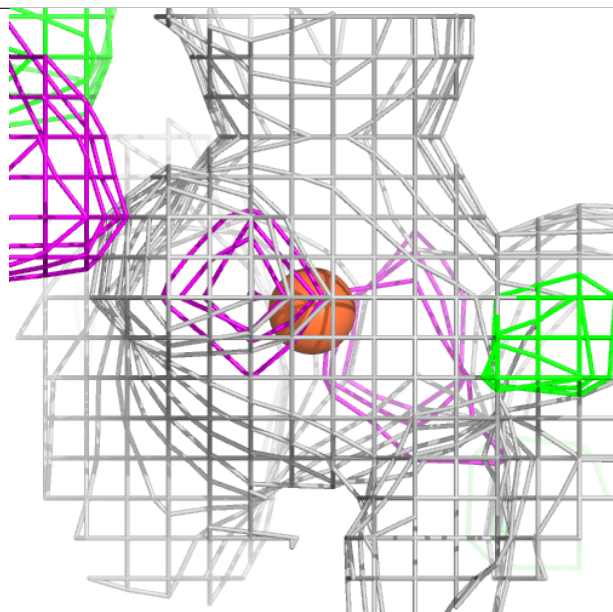
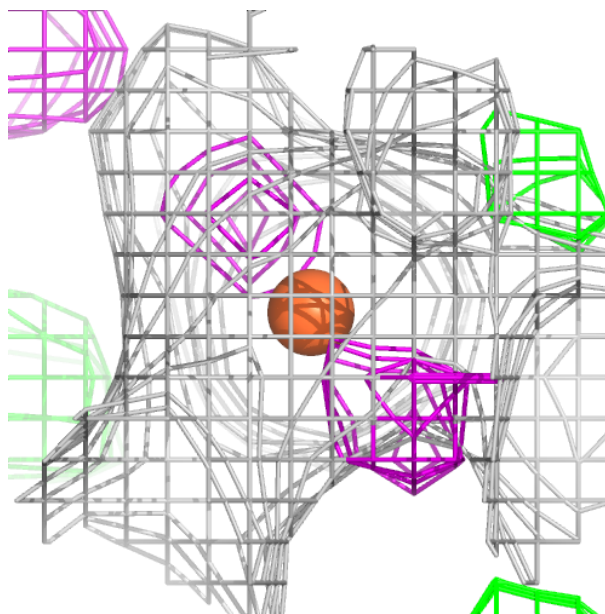
Electron density around CL A 202:

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



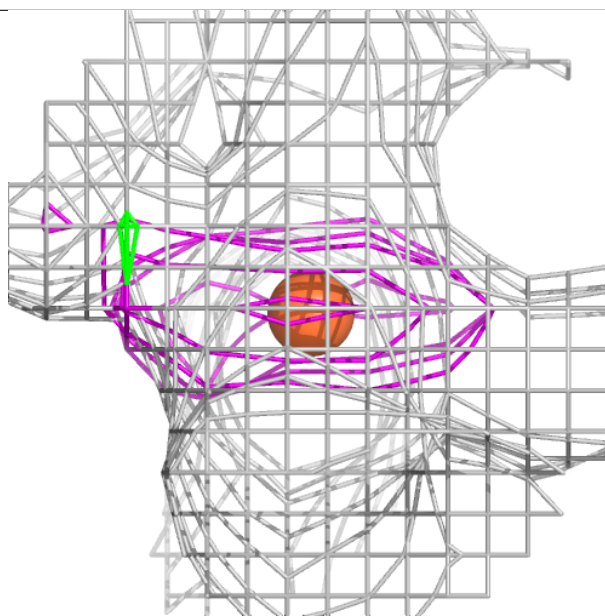
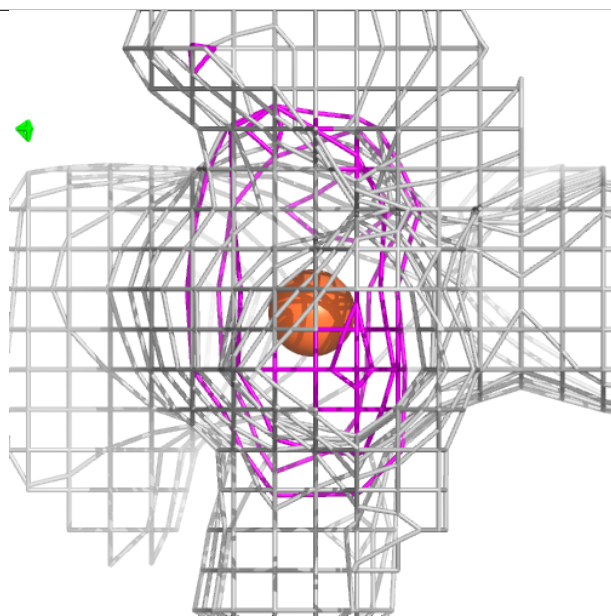
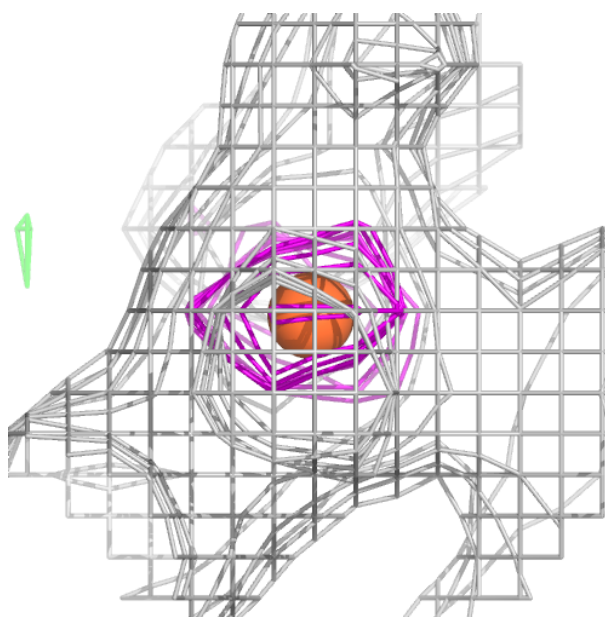
Electron density around FE L 203:

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



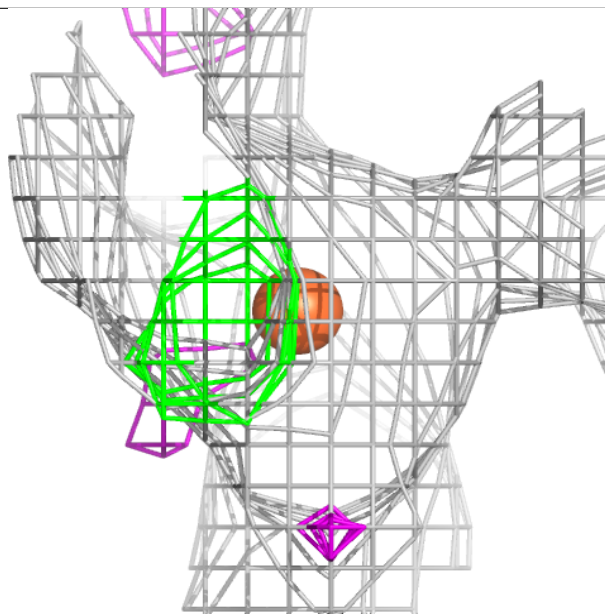
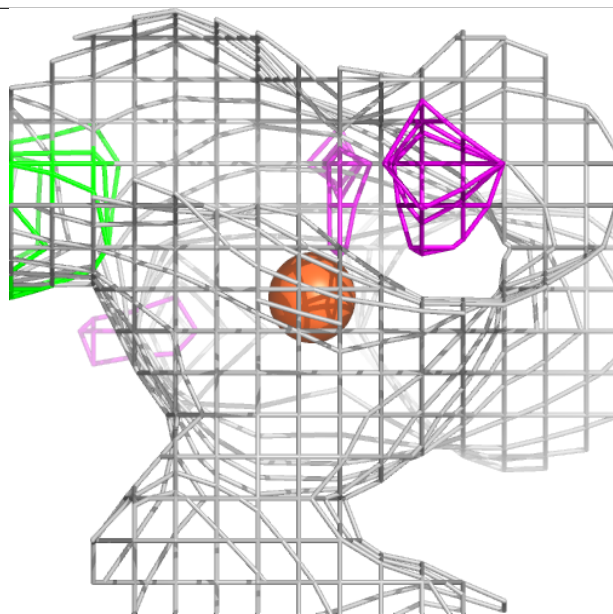
Electron density around FE F 201:

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



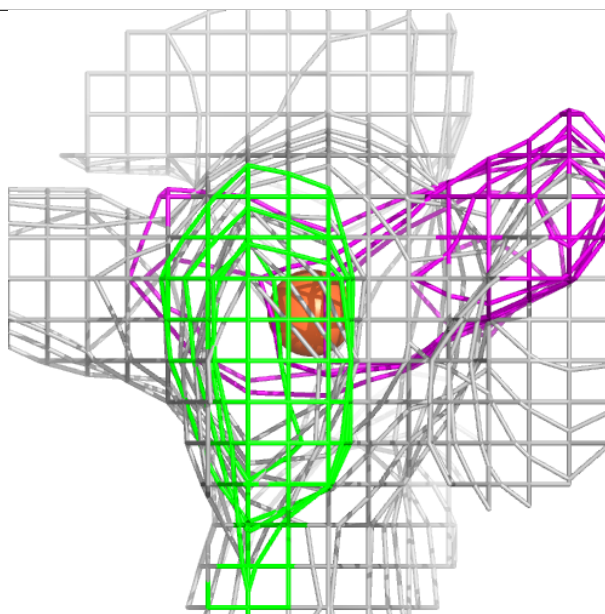
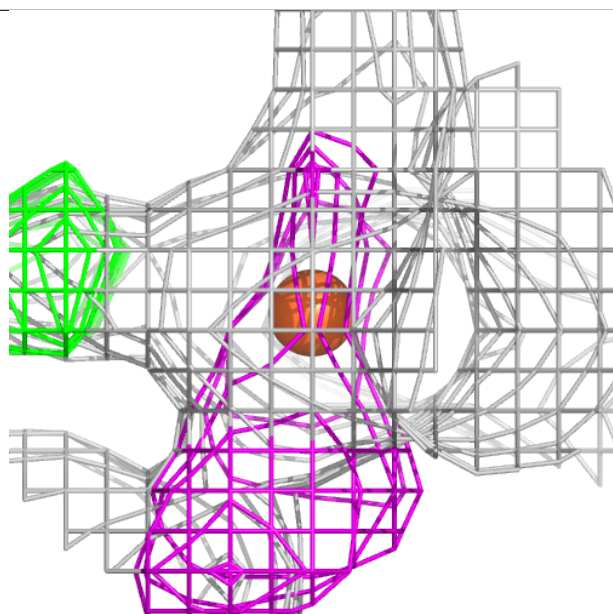
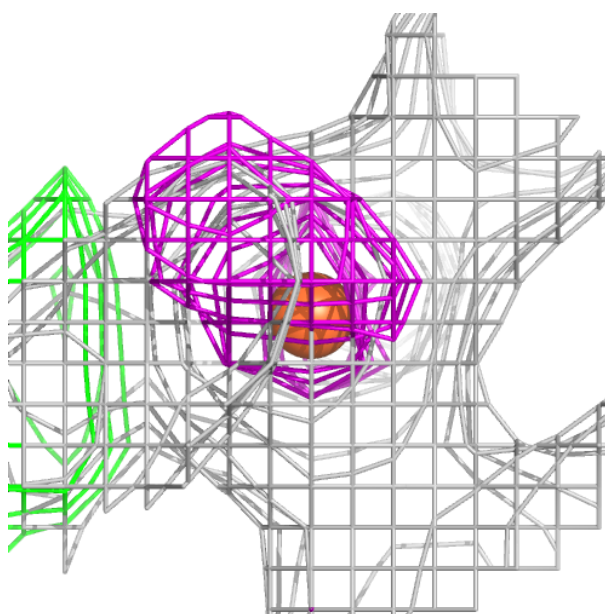
Electron density around FE C 202:

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



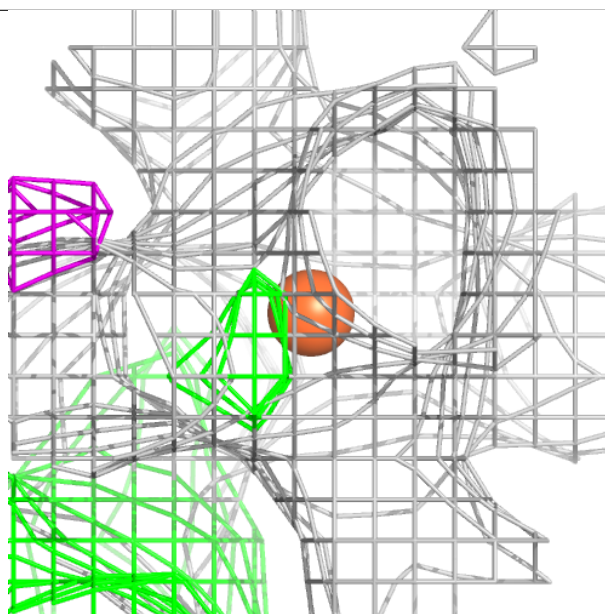
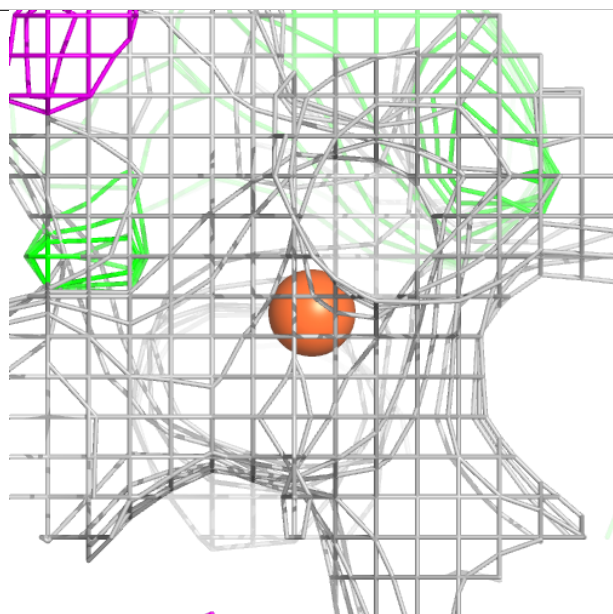
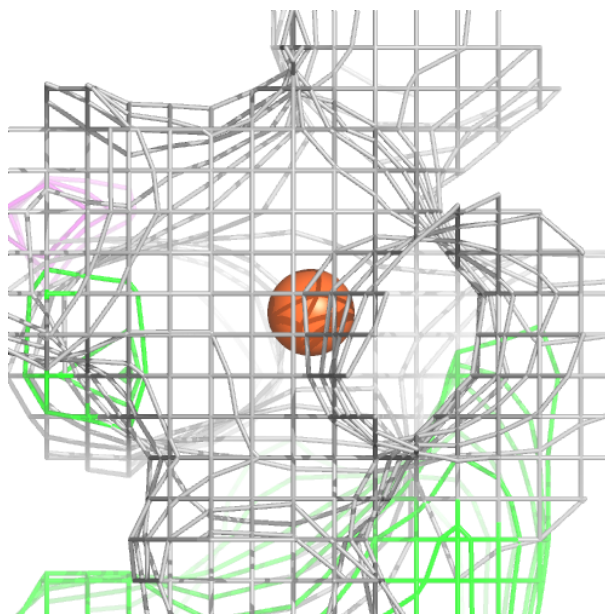
Electron density around FE H 202:

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



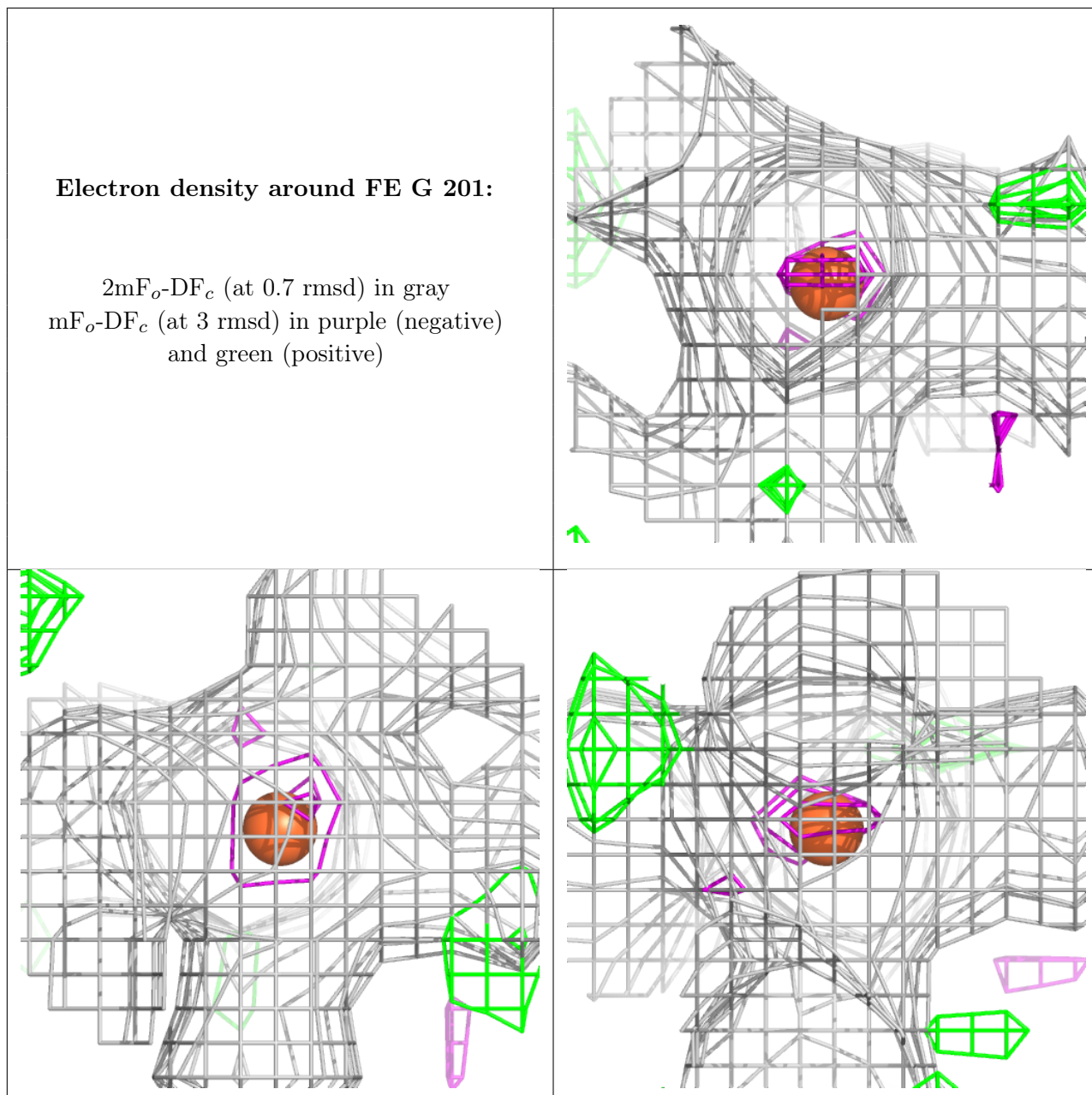
Electron density around FE B 201:

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



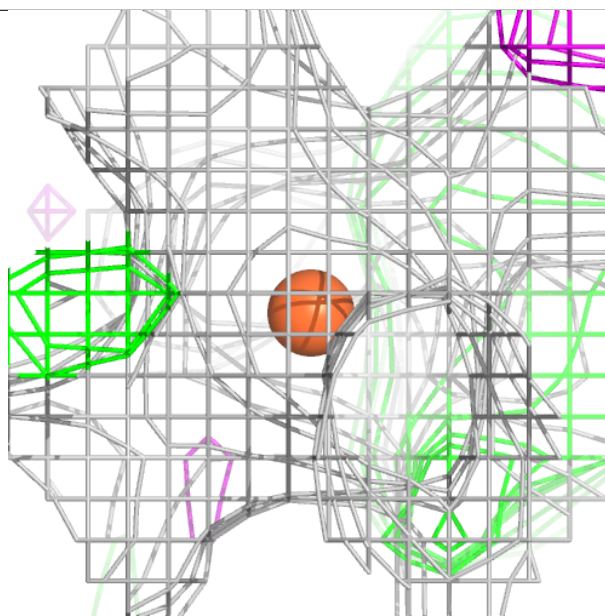
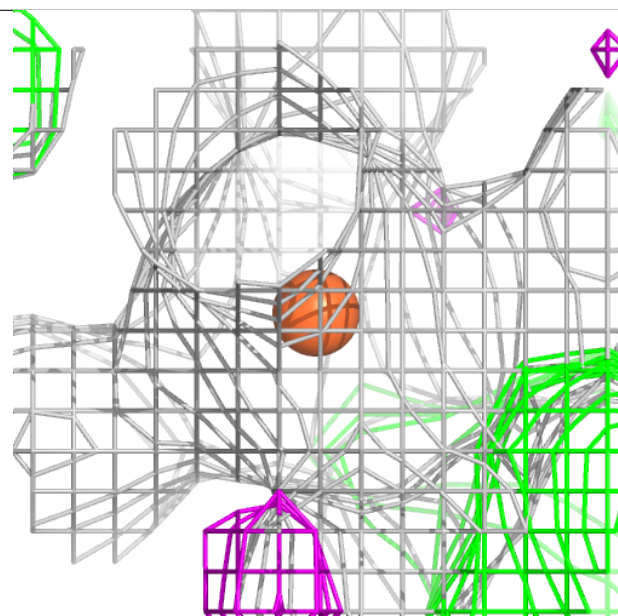
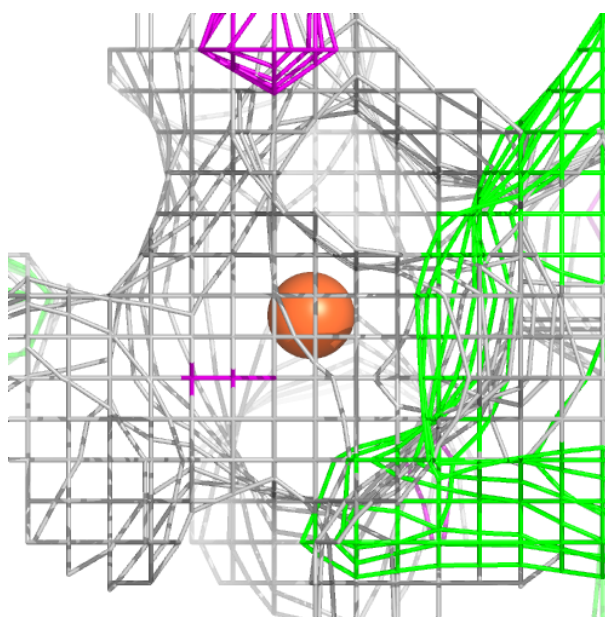
Electron density around FE G 201:

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



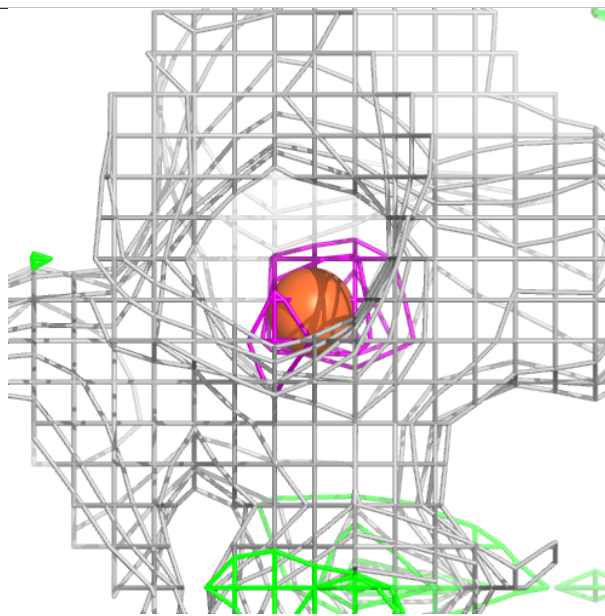
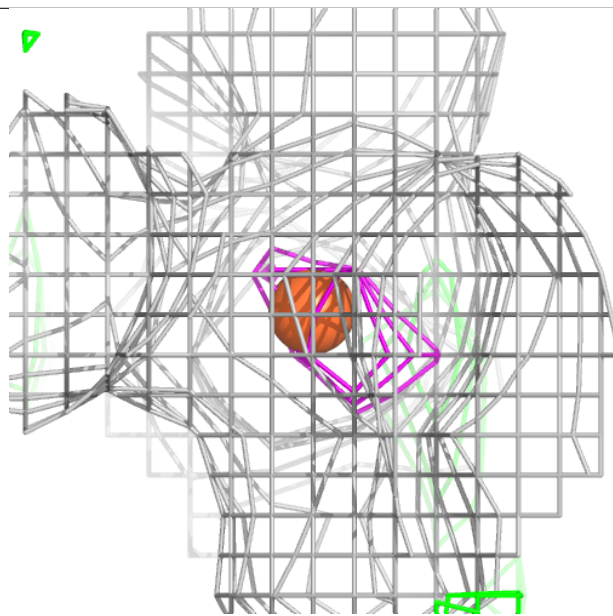
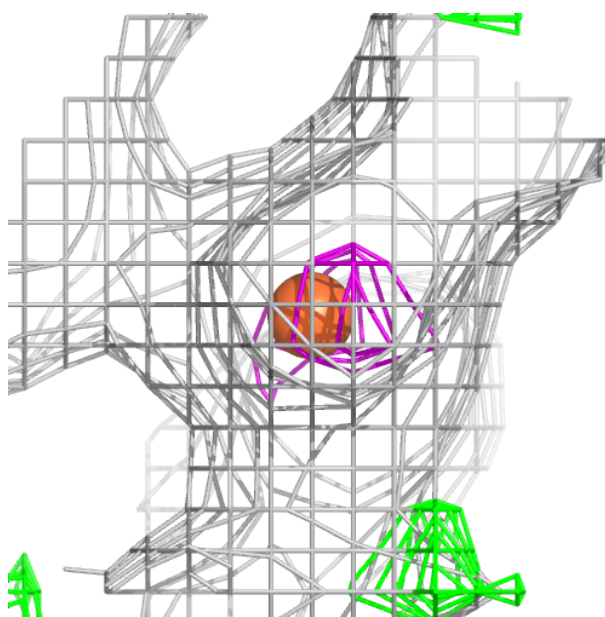
Electron density around FE K 201:

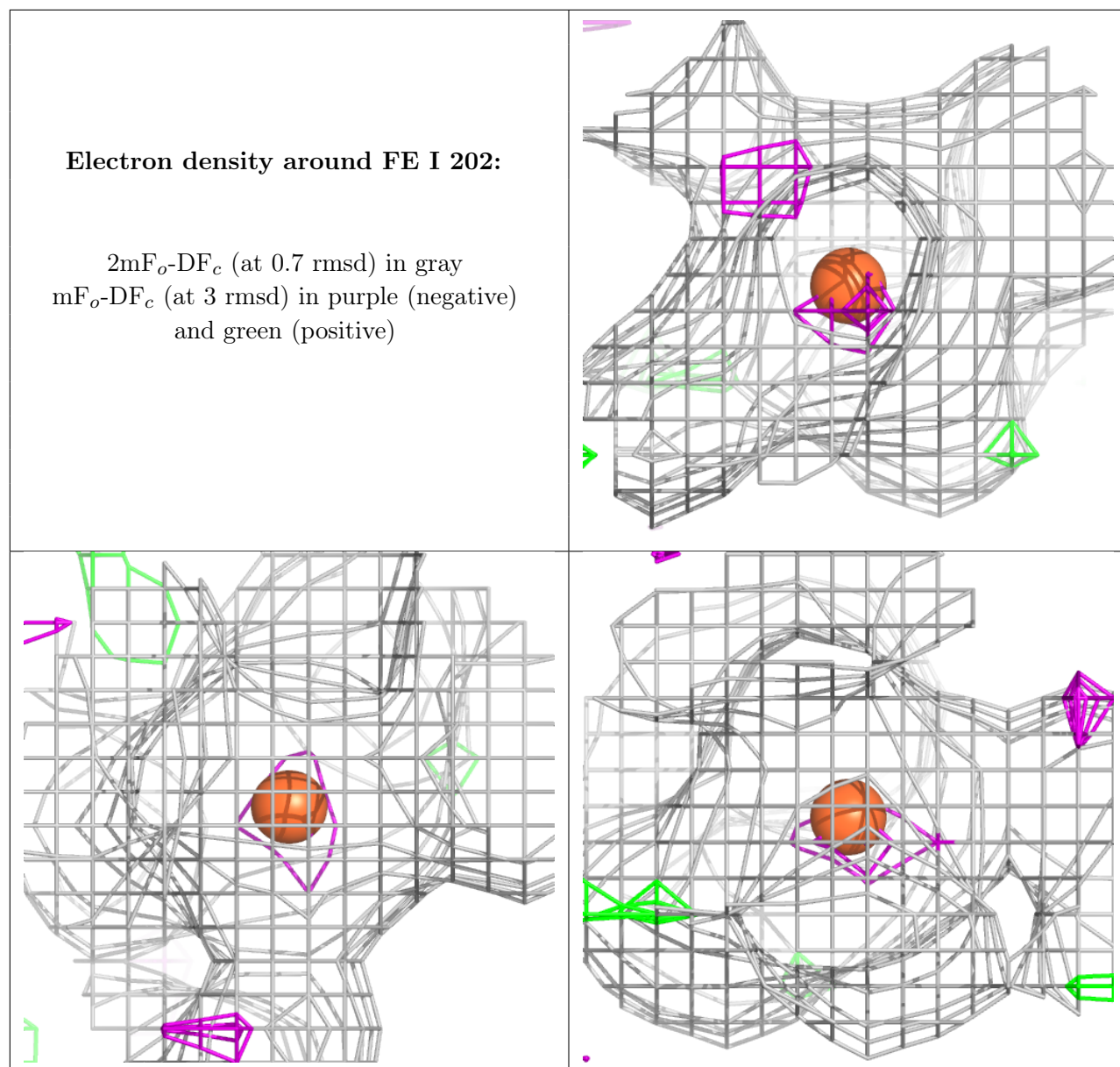
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.