wwPDB X-ray Structure Validation Summary Report (i)

Apr 5, 2026 – 02:49 AM UTC

PDB ID	:	9LUW / pdb_00009luw
Title	:	Enhancing Monodispersity and Thermal Stability of Human H-Ferritin for Improved Applications in Nanocarrier Systems
Authors	:	Gu, C.K.; Wang, S.J.
Deposited on	:	2025-02-10
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

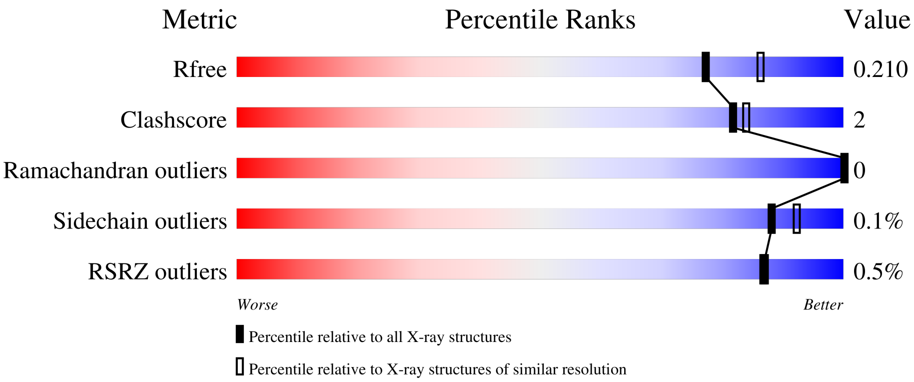
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 <=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	183	% 89% 5% 6%
1	B	183	% 85% 9% 6%
1	C	183	% 85% 9% 7%
1	D	183	% 89% 5% 6%
1	E	183	% 91% • 6%

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Mol	Chain	Length	Quality of chain
1	F	183	90% • 6%
1	G	183	% 91% • 6%
1	H	183	91% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11854 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	172	1406	882	250	270	4	0	0	0
1	B	172	1406	882	250	270	4	0	0	0
1	C	171	1398	878	249	267	4	0	0	0
1	D	172	1406	882	250	270	4	0	0	0
1	E	172	1406	882	250	270	4	0	0	0
1	F	172	1406	882	250	270	4	0	0	0
1	G	172	1406	882	250	270	4	0	0	0
1	H	172	1406	882	250	270	4	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
A	90	ALA	CYS	engineered mutation	UNP P02794
A	102	ALA	CYS	engineered mutation	UNP P02794
A	105	ALA	HIS	engineered mutation	UNP P02794
A	116	ALA	GLU	engineered mutation	UNP P02794
A	122	HIS	THR	engineered mutation	UNP P02794
A	130	ALA	CYS	engineered mutation	UNP P02794
A	165	HIS	LEU	engineered mutation	UNP P02794
B	86	GLN	LYS	conflict	UNP P02794
B	90	ALA	CYS	engineered mutation	UNP P02794
B	102	ALA	CYS	engineered mutation	UNP P02794
B	105	ALA	HIS	engineered mutation	UNP P02794
B	116	ALA	GLU	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	122	HIS	THR	engineered mutation	UNP P02794
B	130	ALA	CYS	engineered mutation	UNP P02794
B	165	HIS	LEU	engineered mutation	UNP P02794
C	86	GLN	LYS	conflict	UNP P02794
C	90	ALA	CYS	engineered mutation	UNP P02794
C	102	ALA	CYS	engineered mutation	UNP P02794
C	105	ALA	HIS	engineered mutation	UNP P02794
C	116	ALA	GLU	engineered mutation	UNP P02794
C	122	HIS	THR	engineered mutation	UNP P02794
C	130	ALA	CYS	engineered mutation	UNP P02794
C	165	HIS	LEU	engineered mutation	UNP P02794
D	86	GLN	LYS	conflict	UNP P02794
D	90	ALA	CYS	engineered mutation	UNP P02794
D	102	ALA	CYS	engineered mutation	UNP P02794
D	105	ALA	HIS	engineered mutation	UNP P02794
D	116	ALA	GLU	engineered mutation	UNP P02794
D	122	HIS	THR	engineered mutation	UNP P02794
D	130	ALA	CYS	engineered mutation	UNP P02794
D	165	HIS	LEU	engineered mutation	UNP P02794
E	86	GLN	LYS	conflict	UNP P02794
E	90	ALA	CYS	engineered mutation	UNP P02794
E	102	ALA	CYS	engineered mutation	UNP P02794
E	105	ALA	HIS	engineered mutation	UNP P02794
E	116	ALA	GLU	engineered mutation	UNP P02794
E	122	HIS	THR	engineered mutation	UNP P02794
E	130	ALA	CYS	engineered mutation	UNP P02794
E	165	HIS	LEU	engineered mutation	UNP P02794
F	86	GLN	LYS	conflict	UNP P02794
F	90	ALA	CYS	engineered mutation	UNP P02794
F	102	ALA	CYS	engineered mutation	UNP P02794
F	105	ALA	HIS	engineered mutation	UNP P02794
F	116	ALA	GLU	engineered mutation	UNP P02794
F	122	HIS	THR	engineered mutation	UNP P02794
F	130	ALA	CYS	engineered mutation	UNP P02794
F	165	HIS	LEU	engineered mutation	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
G	90	ALA	CYS	engineered mutation	UNP P02794
G	102	ALA	CYS	engineered mutation	UNP P02794
G	105	ALA	HIS	engineered mutation	UNP P02794
G	116	ALA	GLU	engineered mutation	UNP P02794
G	122	HIS	THR	engineered mutation	UNP P02794
G	130	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
G	165	HIS	LEU	engineered mutation	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
H	90	ALA	CYS	engineered mutation	UNP P02794
H	102	ALA	CYS	engineered mutation	UNP P02794
H	105	ALA	HIS	engineered mutation	UNP P02794
H	116	ALA	GLU	engineered mutation	UNP P02794
H	122	HIS	THR	engineered mutation	UNP P02794
H	130	ALA	CYS	engineered mutation	UNP P02794
H	165	HIS	LEU	engineered mutation	UNP P02794

- 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	3	Total Fe 3 3	0	0
2	B	3	Total Fe 3 3	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	2	Total Fe 2 2	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	2	Total Fe 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	79	Total O 79 79	0	0
3	C	76	Total O 76 76	0	0
3	D	76	Total O 76 76	0	0

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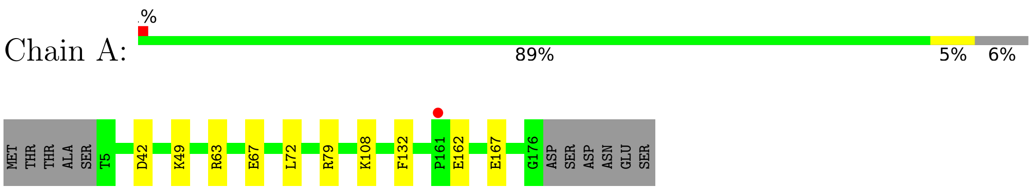
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	74	Total O 74 74	0	0
3	F	68	Total O 68 68	0	0
3	G	71	Total O 71 71	0	0
3	H	81	Total O 81 81	0	0

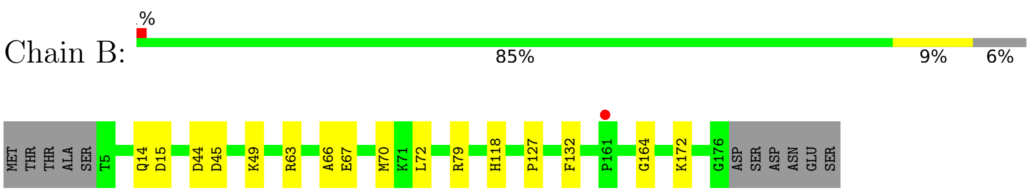
3 Residue-property plots (i)

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.

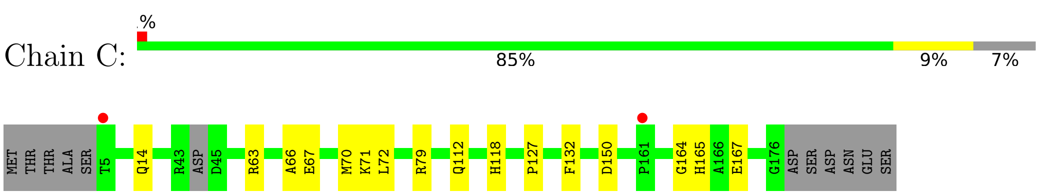
- Molecule 1: Ferritin heavy chain



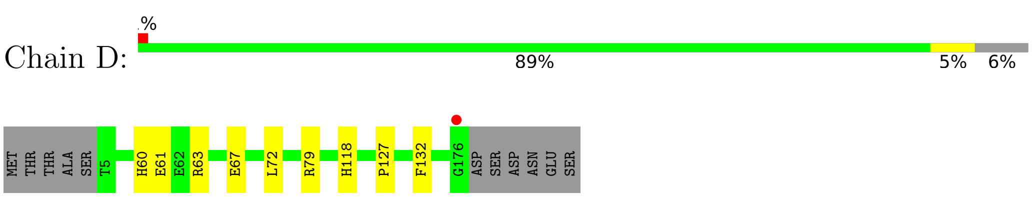
- Molecule 1: Ferritin heavy chain



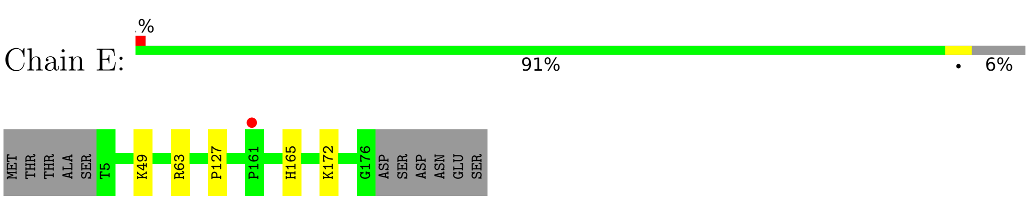
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

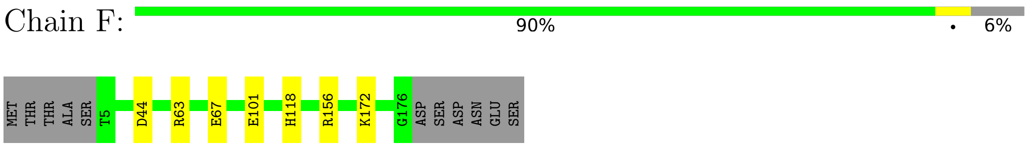


- Molecule 1: Ferritin heavy chain



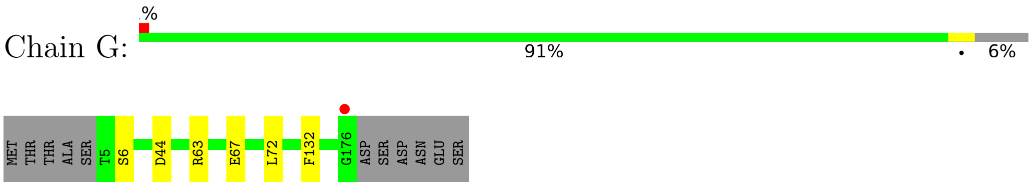
- Molecule 1: Ferritin heavy chain

Chain F:



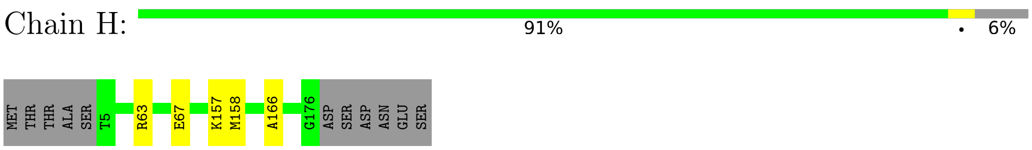
• Molecule 1: Ferritin heavy chain

Chain G:



• Molecule 1: Ferritin heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	180.59Å 180.59Å 180.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.00 29.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.69-2.00) 99.9 (29.69-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.179 , 0.209 0.179 , 0.210	Depositor DCC
R_{free} test set	1998 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 39.3	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.50, $< L^2 >$ = 0.34	Xtriage
Estimated twinning fraction	0.117 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11854	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 40.28 % 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 2.8008e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/1436	0.51	0/1936
1	B	0.28	0/1436	0.51	0/1936
1	C	0.28	0/1427	0.47	0/1922
1	D	0.29	0/1436	0.56	3/1936 (0.2%)
1	E	0.29	0/1436	0.48	0/1936
1	F	0.28	0/1436	0.52	0/1936
1	G	0.29	0/1436	0.46	0/1936
1	H	0.29	0/1436	0.46	0/1936
All	All	0.29	0/11479	0.50	3/15474 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	GLU	CA-CB-CG	7.39	128.88	114.10
1	D	60	HIS	CA-C-N	5.69	127.84	120.44
1	D	60	HIS	C-N-CA	5.69	127.84	120.44

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	1406	0	1345	9	0
1	B	1406	0	1345	14	0
1	C	1398	0	1340	13	0
1	D	1406	0	1345	8	0
1	E	1406	0	1345	7	0
1	F	1406	0	1345	5	0
1	G	1406	0	1345	4	0
1	H	1406	0	1345	3	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
3	A	75	0	0	4	0
3	B	79	0	0	3	0
3	C	76	0	0	4	0
3	D	76	0	0	0	0
3	E	74	0	0	2	0
3	F	68	0	0	1	0
3	G	71	0	0	0	0
3	H	81	0	0	1	0
All	All	11854	0	10755	54	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 2.

The worst 5 of 54 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:A:72:LEU:HD12	1:A:132:PHE:CE2	2.18	0.77
1:H:157:LYS:NZ	3:H:301:HOH:O	2.12	0.71
1:D:72:LEU:HD12	1:D:132:PHE:CD2	2.26	0.70
1:D:72:LEU:HD12	1:D:132:PHE:CE2	2.28	0.68
1:B:49:LYS:HD3	3:B:312:HOH:O	1.94	0.68

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	B	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	C	167/183 (91%)	164 (98%)	3 (2%)	0	100	100
1	D	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	E	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	F	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	G	170/183 (93%)	167 (98%)	3 (2%)	0	100	100
1	H	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
All	All	1357/1464 (93%)	1334 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/158 (94%)	148 (100%)	0	100	100
1	B	148/158 (94%)	148 (100%)	0	100	100
1	C	147/158 (93%)	147 (100%)	0	100	100
1	D	148/158 (94%)	148 (100%)	0	100	100
1	E	148/158 (94%)	148 (100%)	0	100	100
1	F	148/158 (94%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	148/158 (94%)	147 (99%)	1 (1%)	76	82
1	H	148/158 (94%)	148 (100%)	0	100	100
All	All	1183/1264 (94%)	1182 (100%)	1 (0%)	88	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	111	ASN
1	H	111	ASN
1	H	154	ASN
1	H	139	ASN
1	D	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	172/183 (93%)	-0.51	1 (0%)	85	85	8, 11, 22, 36	0
1	B	172/183 (93%)	-0.49	1 (0%)	85	85	7, 12, 23, 37	0
1	C	171/183 (93%)	-0.52	2 (1%)	76	76	7, 11, 22, 42	0
1	D	172/183 (93%)	-0.52	1 (0%)	85	85	7, 11, 22, 35	0
1	E	172/183 (93%)	-0.51	1 (0%)	85	85	8, 11, 22, 34	0
1	F	172/183 (93%)	-0.54	0	100	100	7, 11, 24, 37	0
1	G	172/183 (93%)	-0.56	1 (0%)	85	85	8, 11, 23, 34	0
1	H	172/183 (93%)	-0.55	0	100	100	7, 11, 23, 34	0
All	All	1375/1464 (93%)	-0.53	7 (0%)	87	87	7, 11, 23, 42	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	PRO	3.6
1	B	161	PRO	2.5
1	C	5	THR	2.4
1	D	176	GLY	2.2
1	G	176	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

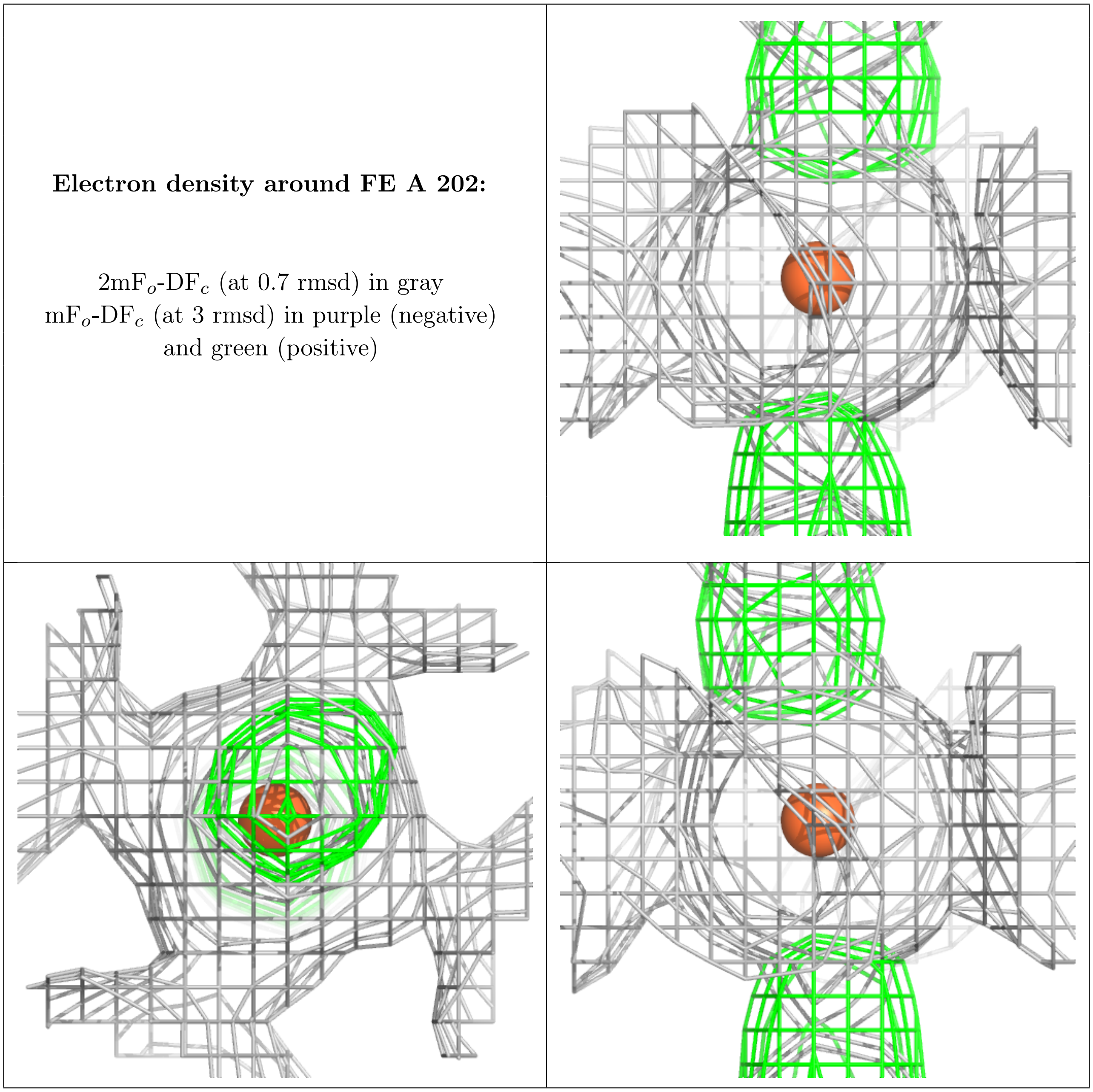
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	A	202	1/1	0.98	0.03	13,13,13,13	0
2	FE	A	203	1/1	0.98	0.02	14,14,14,14	1
2	FE	B	203	1/1	0.98	0.02	12,12,12,12	0
2	FE	B	201	1/1	0.99	0.01	12,12,12,12	0
2	FE	B	202	1/1	0.99	0.02	13,13,13,13	0
2	FE	A	201	1/1	0.99	0.02	11,11,11,11	0
2	FE	C	201	1/1	0.99	0.02	12,12,12,12	0
2	FE	D	201	1/1	0.99	0.02	11,11,11,11	0
2	FE	E	201	1/1	0.99	0.02	12,12,12,12	0
2	FE	E	202	1/1	0.99	0.02	14,14,14,14	0
2	FE	F	201	1/1	0.99	0.01	11,11,11,11	0
2	FE	H	201	1/1	0.99	0.02	12,12,12,12	0
2	FE	G	201	1/1	1.00	0.02	12,12,12,12	0
2	FE	H	202	1/1	1.00	0.04	13,13,13,13	1

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.

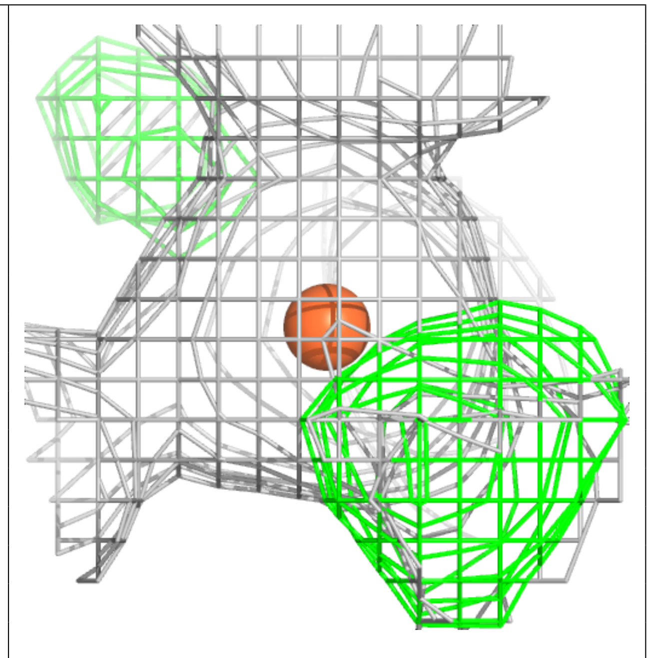
Electron density around FE A 202:

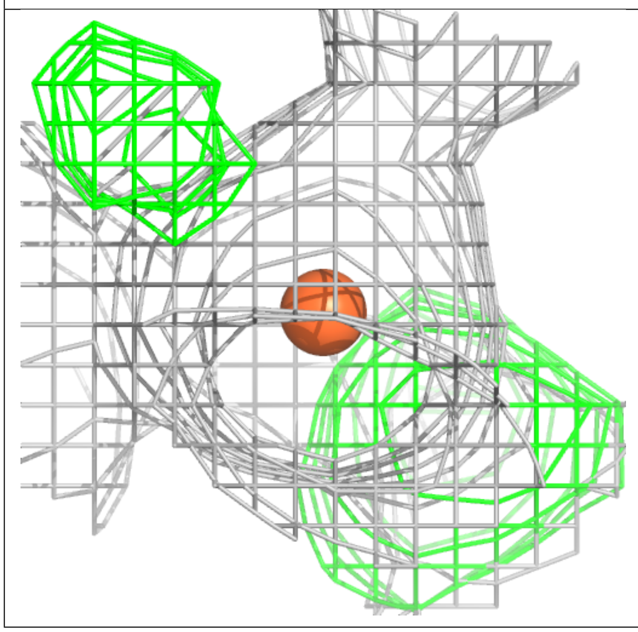
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

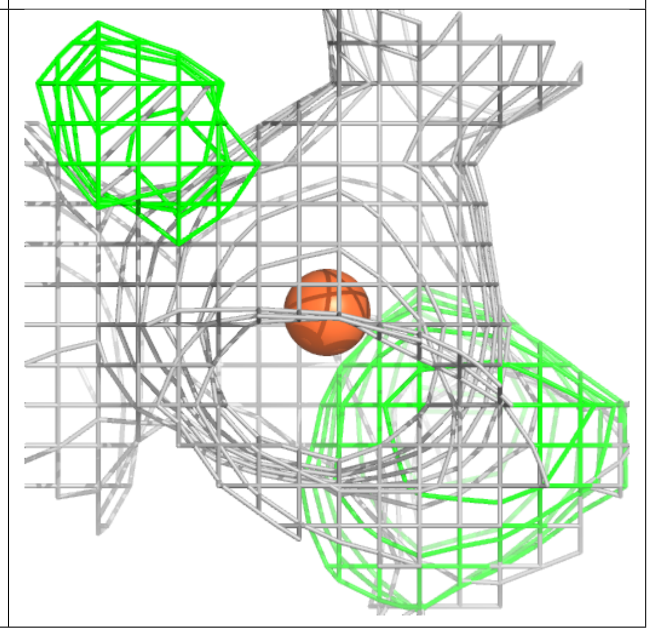


Electron density around FE A 203:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

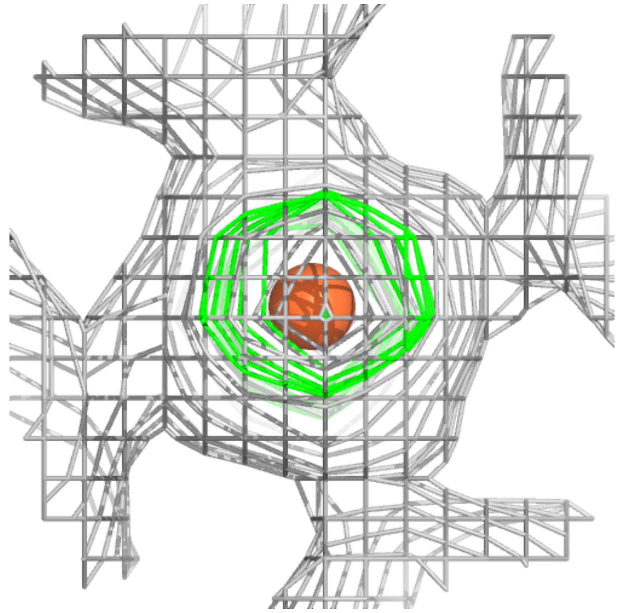


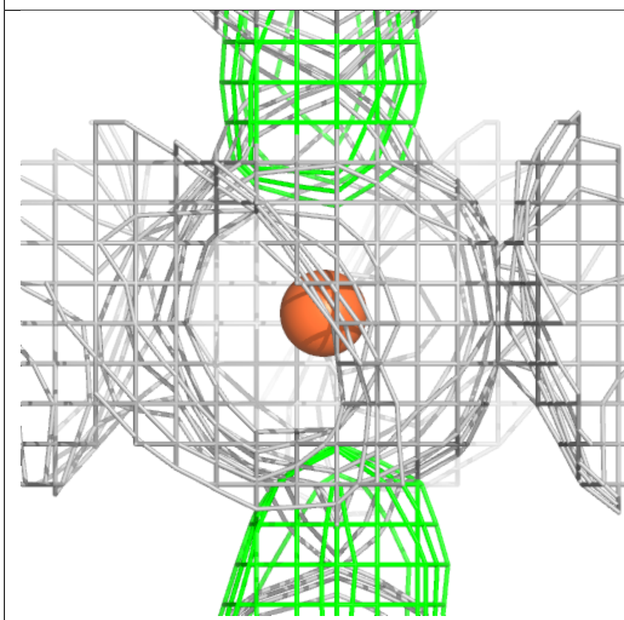


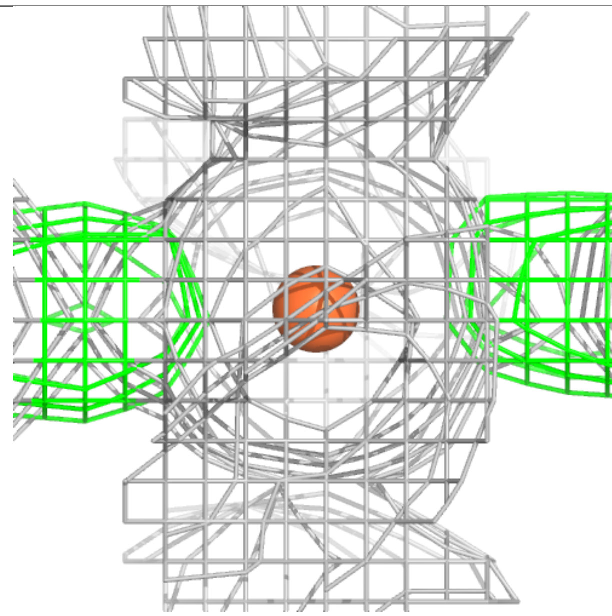


Electron density around FE B 203:

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

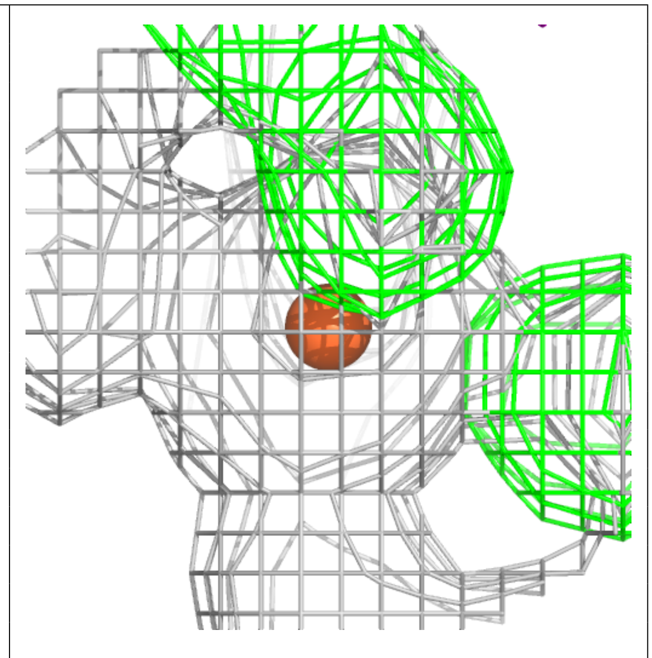


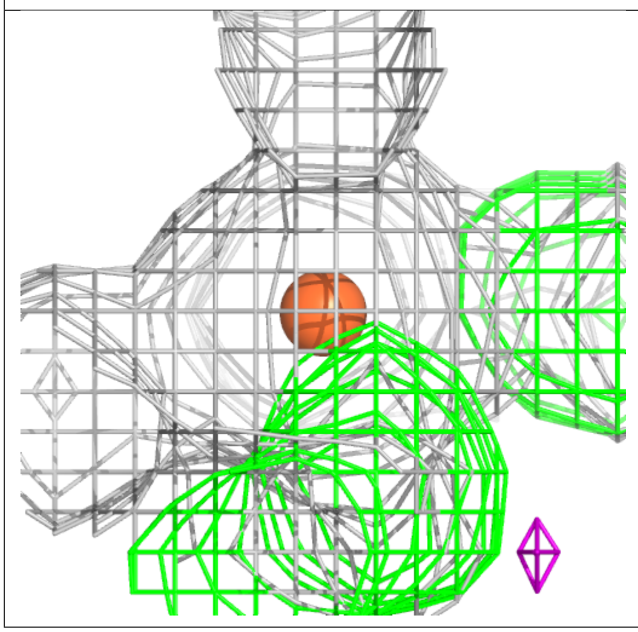


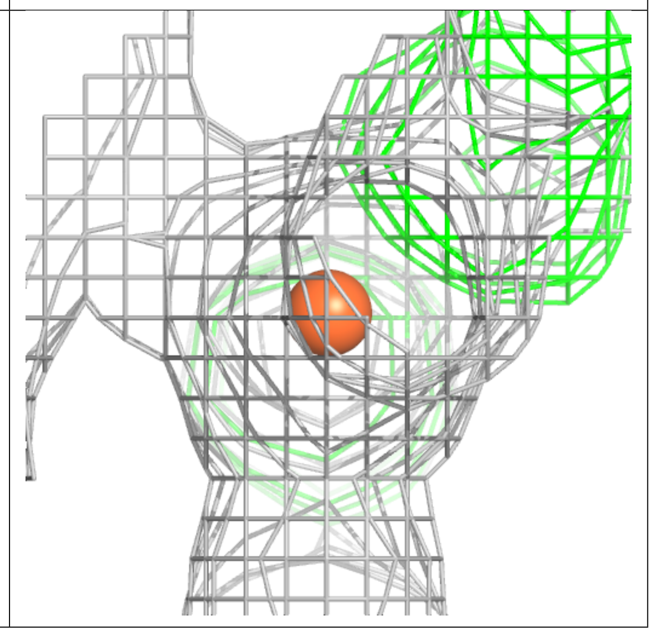


Electron density around FE B 201:

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

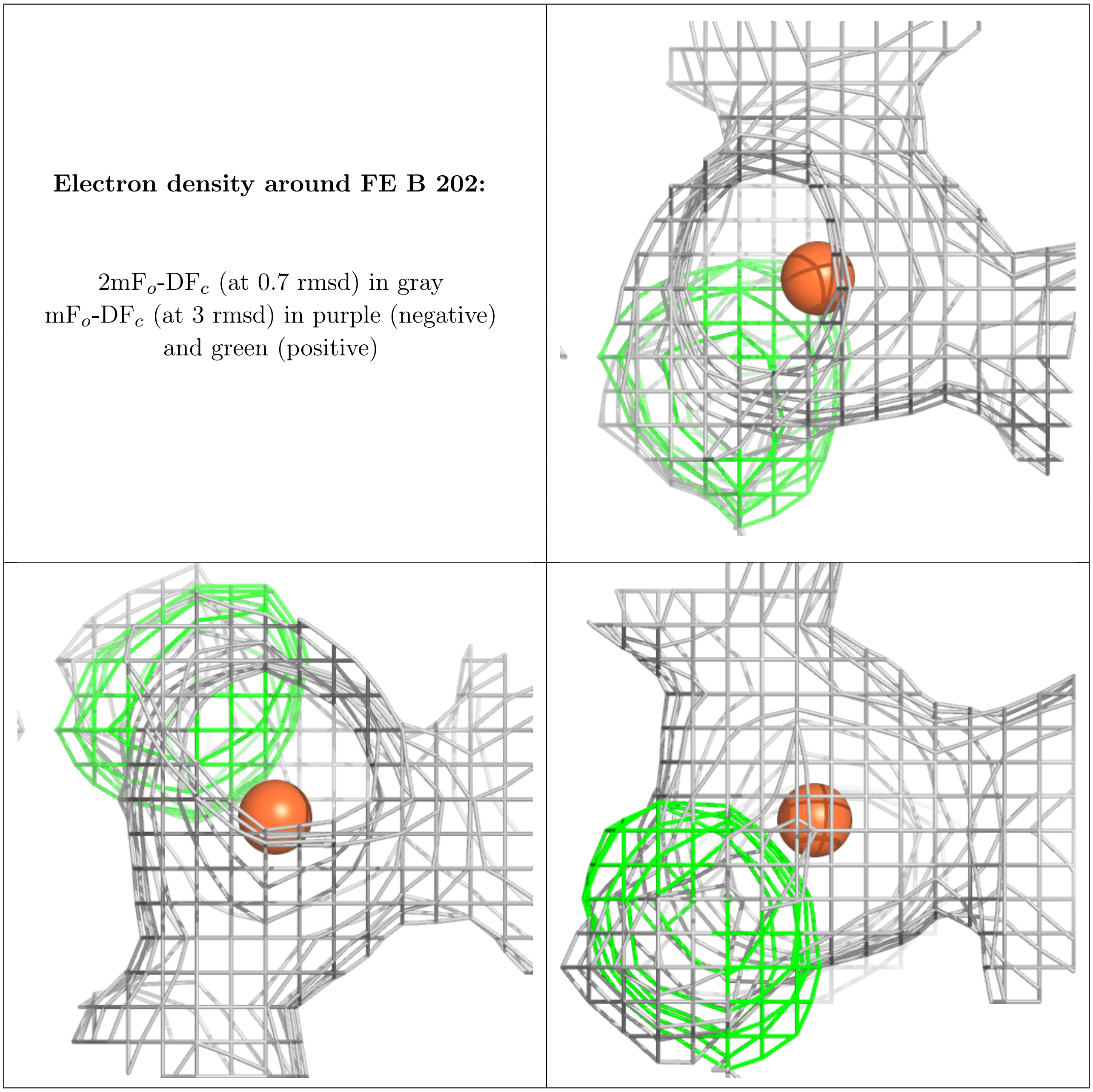






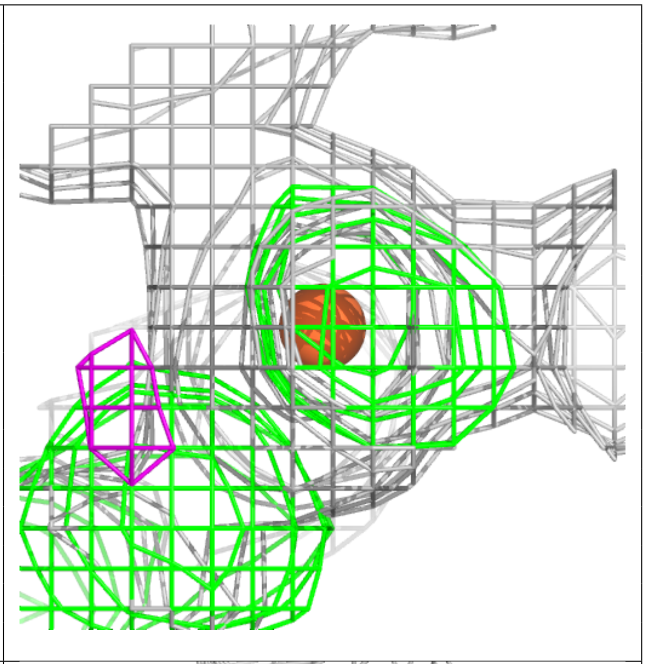
Electron density around FE B 202:

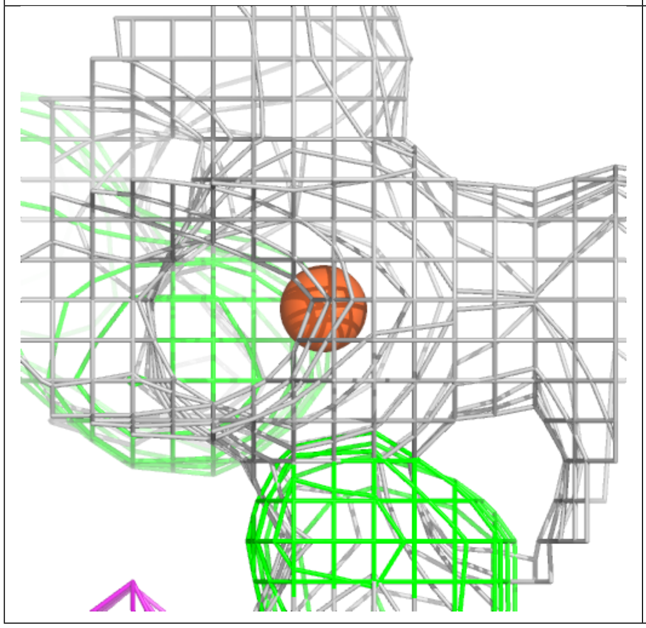
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

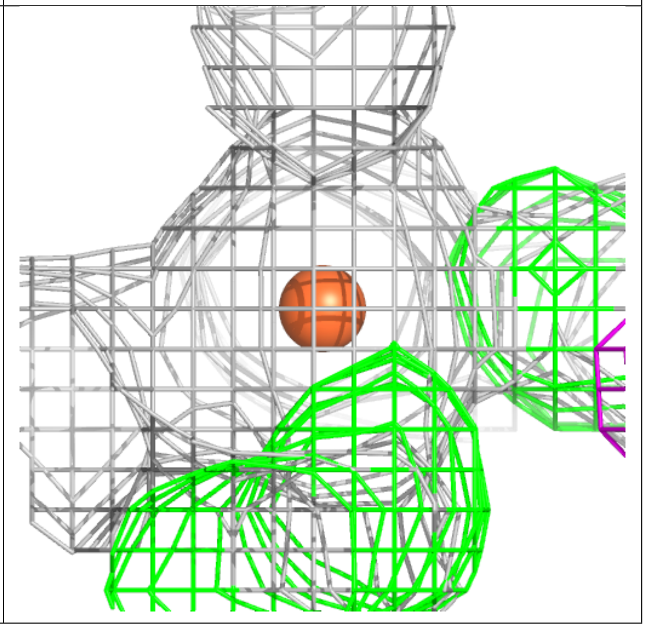


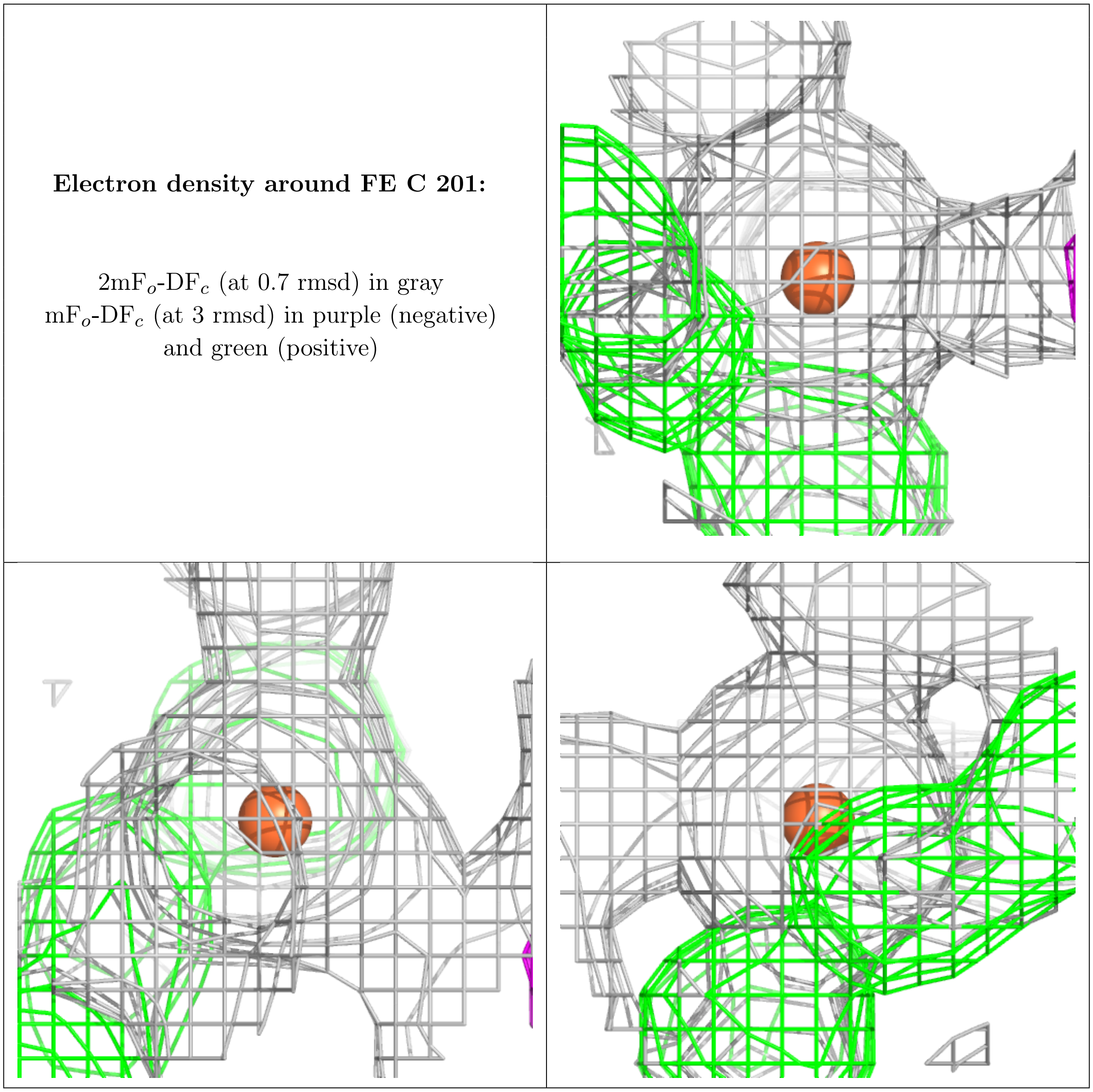
Electron density around FE A 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







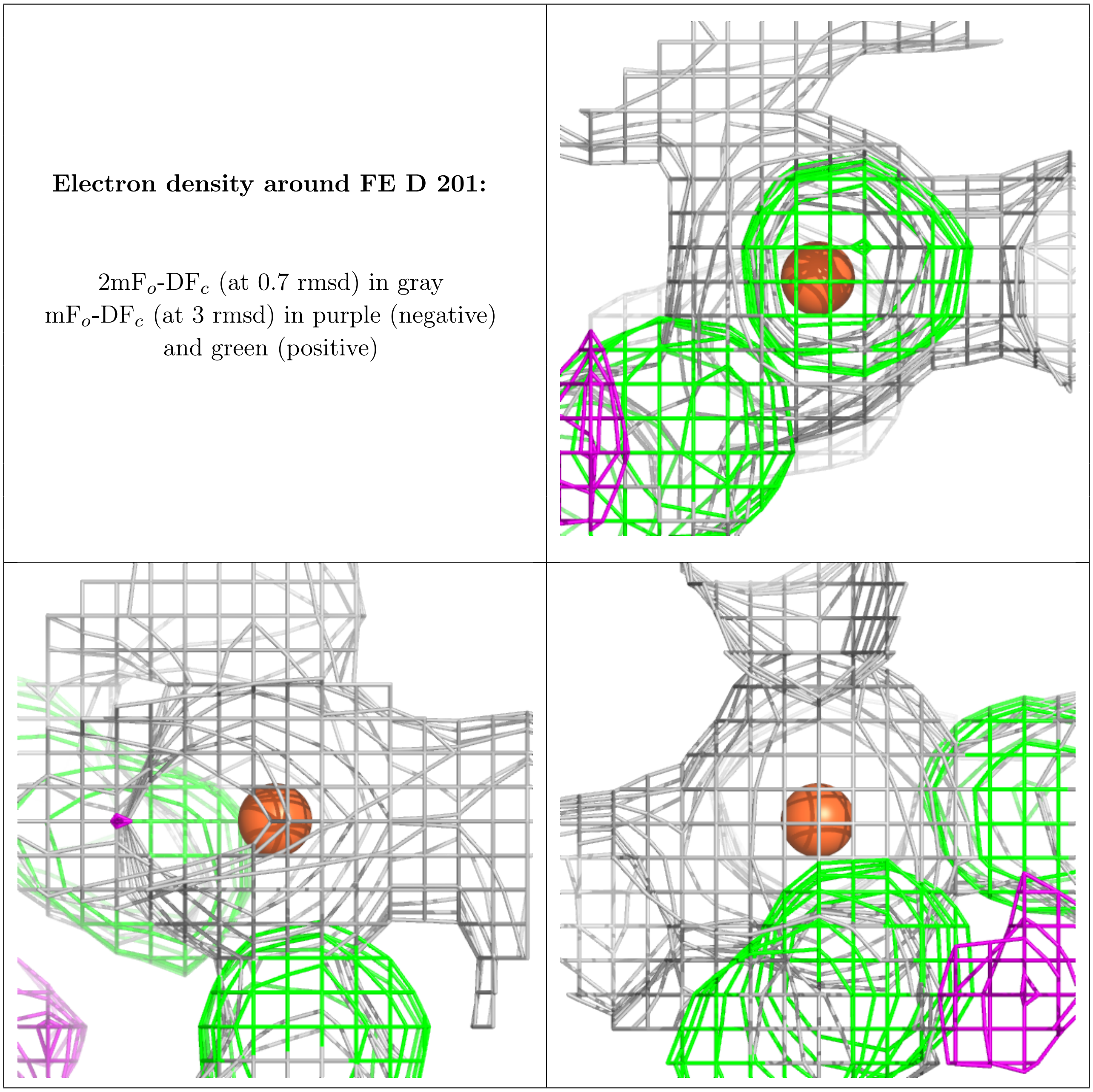


Electron density around FE C 201:

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

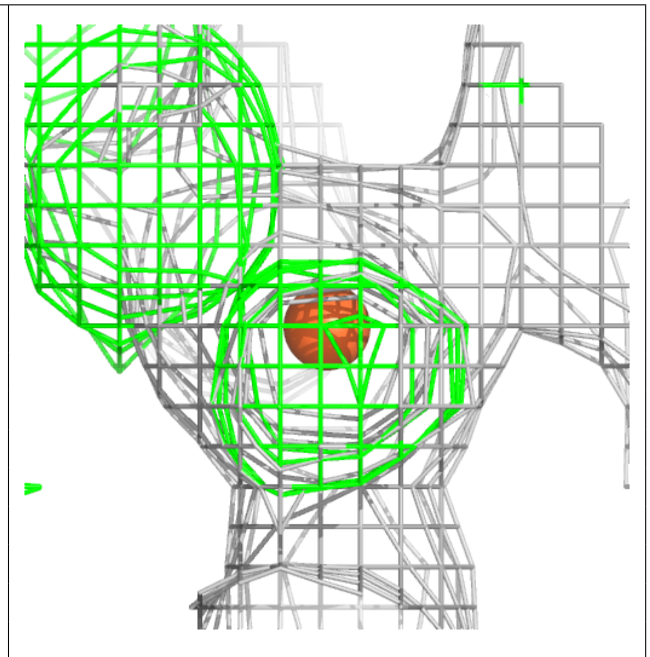
Electron density around FE D 201:

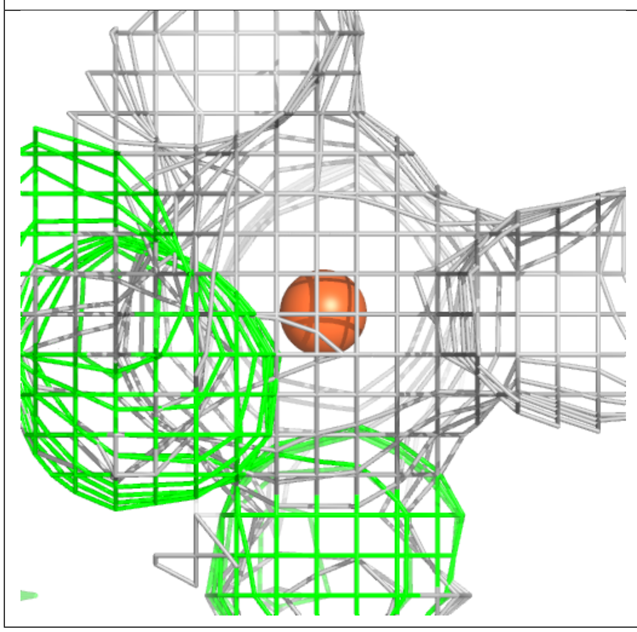
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

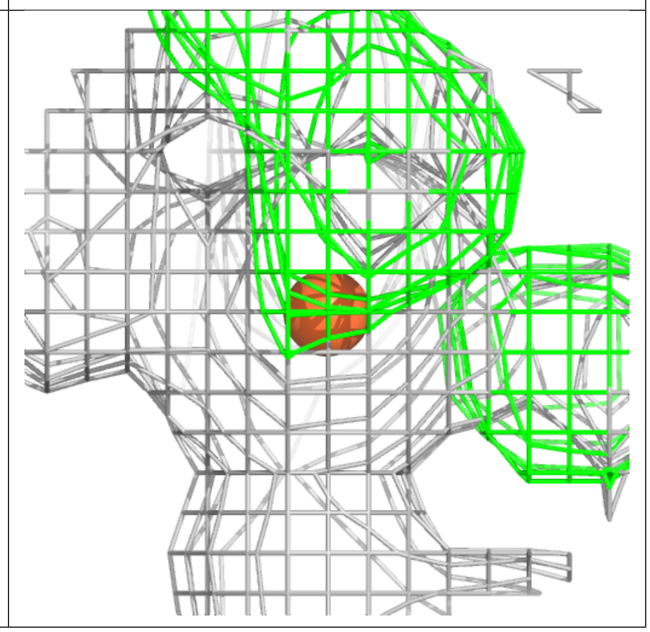


Electron density around FE E 201:

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

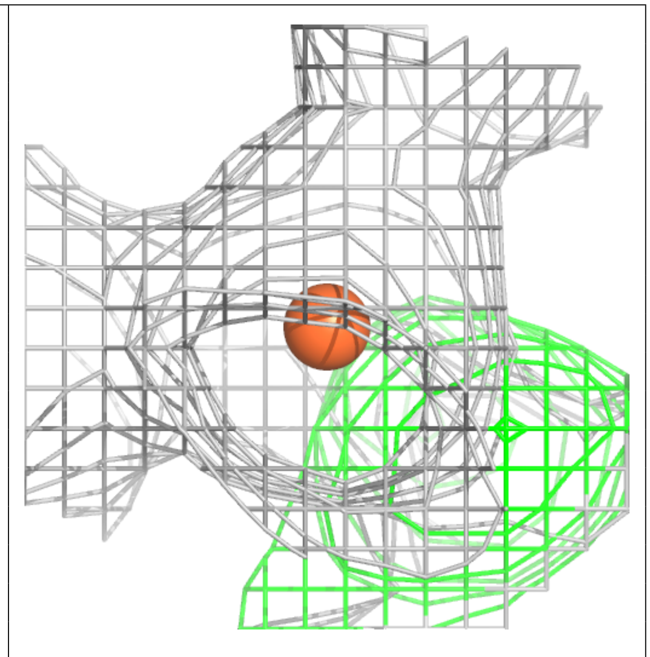


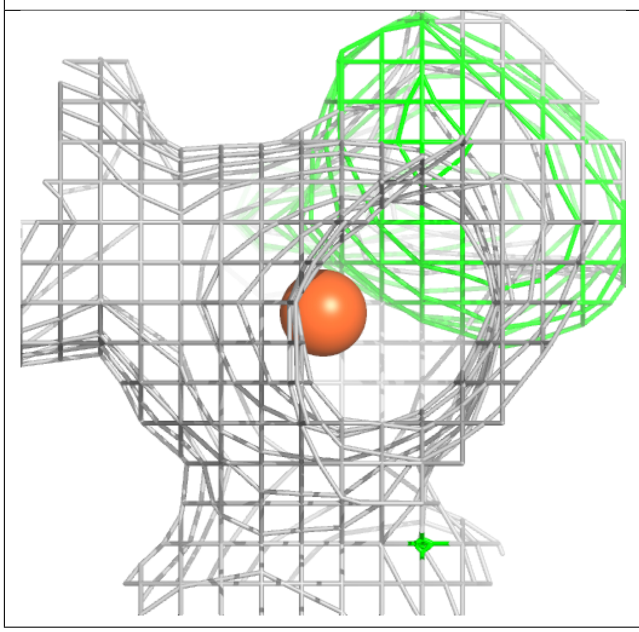


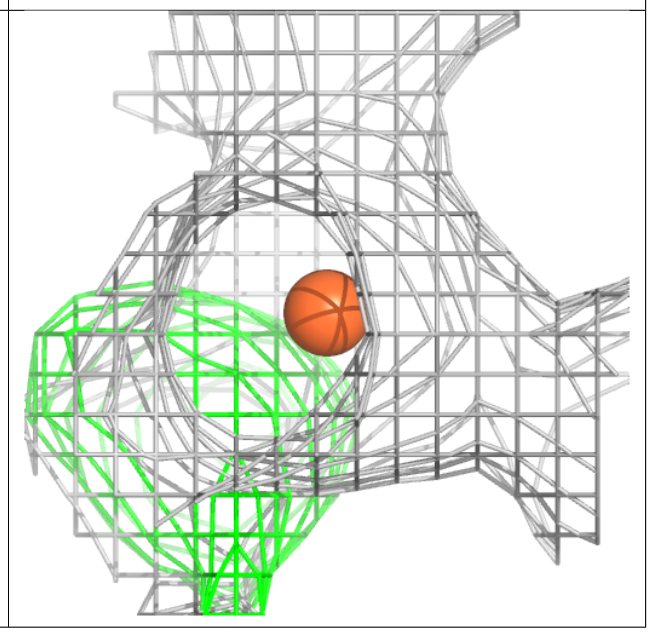


Electron density around FE E 202:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

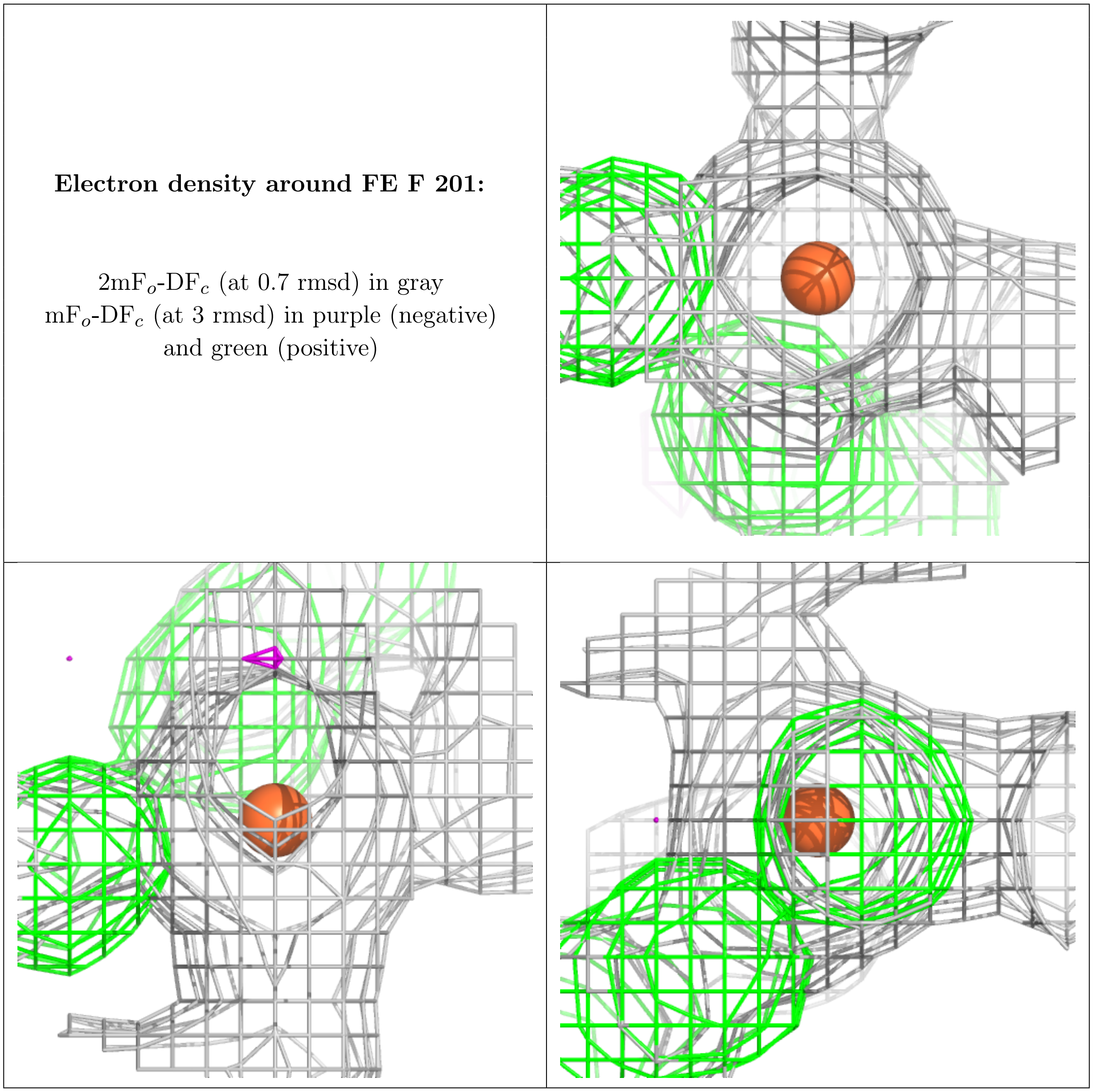






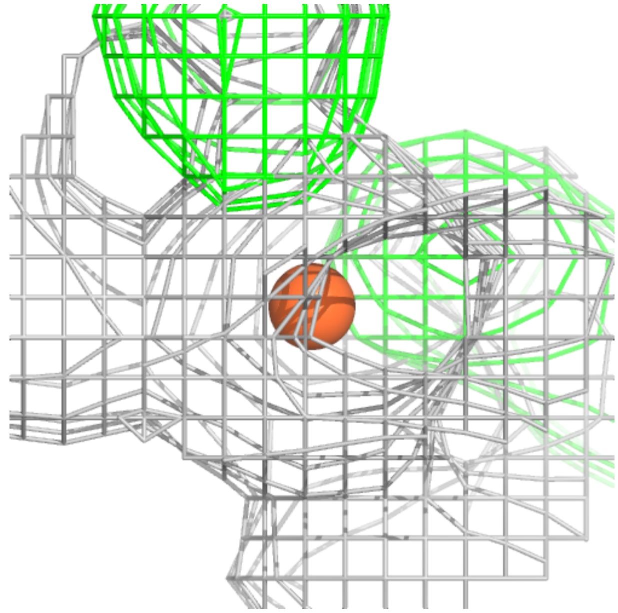
Electron density around FE F 201:

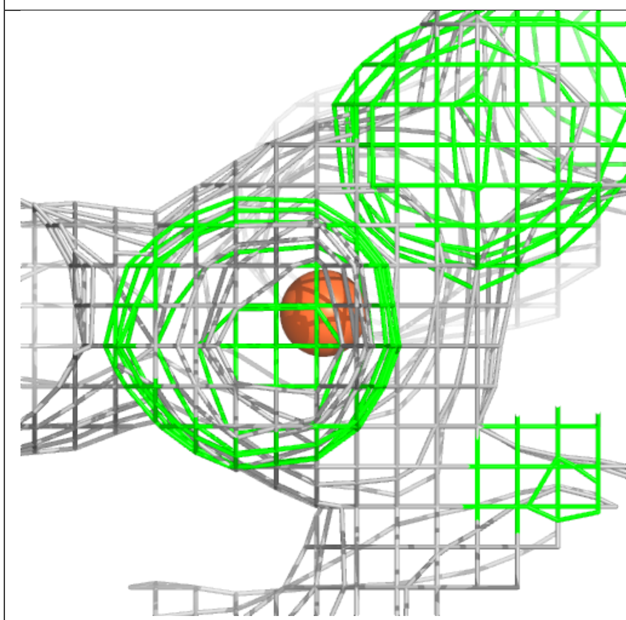
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

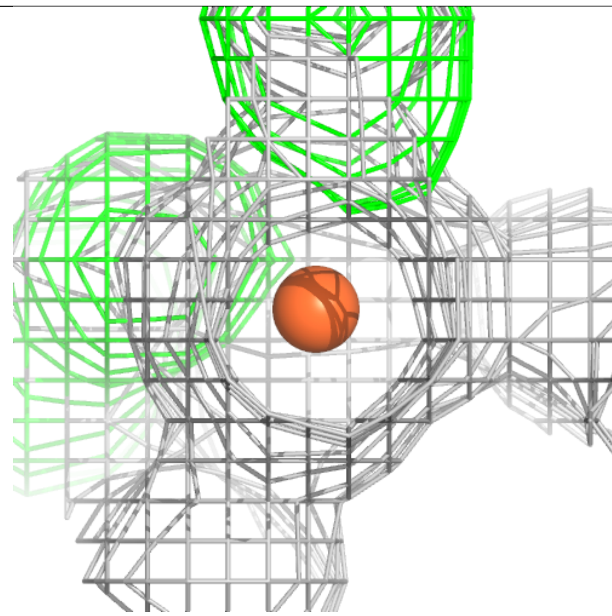


Electron density around FE H 201:

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

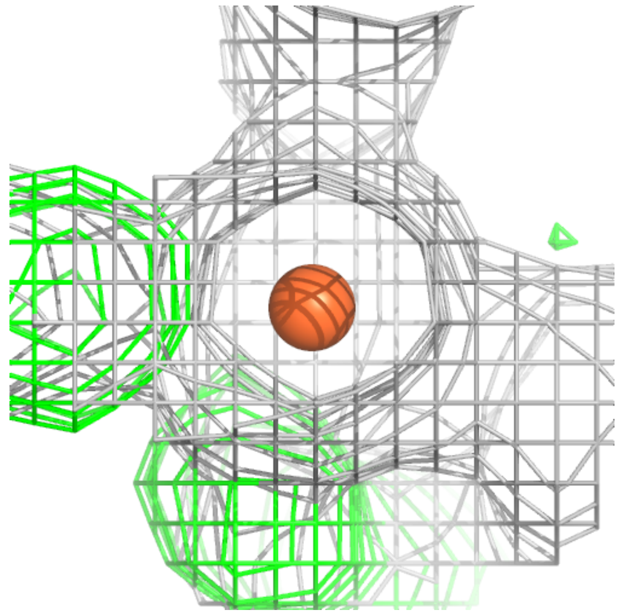


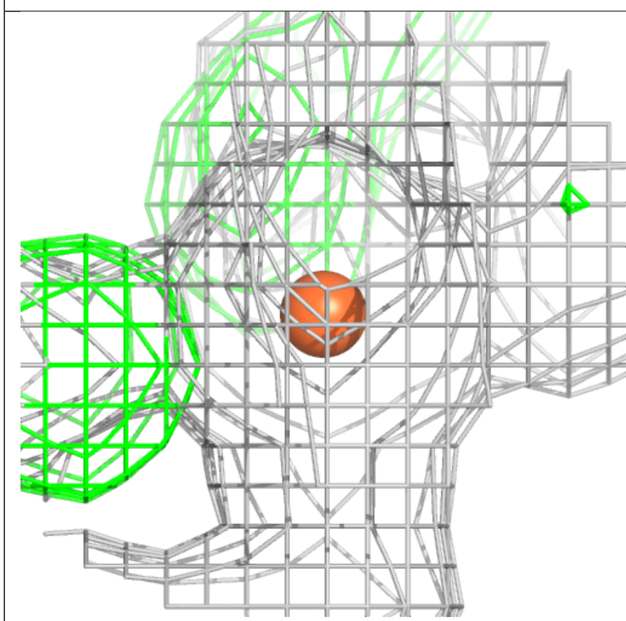


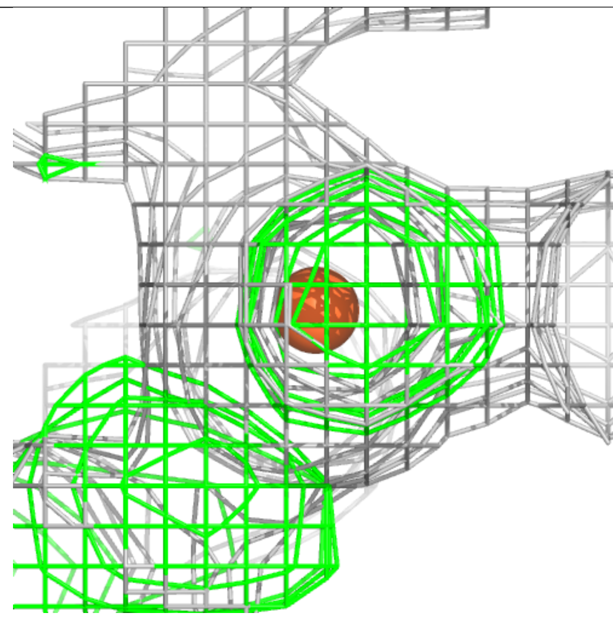


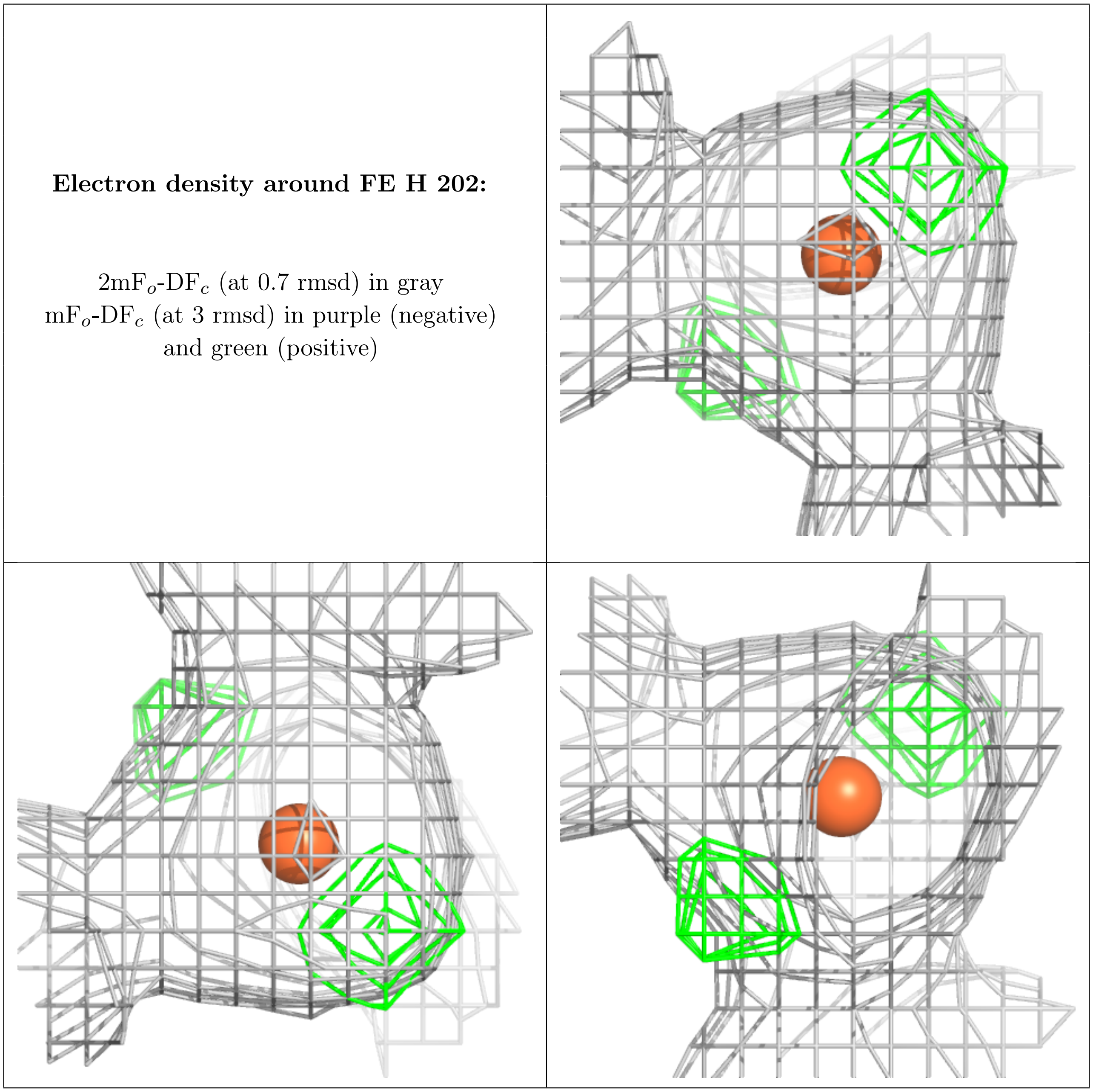
Electron density around FE G 201:

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 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)

6.5 Other polymers (i)

There are no such residues in this entry.