



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2024 – 08:18 PM JST

PDB ID : 8JAI
Title : Crystal Structure of Human H-Ferritin variant 123F assembling in solution 1
Authors : Chen, X.; Zhao, G.
Deposited on : 2023-05-06
Resolution : 2.56 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

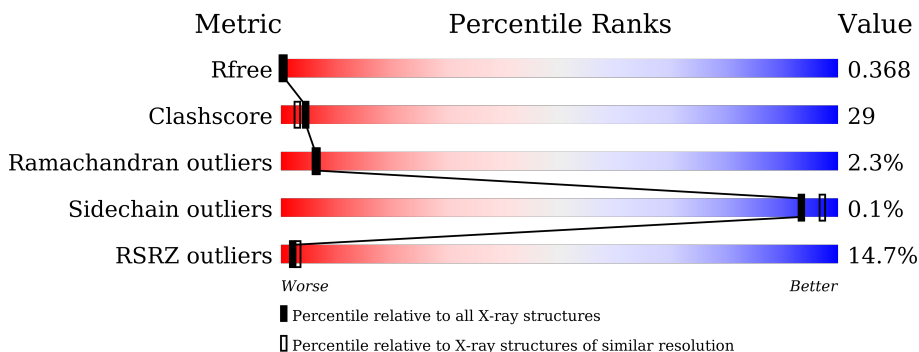
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




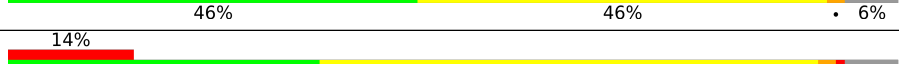
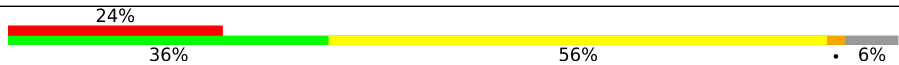
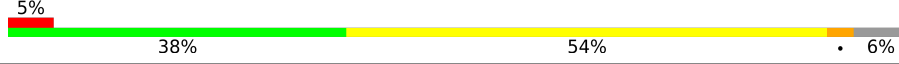
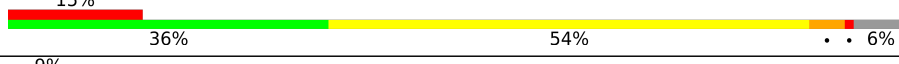
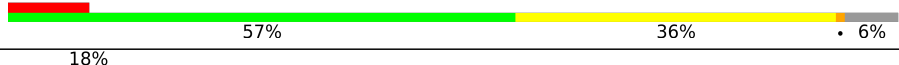

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	183	 7% 48% 45% 6%
1	B	183	 3% 48% 46% 6%
1	C	183	 19% 42% 51% 6%
1	D	183	 20% 33% 60% 6%
1	E	183	 4% 51% 42% 6%
1	F	183	 22% 36% 56% 6%

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Mol	Chain	Length	Quality of chain
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	
1	M	183	
1	N	183	
1	O	183	
1	P	183	
1	Q	183	
1	R	183	
1	S	183	
1	T	183	
1	U	183	
1	V	183	
1	W	183	
1	X	183	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34001 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	1416	891	248	270	7	0	0	0
1	B	172	1416	891	248	270	7	0	0	0
1	C	172	1416	891	248	270	7	0	0	0
1	D	172	1416	891	248	270	7	0	0	0
1	E	172	1416	891	248	270	7	0	0	0
1	F	172	1416	891	248	270	7	0	0	0
1	G	172	1416	891	248	270	7	0	0	0
1	H	172	1416	891	248	270	7	0	0	0
1	I	172	1416	891	248	270	7	0	0	0
1	J	172	1416	891	248	270	7	0	0	0
1	K	172	1416	891	248	270	7	0	0	0
1	L	172	1416	891	248	270	7	0	0	0
1	M	172	1416	891	248	270	7	0	0	0
1	N	172	1416	891	248	270	7	0	0	0
1	O	172	1413	889	248	270	6	0	0	0
1	P	172	1416	891	248	270	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	172	1416	891	248	270	7	0	0	0
1	R	172	1416	891	248	270	7	0	0	0
1	S	172	1416	891	248	270	7	0	0	0
1	T	172	1416	891	248	270	7	0	0	0
1	U	172	1416	891	248	270	7	0	0	0
1	V	172	1416	891	248	270	7	0	0	0
1	W	172	1416	891	248	270	7	0	0	0
1	X	172	1416	891	248	270	7	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	ASP	engineered mutation	UNP P02794
B	123	PHE	ASP	engineered mutation	UNP P02794
C	123	PHE	ASP	engineered mutation	UNP P02794
D	123	PHE	ASP	engineered mutation	UNP P02794
E	123	PHE	ASP	engineered mutation	UNP P02794
F	123	PHE	ASP	engineered mutation	UNP P02794
G	123	PHE	ASP	engineered mutation	UNP P02794
H	123	PHE	ASP	engineered mutation	UNP P02794
I	123	PHE	ASP	engineered mutation	UNP P02794
J	123	PHE	ASP	engineered mutation	UNP P02794
K	123	PHE	ASP	engineered mutation	UNP P02794
L	123	PHE	ASP	engineered mutation	UNP P02794
M	123	PHE	ASP	engineered mutation	UNP P02794
N	123	PHE	ASP	engineered mutation	UNP P02794
O	123	PHE	ASP	engineered mutation	UNP P02794
P	123	PHE	ASP	engineered mutation	UNP P02794
Q	123	PHE	ASP	engineered mutation	UNP P02794
R	123	PHE	ASP	engineered mutation	UNP P02794
S	123	PHE	ASP	engineered mutation	UNP P02794
T	123	PHE	ASP	engineered mutation	UNP P02794
U	123	PHE	ASP	engineered mutation	UNP P02794
V	123	PHE	ASP	engineered mutation	UNP P02794
W	123	PHE	ASP	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
X	123	PHE	ASP	engineered mutation	UNP P02794

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	2	Total Fe 2 2	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	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0
2	P	2	Total Fe 2 2	0	0
2	Q	1	Total Fe 1 1	0	0
2	S	2	Total Fe 2 2	0	0
2	W	1	Total Fe 1 1	0	0

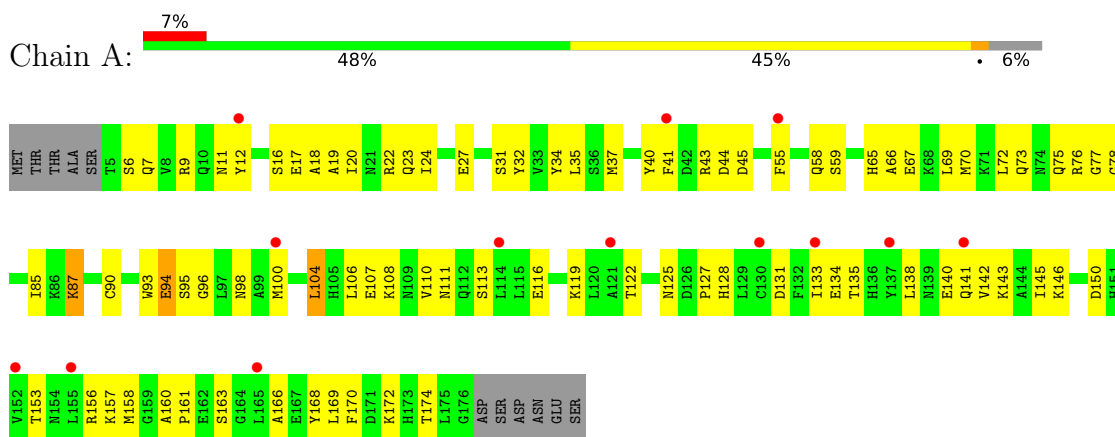
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0

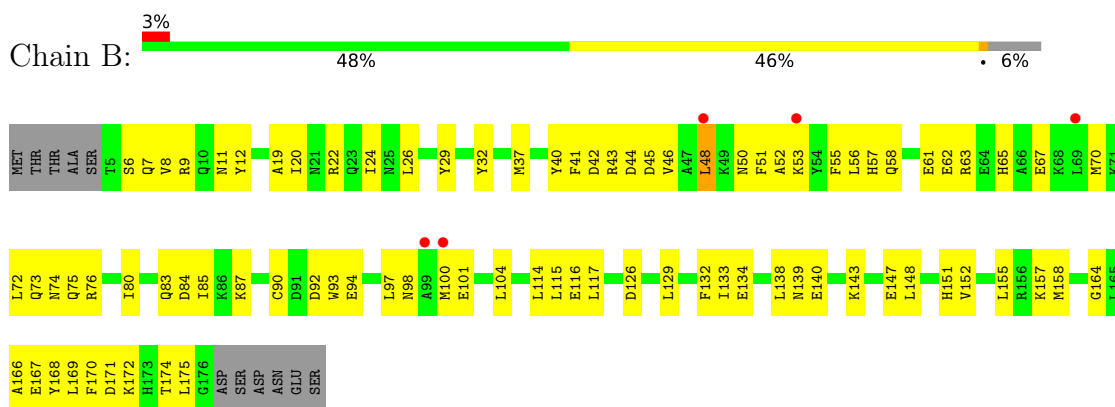
3 Residue-property plots [i](#)

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.

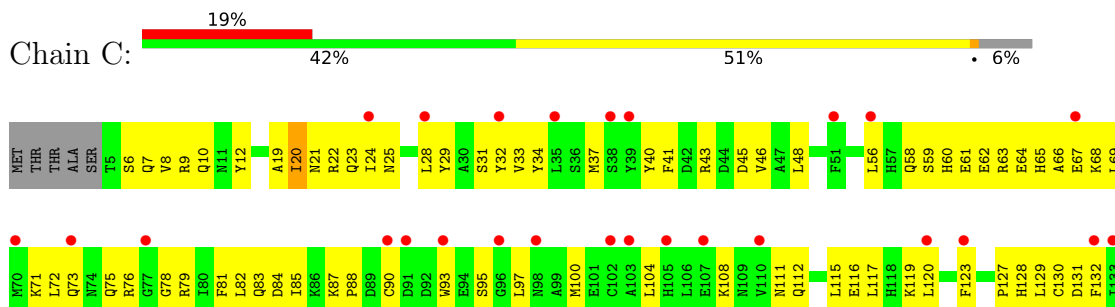
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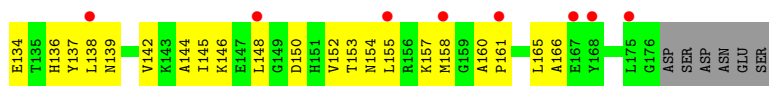


- Molecule 1: Ferritin heavy chain

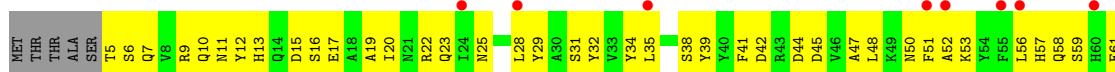


- Molecule 1: Ferritin heavy chain





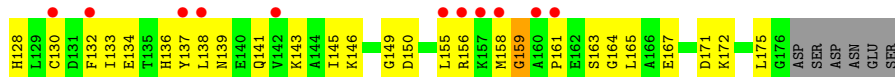
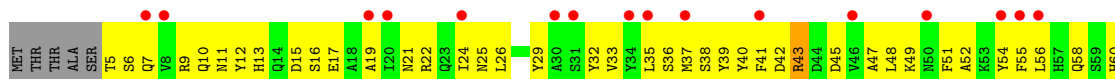
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain

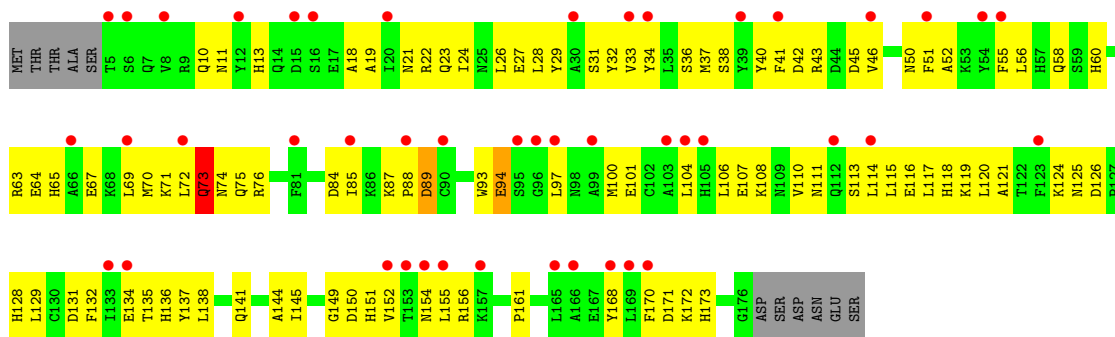


• Molecule 1: Ferritin heavy chain

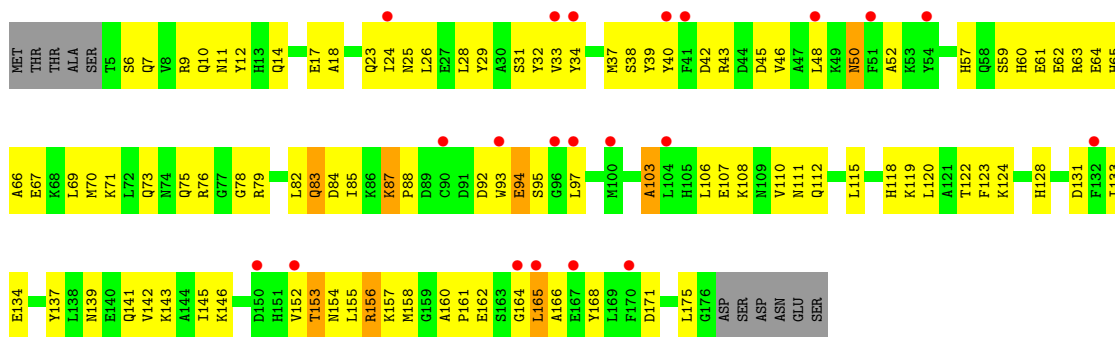
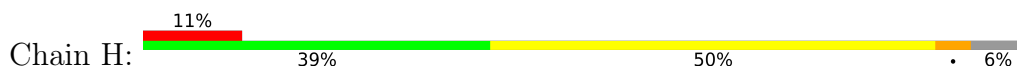


• Molecule 1: Ferritin heavy chain

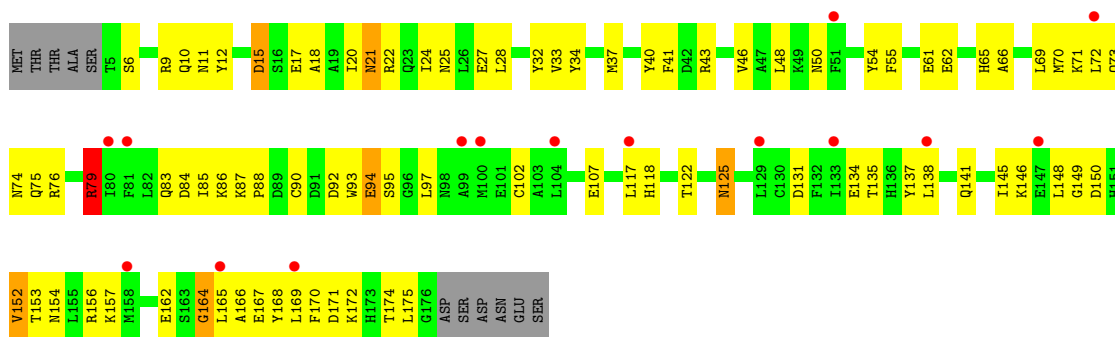




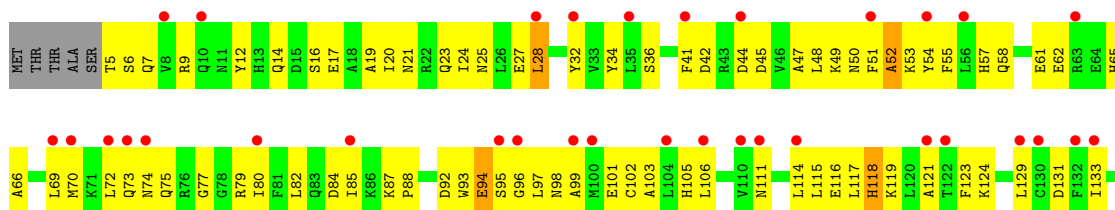
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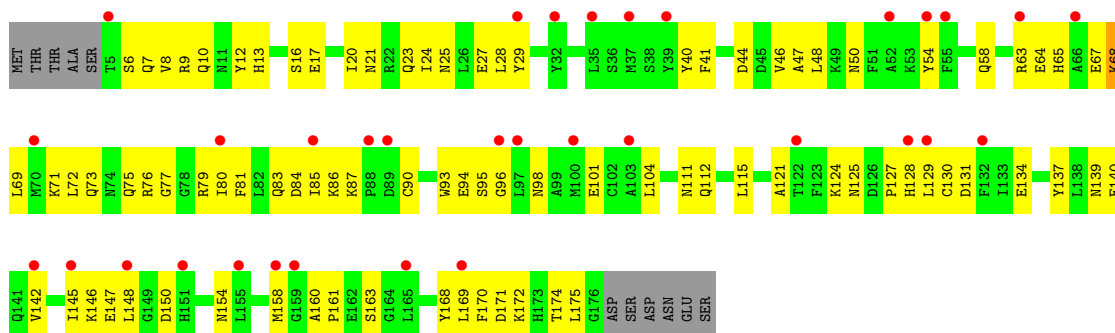


• Molecule 1: Ferritin heavy chain

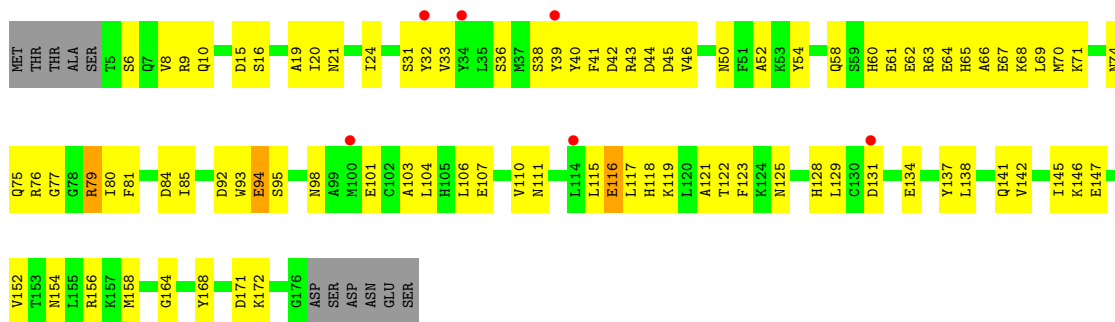




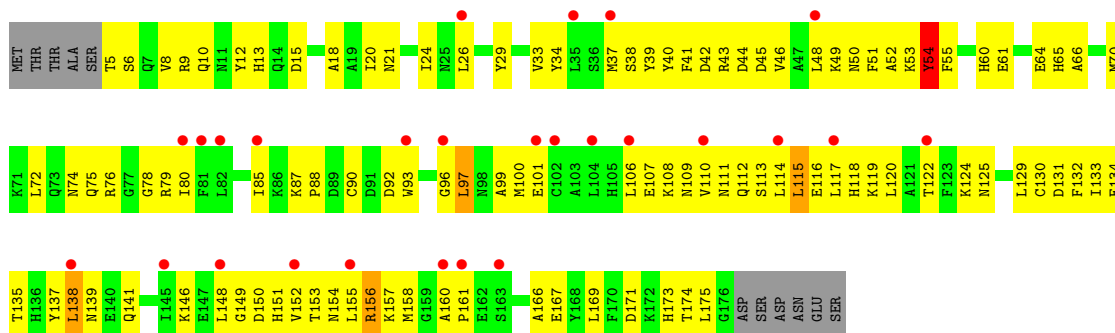
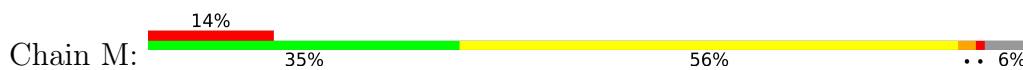
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

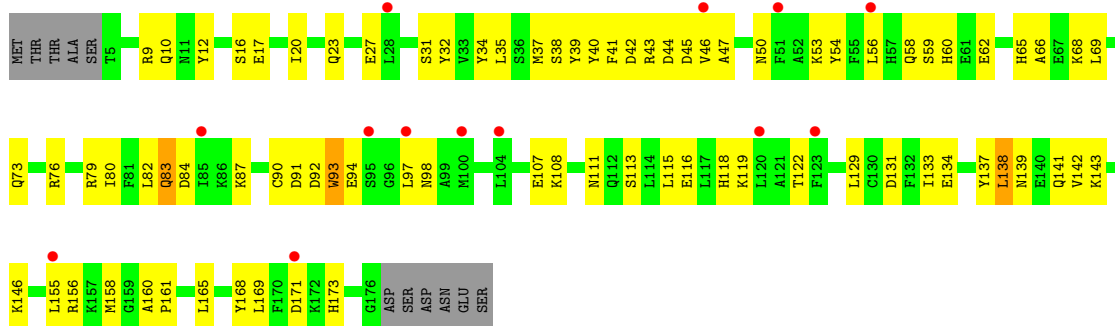


- Molecule 1: Ferritin heavy chain

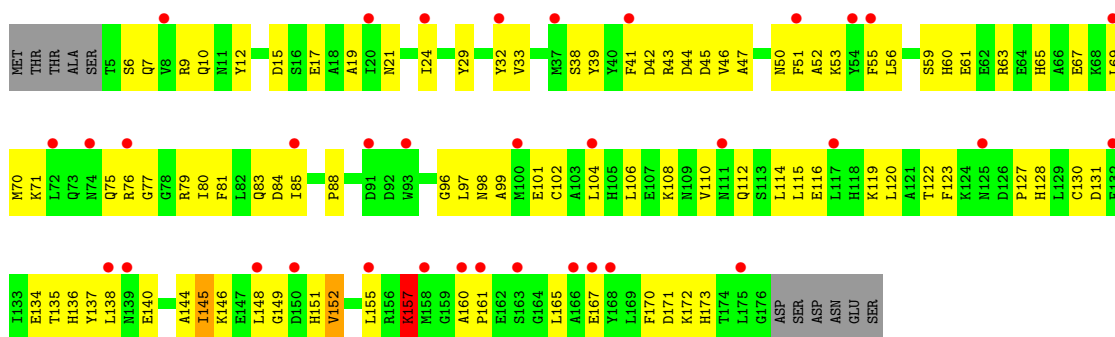
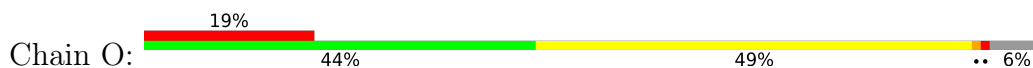


- Molecule 1: Ferritin heavy chain

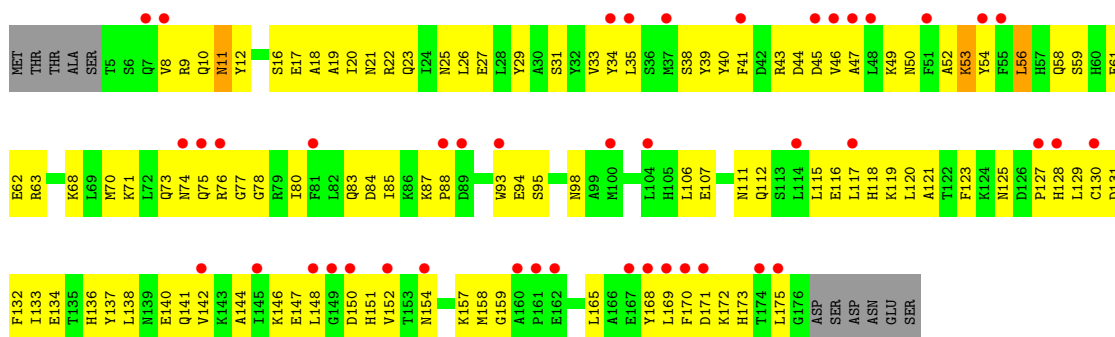




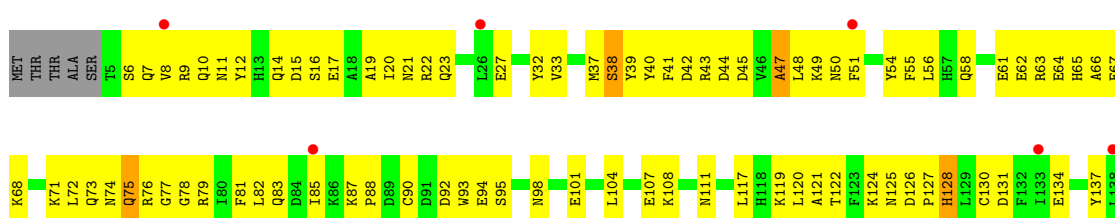
• Molecule 1: Ferritin heavy chain

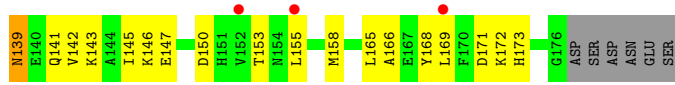


• Molecule 1: Ferritin heavy chain

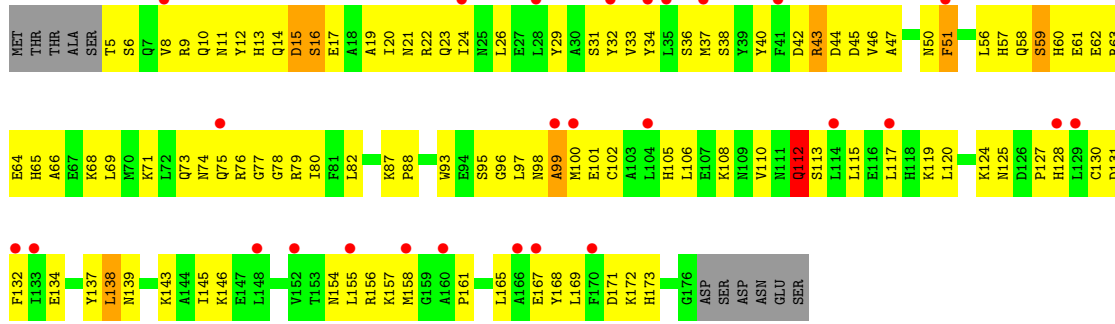


• Molecule 1: Ferritin heavy chain

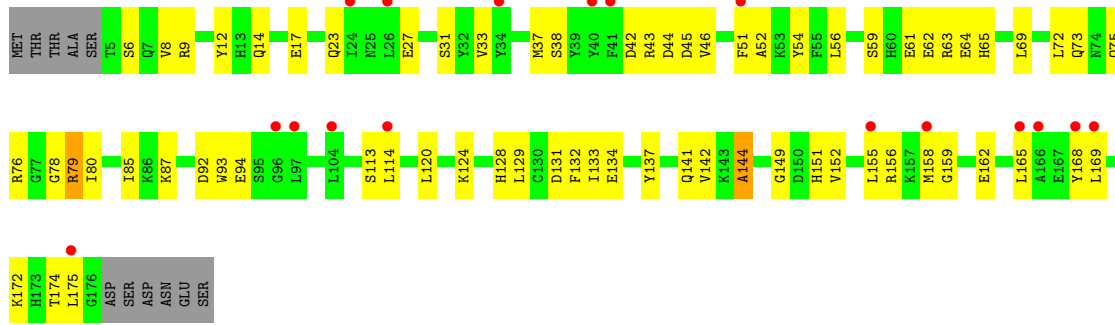




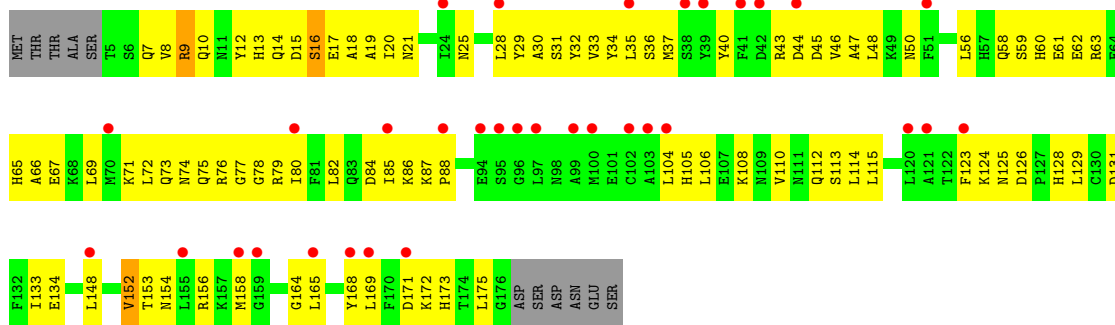
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain

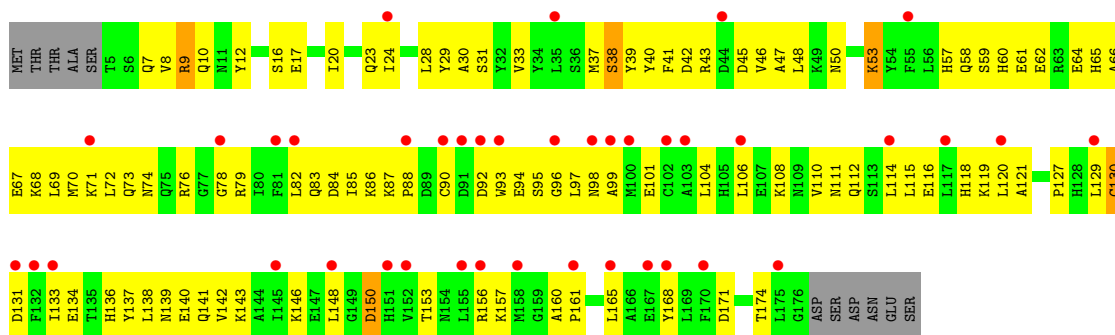


• Molecule 1: Ferritin heavy chain

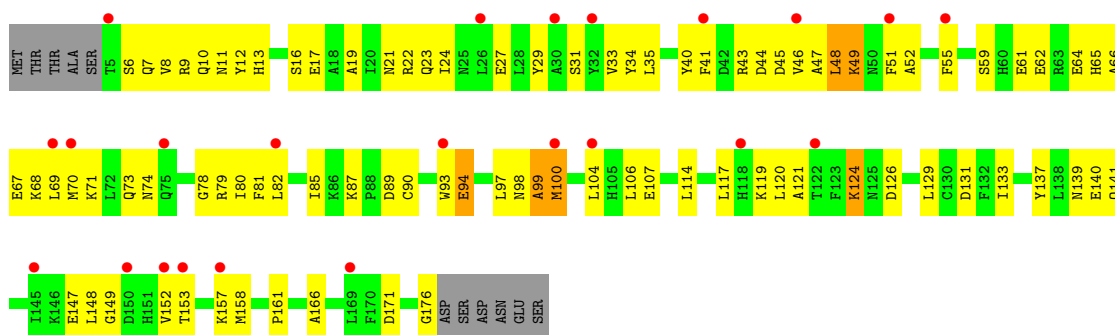


• Molecule 1: Ferritin heavy chain

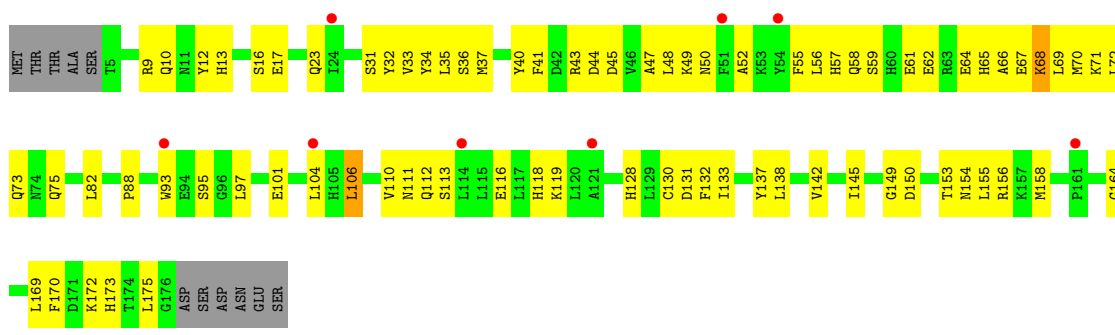




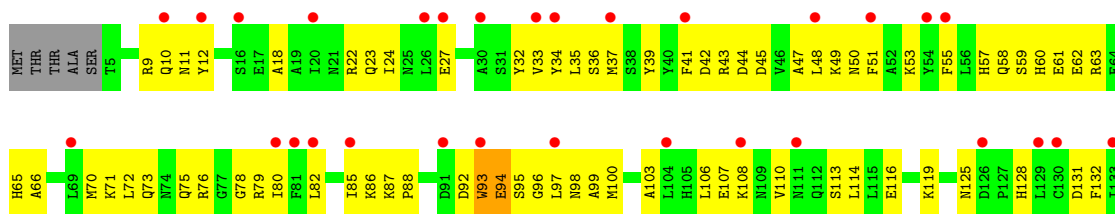
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	301.66Å 301.66Å 316.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.59 – 2.56 65.59 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.59-2.56) 93.3 (65.59-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.335 , 0.368 0.335 , 0.368	Depositor DCC
R_{free} test set	11628 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.089 for -l,-k,-h 0.095 for -h,l,k	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.55	0/1446	0.69	2/1947 (0.1%)
1	B	0.62	2/1446 (0.1%)	0.69	1/1947 (0.1%)
1	C	0.55	0/1446	0.67	0/1947
1	D	0.69	4/1446 (0.3%)	0.71	2/1947 (0.1%)
1	E	0.53	0/1446	0.66	0/1947
1	F	0.55	0/1446	0.70	1/1947 (0.1%)
1	G	0.52	0/1446	0.72	2/1947 (0.1%)
1	H	0.57	1/1446 (0.1%)	0.74	1/1947 (0.1%)
1	I	0.76	2/1446 (0.1%)	0.78	6/1947 (0.3%)
1	J	0.54	0/1446	0.68	1/1947 (0.1%)
1	K	0.50	0/1446	0.67	1/1947 (0.1%)
1	L	0.61	1/1446 (0.1%)	0.72	0/1947
1	M	0.69	3/1446 (0.2%)	0.87	7/1947 (0.4%)
1	N	0.60	1/1446 (0.1%)	0.68	2/1947 (0.1%)
1	O	0.60	2/1443 (0.1%)	0.67	0/1944
1	P	0.54	1/1446 (0.1%)	0.64	1/1947 (0.1%)
1	Q	0.55	0/1446	0.70	2/1947 (0.1%)
1	R	0.65	1/1446 (0.1%)	0.76	2/1947 (0.1%)
1	S	0.58	0/1446	0.72	2/1947 (0.1%)
1	T	0.55	0/1446	0.68	2/1947 (0.1%)
1	U	0.53	0/1446	0.75	3/1947 (0.2%)
1	V	0.63	1/1446 (0.1%)	0.73	1/1947 (0.1%)
1	W	0.65	1/1446 (0.1%)	0.67	0/1947
1	X	0.62	2/1446 (0.1%)	0.67	2/1947 (0.1%)
All	All	0.59	22/34701 (0.1%)	0.71	41/46725 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	M	0	1
1	V	0	1
All	All	0	4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	79	ARG	NE-CZ	14.76	1.52	1.33
1	I	79	ARG	CZ-NH1	12.61	1.49	1.33
1	W	68	LYS	CE-NZ	12.52	1.80	1.49
1	X	167	GLU	CB-CG	10.26	1.71	1.52
1	R	112	GLN	CG-CD	9.96	1.74	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	79	ARG	CG-CD-NE	12.76	138.60	111.80
1	M	156	ARG	NE-CZ-NH2	11.37	125.98	120.30
1	U	53	LYS	CD-CE-NZ	10.29	135.36	111.70
1	I	79	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	S	79	ARG	NE-CZ-NH2	8.11	124.36	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	50	ASN	Peptide
1	I	79	ARG	Sidechain
1	M	54	TYR	Sidechain
1	V	124	LYS	Mainchain

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1416	0	1362	74	0
1	B	1416	0	1362	78	0
1	C	1416	0	1362	98	0
1	D	1416	0	1362	120	0
1	E	1416	0	1362	63	0
1	F	1416	0	1362	109	0
1	G	1416	0	1362	100	0
1	H	1416	0	1362	93	0
1	I	1416	0	1362	87	0
1	J	1416	0	1362	103	0
1	K	1416	0	1362	86	0
1	L	1416	0	1362	75	0
1	M	1416	0	1362	112	1
1	N	1416	0	1362	83	0
1	O	1413	0	1355	98	1
1	P	1416	0	1361	108	0
1	Q	1416	0	1362	106	0
1	R	1416	0	1362	111	0
1	S	1416	0	1362	59	0
1	T	1416	0	1362	96	0
1	U	1416	0	1362	98	0
1	V	1416	0	1362	87	0
1	W	1416	0	1362	69	0
1	X	1416	0	1362	114	0
2	A	1	0	0	0	0
2	B	2	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	1	0	0	0	0
2	I	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	S	2	0	0	0	0
2	W	1	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
All	All	34001	0	32680	1919	1

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 29.

The worst 5 of 1919 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:O:157:LYS:NZ	1:O:157:LYS:CE	1.68	1.55
1:W:68:LYS:NZ	1:W:68:LYS:CE	1.80	1.43
1:M:101:GLU:OE2	1:M:156:ARG:NH1	1.94	1.00
1:D:10:GLN:O	1:D:76:ARG:NH2	1.93	0.99
1:N:83:GLN:OE1	1:N:84:ASP:N	1.95	0.99

All (1) 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)
1:M:124:LYS:NZ	1:O:123:PHE:O[3_545]	2.14	0.06

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%)	144 (85%)	23 (14%)	3 (2%)	8	10
1	B	170/183 (93%)	149 (88%)	18 (11%)	3 (2%)	8	10
1	C	170/183 (93%)	148 (87%)	20 (12%)	2 (1%)	13	17
1	D	170/183 (93%)	144 (85%)	24 (14%)	2 (1%)	13	17
1	E	170/183 (93%)	154 (91%)	13 (8%)	3 (2%)	8	10
1	F	170/183 (93%)	144 (85%)	22 (13%)	4 (2%)	6	6
1	G	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	6	6
1	H	170/183 (93%)	144 (85%)	17 (10%)	9 (5%)	2	1
1	I	170/183 (93%)	145 (85%)	18 (11%)	7 (4%)	3	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	170/183 (93%)	145 (85%)	21 (12%)	4 (2%)	6	6
1	K	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	13	17
1	L	170/183 (93%)	148 (87%)	18 (11%)	4 (2%)	6	6
1	M	170/183 (93%)	153 (90%)	15 (9%)	2 (1%)	13	17
1	N	170/183 (93%)	153 (90%)	14 (8%)	3 (2%)	8	10
1	O	170/183 (93%)	146 (86%)	21 (12%)	3 (2%)	8	10
1	P	170/183 (93%)	143 (84%)	23 (14%)	4 (2%)	6	6
1	Q	170/183 (93%)	138 (81%)	26 (15%)	6 (4%)	3	2
1	R	170/183 (93%)	134 (79%)	28 (16%)	8 (5%)	2	1
1	S	170/183 (93%)	151 (89%)	18 (11%)	1 (1%)	25	33
1	T	170/183 (93%)	139 (82%)	27 (16%)	4 (2%)	6	6
1	U	170/183 (93%)	143 (84%)	22 (13%)	5 (3%)	4	4
1	V	170/183 (93%)	135 (79%)	30 (18%)	5 (3%)	4	4
1	W	170/183 (93%)	143 (84%)	25 (15%)	2 (1%)	13	17
1	X	170/183 (93%)	144 (85%)	23 (14%)	3 (2%)	8	10
All	All	4080/4392 (93%)	3473 (85%)	514 (13%)	93 (2%)	6	6

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	B	115	LEU
1	I	21	ASN
1	K	68	LYS
1	N	158	MET

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	153/163 (94%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	153/163 (94%)	153 (100%)	0	100	100
1	C	153/163 (94%)	153 (100%)	0	100	100
1	D	153/163 (94%)	153 (100%)	0	100	100
1	E	153/163 (94%)	152 (99%)	1 (1%)	84	90
1	F	153/163 (94%)	153 (100%)	0	100	100
1	G	153/163 (94%)	153 (100%)	0	100	100
1	H	153/163 (94%)	153 (100%)	0	100	100
1	I	153/163 (94%)	153 (100%)	0	100	100
1	J	153/163 (94%)	153 (100%)	0	100	100
1	K	153/163 (94%)	153 (100%)	0	100	100
1	L	153/163 (94%)	153 (100%)	0	100	100
1	M	153/163 (94%)	152 (99%)	1 (1%)	84	90
1	N	153/163 (94%)	153 (100%)	0	100	100
1	O	152/163 (93%)	152 (100%)	0	100	100
1	P	153/163 (94%)	153 (100%)	0	100	100
1	Q	153/163 (94%)	153 (100%)	0	100	100
1	R	153/163 (94%)	152 (99%)	1 (1%)	84	90
1	S	153/163 (94%)	153 (100%)	0	100	100
1	T	153/163 (94%)	153 (100%)	0	100	100
1	U	153/163 (94%)	153 (100%)	0	100	100
1	V	153/163 (94%)	153 (100%)	0	100	100
1	W	153/163 (94%)	153 (100%)	0	100	100
1	X	153/163 (94%)	153 (100%)	0	100	100
All	All	3671/3912 (94%)	3668 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	LYS
1	M	54	TYR
1	R	51	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	111	ASN
1	X	136	HIS
1	O	173	HIS
1	X	73	GLN
1	V	139	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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	172/183 (93%)	0.73	13 (7%) 13 18	26, 49, 65, 73	0
1	B	172/183 (93%)	0.59	5 (2%) 51 61	21, 41, 59, 75	0
1	C	172/183 (93%)	1.25	34 (19%) 1 1	41, 60, 77, 90	0
1	D	172/183 (93%)	1.25	36 (20%) 1 1	43, 61, 73, 83	0
1	E	172/183 (93%)	0.60	8 (4%) 31 40	28, 51, 68, 80	0
1	F	172/183 (93%)	1.35	40 (23%) 0 0	42, 61, 73, 83	0
1	G	172/183 (93%)	1.35	45 (26%) 0 0	46, 61, 77, 94	0
1	H	172/183 (93%)	0.91	21 (12%) 4 6	28, 55, 70, 84	0
1	I	172/183 (93%)	0.82	15 (8%) 10 14	29, 55, 71, 78	0
1	J	172/183 (93%)	1.19	40 (23%) 0 0	40, 56, 72, 83	0
1	K	172/183 (93%)	1.12	33 (19%) 1 1	44, 60, 73, 90	0
1	L	172/183 (93%)	0.52	6 (3%) 44 53	26, 40, 60, 72	0
1	M	172/183 (93%)	1.00	26 (15%) 2 3	31, 53, 71, 81	0
1	N	172/183 (93%)	0.66	13 (7%) 13 18	27, 43, 63, 80	0
1	O	172/183 (93%)	1.12	35 (20%) 1 1	38, 59, 72, 84	0
1	P	172/183 (93%)	1.37	44 (25%) 0 0	43, 59, 75, 92	0
1	Q	172/183 (93%)	0.69	9 (5%) 27 34	26, 48, 66, 81	0
1	R	172/183 (93%)	1.04	27 (15%) 2 3	39, 58, 72, 89	0
1	S	172/183 (93%)	0.68	17 (9%) 7 10	24, 48, 65, 78	0
1	T	172/183 (93%)	1.15	33 (19%) 1 1	44, 57, 73, 85	0
1	U	172/183 (93%)	1.29	40 (23%) 0 0	43, 57, 72, 94	0
1	V	172/183 (93%)	1.05	23 (13%) 3 4	40, 57, 71, 82	0
1	W	172/183 (93%)	0.63	8 (4%) 31 40	27, 42, 61, 82	0
1	X	172/183 (93%)	1.08	35 (20%) 1 1	41, 60, 73, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4128/4392 (93%)	0.98	606 (14%) 2 3	21, 55, 72, 94	0

The worst 5 of 606 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	129	LEU	8.2
1	D	24	ILE	7.8
1	G	165	LEU	7.8
1	D	99	ALA	7.6
1	U	99	ALA	7.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

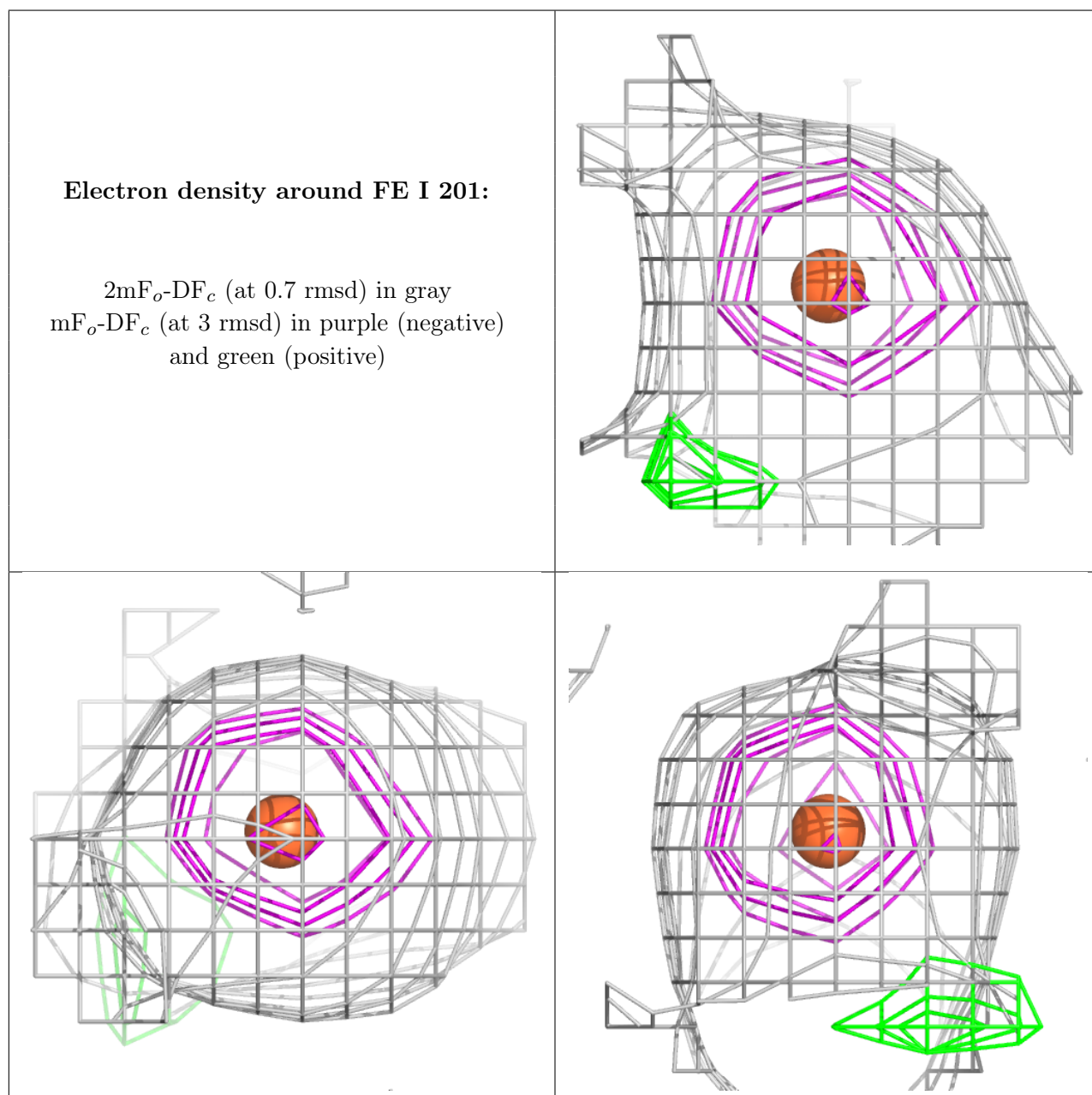
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	I	201	1/1	0.96	0.04	30,30,30,30	0
2	FE	D	201	1/1	0.97	0.07	30,30,30,30	0
2	FE	F	201	1/1	0.97	0.08	30,30,30,30	0
2	FE	G	201	1/1	0.97	0.06	30,30,30,30	0
2	FE	B	201	1/1	0.97	0.06	30,30,30,30	0
2	FE	P	201	1/1	0.97	0.10	30,30,30,30	0
2	FE	P	202	1/1	0.97	0.08	30,30,30,30	0
2	FE	W	201	1/1	0.97	0.04	30,30,30,30	0
2	FE	H	201	1/1	0.98	0.06	30,30,30,30	0
2	FE	B	202	1/1	0.98	0.07	30,30,30,30	0
2	FE	Q	201	1/1	0.98	0.04	30,30,30,30	0
2	FE	S	202	1/1	0.98	0.05	30,30,30,30	0
2	FE	L	201	1/1	0.98	0.09	30,30,30,30	0

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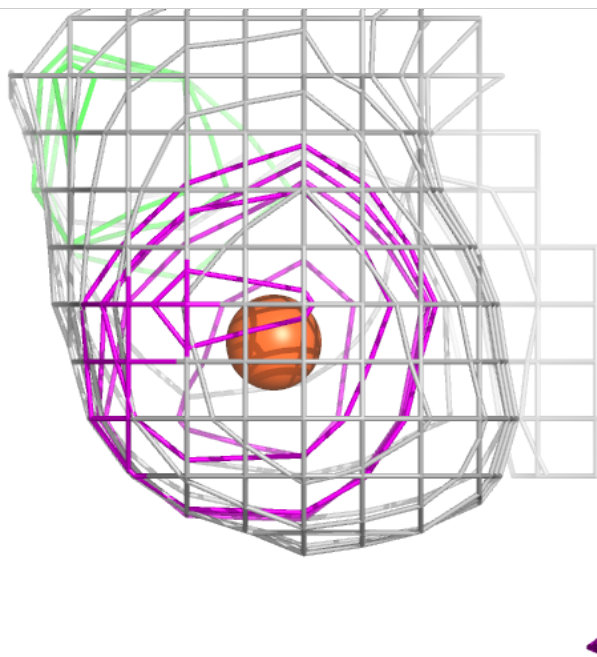
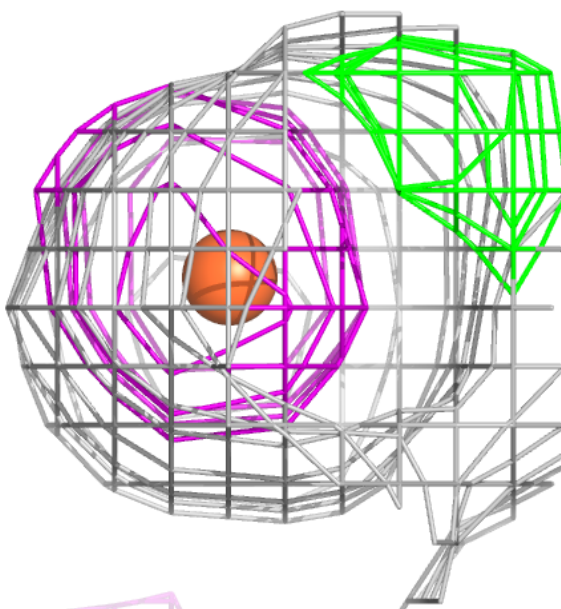
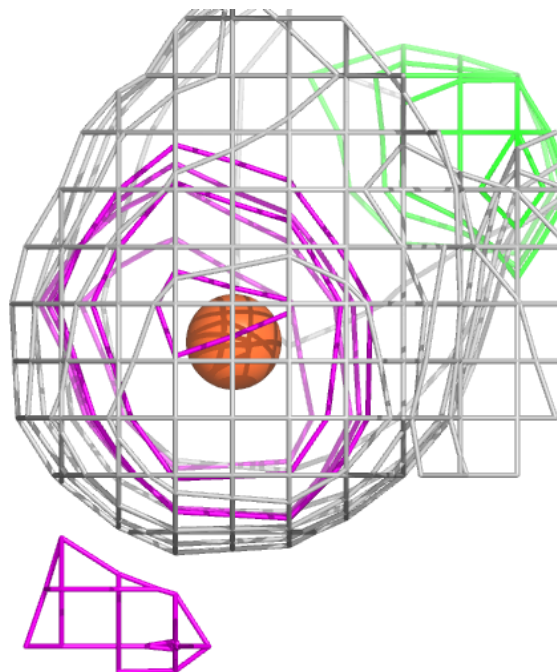
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	201	1/1	0.99	0.04	30,30,30,30	0
2	FE	E	201	1/1	0.99	0.08	30,30,30,30	0
2	FE	S	201	1/1	0.99	0.02	30,30,30,30	0
2	FE	M	201	1/1	0.99	0.02	30,30,30,30	0
2	FE	E	202	1/1	0.99	0.06	30,30,30,30	0

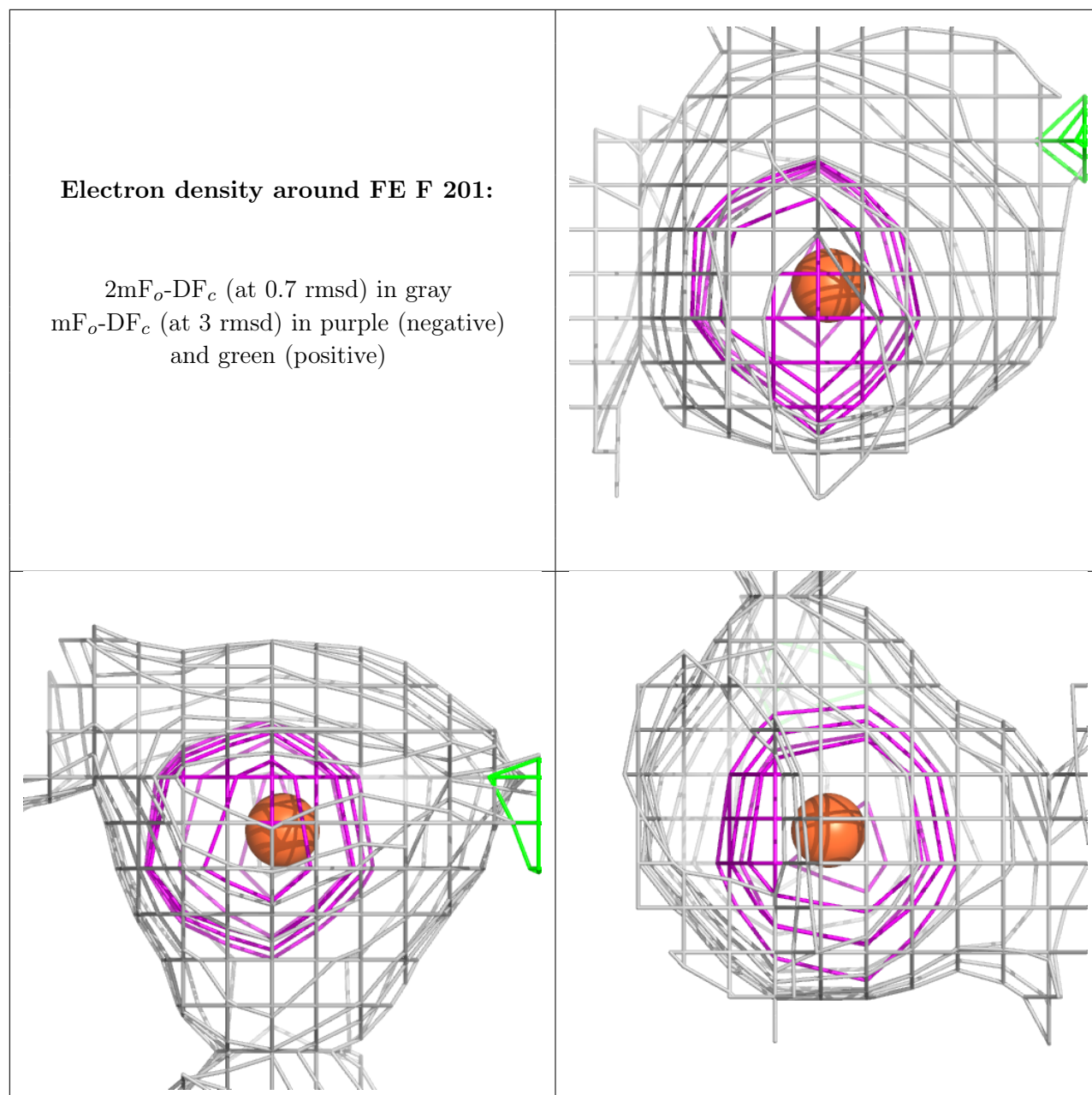
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around FE D 201:

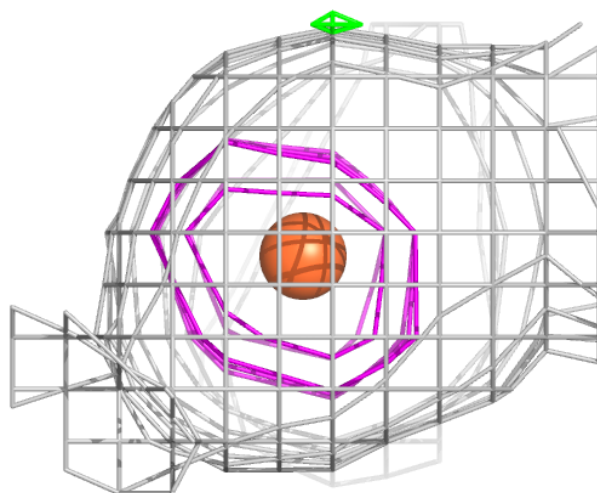
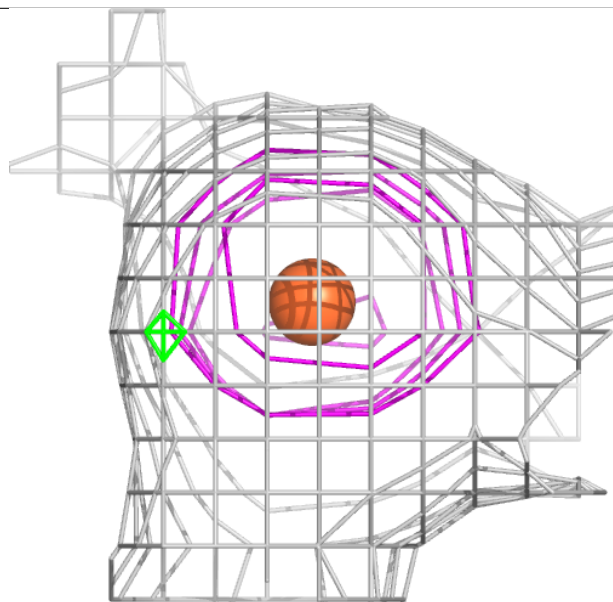
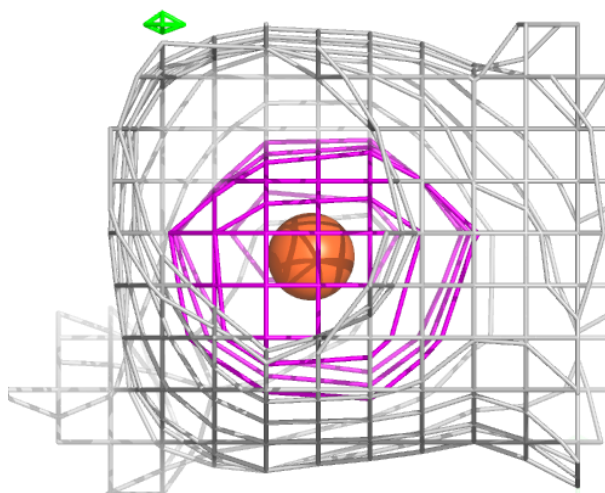
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

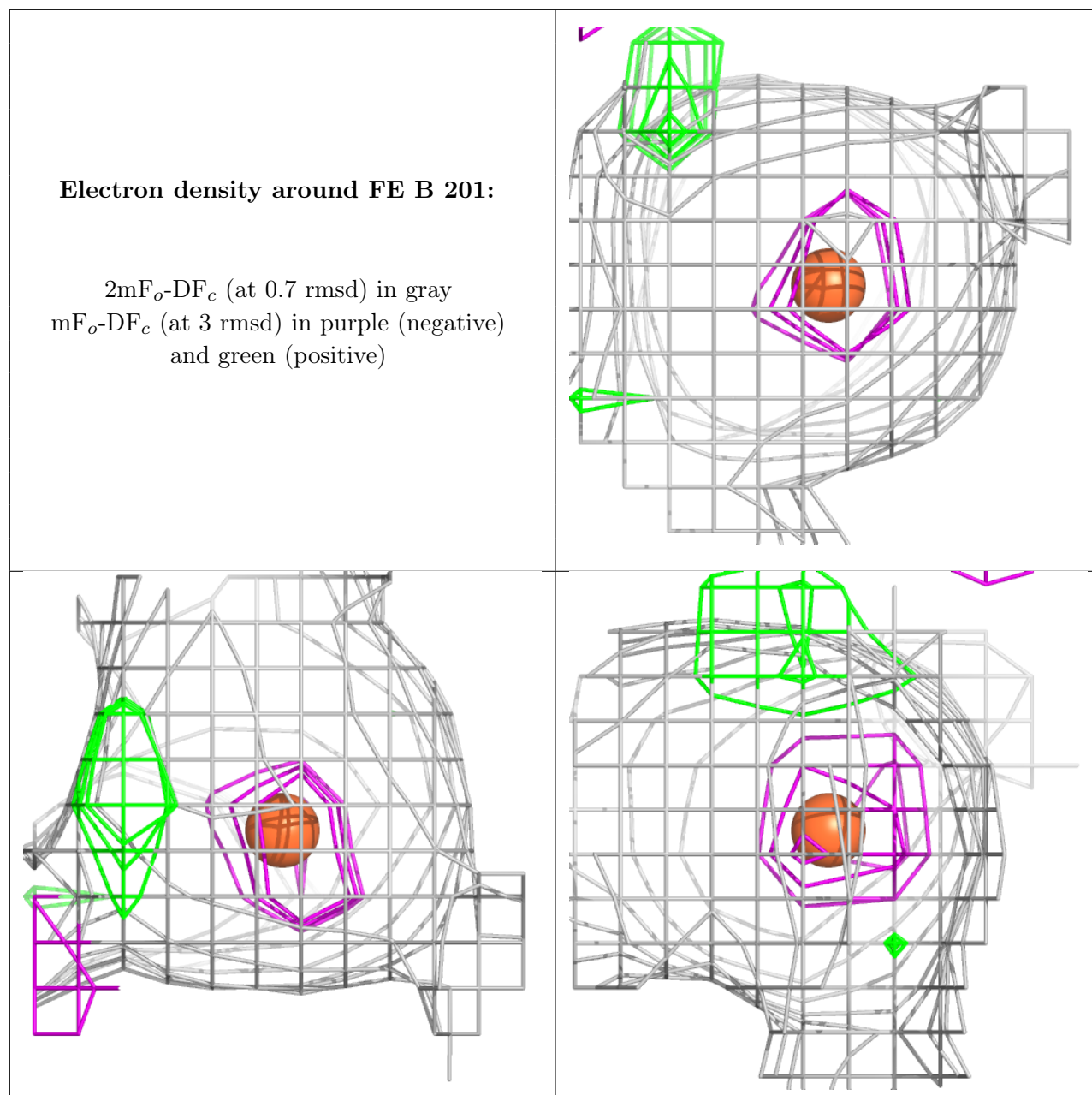


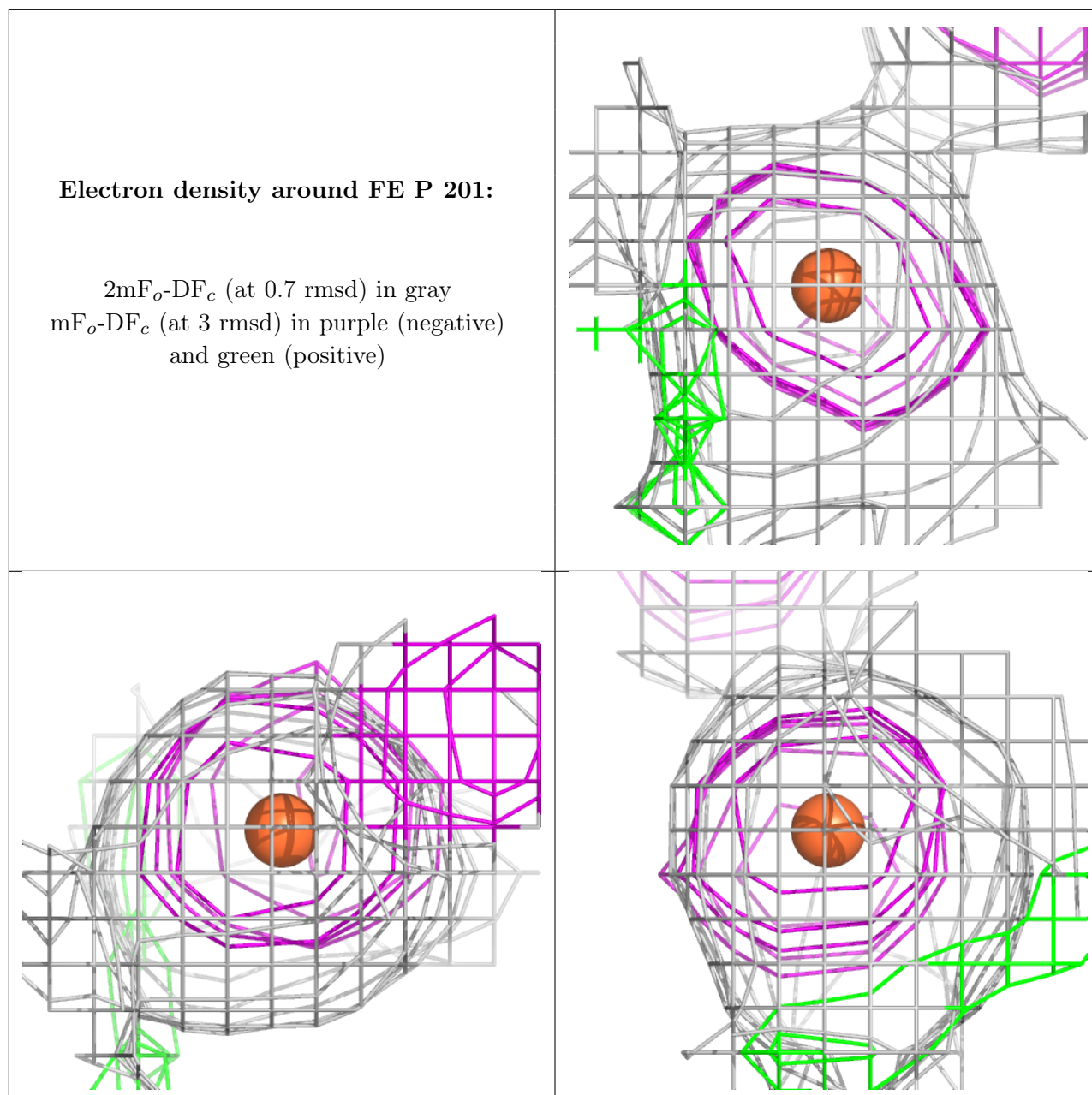


Electron density around FE G 201:

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

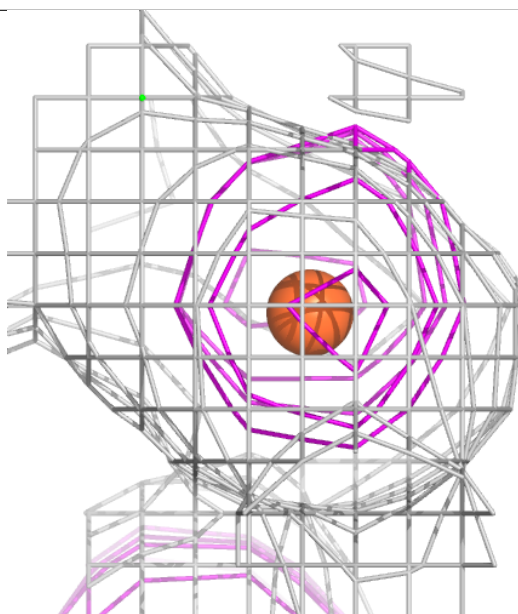
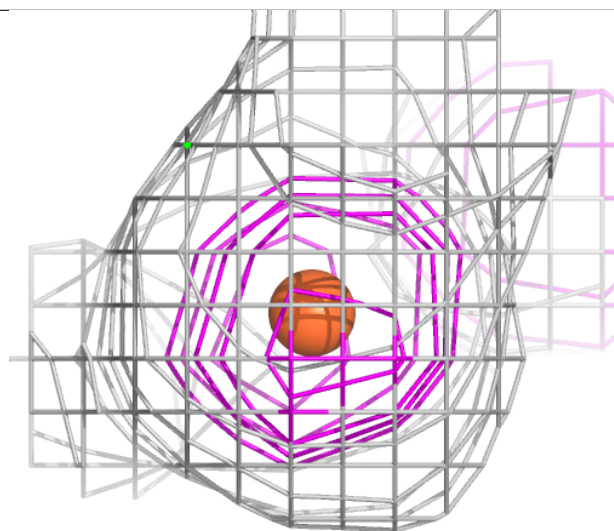
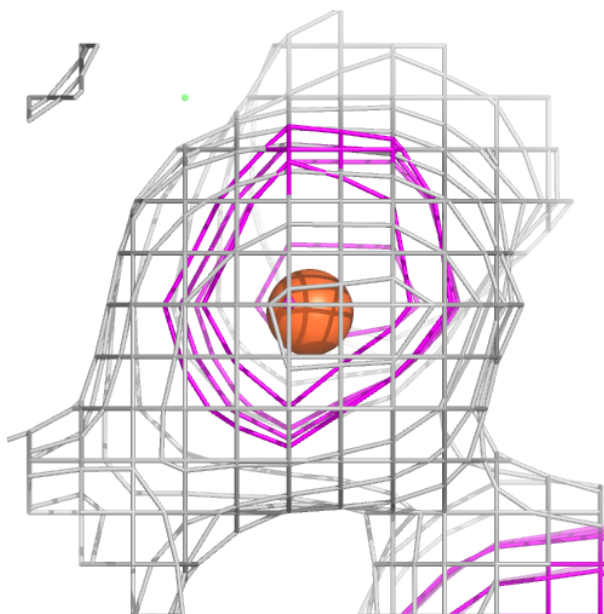






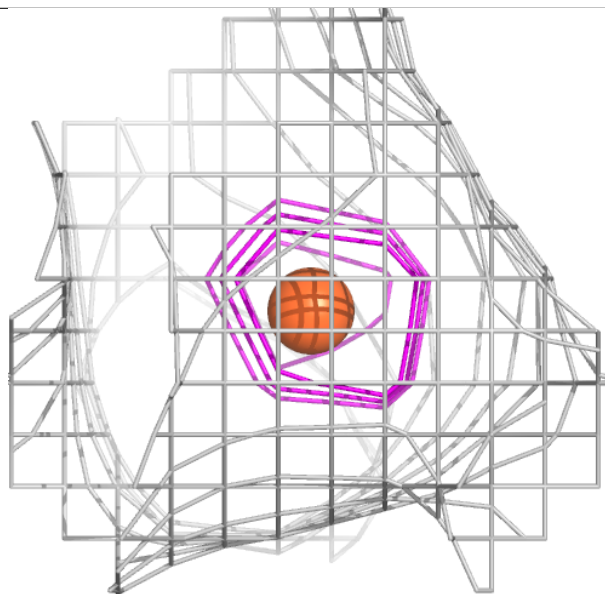
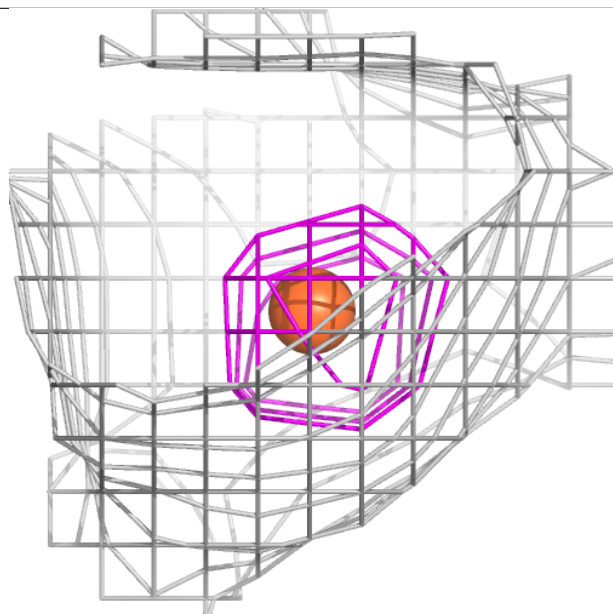
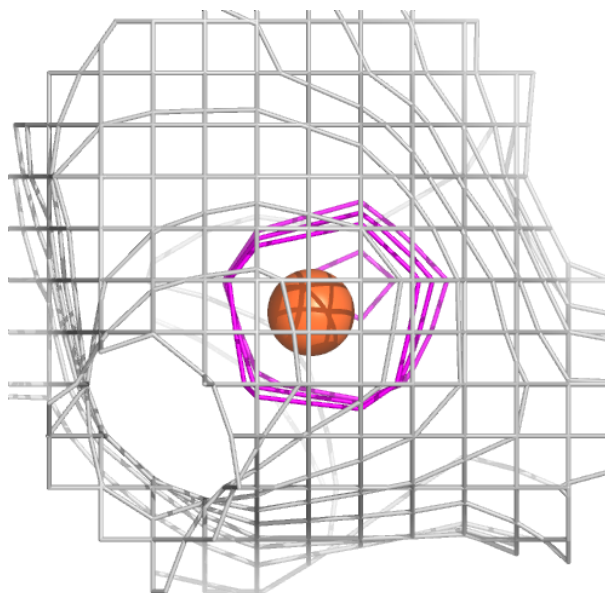
Electron density around FE P 202:

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



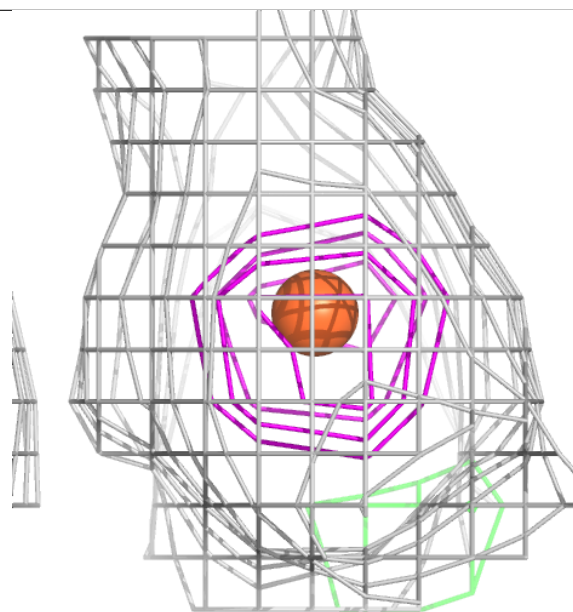
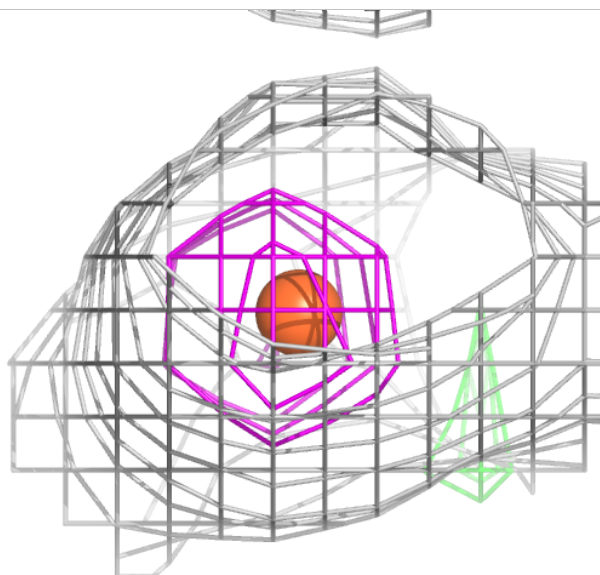
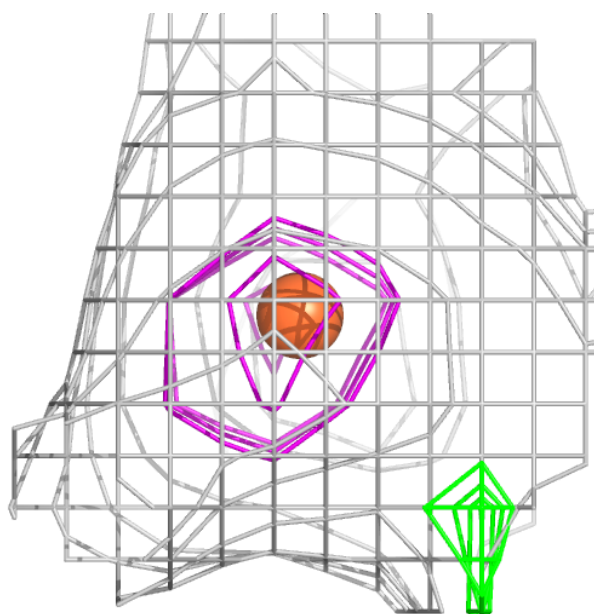
Electron density around FE W 201:

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and green (positive)



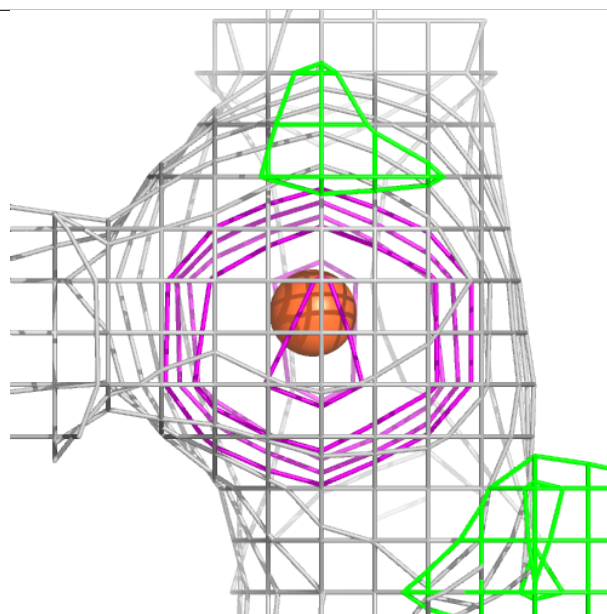
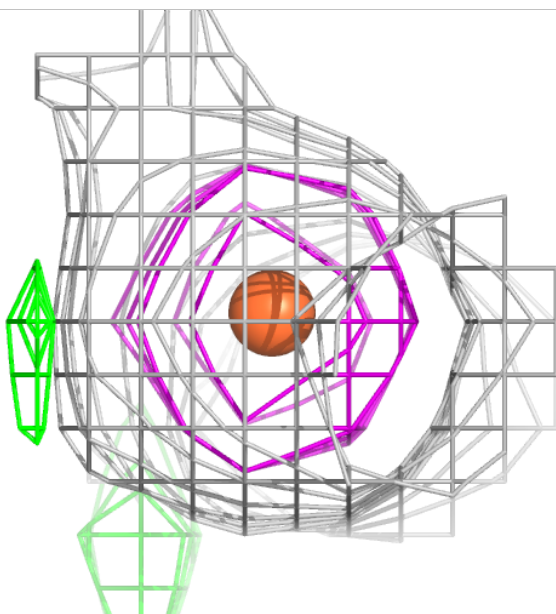
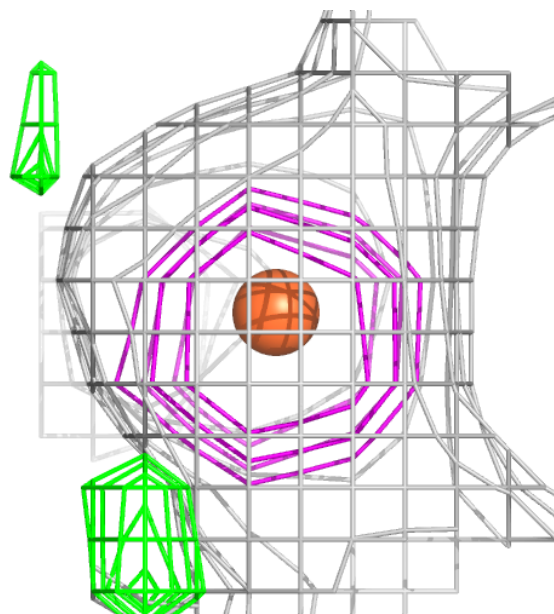
Electron density around FE H 201:

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and green (positive)



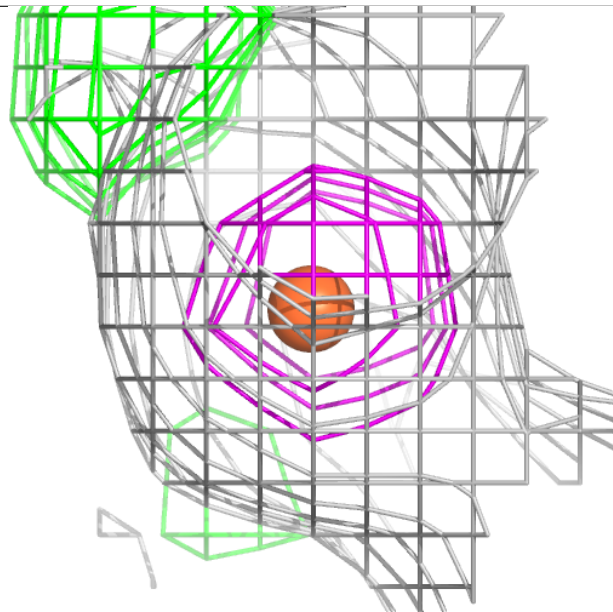
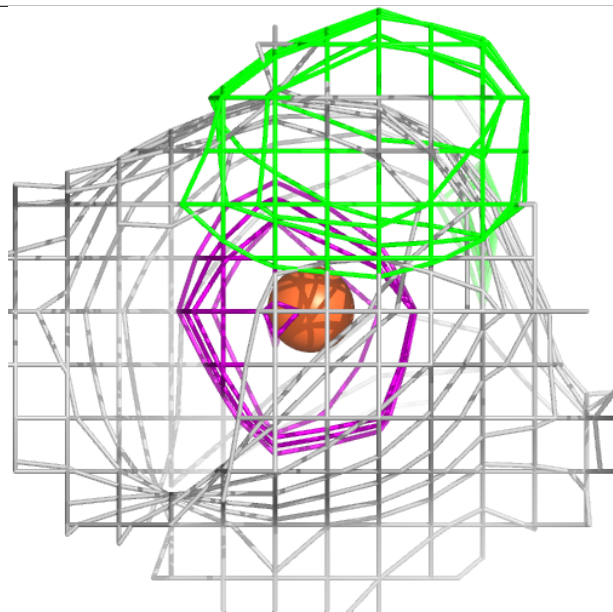
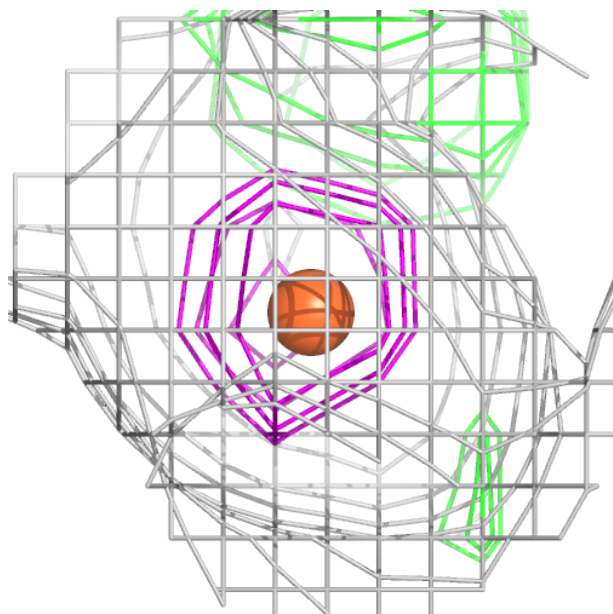
Electron density around FE B 202:

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and green (positive)



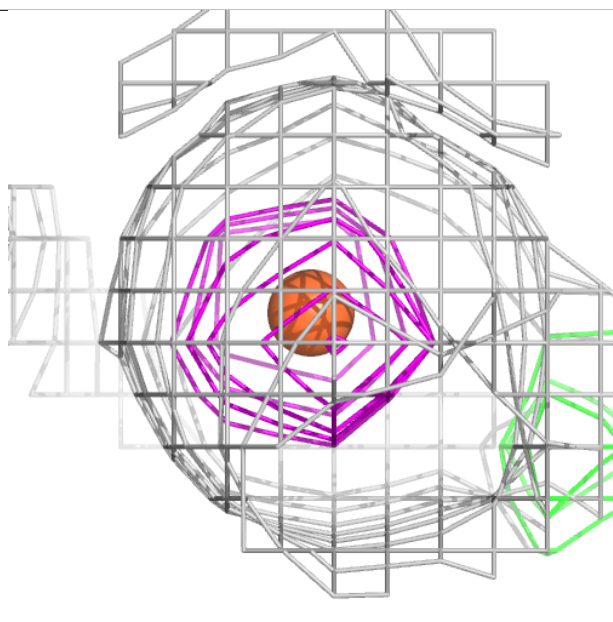
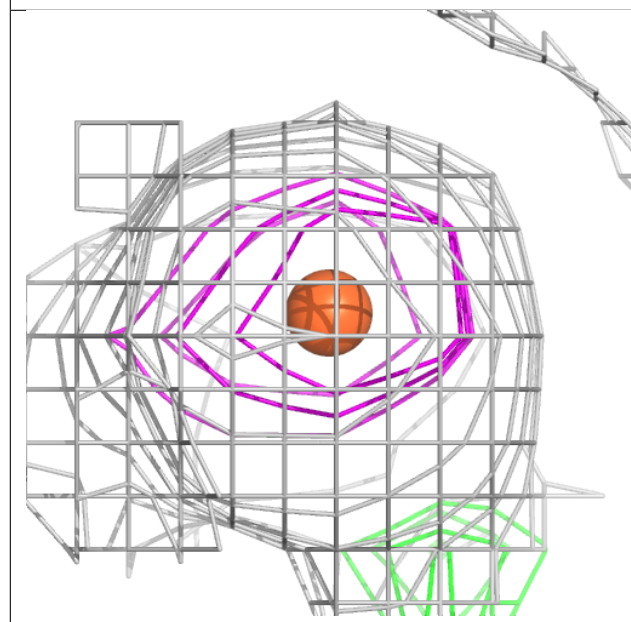
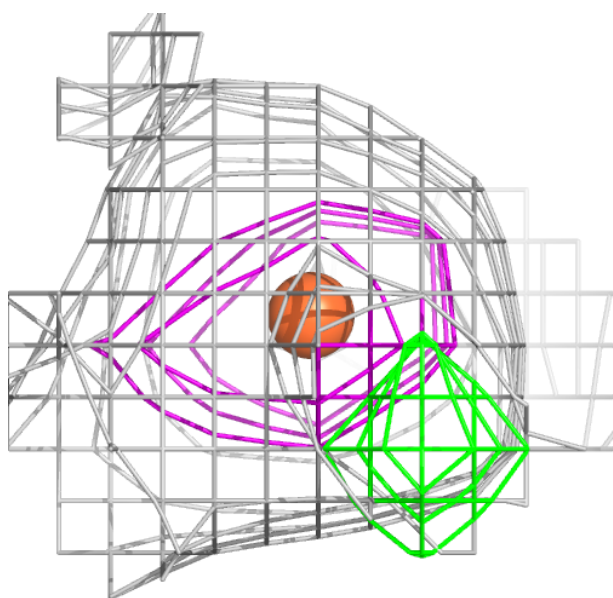
Electron density around FE Q 201:

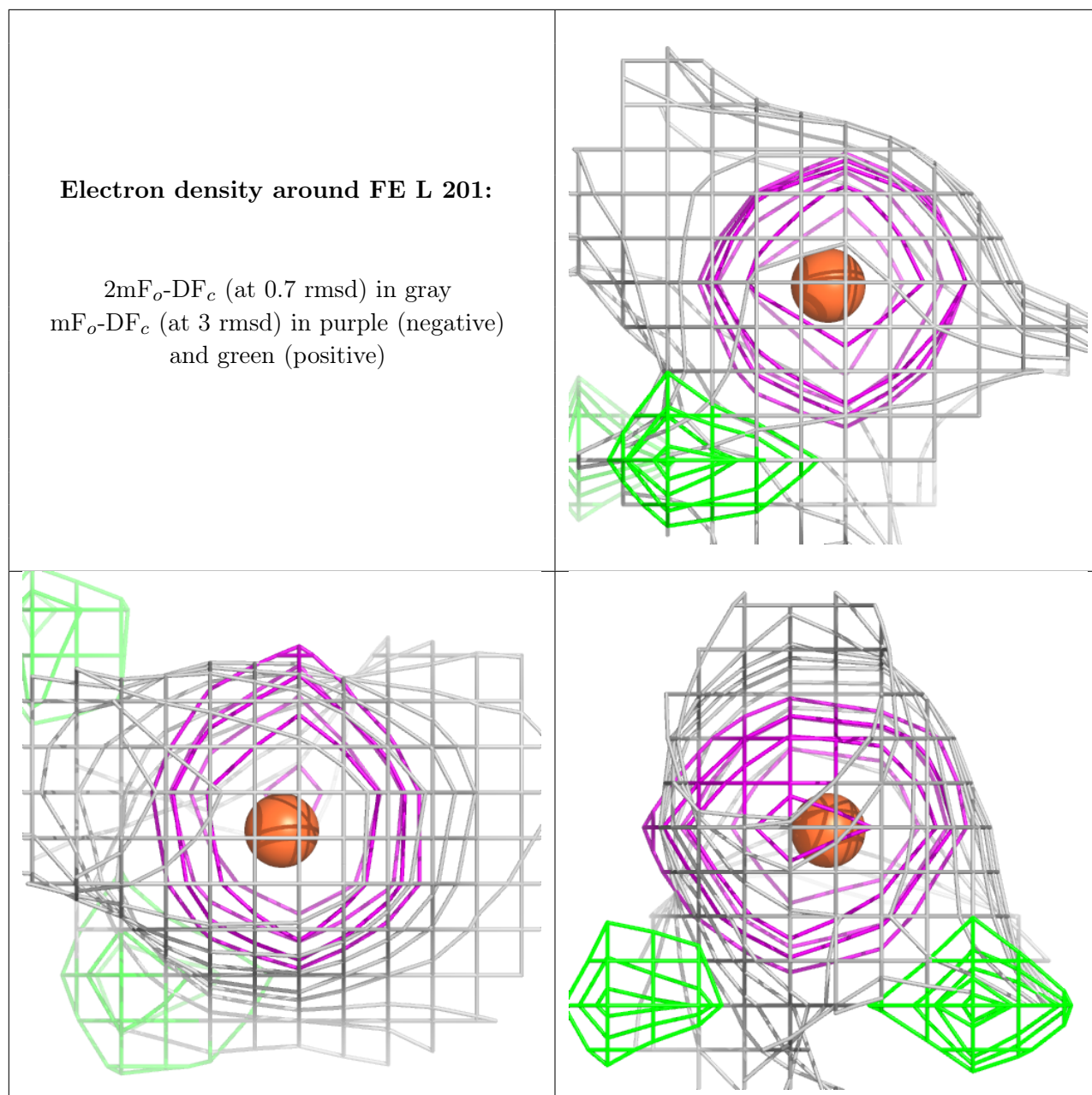
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE S 202:

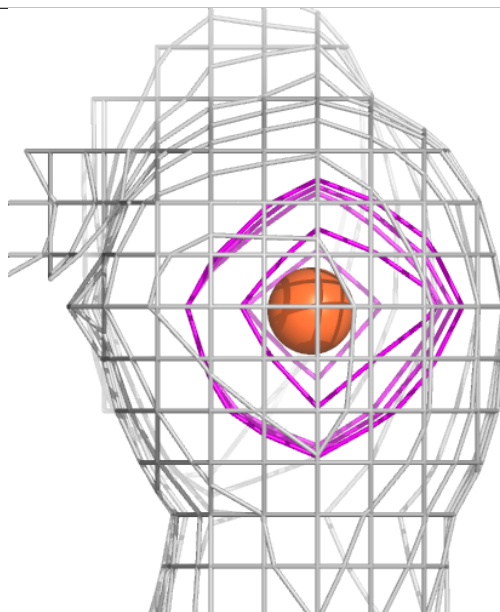
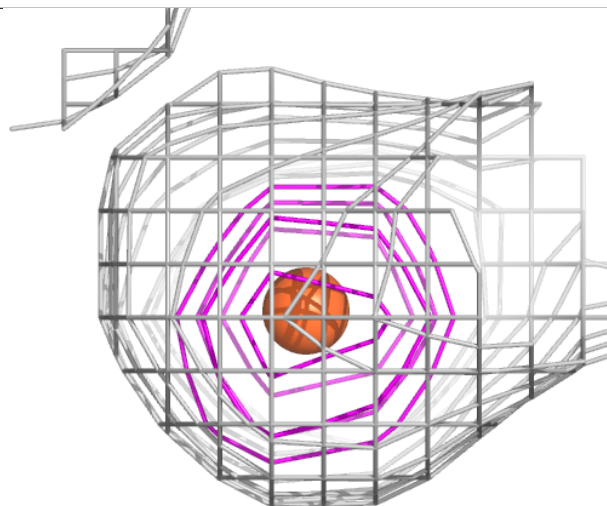
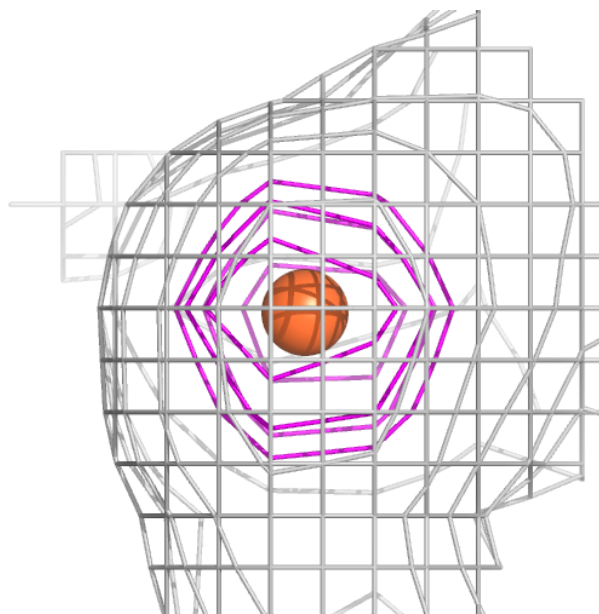
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

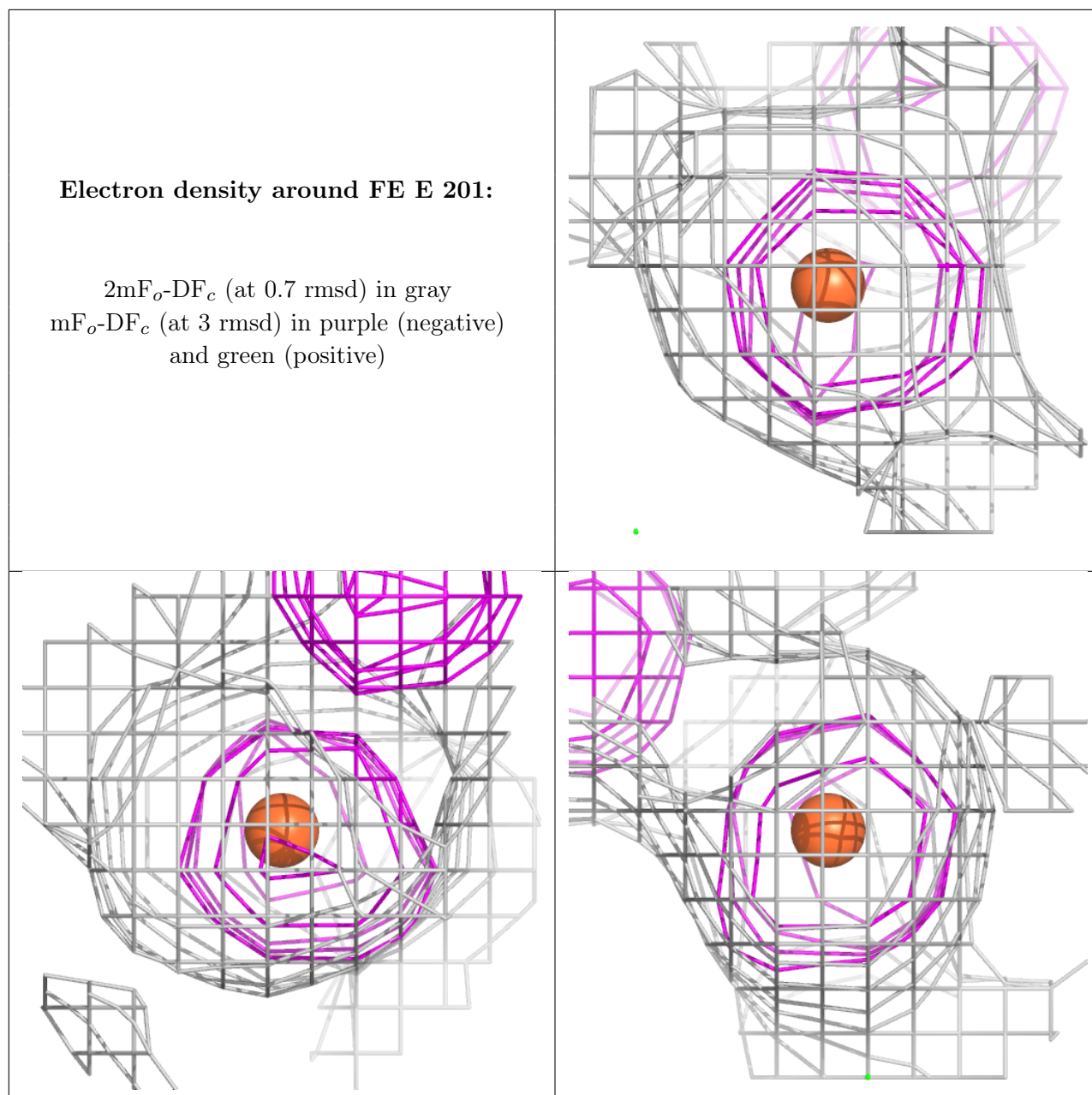


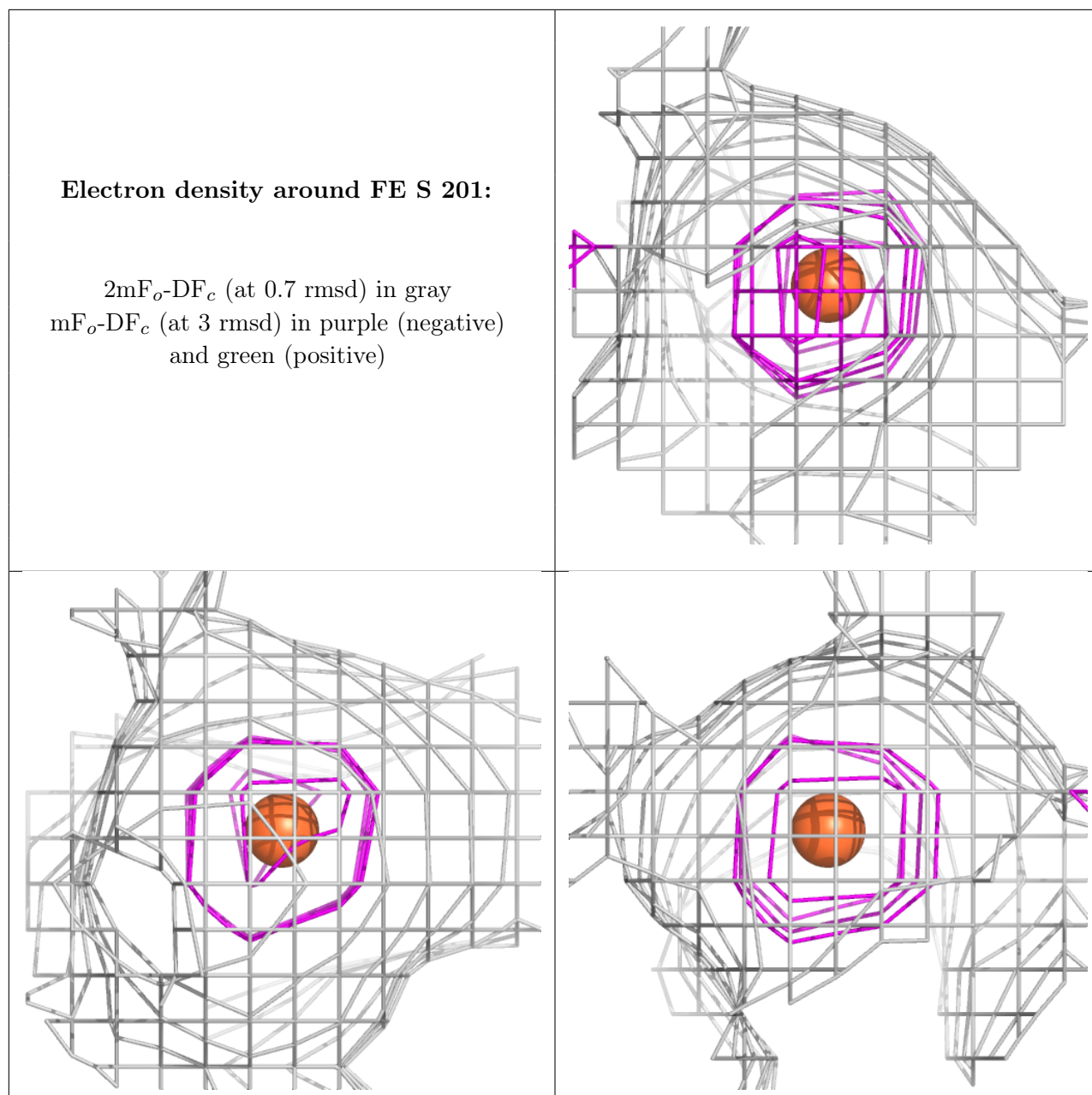


Electron density around FE A 201:

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

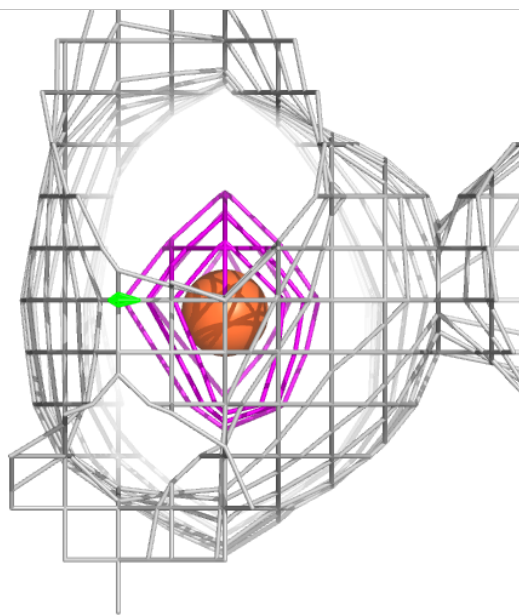
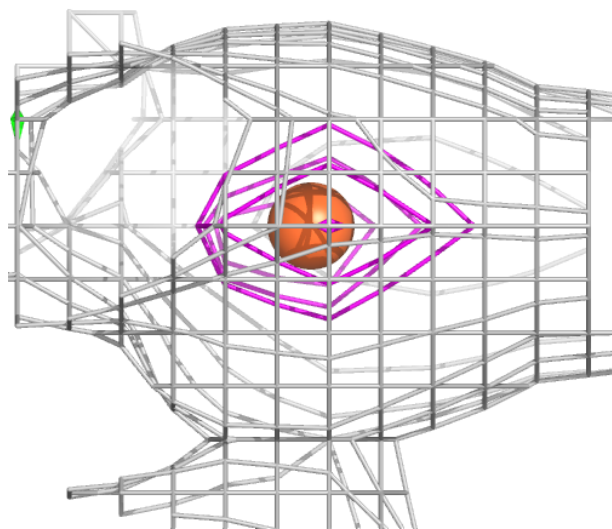
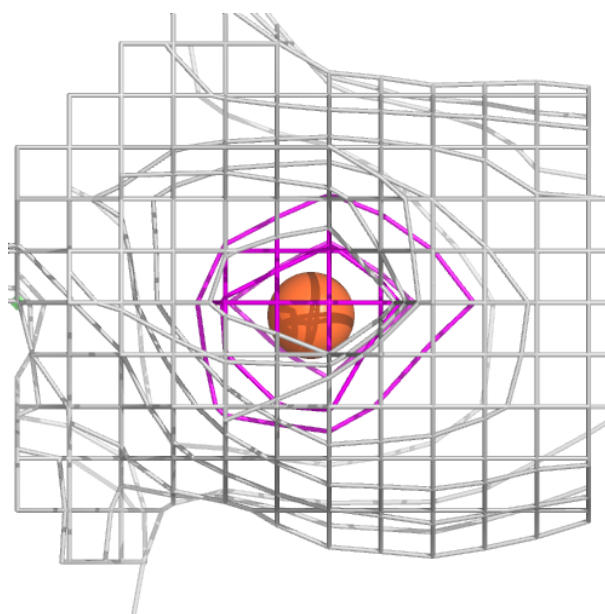


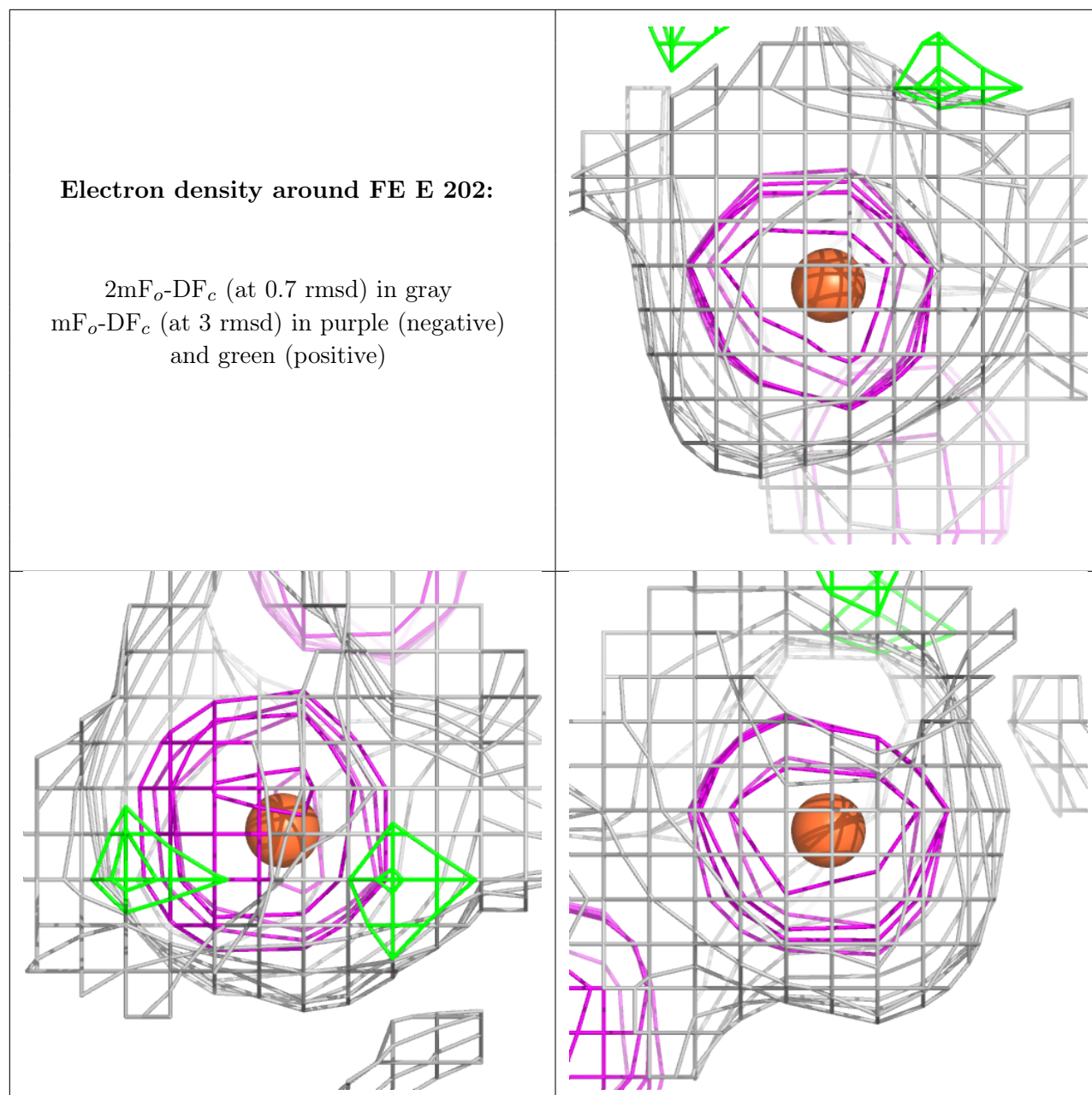




Electron density around FE M 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.