



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 01:16 pm BST

PDB ID : 9S4O / pdb_00009s4o
Title : diFe-Sulerythin_wildtype_O2-reacted
Authors : Jeoung, J.-H.; Dobbek, H.
Deposited on : 2025-07-28
Resolution : 1.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

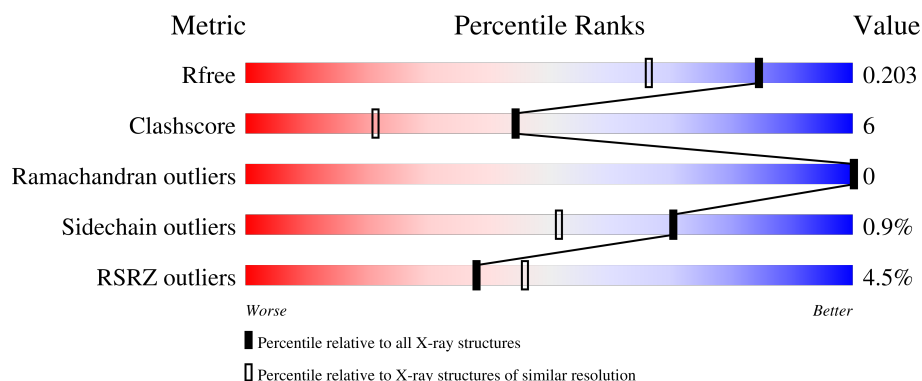
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	146	
1	B	146	
1	C	146	
1	D	146	
1	E	146	

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Mol	Chain	Length	Quality of chain
1	F	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	A	205	-	-	X	-
5	CL	F	201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14351 atoms, of which 6711 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 Sulerythrin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	H	N	O	S	0	6	0
			2313	741	1145	198	224	5			
1	B	145	Total	C	H	N	O	S	0	6	0
			2315	742	1143	197	228	5			
1	C	143	Total	C	H	N	O	S	0	7	0
			2327	745	1152	199	226	5			
1	D	141	Total	C	H	N	O	S	0	0	0
			2196	707	1082	190	214	3			
1	E	138	Total	C	H	N	O	S	0	4	0
			2209	711	1089	190	215	4			
1	F	140	Total	C	H	N	O	S	0	3	0
			2228	715	1100	193	216	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP F9VPE5
A	0	ASN	-	expression tag	UNP F9VPE5
B	-1	GLY	-	expression tag	UNP F9VPE5
B	0	ASN	-	expression tag	UNP F9VPE5
C	-1	GLY	-	expression tag	UNP F9VPE5
C	0	ASN	-	expression tag	UNP F9VPE5
D	-1	GLY	-	expression tag	UNP F9VPE5
D	0	ASN	-	expression tag	UNP F9VPE5
E	-1	GLY	-	expression tag	UNP F9VPE5
E	0	ASN	-	expression tag	UNP F9VPE5
F	-1	GLY	-	expression tag	UNP F9VPE5
F	0	ASN	-	expression tag	UNP F9VPE5

- 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	2	Total Fe 2 2	0	1
2	B	2	Total Fe 2 2	0	1
2	C	2	Total Fe 2 2	0	1
2	D	2	Total Fe 2 2	0	1
2	E	2	Total Fe 2 2	0	1
2	F	2	Total Fe 2 2	0	1

- Molecule 3 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	2	Total 2	Cl 2	0	0
5	F	2	Total 2	Cl 2	0	0

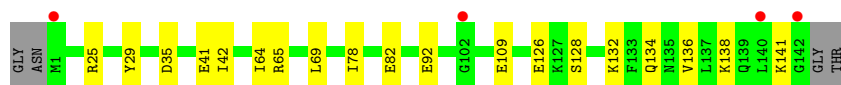
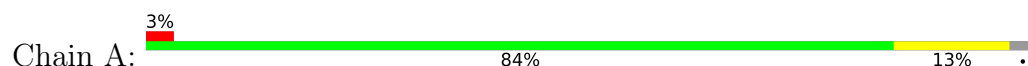
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total 148	O 148	0	0
6	B	124	Total 124	O 124	0	0
6	C	126	Total 126	O 126	0	0
6	D	115	Total 115	O 115	0	0
6	E	116	Total 116	O 116	0	0
6	F	102	Total 102	O 102	0	0

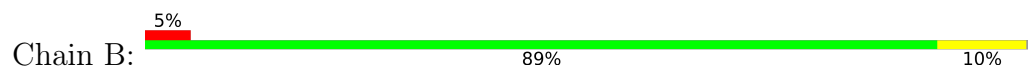
3 Residue-property plots [i](#)

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.

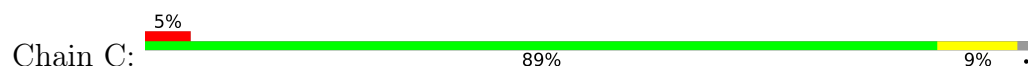
- Molecule 1: Sulerythrin



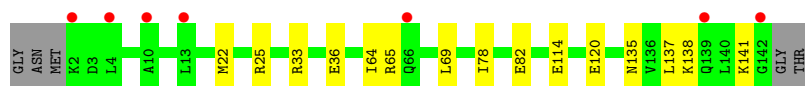
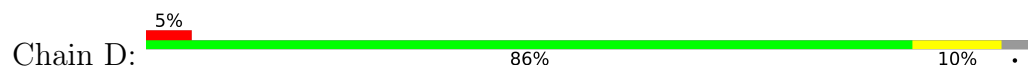
- Molecule 1: Sulerythrin



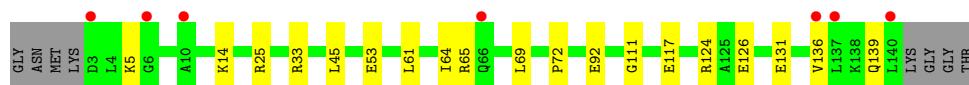
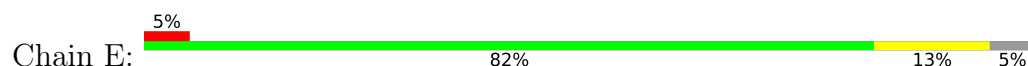
- Molecule 1: Sulerythrin



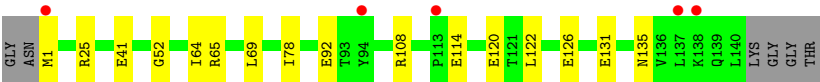
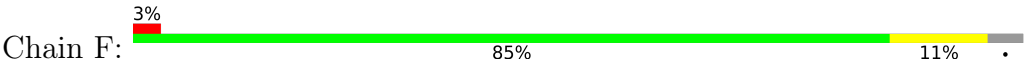
- Molecule 1: Sulerythrin



- Molecule 1: Sulerythrin



- Molecule 1: Sulerythrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.90Å 88.23Å 100.24Å 90.00° 114.56° 90.00°	Depositor
Resolution (Å)	34.07 – 1.55 34.07 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.07-1.55) 97.8 (34.07-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.176 , 0.203 0.176 , 0.203	Depositor DCC
R_{free} test set	6607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14351	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 69.24 % 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 3.8210e-06. 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: CL, FE2, FE, O

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	0.40	0/1201	0.57	0/1611
1	B	0.38	0/1211	0.53	0/1626
1	C	0.36	0/1211	0.52	0/1625
1	D	0.38	0/1138	0.55	0/1530
1	E	0.41	0/1153	0.57	0/1551
1	F	0.40	0/1158	0.58	0/1557
All	All	0.39	0/7072	0.55	0/9500

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1168	1145	1144	16	0
1	B	1172	1143	1143	15	0
1	C	1175	1152	1149	12	0
1	D	1114	1082	1082	13	0
1	E	1120	1089	1088	19	0
1	F	1128	1100	1101	15	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	3	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	3	0
6	A	148	0	0	2	0
6	B	124	0	0	1	0
6	C	126	0	0	6	0
6	D	115	0	0	1	0
6	E	116	0	0	6	0
6	F	102	0	0	4	0
All	All	7640	6711	6707	81	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 6.

All (81) 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:5:LYS:NZ	6:C:301:HOH:O	1.74	1.16
1:C:2:LYS:NZ	6:C:302:HOH:O	1.94	1.00
1:C:14:LYS:NZ	6:C:304:HOH:O	2.10	0.84
1:C:135[B]:ASN:ND2	6:C:303:HOH:O	2.08	0.84
1:E:117:GLU:OE2	6:E:301:HOH:O	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLU:OE1	1:E:126:GLU:OE1	2.00	0.80
1:E:131:GLU:OE2	6:E:302:HOH:O	2.01	0.76
1:A:109:GLU:OE1	6:A:301:HOH:O	2.04	0.75
1:F:135[A]:ASN:ND2	6:F:302:HOH:O	2.20	0.75
1:F:131:GLU:OE2	6:F:301:HOH:O	2.07	0.73
1:D:135:ASN:HA	1:D:138:LYS:HD2	1.74	0.69
1:D:33:ARG:NH1	1:D:36:GLU:OE2	2.26	0.68
1:E:117:GLU:OE1	6:E:303:HOH:O	2.10	0.67
1:C:135[A]:ASN:OD1	6:C:305:HOH:O	2.12	0.66
1:E:111:GLY:O	6:E:304:HOH:O	2.14	0.65
1:A:82[A]:GLU:OE1	1:A:141:LYS:NZ	2.29	0.65
1:B:1:MET:HE3	5:F:201:CL:CL	2.37	0.62
1:B:114:GLU:H	1:B:114:GLU:CD	2.10	0.60
1:B:1:MET:HA	1:B:1:MET:HE2	1.85	0.58
1:E:64:ILE:HG23	1:E:69:LEU:HB2	1.87	0.56
1:E:131:GLU:CG	6:E:302:HOH:O	2.53	0.56
1:D:33:ARG:NH1	1:D:36:GLU:CD	2.64	0.56
1:E:124:ARG:NH2	6:E:303:HOH:O	2.39	0.56
1:F:1:MET:SD	1:F:1:MET:O	2.64	0.56
1:A:65[B]:ARG:HH22	1:E:33:ARG:NH2	2.04	0.54
1:F:65[A]:ARG:HG2	1:F:78:ILE:HG13	1.89	0.54
1:E:5:LYS:HE2	1:E:69:LEU:HA	1.91	0.52
1:D:65:ARG:HG2	1:D:78:ILE:HG13	1.91	0.52
1:F:131:GLU:CG	6:F:301:HOH:O	2.57	0.51
1:B:1:MET:SD	1:F:114:GLU:OE1	2.69	0.50
1:B:80:THR:O	1:B:84:MET:HG3	2.12	0.50
1:B:92:GLU:OE1	1:B:126:GLU:OE1	2.30	0.49
1:D:64:ILE:HG23	1:D:69:LEU:HB2	1.94	0.49
1:A:65[B]:ARG:HG2	1:A:78:ILE:HG13	1.93	0.49
1:F:92:GLU:OE1	1:F:126:GLU:OE1	2.30	0.49
1:D:33:ARG:CZ	1:D:36:GLU:OE2	2.60	0.49
1:B:95:GLU:OE1	3:B:203:O:O	2.31	0.49
1:F:108:ARG:NH1	1:F:120:GLU:OE2	2.43	0.48
1:B:64:ILE:HG23	1:B:69:LEU:HB2	1.96	0.48
1:F:65[A]:ARG:HD2	1:F:78:ILE:HD12	1.96	0.48
1:D:114:GLU:H	1:D:114:GLU:CD	2.21	0.48
1:A:134:GLN:O	1:A:138:LYS:HG3	2.14	0.48
1:A:29:TYR:HE2	1:E:65[B]:ARG:HD3	1.79	0.47
1:C:122:LEU:O	1:C:126:GLU:HG2	2.14	0.47
1:C:72:PRO:HB2	1:D:22:MET:CE	2.45	0.47
1:D:82:GLU:OE2	1:D:141:LYS:NZ	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG23	1:A:69:LEU:HB2	1.96	0.47
1:D:33:ARG:NH2	1:D:36:GLU:OE2	2.48	0.47
1:F:122:LEU:O	1:F:126:GLU:HG2	2.14	0.47
1:C:64:ILE:HG23	1:C:69:LEU:HB2	1.97	0.46
1:A:42:ILE:HG12	1:E:136:VAL:CG2	2.46	0.46
1:B:127:LYS:NZ	1:B:131:GLU:OE1	2.45	0.46
1:A:41[B]:GLU:HB2	5:A:205:CL:CL	2.53	0.46
1:A:65[B]:ARG:NH2	1:E:33:ARG:NH2	2.64	0.45
1:F:64:ILE:HG23	1:F:69:LEU:HB2	1.98	0.45
1:A:92:GLU:OE1	1:A:126:GLU:OE1	2.34	0.45
1:D:120:GLU:OE1	6:D:301:HOH:O	2.21	0.45
1:F:135[A]:ASN:CG	6:F:302:HOH:O	2.57	0.44
1:A:41[B]:GLU:HG2	6:A:424:HOH:O	2.16	0.44
1:B:108:ARG:NH2	1:B:120:GLU:HG3	2.33	0.44
1:B:108:ARG:HH22	1:B:120:GLU:CD	2.25	0.44
1:C:36:GLU:HG3	6:C:349:HOH:O	2.18	0.44
1:D:137:LEU:HD11	1:D:141:LYS:HE2	1.99	0.44
1:B:108:ARG:HH22	1:B:120:GLU:CG	2.31	0.43
1:C:33:ARG:NH1	1:D:65:ARG:HH22	2.16	0.43
1:B:108:ARG:HH22	1:B:120:GLU:HG3	1.82	0.43
1:E:14:LYS:HG3	1:E:72:PRO:HB3	2.01	0.43
1:E:61:LEU:O	1:E:65[B]:ARG:HG3	2.18	0.43
1:C:92:GLU:OE1	1:C:126:GLU:OE1	2.37	0.43
1:A:136:VAL:HG21	1:E:45:LEU:HD23	2.01	0.42
1:B:1:MET:HG3	1:F:114:GLU:OE1	2.21	0.41
1:A:41[A]:GLU:HB3	5:A:205:CL:CL	2.57	0.41
1:C:5:LYS:HD3	1:C:5:LYS:HA	1.94	0.41
5:A:205:CL:CL	1:E:139:GLN:NE2	2.86	0.41
1:F:41:GLU:HB2	5:F:205:CL:CL	2.58	0.41
1:A:128:SER:O	1:A:132:LYS:HG2	2.21	0.41
1:A:35:ASP:HB3	1:F:52:GLY:HA2	2.02	0.41
6:B:394:HOH:O	5:F:201:CL:CL	2.59	0.41
1:E:136:VAL:O	1:E:139:GLN:HG3	2.21	0.41
1:B:122:LEU:O	1:B:126:GLU:HG2	2.21	0.40
1:E:53:GLU:HA	1:E:53:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/146 (100%)	144 (99%)	2 (1%)	0	100	100
1	B	149/146 (102%)	146 (98%)	3 (2%)	0	100	100
1	C	148/146 (101%)	144 (97%)	4 (3%)	0	100	100
1	D	139/146 (95%)	136 (98%)	3 (2%)	0	100	100
1	E	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
1	F	141/146 (97%)	139 (99%)	2 (1%)	0	100	100
All	All	863/876 (98%)	847 (98%)	16 (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	117/113 (104%)	116 (99%)	1 (1%)	70	51
1	B	118/113 (104%)	117 (99%)	1 (1%)	73	56
1	C	118/113 (104%)	117 (99%)	1 (1%)	73	56
1	D	110/113 (97%)	109 (99%)	1 (1%)	70	51
1	E	112/113 (99%)	111 (99%)	1 (1%)	70	51
1	F	113/113 (100%)	112 (99%)	1 (1%)	70	51
All	All	688/678 (102%)	682 (99%)	6 (1%)	70	51

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	B	25	ARG
1	C	25	ARG
1	D	25	ARG
1	E	25	ARG
1	F	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	15	GLN
1	E	66	GLN
1	F	98	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	142/146 (97%)	0.05	4 (2%)	55	63	9, 24, 50, 68	6 (4%)
1	B	145/146 (99%)	0.36	7 (4%)	35	43	11, 27, 56, 69	6 (4%)
1	C	143/146 (97%)	0.42	8 (5%)	30	36	13, 29, 64, 86	7 (4%)
1	D	141/146 (96%)	0.43	7 (4%)	34	41	16, 31, 59, 91	0
1	E	138/146 (94%)	0.21	7 (5%)	33	40	10, 27, 50, 63	4 (2%)
1	F	140/146 (95%)	0.40	5 (3%)	46	54	16, 30, 51, 104	3 (2%)
All	All	849/876 (96%)	0.31	38 (4%)	38	46	9, 29, 57, 104	26 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	5.7
1	B	143	GLY	4.1
1	E	140	LEU	3.8
1	D	142	GLY	3.5
1	F	1	MET	3.2
1	A	142	GLY	3.2
1	C	2	LYS	3.1
1	D	13	LEU	3.1
1	D	2	LYS	3.1
1	B	1	MET	2.9
1	E	10	ALA	2.8
1	C	113	PRO	2.7
1	D	10	ALA	2.6
1	E	6	GLY	2.6
1	F	138	LYS	2.6
1	A	1	MET	2.6
1	F	94	TYR	2.6
1	C	114	GLU	2.6
1	C	136	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	66	GLN	2.5
1	C	112	PHE	2.5
1	C	115	VAL	2.5
1	A	102	GLY	2.4
1	B	140	LEU	2.4
1	F	137	LEU	2.4
1	E	137	LEU	2.3
1	D	4	LEU	2.2
1	B	135[A]	ASN	2.2
1	C	3	ASP	2.2
1	B	114	GLU	2.2
1	D	139	GLN	2.2
1	E	3	ASP	2.2
1	B	142	GLY	2.1
1	A	140	LEU	2.1
1	E	136	VAL	2.1
1	C	144	THR	2.1
1	F	113	PRO	2.0
1	D	66	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	O	B	202	1/1	0.79	0.30	26,26,26,26	1
3	O	A	202	1/1	0.80	0.39	27,27,27,27	1
3	O	C	205	1/1	0.86	0.41	24,24,24,24	1
3	O	D	205	1/1	0.87	0.29	29,29,29,29	1

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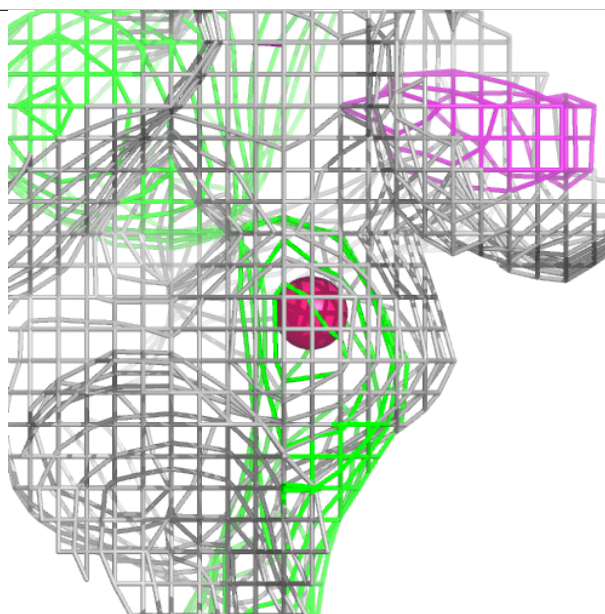
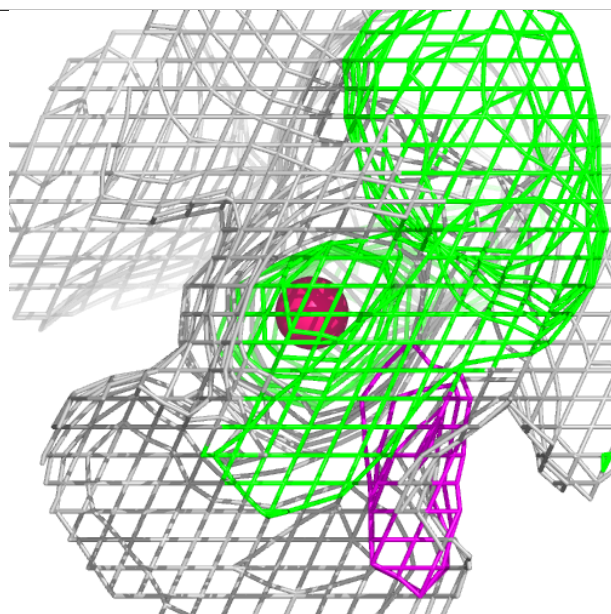
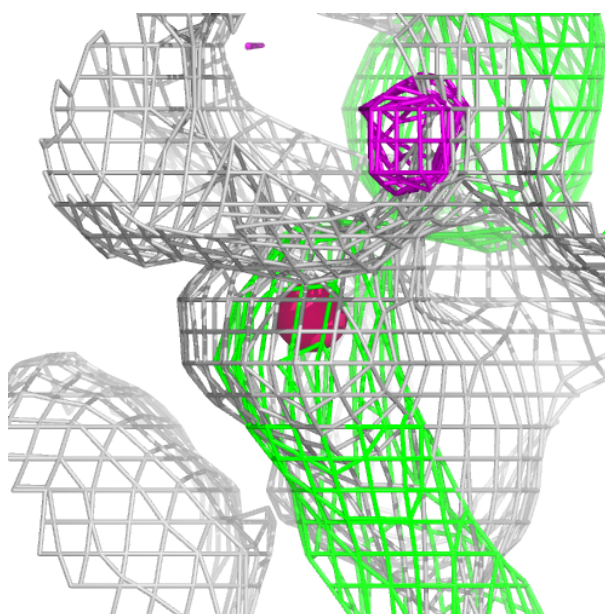
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	O	B	203	1/1	0.88	0.33	28,28,28,28	1
4	FE2	A	204[B]	1/1	0.88	0.09	33,33,33,33	1
2	FE	E	203[B]	1/1	0.90	0.12	33,33,33,33	1
3	O	E	201	1/1	0.91	0.30	24,24,24,24	1
4	FE2	B	206[B]	1/1	0.91	0.08	34,34,34,34	1
2	FE	F	204[B]	1/1	0.93	0.09	31,31,31,31	1
2	FE	C	203[B]	1/1	0.94	0.07	33,33,33,33	1
2	FE	D	202[B]	1/1	0.94	0.08	38,38,38,38	1
5	CL	A	205	1/1	0.94	0.11	28,28,28,28	0
5	CL	C	204	1/1	0.95	0.13	26,26,26,26	0
4	FE2	C	202[A]	1/1	0.96	0.05	23,23,23,23	1
4	FE2	F	203[A]	1/1	0.96	0.04	21,21,21,21	1
2	FE	D	203	1/1	0.97	0.04	20,20,20,20	1
4	FE2	E	202[A]	1/1	0.97	0.04	18,18,18,18	1
2	FE	A	201	1/1	0.97	0.04	17,17,17,17	1
2	FE	E	204	1/1	0.97	0.04	20,20,20,20	1
5	CL	B	201	1/1	0.97	0.11	29,29,29,29	0
2	FE	B	205[A]	1/1	0.97	0.05	22,22,22,22	1
2	FE	A	203[A]	1/1	0.98	0.04	22,22,22,22	1
2	FE	F	202	1/1	0.98	0.03	19,19,19,19	1
2	FE	C	201	1/1	0.98	0.04	22,22,22,22	1
2	FE	B	204	1/1	0.98	0.04	19,19,19,19	1
4	FE2	D	201[A]	1/1	0.98	0.04	22,22,22,22	1
5	CL	E	205	1/1	0.98	0.07	26,26,26,26	0
5	CL	F	201	1/1	0.98	0.12	36,36,36,36	0
5	CL	F	205	1/1	0.98	0.06	29,29,29,29	0
5	CL	D	204	1/1	0.99	0.05	19,19,19,19	0
5	CL	E	206	1/1	0.99	0.18	25,25,25,25	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.

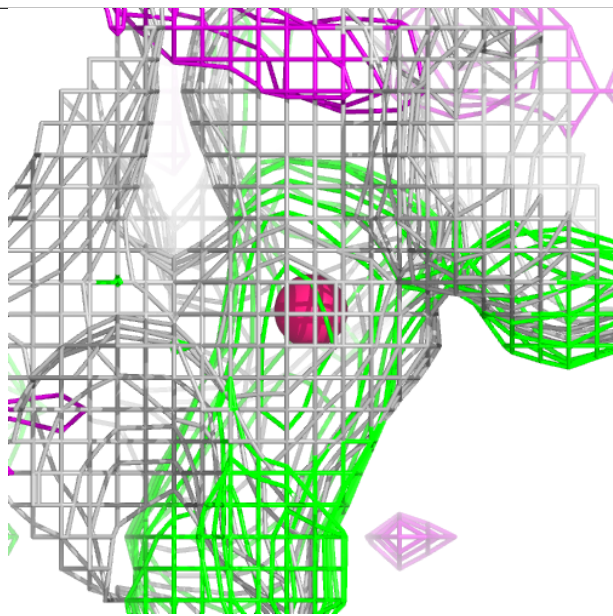
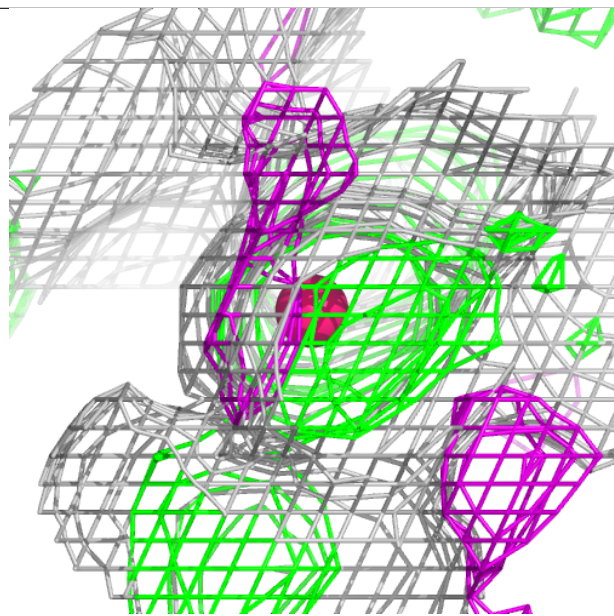
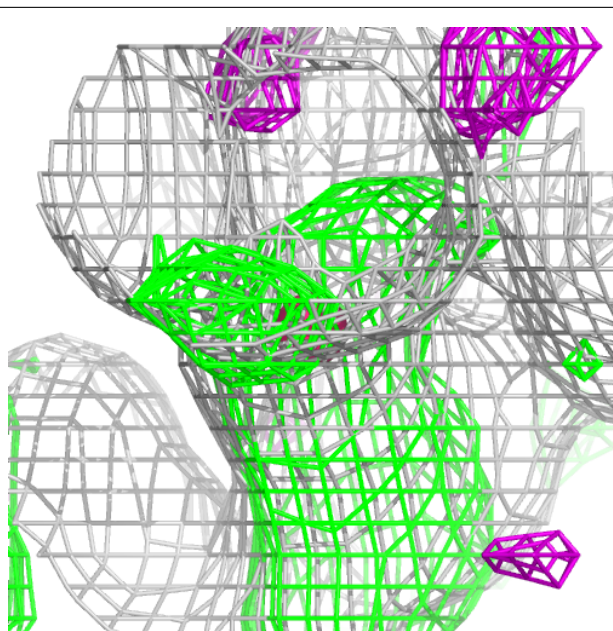
Electron density around O B 202:

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



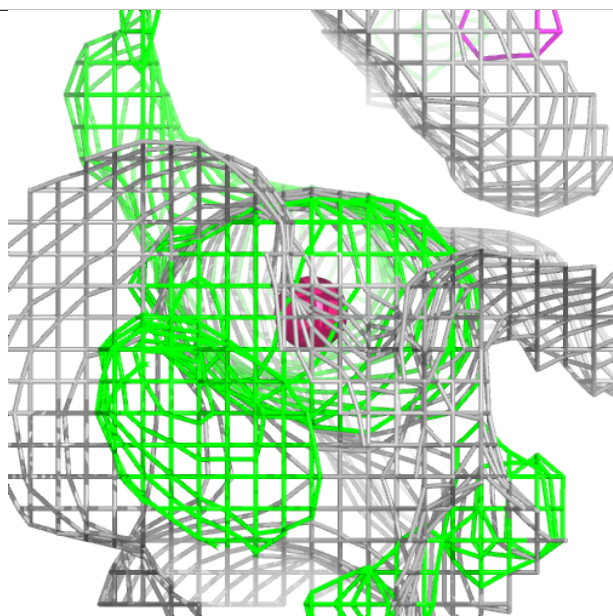
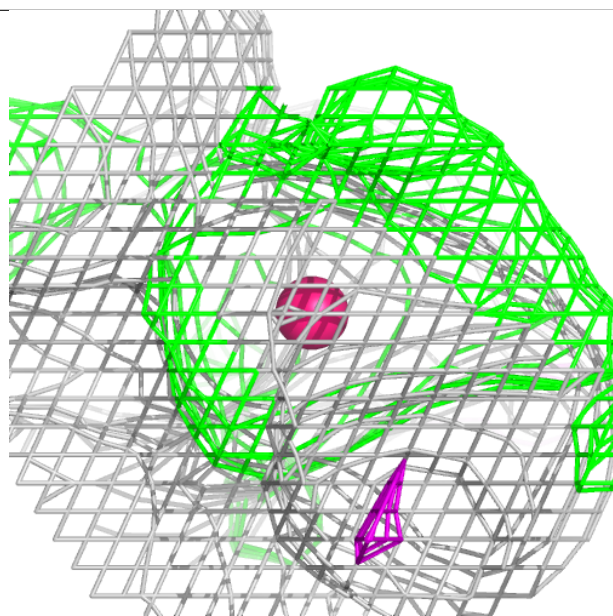
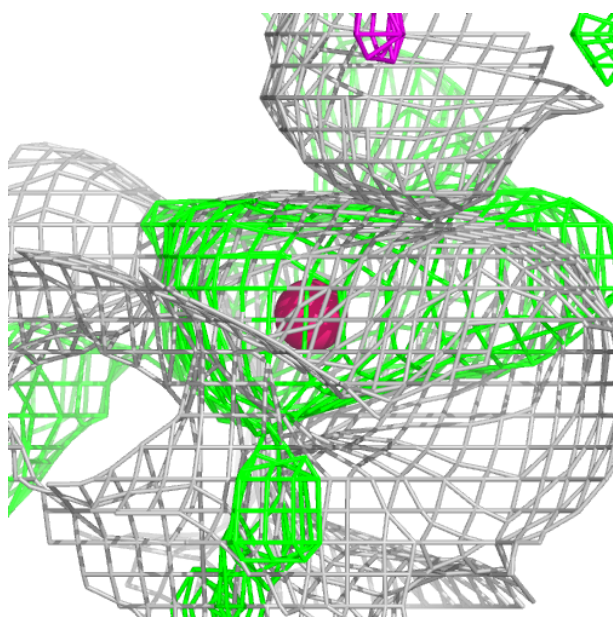
Electron density around O A 202:

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



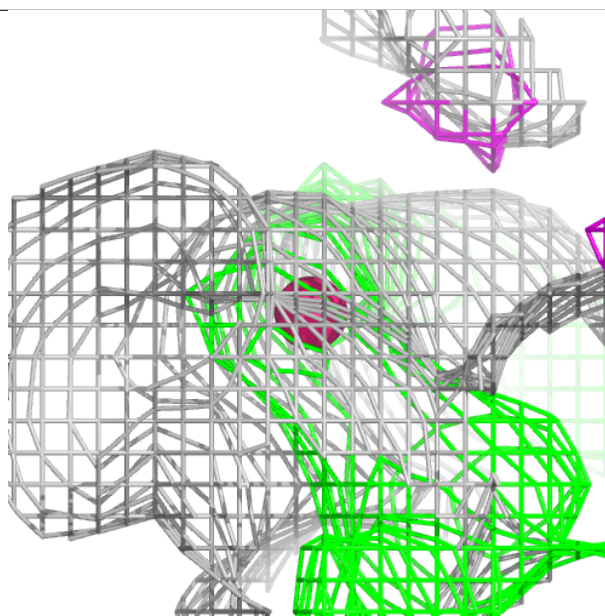
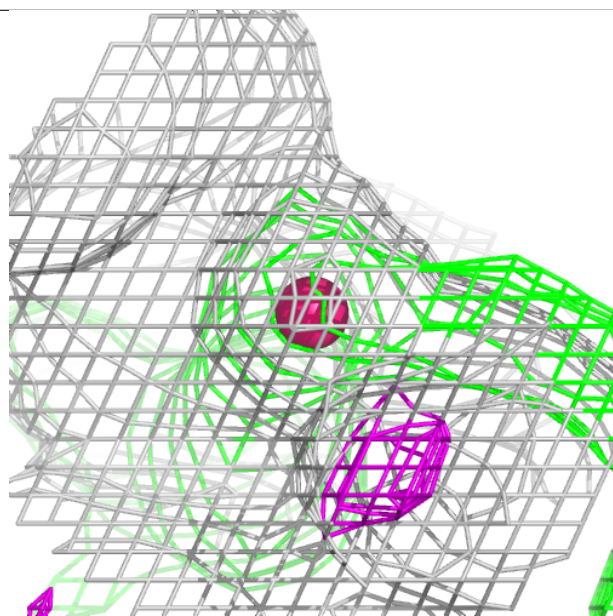
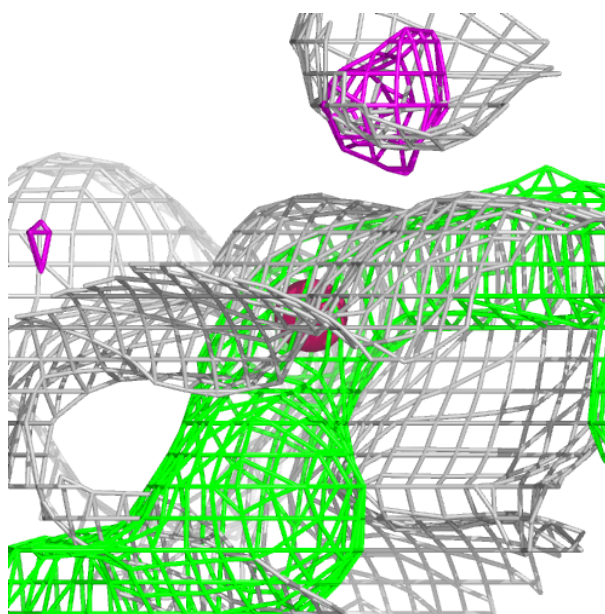
Electron density around O C 205:

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



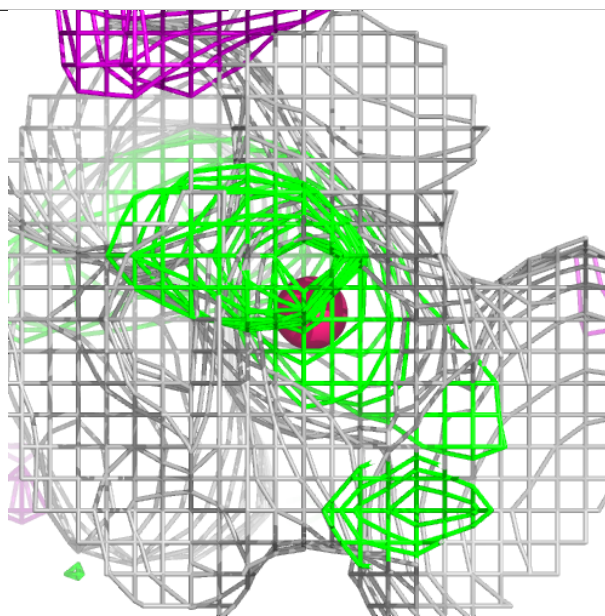
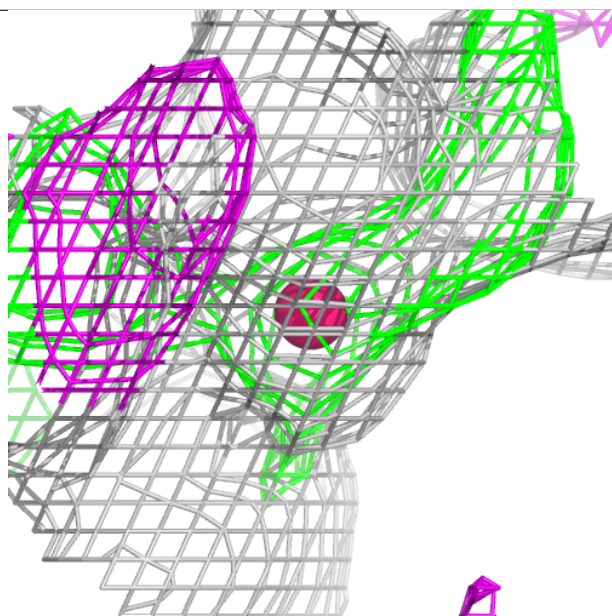
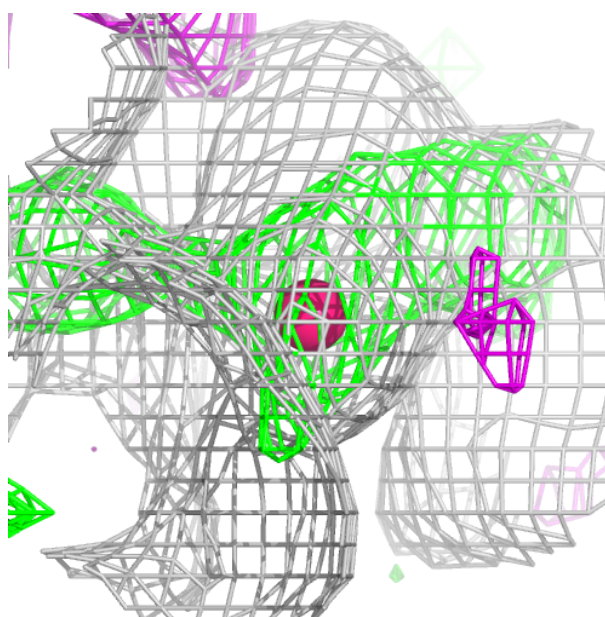
Electron density around O D 205:

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and green (positive)



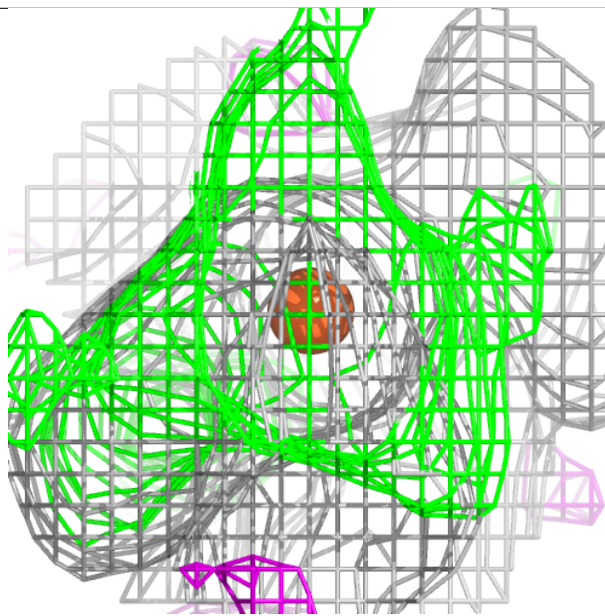
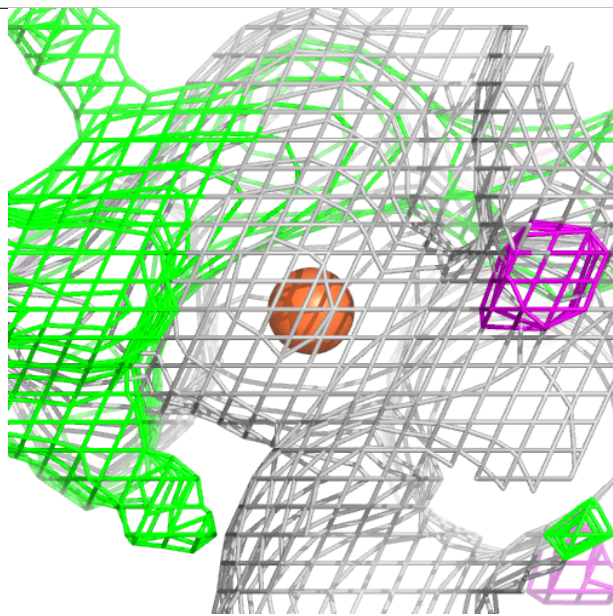
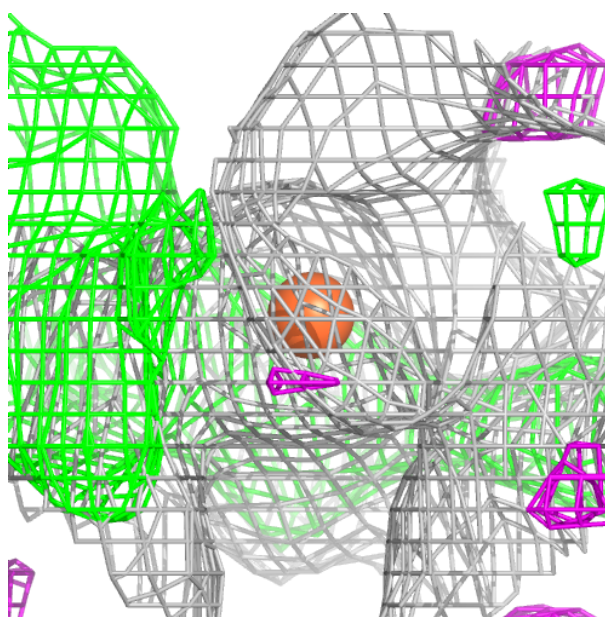
Electron density around O B 203:

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and green (positive)



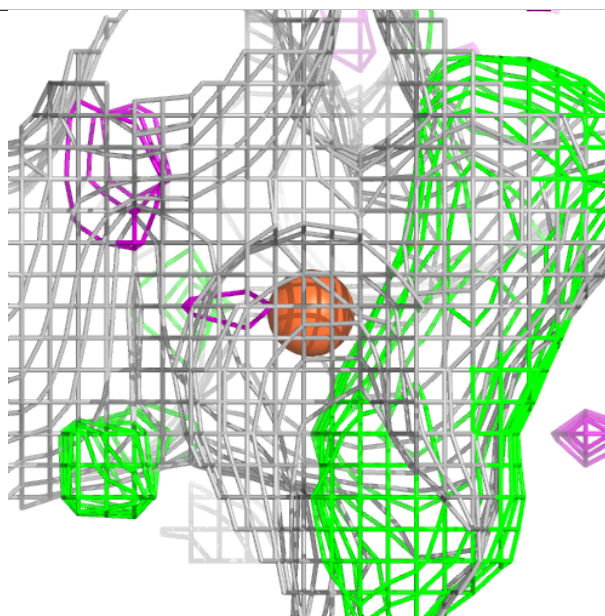
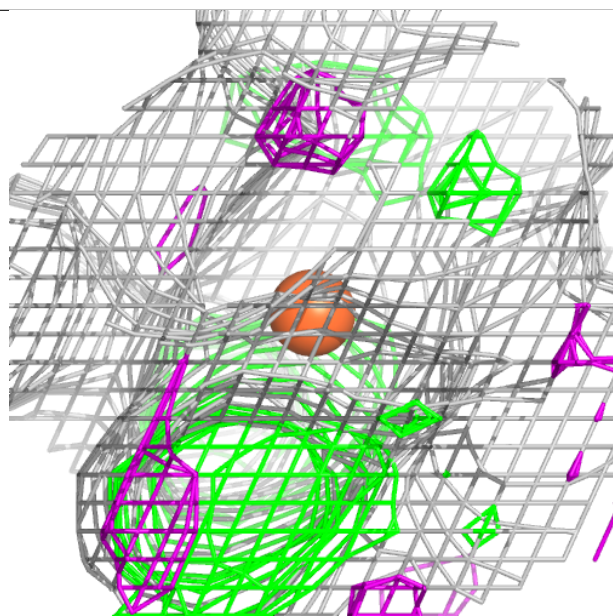
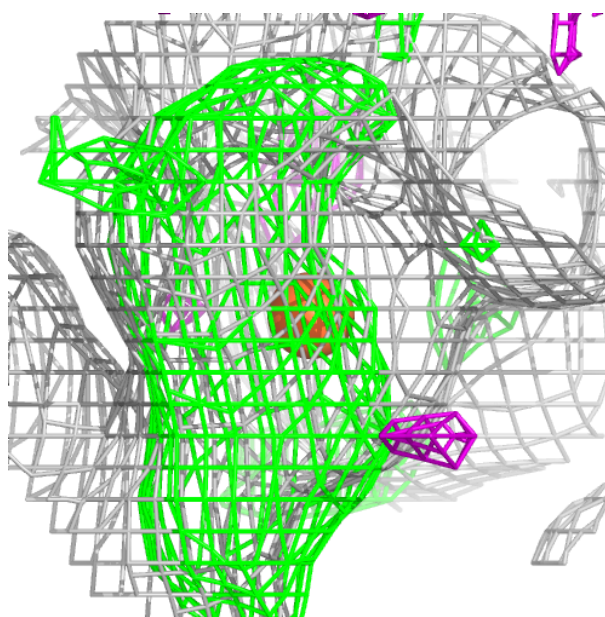
Electron density around FE2 A 204 (B):

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and green (positive)



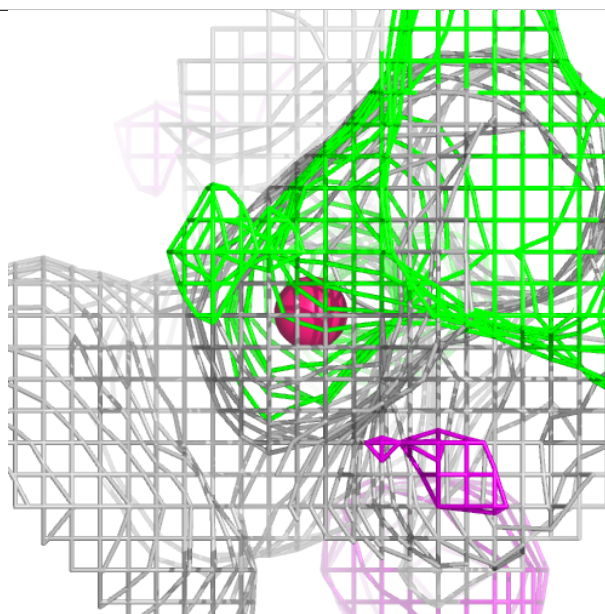
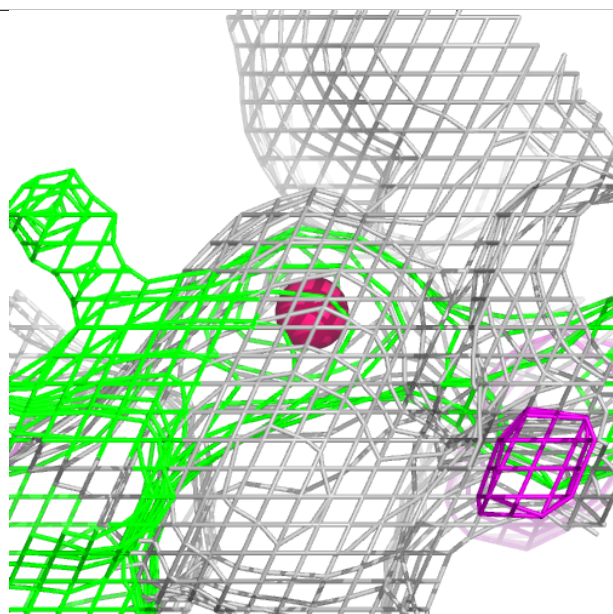
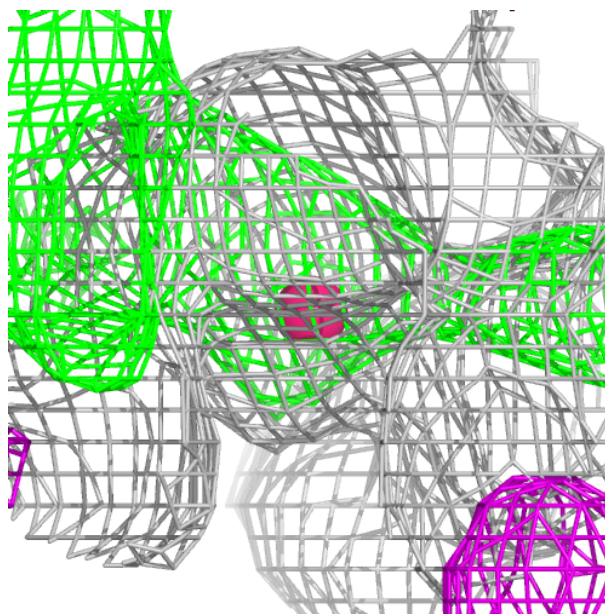
Electron density around FE E 203 (B):

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



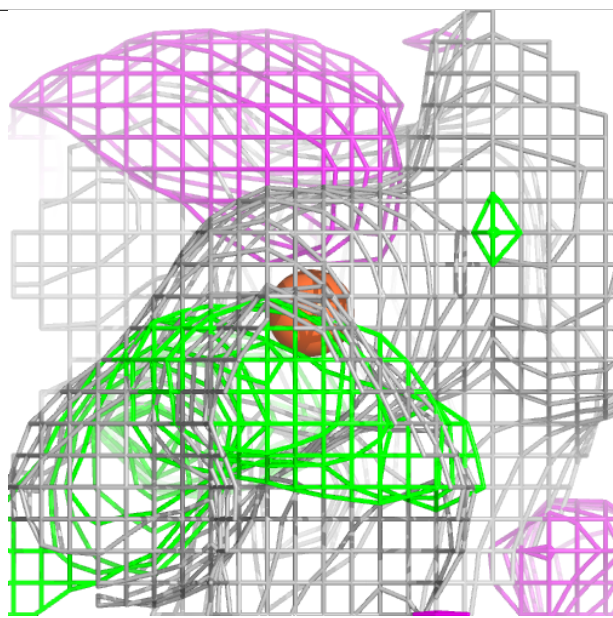
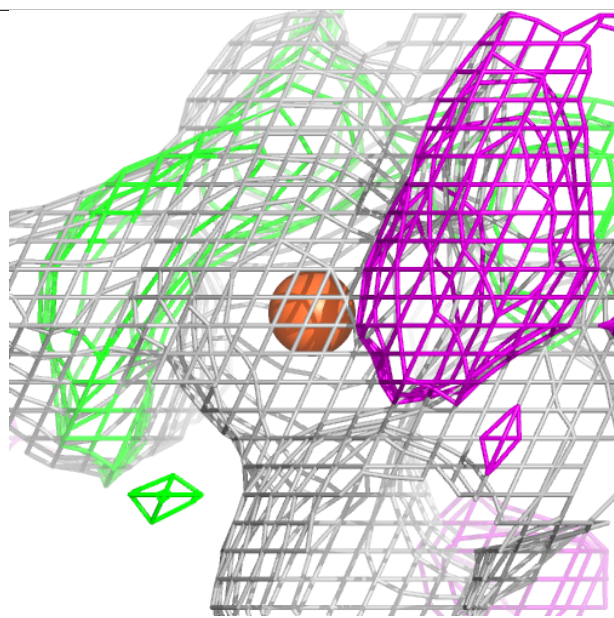
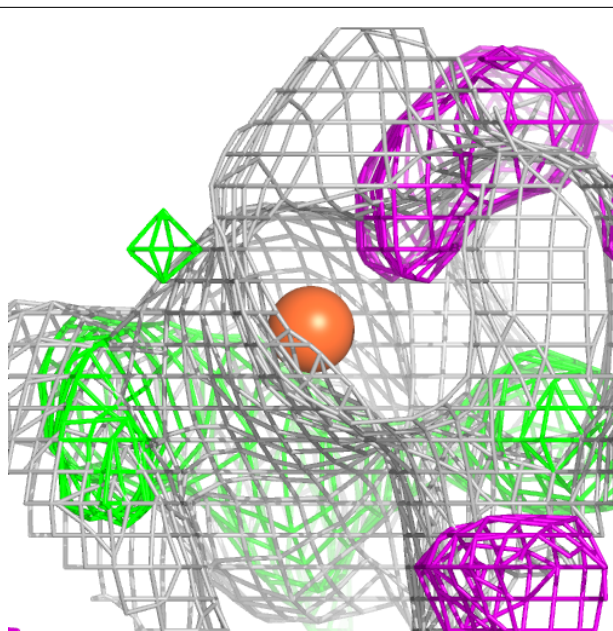
Electron density around O E 201:

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and green (positive)



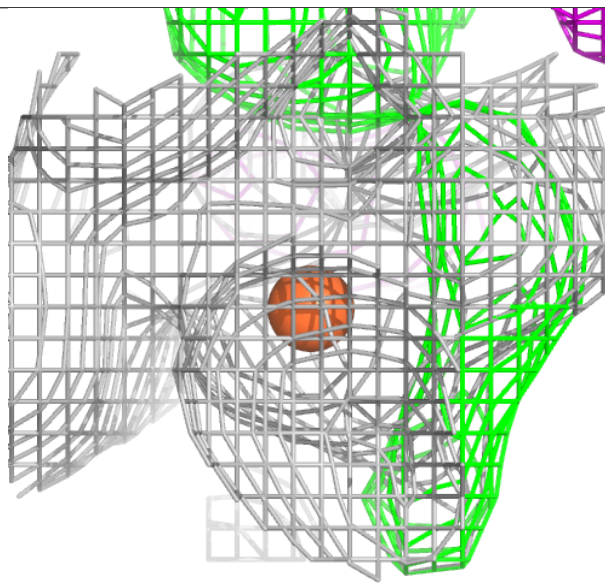
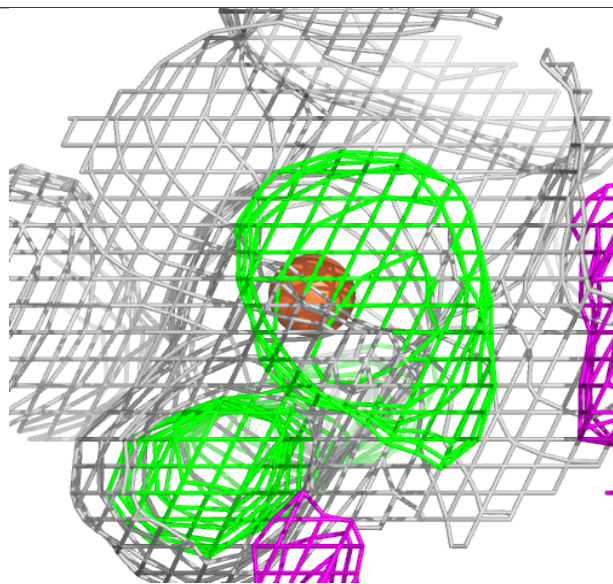
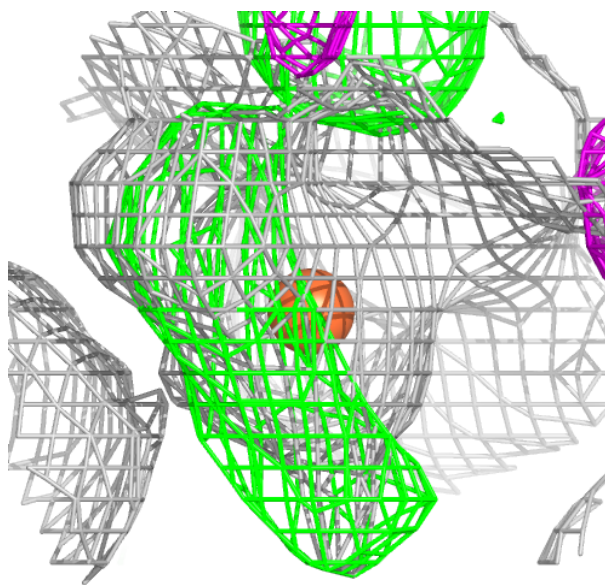
Electron density around FE2 B 206 (B):

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



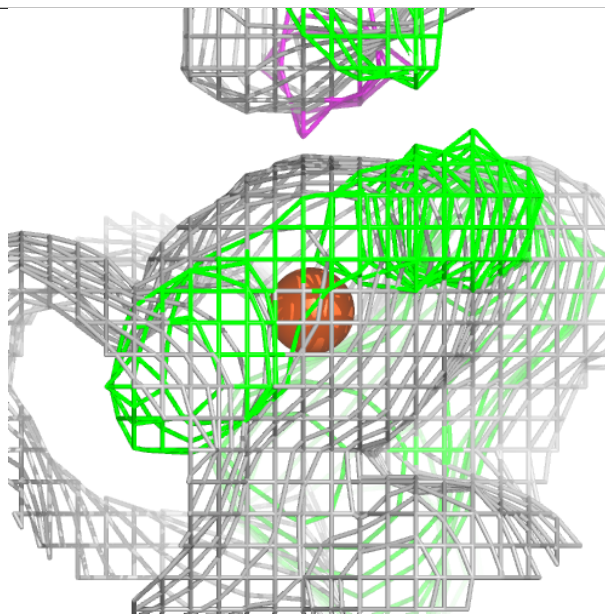
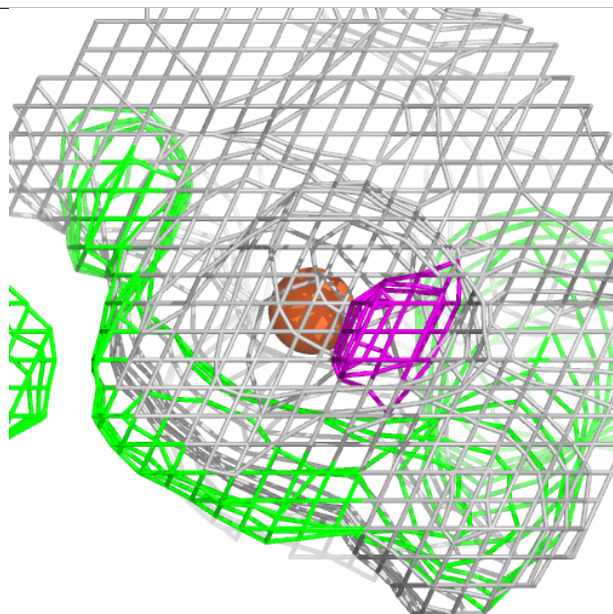
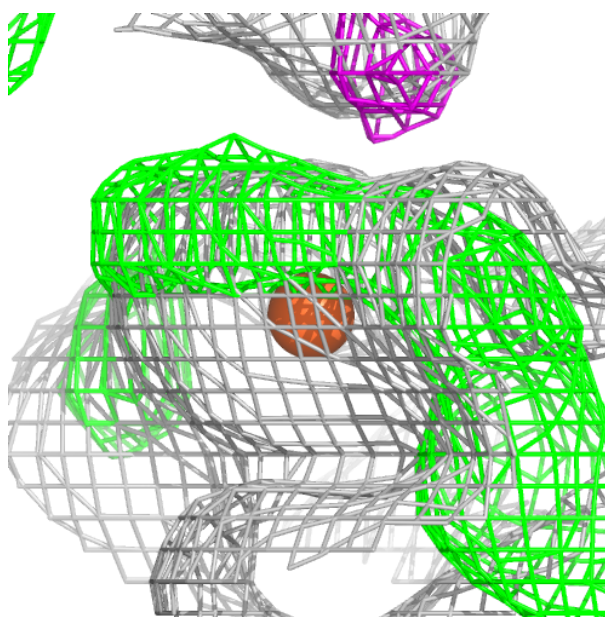
Electron density around FE F 204 (B):

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



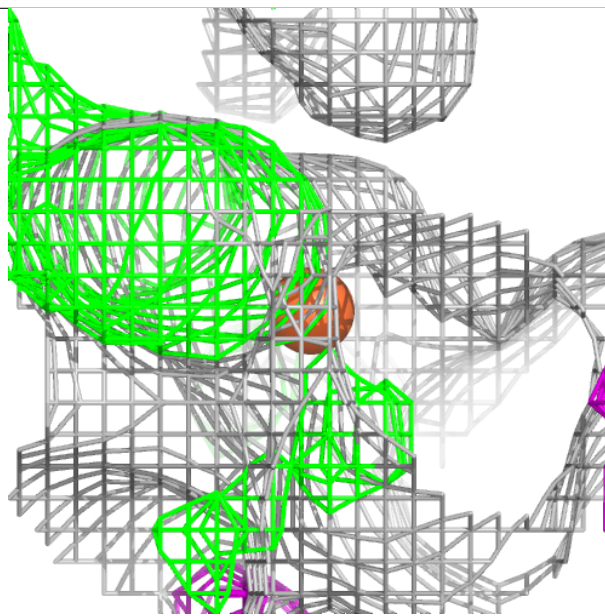
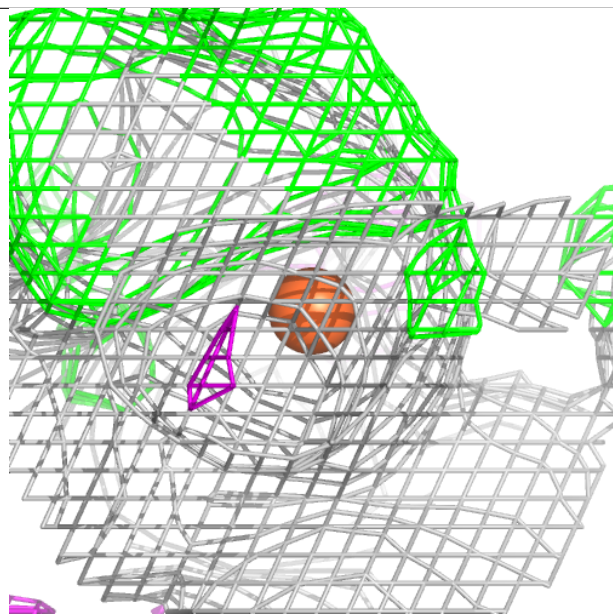
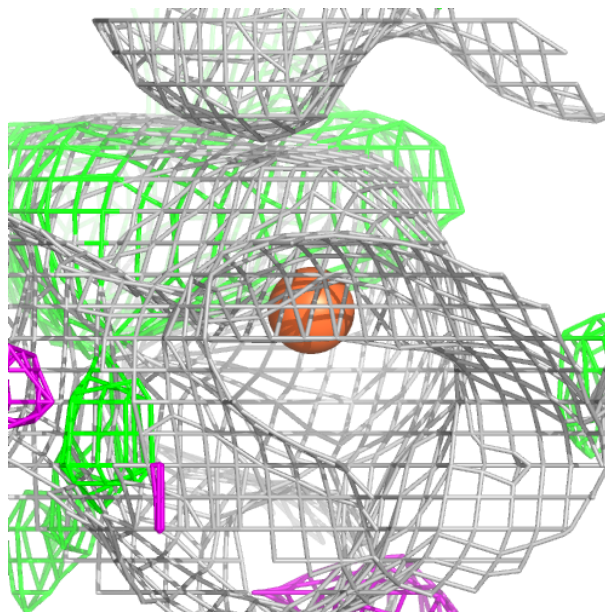
Electron density around FE C 203 (B):

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



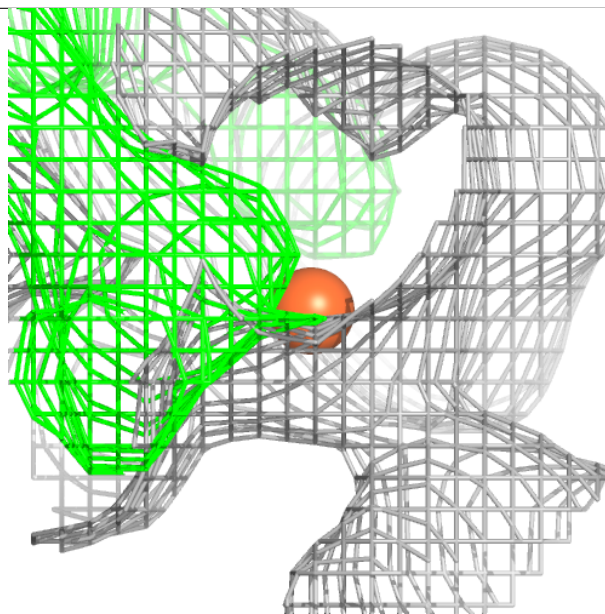
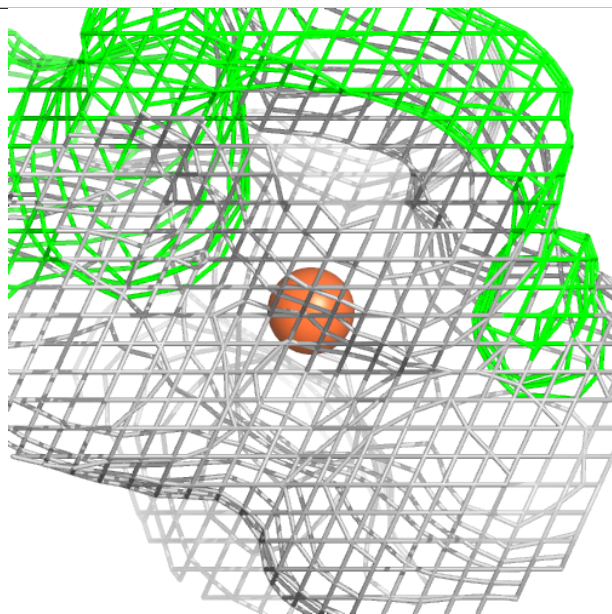
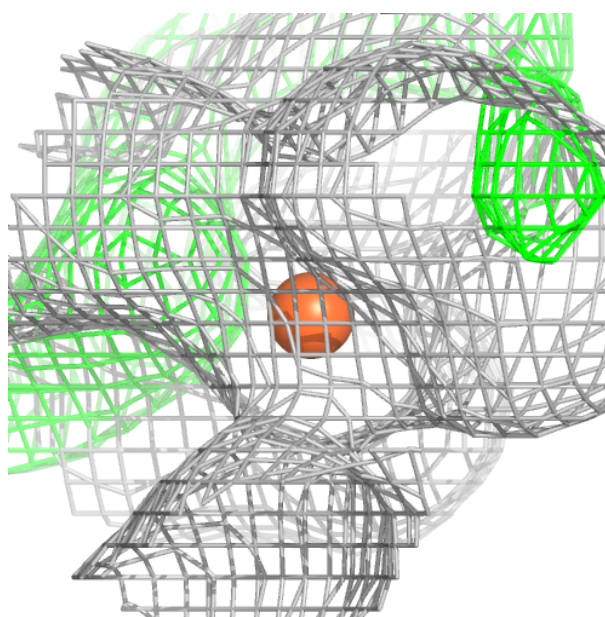
Electron density around FE D 202 (B):

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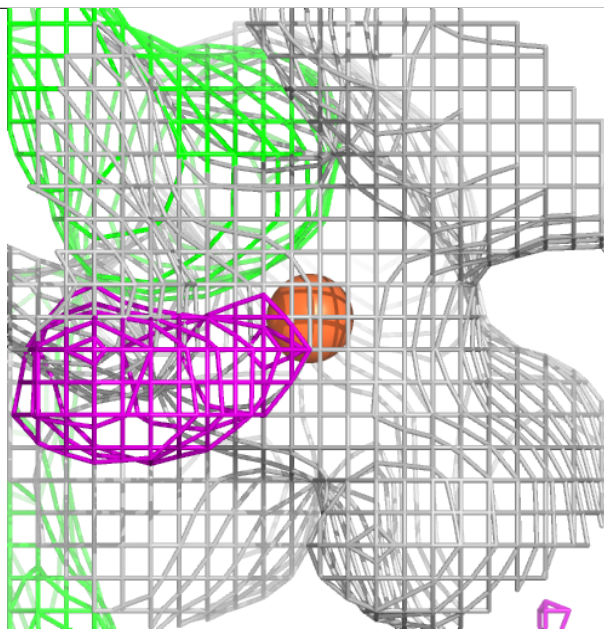
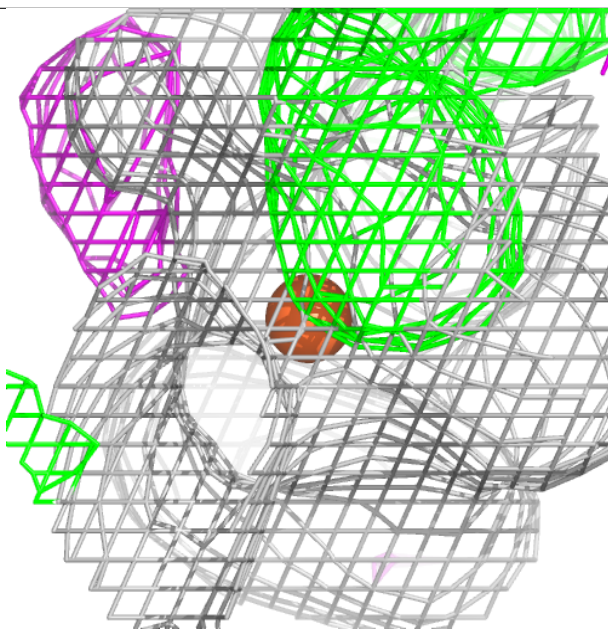
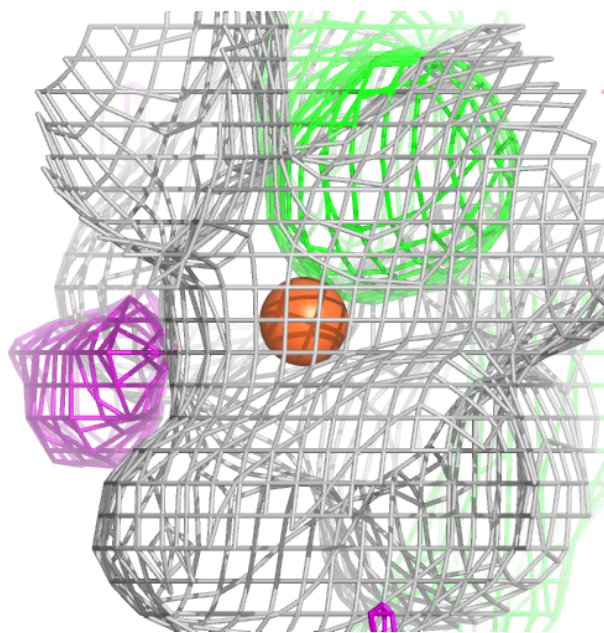
Electron density around FE2 C 202 (A):

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



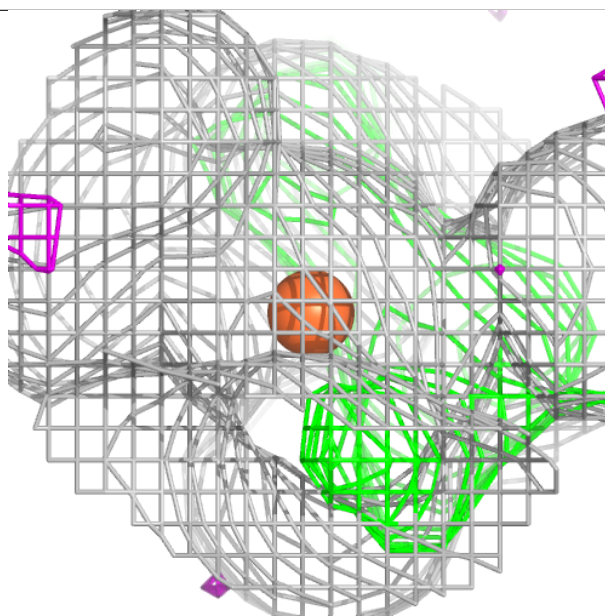
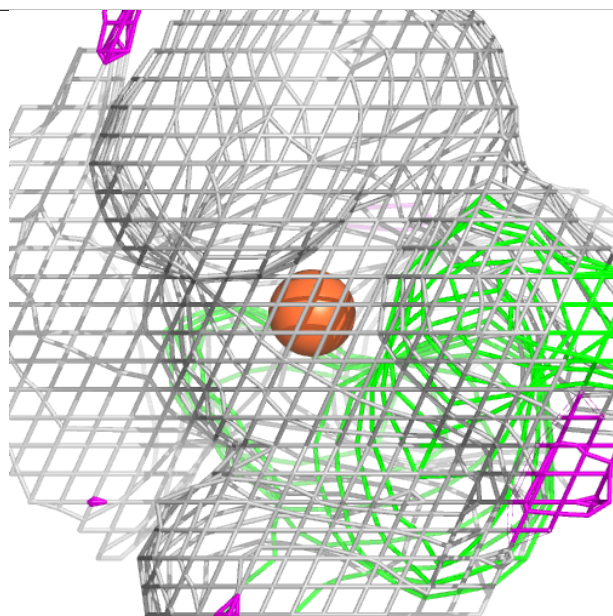
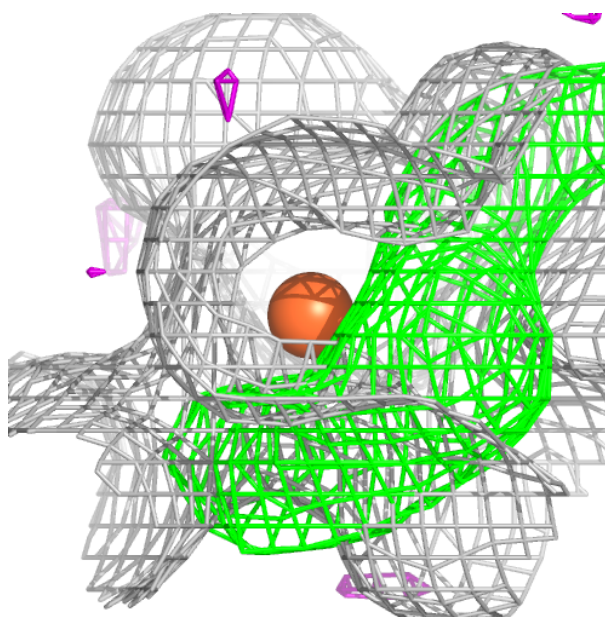
Electron density around FE2 F 203 (A):

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



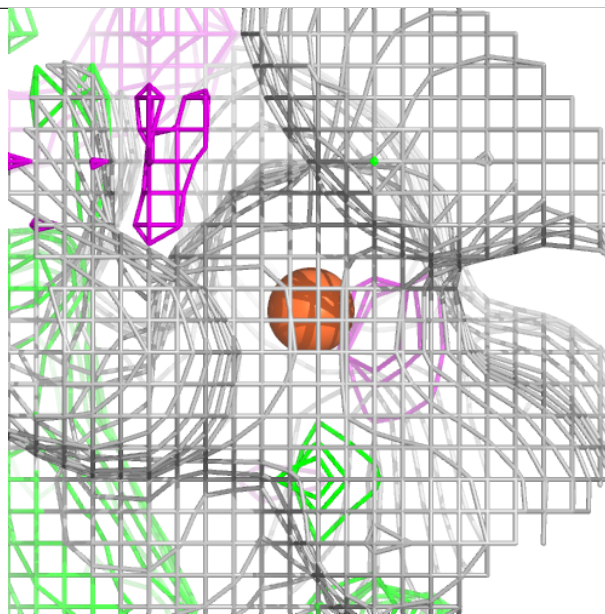
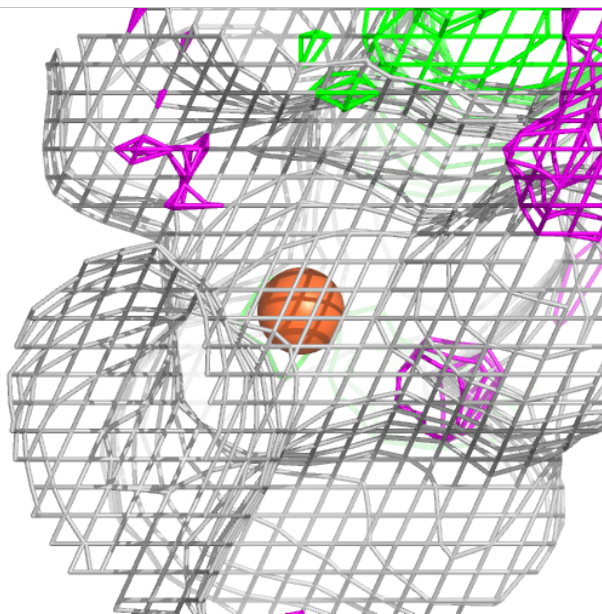
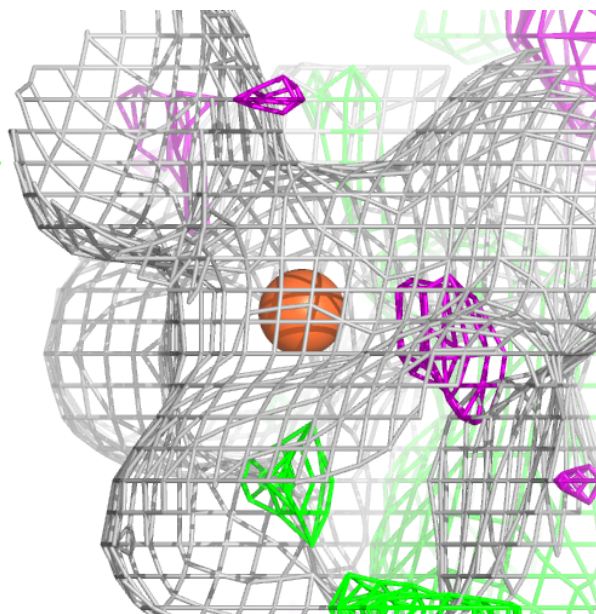
Electron density around FE D 203:

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and green (positive)



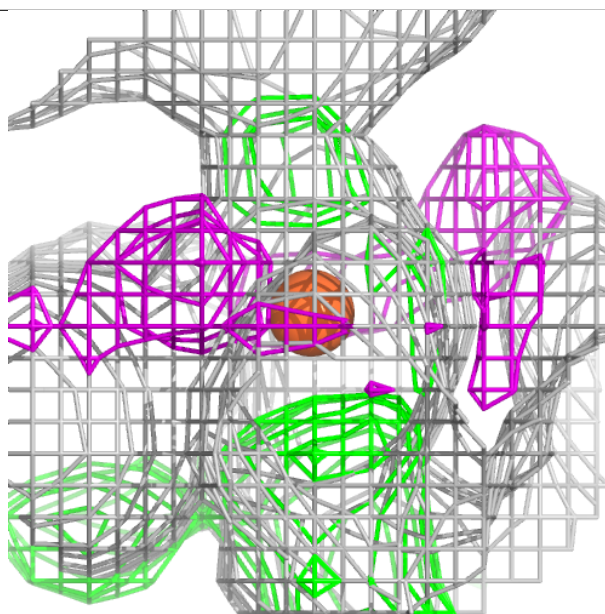
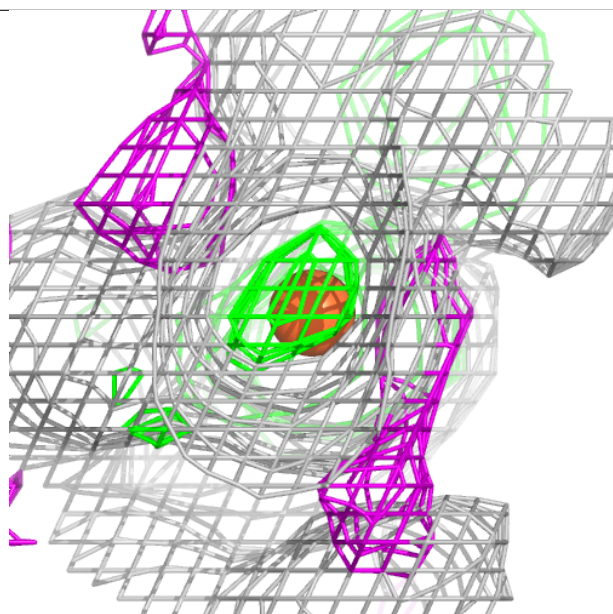
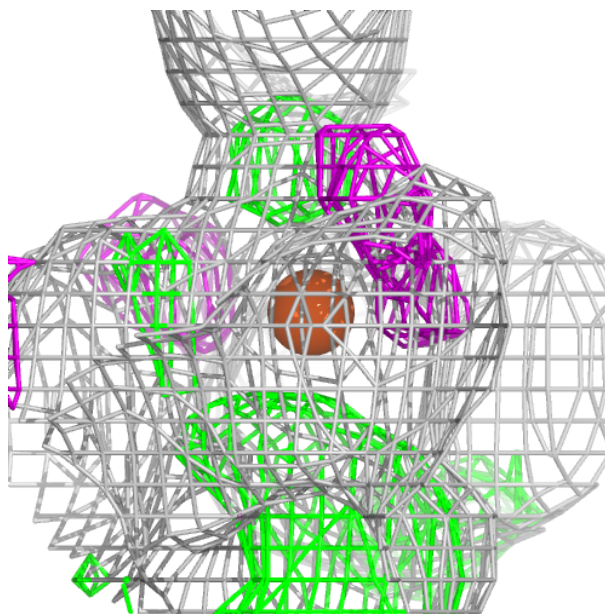
Electron density around FE2 E 202 (A):

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



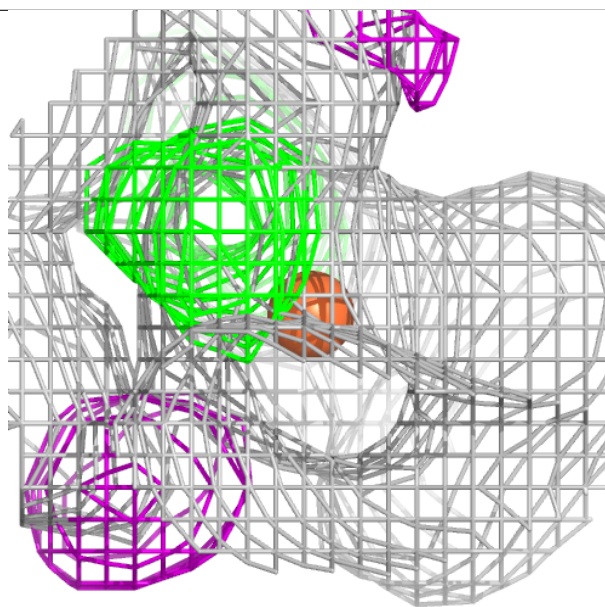
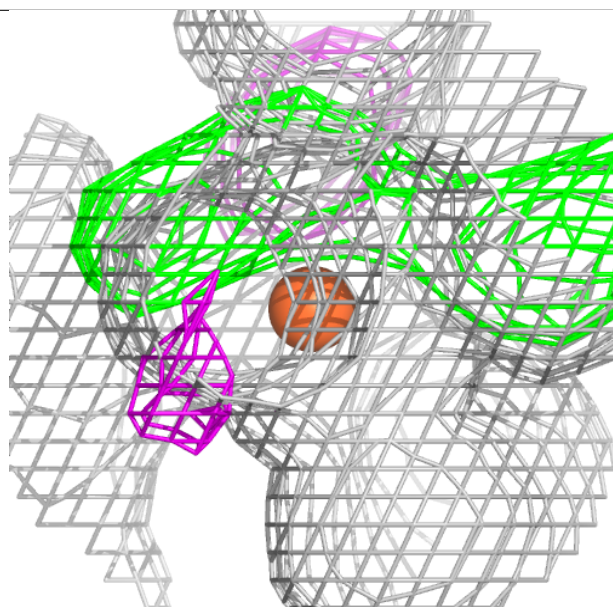
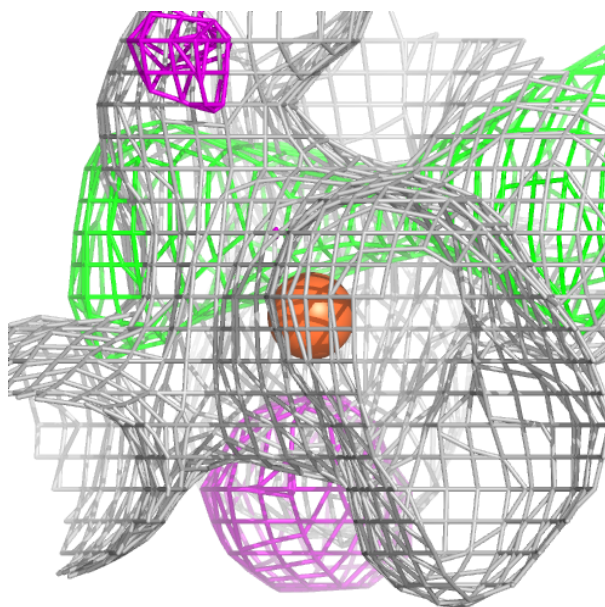
Electron density around FE A 201:

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



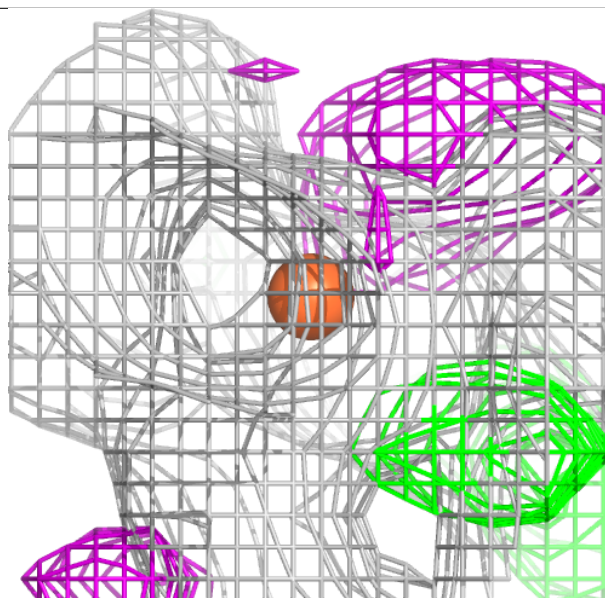
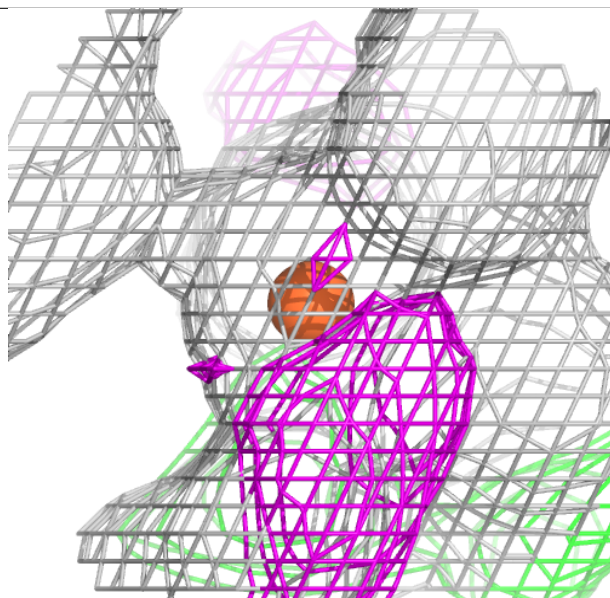
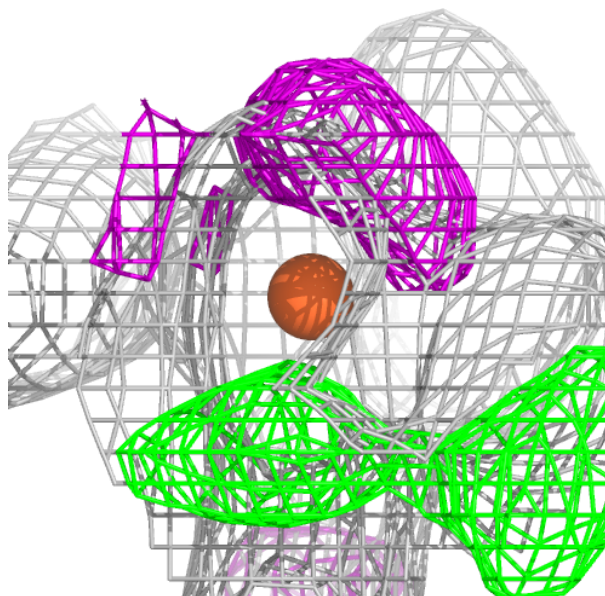
Electron density around FE E 204:

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



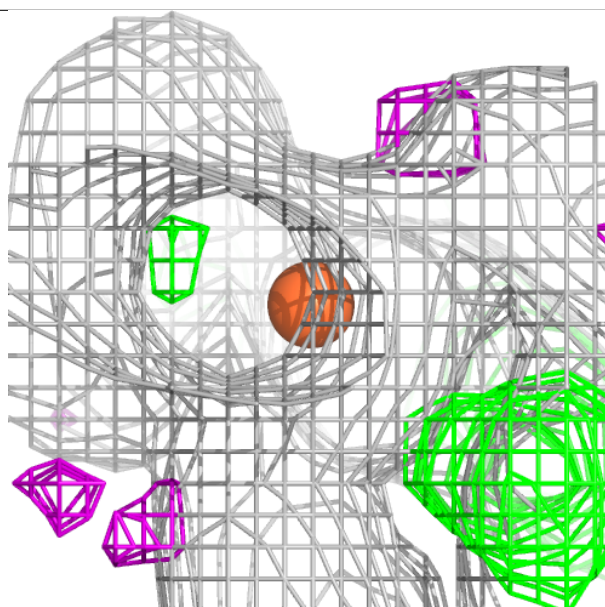
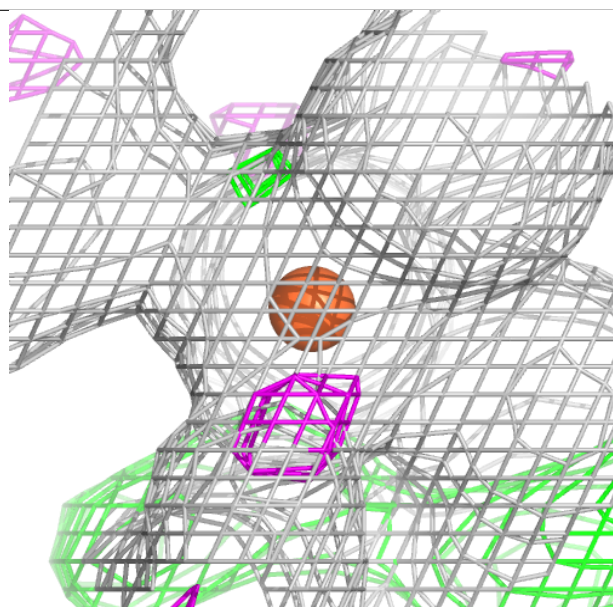
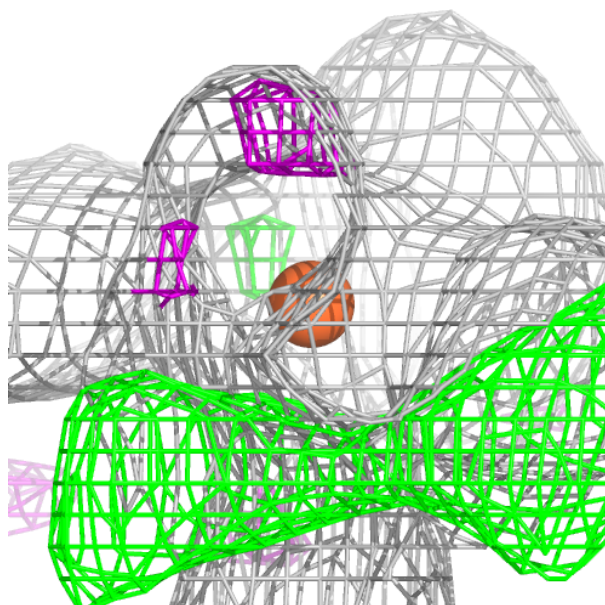
Electron density around FE B 205 (A):

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



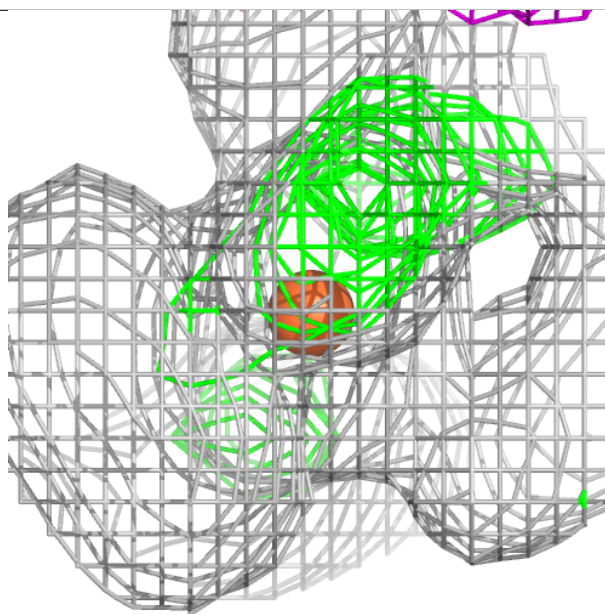
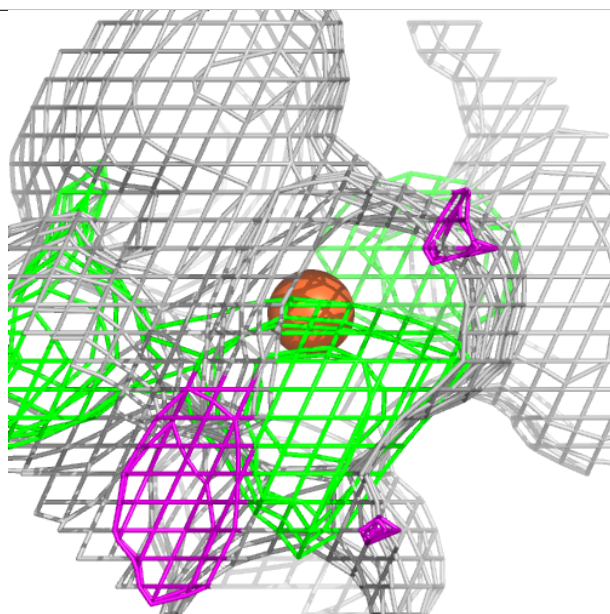
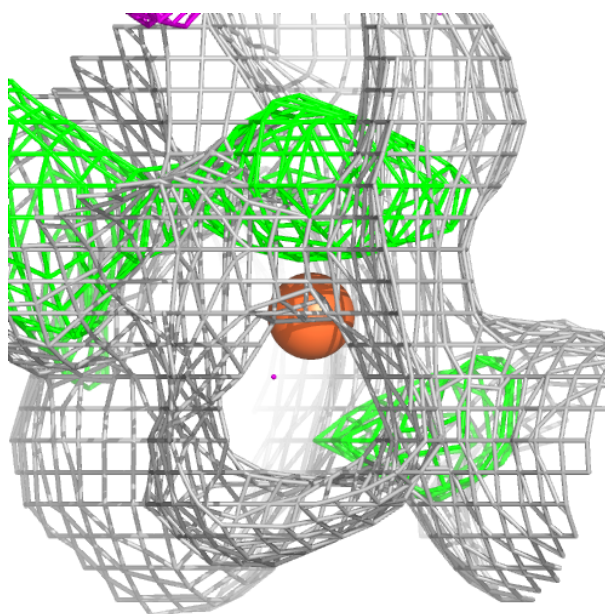
Electron density around FE A 203 (A):

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



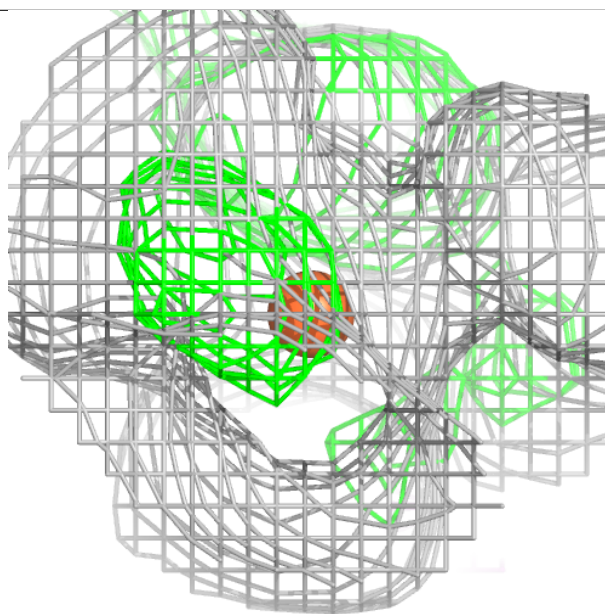
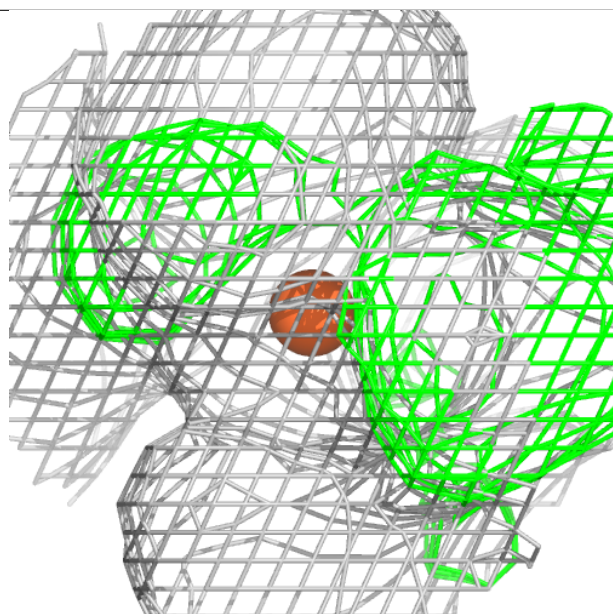
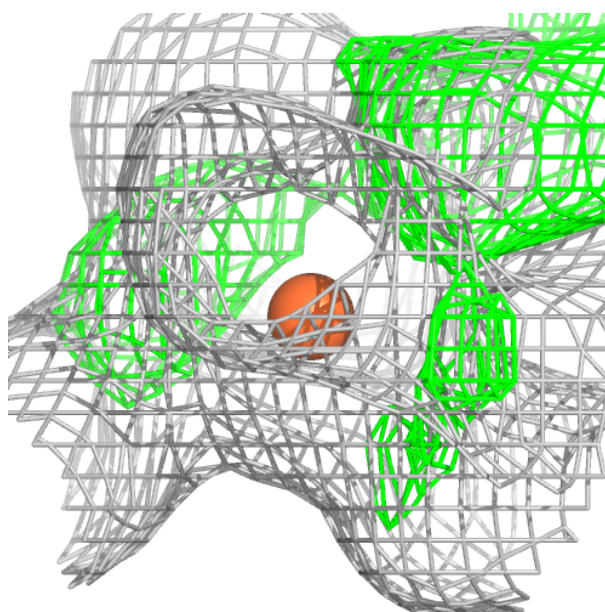
Electron density around FE F 202:

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



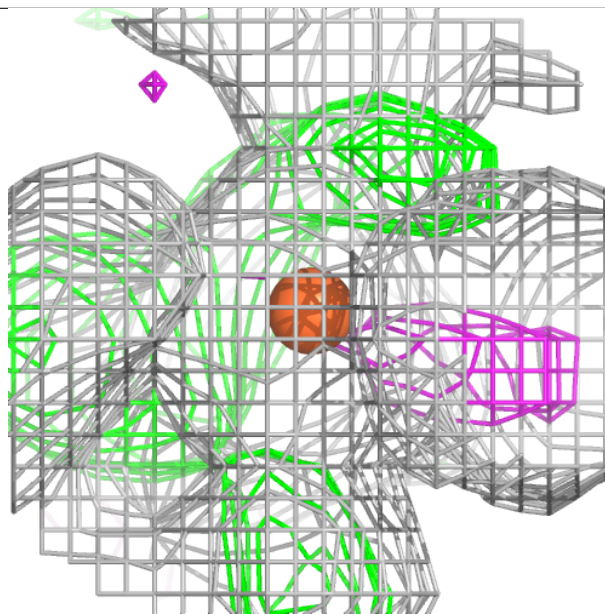
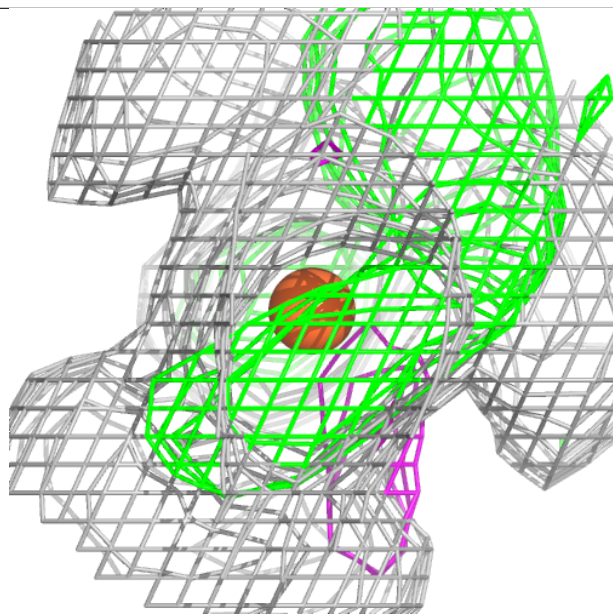
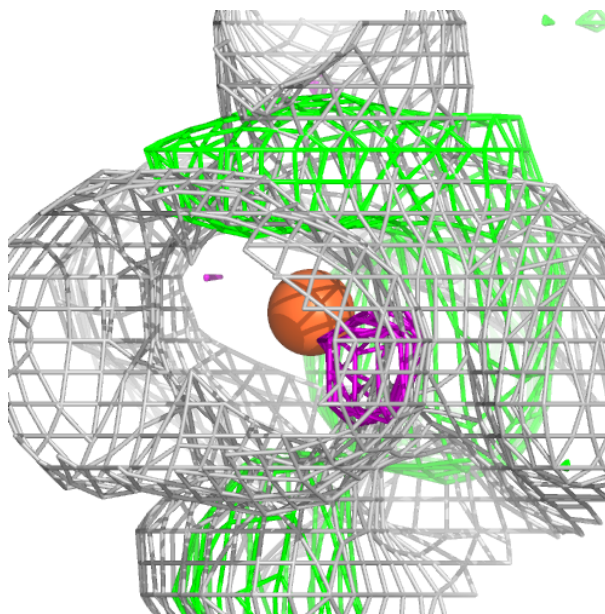
Electron density around FE C 201:

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



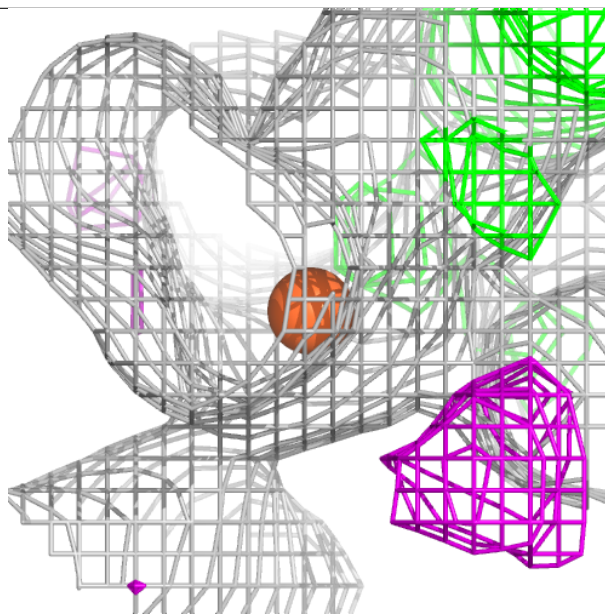
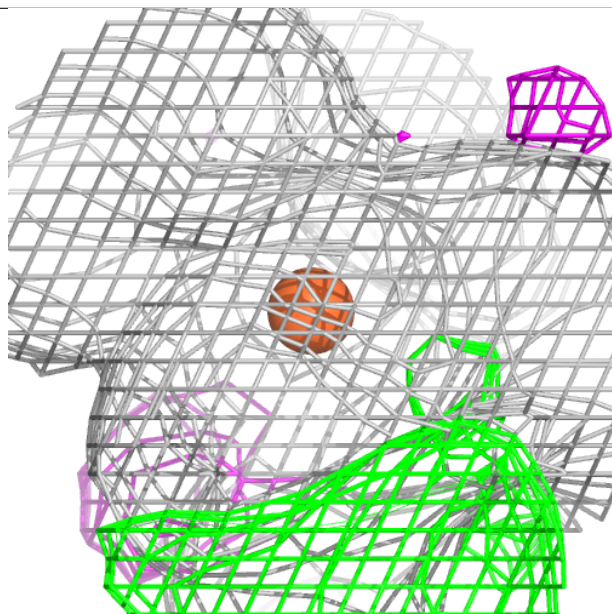
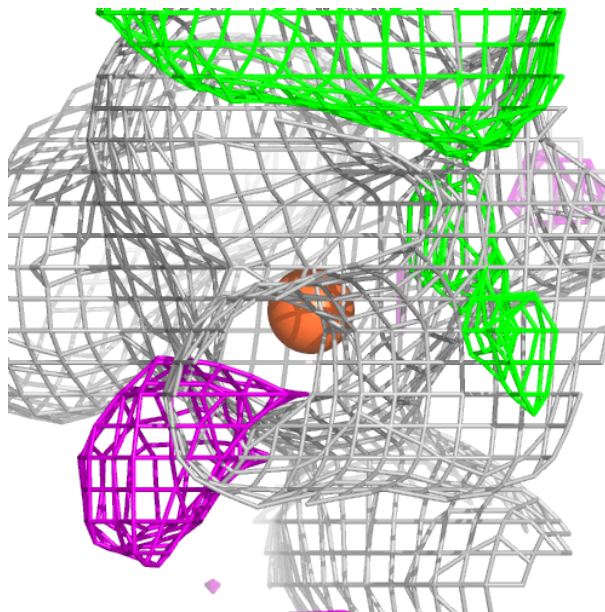
Electron density around FE B 204:

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



Electron density around FE2 D 201 (A):

$2mF_o-DF_c$ (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.