



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:48 PM UTC

PDB ID : 9FJ2 / pdb_00009fj2
Title : Rubrerythrin from Clostridium difficile P28
Authors : Salgueiro, B.A.; Matias, P.M.; Romao, C.V.
Deposited on : 2024-05-30
Resolution : 2.19 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:

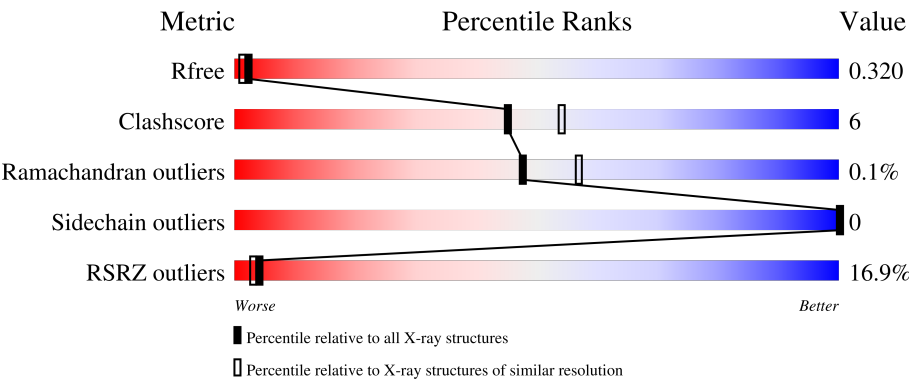
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	178	21% 81% 17% .
1	B	178	16% 87% 12% .
1	C	178	16% 85% 14% .
1	D	178	14% 86% 12% .
1	E	178	16% 87% 13% .

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Mol	Chain	Length	Quality of chain
1	F	178	
1	G	178	
1	H	178	

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
3	O	D	204	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11797 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 Rubrerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1407	880	240	278	9			
1	B	175	Total	C	N	O	S	0	0	0
			1407	880	240	278	9			
1	C	176	Total	C	N	O	S	0	0	0
			1415	886	241	279	9			
1	D	175	Total	C	N	O	S	0	0	0
			1407	880	240	278	9			
1	E	178	Total	C	N	O	S	0	0	0
			1431	895	244	282	10			
1	F	175	Total	C	N	O	S	0	0	0
			1407	880	240	278	9			
1	G	175	Total	C	N	O	S	0	0	0
			1407	880	240	278	9			
1	H	176	Total	C	N	O	S	0	0	0
			1415	886	241	279	9			

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total 3	Fe 3	0	0
2	H	3	Total 3	Fe 3	0	0

- 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 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	D	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0

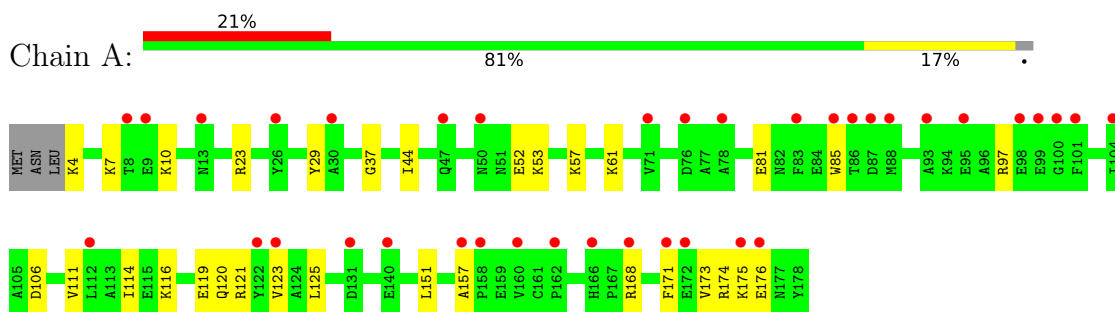
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total 75	O 75	0	0
4	B	60	Total 60	O 60	0	0
4	C	63	Total 63	O 63	0	0
4	D	52	Total 52	O 52	0	0
4	E	53	Total 53	O 53	0	0
4	F	66	Total 66	O 66	0	0
4	G	42	Total 42	O 42	0	0
4	H	61	Total 61	O 61	0	0

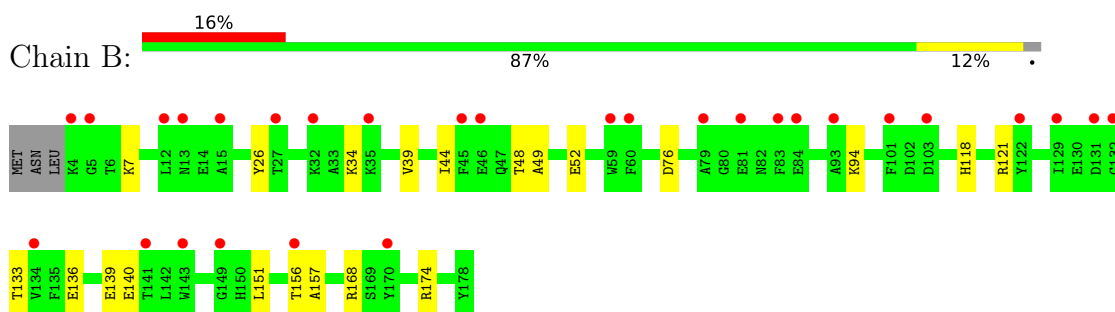
3 Residue-property plots [i](#)

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.

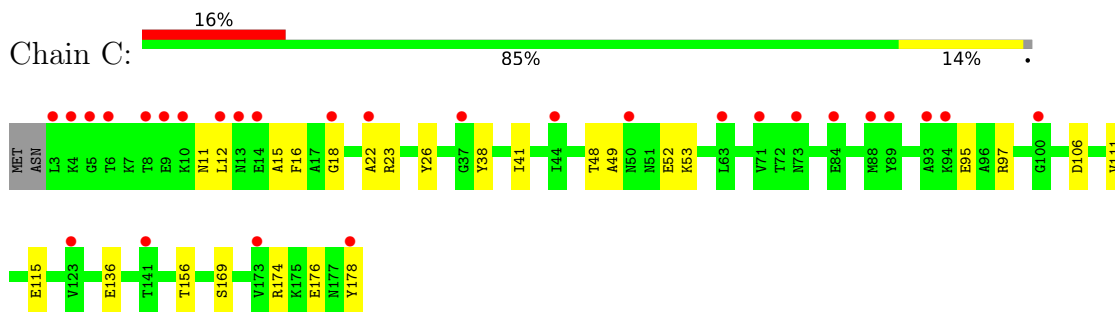
• Molecule 1: Rubrerythrin



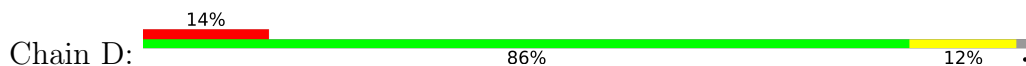
• Molecule 1: Rubrerythrin

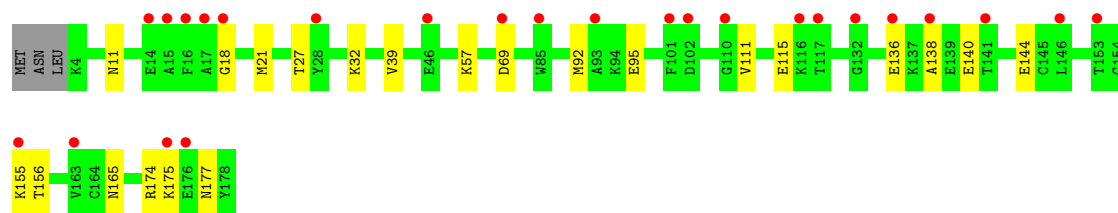


• Molecule 1: Rubrerythrin

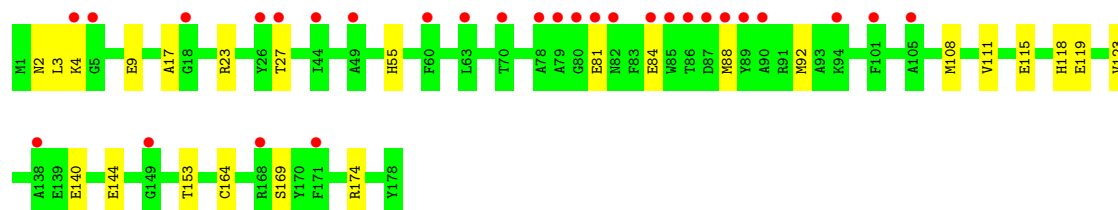
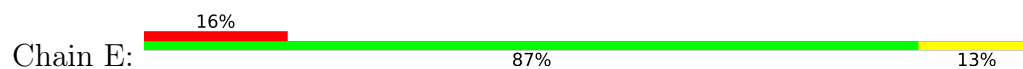


• Molecule 1: Rubrerythrin

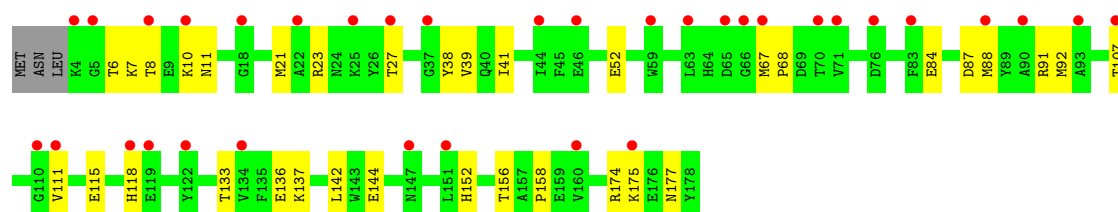
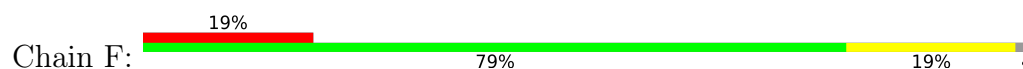




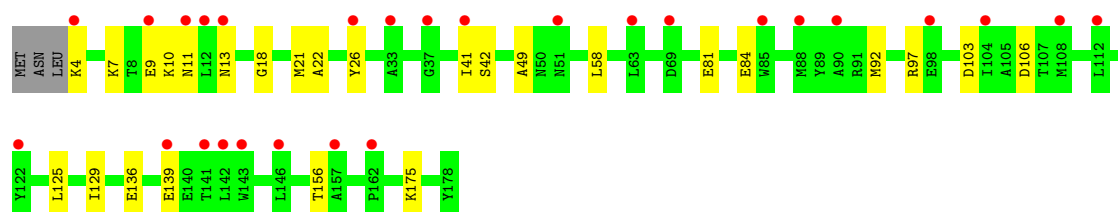
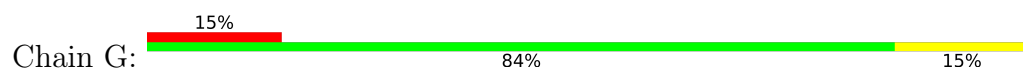
• Molecule 1: Rubrerythrin



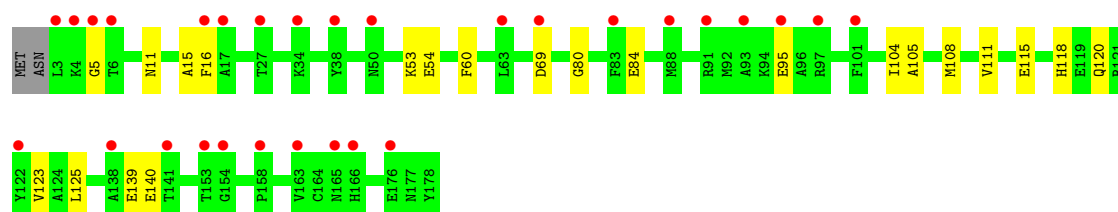
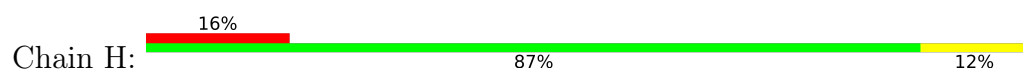
• Molecule 1: Rubrerythrin



• Molecule 1: Rubrerythrin



• Molecule 1: Rubrerythrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.77Å 67.67Å 95.33Å 93.29° 98.34° 106.88°	Depositor
Resolution (Å)	36.15 – 2.19 36.15 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.9 (36.15-2.19) 93.9 (36.15-2.19)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.264 , 0.321 0.264 , 0.320	Depositor DCC
R_{free} test set	3466 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11797	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 20.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7360e-03. 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: O, 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	0.11	0/1437	0.28	0/1938
1	B	0.12	0/1437	0.28	0/1938
1	C	0.11	0/1445	0.32	0/1949
1	D	0.14	0/1437	0.32	0/1938
1	E	0.13	0/1461	0.28	0/1970
1	F	0.10	0/1437	0.26	0/1938
1	G	0.15	0/1437	0.35	0/1938
1	H	0.12	0/1445	0.28	0/1949
All	All	0.12	0/11536	0.30	0/15558

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	1407	0	1330	22	0
1	B	1407	0	1330	19	0
1	C	1415	0	1341	19	0
1	D	1407	0	1330	19	0
1	E	1431	0	1359	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1407	0	1330	28	0
1	G	1407	0	1330	20	0
1	H	1415	0	1341	14	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	75	0	0	3	0
4	B	60	0	0	4	0
4	C	63	0	0	2	0
4	D	52	0	0	3	0
4	E	53	0	0	0	0
4	F	66	0	0	7	0
4	G	42	0	0	2	0
4	H	61	0	0	2	0
All	All	11797	0	10691	130	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 (130) 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:136:GLU:HG3	1:C:156:THR:HG22	1.56	0.87
1:G:92:MET:HE1	1:H:15:ALA:HB2	1.64	0.79
1:F:107:THR:O	4:F:301:HOH:O	2.06	0.74
1:C:12:LEU:O	4:C:301:HOH:O	2.07	0.71
1:D:165:ASN:ND2	4:D:302:HOH:O	2.24	0.70
1:F:111:VAL:N	4:F:301:HOH:O	2.20	0.70
1:F:118:HIS:O	4:F:302:HOH:O	2.10	0.69
1:G:92:MET:HE3	1:H:11:ASN:HB3	1.77	0.66
1:E:88:MET:SD	4:F:322:HOH:O	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:GLU:HG3	1:G:156:THR:HG22	1.79	0.65
1:A:52:GLU:OE2	4:A:301:HOH:O	2.15	0.64
1:F:136:GLU:HG3	1:F:156:THR:HG22	1.78	0.64
1:G:97:ARG:NH2	1:G:106:ASP:OD1	2.31	0.64
1:E:55:HIS:CE1	1:F:115:GLU:OE2	2.52	0.61
1:C:16:PHE:N	4:C:301:HOH:O	2.33	0.61
1:D:136:GLU:HG3	1:D:156:THR:HG22	1.83	0.61
1:C:15:ALA:HB2	1:D:92:MET:HE1	1.83	0.60
1:D:32:LYS:NZ	4:D:308:HOH:O	2.34	0.60
1:H:104:ILE:HG22	1:H:108:MET:HE2	1.83	0.59
1:A:44:ILE:HG23	1:B:121:ARG:HH21	1.66	0.59
1:G:139:GLU:OE1	1:G:139:GLU:N	2.31	0.57
1:A:121:ARG:HH11	1:D:174:ARG:HH22	1.51	0.57
1:B:168:ARG:HH11	1:E:4:LYS:HD2	1.69	0.56
1:F:67:MET:HE3	1:F:68:PRO:HD2	1.88	0.56
1:E:118:HIS:ND1	4:F:304:HOH:O	2.26	0.55
1:F:52:GLU:OE2	4:F:304:HOH:O	2.17	0.55
1:A:57:LYS:O	1:A:61:LYS:HG3	2.07	0.55
1:B:133:THR:N	4:B:306:HOH:O	2.34	0.54
1:G:4:LYS:N	4:G:309:HOH:O	2.41	0.53
1:G:9:GLU:O	1:G:13:ASN:N	2.41	0.52
1:A:120:GLN:HA	1:A:123:VAL:HG22	1.90	0.52
1:C:38:TYR:HB3	1:C:41:ILE:HD12	1.91	0.52
1:C:11:ASN:ND2	1:D:95:GLU:OE1	2.42	0.52
1:E:92:MET:HG2	1:F:11:ASN:HB3	1.91	0.52
1:E:3:LEU:HB3	1:E:9:GLU:HB2	1.92	0.52
1:G:42:SER:N	4:G:301:HOH:O	2.23	0.52
1:C:11:ASN:HD22	1:D:92:MET:HA	1.75	0.52
1:B:139:GLU:HG2	1:B:140:GLU:N	2.26	0.51
1:F:7:LYS:O	1:F:11:ASN:ND2	2.44	0.51
1:B:136:GLU:HG2	1:B:156:THR:HG22	1.93	0.50
1:C:18:GLY:O	1:C:22:ALA:N	2.37	0.50
1:A:81:GLU:OE1	1:B:26:TYR:OH	2.16	0.50
4:A:301:HOH:O	1:B:118:HIS:ND1	2.23	0.50
1:B:26:TYR:HB2	1:B:49:ALA:HB2	1.94	0.50
1:E:169:SER:HB2	1:F:39:VAL:HG23	1.93	0.50
1:E:17:ALA:HB2	1:F:21:MET:HE2	1.93	0.49
1:E:23:ARG:O	1:E:27:THR:HG23	2.12	0.49
1:E:140:GLU:OE1	1:E:153:THR:OG1	2.28	0.49
1:F:87:ASP:O	1:F:91:ARG:HG2	2.13	0.49
1:D:57:LYS:NZ	4:D:318:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:O	1:B:168:ARG:NH2	2.46	0.49
1:G:41:ILE:HG23	1:H:125:LEU:HD13	1.95	0.49
1:B:151:LEU:HD21	1:B:174:ARG:HH11	1.76	0.49
1:A:157:ALA:HB3	1:A:168:ARG:HD2	1.95	0.48
1:F:111:VAL:O	1:F:115:GLU:HG2	2.13	0.48
1:G:103:ASP:N	1:G:103:ASP:OD1	2.46	0.48
1:C:97:ARG:NH2	1:C:106:ASP:OD1	2.45	0.48
1:G:7:LYS:HD2	1:G:10:LYS:HE3	1.95	0.48
1:A:168:ARG:HA	1:A:171:PHE:HD2	1.78	0.48
1:A:175:LYS:HB3	1:D:175:LYS:HD2	1.96	0.48
1:C:23:ARG:HH12	1:D:27:THR:HG21	1.79	0.48
1:A:23:ARG:HD2	1:A:53:LYS:HB2	1.96	0.48
1:G:11:ASN:ND2	1:H:95:GLU:OE2	2.37	0.47
1:H:5:GLY:N	4:H:301:HOH:O	2.26	0.47
1:D:18:GLY:HA2	1:D:21:MET:HB2	1.96	0.47
1:E:92:MET:HB3	1:E:108:MET:SD	2.55	0.47
1:A:4:LYS:N	4:A:308:HOH:O	2.48	0.47
1:A:7:LYS:HE3	1:A:10:LYS:HD3	1.97	0.47
1:B:48:THR:O	1:B:52:GLU:HG2	2.15	0.47
1:B:121:ARG:HD2	1:C:174:ARG:HH22	1.80	0.46
1:F:91:ARG:NH1	4:F:311:HOH:O	2.43	0.46
1:A:85:TRP:NE1	1:A:119:GLU:OE1	2.29	0.46
1:D:140:GLU:HA	1:D:155:LYS:HA	1.98	0.46
1:A:174:ARG:HG2	1:A:176:GLU:OE2	2.15	0.46
1:D:138:ALA:O	1:D:155:LYS:NZ	2.49	0.46
1:B:7:LYS:NZ	4:B:315:HOH:O	2.49	0.46
1:E:81:GLU:CD	1:E:84:GLU:OE1	2.59	0.46
1:B:34:LYS:HE3	1:B:39:VAL:HG22	1.98	0.45
1:D:69:ASP:N	1:D:69:ASP:OD1	2.47	0.45
1:E:144:GLU:HB2	1:E:174:ARG:HB2	1.99	0.45
1:F:175:LYS:HB2	1:G:175:LYS:HG2	1.99	0.45
1:D:111:VAL:O	1:D:115:GLU:HG2	2.16	0.45
1:H:111:VAL:O	1:H:115:GLU:HG2	2.16	0.45
1:F:115:GLU:HA	1:F:118:HIS:HB2	1.97	0.45
1:B:121:ARG:NH1	4:B:303:HOH:O	2.33	0.44
1:F:152:HIS:CG	1:F:158:PRO:HG3	2.52	0.44
1:A:173:VAL:O	1:D:177:ASN:ND2	2.46	0.44
1:H:16:PHE:CE1	1:H:60:PHE:HB2	2.52	0.44
1:B:121:ARG:HG2	1:C:178:TYR:OH	2.18	0.44
1:C:95:GLU:OE1	1:D:11:ASN:ND2	2.36	0.44
1:F:87:ASP:HA	1:F:91:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:HIS:ND1	4:H:303:HOH:O	2.29	0.43
1:F:144:GLU:OE2	1:F:174:ARG:NH1	2.42	0.43
1:A:97:ARG:NH2	1:A:106:ASP:OD1	2.52	0.43
1:C:48:THR:O	1:C:52:GLU:HG2	2.19	0.43
1:C:53:LYS:HB3	1:C:53:LYS:HE3	1.80	0.43
1:G:125:LEU:O	1:G:129:ILE:HG13	2.18	0.43
1:C:174:ARG:NH2	1:C:176:GLU:OE1	2.39	0.42
1:F:177:ASN:HB3	1:G:175:LYS:HB2	2.01	0.42
1:G:26:TYR:HB2	1:G:49:ALA:HB2	2.01	0.42
1:D:144:GLU:HB2	1:D:174:ARG:HB2	2.01	0.42
1:E:111:VAL:O	1:E:115:GLU:HG2	2.19	0.42
1:E:119:GLU:O	1:E:123:VAL:HG22	2.19	0.42
1:F:88:MET:O	1:F:92:MET:HG3	2.19	0.42
1:A:111:VAL:HA	1:A:114:ILE:HD12	2.02	0.42
1:F:84:GLU:HA	1:F:88:MET:HB3	2.01	0.42
1:F:7:LYS:HA	1:F:10:LYS:HE2	2.01	0.42
1:G:81:GLU:HA	1:G:84:GLU:OE1	2.20	0.42
1:A:151:LEU:HD21	1:A:174:ARG:HD2	2.01	0.42
1:F:142:LEU:HD12	1:F:142:LEU:HA	1.89	0.41
1:C:169:SER:HB2	1:D:39:VAL:HG23	2.02	0.41
1:F:38:TYR:HB3	1:F:41:ILE:HB	2.02	0.41
1:A:29:TYR:OH	1:B:76:ASP:OD2	2.32	0.41
1:A:125:LEU:HD11	1:B:44:ILE:HG21	2.03	0.41
1:B:94:LYS:NZ	4:B:307:HOH:O	2.36	0.41
1:H:105:ALA:HA	1:H:108:MET:HE3	2.03	0.41
1:H:120:GLN:HA	1:H:123:VAL:HG22	2.02	0.41
1:G:18:GLY:HA2	1:G:21:MET:HE3	2.03	0.41
1:C:26:TYR:HB2	1:C:49:ALA:HB2	2.02	0.41
1:F:23:ARG:O	1:F:27:THR:HG23	2.20	0.41
1:G:18:GLY:O	1:G:22:ALA:N	2.40	0.41
1:C:111:VAL:O	1:C:115:GLU:HG2	2.21	0.41
1:H:53:LYS:NZ	1:H:54:GLU:OE2	2.54	0.41
1:E:164:CYS:HA	1:G:58:LEU:HD21	2.03	0.40
1:F:6:THR:HG22	1:F:8:THR:H	1.84	0.40
1:H:139:GLU:HG2	1:H:140:GLU:N	2.36	0.40
1:F:133:THR:O	1:F:137:LYS:NZ	2.45	0.40
1:H:80:GLY:O	1:H:84:GLU:HG3	2.22	0.40
1:A:37:GLY:HA3	1:E:2:ASN:HB3	2.03	0.40
1:A:116:LYS:O	1:A:120:GLN:HG2	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	173/178 (97%)	169 (98%)	4 (2%)	0	100	100
1	B	173/178 (97%)	167 (96%)	6 (4%)	0	100	100
1	C	174/178 (98%)	169 (97%)	5 (3%)	0	100	100
1	D	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
1	E	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
1	F	173/178 (97%)	168 (97%)	5 (3%)	0	100	100
1	G	173/178 (97%)	169 (98%)	4 (2%)	0	100	100
1	H	174/178 (98%)	169 (97%)	4 (2%)	1 (1%)	21	23
All	All	1389/1424 (98%)	1345 (97%)	43 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	69	ASP

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	147/150 (98%)	147 (100%)	0	100	100
1	B	147/150 (98%)	147 (100%)	0	100	100
1	C	148/150 (99%)	148 (100%)	0	100	100
1	D	147/150 (98%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	150/150 (100%)	150 (100%)	0	100	100
1	F	147/150 (98%)	147 (100%)	0	100	100
1	G	147/150 (98%)	147 (100%)	0	100	100
1	H	148/150 (99%)	148 (100%)	0	100	100
All	All	1181/1200 (98%)	1181 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	147	ASN
1	A	165	ASN
1	A	166	HIS
1	B	64	HIS
1	C	11	ASN
1	C	82	ASN
1	D	118	HIS
1	D	147	ASN
1	F	82	ASN
1	G	47	GLN
1	G	50	ASN
1	G	127	ASN
1	H	13	ASN
1	H	150	HIS

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 29 ligands modelled in this entry, 29 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	175/178 (98%)	1.30	37 (21%) 2 2	22, 35, 51, 61	0
1	B	175/178 (98%)	1.25	29 (16%) 4 3	22, 33, 46, 55	0
1	C	176/178 (98%)	1.26	28 (15%) 5 3	24, 33, 46, 57	0
1	D	175/178 (98%)	1.26	25 (14%) 6 4	23, 34, 49, 54	0
1	E	178/178 (100%)	1.19	29 (16%) 4 3	22, 32, 48, 59	0
1	F	175/178 (98%)	1.28	34 (19%) 3 2	22, 33, 48, 56	0
1	G	175/178 (98%)	1.15	27 (15%) 5 4	24, 33, 47, 64	0
1	H	176/178 (98%)	1.24	29 (16%) 4 3	24, 34, 47, 58	0
All	All	1405/1424 (98%)	1.24	238 (16%) 4 3	22, 33, 48, 64	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	ALA	5.2
1	A	176	GLU	5.2
1	F	5	GLY	4.7
1	F	22	ALA	4.6
1	H	3	LEU	4.5
1	D	175	LYS	4.1
1	C	94	LYS	4.0
1	C	178	TYR	4.0
1	A	93	ALA	3.9
1	A	104	ILE	3.8
1	H	153	THR	3.8
1	C	18	GLY	3.8
1	E	79	ALA	3.7
1	C	84	GLU	3.6
1	F	46	GLU	3.6
1	H	83	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	88	MET	3.4
1	E	70	THR	3.4
1	B	134	VAL	3.4
1	D	16	PHE	3.4
1	H	16	PHE	3.4
1	H	50	ASN	3.3
1	D	14	GLU	3.3
1	E	18	GLY	3.2
1	C	123	VAL	3.2
1	D	138	ALA	3.2
1	E	101	PHE	3.2
1	E	94	LYS	3.2
1	F	134	VAL	3.2
1	D	101	PHE	3.2
1	E	27	THR	3.2
1	A	26	TYR	3.1
1	C	3	LEU	3.1
1	A	86	THR	3.1
1	B	13	ASN	3.1
1	D	102	ASP	3.1
1	F	65	ASP	3.1
1	B	35	LYS	3.1
1	F	10	LYS	3.1
1	G	63	LEU	3.1
1	G	9	GLU	3.0
1	G	139	GLU	3.0
1	F	110	GLY	3.0
1	H	165	ASN	3.0
1	D	141	THR	3.0
1	G	11	ASN	3.0
1	D	28	TYR	3.0
1	F	122	TYR	3.0
1	B	81	GLU	2.9
1	G	4	LYS	2.9
1	A	78	ALA	2.9
1	C	37	GLY	2.9
1	E	80	GLY	2.9
1	A	122	TYR	2.9
1	E	87	ASP	2.9
1	A	88	MET	2.9
1	H	141	THR	2.9
1	C	13	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	163	VAL	2.8
1	A	99	GLU	2.8
1	B	5	GLY	2.8
1	D	153	THR	2.8
1	E	4	LYS	2.8
1	F	175	LYS	2.8
1	A	171	PHE	2.8
1	E	81	GLU	2.8
1	G	157	ALA	2.8
1	F	63	LEU	2.8
1	A	162	PRO	2.8
1	C	173	VAL	2.8
1	A	175	LYS	2.8
1	H	91	ARG	2.8
1	D	18	GLY	2.8
1	E	89	TYR	2.8
1	G	112	LEU	2.8
1	A	13	ASN	2.7
1	A	87	ASP	2.7
1	D	136	GLU	2.7
1	D	110	GLY	2.7
1	A	123	VAL	2.7
1	F	44	ILE	2.7
1	H	69	ASP	2.7
1	B	83	PHE	2.7
1	D	93	ALA	2.7
1	G	90	ALA	2.7
1	C	63	LEU	2.7
1	D	176	GLU	2.7
1	B	129	ILE	2.7
1	E	78	ALA	2.6
1	D	117	THR	2.6
1	F	111	VAL	2.6
1	A	95	GLU	2.6
1	H	17	ALA	2.6
1	F	151	LEU	2.6
1	H	5	GLY	2.6
1	G	98	GLU	2.6
1	C	12	LEU	2.6
1	E	171	PHE	2.6
1	F	88	MET	2.6
1	H	63	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	160	VAL	2.5
1	B	132	GLY	2.5
1	F	18	GLY	2.5
1	D	46	GLU	2.5
1	A	83	PHE	2.5
1	A	101	PHE	2.5
1	D	163	VAL	2.5
1	H	4	LYS	2.5
1	E	86	THR	2.5
1	F	8	THR	2.5
1	F	27	THR	2.5
1	A	172	GLU	2.5
1	G	13	ASN	2.5
1	E	26	TYR	2.5
1	A	140	GLU	2.5
1	F	107	THR	2.5
1	B	79	ALA	2.5
1	G	33	ALA	2.5
1	B	4	LYS	2.5
1	B	32	LYS	2.5
1	E	82	ASN	2.5
1	F	147	ASN	2.5
1	F	71	VAL	2.4
1	B	84	GLU	2.4
1	C	14	GLU	2.4
1	H	27	THR	2.4
1	F	119	GLU	2.4
1	H	6	THR	2.4
1	A	157	ALA	2.4
1	D	15	ALA	2.4
1	D	116	LYS	2.4
1	G	142	LEU	2.4
1	A	100	GLY	2.4
1	H	154	GLY	2.4
1	C	9	GLU	2.4
1	D	85	TRP	2.4
1	G	26	TYR	2.4
1	F	83	PHE	2.4
1	F	25	LYS	2.4
1	A	85	TRP	2.4
1	A	166	HIS	2.4
1	B	141	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	85	TRP	2.4
1	H	158	PRO	2.4
1	H	166	HIS	2.4
1	C	89	TYR	2.3
1	C	22	ALA	2.3
1	H	93	ALA	2.3
1	E	60	PHE	2.3
1	G	104	ILE	2.3
1	A	8	THR	2.3
1	A	158	PRO	2.3
1	B	27	THR	2.3
1	C	6	THR	2.3
1	B	46	GLU	2.3
1	H	95	GLU	2.3
1	B	170	TYR	2.3
1	E	90	ALA	2.3
1	H	138	ALA	2.3
1	E	5	GLY	2.3
1	D	155	LYS	2.3
1	B	101	PHE	2.3
1	D	146	LEU	2.3
1	H	176	GLU	2.3
1	B	103	ASP	2.3
1	E	138	ALA	2.3
1	B	149	GLY	2.3
1	D	132	GLY	2.3
1	F	66	GLY	2.3
1	B	60	PHE	2.2
1	C	44	ILE	2.2
1	G	141	THR	2.2
1	C	50	ASN	2.2
1	C	10	LYS	2.2
1	A	76	ASP	2.2
1	A	30	ALA	2.2
1	G	146	LEU	2.2
1	G	51	ASN	2.2
1	G	88	MET	2.2
1	F	37	GLY	2.2
1	A	98	GLU	2.2
1	B	15	ALA	2.2
1	C	93	ALA	2.2
1	E	84	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	12	LEU	2.2
1	G	122	TYR	2.2
1	B	143	TRP	2.2
1	G	143	TRP	2.2
1	G	108	MET	2.2
1	C	71	VAL	2.2
1	F	118	HIS	2.2
1	B	12	LEU	2.2
1	C	4	LYS	2.2
1	G	41	ILE	2.1
1	A	71	VAL	2.1
1	F	90	ALA	2.1
1	F	93	ALA	2.1
1	E	168	ARG	2.1
1	H	38	TYR	2.1
1	F	76	ASP	2.1
1	B	59	TRP	2.1
1	E	105	ALA	2.1
1	A	112	LEU	2.1
1	E	63	LEU	2.1
1	C	8	THR	2.1
1	F	70	THR	2.1
1	C	5	GLY	2.1
1	E	44	ILE	2.1
1	F	59	TRP	2.1
1	A	160	VAL	2.1
1	F	4	LYS	2.1
1	H	34	LYS	2.1
1	B	93	ALA	2.1
1	F	67	MET	2.1
1	A	47	GLN	2.1
1	A	168	ARG	2.1
1	B	156	THR	2.1
1	H	122	TYR	2.1
1	C	100	GLY	2.1
1	E	149	GLY	2.1
1	B	45	PHE	2.1
1	H	101	PHE	2.1
1	E	49	ALA	2.1
1	C	88	MET	2.0
1	H	88	MET	2.0
1	B	131	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	162	PRO	2.0
1	B	122	TYR	2.0
1	A	9	GLU	2.0
1	G	85	TRP	2.0
1	A	50	ASN	2.0
1	C	73	ASN	2.0
1	A	131	ASP	2.0
1	D	69	ASP	2.0
1	G	69	ASP	2.0
1	H	97	ARG	2.0
1	C	141	THR	2.0
1	G	37	GLY	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	D	204	1/1	0.60	0.49	43,43,43,43	0
3	O	F	204	1/1	0.80	0.13	42,42,42,42	0
2	FE	B	203	1/1	0.82	0.12	55,55,55,55	0
2	FE	D	202	1/1	0.88	0.10	41,41,41,41	0
2	FE	F	201	1/1	0.88	0.09	44,44,44,44	0
2	FE	A	203	1/1	0.89	0.08	41,41,41,41	0
2	FE	G	201	1/1	0.89	0.08	40,40,40,40	0
3	O	B	204	1/1	0.90	0.29	41,41,41,41	0
2	FE	G	203	1/1	0.91	0.12	47,47,47,47	0
2	FE	H	202	1/1	0.91	0.10	35,35,35,35	0
2	FE	E	201	1/1	0.91	0.07	46,46,46,46	0

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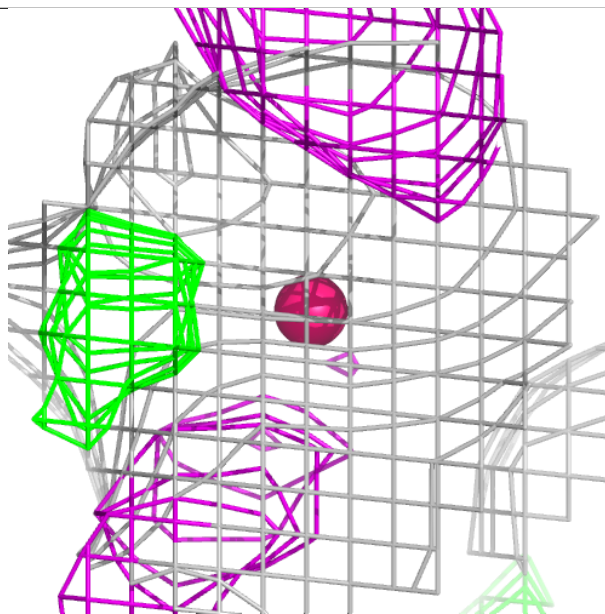
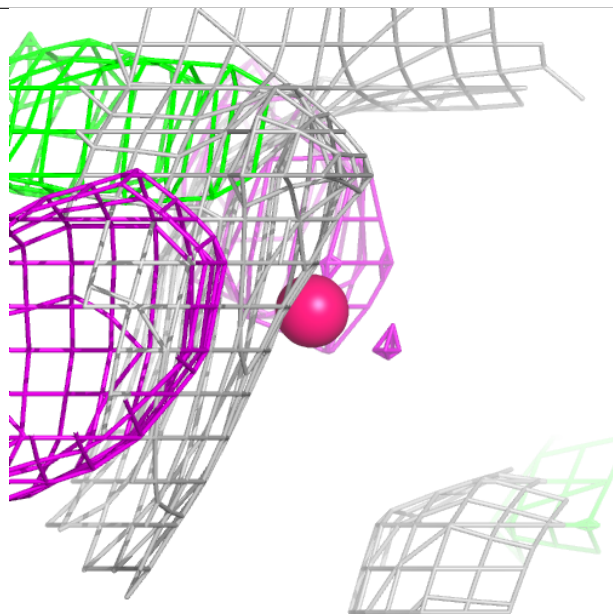
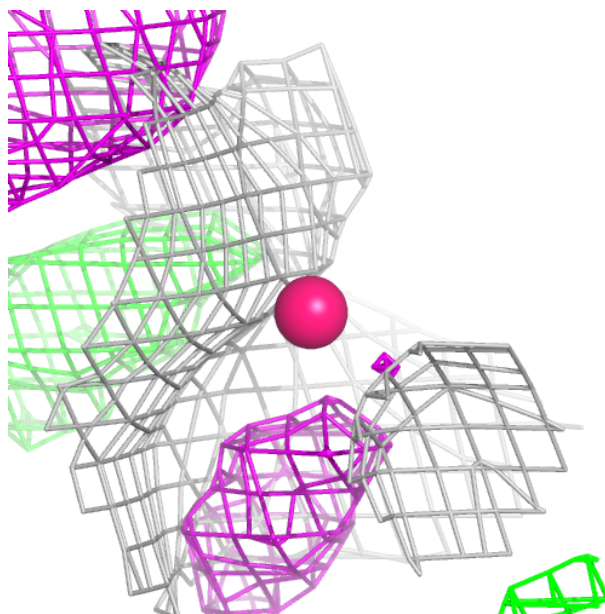
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	C	203	1/1	0.91	0.09	36,36,36,36	0
2	FE	A	201	1/1	0.91	0.06	45,45,45,45	0
3	O	A	204	1/1	0.92	0.07	39,39,39,39	0
2	FE	C	201	1/1	0.92	0.06	35,35,35,35	0
2	FE	B	201	1/1	0.93	0.06	35,35,35,35	0
2	FE	E	202	1/1	0.94	0.07	43,43,43,43	0
3	O	G	204	1/1	0.94	0.07	32,32,32,32	0
2	FE	F	203	1/1	0.96	0.04	26,26,26,26	0
2	FE	H	201	1/1	0.96	0.05	43,43,43,43	0
2	FE	D	203	1/1	0.97	0.04	27,27,27,27	0
2	FE	A	202	1/1	0.97	0.03	29,29,29,29	0
2	FE	D	201	1/1	0.97	0.05	40,40,40,40	0
2	FE	B	202	1/1	0.97	0.05	27,27,27,27	0
2	FE	F	202	1/1	0.97	0.05	40,40,40,40	0
2	FE	C	202	1/1	0.98	0.07	25,25,25,25	0
2	FE	H	203	1/1	0.99	0.02	26,26,26,26	0
2	FE	G	202	1/1	0.99	0.06	26,26,26,26	0
2	FE	E	203	1/1	0.99	0.02	27,27,27,27	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.

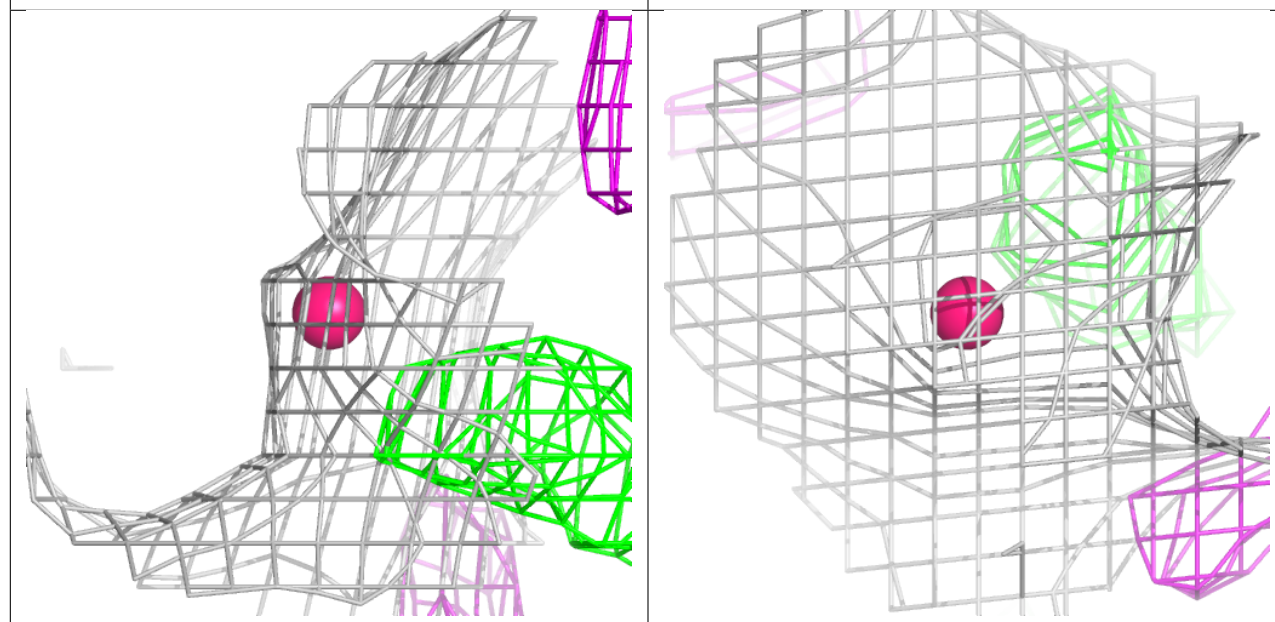
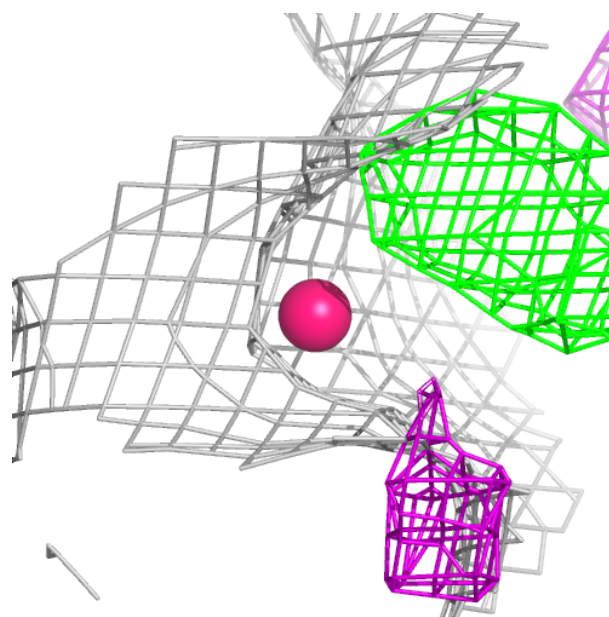
Electron density around O D 204:

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



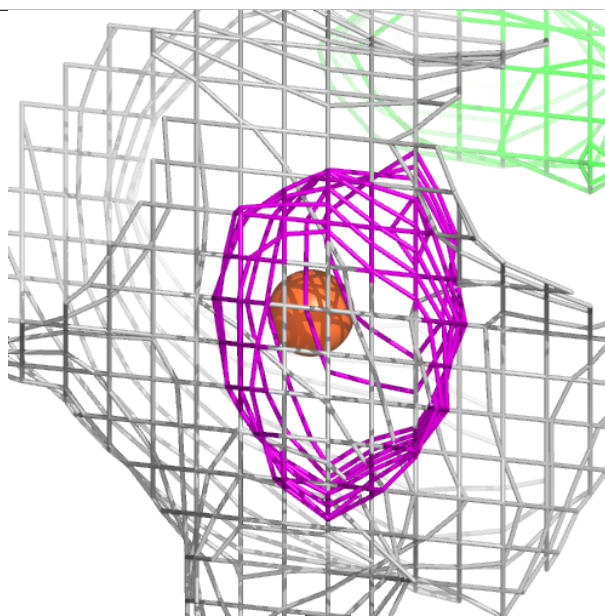
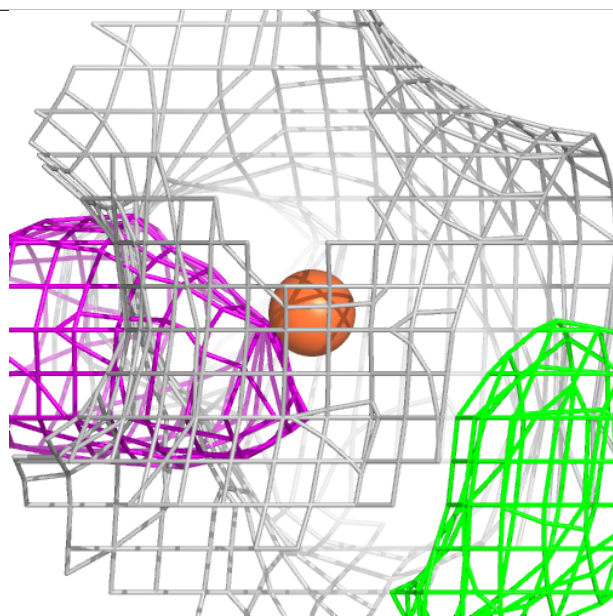
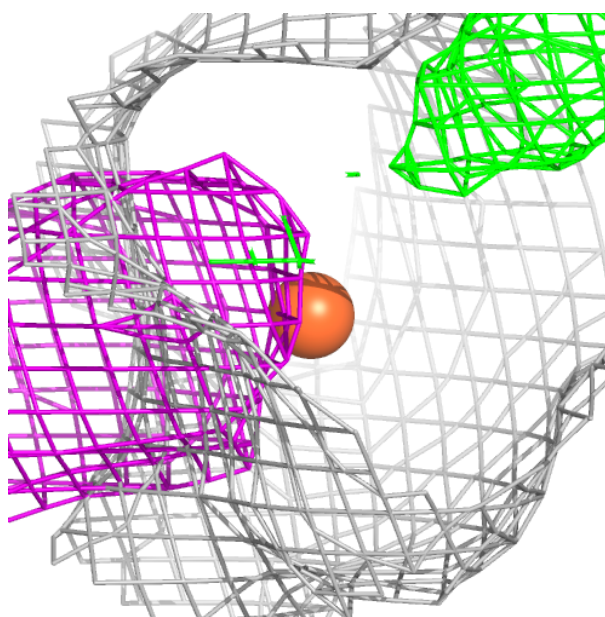
Electron density around O F 204:

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



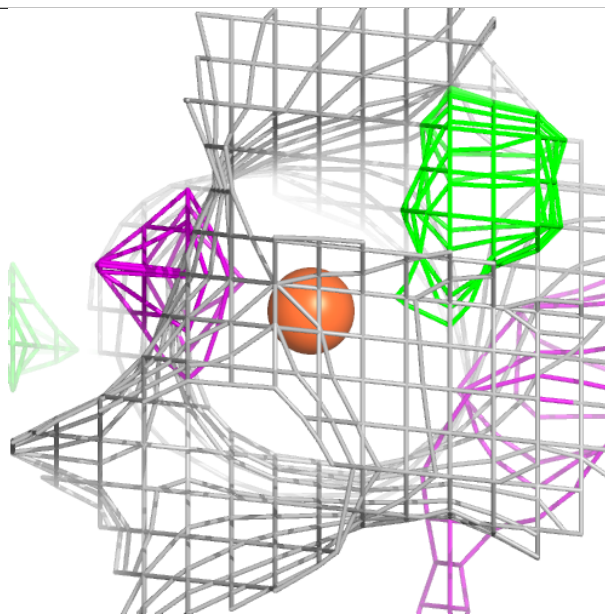
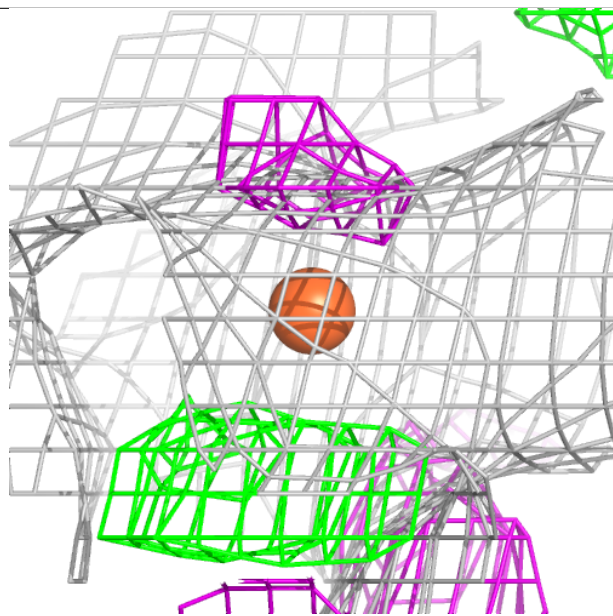
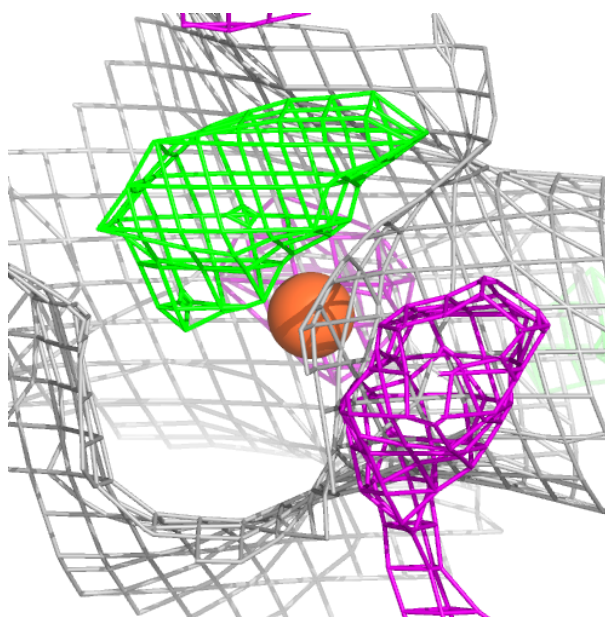
Electron density around FE B 203:

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



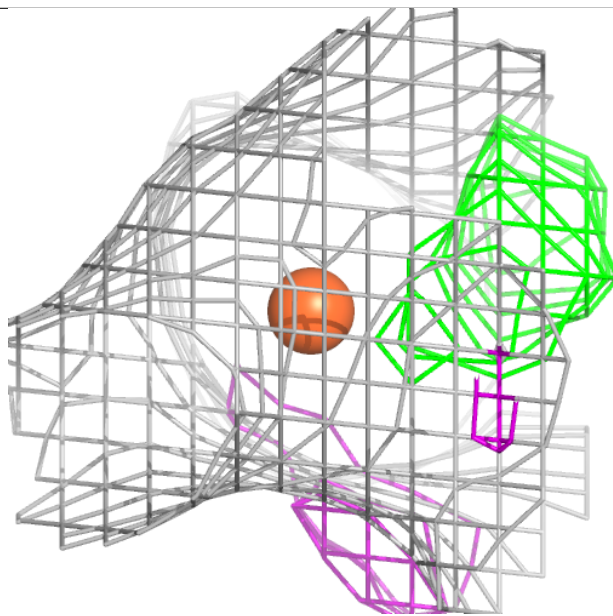
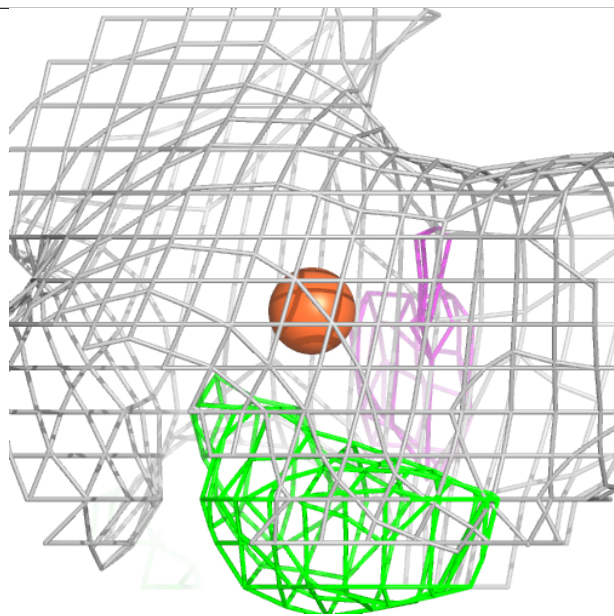
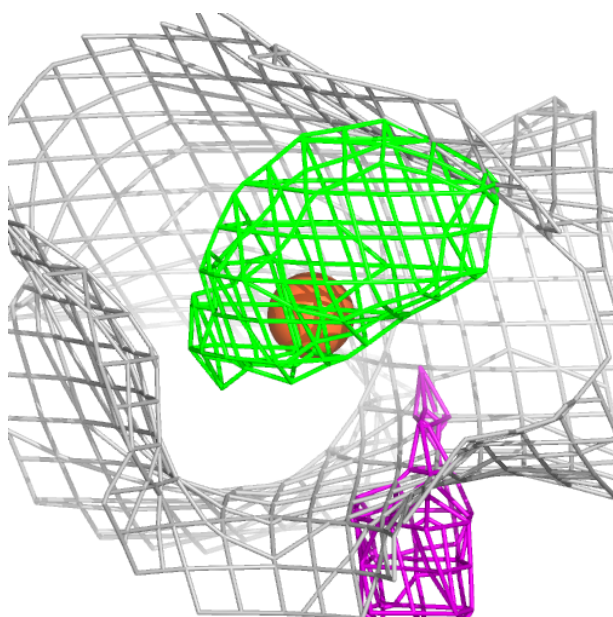
Electron density around FE D 202:

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



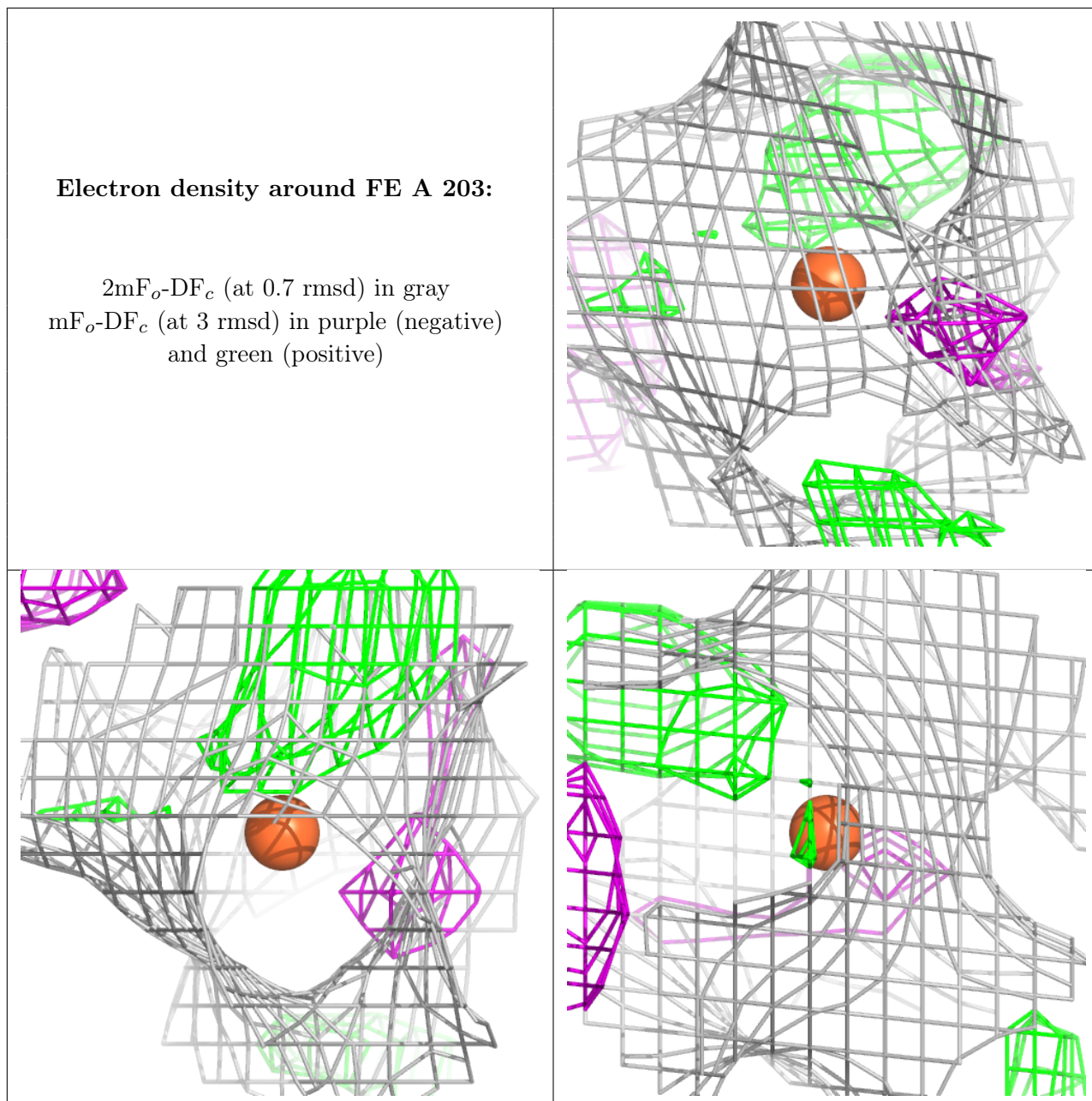
Electron density around FE F 201:

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



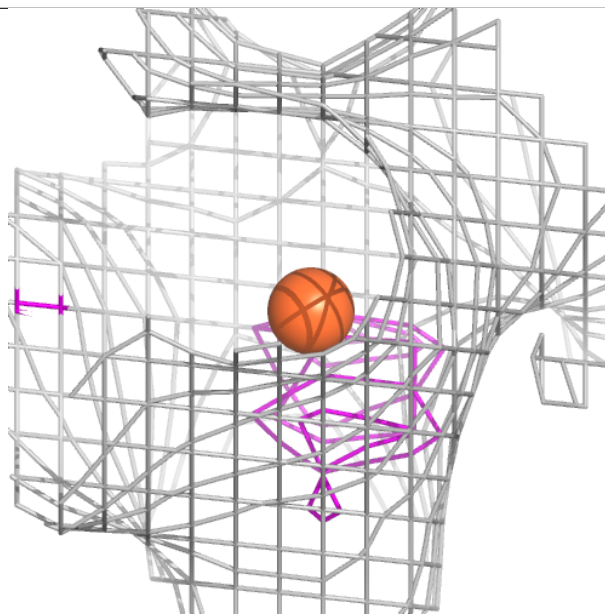
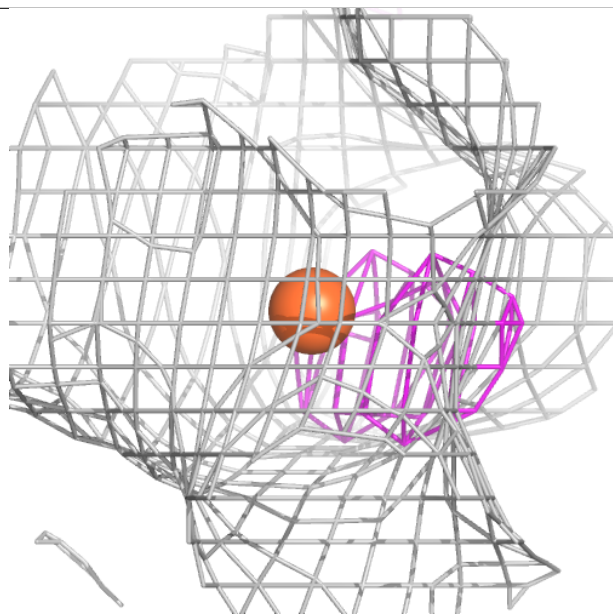
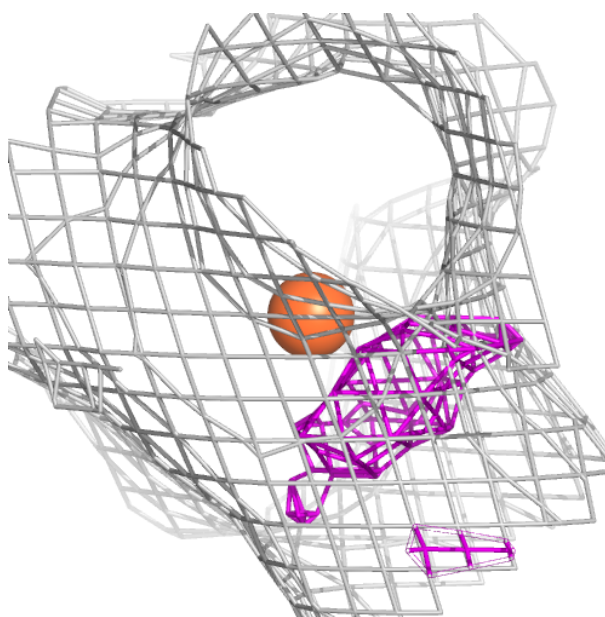
Electron density around FE A 203:

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



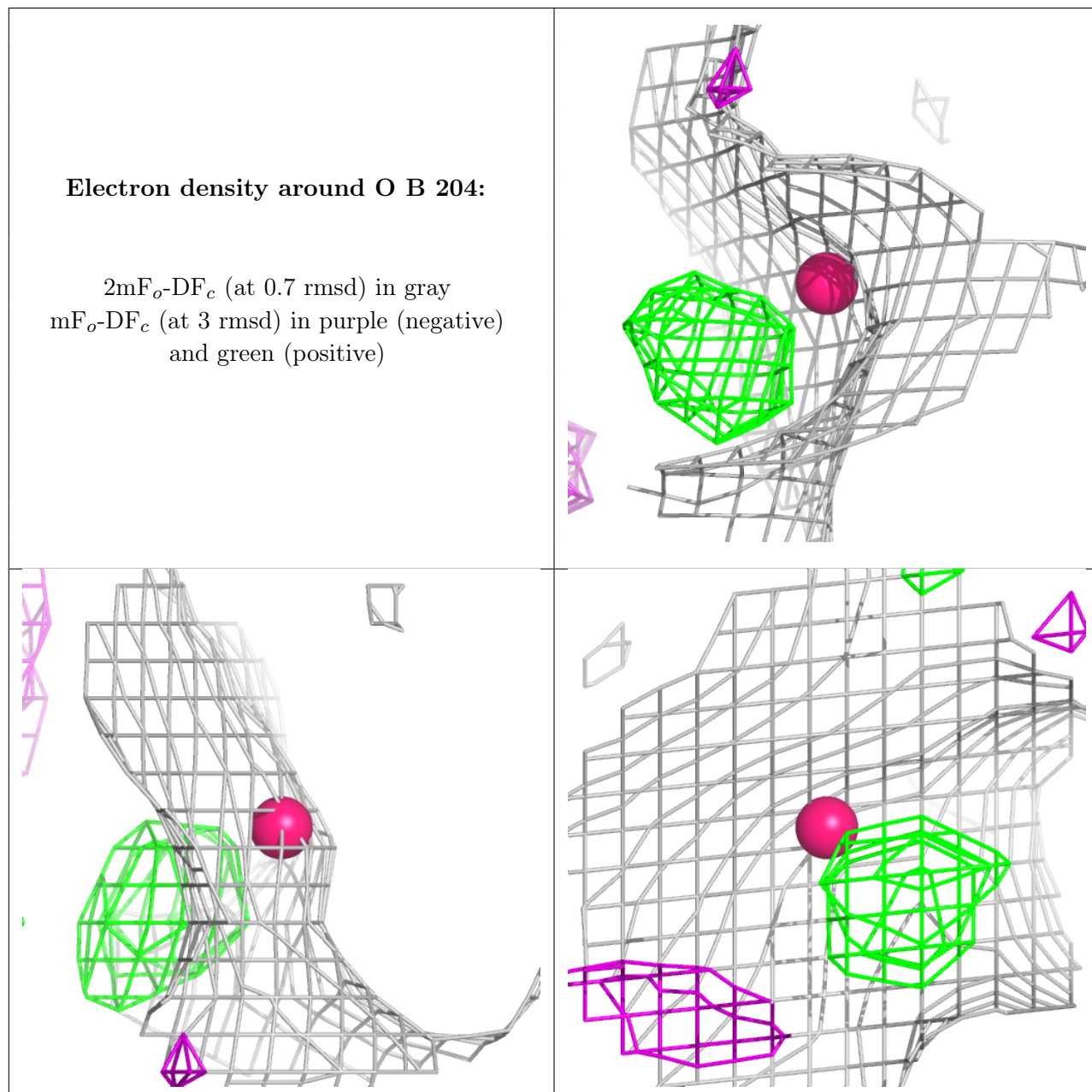
Electron density around FE G 201:

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



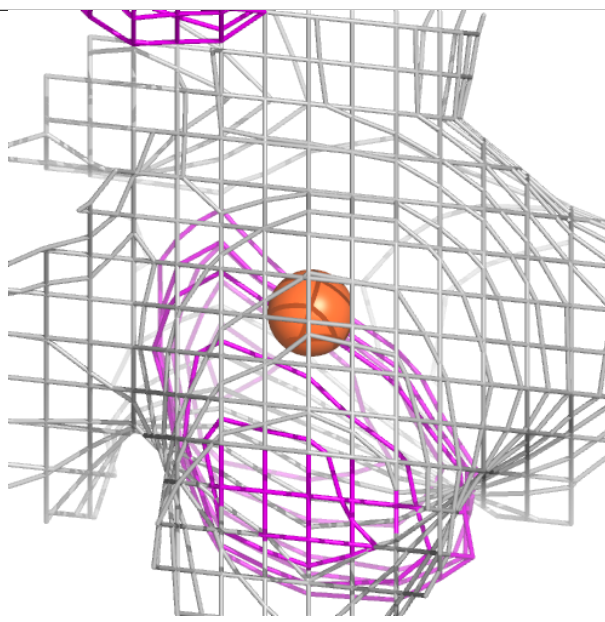
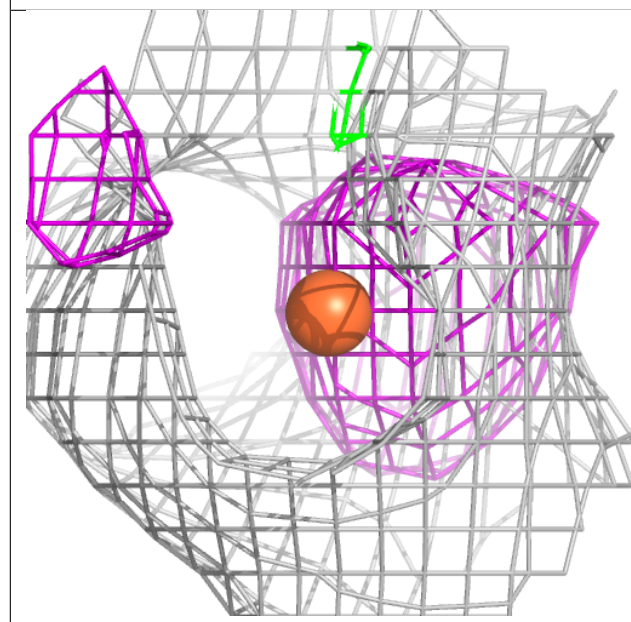
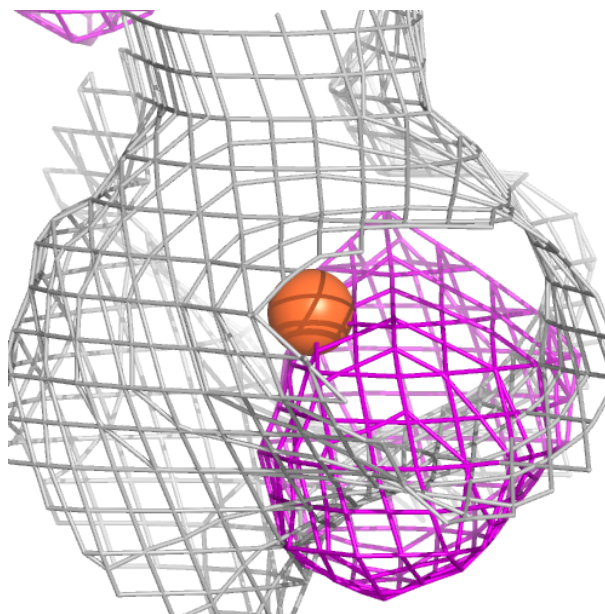
Electron density around O B 204:

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



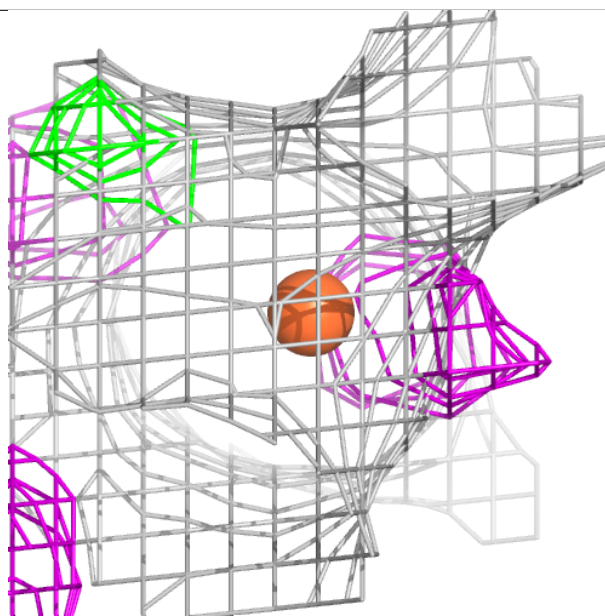
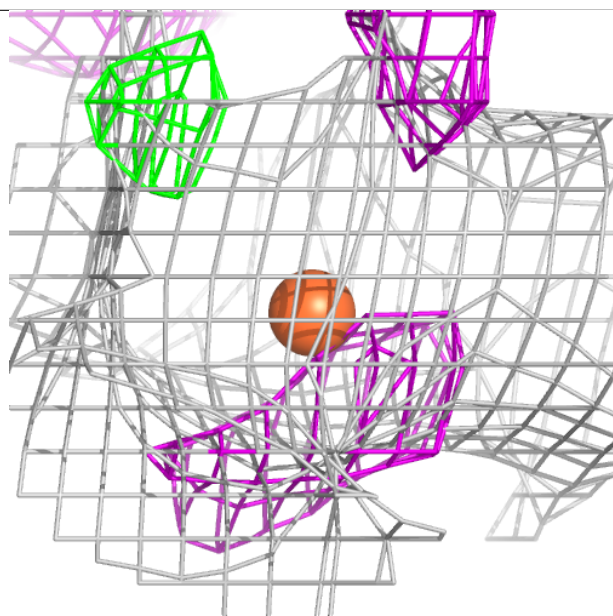
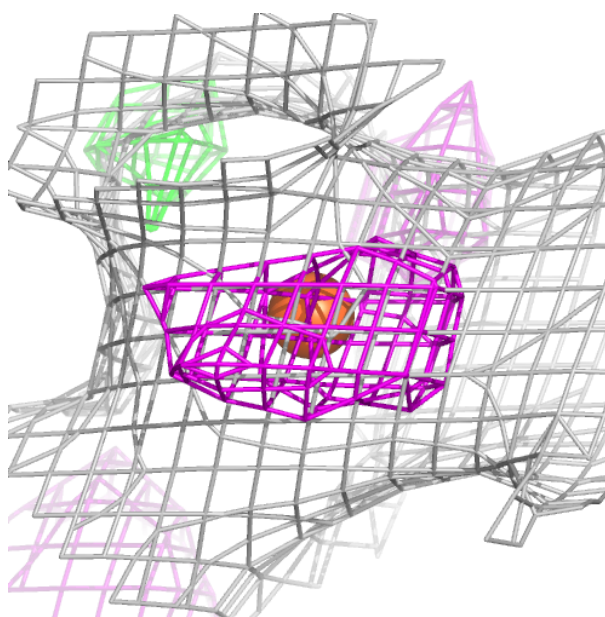
Electron density around FE G 203:

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



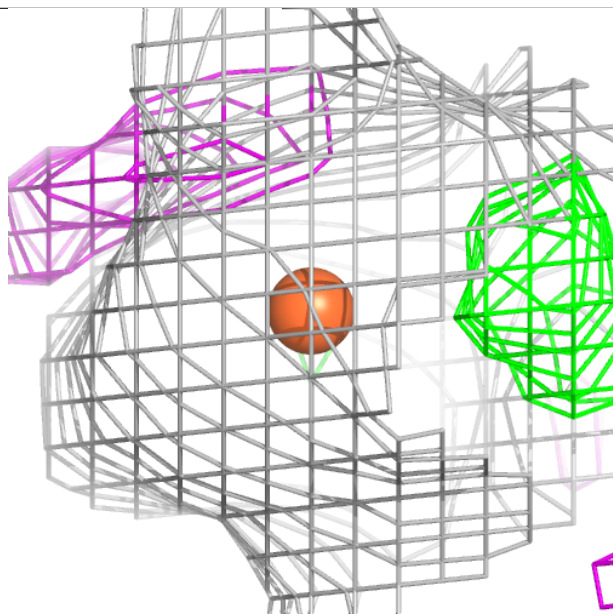
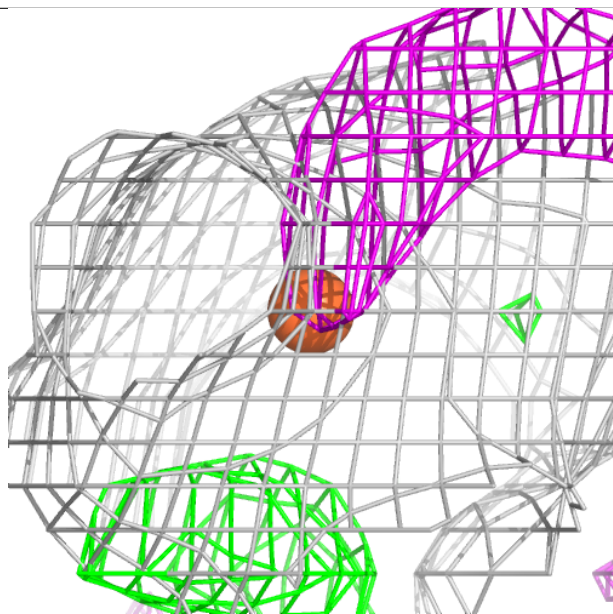
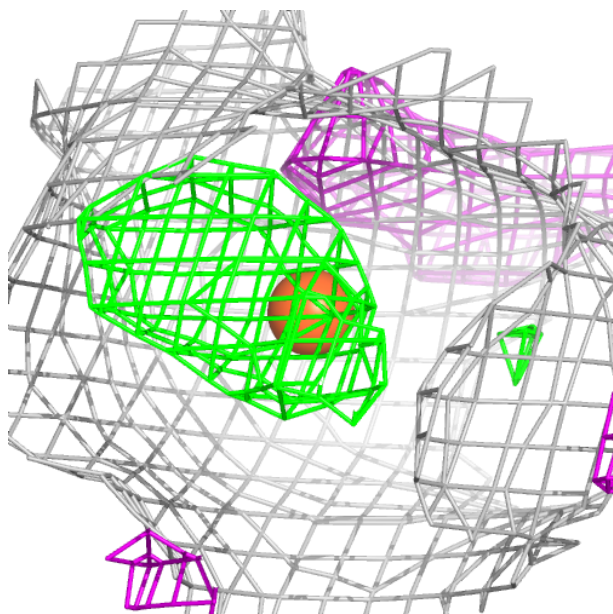
Electron density around FE H 202:

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



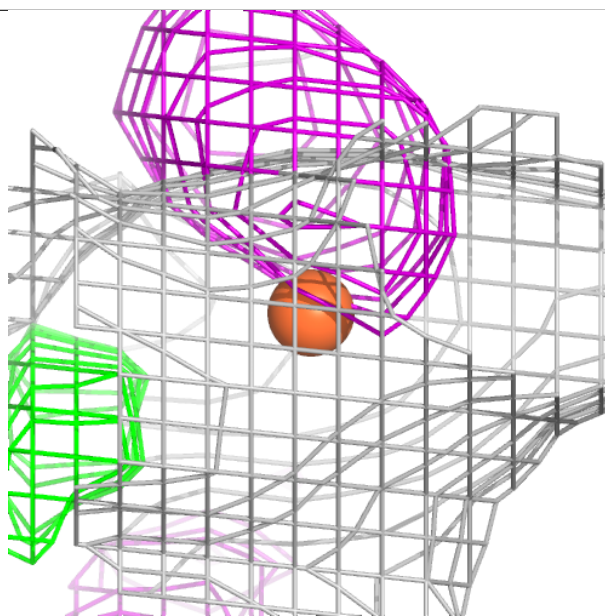
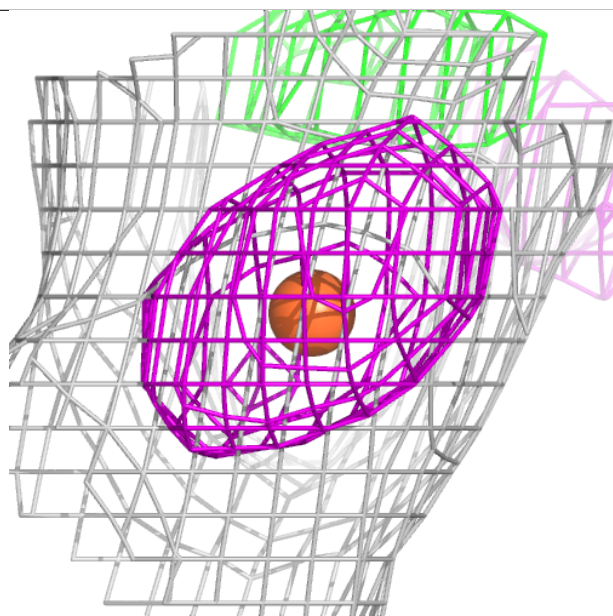
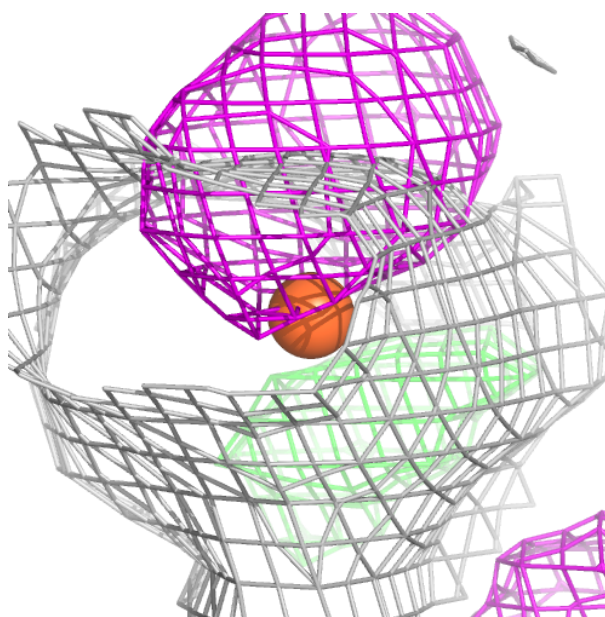
Electron density around FE E 201:

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



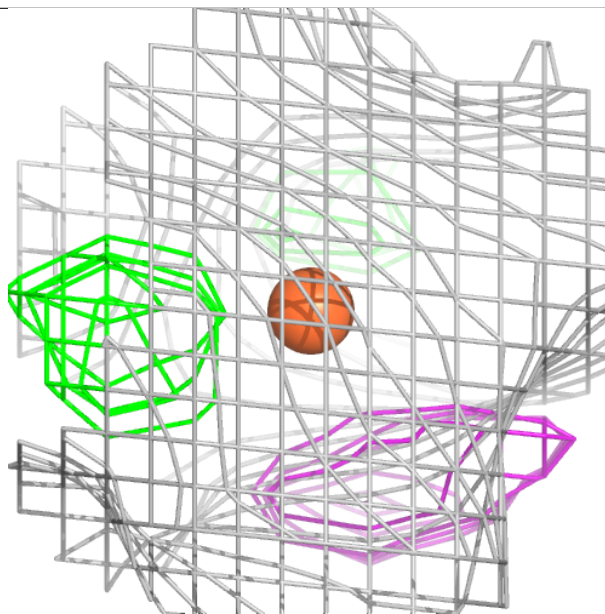
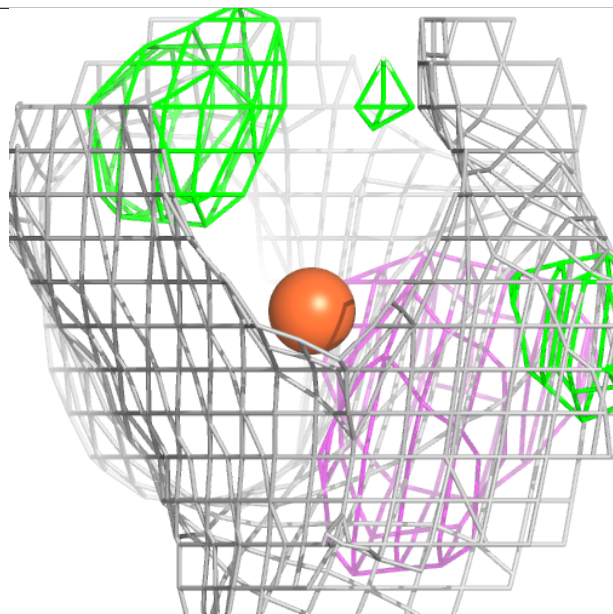
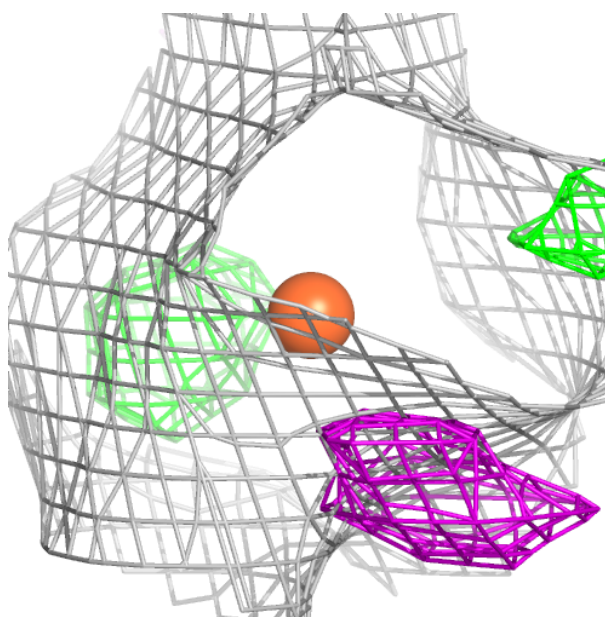
Electron density around FE C 203:

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



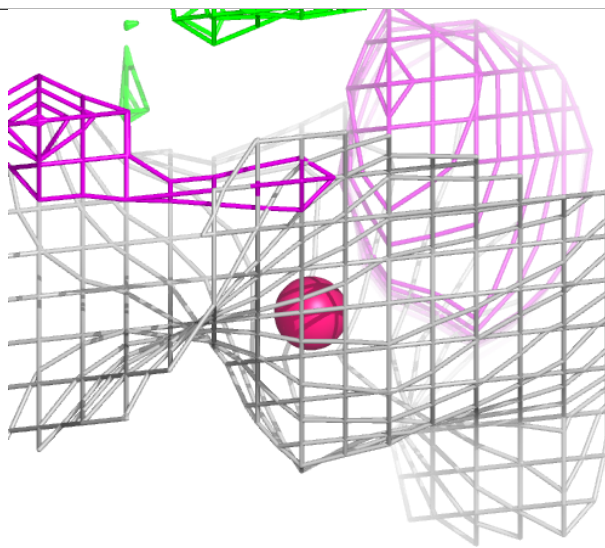
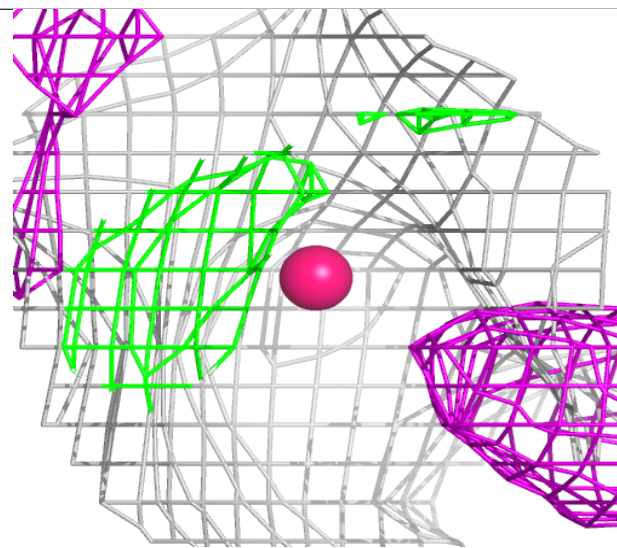
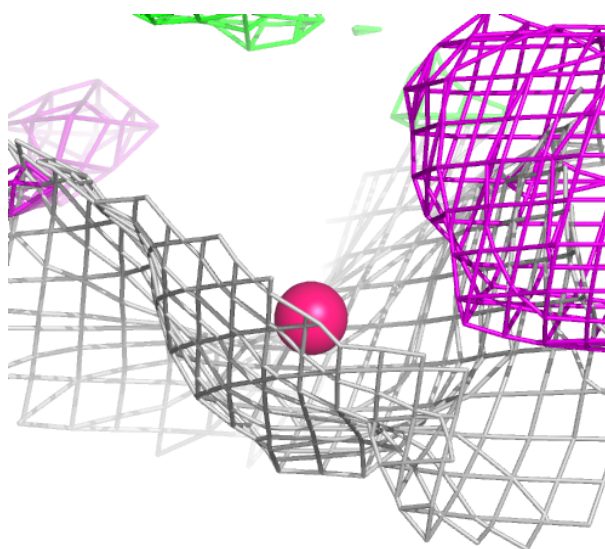
Electron density around FE A 201:

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



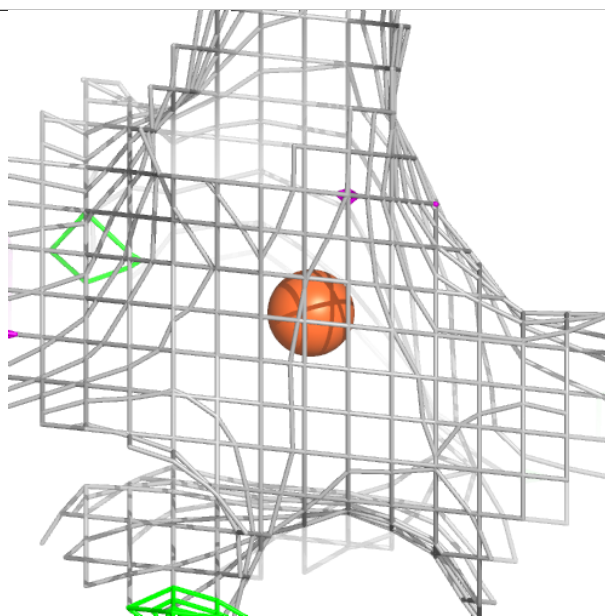
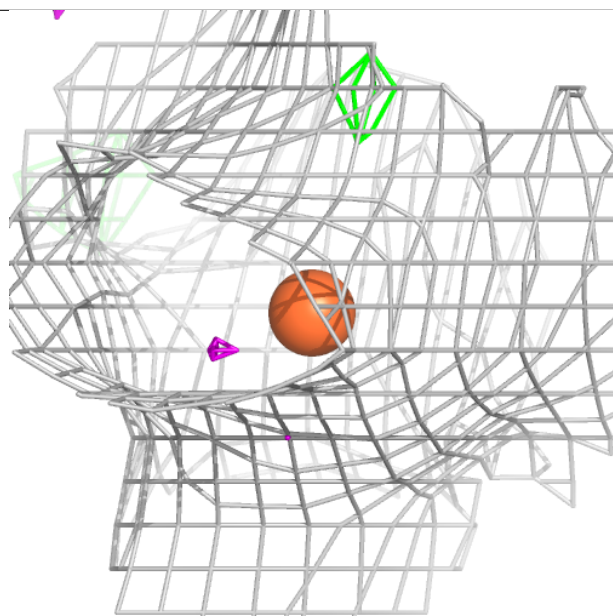
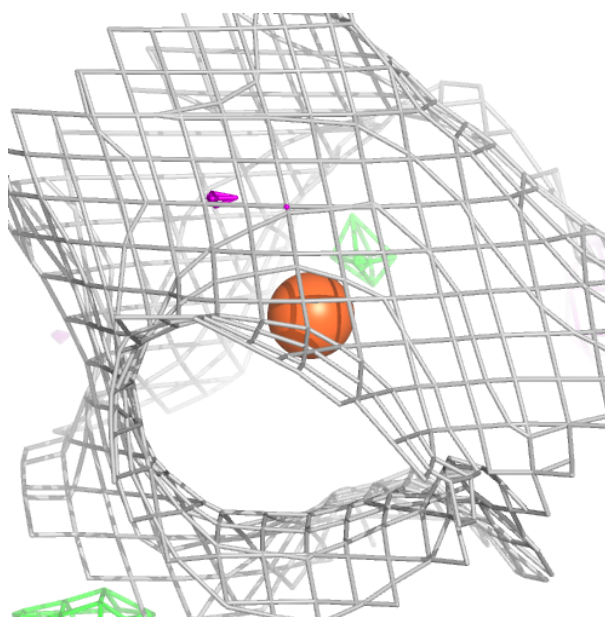
Electron density around O A 204:

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



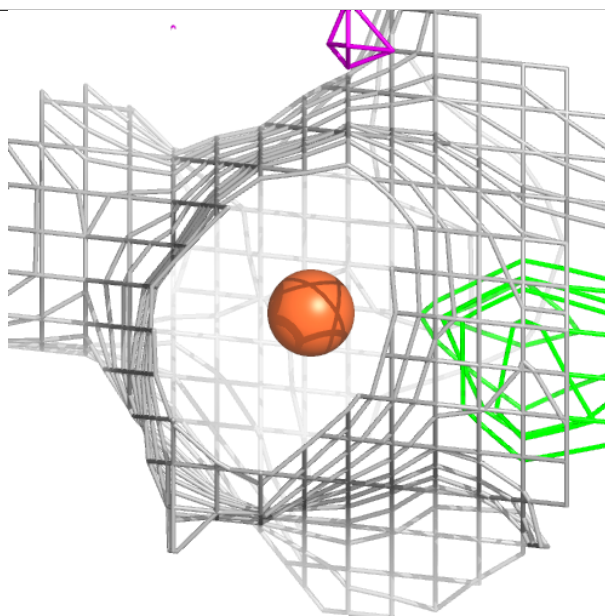
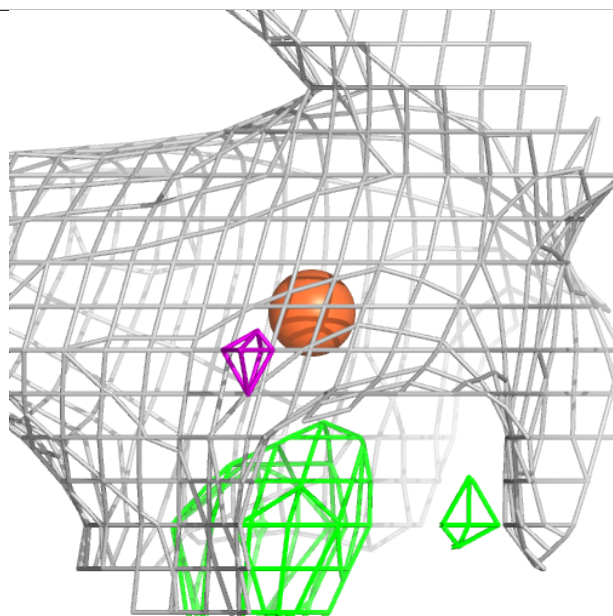
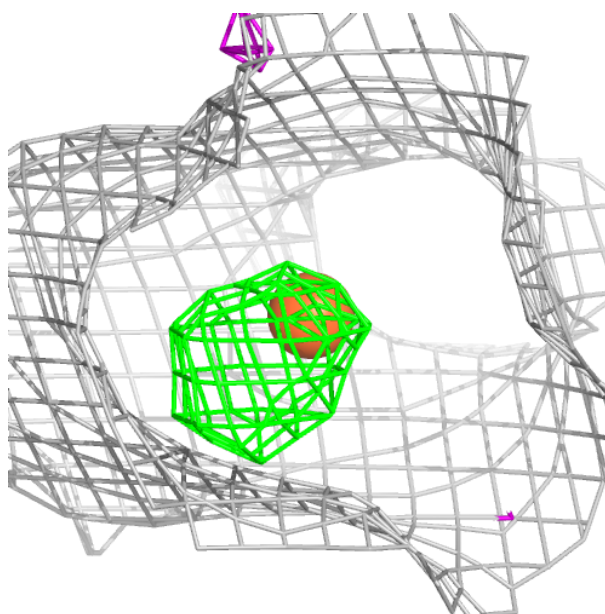
Electron density around FE C 201:

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



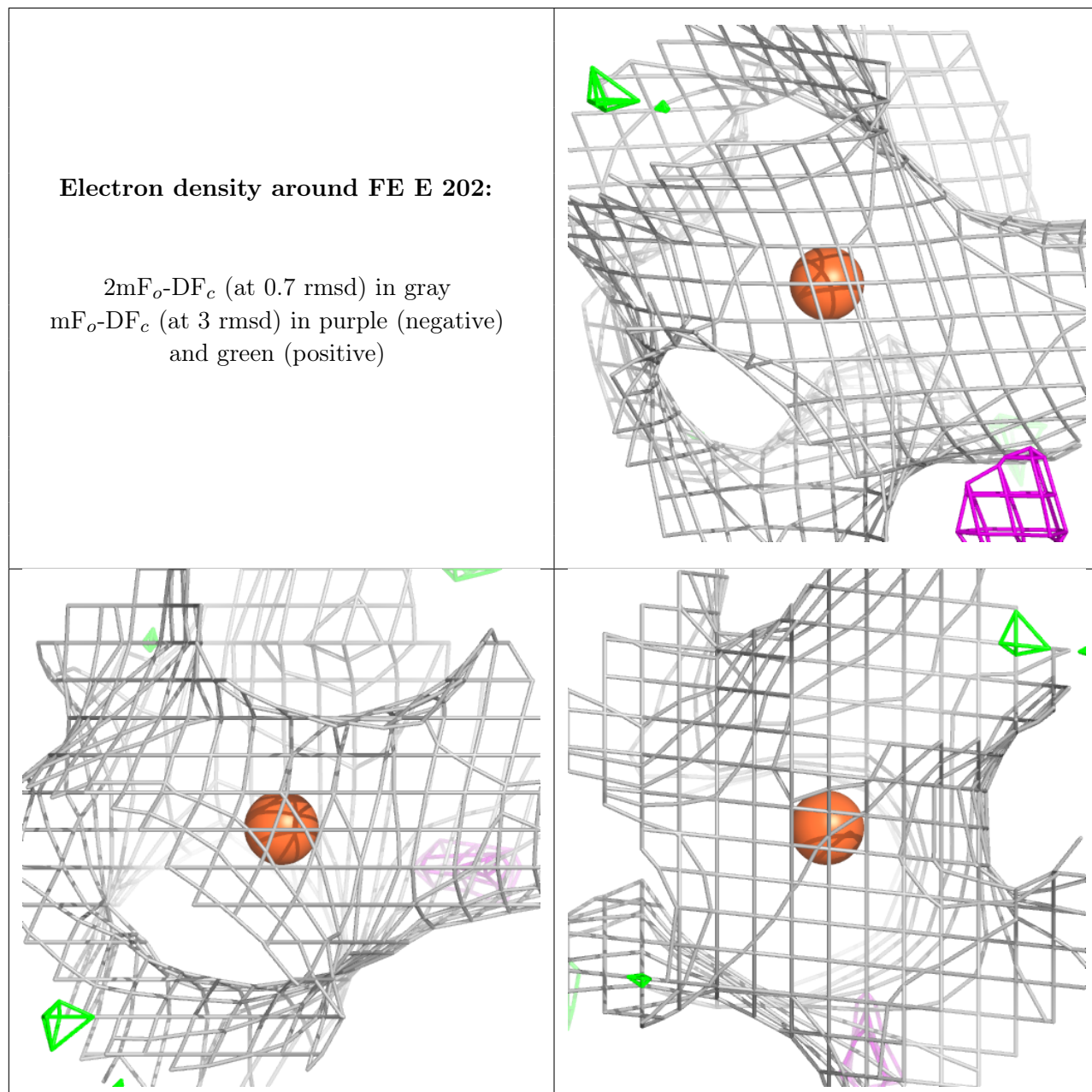
Electron density around FE B 201:

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



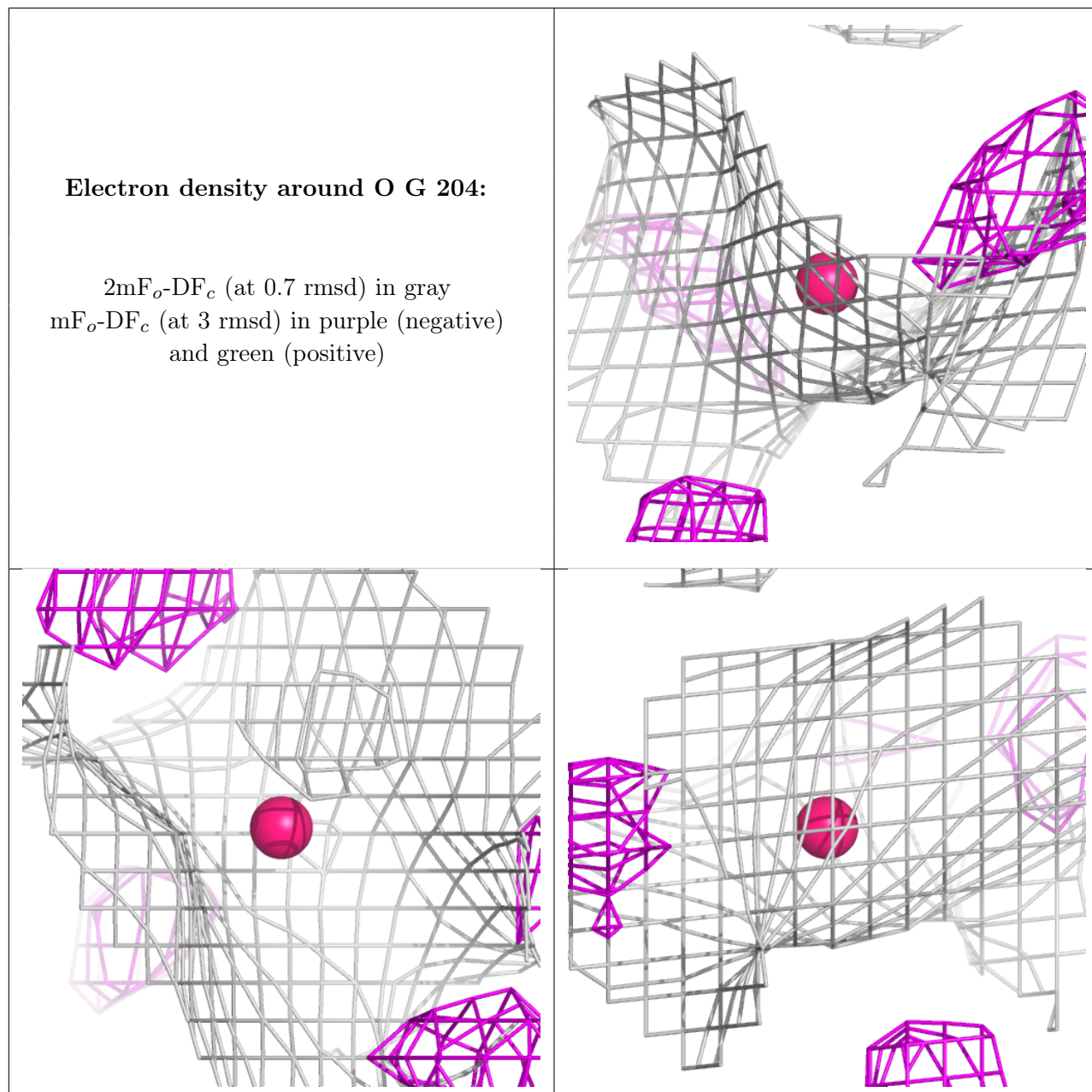
Electron density around FE E 202:

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



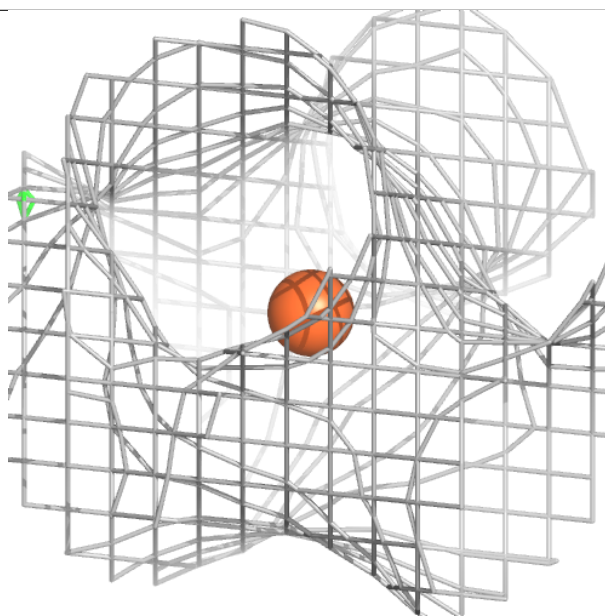
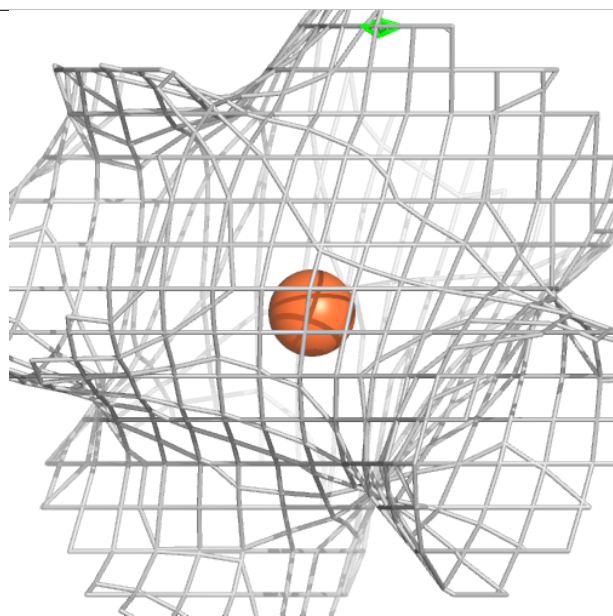
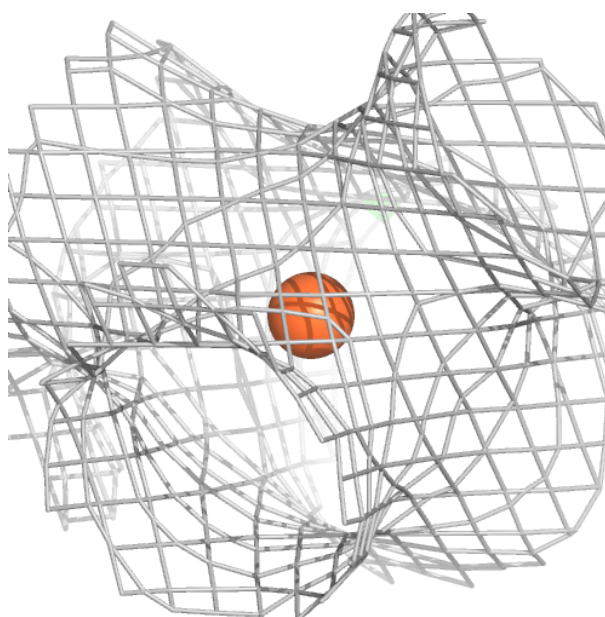
Electron density around O G 204:

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



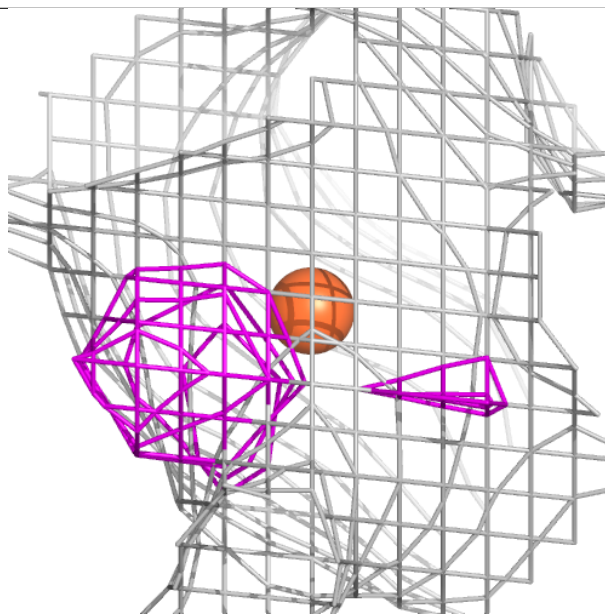
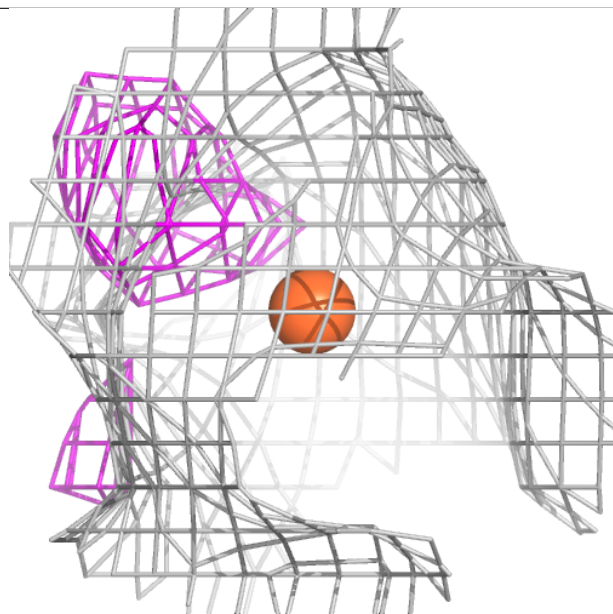
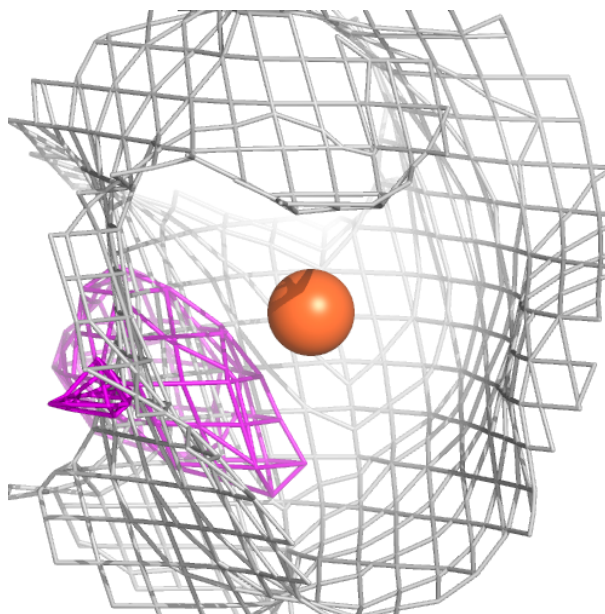
Electron density around FE F 203:

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



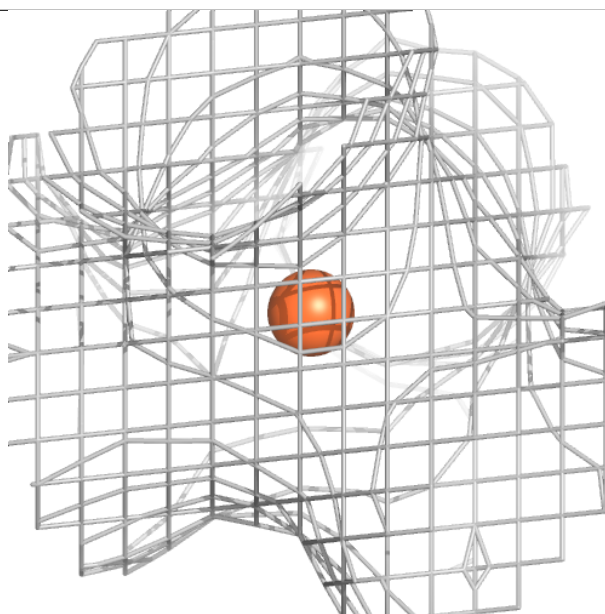
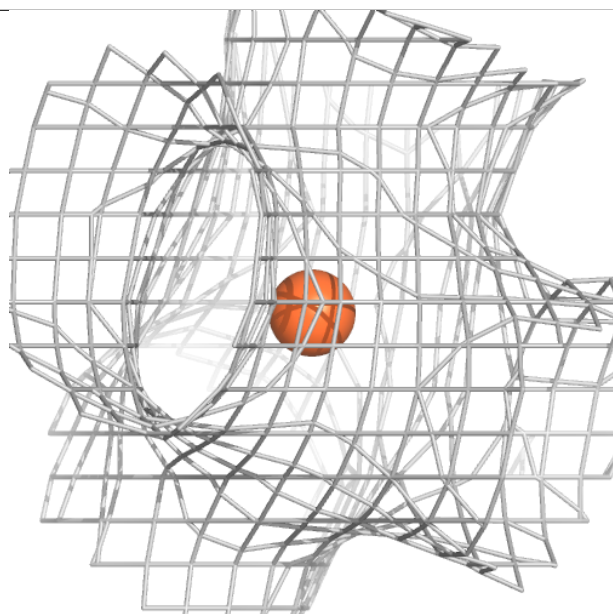
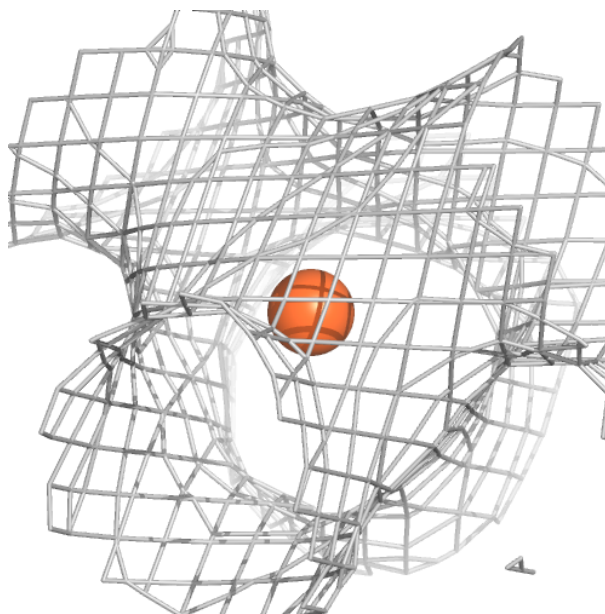
Electron density around FE H 201:

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



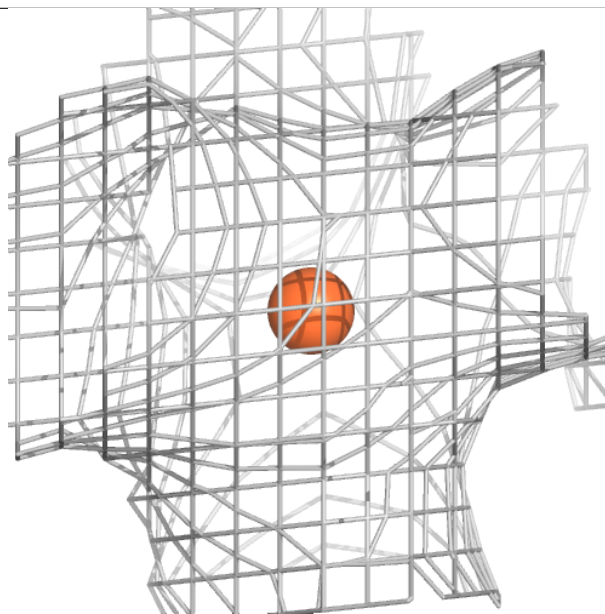
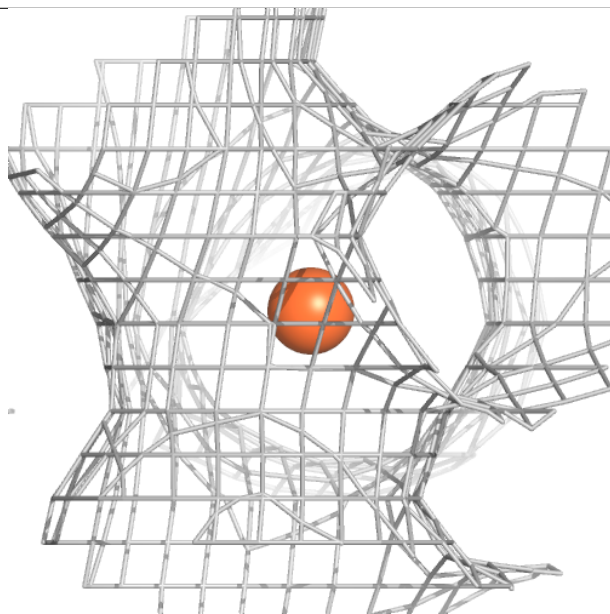
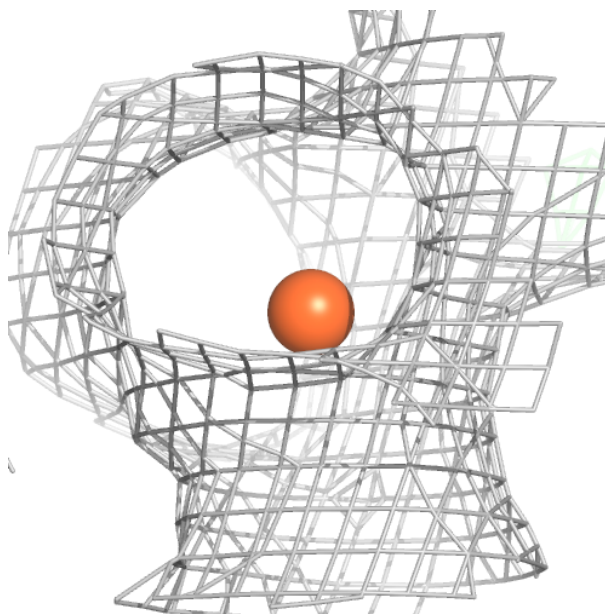
Electron density around FE D 203:

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



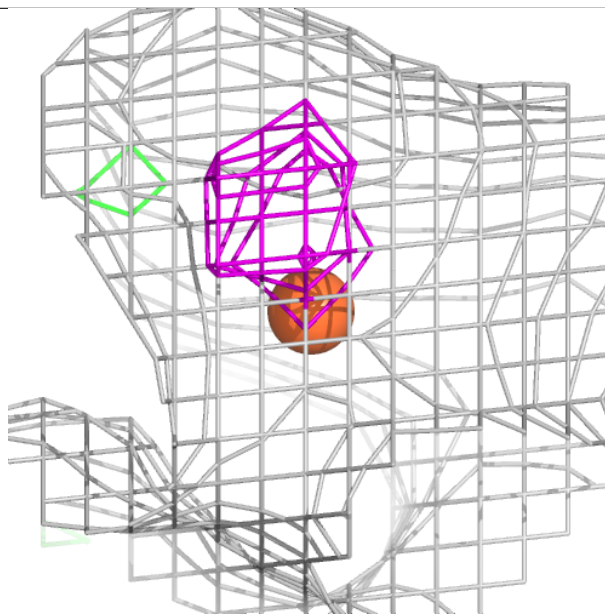
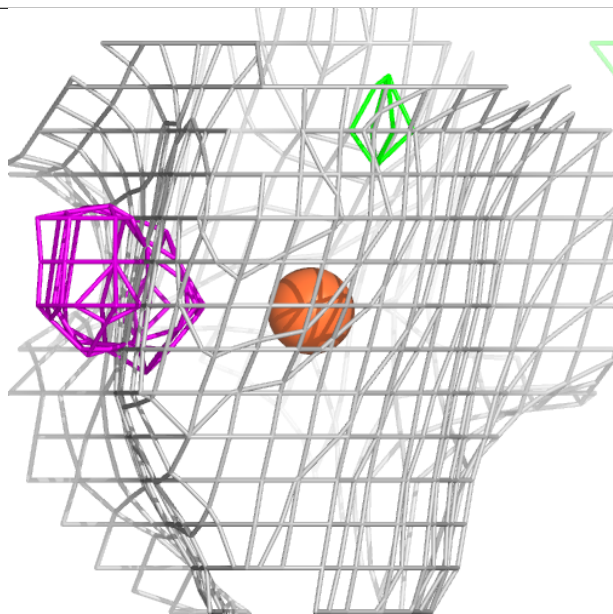
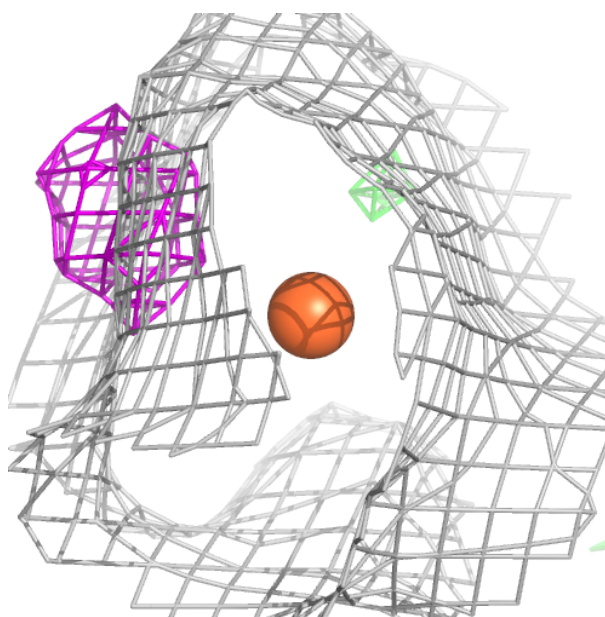
Electron density around FE A 202:

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



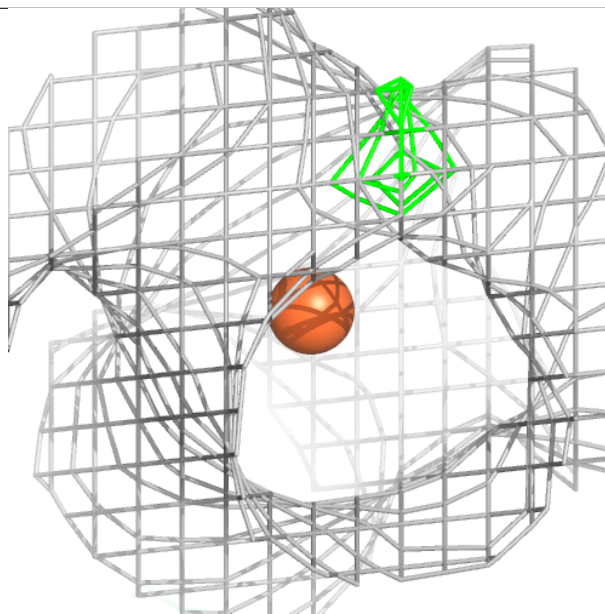
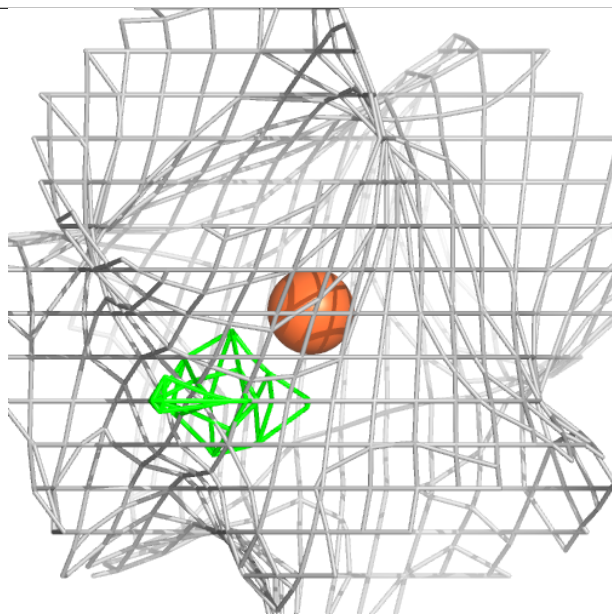
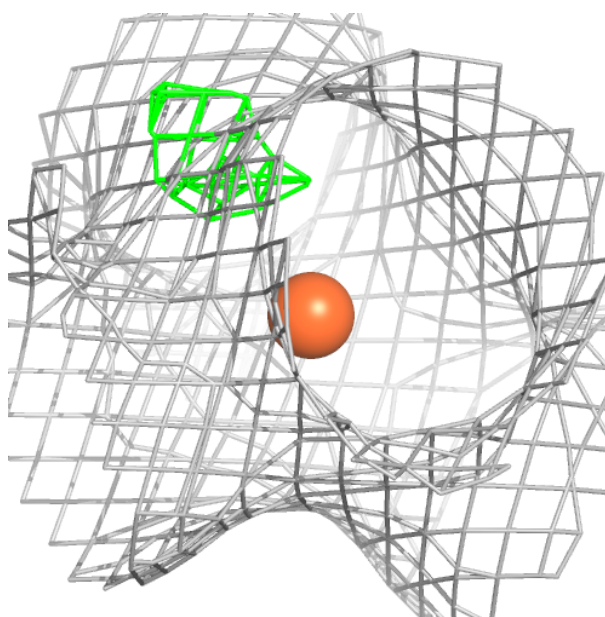
Electron density around FE D 201:

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



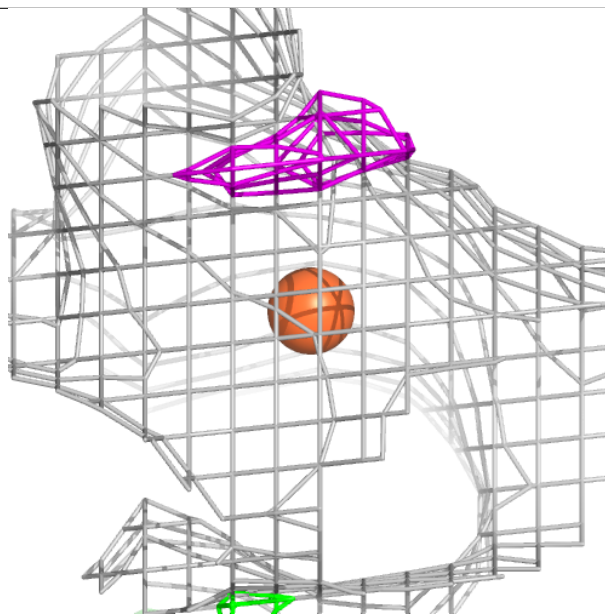
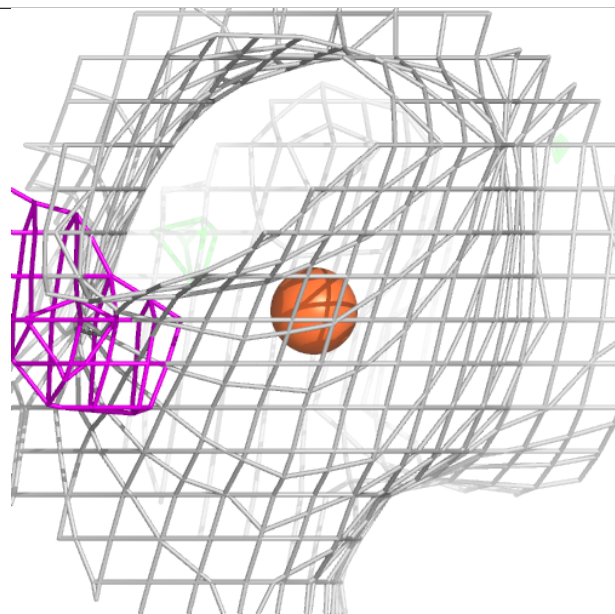
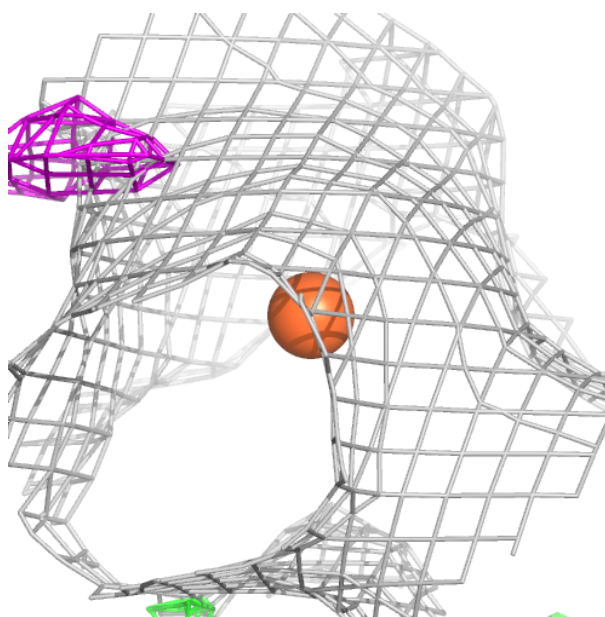
Electron density around FE B 202:

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



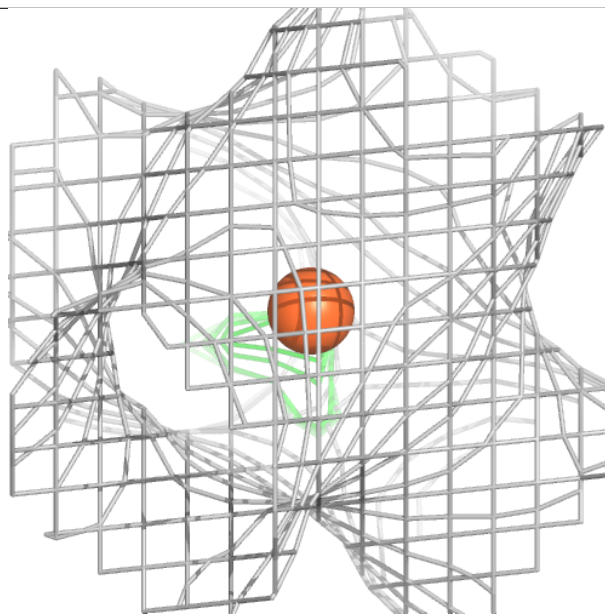
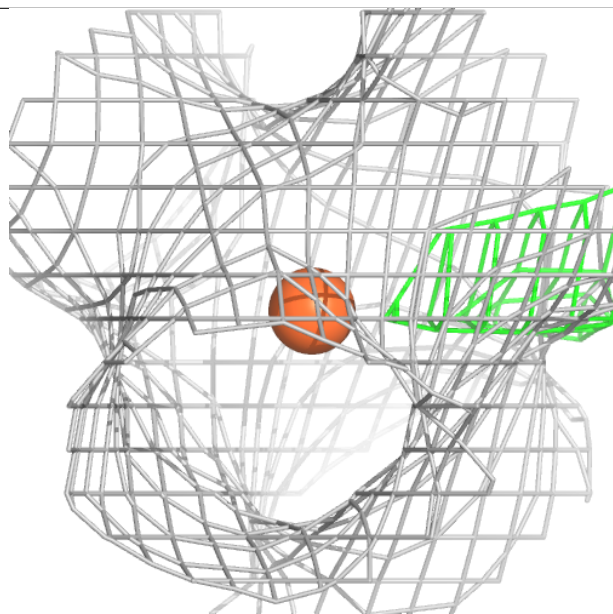
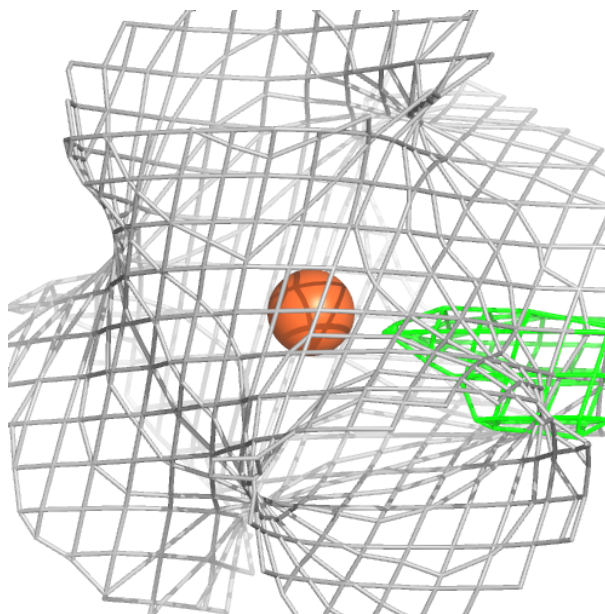
Electron density around FE F 202:

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



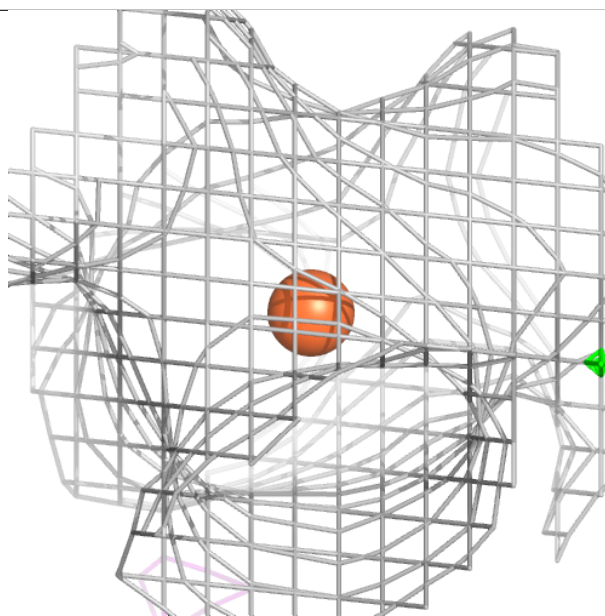
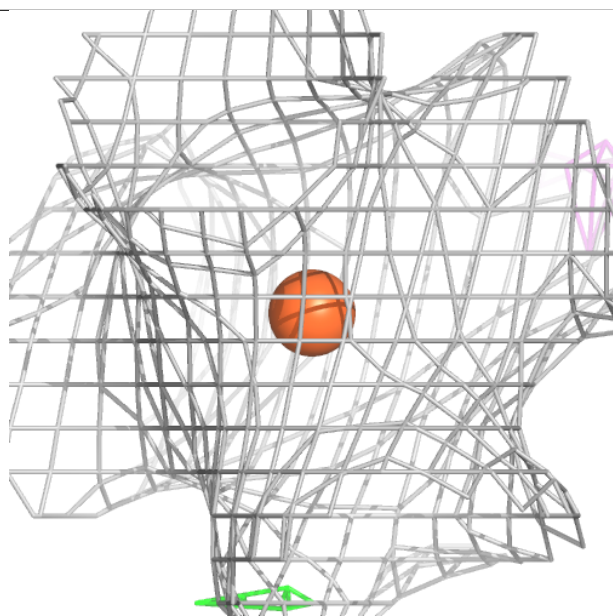
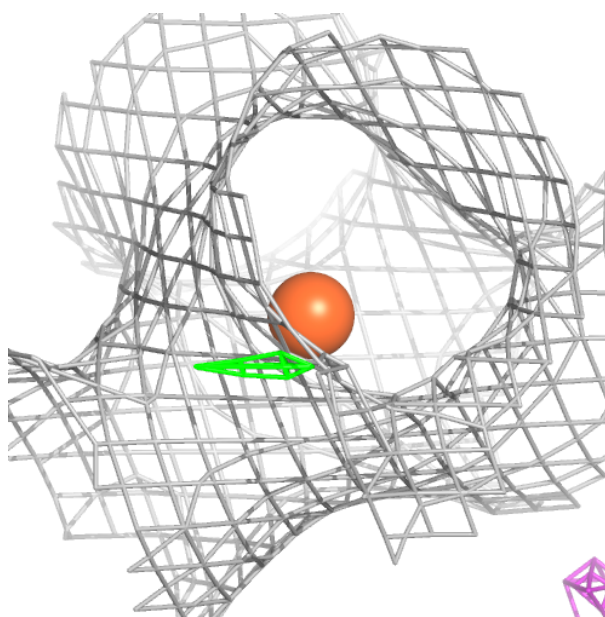
Electron density around FE C 202:

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



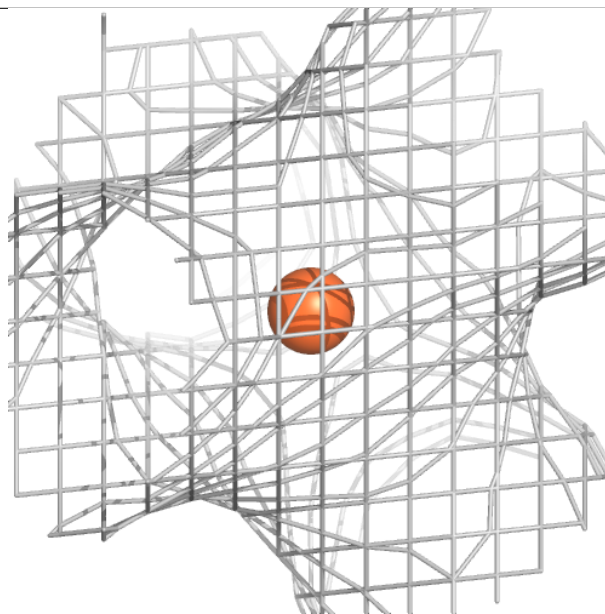
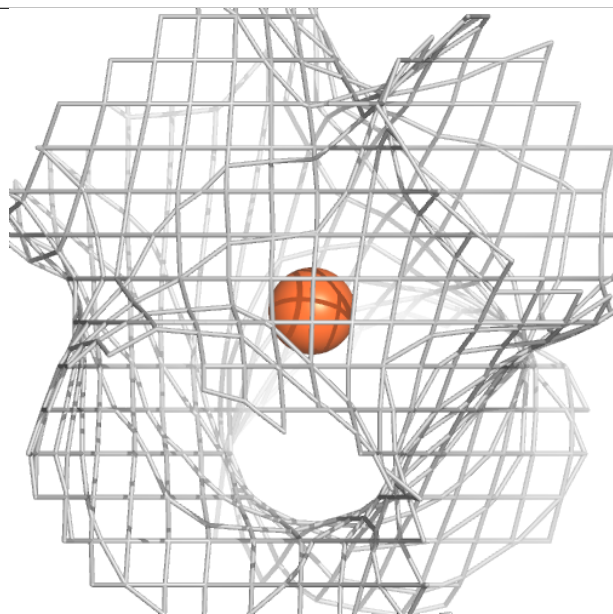
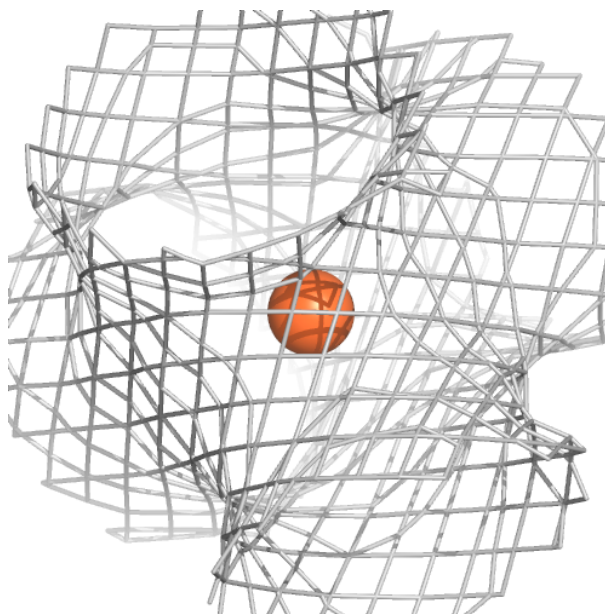
Electron density around FE H 203:

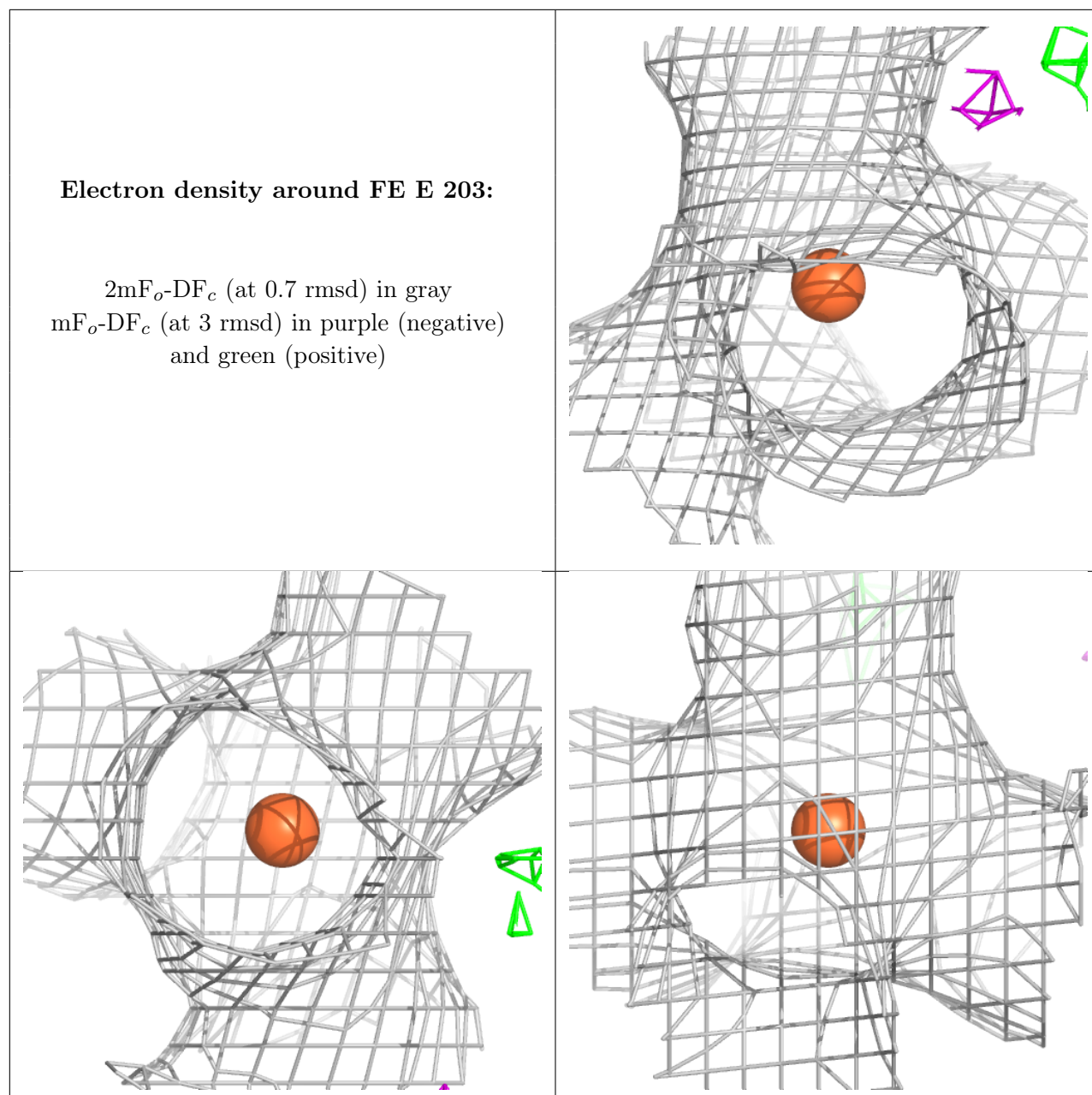
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE G 202:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.