



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:38 PM UTC

PDB ID : 8FFB / pdb_00008ffb
Title : Crystal structure of iron bound Dps protein (PA0962) from *Pseudomonas aeruginosa* (orthorhombic form)
Authors : Lovell, S.; Kashipathy, M.M.; Battaile, K.P.; Rivera, M.
Deposited on : 2022-12-08
Resolution : 2.25 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

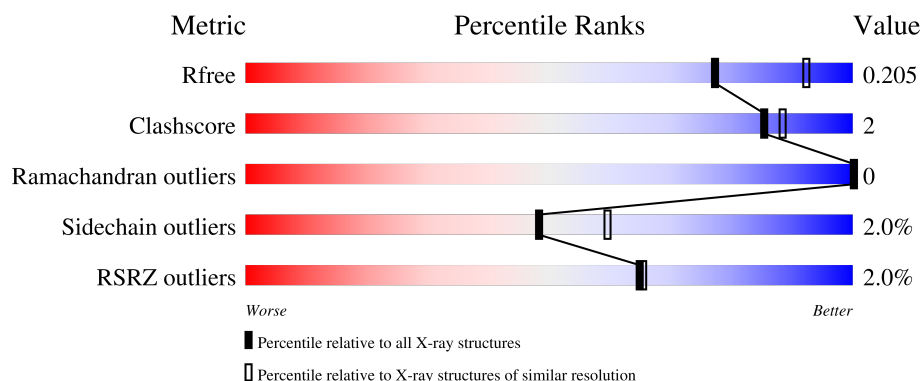
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	156	% 92% 6% ..
1	B	156	% 96% ..
1	C	156	3% 90% 9% .
1	D	156	% 93% 6% .
1	E	156	90% 10% .

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Mol	Chain	Length	Quality of chain
1	F	156	4% 92% 8% .
1	G	156	5% 94% 6% .
1	H	156	% 94% 6% .
1	I	156	% 89% 10% ..
1	J	156	5% 90% 9% .
1	K	156	94% 6% .
1	L	156	2% 91% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15155 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 Probable dna-binding stress protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1188	757	204	221	6			
1	B	155	Total	C	N	O	S	0	0	0
			1200	764	207	223	6			
1	C	155	Total	C	N	O	S	0	0	0
			1199	764	208	221	6			
1	D	155	Total	C	N	O	S	0	0	0
			1208	767	209	226	6			
1	E	155	Total	C	N	O	S	0	0	0
			1192	759	204	223	6			
1	F	155	Total	C	N	O	S	0	0	0
			1191	759	201	225	6			
1	G	155	Total	C	N	O	S	0	0	0
			1191	758	204	223	6			
1	H	155	Total	C	N	O	S	0	0	0
			1201	762	204	229	6			
1	I	155	Total	C	N	O	S	0	0	0
			1208	766	208	228	6			
1	J	155	Total	C	N	O	S	0	0	0
			1189	757	204	223	5			
1	K	155	Total	C	N	O	S	0	0	0
			1201	763	207	225	6			
1	L	155	Total	C	N	O	S	0	0	0
			1198	761	205	226	6			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (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	2	Total	Fe	0	0
			2	2		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	88	Total 88	O 88	0	0
3	C	48	Total 48	O 48	0	0
3	D	68	Total 68	O 68	0	0
3	E	67	Total 67	O 67	0	0
3	F	53	Total 53	O 53	0	0
3	G	42	Total 42	O 42	0	0
3	H	82	Total 82	O 82	0	0
3	I	80	Total 80	O 80	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	42	Total 42	O 42	0	0
3	K	81	Total 81	O 81	0	0
3	L	65	Total 65	O 65	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: Probable dna-binding stress protein



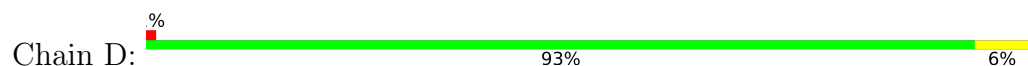
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



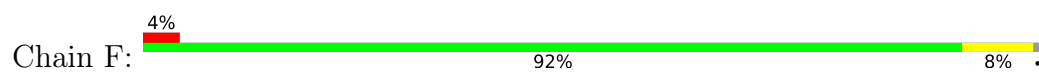
- Molecule 1: Probable dna-binding stress protein



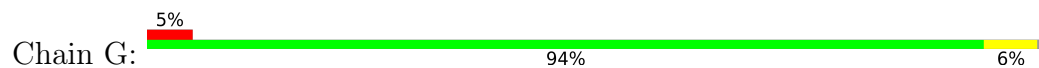
- Molecule 1: Probable dna-binding stress protein



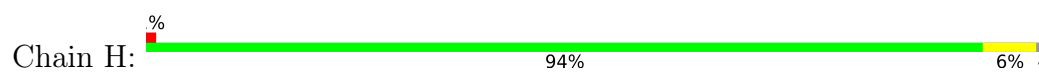
- Molecule 1: Probable dna-binding stress protein



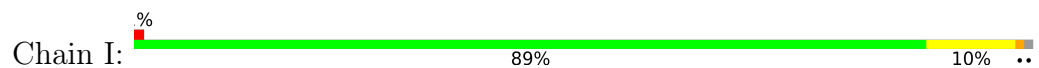
- Molecule 1: Probable dna-binding stress protein



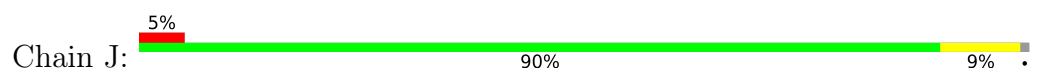
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



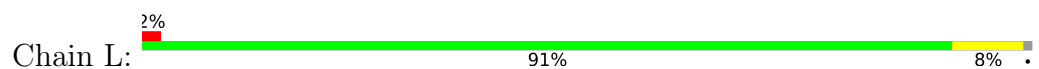
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.08Å 131.84Å 157.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.25 48.86 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.86-2.25) 100.0 (48.86-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.24Å)	Xtriage
Refinement program	PHENIX dev_4126	Depositor
R, R_{free}	0.183 , 0.233 (Not available) , 0.205	Depositor DCC
R_{free} test set	6435 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15155	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: FE2

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	0.37	0/1211	0.53	0/1648
1	B	0.46	0/1223	0.58	0/1662
1	C	0.36	0/1222	0.52	0/1660
1	D	0.39	0/1231	0.52	0/1672
1	E	0.39	0/1215	0.54	0/1653
1	F	0.36	0/1214	0.51	0/1652
1	G	0.37	0/1214	0.53	0/1652
1	H	0.45	0/1224	0.60	0/1665
1	I	0.41	0/1231	0.56	0/1673
1	J	0.37	0/1212	0.52	0/1650
1	K	0.43	0/1224	0.58	0/1664
1	L	0.41	0/1221	0.56	0/1661
All	All	0.40	0/14642	0.55	0/19912

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	1188	0	1165	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1200	0	1184	2	0
1	C	1199	0	1189	6	0
1	D	1208	0	1197	4	0
1	E	1192	0	1169	8	0
1	F	1191	0	1164	7	0
1	G	1191	0	1167	6	0
1	H	1201	0	1175	4	0
1	I	1208	0	1190	9	0
1	J	1189	0	1162	7	0
1	K	1201	0	1182	3	0
1	L	1198	0	1175	6	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	49	0	0	0	0
3	B	88	0	0	0	0
3	C	48	0	0	0	0
3	D	68	0	0	1	0
3	E	67	0	0	1	0
3	F	53	0	0	1	0
3	G	42	0	0	0	0
3	H	82	0	0	0	0
3	I	80	0	0	0	0
3	J	42	0	0	0	0
3	K	81	0	0	0	0
3	L	65	0	0	0	0
All	All	15155	0	14119	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (63) 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:G:7:ILE:HG23	1:G:127:VAL:HG11	1.60	0.83
1:F:7:ILE:HG23	1:F:127:VAL:HG11	1.78	0.64
1:G:7:ILE:HG23	1:G:127:VAL:CG1	2.32	0.57
1:C:83:ALA:O	1:C:87:LEU:HD12	2.06	0.56
1:J:37:HIS:CE1	1:J:49:HIS:CE1	2.94	0.55
1:G:106:LEU:O	1:G:110:GLN:HG2	2.08	0.54
1:E:118:ARG:NH1	3:E:301:HOH:O	2.40	0.54
1:E:7:ILE:HG23	1:E:127:VAL:HG11	1.90	0.53
1:K:106:LEU:O	1:K:110:GLN:HG2	2.09	0.52
1:E:106:LEU:O	1:E:110:GLN:HG2	2.11	0.51
1:F:37:HIS:CE1	1:F:49:HIS:CE1	3.00	0.50
1:L:37:HIS:CE1	1:L:49:HIS:CE1	3.00	0.50
1:A:53:GLU:HA	1:A:56:TYR:CE2	2.46	0.50
1:B:37:HIS:CE1	1:B:49:HIS:CE1	3.00	0.49
1:I:15:ILE:HD11	1:I:127:VAL:HG21	1.94	0.49
1:D:46:ASN:OD1	1:J:51:MET:HE3	2.13	0.49
1:A:13:ALA:HB2	1:A:75:PHE:CZ	2.48	0.48
1:I:22:LEU:HD22	1:I:136:LEU:CD2	2.44	0.47
1:E:7:ILE:HG23	1:E:127:VAL:CG1	2.44	0.47
1:F:106:LEU:O	1:F:110:GLN:HG2	2.15	0.47
1:E:37:HIS:CE1	1:E:49:HIS:CE1	3.03	0.47
1:H:37:HIS:CE1	1:H:49:HIS:CE1	3.03	0.47
1:I:106:LEU:O	1:I:110:GLN:HG2	2.15	0.46
1:G:127:VAL:HG12	1:G:127:VAL:O	2.15	0.46
1:L:124:LEU:HD22	1:L:129:ASP:HB3	1.97	0.46
1:F:7:ILE:HG23	1:F:127:VAL:CG1	2.43	0.46
1:F:21:ARG:NH1	3:F:304:HOH:O	2.48	0.46
1:A:127:VAL:O	1:A:127:VAL:CG1	2.64	0.45
1:B:124:LEU:HD11	1:B:136:LEU:HD22	1.98	0.45
1:C:37:HIS:CE1	1:C:49:HIS:CE1	3.05	0.45
1:F:51:MET:HE3	1:I:46:ASN:OD1	2.17	0.45
1:E:79:GLY:HA2	1:E:84:TYR:CZ	2.52	0.44
1:D:53:GLU:HA	1:D:56:TYR:CE2	2.52	0.44
1:E:53:GLU:HA	1:E:56:TYR:CE2	2.53	0.44
1:J:154:LEU:O	1:J:155:ALA:C	2.60	0.44
1:D:13:ALA:HB2	1:D:75:PHE:CZ	2.52	0.44
1:I:59:LEU:O	1:I:63:VAL:HG13	2.18	0.44
1:C:106:LEU:O	1:C:110:GLN:HG2	2.18	0.43
1:G:13:ALA:HB2	1:G:75:PHE:CZ	2.53	0.43
1:L:106:LEU:O	1:L:110:GLN:HG2	2.17	0.43
1:I:27:TYR:O	1:I:30:TYR:HB3	2.18	0.43
1:I:26:THR:HG22	1:I:63:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:GLN:O	1:E:59:LEU:HG	2.19	0.43
1:H:106:LEU:O	1:H:110:GLN:HG2	2.19	0.43
1:A:37:HIS:CE1	1:A:49:HIS:CE1	3.07	0.43
1:L:127:VAL:O	1:L:128:SER:HB2	2.19	0.43
1:C:154:LEU:O	1:C:155:ALA:C	2.62	0.43
1:H:154:LEU:O	1:H:155:ALA:C	2.62	0.42
1:G:27:TYR:CZ	1:I:31:LEU:HD13	2.53	0.42
1:J:60:ALA:O	1:J:63:VAL:HG22	2.19	0.42
1:L:53:GLU:HA	1:L:56:TYR:CE2	2.55	0.42
1:J:79:GLY:HA2	1:J:84:TYR:CZ	2.54	0.41
1:A:148:TRP:HB2	1:C:72:ALA:HA	2.02	0.41
1:H:53:GLU:HA	1:H:56:TYR:CE2	2.55	0.41
1:D:91:LYS:N	3:D:301:HOH:O	2.23	0.41
1:J:59:LEU:O	1:J:63:VAL:HG13	2.20	0.41
1:C:53:GLU:HA	1:C:56:TYR:CE2	2.55	0.41
1:K:53:GLU:HA	1:K:56:TYR:CE2	2.55	0.41
1:J:106:LEU:O	1:J:110:GLN:HG2	2.21	0.41
1:K:15:ILE:HD11	1:K:127:VAL:HG21	2.03	0.40
1:L:79:GLY:HA2	1:L:84:TYR:CZ	2.56	0.40
1:F:56:TYR:CD1	1:F:56:TYR:C	2.99	0.40
1:I:37:HIS:CE1	1:I:49:HIS:CE1	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
1	B	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	C	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	D	153/156 (98%)	150 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
1	F	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
1	G	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	H	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	I	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
1	J	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
1	K	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
1	L	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
All	All	1836/1872 (98%)	1800 (98%)	36 (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	119/129 (92%)	115 (97%)	4 (3%)	32	40
1	B	121/129 (94%)	119 (98%)	2 (2%)	53	65
1	C	121/129 (94%)	118 (98%)	3 (2%)	42	52
1	D	124/129 (96%)	120 (97%)	4 (3%)	34	43
1	E	120/129 (93%)	118 (98%)	2 (2%)	53	65
1	F	120/129 (93%)	117 (98%)	3 (2%)	42	52
1	G	120/129 (93%)	118 (98%)	2 (2%)	53	65
1	H	123/129 (95%)	122 (99%)	1 (1%)	73	80
1	I	124/129 (96%)	122 (98%)	2 (2%)	55	66
1	J	119/129 (92%)	117 (98%)	2 (2%)	53	65
1	K	122/129 (95%)	119 (98%)	3 (2%)	42	52
1	L	122/129 (95%)	121 (99%)	1 (1%)	73	80
All	All	1455/1548 (94%)	1426 (98%)	29 (2%)	48	59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	47	THR
1	A	92	GLU
1	A	127	VAL
1	B	56	TYR
1	B	92	GLU
1	C	34	HIS
1	C	104	ARG
1	C	123	LEU
1	D	34	HIS
1	D	63	VAL
1	D	90	ILE
1	D	92	GLU
1	E	63	VAL
1	E	92	GLU
1	F	34	HIS
1	F	92	GLU
1	F	119	SER
1	G	47	THR
1	G	123	LEU
1	H	47	THR
1	I	10	GLN
1	I	127	VAL
1	J	47	THR
1	J	119	SER
1	K	34	HIS
1	K	47	THR
1	K	92	GLU
1	L	10	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	ASN
1	C	4	ASN
1	F	34	HIS
1	G	4	ASN
1	H	4	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 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 ⓘ

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	155/156 (99%)	0.14	2 (1%) 75 76	31, 41, 54, 66	0
1	B	155/156 (99%)	-0.37	1 (0%) 85 86	23, 31, 45, 60	0
1	C	155/156 (99%)	0.26	4 (2%) 57 58	33, 43, 60, 73	0
1	D	155/156 (99%)	-0.16	1 (0%) 85 86	26, 37, 48, 66	0
1	E	155/156 (99%)	-0.11	0 100 100	27, 37, 52, 59	0
1	F	155/156 (99%)	0.17	7 (4%) 38 37	30, 42, 62, 86	0
1	G	155/156 (99%)	0.24	8 (5%) 33 31	32, 44, 66, 79	0
1	H	155/156 (99%)	-0.36	1 (0%) 85 86	23, 31, 47, 66	0
1	I	155/156 (99%)	-0.16	2 (1%) 75 76	27, 36, 50, 56	0
1	J	155/156 (99%)	0.34	8 (5%) 33 31	33, 46, 62, 78	0
1	K	155/156 (99%)	-0.29	0 100 100	25, 33, 47, 65	0
1	L	155/156 (99%)	-0.11	3 (1%) 66 67	26, 35, 55, 72	0
All	All	1860/1872 (99%)	-0.03	37 (1%) 65 65	23, 38, 56, 86	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	155	ALA	4.0
1	F	123	LEU	3.5
1	A	155	ALA	3.1
1	J	1	MET	3.1
1	J	126	LYS	3.1
1	C	123	LEU	2.9
1	G	123	LEU	2.9
1	J	127	VAL	2.9
1	D	155	ALA	2.9
1	L	128	SER	2.8
1	C	125	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	2	GLU	2.8
1	L	155	ALA	2.8
1	I	155	ALA	2.7
1	G	128	SER	2.7
1	J	155	ALA	2.7
1	F	126	LYS	2.7
1	F	125	ASP	2.7
1	H	155	ALA	2.6
1	L	125	ASP	2.6
1	F	2	GLU	2.5
1	A	125	ASP	2.5
1	G	125	ASP	2.5
1	G	127	VAL	2.5
1	G	27	TYR	2.5
1	J	2	GLU	2.5
1	F	127	VAL	2.4
1	F	155	ALA	2.4
1	J	125	ASP	2.3
1	G	126	LYS	2.3
1	B	2	GLU	2.3
1	J	128	SER	2.3
1	F	128	SER	2.2
1	I	85	ALA	2.2
1	J	123	LEU	2.2
1	C	2	GLU	2.2
1	C	128	SER	2.2

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](#)

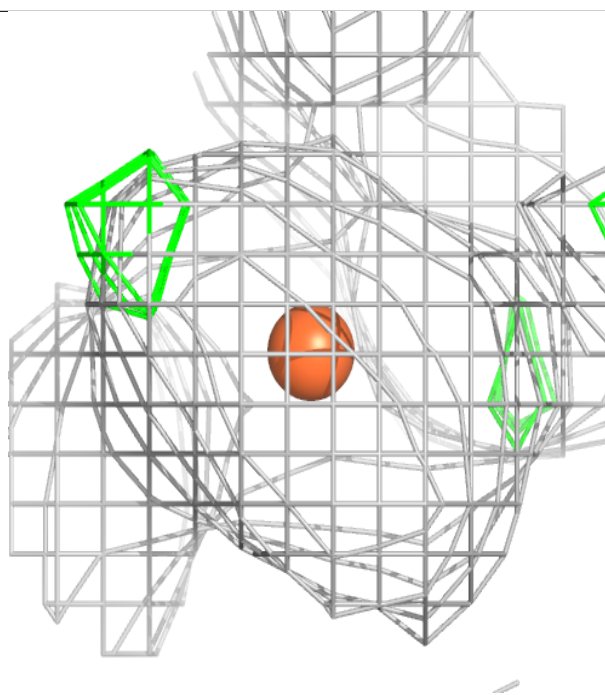
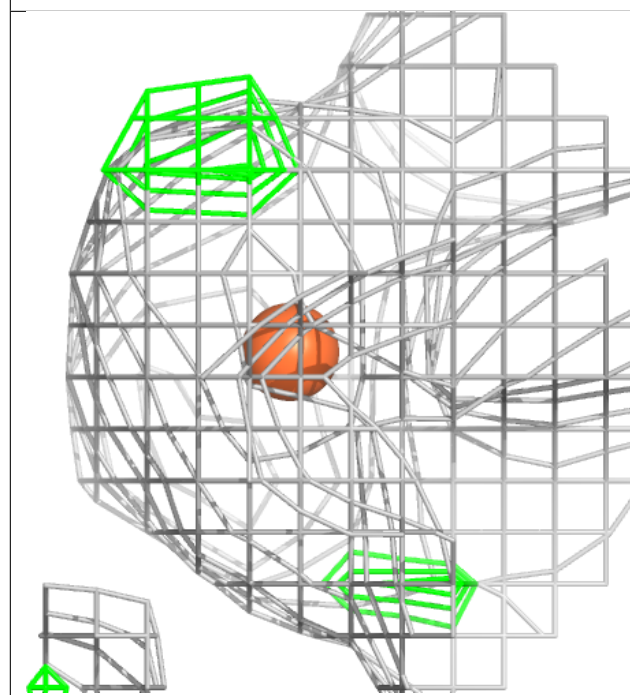
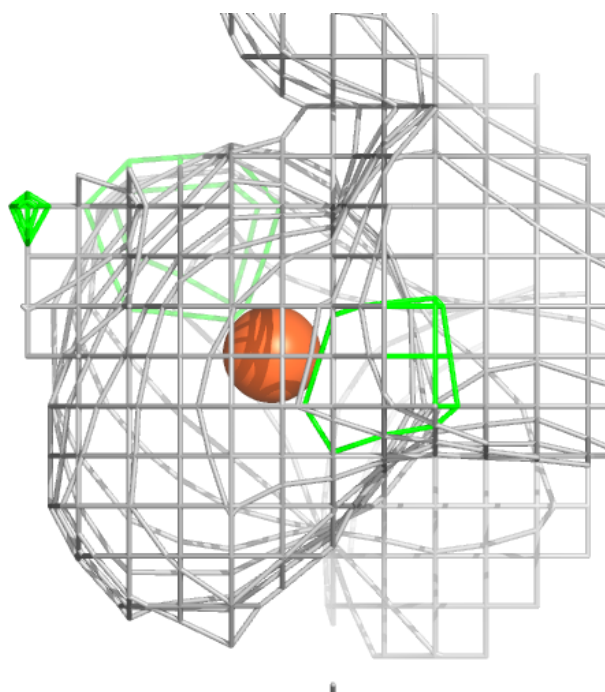
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE2	K	202	1/1	0.82	0.14	79,79,79,79	1
2	FE2	D	203	1/1	0.84	0.12	77,77,77,77	1
2	FE2	A	202	1/1	0.84	0.14	79,79,79,79	1
2	FE2	H	202	1/1	0.85	0.14	82,82,82,82	1
2	FE2	A	203	1/1	0.85	0.13	65,65,65,65	1
2	FE2	I	202	1/1	0.86	0.10	76,76,76,76	1
2	FE2	C	202	1/1	0.87	0.11	71,71,71,71	1
2	FE2	B	202	1/1	0.89	0.12	71,71,71,71	1
2	FE2	L	202	1/1	0.89	0.11	68,68,68,68	1
2	FE2	D	202	1/1	0.90	0.09	73,73,73,73	1
2	FE2	G	202	1/1	0.92	0.09	60,60,60,60	1
2	FE2	C	203	1/1	0.94	0.07	65,65,65,65	1
2	FE2	A	201	1/1	0.97	0.06	55,55,55,55	0
2	FE2	H	201	1/1	0.98	0.03	37,37,37,37	1
2	FE2	C	201	1/1	0.98	0.05	58,58,58,58	0
2	FE2	E	201	1/1	0.98	0.03	44,44,44,44	1
2	FE2	K	201	1/1	0.98	0.03	48,48,48,48	0
2	FE2	G	201	1/1	0.98	0.05	55,55,55,55	0
2	FE2	L	201	1/1	0.98	0.05	37,37,37,37	1
2	FE2	B	201	1/1	0.98	0.04	40,40,40,40	1
2	FE2	I	201	1/1	0.99	0.03	43,43,43,43	1
2	FE2	D	201	1/1	0.99	0.04	53,53,53,53	0
2	FE2	F	201	1/1	0.99	0.04	54,54,54,54	1
2	FE2	J	201	1/1	1.00	0.03	55,55,55,55	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.

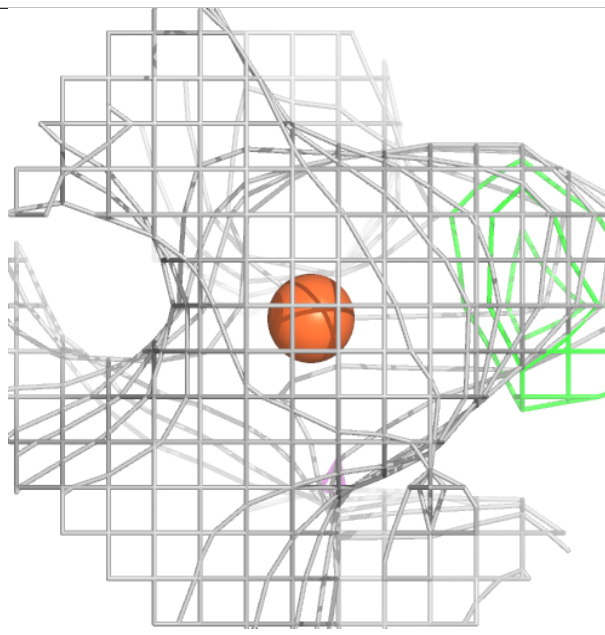
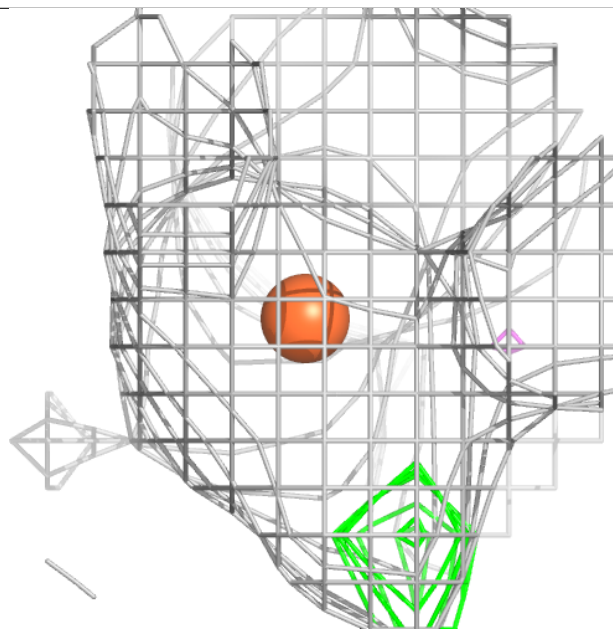
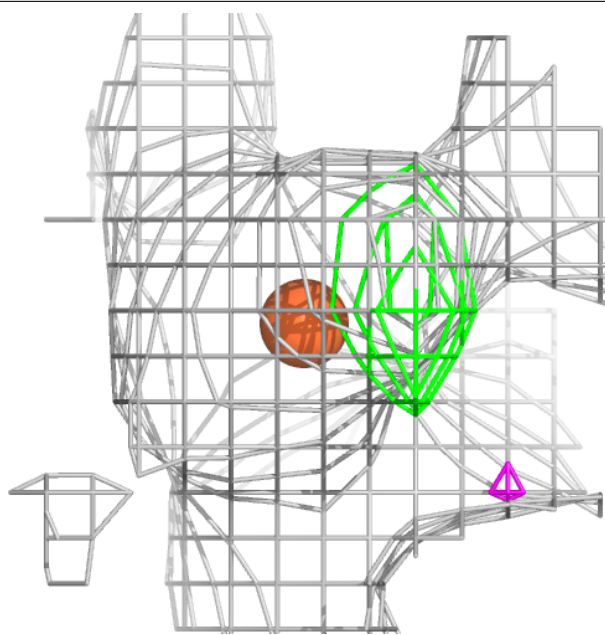
Electron density around FE2 K 202:

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



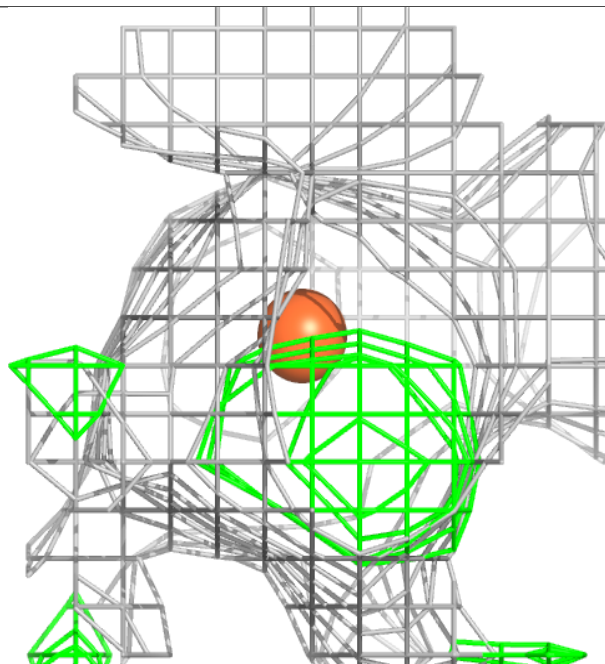
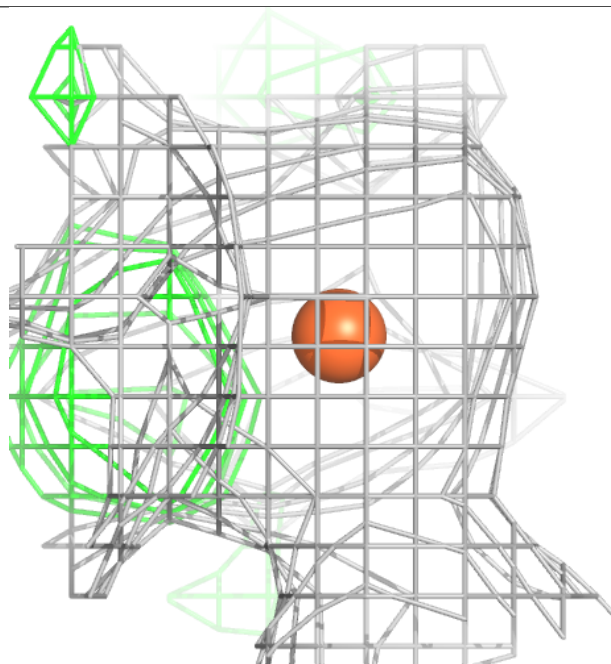
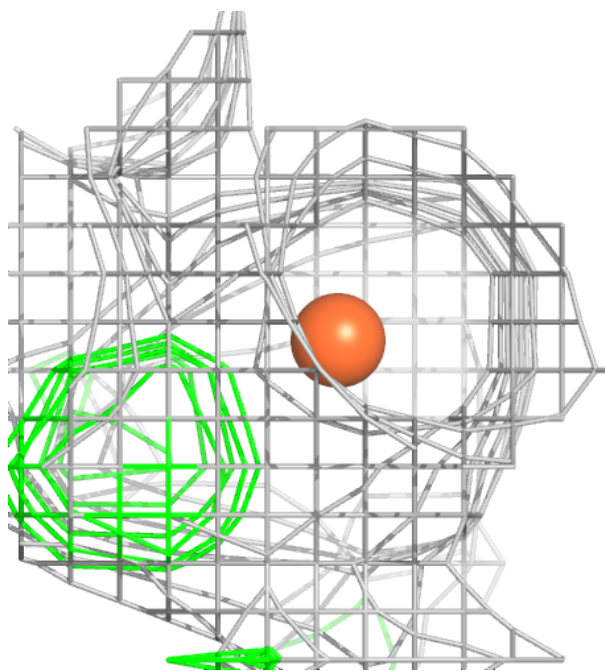
Electron density around FE2 D 203:

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and green (positive)



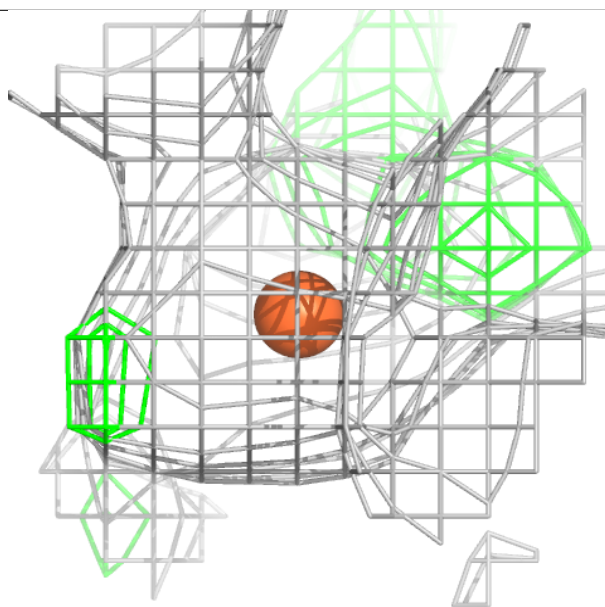
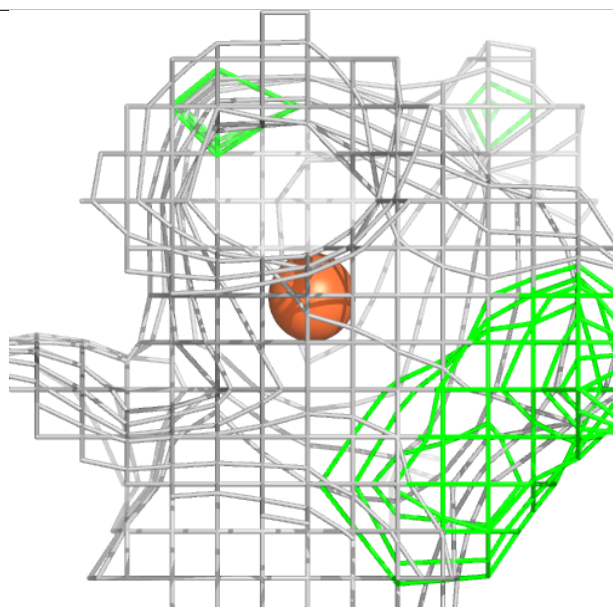
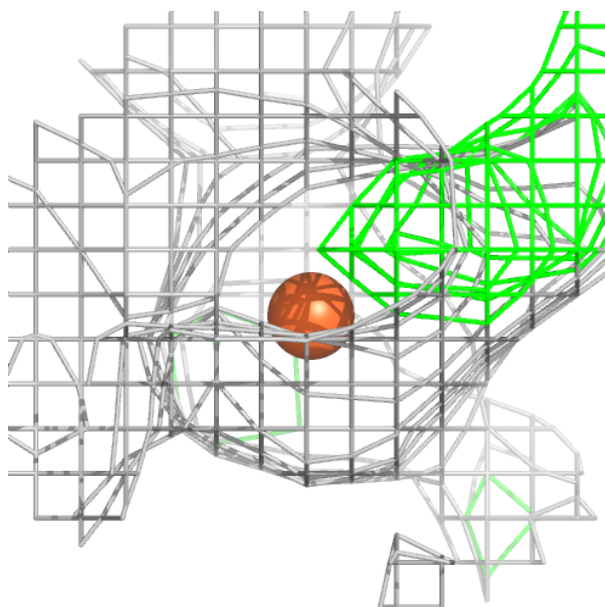
Electron density around FE2 A 202:

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and green (positive)



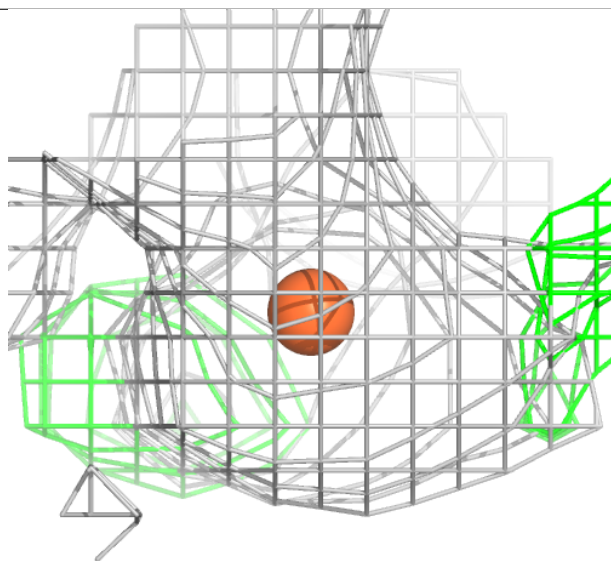
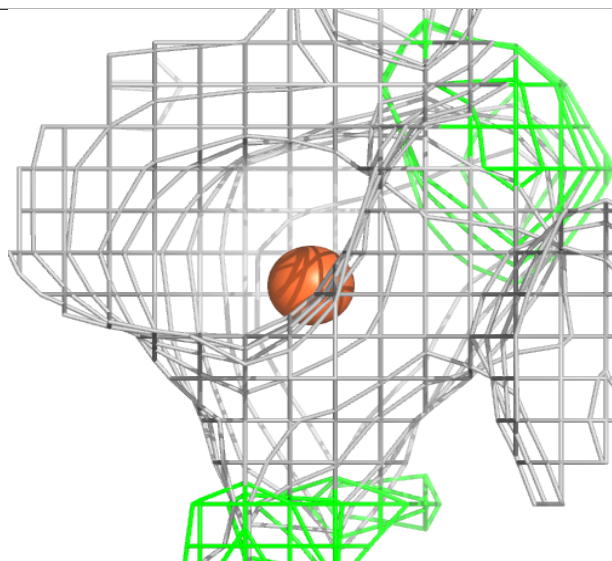
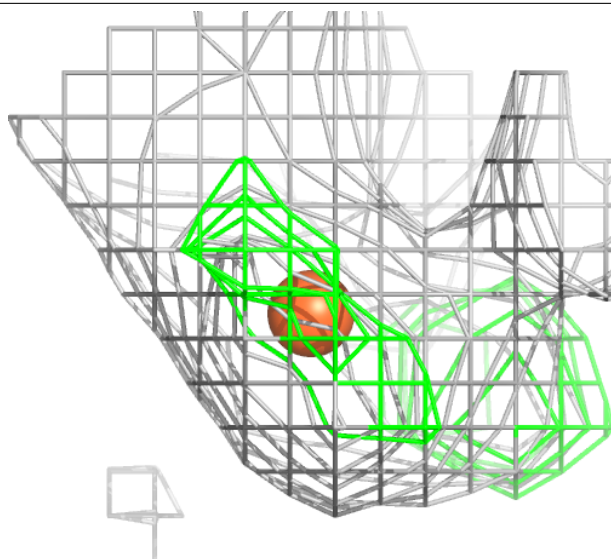
Electron density around FE2 H 202:

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and green (positive)



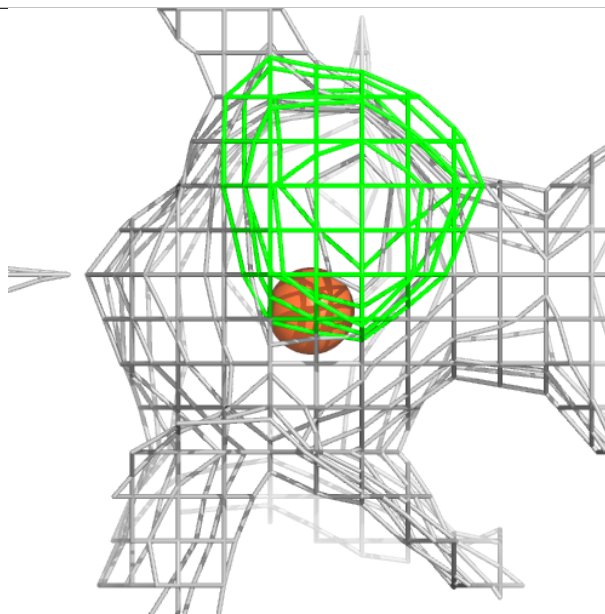
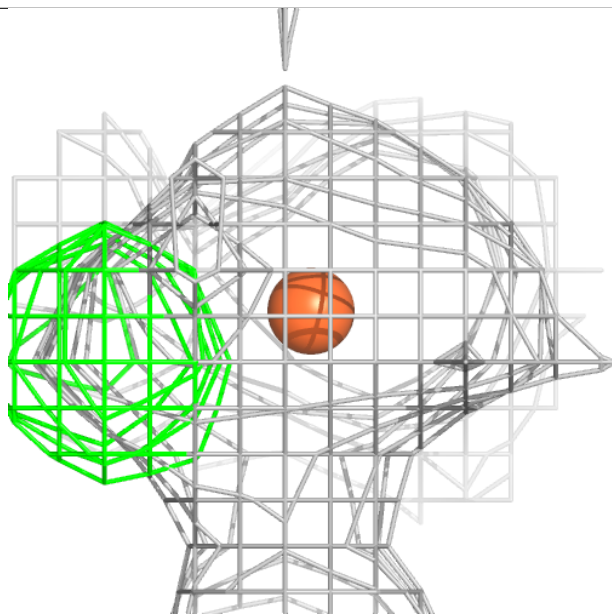
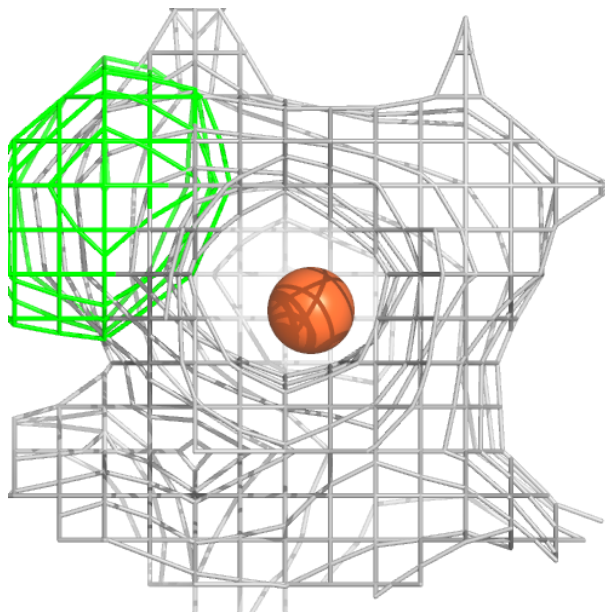
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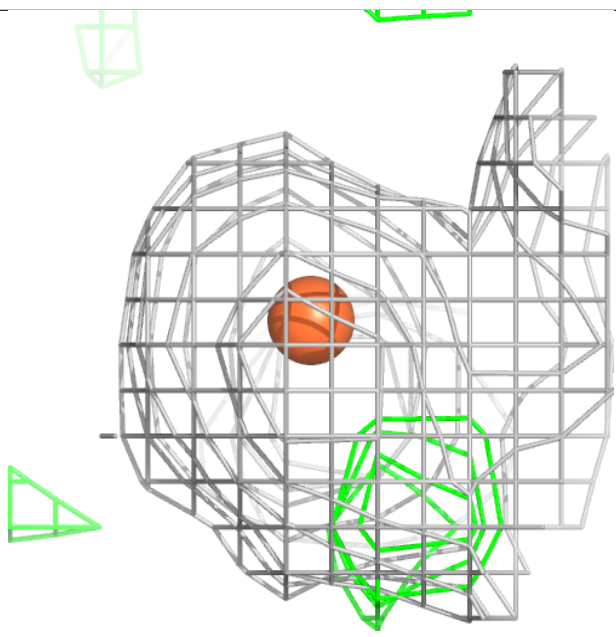
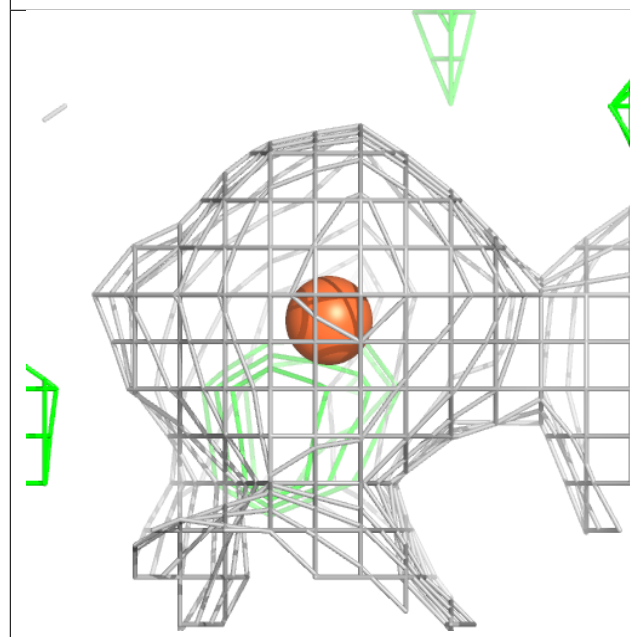
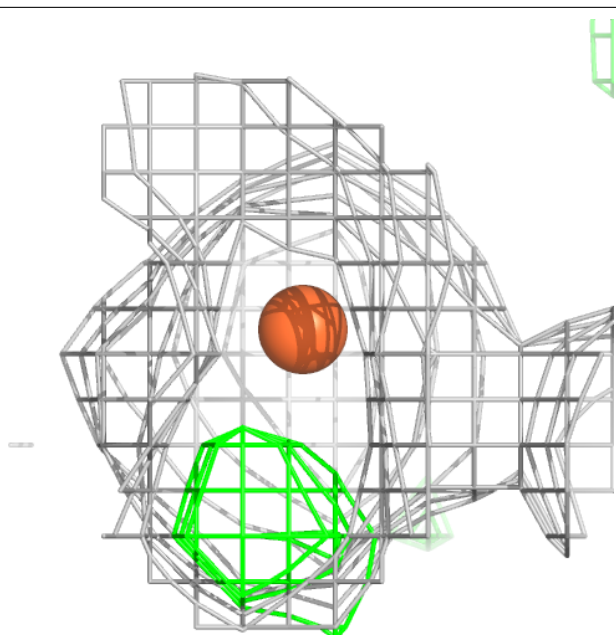
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and green (positive)



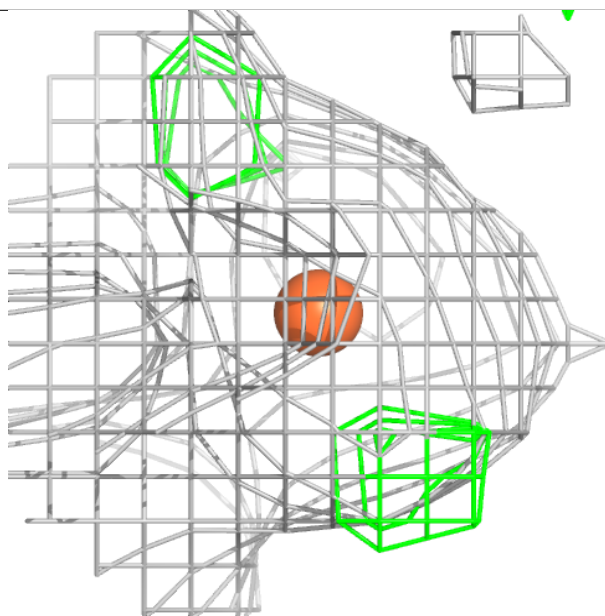
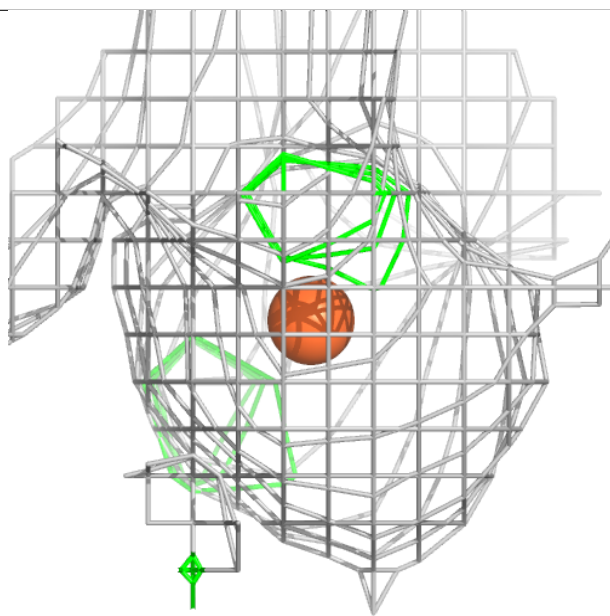
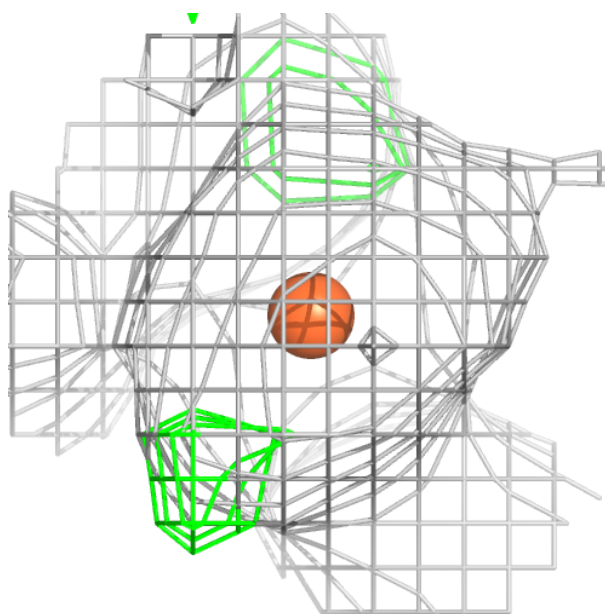
Electron density around FE2 C 202:

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and green (positive)



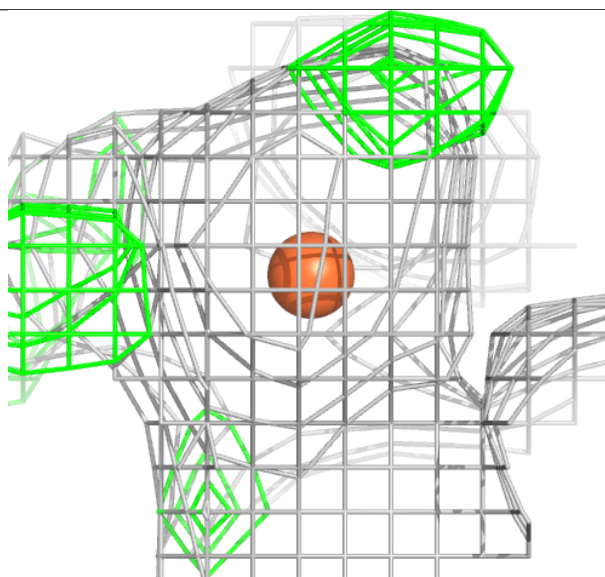
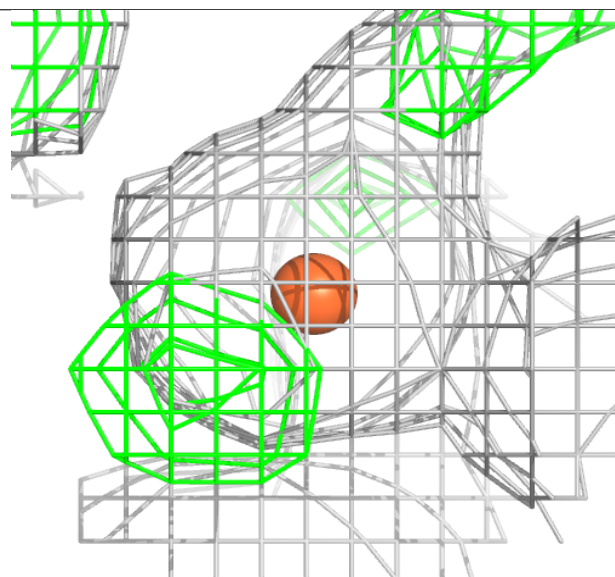
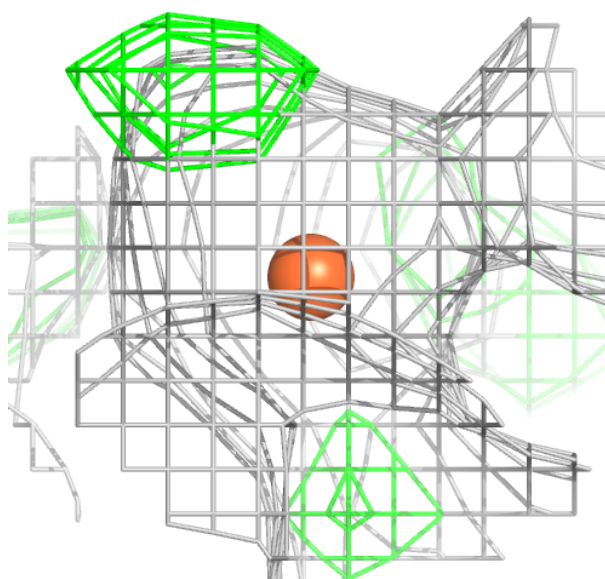
Electron density around FE2 B 202:

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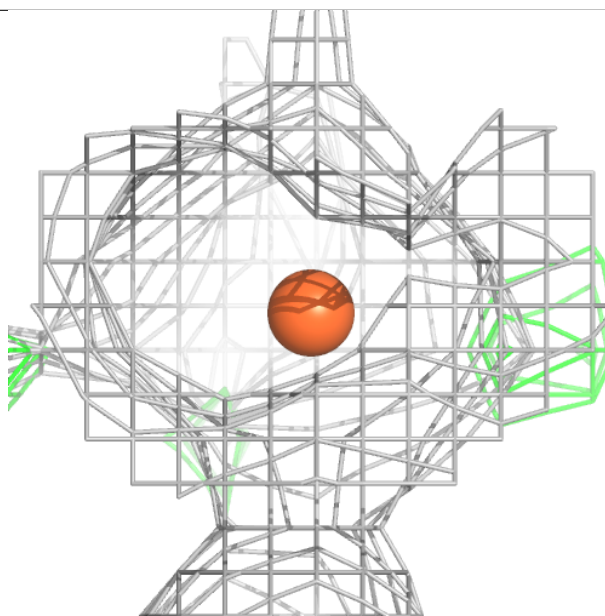
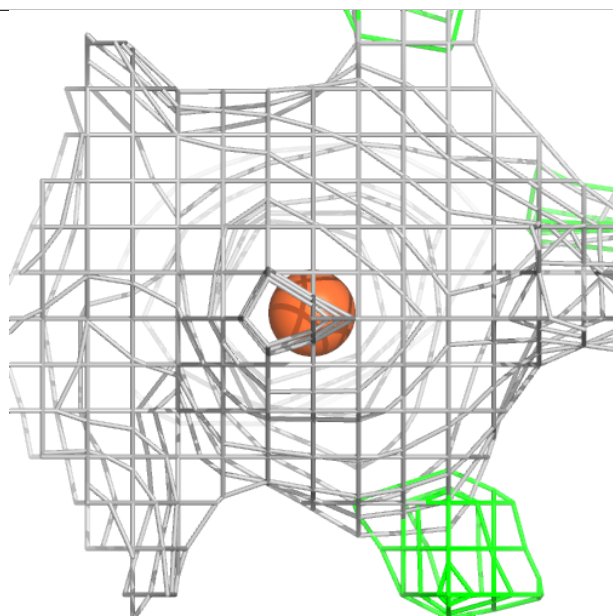
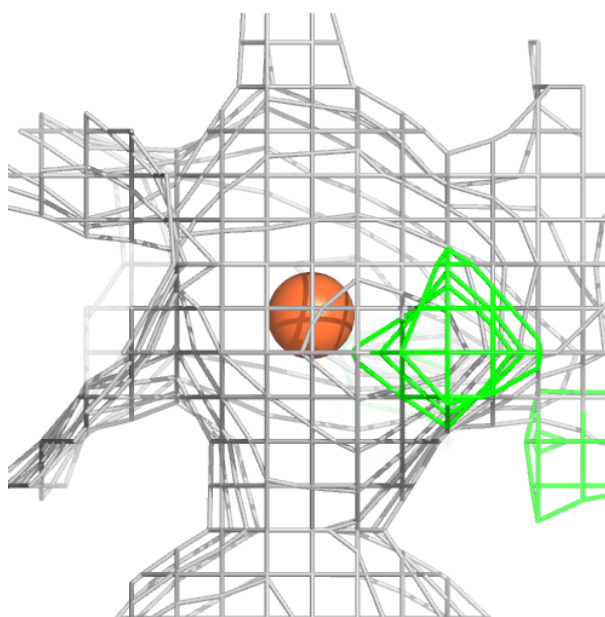
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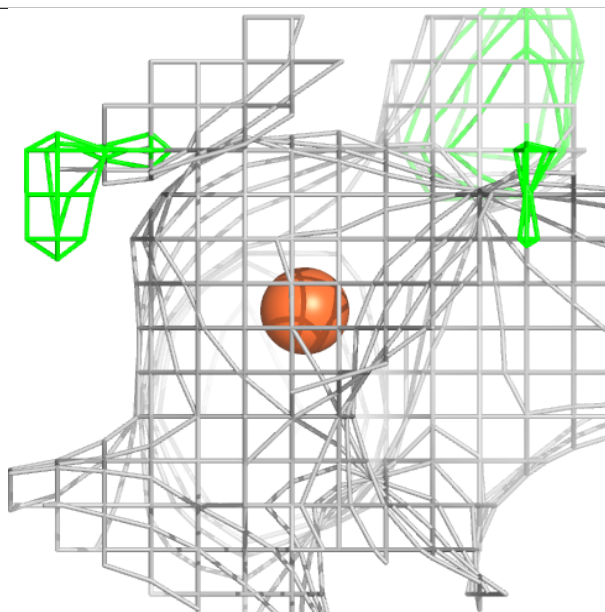
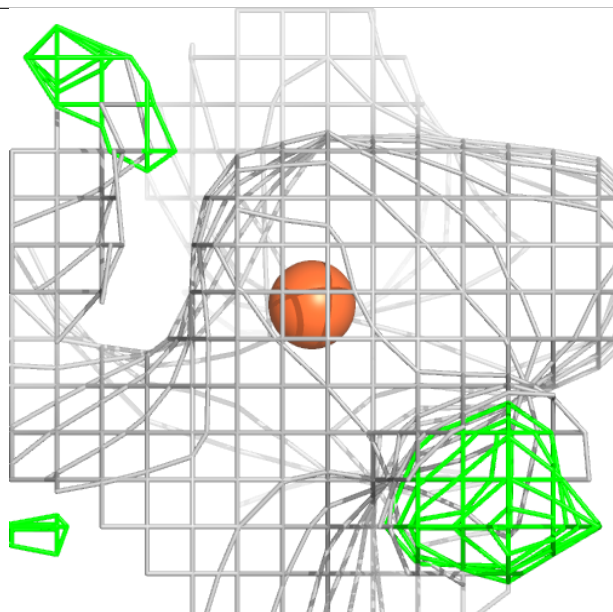
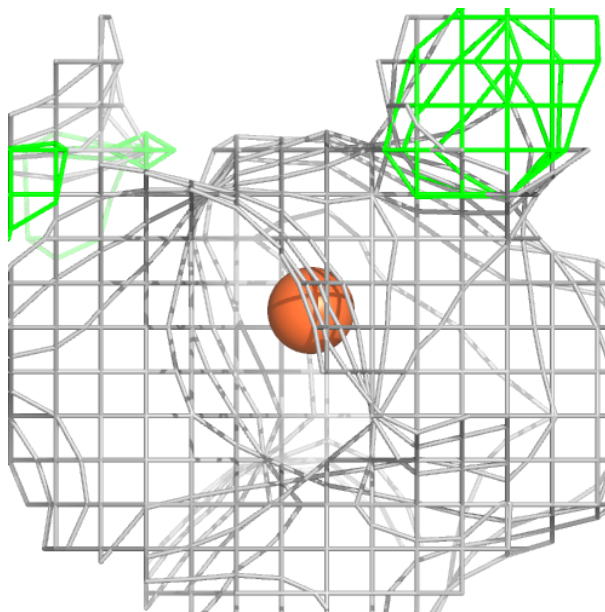
Electron density around FE2 D 202:

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and green (positive)



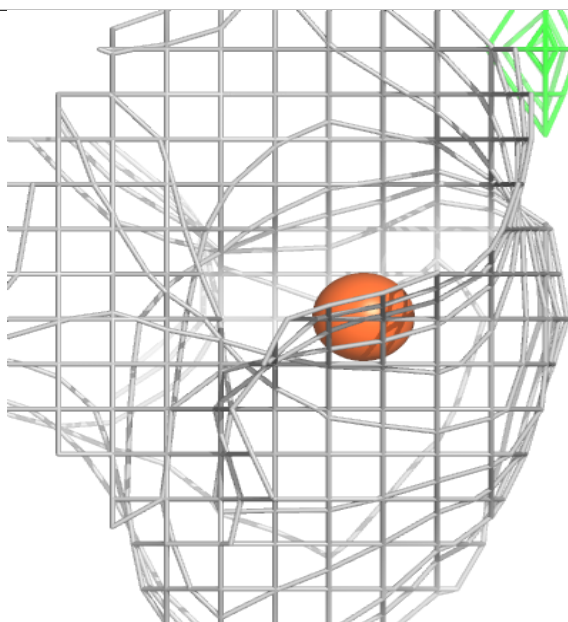
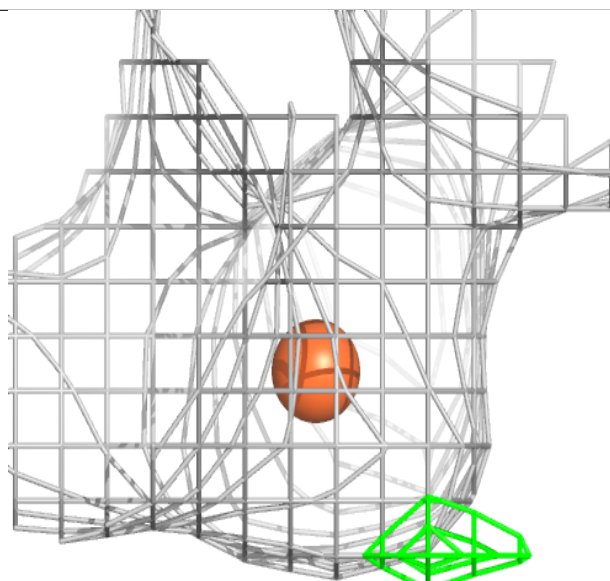
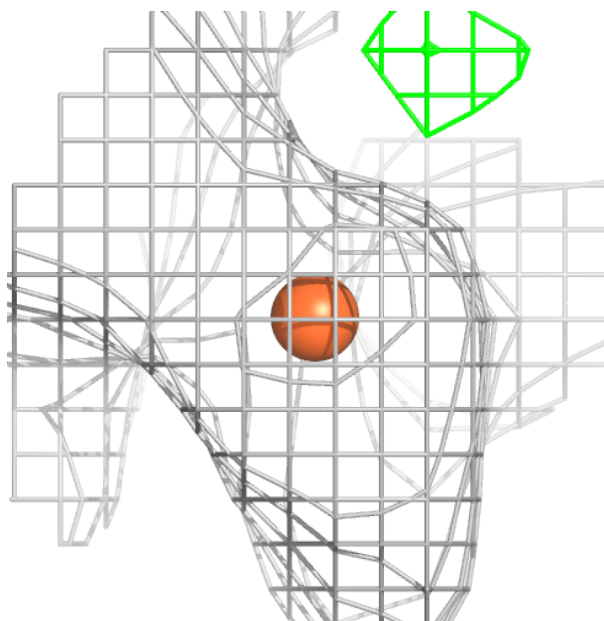
Electron density around FE2 G 202:

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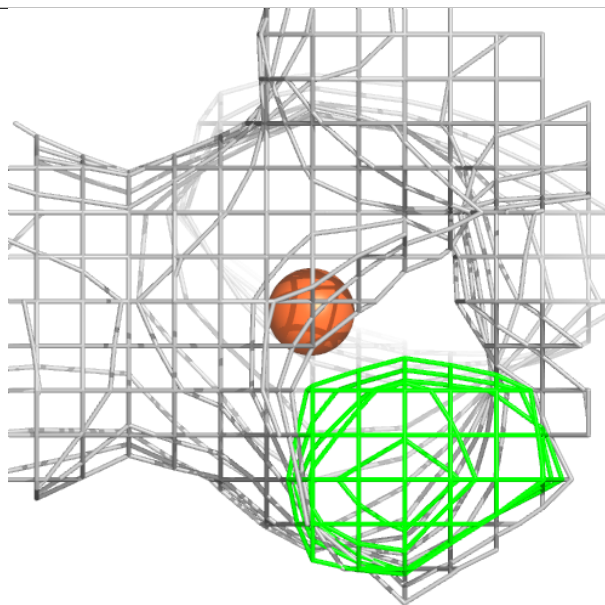
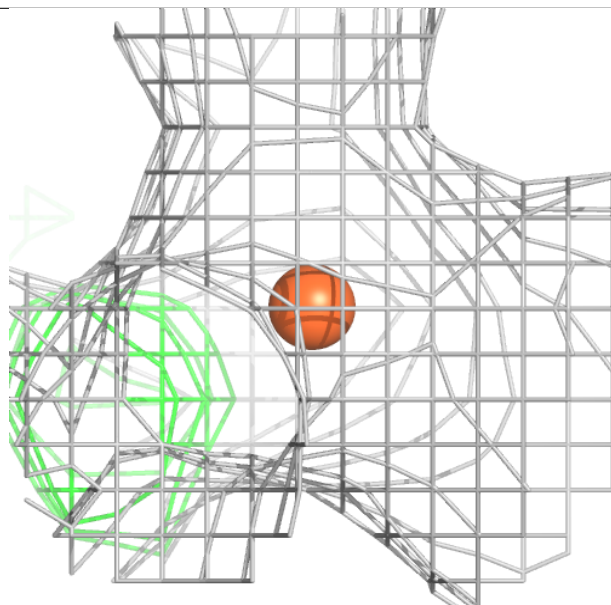
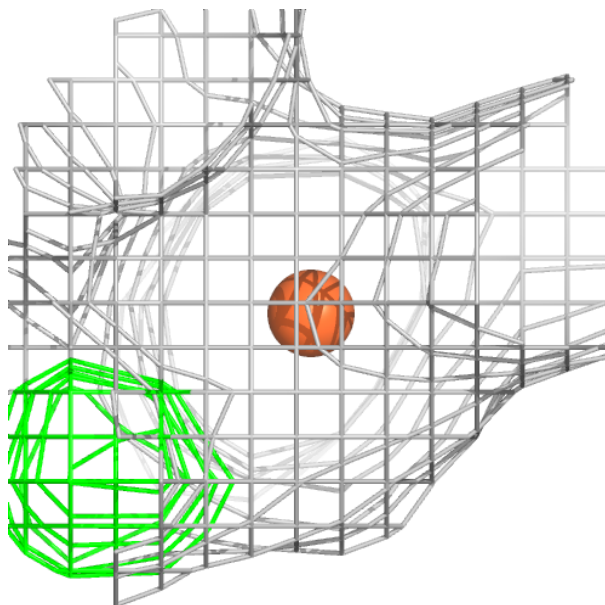
Electron density around FE2 C 203:

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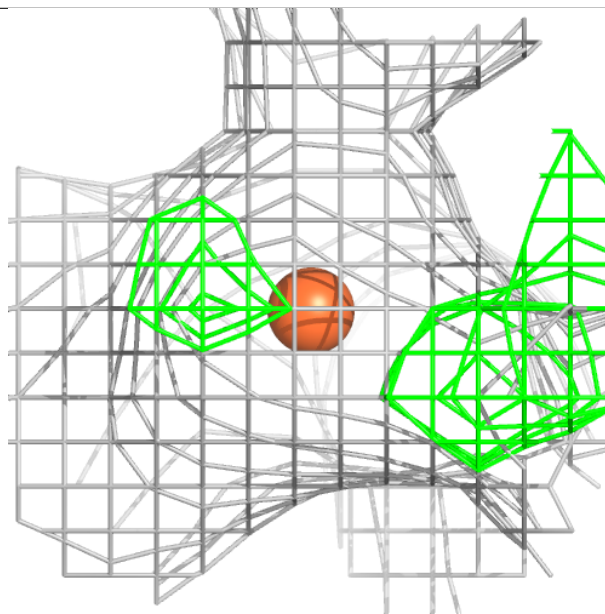
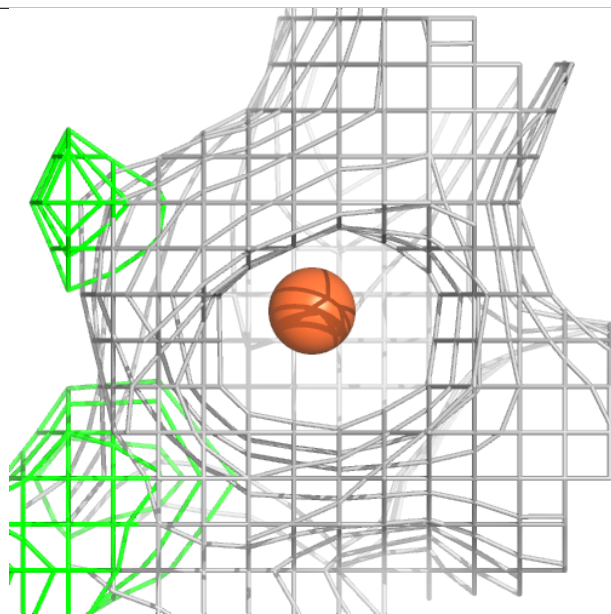
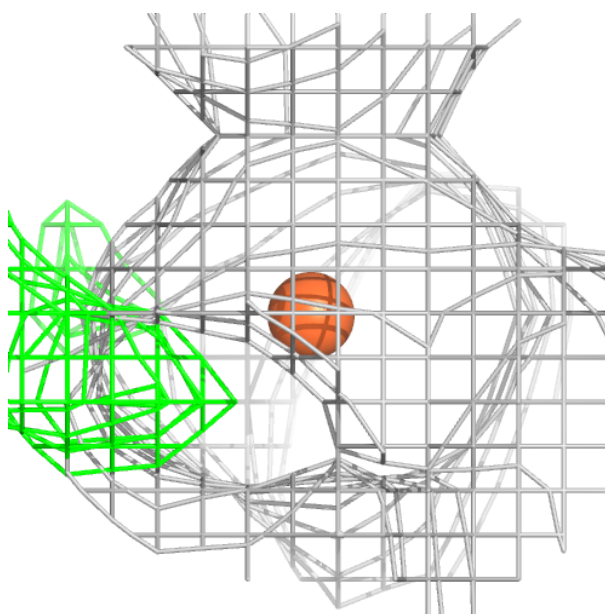
Electron density around FE2 A 201:

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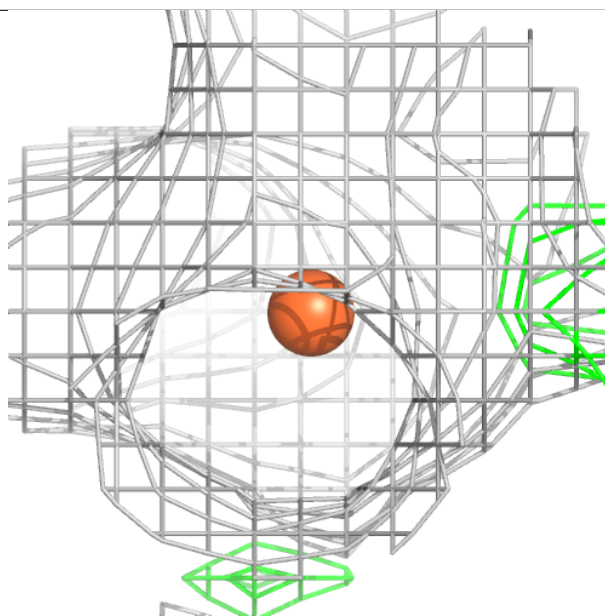
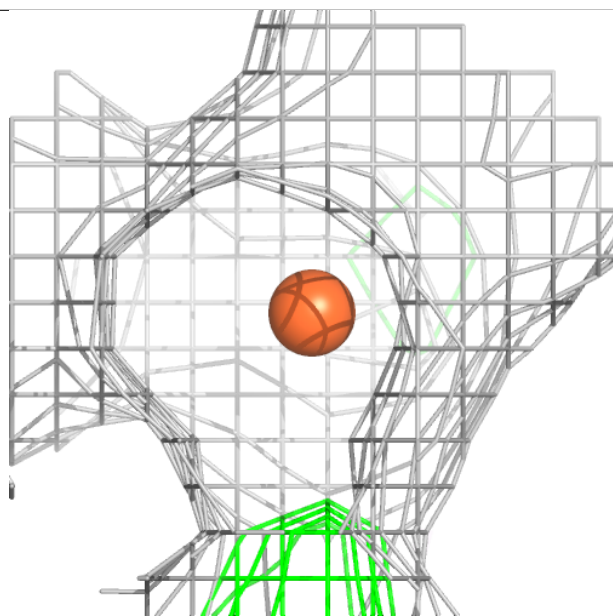
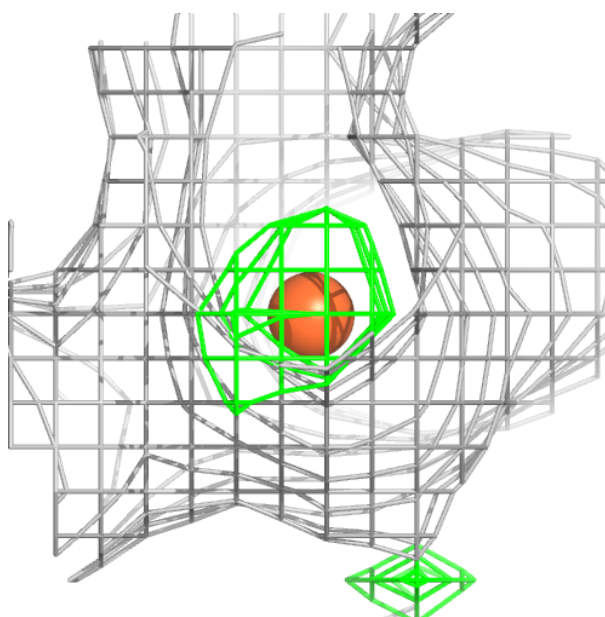
Electron density around FE2 H 201:

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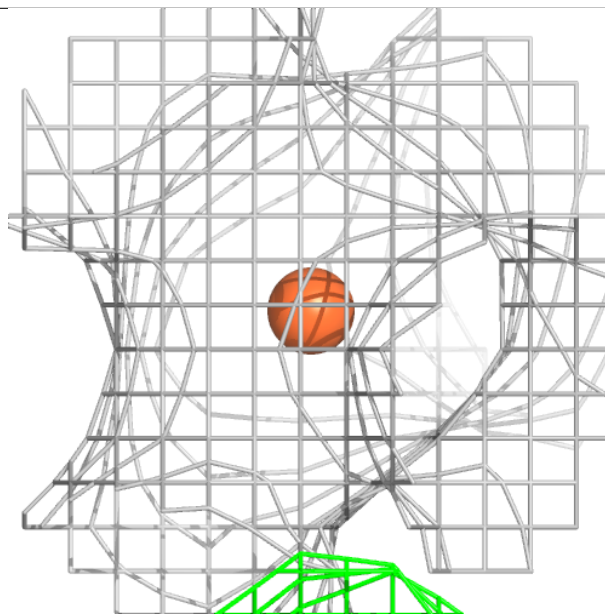
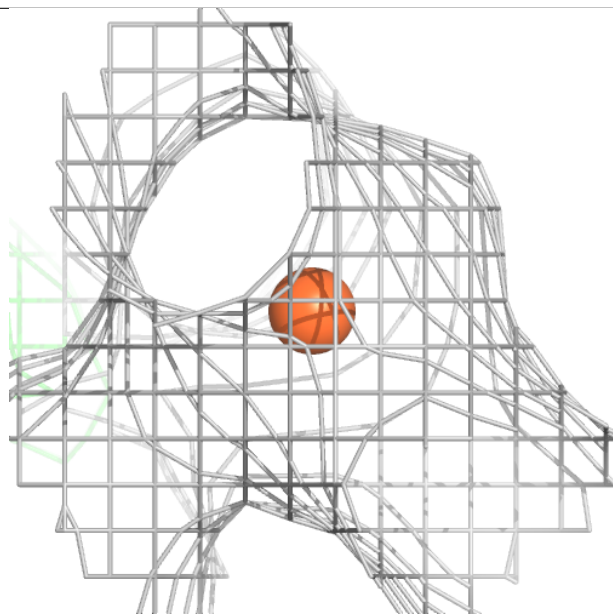
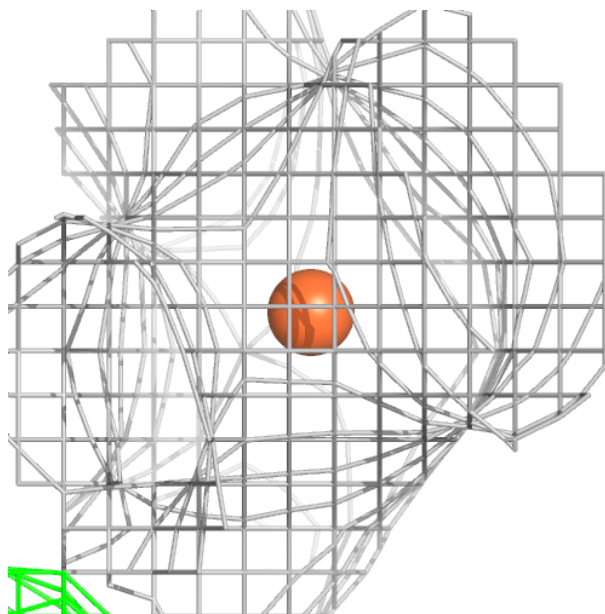
Electron density around FE2 C 201:

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and green (positive)



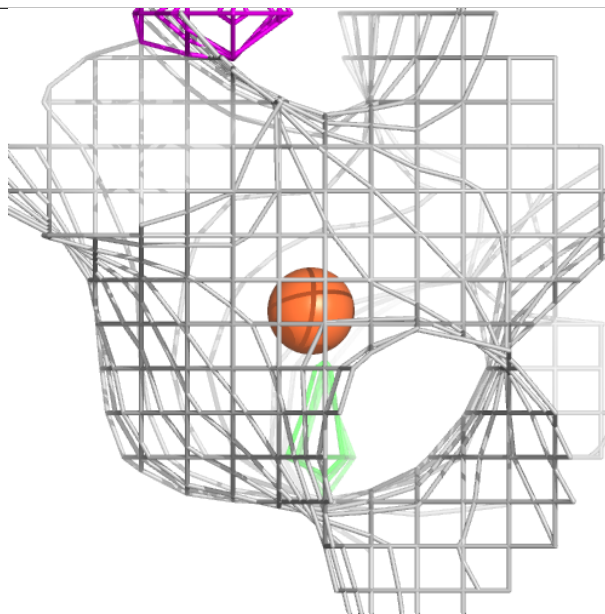
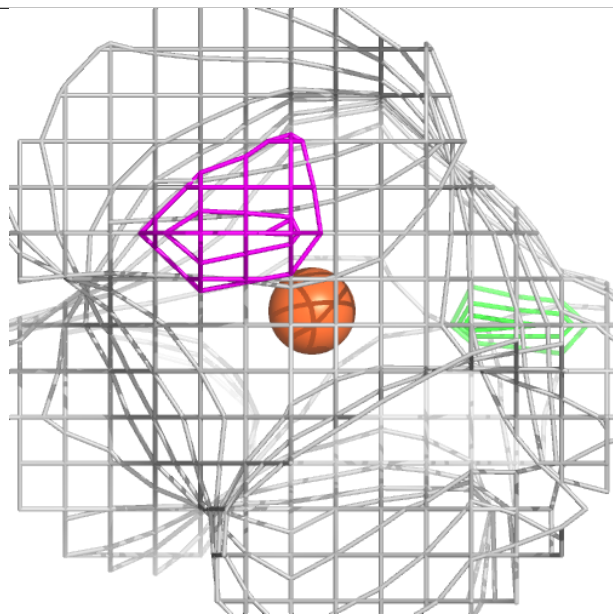
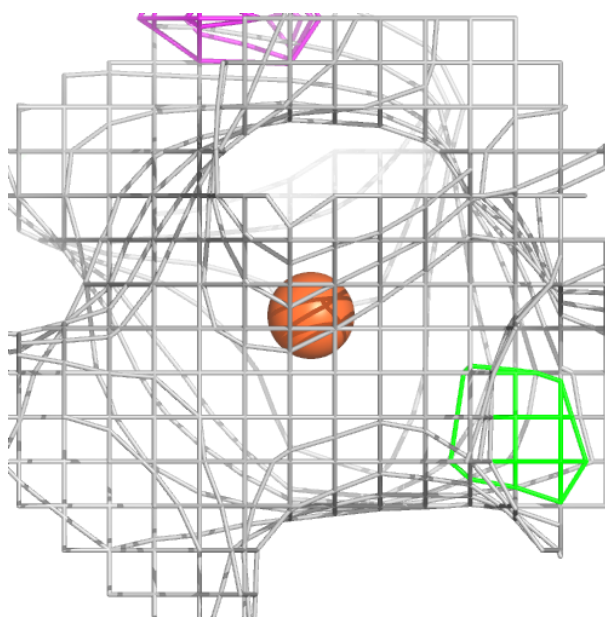
Electron density around FE2 E 201:

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



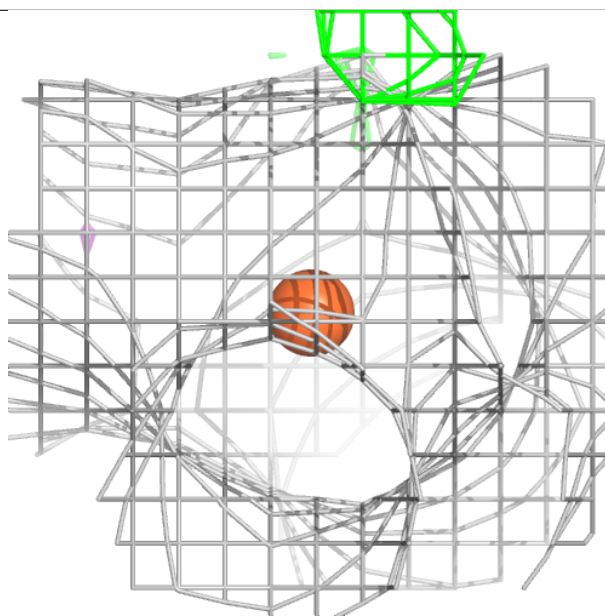
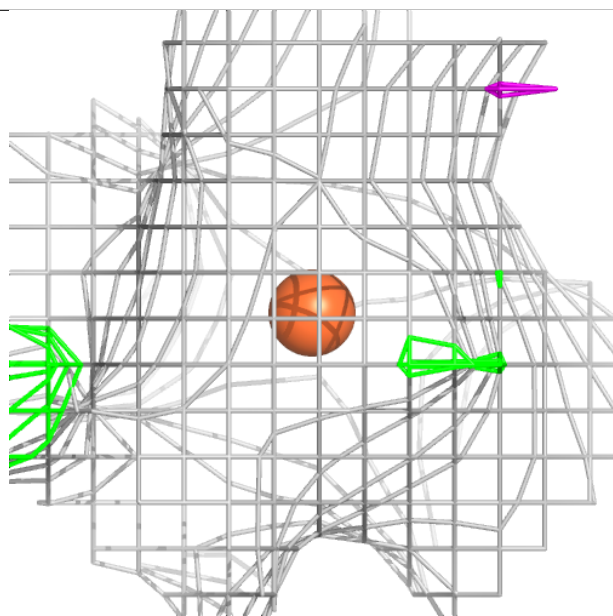
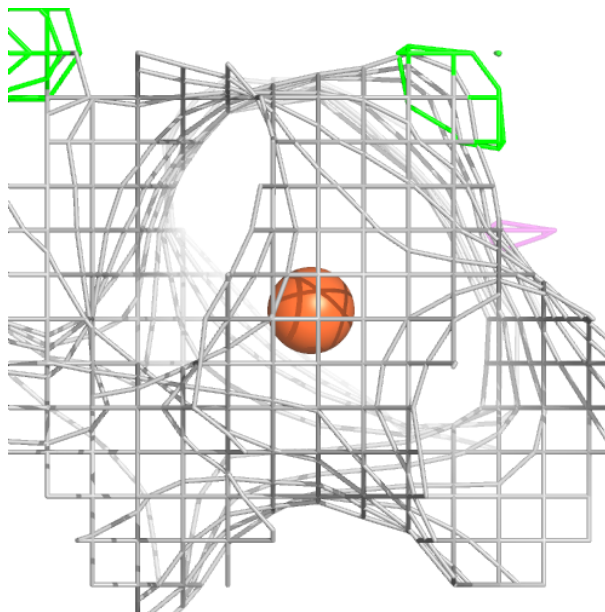
Electron density around FE2 K 201:

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



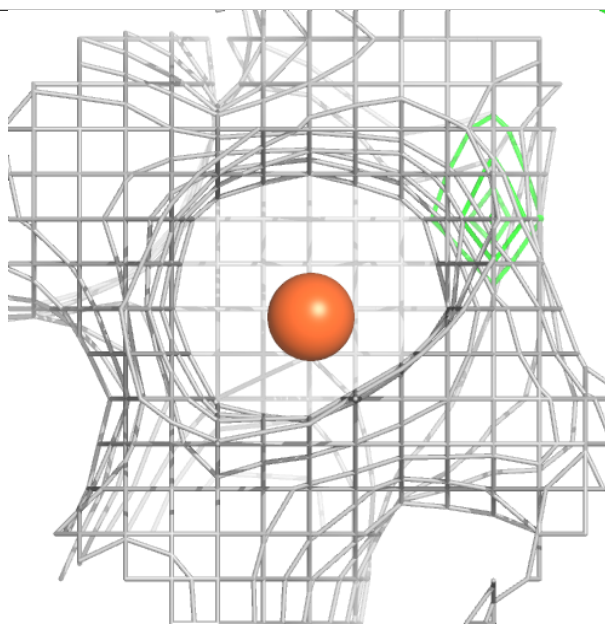
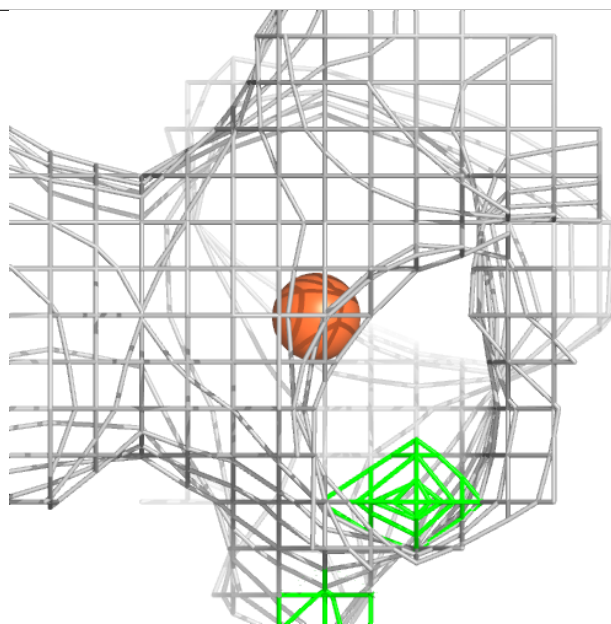
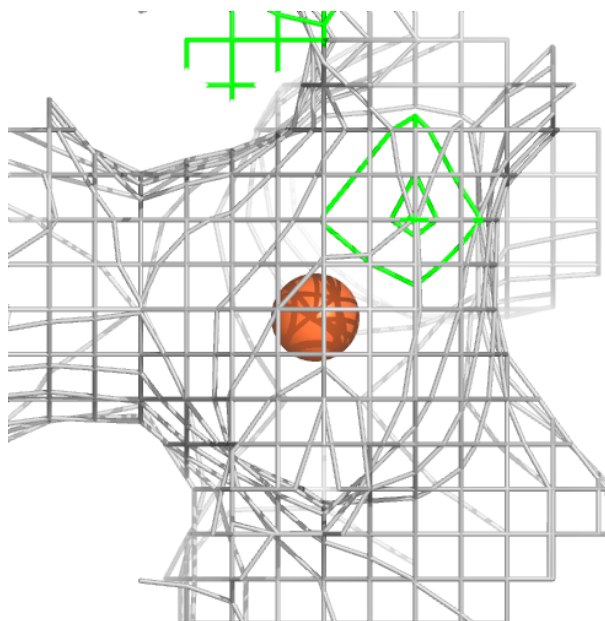
Electron density around FE2 G 201:

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



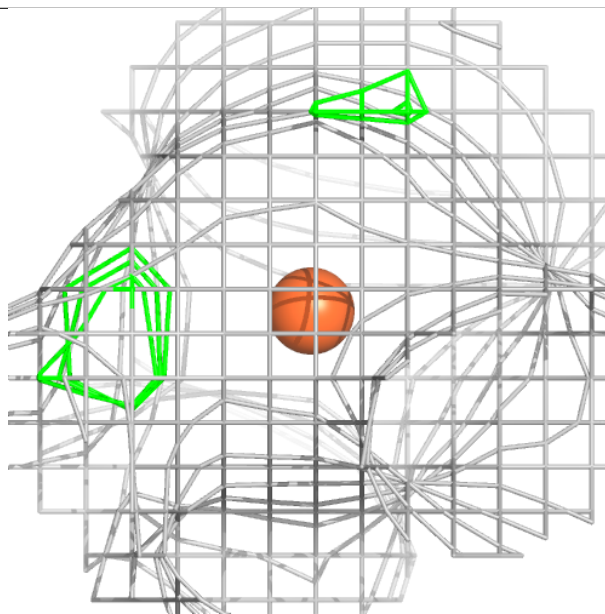
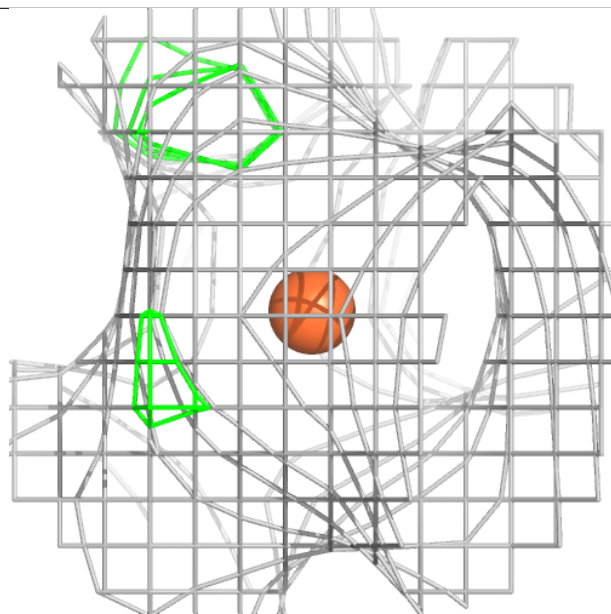
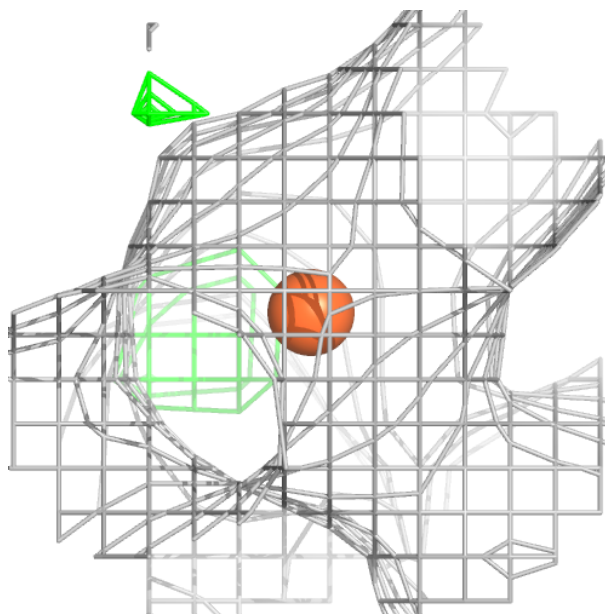
Electron density around FE2 L 201:

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



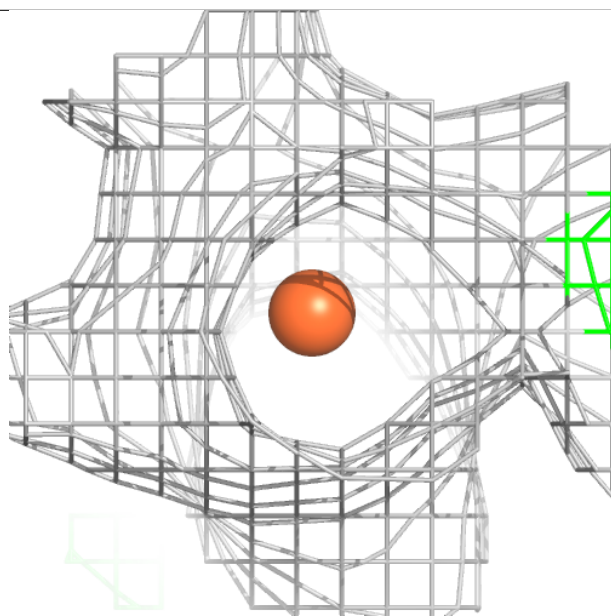
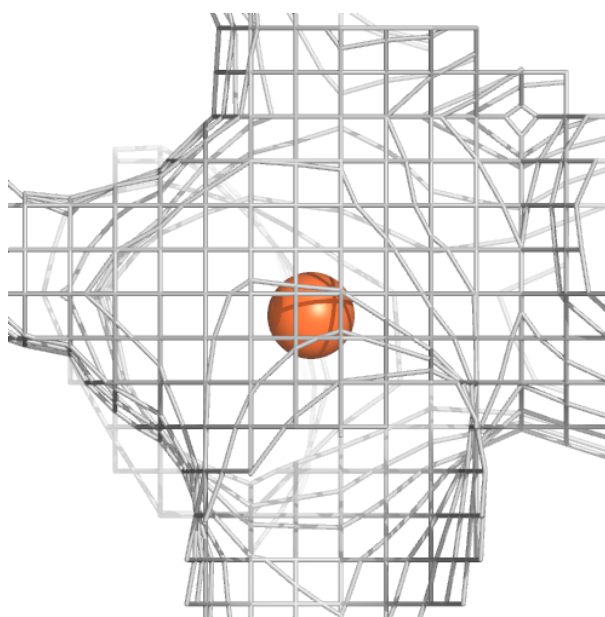
Electron density around FE2 B 201:

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



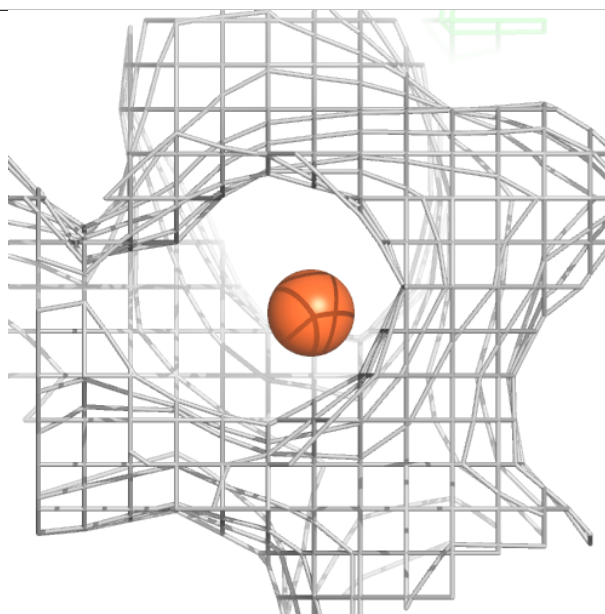
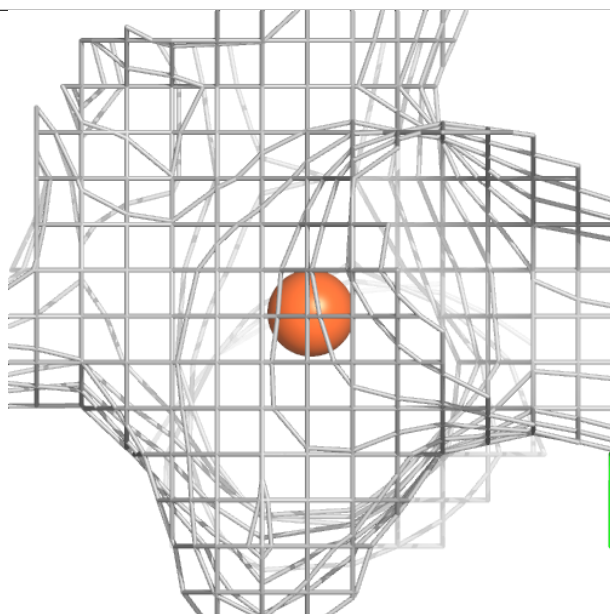
Electron density around FE2 I 201:

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



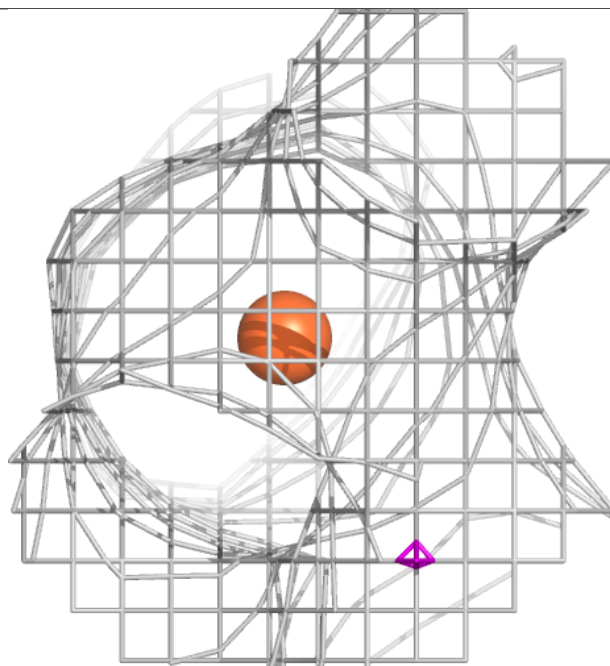
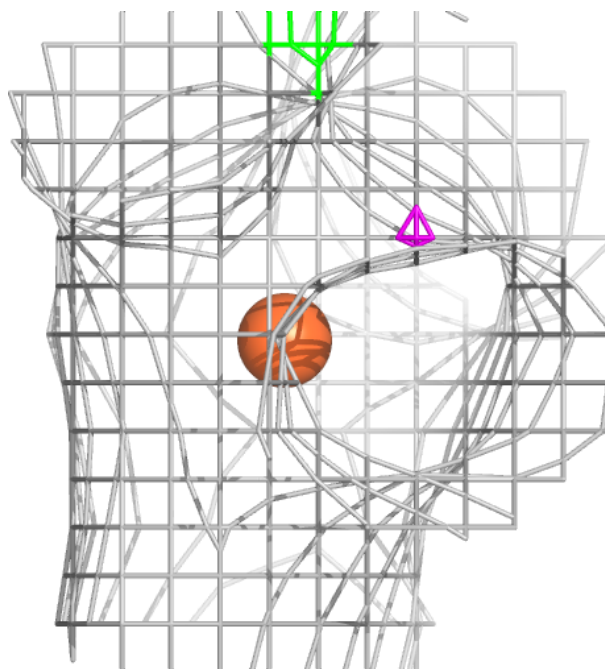
Electron density around FE2 D 201:

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



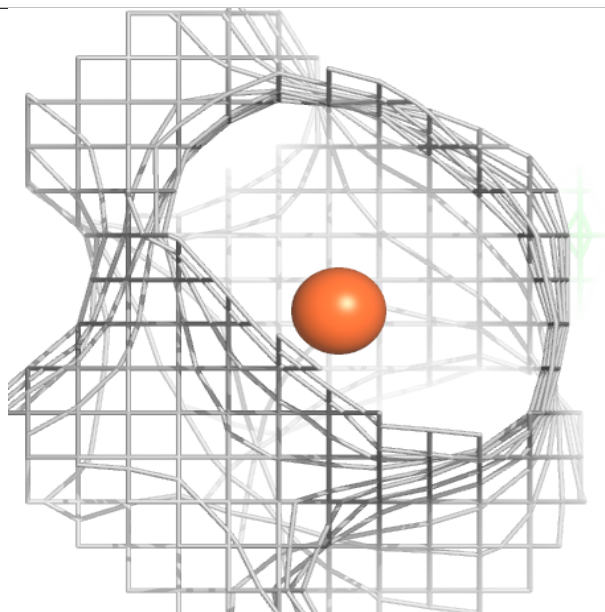
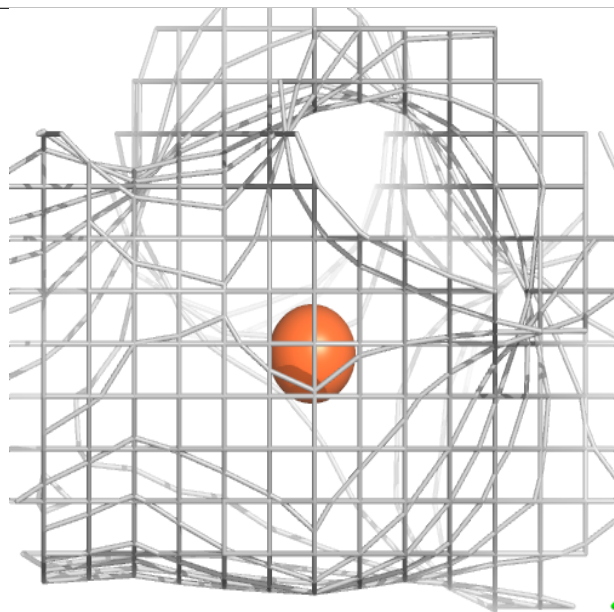
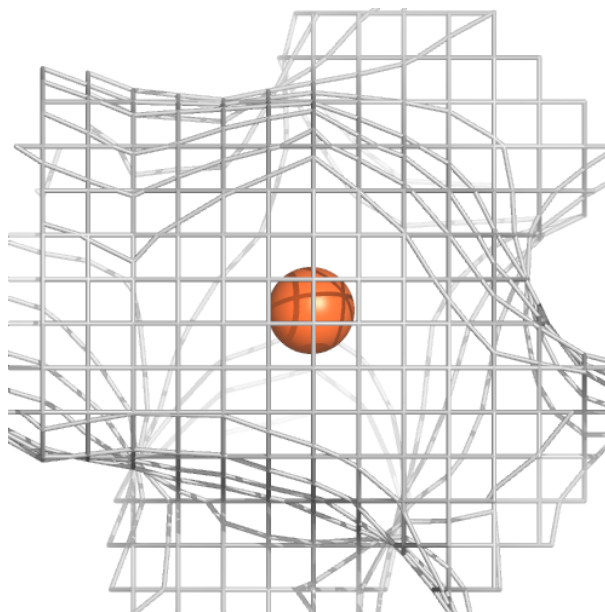
Electron density around FE2 F 201:

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



Electron density around FE2 J 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.