



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:41 PM UTC

PDB ID : 6LPD / pdb_00006lpd
Title : Phascolosoma esculenta
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Deposited on : 2020-01-09
Resolution : 1.65 Å(reported)

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

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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

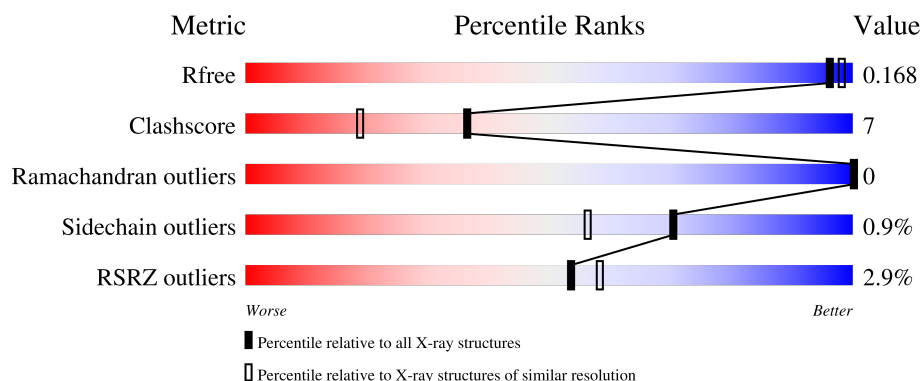
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	174	3% 75% 21% ...
1	B	174	3% 82% 14% ..
1	C	174	3% 79% 16% ..
1	D	174	3% 81% 16% ...
1	E	174	% 78% 20% .

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Mol	Chain	Length	Quality of chain
1	F	174	3% 80% 16% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	23	0
			1562	972	264	320	6			
1	B	170	Total	C	N	O	S	0	20	0
			1550	959	267	317	7			
1	C	170	Total	C	N	O	S	0	18	0
			1542	952	268	315	7			
1	D	170	Total	C	N	O	S	0	19	0
			1551	958	267	320	6			
1	E	170	Total	C	N	O	S	0	17	0
			1521	944	264	306	7			
1	F	170	Total	C	N	O	S	0	16	0
			1494	929	256	303	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	2	Total	Fe	0	0
			2	2		
2	B	3	Total	Fe	0	0
			3	3		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	F	2	Total	Fe	0	0
			2	2		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Fe 1	0	0

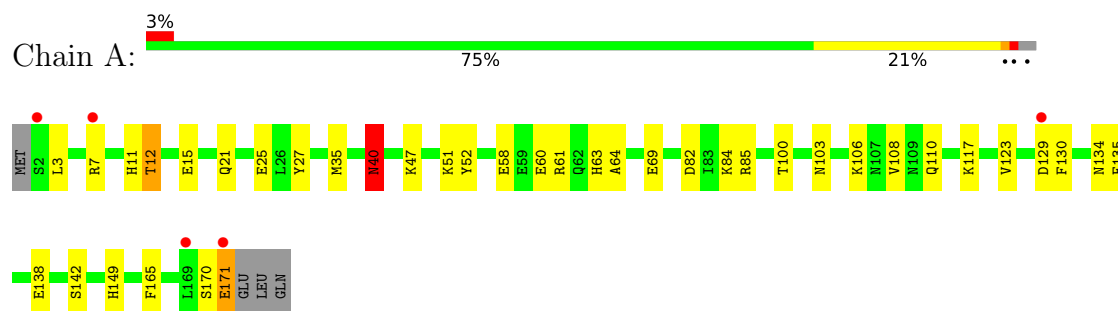
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total 256	O 256	0	0
4	B	232	Total 232	O 232	0	0
4	C	247	Total 247	O 247	0	0
4	D	241	Total 241	O 241	0	0
4	E	238	Total 238	O 238	0	0
4	F	245	Total 245	O 245	0	0

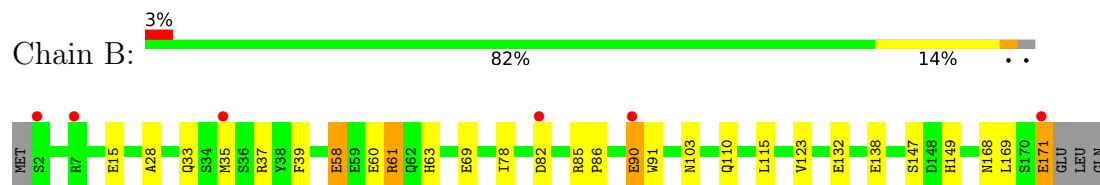
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

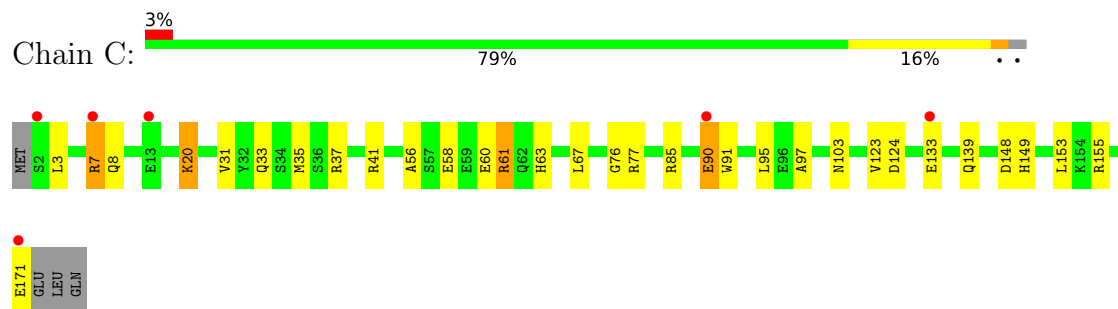
- Molecule 1: Ferritin



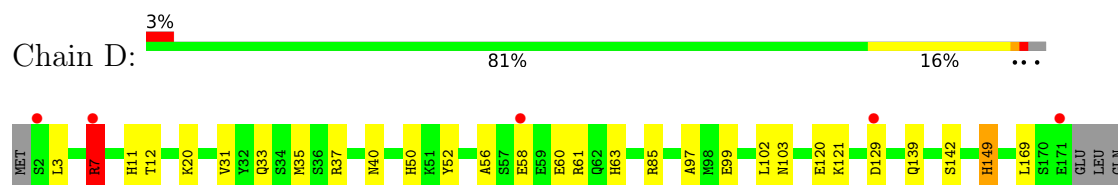
- Molecule 1: Ferritin



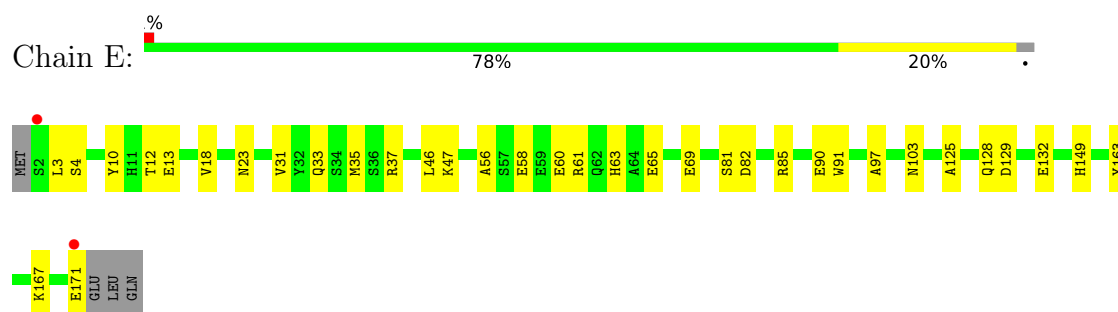
- Molecule 1: Ferritin



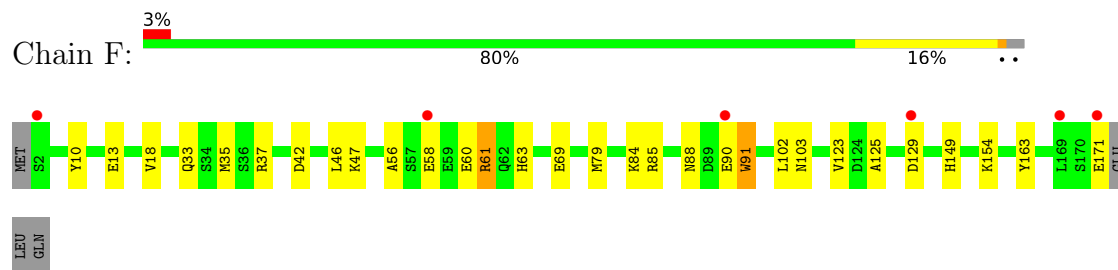
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.00Å 153.49Å 153.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.65 – 1.65 108.65 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.4 (108.65-1.65) 96.4 (108.65-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.74 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.108 , 0.153 0.134 , 0.168	Depositor DCC
R_{free} test set	10411 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.427 for -h,-l,-k 0.399 for l,-k,h 0.419 for -k,-h,-l 0.400 for k,-l,-h 0.400 for -l,h,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10693	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	1.56	17/1623 (1.0%)	1.26	4/2179 (0.2%)
1	B	1.56	16/1593 (1.0%)	1.30	11/2140 (0.5%)
1	C	1.53	8/1571 (0.5%)	1.20	4/2108 (0.2%)
1	D	1.56	8/1589 (0.5%)	1.31	7/2134 (0.3%)
1	E	1.67	15/1571 (1.0%)	1.35	6/2108 (0.3%)
1	F	1.65	14/1552 (0.9%)	1.30	7/2084 (0.3%)
All	All	1.59	78/9499 (0.8%)	1.29	39/12753 (0.3%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	90[A]	GLU	CA-C	11.68	1.66	1.52
1	E	90[B]	GLU	CA-C	11.68	1.66	1.52
1	B	90[A]	GLU	CA-C	8.72	1.63	1.52
1	B	90[B]	GLU	CA-C	8.72	1.63	1.52
1	B	35[A]	MET	CA-C	7.33	1.62	1.52
1	B	35[B]	MET	CA-C	7.33	1.62	1.52
1	A	35	MET	SD-CE	-7.18	1.61	1.79
1	D	3	LEU	N-CA	-7.04	1.36	1.45
1	A	3	LEU	N-CA	-6.74	1.36	1.45
1	F	91	TRP	N-CA	6.73	1.52	1.46
1	A	69	GLU	C-O	-6.68	1.16	1.24
1	A	123	VAL	CA-C	6.59	1.61	1.52
1	F	129[A]	ASP	CA-C	6.54	1.61	1.52
1	F	129[B]	ASP	CA-C	6.54	1.61	1.52
1	B	169	LEU	CB-CG	-6.46	1.40	1.53
1	A	110	GLN	C-O	-6.42	1.16	1.24
1	F	13	GLU	C-O	-6.31	1.16	1.24
1	F	46	LEU	C-O	6.26	1.30	1.23
1	A	100	THR	N-CA	6.16	1.53	1.46
1	C	8	GLN	CA-C	6.13	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	N-CA	-6.09	1.39	1.46
1	B	115	LEU	C-O	5.97	1.31	1.24
1	A	15	GLU	CA-C	5.92	1.60	1.52
1	F	69	GLU	C-O	-5.88	1.17	1.24
1	B	69	GLU	C-O	-5.85	1.17	1.24
1	E	69	GLU	C-O	-5.83	1.17	1.24
1	D	102	LEU	C-O	5.82	1.30	1.24
1	E	132	GLU	C-O	5.80	1.30	1.24
1	F	18	VAL	C-O	5.76	1.30	1.24
1	F	10	TYR	C-O	-5.76	1.17	1.24
1	A	82	ASP	CA-C	5.73	1.59	1.52
1	B	61	ARG	C-O	-5.65	1.17	1.24
1	C	95	LEU	N-CA	-5.64	1.39	1.46
1	E	128	GLN	CD-OE1	5.64	1.34	1.23
1	D	121	LYS	CA-C	5.63	1.60	1.52
1	E	46	LEU	C-O	5.59	1.30	1.23
1	C	67	LEU	CA-C	5.56	1.59	1.52
1	E	18	VAL	C-O	5.54	1.30	1.24
1	A	12[A]	THR	C-N	5.50	1.41	1.33
1	A	12[B]	THR	C-N	5.50	1.41	1.33
1	E	163	TYR	C-O	-5.50	1.17	1.24
1	F	79	MET	N-CA	5.49	1.52	1.46
1	E	125	ALA	CA-CB	5.47	1.61	1.53
1	B	147	SER	N-CA	-5.47	1.39	1.46
1	E	10	TYR	C-O	-5.45	1.17	1.24
1	D	169	LEU	C-O	-5.44	1.17	1.24
1	A	40	ASN	CG-OD1	5.43	1.33	1.23
1	E	4	SER	N-CA	-5.39	1.38	1.45
1	C	153	LEU	C-O	5.38	1.30	1.24
1	A	106	LYS	C-O	-5.38	1.17	1.24
1	F	102	LEU	N-CA	5.34	1.52	1.46
1	B	86	PRO	N-CA	5.33	1.53	1.47
1	C	77	ARG	CA-C	5.33	1.58	1.52
1	B	78	ILE	CA-C	5.30	1.58	1.52
1	B	110	GLN	C-N	5.29	1.40	1.33
1	D	11	HIS	C-O	5.28	1.30	1.23
1	E	91	TRP	N-CA	5.28	1.52	1.46
1	B	132	GLU	CA-C	5.26	1.59	1.52
1	C	124	ASP	CA-CB	-5.25	1.43	1.53
1	F	61	ARG	C-O	-5.24	1.18	1.24
1	A	11	HIS	CA-C	5.22	1.60	1.53
1	B	15	GLU	C-O	-5.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	TYR	C-O	-5.20	1.18	1.24
1	E	13	GLU	C-O	-5.19	1.18	1.24
1	C	76	GLY	C-O	5.14	1.30	1.23
1	A	52	TYR	C-O	-5.14	1.18	1.24
1	E	23	ASN	CG-ND2	-5.10	1.22	1.33
1	F	56	ALA	N-CA	-5.10	1.40	1.46
1	D	20	LYS	N-CA	5.09	1.52	1.46
1	F	163	TYR	C-O	-5.08	1.18	1.24
1	B	58	GLU	C-O	-5.08	1.18	1.24
1	B	28	ALA	CA-C	5.07	1.59	1.52
1	E	3	LEU	N-CA	-5.06	1.39	1.45
1	F	123	VAL	CA-C	5.06	1.59	1.52
1	D	149	HIS	CE1-NE2	-5.05	1.27	1.32
1	C	61	ARG	C-O	-5.04	1.18	1.24
1	A	27	TYR	N-CA	-5.03	1.40	1.46
1	A	165	PHE	CA-C	5.01	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	129[A]	ASP	CA-C-O	10.71	132.20	120.10
1	F	129[B]	ASP	CA-C-O	10.71	132.20	120.10
1	B	35[A]	MET	CA-C-O	10.28	131.44	120.55
1	B	35[B]	MET	CA-C-O	10.28	131.44	120.55
1	A	117[A]	LYS	CA-C-O	9.45	130.77	120.10
1	A	117[B]	LYS	CA-C-O	9.45	130.77	120.10
1	D	129[A]	ASP	CA-C-O	8.23	129.43	119.97
1	D	129[B]	ASP	CA-C-O	8.23	129.43	119.97
1	E	129[A]	ASP	CA-C-O	7.87	129.02	119.97
1	E	129[B]	ASP	CA-C-O	7.87	129.02	119.97
1	E	129[A]	ASP	N-CA-C	7.15	120.11	111.82
1	E	129[B]	ASP	N-CA-C	7.15	120.11	111.82
1	E	171	GLU	CA-CB-CG	-6.92	100.26	114.10
1	F	129[A]	ASP	N-CA-C	6.82	119.55	111.71
1	F	129[B]	ASP	N-CA-C	6.82	119.55	111.71
1	B	171	GLU	CA-CB-CG	-6.73	100.63	114.10
1	C	171	GLU	CA-CB-CG	-6.72	100.65	114.10
1	F	171	GLU	CA-CB-CG	-6.68	100.74	114.10
1	A	171	GLU	CA-CB-CG	-6.43	101.24	114.10
1	F	154	LYS	N-CA-C	6.34	118.19	111.28
1	D	129[A]	ASP	N-CA-C	6.30	118.96	111.71
1	D	129[B]	ASP	N-CA-C	6.30	118.96	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	125	ALA	N-CA-C	6.17	118.01	111.28
1	B	35[A]	MET	N-CA-C	6.14	117.97	111.28
1	B	35[B]	MET	N-CA-C	6.14	117.97	111.28
1	D	139	GLN	CB-CG-CD	5.81	122.48	112.60
1	B	90[A]	GLU	CA-C-N	-5.71	113.01	122.08
1	B	90[A]	GLU	C-N-CA	-5.71	113.01	122.08
1	B	90[B]	GLU	CA-C-N	-5.71	113.01	122.08
1	B	90[B]	GLU	C-N-CA	-5.71	113.01	122.08
1	B	90[A]	GLU	CA-C-O	5.69	128.44	121.56
1	B	90[B]	GLU	CA-C-O	5.69	128.44	121.56
1	C	139	GLN	CB-CG-CD	5.42	121.81	112.60
1	E	85	ARG	CG-CD-NE	-5.29	100.36	112.00
1	C	155	ARG	CD-NE-CZ	5.29	131.81	124.40
1	A	51	LYS	CG-CD-CE	5.16	123.17	111.30
1	C	171	GLU	CB-CA-C	5.13	119.85	110.10
1	D	7	ARG	N-CA-C	5.10	118.19	110.64
1	D	20	LYS	CB-CA-C	5.09	118.87	110.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1562	0	1474	21	0
1	B	1550	0	1446	17	0
1	C	1542	0	1445	29	0
1	D	1551	0	1449	21	0
1	E	1521	0	1455	21	0
1	F	1494	0	1432	24	0
2	A	2	0	0	0	0
2	B	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
4	A	256	0	0	10	0
4	B	232	0	0	8	0
4	C	247	0	0	10	0
4	D	241	0	0	9	0
4	E	238	0	0	9	0
4	F	245	0	0	12	0
All	All	10693	0	8701	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 7.

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:E:63[C]:HIS:CE1	4:E:306:HOH:O	1.80	1.24
1:F:63[B]:HIS:CE1	4:F:333:HOH:O	1.89	1.22
1:A:63[B]:HIS:CE1	4:A:329:HOH:O	1.93	1.20
1:D:63[B]:HIS:CE1	4:D:330:HOH:O	1.97	1.16
1:B:63[B]:HIS:CE1	4:B:412:HOH:O	1.97	1.15
1:D:63[B]:HIS:HE1	4:D:330:HOH:O	1.31	1.08
1:C:90[A]:GLU:O	1:C:91:TRP:CG	2.10	1.04
1:C:63[B]:HIS:CE1	4:C:388:HOH:O	2.10	1.02
1:F:33[B]:GLN:NE2	4:F:301:HOH:O	1.90	1.02
1:D:12[A]:THR:HG22	4:D:334:HOH:O	1.70	0.92
1:F:90[A]:GLU:O	1:F:91:TRP:CG	2.25	0.89
1:A:12[A]:THR:HG22	4:A:323:HOH:O	1.75	0.86
1:C:33[B]:GLN:HE21	1:C:37:ARG:HE	1.21	0.85
1:B:60[B]:GLU:OE1	4:B:401:HOH:O	1.94	0.85
1:C:90[A]:GLU:O	1:C:91:TRP:CD1	2.31	0.83
1:E:33[B]:GLN:HE21	1:E:37:ARG:HE	1.26	0.83
1:B:63[B]:HIS:HE1	4:B:412:HOH:O	1.44	0.83
1:D:33[B]:GLN:HE21	1:D:37:ARG:HE	1.28	0.81
1:D:99[B]:GLU:OE1	4:D:301:HOH:O	2.00	0.79
1:B:33[B]:GLN:HE21	1:B:37:ARG:HE	1.30	0.79
1:C:33[B]:GLN:OE1	4:C:301:HOH:O	2.02	0.77
1:C:41:ARG:NH1	1:C:90[A]:GLU:OE1	2.17	0.76
1:F:63[B]:HIS:HE1	4:F:333:HOH:O	1.48	0.72
1:A:60:GLU:OE2	4:A:301:HOH:O	2.08	0.71
1:C:60[A]:GLU:OE2	4:C:302:HOH:O	2.07	0.70
1:F:84[A]:LYS:NZ	4:F:304:HOH:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12[B]:THR:HG23	4:A:306:HOH:O	1.91	0.70
1:C:33[B]:GLN:CD	4:C:301:HOH:O	2.36	0.69
1:C:90[A]:GLU:O	1:C:91:TRP:CD2	2.47	0.68
1:F:33[B]:GLN:CD	4:F:301:HOH:O	2.31	0.67
1:A:134:ASN:HB2	1:A:135[B]:PHE:CE1	2.30	0.67
1:E:33[B]:GLN:HE22	1:E:37:ARG:HH21	1.43	0.66
1:E:33[B]:GLN:NE2	1:E:37:ARG:HE	1.92	0.66
1:F:90[A]:GLU:O	1:F:91:TRP:CD1	2.49	0.66
1:D:142[A]:SER:OG	4:D:303:HOH:O	2.13	0.66
1:F:60:GLU:OE2	4:F:302:HOH:O	2.15	0.64
1:B:90[B]:GLU:CA	1:B:91:TRP:N	2.55	0.64
1:C:90[A]:GLU:C	1:C:91:TRP:CG	2.76	0.64
1:D:120:GLU:OE1	4:D:304:HOH:O	2.15	0.63
1:B:33[B]:GLN:NE2	1:B:37:ARG:HE	1.97	0.62
1:C:31:VAL:O	1:C:35[B]:MET:HG3	1.99	0.62
1:F:85:ARG:NH1	4:F:306:HOH:O	2.33	0.61
1:C:33[B]:GLN:NE2	1:C:37:ARG:HE	1.94	0.61
1:A:138[B]:GLU:HG2	4:A:403:HOH:O	2.00	0.61
1:C:33[B]:GLN:NE2	4:C:301:HOH:O	2.35	0.59
1:C:148:ASP:OD1	1:F:42:ASP:HA	2.02	0.59
1:F:90[A]:GLU:O	1:F:91:TRP:CD2	2.56	0.59
1:B:82:ASP:OD1	1:D:85:ARG:HG2	2.02	0.58
1:B:58:GLU:CD	1:B:61:ARG:HH22	2.12	0.58
1:C:33[B]:GLN:NE2	1:C:37:ARG:HH21	2.03	0.57
1:D:7:ARG:HD2	4:D:382:HOH:O	2.04	0.57
1:D:31:VAL:O	1:D:35:MET:HG3	2.04	0.57
1:D:33[B]:GLN:HE22	1:D:37:ARG:HH21	1.53	0.57
1:C:33[B]:GLN:HE22	1:C:37:ARG:HH21	1.54	0.56
1:E:61[B]:ARG:NH1	1:F:58:GLU:OE2	2.39	0.55
1:B:85:ARG:NH1	4:B:406:HOH:O	2.40	0.55
1:A:58:GLU:CD	1:A:61:ARG:HH12	2.15	0.55
1:D:33[B]:GLN:NE2	1:D:37:ARG:HH21	2.05	0.55
1:F:103:ASN:ND2	4:F:308:HOH:O	2.39	0.54
1:E:103:ASN:ND2	4:E:305:HOH:O	2.41	0.54
1:C:85:ARG:NH1	4:C:305:HOH:O	2.41	0.54
1:D:33[B]:GLN:NE2	1:D:37:ARG:HE	2.01	0.53
1:B:103[A]:ASN:ND2	4:B:407:HOH:O	2.41	0.53
1:C:103:ASN:ND2	4:C:306:HOH:O	2.41	0.53
1:E:31:VAL:O	1:E:35[A]:MET:HG3	2.09	0.52
1:C:133:GLU:O	1:C:133:GLU:HG3	2.08	0.52
1:D:103:ASN:ND2	4:D:306:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLU:CD	1:F:61:ARG:HH12	2.17	0.52
1:E:33[B]:GLN:NE2	1:E:37:ARG:HH21	2.06	0.51
1:E:61[B]:ARG:NH1	1:E:65:GLU:OE2	2.44	0.51
1:F:90[A]:GLU:C	1:F:91:TRP:CG	2.85	0.51
1:B:138[B]:GLU:HG2	4:B:515:HOH:O	2.11	0.50
4:E:352:HOH:O	1:F:84[A]:LYS:HE3	2.11	0.50
1:A:40:ASN:HD21	1:A:47:LYS:NZ	2.09	0.50
1:C:58:GLU:CD	1:C:61:ARG:HH12	2.20	0.50
1:C:90[A]:GLU:C	1:C:91:TRP:CD1	2.91	0.49
1:F:149:HIS:HD2	4:F:457:HOH:O	1.95	0.49
1:E:35[A]:MET:HE2	1:E:97:ALA:HB1	1.94	0.49
1:D:56:ALA:O	1:D:60[B]:GLU:HG2	2.13	0.48
1:A:142[A]:SER:OG	4:A:302:HOH:O	2.20	0.48
1:E:12[B]:THR:HG23	4:E:440:HOH:O	2.15	0.47
1:F:84[A]:LYS:CE	4:F:304:HOH:O	2.63	0.47
1:C:37:ARG:HD3	1:C:37:ARG:HA	1.63	0.47
1:E:58:GLU:CD	1:E:61[A]:ARG:HH12	2.23	0.46
1:A:84[B]:LYS:CD	4:C:317:HOH:O	2.64	0.46
1:D:149:HIS:HD2	4:D:463:HOH:O	1.99	0.46
1:F:58:GLU:OE1	1:F:61:ARG:NH2	2.34	0.46
1:A:149:HIS:HD2	4:A:464:HOH:O	1.98	0.46
1:E:47:LYS:CG	4:E:302:HOH:O	2.64	0.46
1:B:149:HIS:HD2	4:B:559:HOH:O	1.98	0.45
1:E:47:LYS:HG2	4:E:302:HOH:O	2.16	0.45
1:A:21:GLN:O	1:A:25[B]:GLU:HG2	2.17	0.45
1:C:149:HIS:HD2	4:C:468:HOH:O	1.99	0.45
1:F:35:MET:HE3	1:F:91:TRP:CE3	2.52	0.45
1:A:25[A]:GLU:OE1	1:A:60:GLU:OE1	2.36	0.44
1:B:58:GLU:HG3	4:B:605:HOH:O	2.17	0.44
1:E:149:HIS:HD2	4:E:460:HOH:O	1.99	0.44
1:B:168[B]:ASN:O	1:B:171:GLU:HG3	2.16	0.44
1:A:103[A]:ASN:ND2	4:A:310:HOH:O	2.51	0.43
1:D:40[B]:ASN:ND2	1:D:50:HIS:CE1	2.86	0.43
1:E:81[A]:SER:O	1:E:82:ASP:C	2.59	0.43
1:E:81[B]:SER:O	1:E:82:ASP:C	2.58	0.43
1:F:47:LYS:HG2	4:F:311:HOH:O	2.16	0.43
1:D:33[B]:GLN:HE21	1:D:37:ARG:NE	2.08	0.43
1:A:134:ASN:C	1:A:135[B]:PHE:CG	2.96	0.43
1:A:129[A]:ASP:O	1:A:130:PHE:C	2.61	0.42
1:C:3:LEU:HD22	1:C:7:ARG:HD2	2.01	0.42
1:D:58:GLU:CD	1:D:61:ARG:HH12	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ARG:HH21	1:C:7:ARG:HG3	1.84	0.42
1:C:33[B]:GLN:HE21	1:C:37:ARG:NE	2.02	0.42
1:E:56:ALA:O	1:E:60[B]:GLU:HG2	2.19	0.42
1:A:170:SER:C	1:A:171:GLU:HG3	2.45	0.42
1:C:35[B]:MET:HE2	1:C:97:ALA:HB1	2.02	0.42
1:E:63[C]:HIS:HE1	4:E:306:HOH:O	1.51	0.42
1:A:103[C]:ASN:OD1	4:A:303:HOH:O	2.21	0.41
1:A:134:ASN:CB	1:A:135[B]:PHE:CE1	3.02	0.41
1:C:20:LYS:CE	4:C:419:HOH:O	2.67	0.41
1:F:37:ARG:HA	1:F:37:ARG:HD3	1.77	0.41
1:D:35:MET:HE2	1:D:97:ALA:HB1	2.02	0.41
1:F:88[B]:ASN:HB3	1:F:90[B]:GLU:O	2.19	0.41
1:E:167:LYS:HE2	4:E:345:HOH:O	2.21	0.41
1:B:33[B]:GLN:NE2	1:B:37:ARG:NE	2.66	0.41
1:D:33[B]:GLN:HE22	1:D:37:ARG:NH2	2.17	0.41
1:A:25[B]:GLU:HB2	1:A:64:ALA:HB2	2.03	0.41
1:C:56:ALA:O	1:C:60[B]:GLU:HG2	2.21	0.41
1:E:33[B]:GLN:HE22	1:E:37:ARG:NH2	2.15	0.40
1:F:47:LYS:CG	4:F:311:HOH:O	2.69	0.40
1:A:85:ARG:NH1	4:A:315:HOH:O	2.53	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	194/174 (112%)	187 (96%)	7 (4%)	0	100	100
1	B	190/174 (109%)	184 (97%)	6 (3%)	0	100	100
1	C	187/174 (108%)	182 (97%)	5 (3%)	0	100	100
1	D	189/174 (109%)	184 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	187/174 (108%)	182 (97%)	5 (3%)	0	100	100
1	F	186/174 (107%)	182 (98%)	4 (2%)	0	100	100
All	All	1133/1044 (108%)	1101 (97%)	32 (3%)	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	173/157 (110%)	171 (99%)	2 (1%)	63	45
1	B	171/157 (109%)	170 (99%)	1 (1%)	78	68
1	C	170/157 (108%)	165 (97%)	5 (3%)	37	14
1	D	171/157 (109%)	170 (99%)	1 (1%)	78	68
1	E	170/157 (108%)	170 (100%)	0	100	100
1	F	167/157 (106%)	167 (100%)	0	100	100
All	All	1022/942 (108%)	1013 (99%)	9 (1%)	70	56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	40	ASN
1	B	123	VAL
1	C	7	ARG
1	C	20	LYS
1	C	90[A]	GLU
1	C	90[C]	GLU
1	C	123	VAL
1	D	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	149	HIS
1	B	126	GLN
1	B	149	HIS
1	C	109	ASN
1	C	128	GLN
1	C	149	HIS
1	D	128	GLN
1	D	149	HIS
1	E	103	ASN
1	E	128	GLN
1	E	149	HIS
1	F	103	ASN
1	F	126	GLN
1	F	128	GLN
1	F	149	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 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	170/174 (97%)	-0.28	5 (2%)	53	58	4, 13, 25, 70	23 (13%)
1	B	170/174 (97%)	-0.25	6 (3%)	47	51	4, 13, 26, 64	20 (11%)
1	C	170/174 (97%)	-0.18	6 (3%)	47	51	4, 13, 25, 65	18 (10%)
1	D	170/174 (97%)	-0.31	5 (2%)	53	58	4, 13, 24, 64	19 (11%)
1	E	170/174 (97%)	-0.33	2 (1%)	76	81	4, 14, 25, 78	17 (10%)
1	F	170/174 (97%)	-0.21	6 (3%)	47	51	6, 14, 23, 48	16 (9%)
All	All	1020/1044 (97%)	-0.26	30 (2%)	53	58	4, 13, 25, 78	113 (11%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90[A]	GLU	7.8
1	F	90[A]	GLU	7.4
1	B	82	ASP	6.2
1	F	2	SER	4.6
1	B	171	GLU	4.6
1	B	7	ARG	4.1
1	E	171	GLU	3.2
1	C	171	GLU	3.1
1	E	2	SER	3.1
1	C	13	GLU	3.0
1	A	2	SER	3.0
1	D	58	GLU	3.0
1	D	7	ARG	3.0
1	C	2	SER	2.9
1	A	169	LEU	2.9
1	A	171	GLU	2.8
1	F	129[A]	ASP	2.8
1	D	171	GLU	2.7
1	D	2	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	129[A]	ASP	2.7
1	F	58	GLU	2.6
1	C	7	ARG	2.6
1	A	129[A]	ASP	2.6
1	B	90[A]	GLU	2.5
1	F	171	GLU	2.3
1	F	169	LEU	2.3
1	A	7	ARG	2.3
1	B	35[A]	MET	2.2
1	B	2	SER	2.2
1	C	133	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE2	B	303	1/1	0.93	0.12	59,59,59,59	1
2	FE2	A	202	1/1	0.95	0.13	60,60,60,60	1
2	FE2	D	202	1/1	0.95	0.14	67,67,67,67	1
2	FE2	F	203	1/1	0.95	0.12	67,67,67,67	1
2	FE2	C	202	1/1	0.97	0.12	58,58,58,58	1
2	FE2	E	202	1/1	0.98	0.09	66,66,66,66	1
2	FE2	B	301	1/1	0.98	0.05	29,29,29,29	1
3	FE	F	202	1/1	0.98	0.08	31,31,31,31	1
2	FE2	D	201	1/1	0.99	0.10	28,28,28,28	1
2	FE2	F	201	1/1	0.99	0.11	29,29,29,29	1
2	FE2	A	201	1/1	0.99	0.10	27,27,27,27	1
2	FE2	E	201	1/1	0.99	0.07	30,30,30,30	1

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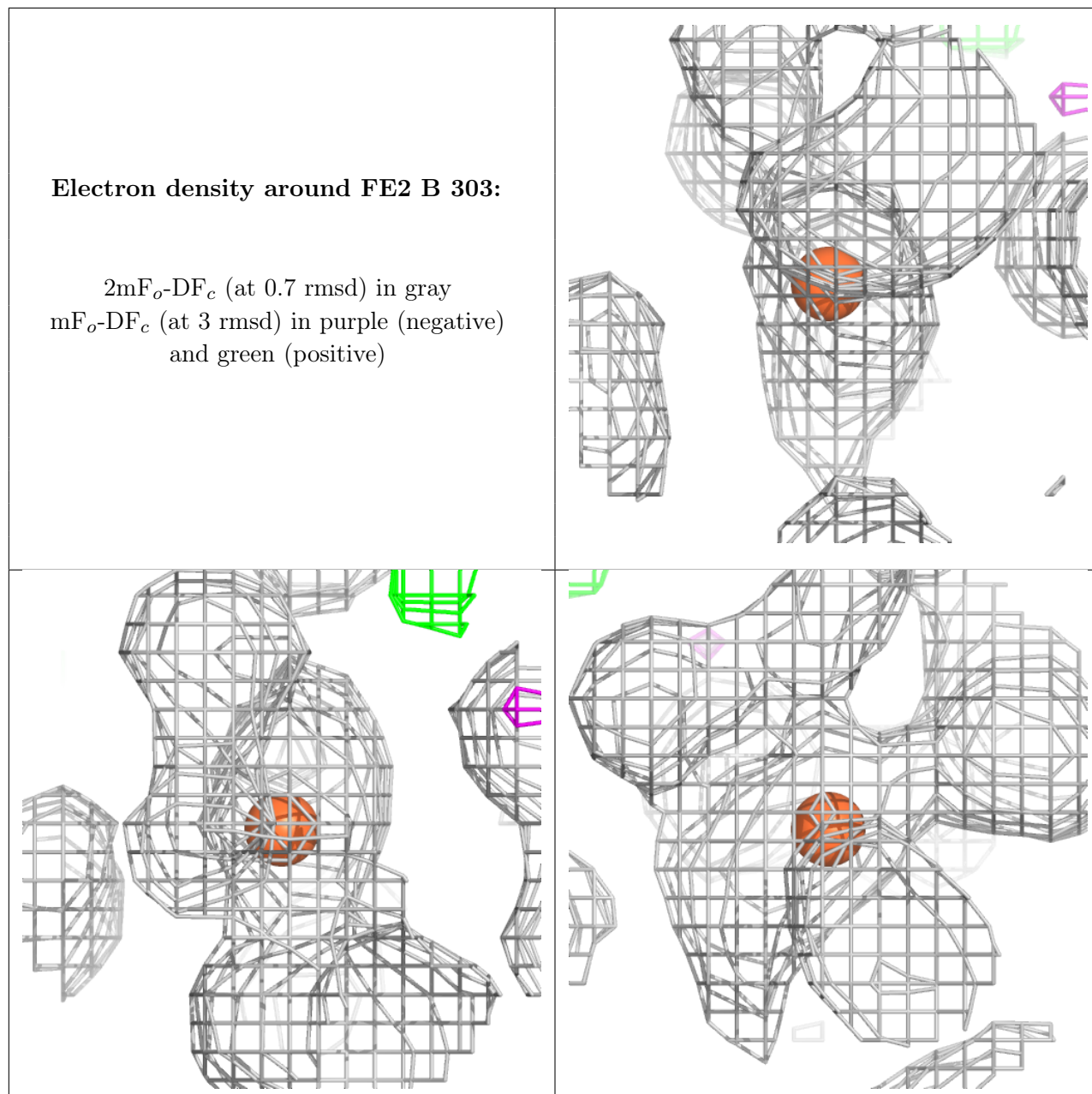
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE2	B	302	1/1	1.00	0.06	28,28,28,28	1
2	FE2	C	201	1/1	1.00	0.08	28,28,28,28	1

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

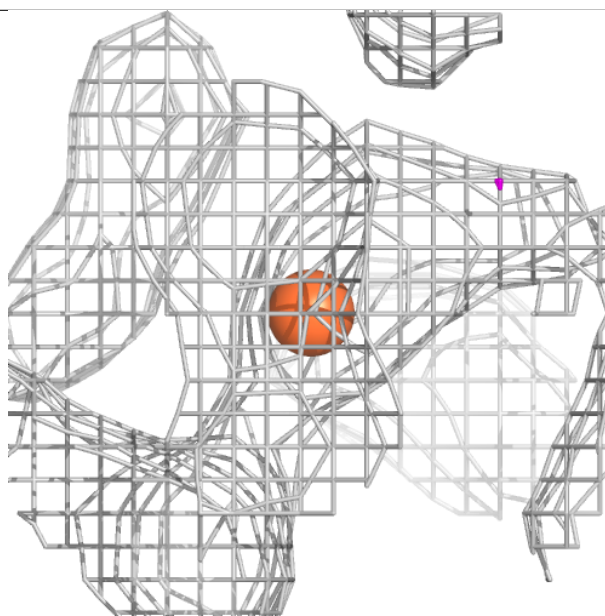
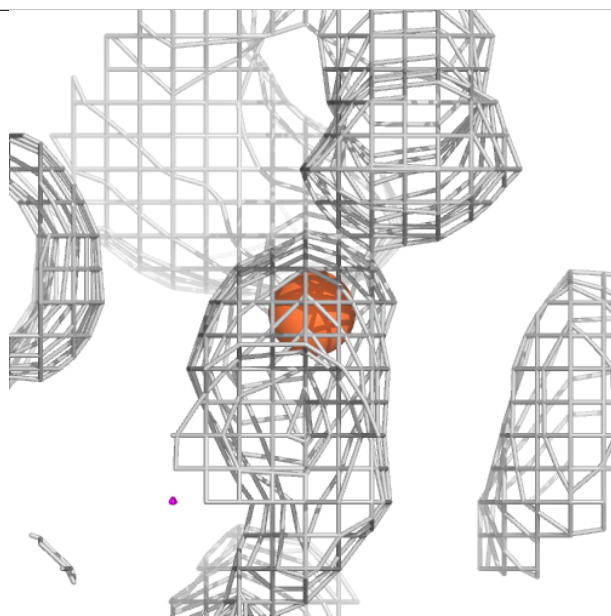
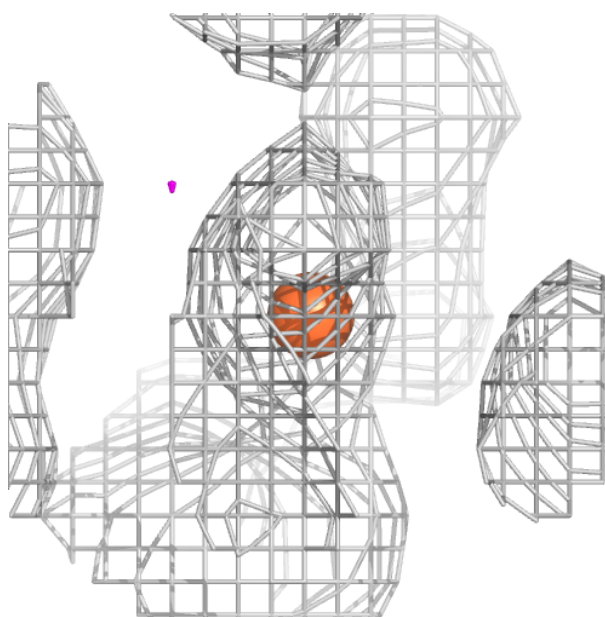
Electron density around FE2 B 303:

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



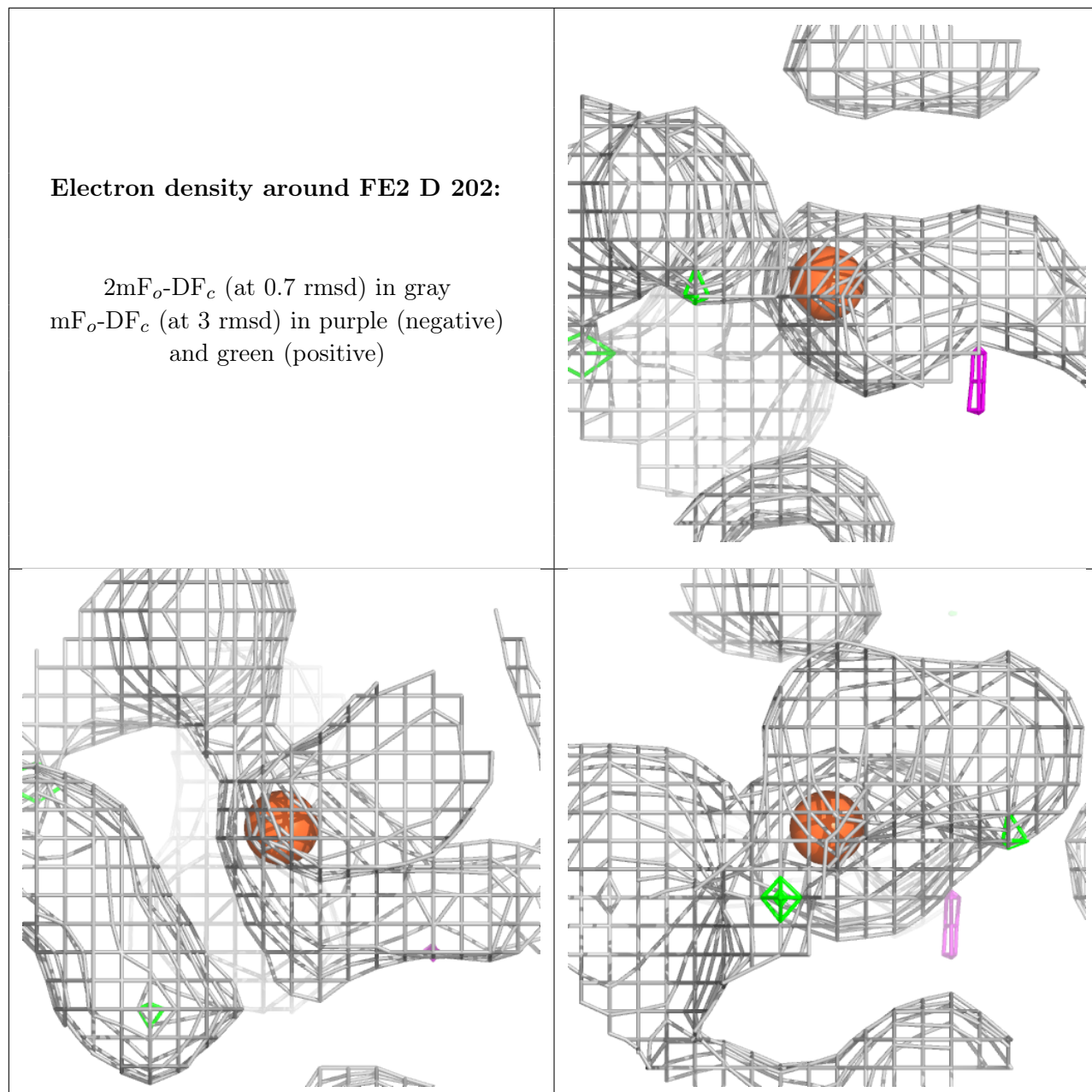
Electron density around FE2 A 202:

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



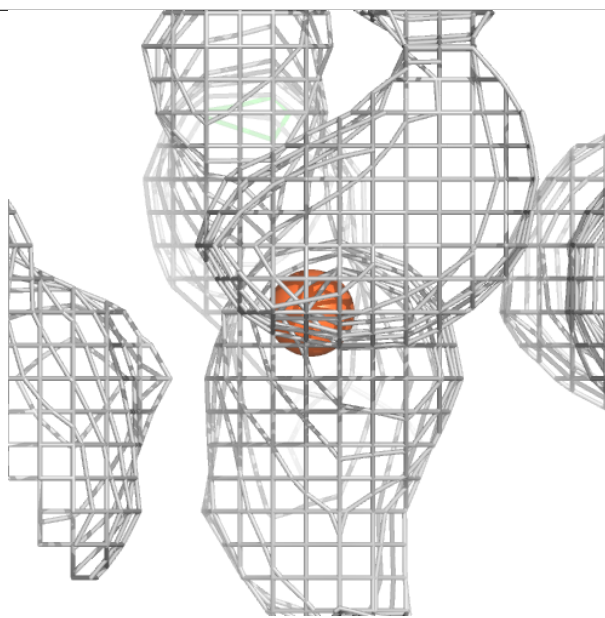
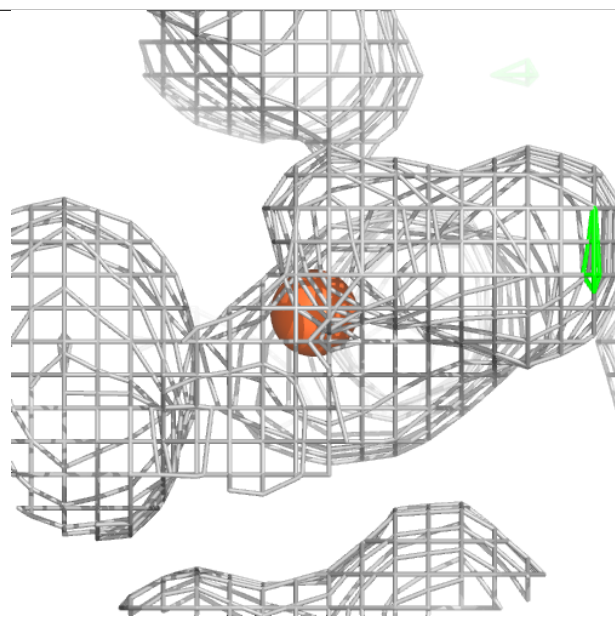
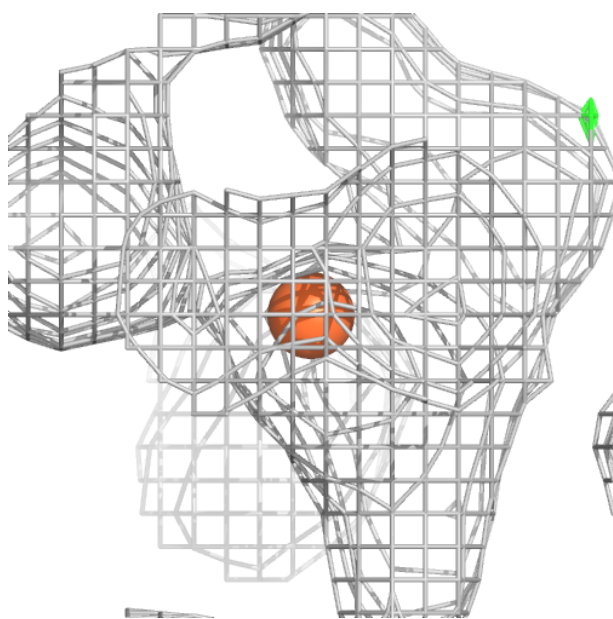
Electron density around FE2 D 202:

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



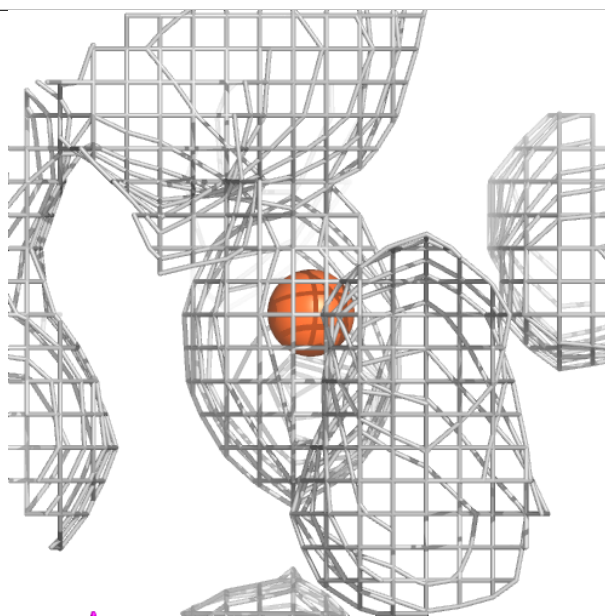
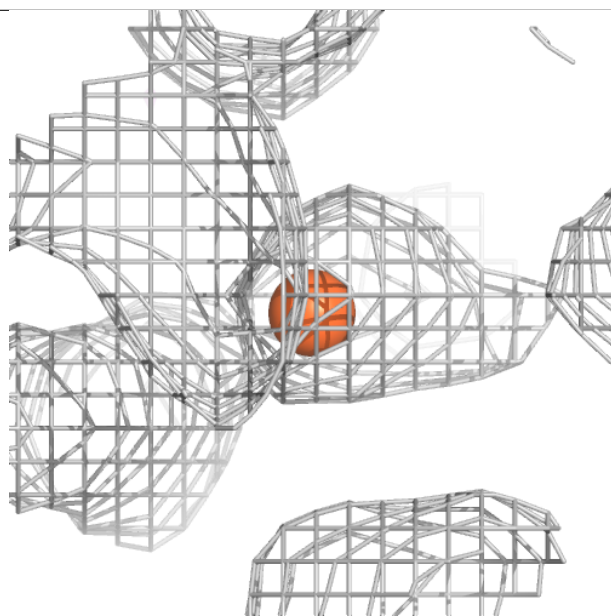
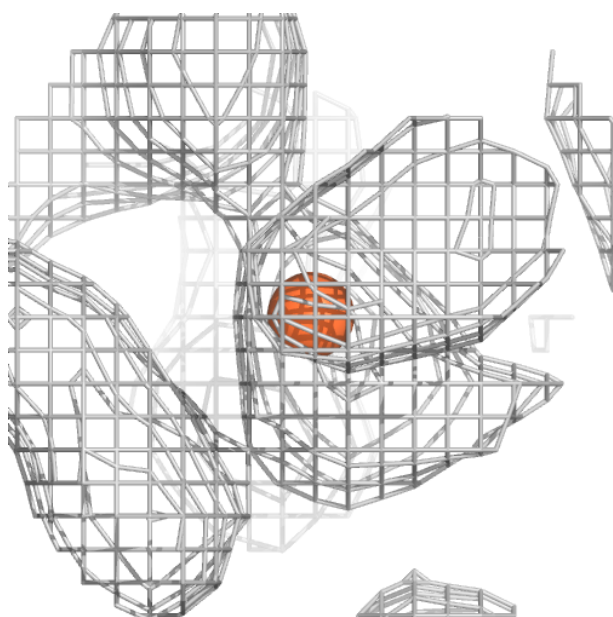
Electron density around FE2 F 203:

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



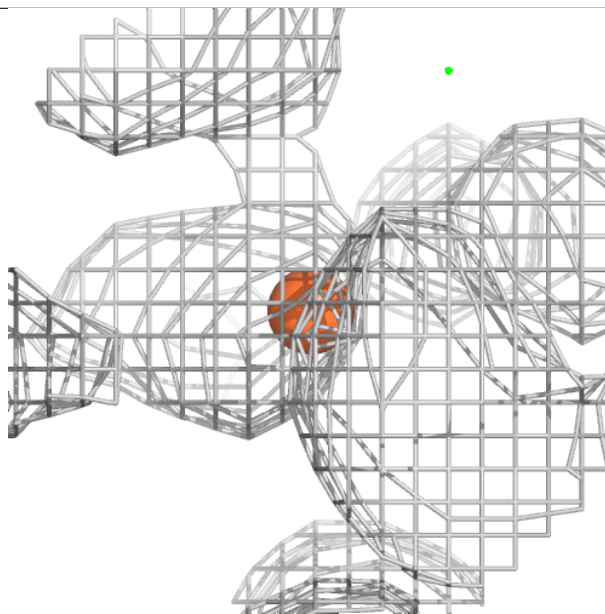
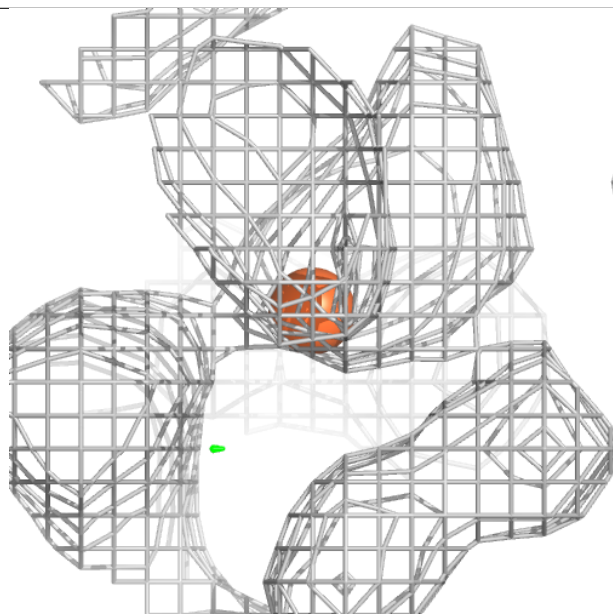
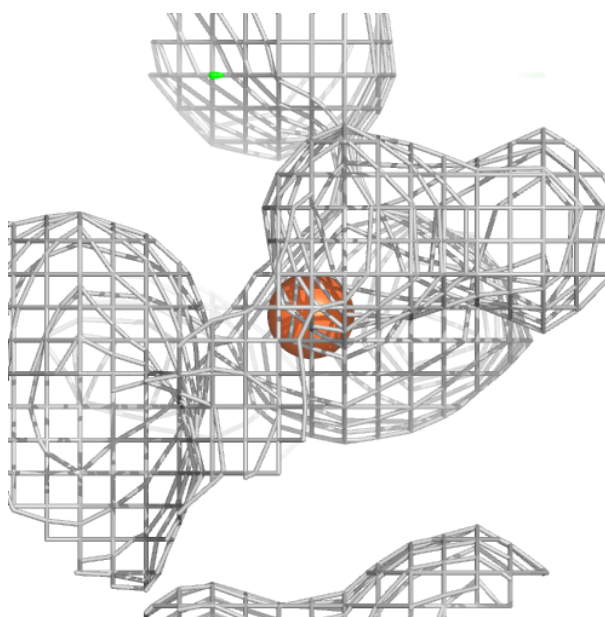
Electron density around FE2 C 202:

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



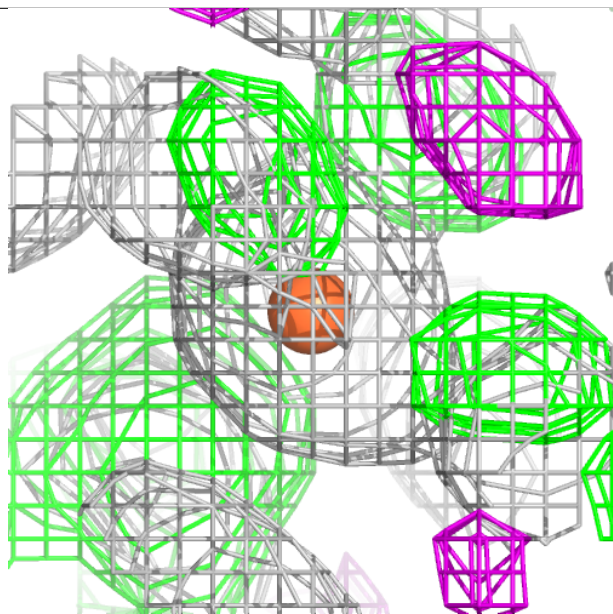
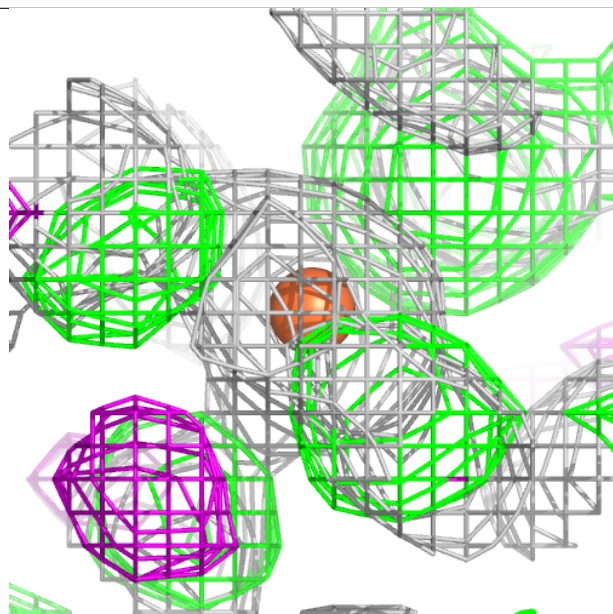
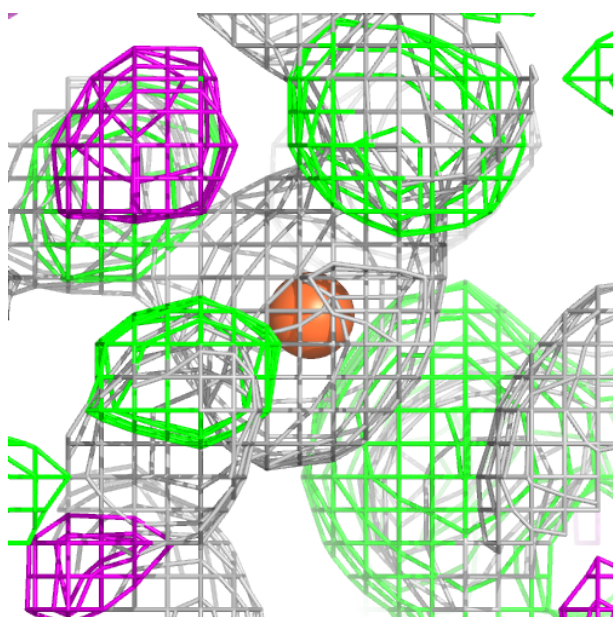
Electron density around FE2 E 202:

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



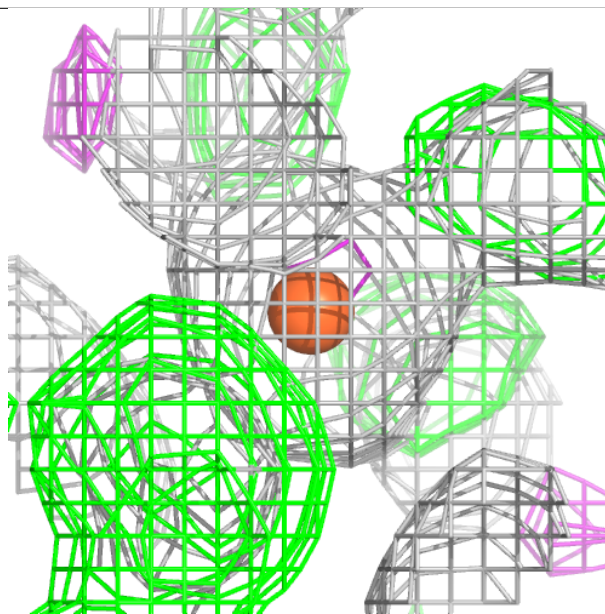
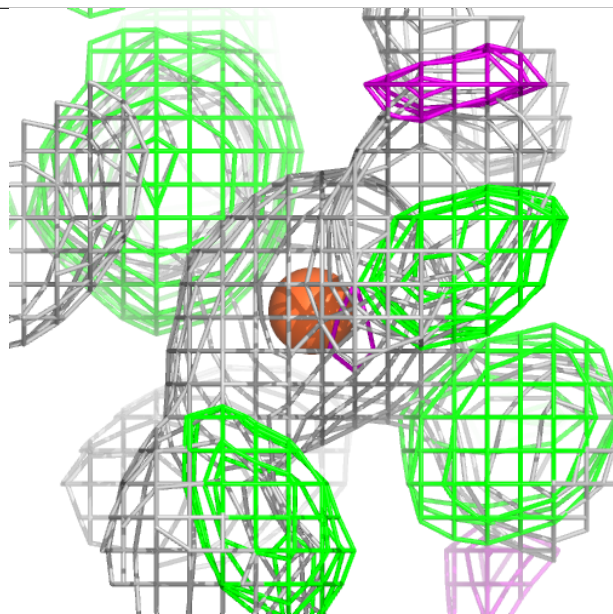
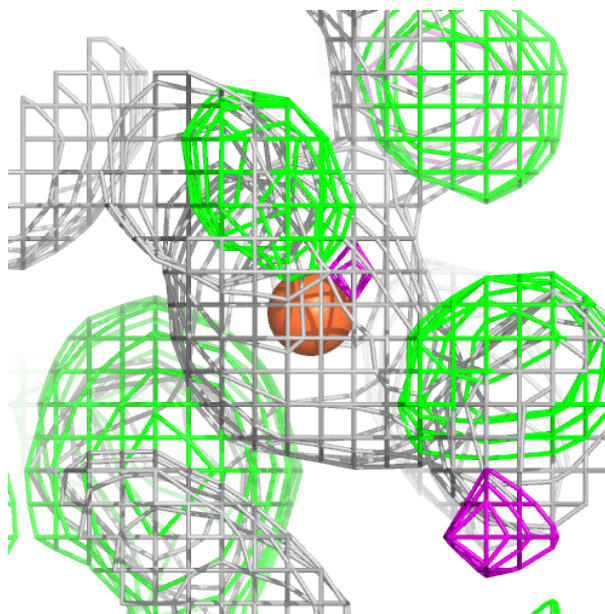
Electron density around FE2 B 301:

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



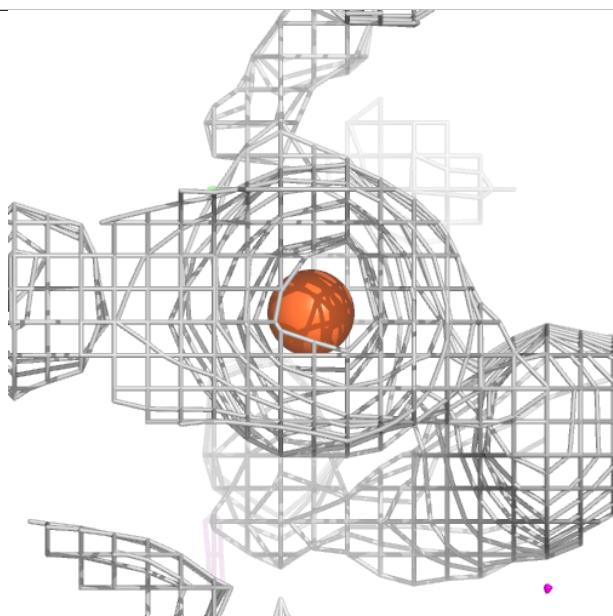
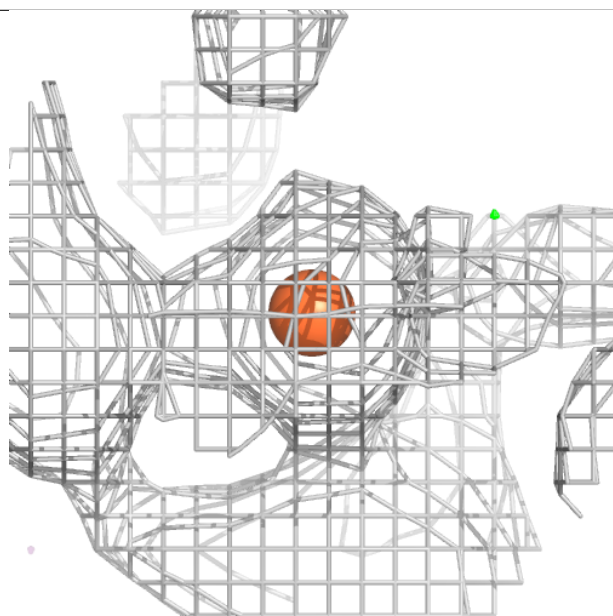
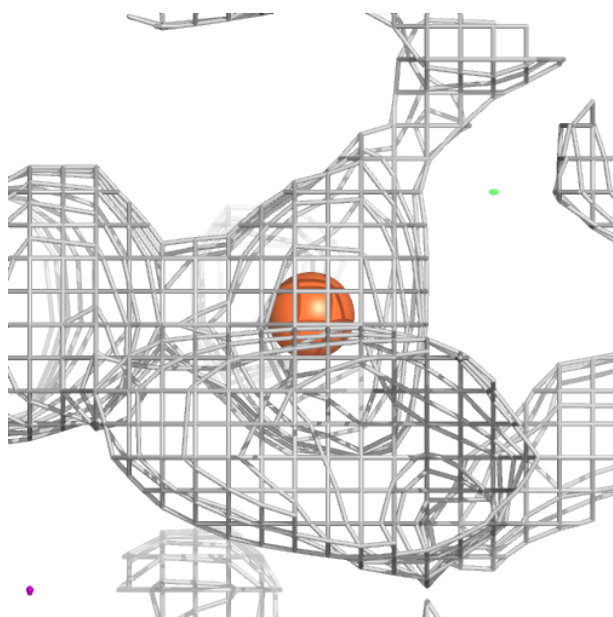
Electron density around FE F 202:

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



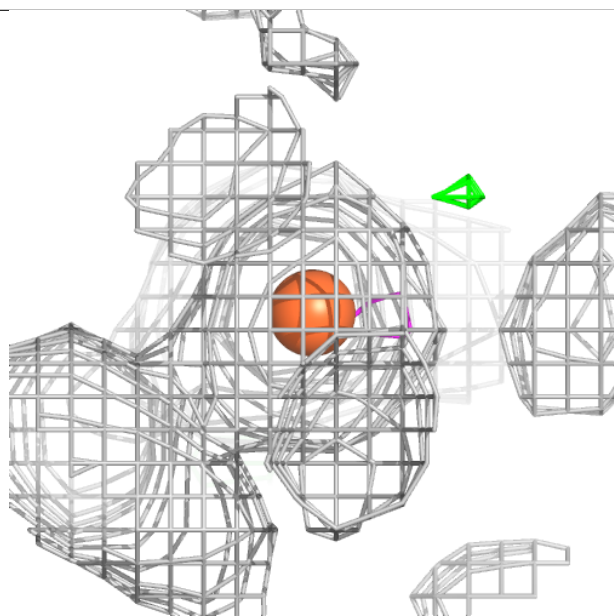
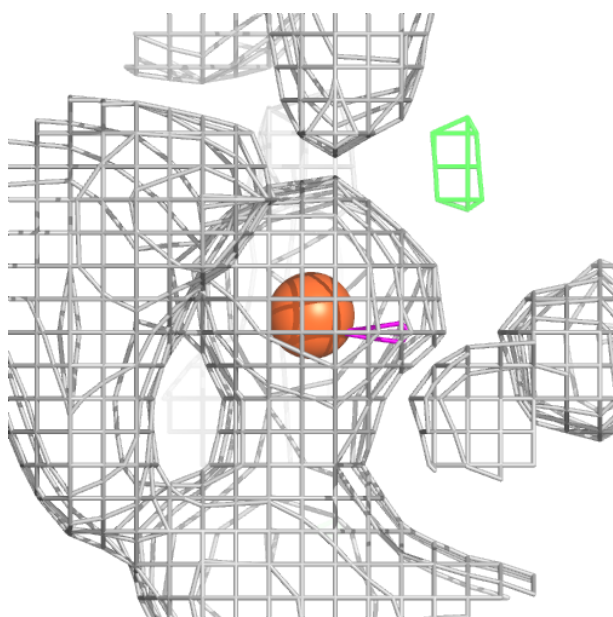
Electron density around FE2 D 201:

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



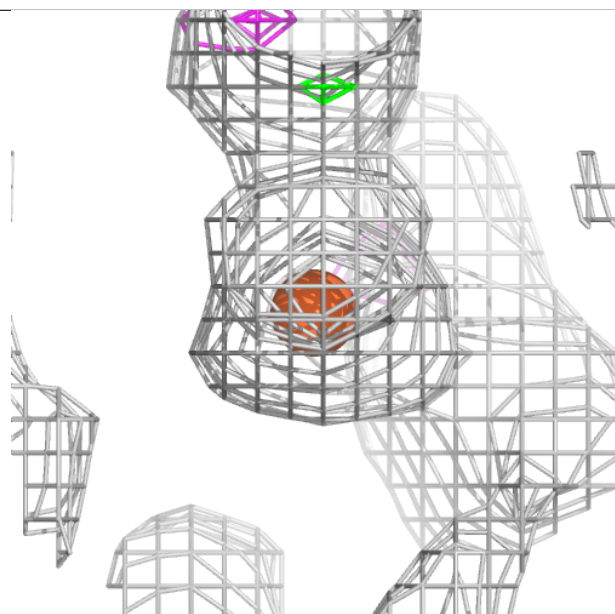
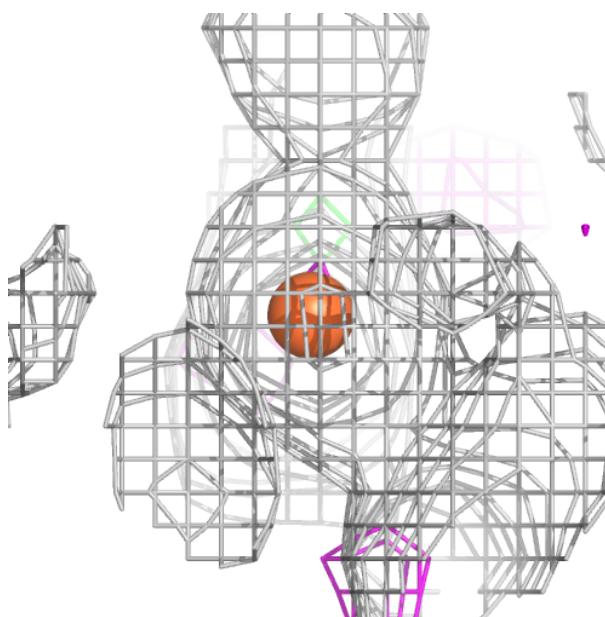
Electron density around FE2 F 201:

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



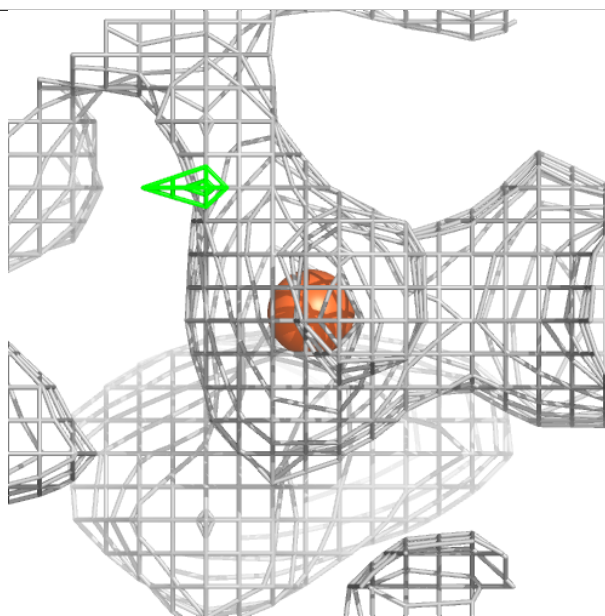
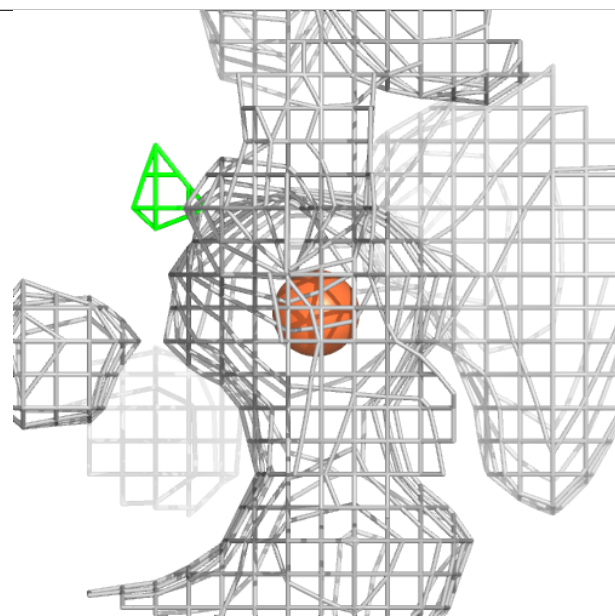
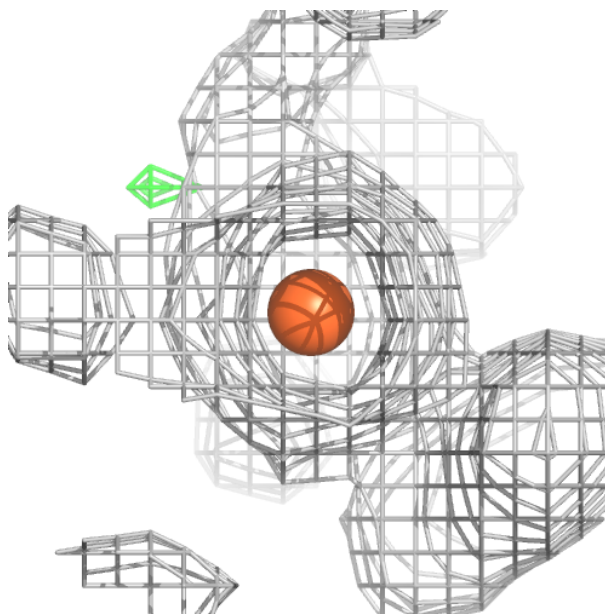
Electron density around FE2 A 201:

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



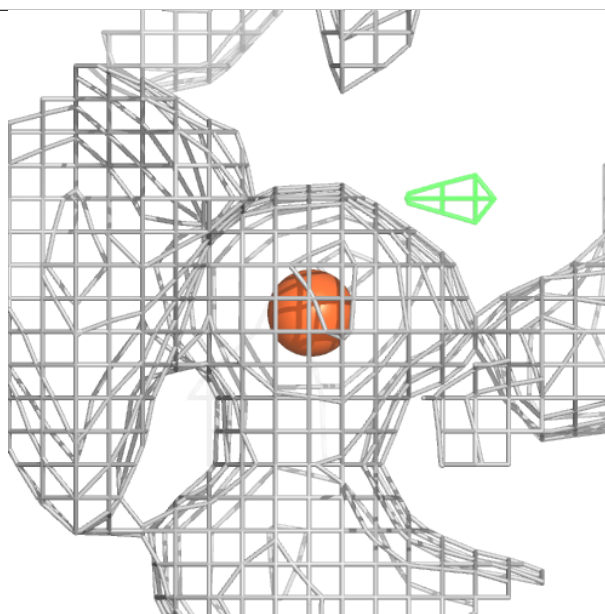
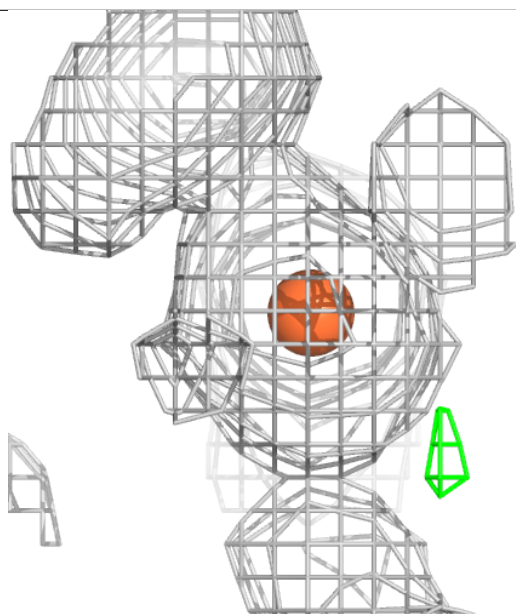
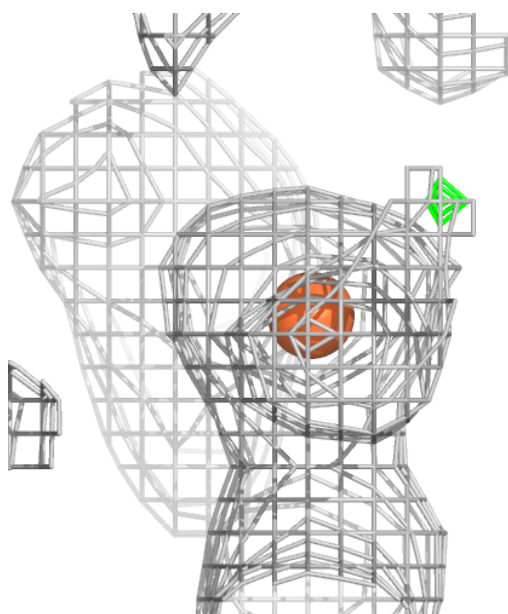
Electron density around FE2 E 201:

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



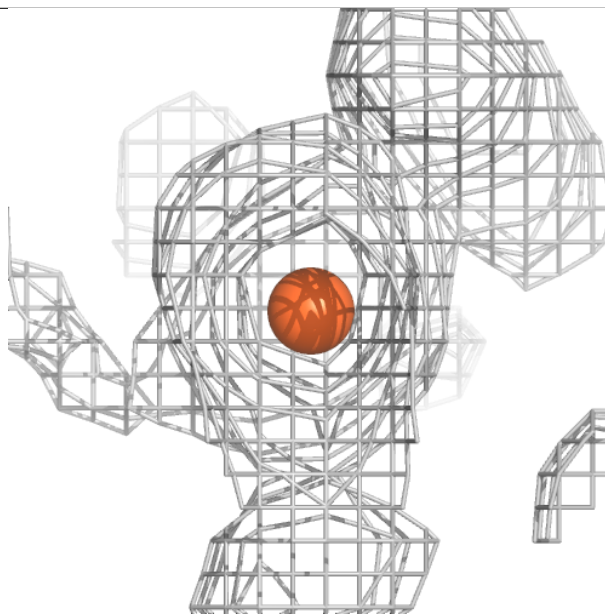
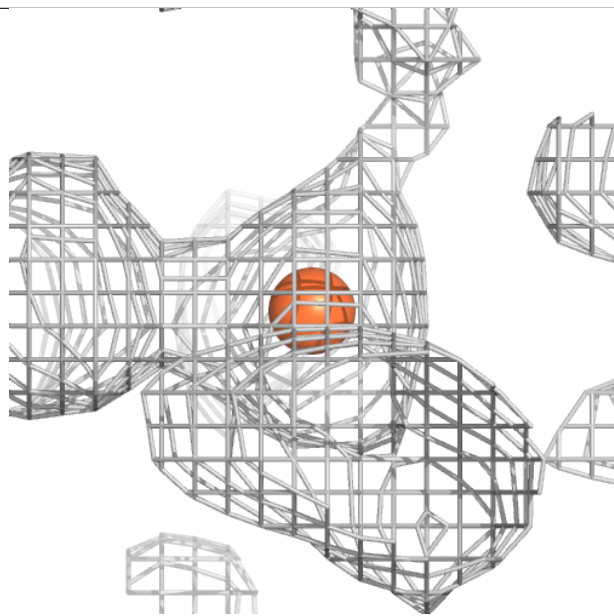
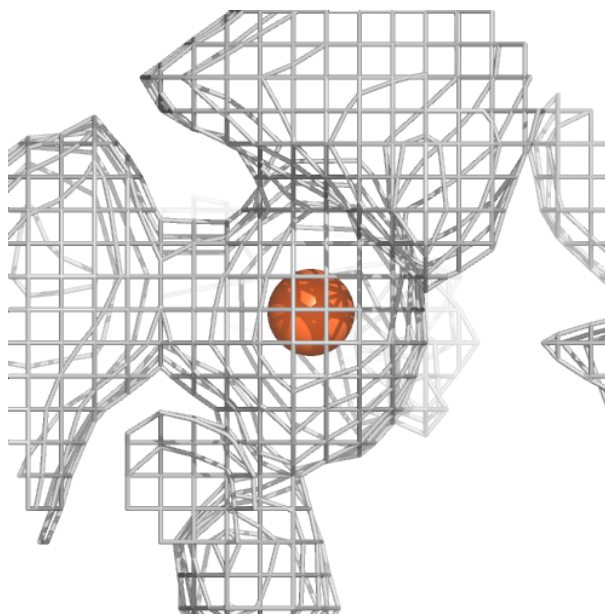
Electron density around FE2 B 302:

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



Electron density around FE2 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.