



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 01:15 pm BST

PDB ID : 9S4P / pdb_00009s4p
Title : diFe-Sulerythin_E53D reduced
Authors : Jeoung, J.-H.; Dobbek, H.
Deposited on : 2025-07-28
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

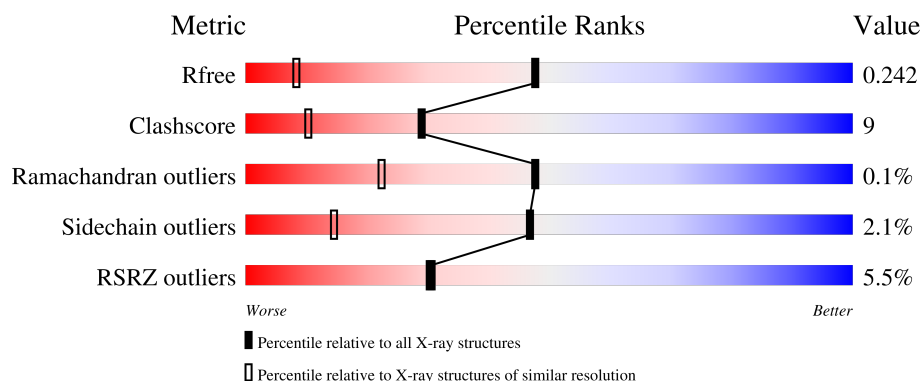
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	145	<div> <div>8%</div> <div>80%</div> <div>13%</div> <div>...</div> </div>
1	B	145	<div> <div>7%</div> <div>74%</div> <div>17%</div> <div>5%</div> <div>.</div> </div>
1	C	145	<div> <div>5%</div> <div>89%</div> <div>10%</div> <div>..</div> </div>
1	D	145	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	E	145	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	145	<div><div></div><div>6%</div><div>83%</div><div>14%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7836 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 Sulerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	4	0
			1140	723	196	217	4			
1	B	140	Total	C	N	O	S	0	6	0
			1145	727	195	219	4			
1	C	144	Total	C	N	O	S	0	8	0
			1176	747	197	227	5			
1	D	140	Total	C	N	O	S	0	2	0
			1113	707	189	214	3			
1	E	140	Total	C	N	O	S	0	6	0
			1138	724	192	218	4			
1	F	142	Total	C	N	O	S	0	5	0
			1143	725	194	221	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASN	-	expression tag	UNP F9VPE5
A	53	ASP	GLU	engineered mutation	UNP F9VPE5
B	0	ASN	-	expression tag	UNP F9VPE5
B	53	ASP	GLU	engineered mutation	UNP F9VPE5
C	0	ASN	-	expression tag	UNP F9VPE5
C	53	ASP	GLU	engineered mutation	UNP F9VPE5
D	0	ASN	-	expression tag	UNP F9VPE5
D	53	ASP	GLU	engineered mutation	UNP F9VPE5
E	0	ASN	-	expression tag	UNP F9VPE5
E	53	ASP	GLU	engineered mutation	UNP F9VPE5
F	0	ASN	-	expression tag	UNP F9VPE5
F	53	ASP	GLU	engineered mutation	UNP F9VPE5

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

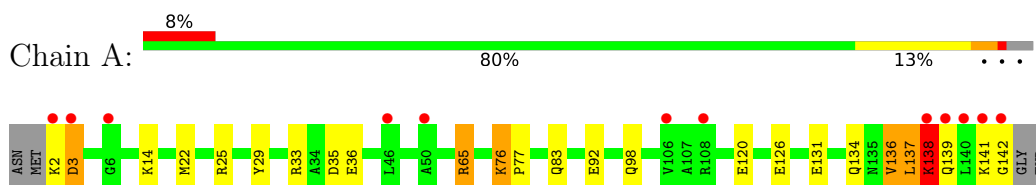
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	178	Total O 178 178	0	0
4	B	149	Total O 149 149	0	0
4	C	163	Total O 163 163	0	0
4	D	153	Total O 153 153	0	0
4	E	163	Total O 163 163	0	0
4	F	156	Total O 156 156	0	0

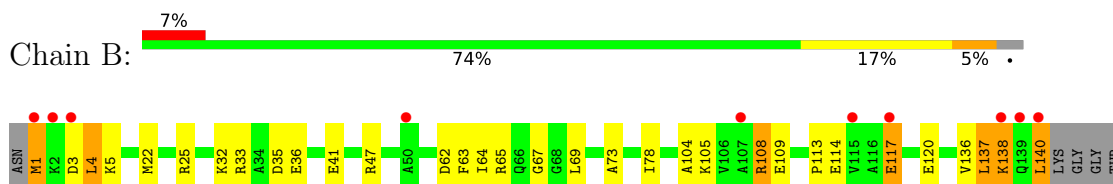
3 Residue-property plots [i](#)

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

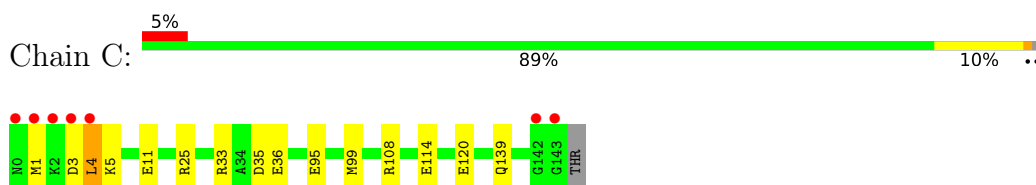
- Molecule 1: Sulerythrin



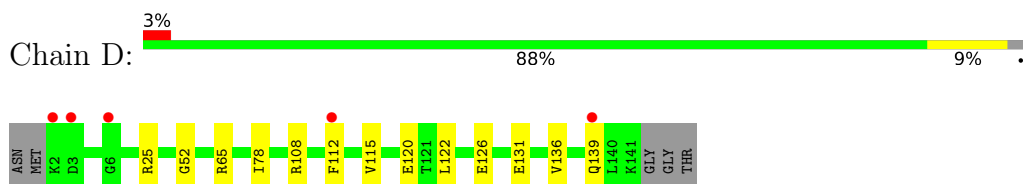
- Molecule 1: Sulerythrin



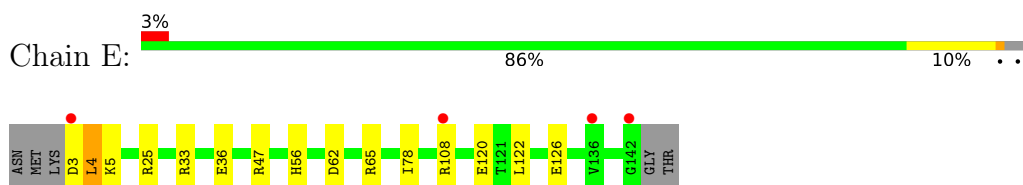
- Molecule 1: Sulerythrin



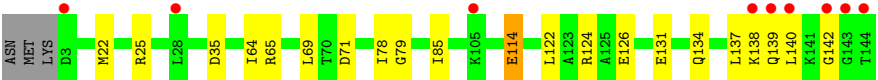
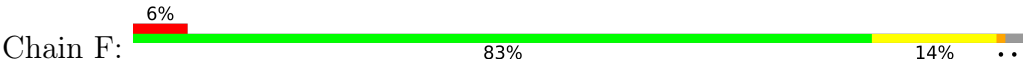
- Molecule 1: Sulerythrin



- Molecule 1: Sulerythrin



- Molecule 1: Sulerythrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 88.68Å 100.99Å 90.00° 114.86° 90.00°	Depositor
Resolution (Å)	45.81 – 1.45 45.81 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.81-1.45) 99.1 (45.81-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.165 , 0.202 0.203 , 0.242	Depositor DCC
R_{free} test set	2101 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7836	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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 63.22 % 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 1.0002e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.69	0/1173	1.16	6/1576 (0.4%)
1	B	0.70	0/1187	1.14	7/1595 (0.4%)
1	C	0.67	0/1224	1.05	3/1644 (0.2%)
1	D	0.66	0/1143	1.06	0/1538
1	E	0.69	1/1180 (0.1%)	1.09	2/1585 (0.1%)
1	F	0.68	0/1182	1.08	5/1589 (0.3%)
All	All	0.68	1/7089 (0.0%)	1.10	23/9527 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	E	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	56	HIS	CE1-NE2	6.15	1.38	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	LYS	N-CA-CB	-12.09	90.06	110.49
1	A	138	LYS	CB-CA-C	8.95	128.24	110.42
1	B	41	GLU	CB-CG-CD	8.43	126.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLU	CB-CG-CD	7.99	126.19	112.60
1	F	139	GLN	CB-CA-C	7.88	124.25	110.85
1	B	22	MET	CG-SD-CE	-7.82	83.70	100.90
1	E	4	LEU	N-CA-CB	6.93	120.73	110.33
1	A	3	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	4	LEU	N-CA-CB	-6.50	100.87	110.49
1	F	71	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	137	LEU	N-CA-C	-6.03	104.71	111.28
1	A	98	GLN	N-CA-CB	5.66	120.05	110.49
1	E	62	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	35	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	98	GLN	CB-CA-C	-5.55	99.37	110.42
1	C	4	LEU	N-CA-CB	-5.54	102.25	110.61
1	A	137	LEU	CA-C-O	5.46	126.40	120.55
1	F	35	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	140	LEU	N-CA-CB	-5.38	101.36	110.50
1	B	35	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	114	GLU	CB-CG-CD	5.28	121.57	112.60
1	F	22	MET	CG-SD-CE	-5.24	89.37	100.90
1	B	62	ASP	CA-CB-CG	5.22	117.82	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65[A]	ARG	Sidechain
1	A	65[B]	ARG	Sidechain
1	B	108[A]	ARG	Sidechain
1	B	108[B]	ARG	Sidechain
1	B	47	ARG	Sidechain
1	E	108	ARG	Sidechain
1	E	47	ARG	Sidechain

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	1140	0	1115	32	0
1	B	1145	0	1127	34	0
1	C	1176	0	1160	20	0
1	D	1113	0	1083	17	0
1	E	1138	0	1119	11	0
1	F	1143	0	1118	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	178	0	0	17	1
4	B	149	0	0	8	0
4	C	163	0	0	12	0
4	D	153	0	0	6	0
4	E	163	0	0	7	0
4	F	156	0	0	7	1
All	All	7836	0	6722	118	2

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 9.

All (118) 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:A:83:GLN:O	4:A:301:HOH:O	1.55	1.20
1:A:131:GLU:OE1	4:A:302:HOH:O	1.56	1.20
1:B:138:LYS:N	4:B:302:HOH:O	1.74	1.18
1:B:137:LEU:C	4:B:302:HOH:O	1.90	1.12
1:B:1:MET:HE3	4:B:338:HOH:O	1.48	1.12
1:B:1:MET:N	4:B:303:HOH:O	1.94	1.00
1:F:131[A]:GLU:HG3	4:F:385:HOH:O	1.67	0.95
1:F:134:GLN:HB3	4:F:386:HOH:O	1.67	0.94
1:E:120:GLU:HG2	4:E:314:HOH:O	1.72	0.89
1:A:33:ARG:NH2	1:B:65[B]:ARG:HH22	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:NH1	4:D:301:HOH:O	2.10	0.84
1:C:36[B]:GLU:CD	4:C:313:HOH:O	2.21	0.82
1:E:65[B]:ARG:HD2	1:E:78:ILE:O	1.80	0.80
1:A:83:GLN:C	4:A:301:HOH:O	2.09	0.80
1:A:120:GLU:OE2	4:A:303:HOH:O	2.03	0.76
1:C:108:ARG:NH2	4:C:304:HOH:O	2.19	0.76
1:A:136:VAL:O	1:A:139[A]:GLN:HB3	1.87	0.75
4:E:433:HOH:O	1:F:114:GLU:HG3	1.85	0.75
1:A:33:ARG:HH22	1:B:65[B]:ARG:HH22	1.34	0.73
1:E:120:GLU:CG	4:E:314:HOH:O	2.34	0.73
1:A:33:ARG:NH2	1:B:65[B]:ARG:NH2	2.39	0.71
1:F:65[B]:ARG:NH1	1:F:79:GLY:O	2.22	0.71
1:B:108[A]:ARG:NH1	1:B:120:GLU:OE2	2.24	0.71
1:C:33:ARG:NH2	1:D:65:ARG:HH22	1.91	0.68
1:D:131:GLU:HG3	4:D:383:HOH:O	1.93	0.67
1:A:76:LYS:HG2	1:A:77:PRO:HD2	1.76	0.67
1:E:120:GLU:OE1	4:E:301:HOH:O	2.11	0.67
1:C:11:GLU:OE1	4:C:301:HOH:O	2.12	0.67
1:C:120:GLU:CD	4:C:304:HOH:O	2.38	0.67
1:F:142:GLY:O	4:F:301:HOH:O	2.13	0.66
1:C:33:ARG:NH2	1:D:65:ARG:NH2	2.42	0.66
1:B:138:LYS:C	1:B:140:LEU:H	2.04	0.65
1:A:36:GLU:HG3	4:A:345:HOH:O	1.97	0.65
1:A:139[B]:GLN:O	4:A:304:HOH:O	2.15	0.64
1:F:85[B]:ILE:HD12	1:F:140:LEU:HD11	1.80	0.64
1:A:2:LYS:O	1:A:2:LYS:HD2	1.98	0.63
1:F:114:GLU:H	1:F:114:GLU:CD	2.06	0.63
1:B:36:GLU:CD	4:B:307:HOH:O	2.42	0.63
1:A:14:LYS:NZ	4:A:309:HOH:O	2.29	0.62
1:B:32:LYS:HD3	4:B:428:HOH:O	2.01	0.61
1:E:33:ARG:HH12	1:F:65[B]:ARG:HH12	1.50	0.59
1:C:95:GLU:OE2	4:C:302:HOH:O	2.17	0.59
1:A:136:VAL:O	1:A:139[B]:GLN:HB2	2.03	0.58
1:C:36[B]:GLU:CG	4:C:313:HOH:O	2.52	0.58
1:A:65[B]:ARG:NH2	1:B:33:ARG:NH2	2.51	0.58
1:D:65:ARG:NH2	4:D:303:HOH:O	2.38	0.57
1:D:65:ARG:HG2	1:D:78:ILE:HG13	1.86	0.56
1:F:85[B]:ILE:HD12	1:F:140:LEU:CD1	2.35	0.56
1:F:131[A]:GLU:CG	4:F:385:HOH:O	2.39	0.56
1:B:136:VAL:O	1:B:138:LYS:N	2.38	0.55
1:A:134:GLN:HG2	4:A:369:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[A]:MET:HE2	1:B:73:ALA:HB2	1.88	0.55
1:A:65[B]:ARG:HH22	1:B:33:ARG:NH2	2.06	0.54
1:A:36:GLU:CD	4:A:345:HOH:O	2.49	0.54
1:E:36[B]:GLU:CD	4:E:330:HOH:O	2.50	0.54
1:C:3:ASP:O	4:C:303:HOH:O	2.19	0.54
1:C:139:GLN:HB2	4:C:396:HOH:O	2.06	0.54
1:E:36[B]:GLU:HG3	4:E:330:HOH:O	2.07	0.53
1:B:1:MET:HE1	1:B:4:LEU:HD11	1.90	0.53
1:E:33:ARG:HH12	1:F:65[B]:ARG:NH1	2.07	0.53
1:D:139:GLN:NE2	4:D:305:HOH:O	2.40	0.53
1:B:138:LYS:O	1:B:140:LEU:N	2.41	0.53
1:E:3:ASP:OD1	1:E:4:LEU:N	2.42	0.52
1:D:139:GLN:HB2	4:D:394:HOH:O	2.09	0.52
1:C:1:MET:HE3	3:C:202:CL:CL	2.47	0.52
1:D:108:ARG:HH21	1:D:120:GLU:CD	2.18	0.52
1:B:65[B]:ARG:HG2	1:B:78:ILE:HG13	1.90	0.52
1:B:138:LYS:C	1:B:140:LEU:N	2.63	0.52
1:C:36[B]:GLU:HG3	4:C:313:HOH:O	2.08	0.51
1:C:99:MET:HE1	4:C:413:HOH:O	2.11	0.51
1:B:136:VAL:C	1:B:138:LYS:H	2.18	0.51
1:A:2:LYS:NZ	4:A:314:HOH:O	2.44	0.50
1:A:3:ASP:HA	4:A:314:HOH:O	2.10	0.50
1:C:33:ARG:HH22	1:D:65:ARG:HH22	1.60	0.50
1:C:139:GLN:NE2	4:C:308:HOH:O	2.37	0.49
1:F:65[B]:ARG:HD2	1:F:78:ILE:O	2.12	0.49
1:A:33:ARG:HH22	1:B:65[B]:ARG:NH2	2.04	0.49
1:A:36:GLU:CG	4:A:345:HOH:O	2.56	0.49
1:F:124:ARG:NH2	4:F:305:HOH:O	2.46	0.48
1:C:4:LEU:HD23	1:D:112:PHE:CE1	2.49	0.48
1:A:141:LYS:O	1:A:142:GLY:C	2.56	0.48
1:A:138:LYS:HG3	4:A:430:HOH:O	2.14	0.47
1:F:134:GLN:CD	4:F:312:HOH:O	2.57	0.47
1:B:114:GLU:HA	1:B:114:GLU:OE2	2.13	0.47
1:A:92:GLU:OE1	1:A:126:GLU:OE1	2.33	0.47
1:B:136:VAL:C	1:B:138:LYS:N	2.74	0.46
1:C:5:LYS:HD3	4:C:408:HOH:O	2.15	0.46
1:A:35:ASP:HB3	1:D:52:GLY:HA2	1.98	0.46
1:C:1:MET:HE1	1:D:115:VAL:HG23	1.98	0.45
1:C:4:LEU:HD23	1:D:112:PHE:CZ	2.50	0.45
1:F:138:LYS:HB3	4:F:439:HOH:O	2.16	0.45
1:B:114:GLU:HB2	4:B:436:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ILE:HG23	1:F:69:LEU:HB2	1.98	0.45
1:B:64:ILE:HG23	1:B:69:LEU:HB2	2.00	0.43
1:F:85[B]:ILE:CD1	1:F:140:LEU:HD11	2.48	0.43
1:A:134:GLN:CB	4:A:310:HOH:O	2.66	0.43
1:B:36:GLU:HG3	4:B:307:HOH:O	2.18	0.43
1:B:104:ALA:O	1:B:108[A]:ARG:HG2	2.18	0.43
1:D:120:GLU:HG2	4:D:437:HOH:O	2.18	0.43
1:E:122:LEU:O	1:E:126:GLU:HG2	2.18	0.43
1:B:1:MET:HE2	1:B:63:PHE:HD1	1.84	0.43
1:C:33:ARG:HH22	1:D:65:ARG:NH2	2.13	0.42
1:E:36[B]:GLU:CG	4:E:330:HOH:O	2.66	0.42
1:B:113:PRO:O	1:B:117:GLU:HG2	2.19	0.42
1:A:137:LEU:C	1:A:139[B]:GLN:N	2.75	0.42
1:F:122:LEU:O	1:F:126:GLU:HG2	2.20	0.42
1:A:138:LYS:CG	4:A:430:HOH:O	2.67	0.42
1:B:105:LYS:HE2	1:B:109:GLU:OE1	2.20	0.41
1:B:1:MET:HE2	1:B:63:PHE:CD1	2.56	0.41
1:A:29:TYR:HE2	1:B:65[B]:ARG:HD2	1.84	0.41
1:B:3:ASP:OD1	1:B:5:LYS:HB2	2.20	0.41
1:A:134:GLN:HB2	4:A:310:HOH:O	2.21	0.41
1:B:4:LEU:HD12	1:B:67:GLY:HA3	2.03	0.41
1:D:122:LEU:O	1:D:126:GLU:HG2	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:343:HOH:O	4:F:416:HOH:O[2_656]	2.04	0.16
4:A:350:HOH:O	4:A:393:HOH:O[2_555]	2.09	0.11

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	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
1	B	144/145 (99%)	138 (96%)	5 (4%)	1 (1%)	18	4
1	C	150/145 (103%)	147 (98%)	3 (2%)	0	100	100
1	D	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
1	E	144/145 (99%)	141 (98%)	3 (2%)	0	100	100
1	F	145/145 (100%)	142 (98%)	3 (2%)	0	100	100
All	All	866/870 (100%)	845 (98%)	20 (2%)	1 (0%)	48	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	LEU

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	114/113 (101%)	110 (96%)	4 (4%)	32	5
1	B	116/113 (103%)	113 (97%)	3 (3%)	40	10
1	C	120/113 (106%)	119 (99%)	1 (1%)	73	50
1	D	111/113 (98%)	109 (98%)	2 (2%)	51	19
1	E	115/113 (102%)	113 (98%)	2 (2%)	53	21
1	F	115/113 (102%)	113 (98%)	2 (2%)	53	21
All	All	691/678 (102%)	677 (98%)	14 (2%)	47	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	76	LYS
1	A	136	VAL
1	A	138	LYS

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Mol	Chain	Res	Type
1	B	1	MET
1	B	25	ARG
1	B	138	LYS
1	C	25	ARG
1	D	25	ARG
1	D	136	VAL
1	E	5	LYS
1	E	25	ARG
1	F	25	ARG
1	F	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	98	GLN
1	C	98	GLN
1	C	134	GLN
1	D	66	GLN
1	F	66	GLN
1	F	139	GLN

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 19 ligands modelled in this entry, 19 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	141/145 (97%)	0.61	12 (8%)	16 17	6, 9, 20, 53	4 (2%)
1	B	140/145 (96%)	0.37	10 (7%)	22 21	5, 9, 20, 43	6 (4%)
1	C	144/145 (99%)	0.35	7 (4%)	35 36	5, 9, 23, 44	8 (5%)
1	D	140/145 (96%)	0.34	5 (3%)	46 48	5, 10, 17, 51	2 (1%)
1	E	140/145 (96%)	0.30	4 (2%)	53 56	6, 9, 18, 38	6 (4%)
1	F	142/145 (97%)	0.50	9 (6%)	26 25	4, 10, 20, 52	5 (3%)
All	All	847/870 (97%)	0.41	47 (5%)	30 30	4, 9, 20, 53	31 (3%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	144	THR	11.7
1	F	143	GLY	8.0
1	C	143	GLY	6.8
1	E	3	ASP	5.9
1	B	140	LEU	5.6
1	A	142	GLY	5.5
1	A	138	LYS	5.1
1	C	142	GLY	5.1
1	F	142	GLY	4.9
1	A	140	LEU	4.6
1	A	141	LYS	4.6
1	B	1	MET	4.6
1	B	2	LYS	4.3
1	B	138	LYS	3.9
1	C	1	MET	3.8
1	E	142	GLY	3.5
1	D	2	LYS	3.5
1	A	6	GLY	3.4
1	F	139	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	2	LYS	3.2
1	D	3	ASP	3.2
1	F	138	LYS	3.2
1	B	139	GLN	3.2
1	A	2	LYS	3.1
1	C	0	ASN	3.1
1	F	3	ASP	3.1
1	D	112	PHE	3.0
1	A	3	ASP	2.9
1	B	107	ALA	2.8
1	B	3	ASP	2.8
1	D	139	GLN	2.7
1	F	105	LYS	2.7
1	E	136	VAL	2.5
1	C	3	ASP	2.5
1	A	50	ALA	2.4
1	A	139[A]	GLN	2.4
1	A	46	LEU	2.3
1	B	50	ALA	2.2
1	F	28	LEU	2.2
1	B	115	VAL	2.2
1	D	6	GLY	2.2
1	B	117	GLU	2.1
1	A	108	ARG	2.1
1	A	106	VAL	2.0
1	C	4	LEU	2.0
1	E	108	ARG	2.0
1	F	140	LEU	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,

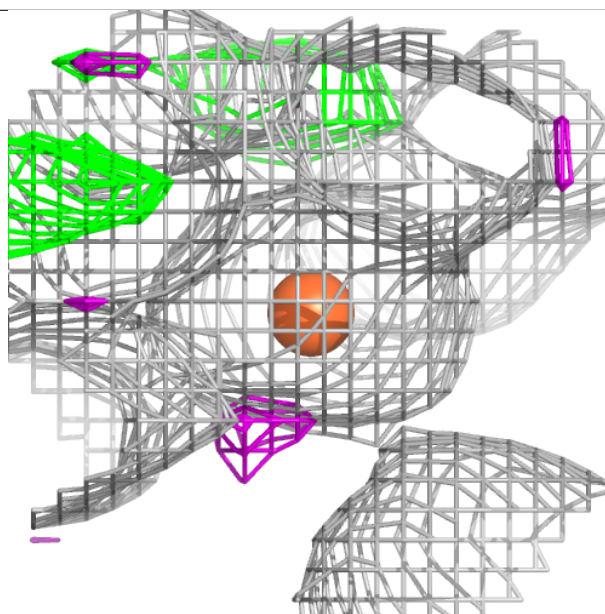
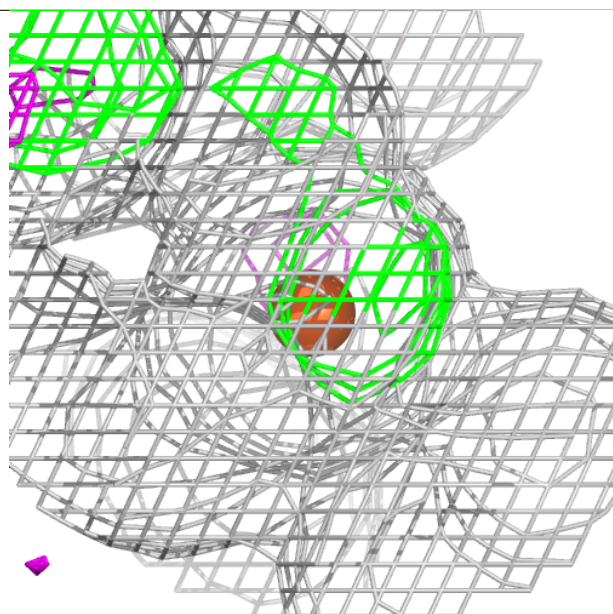
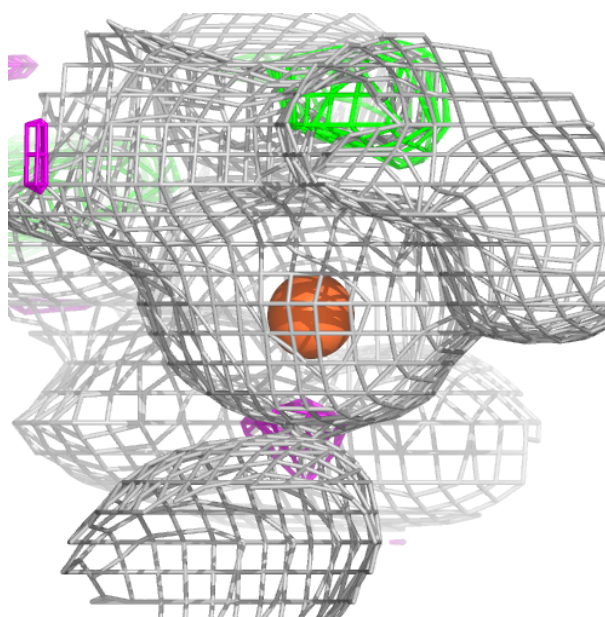
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	C	202	1/1	0.78	0.22	55,55,55,55	0
3	CL	B	203	1/1	0.97	0.09	17,17,17,17	0
3	CL	A	203	1/1	0.97	0.05	9,9,9,9	0
3	CL	F	203	1/1	0.98	0.04	11,11,11,11	0
2	FE2	C	201	1/1	0.99	0.02	14,14,14,14	1
2	FE2	C	203	1/1	0.99	0.04	8,8,8,8	0
2	FE2	D	201	1/1	0.99	0.09	18,18,18,18	0
2	FE2	D	202	1/1	0.99	0.05	9,9,9,9	0
2	FE2	E	201	1/1	0.99	0.08	9,9,9,9	0
2	FE2	E	202	1/1	0.99	0.02	15,15,15,15	1
2	FE2	F	201	1/1	0.99	0.03	15,15,15,15	1
2	FE2	F	202	1/1	0.99	0.09	9,9,9,9	0
2	FE2	A	201	1/1	0.99	0.06	15,15,15,15	1
2	FE2	A	202	1/1	0.99	0.07	9,9,9,9	0
2	FE2	B	201	1/1	0.99	0.03	14,14,14,14	1
3	CL	C	204	1/1	0.99	0.05	6,6,6,6	0
3	CL	E	203	1/1	0.99	0.05	13,13,13,13	0
2	FE2	B	202	1/1	0.99	0.06	9,9,9,9	0
3	CL	D	203	1/1	1.00	0.05	9,9,9,9	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.

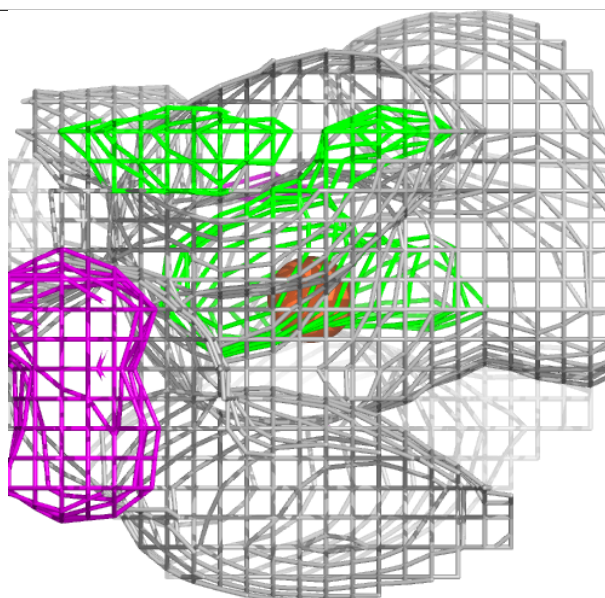
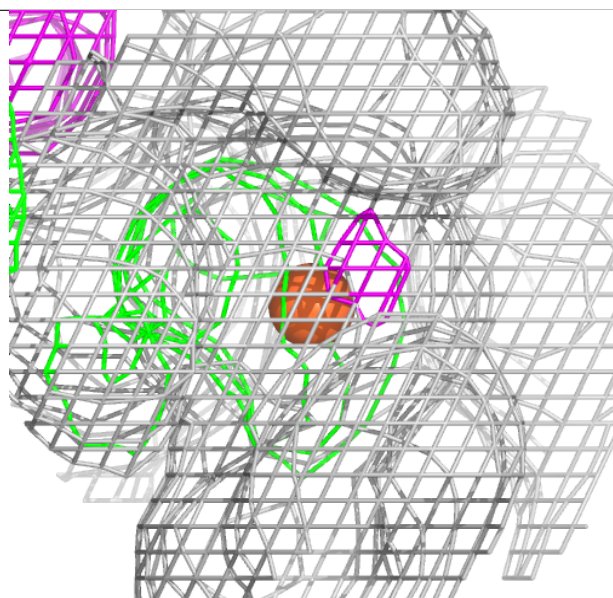
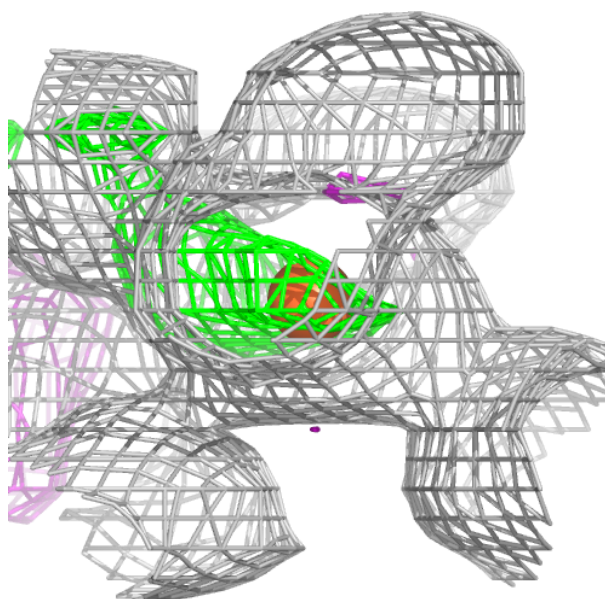
Electron density around FE2 C 201:

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



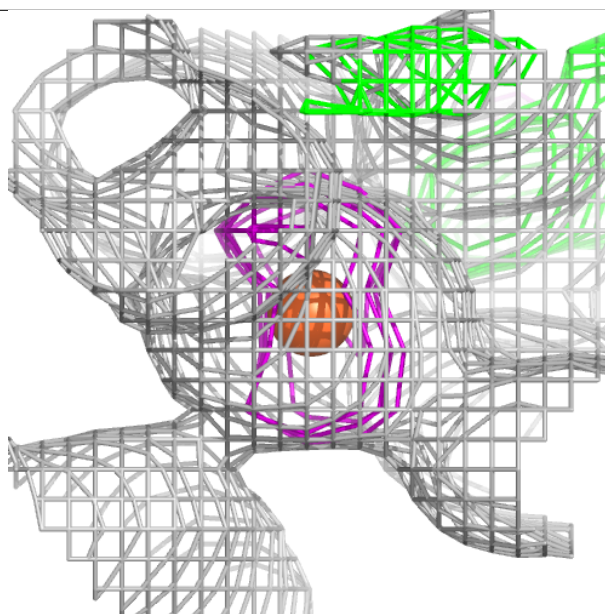
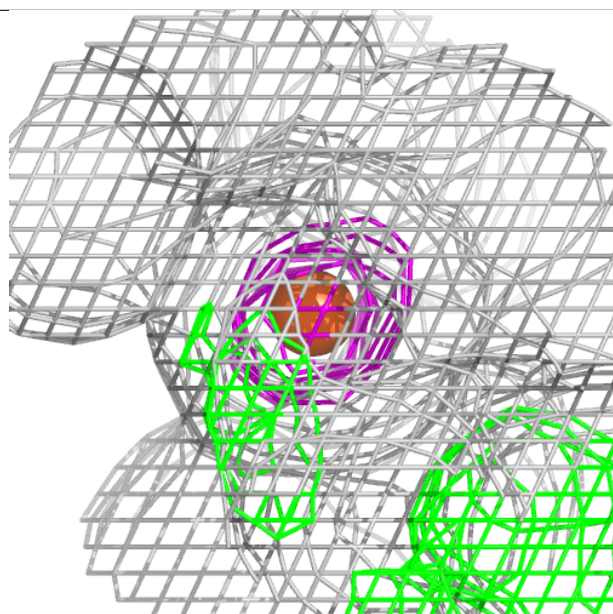
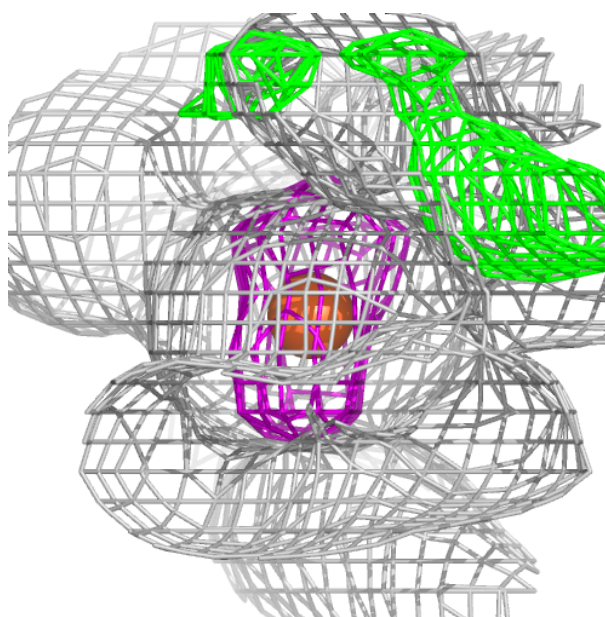
Electron density around FE2 C 203:

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and green (positive)



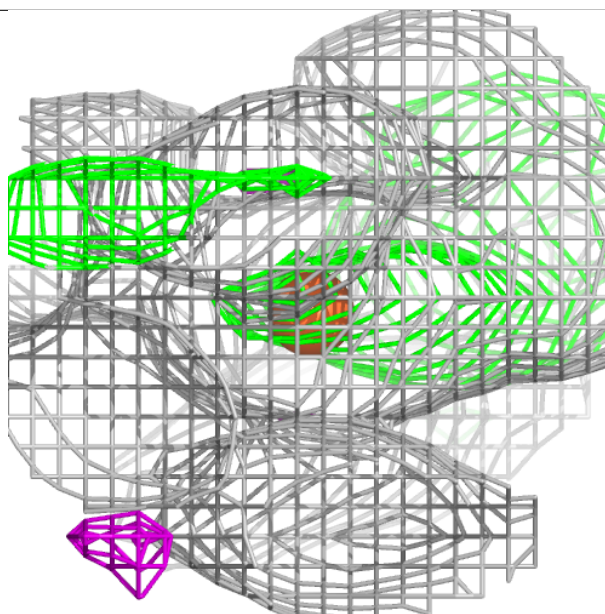
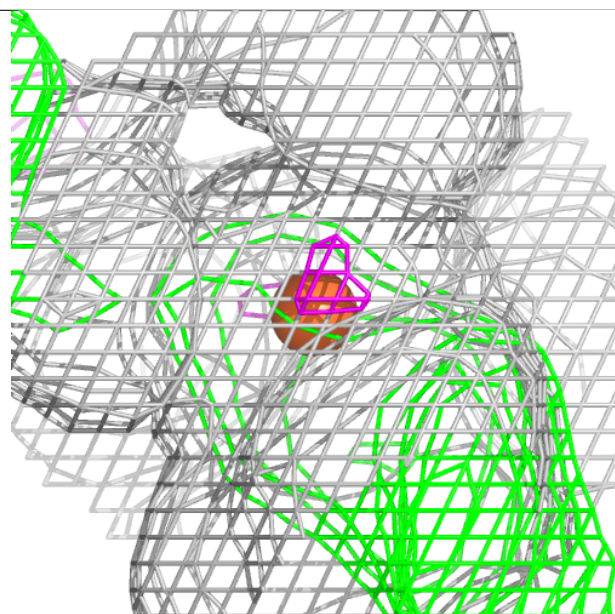
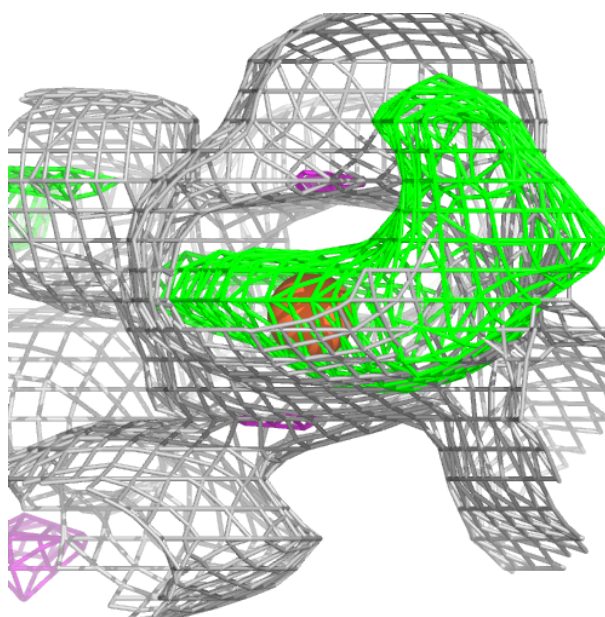
Electron density around FE2 D 201:

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and green (positive)



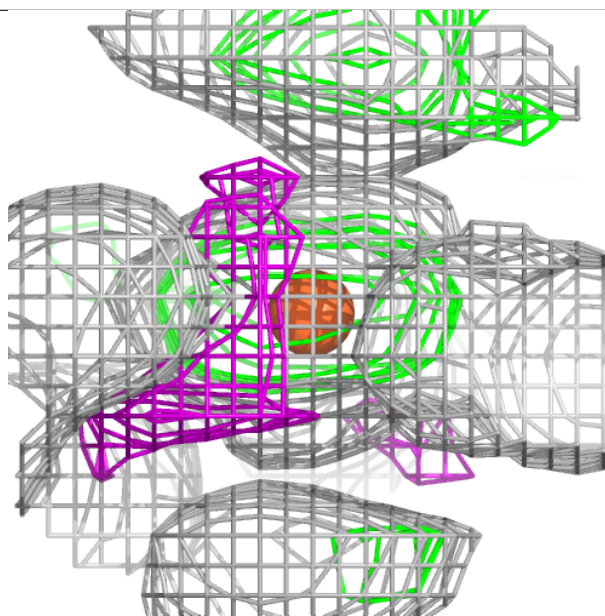
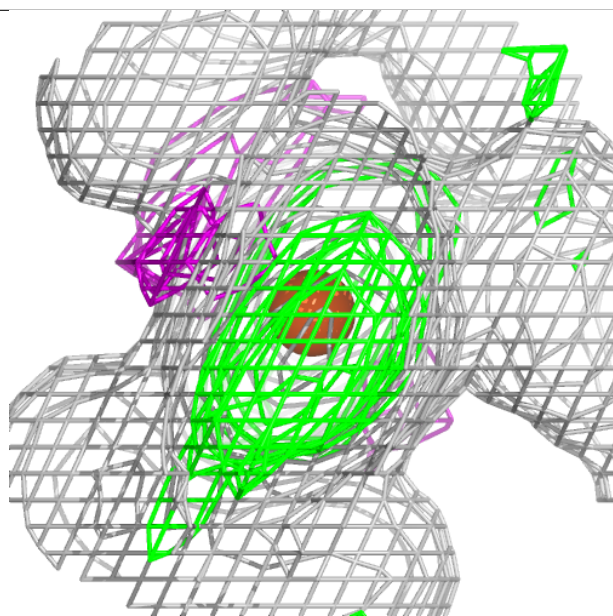
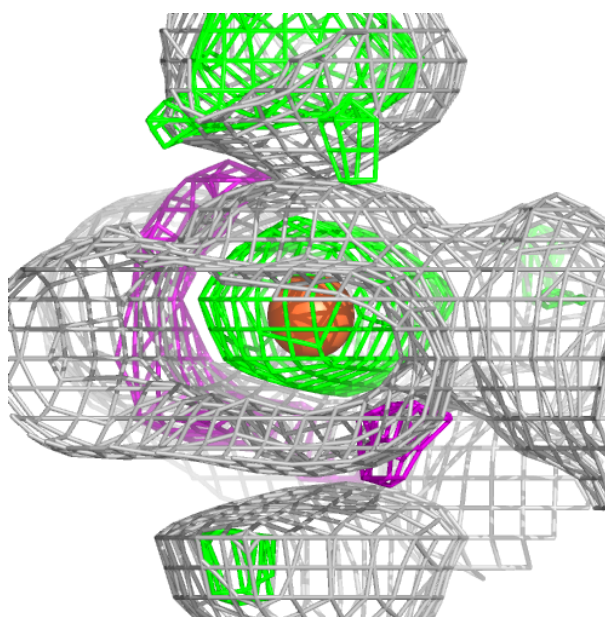
Electron density around FE2 D 202:

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and green (positive)



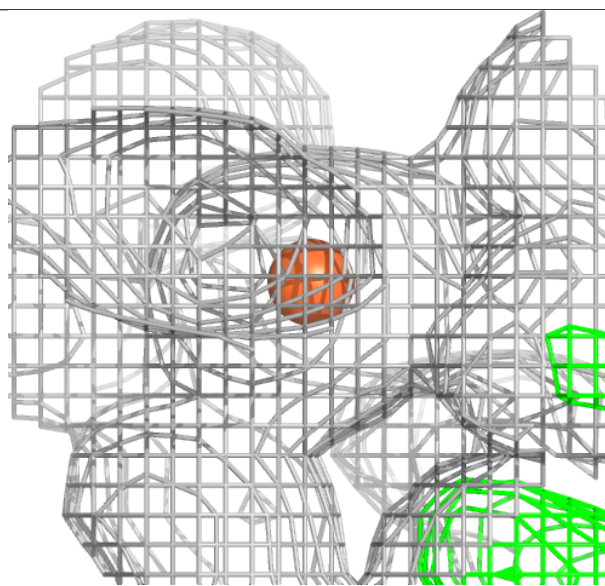
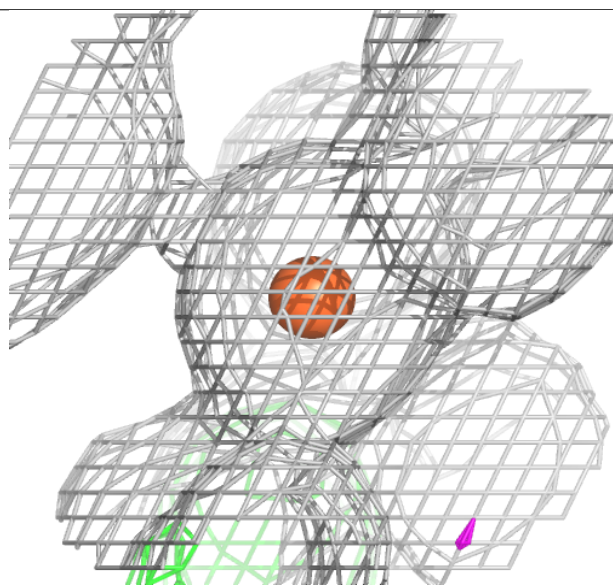
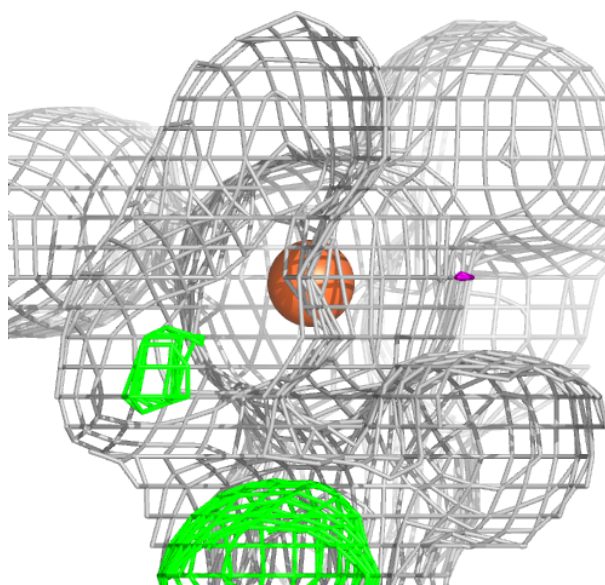
Electron density around FE2 E 201:

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and green (positive)



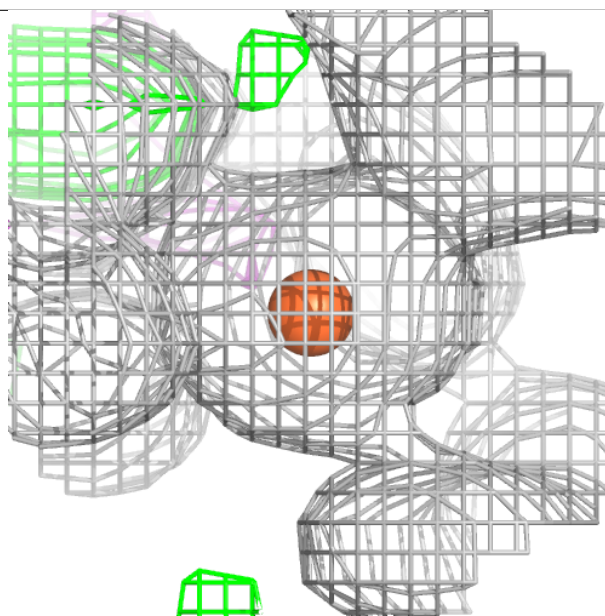
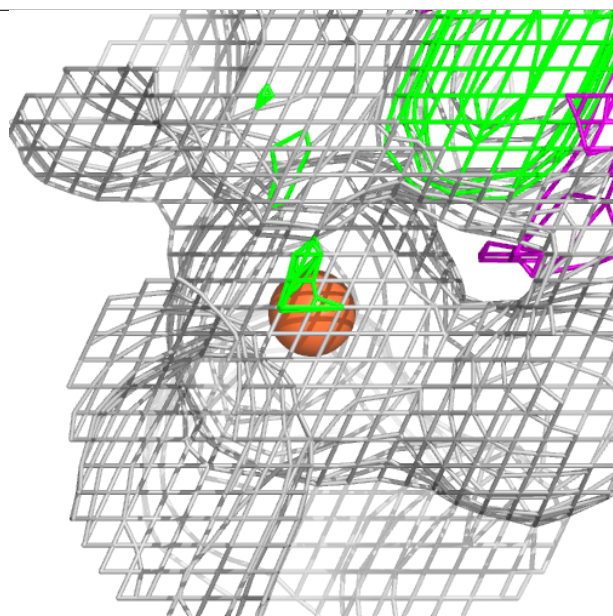
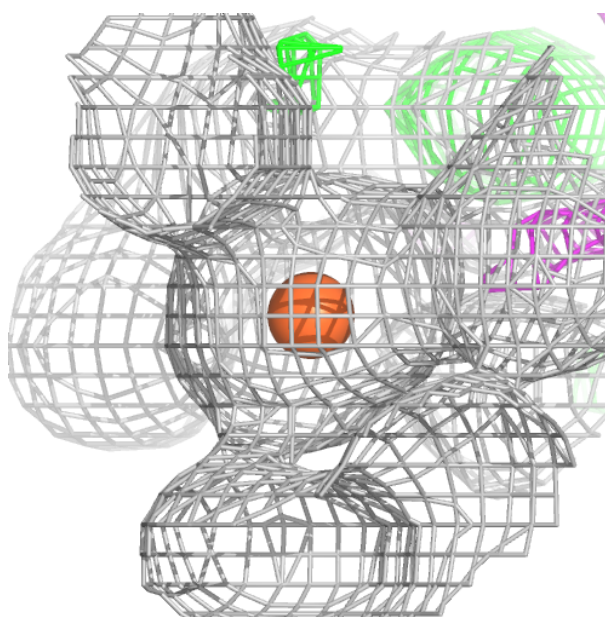
Electron density around FE2 E 202:

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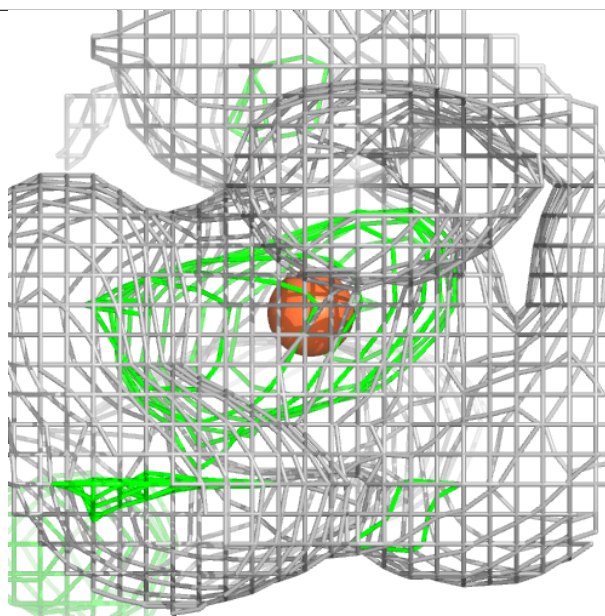
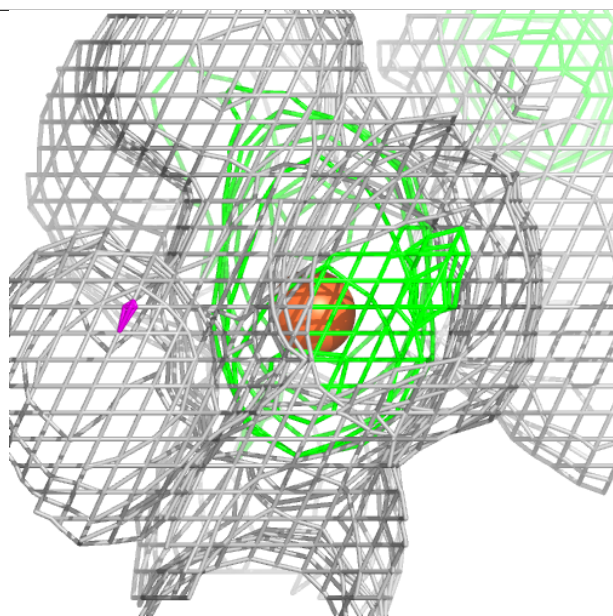
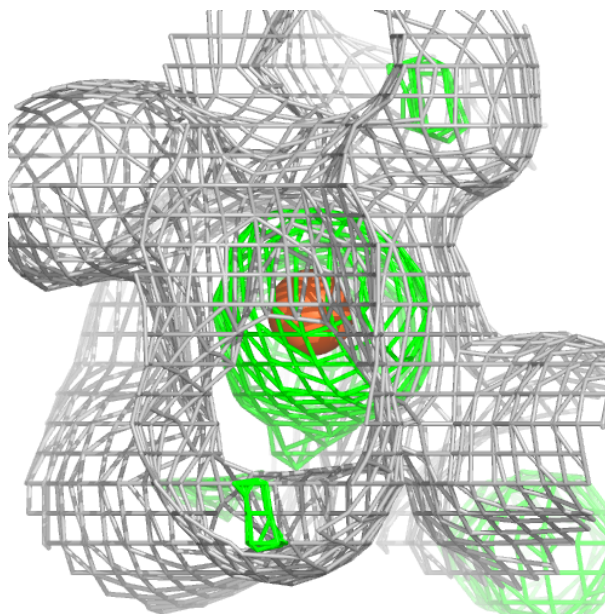
Electron density around FE2 F 201:

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and green (positive)



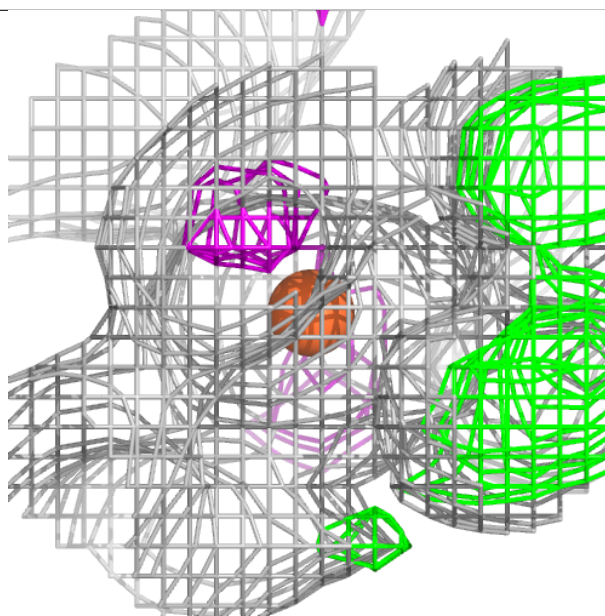
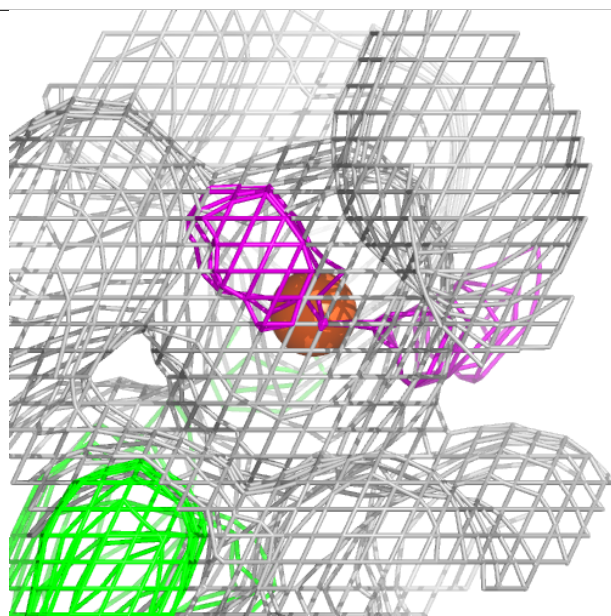
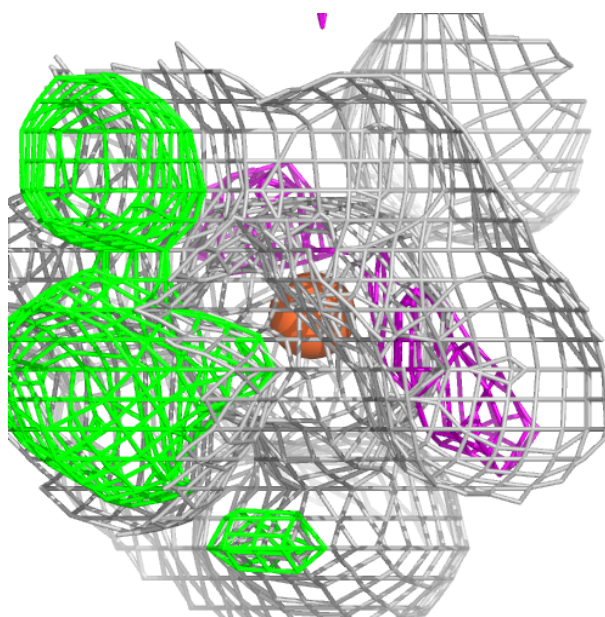
Electron density around FE2 F 202:

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and green (positive)



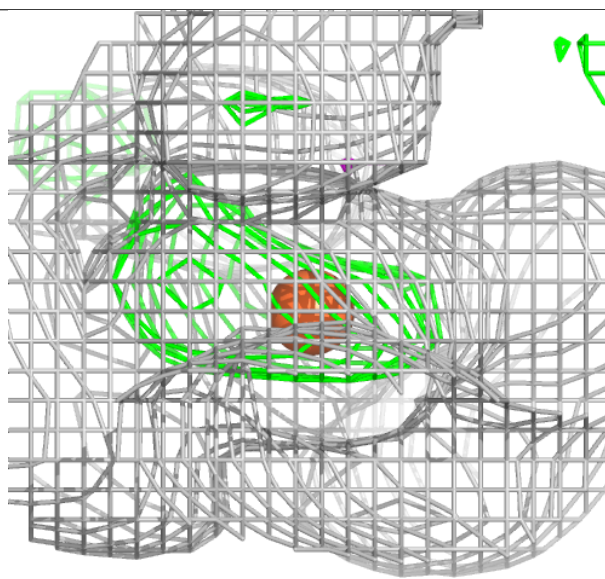
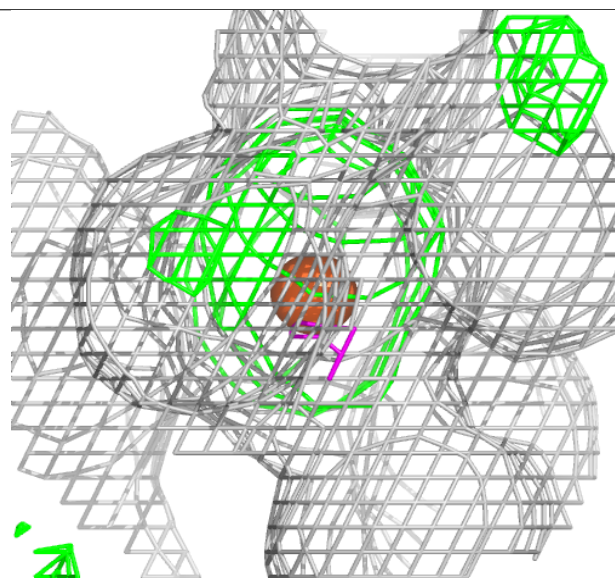
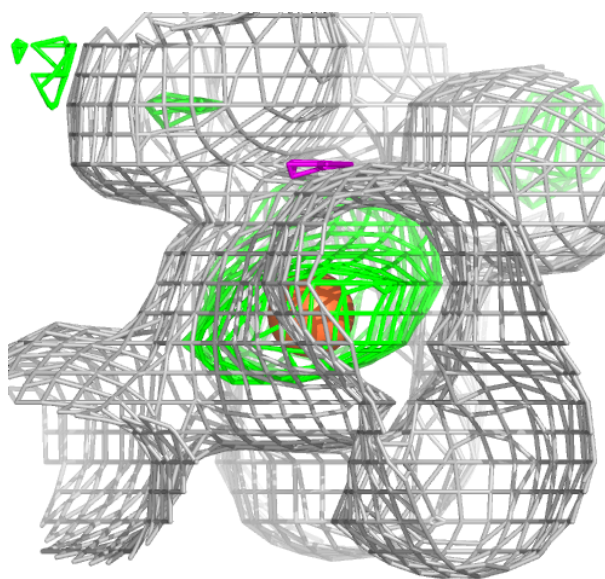
Electron density around FE2 A 201:

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and green (positive)



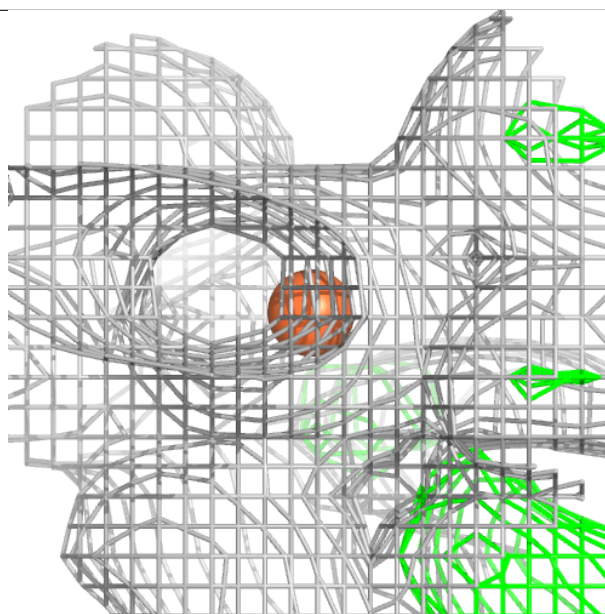
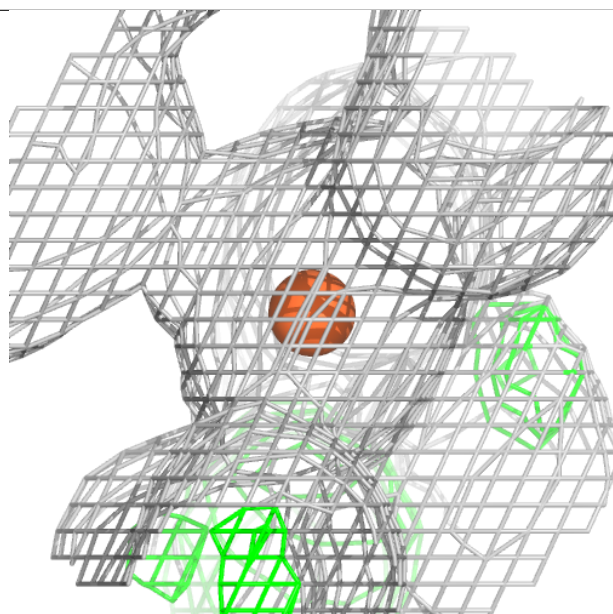
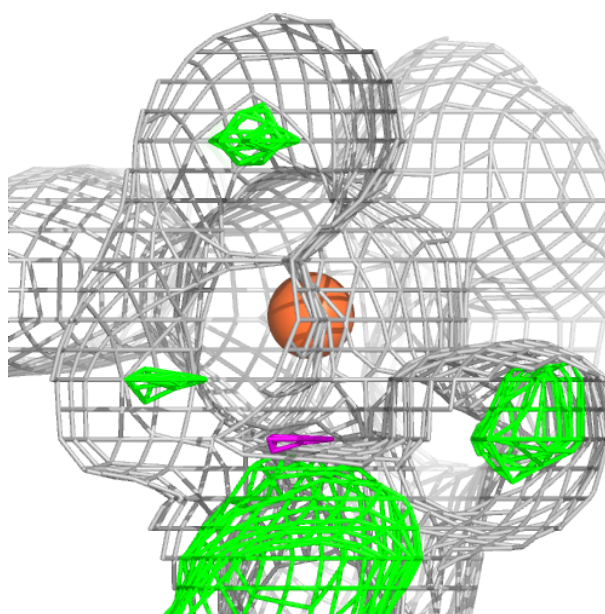
Electron density around FE2 A 202:

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and green (positive)



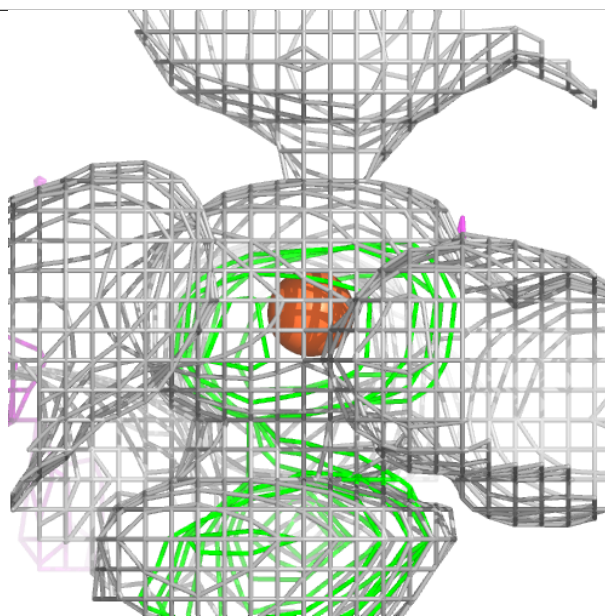
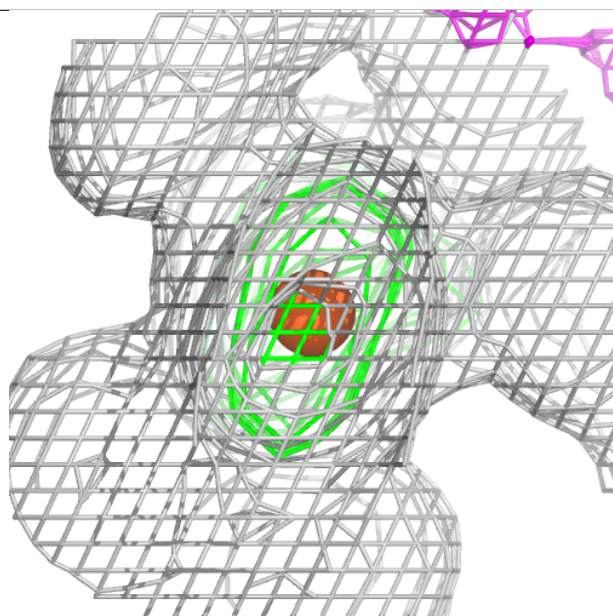
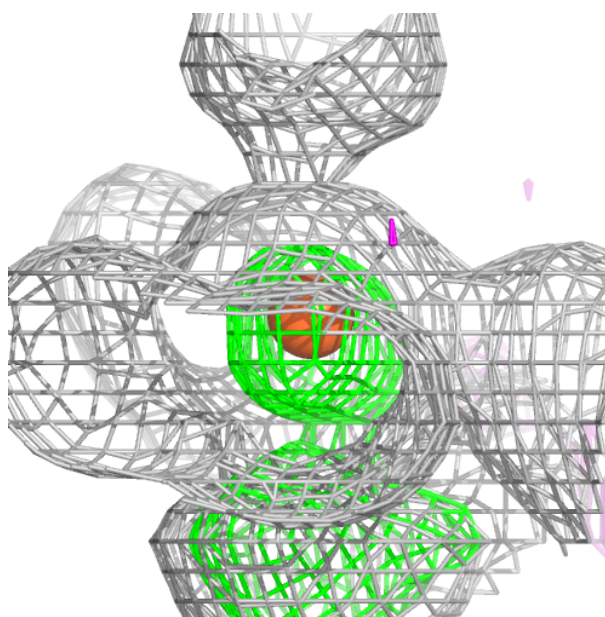
Electron density around FE2 B 201:

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



Electron density around FE2 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.