



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 PM UTC

PDB ID : 8SM9 / pdb_00008sm9
Title : Air-oxidized C. fi TruffO expressed from M9 minimal medium supplemented with Fe
Authors : Liu, C.; Rittle, J.
Deposited on : 2023-04-25
Resolution : 2.30 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

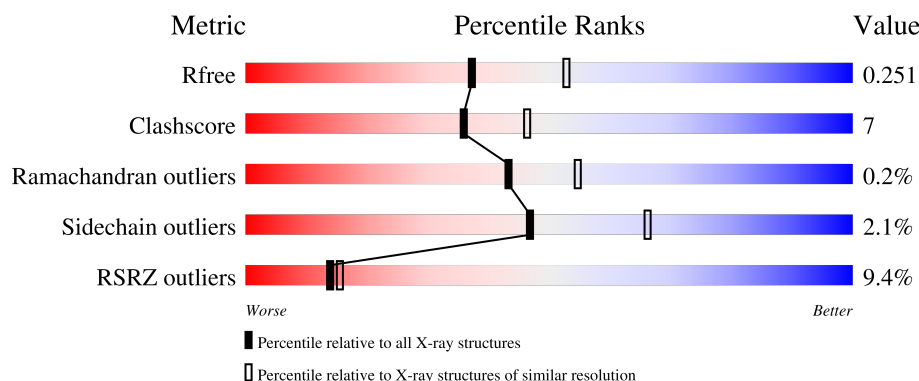
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	B	361	4% 78% 17% • 5%
1	D	361	11% 77% 18% 5%
1	F	361	5% 76% 18% • 5%
1	H	361	15% 77% 17% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11527 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 Amidohydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	344	Total	C	N	O	S	0	0	0
			2816	1816	479	507	14			
1	B	344	Total	C	N	O	S	0	0	0
			2816	1817	480	505	14			
1	D	344	Total	C	N	O	S	0	0	0
			2816	1817	480	505	14			
1	H	344	Total	C	N	O	S	0	0	0
			2820	1819	480	507	14			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	H	2	Total	Fe	0	0
			2	2		

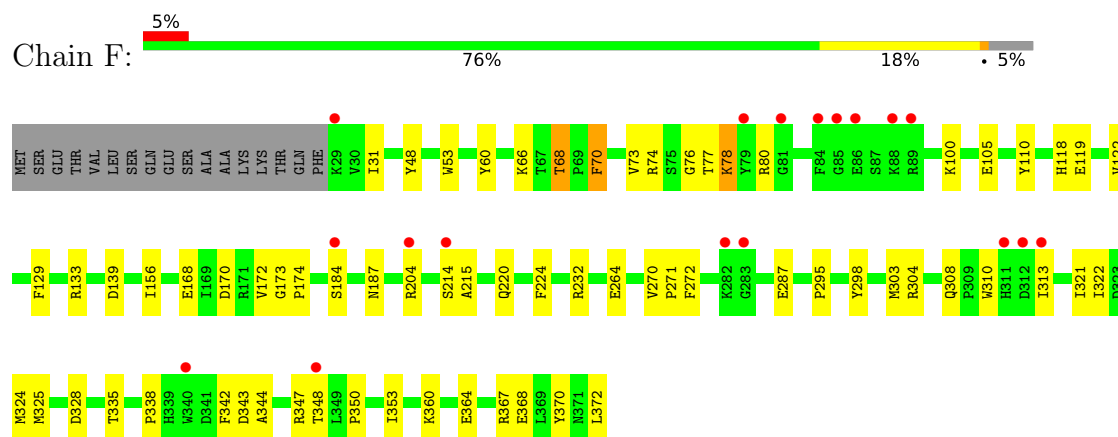
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	77	Total	O	0	0
			77	77		
3	B	75	Total	O	0	0
			75	75		
3	D	47	Total	O	0	0
			47	47		
3	H	52	Total	O	0	0
			52	52		

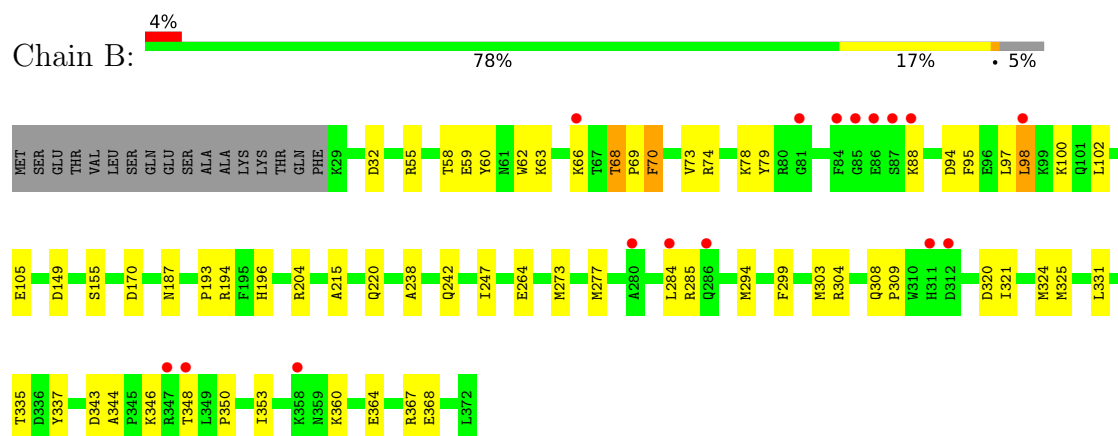
3 Residue-property plots [i](#)

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.

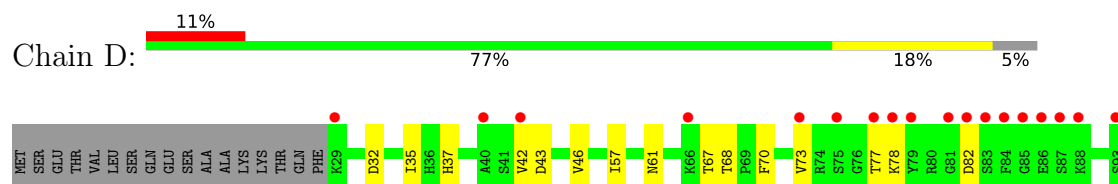
• Molecule 1: Amidohydrolase 2

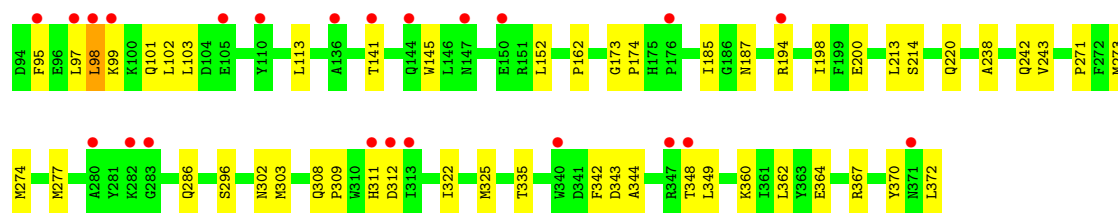


• Molecule 1: Amidohydrolase 2

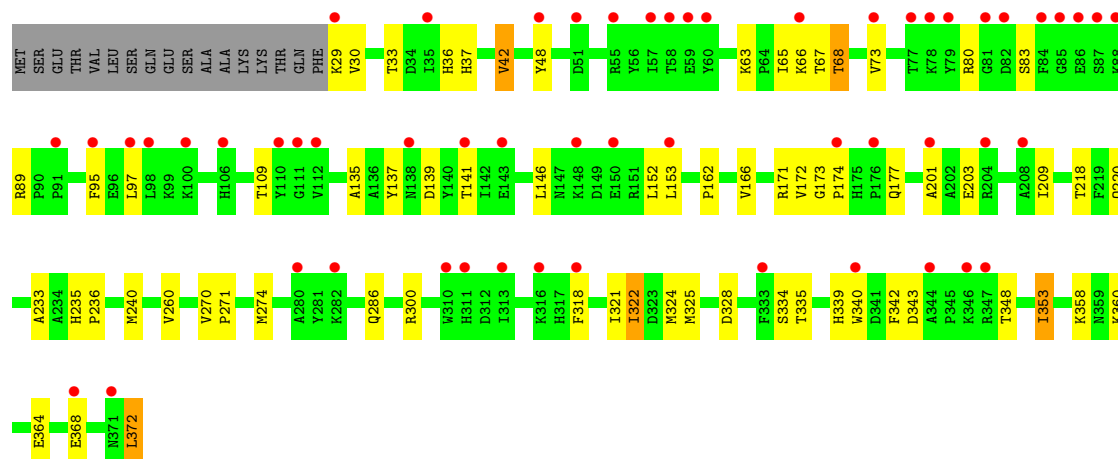
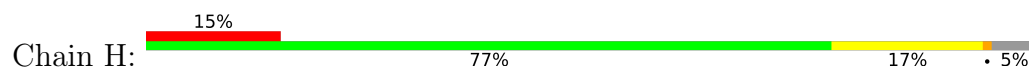


• Molecule 1: Amidohydrolase 2





● Molecule 1: Amidohydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.82Å 67.88Å 138.51Å 90.00° 111.74° 90.00°	Depositor
Resolution (Å)	60.04 – 2.30 60.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (60.04-2.30) 86.0 (60.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.203 , 0.251 0.205 , 0.251	Depositor DCC
R_{free} test set	1992 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11527	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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

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	B	0.43	0/2907	0.62	0/3947
1	D	0.43	0/2907	0.63	1/3947 (0.0%)
1	F	0.52	0/2907	0.70	0/3948
1	H	0.40	0/2911	0.58	0/3952
All	All	0.45	0/11632	0.63	1/15794 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	SER	N-CA-C	-6.99	99.62	109.69

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	B	2816	0	2707	40	0
1	D	2816	0	2707	41	0
1	F	2816	0	2700	47	0
1	H	2820	0	2711	43	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
2	H	2	0	0	0	0
3	B	75	0	0	1	0
3	D	47	0	0	1	0
3	F	77	0	0	1	0
3	H	52	0	0	1	0
All	All	11527	0	10825	161	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 (161) 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:F:343:ASP:HB3	1:F:348:THR:HG21	1.49	0.94
1:F:66:LYS:HD2	1:F:68:THR:HG23	1.59	0.84
1:F:344:ALA:HB3	1:F:347:ARG:HG2	1.62	0.82
1:B:343:ASP:HB3	1:B:348:THR:HG21	1.64	0.78
1:D:77:THR:HG23	1:D:78:LYS:H	1.48	0.77
1:B:285:ARG:HH21	1:B:294:MET:HE2	1.51	0.75
1:F:31:ILE:HG12	1:F:110:TYR:HB2	1.69	0.73
1:D:37:HIS:NE2	1:D:141:THR:HG22	2.04	0.72
1:F:170:ASP:OD1	1:F:204:ARG:NH2	2.23	0.71
1:D:343:ASP:HB3	1:D:348:THR:HG21	1.73	0.71
1:H:166:VAL:HG13	1:H:201:ALA:HB2	1.73	0.70
1:F:321:ILE:HG22	1:F:325:MET:HE3	1.74	0.69
1:B:284:LEU:HD21	1:H:340:TRP:CH2	2.27	0.69
1:F:66:LYS:HD2	1:F:68:THR:CG2	2.21	0.69
1:D:335:THR:HB	1:D:342:PHE:CE1	2.29	0.67
1:D:35:ILE:HD13	1:D:102:LEU:HD21	1.77	0.66
1:H:360:LYS:HA	1:H:364:GLU:HB3	1.79	0.63
1:H:137:TYR:O	1:H:141:THR:HG23	1.98	0.63
1:B:170:ASP:OD1	1:B:204:ARG:NH2	2.34	0.61
1:B:285:ARG:NH2	1:B:294:MET:HE2	2.16	0.60
1:H:353:ILE:HD11	1:H:358:LYS:HG3	1.84	0.60
1:B:98:LEU:HD23	1:B:337:TYR:CE2	2.37	0.60
1:F:344:ALA:O	1:F:348:THR:HG23	2.00	0.59
1:H:270:VAL:O	1:H:274:MET:HG3	2.02	0.59
1:D:243:VAL:HB	1:D:303:MET:HE1	1.85	0.59
1:H:343:ASP:HB3	1:H:348:THR:HG21	1.83	0.59
1:B:321:ILE:HA	1:B:324:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:PRO:O	1:H:166:VAL:HG23	2.04	0.58
1:F:68:THR:CG2	1:F:215:ALA:HB1	2.34	0.57
1:B:344:ALA:O	1:B:348:THR:HG23	2.05	0.57
1:B:100:LYS:O	1:B:105:GLU:HB2	2.05	0.57
1:F:73:VAL:HG23	1:B:60:TYR:CE2	2.41	0.56
1:B:303:MET:O	1:B:304:ARG:HD3	2.06	0.55
1:H:171:ARG:HG2	1:H:172:VAL:HG13	1.88	0.55
1:D:113:LEU:HD11	1:D:152:LEU:HD13	1.88	0.55
1:F:220:GLN:HB3	1:D:187:ASN:HA	1.89	0.55
1:H:335:THR:HB	1:H:342:PHE:CE1	2.42	0.55
1:H:300:ARG:HD2	3:H:506:HOH:O	2.07	0.55
1:D:311:HIS:HD2	3:D:543:HOH:O	1.89	0.54
1:H:328:ASP:OD2	1:H:360:LYS:NZ	2.30	0.54
1:H:153:LEU:HD11	1:H:372:LEU:HD11	1.89	0.54
1:B:98:LEU:HD22	1:B:102:LEU:HB3	1.90	0.53
1:F:303:MET:O	1:F:304:ARG:HD3	2.08	0.53
1:B:308:GLN:HG2	1:B:309:PRO:HA	1.91	0.52
1:D:367:ARG:NH1	1:D:372:LEU:O	2.42	0.52
1:F:287:GLU:HB2	1:D:73:VAL:HG11	1.92	0.52
1:H:364:GLU:O	1:H:368:GLU:HG3	2.09	0.52
1:B:350:PRO:O	1:B:353:ILE:HG13	2.10	0.51
1:D:42:VAL:HG22	1:D:57:ILE:HD13	1.93	0.51
1:D:360:LYS:HA	1:D:364:GLU:HB3	1.92	0.51
1:H:66:LYS:HE3	1:H:68:THR:HB	1.91	0.51
1:F:335:THR:HB	1:F:342:PHE:CE1	2.46	0.51
1:B:325:MET:HE1	1:B:331:LEU:HD11	1.92	0.51
1:B:220:GLN:HG3	1:H:218:THR:O	2.10	0.51
1:F:100:LYS:O	1:F:105:GLU:HB2	2.12	0.50
1:D:43:ASP:HA	1:D:46:VAL:HG23	1.93	0.50
1:F:66:LYS:CD	1:F:68:THR:HG23	2.37	0.50
1:B:193:PRO:HA	1:B:196:HIS:CD2	2.47	0.50
1:B:284:LEU:HD21	1:H:340:TRP:HH2	1.75	0.49
1:B:364:GLU:HG3	1:B:368:GLU:OE1	2.12	0.49
1:D:82:ASP:O	1:D:101:GLN:NE2	2.32	0.49
1:F:232:ARG:NH1	3:F:502:HOH:O	2.45	0.49
1:B:94:ASP:OD2	1:B:97:LEU:HD23	2.13	0.49
1:D:286:GLN:H	1:D:286:GLN:CD	2.21	0.49
1:D:98:LEU:HG	1:D:145:TRP:HZ3	1.78	0.48
1:D:103:LEU:HD11	1:D:152:LEU:HD21	1.95	0.48
1:F:187:ASN:HA	1:D:220:GLN:HB3	1.95	0.48
1:D:273:MET:O	1:D:277:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:THR:HG22	1:F:215:ALA:HB1	1.95	0.48
1:B:273:MET:HE1	1:H:233:ALA:O	2.14	0.48
1:H:42:VAL:HG21	1:H:63:LYS:HD3	1.96	0.47
1:B:32:ASP:OD2	1:B:335:THR:OG1	2.27	0.47
1:F:70:PHE:CZ	1:F:224:PHE:HB3	2.50	0.47
1:B:367:ARG:NH2	1:B:368:GLU:HG3	2.29	0.47
1:D:344:ALA:O	1:D:348:THR:HG23	2.15	0.47
1:F:321:ILE:HA	1:F:324:MET:HE3	1.97	0.47
1:D:271:PRO:HD3	1:D:325:MET:HE2	1.96	0.47
1:H:48:TYR:CD1	1:H:139:ASP:HB3	2.50	0.47
1:F:119:GLU:OE1	1:F:133:ARG:NH2	2.45	0.46
1:B:74:ARG:NH2	1:B:79:TYR:O	2.47	0.46
1:D:35:ILE:HB	1:D:113:LEU:HD23	1.97	0.46
1:B:320:ASP:O	1:B:324:MET:HG3	2.16	0.46
1:H:209:ILE:HB	1:H:260:VAL:HG22	1.97	0.46
1:B:187:ASN:HA	1:H:220:GLN:HB3	1.97	0.46
1:F:367:ARG:NH2	1:F:368:GLU:HG3	2.30	0.46
1:B:360:LYS:HA	1:B:364:GLU:HB3	1.98	0.46
1:H:33:THR:OG1	1:H:334:SER:HB3	2.16	0.46
1:F:68:THR:HG21	1:F:215:ALA:HB1	1.98	0.46
1:H:37:HIS:NE2	1:H:141:THR:HG22	2.31	0.46
1:B:88:LYS:HD2	1:B:88:LYS:N	2.30	0.45
1:D:185:ILE:HB	1:D:213:LEU:HA	1.97	0.45
1:H:286:GLN:H	1:H:286:GLN:CD	2.23	0.45
1:B:62:TRP:O	1:B:63:LYS:HD3	2.17	0.45
1:F:364:GLU:HG3	1:F:368:GLU:OE2	2.16	0.45
1:D:349:LEU:HD12	1:D:349:LEU:H	1.81	0.45
1:H:89:ARG:HD3	1:H:89:ARG:H	1.81	0.45
1:D:95:PHE:CZ	1:D:99:LYS:HD3	2.51	0.45
1:D:302:ASN:C	1:D:303:MET:HG2	2.41	0.45
1:F:122:VAL:HG11	1:F:214:SER:OG	2.16	0.45
1:D:67:THR:HG22	1:H:67:THR:HG22	1.97	0.45
1:H:146:LEU:HD13	1:H:177:GLN:HB2	1.99	0.45
1:H:235:HIS:CD2	1:H:236:PRO:HD3	2.52	0.45
1:B:68:THR:OG1	1:B:215:ALA:HB1	2.17	0.45
1:F:80:ARG:HG3	1:F:338:PRO:O	2.17	0.44
1:F:310:TRP:CZ2	1:F:350:PRO:HD3	2.52	0.44
1:H:321:ILE:O	1:H:325:MET:HG3	2.17	0.44
1:F:78:LYS:H	1:F:78:LYS:HG3	1.37	0.44
1:F:270:VAL:N	1:F:271:PRO:HD2	2.33	0.44
1:F:370:TYR:HB2	1:F:372:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ARG:O	1:H:83:SER:OG	2.34	0.44
1:F:156:ILE:HG12	1:F:172:VAL:HG23	1.99	0.44
1:B:95:PHE:HZ	1:B:149:ASP:HB2	1.82	0.44
1:F:328:ASP:OD2	1:F:360:LYS:NZ	2.46	0.44
1:D:173:GLY:N	1:D:174:PRO:HD2	2.32	0.44
1:D:277:MET:HE2	1:D:277:MET:HB3	1.75	0.44
1:D:308:GLN:HG2	1:D:309:PRO:HA	2.00	0.43
1:B:69:PRO:HG2	1:B:70:PHE:CE2	2.54	0.43
1:B:78:LYS:HE2	1:B:79:TYR:CZ	2.53	0.43
1:B:346:LYS:HB2	3:B:533:HOH:O	2.19	0.43
1:D:162:PRO:HA	1:D:198:ILE:HD11	2.01	0.43
1:F:310:TRP:CZ2	1:F:313:ILE:HG22	2.54	0.43
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.76	0.43
1:H:173:GLY:N	1:H:174:PRO:HD2	2.34	0.43
1:H:95:PHE:CD1	1:H:95:PHE:C	2.96	0.43
1:H:89:ARG:HD3	1:H:89:ARG:N	2.33	0.43
1:D:32:ASP:OD2	1:D:335:THR:OG1	2.32	0.42
1:F:76:GLY:C	1:F:77:THR:HG1	2.26	0.42
1:B:299:PHE:HA	1:B:303:MET:HB2	2.01	0.42
1:F:168:GLU:O	1:F:172:VAL:HG22	2.20	0.42
1:H:340:TRP:CD1	1:H:340:TRP:H	2.37	0.42
1:H:135:ALA:HB1	1:H:171:ARG:NH2	2.35	0.42
1:B:55:ARG:HG2	1:B:59:GLU:CD	2.43	0.42
1:B:247:ILE:HB	1:B:277:MET:HE1	2.02	0.42
1:F:118:HIS:HB3	1:F:184:SER:OG	2.20	0.42
1:H:271:PRO:HB3	1:H:324:MET:HB3	2.02	0.42
1:D:61:ASN:CG	1:D:61:ASN:O	2.63	0.42
1:F:173:GLY:N	1:F:174:PRO:HD2	2.35	0.41
1:D:97:LEU:HD12	1:D:97:LEU:HA	1.86	0.41
1:F:321:ILE:O	1:F:325:MET:HG3	2.19	0.41
1:F:264:GLU:HG3	1:F:308:GLN:OE1	2.20	0.41
1:D:77:THR:HG23	1:D:78:LYS:N	2.25	0.41
1:D:335:THR:O	1:D:342:PHE:HA	2.20	0.41
1:F:360:LYS:HA	1:F:364:GLU:HB3	2.03	0.41
1:F:350:PRO:O	1:F:353:ILE:HG12	2.21	0.41
1:F:295:PRO:HA	1:F:298:TYR:HD2	1.86	0.41
1:B:238:ALA:O	1:B:242:GLN:HG2	2.19	0.41
1:B:58:THR:HG22	1:B:59:GLU:HG3	2.03	0.41
1:B:73:VAL:O	1:B:73:VAL:HG23	2.21	0.41
1:D:274:MET:HE3	1:D:296:SER:HB2	2.02	0.41
1:H:36:HIS:CD2	1:H:339:HIS:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:LEU:HD12	1:H:97:LEU:HA	1.90	0.41
1:H:236:PRO:O	1:H:240:MET:HG3	2.21	0.41
1:F:48:TYR:CD1	1:F:139:ASP:HB3	2.56	0.40
1:F:53:TRP:CZ3	1:F:129:PHE:HB2	2.55	0.40
1:F:74:ARG:NH1	1:F:77:THR:O	2.53	0.40
1:F:60:TYR:CD1	1:F:60:TYR:N	2.83	0.40
1:D:370:TYR:HB2	1:D:372:LEU:HG	2.03	0.40
1:H:30:VAL:O	1:H:109:THR:HB	2.21	0.40
1:D:238:ALA:O	1:D:242:GLN:HG2	2.21	0.40
1:H:152:LEU:HD23	1:H:152:LEU:HA	1.88	0.40
1:H:318:PHE:O	1:H:322:ILE:HD12	2.21	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	B	342/361 (95%)	323 (94%)	18 (5%)	1 (0%)	36	46
1	D	342/361 (95%)	325 (95%)	16 (5%)	1 (0%)	36	46
1	F	342/361 (95%)	325 (95%)	17 (5%)	0	100	100
1	H	342/361 (95%)	312 (91%)	29 (8%)	1 (0%)	36	46
All	All	1368/1444 (95%)	1285 (94%)	80 (6%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	GLU
1	D	312	ASP
1	H	73	VAL

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	B	295/311 (95%)	289 (98%)	6 (2%)	48	67
1	D	295/311 (95%)	289 (98%)	6 (2%)	48	67
1	F	295/311 (95%)	290 (98%)	5 (2%)	53	72
1	H	296/311 (95%)	288 (97%)	8 (3%)	39	58
All	All	1181/1244 (95%)	1156 (98%)	25 (2%)	47	66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	68	THR
1	F	70	PHE
1	F	78	LYS
1	F	272	PHE
1	F	322	ILE
1	B	66	LYS
1	B	68	THR
1	B	70	PHE
1	B	98	LEU
1	B	155	SER
1	B	194	ARG
1	D	68	THR
1	D	70	PHE
1	D	98	LEU
1	D	194	ARG
1	D	200	GLU
1	D	322	ILE
1	H	29	LYS
1	H	42	VAL
1	H	65	ILE
1	H	68	THR
1	H	203	GLU
1	H	322	ILE
1	H	353	ILE
1	H	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	237	GLN
1	F	257	ASN
1	F	311	HIS
1	B	257	ASN
1	B	311	HIS
1	B	371	ASN
1	D	106	HIS
1	D	257	ASN
1	D	339	HIS
1	H	61	ASN
1	H	147	ASN
1	H	275	ASN
1	H	311	HIS
1	H	339	HIS

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 8 ligands modelled in this entry, 8 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	344/361 (95%)	0.59	16 (4%) 36 38	33, 46, 63, 97	0
1	D	344/361 (95%)	1.09	41 (11%) 9 10	36, 55, 77, 112	0
1	F	344/361 (95%)	0.59	18 (5%) 33 34	33, 45, 63, 94	0
1	H	344/361 (95%)	1.21	55 (15%) 5 5	38, 57, 79, 105	0
All	All	1376/1444 (95%)	0.87	130 (9%) 14 15	33, 49, 74, 112	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	GLY	5.1
1	D	86	GLU	5.0
1	F	311	HIS	4.8
1	H	282	LYS	4.8
1	B	311	HIS	4.7
1	D	312	ASP	4.4
1	D	84	PHE	4.4
1	H	81	GLY	4.3
1	D	99	LYS	4.2
1	D	85	GLY	4.1
1	H	311	HIS	3.9
1	D	87	SER	3.9
1	D	88	LYS	3.8
1	D	77	THR	3.7
1	H	84	PHE	3.7
1	D	66	LYS	3.5
1	D	282	LYS	3.4
1	D	150	GLU	3.4
1	B	86	GLU	3.4
1	F	84	PHE	3.4
1	D	311	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	79	TYR	3.2
1	B	85	GLY	3.2
1	F	282	LYS	3.2
1	H	88	LYS	3.2
1	F	184	SER	3.2
1	D	75	SER	3.1
1	H	340	TRP	3.1
1	D	95	PHE	3.0
1	H	95	PHE	3.0
1	H	79	TYR	3.0
1	H	110	TYR	3.0
1	H	87	SER	3.0
1	H	150	GLU	3.0
1	H	176	PRO	2.9
1	F	88	LYS	2.9
1	D	82	ASP	2.9
1	D	105	GLU	2.9
1	D	98	LEU	2.8
1	H	98	LEU	2.8
1	F	89	ARG	2.8
1	H	85	GLY	2.8
1	B	88	LYS	2.8
1	H	112	VAL	2.8
1	H	347	ARG	2.8
1	H	316	LYS	2.8
1	H	82	ASP	2.7
1	D	347	ARG	2.7
1	D	29	LYS	2.7
1	B	81	GLY	2.7
1	H	148	LYS	2.7
1	F	348	THR	2.7
1	B	358	LYS	2.7
1	H	344	ALA	2.6
1	D	42	VAL	2.6
1	F	340	TRP	2.6
1	H	310	TRP	2.6
1	F	29	LYS	2.6
1	H	29	LYS	2.6
1	H	346	LYS	2.6
1	B	348	THR	2.6
1	D	73	VAL	2.6
1	H	313	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	368	GLU	2.5
1	B	312	ASP	2.5
1	F	283	GLY	2.5
1	H	66	LYS	2.5
1	H	204	ARG	2.5
1	H	100	LYS	2.4
1	H	86	GLU	2.4
1	D	83	SER	2.4
1	H	35	ILE	2.4
1	B	98	LEU	2.4
1	D	176	PRO	2.4
1	H	141	THR	2.4
1	F	79	TYR	2.4
1	B	66	LYS	2.4
1	D	348	THR	2.4
1	H	78	LYS	2.4
1	H	106	HIS	2.4
1	D	371	ASN	2.3
1	D	78	LYS	2.3
1	D	141	THR	2.3
1	H	97	LEU	2.3
1	H	208	ALA	2.3
1	H	55	ARG	2.3
1	F	85	GLY	2.3
1	F	81	GLY	2.3
1	D	136	ALA	2.3
1	D	340	TRP	2.3
1	H	59	GLU	2.3
1	D	313	ILE	2.3
1	H	333	PHE	2.2
1	H	51	ASP	2.2
1	H	138	ASN	2.2
1	D	283	GLY	2.2
1	B	280	ALA	2.2
1	H	111	GLY	2.2
1	F	86	GLU	2.2
1	D	110	TYR	2.2
1	F	313	ILE	2.2
1	B	284	LEU	2.2
1	H	153	LEU	2.2
1	H	371	ASN	2.2
1	D	97	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	214	SER	2.2
1	D	93	SER	2.2
1	F	312	ASP	2.1
1	H	73	VAL	2.1
1	B	84	PHE	2.1
1	D	194	ARG	2.1
1	D	40	ALA	2.1
1	H	60	TYR	2.1
1	F	204	ARG	2.1
1	B	347	ARG	2.1
1	D	280	ALA	2.1
1	H	201	ALA	2.1
1	H	174	PRO	2.1
1	H	58	THR	2.0
1	H	143	GLU	2.0
1	H	280	ALA	2.0
1	H	57	ILE	2.0
1	H	91	PRO	2.0
1	H	48	TYR	2.0
1	H	318	PHE	2.0
1	B	87	SER	2.0
1	H	77	THR	2.0
1	B	286	GLN	2.0
1	D	144	GLN	2.0
1	D	147	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

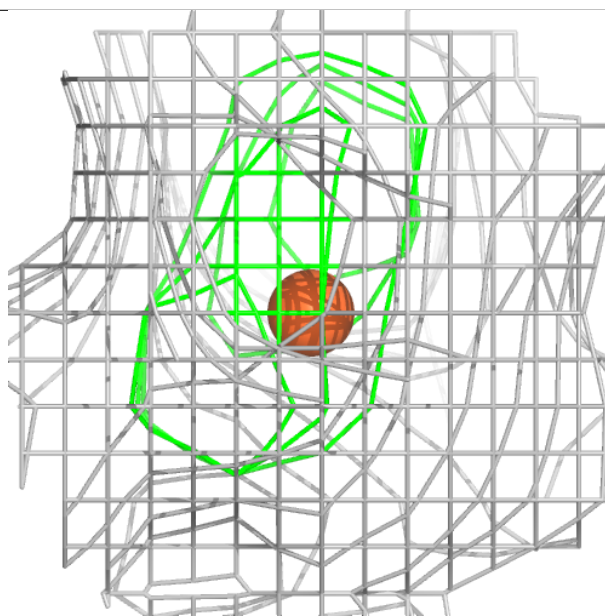
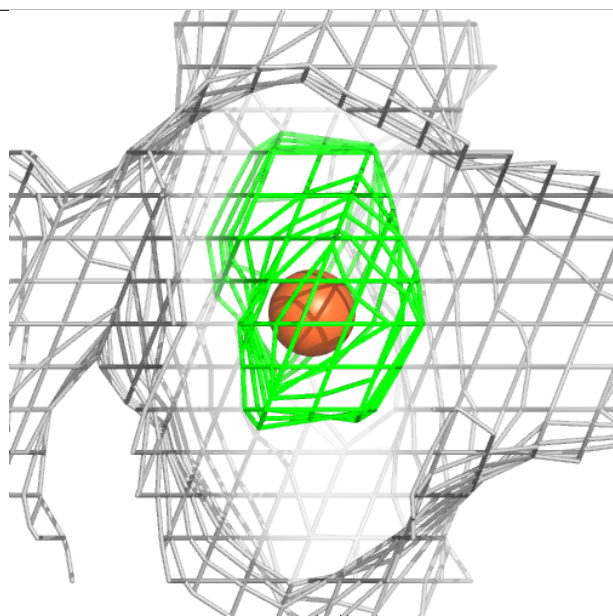
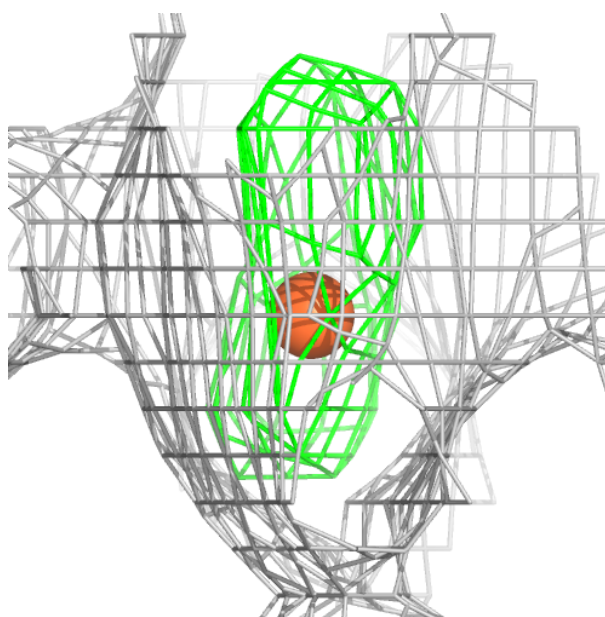
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FE	D	402	1/1	0.94	0.19	63,63,63,63	1
2	FE	B	402	1/1	0.96	0.20	63,63,63,63	1
2	FE	F	402	1/1	0.96	0.17	46,46,46,46	1
2	FE	B	401	1/1	0.97	0.18	44,44,44,44	1
2	FE	H	401	1/1	0.97	0.08	72,72,72,72	0
2	FE	H	402	1/1	0.97	0.15	58,58,58,58	1
2	FE	D	401	1/1	0.98	0.09	63,63,63,63	0
2	FE	F	401	1/1	0.99	0.12	59,59,59,59	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.

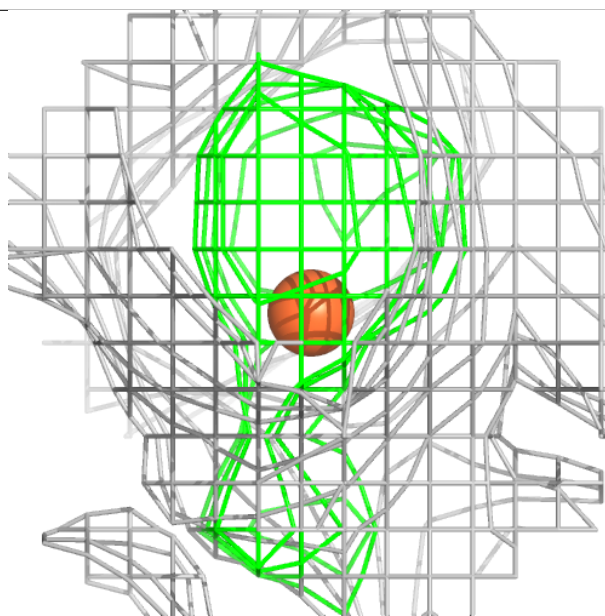
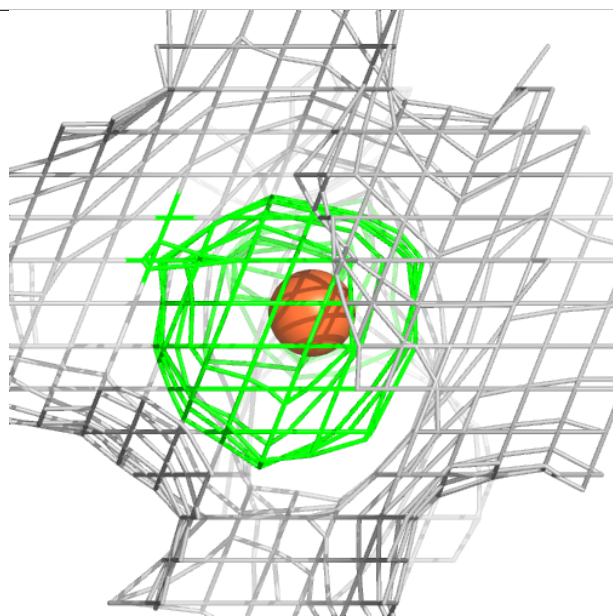
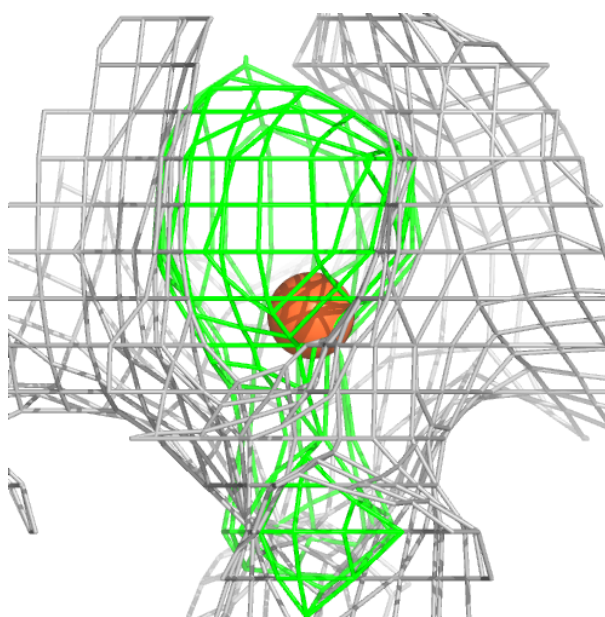
Electron density around FE D 402:

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



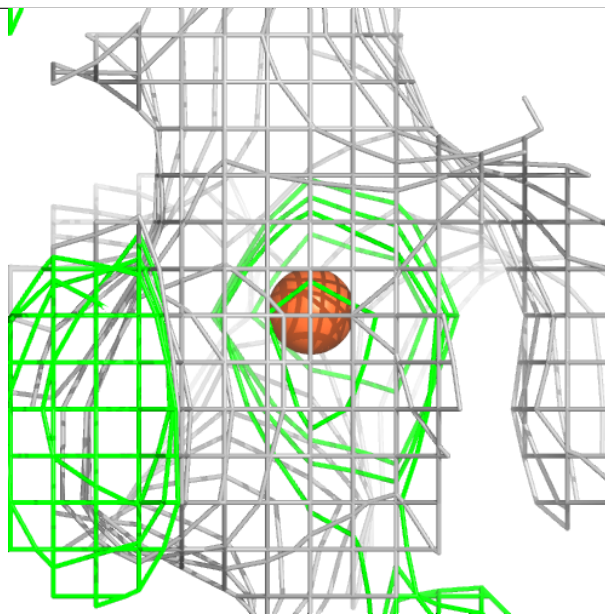
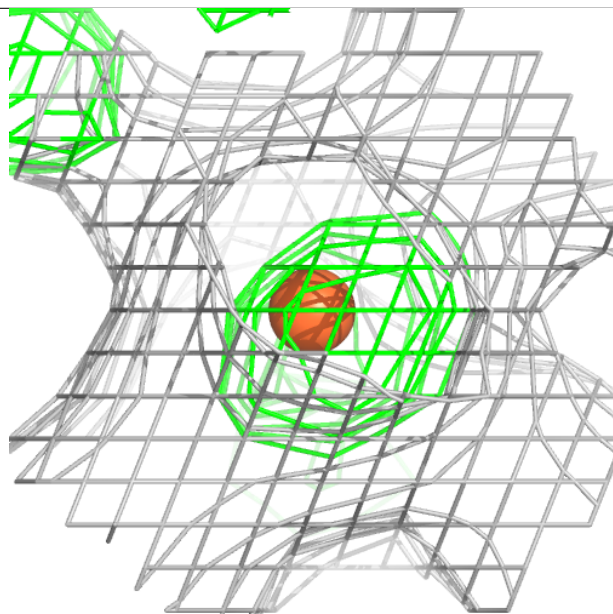
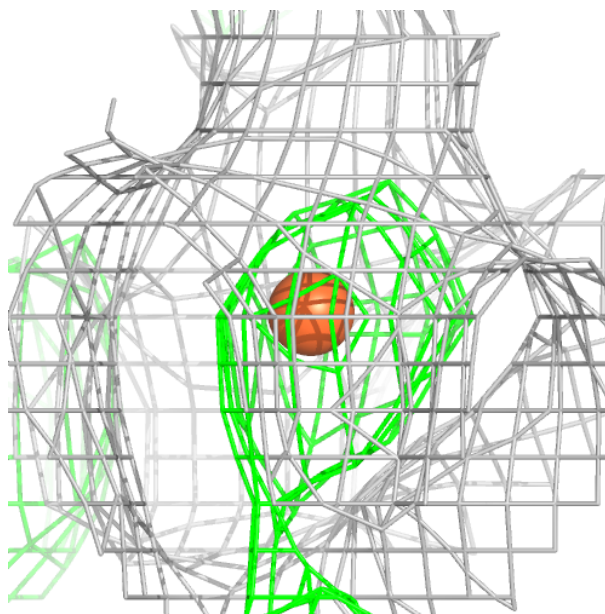
Electron density around FE B 402:

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and green (positive)



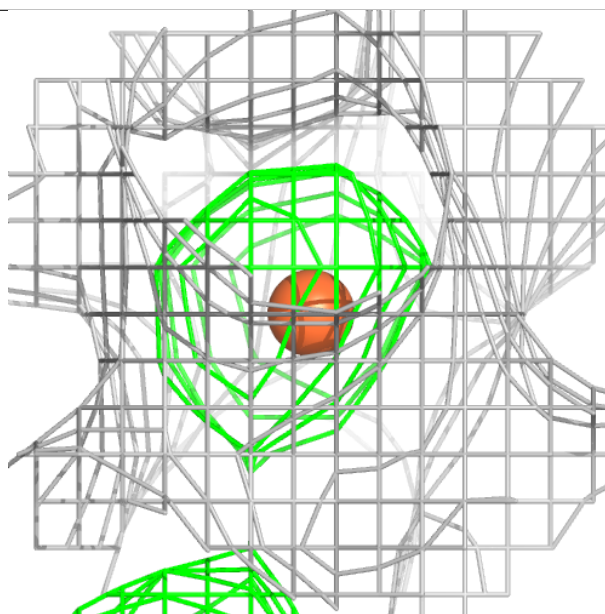
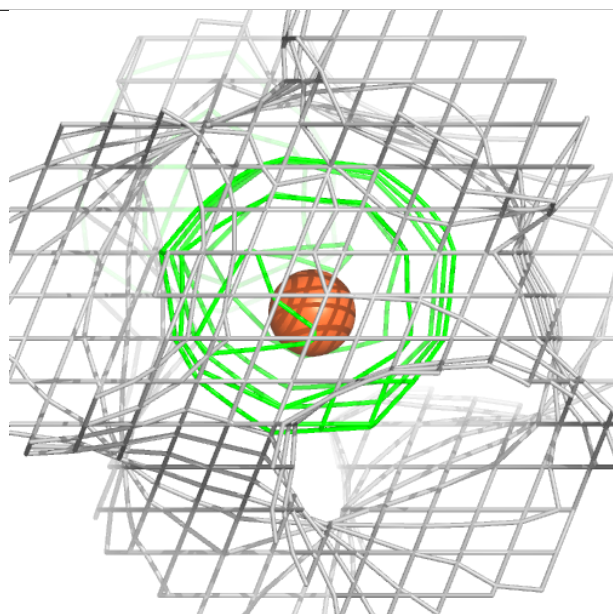
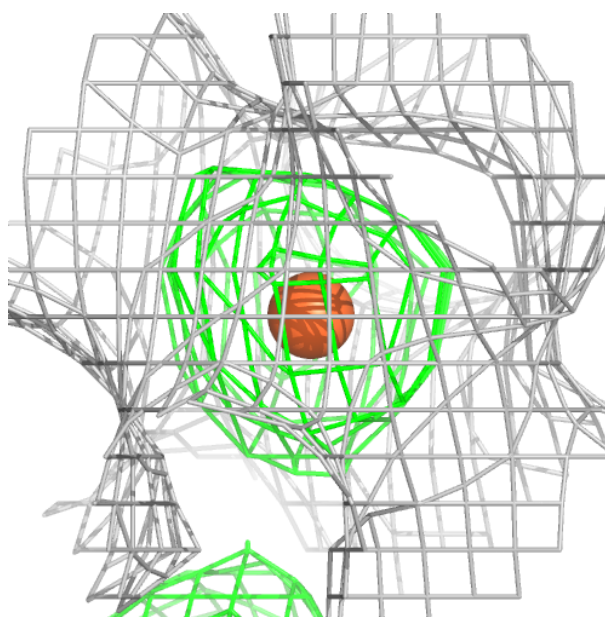
Electron density around FE F 402:

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and green (positive)



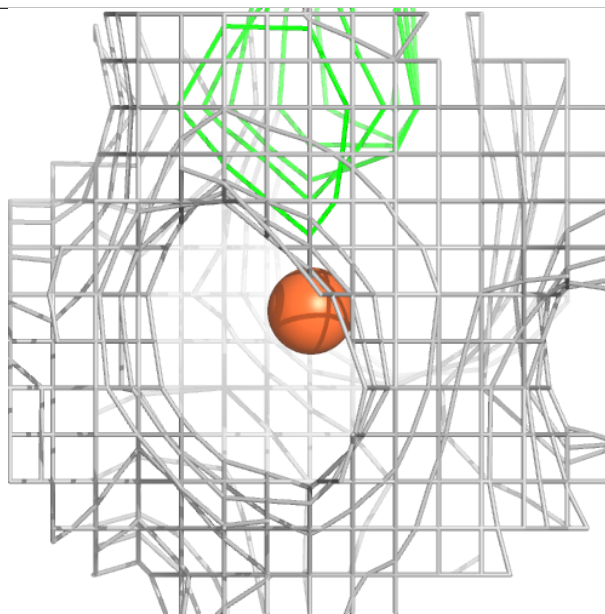
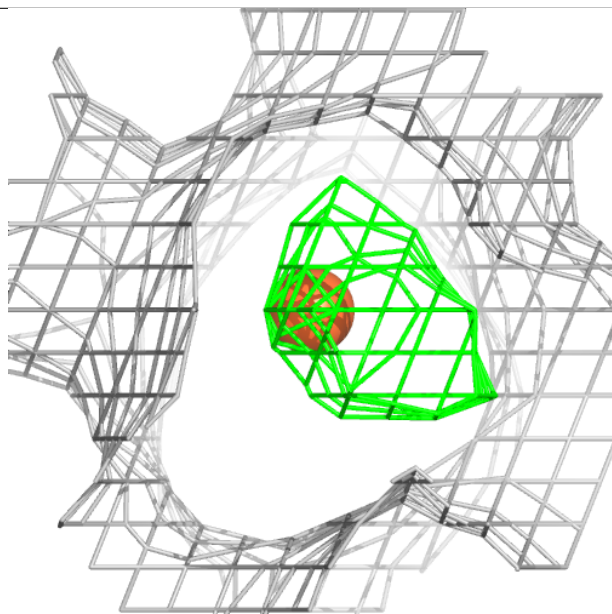
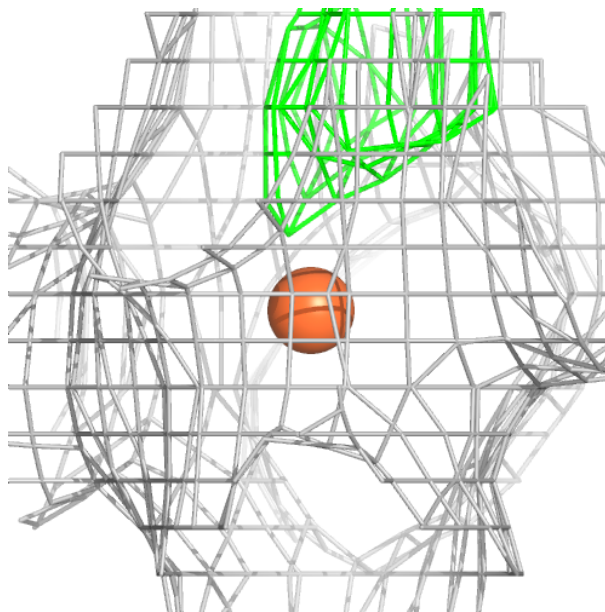
Electron density around FE B 401:

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



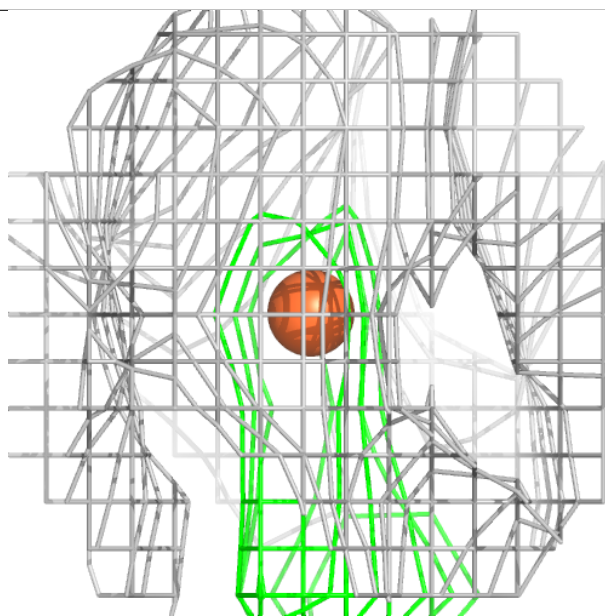
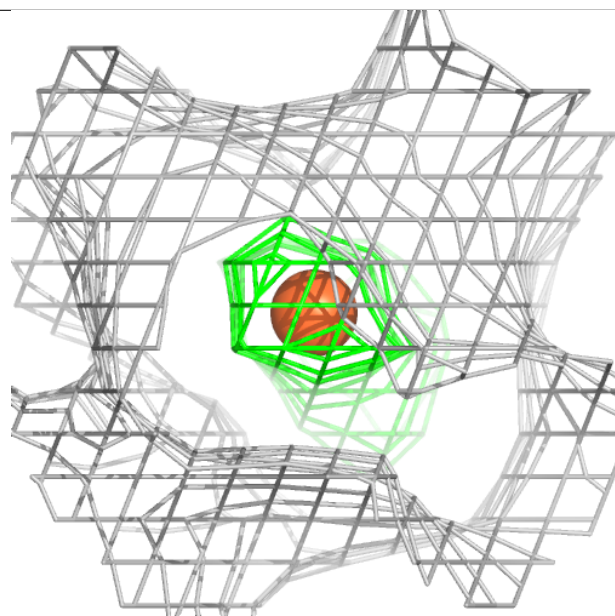
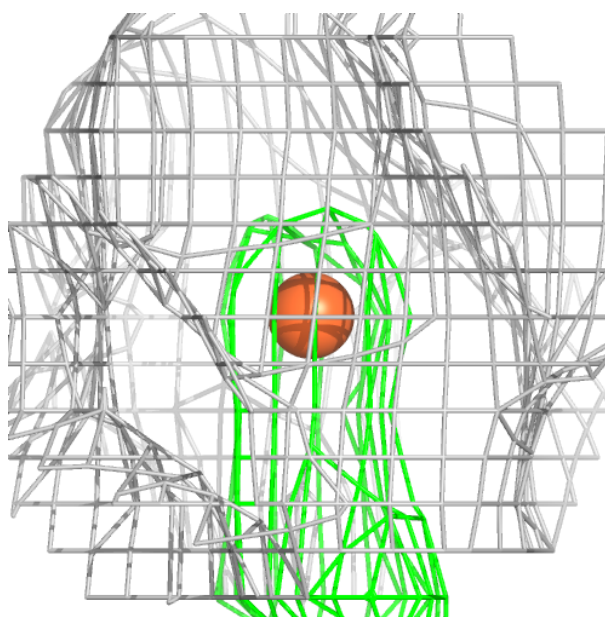
Electron density around FE H 401:

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



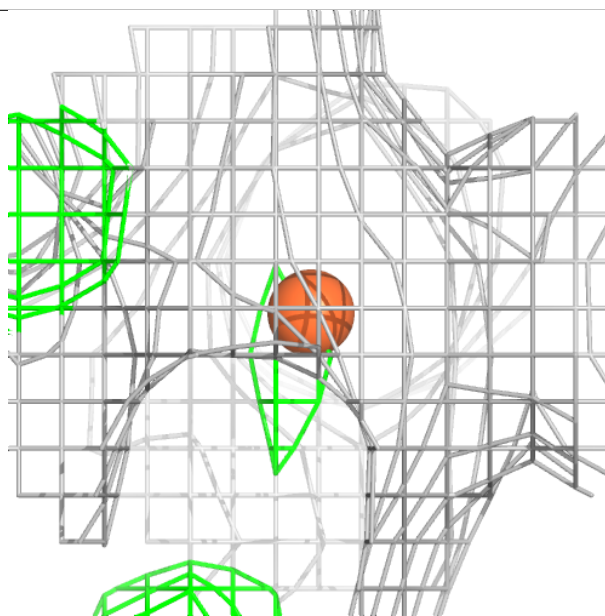
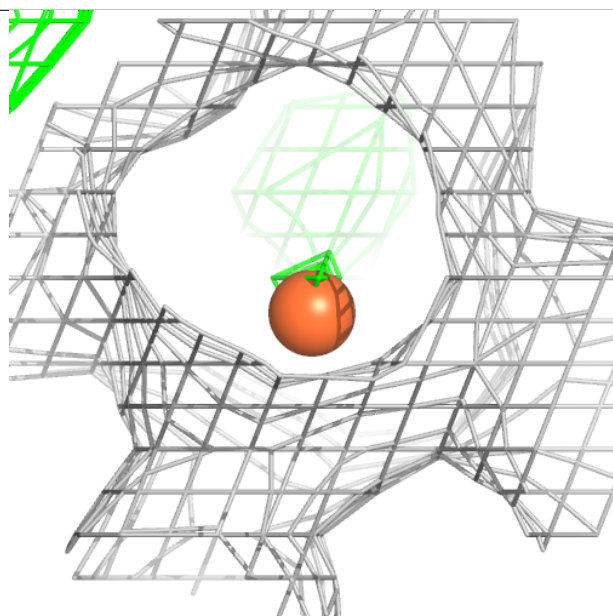
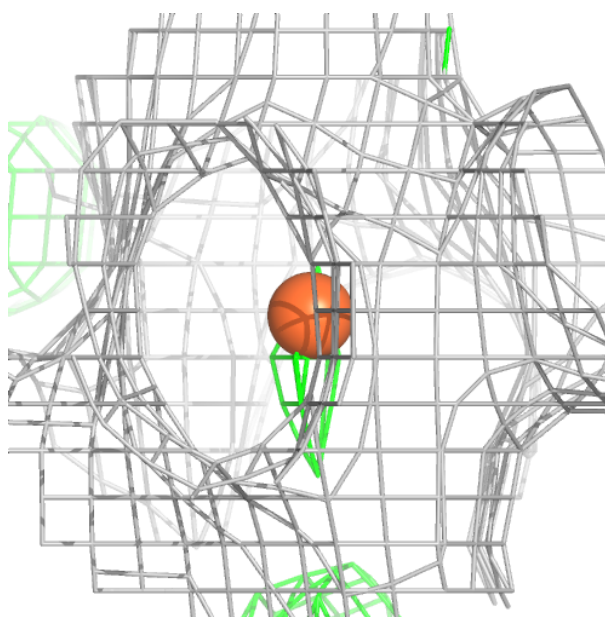
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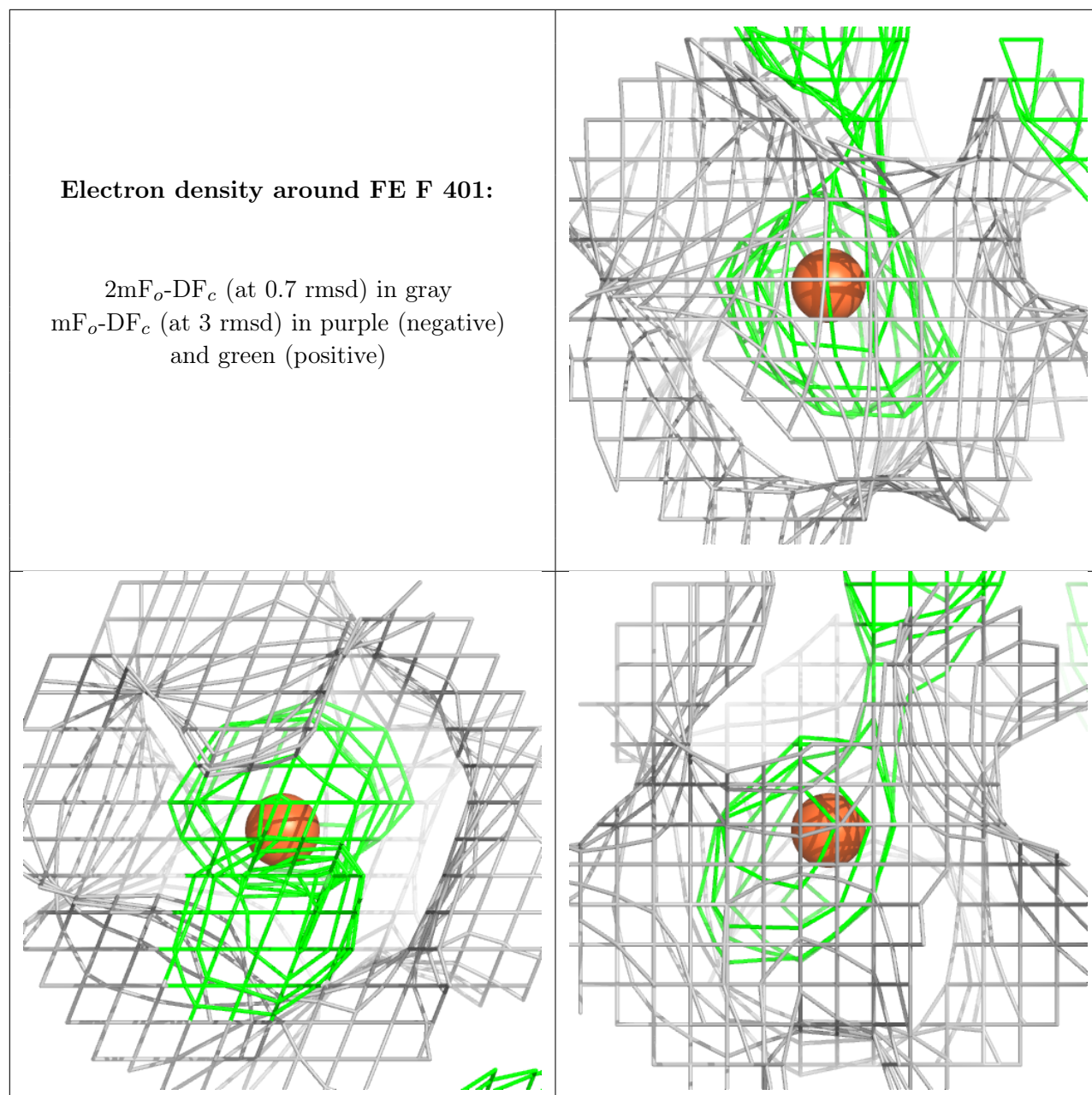
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE D 401:

$2mF_o-DF_c$ (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.