



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 AM UTC

PDB ID : 8B7O / pdb_00008b7o
Title : X-ray structure of Auranofin-human H-chain ferritin
Authors : Ferraro, G.; Merlino, A.
Deposited on : 2022-09-30
Resolution : 1.17 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

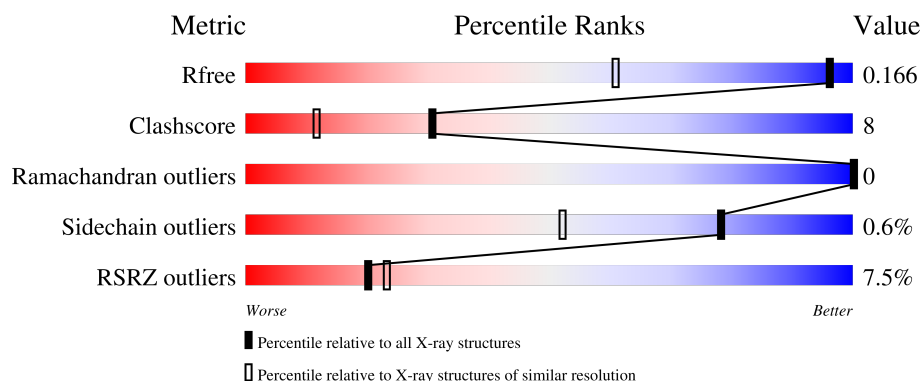
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.17 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	1789 (1.20-1.16)
Clashscore	190562	1845 (1.20-1.16)
Ramachandran outliers	187476	1789 (1.20-1.16)
Sidechain outliers	187428	1789 (1.20-1.16)
RSRZ outliers	180081	1787 (1.20-1.16)

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	AAA	183	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2063 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 heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	174	Total	C	N	O	S	0	26	0
			1631	1022	286	315	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	183	GLY	-	expression tag	UNP P02794

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	6	Total	Cl	0	0
			6	6		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	8	Total	Mg	0	2
			10	10		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Fe	0	0
			1	1		

- Molecule 5 is GOLD ION (CCD ID: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	5	Total 8	Au 8	0	3

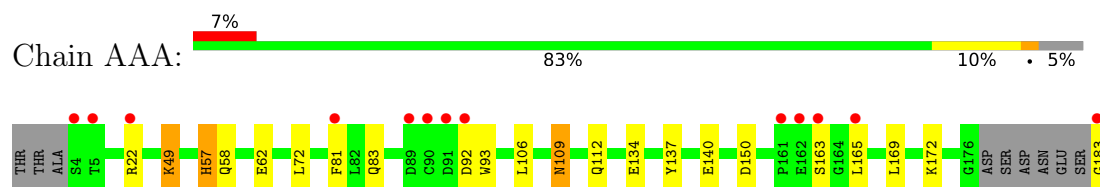
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	394	Total 407	O 407	0	20

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 heavy chain, N-terminally processed



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.03Å 184.03Å 184.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 1.17 46.05 – 1.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.05-1.17) 100.0 (46.05-1.17)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.17Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.149 , 0.167 0.149 , 0.166	Depositor DCC
R_{free} test set	4432 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2063	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, AU, 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	AAA	1.17	4/1676 (0.2%)	1.15	5/2246 (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	AAA	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	163	SER	C-O	6.49	1.32	1.23
1	AAA	134[A]	GLU	C-O	5.32	1.30	1.24
1	AAA	134[B]	GLU	C-O	5.32	1.30	1.24
1	AAA	57	HIS	CE1-NE2	-5.17	1.27	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	183[C]	GLY	CA-C-O	-7.45	105.16	120.80
1	AAA	109[A]	ASN	O-C-N	-6.95	114.86	122.09
1	AAA	109[B]	ASN	O-C-N	-6.95	114.86	122.09
1	AAA	93	TRP	N-CA-CB	-6.11	101.59	110.45
1	AAA	150	ASP	CA-CB-CG	5.33	117.93	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	TYR	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	AAA	1631	0	1571	24	0
2	AAA	6	0	0	0	0
3	AAA	10	0	0	0	0
4	AAA	1	0	0	0	0
5	AAA	8	0	0	0	0
6	AAA	407	0	0	13	1
All	All	2063	0	1571	24	1

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 8.

All (24) 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:AAA:81[B]:PHE:CE2	1:AAA:83:GLN:OE1	1.89	1.25
1:AAA:140[A]:GLU:CD	6:AAA:301[A]:HOH:O	2.12	0.91
1:AAA:140[A]:GLU:OE2	6:AAA:301[A]:HOH:O	1.93	0.83
1:AAA:81[B]:PHE:HE2	1:AAA:83:GLN:OE1	1.57	0.82
1:AAA:165[B]:LEU:HD23	1:AAA:165[B]:LEU:C	2.07	0.79
1:AAA:58:GLN:NE2	6:AAA:302:HOH:O	2.15	0.74
1:AAA:22[A]:ARG:HD2	6:AAA:411:HOH:O	1.94	0.66
1:AAA:49[B]:LYS:HG2	6:AAA:367:HOH:O	1.99	0.63
1:AAA:49[B]:LYS:NZ	1:AAA:49[B]:LYS:HB3	2.14	0.61
1:AAA:81[B]:PHE:CD2	1:AAA:83:GLN:OE1	2.56	0.55
1:AAA:49[B]:LYS:CG	6:AAA:367:HOH:O	2.55	0.54
1:AAA:92:ASP:O	6:AAA:304:HOH:O	2.18	0.54
1:AAA:62[B]:GLU:OE2	6:AAA:303:HOH:O	2.16	0.53
1:AAA:172[B]:LYS:HE2	6:AAA:391:HOH:O	2.07	0.53
1:AAA:49[B]:LYS:HB3	1:AAA:49[B]:LYS:HZ1	1.73	0.53
1:AAA:172[C]:LYS:HD2	6:AAA:345:HOH:O	2.09	0.52
1:AAA:57:HIS:CE1	6:AAA:322:HOH:O	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:106:LEU:O	1:AAA:109[B]:ASN:HB3	2.13	0.48
1:AAA:165[B]:LEU:C	1:AAA:165[B]:LEU:CD2	2.81	0.48
1:AAA:112[A]:GLN:NE2	6:AAA:316:HOH:O	2.48	0.47
1:AAA:165[B]:LEU:HD21	1:AAA:169:LEU:HD12	1.96	0.47
1:AAA:49[B]:LYS:HG2	6:AAA:484:HOH:O	2.15	0.46
1:AAA:72:LEU:HD13	1:AAA:72:LEU:C	2.43	0.43
1:AAA:165[B]:LEU:HD21	1:AAA:169:LEU:CD1	2.52	0.41

All (1) 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)
6:AAA:580:HOH:O	6:AAA:624:HOH:O[54_554]	1.89	0.31

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	AAA	196/183 (107%)	192 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	AAA	179/162 (110%)	177 (99%)	2 (1%)	65 31

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	49[A]	LYS
1	AAA	49[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	AAA	174/183 (95%)	0.22	13 (7%)	20 23	4, 10, 19, 60	26 (14%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	90[A]	CYS	5.7
1	AAA	92	ASP	4.6
1	AAA	91	ASP	4.4
1	AAA	5	THR	4.4
1	AAA	89	ASP	4.2
1	AAA	4	SER	3.8
1	AAA	161	PRO	3.2
1	AAA	165[A]	LEU	2.5
1	AAA	81[A]	PHE	2.5
1	AAA	163	SER	2.2
1	AAA	162	GLU	2.1
1	AAA	183[C]	GLY	2.1
1	AAA	22[A]	ARG	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 ⓘ

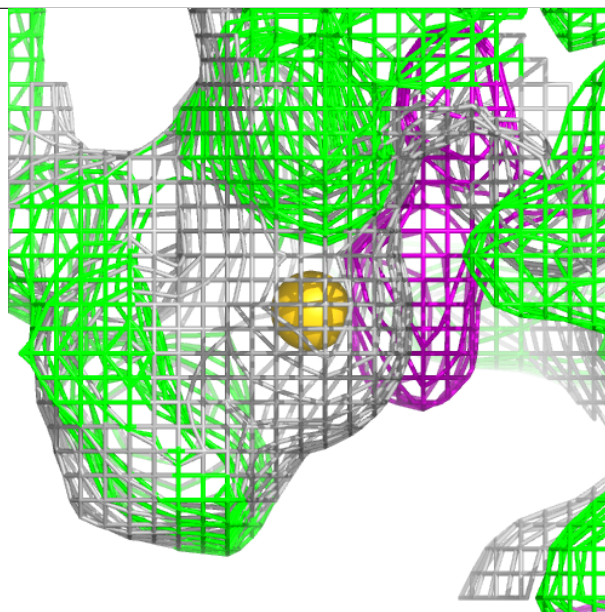
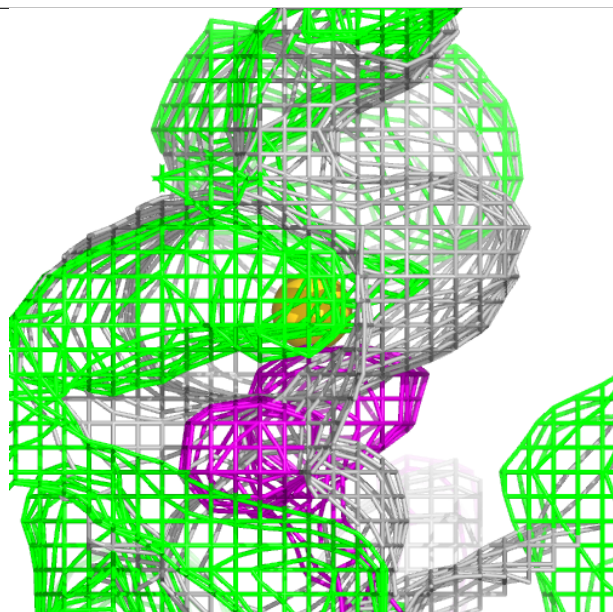
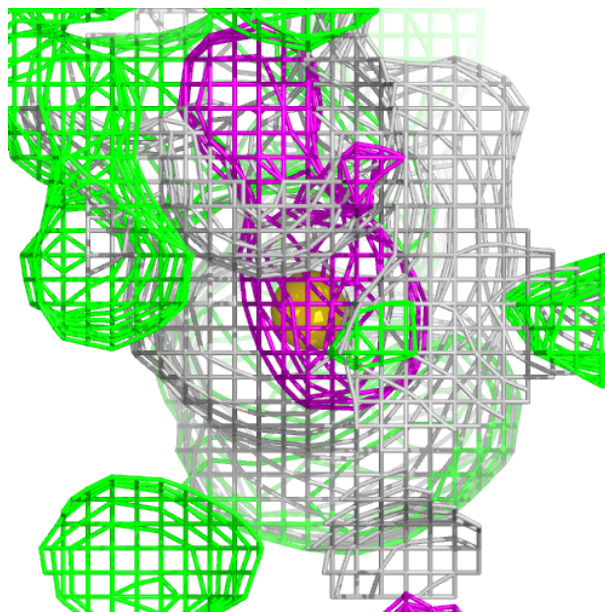
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CL	AAA	214	1/1	0.76	0.30	15,15,15,15	1
3	MG	AAA	212	1/1	0.81	0.12	14,14,14,14	1
5	AU	AAA	219	1/1	0.83	0.14	35,35,35,35	1
5	AU	AAA	218	1/1	0.87	0.12	34,34,34,34	1
5	AU	AAA	220[A]	1/1	0.92	0.08	16,16,16,16	1
5	AU	AAA	220[B]	1/1	0.92	0.08	22,22,22,22	1
5	AU	AAA	220[C]	1/1	0.92	0.08	23,23,23,23	1
3	MG	AAA	210	1/1	0.93	0.16	10,10,10,10	1
5	AU	AAA	216[A]	1/1	0.96	0.07	16,16,16,16	1
3	MG	AAA	209[B]	1/1	0.96	0.17	21,21,21,21	1
3	MG	AAA	206	1/1	0.96	0.07	12,12,12,12	1
3	MG	AAA	211[A]	1/1	0.96	0.05	14,14,14,14	1
3	MG	AAA	211[B]	1/1	0.96	0.05	13,13,13,13	1
3	MG	AAA	209[A]	1/1	0.96	0.17	11,11,11,11	1
2	CL	AAA	203	1/1	0.97	0.08	19,19,19,19	1
2	CL	AAA	202	1/1	0.98	0.04	14,14,14,14	1
5	AU	AAA	217[A]	1/1	0.98	0.04	17,17,17,17	1
5	AU	AAA	217[B]	1/1	0.98	0.04	43,43,43,43	1
3	MG	AAA	208	1/1	0.98	0.10	14,14,14,14	1
3	MG	AAA	207	1/1	0.99	0.05	12,12,12,12	1
2	CL	AAA	213	1/1	0.99	0.04	15,15,15,15	1
2	CL	AAA	201	1/1	0.99	0.05	11,11,11,11	1
2	CL	AAA	204	1/1	0.99	0.09	15,15,15,15	1
3	MG	AAA	205	1/1	1.00	0.03	9,9,9,9	1
4	FE	AAA	215	1/1	1.00	0.02	10,10,10,10	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.

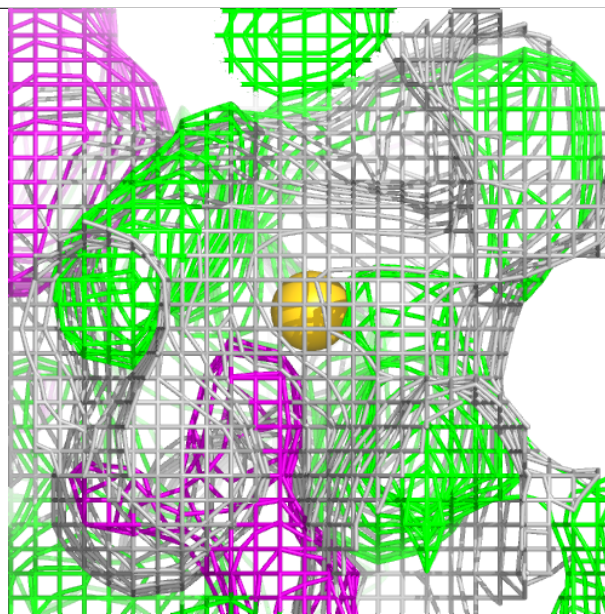
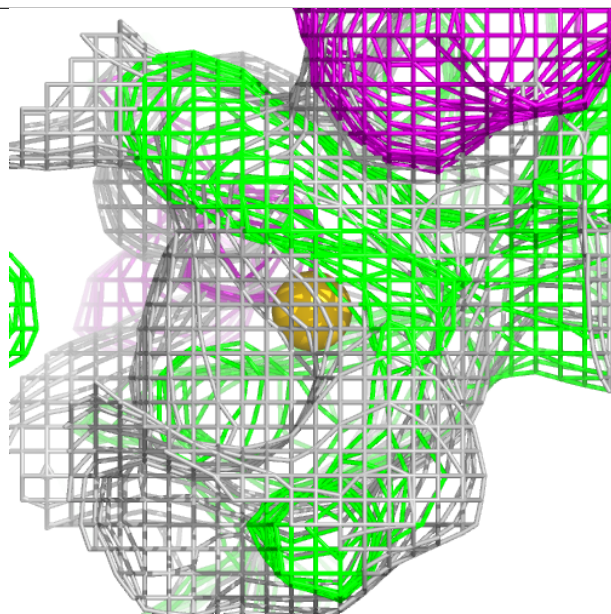
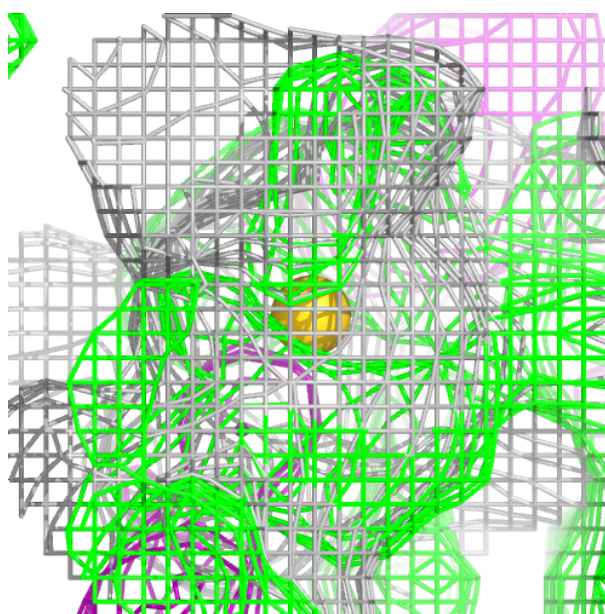
Electron density around AU AAA 219:

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



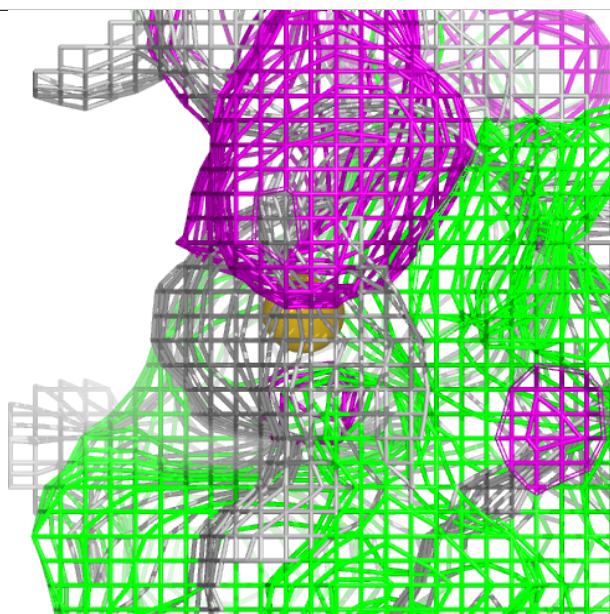
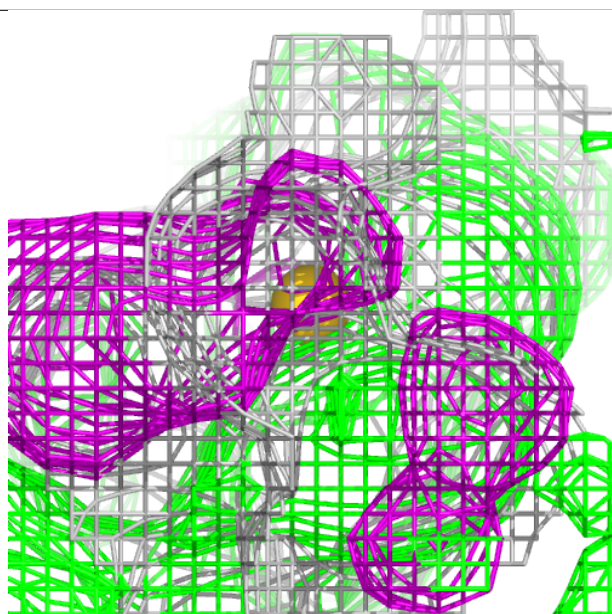
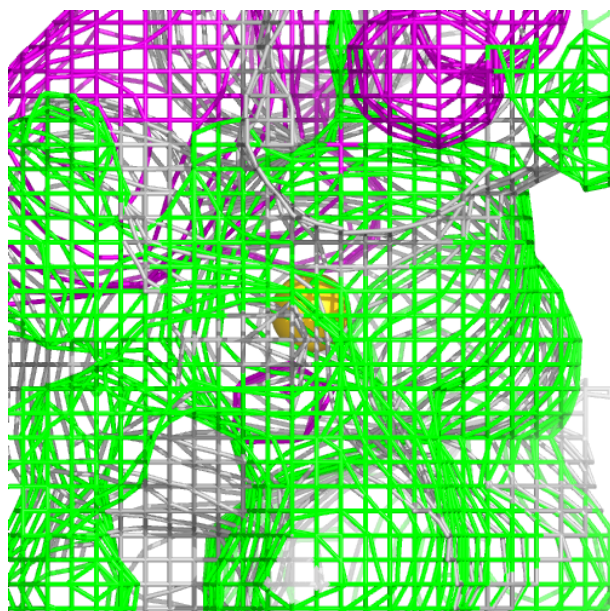
Electron density around AU AAA 218:

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



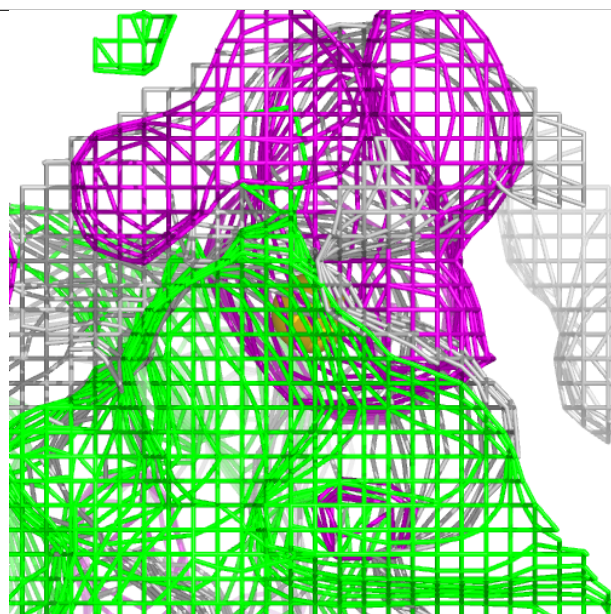
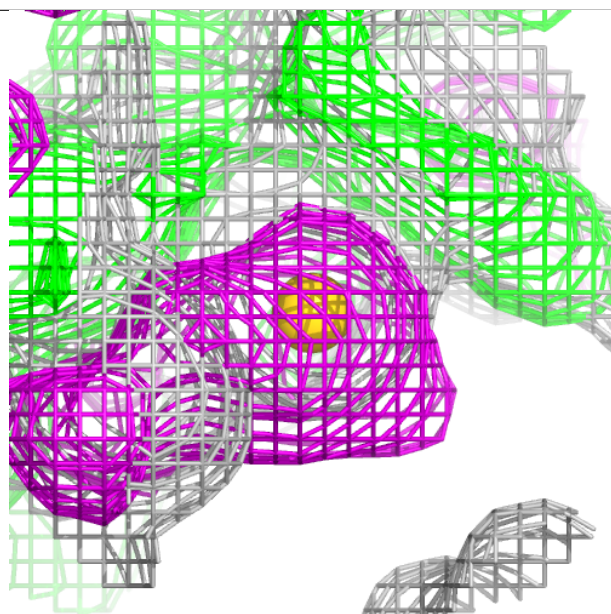
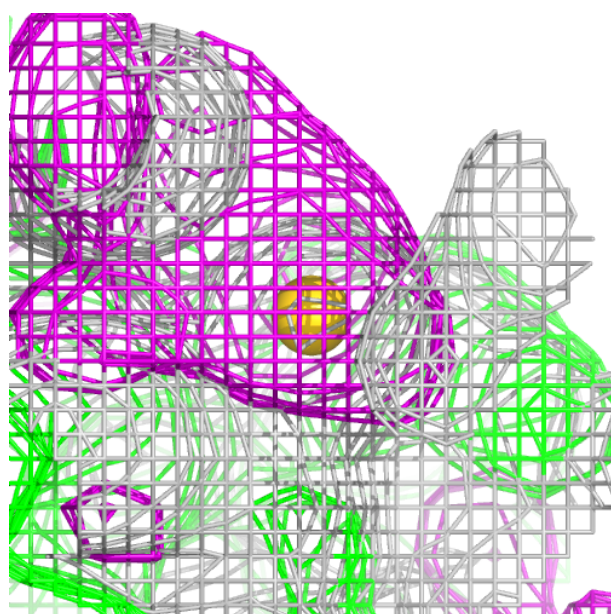
Electron density around AU AAA 220 (A):

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



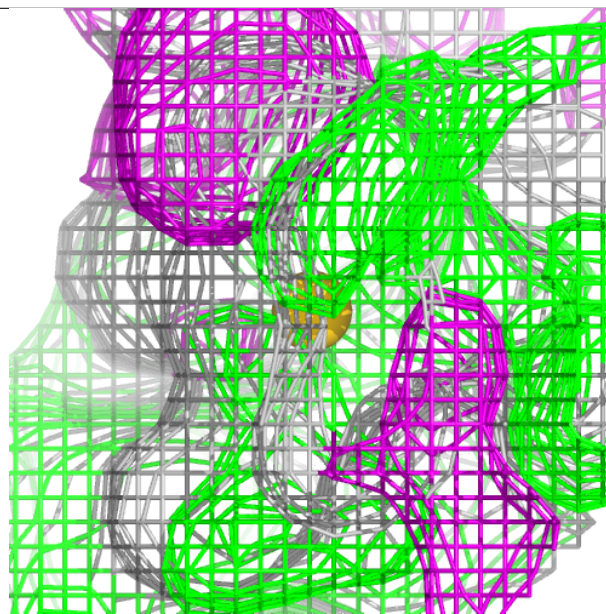
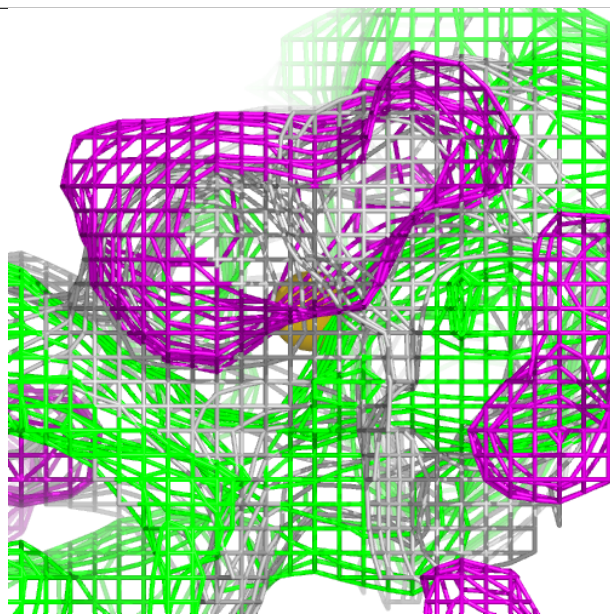
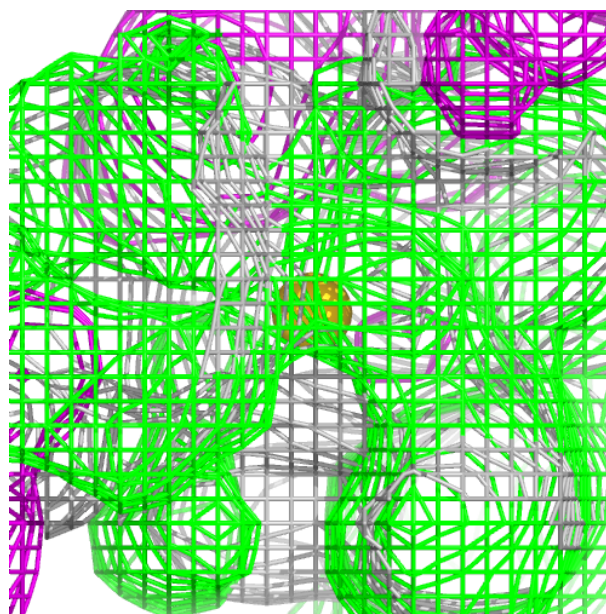
Electron density around AU AAA 220 (B):

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



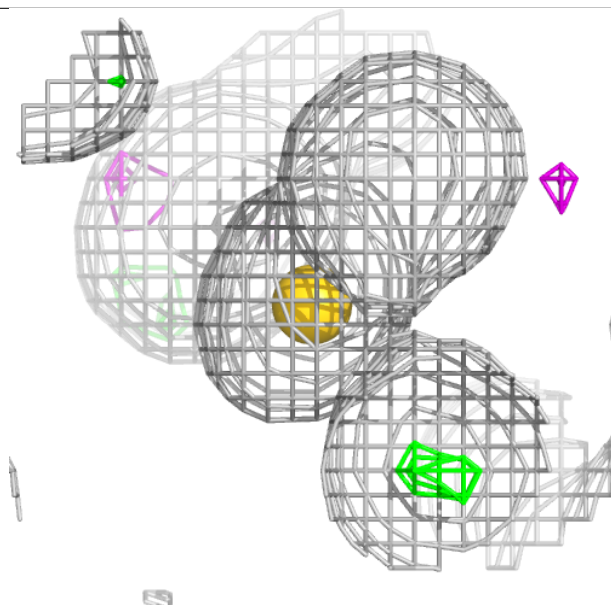
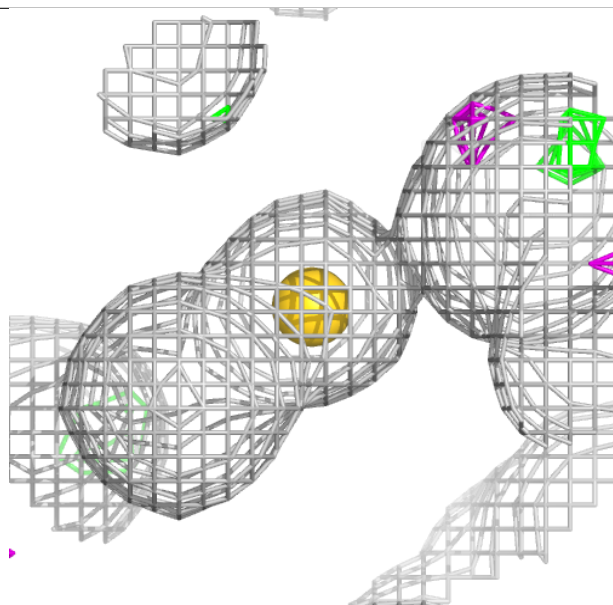
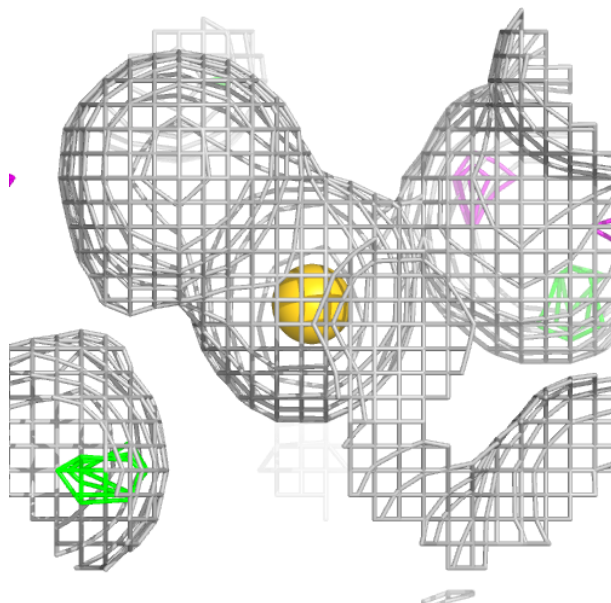
Electron density around AU AAA 220 (C):

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



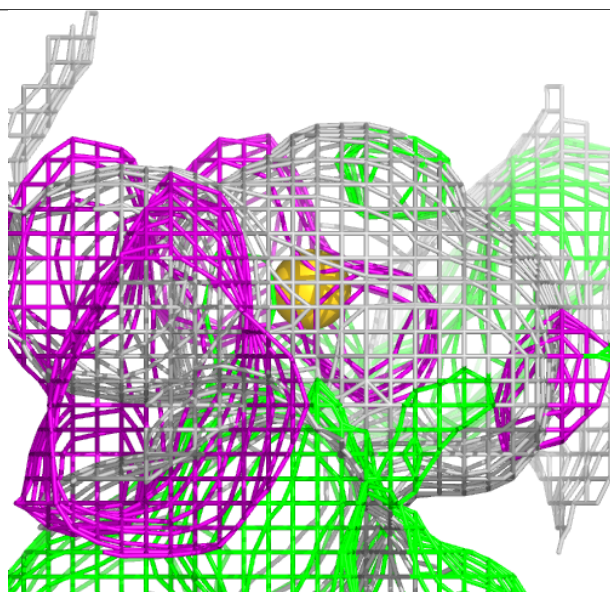
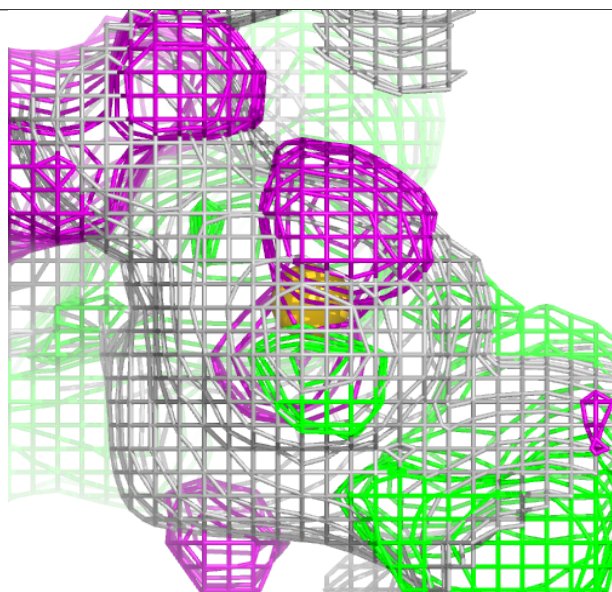
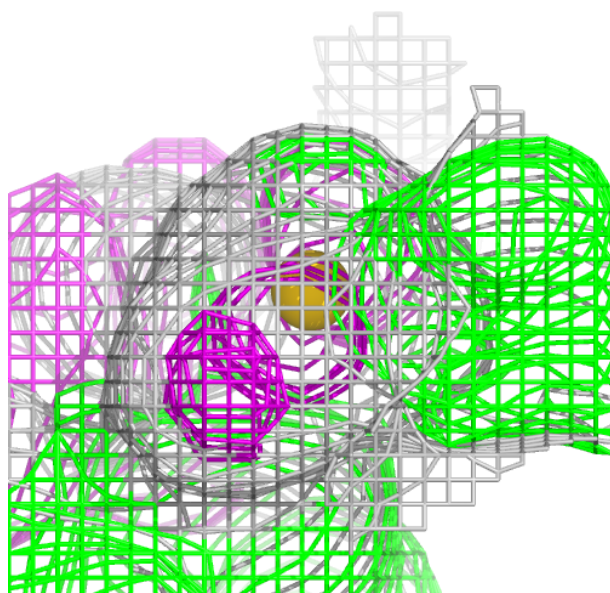
Electron density around AU AAA 216 (A):

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



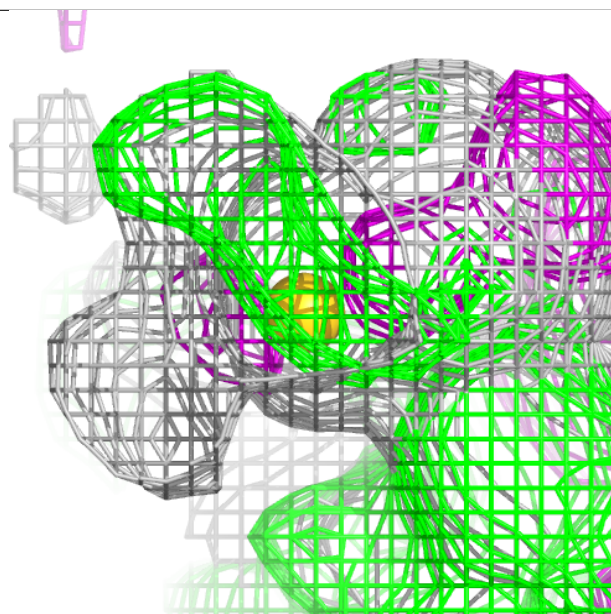
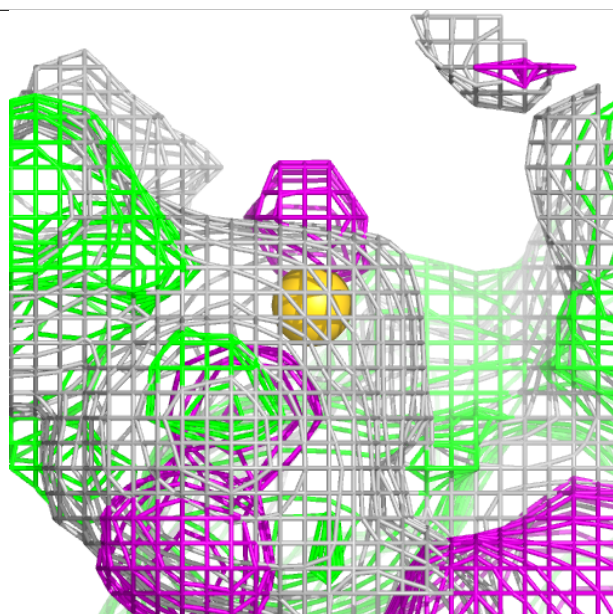
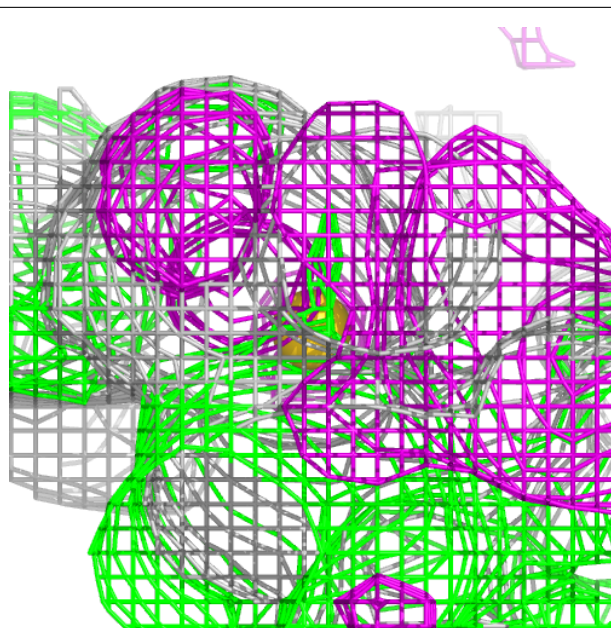
Electron density around AU AAA 217 (A):

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



Electron density around AU AAA 217 (B):

$2mF_o-DF_c$ (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.