



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 06:33 PM JST

PDB ID : 7E3V  
Title : Metallo beta-lactamase fold protein (cAMP free)  
Authors : Lee, K.-Y.; Kim, D.-G.; Lee, B.-J.  
Deposited on : 2021-02-09  
Resolution : 2.05 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

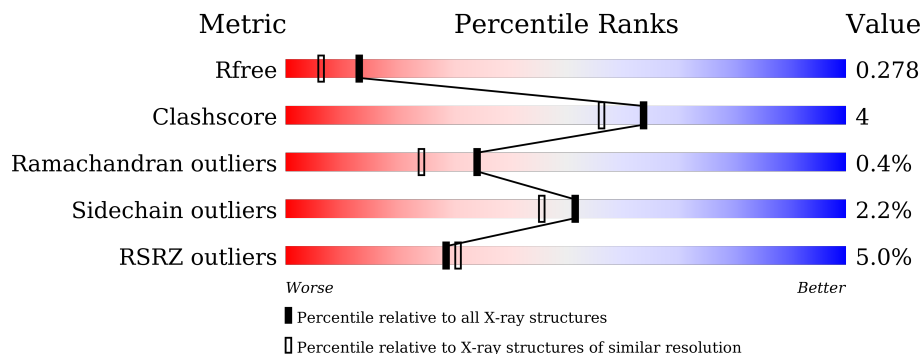
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	246	
1	B	246	
1	C	246	
1	D	246	
1	E	246	
1	F	246	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	CL	D	302	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11016 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 UPF0173 metal-dependent hydrolase C7P97\_11315.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1788	1149	289	340	10	0	0	0
1	B	230	1788	1149	289	340	10	0	0	0
1	C	230	1788	1149	289	340	10	0	0	0
1	D	230	1788	1149	289	340	10	0	0	0
1	E	230	1788	1149	289	340	10	0	0	0
1	F	230	1788	1149	289	340	10	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP W8UA39
A	-15	HIS	-	expression tag	UNP W8UA39
A	-14	HIS	-	expression tag	UNP W8UA39
A	-13	HIS	-	expression tag	UNP W8UA39
A	-12	HIS	-	expression tag	UNP W8UA39
A	-11	HIS	-	expression tag	UNP W8UA39
A	-10	SER	-	expression tag	UNP W8UA39
A	-9	SER	-	expression tag	UNP W8UA39
A	-8	GLY	-	expression tag	UNP W8UA39
A	-7	LEU	-	expression tag	UNP W8UA39
A	-6	VAL	-	expression tag	UNP W8UA39
A	-5	PRO	-	expression tag	UNP W8UA39
A	-4	ARG	-	expression tag	UNP W8UA39
A	-3	GLY	-	expression tag	UNP W8UA39
A	-2	SER	-	expression tag	UNP W8UA39
A	-1	HIS	-	expression tag	UNP W8UA39
A	0	MET	-	expression tag	UNP W8UA39

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP W8UA39
B	-15	HIS	-	expression tag	UNP W8UA39
B	-14	HIS	-	expression tag	UNP W8UA39
B	-13	HIS	-	expression tag	UNP W8UA39
B	-12	HIS	-	expression tag	UNP W8UA39
B	-11	HIS	-	expression tag	UNP W8UA39
B	-10	SER	-	expression tag	UNP W8UA39
B	-9	SER	-	expression tag	UNP W8UA39
B	-8	GLY	-	expression tag	UNP W8UA39
B	-7	LEU	-	expression tag	UNP W8UA39
B	-6	VAL	-	expression tag	UNP W8UA39
B	-5	PRO	-	expression tag	UNP W8UA39
B	-4	ARG	-	expression tag	UNP W8UA39
B	-3	GLY	-	expression tag	UNP W8UA39
B	-2	SER	-	expression tag	UNP W8UA39
B	-1	HIS	-	expression tag	UNP W8UA39
B	0	MET	-	expression tag	UNP W8UA39
C	-16	HIS	-	expression tag	UNP W8UA39
C	-15	HIS	-	expression tag	UNP W8UA39
C	-14	HIS	-	expression tag	UNP W8UA39
C	-13	HIS	-	expression tag	UNP W8UA39
C	-12	HIS	-	expression tag	UNP W8UA39
C	-11	HIS	-	expression tag	UNP W8UA39
C	-10	SER	-	expression tag	UNP W8UA39
C	-9	SER	-	expression tag	UNP W8UA39
C	-8	GLY	-	expression tag	UNP W8UA39
C	-7	LEU	-	expression tag	UNP W8UA39
C	-6	VAL	-	expression tag	UNP W8UA39
C	-5	PRO	-	expression tag	UNP W8UA39
C	-4	ARG	-	expression tag	UNP W8UA39
C	-3	GLY	-	expression tag	UNP W8UA39
C	-2	SER	-	expression tag	UNP W8UA39
C	-1	HIS	-	expression tag	UNP W8UA39
C	0	MET	-	expression tag	UNP W8UA39
D	-16	HIS	-	expression tag	UNP W8UA39
D	-15	HIS	-	expression tag	UNP W8UA39
D	-14	HIS	-	expression tag	UNP W8UA39
D	-13	HIS	-	expression tag	UNP W8UA39
D	-12	HIS	-	expression tag	UNP W8UA39
D	-11	HIS	-	expression tag	UNP W8UA39
D	-10	SER	-	expression tag	UNP W8UA39
D	-9	SER	-	expression tag	UNP W8UA39

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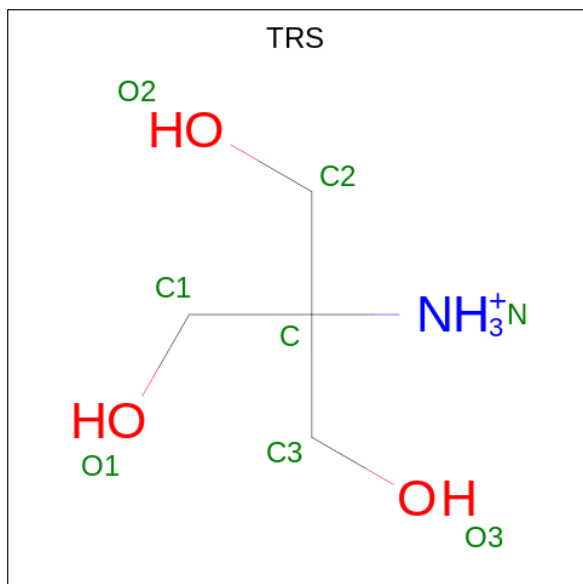
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP W8UA39
D	-7	LEU	-	expression tag	UNP W8UA39
D	-6	VAL	-	expression tag	UNP W8UA39
D	-5	PRO	-	expression tag	UNP W8UA39
D	-4	ARG	-	expression tag	UNP W8UA39
D	-3	GLY	-	expression tag	UNP W8UA39
D	-2	SER	-	expression tag	UNP W8UA39
D	-1	HIS	-	expression tag	UNP W8UA39
D	0	MET	-	expression tag	UNP W8UA39
E	-16	HIS	-	expression tag	UNP W8UA39
E	-15	HIS	-	expression tag	UNP W8UA39
E	-14	HIS	-	expression tag	UNP W8UA39
E	-13	HIS	-	expression tag	UNP W8UA39
E	-12	HIS	-	expression tag	UNP W8UA39
E	-11	HIS	-	expression tag	UNP W8UA39
E	-10	SER	-	expression tag	UNP W8UA39
E	-9	SER	-	expression tag	UNP W8UA39
E	-8	GLY	-	expression tag	UNP W8UA39
E	-7	LEU	-	expression tag	UNP W8UA39
E	-6	VAL	-	expression tag	UNP W8UA39
E	-5	PRO	-	expression tag	UNP W8UA39
E	-4	ARG	-	expression tag	UNP W8UA39
E	-3	GLY	-	expression tag	UNP W8UA39
E	-2	SER	-	expression tag	UNP W8UA39
E	-1	HIS	-	expression tag	UNP W8UA39
E	0	MET	-	expression tag	UNP W8UA39
F	-16	HIS	-	expression tag	UNP W8UA39
F	-15	HIS	-	expression tag	UNP W8UA39
F	-14	HIS	-	expression tag	UNP W8UA39
F	-13	HIS	-	expression tag	UNP W8UA39
F	-12	HIS	-	expression tag	UNP W8UA39
F	-11	HIS	-	expression tag	UNP W8UA39
F	-10	SER	-	expression tag	UNP W8UA39
F	-9	SER	-	expression tag	UNP W8UA39
F	-8	GLY	-	expression tag	UNP W8UA39
F	-7	LEU	-	expression tag	UNP W8UA39
F	-6	VAL	-	expression tag	UNP W8UA39
F	-5	PRO	-	expression tag	UNP W8UA39
F	-4	ARG	-	expression tag	UNP W8UA39
F	-3	GLY	-	expression tag	UNP W8UA39
F	-2	SER	-	expression tag	UNP W8UA39
F	-1	HIS	-	expression tag	UNP W8UA39

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	expression tag	UNP W8UA39

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0
2	D	1	8	4	1	3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	A	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ni 2	0	0
4	C	2	Total 2	Ni 2	0	0
4	D	2	Total 2	Ni 2	0	0
4	E	2	Total 2	Ni 2	0	0
4	F	2	Total 2	Ni 2	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Zn 2	0	0
5	B	2	Total 2	Zn 2	0	0
5	C	2	Total 2	Zn 2	0	0
5	D	2	Total 2	Zn 2	0	0
5	E	2	Total 2	Zn 2	0	0
5	F	2	Total 2	Zn 2	0	0

- Molecule 6 is water.

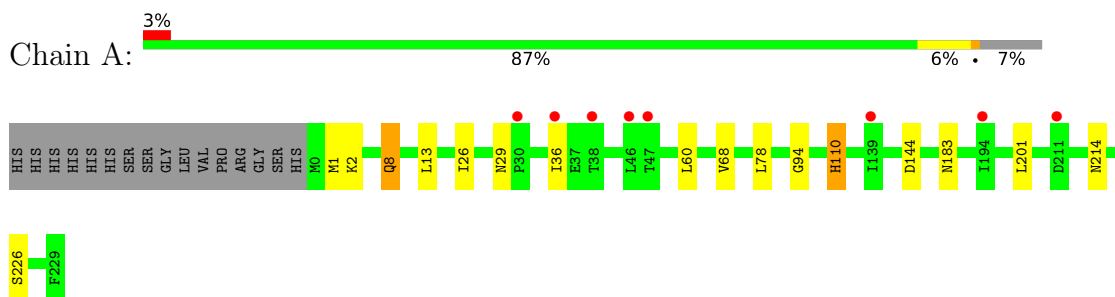
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	35	Total 35	O 35	0	0
6	C	40	Total 40	O 40	0	0
6	D	43	Total 43	O 43	0	0
6	E	44	Total 44	O 44	0	0
6	F	36	Total 36	O 36	0	0



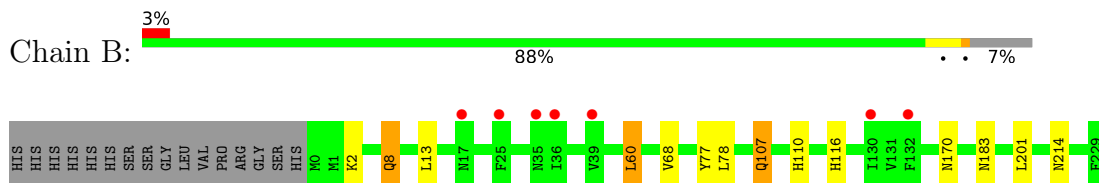
### 3 Residue-property plots [i](#)

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.

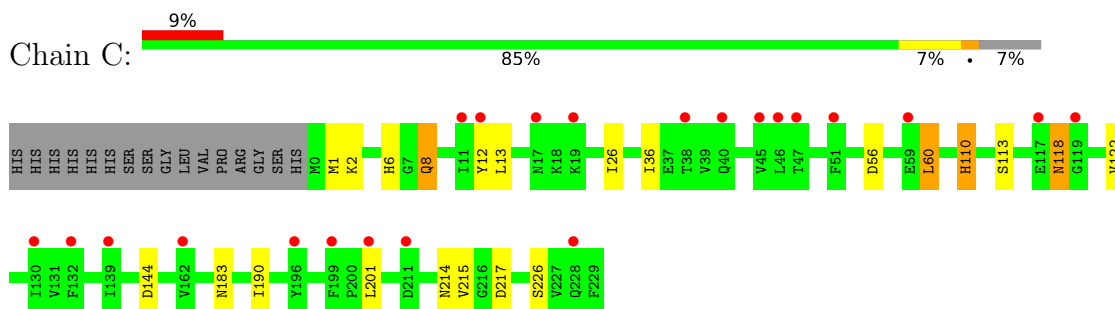
- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315



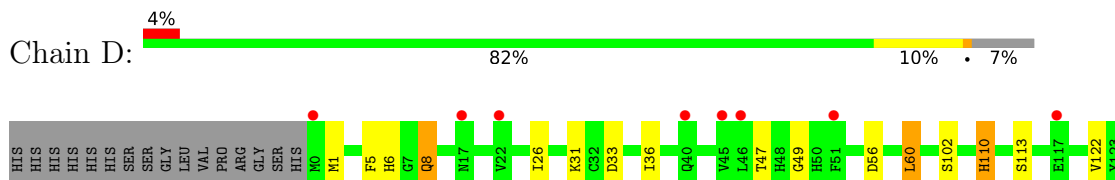
- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315



- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315

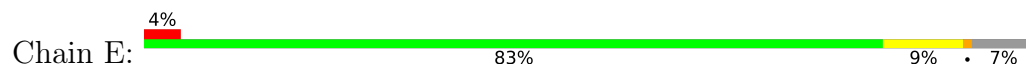


- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315

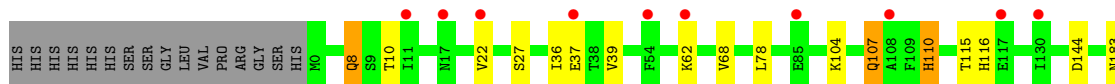
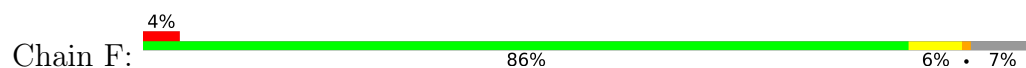




- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315



- Molecule 1: UPF0173 metal-dependent hydrolase C7P97\_11315



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.95Å 120.81Å 186.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.05 29.81 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.83-2.05) 93.7 (29.81-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.04Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.238 , 0.277 0.244 , 0.278	Depositor DCC
$R_{free}$ test set	4636 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.40 % 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 2.3729e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CL, TRS, NI

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	0.66	0/1834	0.75	0/2486
1	B	0.64	0/1834	0.74	0/2486
1	C	0.64	0/1834	0.74	0/2486
1	D	0.64	0/1834	0.75	0/2486
1	E	0.65	0/1834	0.75	0/2486
1	F	0.64	0/1834	0.75	0/2486
All	All	0.64	0/11004	0.75	0/14916

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1788	0	1730	10	0
1	B	1788	0	1730	11	0
1	C	1788	0	1730	19	0
1	D	1788	0	1730	17	0
1	E	1788	0	1730	17	0
1	F	1788	0	1730	14	0
2	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	0	12	1	0
3	A	1	0	0	1	0
3	D	1	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
6	A	48	0	0	0	0
6	B	35	0	0	1	0
6	C	40	0	0	1	0
6	D	43	0	0	0	0
6	E	44	0	0	0	0
6	F	36	0	0	0	0
All	All	11016	0	10404	88	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 4.

All (88) 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:8:GLN:HA	1:E:8:GLN:HE21	1.24	1.03
2:A:301:TRS:N	3:A:302:CL:CL	2.33	0.97
2:D:301:TRS:N	3:D:302:CL:CL	2.38	0.93
1:B:107:GLN:HE21	1:B:107:GLN:H	1.17	0.93
1:D:8:GLN:HE21	1:D:8:GLN:HA	1.36	0.89
1:A:8:GLN:HE21	1:A:8:GLN:HA	1.39	0.87
1:F:8:GLN:HE21	1:F:8:GLN:HA	1.44	0.82
1:B:183:ASN:HD21	1:B:214:ASN:H	1.27	0.81
1:A:183:ASN:HD21	1:A:214:ASN:H	1.29	0.79
1:C:8:GLN:HE21	1:C:8:GLN:HA	1.49	0.78
1:B:8:GLN:HE21	1:B:8:GLN:HA	1.48	0.77
1:E:8:GLN:HA	1:E:8:GLN:NE2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ASN:HD21	1:F:214:ASN:H	1.36	0.74
1:F:107:GLN:HE21	1:F:107:GLN:H	1.36	0.73
1:E:183:ASN:HD21	1:E:214:ASN:H	1.35	0.72
1:C:183:ASN:HD21	1:C:214:ASN:H	1.39	0.70
1:D:183:ASN:HD21	1:D:214:ASN:H	1.41	0.68
1:D:8:GLN:HA	1:D:8:GLN:NE2	2.13	0.62
1:B:183:ASN:ND2	1:B:214:ASN:H	1.98	0.61
1:B:8:GLN:HA	1:B:8:GLN:NE2	2.16	0.60
1:E:8:GLN:HE21	1:E:8:GLN:CA	2.03	0.60
1:A:8:GLN:HA	1:A:8:GLN:NE2	2.13	0.59
1:E:110:HIS:CE1	1:E:144:ASP:HB3	2.38	0.59
1:F:8:GLN:HA	1:F:8:GLN:NE2	2.17	0.57
1:C:201:LEU:HB2	6:C:435:HOH:O	2.05	0.56
1:B:68:VAL:HG11	1:B:78:LEU:CD1	2.36	0.56
1:F:183:ASN:ND2	1:F:214:ASN:H	2.03	0.54
1:A:183:ASN:ND2	1:A:214:ASN:H	2.02	0.54
1:C:183:ASN:ND2	1:C:214:ASN:H	2.04	0.54
1:E:183:ASN:ND2	1:E:214:ASN:H	2.07	0.53
1:E:68:VAL:HG11	1:E:78:LEU:CD1	2.40	0.52
1:F:68:VAL:HG11	1:F:78:LEU:HD13	1.91	0.51
1:C:118:ASN:H	1:C:118:ASN:HD22	1.59	0.51
1:E:4:SER:OG	1:E:6:HIS:HE1	1.92	0.51
1:B:77:TYR:OH	1:B:116:HIS:HE1	1.94	0.50
1:F:27:SER:HB3	1:F:36:ILE:CD1	2.41	0.50
1:D:6:HIS:HD2	1:D:33:ASP:OD1	1.95	0.50
1:C:8:GLN:HA	1:C:8:GLN:NE2	2.23	0.50
1:E:6:HIS:HD2	1:E:33:ASP:OD1	1.96	0.49
1:D:183:ASN:ND2	1:D:214:ASN:H	2.08	0.49
1:C:118:ASN:HD22	1:C:118:ASN:N	2.11	0.49
1:C:26:ILE:HB	1:C:36:ILE:HD11	1.95	0.48
1:D:31:LYS:HE3	1:D:197:ASP:O	2.13	0.48
1:D:5:PHE:CE1	1:D:194:ILE:HG22	2.48	0.48
1:F:8:GLN:HE21	1:F:8:GLN:CA	2.20	0.48
1:A:110:HIS:CE1	1:A:144:ASP:HB3	2.50	0.47
1:A:68:VAL:HG11	1:A:78:LEU:CD1	2.44	0.47
1:D:26:ILE:HB	1:D:36:ILE:HD11	1.97	0.47
1:C:183:ASN:HD22	1:C:215:VAL:HG12	1.79	0.47
1:E:4:SER:OG	1:E:6:HIS:CE1	2.68	0.47
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.83	0.47
1:E:102:SER:OG	1:E:133:GLU:HB2	2.14	0.46
1:C:110:HIS:CE1	1:C:144:ASP:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:C	1:B:13:LEU:HD12	2.36	0.46
1:D:49:GLY:HA3	1:D:124:LEU:HD12	1.98	0.45
1:C:113:SER:HA	1:C:122:VAL:O	2.17	0.45
1:D:183:ASN:HD22	1:D:215:VAL:HG12	1.81	0.45
1:E:77:TYR:OH	1:E:116:HIS:HE1	2.00	0.45
1:C:56:ASP:O	1:C:60:LEU:HB2	2.17	0.44
1:F:27:SER:HB3	1:F:36:ILE:HD11	1.99	0.44
1:F:110:HIS:CE1	1:F:144:ASP:HB3	2.53	0.44
1:C:6:HIS:CE1	1:C:12:TYR:HB3	2.53	0.44
1:E:35:ASN:O	1:E:39:VAL:HG23	2.17	0.44
1:E:10:THR:HA	1:E:22:VAL:O	2.17	0.43
1:F:115:THR:HG22	1:F:116:HIS:O	2.18	0.43
1:D:113:SER:HA	1:D:122:VAL:O	2.18	0.43
1:D:102:SER:OG	1:D:133:GLU:HB2	2.17	0.43
1:D:56:ASP:O	1:D:60:LEU:HB2	2.19	0.43
1:F:68:VAL:HG11	1:F:78:LEU:CD1	2.48	0.43
1:A:2:LYS:NZ	1:A:226:SER:OG	2.52	0.43
1:C:13:LEU:C	1:C:13:LEU:HD12	2.39	0.43
1:C:2:LYS:NZ	1:C:226:SER:OG	2.52	0.42
1:A:26:ILE:HB	1:A:36:ILE:HD11	2.01	0.42
3:D:302:CL:CL	1:E:149:SER:OG	2.74	0.42
1:C:190:ILE:HA	1:C:217:ASP:O	2.19	0.42
1:B:201:LEU:HB2	6:B:427:HOH:O	2.19	0.42
1:C:6:HIS:HE1	1:C:12:TYR:HB3	1.85	0.41
1:F:10:THR:HA	1:F:22:VAL:O	2.20	0.41
1:D:177:ASP:OD2	1:F:104:LYS:NZ	2.44	0.41
1:C:201:LEU:HD12	1:C:201:LEU:HA	1.89	0.41
1:E:140:TYR:O	1:E:163:CYS:HA	2.20	0.41
1:D:110:HIS:CE1	1:D:144:ASP:HB3	2.56	0.41
1:E:183:ASN:HD22	1:E:215:VAL:HG12	1.86	0.41
1:A:13:LEU:C	1:A:13:LEU:HD12	2.41	0.40
1:A:94:GLY:HA3	1:B:170:ASN:O	2.21	0.40
1:C:118:ASN:H	1:C:118:ASN:ND2	2.16	0.40
1:D:47:THR:HB	1:D:128:MET:O	2.22	0.40
1:D:201:LEU:HD12	1:D:201:LEU:HA	1.91	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	228/246 (93%)	218 (96%)	9 (4%)	1 (0%)	34	24
1	B	228/246 (93%)	219 (96%)	8 (4%)	1 (0%)	34	24
1	C	228/246 (93%)	218 (96%)	9 (4%)	1 (0%)	34	24
1	D	228/246 (93%)	219 (96%)	8 (4%)	1 (0%)	34	24
1	E	228/246 (93%)	219 (96%)	8 (4%)	1 (0%)	34	24
1	F	228/246 (93%)	218 (96%)	9 (4%)	1 (0%)	34	24
All	All	1368/1476 (93%)	1311 (96%)	51 (4%)	6 (0%)	34	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	110	HIS
1	A	110	HIS
1	C	110	HIS
1	B	110	HIS
1	E	110	HIS
1	F	110	HIS

### 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	A	199/213 (93%)	194 (98%)	5 (2%)	47	40
1	B	199/213 (93%)	195 (98%)	4 (2%)	55	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	199/213 (93%)	195 (98%)	4 (2%)	55	50
1	D	199/213 (93%)	195 (98%)	4 (2%)	55	50
1	E	199/213 (93%)	195 (98%)	4 (2%)	55	50
1	F	199/213 (93%)	194 (98%)	5 (2%)	47	40
All	All	1194/1278 (93%)	1168 (98%)	26 (2%)	52	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	GLN
1	A	29	ASN
1	A	60	LEU
1	A	201	LEU
1	B	2	LYS
1	B	8	GLN
1	B	60	LEU
1	B	107	GLN
1	C	1	MET
1	C	8	GLN
1	C	60	LEU
1	C	118	ASN
1	D	1	MET
1	D	8	GLN
1	D	60	LEU
1	D	187	LYS
1	E	2	LYS
1	E	8	GLN
1	E	36	ILE
1	E	60	LEU
1	F	8	GLN
1	F	37	GLU
1	F	39	VAL
1	F	62	LYS
1	F	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	29	ASN
1	A	183	ASN
1	A	204	GLN
1	B	6	HIS
1	B	8	GLN
1	B	16	ASN
1	B	107	GLN
1	B	116	HIS
1	B	170	ASN
1	B	183	ASN
1	B	204	GLN
1	C	6	HIS
1	C	8	GLN
1	C	16	ASN
1	C	40	GLN
1	C	118	ASN
1	C	170	ASN
1	C	183	ASN
1	C	204	GLN
1	D	6	HIS
1	D	8	GLN
1	D	16	ASN
1	D	170	ASN
1	D	183	ASN
1	D	204	GLN
1	D	207	GLN
1	D	214	ASN
1	E	6	HIS
1	E	8	GLN
1	E	16	ASN
1	E	40	GLN
1	E	82	HIS
1	E	116	HIS
1	E	183	ASN
1	E	204	GLN
1	E	207	GLN
1	F	6	HIS
1	F	8	GLN
1	F	16	ASN
1	F	28	ASN
1	F	107	GLN
1	F	170	ASN

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Mol	Chain	Res	Type
1	F	183	ASN
1	F	204	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 26 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TRS	A	301	-	7,7,7	0.21	0	9,9,9	0.30	0
2	TRS	D	301	-	7,7,7	0.19	0	9,9,9	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	301	-	-	3/9/9/9	-
2	TRS	D	301	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	TRS	N-C-C2-O2
2	D	301	TRS	N-C-C3-O3
2	A	301	TRS	C2-C-C1-O1
2	A	301	TRS	C3-C-C1-O1
2	D	301	TRS	C1-C-C2-O2
2	D	301	TRS	C3-C-C2-O2
2	D	301	TRS	C1-C-C3-O3
2	D	301	TRS	C2-C-C3-O3
2	A	301	TRS	N-C-C1-O1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	TRS	1	0
2	D	301	TRS	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	230/246 (93%)	0.29	8 (3%) 44 48	21, 31, 45, 62	0
1	B	230/246 (93%)	0.42	7 (3%) 50 54	21, 34, 53, 63	0
1	C	230/246 (93%)	0.58	22 (9%) 8 8	22, 34, 51, 64	0
1	D	230/246 (93%)	0.45	11 (4%) 30 33	20, 32, 49, 69	0
1	E	230/246 (93%)	0.25	11 (4%) 30 33	21, 30, 45, 58	0
1	F	230/246 (93%)	0.40	10 (4%) 35 38	21, 34, 51, 67	0
All	All	1380/1476 (93%)	0.40	69 (5%) 28 31	20, 32, 50, 69	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	GLU	5.1
1	A	36	ILE	5.0
1	B	36	ILE	4.8
1	C	119	GLY	4.2
1	F	22	VAL	4.1
1	F	85	GLU	4.0
1	E	117	GLU	3.9
1	E	30	PRO	3.8
1	D	199	PHE	3.8
1	E	0	MET	3.6
1	E	22	VAL	3.5
1	F	17	ASN	3.3
1	D	51	PHE	3.3
1	F	117	GLU	3.2
1	F	62	LYS	3.2
1	B	39	VAL	3.2
1	D	46	LEU	3.1
1	C	117	GLU	3.1
1	D	17	ASN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	30	PRO	3.0
1	C	19	LYS	3.0
1	A	46	LEU	3.0
1	A	211	ASP	2.9
1	C	46	LEU	2.9
1	E	36	ILE	2.9
1	F	54	PHE	2.9
1	C	38	THR	2.9
1	C	130	ILE	2.9
1	C	51	PHE	2.8
1	D	45	VAL	2.8
1	C	199	PHE	2.8
1	B	132	PHE	2.7
1	D	130	ILE	2.7
1	A	38	THR	2.7
1	C	12	TYR	2.7
1	C	11	ILE	2.7
1	C	162	VAL	2.6
1	C	40	GLN	2.6
1	B	25	PHE	2.6
1	C	17	ASN	2.6
1	B	130	ILE	2.6
1	E	40	GLN	2.5
1	B	17	ASN	2.5
1	C	132	PHE	2.5
1	A	139	ILE	2.5
1	D	22	VAL	2.5
1	C	196	TYR	2.5
1	D	0	MET	2.4
1	C	211	ASP	2.4
1	F	11	ILE	2.4
1	F	130	ILE	2.4
1	C	47	THR	2.4
1	D	40	GLN	2.3
1	C	139	ILE	2.3
1	E	99	ASP	2.3
1	A	194	ILE	2.2
1	C	45	VAL	2.2
1	D	143	GLY	2.2
1	C	59	GLU	2.2
1	A	47	THR	2.2
1	F	37	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	2.1
1	F	108	ALA	2.1
1	B	35	ASN	2.1
1	E	17	ASN	2.1
1	E	194	ILE	2.0
1	E	85	GLU	2.0
1	E	45	VAL	2.0
1	C	228	GLN	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TRS	A	301	8/8	0.88	0.15	32,34,38,41	0
2	TRS	D	301	8/8	0.96	0.11	32,34,36,36	0
4	NI	A	304	1/1	0.97	0.06	41,41,41,41	1
5	ZN	A	306	1/1	0.97	0.06	39,39,39,39	1
3	CL	A	302	1/1	0.98	0.07	27,27,27,27	0
4	NI	B	302	1/1	0.98	0.05	50,50,50,50	1
4	NI	C	302	1/1	0.98	0.05	47,47,47,47	1
3	CL	D	302	1/1	0.98	0.10	30,30,30,30	0
5	ZN	B	304	1/1	0.98	0.05	44,44,44,44	1
5	ZN	C	304	1/1	0.98	0.05	44,44,44,44	1
5	ZN	F	304	1/1	0.98	0.04	45,45,45,45	1
4	NI	D	304	1/1	0.99	0.04	44,44,44,44	1
4	NI	E	301	1/1	0.99	0.05	34,34,34,34	1
4	NI	E	302	1/1	0.99	0.04	38,38,38,38	1
4	NI	F	301	1/1	0.99	0.07	36,36,36,36	1

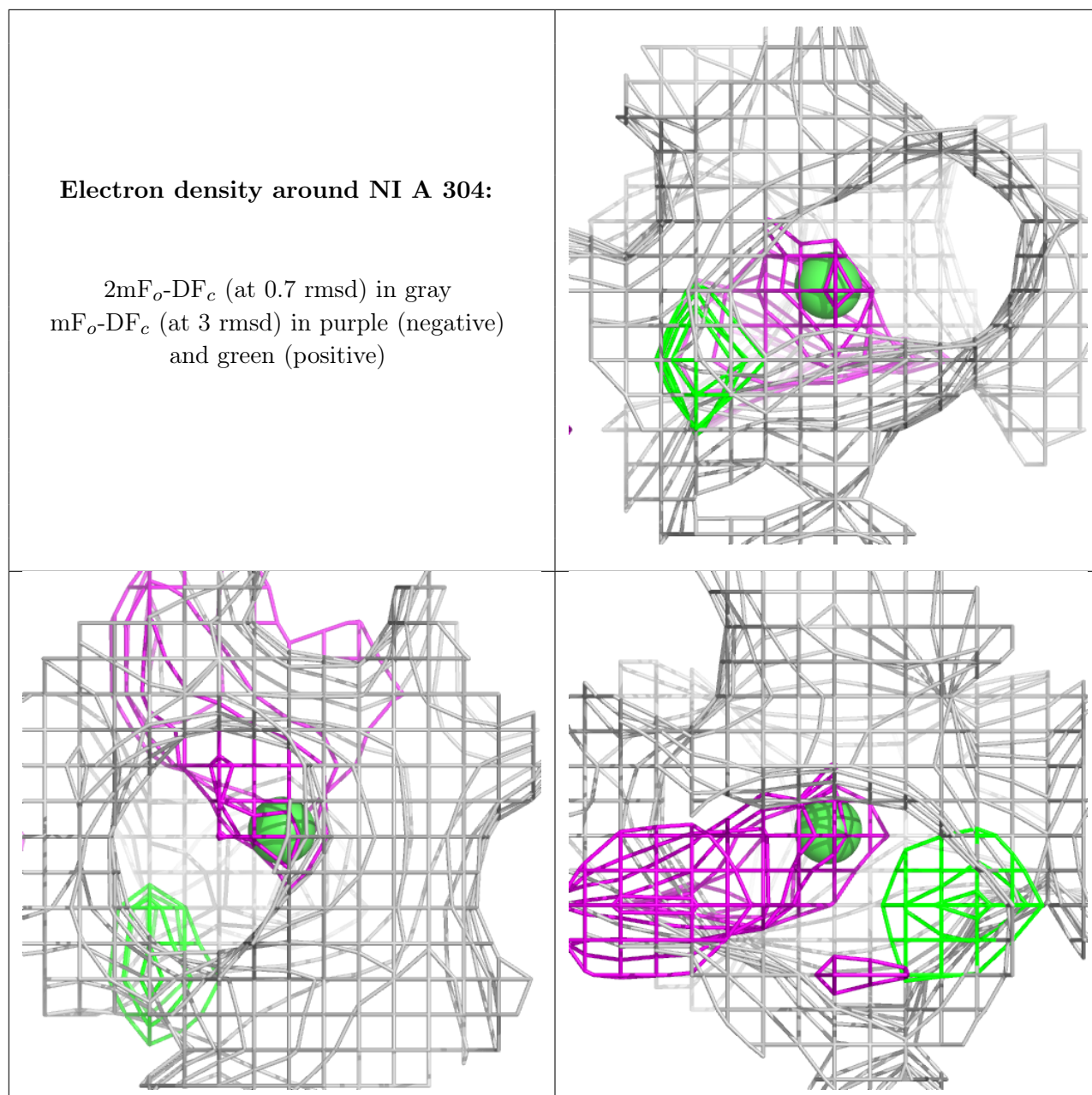
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NI	F	302	1/1	0.99	0.06	49,49,49,49	1
5	ZN	A	305	1/1	0.99	0.09	33,33,33,33	1
4	NI	A	303	1/1	0.99	0.09	33,33,33,33	1
5	ZN	B	303	1/1	0.99	0.06	34,34,34,34	1
4	NI	C	301	1/1	0.99	0.07	35,35,35,35	1
5	ZN	C	303	1/1	0.99	0.08	34,34,34,34	1
4	NI	B	301	1/1	0.99	0.06	35,35,35,35	1
5	ZN	D	305	1/1	0.99	0.06	32,32,32,32	1
5	ZN	D	306	1/1	0.99	0.04	42,42,42,42	1
5	ZN	E	303	1/1	0.99	0.05	33,33,33,33	1
5	ZN	E	304	1/1	0.99	0.04	36,36,36,36	1
5	ZN	F	303	1/1	0.99	0.07	35,35,35,35	1
4	NI	D	303	1/1	0.99	0.06	33,33,33,33	1

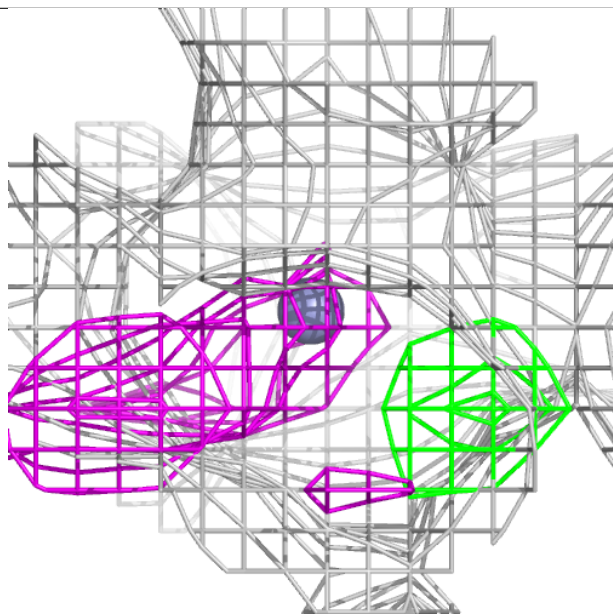
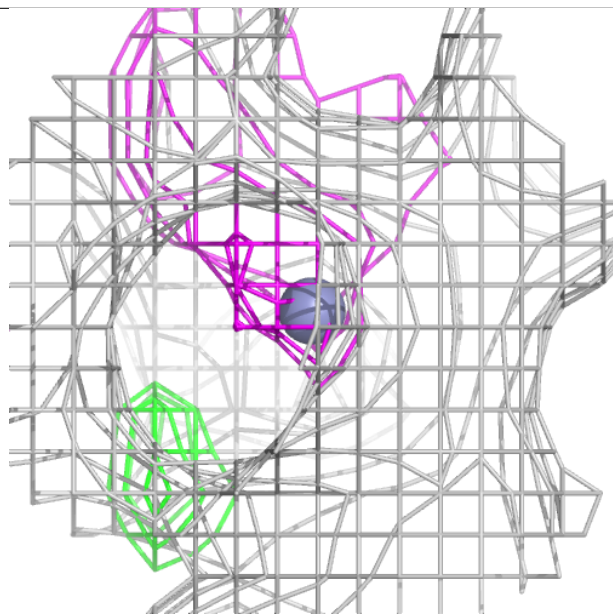
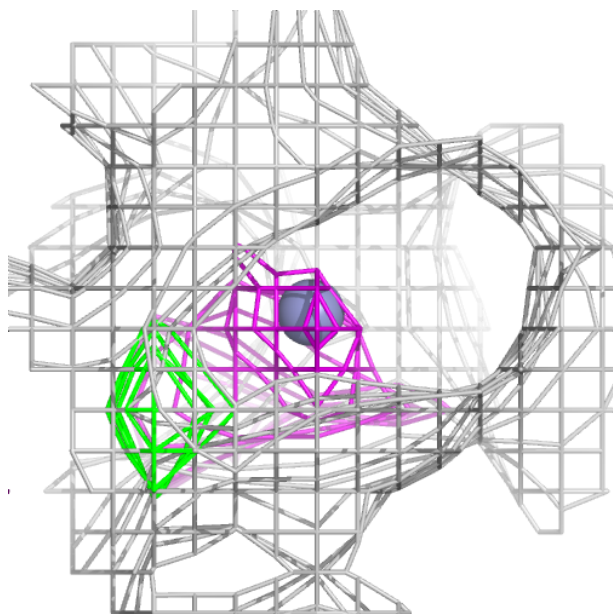
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

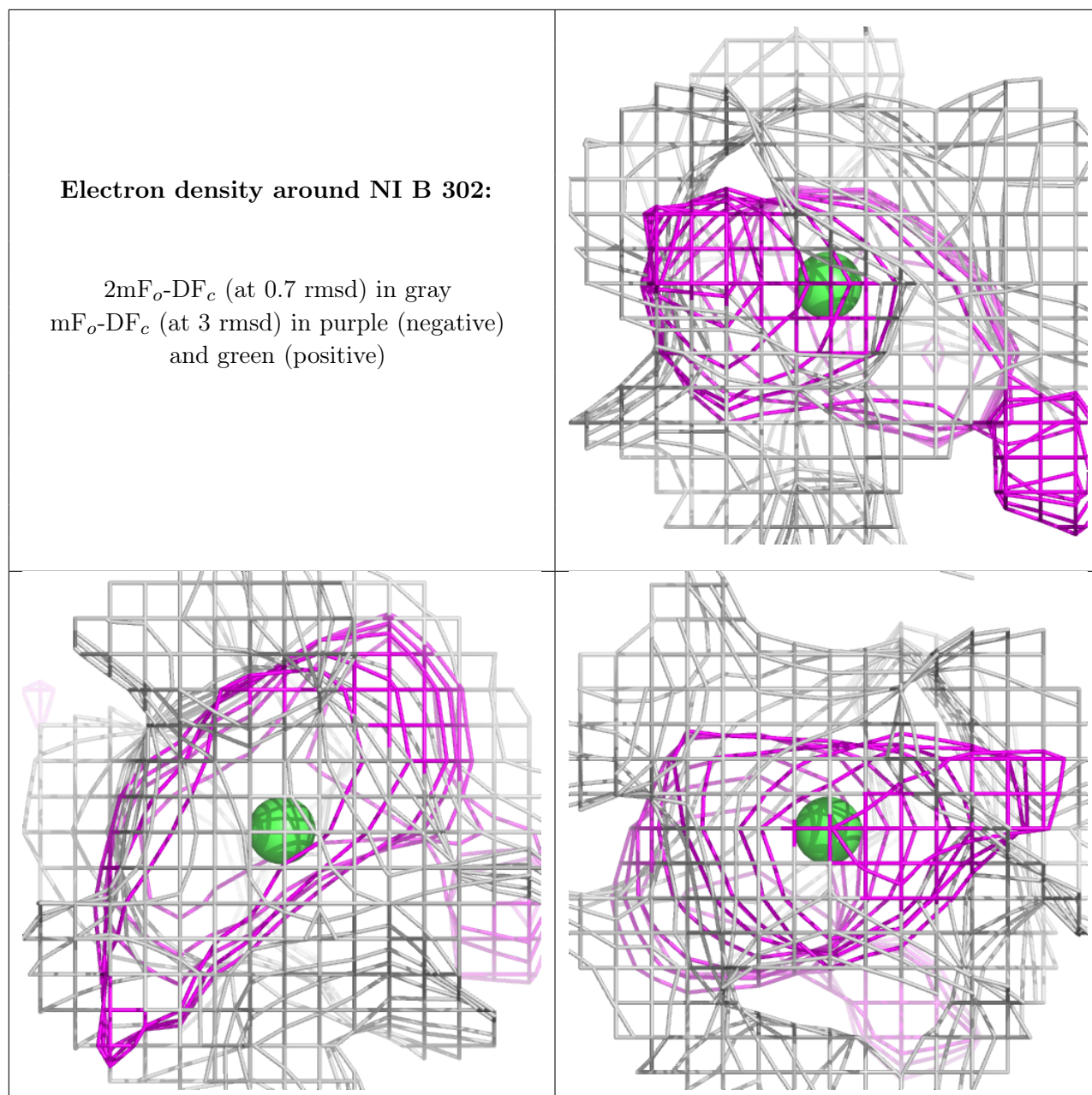


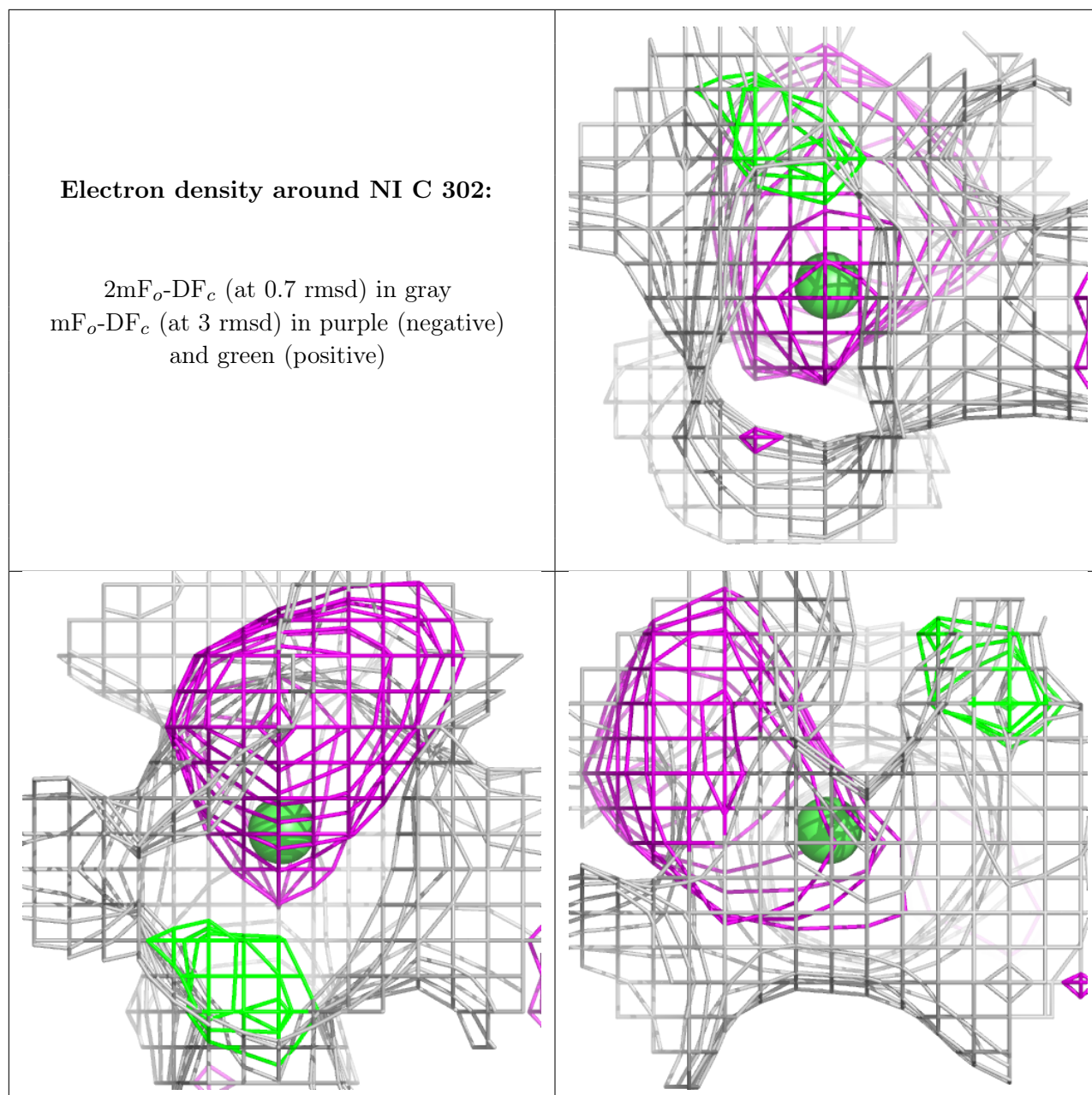


**Electron density around ZN A 306:**

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

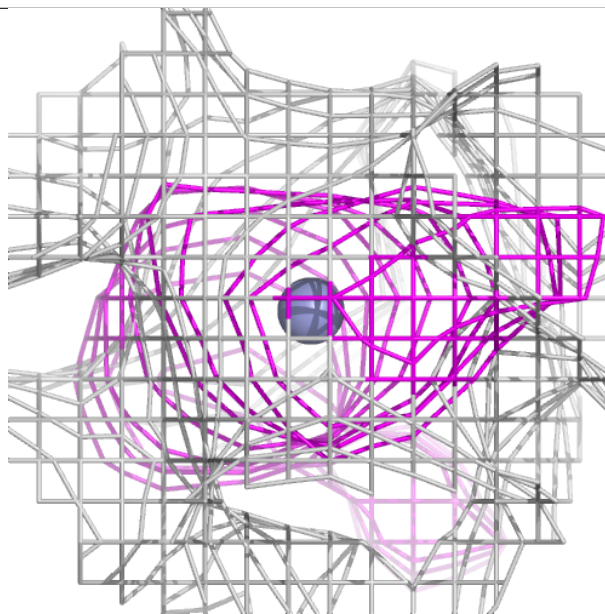
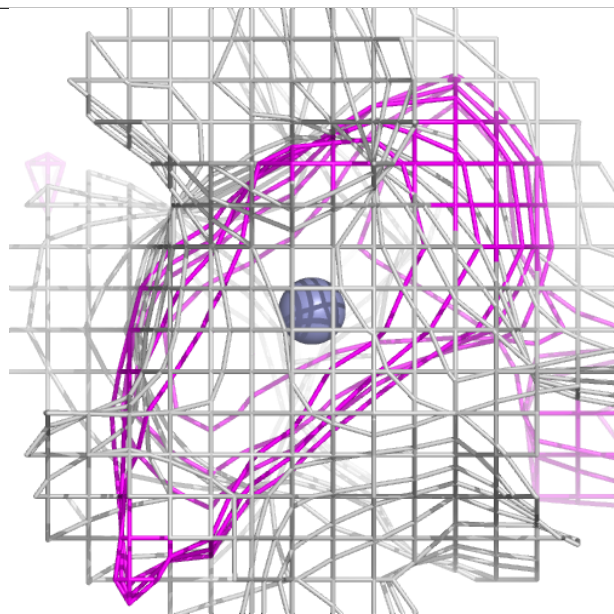
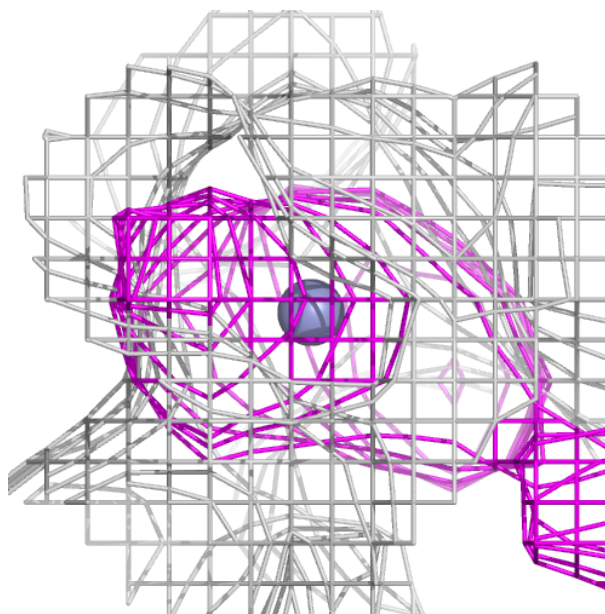






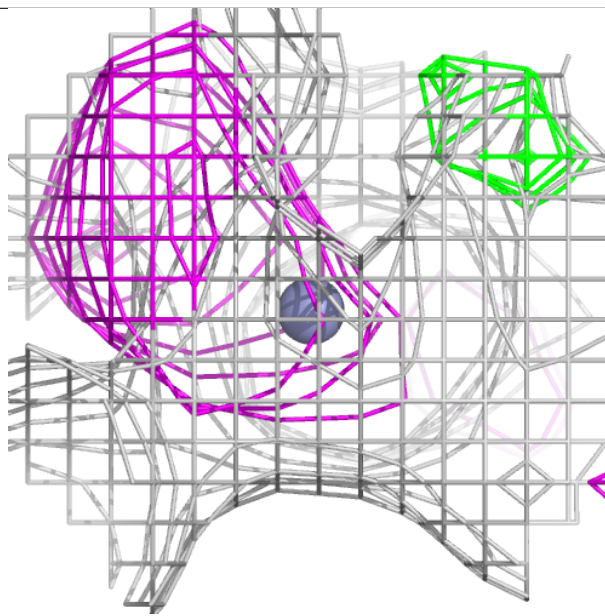
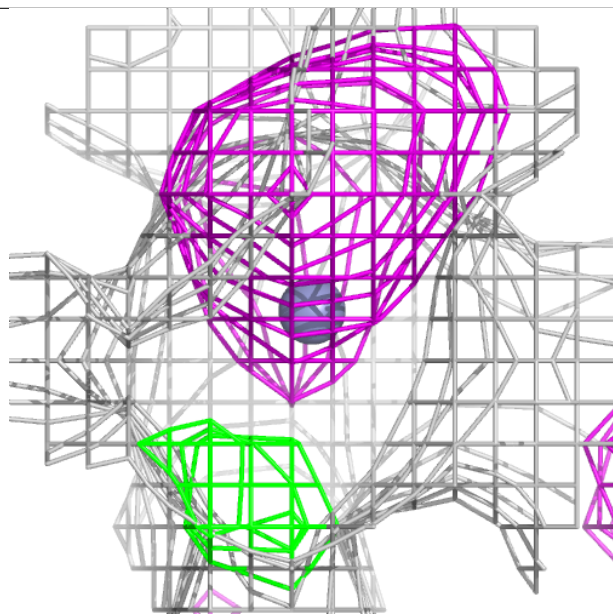
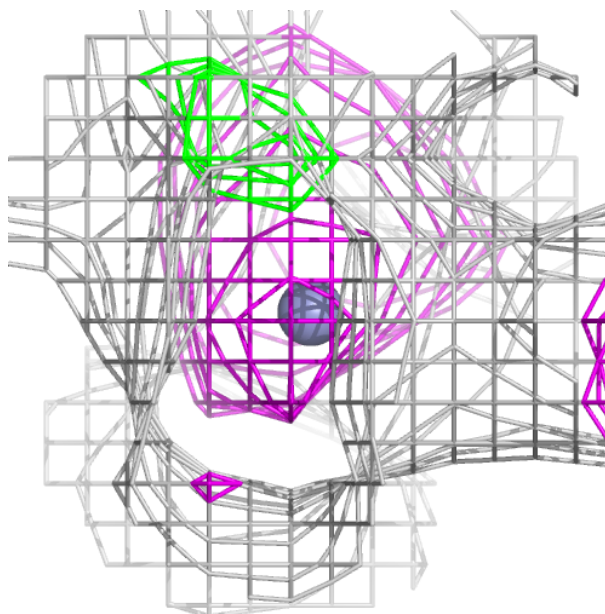
**Electron density around ZN B 304:**

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



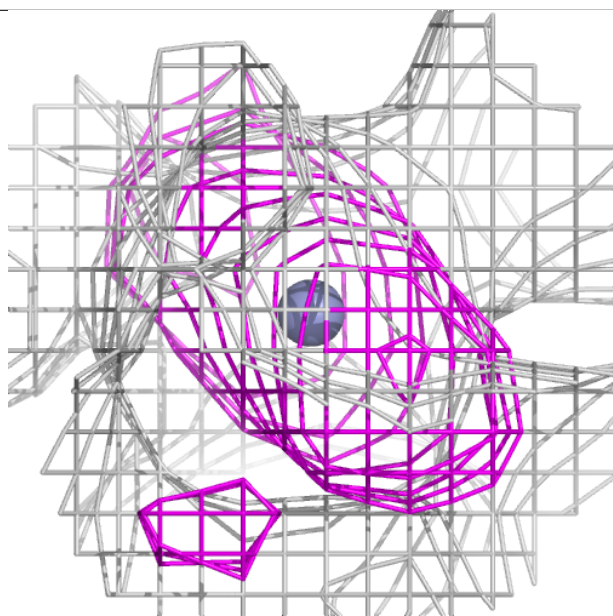
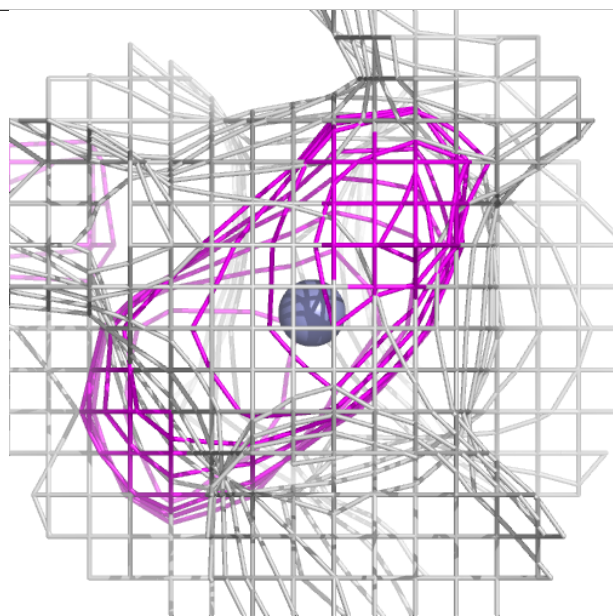
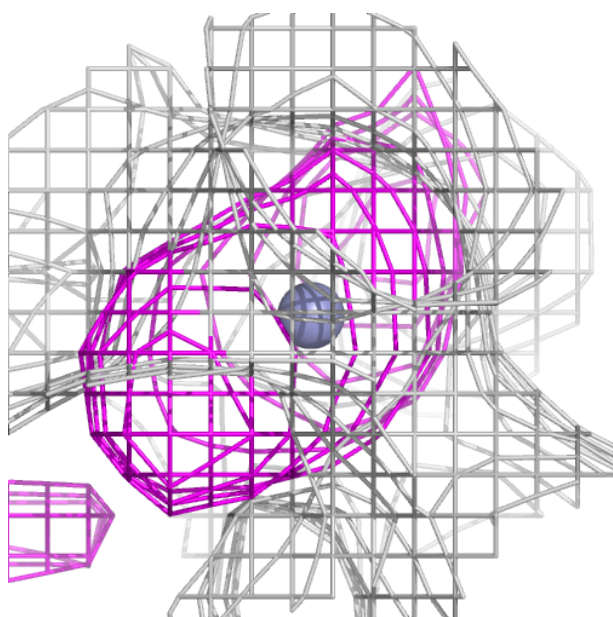
**Electron density around ZN C 304:**

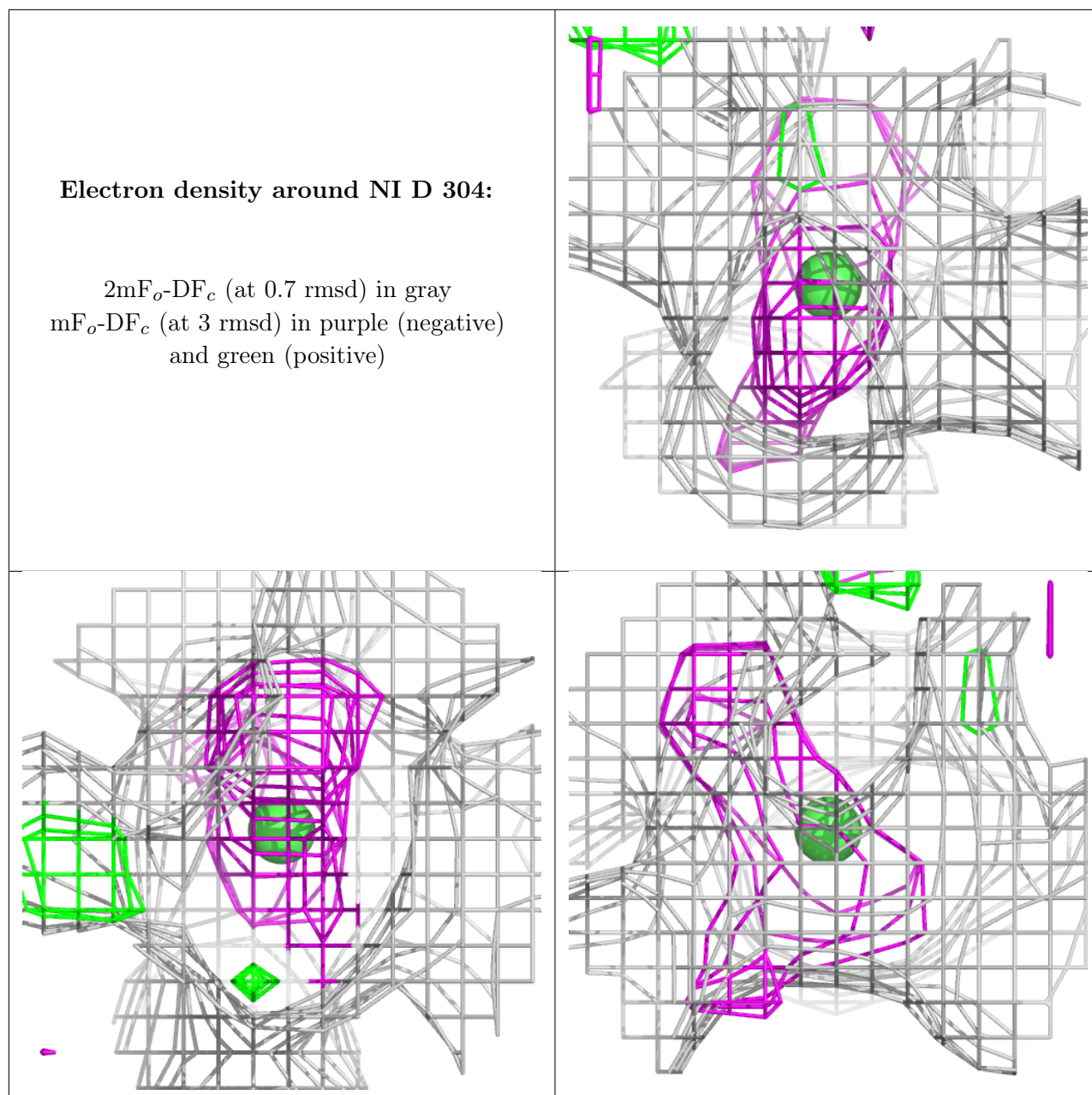
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN F 304:**

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

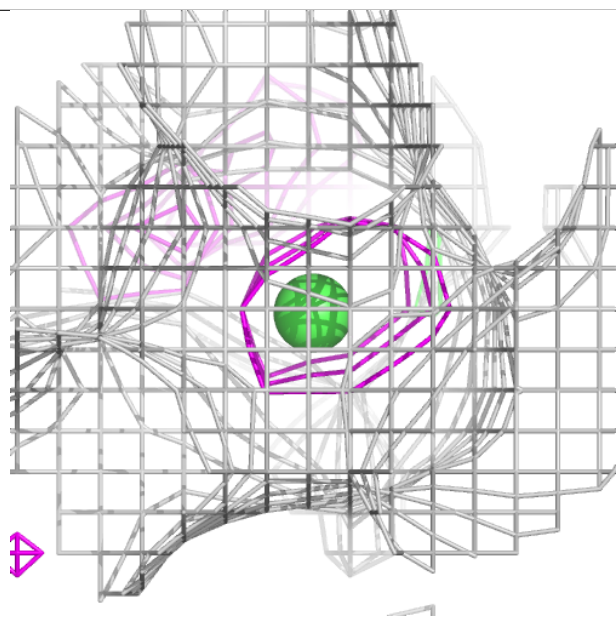
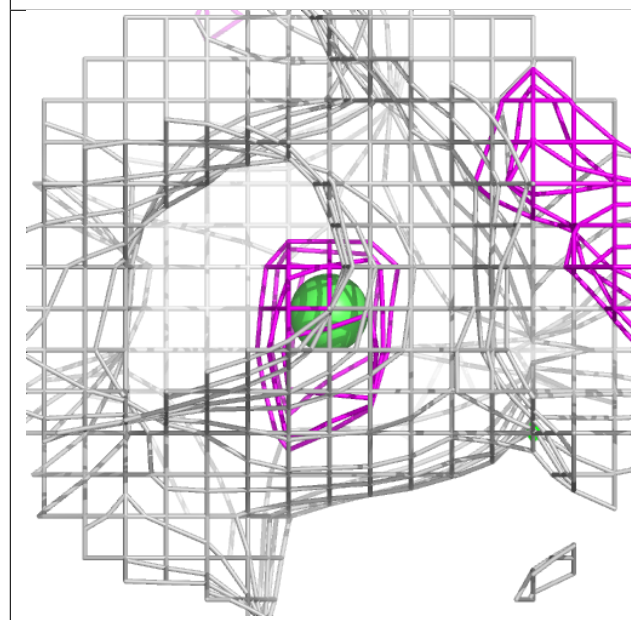
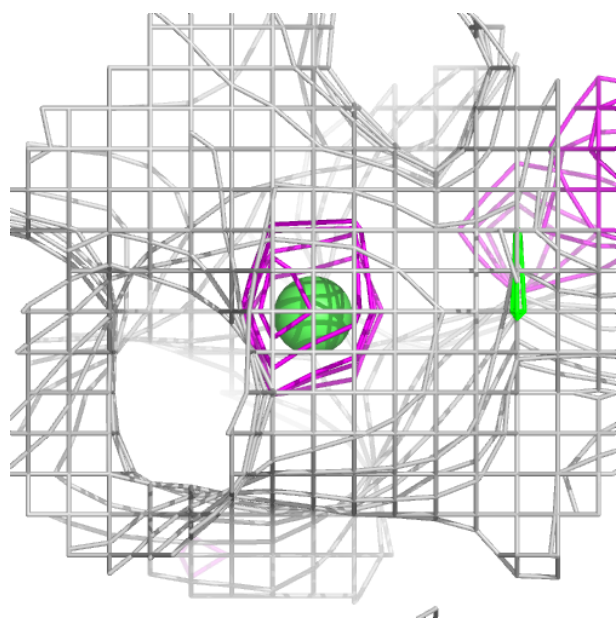






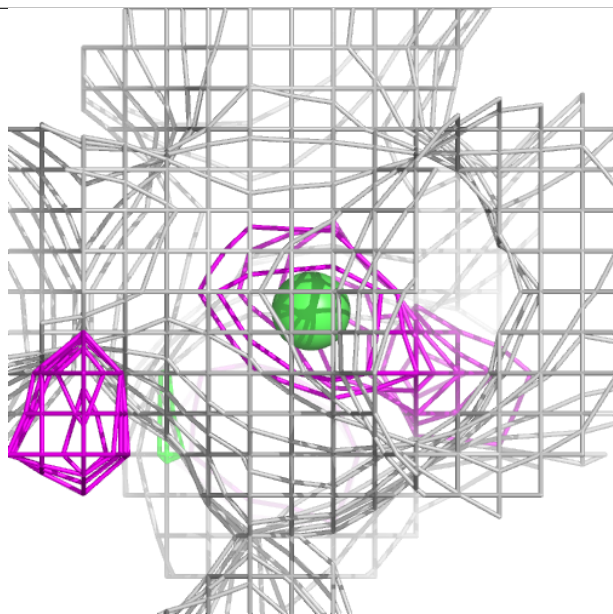
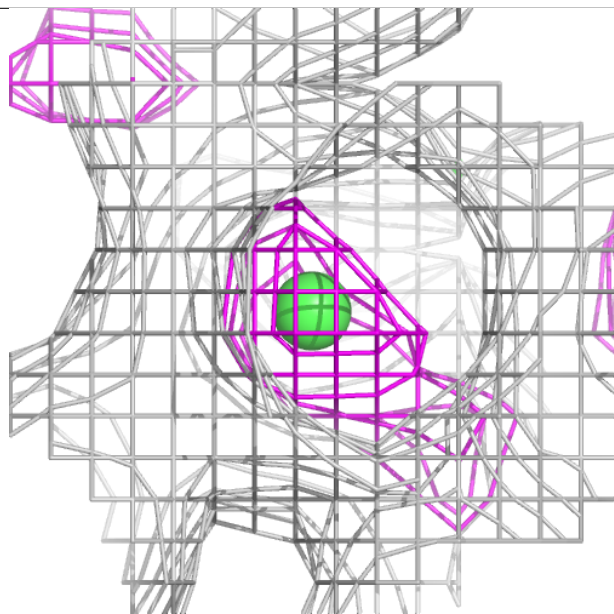
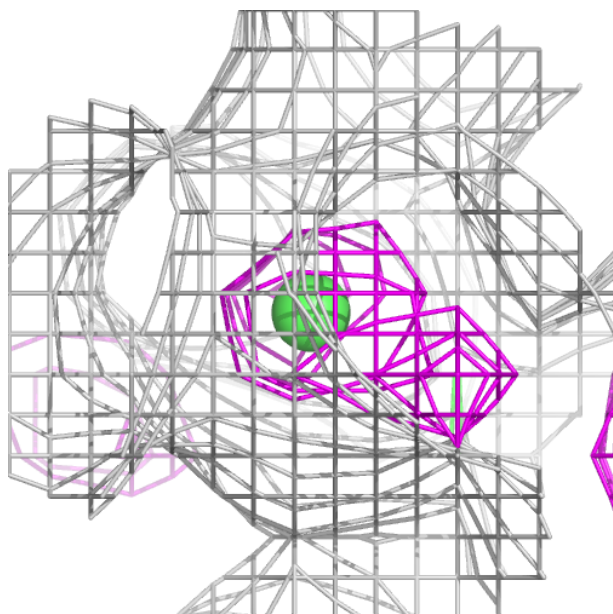
**Electron density around NI E 301:**

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



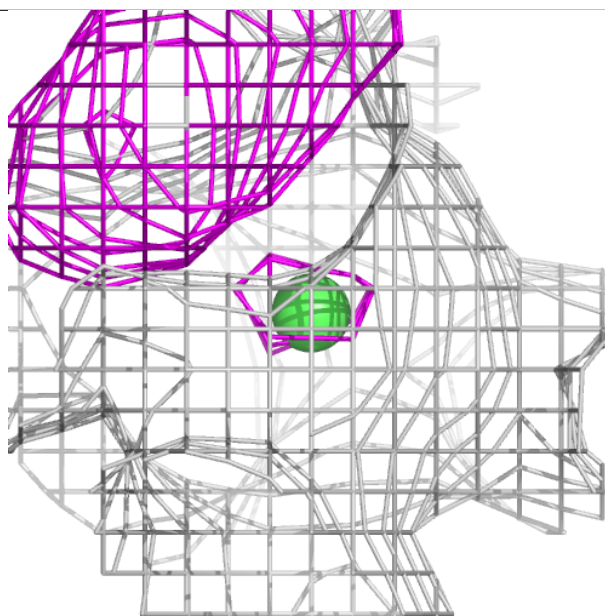
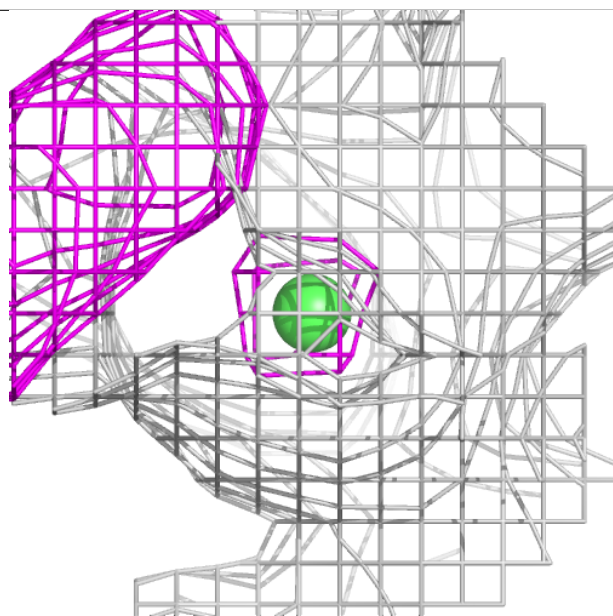
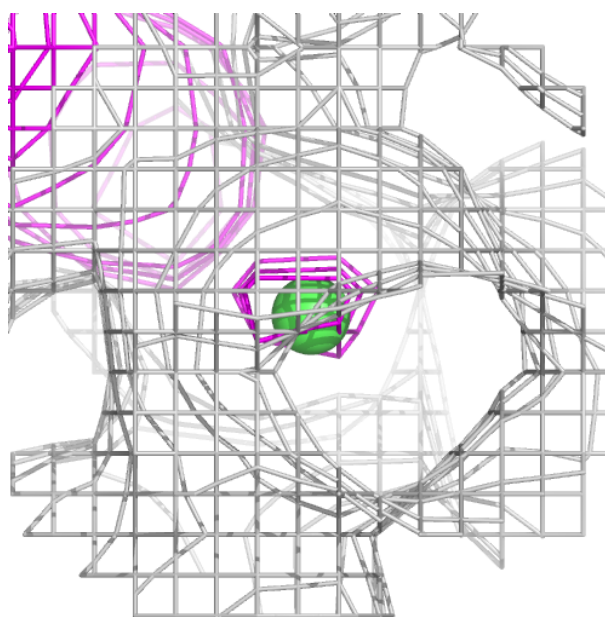
**Electron density around NI E 302:**

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



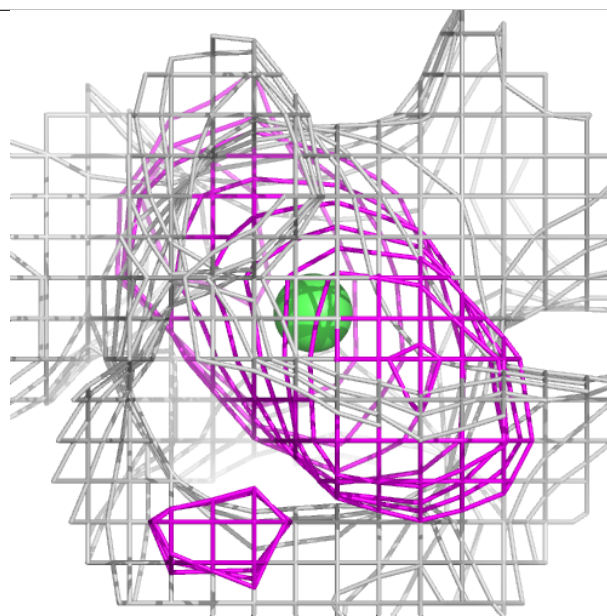
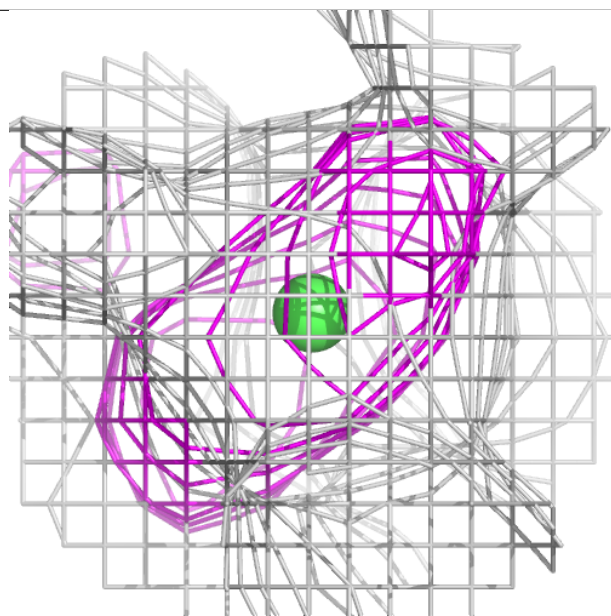
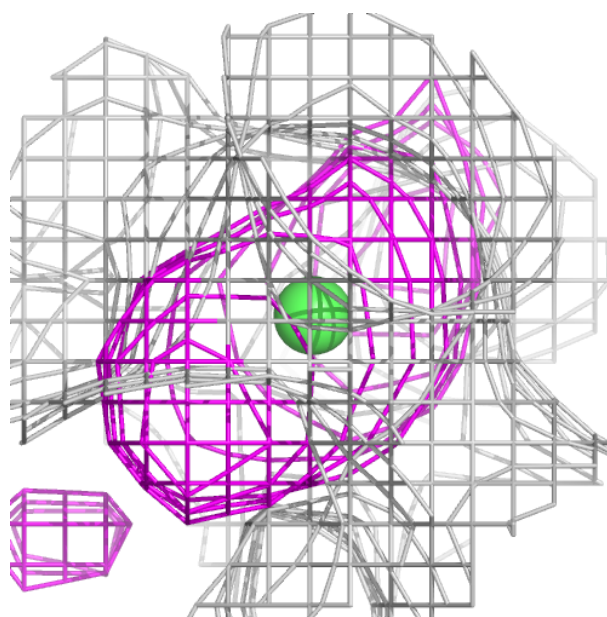
**Electron density around NI F 301:**

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



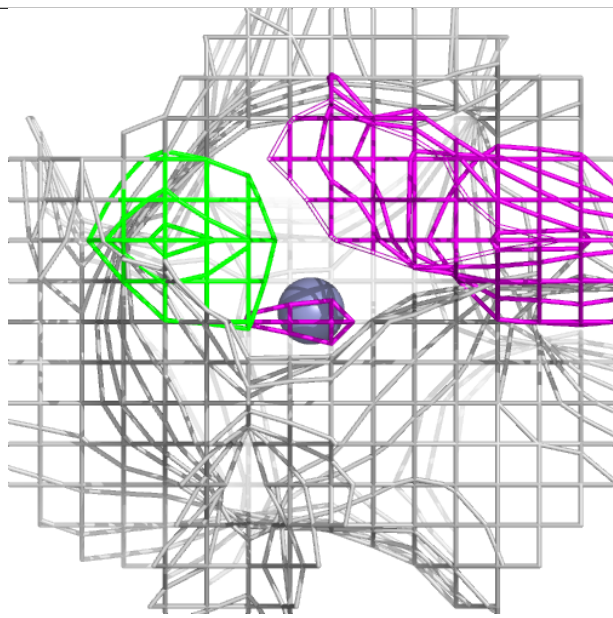
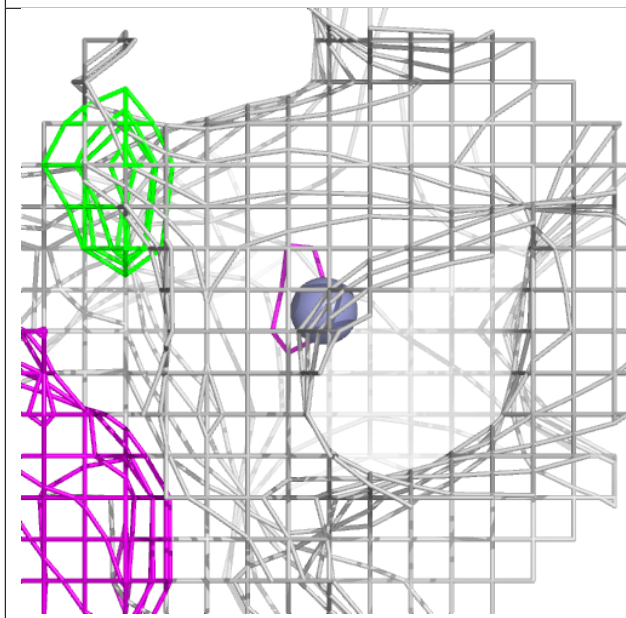
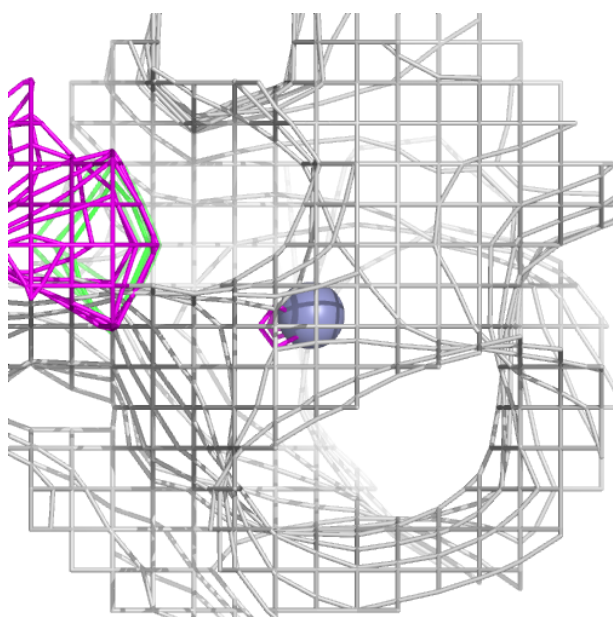
**Electron density around NI F 302:**

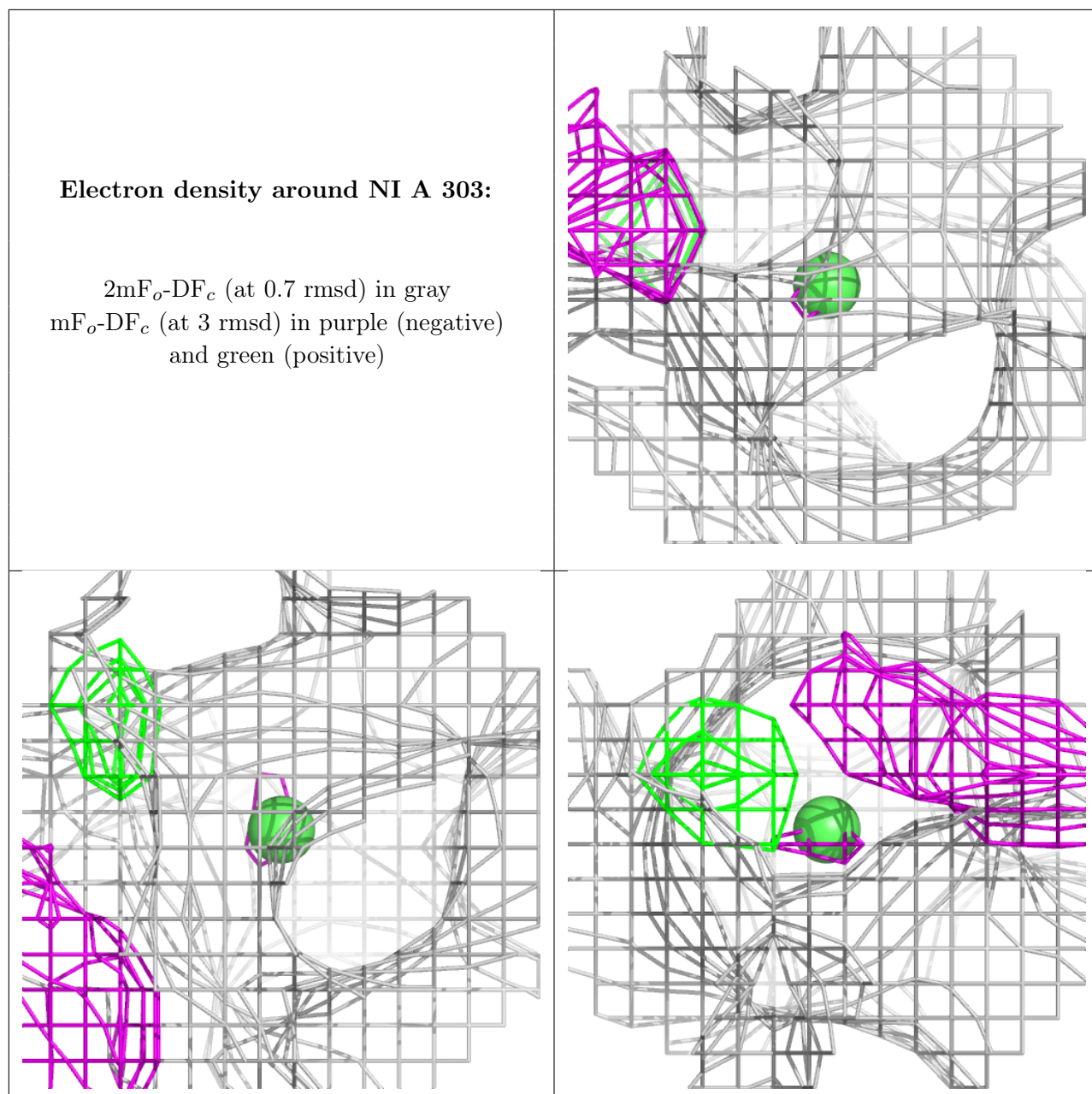
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN A 305:**

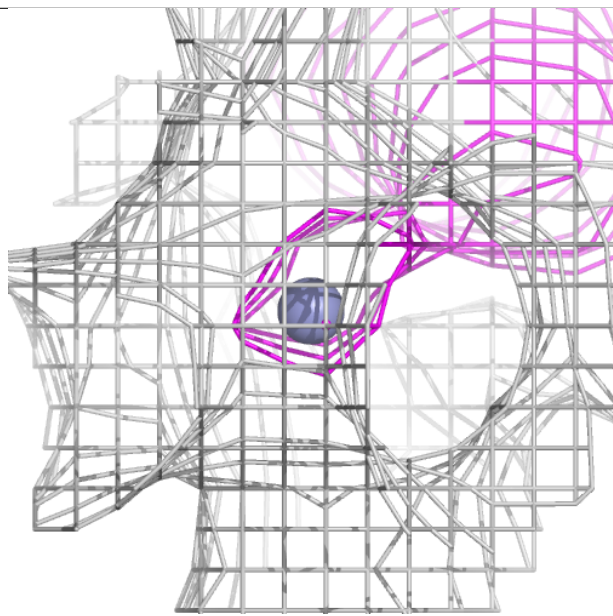
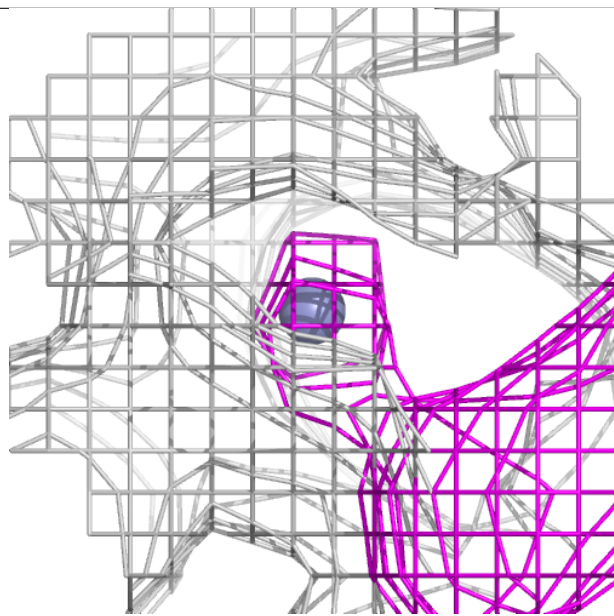
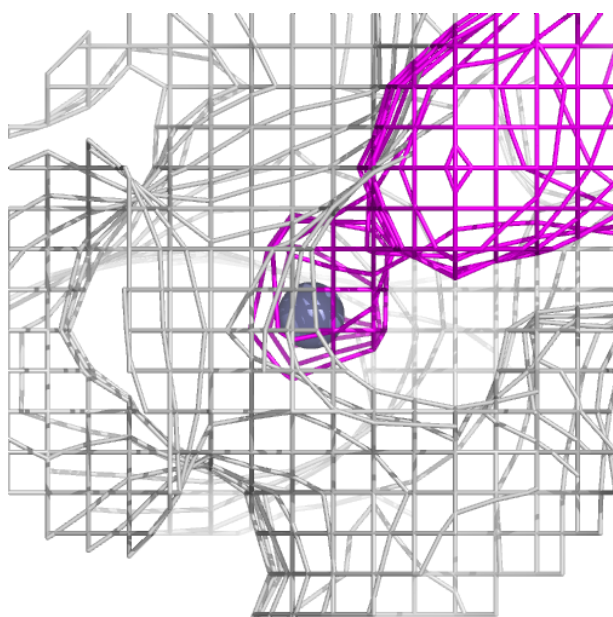
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

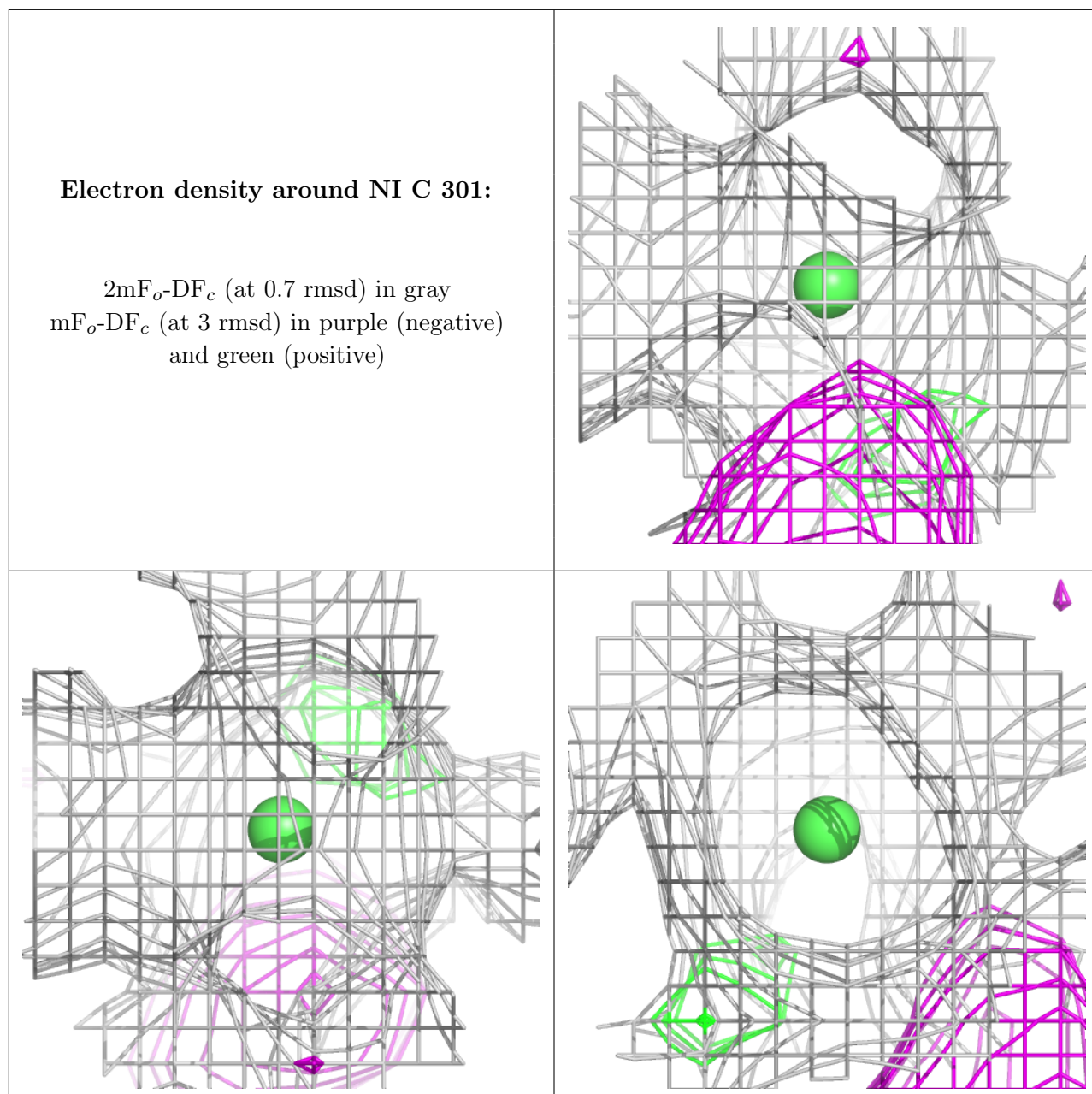




**Electron density around ZN B 303:**

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

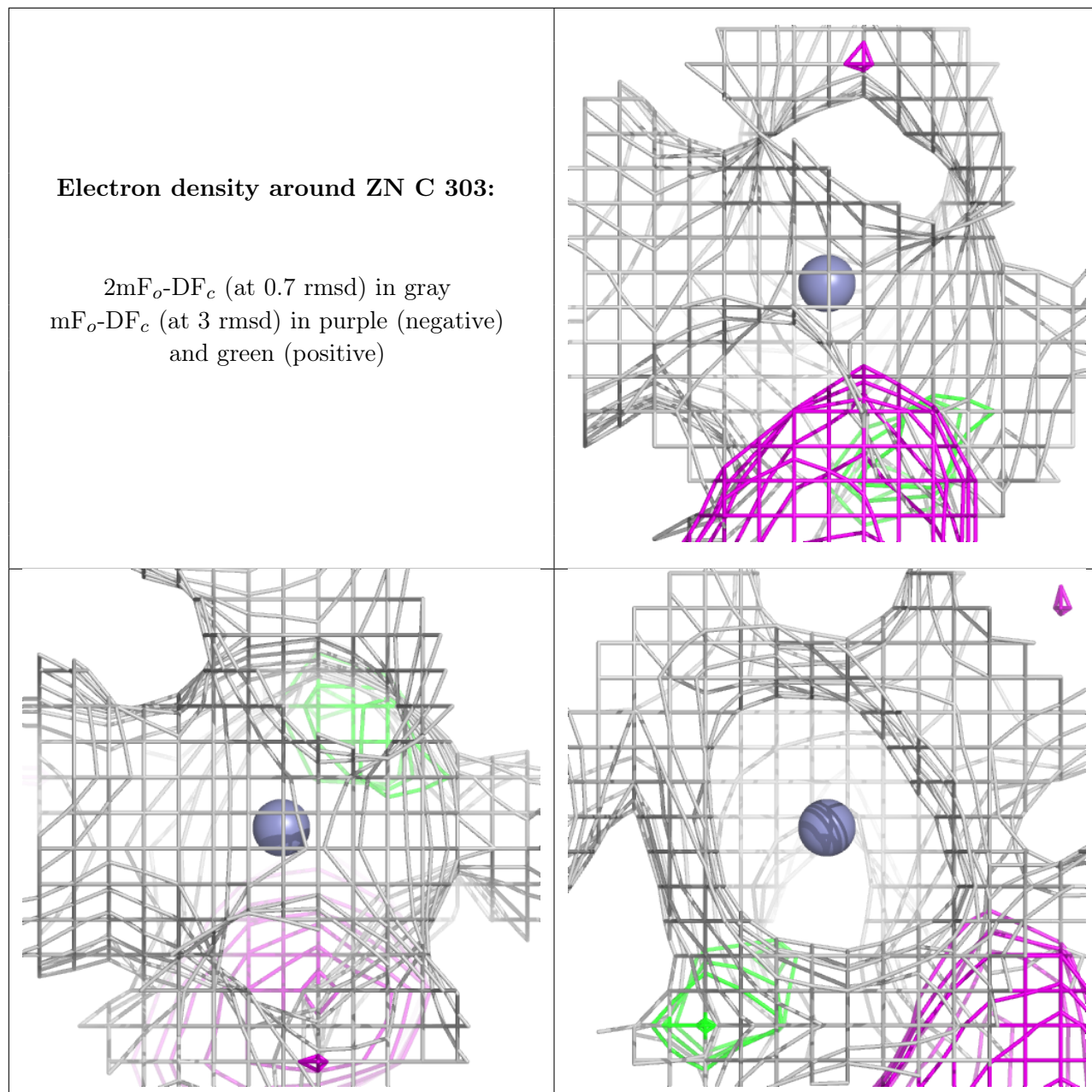


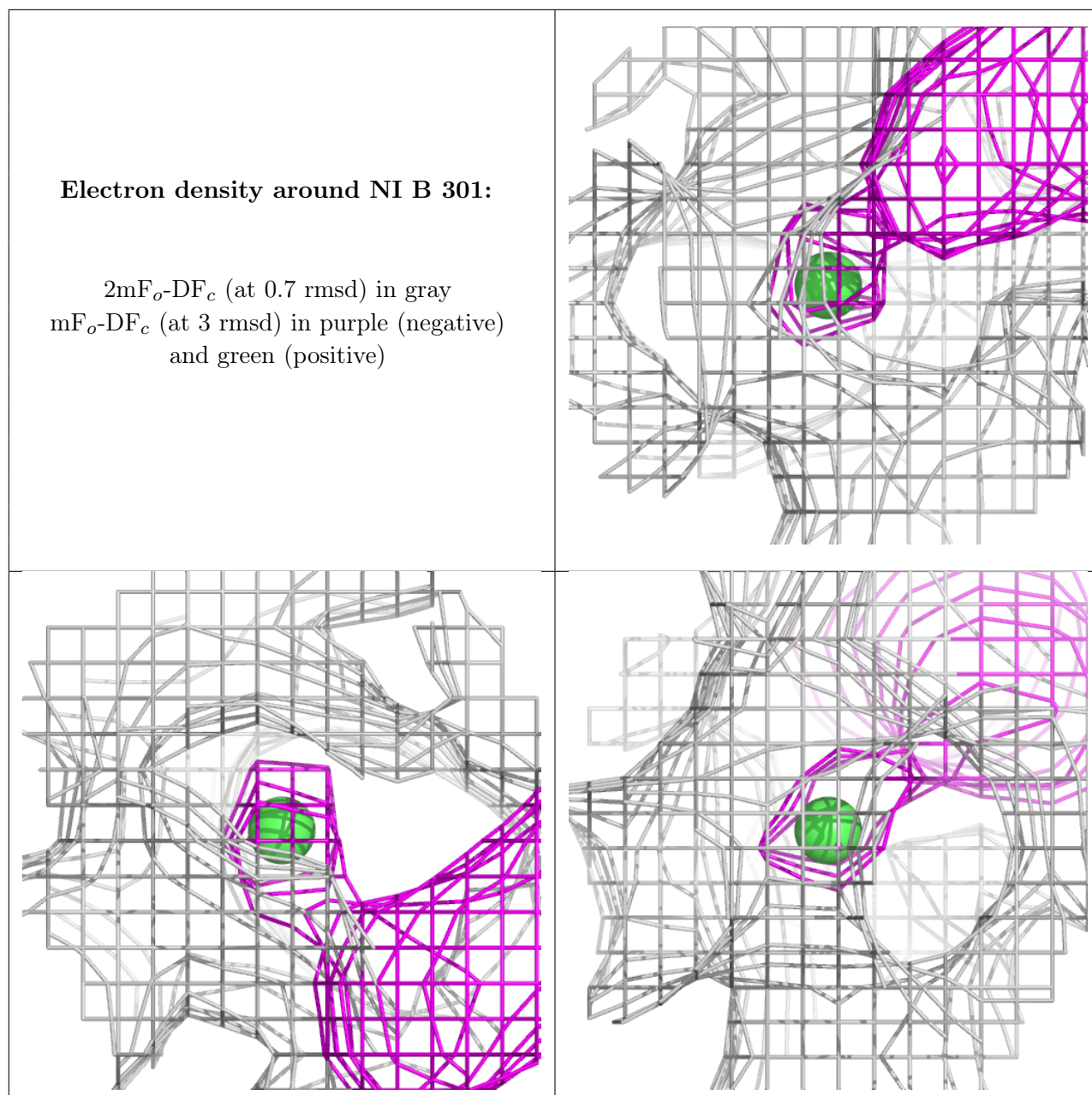




**Electron density around ZN C 303:**

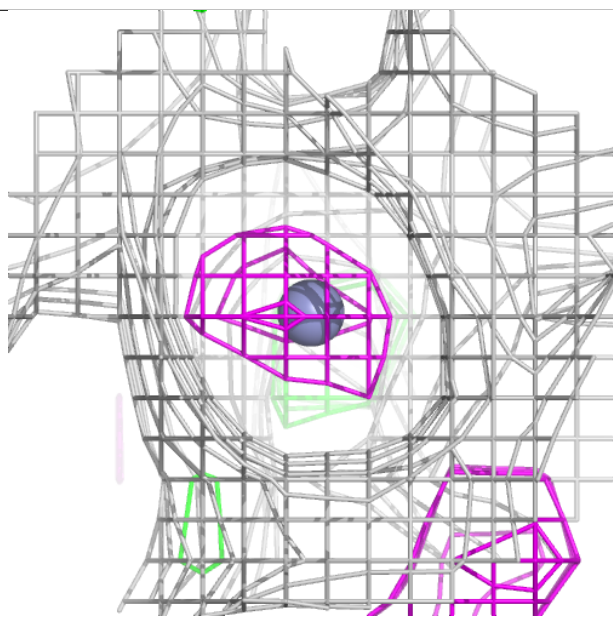
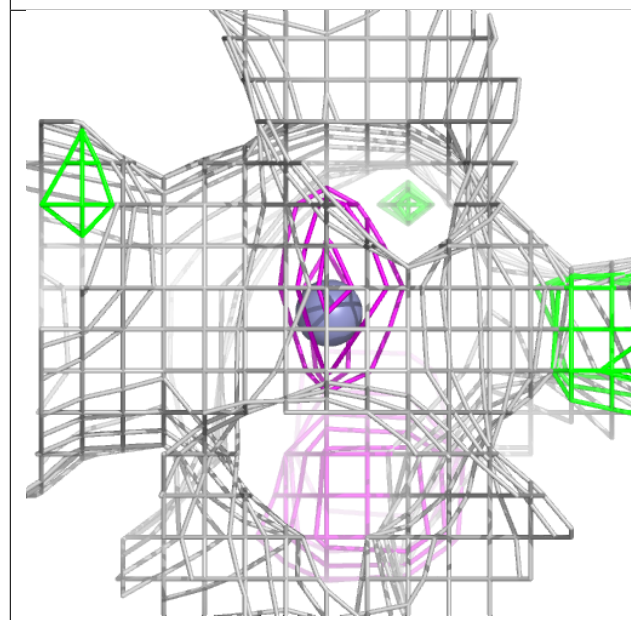
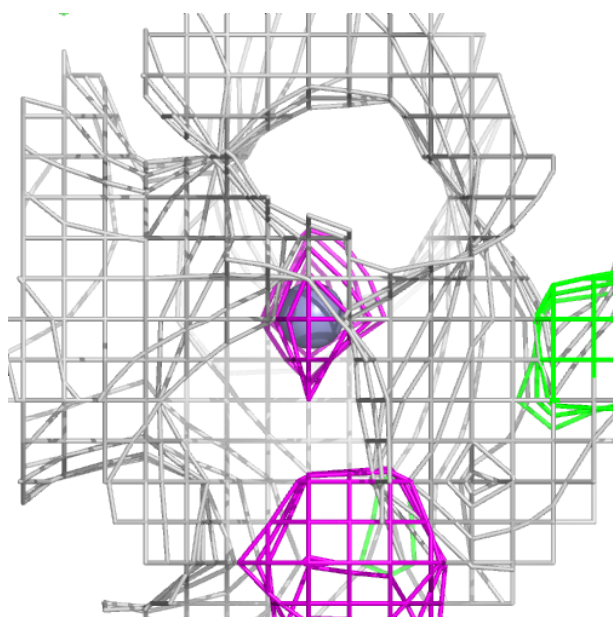
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





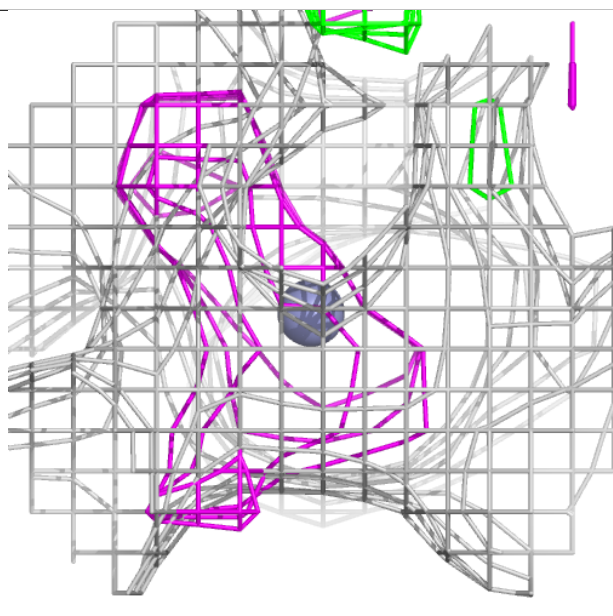
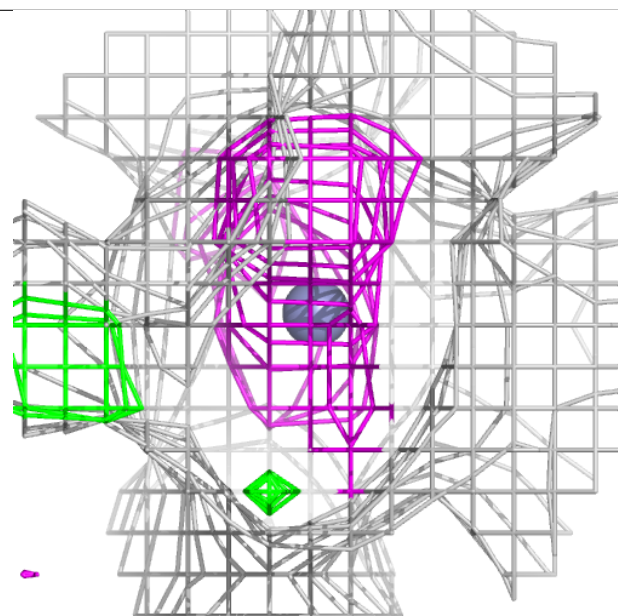
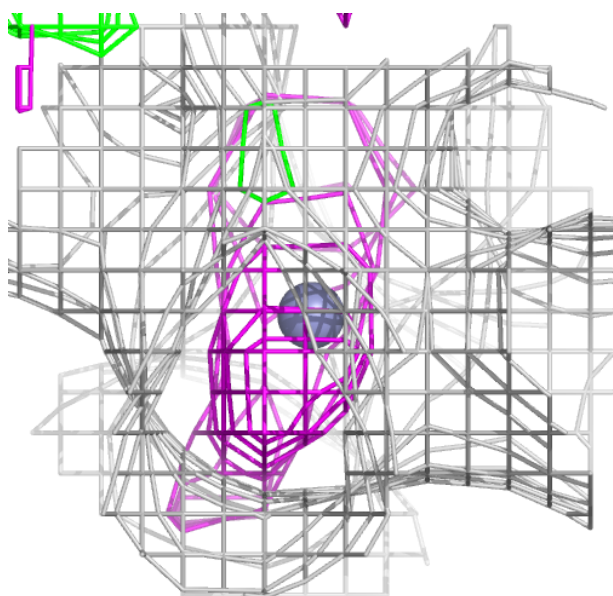
**Electron density around ZN D 305:**

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



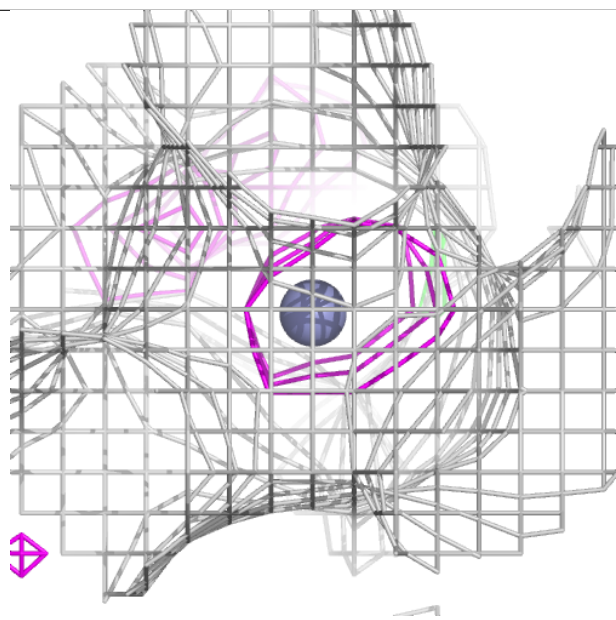
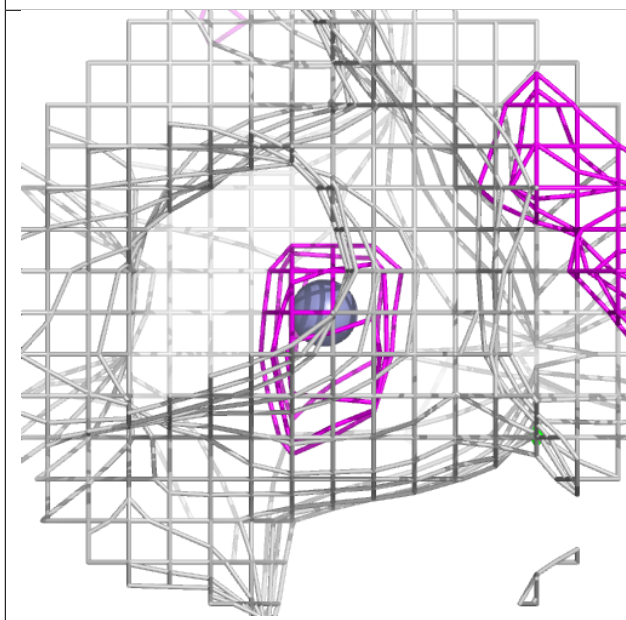
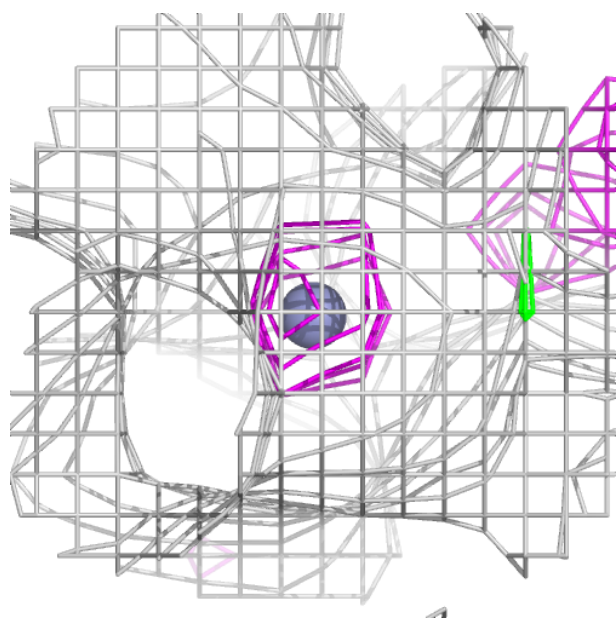
**Electron density around ZN D 306:**

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



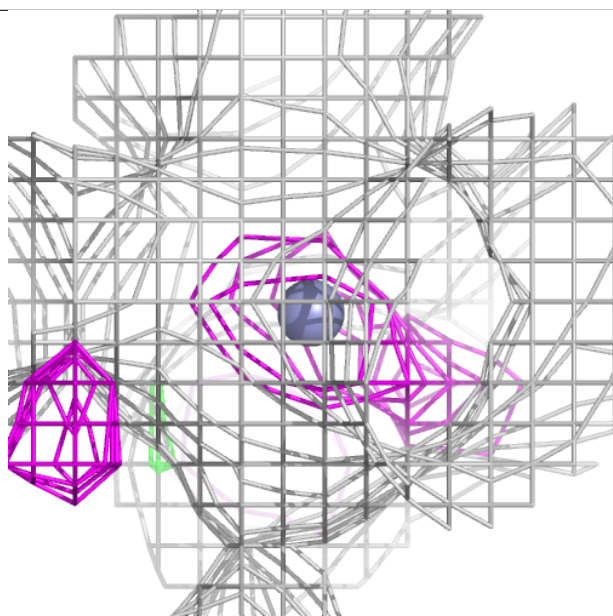
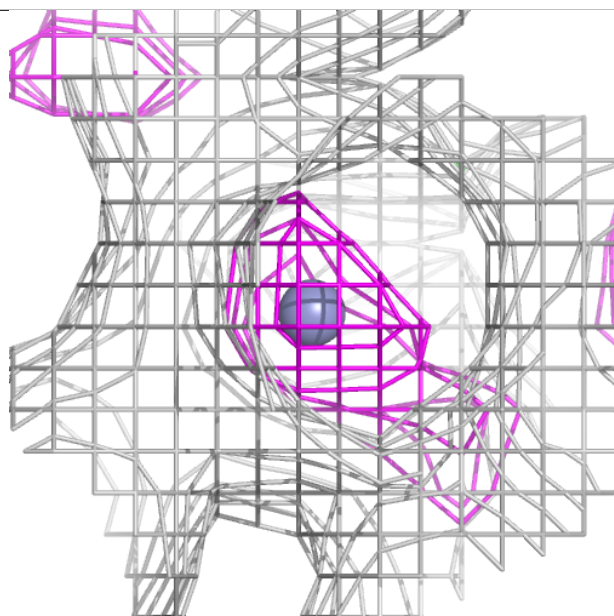
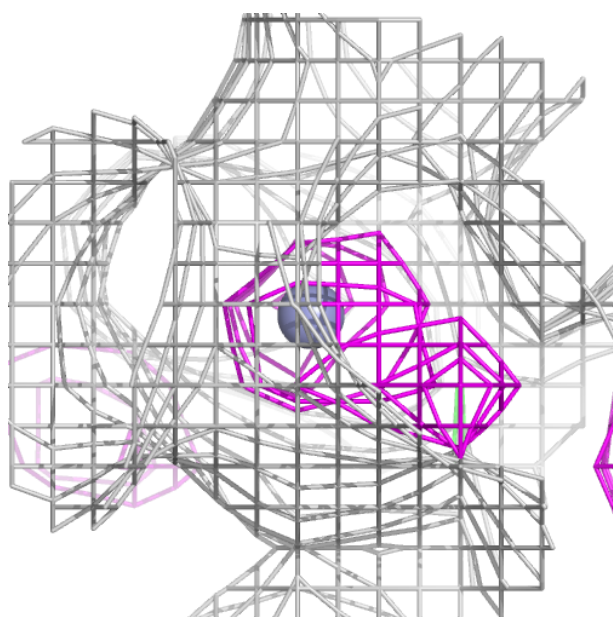
**Electron density around ZN E 303:**

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



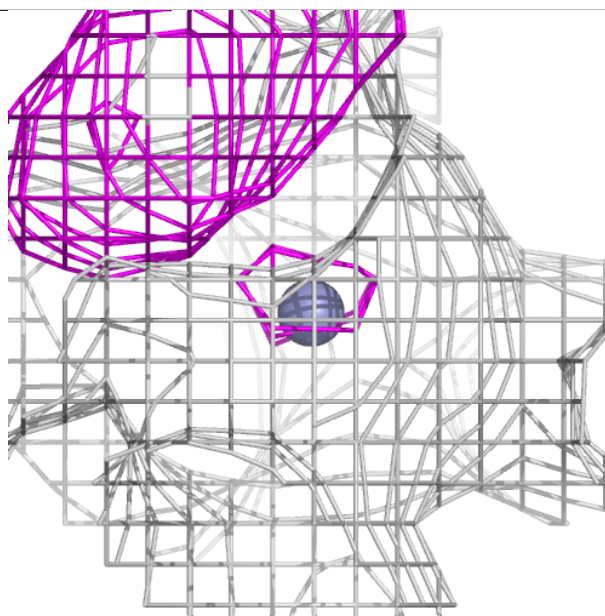
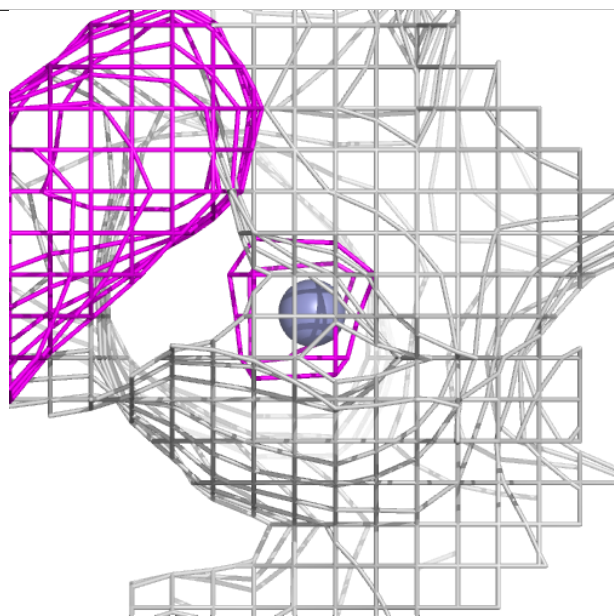
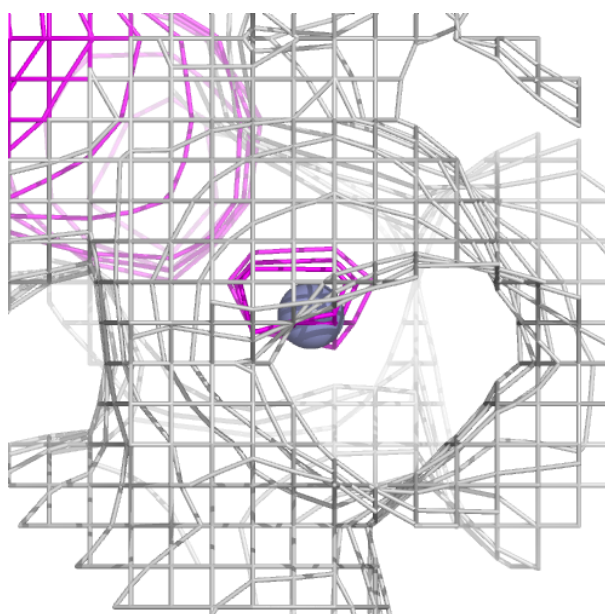
**Electron density around ZN E 304:**

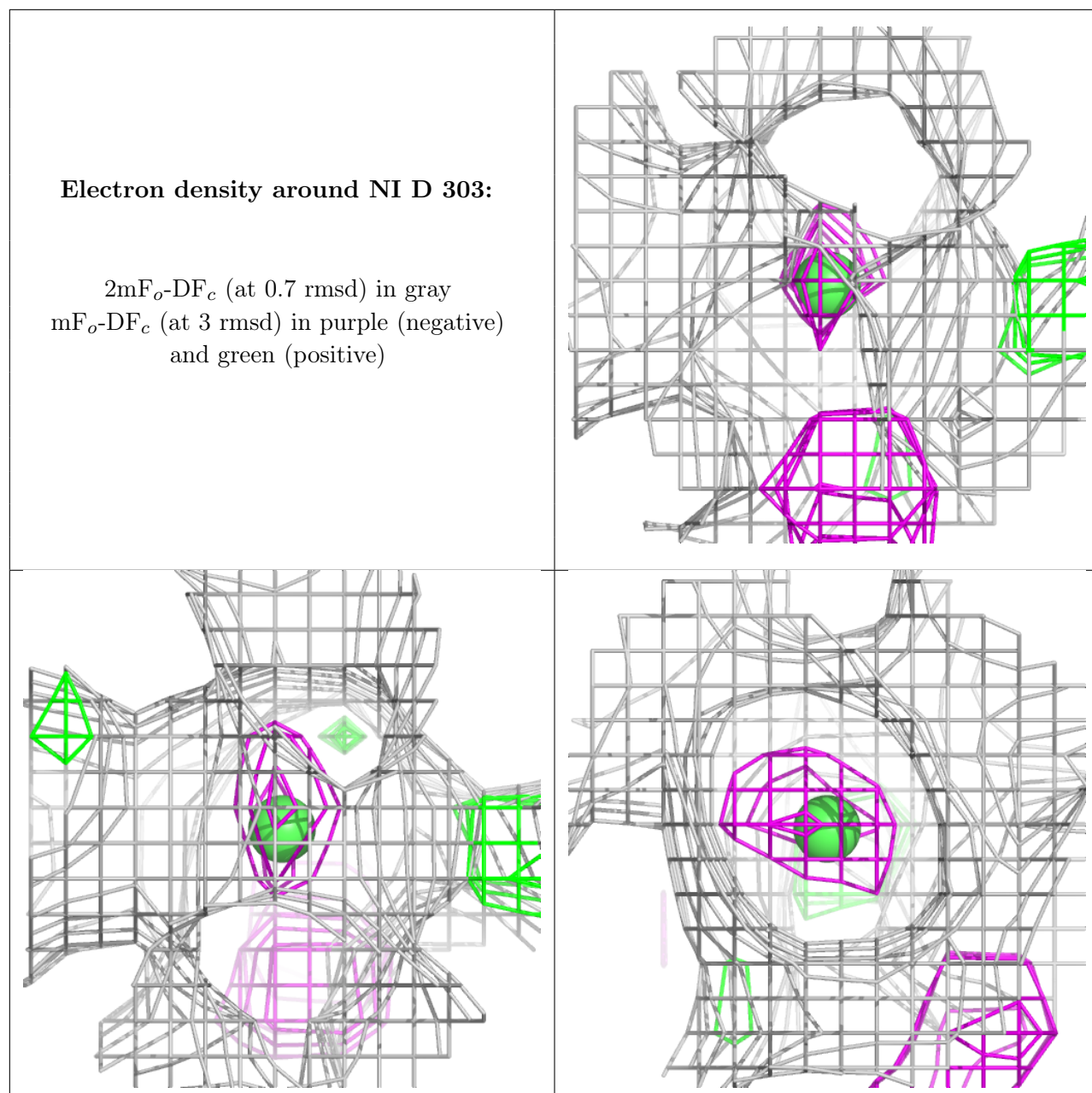
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN F 303:**

$2mF_o-DF_c$  (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.