wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2026 – 05:07 pm BST

PDB ID	:	31NR / pdb_000031nr
Title	:	Crystal structure of nickel-bound deoxyhypusine hydroxylase
Authors	:	Zakaszewski, D.; Wilk, P.; Wator-Wilk, E.; Grudnik, P.
Deposited on	:	2026-06-15
Resolution	:	2.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

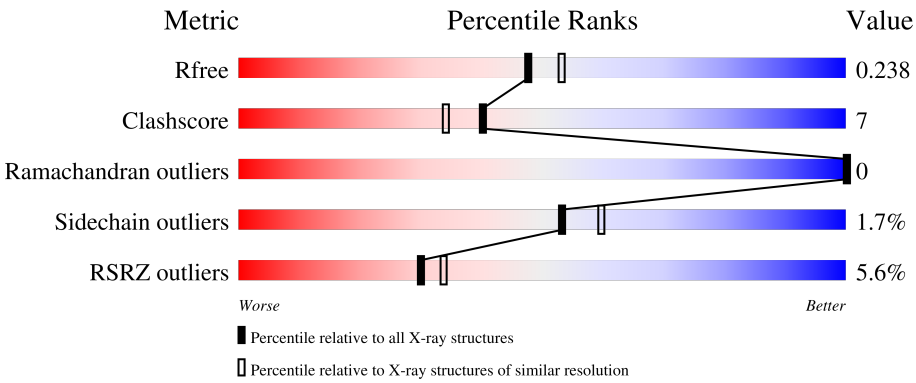
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 <=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	291	7% 83% 15% ••
1	B	291	3% 83% 14% •
1	C	291	6% 81% 18% •
1	D	291	5% 84% 13% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9640 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 Deoxyhypusine hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2207	1374	400	420	13	0	1	0
1	B	282	2159	1344	390	412	13	0	0	0
1	C	288	2210	1376	400	420	14	0	1	0
1	D	282	2167	1349	393	412	13	0	1	0

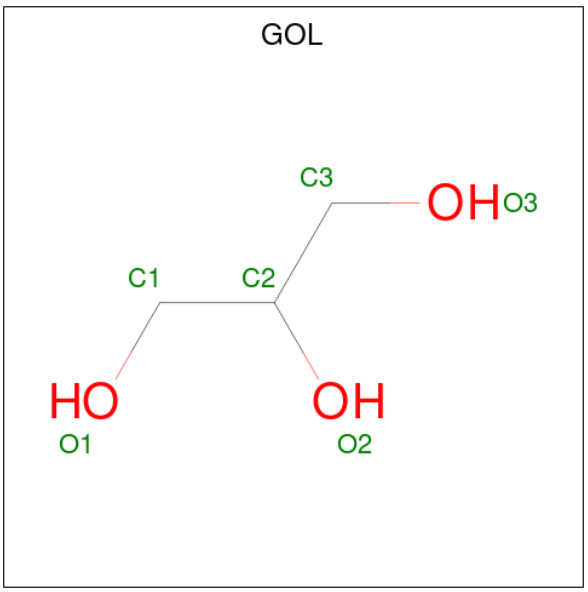
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9BU89
A	-1	SER	-	expression tag	UNP Q9BU89
B	-2	GLY	-	expression tag	UNP Q9BU89
B	-1	SER	-	expression tag	UNP Q9BU89
C	-2	GLY	-	expression tag	UNP Q9BU89
C	-1	SER	-	expression tag	UNP Q9BU89
D	-2	GLY	-	expression tag	UNP Q9BU89
D	-1	SER	-	expression tag	UNP Q9BU89

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	3	3	3	0	0
2	B	4	4	4	0	0
2	C	3	3	3	0	0
2	D	4	4	4	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	231	231	231	0	0
			Total	O		
4	B	192	192	192	0	0
			Total	O		
4	C	236	236	236	0	0

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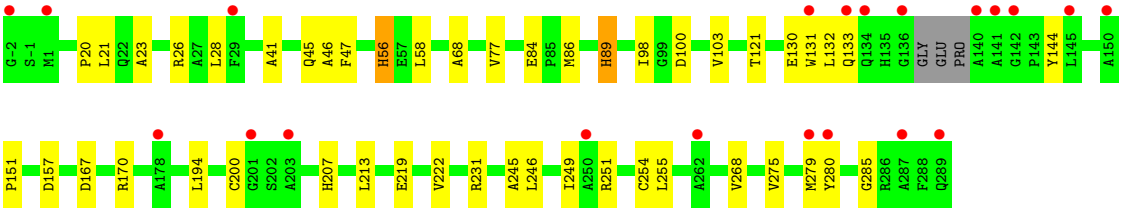
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	176	176	176	0	0

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.

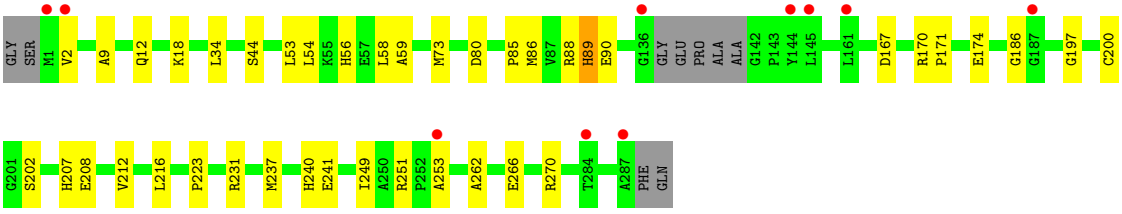
• Molecule 1: Deoxyhypusine hydroxylase

Chain A:



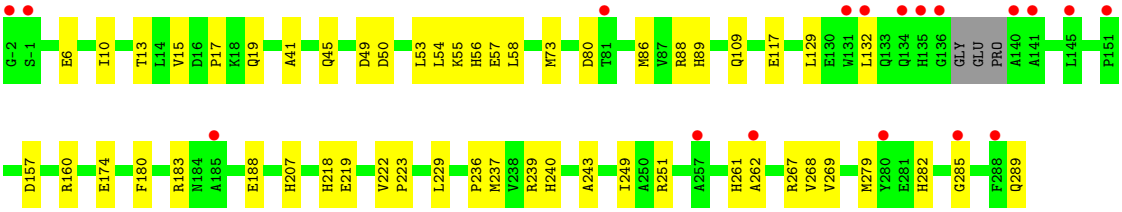
• Molecule 1: Deoxyhypusine hydroxylase

Chain B:



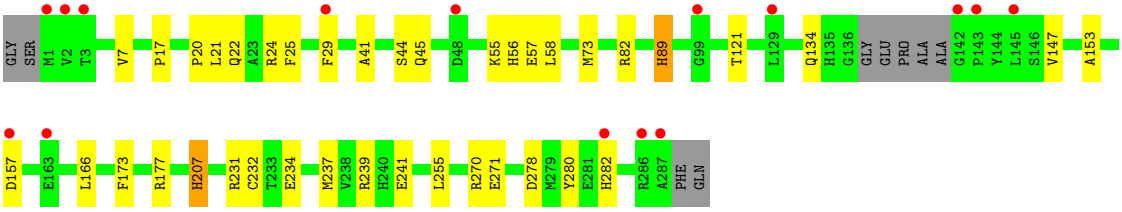
• Molecule 1: Deoxyhypusine hydroxylase

Chain C:



• Molecule 1: Deoxyhypusine hydroxylase

Chain D:


GLY SER M1 V2 T3 V7 P17 P20 L21 Q22 A23 R24 F25 F29 A41 S44 Q45 D48 K55 H56 E57 L58 M73 R82 H89 G99 T121 L129 Q134 H135 G136 GLY GLU PRO ALA ALA G142 P143 Y144 L145 S146 V147 A153
D157 E163 L166 F173 R177 H207 R231 C232 T233 E234 M237 V238 R239 H240 E241 L255 R270 E271 D278 M279 Y280 E281 H282 R286 A287 PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.21Å 60.28Å 88.91Å 93.48° 100.50° 101.65°	Depositor
Resolution (Å)	37.34 – 2.16 37.34 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.34-2.16) 99.7 (37.34-2.16)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.16Å)	Xtriage
Refinement program	PHENIX 2.0	Depositor
R, R_{free}	0.227 , 0.239 0.227 , 0.238	Depositor DCC
R_{free} test set	1920 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 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	0.48	0/2250	0.64	0/3052
1	B	0.47	0/2198	0.68	0/2983
1	C	0.43	0/2253	0.61	0/3055
1	D	0.52	0/2209	0.72	0/2997
All	All	0.47	0/8910	0.66	0/12087

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	ARG	Sidechain
1	B	231	ARG	Sidechain
1	D	270	ARG	Sidechain

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	A	2207	0	2161	30	0
1	B	2159	0	2113	24	0
1	C	2210	0	2168	34	0
1	D	2167	0	2126	27	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
3	A	12	0	14	0	0
3	B	18	0	22	0	0
3	C	6	0	6	0	0
3	D	12	0	14	0	0
4	A	231	0	0	7	0
4	B	192	0	0	6	0
4	C	236	0	0	12	0
4	D	176	0	0	10	0
All	All	9640	0	8624	115	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.

The worst 5 of 115 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:D:282:HIS:HE1	4:D:501:HOH:O	1.35	1.09
1:D:29:PHE:CZ	4:D:560:HOH:O	2.32	0.81
1:B:186:GLY:HA2	1:B:216:LEU:HD11	1.65	0.77
1:D:29:PHE:HZ	4:D:560:HOH:O	1.68	0.74
1:A:279:MET:HG2	4:A:602:HOH:O	1.91	0.70

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	285/291 (98%)	280 (98%)	5 (2%)	0	100	100
1	B	278/291 (96%)	277 (100%)	1 (0%)	0	100	100
1	C	285/291 (98%)	281 (99%)	4 (1%)	0	100	100
1	D	279/291 (96%)	275 (99%)	4 (1%)	0	100	100
All	All	1127/1164 (97%)	1113 (99%)	14 (1%)	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	A	222/224 (99%)	219 (99%)	3 (1%)	59	66
1	B	218/224 (97%)	214 (98%)	4 (2%)	51	58
1	C	223/224 (100%)	220 (99%)	3 (1%)	61	68
1	D	219/224 (98%)	214 (98%)	5 (2%)	44	49
All	All	882/896 (98%)	867 (98%)	15 (2%)	53	60

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	56	HIS
1	D	134	GLN
1	C	89	HIS

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Mol	Chain	Res	Type
1	D	207	HIS
1	D	56	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	C	133	GLN
1	D	45	GLN
1	D	135	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 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	GOL	A	305	-	5,5,5	0.09	0	5,5,5	0.37	0
3	GOL	B	305	2	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	A	304	2	5,5,5	0.28	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	307	-	5,5,5	0.09	0	5,5,5	0.32	0
3	GOL	B	306	-	5,5,5	0.08	0	5,5,5	0.26	0
3	GOL	D	305	2	5,5,5	0.27	0	5,5,5	0.56	0
3	GOL	C	304	2	5,5,5	0.31	0	5,5,5	0.56	0
3	GOL	D	306	-	5,5,5	0.09	0	5,5,5	0.31	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
3	GOL	A	305	-	-	0/4/4/4	-
3	GOL	B	305	2	-	0/4/4/4	-
3	GOL	A	304	2	-	0/4/4/4	-
3	GOL	B	307	-	-	0/4/4/4	-
3	GOL	B	306	-	-	0/4/4/4	-
3	GOL	D	305	2	-	0/4/4/4	-
3	GOL	C	304	2	-	2/4/4/4	-
3	GOL	D	306	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	304	GOL	O1-C1-C2-C3
3	C	304	GOL	O1-C1-C2-O2

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	A	288/291 (98%)	0.67	21 (7%)	21	24	15, 29, 44, 65	1 (0%)
1	B	282/291 (96%)	0.60	10 (3%)	47	51	22, 30, 49, 70	0
1	C	288/291 (98%)	0.63	18 (6%)	26	29	16, 29, 45, 70	1 (0%)
1	D	282/291 (96%)	0.58	15 (5%)	32	36	17, 29, 48, 67	1 (0%)
All	All	1140/1164 (97%)	0.62	64 (5%)	30	34	15, 29, 48, 70	3 (0%)

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	ALA	4.5
1	B	253	ALA	4.1
1	C	140	ALA	3.9
1	D	287	ALA	3.7
1	D	286	ARG	3.6

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

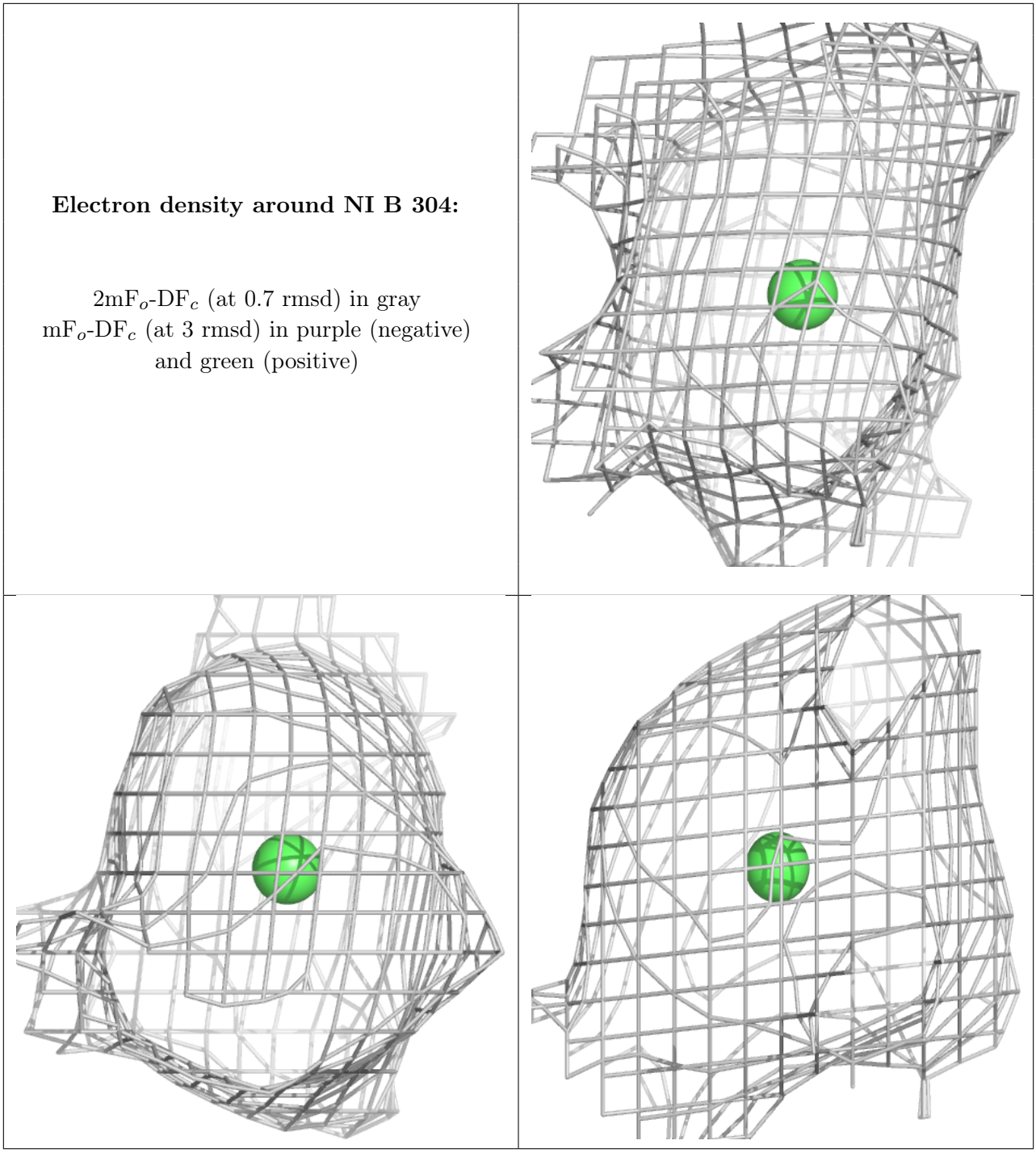
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	307	6/6	0.72	0.20	44,46,48,49	0
3	GOL	B	306	6/6	0.79	0.14	36,39,42,44	0
3	GOL	A	305	6/6	0.83	0.13	39,40,42,46	0
3	GOL	D	306	6/6	0.84	0.12	33,34,35,44	0
3	GOL	C	304	6/6	0.91	0.13	21,24,28,29	0
2	NI	B	304	1/1	0.92	0.09	77,77,77,77	0
2	NI	D	301	1/1	0.92	0.08	83,83,83,83	0
3	GOL	A	304	6/6	0.92	0.12	17,24,25,28	0
2	NI	B	301	1/1	0.92	0.12	76,76,76,76	0
3	GOL	D	305	6/6	0.93	0.09	24,26,28,29	0
3	GOL	B	305	6/6	0.95	0.08	19,26,27,27	0
2	NI	A	303	1/1	0.95	0.05	64,64,64,64	0
2	NI	D	304	1/1	0.95	0.11	78,78,78,78	0
2	NI	C	303	1/1	0.96	0.05	61,61,61,61	0
2	NI	A	302	1/1	0.98	0.03	32,32,32,32	0
2	NI	D	303	1/1	0.99	0.03	31,31,31,31	0
2	NI	C	301	1/1	0.99	0.02	24,24,24,24	0
2	NI	C	302	1/1	0.99	0.02	34,34,34,34	0
2	NI	B	302	1/1	0.99	0.01	23,23,23,23	0
2	NI	A	301	1/1	0.99	0.02	23,23,23,23	0
2	NI	B	303	1/1	1.00	0.01	31,31,31,31	0
2	NI	D	302	1/1	1.00	0.01	22,22,22,22	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.

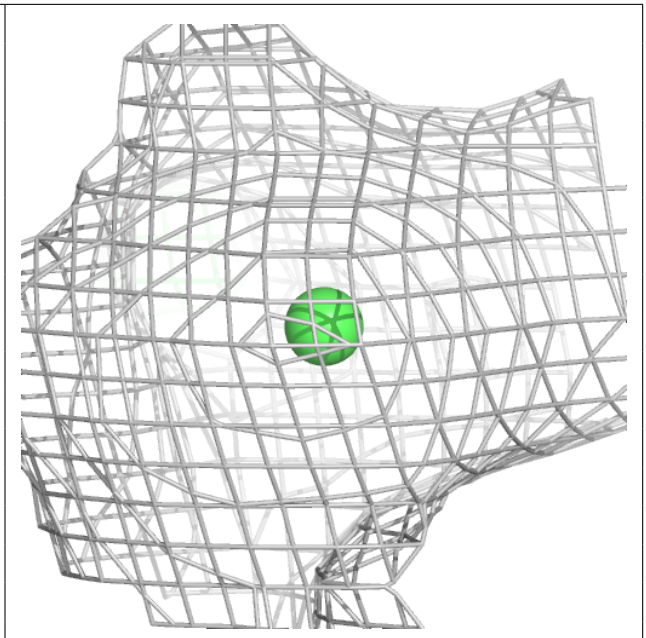
Electron density around NI B 304:

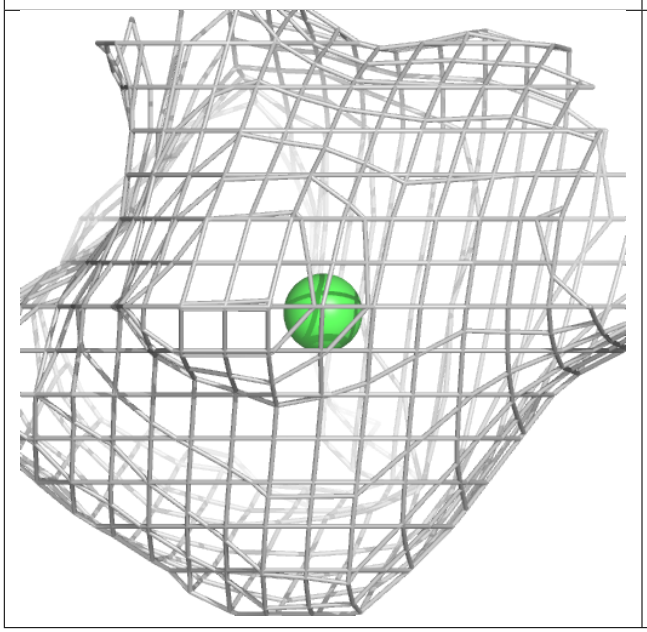
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

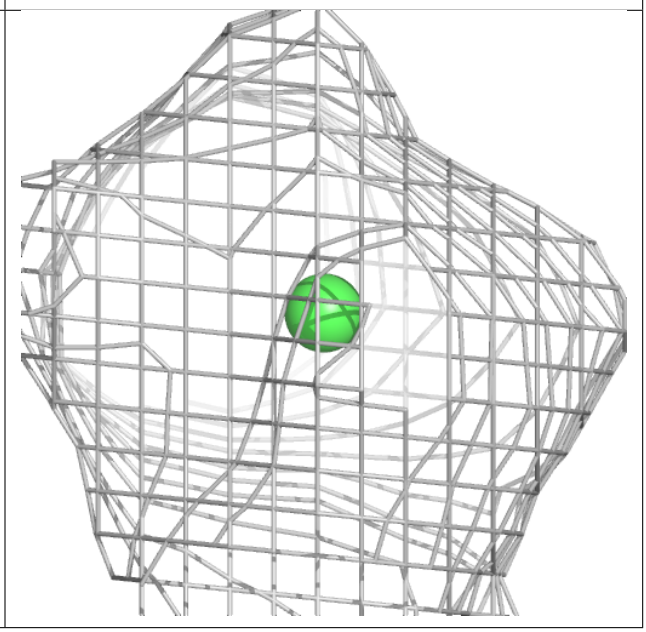


Electron density around NI D 301:

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

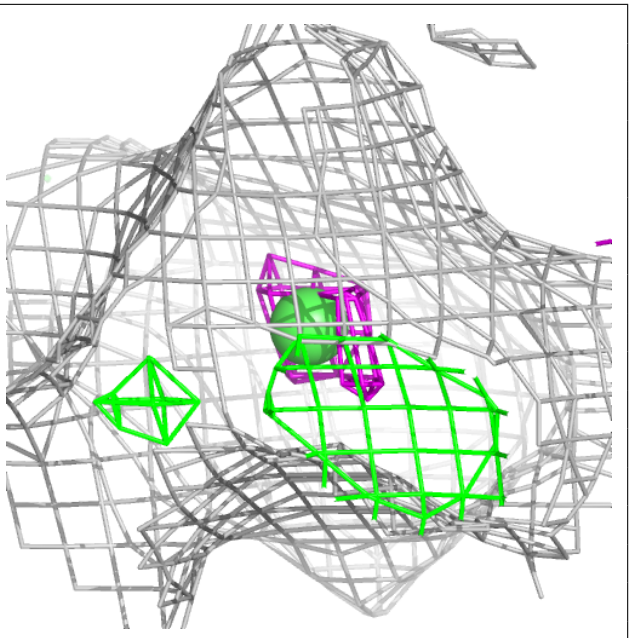


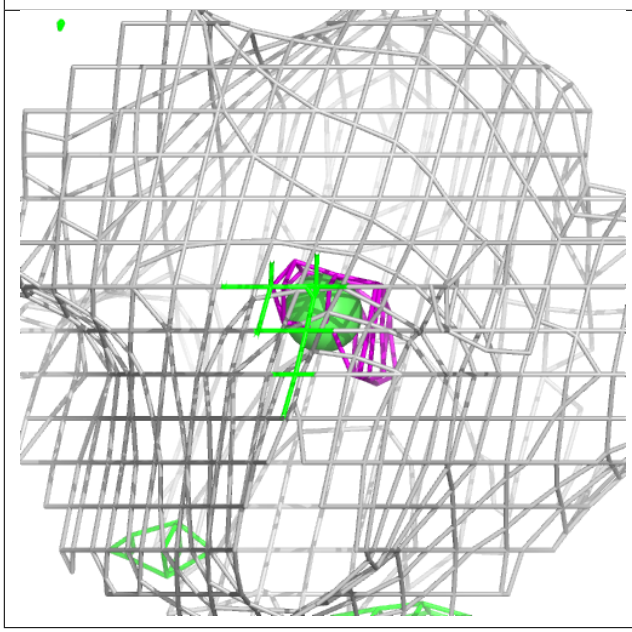


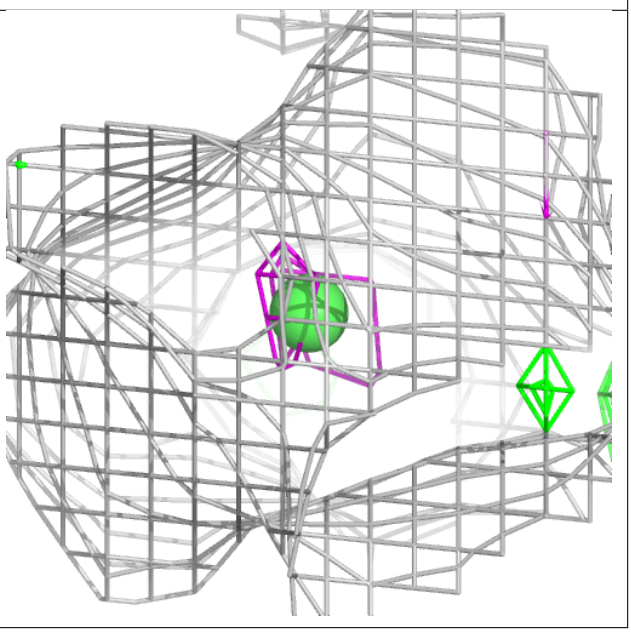


Electron density around NI B 301:

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

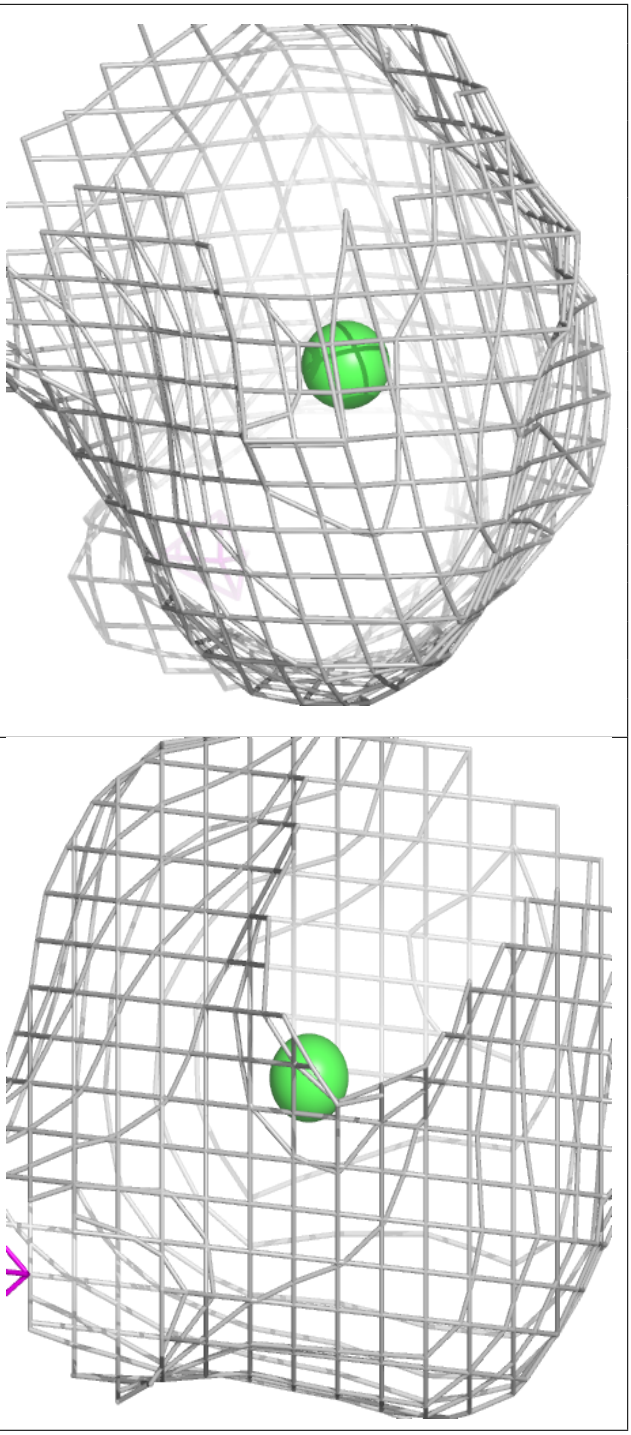






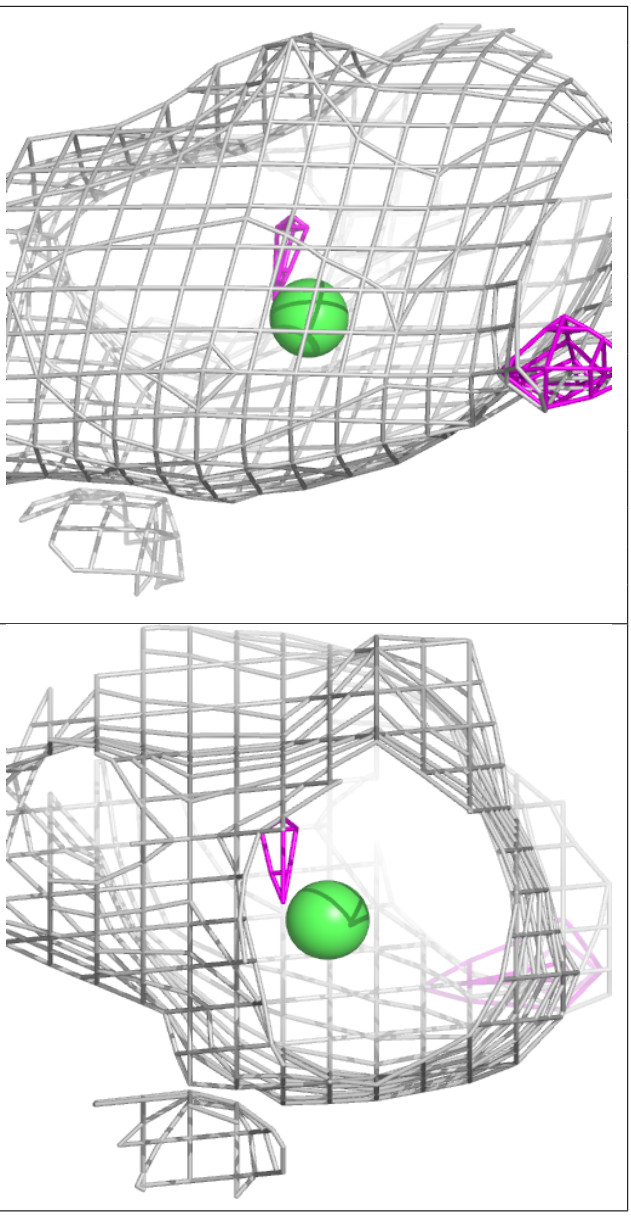
Electron density around NI A 303:

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



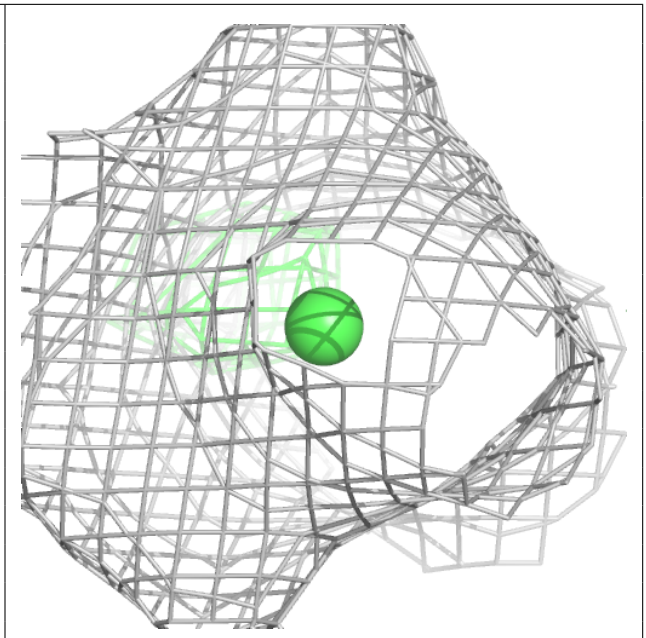
Electron density around NI D 304:

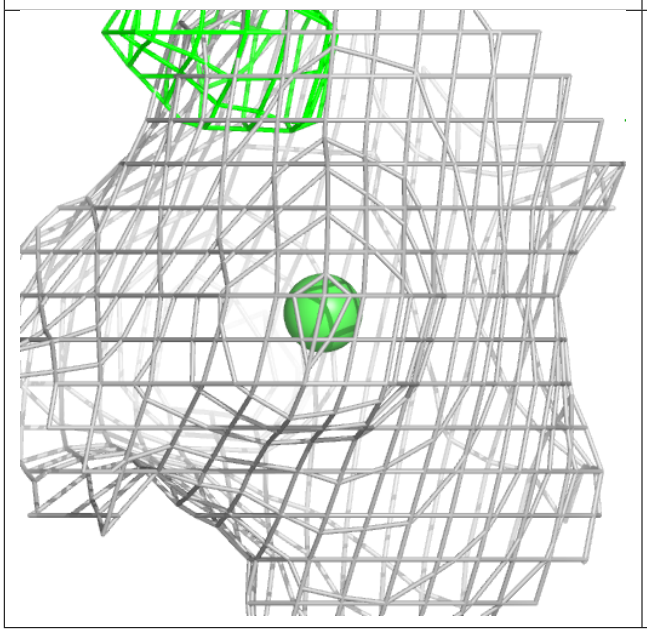
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

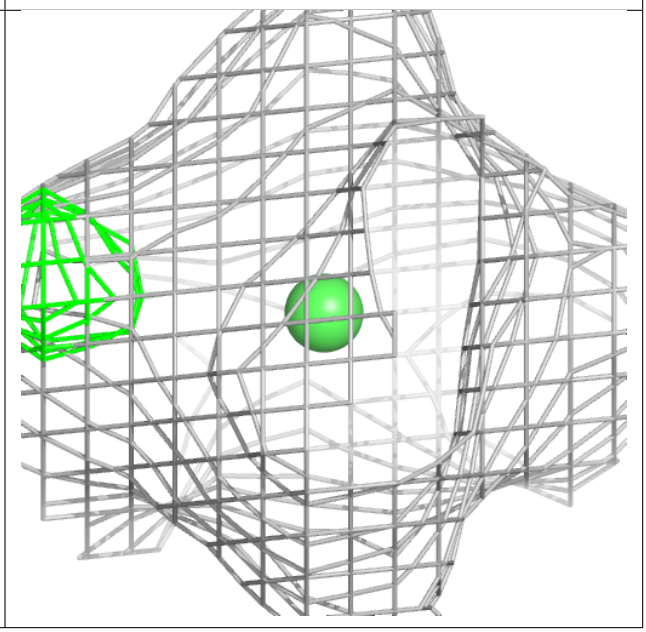


Electron density around NI C 303:

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

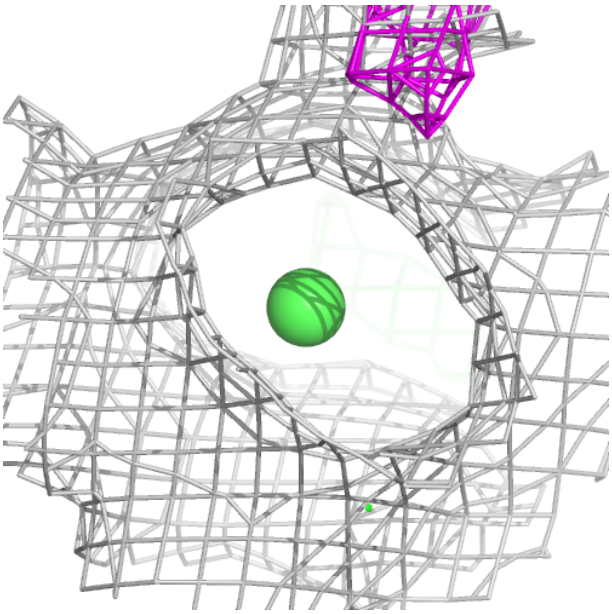


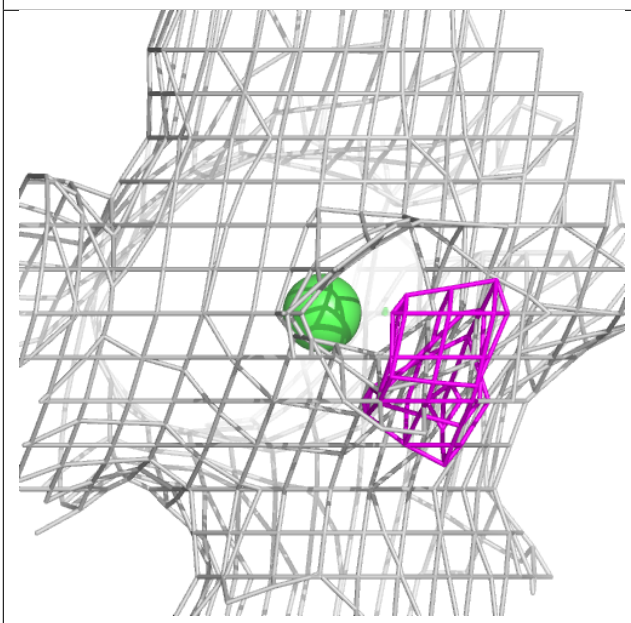


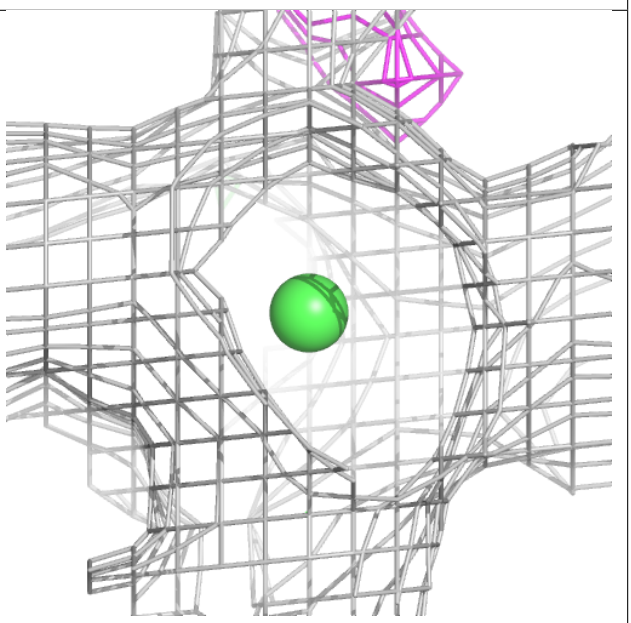


Electron density around NI A 302:

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

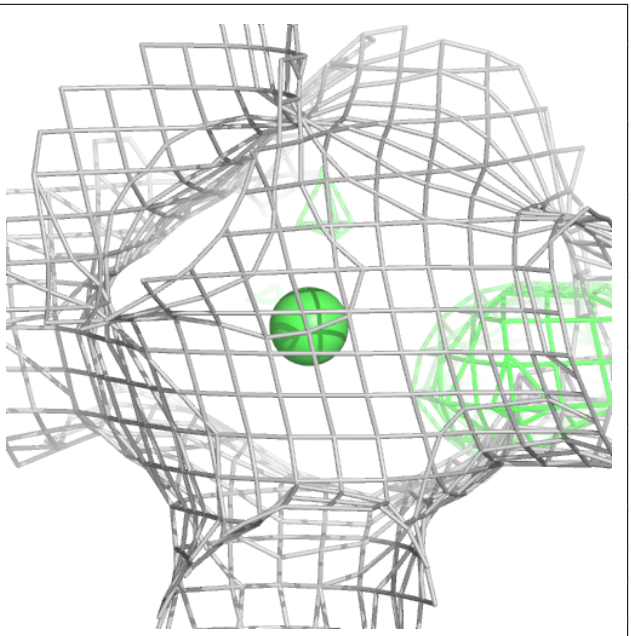


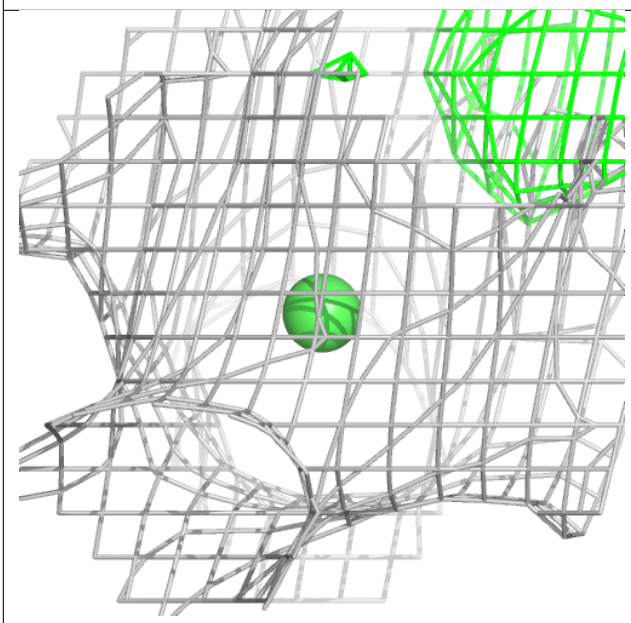


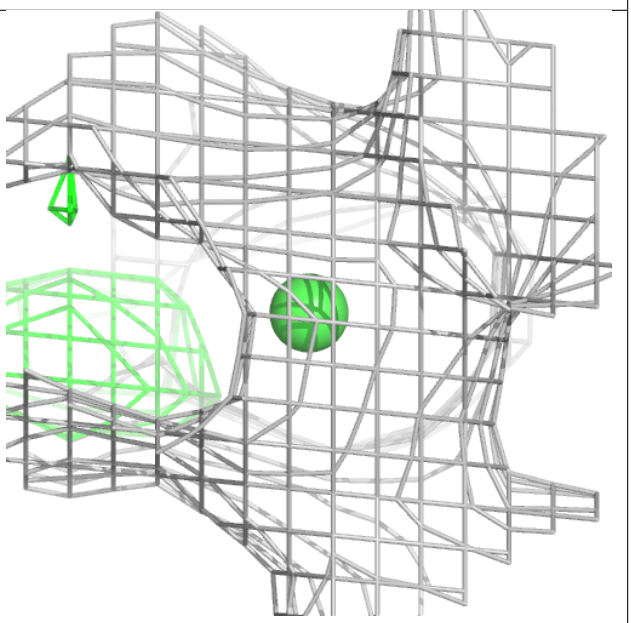


Electron density around NI D 303:

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

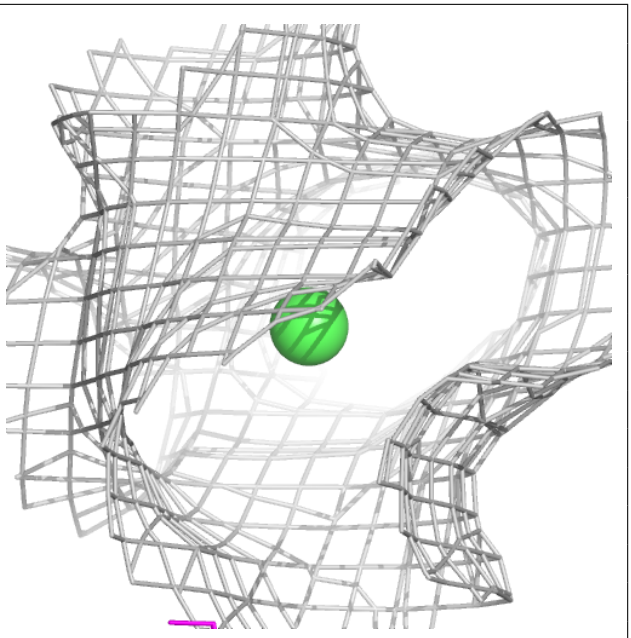


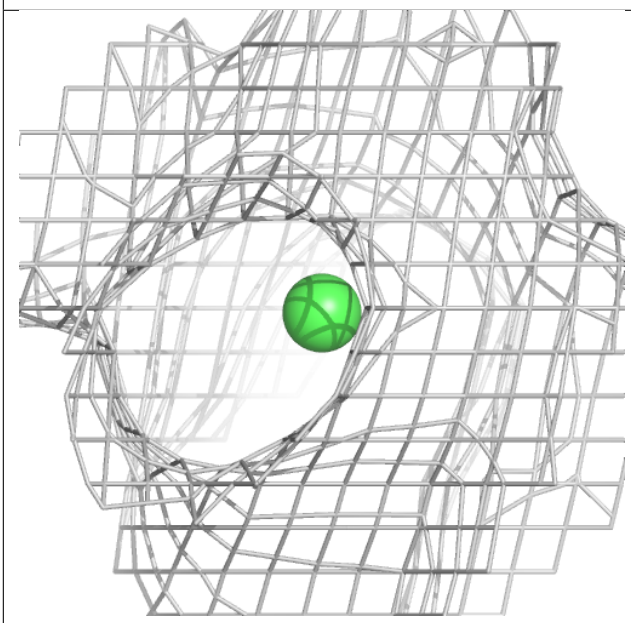


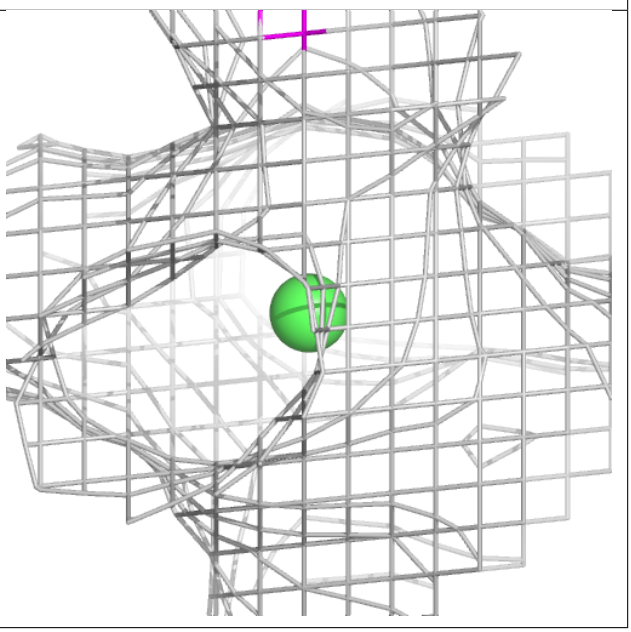


Electron density around NI C 301:

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

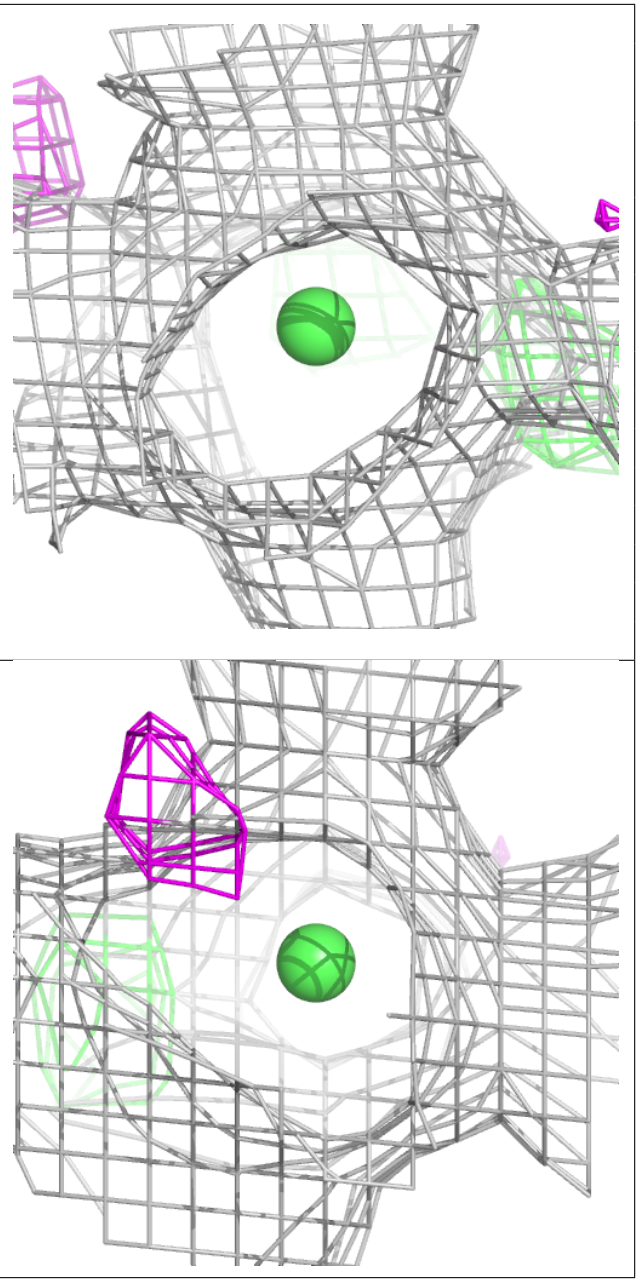






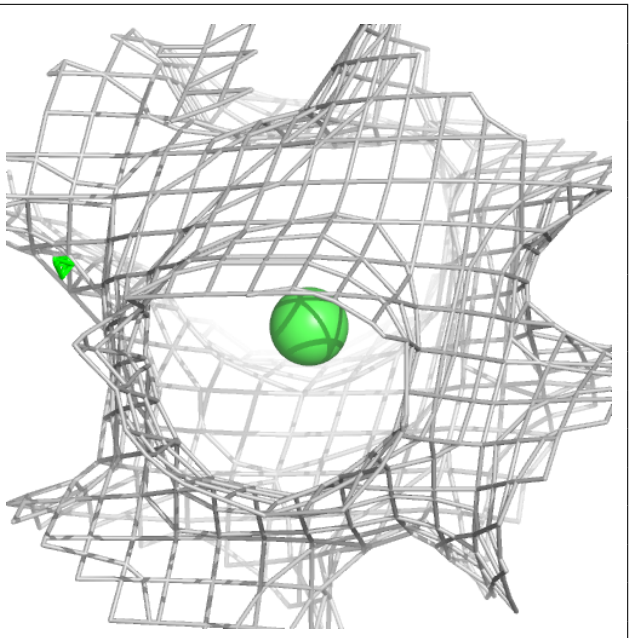
Electron density around NI C 302:

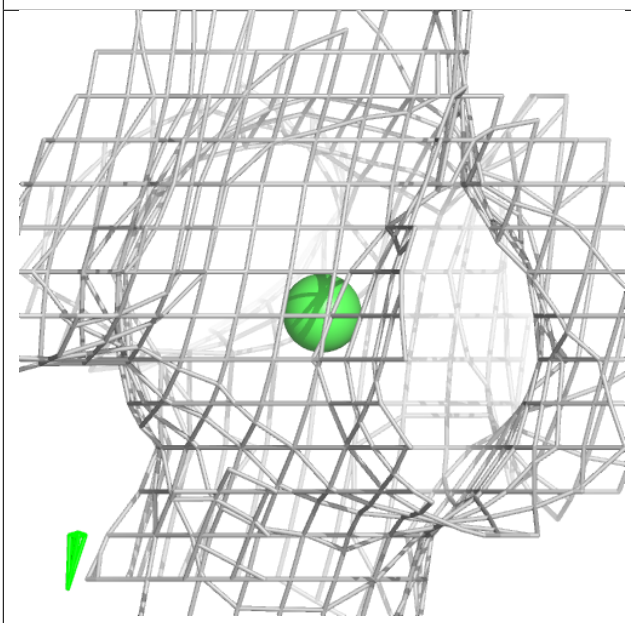
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

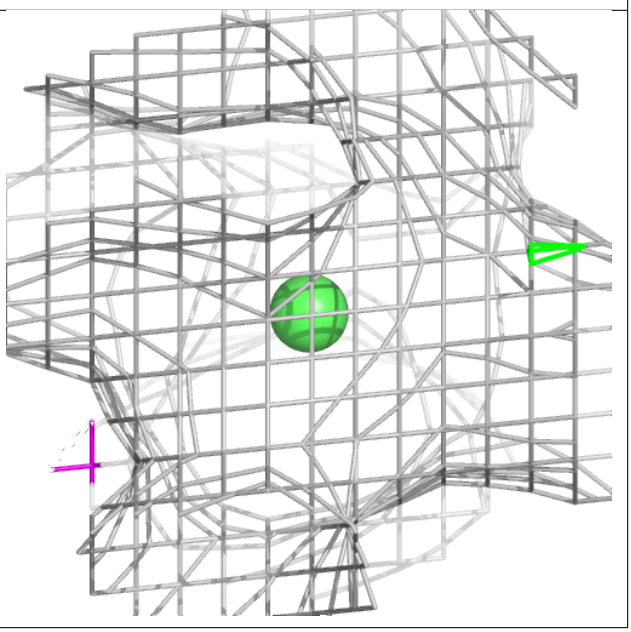


Electron density around NI B 302:

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

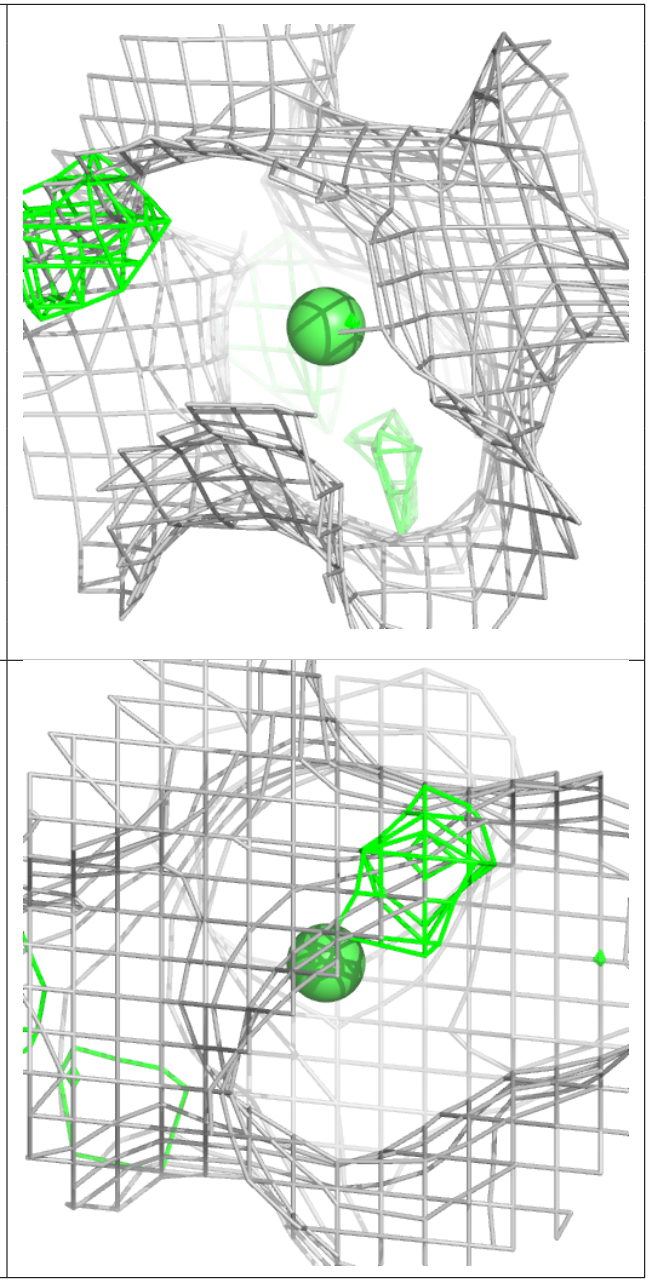






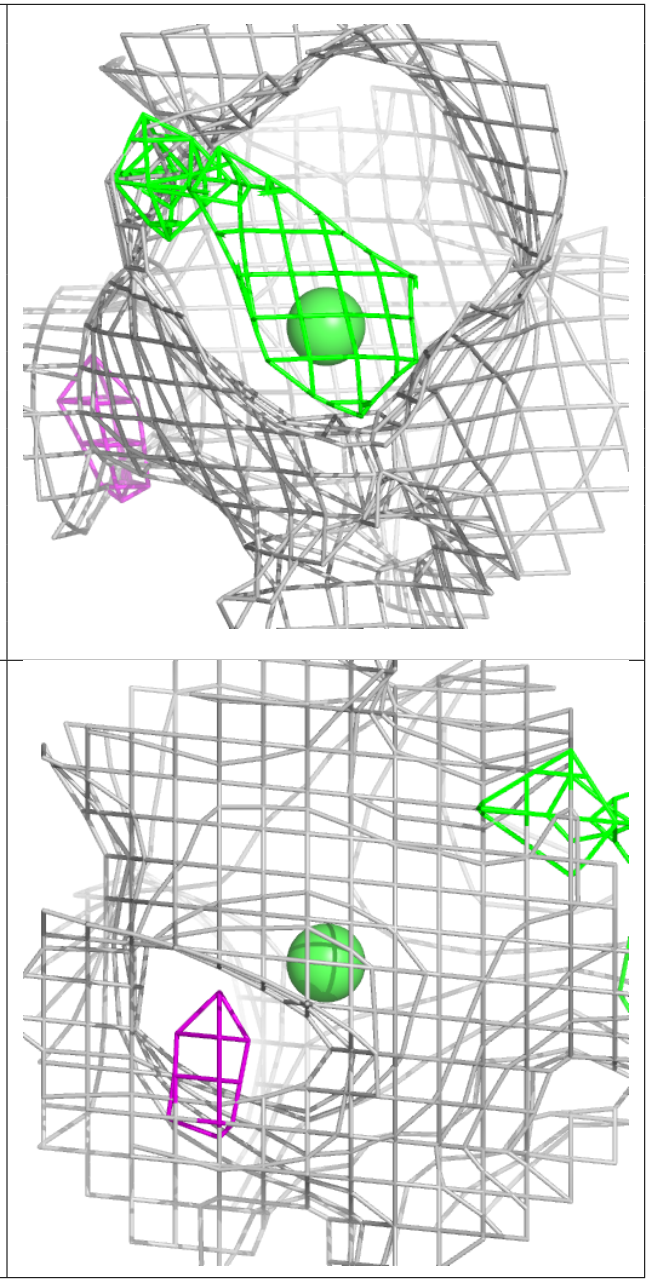
Electron density around NI A 301:

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



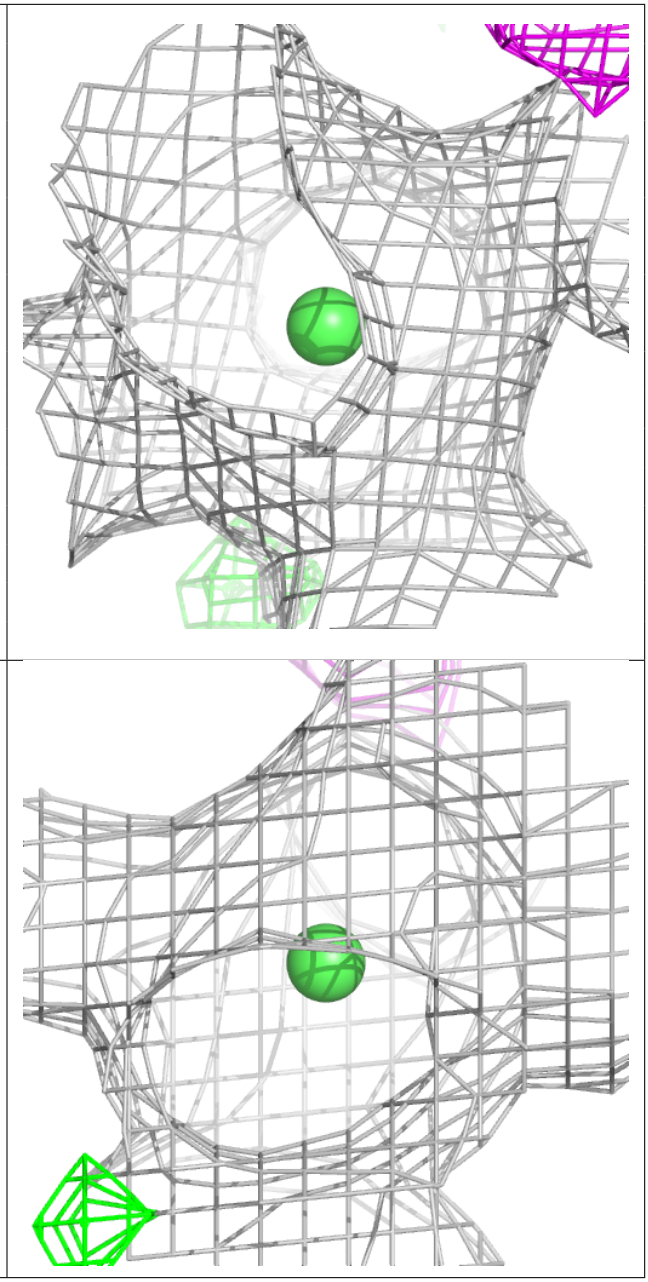
Electron density around NI B 303:

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



Electron density around NI D 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.