



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2025 – 12:34 PM EDT

PDB ID : 9MYP / pdb_00009myp
Title : Structure of Patiria miniata Hop1 chromatin binding region
Authors : Rodriguez, A.R.; Ye, Q.; Nguyen, J.; Chau, K.; Corbett, K.D.
Deposited on : 2025-01-22
Resolution : 1.84 Å(reported)

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

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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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

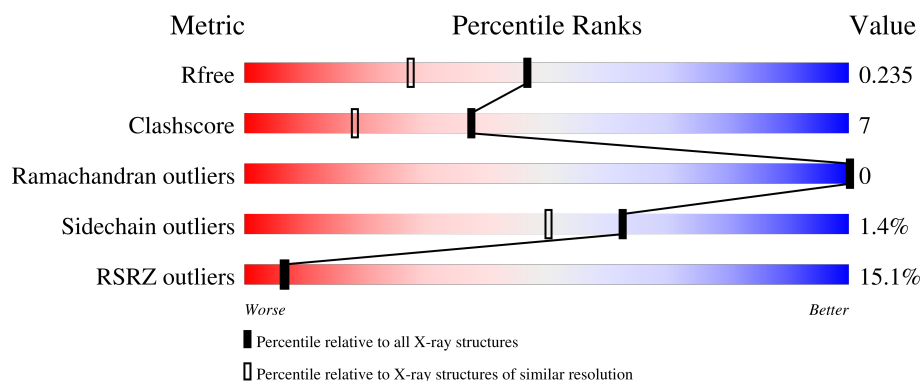
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	167	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	B	167	<div> <div>14%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	C	167	<div> <div>27%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7970 atoms, of which 3780 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 HORMA domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	H	N	O	S	0	0	0
			2553	808	1263	238	230	14			
1	C	159	Total	C	H	N	O	S	0	0	0
			2530	801	1253	235	227	14			
1	B	161	Total	C	H	N	O	S	0	0	0
			2554	808	1264	238	230	14			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	MET	-	initiating methionine	UNP A0A913ZKG6
A	334	LYS	-	expression tag	UNP A0A913ZKG6
A	335	SER	-	expression tag	UNP A0A913ZKG6
A	336	SER	-	expression tag	UNP A0A913ZKG6
A	337	HIS	-	expression tag	UNP A0A913ZKG6
A	338	HIS	-	expression tag	UNP A0A913ZKG6
A	339	HIS	-	expression tag	UNP A0A913ZKG6
A	340	HIS	-	expression tag	UNP A0A913ZKG6
A	341	HIS	-	expression tag	UNP A0A913ZKG6
A	342	HIS	-	expression tag	UNP A0A913ZKG6
A	343	GLU	-	expression tag	UNP A0A913ZKG6
A	344	ASN	-	expression tag	UNP A0A913ZKG6
A	345	LEU	-	expression tag	UNP A0A913ZKG6
A	346	TYR	-	expression tag	UNP A0A913ZKG6
A	347	PHE	-	expression tag	UNP A0A913ZKG6
A	348	GLN	-	expression tag	UNP A0A913ZKG6
A	349	SER	-	expression tag	UNP A0A913ZKG6
A	350	ASN	-	expression tag	UNP A0A913ZKG6
A	351	ALA	-	expression tag	UNP A0A913ZKG6
C	333	MET	-	initiating methionine	UNP A0A913ZKG6
C	334	LYS	-	expression tag	UNP A0A913ZKG6
C	335	SER	-	expression tag	UNP A0A913ZKG6
C	336	SER	-	expression tag	UNP A0A913ZKG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	337	HIS	-	expression tag	UNP A0A913ZKG6
C	338	HIS	-	expression tag	UNP A0A913ZKG6
C	339	HIS	-	expression tag	UNP A0A913ZKG6
C	340	HIS	-	expression tag	UNP A0A913ZKG6
C	341	HIS	-	expression tag	UNP A0A913ZKG6
C	342	HIS	-	expression tag	UNP A0A913ZKG6
C	343	GLU	-	expression tag	UNP A0A913ZKG6
C	344	ASN	-	expression tag	UNP A0A913ZKG6
C	345	LEU	-	expression tag	UNP A0A913ZKG6
C	346	TYR	-	expression tag	UNP A0A913ZKG6
C	347	PHE	-	expression tag	UNP A0A913ZKG6
C	348	GLN	-	expression tag	UNP A0A913ZKG6
C	349	SER	-	expression tag	UNP A0A913ZKG6
C	350	ASN	-	expression tag	UNP A0A913ZKG6
C	351	ALA	-	expression tag	UNP A0A913ZKG6
B	333	MET	-	initiating methionine	UNP A0A913ZKG6
B	334	LYS	-	expression tag	UNP A0A913ZKG6
B	335	SER	-	expression tag	UNP A0A913ZKG6
B	336	SER	-	expression tag	UNP A0A913ZKG6
B	337	HIS	-	expression tag	UNP A0A913ZKG6
B	338	HIS	-	expression tag	UNP A0A913ZKG6
B	339	HIS	-	expression tag	UNP A0A913ZKG6
B	340	HIS	-	expression tag	UNP A0A913ZKG6
B	341	HIS	-	expression tag	UNP A0A913ZKG6
B	342	HIS	-	expression tag	UNP A0A913ZKG6
B	343	GLU	-	expression tag	UNP A0A913ZKG6
B	344	ASN	-	expression tag	UNP A0A913ZKG6
B	345	LEU	-	expression tag	UNP A0A913ZKG6
B	346	TYR	-	expression tag	UNP A0A913ZKG6
B	347	PHE	-	expression tag	UNP A0A913ZKG6
B	348	GLN	-	expression tag	UNP A0A913ZKG6
B	349	SER	-	expression tag	UNP A0A913ZKG6
B	350	ASN	-	expression tag	UNP A0A913ZKG6
B	351	ALA	-	expression tag	UNP A0A913ZKG6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

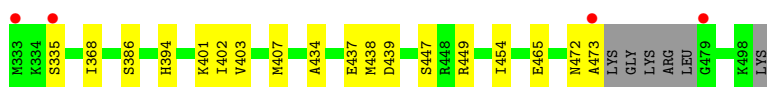
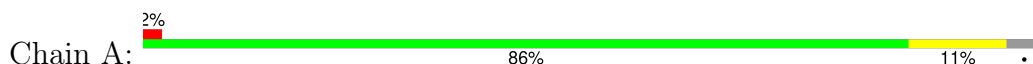
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	C	80	Total	O	0	0
			80	80		
4	B	95	Total	O	0	0
			95	95		

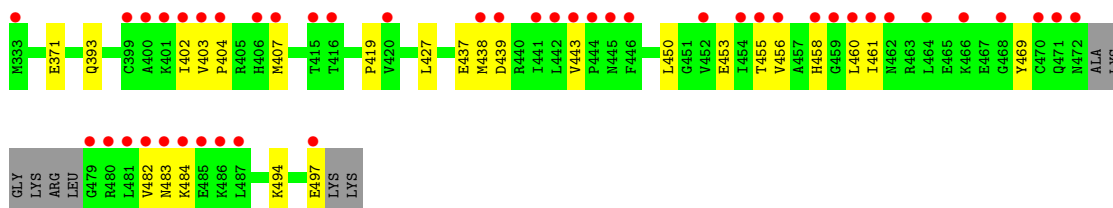
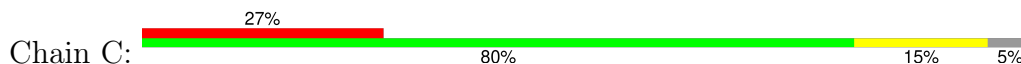
3 Residue-property plots [i](#)

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.

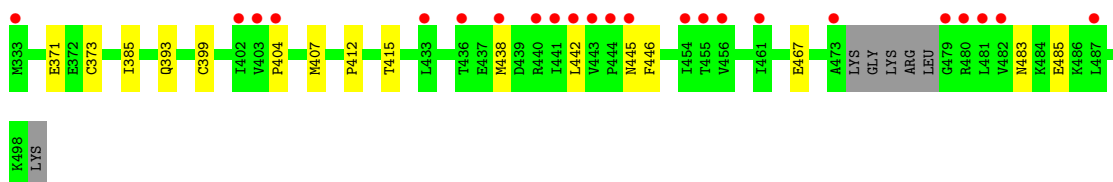
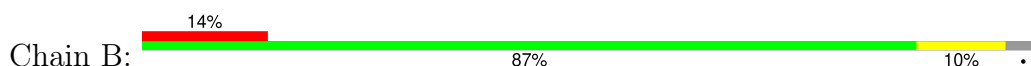
- Molecule 1: HORMA domain-containing protein



- Molecule 1: HORMA domain-containing protein



- Molecule 1: HORMA domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.65Å 106.95Å 131.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.95 – 1.84 82.95 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.6 (82.95-1.84) 98.9 (82.95-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.198 , 0.235 0.198 , 0.235	Depositor DCC
R_{free} test set	2424 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7970	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: MLY, ZN, 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	0.64	0/1307	0.70	0/1765
1	B	0.53	0/1307	0.64	0/1765
1	C	0.52	0/1294	0.62	0/1747
All	All	0.57	0/3908	0.65	0/5277

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	1290	1263	1262	15	0
1	B	1290	1264	1262	14	0
1	C	1277	1253	1251	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	1	0	0	0	0
4	A	151	0	0	5	0
4	B	95	0	0	9	0
4	C	80	0	0	10	0
All	All	4190	3780	3775	53	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 53 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:C:450:LEU:O	4:C:601:HOH:O	1.66	1.11
1:B:399:CYS:SG	4:B:665:HOH:O	2.11	1.06
1:A:401:LYS:NZ	4:A:603:HOH:O	2.09	0.85
1:C:439:ASP:O	4:C:603:HOH:O	1.95	0.83
1:C:482:VAL:O	4:C:604:HOH:O	1.98	0.80

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	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
1	B	156/167 (93%)	150 (96%)	6 (4%)	0	100	100
1	C	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
All	All	466/501 (93%)	448 (96%)	18 (4%)	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	140/146 (96%)	138 (99%)	2 (1%)	62	50
1	B	140/146 (96%)	138 (99%)	2 (1%)	62	50
1	C	139/146 (95%)	137 (99%)	2 (1%)	62	50
All	All	419/438 (96%)	413 (99%)	6 (1%)	62	50

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	497	GLU
1	B	385	ILE
1	B	446	PHE
1	A	386	SER
1	A	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN
1	A	472	ASN
1	B	458	HIS
1	B	393	GLN
1	A	458	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	MLY	B	494	1	9,10,11	0.87	0	6,11,13	0.45	0
1	MLY	A	494	1	9,10,11	0.58	0	6,11,13	0.86	0
1	MLY	C	494	1	9,10,11	0.75	0	6,11,13	0.95	1 (16%)

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
1	MLY	B	494	1	-	0/8/9/11	-
1	MLY	A	494	1	-	0/8/9/11	-
1	MLY	C	494	1	-	0/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	494	MLY	CH2-NZ-CH1	2.09	115.07	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	A	160/167 (95%)	0.00	4 (2%) 58 64	24, 36, 77, 115	0
1	B	160/167 (95%)	0.69	23 (14%) 7 7	25, 51, 100, 149	0
1	C	158/167 (94%)	1.15	45 (28%) 1 1	26, 58, 106, 158	0
All	All	478/501 (95%)	0.61	72 (15%) 6 7	24, 46, 100, 158	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	472	ASN	5.3
1	A	473	ALA	4.8
1	C	333	MET	4.2
1	C	442	LEU	4.2
1	C	400	ALA	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	B	494	11/12	0.93	0.09	38,50,60,60	0
1	MLY	C	494	11/12	0.94	0.08	31,48,57,57	0
1	MLY	A	494	11/12	0.95	0.07	28,37,54,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

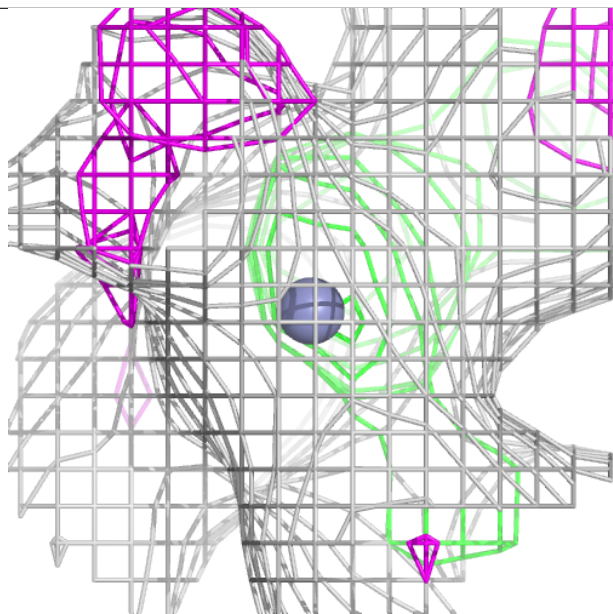
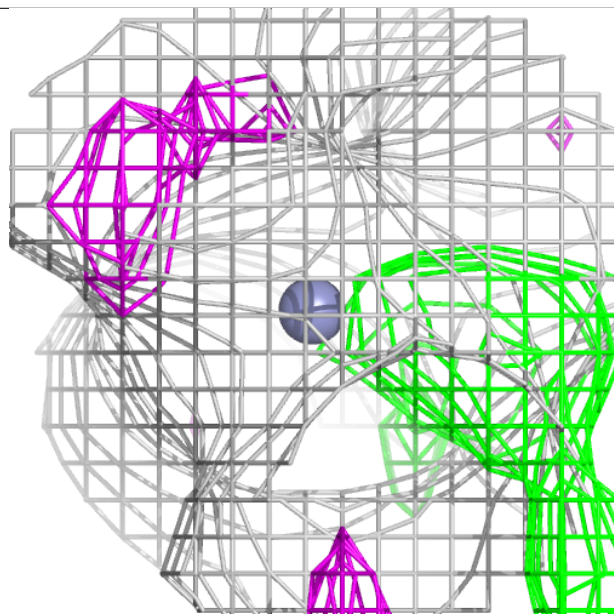
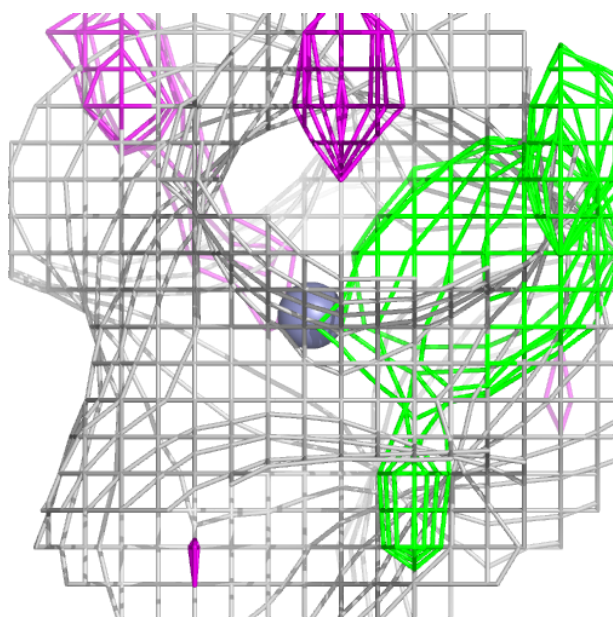
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZN	C	501	1/1	0.94	0.07	47,47,47,47	0
2	ZN	C	502	1/1	0.98	0.06	46,46,46,46	0
2	ZN	B	501	1/1	0.98	0.08	42,42,42,42	0
2	ZN	A	502	1/1	0.99	0.09	31,31,31,31	0
2	ZN	A	501	1/1	0.99	0.09	37,37,37,37	0
2	ZN	B	502	1/1	0.99	0.09	39,39,39,39	0
3	NI	A	503	1/1	1.00	0.03	24,24,24,24	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.

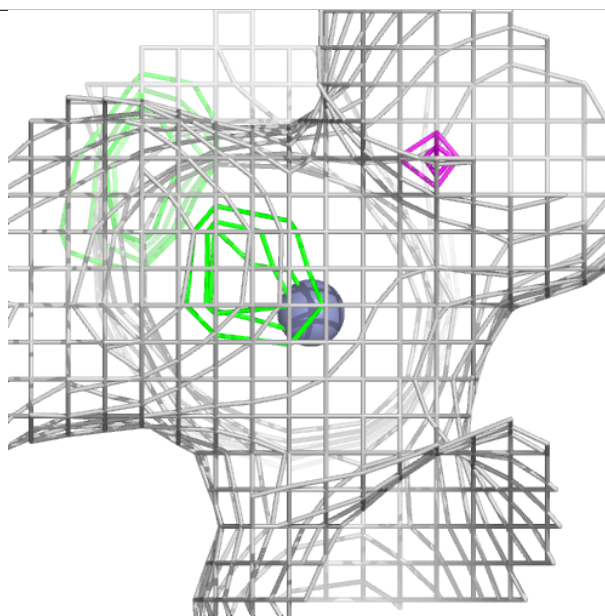
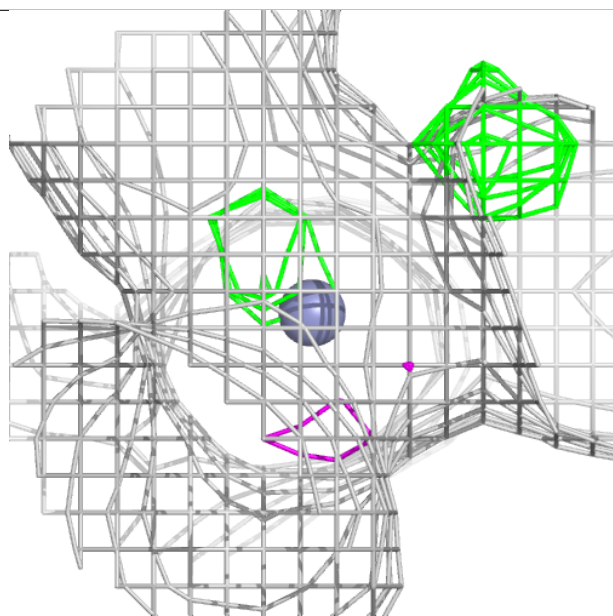
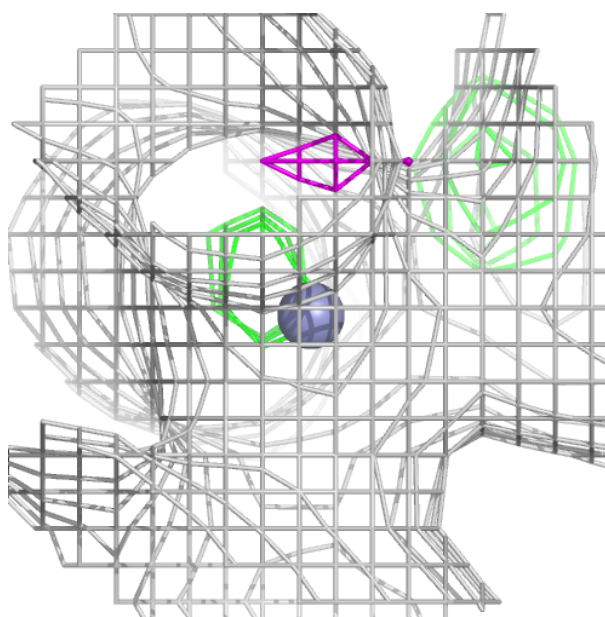
Electron density around ZN C 501:

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



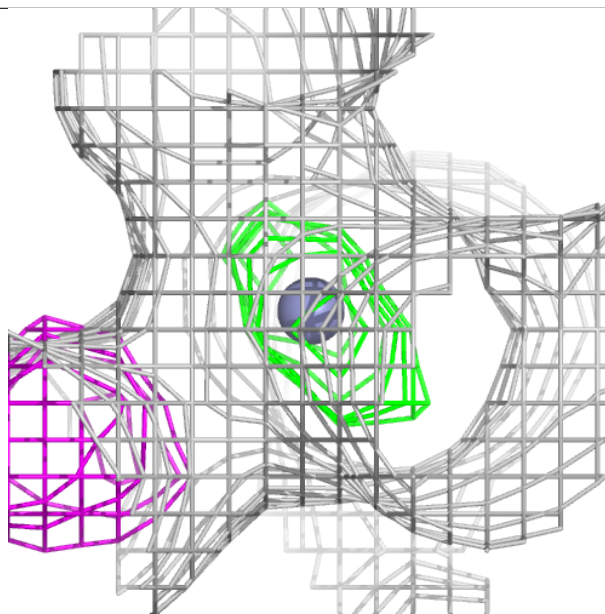
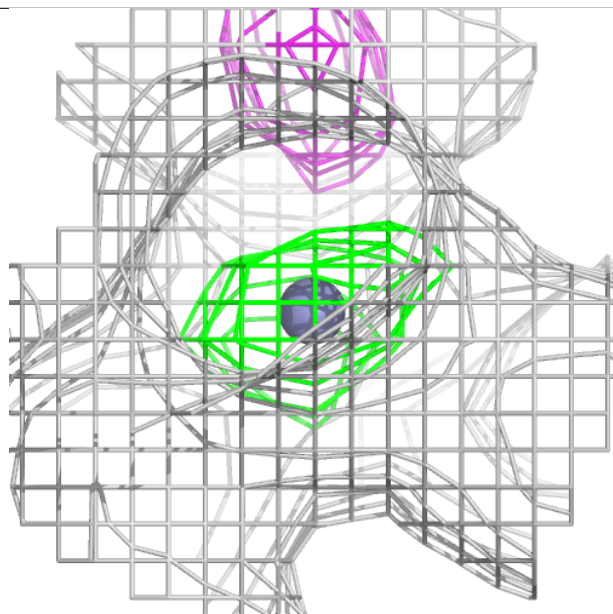
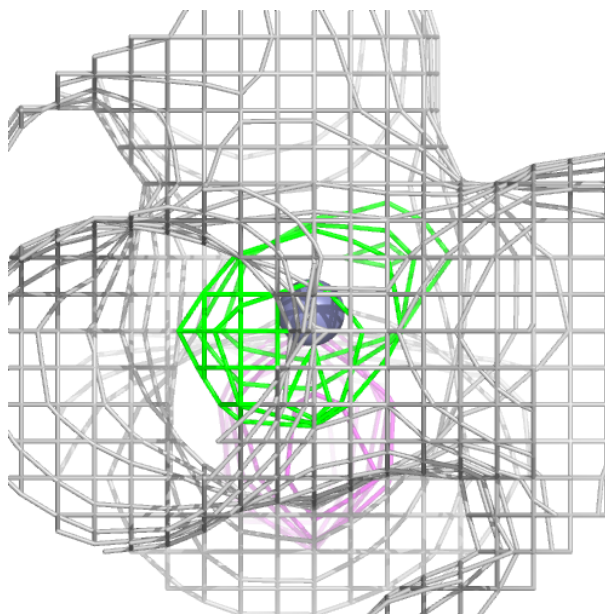
Electron density around ZN C 502:

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



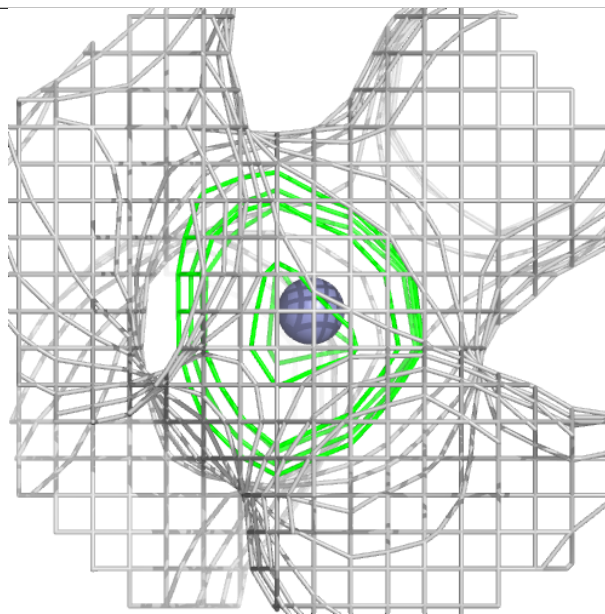
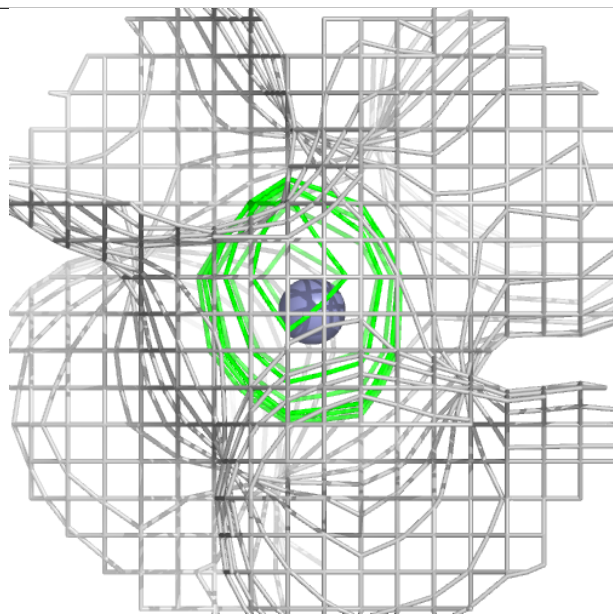
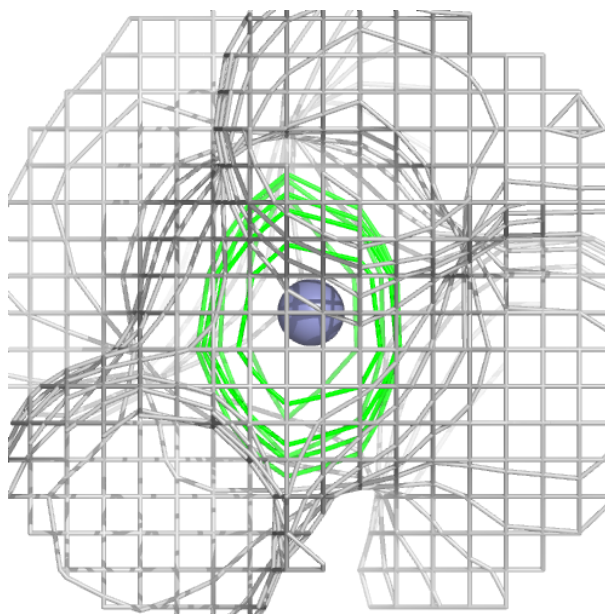
Electron density around ZN B 501:

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



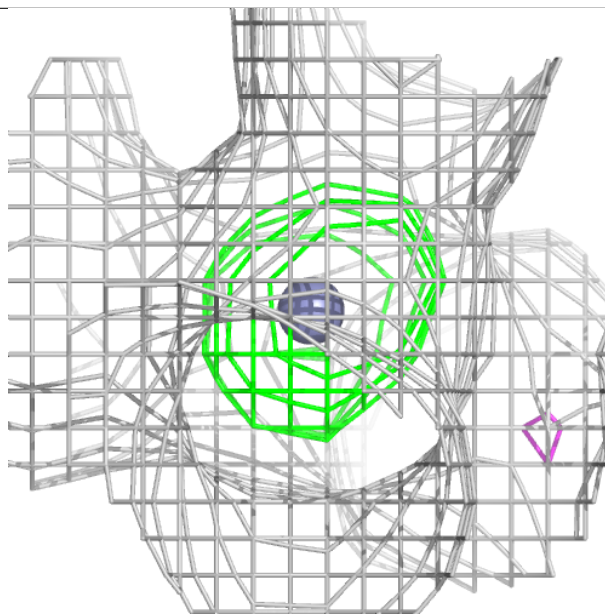
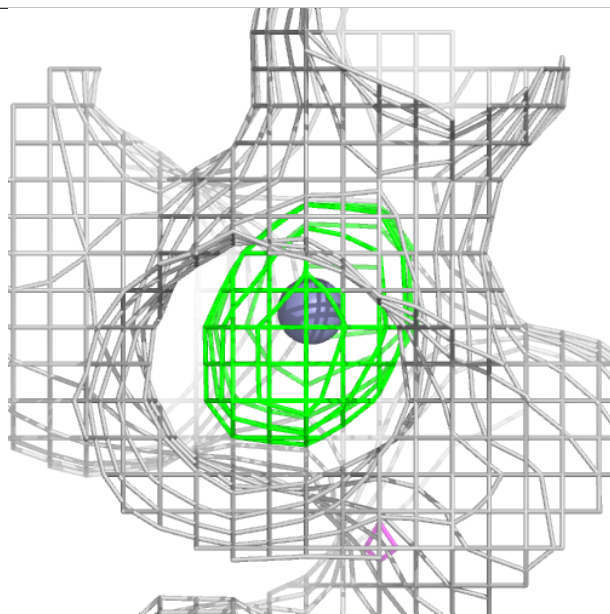
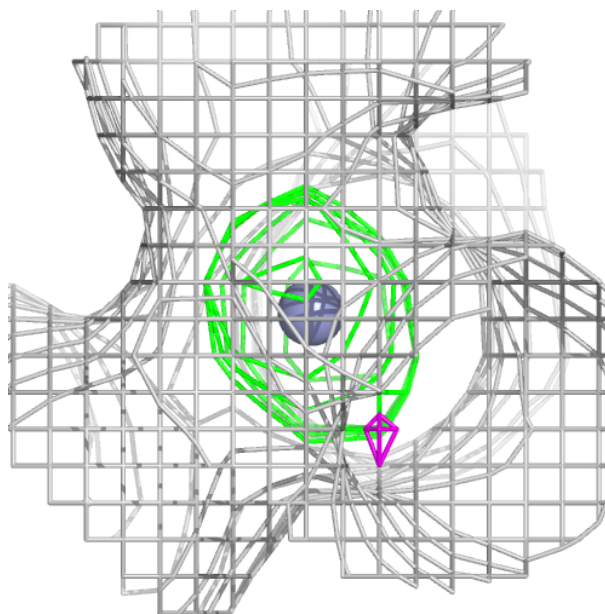
Electron density around ZN A 502:

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



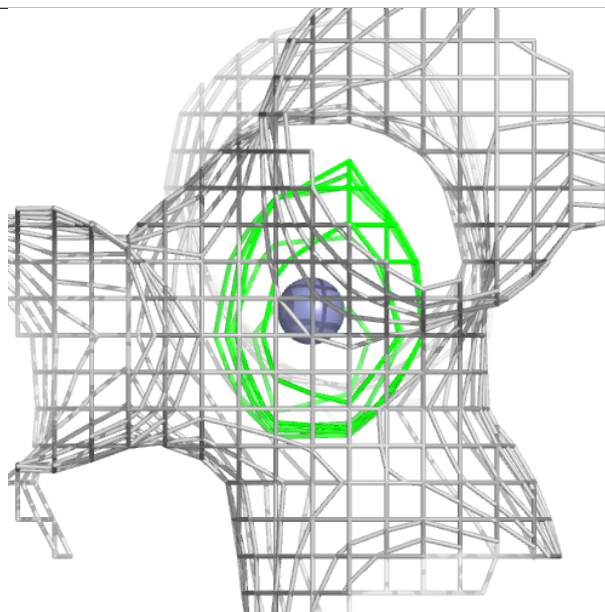
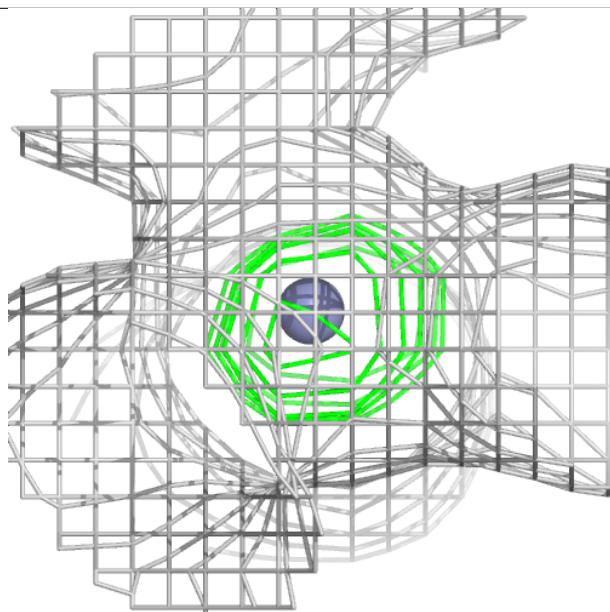
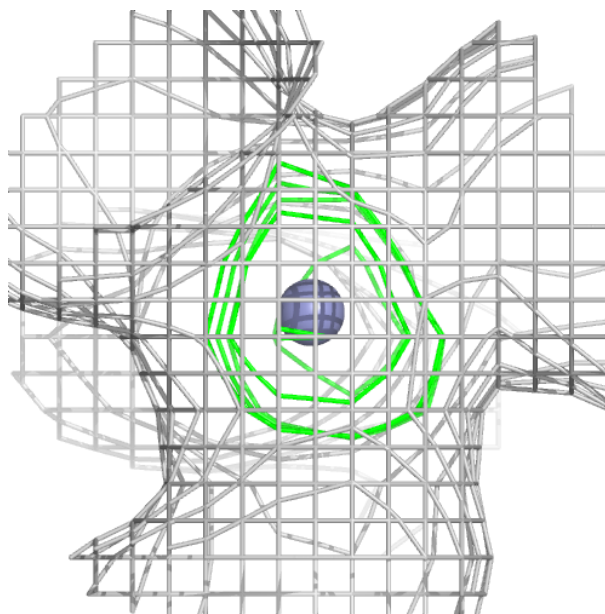
Electron density around ZN A 501:

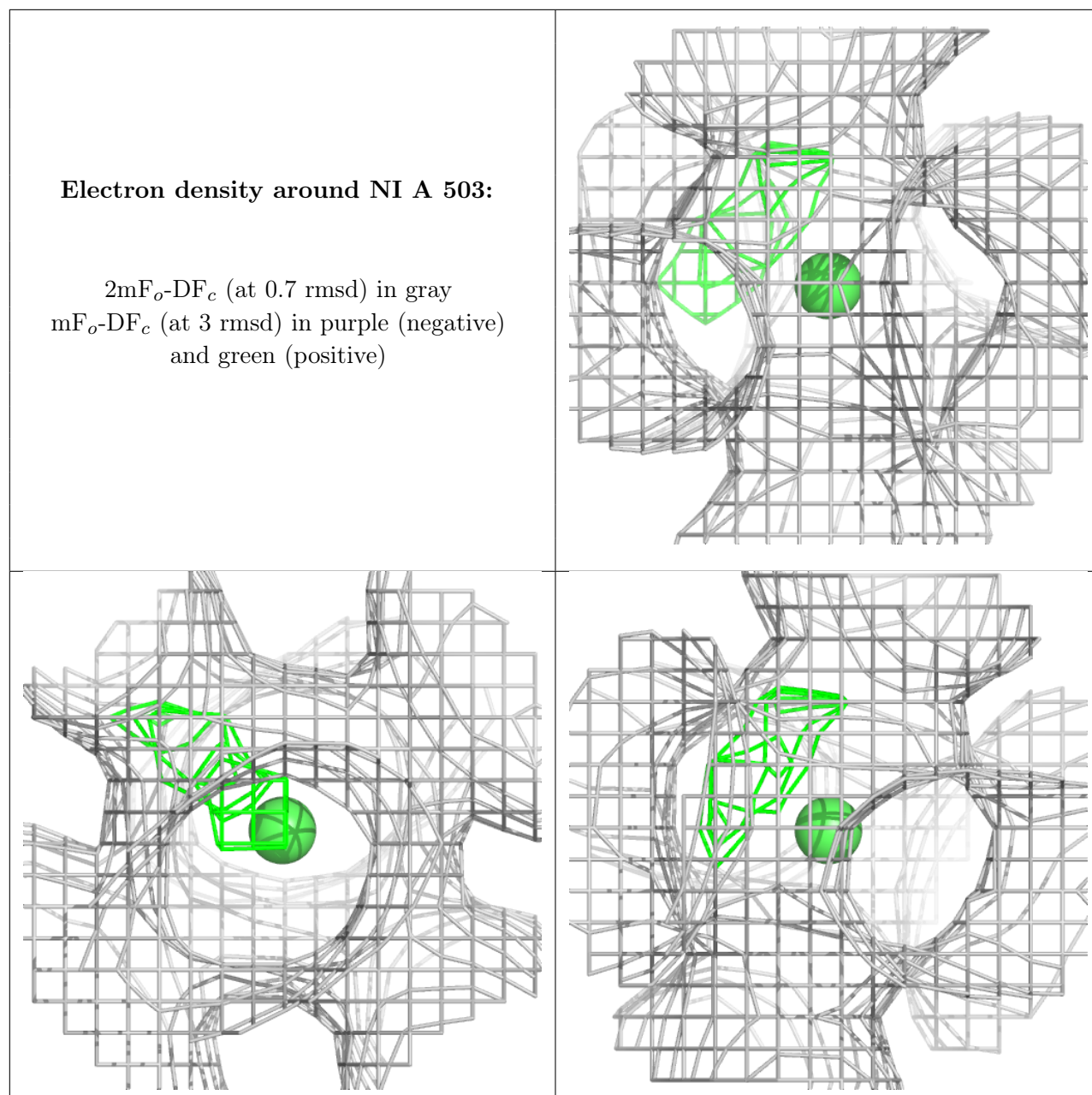
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 502:

$2mF_o-DF_c$ (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.