wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 06:32 PM JST

PDB ID	:	7WI1
Title	:	The mutant variant of PNGM-1, H93 was substituuted for alanine to study metal coordination
Authors	:	Park, Y.S.; Kang, L.W.; Lee, J.H.
Deposited on	:	2022-01-01
Resolution	:	1.61 Å(reported)

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

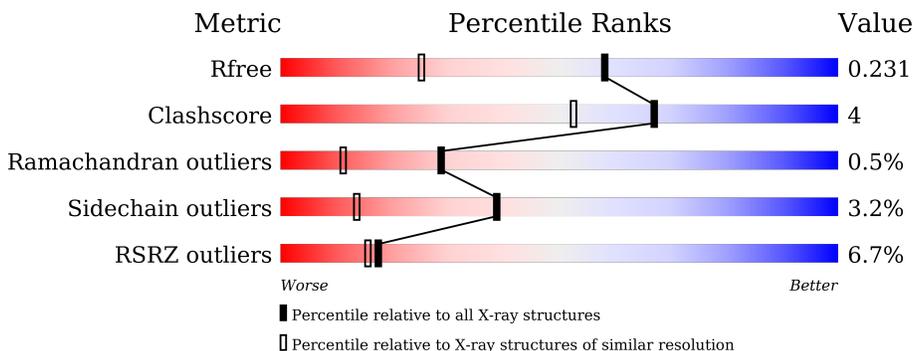|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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:
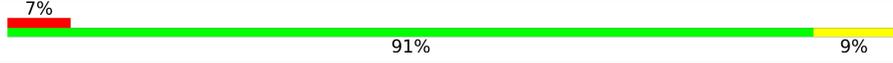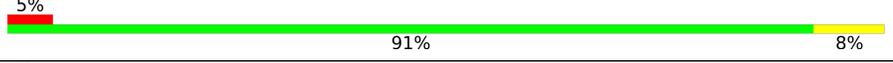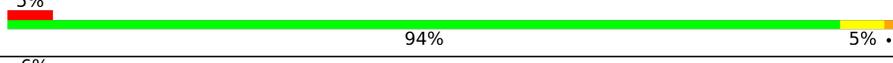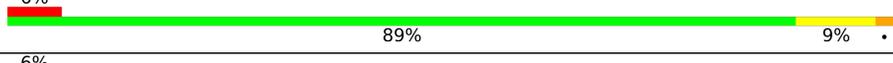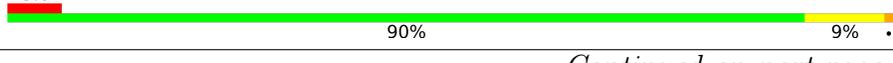*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.61 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.
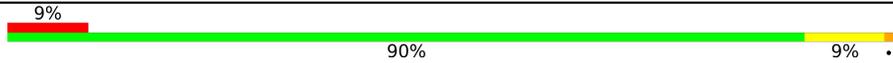
Metric	Percentile Ranks	Value
Rfree		0.231
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		3.2%
RSRZ outliers		6.7%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	372	7% — 89% / 10% ·
1	B	372	7% — 91% / 9% ·
1	C	372	5% — 91% / 8%
1	D	372	5% — 94% / 5% ·
1	E	372	6% — 89% / 9% ·
1	F	372	6% — 90% / 9% ··

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Mol	Chain	Length	Quality of chain
1	G	372	9% 90% 9%
1	H	372	8% 90% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24542 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 Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	G	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	C	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	E	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	D	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	F	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	B	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			
1	H	372	Total	C	N	O	S	0	0	0
			2928	1850	504	554	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
G	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
E	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
F	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
H	93	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	G	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total 177	O 177	0	0
3	G	96	Total 96	O 96	0	0
3	C	182	Total 182	O 182	0	0
3	E	105	Total 105	O 105	0	0
3	D	171	Total 171	O 171	0	0
3	F	95	Total 95	O 95	0	0
3	B	181	Total 181	O 181	0	0
3	H	103	Total 103	O 103	0	0

# 3   Residue-property plots ⓘ

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.
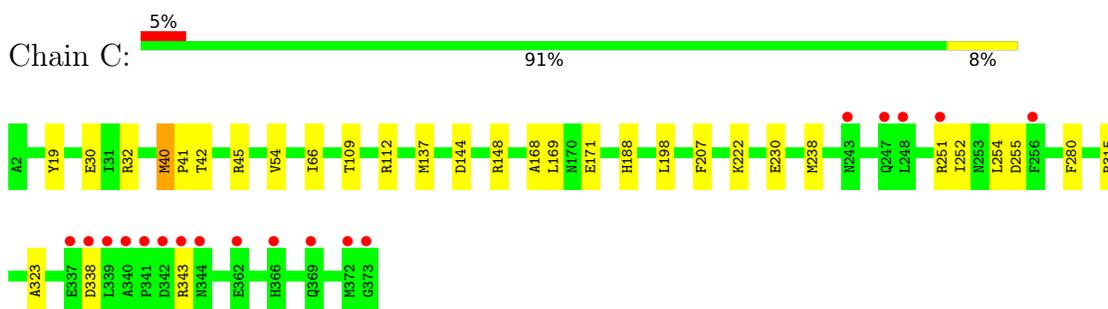
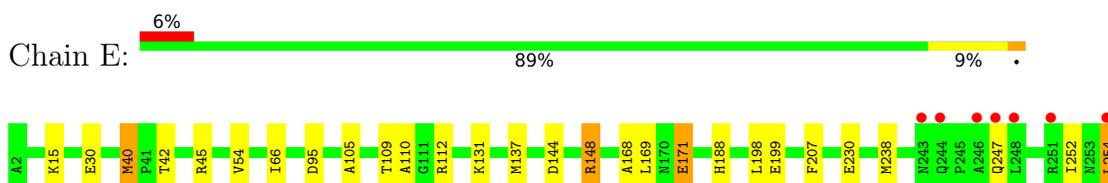- Molecule 1: Metallo-beta-lactamase PNGM-1
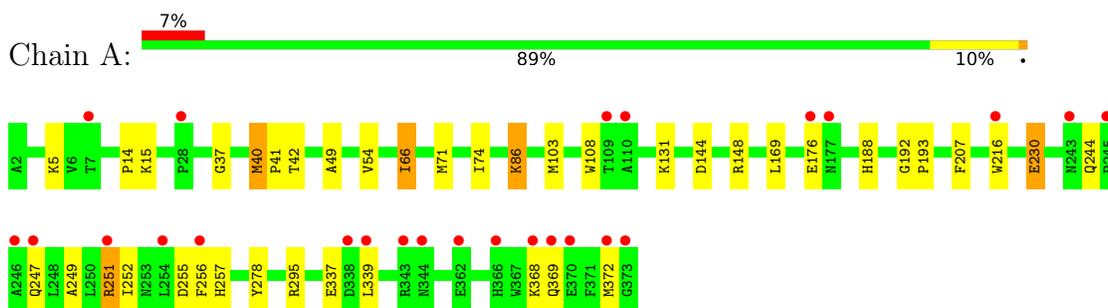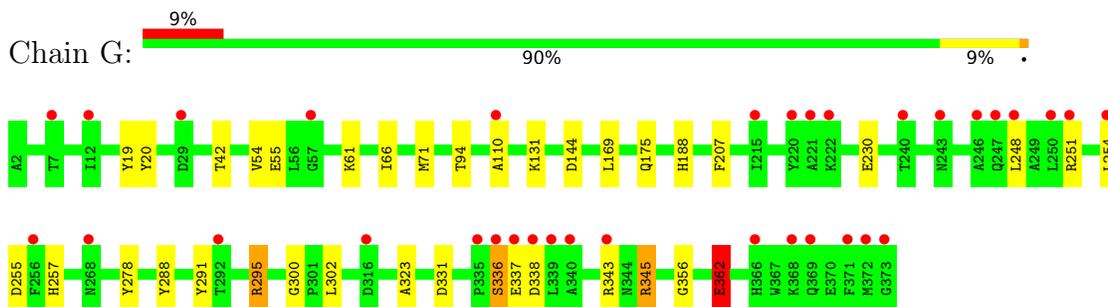
Chain A:

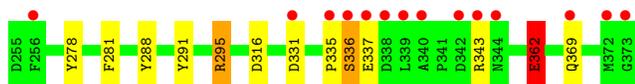- Molecule 1: Metallo-beta-lactamase PNGM-1

Chain G:

- Molecule 1: Metallo-beta-lactamase PNGM-1
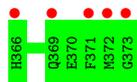
Chain C:

- Molecule 1: Metallo-beta-lactamase PNGM-1

Chain E:

• Molecule 1: Metallo-beta-lactamase PNGM-1

Chain D:

• Molecule 1: Metallo-beta-lactamase PNGM-1

Chain F:
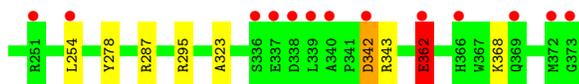

• Molecule 1: Metallo-beta-lactamase PNGM-1
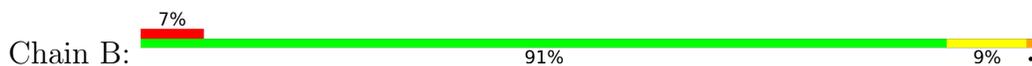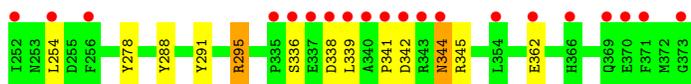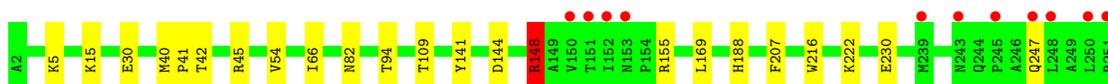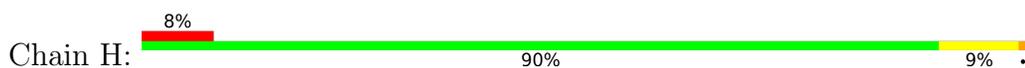
Chain B:

• Molecule 1: Metallo-beta-lactamase PNGM-1

Chain H:

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.75Å 82.79Å 164.05Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	41.51 – 1.61 41.47 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.51-1.61) 99.0 (41.47-1.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.223 0.205 , 0.231	Depositor DCC
R_{free} test set	19534 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	10.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.0	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24542	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.34 % 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 2.8594e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.80	0/3013	0.94	2/4107 (0.0%)
1	B	0.83	3/3013 (0.1%)	0.93	1/4107 (0.0%)
1	C	0.77	1/3013 (0.0%)	0.94	5/4107 (0.1%)
1	D	0.78	1/3013 (0.0%)	0.96	6/4107 (0.1%)
1	E	0.83	4/3013 (0.1%)	1.05	10/4107 (0.2%)
1	F	0.78	1/3013 (0.0%)	0.96	6/4107 (0.1%)
1	G	0.81	1/3013 (0.0%)	1.02	6/4107 (0.1%)
1	H	0.79	2/3013 (0.1%)	1.07	11/4107 (0.3%)
All	All	0.80	13/24104 (0.1%)	0.98	47/32856 (0.1%)

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	B	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	GLU	CD-OE1	13.36	1.40	1.25
1	E	199	GLU	CD-OE1	11.02	1.37	1.25
1	E	362	GLU	CD-OE2	9.13	1.35	1.25
1	B	199	GLU	CD-OE2	8.29	1.34	1.25
1	B	362	GLU	CD-OE1	6.69	1.33	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	295	ARG	NE-CZ-NH1	20.95	130.77	120.30
1	H	295	ARG	NE-CZ-NH1	19.26	129.93	120.30
1	E	295	ARG	NE-CZ-NH2	-17.65	111.47	120.30
1	H	345	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	H	295	ARG	NE-CZ-NH2	-14.00	113.30	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	TYR	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	2928	0	2752	34	0
1	B	2928	0	2752	25	0
1	C	2928	0	2752	18	0
1	D	2928	0	2752	13	0
1	E	2928	0	2752	24	0
1	F	2928	0	2752	26	0
1	G	2928	0	2752	23	0
1	H	2928	0	2752	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	177	0	0	9	2
3	B	181	0	0	5	2
3	C	182	0	0	4	0
3	D	171	0	0	6	0
3	E	105	0	0	5	0
3	F	95	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	96	0	0	6	0
3	H	103	0	0	5	0
All	All	24542	0	22016	175	2

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.

The worst 5 of 175 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:G:42:THR:HG22	3:G:526:HOH:O	1.27	1.31
1:A:42:THR:HG22	3:A:585:HOH:O	1.29	1.25
1:C:42:THR:HG22	3:C:534:HOH:O	1.44	1.16
1:A:257:HIS:HD2	3:A:504:HOH:O	1.33	1.09
1:E:42:THR:HG22	3:E:523:HOH:O	1.54	1.08

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:665:HOH:O	3:B:654:HOH:O[2_555]	2.03	0.17
3:A:518:HOH:O	3:B:551:HOH:O[2_545]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	370/372 (100%)	358 (97%)	11 (3%)	1 (0%)	41	21
1	B	370/372 (100%)	357 (96%)	9 (2%)	4 (1%)	14	2
1	C	370/372 (100%)	360 (97%)	9 (2%)	1 (0%)	41	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	370/372 (100%)	359 (97%)	10 (3%)	1 (0%)	41	21
1	E	370/372 (100%)	360 (97%)	8 (2%)	2 (0%)	29	11
1	F	370/372 (100%)	359 (97%)	10 (3%)	1 (0%)	41	21
1	G	370/372 (100%)	357 (96%)	11 (3%)	2 (0%)	29	11
1	H	370/372 (100%)	356 (96%)	10 (3%)	4 (1%)	14	2
All	All	2960/2976 (100%)	2866 (97%)	78 (3%)	16 (0%)	29	11

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	336	SER
1	E	336	SER
1	B	339	LEU
1	H	341	PRO
1	H	338	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/301 (100%)	288 (96%)	13 (4%)	29	8
1	B	301/301 (100%)	293 (97%)	8 (3%)	44	18
1	C	301/301 (100%)	294 (98%)	7 (2%)	50	24
1	D	301/301 (100%)	292 (97%)	9 (3%)	41	15
1	E	301/301 (100%)	289 (96%)	12 (4%)	31	9
1	F	301/301 (100%)	292 (97%)	9 (3%)	41	15
1	G	301/301 (100%)	290 (96%)	11 (4%)	34	10
1	H	301/301 (100%)	293 (97%)	8 (3%)	44	18
All	All	2408/2408 (100%)	2331 (97%)	77 (3%)	39	14

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	254	LEU
1	H	169	LEU
1	F	342	ASP
1	B	254	LEU
1	H	278	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	247	GLN
1	B	244	GLN
1	H	344	ASN
1	H	153	ASN
1	E	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 ⓘ

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, 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	372/372 (100%)	0.58	25 (6%)	17	16	6, 14, 30, 50	0
1	B	372/372 (100%)	0.29	27 (7%)	15	13	4, 10, 40, 84	0
1	C	372/372 (100%)	0.14	18 (4%)	30	27	3, 8, 32, 69	0
1	D	372/372 (100%)	0.31	19 (5%)	28	25	5, 12, 30, 60	0
1	E	372/372 (100%)	0.15	21 (5%)	24	21	3, 9, 30, 71	0
1	F	372/372 (100%)	0.25	24 (6%)	18	16	5, 12, 31, 49	0
1	G	372/372 (100%)	0.67	34 (9%)	9	7	6, 15, 31, 61	0
1	H	372/372 (100%)	0.36	31 (8%)	11	9	4, 10, 41, 84	0
All	All	2976/2976 (100%)	0.34	199 (6%)	17	16	3, 11, 34, 84	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	343	ARG	12.7
1	B	338	ASP	10.3
1	C	338	ASP	9.6
1	H	152	ILE	8.5
1	H	151	THR	8.5

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

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

6.3 Carbohydrates ⓘ

There are no 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, 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	A	401	1/1	0.96	0.06	11,11,11,11	0
2	ZN	G	401	1/1	0.99	0.04	10,10,10,10	0
2	ZN	C	401	1/1	0.99	0.06	7,7,7,7	0
2	ZN	E	401	1/1	0.99	0.07	8,8,8,8	0
2	ZN	H	401	1/1	0.99	0.04	9,9,9,9	0
2	ZN	F	401	1/1	1.00	0.05	8,8,8,8	0
2	ZN	B	401	1/1	1.00	0.05	9,9,9,9	0
2	ZN	D	401	1/1	1.00	0.05	9,9,9,9	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 A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
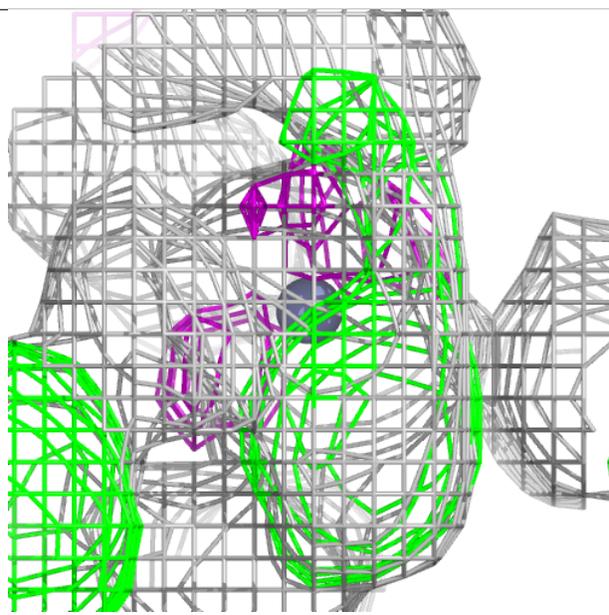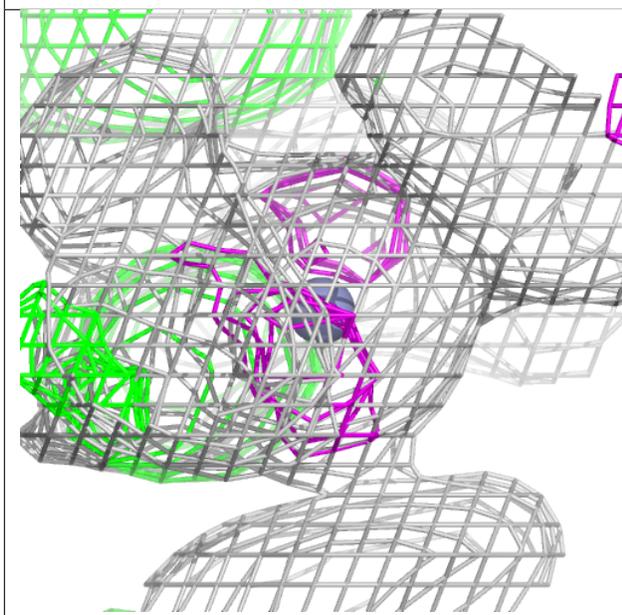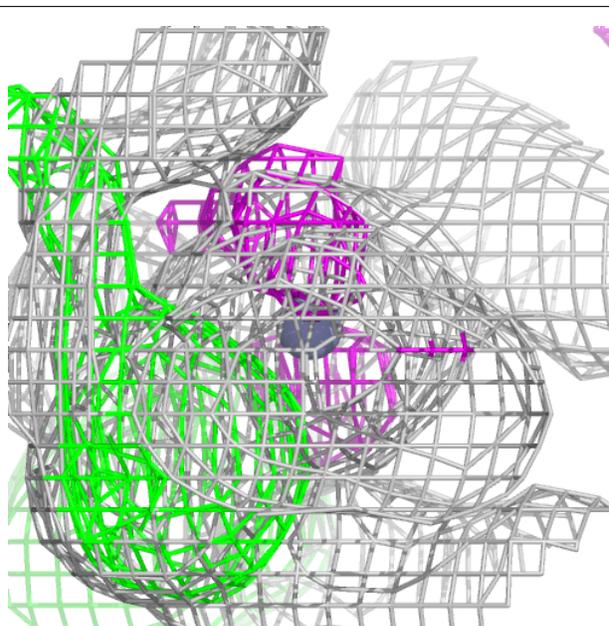
Electron density around ZN G 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
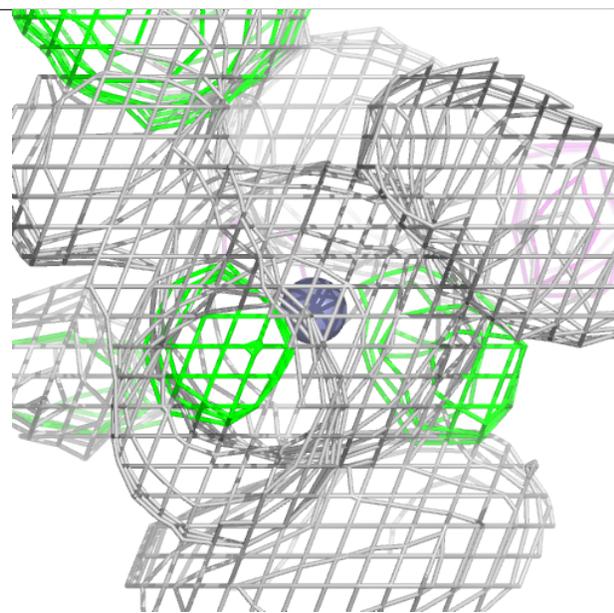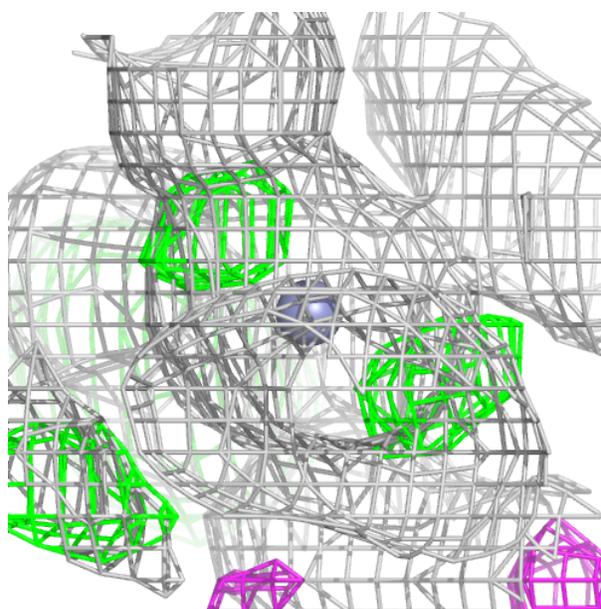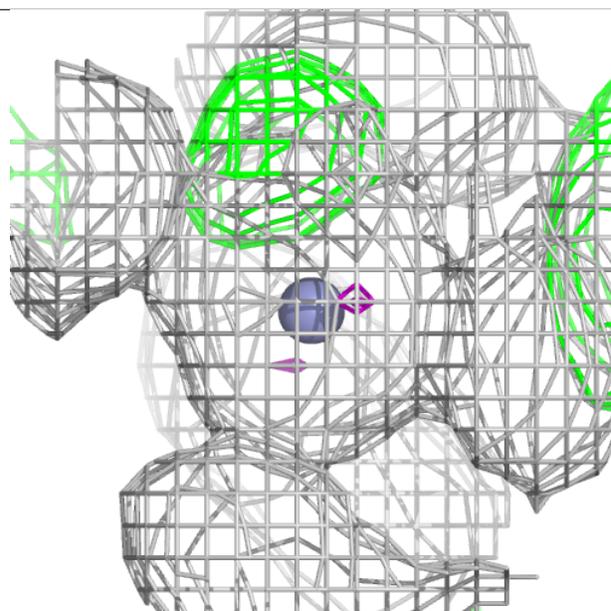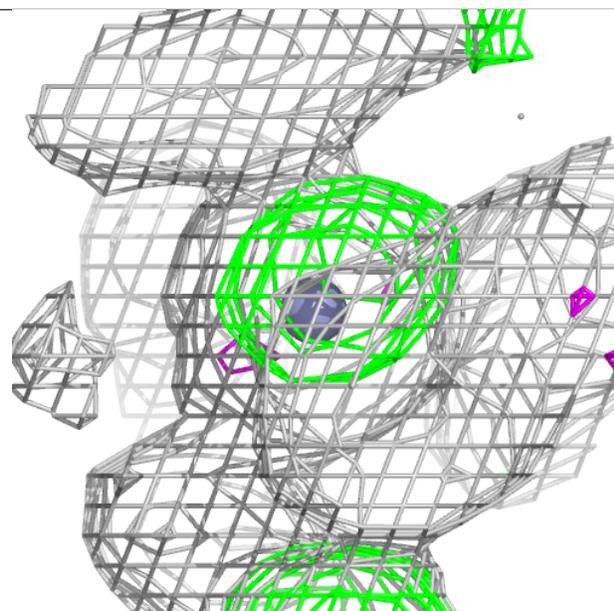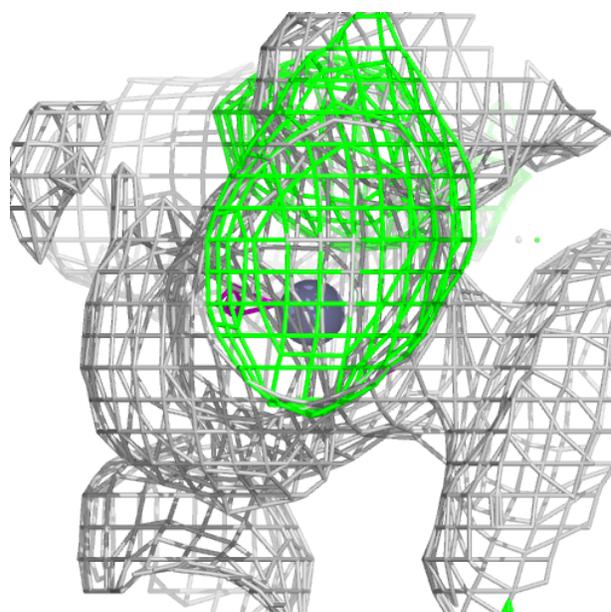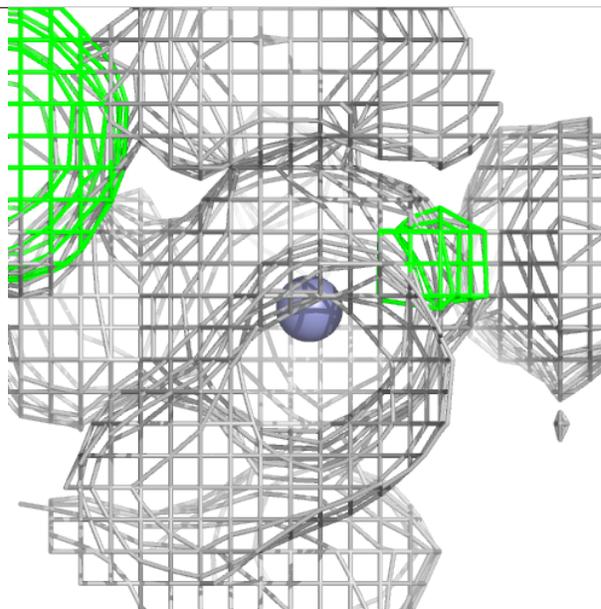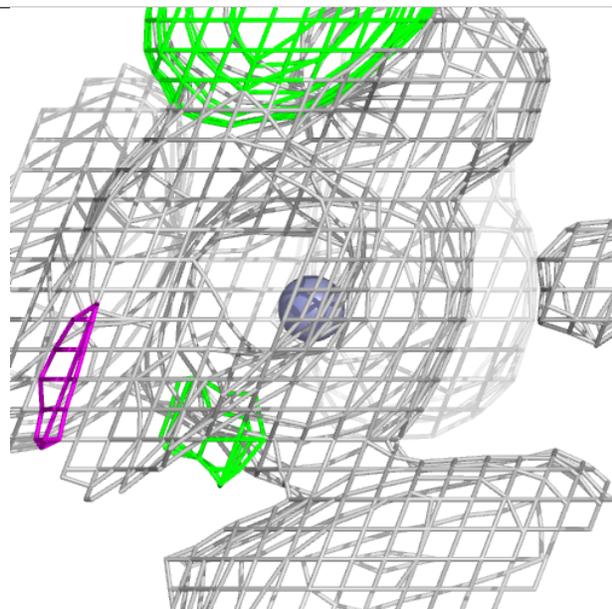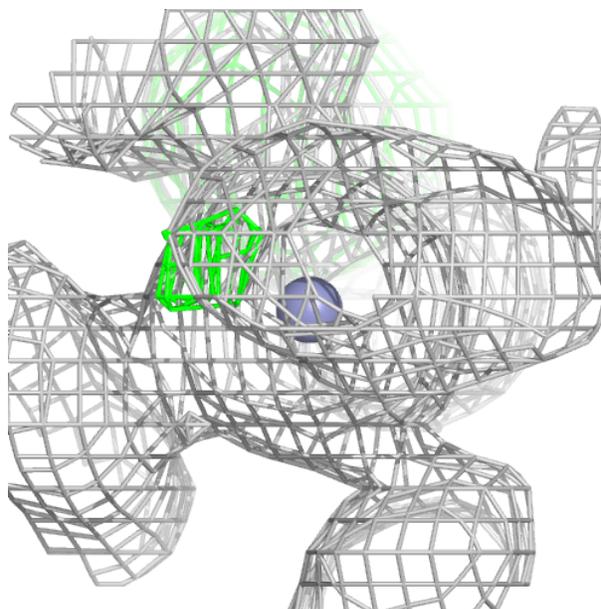and green (positive)
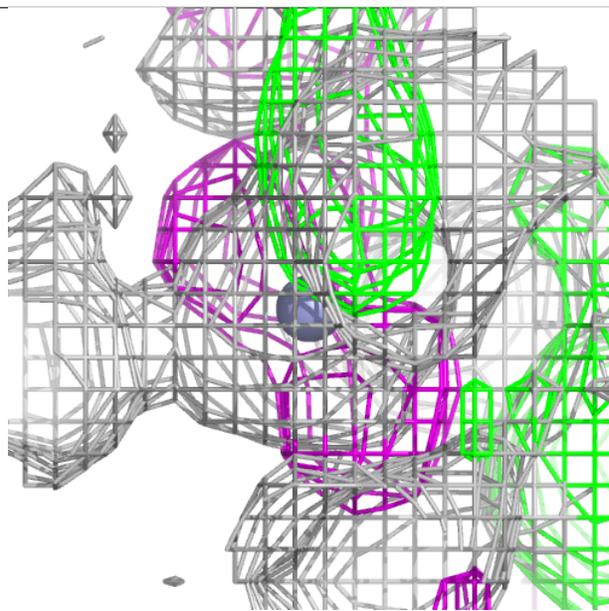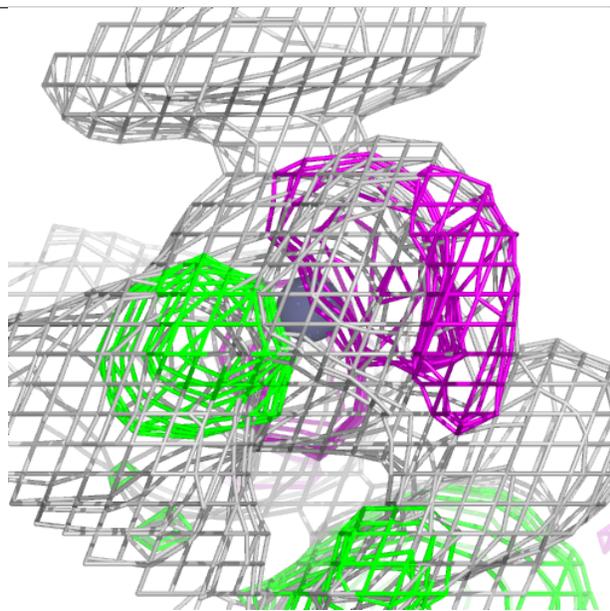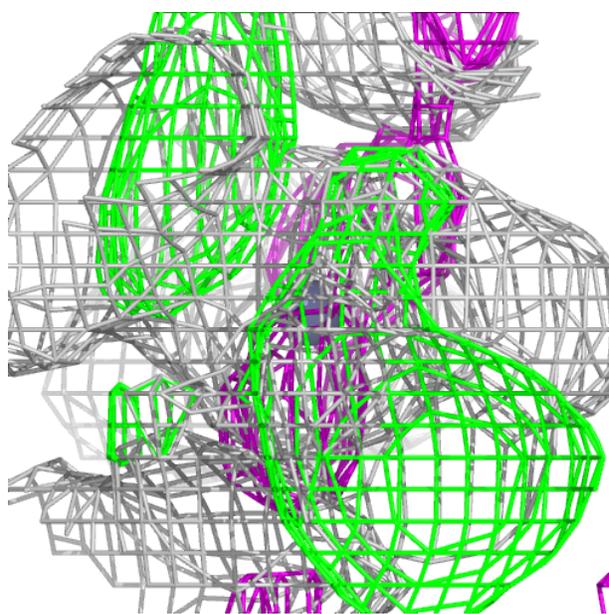
Electron density around ZN C 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
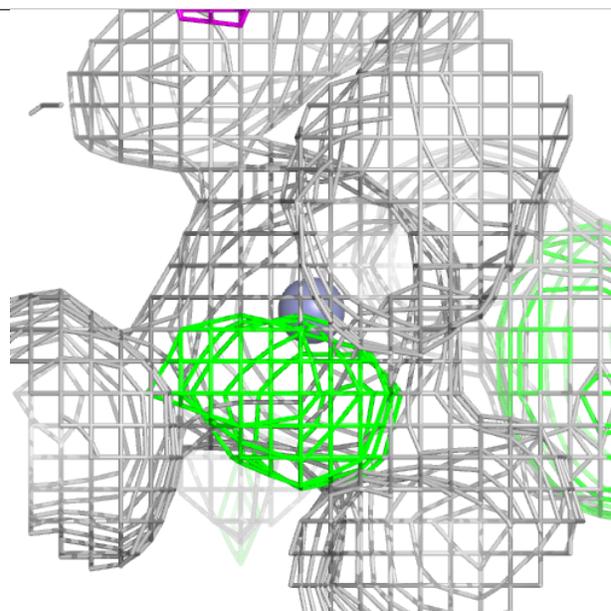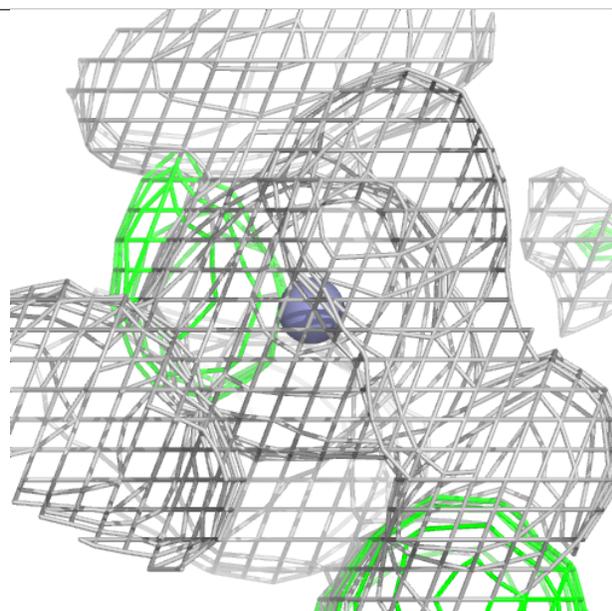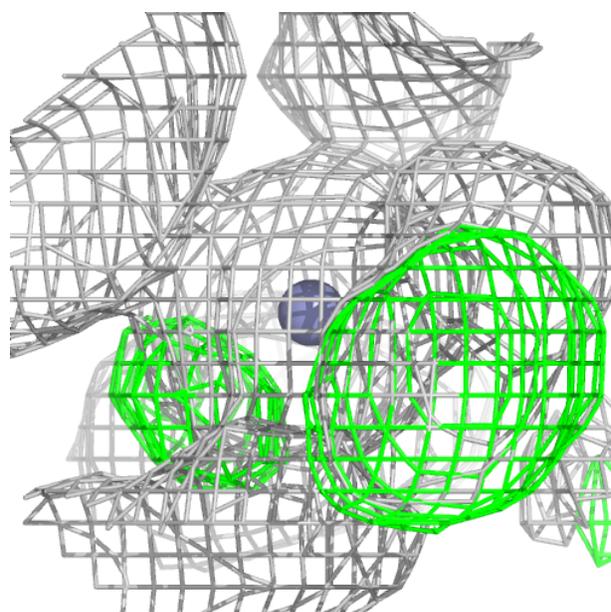
Electron density around ZN E 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
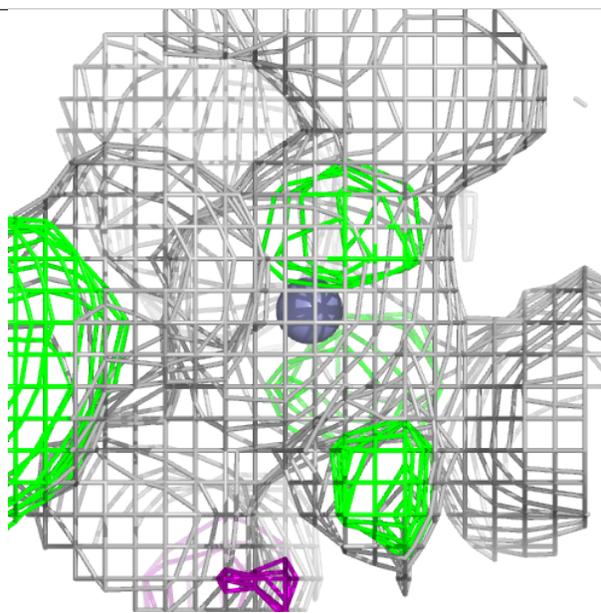
Electron density around ZN H 401:

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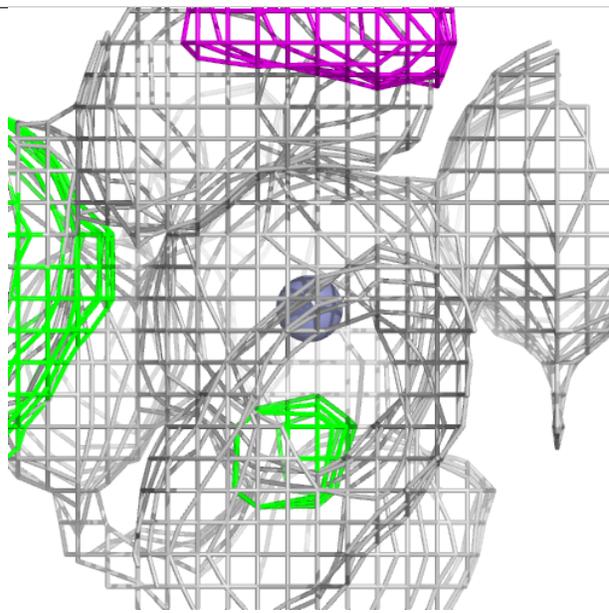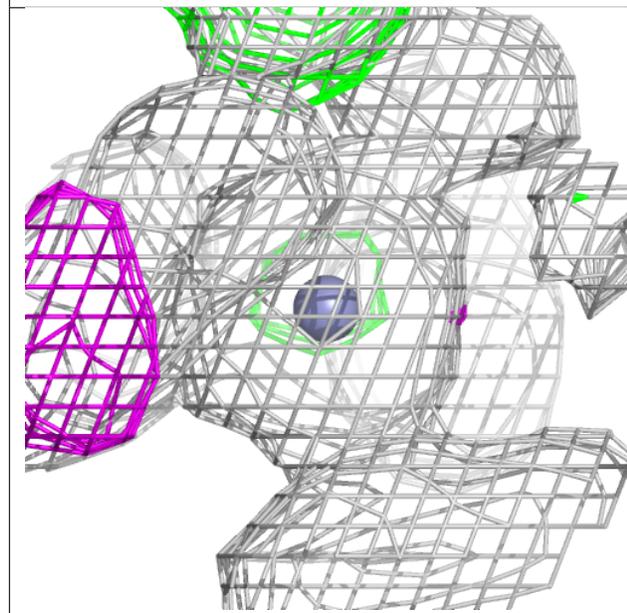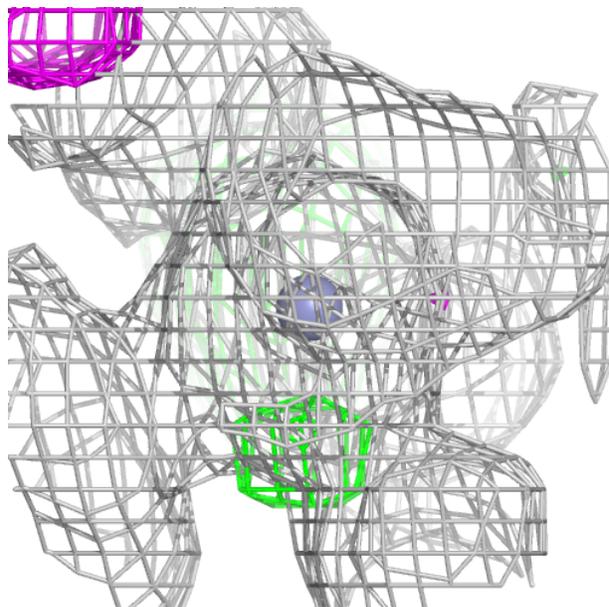and green (positive)

Electron density around ZN F 401:

$2mF_o$-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 401:

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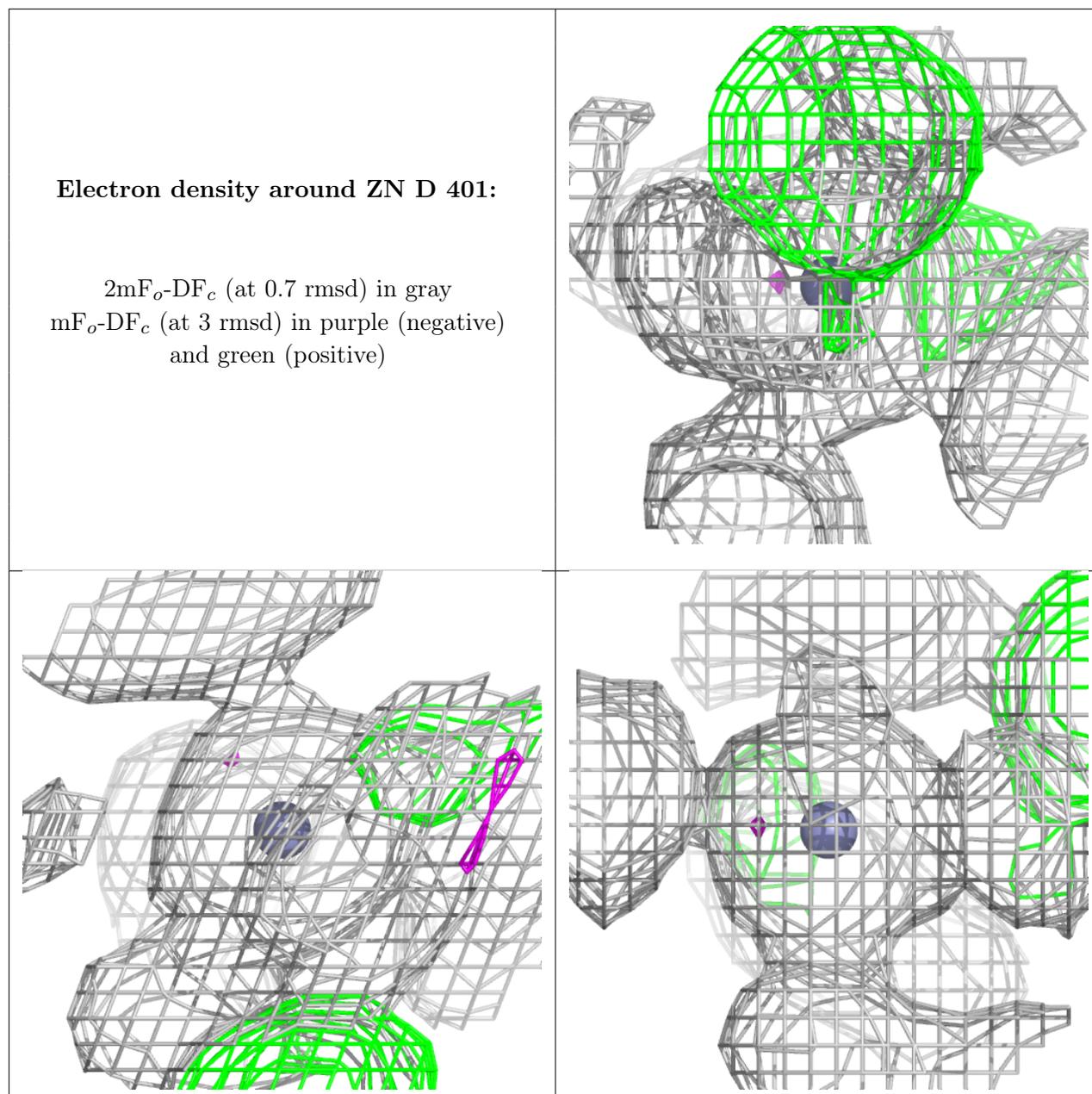and green (positive)

Electron density around ZN D 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.