



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 PM UTC

PDB ID : 7O45 / pdb_00007o45
Title : Crystal structure of ADD domain of the human DNMT3B methyltransferase
Authors : Boyko, K.M.; Nikolaeva, A.Y.; Bonchuk, A.N.; Georgiev, P.G.; Popov, V.O.
Deposited on : 2021-04-05
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

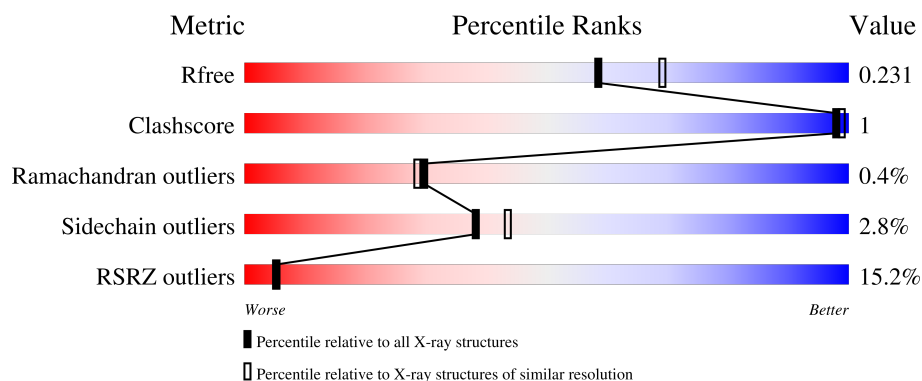
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	146	5% 96% ..
1	B	146	6% 91% 5% ..
1	C	146	3% 89% 7% ..
1	D	146	38% 58% 42%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4065 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 Isoform 6 of DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1105	680	194	212	19			
1	B	141	Total	C	N	O	S	0	2	0
			1109	681	194	214	20			
1	C	141	Total	C	N	O	S	0	3	0
			1111	682	196	214	19			
1	D	84	Total	C	N	O	S	0	0	0
			596	367	110	105	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	SER	-	expression tag	UNP Q9UBC3
A	410	GLY	-	expression tag	UNP Q9UBC3
A	411	SER	-	expression tag	UNP Q9UBC3
B	409	SER	-	expression tag	UNP Q9UBC3
B	410	GLY	-	expression tag	UNP Q9UBC3
B	411	SER	-	expression tag	UNP Q9UBC3
C	409	SER	-	expression tag	UNP Q9UBC3
C	410	GLY	-	expression tag	UNP Q9UBC3
C	411	SER	-	expression tag	UNP Q9UBC3
D	409	SER	-	expression tag	UNP Q9UBC3
D	410	GLY	-	expression tag	UNP Q9UBC3
D	411	SER	-	expression tag	UNP Q9UBC3

- 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	3	Total	Zn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Zn 3	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	3	Total 3	Zn 3	0	0

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Br 2	0	0
3	C	1	Total 1	Br 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total 46	O 46	0	0
4	B	38	Total 38	O 38	0	0
4	C	45	Total 45	O 45	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.

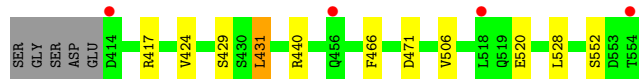
- Molecule 1: Isoform 6 of DNA (cytosine-5)-methyltransferase 3B



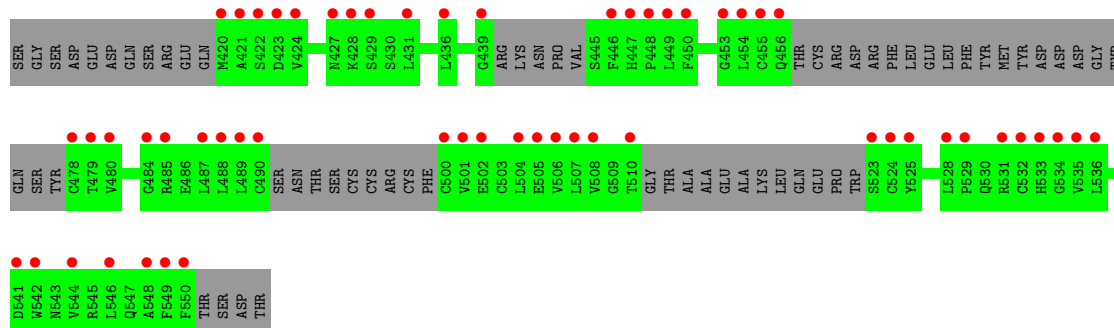
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- Molecule 1: Isoform 6 of DNA (cytosine-5)-methyltransferase 3B



- Molecule 1: Isoform 6 of DNA (cytosine-5)-methyltransferase 3B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.28Å 89.94Å 92.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.38 – 2.10 64.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (64.38-2.10) 92.1 (64.38-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.228 0.202 , 0.231	Depositor DCC
R_{free} test set	1811 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4065	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.09	0/1130	1.46	0/1523
1	B	1.12	0/1138	1.51	1/1534 (0.1%)
1	C	1.11	0/1144	1.44	0/1544
1	D	1.30	0/601	1.71	0/806
All	All	1.14	0/4013	1.51	1/5407 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	442	ASN	CB-CA-C	5.03	115.38	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1105	0	1026	1	0
1	B	1109	0	1027	1	0
1	C	1111	0	1025	3	0
1	D	596	0	531	0	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	A	46	0	0	1	0
4	B	38	0	0	0	0
4	C	45	0	0	0	0
All	All	4065	0	3609	5	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 1.

All (5) 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:424:VAL:HG21	1:C:431:LEU:HD13	1.89	0.55
1:A:459:ARG:NH1	4:A:702:HOH:O	2.45	0.49
1:B:488:LEU:HD13	1:B:504:LEU:HD22	1.96	0.47
1:C:424:VAL:HG11	1:C:431:LEU:HD13	1.95	0.47
1:C:417:ARG:HB3	1:C:506:VAL:HG11	2.03	0.41

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	140/146 (96%)	137 (98%)	3 (2%)	0	100	100
1	B	141/146 (97%)	133 (94%)	7 (5%)	1 (1%)	18	15
1	C	142/146 (97%)	139 (98%)	2 (1%)	1 (1%)	18	15
1	D	74/146 (51%)	69 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	497/584 (85%)	478 (96%)	17 (3%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	415	GLN
1	C	466	PHE

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	124/130 (95%)	124 (100%)	0	100	100
1	B	126/130 (97%)	121 (96%)	5 (4%)	28	29
1	C	126/130 (97%)	119 (94%)	7 (6%)	19	18
1	D	60/130 (46%)	60 (100%)	0	100	100
All	All	436/520 (84%)	424 (97%)	12 (3%)	38	43

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	442	ASN
1	B	465	LEU
1	B	486	GLU
1	B	487	LEU
1	B	528	LEU
1	C	429	SER
1	C	431	LEU
1	C	440	ARG
1	C	471	ASP
1	C	520	GLU
1	C	528	LEU
1	C	552	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	C	519	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 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	141/146 (96%)	0.45	8 (5%) 29 31	35, 47, 71, 81	1 (0%)
1	B	141/146 (96%)	0.53	9 (6%) 25 27	31, 50, 80, 96	2 (1%)
1	C	141/146 (96%)	0.27	4 (2%) 55 57	28, 45, 70, 105	3 (2%)
1	D	84/146 (57%)	2.37	56 (66%) 0 0	66, 106, 140, 152	0
All	All	507/584 (86%)	0.74	77 (15%) 5 5	28, 51, 113, 152	6 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	544	VAL	6.1
1	D	487	LEU	5.4
1	D	454	LEU	5.3
1	D	423	ASP	4.7
1	D	480	VAL	4.5
1	D	525	TYR	4.3
1	D	501	VAL	4.0
1	B	518	LEU	3.9
1	C	554	THR	3.9
1	D	456	GLN	3.7
1	A	484	GLY	3.6
1	D	489	LEU	3.6
1	D	448	PRO	3.6
1	D	505	GLU	3.3
1	D	431	LEU	3.3
1	D	450	PHE	3.3
1	D	534	GLY	3.3
1	D	446	PHE	3.3
1	B	414	ASP	3.2
1	D	507	LEU	3.2
1	A	414	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	518	LEU	3.1
1	D	455	CYS	3.1
1	D	550	PHE	3.0
1	D	532	CYS	3.0
1	D	449	LEU	2.9
1	A	467	TYR	2.9
1	D	424	VAL	2.9
1	D	436	LEU	2.9
1	D	502	GLU	2.9
1	A	485	ARG	2.8
1	D	421	ALA	2.8
1	D	510	THR	2.8
1	D	427	ASN	2.7
1	D	528	LEU	2.7
1	D	548	ALA	2.6
1	D	479	THR	2.6
1	D	428	LYS	2.6
1	D	504	LEU	2.6
1	D	478	CYS	2.6
1	D	542	TRP	2.6
1	D	439	GLY	2.5
1	D	453	GLY	2.5
1	D	429	SER	2.5
1	D	529	PRO	2.5
1	D	533	HIS	2.5
1	D	536	LEU	2.5
1	D	484	GLY	2.5
1	D	506	VAL	2.4
1	D	524	CYS	2.4
1	D	523	SER	2.4
1	D	490	CYS	2.4
1	A	418	GLU	2.4
1	B	485	ARG	2.3
1	D	508	VAL	2.3
1	C	456	GLN	2.3
1	B	515	GLU	2.3
1	D	420	MET	2.3
1	B	437	SER	2.3
1	D	549	PHE	2.3
1	B	510	THR	2.2
1	B	442	ASN	2.2
1	A	465	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	488	LEU	2.2
1	D	546	LEU	2.2
1	D	541	ASP	2.2
1	D	531	ARG	2.2
1	B	467	TYR	2.1
1	D	485	ARG	2.1
1	A	543	ASN	2.1
1	A	466	PHE	2.1
1	B	519	GLN	2.0
1	D	447	HIS	2.0
1	D	535	VAL	2.0
1	D	422	SER	2.0
1	C	414	ASP	2.0
1	D	500	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

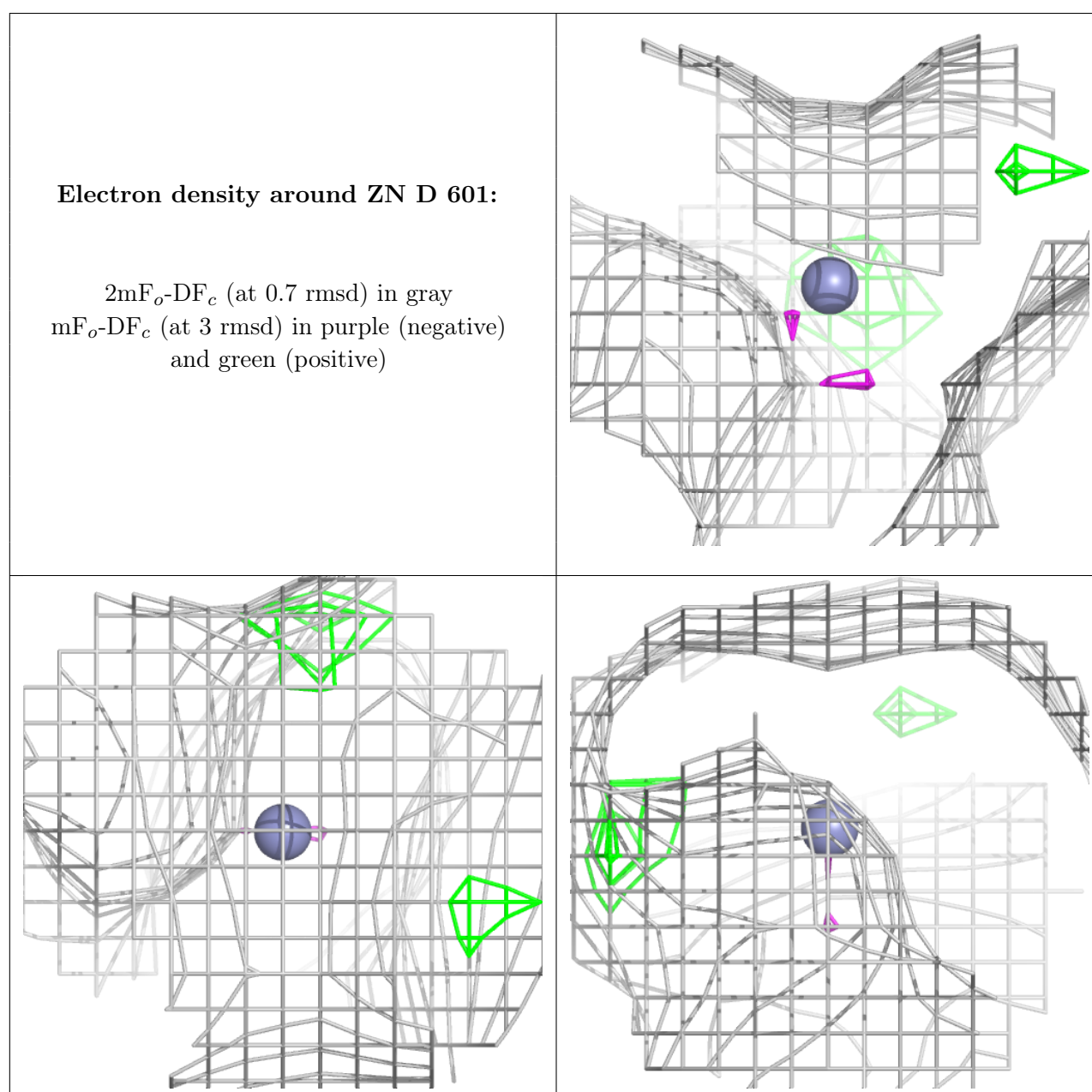
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	D	601	1/1	0.59	0.12	89,89,89,89	1
2	ZN	D	603	1/1	0.82	0.10	80,80,80,80	1
3	BR	C	604	1/1	0.91	0.17	86,86,86,86	0
3	BR	A	604	1/1	0.92	0.09	107,107,107,107	0
2	ZN	B	601	1/1	0.97	0.06	47,47,47,47	0
2	ZN	D	602	1/1	0.98	0.05	77,77,77,77	1
2	ZN	B	602	1/1	0.98	0.04	45,45,45,45	0
2	ZN	B	603	1/1	0.98	0.03	43,43,43,43	0
3	BR	A	605	1/1	0.98	0.13	78,78,78,78	0

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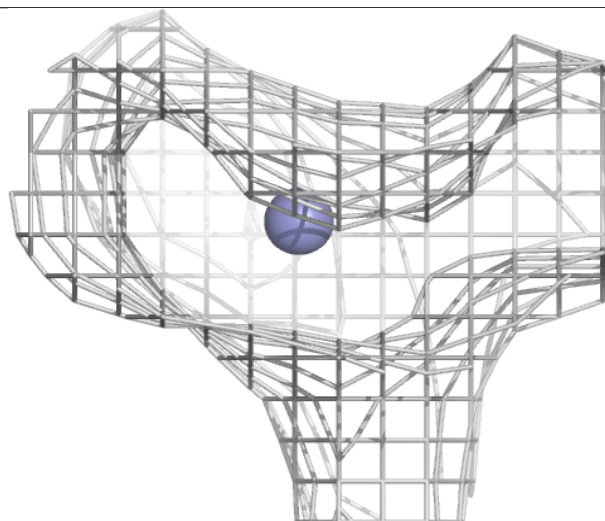
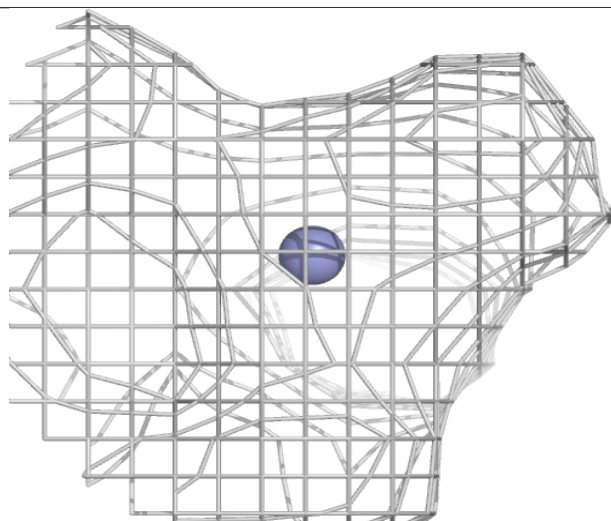
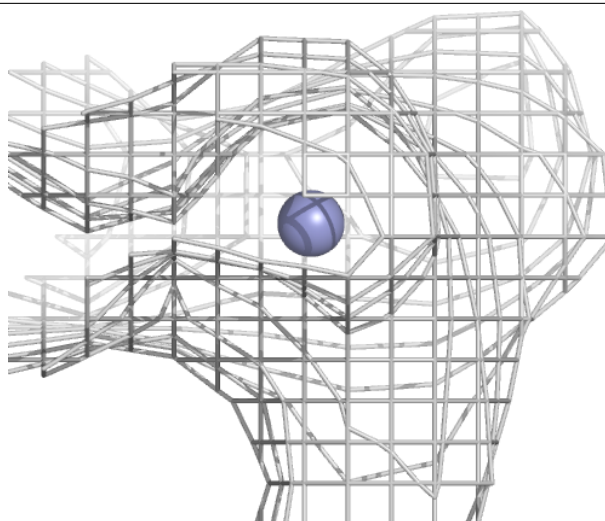
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	601	1/1	0.98	0.03	43,43,43,43	0
2	ZN	C	601	1/1	0.99	0.04	40,40,40,40	0
2	ZN	C	602	1/1	0.99	0.03	40,40,40,40	0
2	ZN	A	603	1/1	0.99	0.03	36,36,36,36	0
2	ZN	A	602	1/1	0.99	0.02	42,42,42,42	0
2	ZN	C	603	1/1	1.00	0.02	38,38,38,38	0

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.



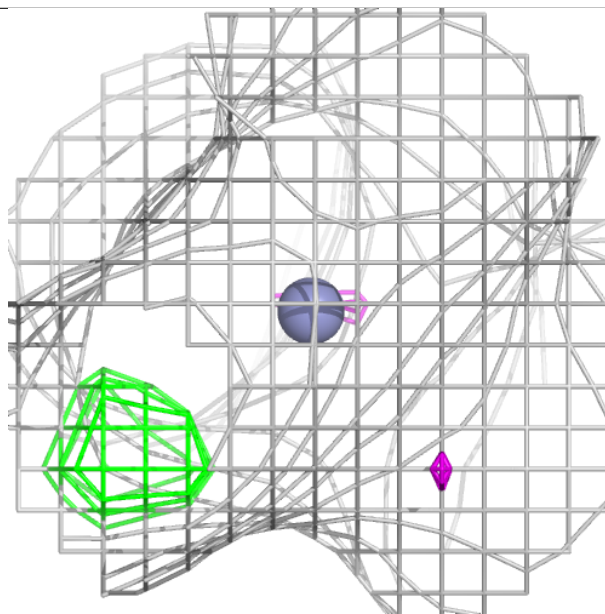
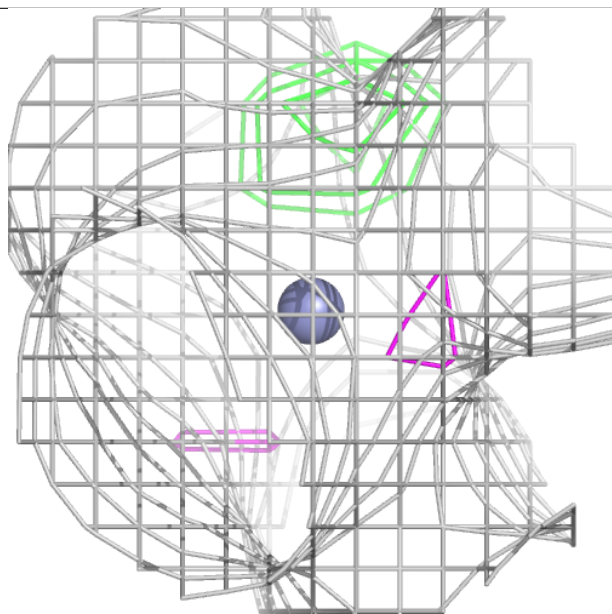
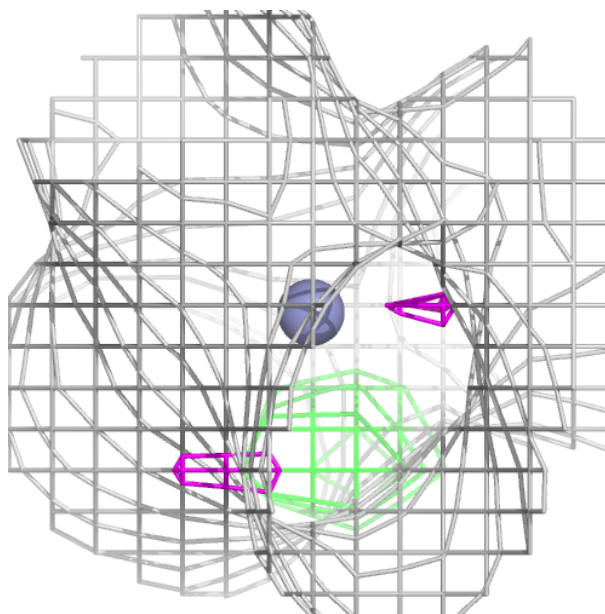
Electron density around ZN D 603:

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



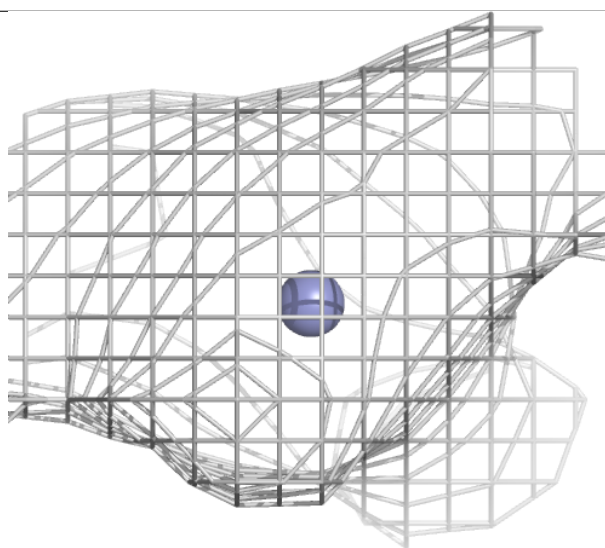
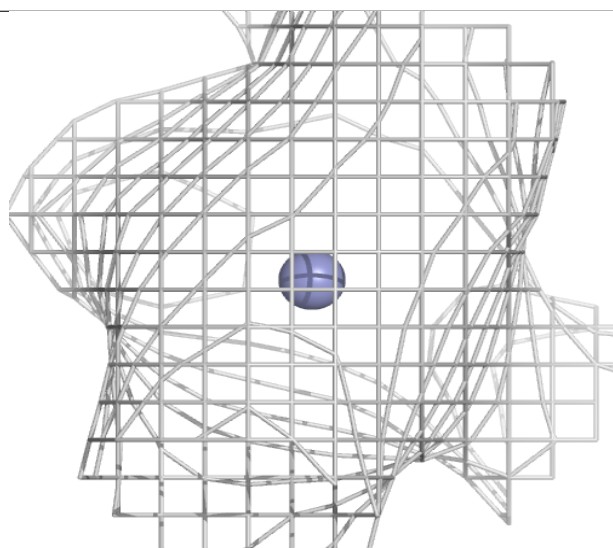
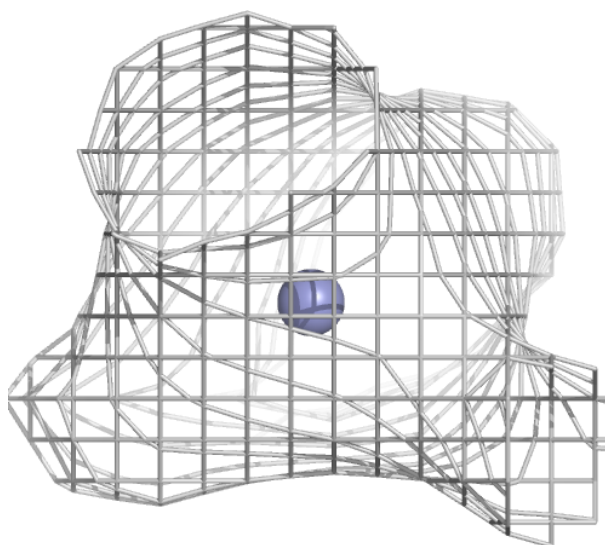
Electron density around ZN B 601:

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



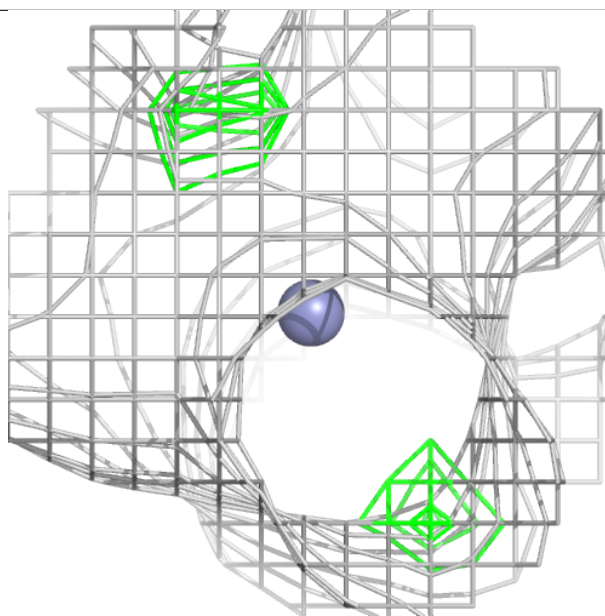
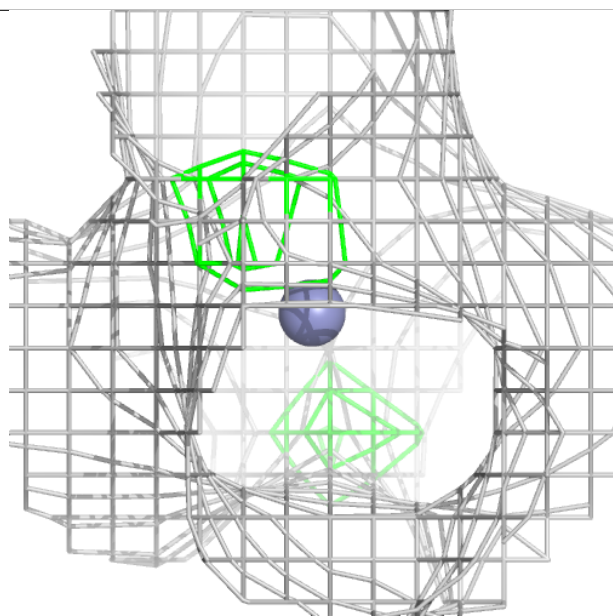
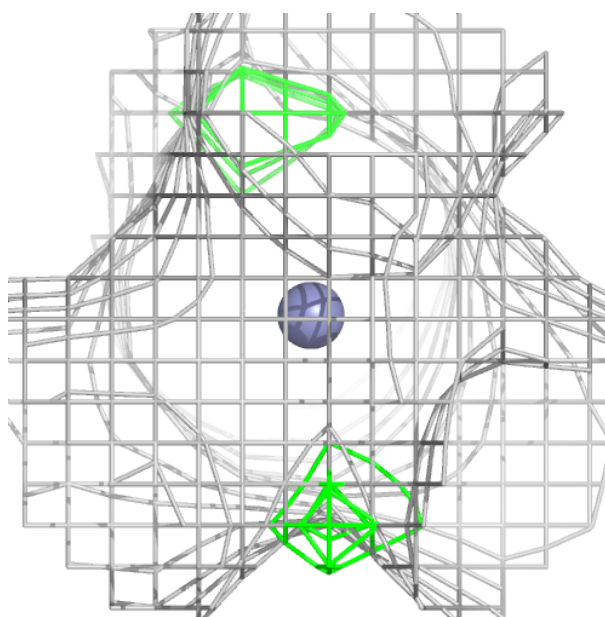
Electron density around ZN D 602:

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



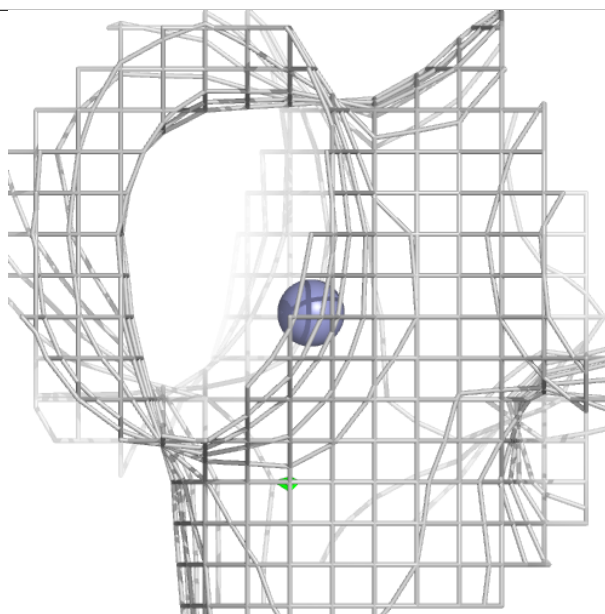
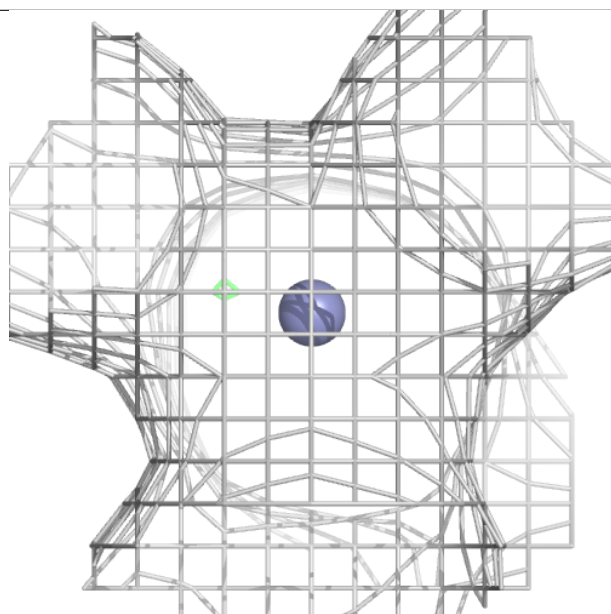
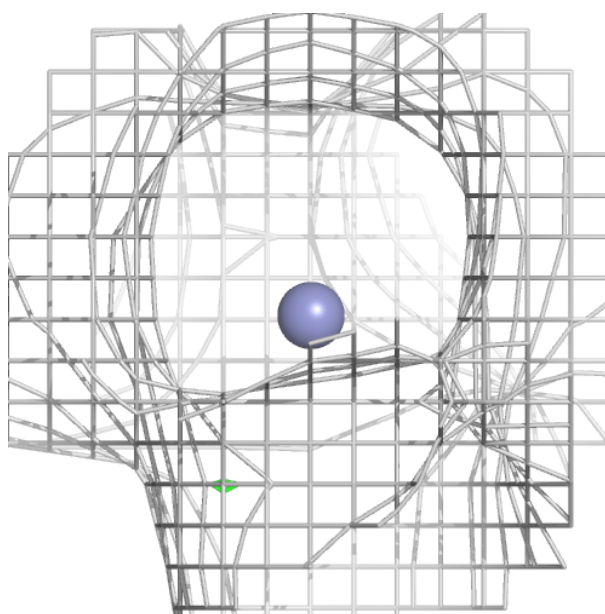
Electron density around ZN B 602:

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



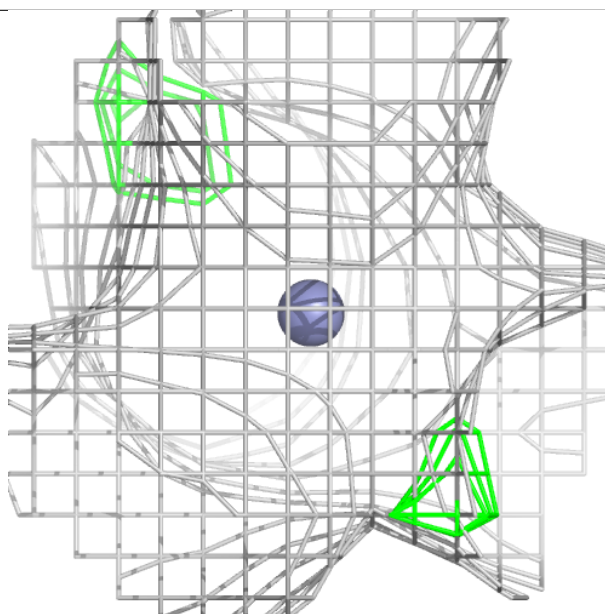
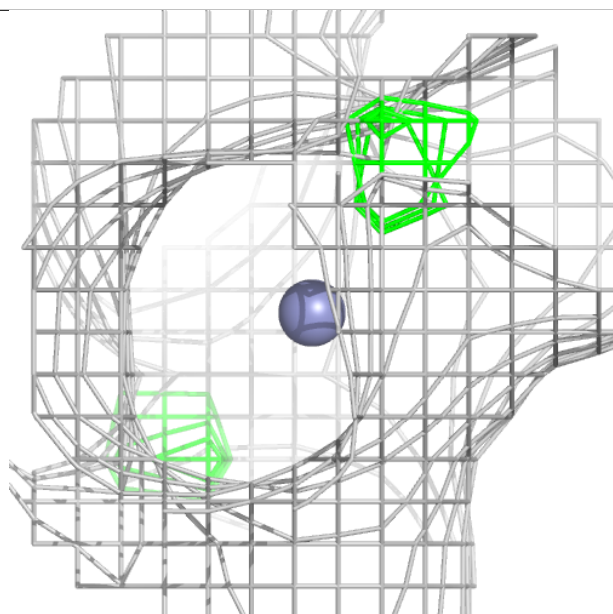
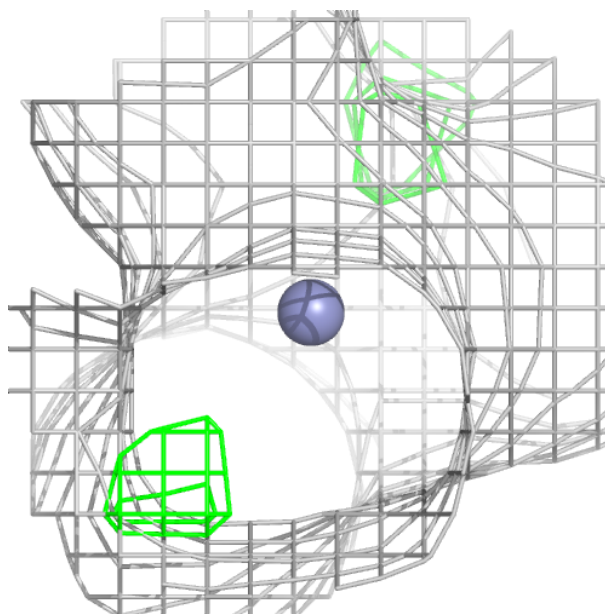
Electron density around ZN B 603:

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



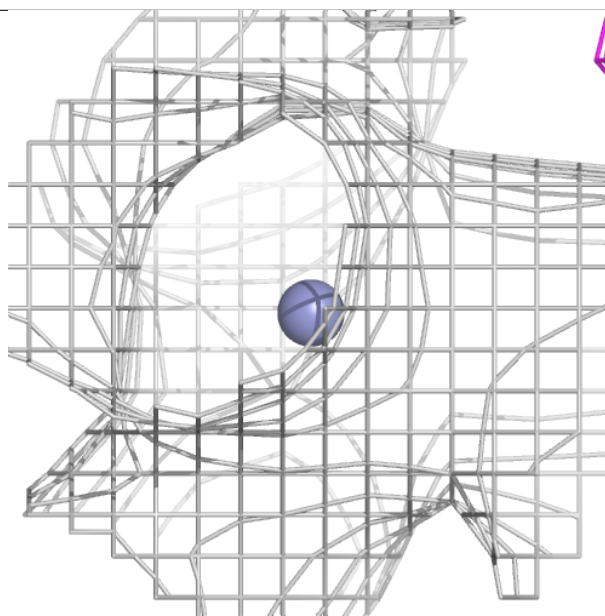
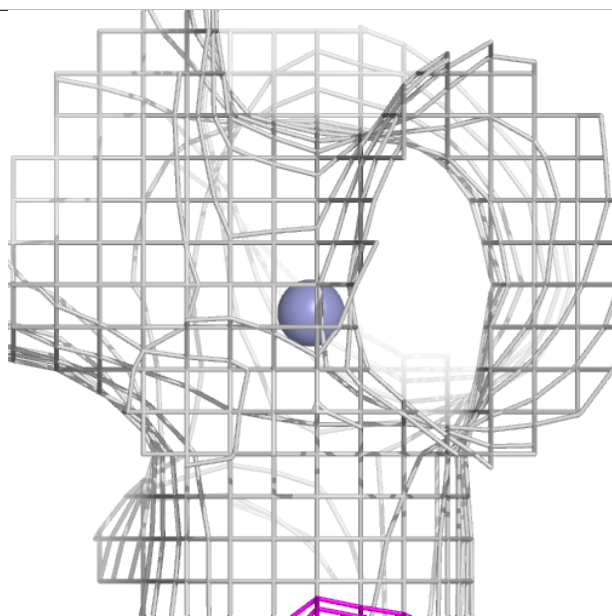
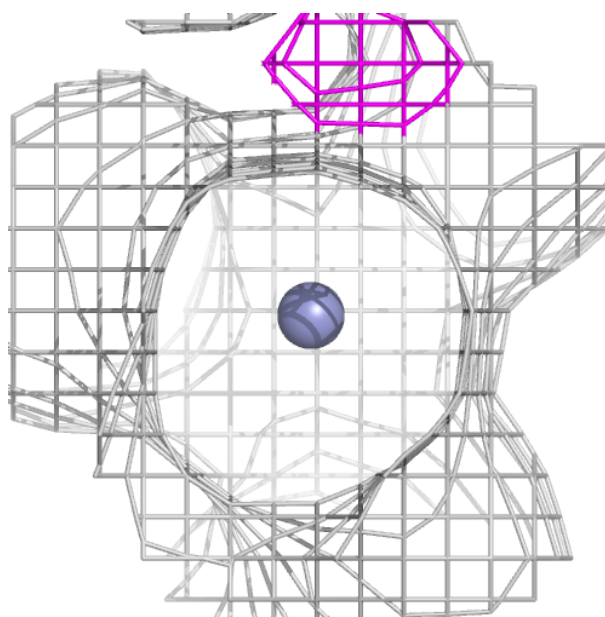
Electron density around ZN A 601:

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



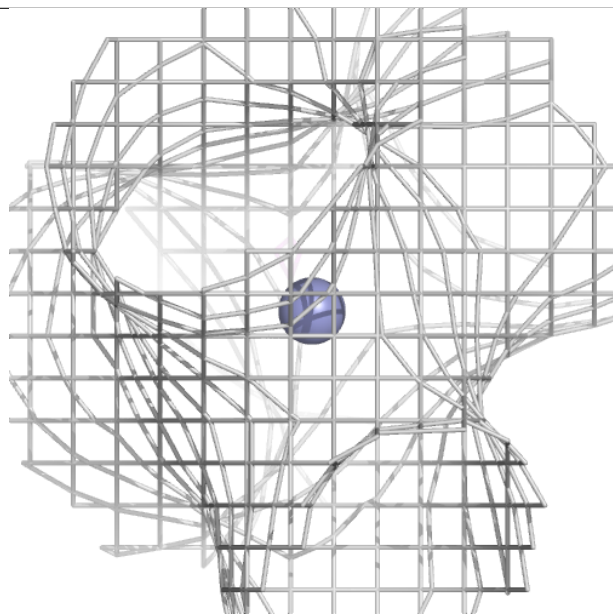
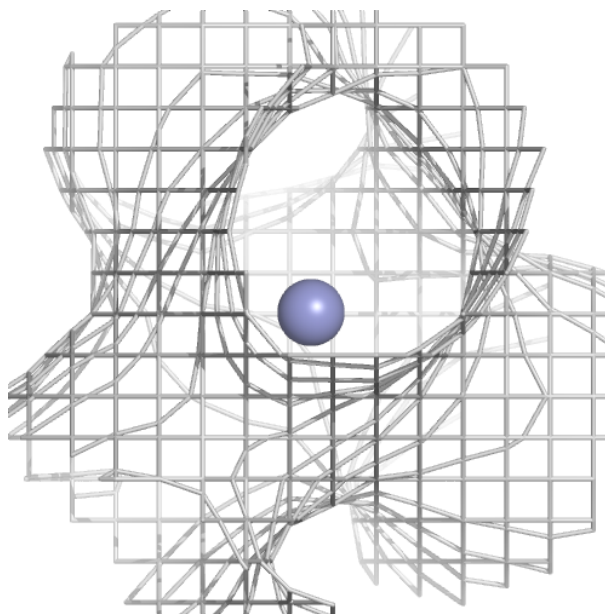
Electron density around ZN C 601:

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



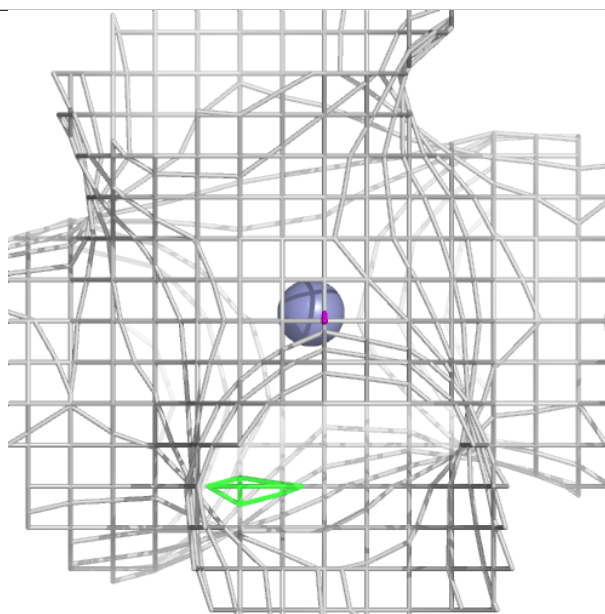
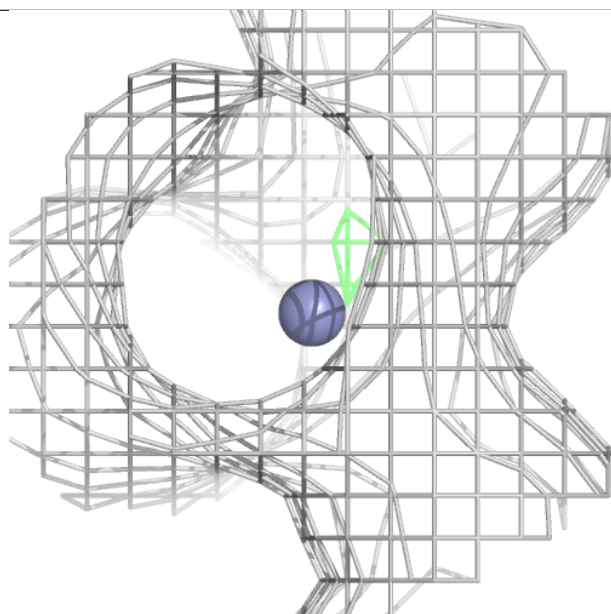
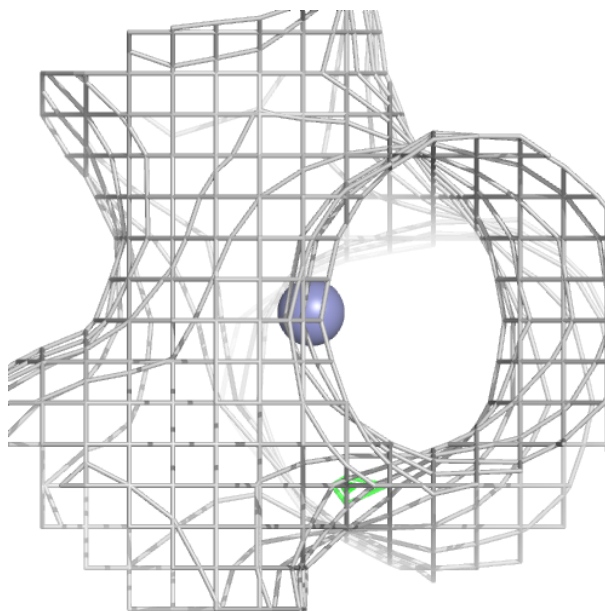
Electron density around ZN C 602:

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



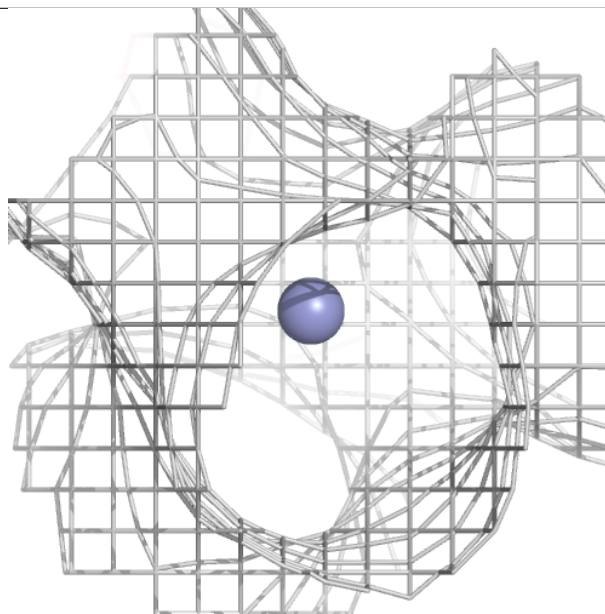
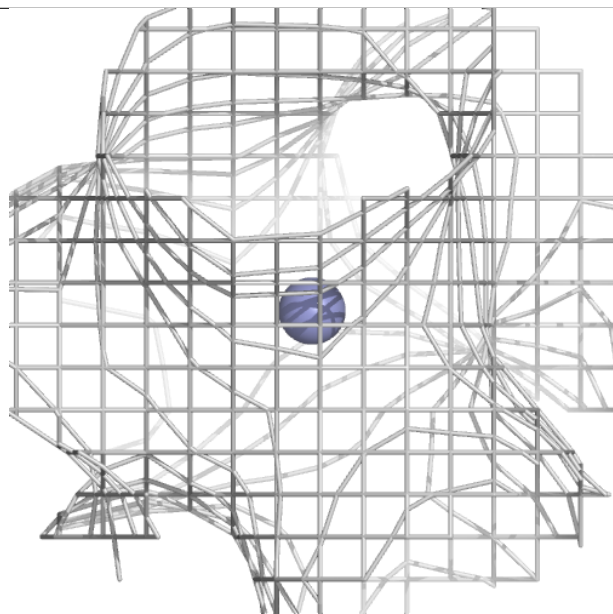
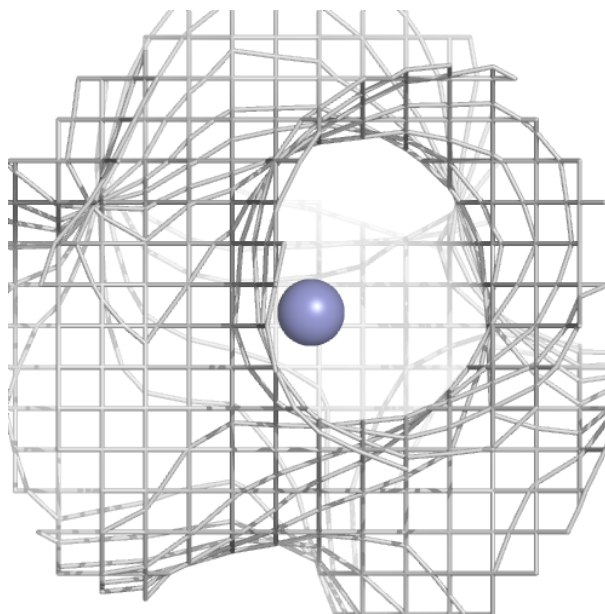
Electron density around ZN A 603:

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



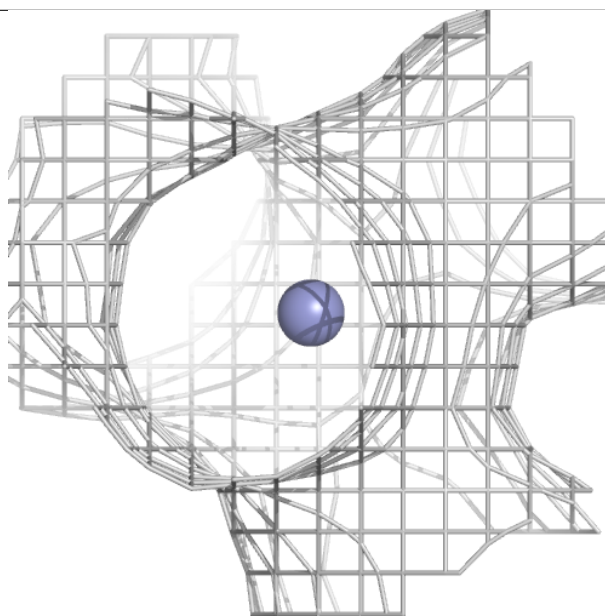
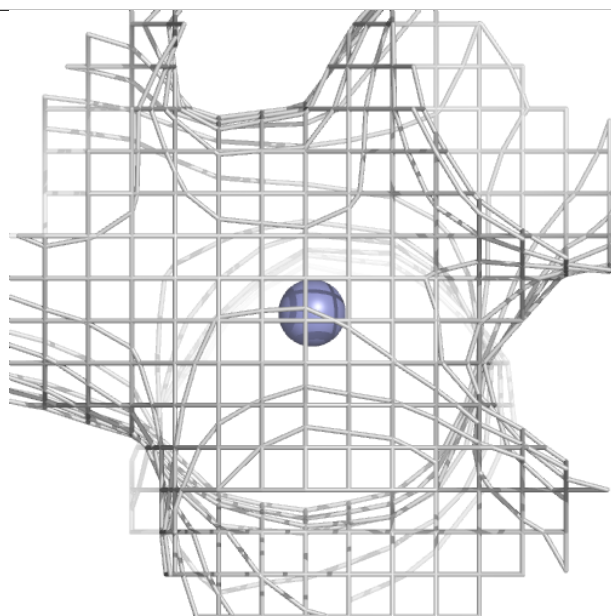
Electron density around ZN A 602:

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



Electron density around ZN C 603:

$2mF_o-DF_c$ (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.