



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 10:06 am BST

PDB ID : 7O45  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

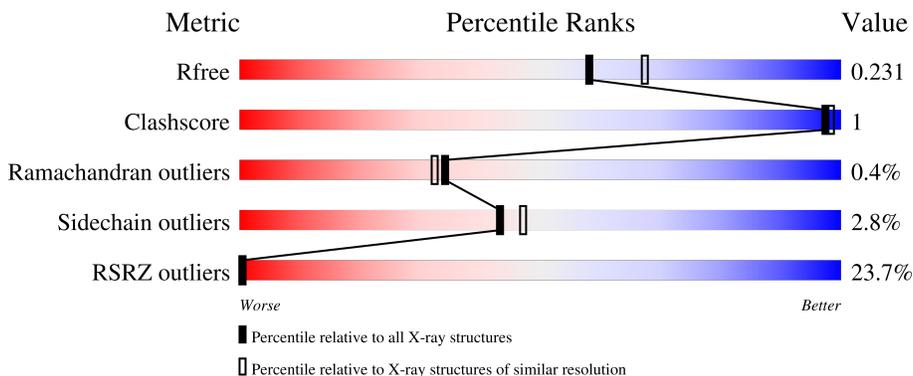
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	 10% 95% ..
1	B	146	 14% 92% 5% ..
1	C	146	 10% 88% 8% ..
1	D	146	 49% 58% 42%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	D	601	-	-	-	X

## 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
			Total	C	N	O	S			
1	A	141	1105	680	194	212	19	0	1	0
1	B	141	1109	681	194	214	20	0	2	0
1	C	141	1111	682	196	214	19	0	3	0
1	D	84	596	367	110	105	14	0	0	0

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 (three-letter code: 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		

*Continued on next page...*

*Continued from previous page...*

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 (three-letter code: 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

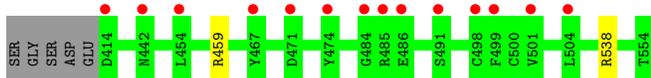
- Molecule 4 is water.

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.

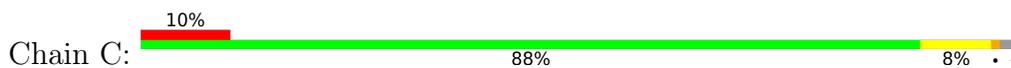
- Molecule 1: Isoform 6 of DNA (cytosine-5)-methyltransferase 3B



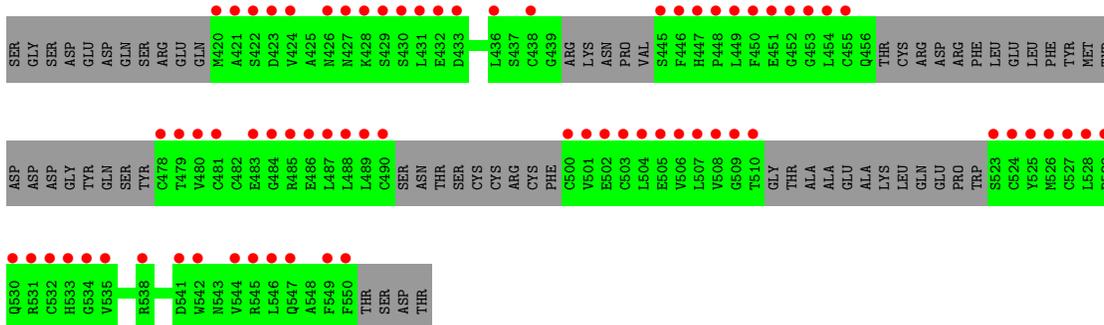
- Molecule 1: Isoform 6 of DNA (cytosine-5)-methyltransferase 3B



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 91.8 (64.38-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.10Å)	Xtrriage
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 <sup>2</sup> )	42.0	Xtrriage
Anisotropy	0.581	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage'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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BR, 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	0.77	0/1130	0.91	1/1523 (0.1%)
1	B	0.78	0/1138	0.94	0/1534
1	C	0.77	0/1144	0.92	1/1544 (0.1%)
1	D	0.92	0/601	0.93	0/806
All	All	0.80	0/4013	0.93	2/5407 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	537	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	4	0
1	D	596	0	531	0	0
2	A	3	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
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	1	0
All	All	4065	0	3609	6	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 (6) 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:492[A]:ASN:OD1	4:C:702:HOH:O	1.84	0.95
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	<a href="#">100</a> <a href="#">100</a>
1	B	141/146 (97%)	133 (94%)	7 (5%)	1 (1%)	<a href="#">22</a> <a href="#">18</a>

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	142/146 (97%)	139 (98%)	2 (1%)	1 (1%)	22	18
1	D	74/146 (51%)	69 (93%)	5 (7%)	0	100	100
All	All	497/584 (85%)	478 (96%)	17 (3%)	2 (0%)	34	32

All (2) Ramachandran outliers are listed below:

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

### 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	124/130 (95%)	124 (100%)	0	100	100
1	B	126/130 (97%)	122 (97%)	4 (3%)	39	41
1	C	126/130 (97%)	118 (94%)	8 (6%)	18	15
1	D	60/130 (46%)	60 (100%)	0	100	100
All	All	436/520 (84%)	424 (97%)	12 (3%)	43	47

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	528	LEU
1	C	417	ARG
1	C	429	SER
1	C	431	LEU
1	C	440	ARG
1	C	471	ASP
1	C	520	GLU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	528	LEU
1	C	552	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	141/146 (96%)	1.20	14 (9%) <b>7</b> <b>9</b>	35, 47, 71, 81	0
1	B	141/146 (96%)	1.32	20 (14%) <b>2</b> <b>3</b>	34, 50, 80, 96	0
1	C	141/146 (96%)	1.13	15 (10%) <b>6</b> <b>7</b>	36, 45, 70, 105	0
1	D	84/146 (57%)	5.13	71 (84%) <b>0</b> <b>0</b>	66, 106, 140, 152	0
All	All	507/584 (86%)	1.87	120 (23%) <b>0</b> <b>0</b>	34, 51, 113, 152	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	484	GLY	20.3
1	D	504	LEU	15.8
1	D	489	LEU	14.9
1	D	428	LYS	13.1
1	D	500	CYS	12.9
1	D	455	CYS	12.1
1	D	532	CYS	10.4
1	D	510	THR	10.3
1	D	503	CYS	10.3
1	D	533	HIS	9.7
1	D	430	SER	8.9
1	D	546	LEU	8.7
1	D	423	ASP	8.5
1	D	525	TYR	8.3
1	D	432	GLU	8.1
1	D	508	VAL	8.1
1	D	501	VAL	7.8
1	D	528	LEU	7.8
1	A	484	GLY	7.0
1	D	480	VAL	6.9
1	D	446	PHE	6.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	486	GLU	6.3
1	D	550	PHE	6.1
1	D	523	SER	6.0
1	D	485	ARG	5.9
1	D	422	SER	5.8
1	D	431	LEU	5.8
1	D	530	GLN	5.7
1	D	488	LEU	5.5
1	D	544	VAL	5.4
1	D	445	SER	5.3
1	D	451	GLU	5.1
1	D	479	THR	5.0
1	D	524	CYS	5.0
1	A	467	TYR	4.8
1	D	478	CYS	4.8
1	D	424	VAL	4.7
1	D	454	LEU	4.7
1	B	554	THR	4.6
1	D	509	GLY	4.6
1	D	487	LEU	4.5
1	B	442	ASN	4.5
1	D	541	ASP	4.5
1	D	433	ASP	4.4
1	D	429	SER	4.2
1	D	427	ASN	4.2
1	B	414	ASP	4.2
1	D	426	ASN	4.1
1	D	542	TRP	4.1
1	D	421	ALA	4.0
1	D	535	VAL	3.9
1	B	444	VAL	3.9
1	D	420	MET	3.9
1	C	554	THR	3.9
1	D	534	GLY	3.9
1	B	518	LEU	3.8
1	D	547	GLN	3.8
1	D	481	CYS	3.8
1	D	447	HIS	3.7
1	B	456	GLN	3.7
1	A	486	GLU	3.6
1	D	538	ARG	3.5
1	D	506	VAL	3.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	518	LEU	3.4
1	D	436	LEU	3.3
1	B	517	LYS	3.3
1	D	531	ARG	3.2
1	D	490	CYS	3.1
1	D	448	PRO	3.1
1	D	438	CYS	3.1
1	C	442	ASN	3.1
1	D	529	PRO	3.0
1	A	491	SER	3.0
1	B	519	GLN	2.9
1	B	496	CYS	2.9
1	D	507	LEU	2.9
1	D	527	CYS	2.9
1	D	505	GLU	2.8
1	C	461[A]	ARG	2.8
1	C	499	PHE	2.8
1	A	442	ASN	2.8
1	B	553	ASP	2.8
1	D	549	PHE	2.8
1	C	519	GLN	2.7
1	D	450	PHE	2.7
1	A	498	CYS	2.7
1	C	429	SER	2.7
1	D	453	GLY	2.6
1	D	483	GLU	2.6
1	C	479	THR	2.5
1	A	414	ASP	2.4
1	A	499	PHE	2.4
1	B	532[A]	CYS	2.4
1	D	502	GLU	2.4
1	A	504	LEU	2.4
1	C	447	HIS	2.4
1	B	501	VAL	2.3
1	C	480	VAL	2.3
1	D	526	MET	2.3
1	B	508	VAL	2.3
1	B	459	ARG	2.3
1	B	467	TYR	2.3
1	A	501	VAL	2.3
1	C	496	CYS	2.2
1	C	521	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	499	PHE	2.1
1	A	485	ARG	2.1
1	A	454	LEU	2.1
1	C	515	GLU	2.1
1	B	504	LEU	2.1
1	B	492[A]	ASN	2.1
1	A	471	ASP	2.1
1	D	545	ARG	2.1
1	B	513	ALA	2.1
1	D	452	GLY	2.1
1	B	544	VAL	2.1
1	C	498	CYS	2.0
1	D	449	LEU	2.0
1	C	466	PHE	2.0
1	A	474	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	601	1/1	0.49	0.83	89,89,89,89	1
3	BR	A	604	1/1	0.51	0.09	107,107,107,107	0
2	ZN	D	602	1/1	0.88	0.15	77,77,77,77	1
2	ZN	B	602	1/1	0.91	0.05	45,45,45,45	0
2	ZN	B	603	1/1	0.92	0.07	43,43,43,43	0
2	ZN	B	601	1/1	0.93	0.07	47,47,47,47	0
3	BR	C	604	1/1	0.93	0.10	86,86,86,86	0
3	BR	A	605	1/1	0.94	0.12	78,78,78,78	0

*Continued on next page...*

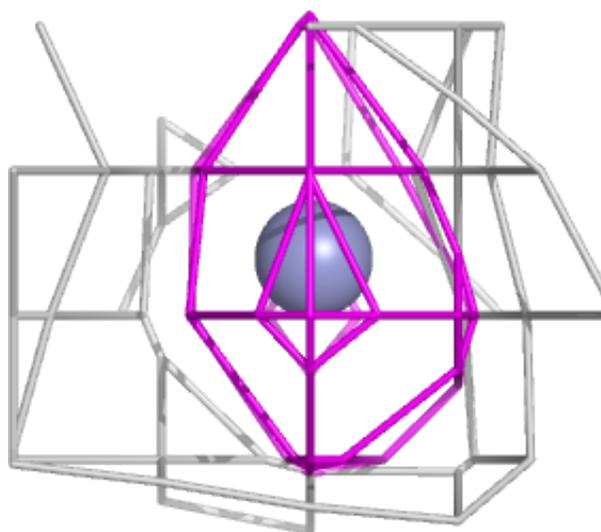
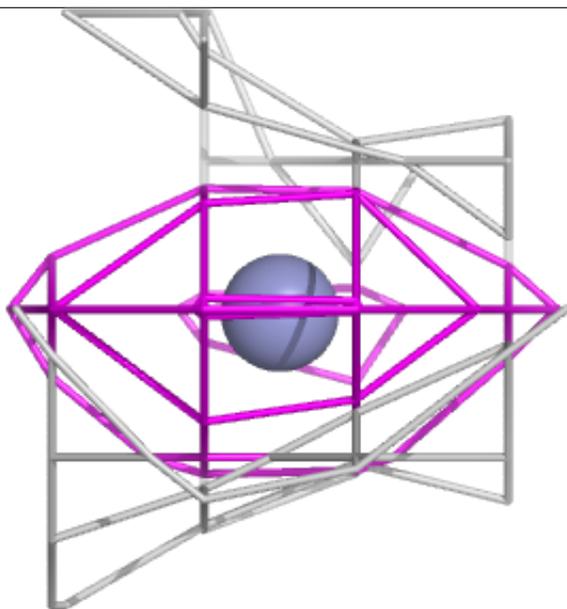
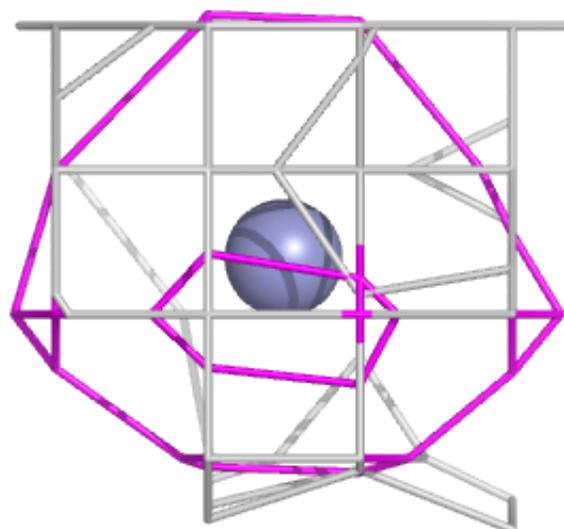
*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Atoms</b>	<b>RSCC</b>	<b>RSR</b>	<b>B-factors(<math>\text{\AA}^2</math>)</b>	<b>Q&lt;0.9</b>
2	ZN	A	601	1/1	0.96	0.07	43,43,43,43	0
2	ZN	C	601	1/1	0.96	0.11	40,40,40,40	0
2	ZN	D	603	1/1	0.96	0.19	80,80,80,80	1
2	ZN	A	602	1/1	0.97	0.07	42,42,42,42	0
2	ZN	A	603	1/1	0.97	0.09	36,36,36,36	0
2	ZN	C	603	1/1	0.97	0.08	38,38,38,38	0
2	ZN	C	602	1/1	0.98	0.05	40,40,40,40	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.

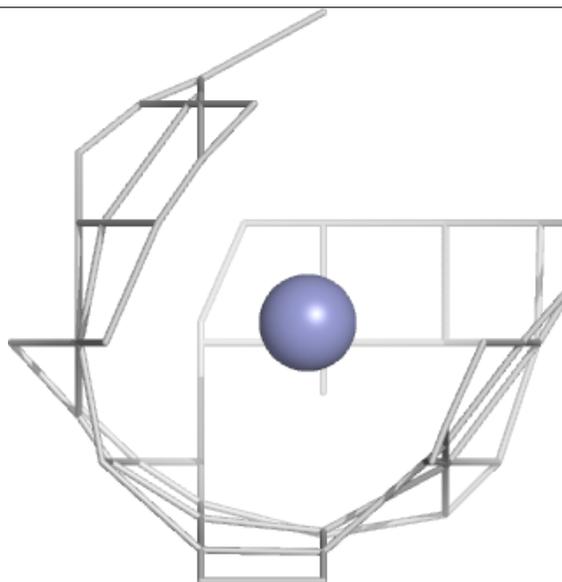
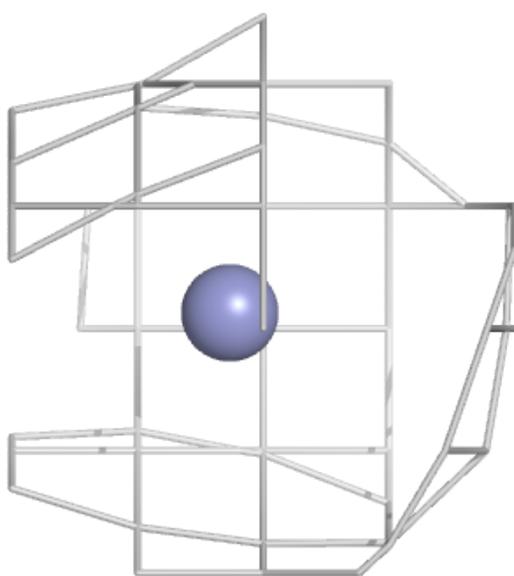
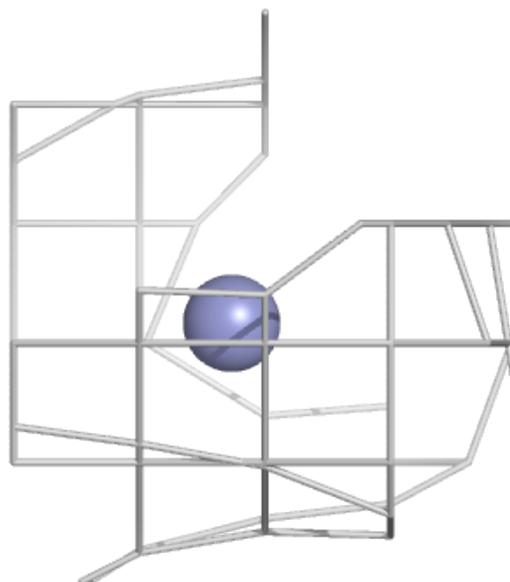
**Electron density around ZN D 601:**

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



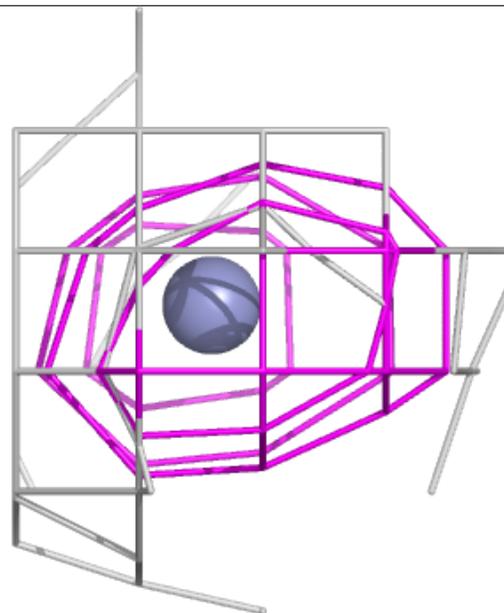
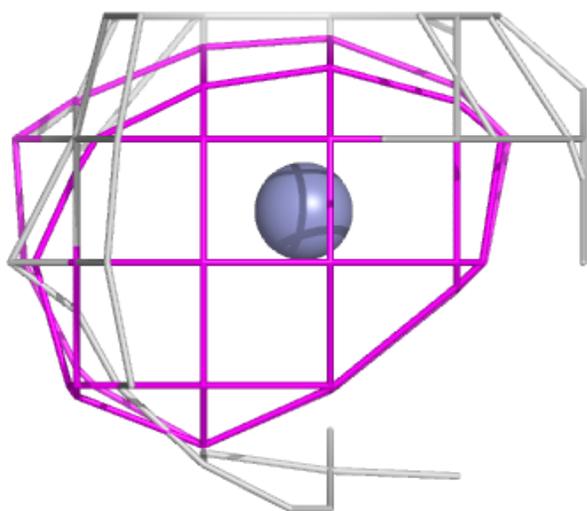
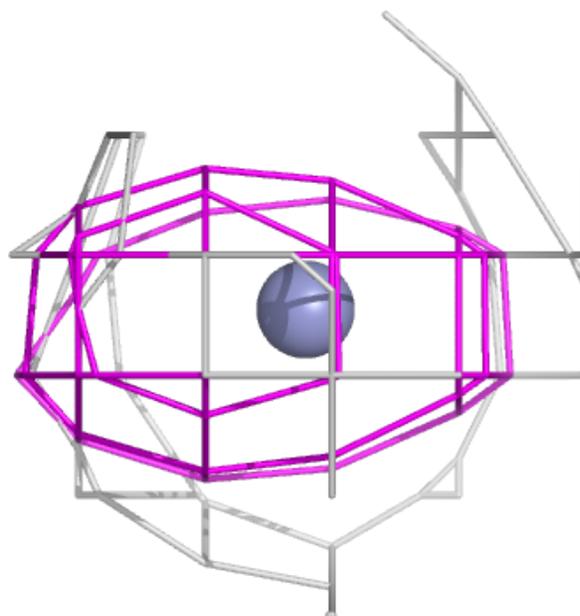
**Electron density around ZN D 602:**

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



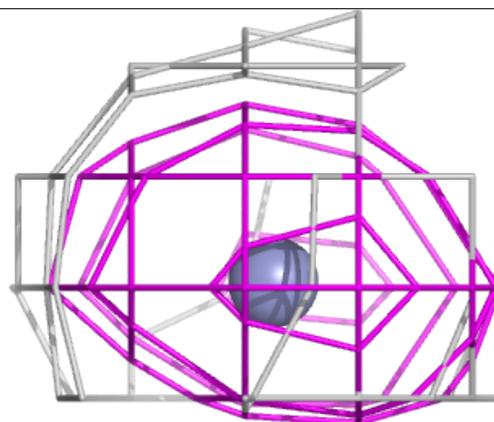
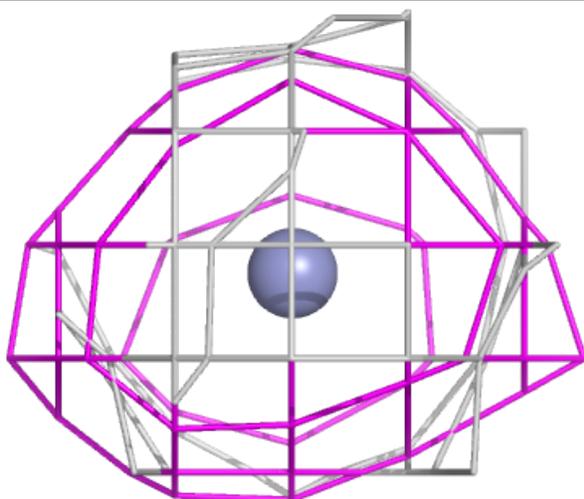
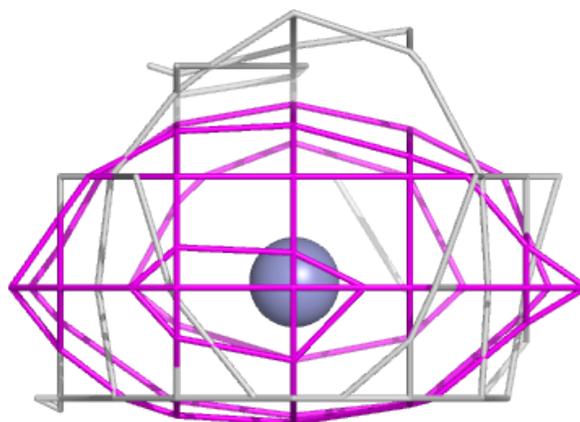
**Electron density around ZN B 602:**

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



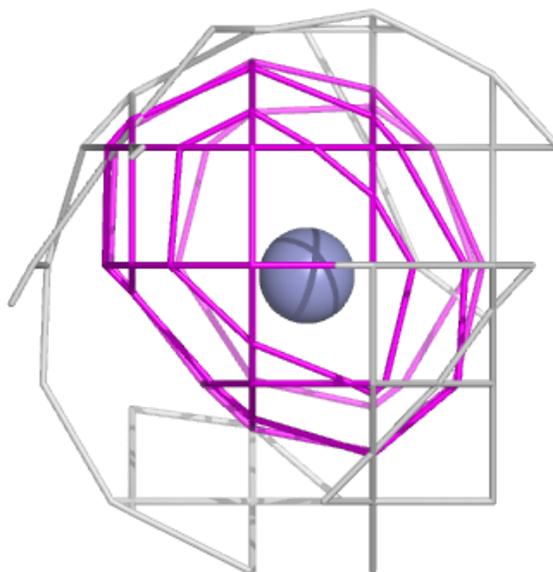
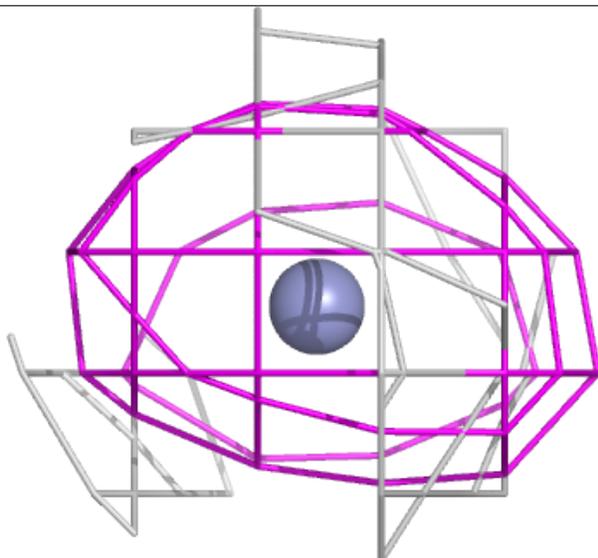
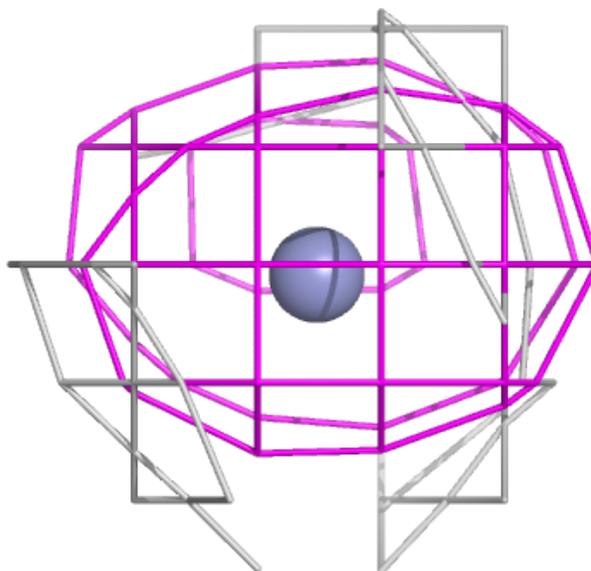
**Electron density around ZN B 603:**

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



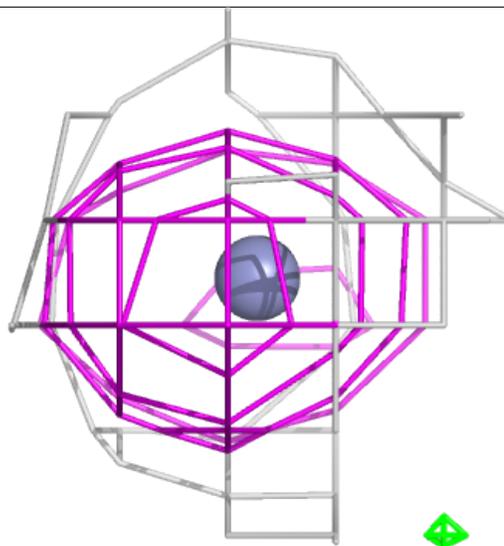
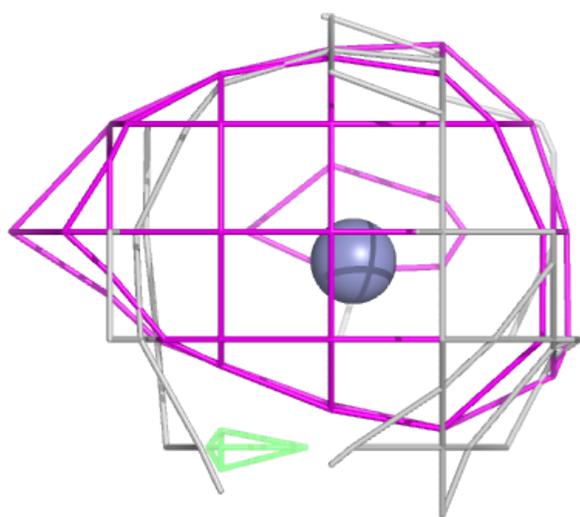
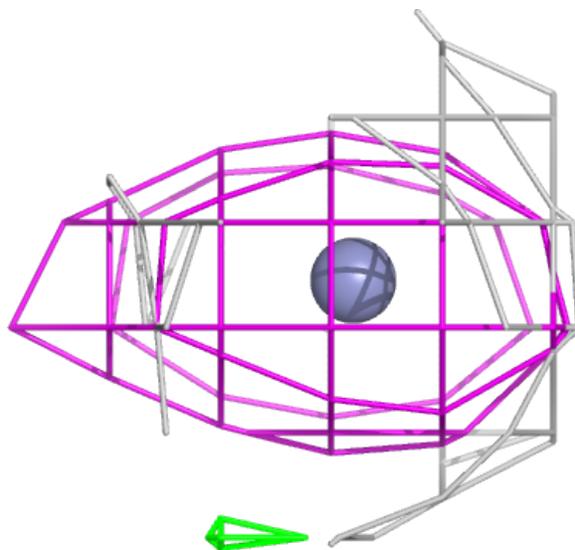
**Electron density around ZN B 601:**

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



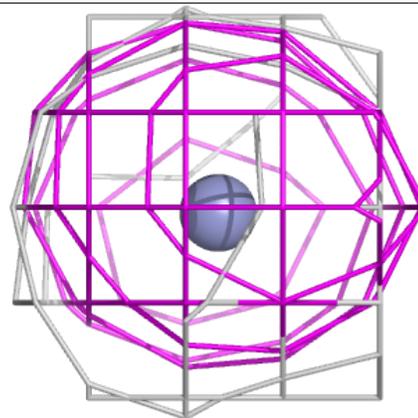
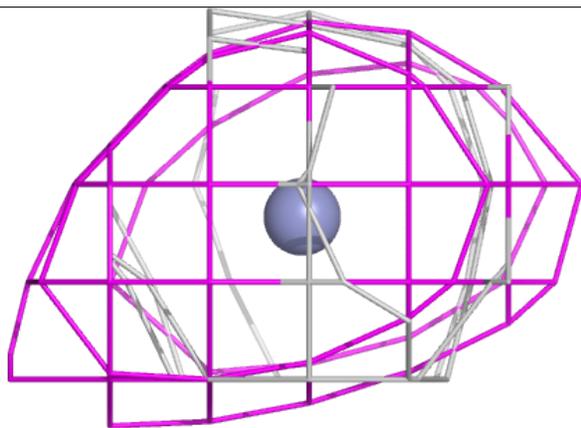
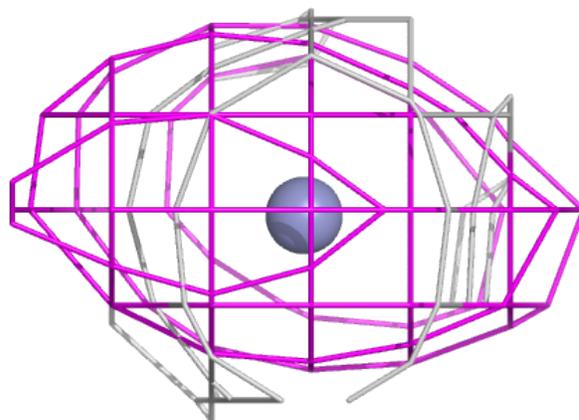
**Electron density around ZN A 601:**

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



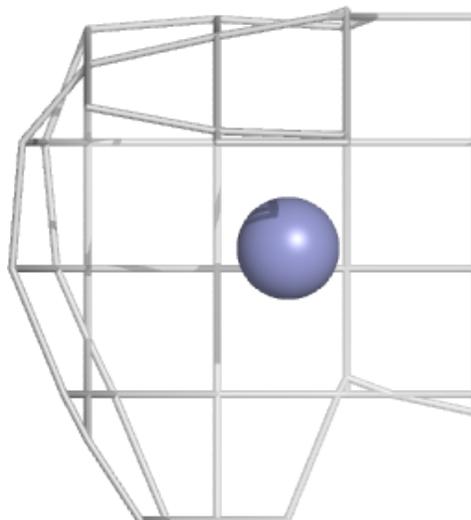
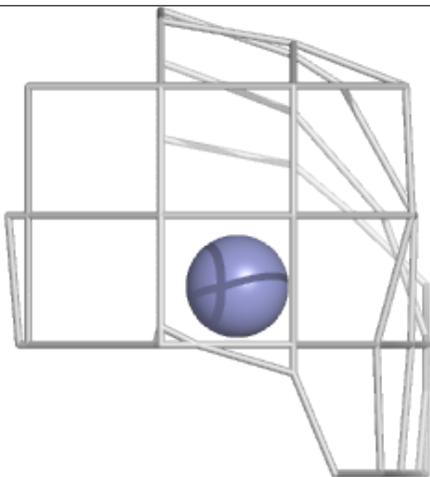
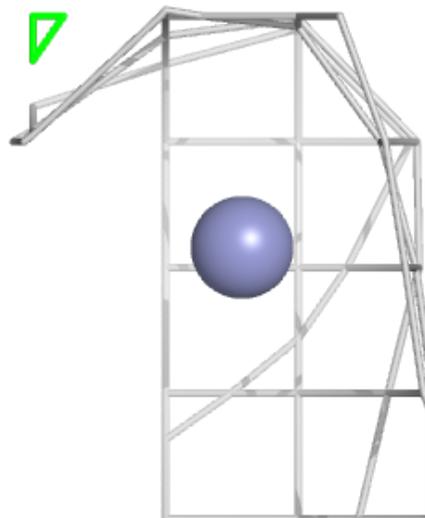
**Electron density around ZN C 601:**

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



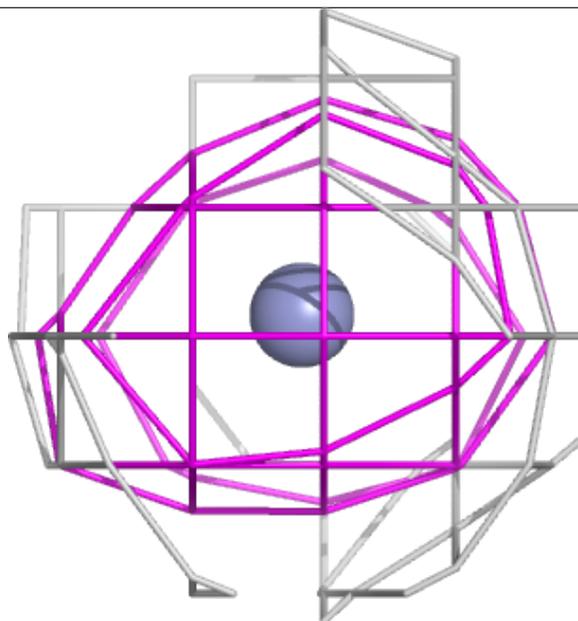
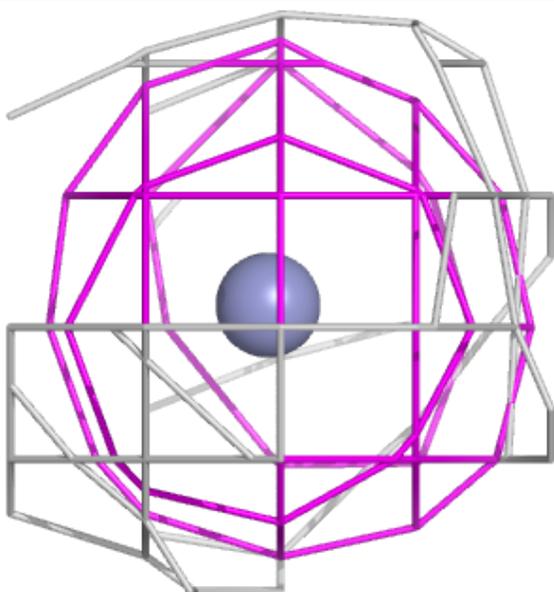
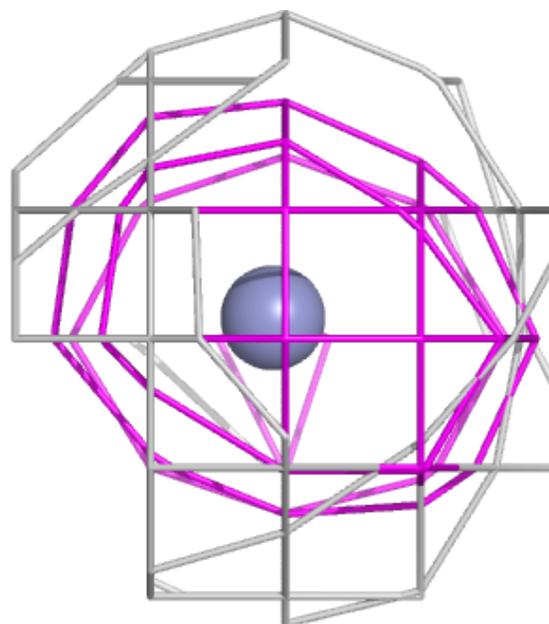
**Electron density around ZN D 603:**

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



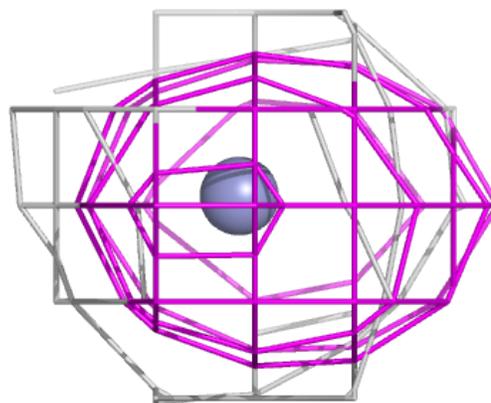
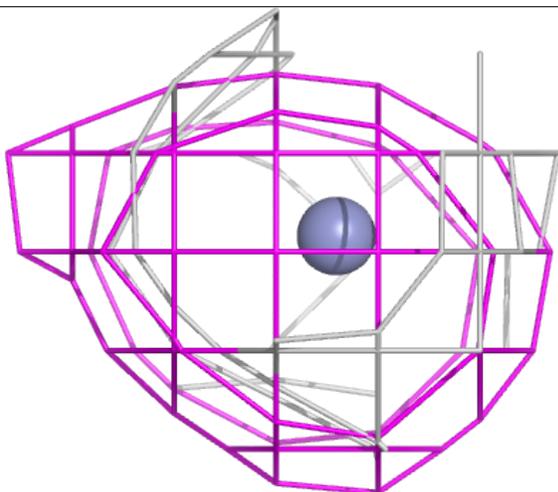
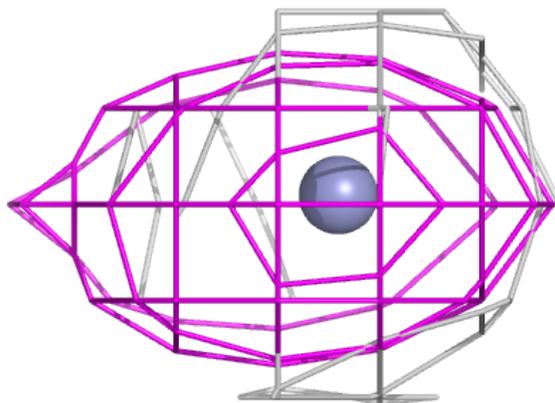
**Electron density around ZN A 602:**

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



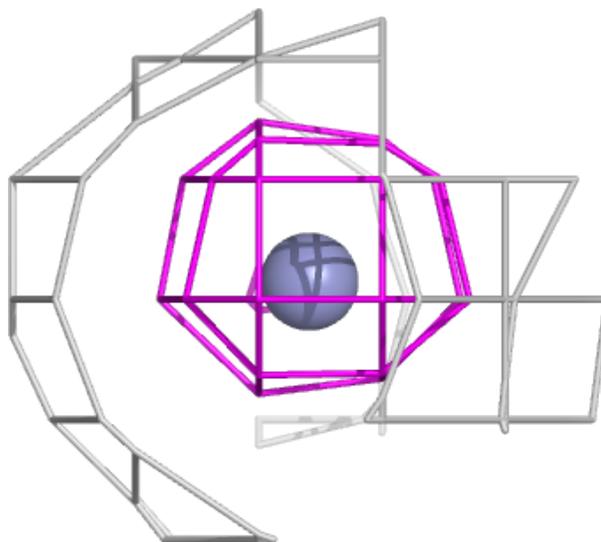
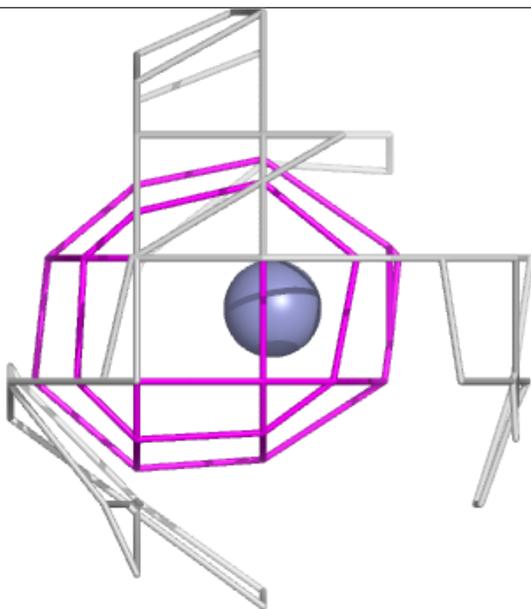
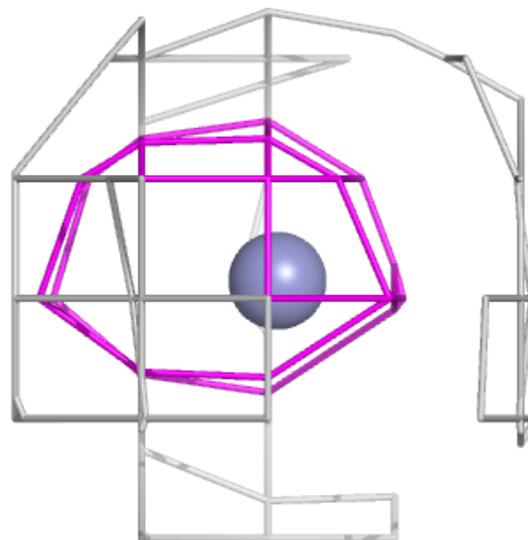
**Electron density around ZN A 603:**

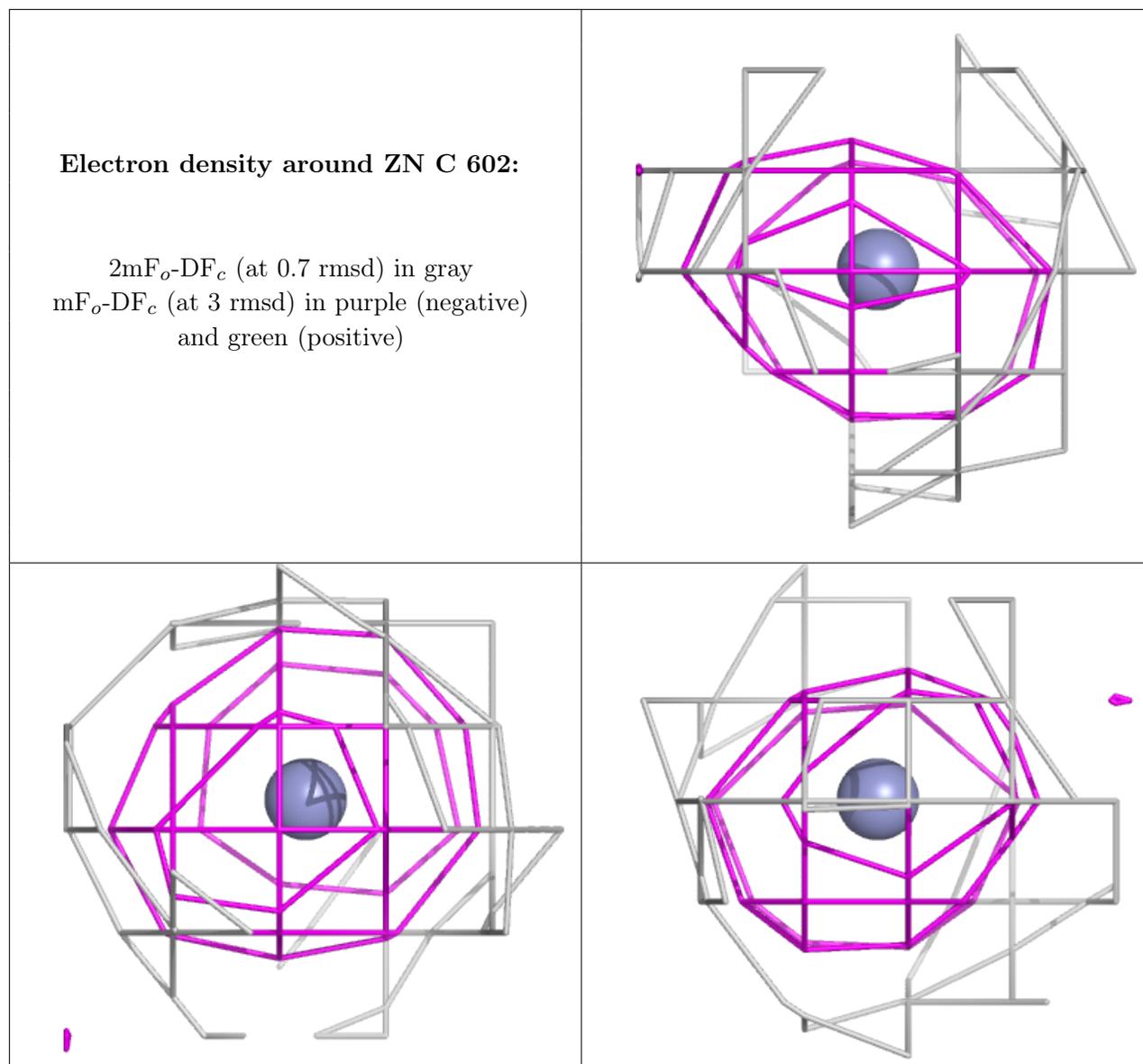
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN 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.