



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:02 AM EDT

PDB ID : 7TD5  
Title : Structure of human PRC2-EZH1 containing phosphorylated SUZ12  
Authors : Gong, L.; Jiao, L.; Liu, X.  
Deposited on : 2021-12-30  
Resolution : 2.99 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

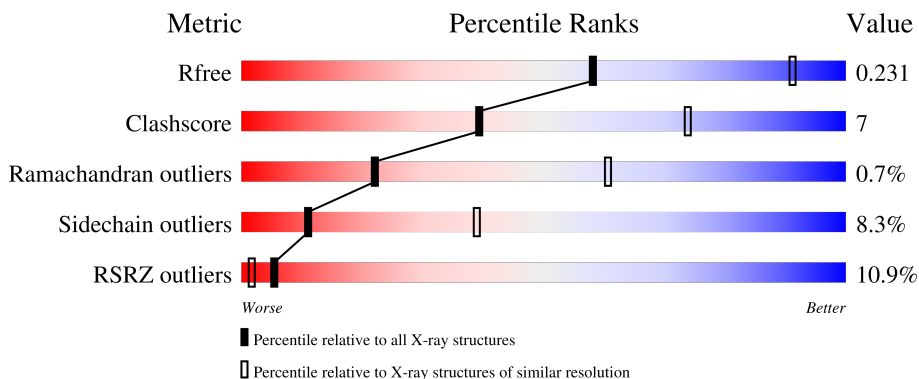
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	747	 3% 53% 13% 33%
1	F	747	 17% 48% 11% 40%
2	B	373	 0% 76% 23%
2	G	373	 4% 76% 22%
3	C	179	 0% 49% 24% 26%

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Mol	Chain	Length	Quality of chain
3	H	179	<p>22% 56% 15% 26%</p>
4	D	10	<p>80% 20%</p>
4	I	10	<p>40% 80% 10% 10%</p>
5	E	10	<p>10% 60% 30% 10%</p>
5	J	10	<p>10% 80% 10% 10%</p>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16191 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 Histone-lysine N-methyltransferase EZH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3999	2524	692	740	43	0	0	0
1	F	447	3597	2262	625	669	41	0	0	0

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	373	3031	1920	533	556	22	0	0	0
2	G	372	3020	1914	529	555	22	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP O75530
B	70	TRP	-	expression tag	UNP O75530
B	71	SER	-	expression tag	UNP O75530
B	72	HIS	-	expression tag	UNP O75530
B	73	PRO	-	expression tag	UNP O75530
B	74	GLN	-	expression tag	UNP O75530
B	75	PHE	-	expression tag	UNP O75530
B	76	GLU	-	expression tag	UNP O75530
G	69	SER	-	expression tag	UNP O75530
G	70	TRP	-	expression tag	UNP O75530
G	71	SER	-	expression tag	UNP O75530
G	72	HIS	-	expression tag	UNP O75530
G	73	PRO	-	expression tag	UNP O75530
G	74	GLN	-	expression tag	UNP O75530
G	75	PHE	-	expression tag	UNP O75530
G	76	GLU	-	expression tag	UNP O75530

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	132	Total	C	N	O	P	S	0	0	0
			1099	689	188	209	1	12			
3	H	132	Total	C	N	O	P	S	0	0	0
			1099	689	188	209	1	12			

- Molecule 4 is a protein called THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	S	0	0	0
			69	41	14	13	1			
4	I	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			

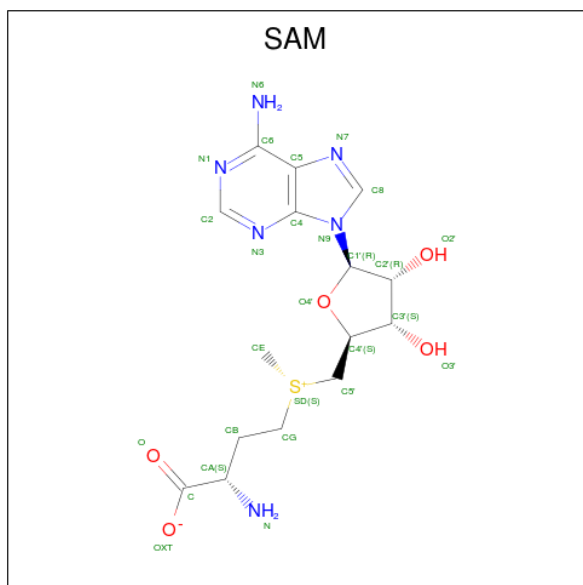
- Molecule 5 is a protein called THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	0	0	0
			72	45	15	12			
5	J	10	Total	C	N	O	0	0	0
			72	45	15	12			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	Zn	0	0
			8	8		
6	F	8	Total	Zn	0	0
			8	8		

- Molecule 7 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).

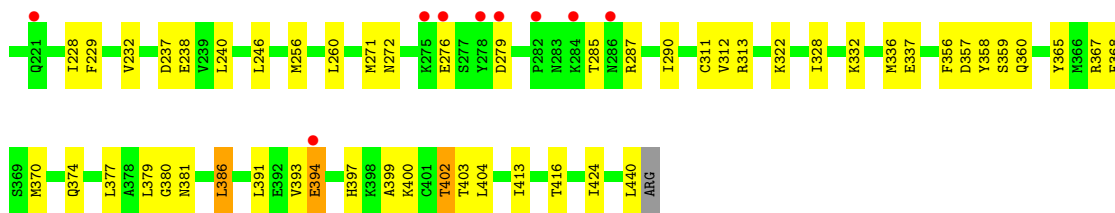


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
7	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

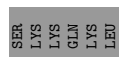
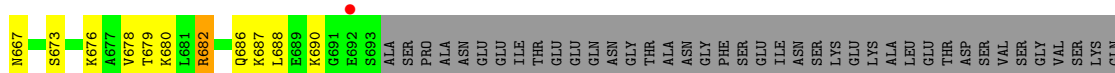




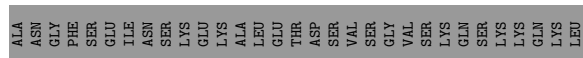
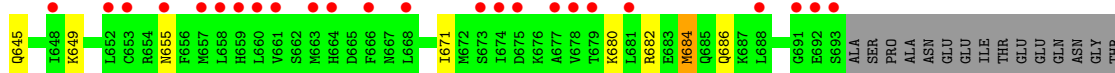
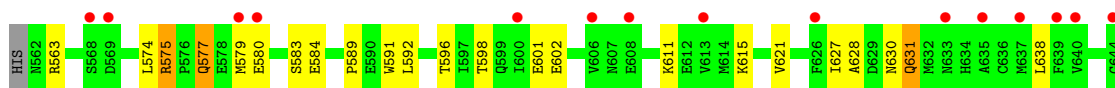




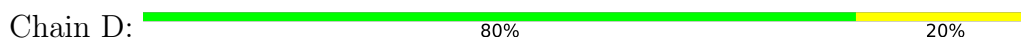
● Molecule 3: Polycomb protein SUZ12



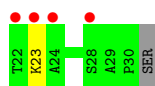
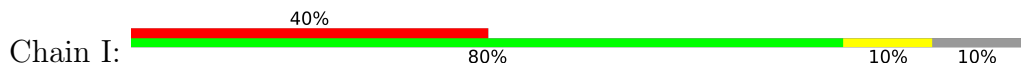
● Molecule 3: Polycomb protein SUZ12



● Molecule 4: THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER



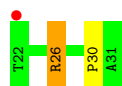
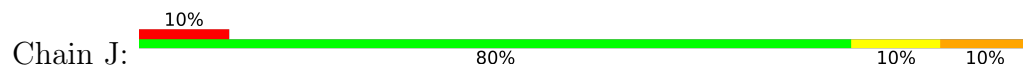
● Molecule 4: THR-LYS-ALA-ALA-ARG-MET-SER-ALA-PRO-SER



● Molecule 5: THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA



● Molecule 5: THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.87Å 64.43Å 254.50Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	42.52 – 2.99 49.62 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.7 (42.52-2.99) 85.7 (49.62-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, $R_{free}$	0.196 , 0.230 0.199 , 0.231	Depositor DCC
$R_{free}$ test set	2988 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: SEP, ZN, SAM, M3L

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	0.47	0/4087	0.63	0/5508
1	F	0.33	0/3673	0.56	0/4946
2	B	0.47	0/3111	0.66	0/4213
2	G	0.38	0/3100	0.63	0/4199
3	C	0.54	0/1108	0.63	0/1483
3	H	0.32	0/1108	0.54	0/1483
4	D	0.53	0/69	0.57	0/91
4	I	0.37	0/63	0.56	0/83
5	E	0.65	0/60	0.71	0/80
5	J	0.47	0/60	0.58	0/80
All	All	0.42	0/16439	0.61	0/22166

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 [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	3999	0	3869	64	0
1	F	3597	0	3468	50	0
2	B	3031	0	2938	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3020	0	2925	51	0
3	C	1099	0	1078	39	0
3	H	1099	0	1078	20	0
4	D	69	0	73	1	0
4	I	63	0	68	0	0
5	E	72	0	83	2	0
5	J	72	0	83	1	0
6	A	8	0	0	0	0
6	F	8	0	0	0	0
7	A	27	0	22	0	0
7	F	27	0	22	0	0
All	All	16191	0	15707	235	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 235 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:A:321:ARG:NH1	3:C:664:HIS:CE1	2.14	1.16
1:A:321:ARG:HH11	3:C:664:HIS:CE1	1.73	1.07
1:F:84:THR:HG22	1:F:96:HIS:HD2	1.21	1.06
1:A:84:THR:HG22	1:A:96:HIS:HD2	1.20	1.00
2:G:70:TRP:HB3	2:G:357:ASP:OD2	1.73	0.88

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	485/747 (65%)	453 (93%)	25 (5%)	7 (1%)	<b>11</b> 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	437/747 (58%)	411 (94%)	25 (6%)	1 (0%)	47	82
2	B	371/373 (100%)	351 (95%)	18 (5%)	2 (0%)	29	68
2	G	370/373 (99%)	355 (96%)	12 (3%)	3 (1%)	19	57
3	C	129/179 (72%)	124 (96%)	5 (4%)	0	100	100
3	H	129/179 (72%)	125 (97%)	4 (3%)	0	100	100
4	D	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
4	I	7/10 (70%)	6 (86%)	1 (14%)	0	100	100
5	E	7/10 (70%)	6 (86%)	0	1 (14%)	0	1
5	J	7/10 (70%)	6 (86%)	1 (14%)	0	100	100
All	All	1950/2638 (74%)	1843 (94%)	93 (5%)	14 (1%)	22	60

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	CYS
1	A	313	HIS
1	F	742	ARG
1	A	314	ALA
1	A	426	GLU

### 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	446/670 (67%)	413 (93%)	33 (7%)	13	44
1	F	402/670 (60%)	371 (92%)	31 (8%)	13	42
2	B	336/336 (100%)	312 (93%)	24 (7%)	14	46
2	G	335/336 (100%)	310 (92%)	25 (8%)	13	43
3	C	124/164 (76%)	109 (88%)	15 (12%)	5	21
3	H	124/164 (76%)	109 (88%)	15 (12%)	5	21
4	D	7/7 (100%)	6 (86%)	1 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	6/7 (86%)	5 (83%)	1 (17%)	2	11
5	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
5	J	5/5 (100%)	4 (80%)	1 (20%)	1	7
All	All	1790/2364 (76%)	1642 (92%)	148 (8%)	11	39

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	180	MET
3	H	649	LYS
2	G	271	MET
2	G	440	LEU
2	B	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	608	GLN
2	G	160	HIS
1	F	636	ASN
1	F	707	HIS
2	G	181	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
5	M3L	J	27	5	10,11,12	0.44	0	9,14,16	0.26	0
3	SEP	H	583	3	8,9,10	1.15	1 (12%)	8,12,14	2.30	3 (37%)
5	M3L	E	27	5	10,11,12	0.45	0	9,14,16	0.27	0
3	SEP	C	583	3	8,9,10	1.22	1 (12%)	8,12,14	4.68	4 (50%)

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
5	M3L	J	27	5	-	0/9/10/12	-
3	SEP	H	583	3	-	1/5/8/10	-
5	M3L	E	27	5	-	0/9/10/12	-
3	SEP	C	583	3	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	583	SEP	P-OG	-2.69	1.51	1.60
3	H	583	SEP	P-OG	-2.42	1.52	1.60

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	583	SEP	OG-CB-CA	10.17	118.04	108.14
3	C	583	SEP	O3P-P-OG	-6.26	90.07	106.73
3	H	583	SEP	OG-CB-CA	5.10	113.11	108.14
3	C	583	SEP	OG-P-O1P	4.47	119.02	106.47
3	H	583	SEP	P-OG-CB	-2.57	111.22	118.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	583	SEP	CA-CB-OG-P
3	H	583	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SAM	F	1009	-	24,29,29	0.72	0	23,42,42	0.92	2 (8%)
7	SAM	A	1009	-	24,29,29	0.72	0	23,42,42	1.01	2 (8%)

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
7	SAM	F	1009	-	-	2/12/33/33	0/3/3/3
7	SAM	A	1009	-	-	2/12/33/33	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1009	SAM	C5-C6-N6	2.49	124.14	120.35
7	F	1009	SAM	C5-C6-N6	2.37	123.95	120.35
7	A	1009	SAM	O-C-CA	-2.18	114.45	122.14
7	F	1009	SAM	O-C-CA	-2.04	114.95	122.14

There are no chirality outliers.

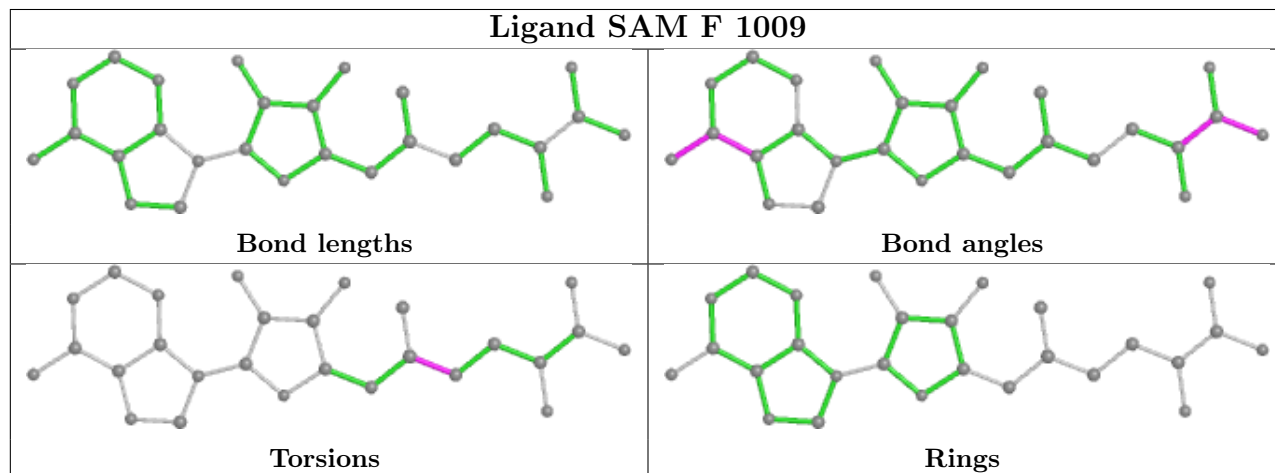
All (4) torsion outliers are listed below:

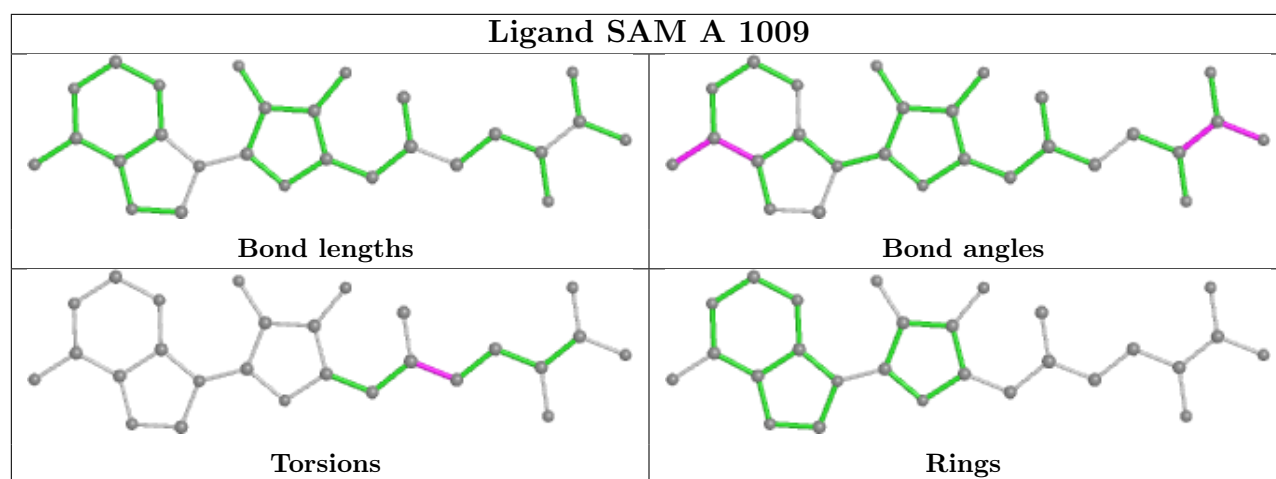
Mol	Chain	Res	Type	Atoms
7	A	1009	SAM	CB-CG-SD-CE
7	A	1009	SAM	CB-CG-SD-C5'
7	F	1009	SAM	CB-CG-SD-CE
7	F	1009	SAM	CB-CG-SD-C5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	497/747 (66%)	0.17	23 (4%) 32 12	16, 53, 96, 130	0
1	F	447/747 (59%)	1.31	129 (28%) 0 0	71, 115, 193, 201	0
2	B	373/373 (100%)	0.04	5 (1%) 77 51	17, 50, 83, 97	0
2	G	372/373 (99%)	0.28	14 (3%) 40 16	38, 78, 115, 146	0
3	C	131/179 (73%)	-0.14	1 (0%) 86 65	18, 35, 73, 88	0
3	H	131/179 (73%)	1.38	39 (29%) 0 0	84, 122, 151, 157	0
4	D	10/10 (100%)	0.16	0 100 100	49, 59, 69, 72	0
4	I	9/10 (90%)	1.77	4 (44%) 0 0	108, 111, 114, 114	0
5	E	9/10 (90%)	0.60	1 (11%) 5 1	55, 63, 78, 79	0
5	J	9/10 (90%)	1.10	1 (11%) 5 1	70, 76, 84, 86	0
All	All	1988/2638 (75%)	0.50	217 (10%) 5 2	16, 72, 152, 201	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	515	SER	7.4
1	F	521	TYR	7.2
1	F	23	TYR	7.0
1	F	538	ILE	6.6
1	A	26	LEU	6.5

### 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, 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( $\text{\AA}^2$ )	Q<0.9
3	SEP	H	583	10/11	0.97	0.21	109,111,117,120	0
5	M3L	E	27	12/13	0.97	0.22	27,32,47,47	0
5	M3L	J	27	12/13	0.98	0.23	56,59,65,65	0
3	SEP	C	583	10/11	0.99	0.15	27,40,42,45	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

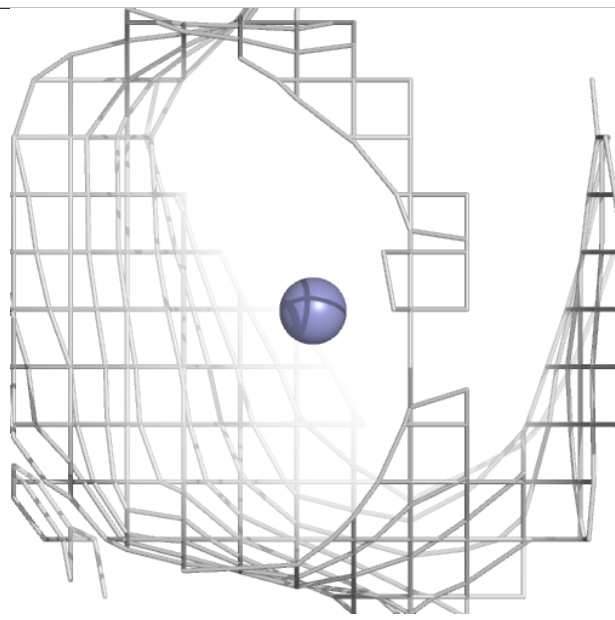
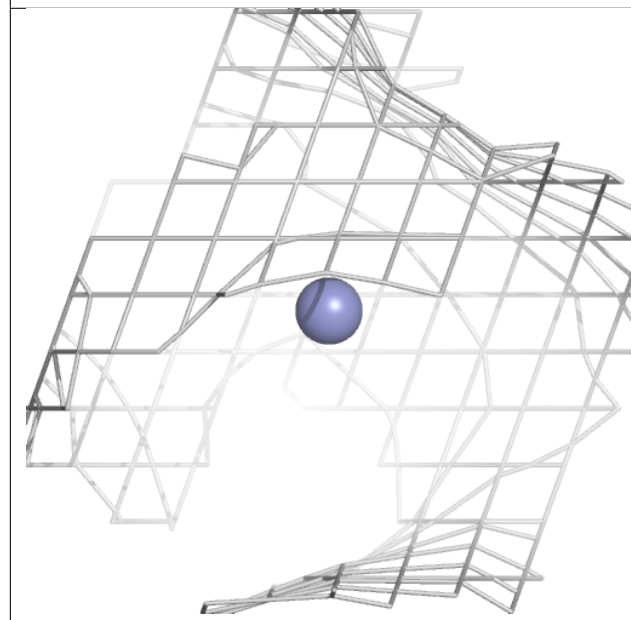
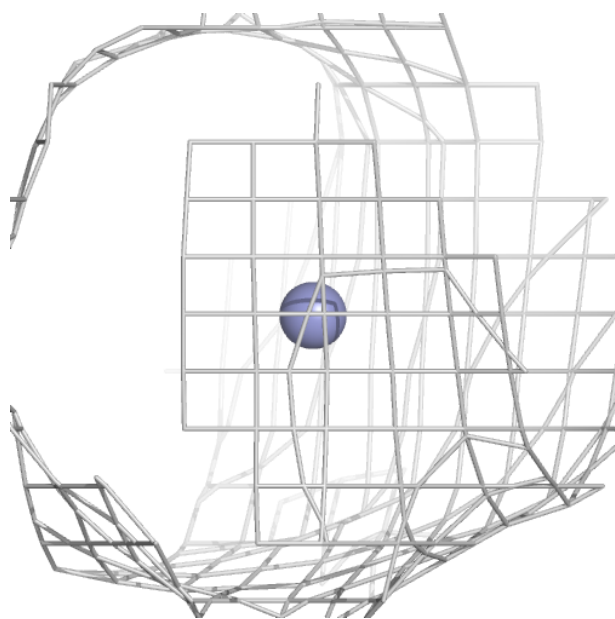
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	F	1002	1/1	0.41	0.16	189,189,189,189	0
7	SAM	F	1009	27/27	0.94	0.19	105,106,106,107	0
6	ZN	F	1005	1/1	0.95	0.06	188,188,188,188	0
6	ZN	F	1004	1/1	0.95	0.05	167,167,167,167	0
6	ZN	F	1003	1/1	0.97	0.04	159,159,159,159	0
7	SAM	A	1009	27/27	0.97	0.20	45,47,49,50	0
6	ZN	F	1001	1/1	0.97	0.08	137,137,137,137	0
6	ZN	F	1006	1/1	0.98	0.09	137,137,137,137	0
6	ZN	F	1008	1/1	0.98	0.09	130,130,130,130	0
6	ZN	A	1001	1/1	0.99	0.14	33,33,33,33	0
6	ZN	A	1004	1/1	0.99	0.11	66,66,66,66	0
6	ZN	F	1007	1/1	0.99	0.05	132,132,132,132	0
6	ZN	A	1007	1/1	1.00	0.13	41,41,41,41	0
6	ZN	A	1008	1/1	1.00	0.14	37,37,37,37	0
6	ZN	A	1003	1/1	1.00	0.12	47,47,47,47	0
6	ZN	A	1002	1/1	1.00	0.10	48,48,48,48	0
6	ZN	A	1005	1/1	1.00	0.11	55,55,55,55	0
6	ZN	A	1006	1/1	1.00	0.14	37,37,37,37	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.

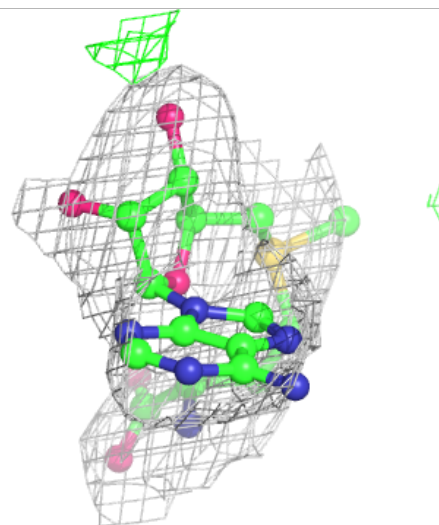
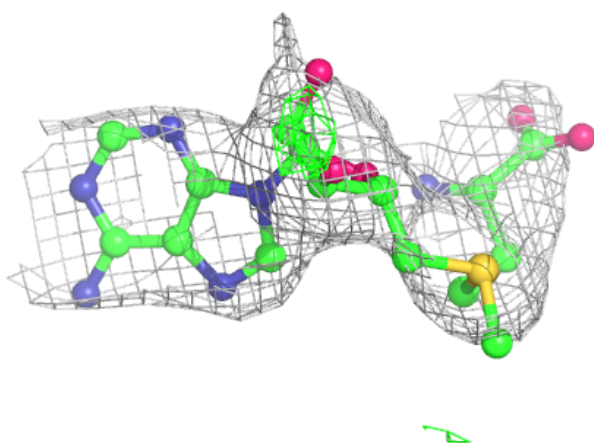
**Electron density around ZN F 1002:**

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



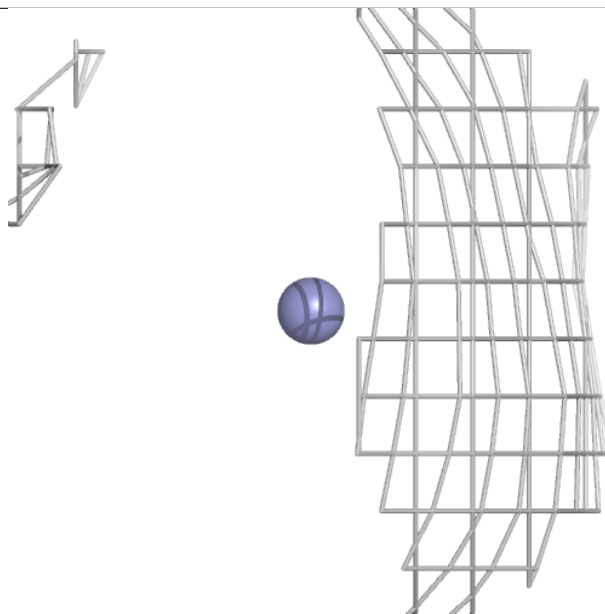
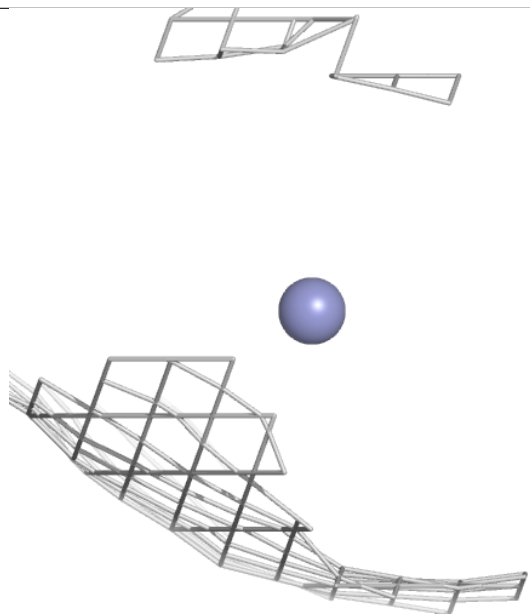
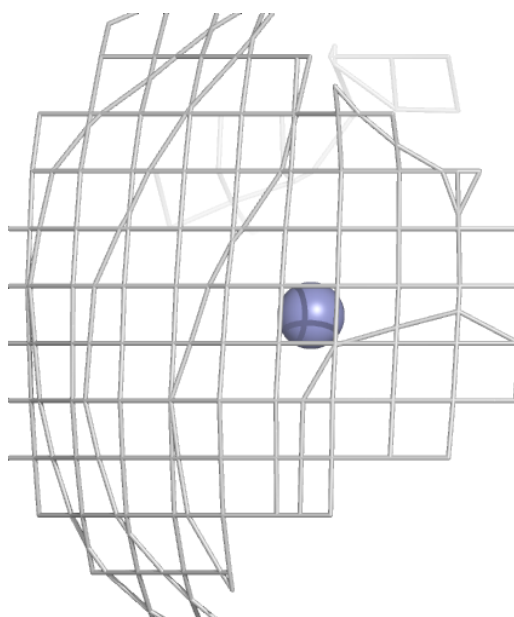
**Electron density around SAM F 1009:**

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



**Electron density around ZN F 1005:**

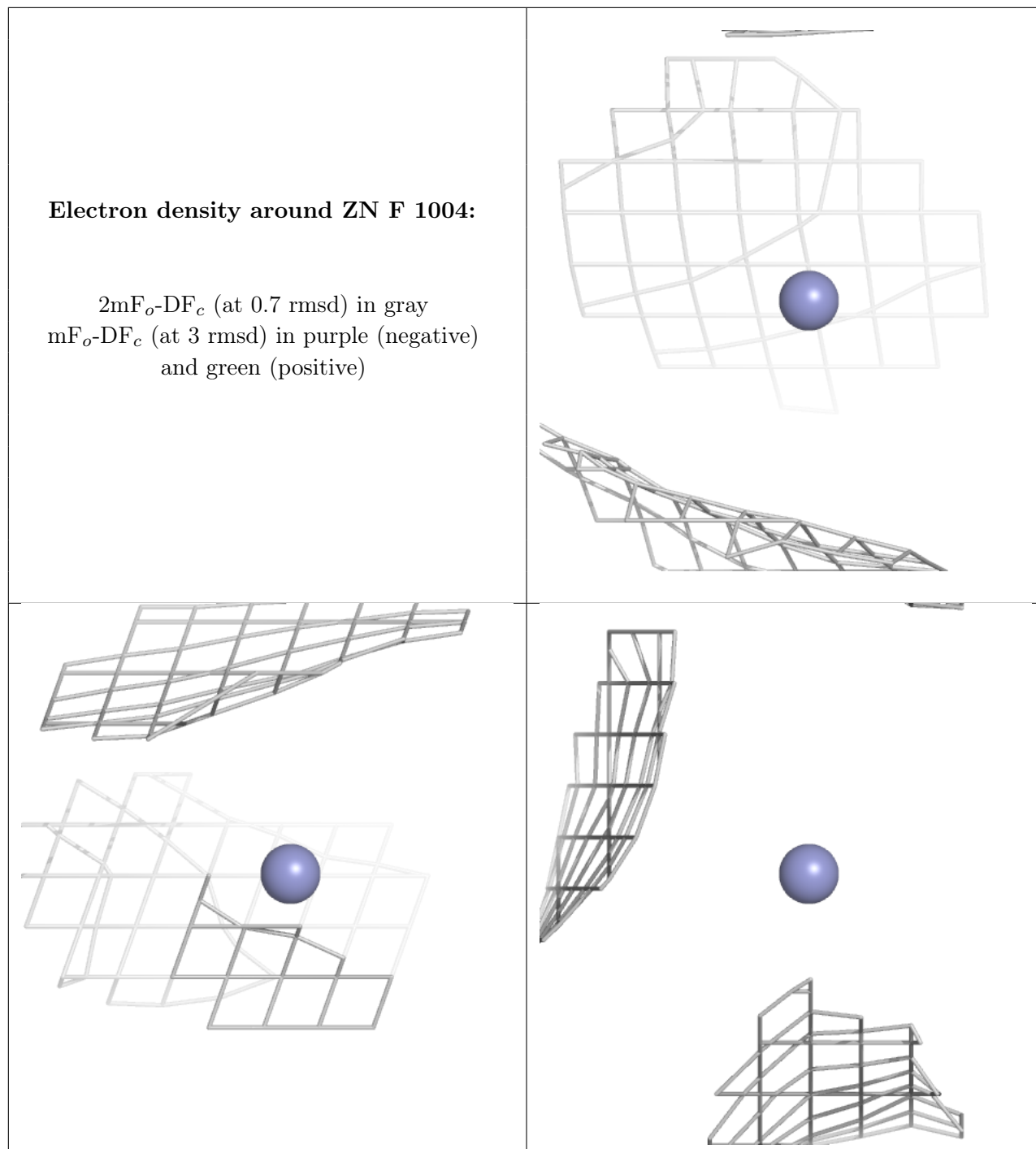
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





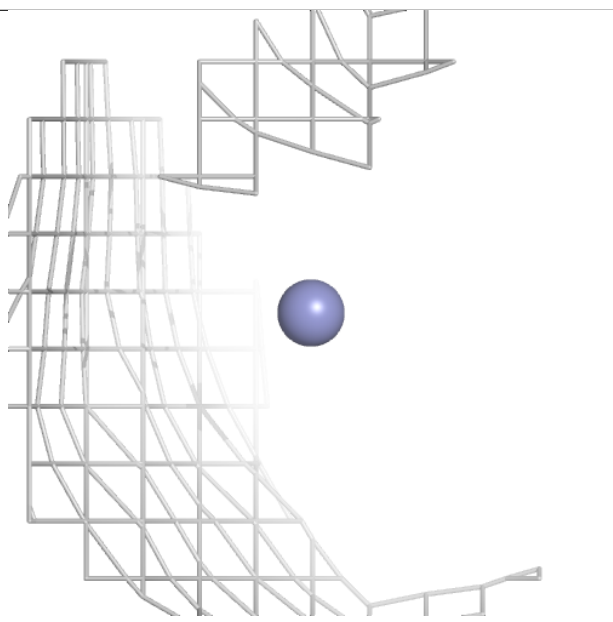
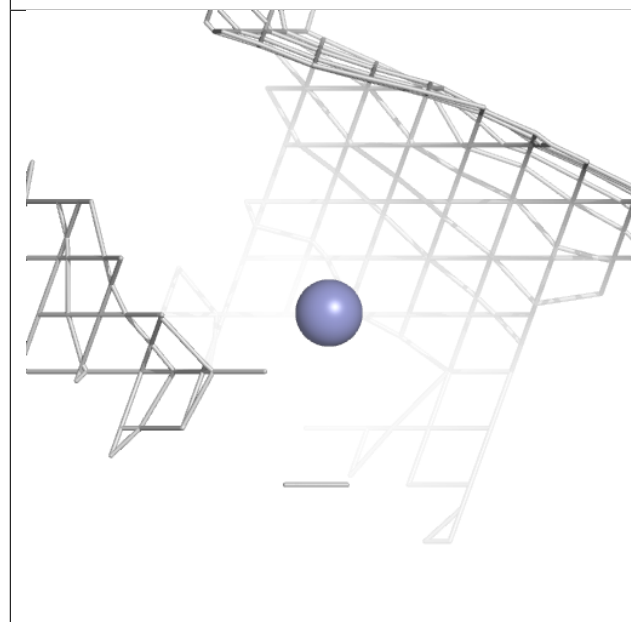
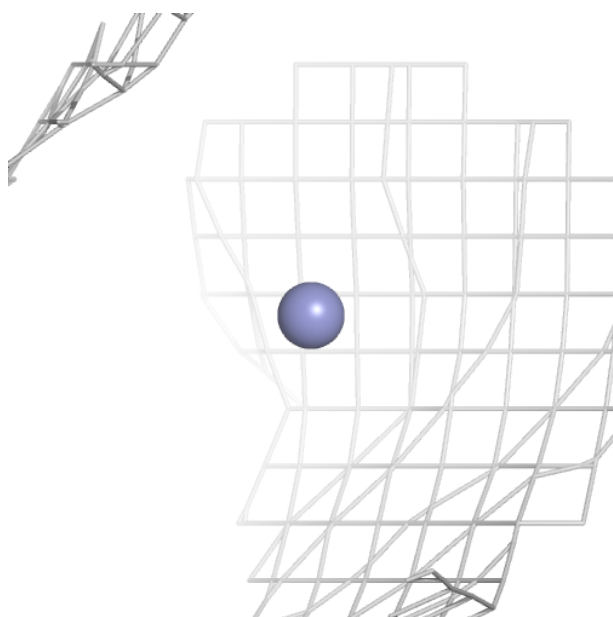
**Electron density around ZN F 1004:**

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



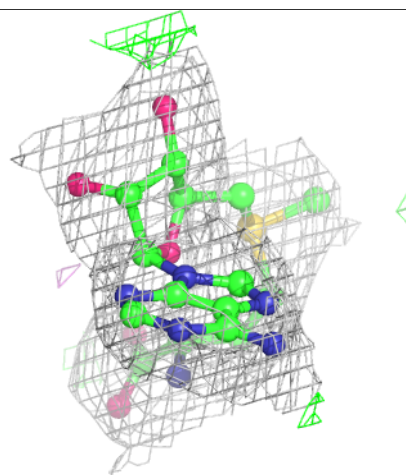
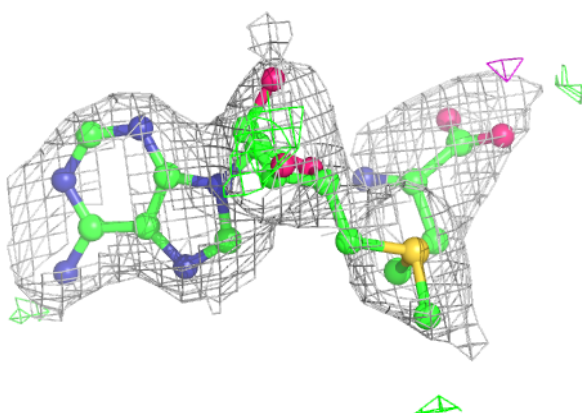
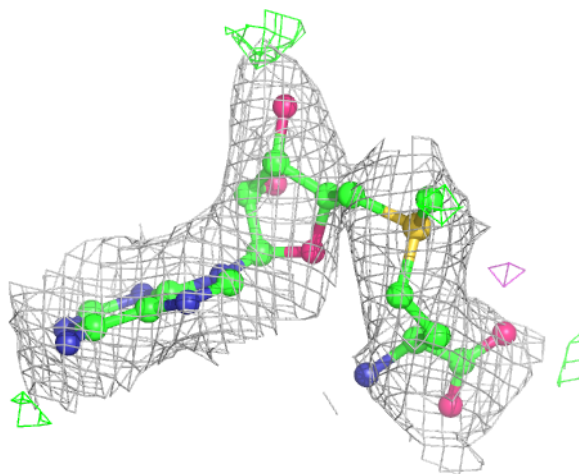
**Electron density around ZN F 1003:**

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



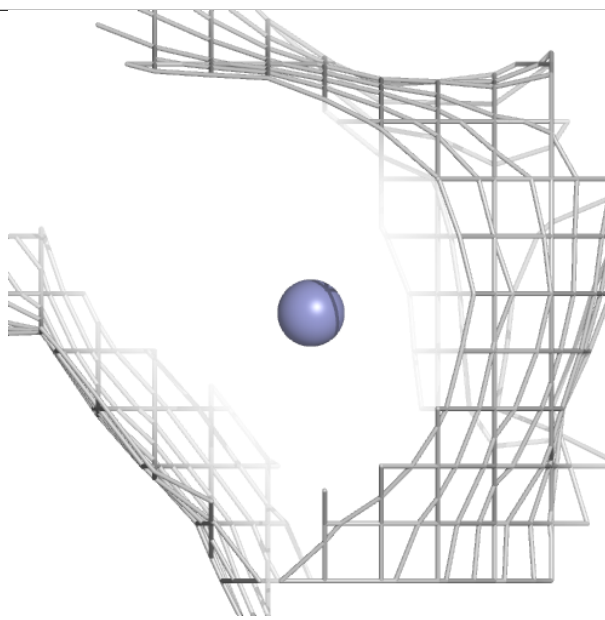
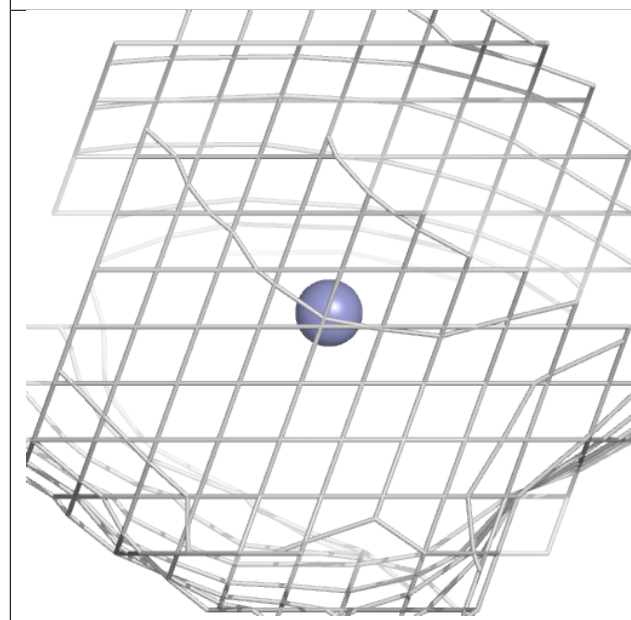
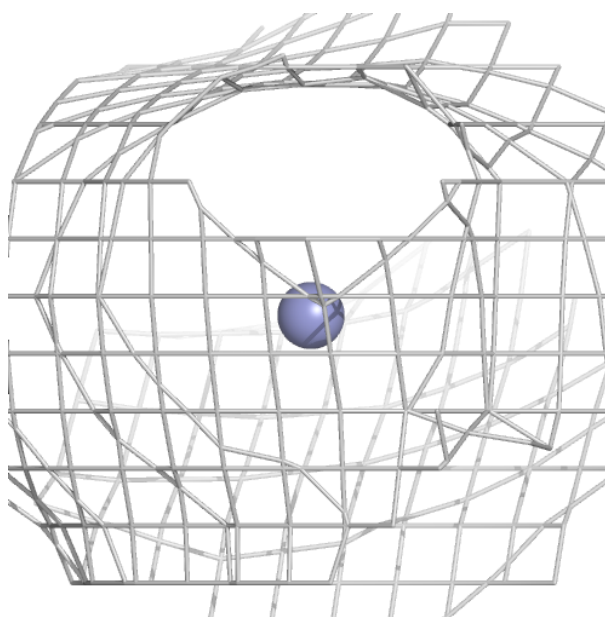
**Electron density around SAM A 1009:**

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



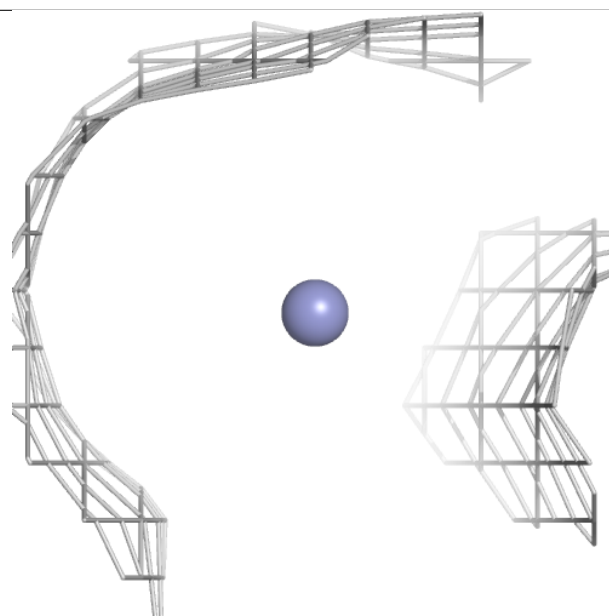
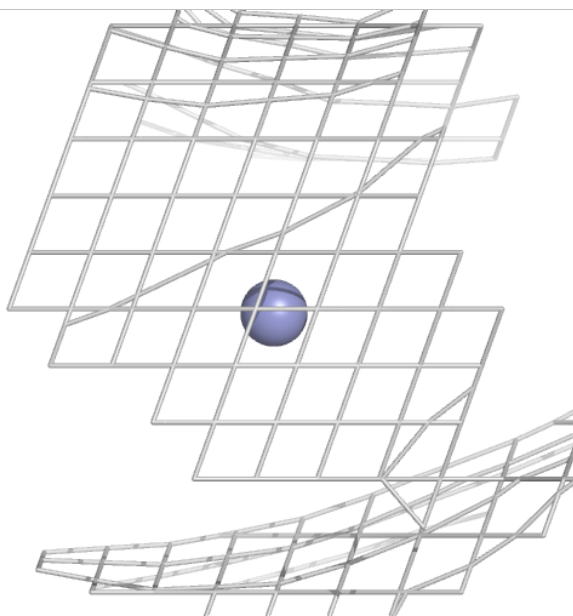
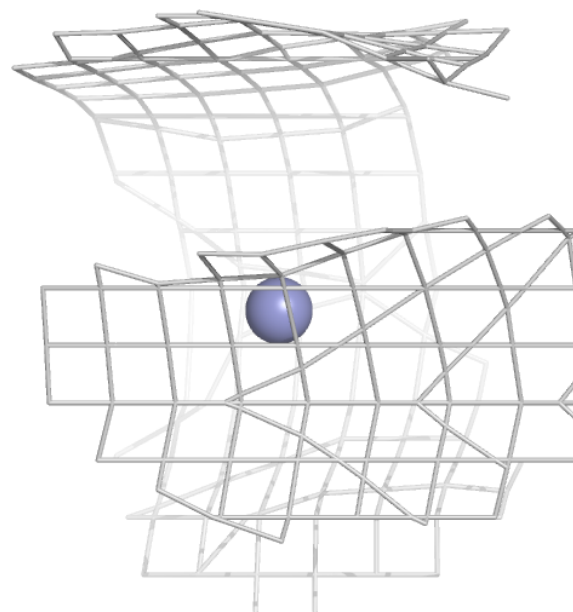
**Electron density around ZN F 1001:**

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



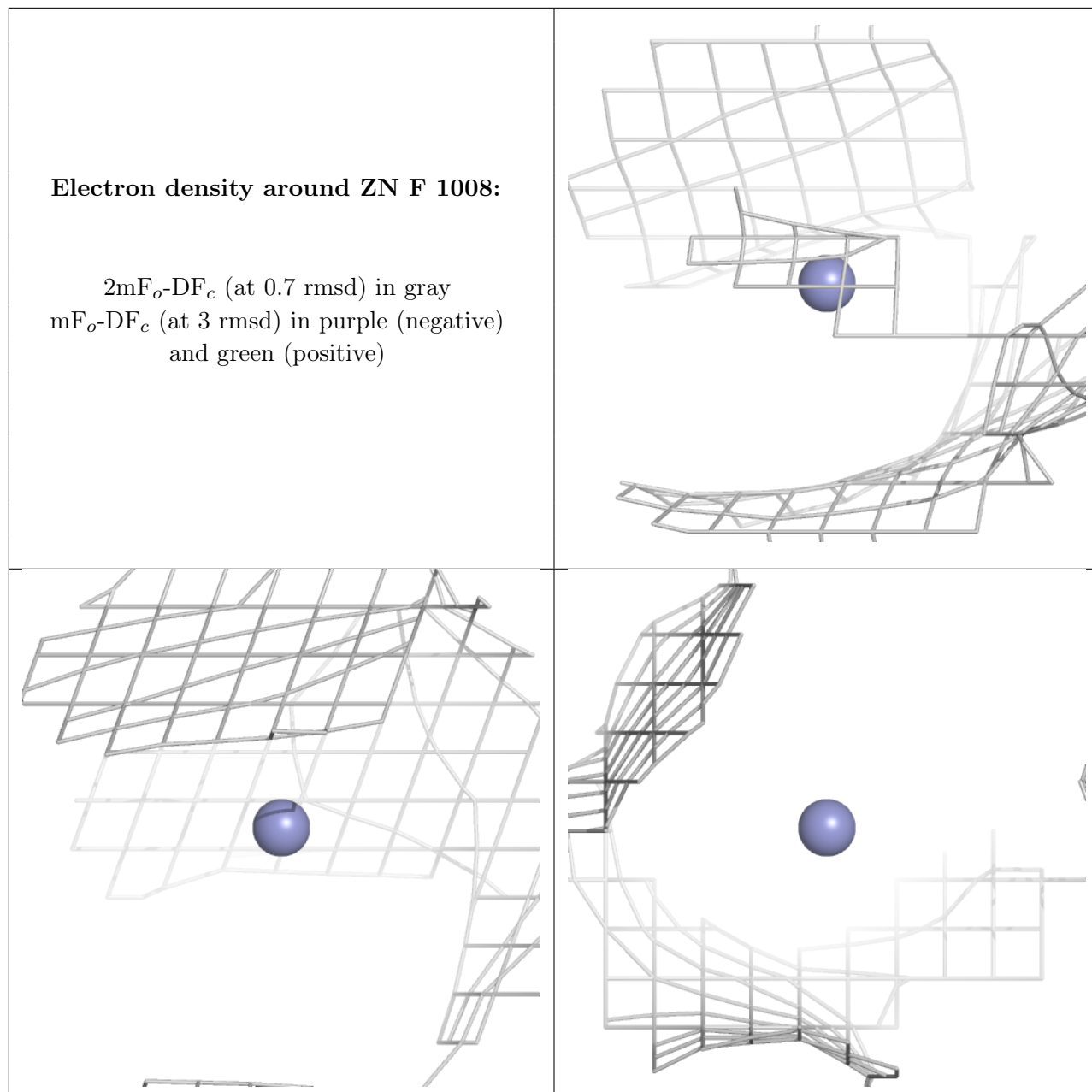
**Electron density around ZN F 1006:**

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



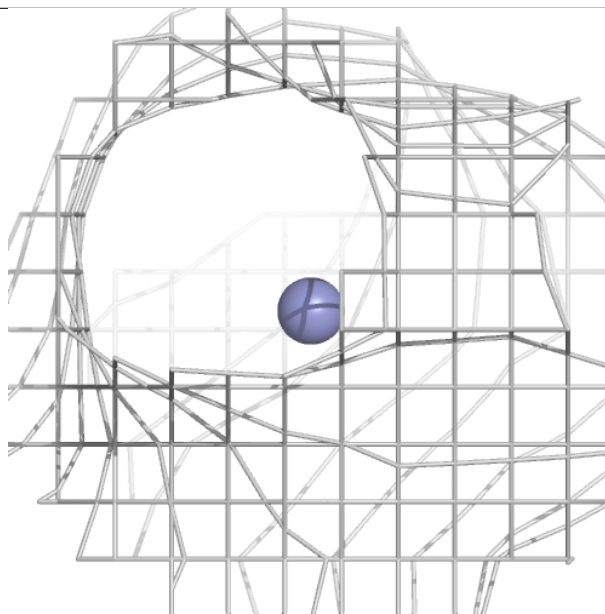
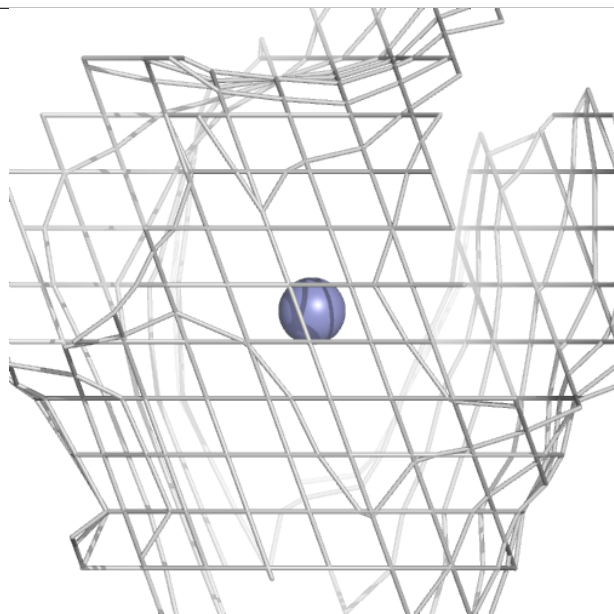
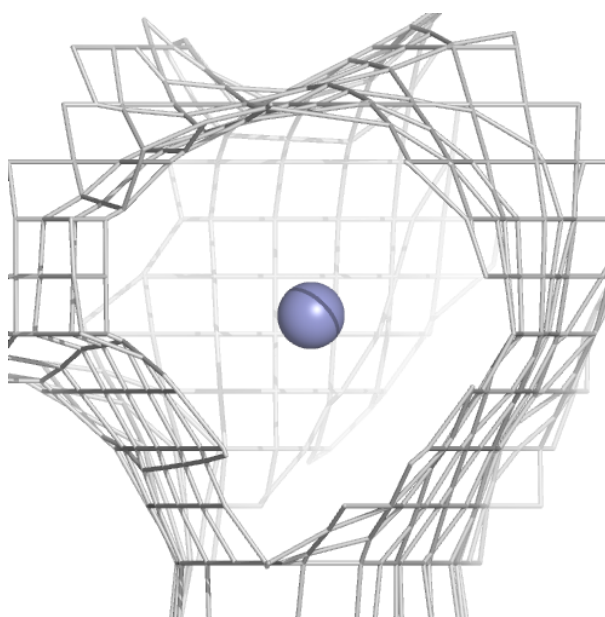
**Electron density around ZN F 1008:**

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and green (positive)



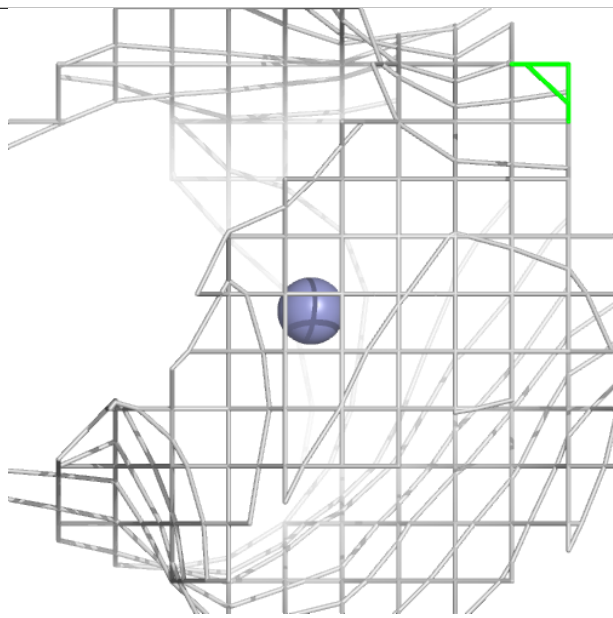
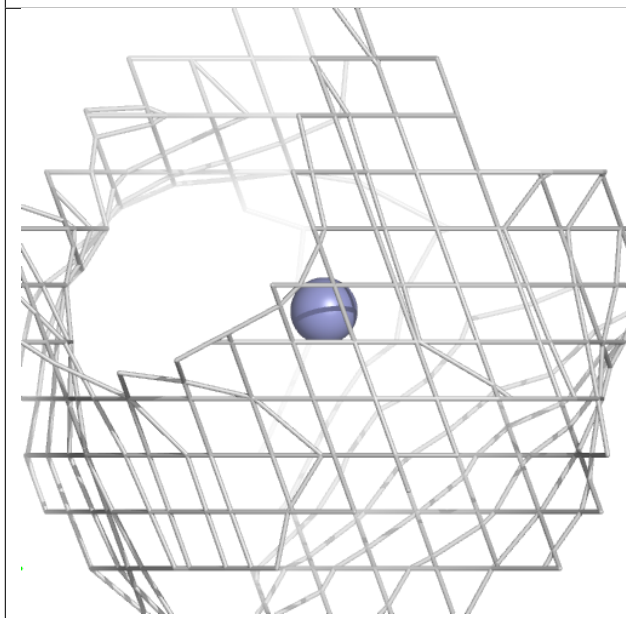
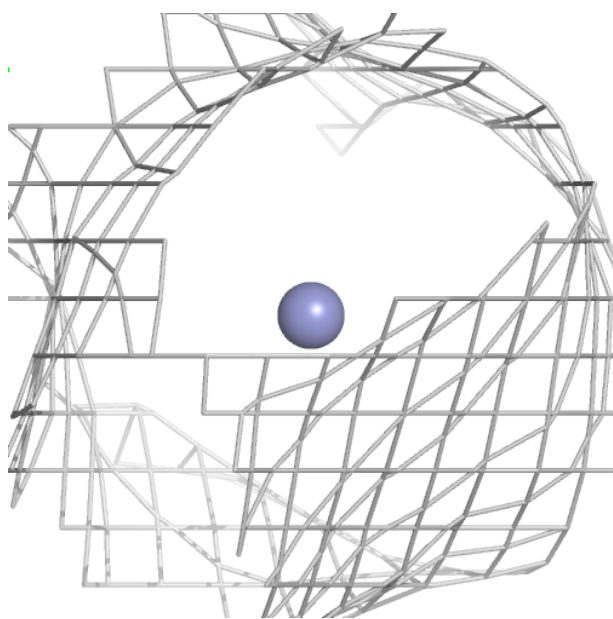
**Electron density around ZN A 1001:**

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



**Electron density around ZN A 1004:**

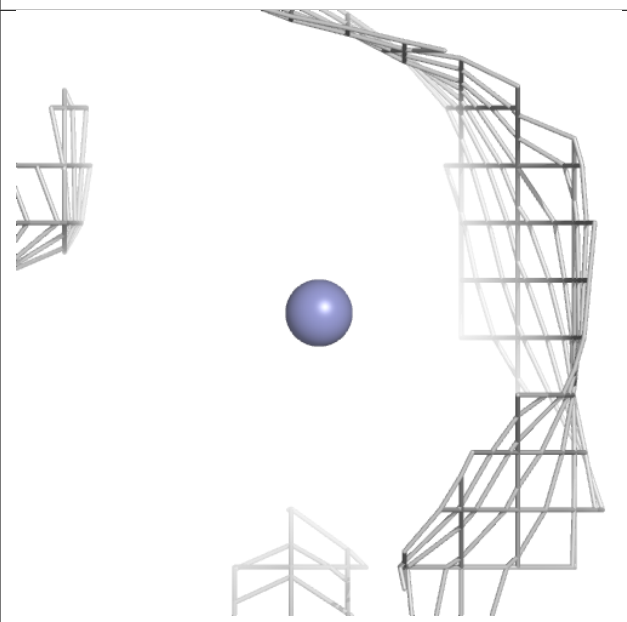
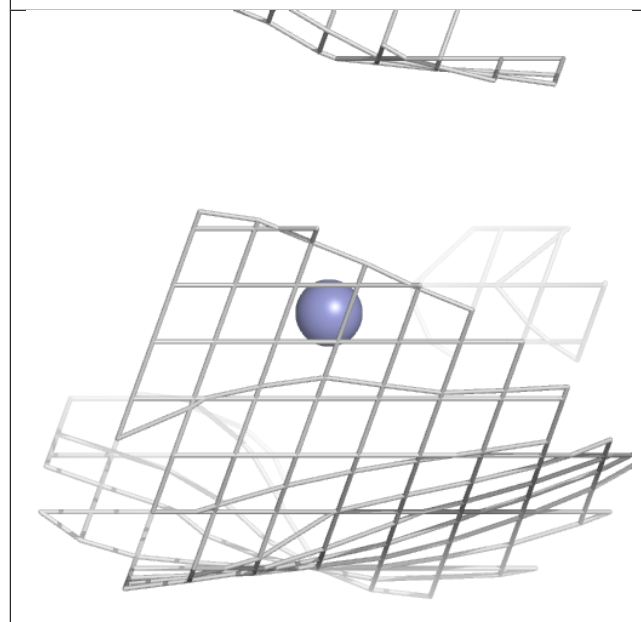
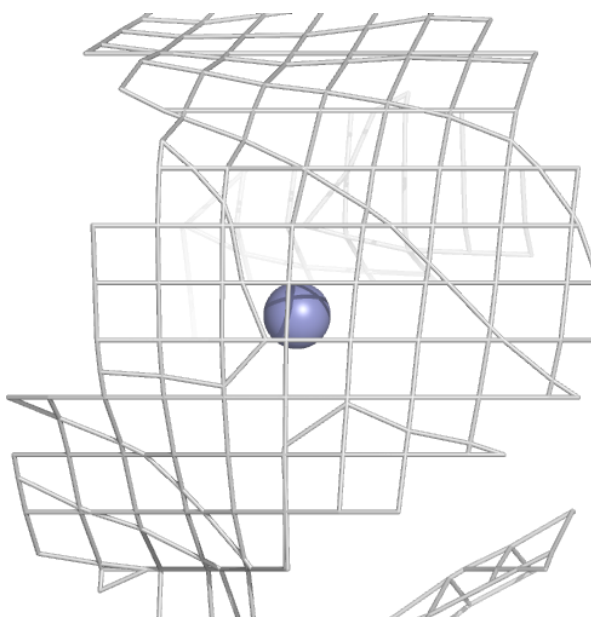
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





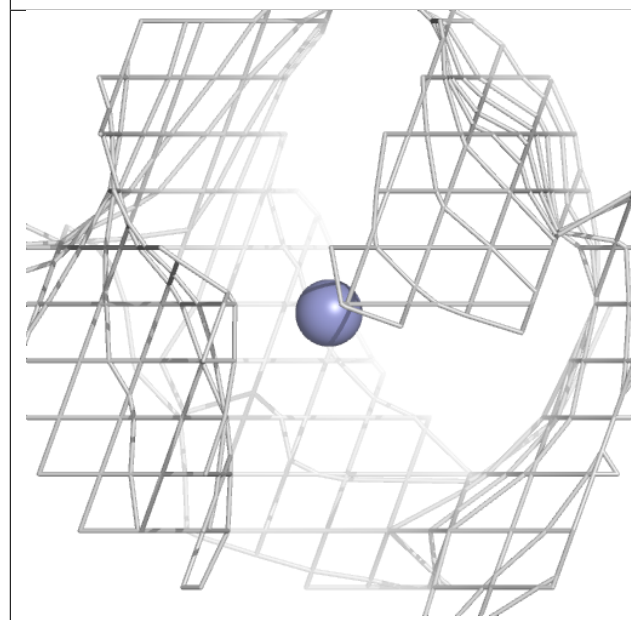
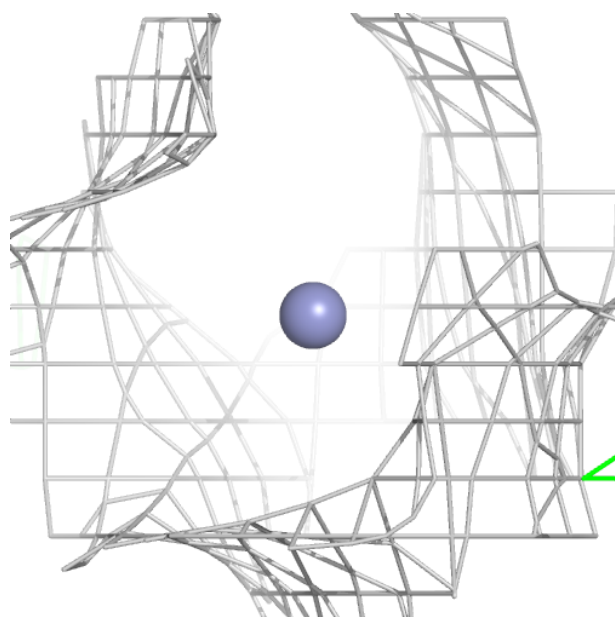
**Electron density around ZN F 1007:**

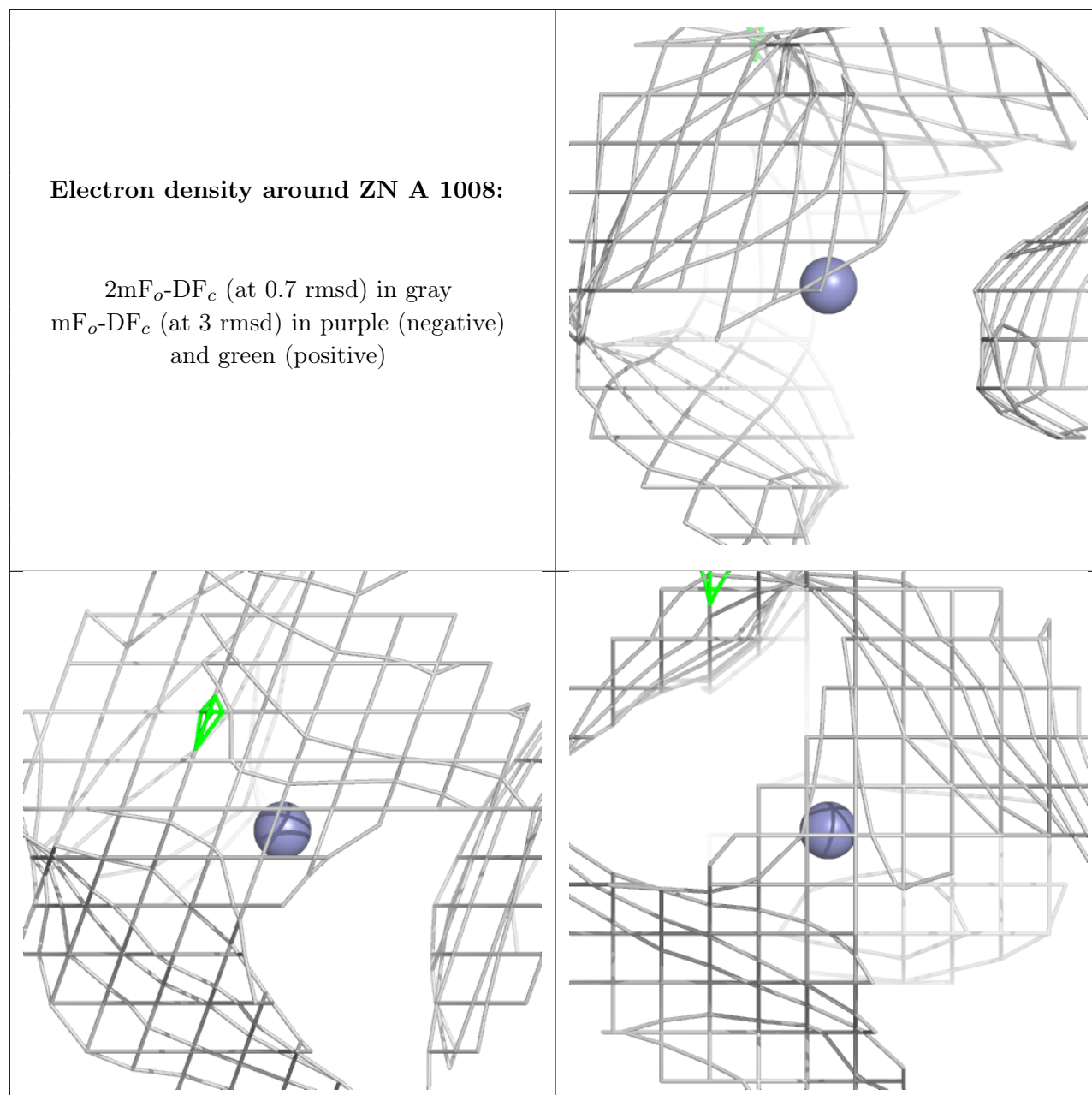
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



**Electron density around ZN A 1007:**

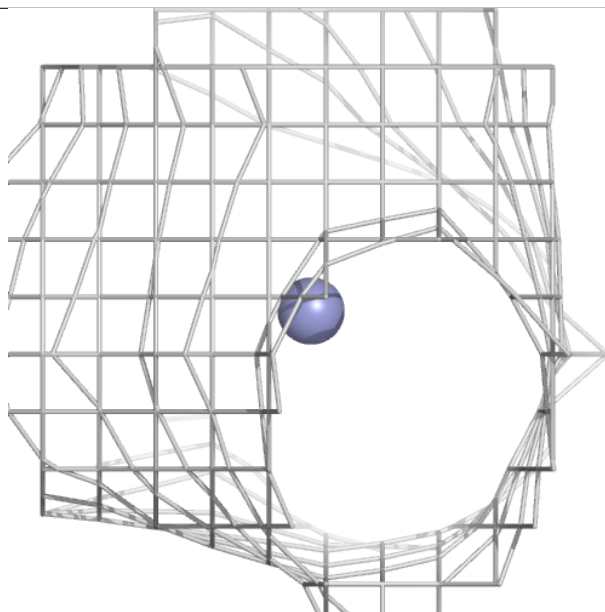
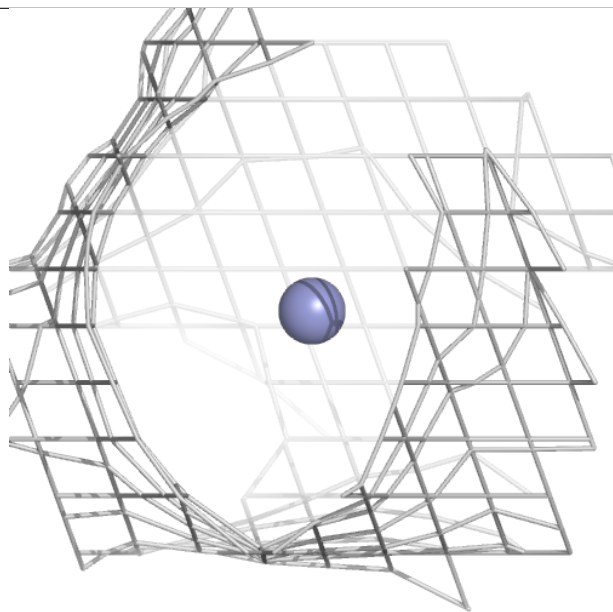
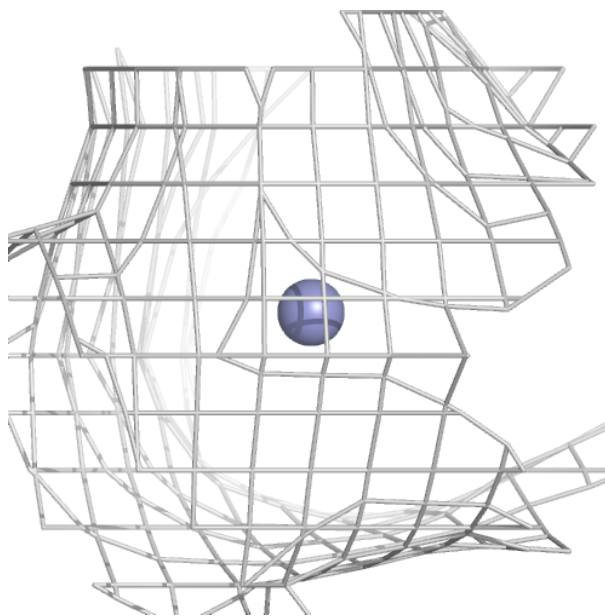
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





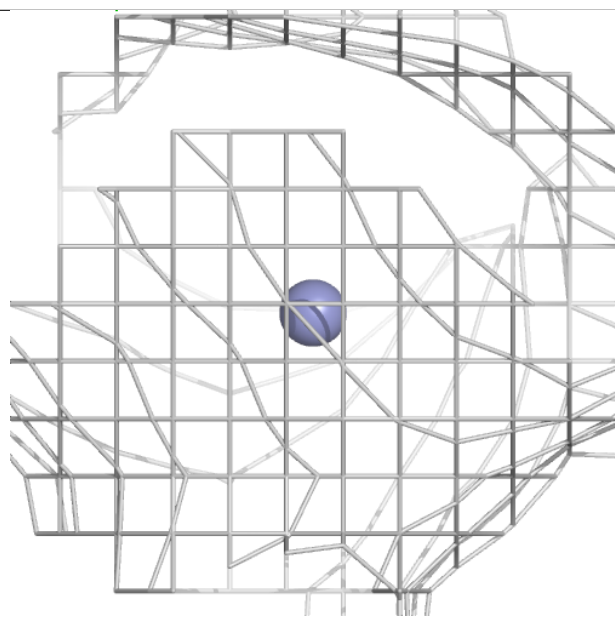
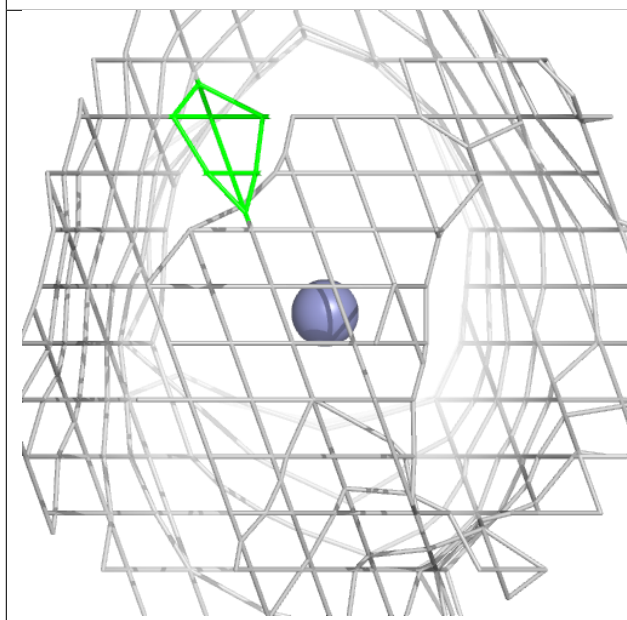
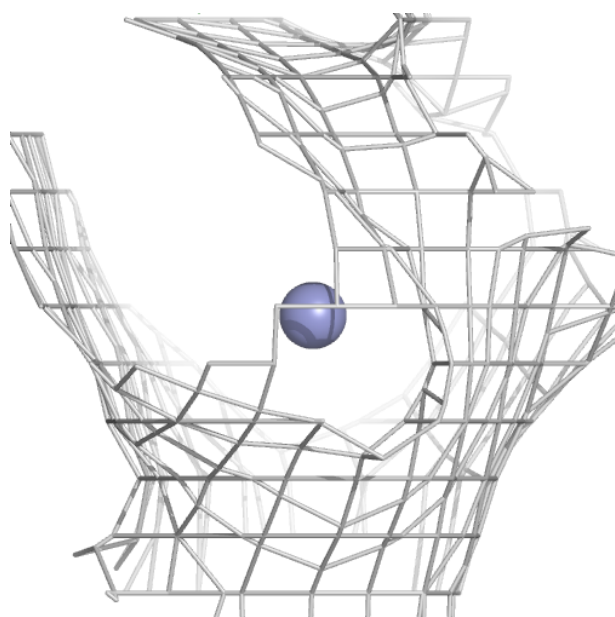
**Electron density around ZN A 1003:**

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



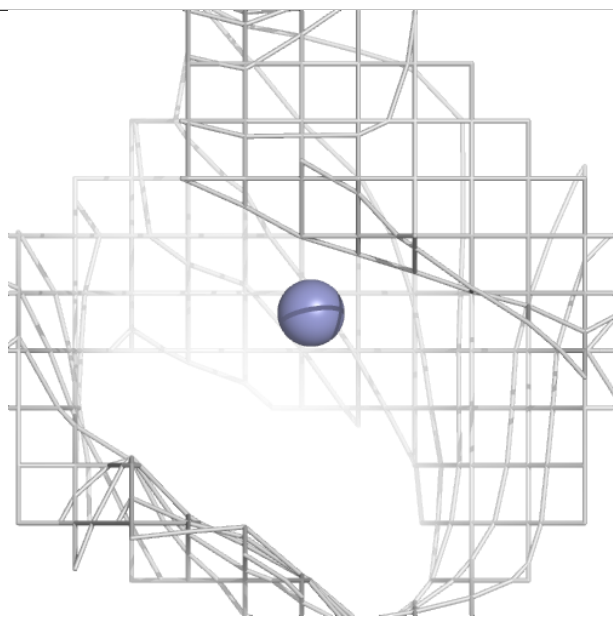
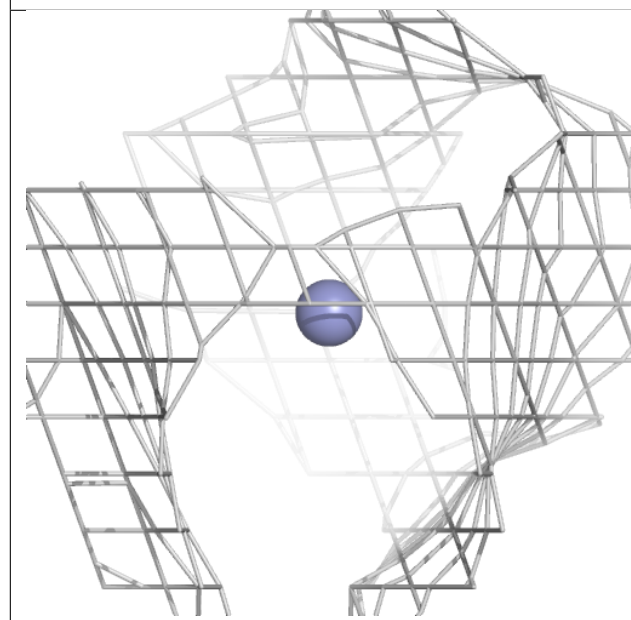
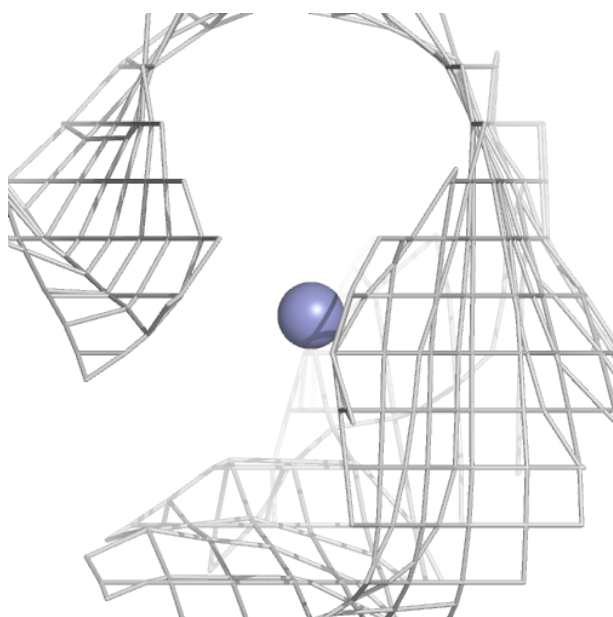
**Electron density around ZN A 1002:**

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

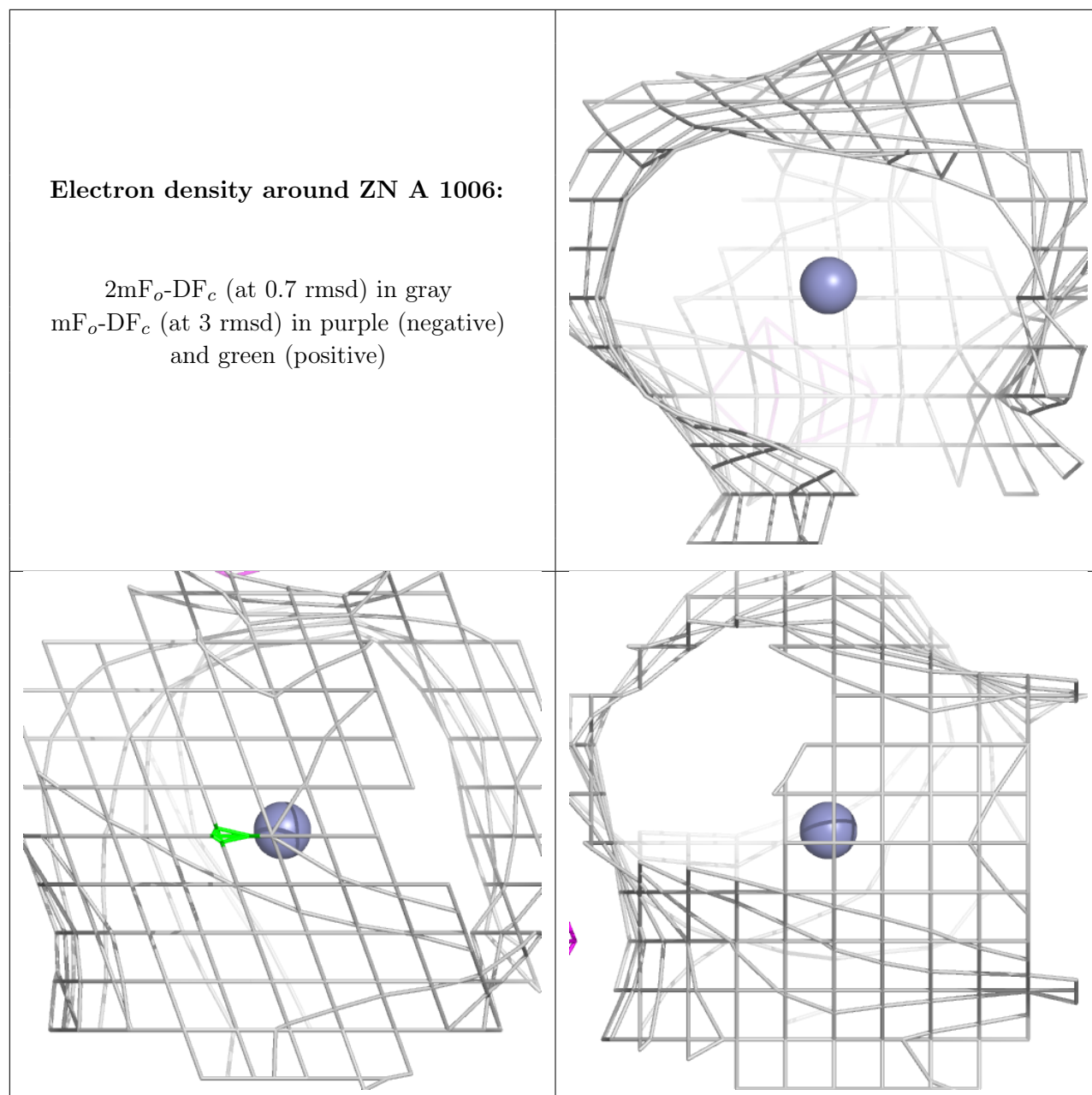


**Electron density around ZN A 1005:**

$2mF_o-DF_c$  (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.