



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 06:28 PM JST

PDB ID : 7D6N
Title : Crystal structure of tick-borne encephalitis virus RNA-dependent RNA polymerase
Authors : Yang, J.; Jing, X.; Gong, P.
Deposited on : 2020-10-01
Resolution : 3.17 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

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 : 4.02b-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

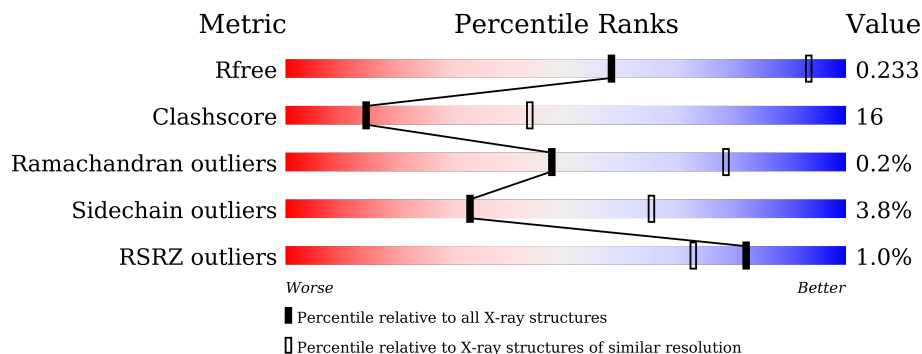
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	638	
1	B	638	
1	C	638	
1	D	638	
1	E	638	
1	F	638	

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Mol	Chain	Length	Quality of chain
1	G	638	 61% 28% • 8%
1	H	638	%  64% 27% • 8%
1	I	638	%  62% 28% • 8%
1	J	638	%  66% 24% • 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45346 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 Tick-borne encephalitis virus RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4569	2887	810	839	33	0	0	0
1	B	584	4571	2882	817	839	33	0	0	0
1	E	588	4519	2850	799	836	34	0	0	0
1	D	589	4549	2868	803	844	34	0	1	0
1	C	586	4514	2852	795	834	33	0	0	0
1	F	583	4544	2870	808	834	32	0	0	0
1	G	584	4560	2873	815	839	33	0	0	0
1	J	582	4441	2811	771	826	33	0	0	0
1	I	586	4535	2860	802	839	34	0	0	0
1	H	588	4514	2853	786	841	34	0	0	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	MET	-	initiating methionine	UNP K4P8A2
A	892	GLY	-	expression tag	UNP K4P8A2
A	893	SER	-	expression tag	UNP K4P8A2
A	894	SER	-	expression tag	UNP K4P8A2
A	895	SER	-	expression tag	UNP K4P8A2
A	896	HIS	-	expression tag	UNP K4P8A2
A	897	HIS	-	expression tag	UNP K4P8A2
A	898	HIS	-	expression tag	UNP K4P8A2
A	899	HIS	-	expression tag	UNP K4P8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	900	HIS	-	expression tag	UNP K4P8A2
A	901	HIS	-	expression tag	UNP K4P8A2
B	264	MET	-	initiating methionine	UNP K4P8A2
B	892	GLY	-	expression tag	UNP K4P8A2
B	893	SER	-	expression tag	UNP K4P8A2
B	894	SER	-	expression tag	UNP K4P8A2
B	895	SER	-	expression tag	UNP K4P8A2
B	896	HIS	-	expression tag	UNP K4P8A2
B	897	HIS	-	expression tag	UNP K4P8A2
B	898	HIS	-	expression tag	UNP K4P8A2
B	899	HIS	-	expression tag	UNP K4P8A2
B	900	HIS	-	expression tag	UNP K4P8A2
B	901	HIS	-	expression tag	UNP K4P8A2
E	264	MET	-	initiating methionine	UNP K4P8A2
E	892	GLY	-	expression tag	UNP K4P8A2
E	893	SER	-	expression tag	UNP K4P8A2
E	894	SER	-	expression tag	UNP K4P8A2
E	895	SER	-	expression tag	UNP K4P8A2
E	896	HIS	-	expression tag	UNP K4P8A2
E	897	HIS	-	expression tag	UNP K4P8A2
E	898	HIS	-	expression tag	UNP K4P8A2
E	899	HIS	-	expression tag	UNP K4P8A2
E	900	HIS	-	expression tag	UNP K4P8A2
E	901	HIS	-	expression tag	UNP K4P8A2
D	264	MET	-	initiating methionine	UNP K4P8A2
D	892	GLY	-	expression tag	UNP K4P8A2
D	893	SER	-	expression tag	UNP K4P8A2
D	894	SER	-	expression tag	UNP K4P8A2
D	895	SER	-	expression tag	UNP K4P8A2
D	896	HIS	-	expression tag	UNP K4P8A2
D	897	HIS	-	expression tag	UNP K4P8A2
D	898	HIS	-	expression tag	UNP K4P8A2
D	899	HIS	-	expression tag	UNP K4P8A2
D	900	HIS	-	expression tag	UNP K4P8A2
D	901	HIS	-	expression tag	UNP K4P8A2
C	264	MET	-	initiating methionine	UNP K4P8A2
C	892	GLY	-	expression tag	UNP K4P8A2
C	893	SER	-	expression tag	UNP K4P8A2
C	894	SER	-	expression tag	UNP K4P8A2
C	895	SER	-	expression tag	UNP K4P8A2
C	896	HIS	-	expression tag	UNP K4P8A2
C	897	HIS	-	expression tag	UNP K4P8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	898	HIS	-	expression tag	UNP K4P8A2
C	899	HIS	-	expression tag	UNP K4P8A2
C	900	HIS	-	expression tag	UNP K4P8A2
C	901	HIS	-	expression tag	UNP K4P8A2
F	264	MET	-	initiating methionine	UNP K4P8A2
F	892	GLY	-	expression tag	UNP K4P8A2
F	893	SER	-	expression tag	UNP K4P8A2
F	894	SER	-	expression tag	UNP K4P8A2
F	895	SER	-	expression tag	UNP K4P8A2
F	896	HIS	-	expression tag	UNP K4P8A2
F	897	HIS	-	expression tag	UNP K4P8A2
F	898	HIS	-	expression tag	UNP K4P8A2
F	899	HIS	-	expression tag	UNP K4P8A2
F	900	HIS	-	expression tag	UNP K4P8A2
F	901	HIS	-	expression tag	UNP K4P8A2
G	264	MET	-	initiating methionine	UNP K4P8A2
G	892	GLY	-	expression tag	UNP K4P8A2
G	893	SER	-	expression tag	UNP K4P8A2
G	894	SER	-	expression tag	UNP K4P8A2
G	895	SER	-	expression tag	UNP K4P8A2
G	896	HIS	-	expression tag	UNP K4P8A2
G	897	HIS	-	expression tag	UNP K4P8A2
G	898	HIS	-	expression tag	UNP K4P8A2
G	899	HIS	-	expression tag	UNP K4P8A2
G	900	HIS	-	expression tag	UNP K4P8A2
G	901	HIS	-	expression tag	UNP K4P8A2
J	264	MET	-	initiating methionine	UNP K4P8A2
J	892	GLY	-	expression tag	UNP K4P8A2
J	893	SER	-	expression tag	UNP K4P8A2
J	894	SER	-	expression tag	UNP K4P8A2
J	895	SER	-	expression tag	UNP K4P8A2
J	896	HIS	-	expression tag	UNP K4P8A2
J	897	HIS	-	expression tag	UNP K4P8A2
J	898	HIS	-	expression tag	UNP K4P8A2
J	899	HIS	-	expression tag	UNP K4P8A2
J	900	HIS	-	expression tag	UNP K4P8A2
J	901	HIS	-	expression tag	UNP K4P8A2
I	264	MET	-	initiating methionine	UNP K4P8A2
I	892	GLY	-	expression tag	UNP K4P8A2
I	893	SER	-	expression tag	UNP K4P8A2
I	894	SER	-	expression tag	UNP K4P8A2
I	895	SER	-	expression tag	UNP K4P8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	896	HIS	-	expression tag	UNP K4P8A2
I	897	HIS	-	expression tag	UNP K4P8A2
I	898	HIS	-	expression tag	UNP K4P8A2
I	899	HIS	-	expression tag	UNP K4P8A2
I	900	HIS	-	expression tag	UNP K4P8A2
I	901	HIS	-	expression tag	UNP K4P8A2
H	264	MET	-	initiating methionine	UNP K4P8A2
H	892	GLY	-	expression tag	UNP K4P8A2
H	893	SER	-	expression tag	UNP K4P8A2
H	894	SER	-	expression tag	UNP K4P8A2
H	895	SER	-	expression tag	UNP K4P8A2
H	896	HIS	-	expression tag	UNP K4P8A2
H	897	HIS	-	expression tag	UNP K4P8A2
H	898	HIS	-	expression tag	UNP K4P8A2
H	899	HIS	-	expression tag	UNP K4P8A2
H	900	HIS	-	expression tag	UNP K4P8A2
H	901	HIS	-	expression tag	UNP K4P8A2

- 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	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

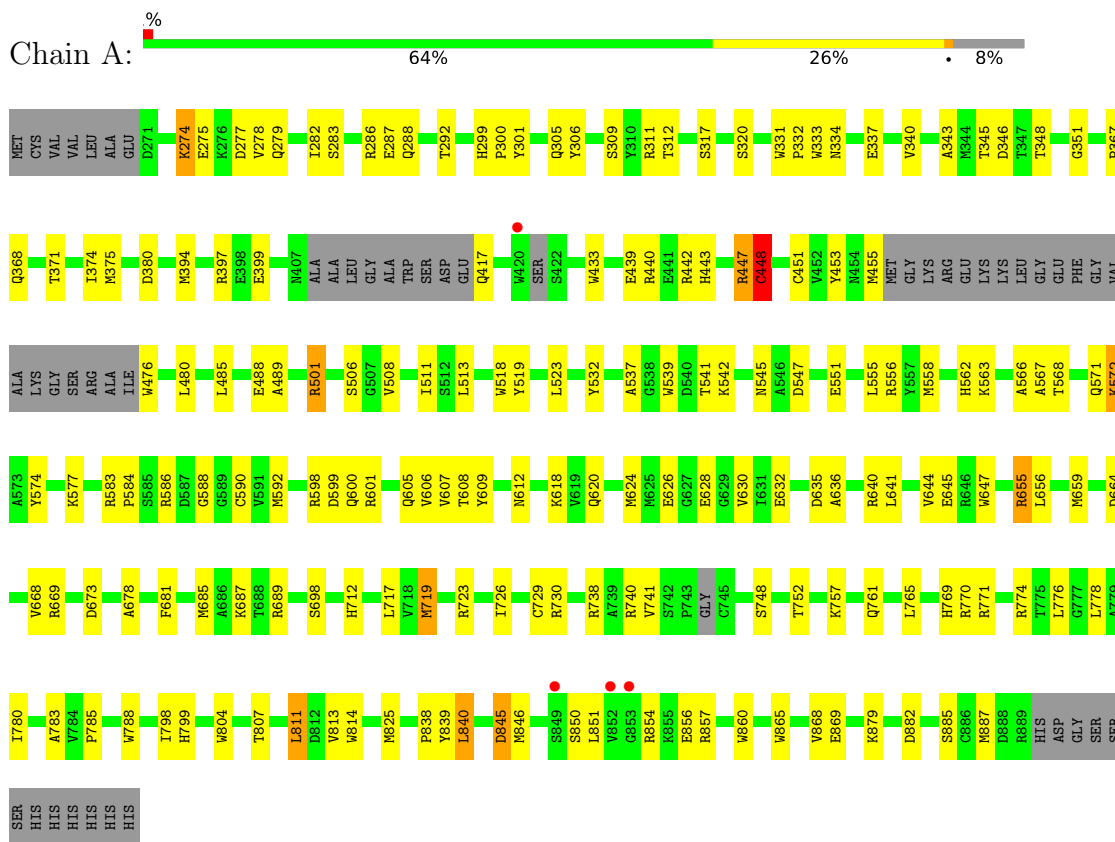
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

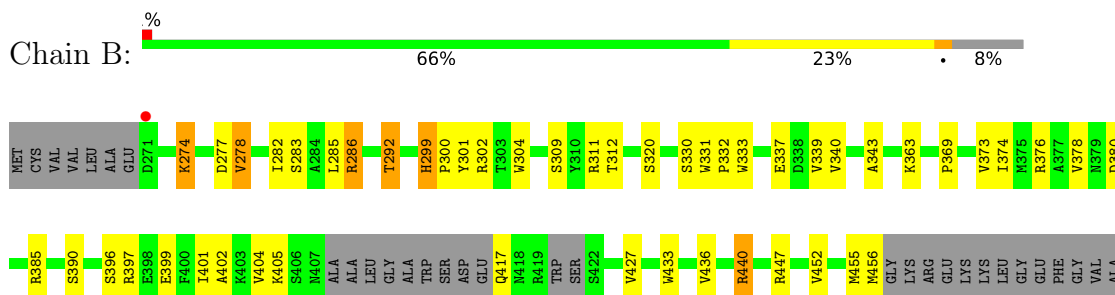
3 Residue-property plots [i](#)

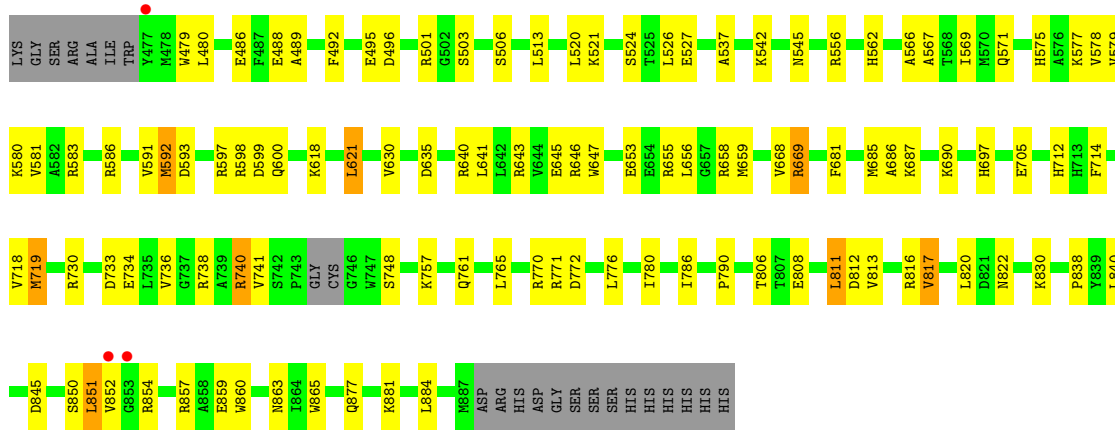
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tick-borne encephalitis virus RNA-dependent RNA polymerase

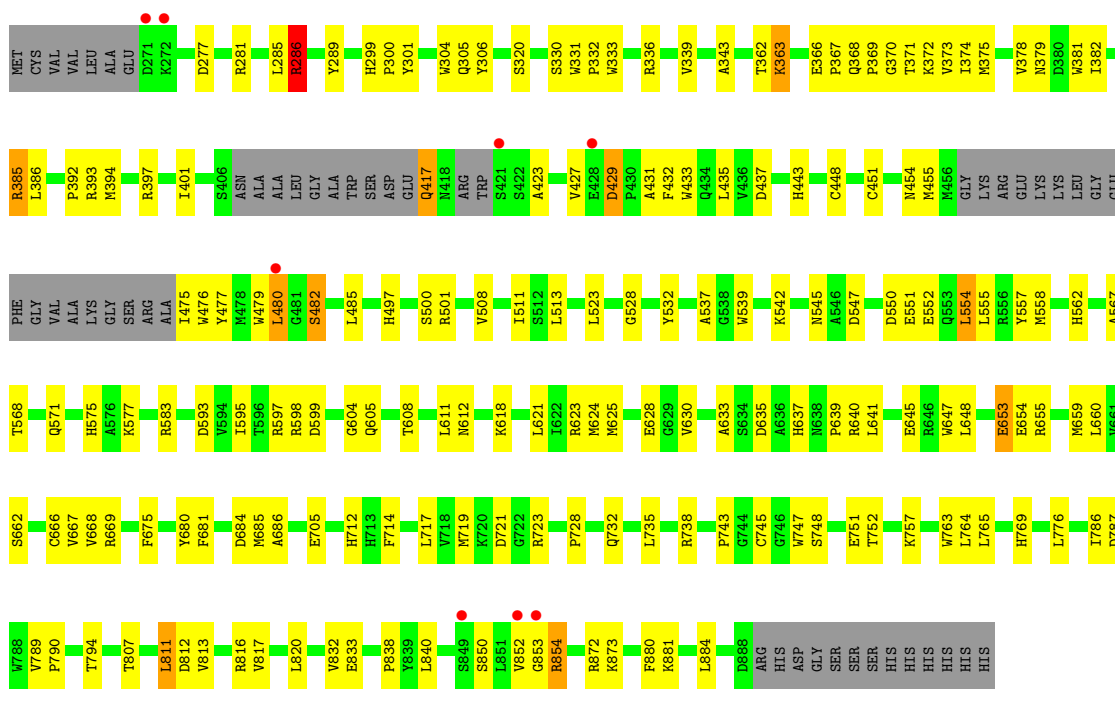


- Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase

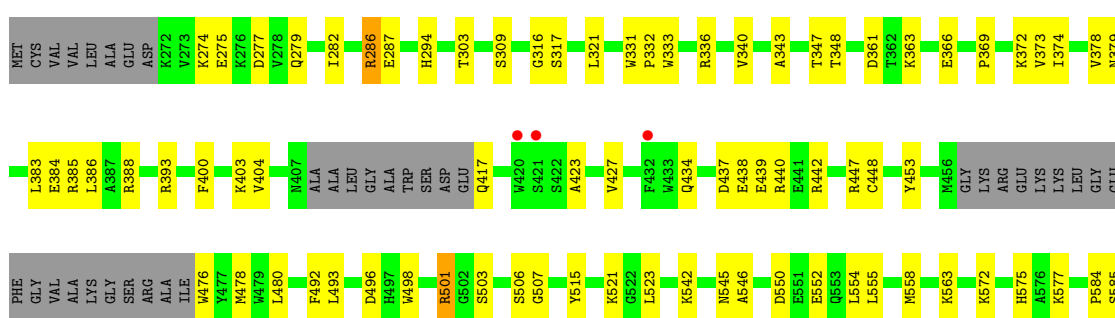


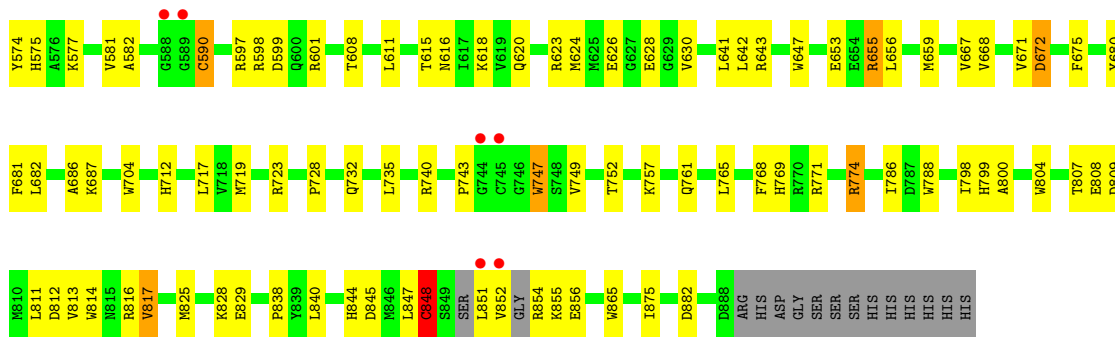


• Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase

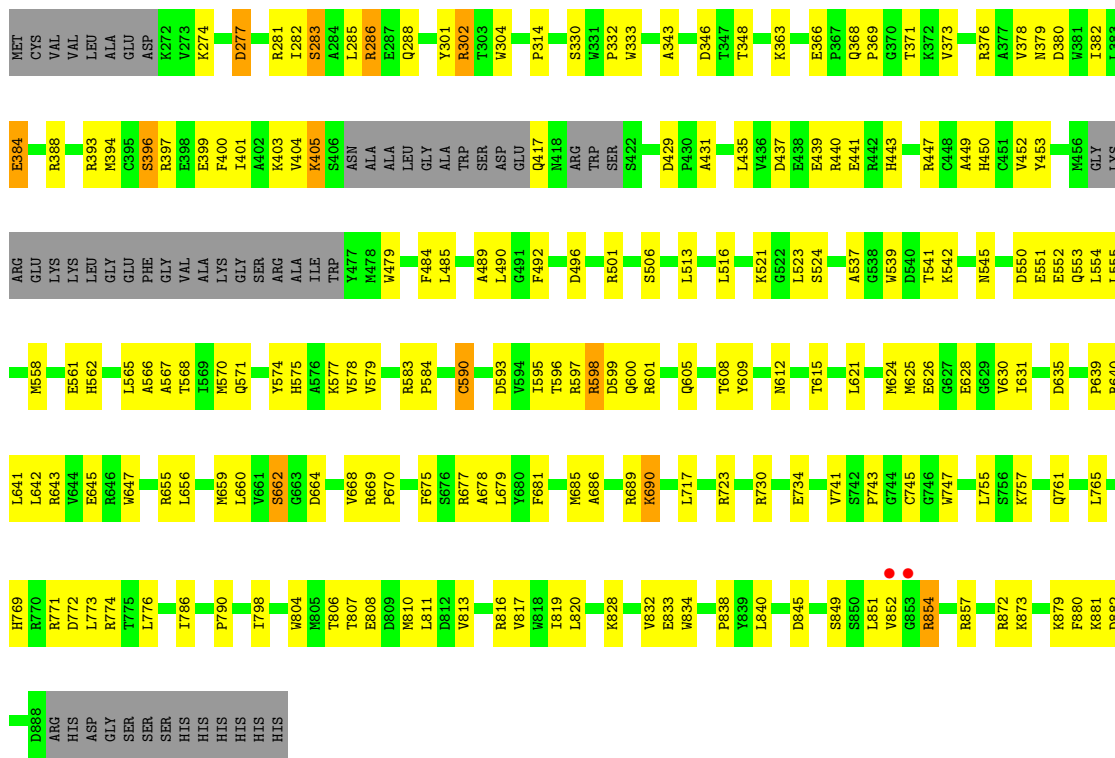


• Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase

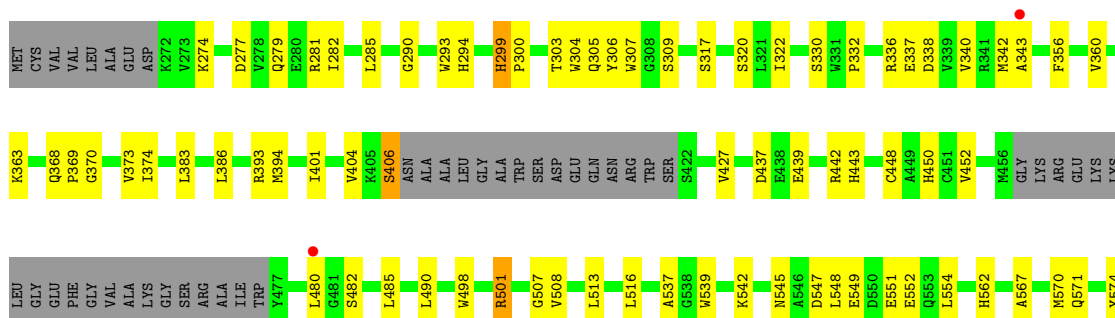


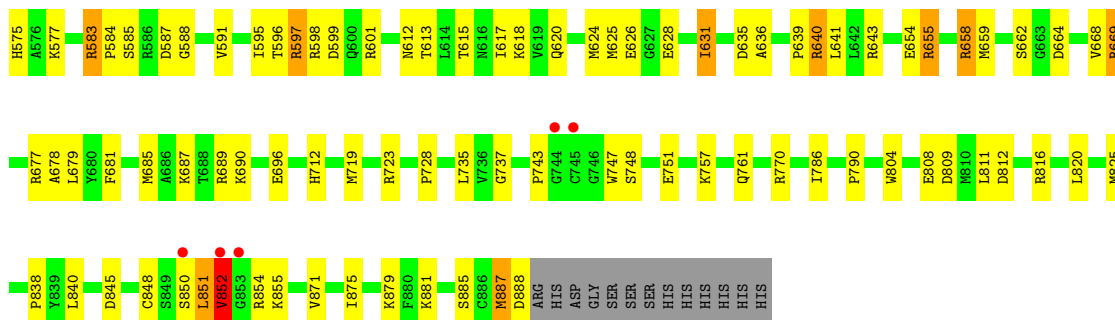


• Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase

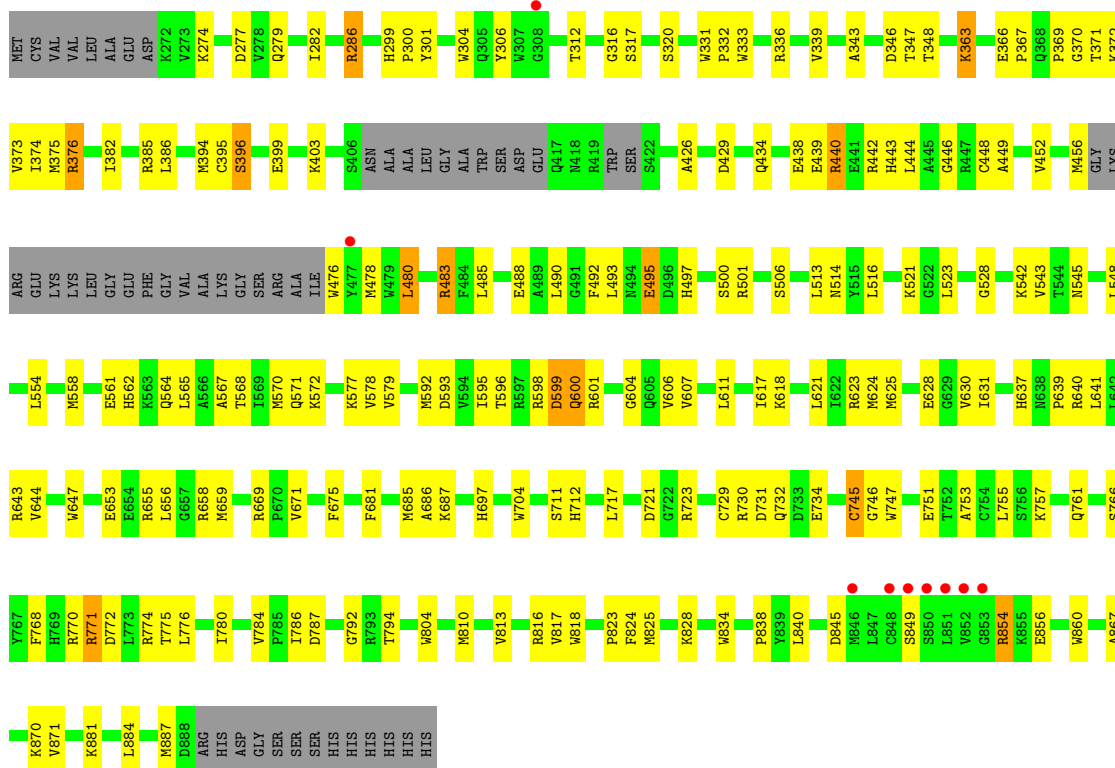


• Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase



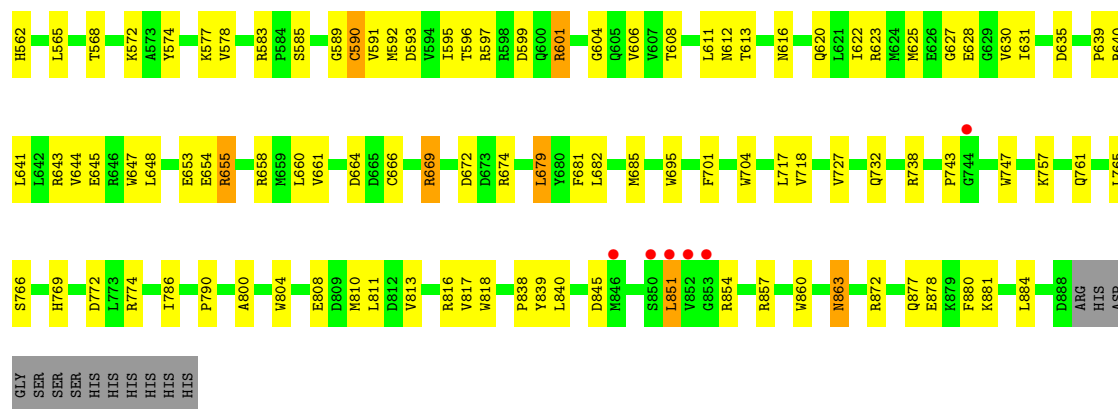


● Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase



● Molecule 1: Tick-borne encephalitis virus RNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	175.99Å 235.18Å 327.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.17 49.99 – 3.17	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.99-3.17) 98.0 (49.99-3.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.12_2829_000	Depositor
R, R_{free}	0.195 , 0.233 0.195 , 0.233	Depositor DCC
R_{free} test set	11329 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45346	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MG, 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	0.61	4/4680 (0.1%)	0.77	4/6356 (0.1%)
1	B	0.61	2/4679 (0.0%)	0.81	6/6345 (0.1%)
1	C	0.55	2/4623 (0.0%)	0.73	2/6286 (0.0%)
1	D	0.56	1/4659 (0.0%)	0.77	4/6334 (0.1%)
1	E	0.57	0/4628	0.77	4/6292 (0.1%)
1	F	0.57	2/4653 (0.0%)	0.75	3/6318 (0.0%)
1	G	0.54	2/4668 (0.0%)	0.73	4/6334 (0.1%)
1	H	0.52	0/4622	0.71	5/6284 (0.1%)
1	I	0.51	0/4644	0.73	2/6307 (0.0%)
1	J	0.52	0/4551	0.73	7/6196 (0.1%)
All	All	0.56	13/46407 (0.0%)	0.75	41/63052 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	848	CYS	CB-SG	7.84	1.95	1.82
1	A	448	CYS	CB-SG	-7.48	1.69	1.82
1	C	848	CYS	CB-SG	6.95	1.94	1.82
1	A	287	GLU	CG-CD	6.58	1.61	1.51
1	C	476	TRP	CB-CG	6.03	1.61	1.50

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	VAL	CG1-CB-CG2	8.95	125.22	110.90
1	J	851	LEU	CB-CG-CD1	8.38	125.24	111.00
1	I	599	ASP	CB-CG-OD1	-8.15	110.97	118.30
1	G	404	VAL	CG1-CB-CG2	7.58	123.02	110.90
1	C	285	LEU	CA-CB-CG	7.25	131.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4569	0	4275	136	0
1	B	4571	0	4324	129	0
1	C	4514	0	4191	131	0
1	D	4549	0	4233	128	0
1	E	4519	0	4188	147	0
1	F	4544	0	4260	124	0
1	G	4560	0	4301	166	0
1	H	4514	0	4194	145	0
1	I	4535	0	4234	147	0
1	J	4441	0	4101	120	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	45346	0	42301	1359	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 16.

The worst 5 of 1359 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:D:279:GLN:HG2	1:D:572:LYS:HE2	1.35	1.07
1:G:417:GLN:HG3	1:G:479:TRP:HZ3	1.16	1.05
1:G:561:GLU:O	1:G:565:LEU:HD12	1.54	1.04
1:H:394:MET:HG3	1:H:562:HIS:HD2	1.23	1.02
1:H:274:LYS:HE2	1:H:363:LYS:HE2	1.47	0.97

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	578/638 (91%)	535 (93%)	43 (7%)	0	100	100
1	B	574/638 (90%)	525 (92%)	48 (8%)	1 (0%)	47	78
1	C	576/638 (90%)	515 (89%)	59 (10%)	2 (0%)	41	73
1	D	584/638 (92%)	529 (91%)	55 (9%)	0	100	100
1	E	580/638 (91%)	524 (90%)	52 (9%)	4 (1%)	22	59
1	F	571/638 (90%)	518 (91%)	53 (9%)	0	100	100
1	G	576/638 (90%)	525 (91%)	49 (8%)	2 (0%)	41	73
1	H	580/638 (91%)	539 (93%)	41 (7%)	0	100	100
1	I	578/638 (91%)	516 (89%)	61 (11%)	1 (0%)	47	78
1	J	576/638 (90%)	528 (92%)	46 (8%)	2 (0%)	41	73
All	All	5773/6380 (90%)	5254 (91%)	507 (9%)	12 (0%)	47	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	852	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	E	854	ARG
1	J	851	LEU
1	B	278	VAL
1	G	849	SER

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	458/543 (84%)	441 (96%)	17 (4%)	34	66
1	B	465/543 (86%)	447 (96%)	18 (4%)	32	64
1	C	450/543 (83%)	432 (96%)	18 (4%)	31	64
1	D	456/543 (84%)	435 (95%)	21 (5%)	27	60
1	E	449/543 (83%)	429 (96%)	20 (4%)	27	61
1	F	457/543 (84%)	440 (96%)	17 (4%)	34	66
1	G	462/543 (85%)	447 (97%)	15 (3%)	39	70
1	H	451/543 (83%)	439 (97%)	12 (3%)	44	73
1	I	455/543 (84%)	439 (96%)	16 (4%)	36	67
1	J	440/543 (81%)	422 (96%)	18 (4%)	30	63
All	All	4543/5430 (84%)	4371 (96%)	172 (4%)	33	65

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	384	GLU
1	J	888	ASP
1	G	590	CYS
1	J	482	SER
1	I	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	761	GLN
1	H	545	ASN
1	G	379	ASN
1	H	616	ASN
1	J	379	ASN

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 30 ligands modelled in this entry, 30 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, 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	588/638 (92%)	-0.29	4 (0%) 87 81	31, 52, 95, 118	0
1	B	584/638 (91%)	-0.33	4 (0%) 87 81	32, 51, 97, 114	0
1	C	586/638 (91%)	-0.26	2 (0%) 94 92	43, 66, 103, 125	0
1	D	589/638 (92%)	-0.27	8 (1%) 75 63	40, 57, 101, 128	0
1	E	588/638 (92%)	-0.26	8 (1%) 75 63	36, 60, 102, 125	0
1	F	583/638 (91%)	-0.23	8 (1%) 75 63	34, 59, 107, 128	0
1	G	584/638 (91%)	-0.27	2 (0%) 94 92	39, 68, 102, 115	0
1	H	588/638 (92%)	-0.15	9 (1%) 73 61	47, 71, 112, 128	0
1	I	586/638 (91%)	-0.20	9 (1%) 73 61	44, 67, 110, 132	0
1	J	582/638 (91%)	-0.20	7 (1%) 79 68	40, 73, 107, 125	0
All	All	5858/6380 (91%)	-0.25	61 (1%) 82 73	31, 63, 104, 132	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	852	VAL	5.1
1	E	852	VAL	4.5
1	D	852	VAL	4.4
1	E	853	GLY	4.1
1	G	853	GLY	3.8

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.

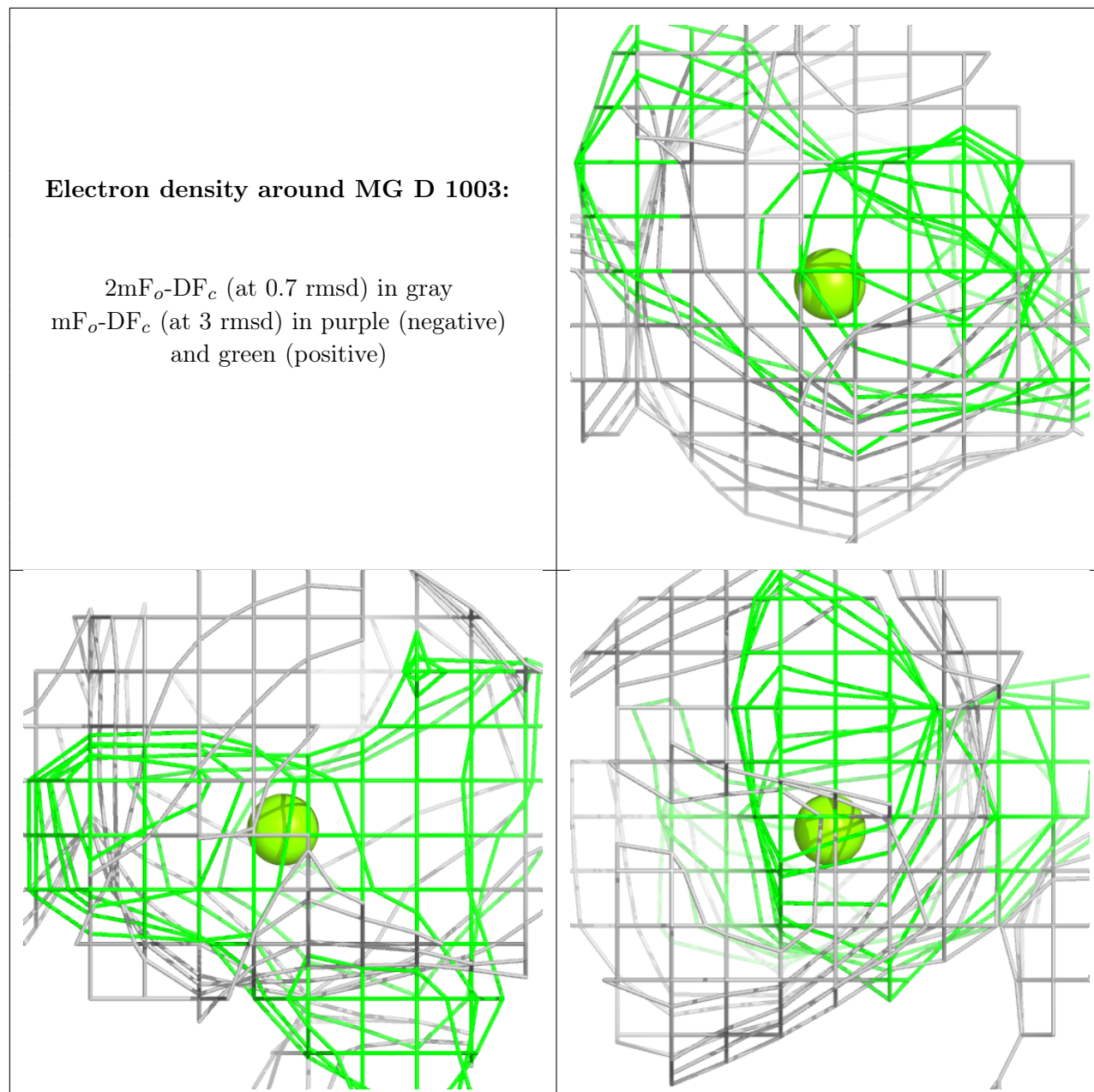
6.4 Ligands [i](#)

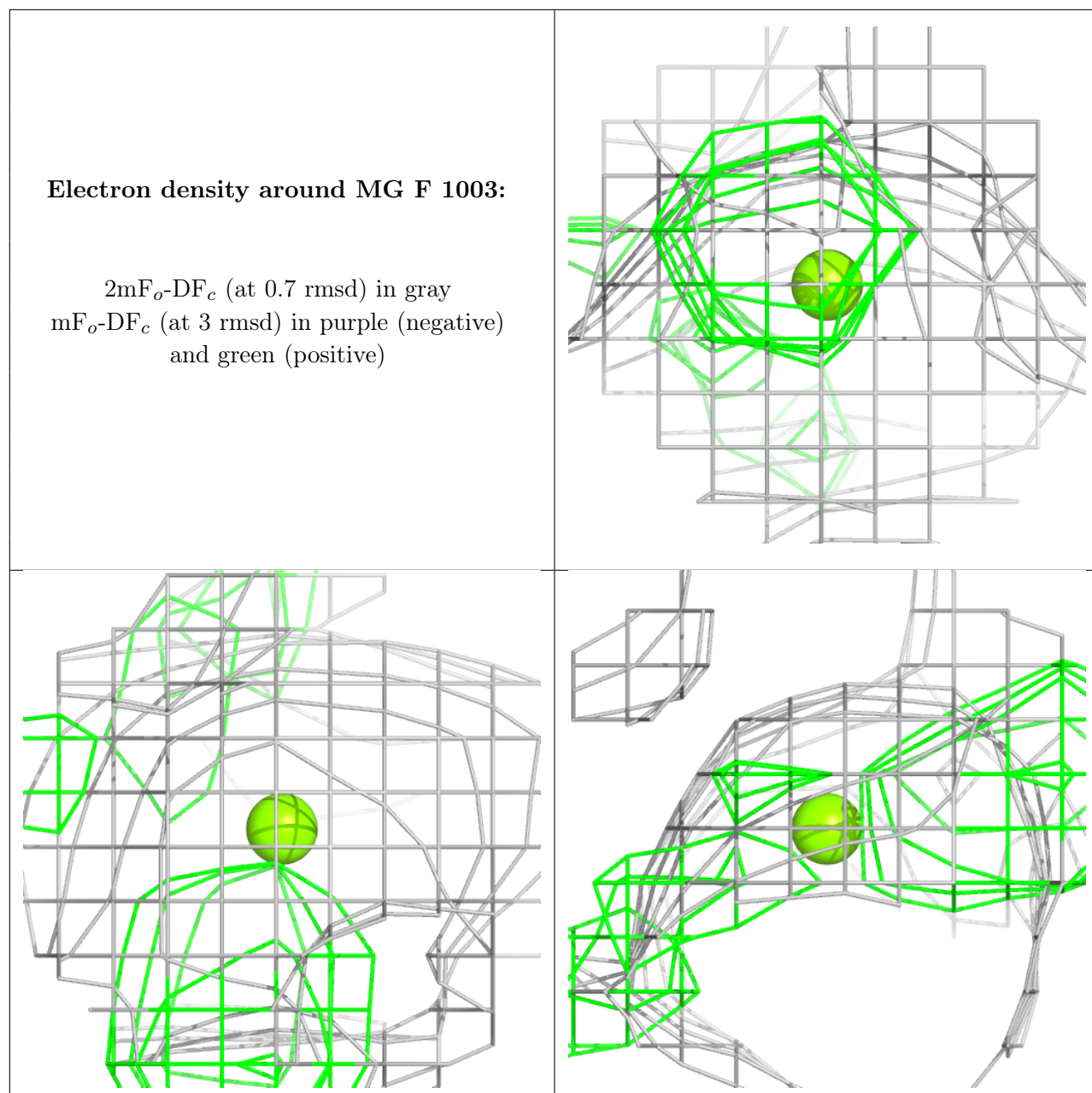
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	D	1003	1/1	0.93	0.27	52,52,52,52	0
3	MG	F	1003	1/1	0.93	0.27	47,47,47,47	0
2	ZN	H	1001	1/1	0.94	0.08	91,91,91,91	1
3	MG	I	1003	1/1	0.94	0.37	73,73,73,73	0
2	ZN	C	1001	1/1	0.95	0.12	80,80,80,80	1
3	MG	B	1003	1/1	0.95	0.24	45,45,45,45	0
3	MG	G	1003	1/1	0.95	0.25	66,66,66,66	0
3	MG	J	1003	1/1	0.95	0.28	75,75,75,75	0
3	MG	E	1003	1/1	0.95	0.31	58,58,58,58	0
3	MG	A	1003	1/1	0.96	0.38	51,51,51,51	0
2	ZN	G	1001	1/1	0.97	0.11	93,93,93,93	1
3	MG	C	1003	1/1	0.97	0.31	61,61,61,61	0
2	ZN	J	1001	1/1	0.97	0.09	84,84,84,84	1
3	MG	H	1003	1/1	0.97	0.23	76,76,76,76	0
2	ZN	F	1001	1/1	0.98	0.09	73,73,73,73	1
2	ZN	A	1002	1/1	0.98	0.13	50,50,50,50	0
2	ZN	B	1001	1/1	0.98	0.09	94,94,94,94	1
2	ZN	A	1001	1/1	0.98	0.11	68,68,68,68	1
2	ZN	H	1002	1/1	0.98	0.10	66,66,66,66	1
2	ZN	C	1002	1/1	0.99	0.07	69,69,69,69	1
2	ZN	E	1001	1/1	0.99	0.09	91,91,91,91	1
2	ZN	F	1002	1/1	0.99	0.09	65,65,65,65	1
2	ZN	E	1002	1/1	0.99	0.10	69,69,69,69	0
2	ZN	G	1002	1/1	0.99	0.12	69,69,69,69	0
2	ZN	D	1001	1/1	0.99	0.08	79,79,79,79	1
2	ZN	J	1002	1/1	0.99	0.12	67,67,67,67	0
2	ZN	I	1001	1/1	0.99	0.09	87,87,87,87	1
2	ZN	D	1002	1/1	0.99	0.14	57,57,57,57	1
2	ZN	B	1002	1/1	0.99	0.10	58,58,58,58	1
2	ZN	I	1002	1/1	1.00	0.10	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all

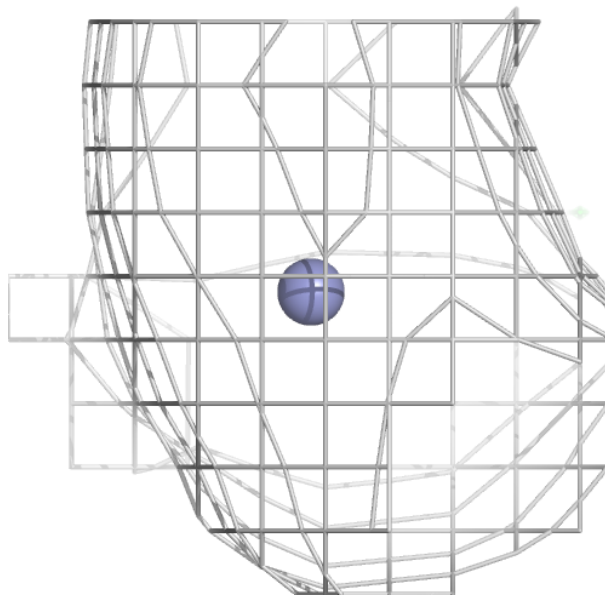
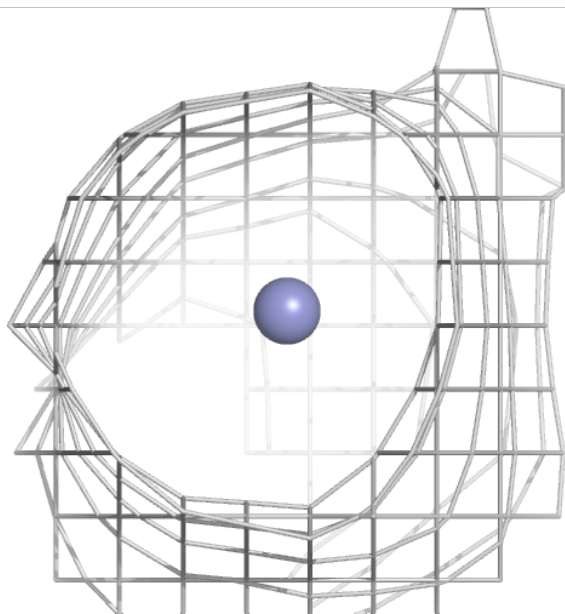
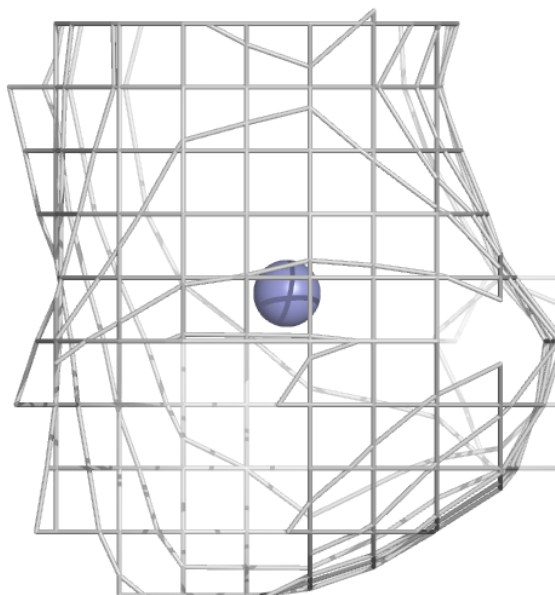
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





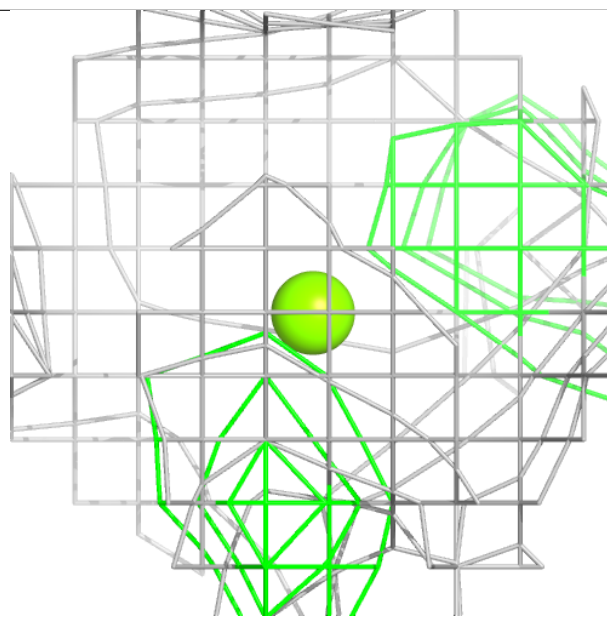
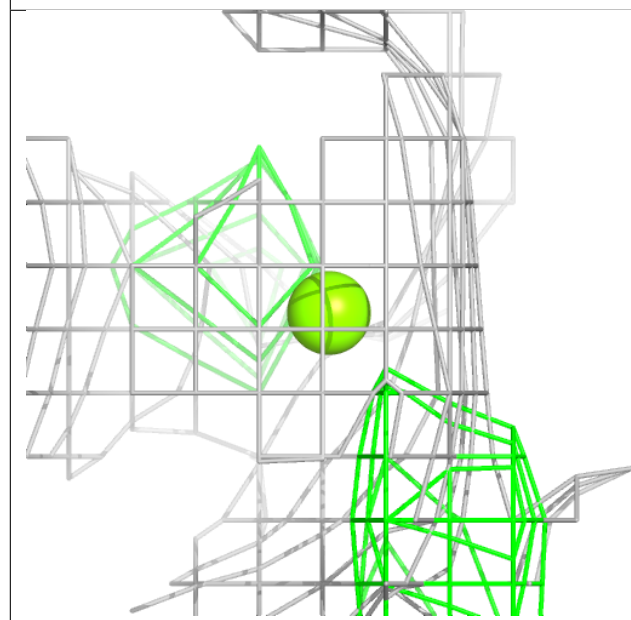
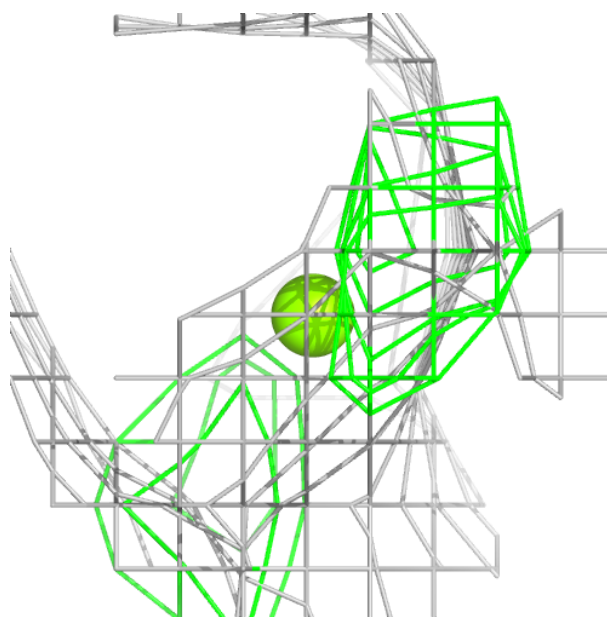
Electron density around ZN H 1001:

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



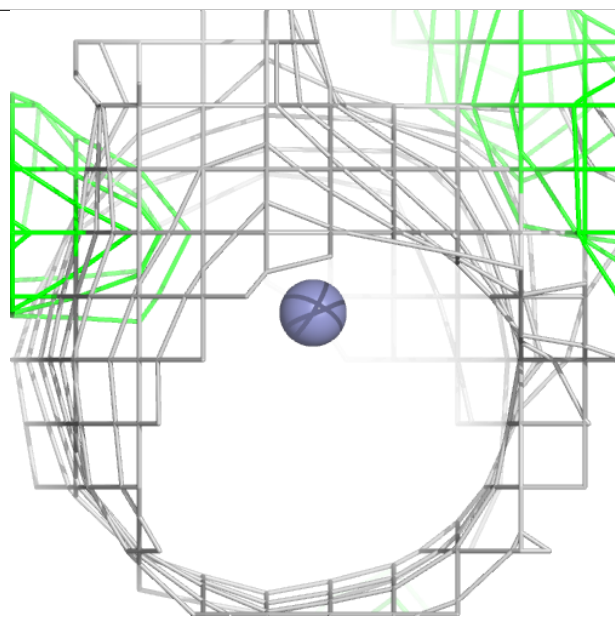
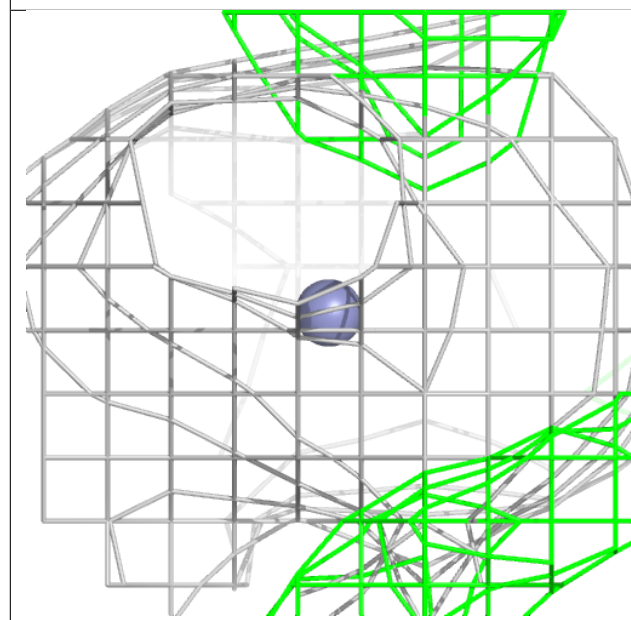
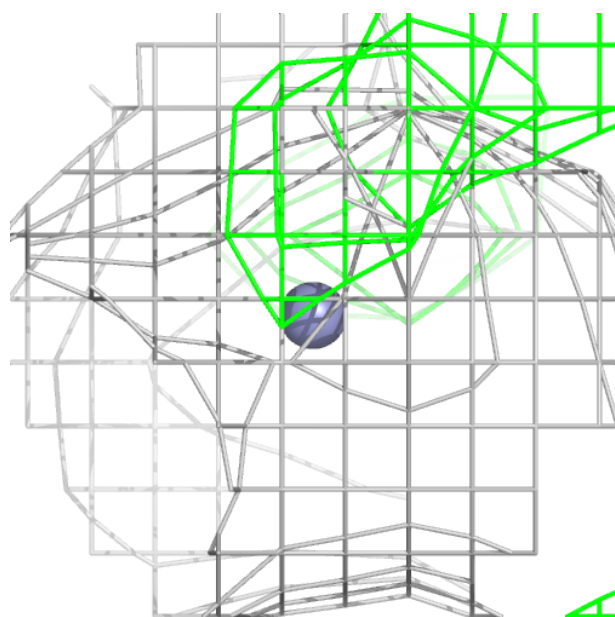
Electron density around MG I 1003:

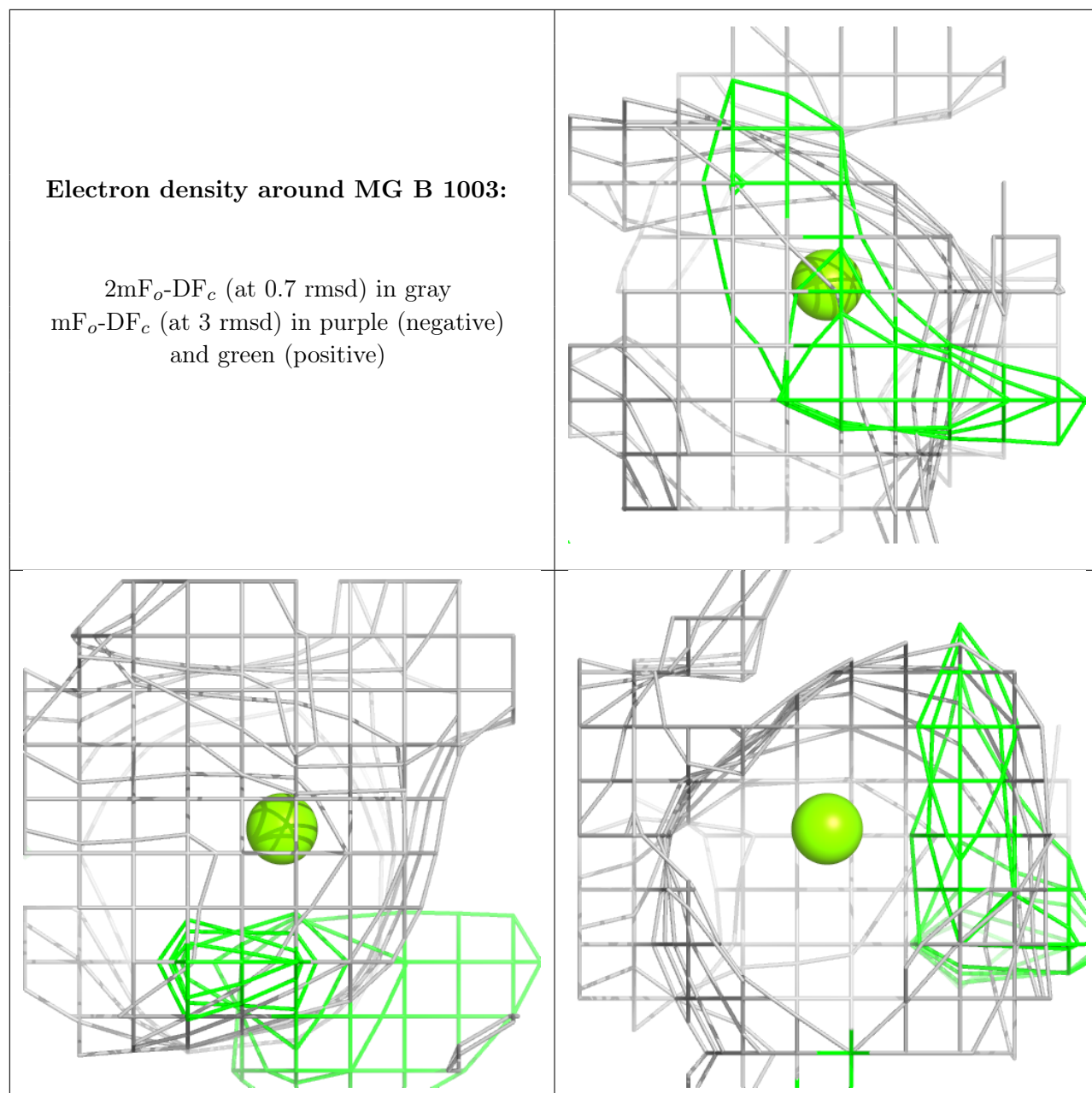
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

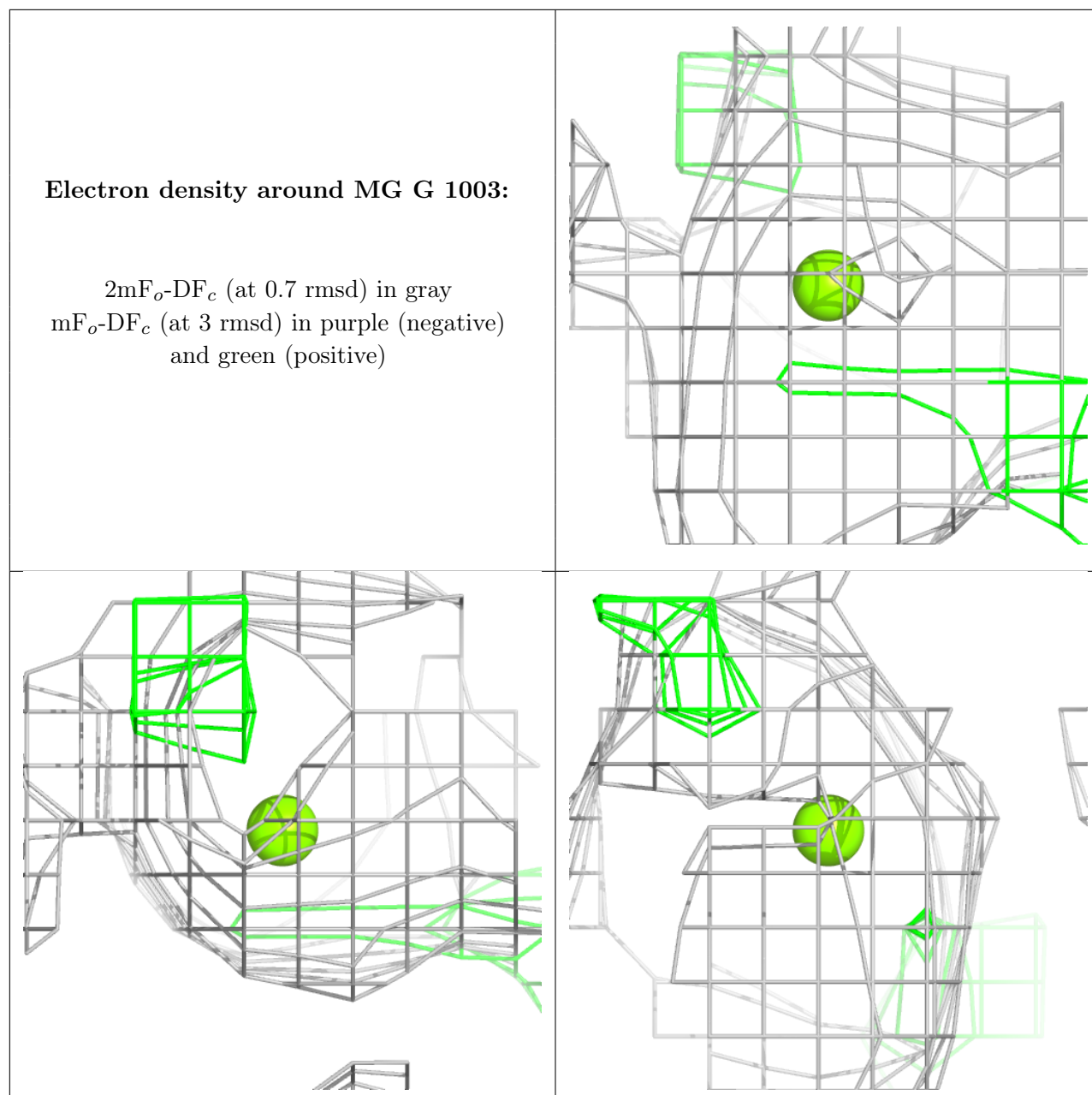


Electron density around ZN C 1001:

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

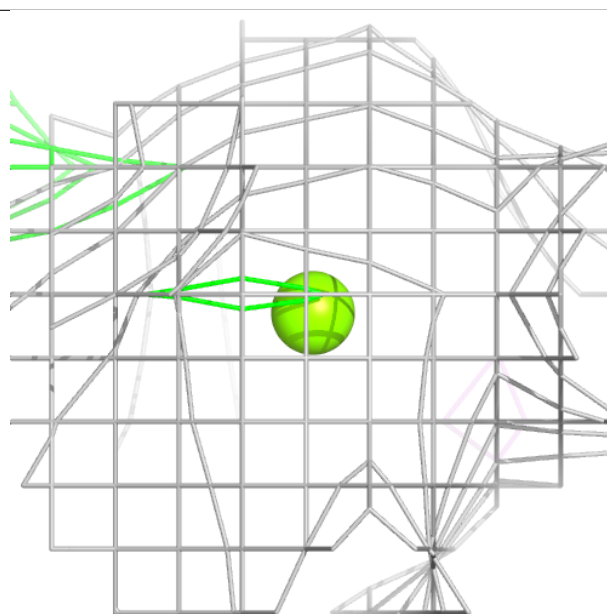
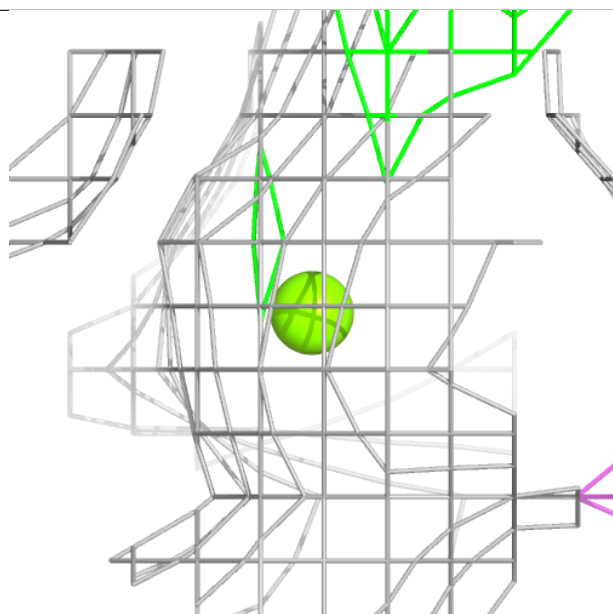
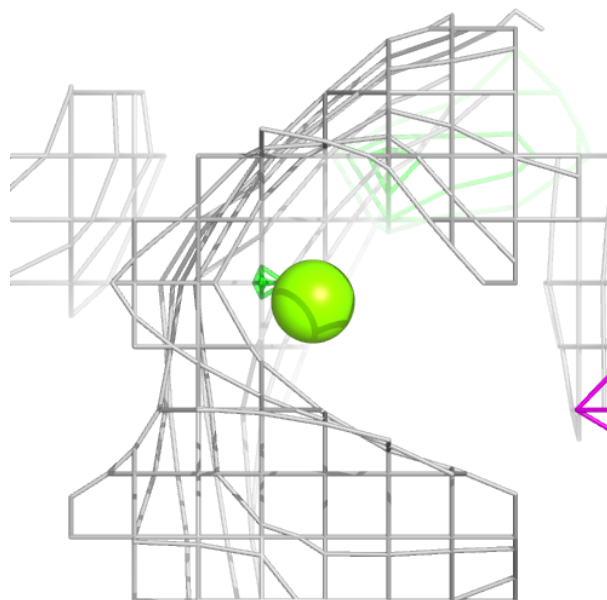


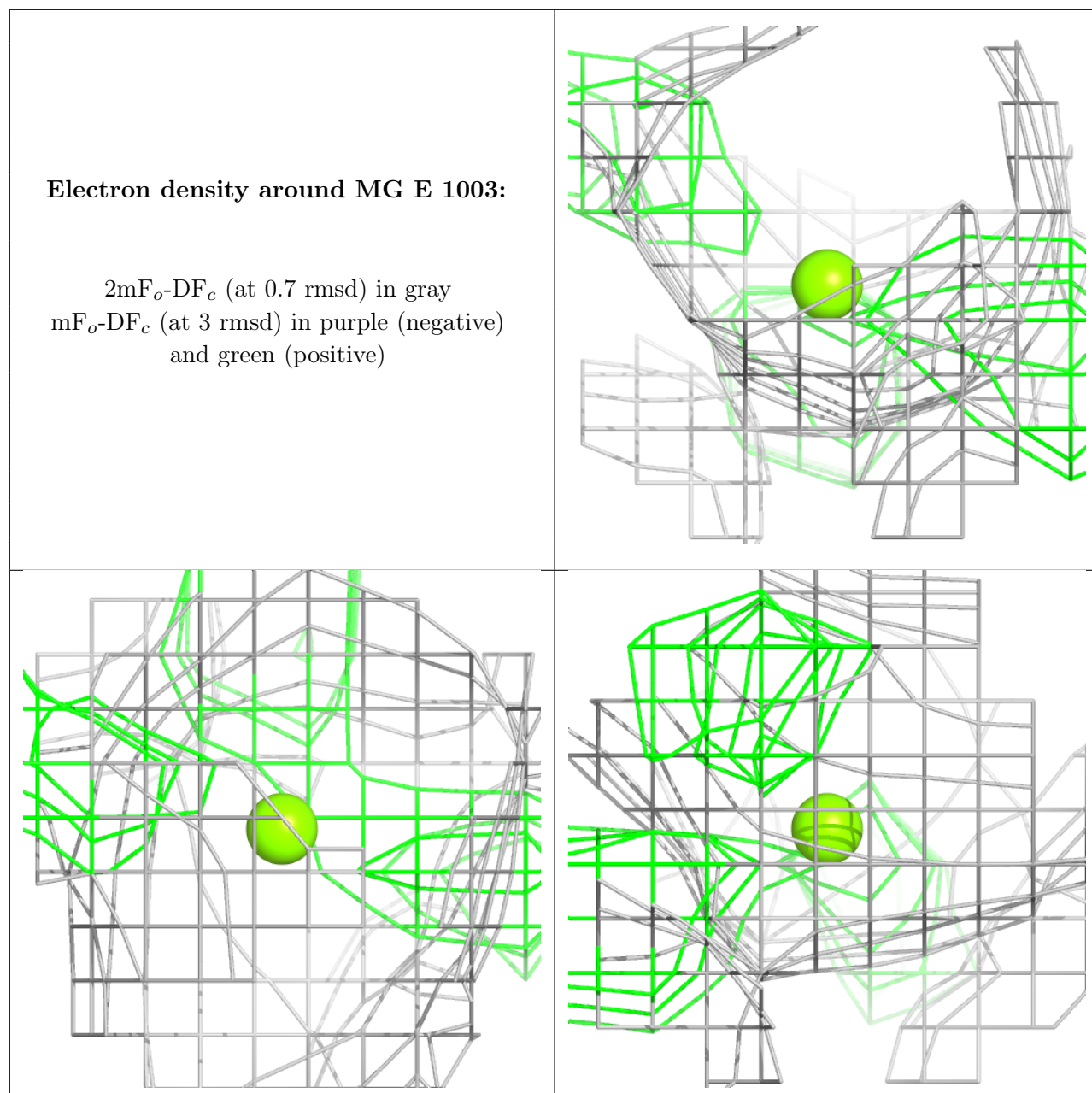




Electron density around MG J 1003:

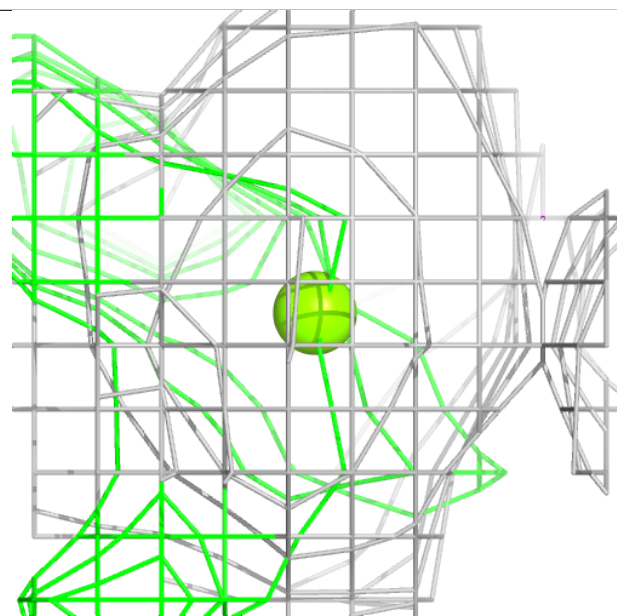
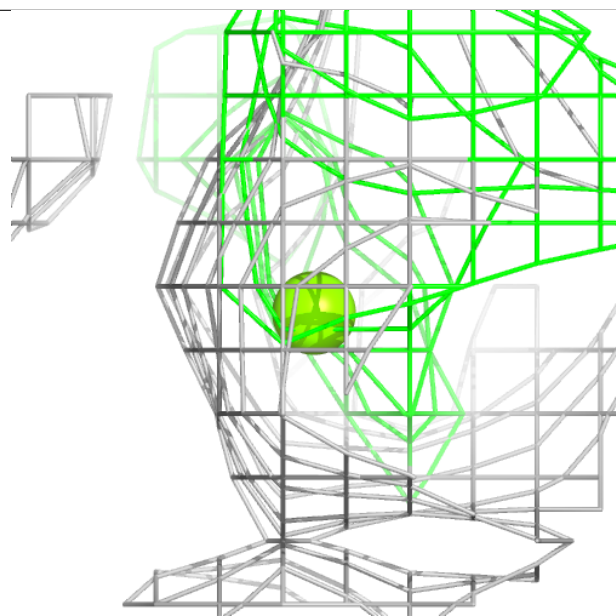
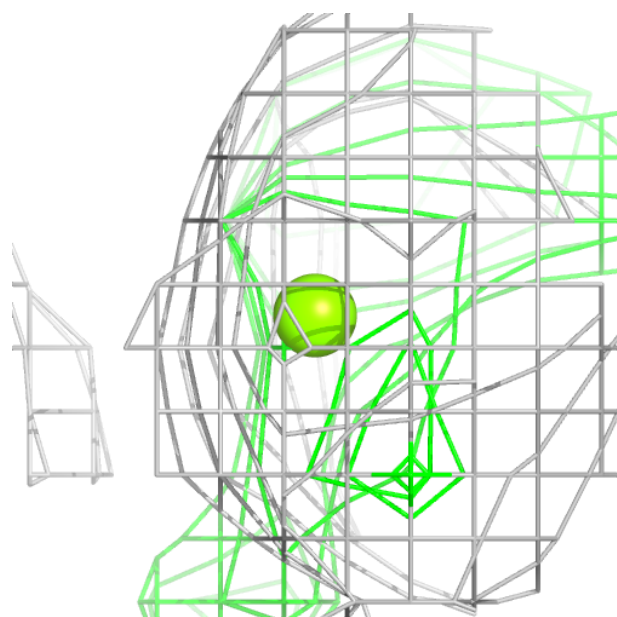
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





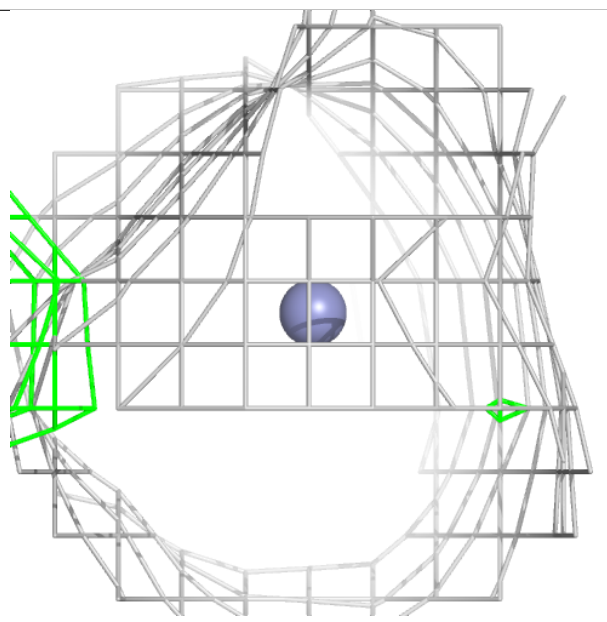
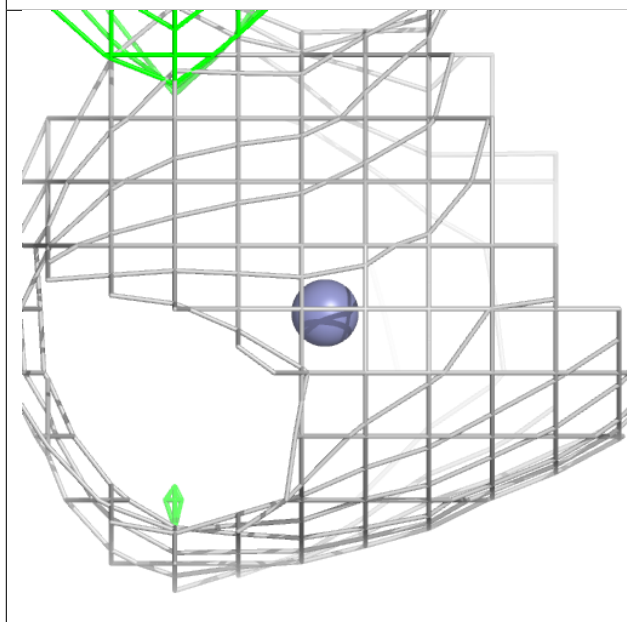
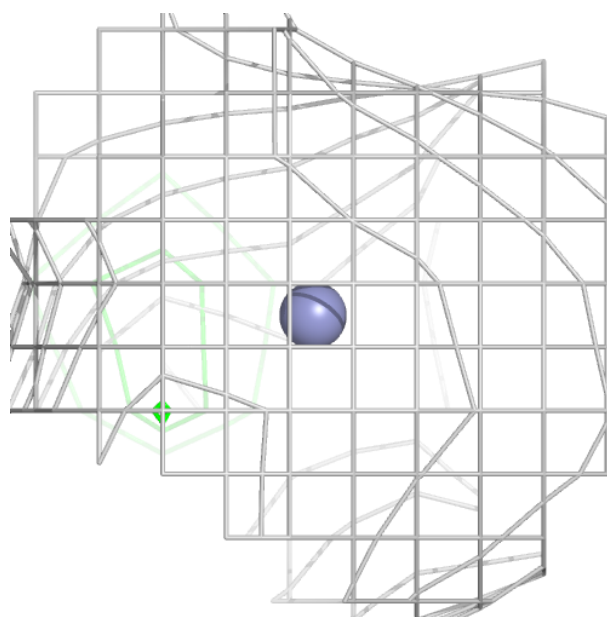
Electron density around MG A 1003:

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and green (positive)



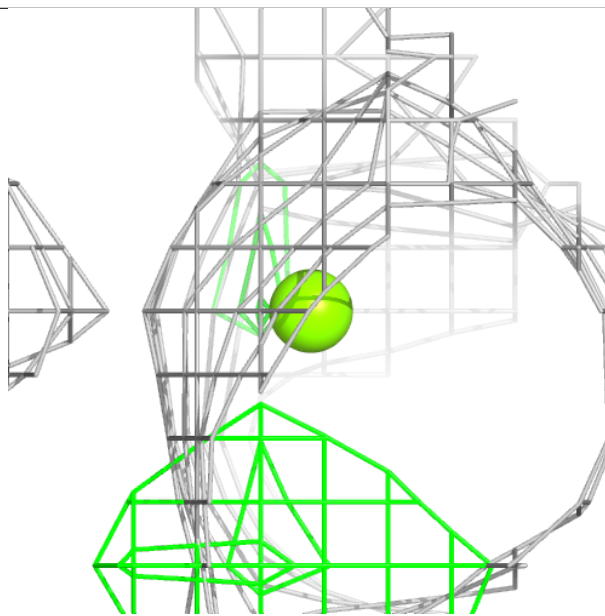
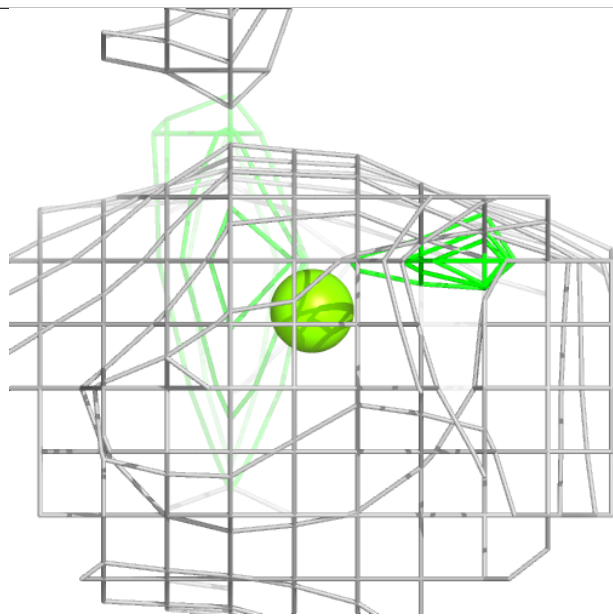
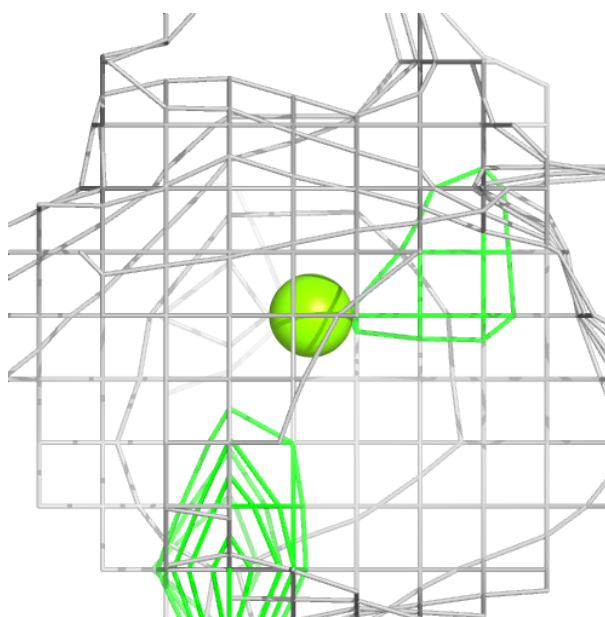
Electron density around ZN G 1001:

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



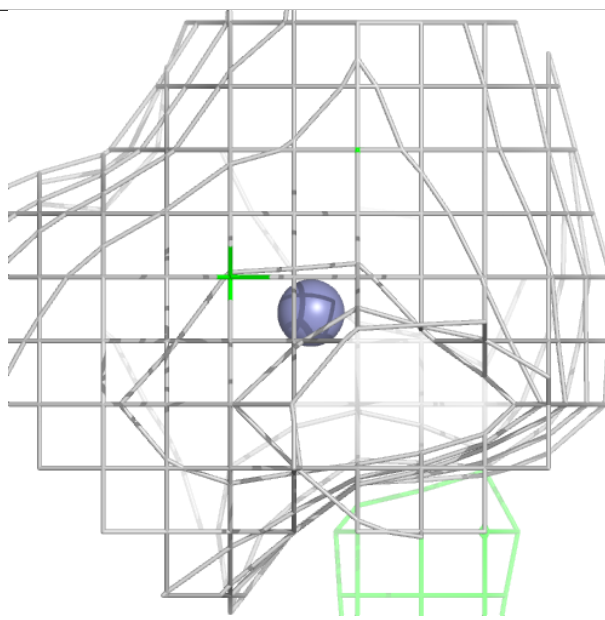
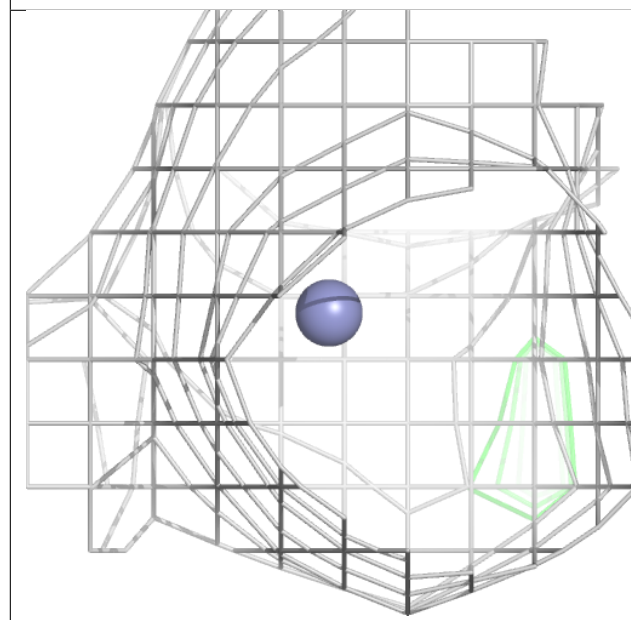
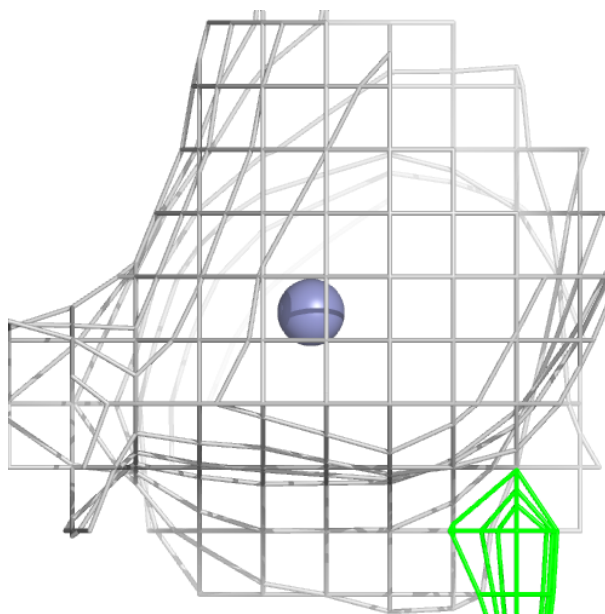
Electron density around MG C 1003:

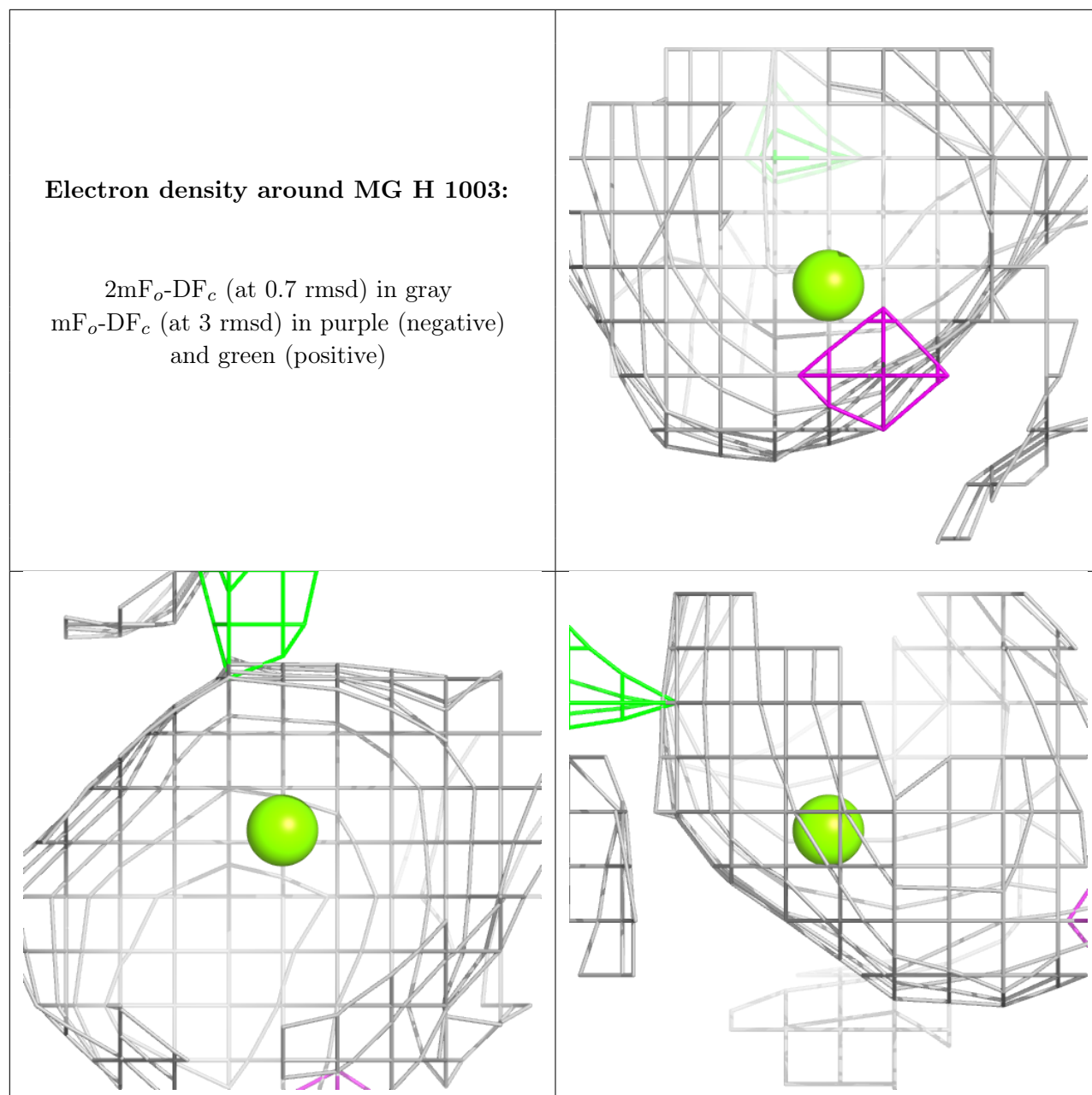
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around ZN J 1001:

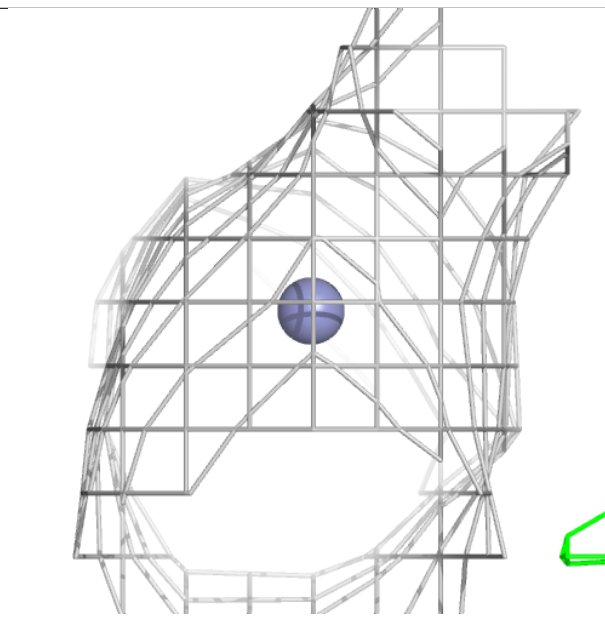
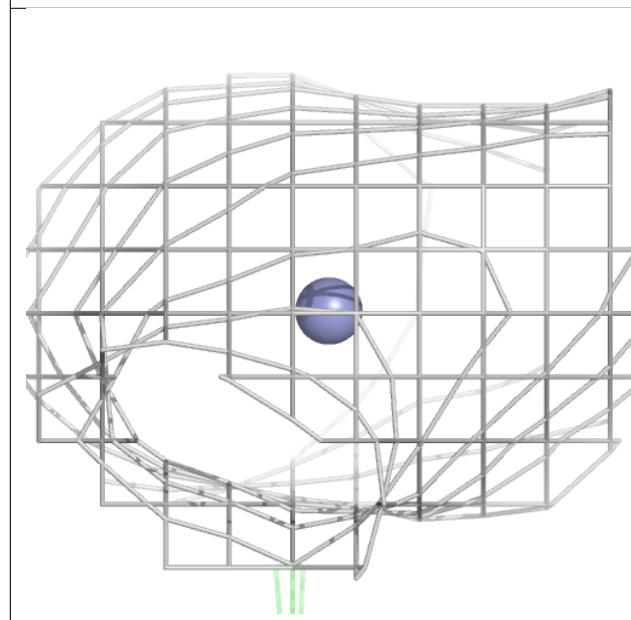
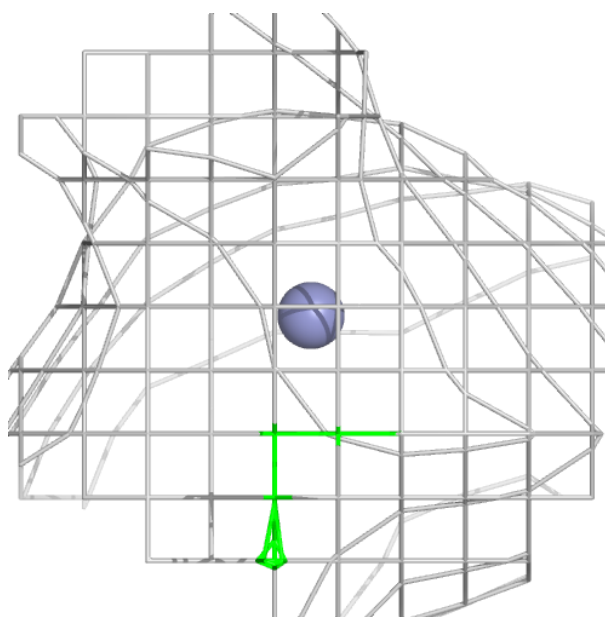
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





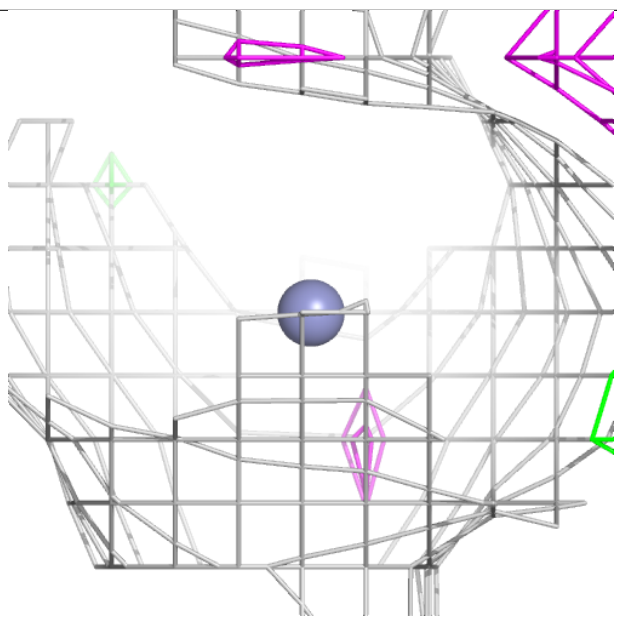
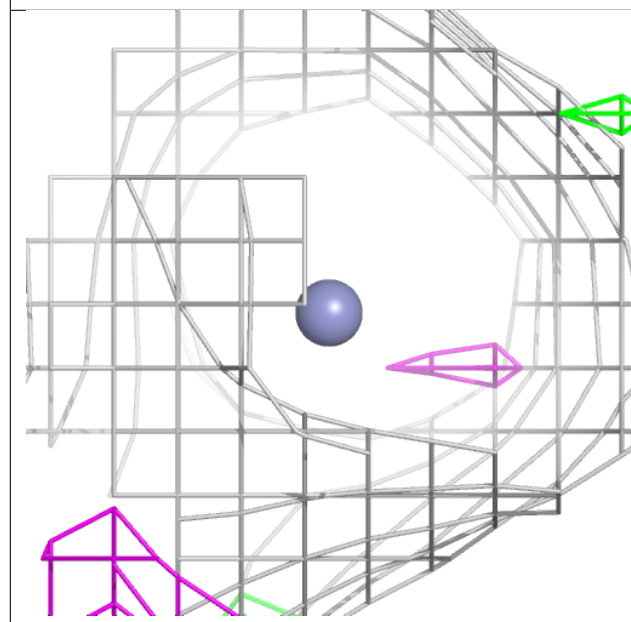
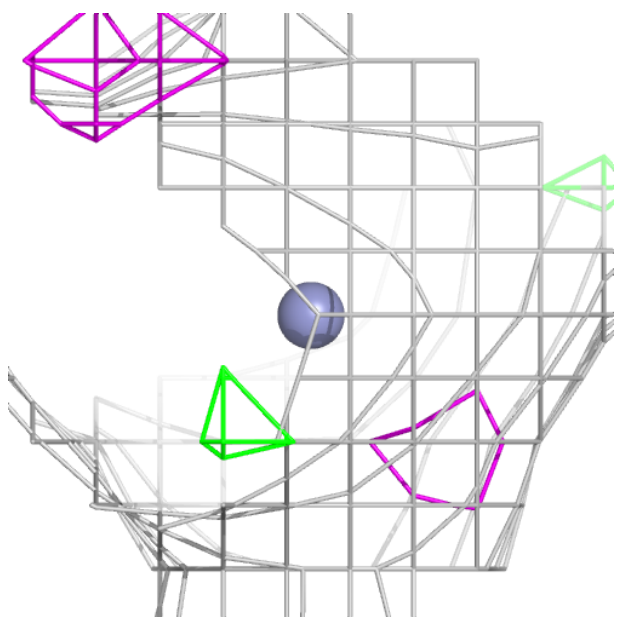
Electron density around ZN F 1001:

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



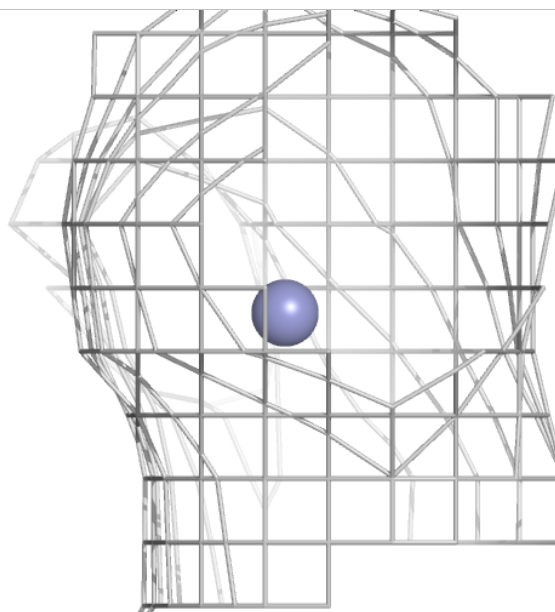
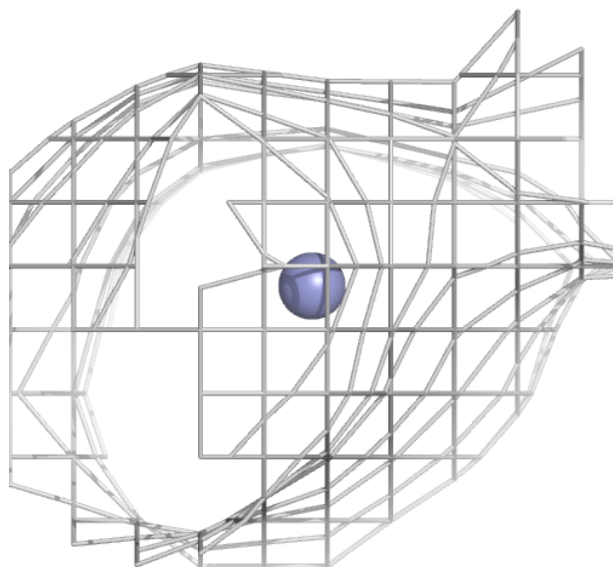
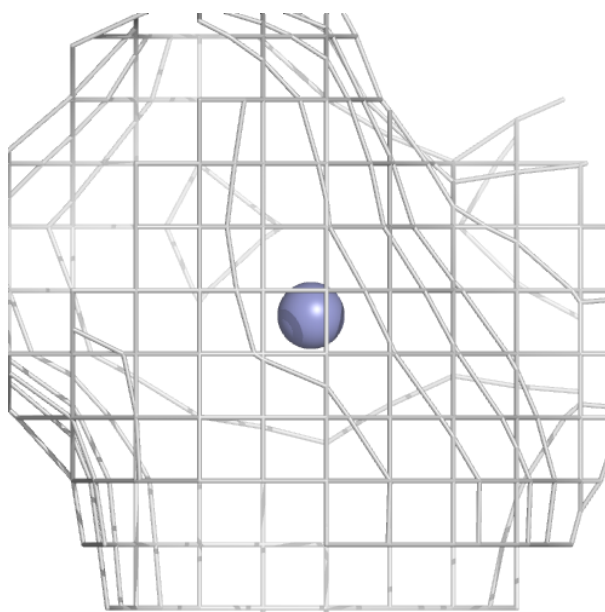
Electron density around ZN A 1002:

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and green (positive)



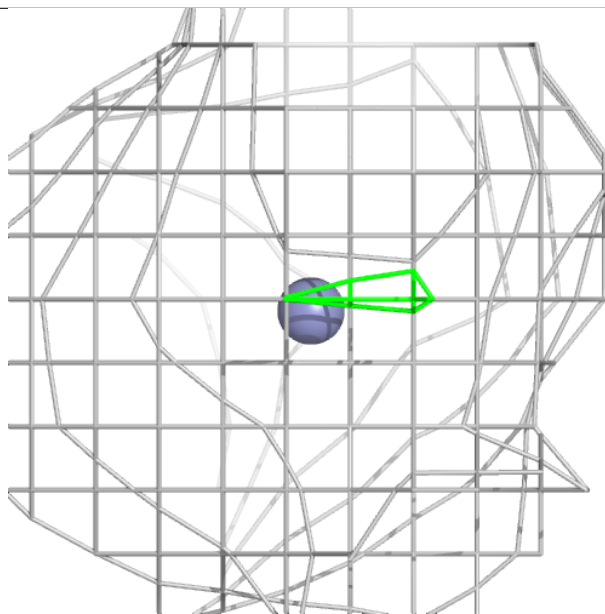
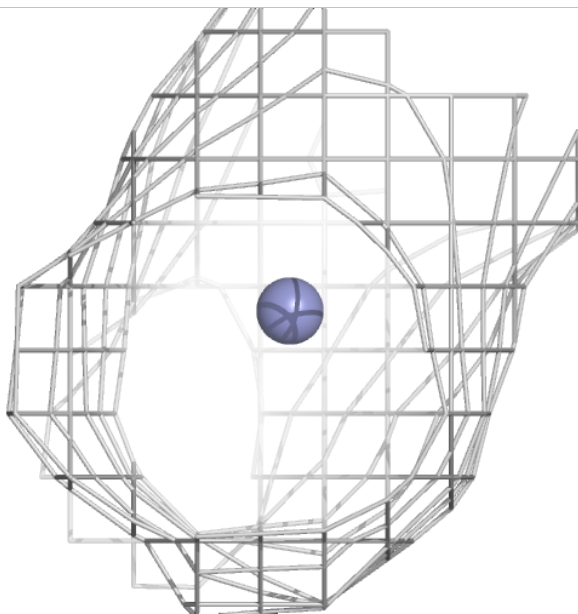
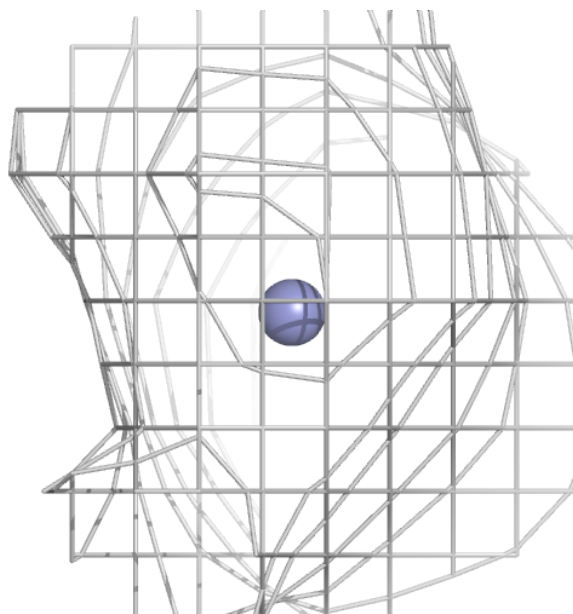
Electron density around ZN B 1001:

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and green (positive)



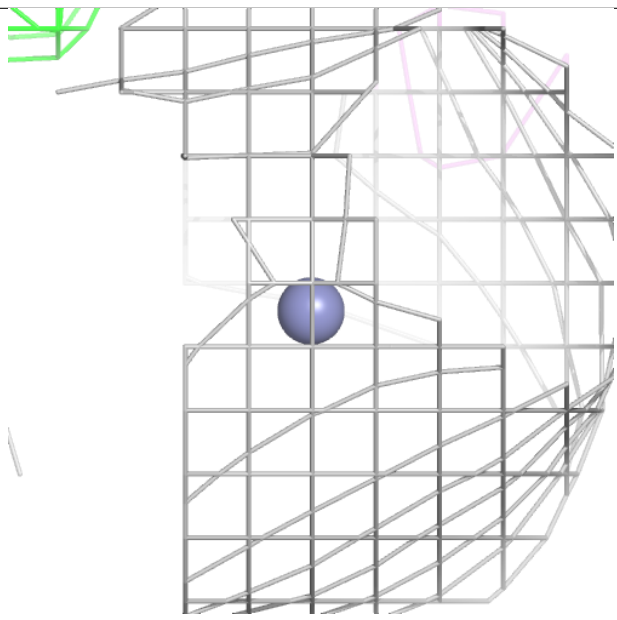
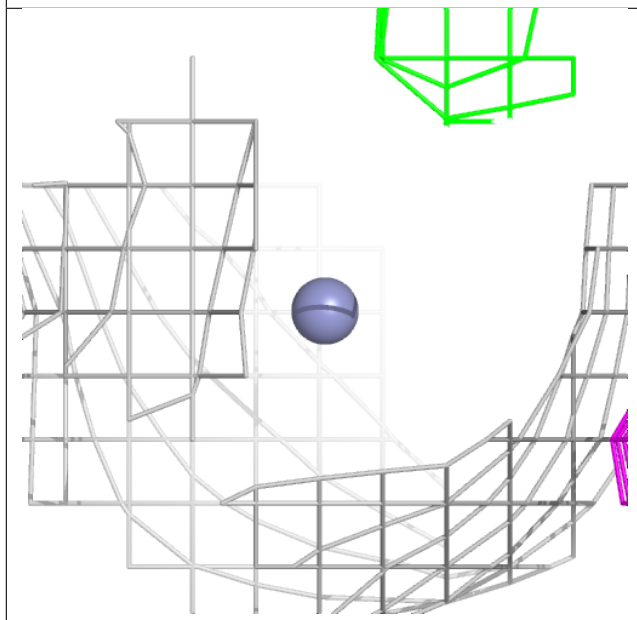
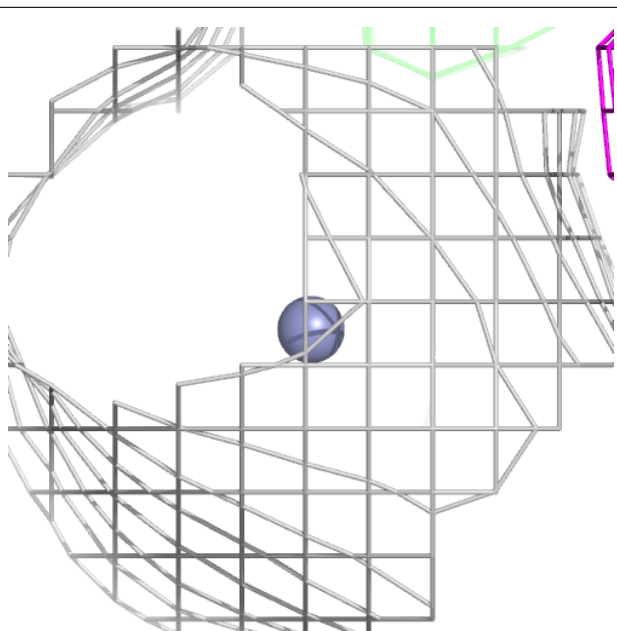
Electron density around ZN A 1001:

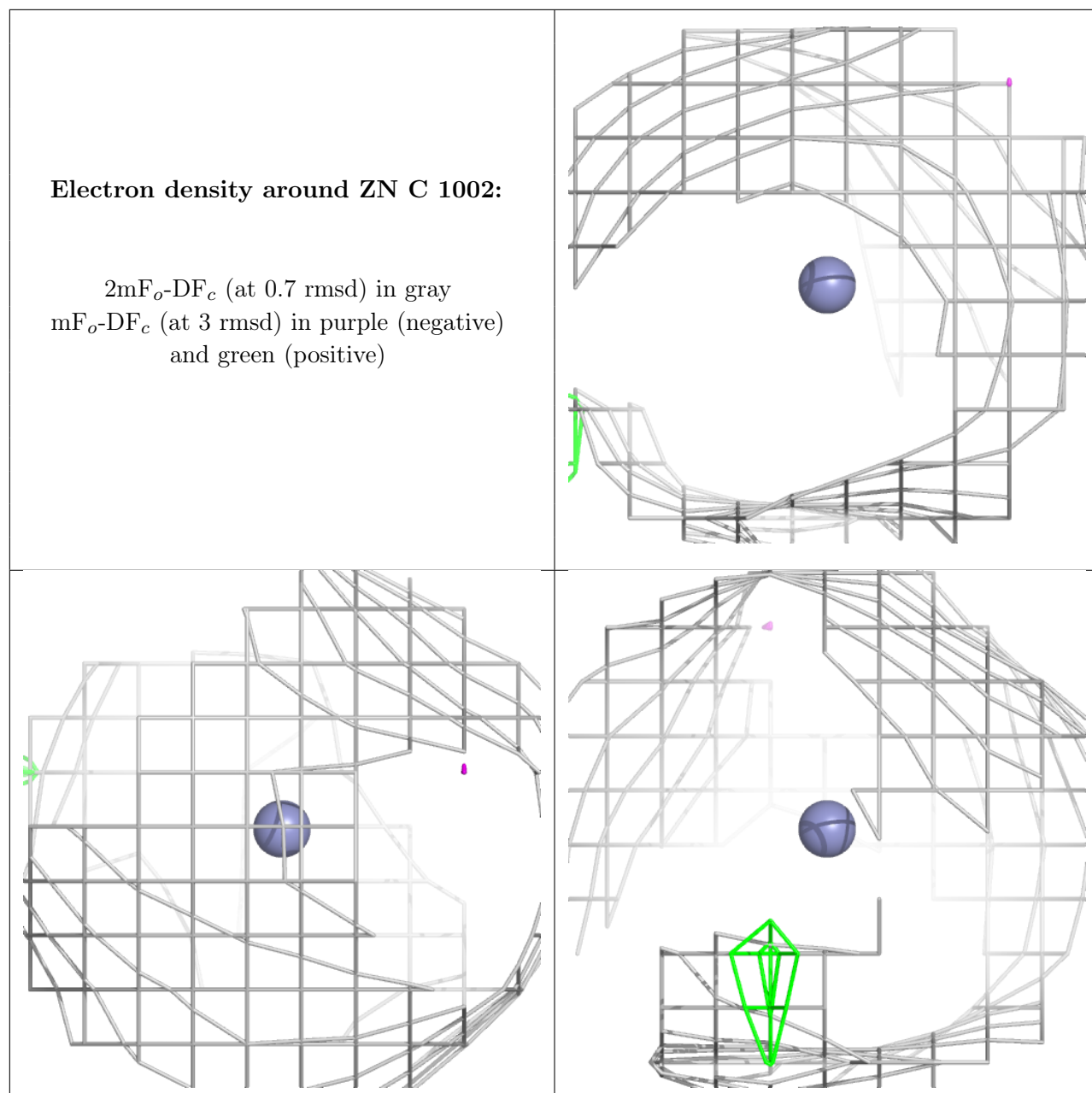
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around ZN H 1002:

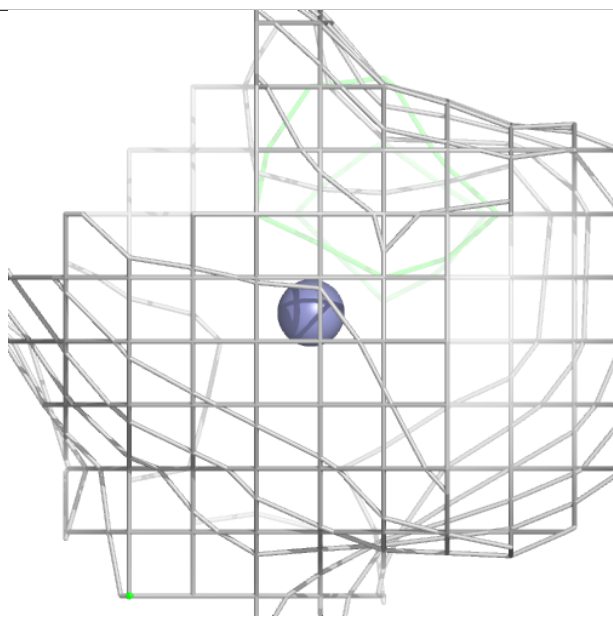
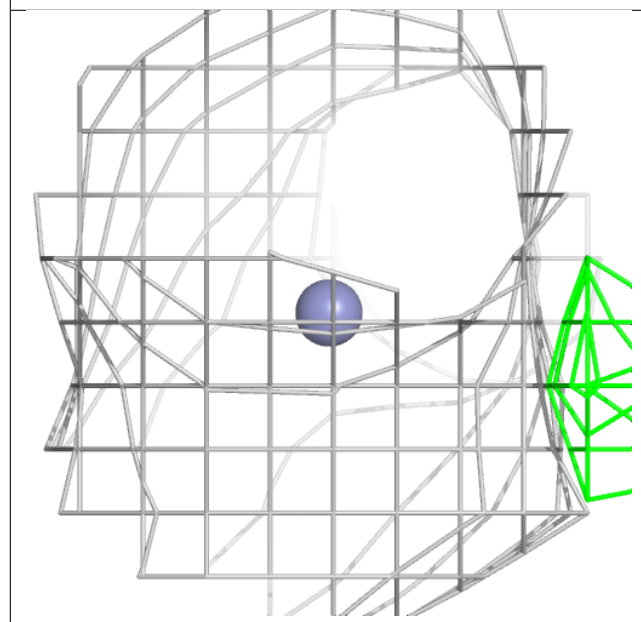
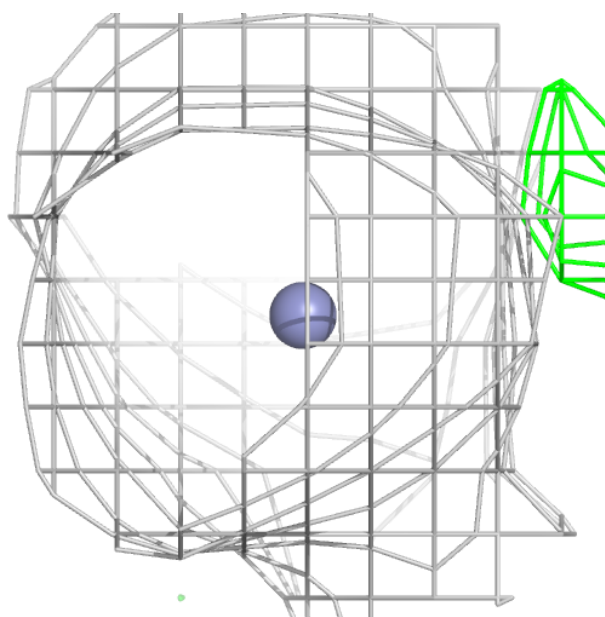
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





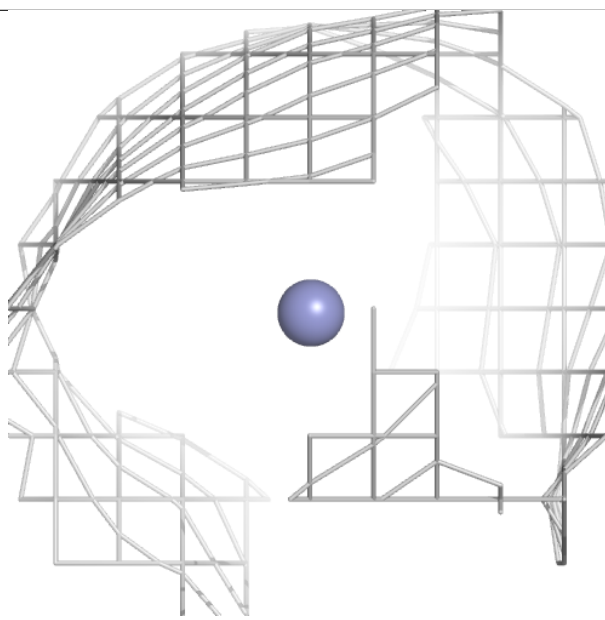
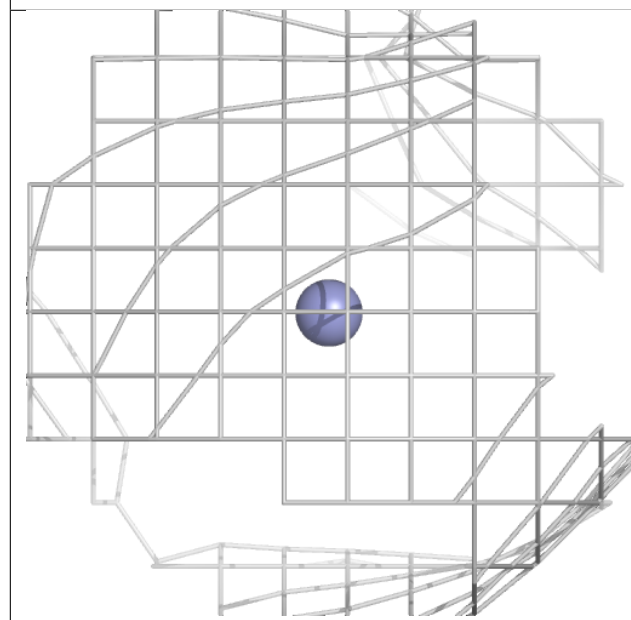
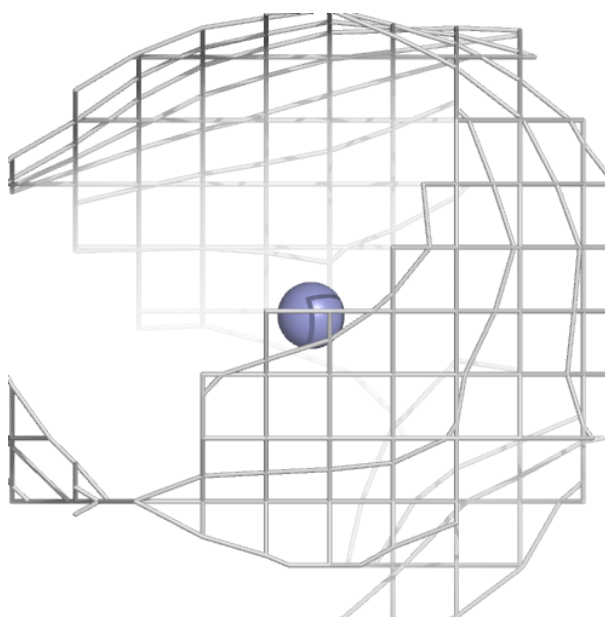
Electron density around ZN E 1001:

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



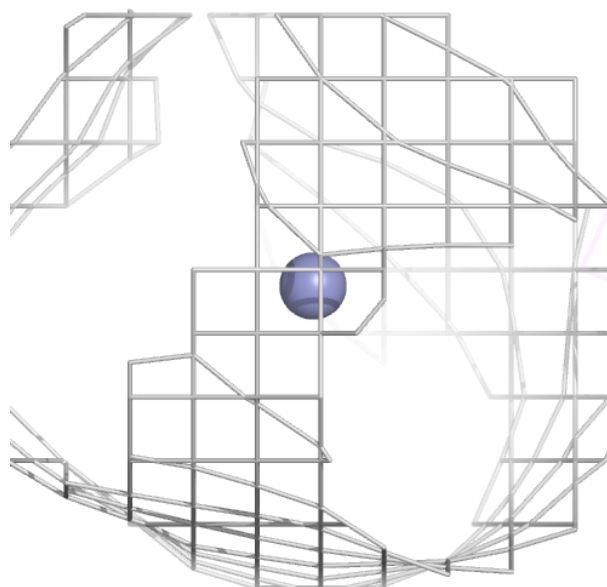
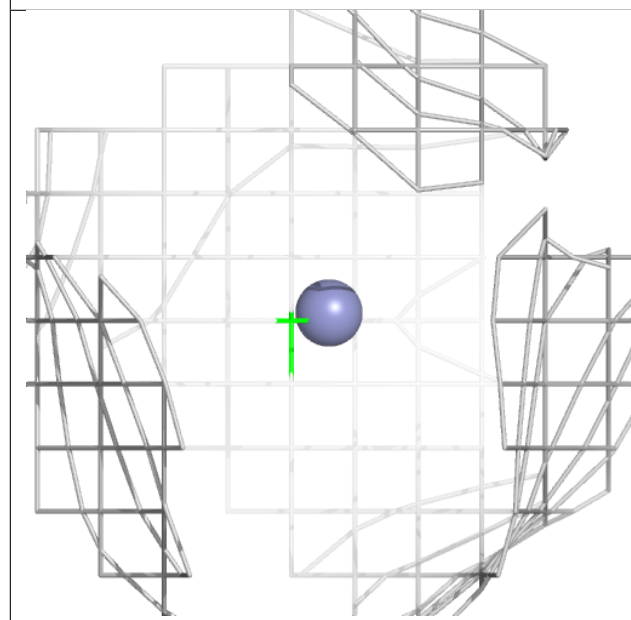
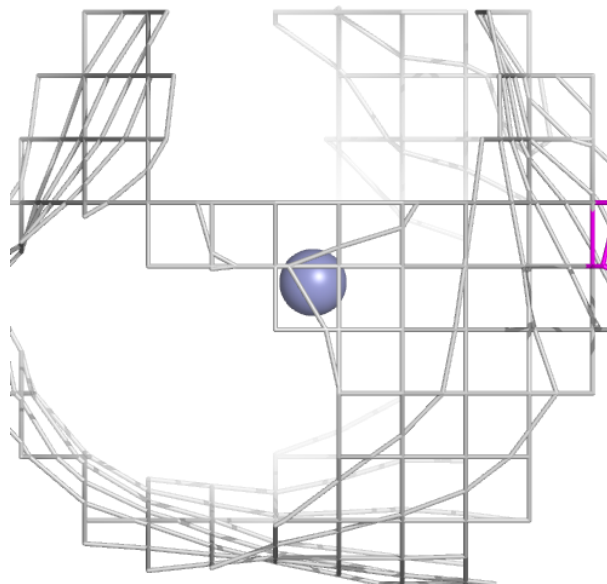
Electron density around ZN F 1002:

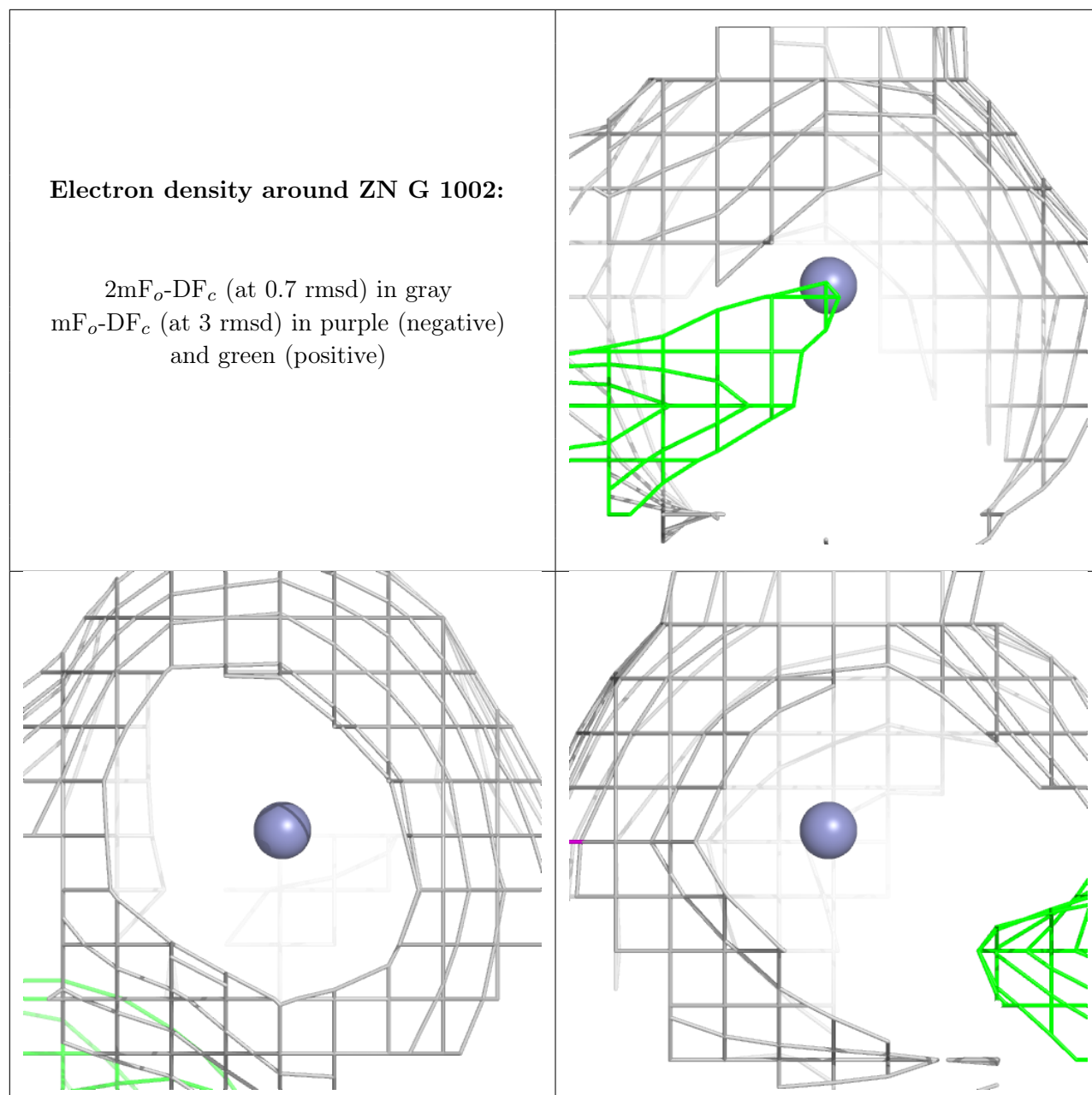
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 1002:

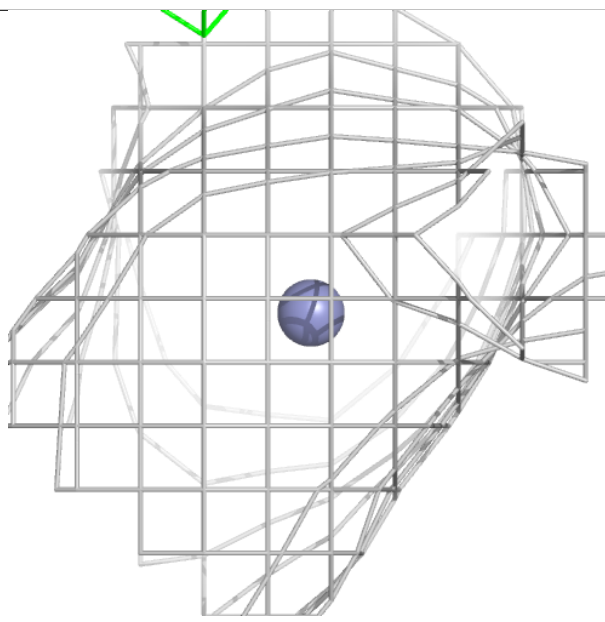
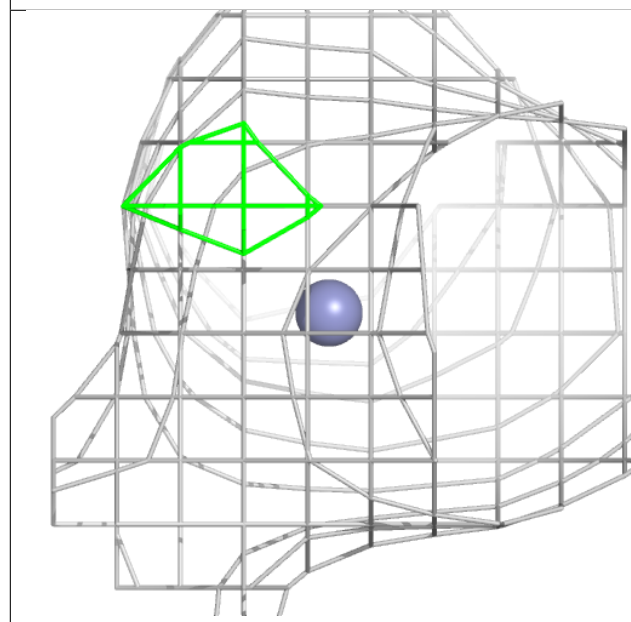
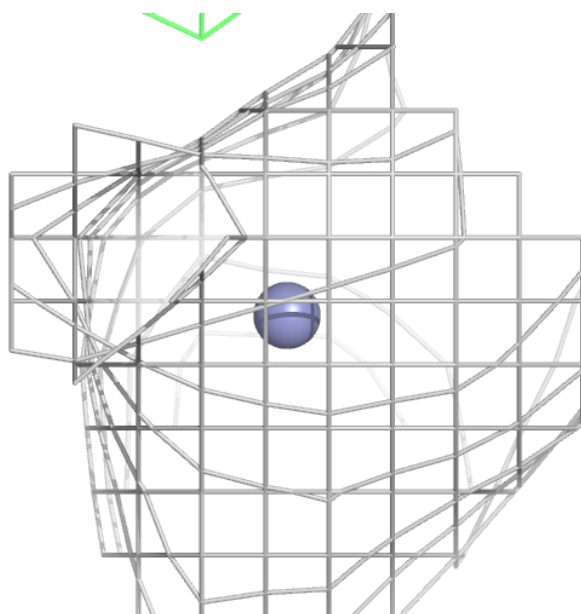
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





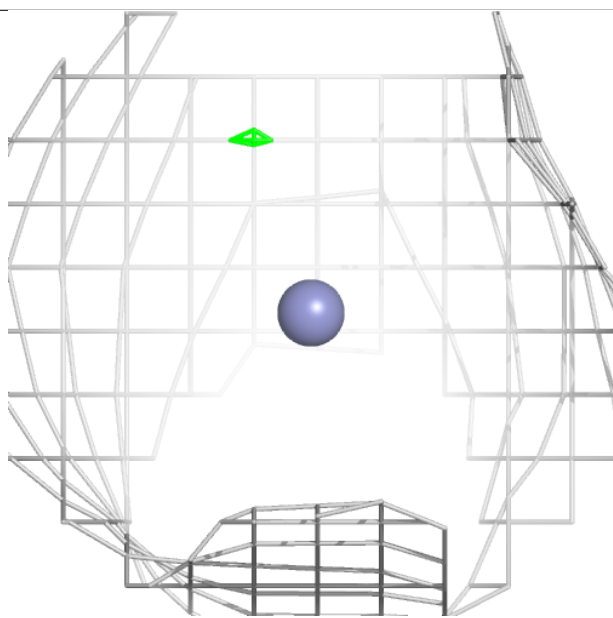
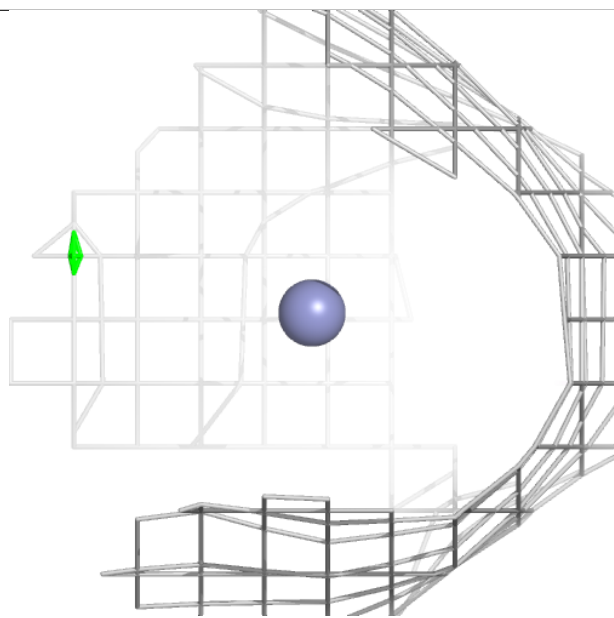
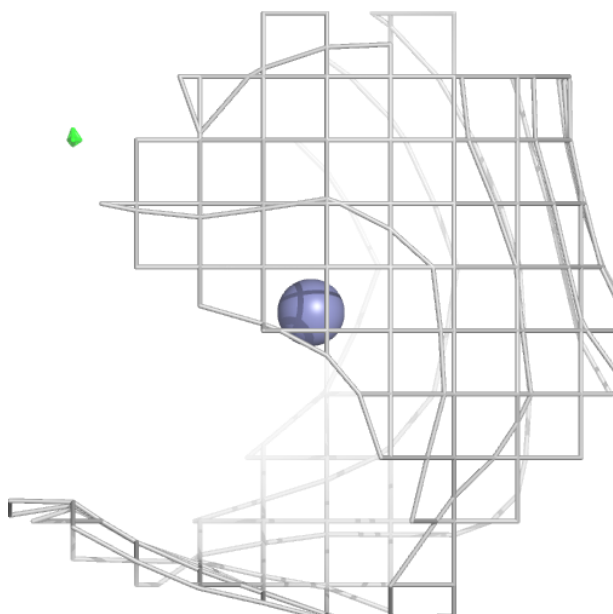
Electron density around ZN D 1001:

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



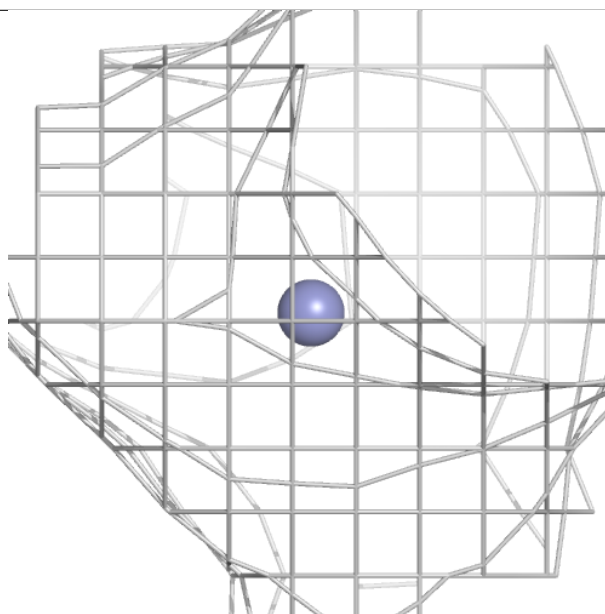
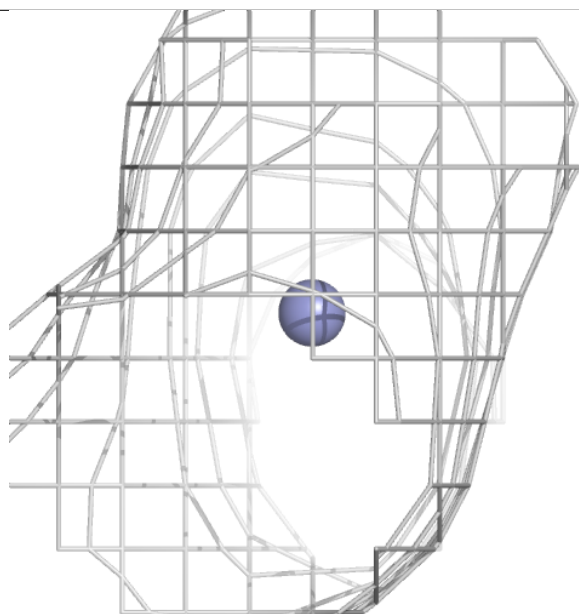
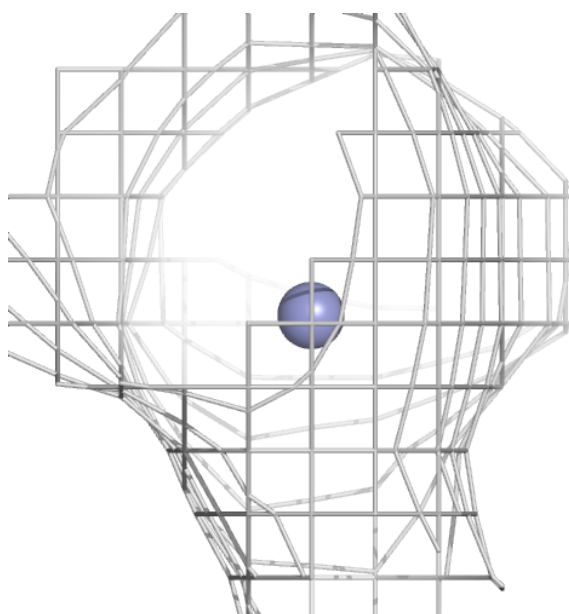
Electron density around ZN J 1002:

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



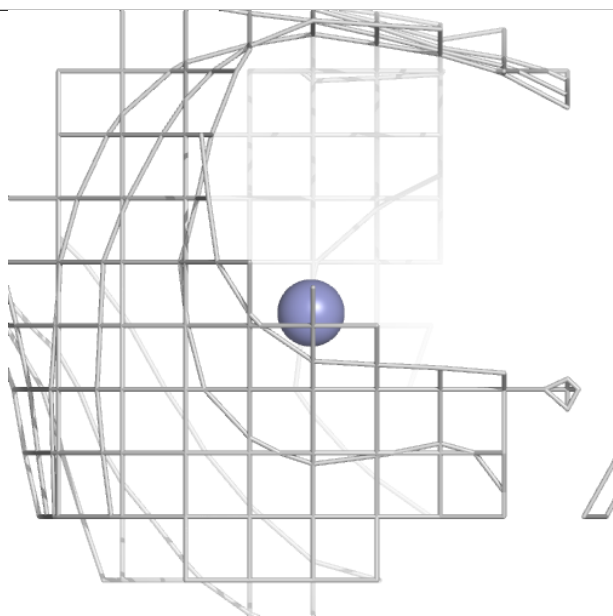
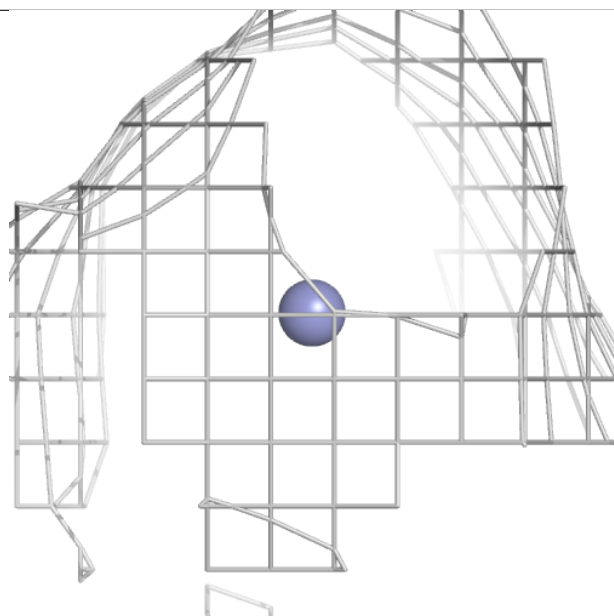
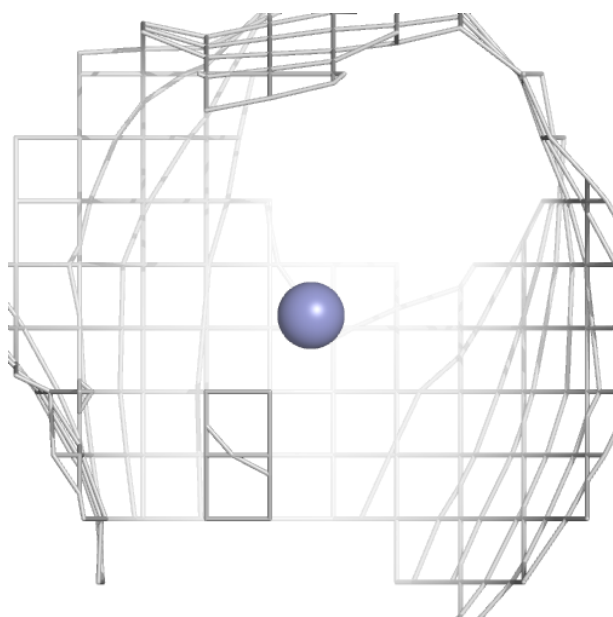
Electron density around ZN I 1001:

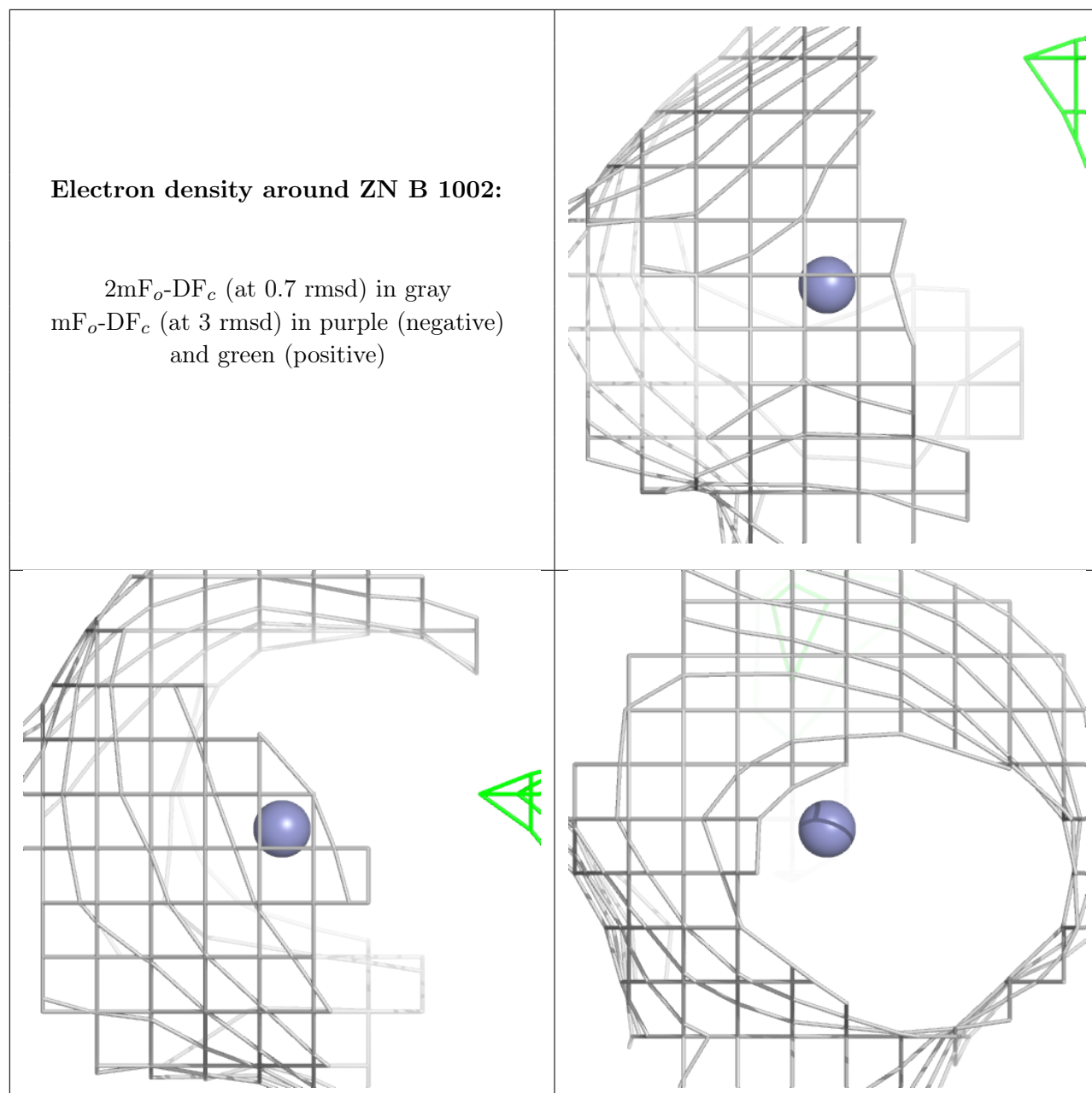
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

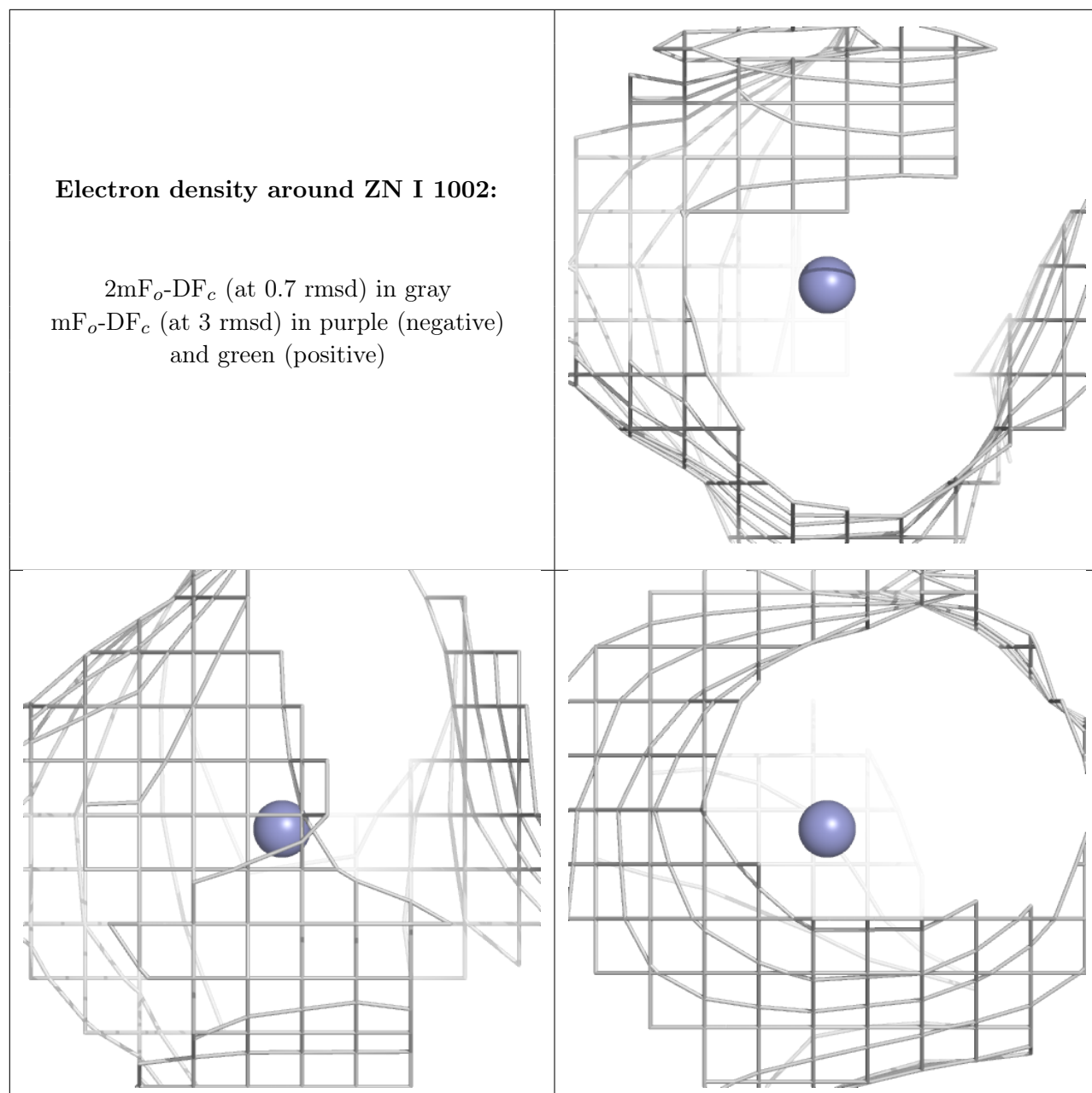


Electron density around ZN D 1002:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.