



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:54 PM JST

PDB ID : 7C07
Title : Crystal structure of yeast U2AF1 complex bound to 5'-AAGGU RNA.
Authors : Yoshida, H.; Park, S.Y.; Urano, T.; Obayashi, E.
Deposited on : 2020-04-30
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtrriage (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

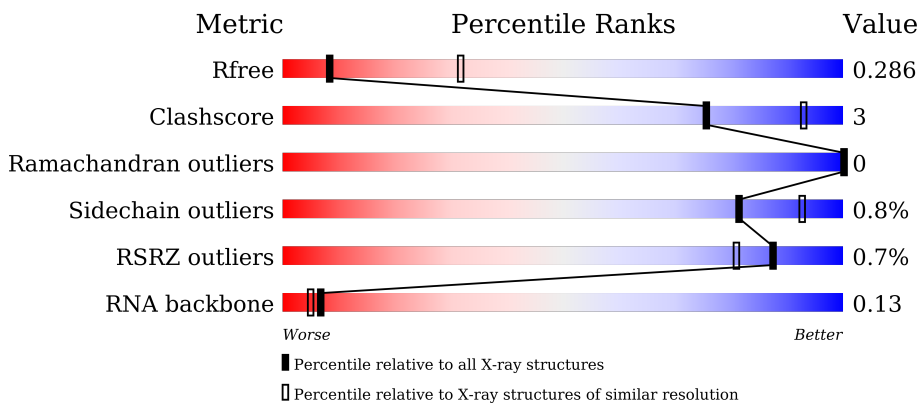
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.20 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.
















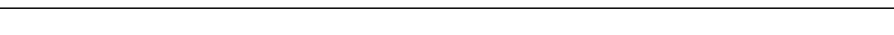

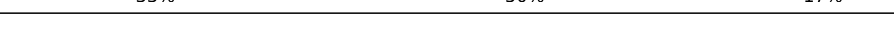
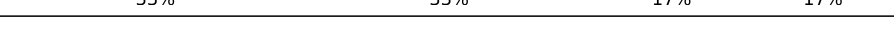
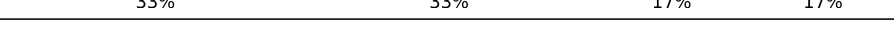





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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	216	 84% 5% 11%
1	D	216	 81% 5% 13%
1	G	216	 81% 8% 11%
1	J	216	 82% 7% 11%

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Mol	Chain	Length	Quality of chain
1	M	216	
1	P	216	
1	S	216	
1	V	216	
1	Y	216	
2	B	69	
2	E	69	
2	H	69	
2	K	69	
2	N	69	
2	Q	69	
2	T	69	
2	W	69	
2	Z	69	
3	1	6	
3	C	6	
3	F	6	
3	I	6	
3	L	6	
3	O	6	
3	R	6	
3	U	6	
3	X	6	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18390 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 Splicing factor U2AF 23 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	Total 1567	C 981	N 278	O 295	S 13	0	0	0
1	D	187	Total 1524	C 955	N 270	O 286	S 13	0	0	0
1	G	193	Total 1567	C 981	N 278	O 295	S 13	0	0	0
1	J	193	Total 1567	C 981	N 278	O 295	S 13	0	0	0
1	M	179	Total 1461	C 916	N 260	O 272	S 13	0	0	0
1	P	189	Total 1534	C 962	N 273	O 286	S 13	0	0	0
1	S	188	Total 1539	C 964	N 274	O 288	S 13	0	1	0
1	V	174	Total 1424	C 895	N 254	O 262	S 13	0	0	0
1	Y	179	Total 1461	C 916	N 260	O 272	S 13	0	0	0

- Molecule 2 is a protein called Splicing factor U2AF 59 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	56	Total 455	C 288	N 82	O 84	S 1	0	0	0
2	E	51	Total 417	C 266	N 74	O 76	S 1	0	0	0
2	H	53	Total 430	C 274	N 76	O 79	S 1	0	0	0
2	K	54	Total 435	C 277	N 77	O 80	S 1	0	0	0
2	N	52	Total 426	C 272	N 75	O 78	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	T	47	Total	C	N	O	S	0	0	0
			383	246	67	69	1			
2	W	53	Total	C	N	O	S	0	0	0
			430	274	76	79	1			
2	Z	44	Total	C	N	O	S	0	0	0
			359	232	63	63	1			

- Molecule 3 is a RNA chain called RNA (5'-R(*U*AP*AP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	F	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	I	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	L	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	O	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	R	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	U	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	X	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			
3	1	5	Total	C	N	O	P	0	0	0
			107	49	22	32	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	J	2	Total	Zn	0	0
			2	2		

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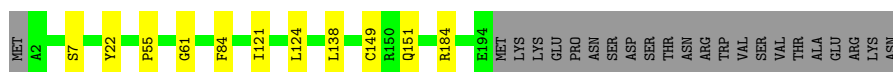
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total 2	Zn 2	0	0
4	P	2	Total 2	Zn 2	0	0
4	S	2	Total 2	Zn 2	0	0
4	V	2	Total 2	Zn 2	0	0
4	Y	2	Total 2	Zn 2	0	0

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: Splicing factor U2AF 23 kDa subunit

Chain A: 




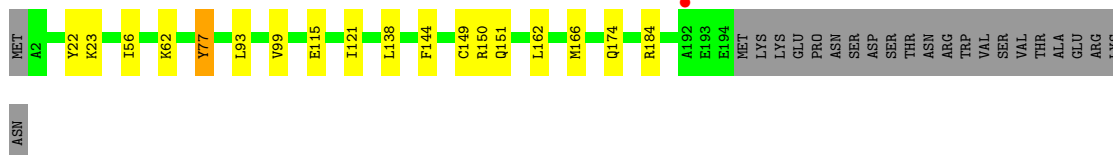
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain D: 




- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain G: 




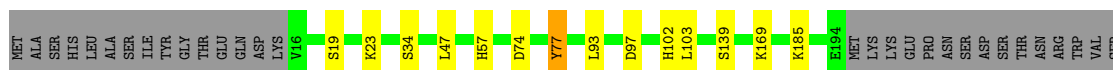
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain J: 




- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain M: 




VAL
THR
ALA
GLU
ARG
LYS
ASN

• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain P:  83% 12%




• Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain S:  79% 8% 13%



VAL
THR
ALA
GLU
ARG
LYS
ASN


• Molecule 1: Splicing factor U2AF 23 kDa subunit

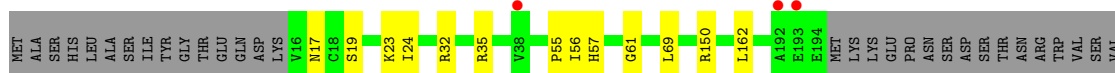
Chain V:  77% 19%



LYS
ASN


• Molecule 1: Splicing factor U2AF 23 kDa subunit

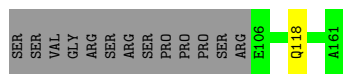
Chain Y:  77% 6% 17%



THR
ALA
GLU
ARG
LYS
ASN

• Molecule 2: Splicing factor U2AF 59 kDa subunit

Chain B:  80% 19%



• Molecule 2: Splicing factor U2AF 59 kDa subunit

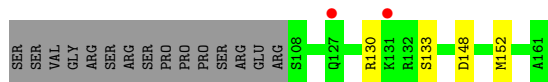
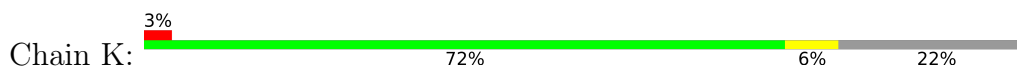
Chain E:  3% 57% 17% 26%



- Molecule 2: Splicing factor U2AF 59 kDa subunit



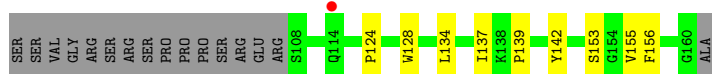
- Molecule 2: Splicing factor U2AF 59 kDa subunit



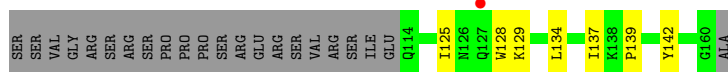
- Molecule 2: Splicing factor U2AF 59 kDa subunit



- Molecule 2: Splicing factor U2AF 59 kDa subunit



- Molecule 2: Splicing factor U2AF 59 kDa subunit



- Molecule 2: Splicing factor U2AF 59 kDa subunit

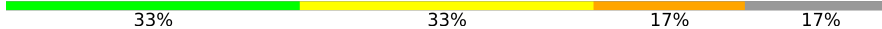


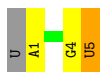
- Molecule 2: Splicing factor U2AF 59 kDa subunit

Chain Z:  55% 9% 36%



• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain C:  33% 33% 17% 17%




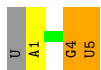
• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain F:  33% 33% 17% 17%




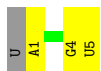
• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain I:  33% 17% 33% 17%



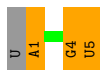
• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain L:  33% 50% 17%



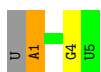
• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain O:  33% 50% 17%




• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain R:  50% 17% 17% 17%

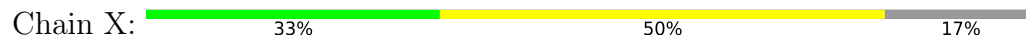


• Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')

Chain U:  33% 17% 33% 17%



- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



- Molecule 3: RNA (5'-R(*U*AP*AP*GP*GP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.49Å 256.95Å 94.59Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.17-3.20) 100.0 (48.17-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.255 , 0.285 0.255 , 0.286	Depositor DCC
R_{free} test set	3656 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtrriage
Anisotropy	0.368	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 10.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.039 for l,-k,h	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18390	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/1604	0.39	0/2163
1	D	0.24	0/1560	0.40	0/2103
1	G	0.24	0/1604	0.39	0/2163
1	J	0.24	0/1604	0.39	0/2163
1	M	0.24	0/1496	0.40	0/2017
1	P	0.24	0/1569	0.38	0/2113
1	S	0.24	0/1576	0.40	0/2125
1	V	0.24	0/1457	0.38	0/1962
1	Y	0.24	0/1496	0.39	0/2017
2	B	0.23	0/465	0.37	0/629
2	E	0.24	0/427	0.39	0/578
2	H	0.24	0/440	0.40	0/596
2	K	0.23	0/445	0.38	0/603
2	N	0.23	0/436	0.43	0/591
2	Q	0.23	0/440	0.39	0/596
2	T	0.23	0/393	0.37	0/533
2	W	0.23	0/440	0.40	0/596
2	Z	0.23	0/368	0.39	0/497
3	1	0.25	0/120	0.87	0/186
3	C	0.21	0/120	0.79	0/186
3	F	0.19	0/120	0.77	0/186
3	I	0.22	0/120	0.84	0/186
3	L	0.23	0/120	0.86	0/186
3	O	0.23	0/120	0.86	0/186
3	R	0.21	0/120	0.83	0/186
3	U	0.18	0/120	0.82	0/186
3	X	0.23	0/120	0.87	0/186
All	All	0.24	0/18900	0.43	0/25719

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

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	1567	0	1487	7	0
1	D	1524	0	1448	8	0
1	G	1567	0	1487	16	0
1	J	1567	0	1488	9	0
1	M	1461	0	1389	10	0
1	P	1534	0	1461	8	0
1	S	1539	0	1459	13	0
1	V	1424	0	1360	5	0
1	Y	1461	0	1389	11	0
2	B	455	0	460	0	0
2	E	417	0	422	7	0
2	H	430	0	436	6	0
2	K	435	0	441	3	0
2	N	426	0	433	7	0
2	Q	430	0	436	5	0
2	T	383	0	387	4	0
2	W	430	0	436	10	0
2	Z	359	0	365	5	0
3	1	107	0	56	4	0
3	C	107	0	56	1	0
3	F	107	0	56	3	0
3	I	107	0	56	3	0
3	L	107	0	56	0	0
3	O	107	0	56	4	0
3	R	107	0	56	1	0
3	U	107	0	56	2	0
3	X	107	0	56	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	2	0	0	0	0
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
All	All	18390	0	17288	112	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 3.

All (112) 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:22:TYR:OH	1:G:184:ARG:NH2	2.22	0.71
1:D:33:CYS:HA	3:F:1:A:H62	1.57	0.70
1:Y:23:LYS:NZ	3:1:4:G:O2'	2.25	0.69
2:W:131:LYS:HD3	2:W:131:LYS:H	1.57	0.69
1:D:23:LYS:NZ	3:F:4:G:O2'	2.31	0.64
1:J:14:ASP:O	1:J:35:ARG:NH2	2.29	0.64
1:G:144:PHE:HD1	1:G:166:MET:HE1	1.62	0.63
1:D:153:GLU:OE1	1:D:153:GLU:N	2.32	0.62
1:Y:23:LYS:HG3	1:Y:24:ILE:HG12	1.83	0.60
1:G:150:ARG:NH1	3:I:5:U:O4	2.34	0.59
2:W:141:GLY:HA2	1:Y:57:HIS:HB3	1.85	0.58
1:Y:55:PRO:O	1:Y:61:GLY:HA3	2.04	0.58
1:P:144:PHE:HD1	1:P:166:MET:HE1	1.69	0.57
2:Q:153:SER:O	1:S:28:ARG:NH2	2.37	0.57
1:D:32:ARG:O	3:F:1:A:N6	2.38	0.56
1:M:34:SER:N	3:O:1:A:H62	2.04	0.56
1:G:62:LYS:HB3	1:P:16:VAL:HG22	1.90	0.53
2:H:139:PRO:HG2	2:H:142:TYR:CD1	2.44	0.53
1:Y:17:ASN:O	1:Y:35:ARG:NH2	2.42	0.53
1:G:149:CYS:SG	1:G:151:GLN:HG2	2.49	0.52
1:J:23:LYS:NZ	1:J:146:GLU:OE1	2.42	0.52
1:P:32:ARG:O	3:R:1:A:N6	2.43	0.52
2:E:153:SER:O	1:P:28:ARG:NH1	2.43	0.51
2:K:152:MET:HG3	1:S:8:ILE:HB	1.92	0.51
1:P:93:LEU:HD13	1:P:109:VAL:HG22	1.92	0.51
1:M:185:LYS:HB2	2:N:119:LEU:HD12	1.93	0.51
1:A:121:ILE:HD13	1:A:138:LEU:HG	1.94	0.50
1:G:23:LYS:NZ	3:I:4:G:O2'	2.44	0.50
1:G:121:ILE:HD13	1:G:138:LEU:HG	1.94	0.50
1:G:115:GLU:OE1	1:G:115:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:184:ARG:HH21	2:W:115:GLU:HG3	1.77	0.49
1:Y:56:ILE:HD11	1:Y:69:LEU:HD13	1.95	0.49
1:Y:19:SER:O	1:Y:23:LYS:HG2	2.13	0.48
1:A:7:SER:HB3	2:H:122:VAL:HG22	1.96	0.48
1:S:47:LEU:HB2	1:S:139:SER:HB2	1.95	0.48
1:Y:150:ARG:HG3	3:1:4:G:N1	2.29	0.48
1:S:29:HIS:O	1:S:32:ARG:HG2	2.14	0.48
2:E:139:PRO:HG2	2:E:142:TYR:CG	2.48	0.47
2:Z:139:PRO:HG2	2:Z:142:TYR:CG	2.49	0.47
2:T:125:ILE:HA	2:T:128:TRP:CD1	2.48	0.47
3:C:5:U:O2'	1:G:174:GLN:HG3	2.14	0.47
1:J:121:ILE:HD13	1:J:138:LEU:HG	1.96	0.47
1:G:77:TYR:CZ	1:G:93:LEU:HD22	2.49	0.47
1:M:57:HIS:ND1	2:Z:143:GLU:OE1	2.47	0.47
2:Z:139:PRO:HG2	2:Z:142:TYR:CD1	2.50	0.47
2:Q:134:LEU:HA	2:Q:137:ILE:HD12	1.97	0.47
2:E:141:GLY:HA2	1:P:57:HIS:HB3	1.96	0.47
1:Y:32:ARG:O	3:1:1:A:N6	2.48	0.46
1:A:149:CYS:SG	1:A:151:GLN:HG2	2.54	0.46
1:D:83:GLU:O	1:D:86:LYS:HG2	2.15	0.46
2:K:148:ASP:OD2	1:S:8:ILE:HG13	2.15	0.46
2:T:139:PRO:HG2	2:T:142:TYR:CG	2.50	0.46
1:S:77:TYR:CE1	1:S:93:LEU:HD23	2.50	0.46
1:A:55:PRO:O	1:A:61:GLY:HA3	2.15	0.45
1:G:62:LYS:O	1:P:16:VAL:HG13	2.15	0.45
1:S:83:GLU:O	1:S:86:LYS:HG2	2.16	0.45
2:E:155:VAL:HG23	2:E:156:PHE:CD2	2.52	0.45
2:Z:129:LYS:HD3	2:Z:129:LYS:HA	1.74	0.45
1:M:102:HIS:CD2	1:M:103:LEU:HG	2.51	0.45
2:Z:134:LEU:HA	2:Z:137:ILE:HD12	1.98	0.45
1:A:184:ARG:NH2	1:G:22:TYR:OH	2.49	0.45
1:S:32:ARG:O	3:U:1:A:N6	2.50	0.45
1:G:150:ARG:HD3	3:I:4:G:N1	2.32	0.45
2:H:155:VAL:HG23	2:H:156:PHE:CD2	2.52	0.45
1:P:62:LYS:HB3	1:P:62:LYS:HE2	1.72	0.45
1:M:19:SER:HB3	3:O:5:U:H1'	1.98	0.45
2:Q:155:VAL:HG23	2:Q:156:PHE:CD2	2.52	0.44
2:Q:139:PRO:HG2	2:Q:142:TYR:CG	2.52	0.44
2:W:134:LEU:HA	2:W:137:ILE:HD12	1.99	0.44
1:D:121:ILE:HD13	1:D:138:LEU:HG	1.99	0.44
1:M:77:TYR:CE1	1:M:93:LEU:HD23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:LEU:HD23	1:J:184:ARG:HH21	1.83	0.44
1:S:121:ILE:HD13	1:S:138:LEU:HG	2.00	0.43
1:J:36:LYS:HD3	1:S:42:PHE:CG	2.53	0.43
2:E:117:GLU:O	2:E:120:ARG:HG3	2.19	0.43
2:H:120:ARG:O	2:H:122:VAL:HG23	2.19	0.43
1:M:97:ASP:HB2	1:M:169:LYS:HB2	2.01	0.43
2:T:134:LEU:HD23	2:T:137:ILE:HD12	2.00	0.42
1:J:154:THR:O	1:J:154:THR:OG1	2.31	0.42
2:K:130:ARG:NH2	2:K:133:SER:OG	2.49	0.42
1:D:77:TYR:CE1	1:D:93:LEU:HD23	2.55	0.42
1:G:99:VAL:HG21	2:N:145:VAL:HG21	2.02	0.42
1:A:84:PHE:HE1	1:A:124:LEU:HD11	1.84	0.42
1:D:155:SER:HA	1:J:59:PRO:HB3	2.01	0.42
2:N:139:PRO:HG2	2:N:142:TYR:CG	2.54	0.42
1:V:90:VAL:HG13	1:V:109:VAL:HG23	2.02	0.42
1:J:83:GLU:O	1:J:86:LYS:HG2	2.20	0.42
2:N:134:LEU:HA	2:N:137:ILE:HD12	2.01	0.42
1:M:34:SER:H	3:O:1:A:H62	1.66	0.42
2:E:111:SER:O	2:E:114:GLN:NE2	2.52	0.42
2:T:134:LEU:HA	2:T:137:ILE:HD12	2.02	0.41
1:G:162:LEU:HD11	2:N:142:TYR:HE2	1.85	0.41
1:S:143:ASP:HB3	1:S:146:GLU:HG2	2.01	0.41
2:W:141:GLY:HA2	1:Y:57:HIS:CB	2.47	0.41
1:G:56:ILE:HD13	2:N:144:LEU:HD11	2.02	0.41
2:Q:124:PRO:O	2:Q:128:TRP:HD1	2.04	0.41
1:V:102:HIS:NE2	2:W:160:GLY:HA3	2.36	0.41
1:V:181:LEU:HD22	2:W:119:LEU:HD21	2.02	0.41
1:S:84:PHE:CD2	1:S:109:VAL:HG21	2.55	0.41
2:E:134:LEU:HA	2:E:137:ILE:HD12	2.02	0.41
2:W:142:TYR:HE2	1:Y:162:LEU:HD21	1.86	0.41
1:J:77:TYR:CE1	1:J:93:LEU:HD23	2.55	0.41
1:S:11:THR:HG22	3:U:5:U:H5'	2.02	0.41
2:H:134:LEU:HA	2:H:137:ILE:HD12	2.02	0.41
2:W:130:ARG:H	2:W:130:ARG:HG2	1.62	0.41
2:H:139:PRO:HG2	2:H:142:TYR:CG	2.57	0.40
2:N:124:PRO:HB2	2:N:126:ASN:OD1	2.21	0.40
1:V:46:ILE:HD11	1:V:136:ALA:HB1	2.03	0.40
2:W:124:PRO:HB2	2:W:126:ASN:OD1	2.21	0.40
3:1:4:G:H3'	3:1:5:U:H5'	2.02	0.40
1:M:23:LYS:NZ	3:O:4:G:O2'	2.53	0.40
1:M:47:LEU:HB2	1:M:139:SER:HB2	2.04	0.40

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	191/216 (88%)	185 (97%)	6 (3%)	0	100	100
1	D	185/216 (86%)	181 (98%)	4 (2%)	0	100	100
1	G	191/216 (88%)	186 (97%)	5 (3%)	0	100	100
1	J	191/216 (88%)	183 (96%)	8 (4%)	0	100	100
1	M	177/216 (82%)	171 (97%)	6 (3%)	0	100	100
1	P	185/216 (86%)	179 (97%)	6 (3%)	0	100	100
1	S	187/216 (87%)	182 (97%)	5 (3%)	0	100	100
1	V	170/216 (79%)	167 (98%)	3 (2%)	0	100	100
1	Y	177/216 (82%)	171 (97%)	6 (3%)	0	100	100
2	B	54/69 (78%)	52 (96%)	2 (4%)	0	100	100
2	E	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
2	H	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	K	52/69 (75%)	48 (92%)	4 (8%)	0	100	100
2	N	50/69 (72%)	47 (94%)	3 (6%)	0	100	100
2	Q	51/69 (74%)	49 (96%)	2 (4%)	0	100	100
2	T	45/69 (65%)	41 (91%)	4 (9%)	0	100	100
2	W	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	Z	40/69 (58%)	36 (90%)	4 (10%)	0	100	100
All	All	2097/2565 (82%)	2021 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	170/192 (88%)	170 (100%)	0	100	100
1	D	166/192 (86%)	165 (99%)	1 (1%)	86	94
1	G	170/192 (88%)	169 (99%)	1 (1%)	86	94
1	J	170/192 (88%)	168 (99%)	2 (1%)	71	88
1	M	159/192 (83%)	157 (99%)	2 (1%)	69	87
1	P	166/192 (86%)	166 (100%)	0	100	100
1	S	167/192 (87%)	166 (99%)	1 (1%)	86	94
1	V	155/192 (81%)	155 (100%)	0	100	100
1	Y	159/192 (83%)	159 (100%)	0	100	100
2	B	50/62 (81%)	49 (98%)	1 (2%)	55	80
2	E	46/62 (74%)	46 (100%)	0	100	100
2	H	48/62 (77%)	47 (98%)	1 (2%)	53	79
2	K	48/62 (77%)	48 (100%)	0	100	100
2	N	48/62 (77%)	46 (96%)	2 (4%)	30	65
2	Q	48/62 (77%)	48 (100%)	0	100	100
2	T	42/62 (68%)	41 (98%)	1 (2%)	49	77
2	W	48/62 (77%)	45 (94%)	3 (6%)	18	52
2	Z	39/62 (63%)	39 (100%)	0	100	100
All	All	1899/2286 (83%)	1884 (99%)	15 (1%)	81	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	118	GLN
1	D	77	TYR
1	G	77	TYR
2	H	120	ARG
1	J	51	MET
1	J	77	TYR

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Mol	Chain	Res	Type
1	M	74	ASP
1	M	77	TYR
2	N	119	LEU
2	N	130	ARG
1	S	77	TYR
2	T	129	LYS
2	W	120	ARG
2	W	130	ARG
2	W	131	LYS

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	1	5/6 (83%)	2 (40%)	1 (20%)
3	C	5/6 (83%)	2 (40%)	1 (20%)
3	F	4/6 (66%)	2 (50%)	0
3	I	5/6 (83%)	2 (40%)	1 (20%)
3	L	5/6 (83%)	2 (40%)	1 (20%)
3	O	5/6 (83%)	2 (40%)	1 (20%)
3	R	5/6 (83%)	1 (20%)	1 (20%)
3	U	5/6 (83%)	2 (40%)	1 (20%)
3	X	5/6 (83%)	2 (40%)	1 (20%)
All	All	44/54 (81%)	17 (38%)	8 (18%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	4	G
3	C	5	U
3	F	2	A
3	F	4	G
3	I	4	G
3	I	5	U
3	L	4	G
3	L	5	U
3	O	4	G
3	O	5	U
3	R	4	G

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Mol	Chain	Res	Type
3	U	4	G
3	U	5	U
3	X	4	G
3	X	5	U
3	1	4	G
3	1	5	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	1	A
3	I	1	A
3	L	1	A
3	O	1	A
3	R	1	A
3	U	1	A
3	X	1	A
3	1	1	A

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 18 ligands modelled in this entry, 18 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	193/216 (89%)	-0.06	0 100 100	45, 68, 108, 136	0
1	D	187/216 (86%)	-0.08	0 100 100	42, 62, 102, 125	0
1	G	193/216 (89%)	-0.06	1 (0%) 91 86	33, 56, 99, 131	0
1	J	193/216 (89%)	0.07	1 (0%) 91 86	43, 72, 106, 130	0
1	M	179/216 (82%)	-0.03	0 100 100	49, 81, 121, 138	0
1	P	189/216 (87%)	0.03	1 (0%) 91 86	42, 67, 92, 122	0
1	S	188/216 (87%)	0.15	2 (1%) 80 69	54, 84, 125, 141	0
1	V	174/216 (80%)	0.00	0 100 100	70, 94, 119, 129	0
1	Y	179/216 (82%)	0.15	3 (1%) 70 57	43, 91, 128, 142	0
2	B	56/69 (81%)	-0.10	0 100 100	48, 72, 111, 119	0
2	E	51/69 (73%)	0.03	2 (3%) 39 25	48, 65, 144, 148	0
2	H	53/69 (76%)	0.01	0 100 100	26, 60, 115, 120	0
2	K	54/69 (78%)	0.07	2 (3%) 41 26	40, 69, 112, 136	0
2	N	52/69 (75%)	0.14	0 100 100	52, 78, 139, 148	0
2	Q	53/69 (76%)	0.12	1 (1%) 66 53	45, 69, 128, 145	0
2	T	47/69 (68%)	0.29	1 (2%) 63 49	66, 89, 150, 156	0
2	W	53/69 (76%)	0.19	1 (1%) 66 53	69, 94, 144, 148	0
2	Z	44/69 (63%)	0.03	0 100 100	48, 71, 124, 137	0
3	I	5/6 (83%)	0.02	0 100 100	105, 115, 126, 146	0
3	C	5/6 (83%)	-0.09	0 100 100	65, 80, 90, 93	0
3	F	5/6 (83%)	0.19	0 100 100	66, 68, 83, 118	0
3	I	5/6 (83%)	-0.13	0 100 100	55, 60, 82, 95	0
3	L	5/6 (83%)	-0.20	0 100 100	66, 87, 92, 101	0
3	O	5/6 (83%)	0.11	0 100 100	100, 108, 130, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	R	5/6 (83%)	0.15	0 100 100	58, 60, 83, 90	0
3	U	5/6 (83%)	0.18	0 100 100	71, 72, 83, 145	0
3	X	5/6 (83%)	-0.47	0 100 100	105, 107, 112, 118	0
All	All	2183/2619 (83%)	0.03	15 (0%) 87 81	26, 76, 125, 156	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	8	ILE	3.5
1	Y	192	ALA	3.2
2	Q	114	GLN	3.2
2	W	108	SER	3.1
1	Y	193	GLU	2.9
2	E	110	ARG	2.8
1	S	92	GLN	2.6
2	E	111	SER	2.5
2	T	127	GLN	2.4
1	G	192	ALA	2.4
1	S	187	LEU	2.4
1	Y	38	VAL	2.4
2	K	127	GLN	2.2
1	P	115	GLU	2.0
2	K	131	LYS	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](#)

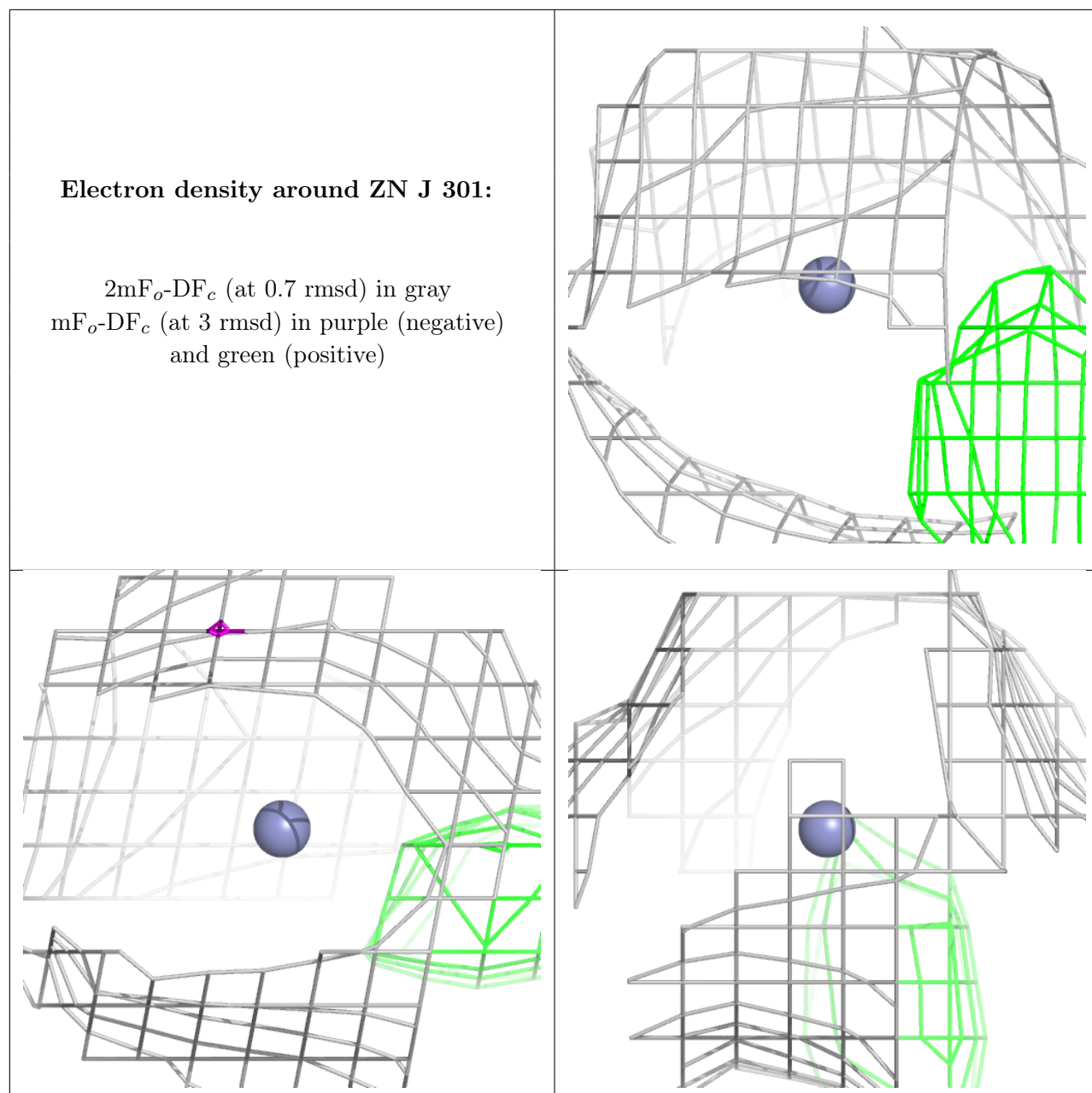
There are no monosaccharides in this entry.

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, 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.

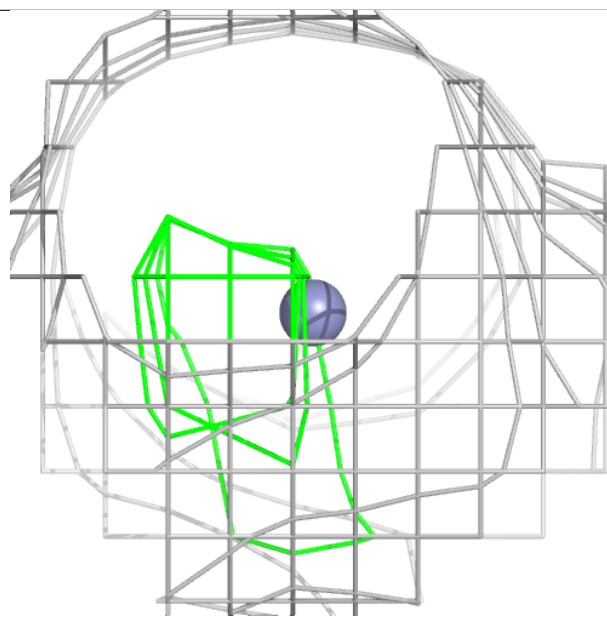
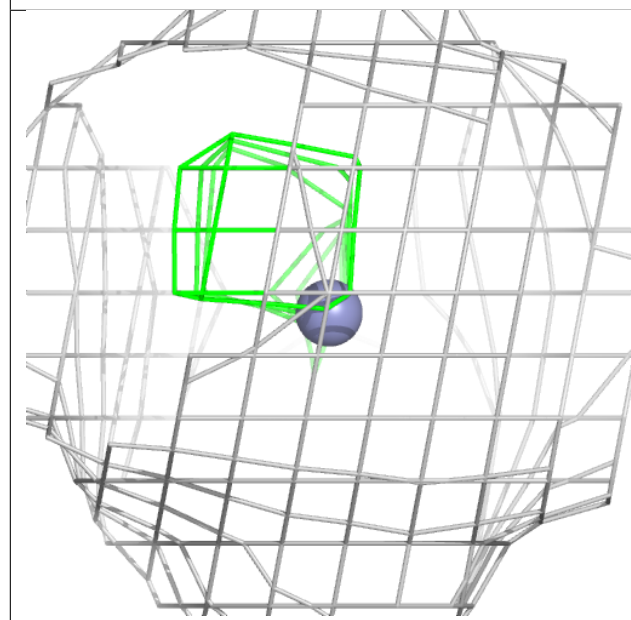
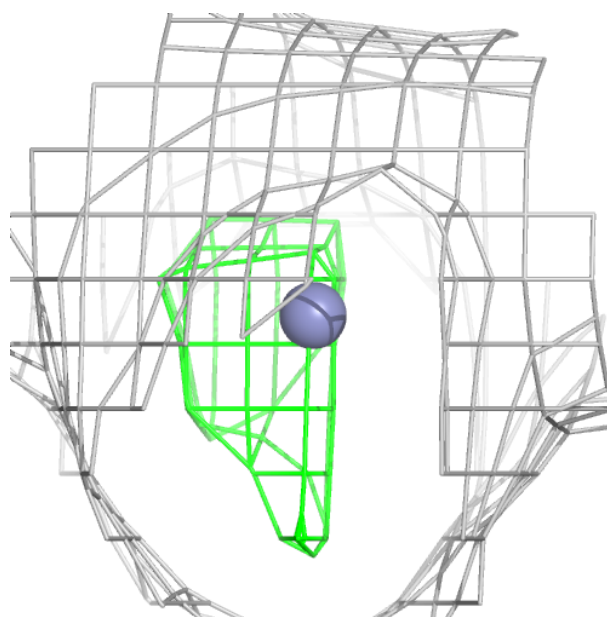
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	J	301	1/1	0.96	0.20	67,67,67,67	0
4	ZN	G	301	1/1	0.98	0.24	48,48,48,48	0
4	ZN	A	302	1/1	0.98	0.22	55,55,55,55	0
4	ZN	J	302	1/1	0.98	0.21	54,54,54,54	0
4	ZN	S	301	1/1	0.98	0.23	59,59,59,59	0
4	ZN	S	302	1/1	0.98	0.21	73,73,73,73	0
4	ZN	A	301	1/1	0.99	0.18	60,60,60,60	0
4	ZN	M	301	1/1	0.99	0.20	70,70,70,70	0
4	ZN	M	302	1/1	0.99	0.18	65,65,65,65	0
4	ZN	P	301	1/1	0.99	0.23	44,44,44,44	0
4	ZN	P	302	1/1	0.99	0.23	45,45,45,45	0
4	ZN	G	302	1/1	0.99	0.22	54,54,54,54	0
4	ZN	D	302	1/1	0.99	0.20	49,49,49,49	0
4	ZN	V	301	1/1	0.99	0.23	72,72,72,72	0
4	ZN	V	302	1/1	0.99	0.17	71,71,71,71	0
4	ZN	Y	301	1/1	0.99	0.19	80,80,80,80	0
4	ZN	Y	302	1/1	0.99	0.17	70,70,70,70	0
4	ZN	D	301	1/1	1.00	0.23	45,45,45,45	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.



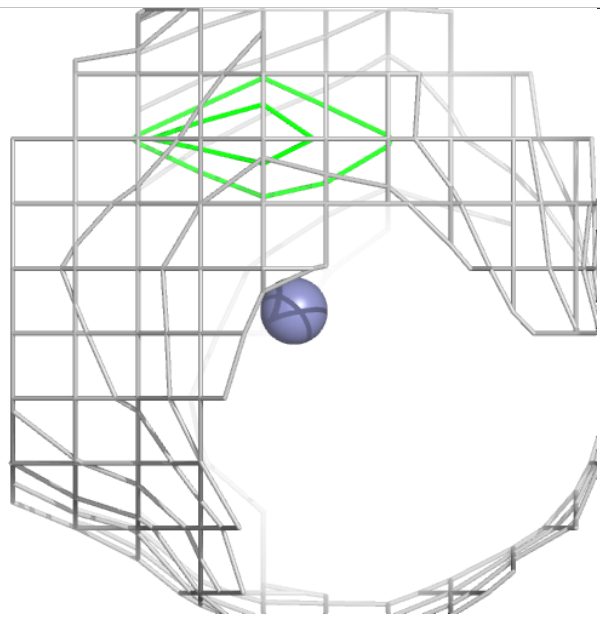
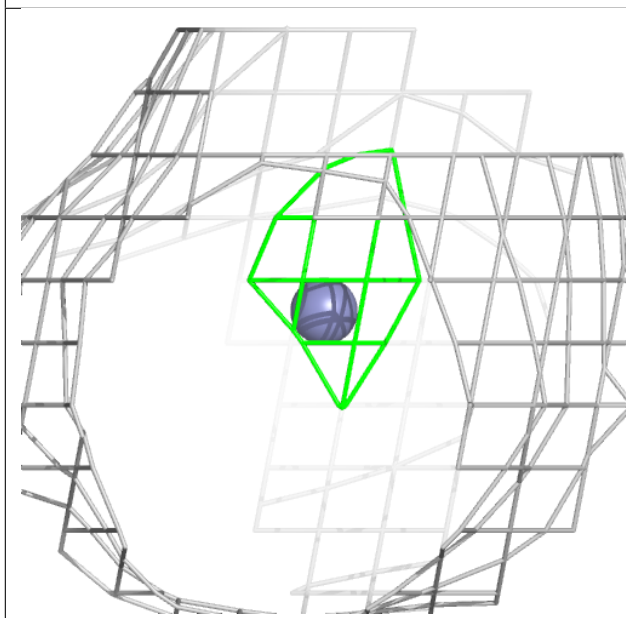
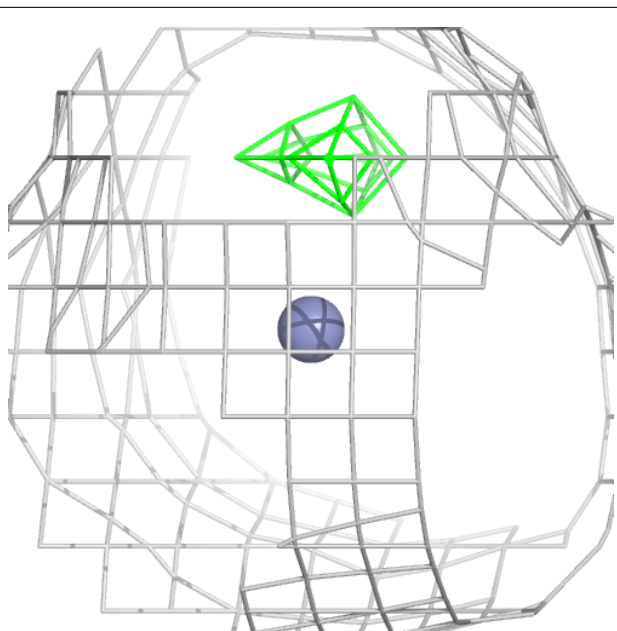
Electron density around ZN G 301:

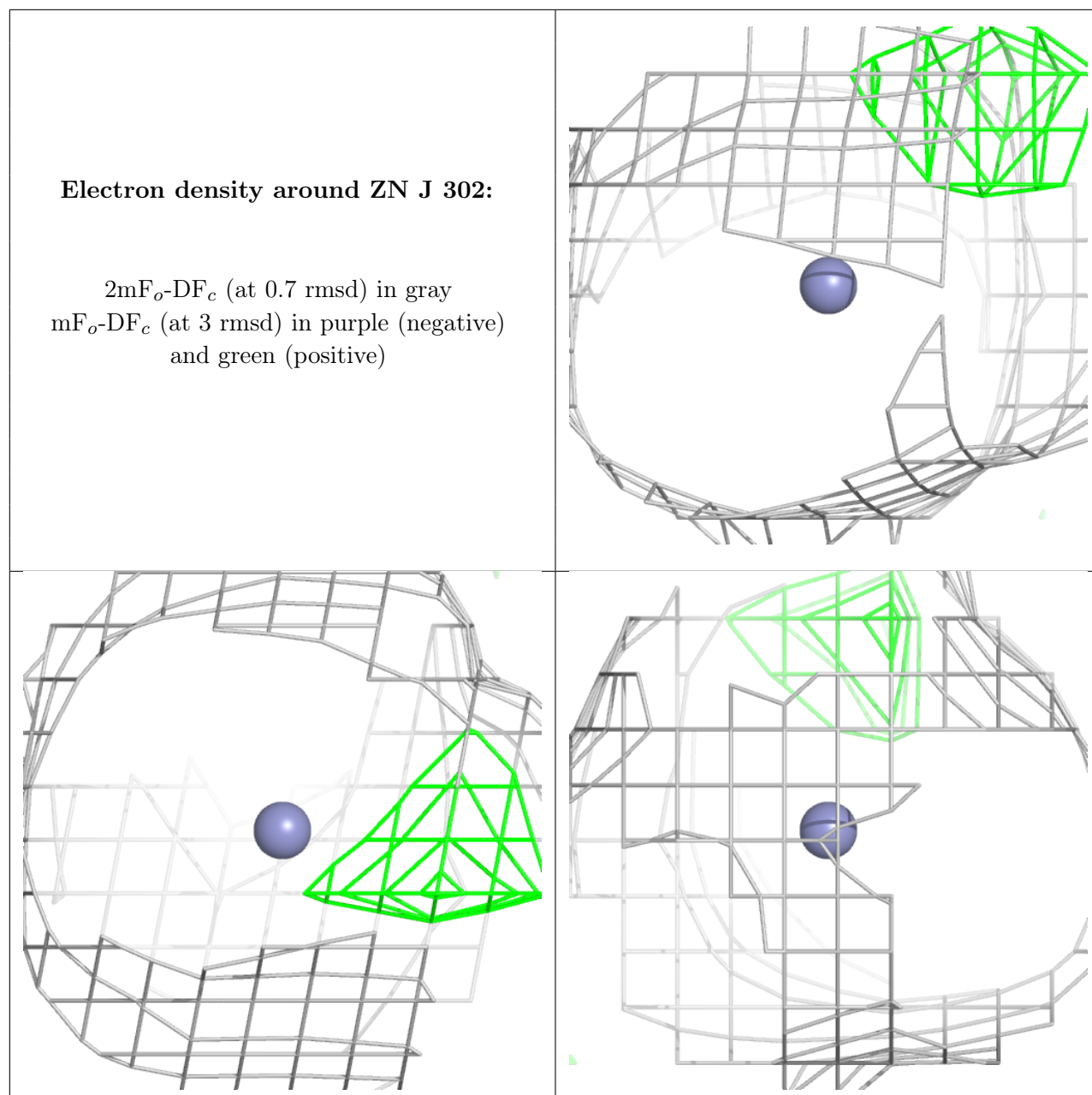
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

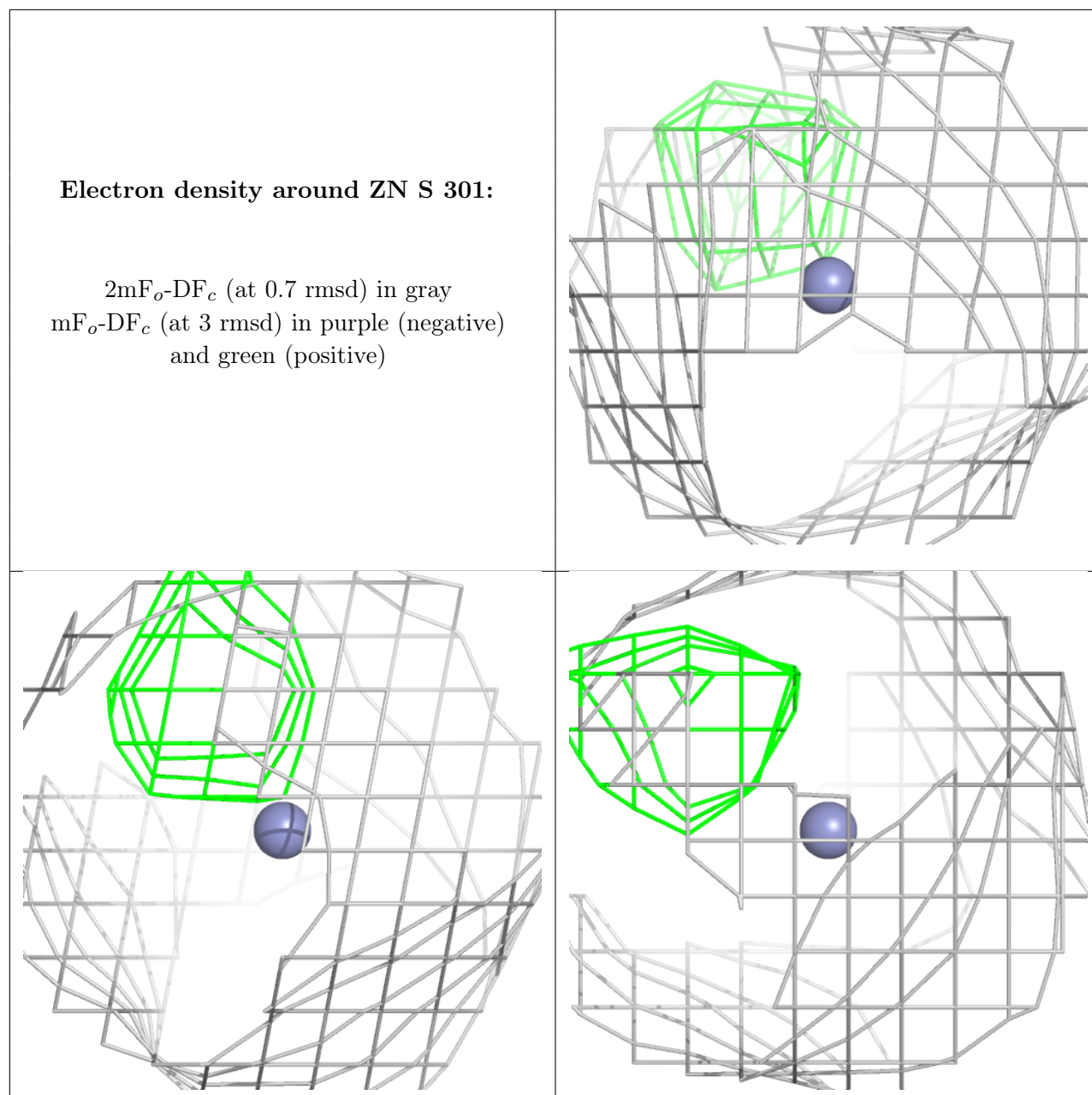


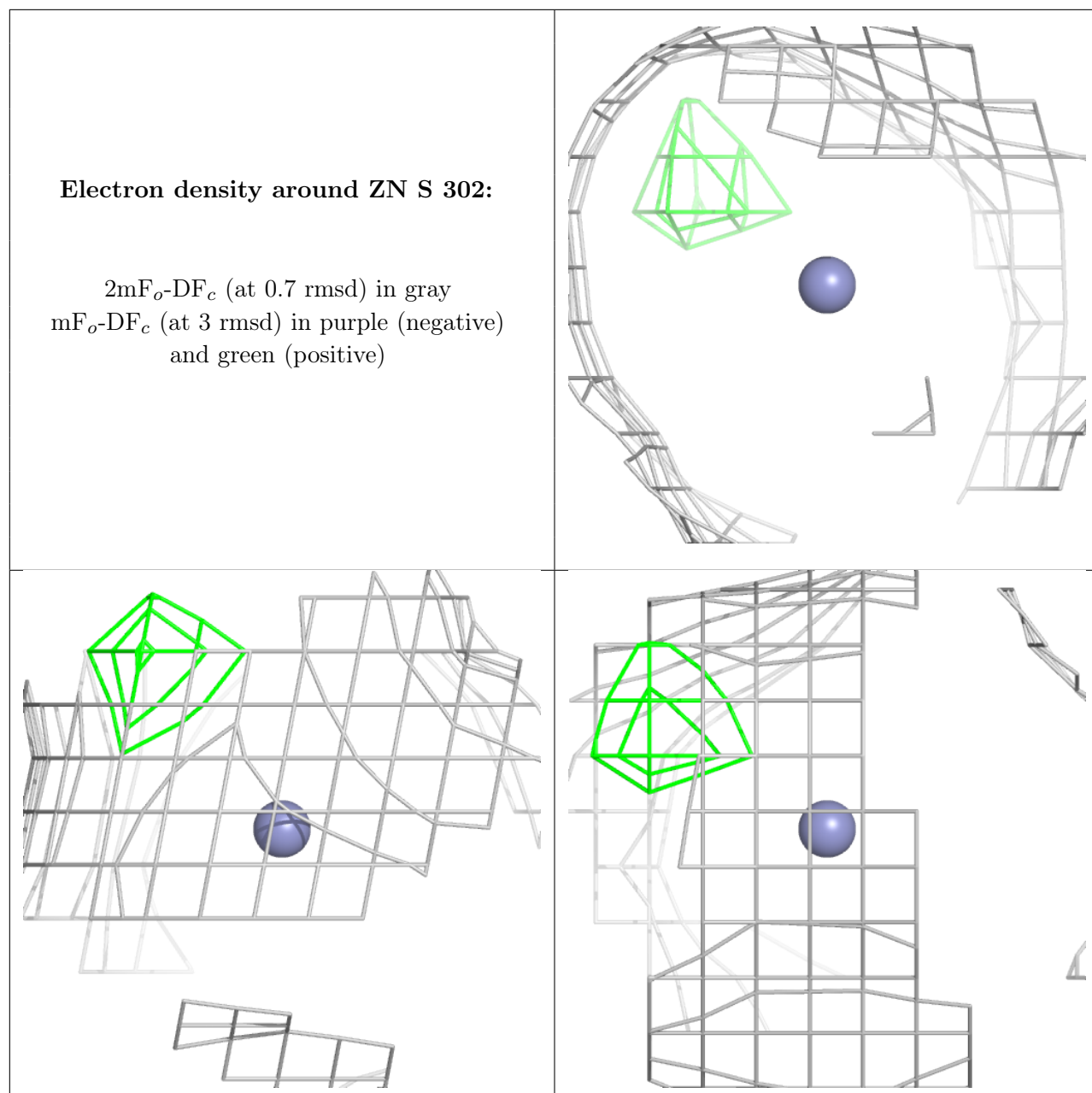
Electron density around ZN A 302:

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



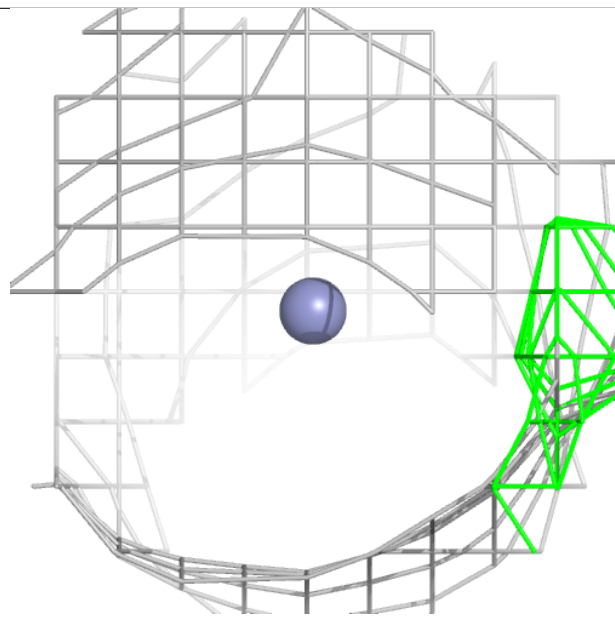
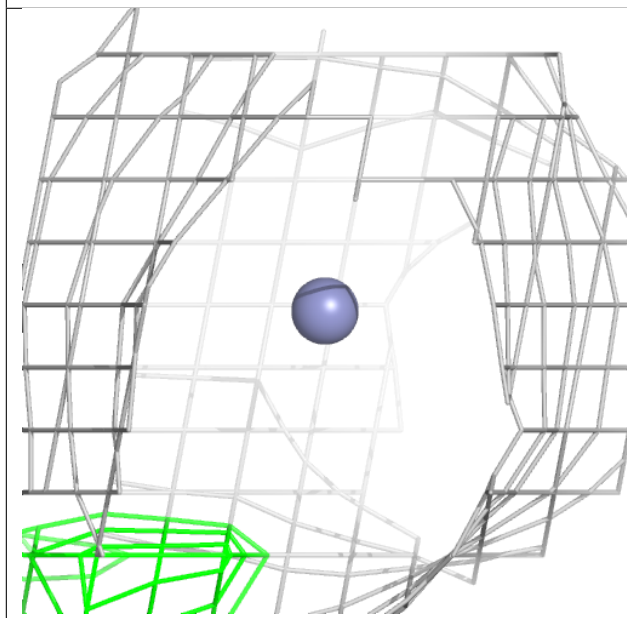
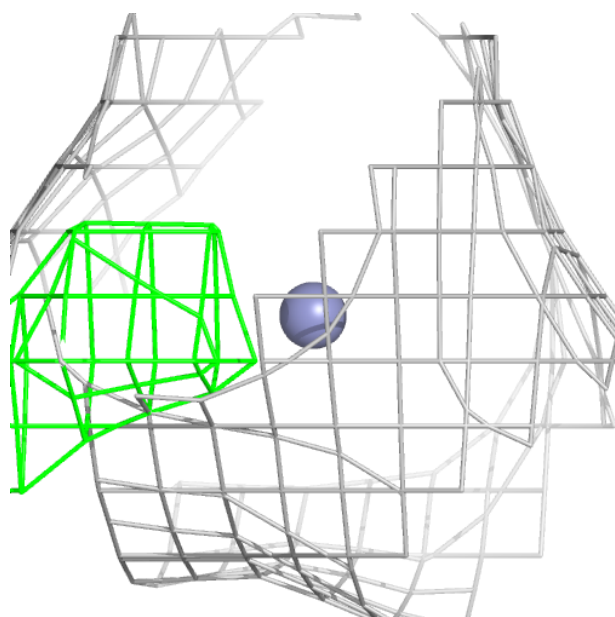


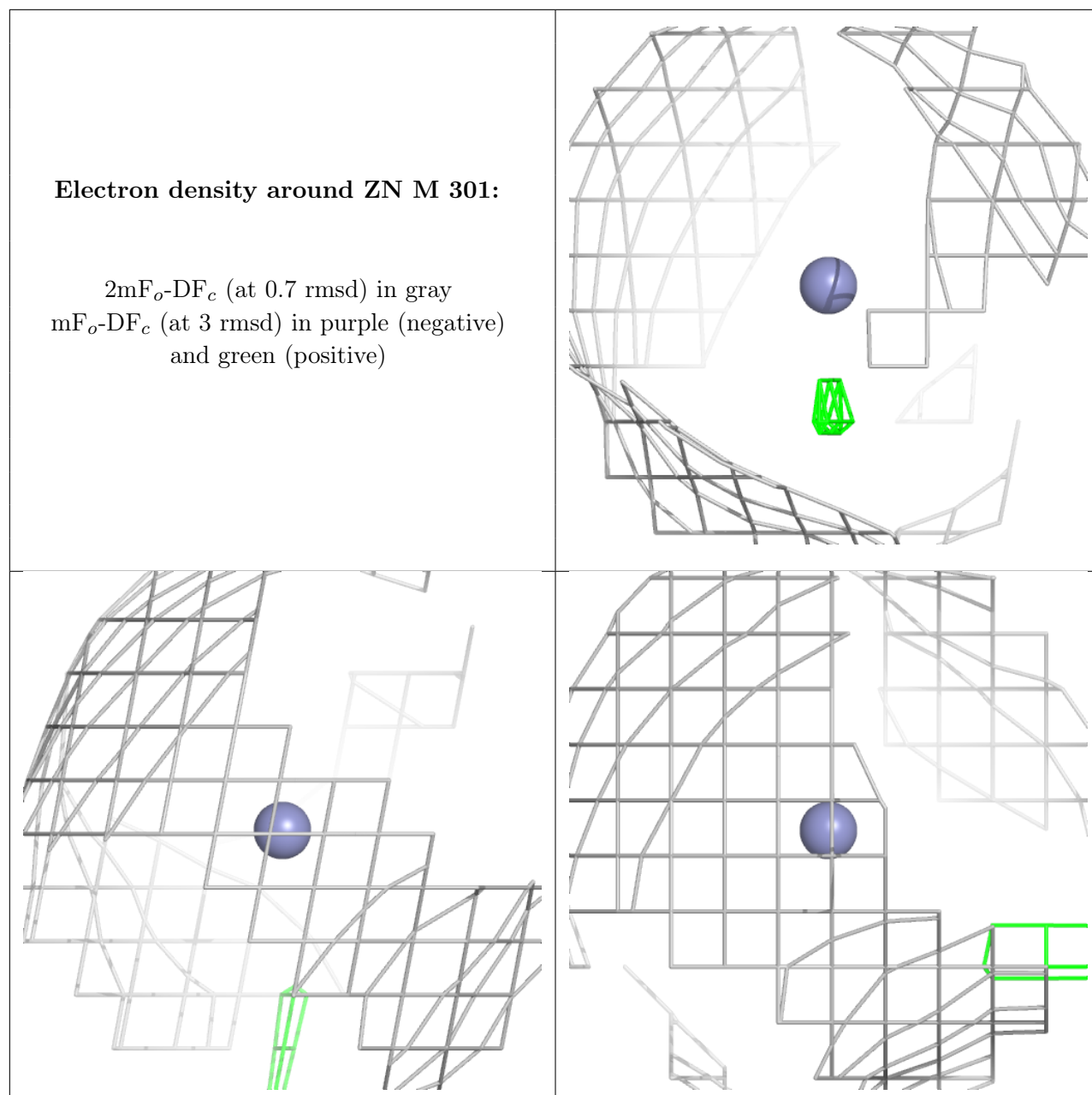




Electron density around ZN A 301:

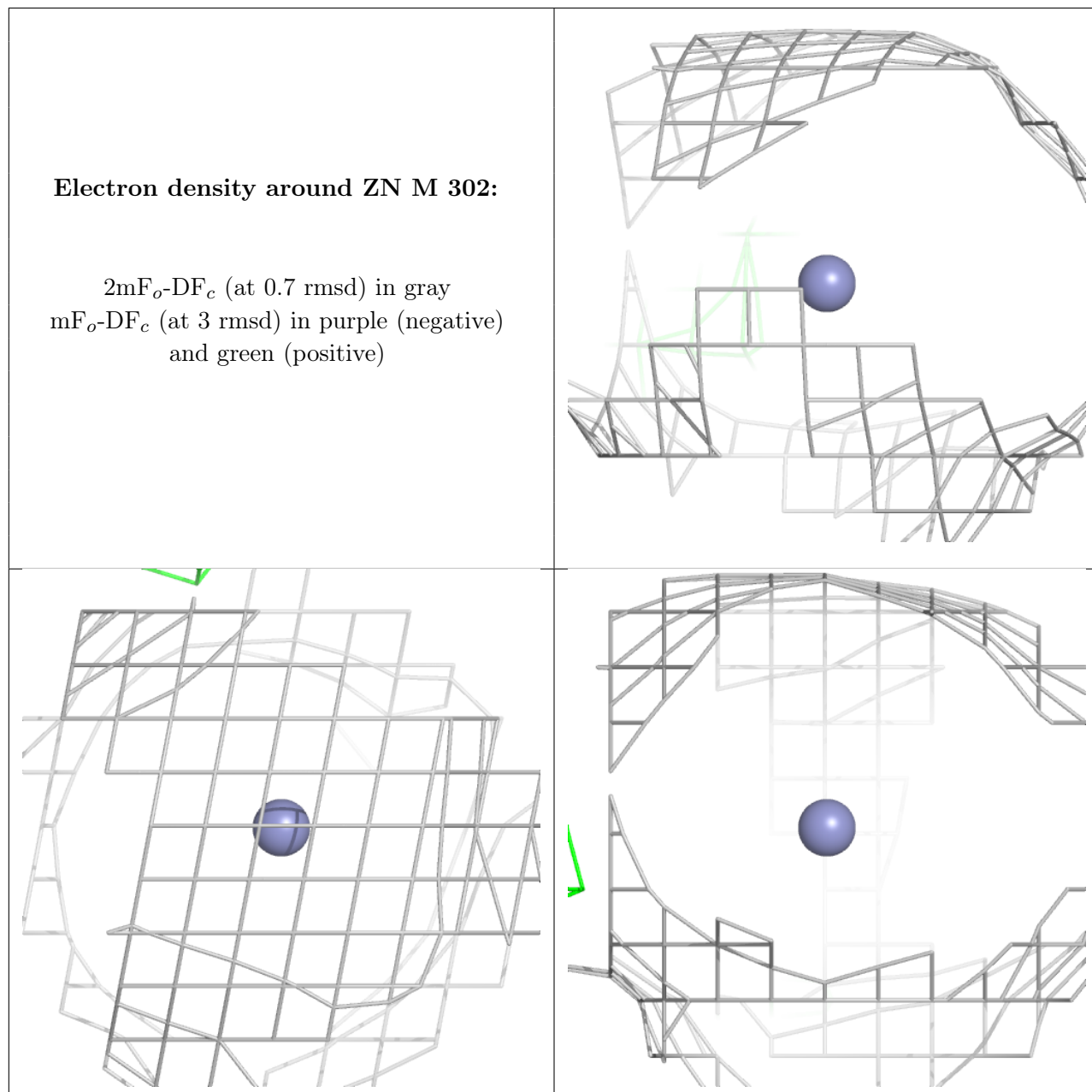
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





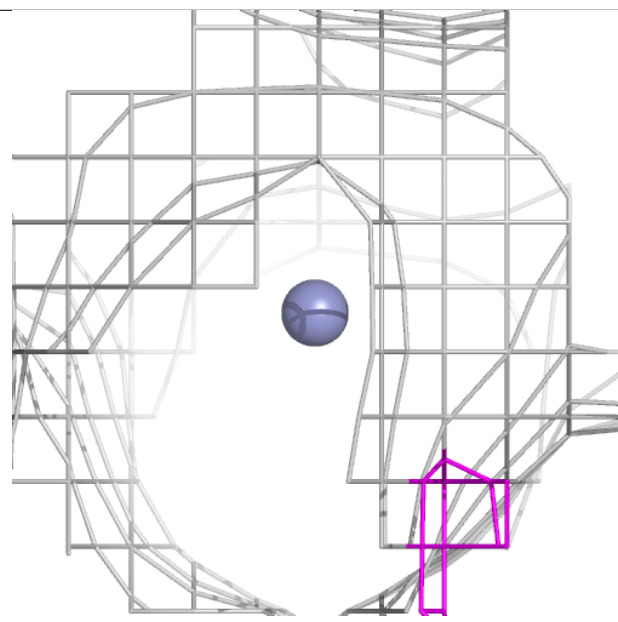
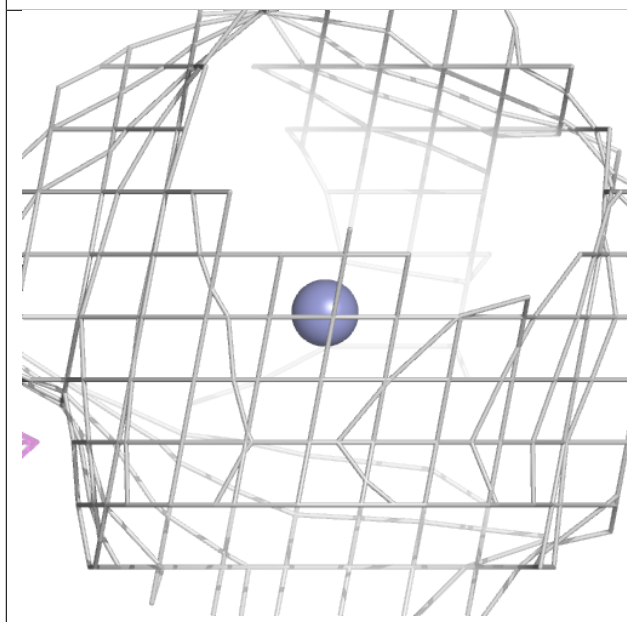
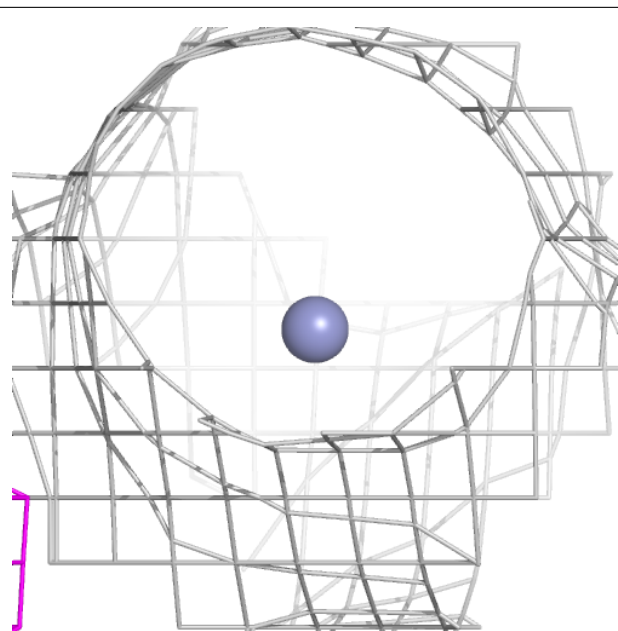
Electron density around ZN M 302:

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



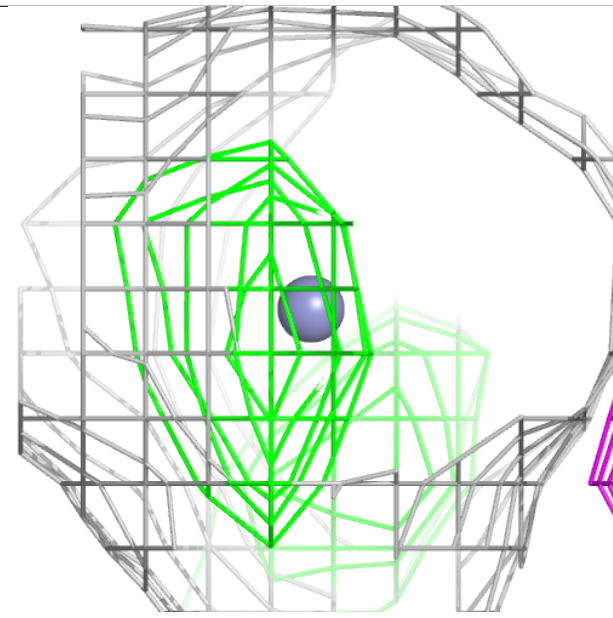
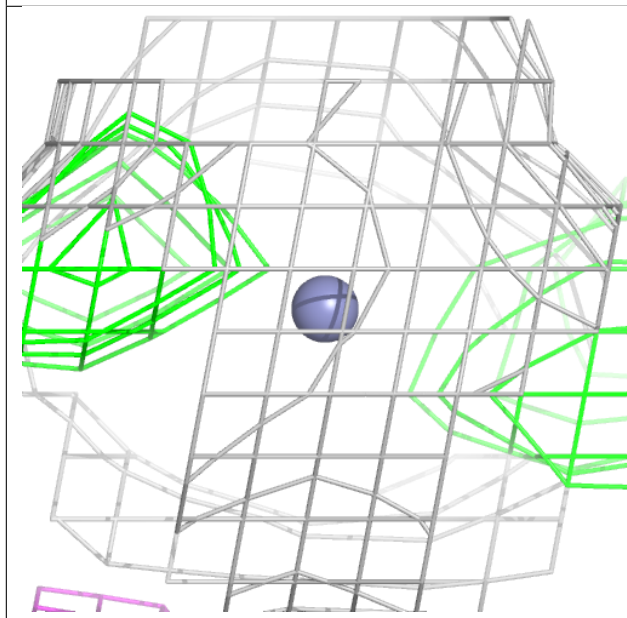
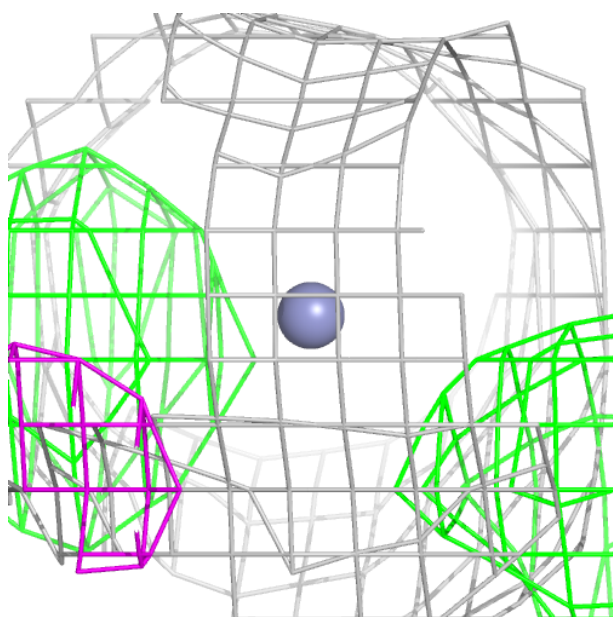
Electron density around ZN P 301:

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



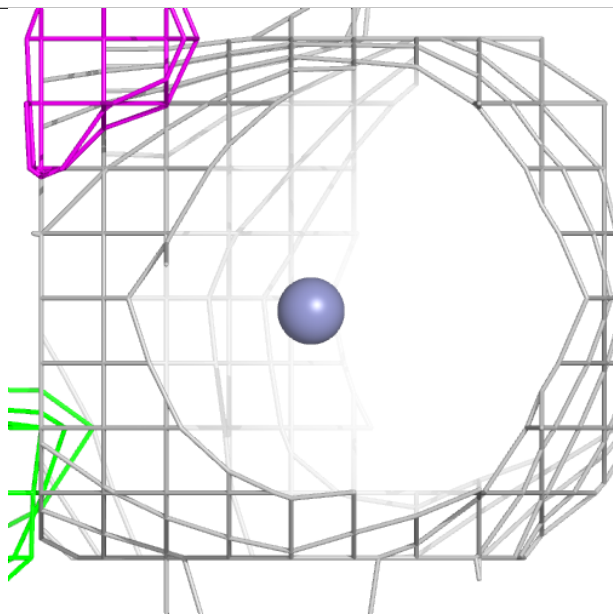
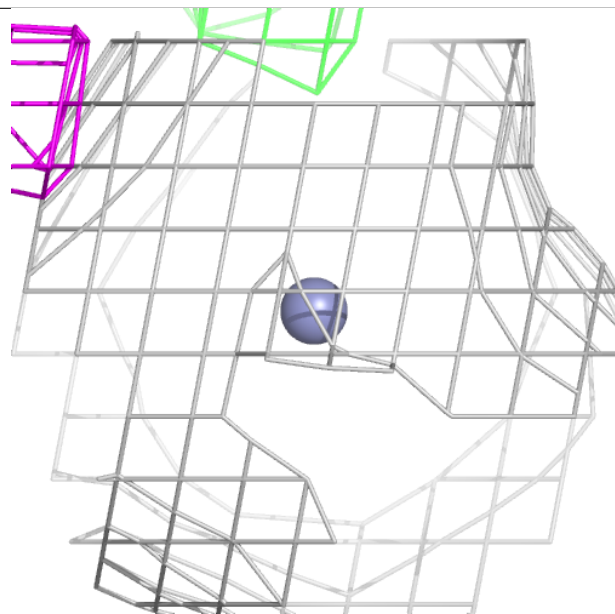
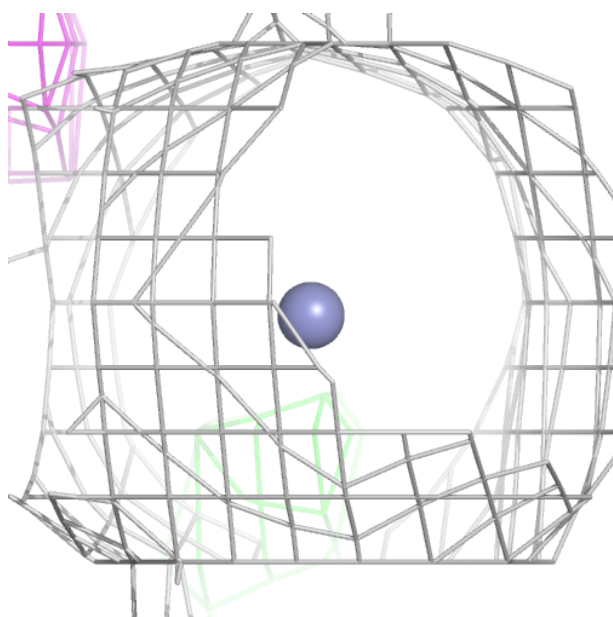
Electron density around ZN P 302:

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



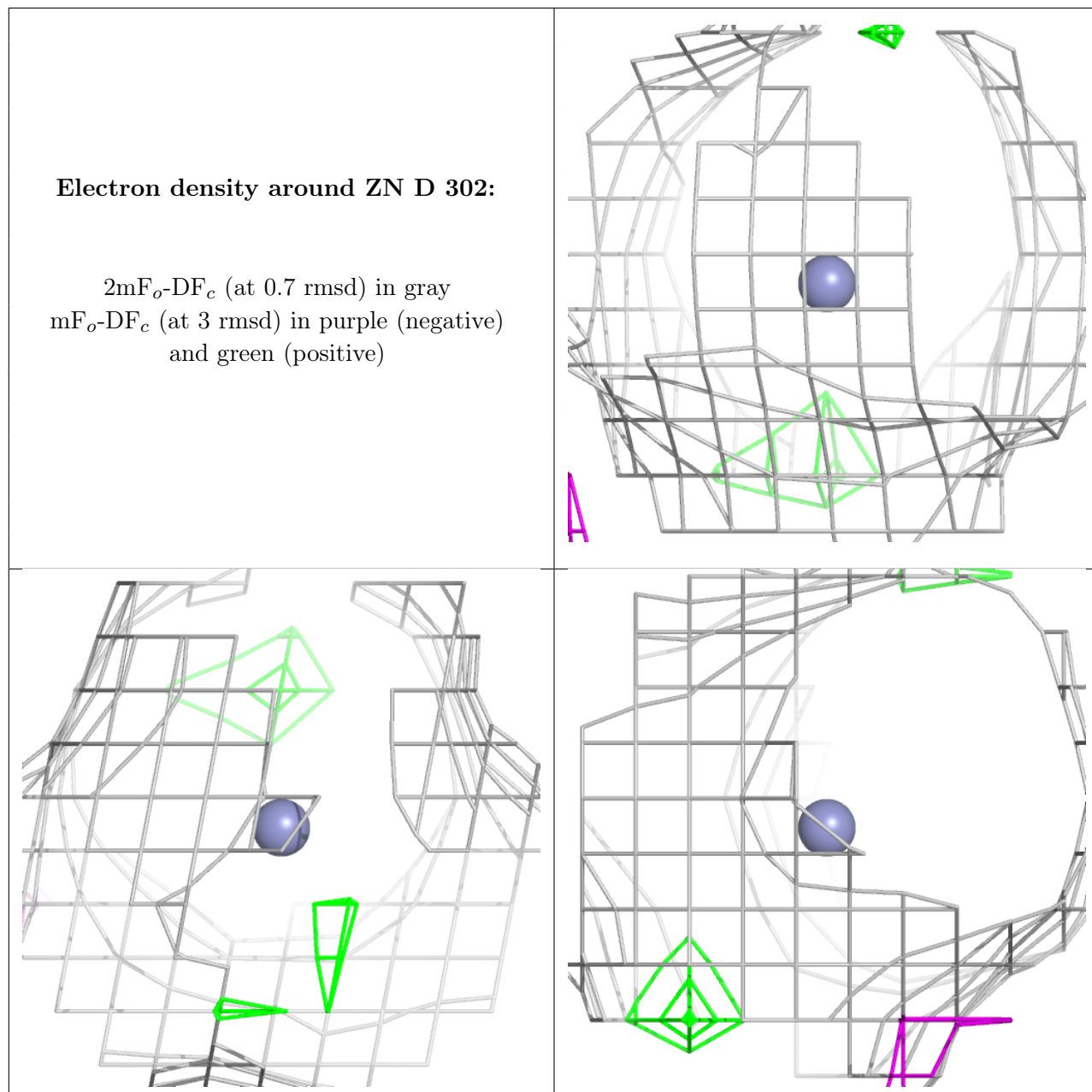
Electron density around ZN G 302:

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



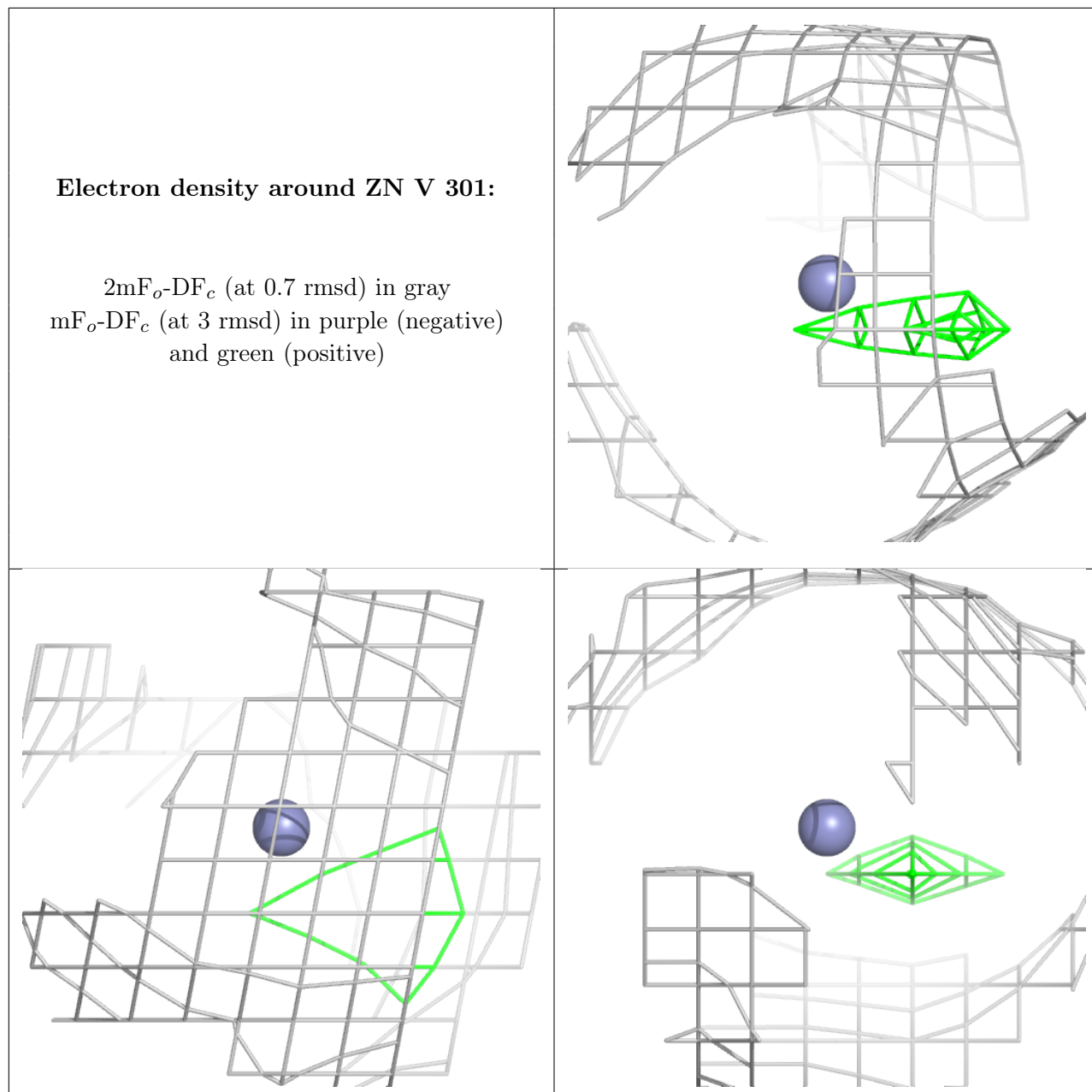
Electron density around ZN D 302:

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



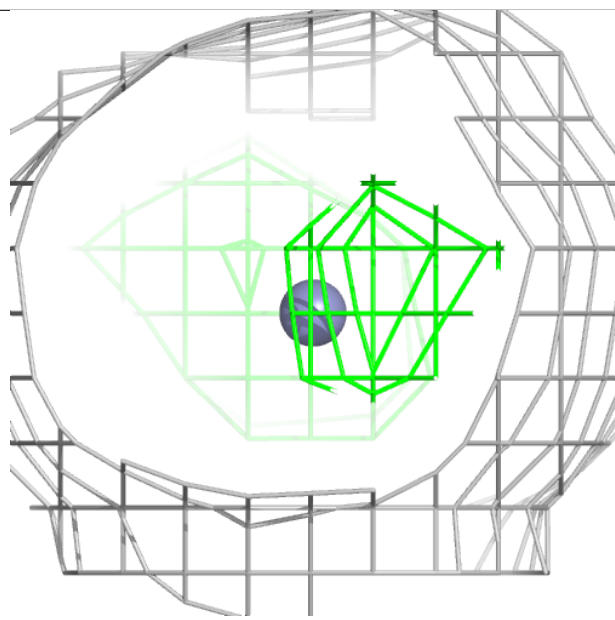
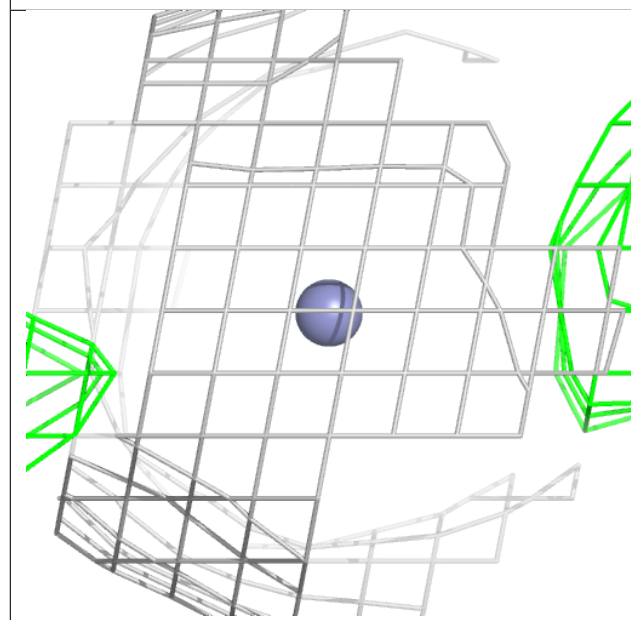
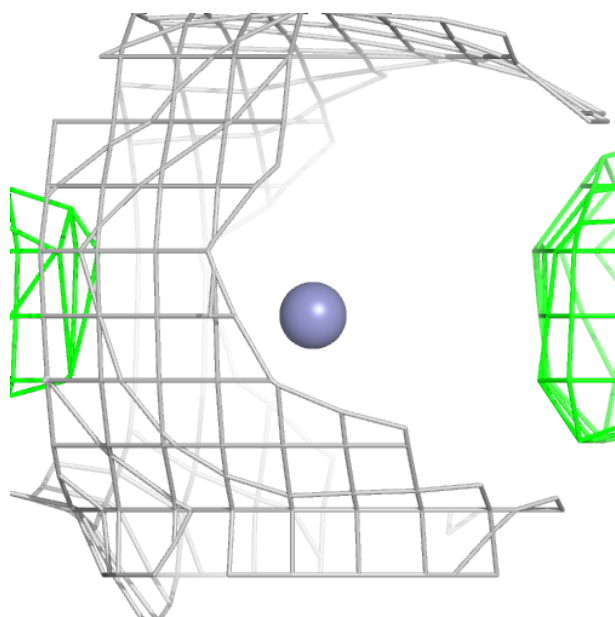
Electron density around ZN V 301:

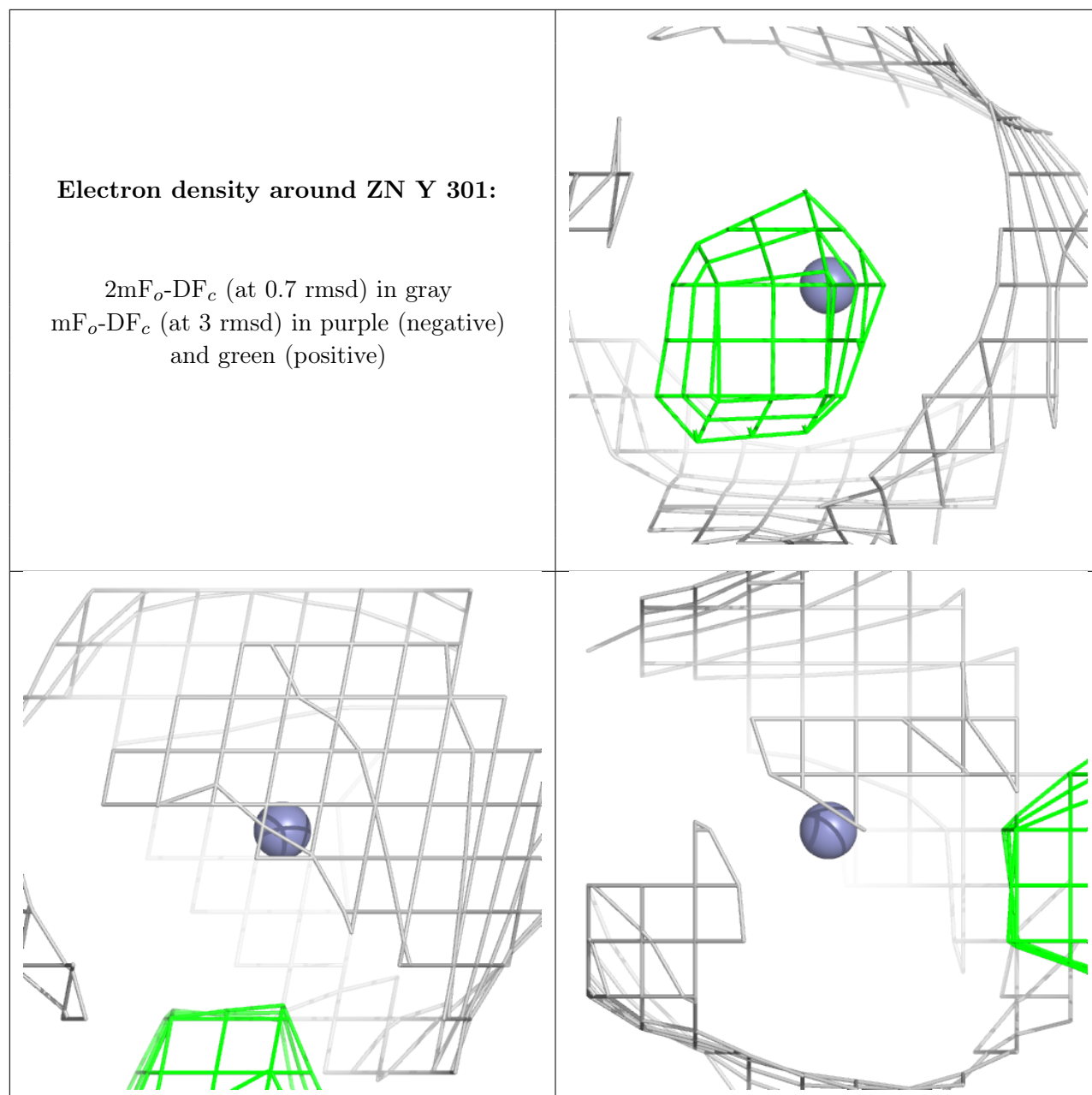
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN V 302:

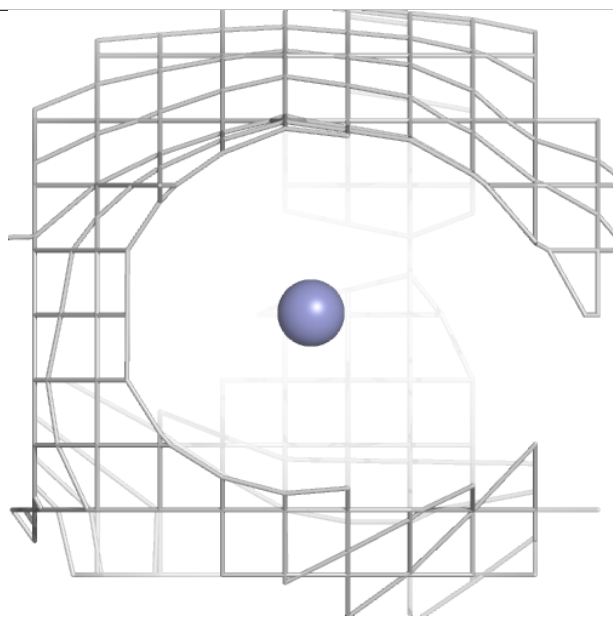
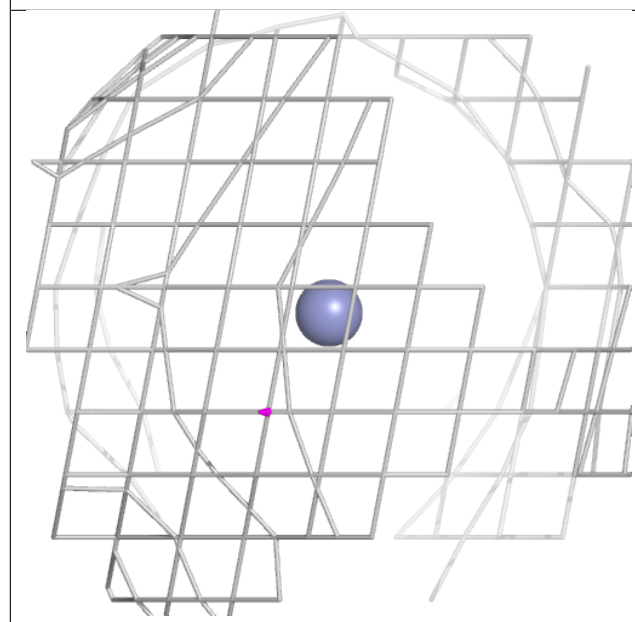
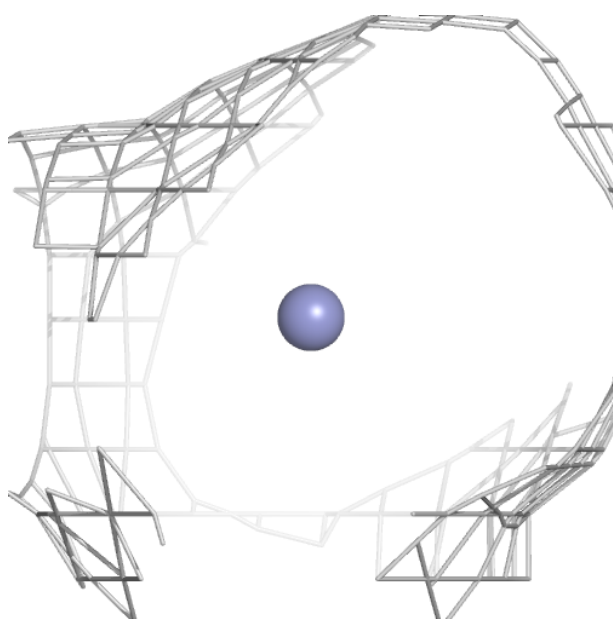
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

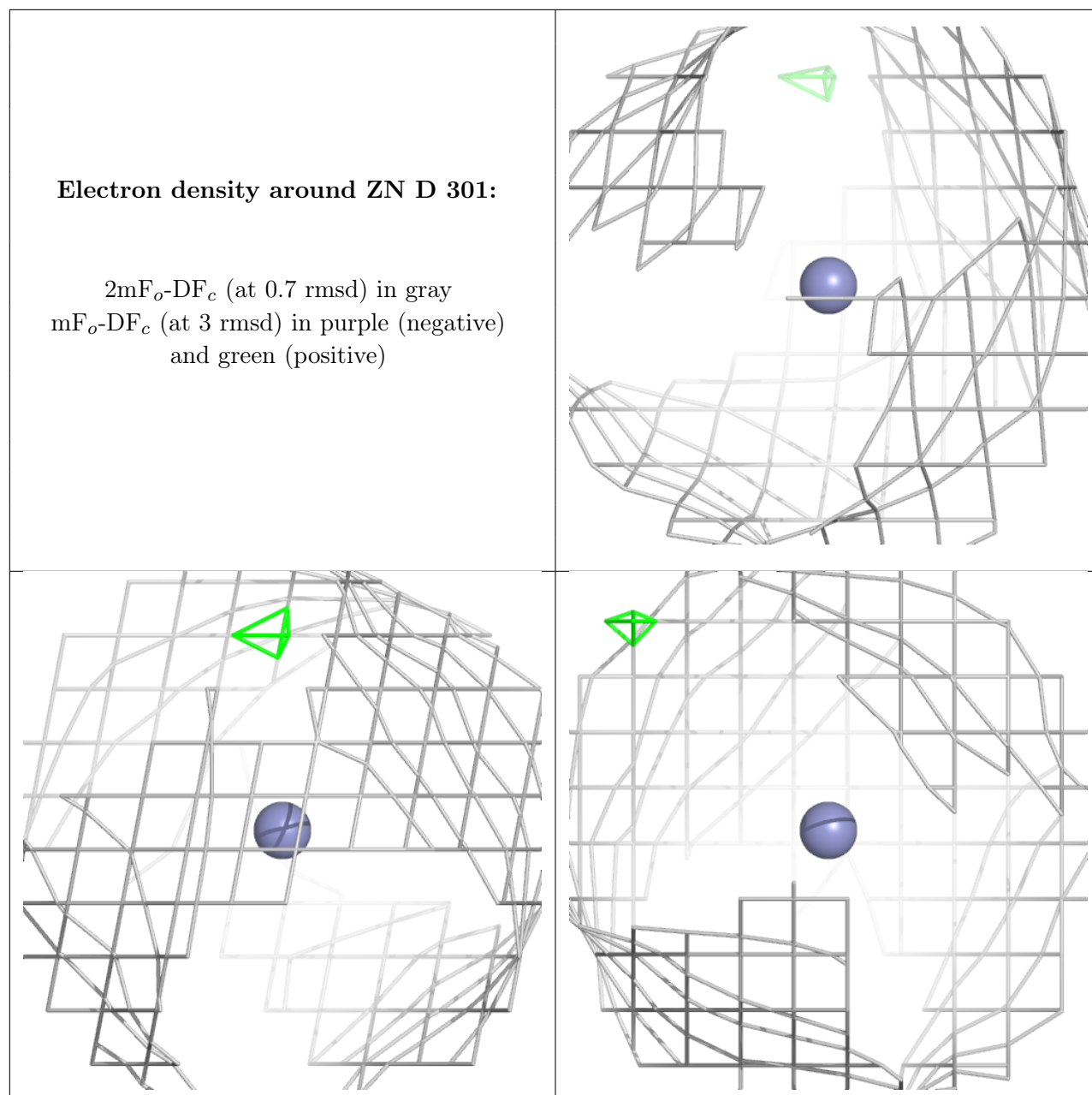




Electron density around ZN Y 302:

$2mF_o-DF_c$ (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.