



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:45 PM JST

PDB ID : 7C08
Title : Crystal structure of S34Y mutant of yeast U2AF1 complex bound to 3' splice site RNA, 5'-UAGGU.
Authors : Yoshida, H.; Park, S.Y.; Urano, T.; Obayashi, E.
Deposited on : 2020-04-30
Resolution : 3.35 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
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

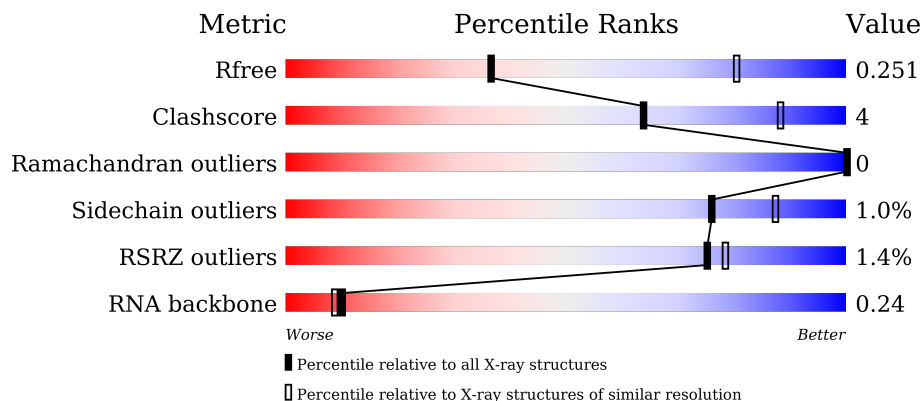
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.35 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.









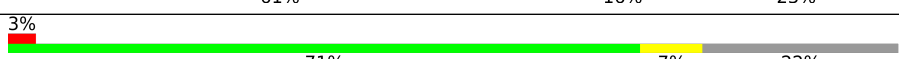


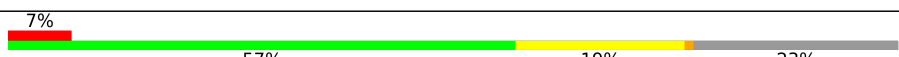

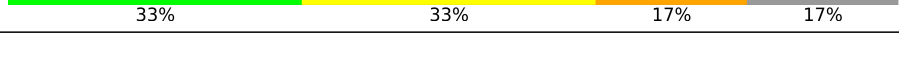



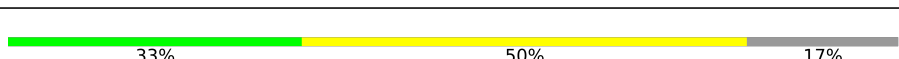
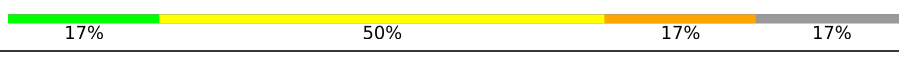
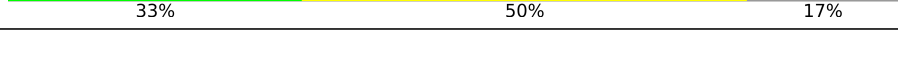




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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	 81% 8% 11%
1	D	216	 78% 9% 13%
1	G	216	 77% 12% 11%
1	J	216	 83% 6% 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

There are 4 unique types of molecules in this entry. The entry contains 18449 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	192	Total 1564	C 982	N 277	O 292	S 13	0	0	0
1	D	187	Total 1530	C 961	N 270	O 286	S 13	0	0	0
1	G	193	Total 1573	C 987	N 278	O 295	S 13	0	0	0
1	J	193	Total 1573	C 987	N 278	O 295	S 13	0	0	0
1	M	177	Total 1449	C 912	N 258	O 266	S 13	0	0	0
1	P	192	Total 1564	C 982	N 277	O 292	S 13	0	0	0
1	S	187	Total 1536	C 965	N 273	O 285	S 13	0	1	0
1	V	174	Total 1425	C 898	N 254	O 260	S 13	0	0	0
1	Y	178	Total 1458	C 917	N 259	O 269	S 13	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	TYR	SER	engineered mutation	UNP Q09176
D	34	TYR	SER	engineered mutation	UNP Q09176
G	34	TYR	SER	engineered mutation	UNP Q09176
J	34	TYR	SER	engineered mutation	UNP Q09176
M	34	TYR	SER	engineered mutation	UNP Q09176
P	34	TYR	SER	engineered mutation	UNP Q09176
S	34	TYR	SER	engineered mutation	UNP Q09176
V	34	TYR	SER	engineered mutation	UNP Q09176
Y	34	TYR	SER	engineered mutation	UNP Q09176

- 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	50	Total 406	C 260	N 70	O 75	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	53	Total 430	C 274	N 76	O 79	S 1	0	0	0
2	Q	53	Total 430	C 274	N 76	O 79	S 1	0	0	0
2	T	50	Total 406	C 260	N 70	O 75	S 1	0	0	0
2	W	53	Total 430	C 274	N 76	O 79	S 1	0	0	0
2	Z	48	Total 392	C 251	N 68	O 72	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	F	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	I	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	L	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	O	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	R	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	U	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	X	5	Total 105	C 48	N 19	O 34	P 4	0	0	0
3	1	5	Total 105	C 48	N 19	O 34	P 4	0	0	0


- 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 2	Zn 2	0	0
4	D	2	Total 2	Zn 2	0	0
4	G	2	Total 2	Zn 2	0	0
4	J	2	Total 2	Zn 2	0	0
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.

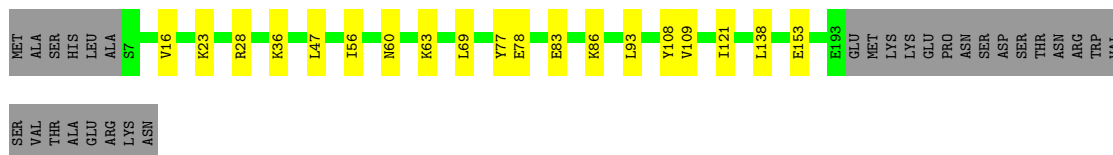
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain A: 




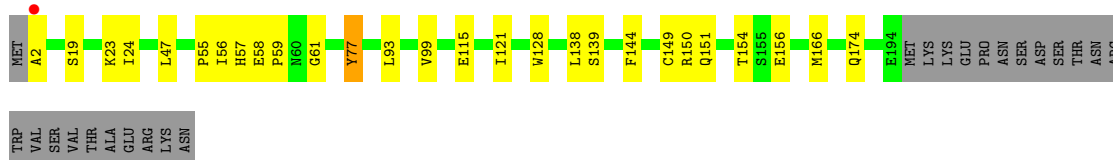
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain D: 




- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain G: 




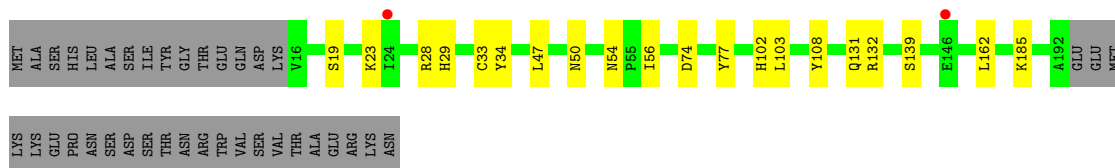
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain J: 



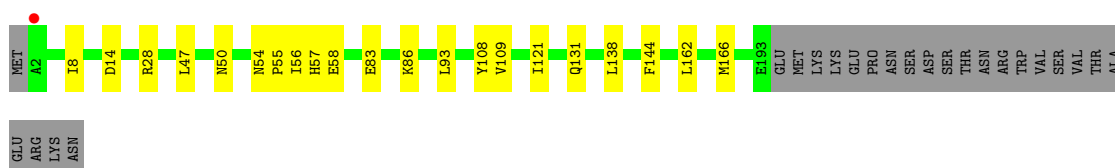
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain M: 



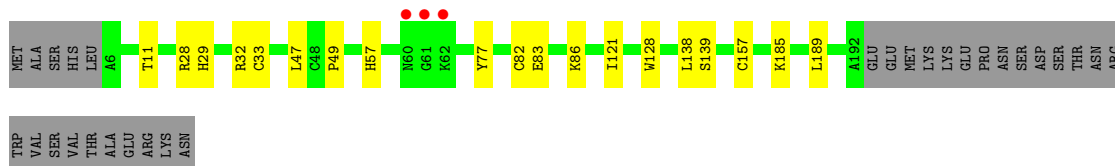
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain P: 79% 10% 11%



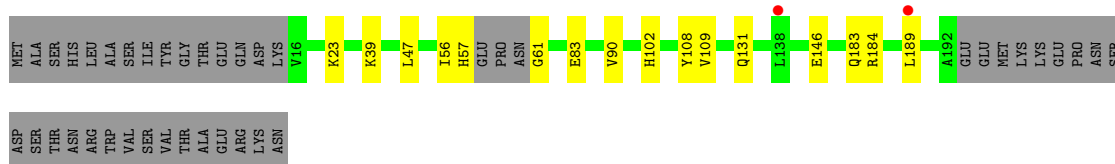
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain S: 78% 9% 13%



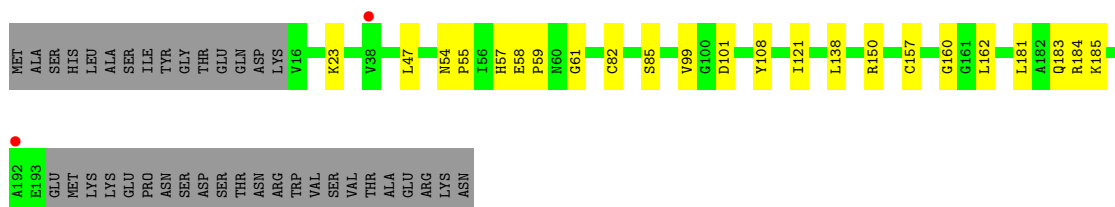
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain V: 73% 7% 19%



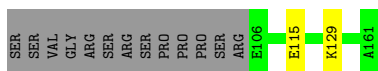
- Molecule 1: Splicing factor U2AF 23 kDa subunit

Chain Y: 72% 11% 18%



- Molecule 2: Splicing factor U2AF 59 kDa subunit

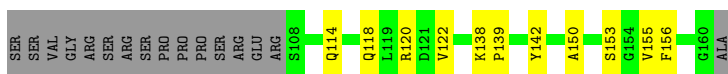
Chain B: 78% 19%



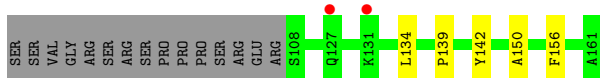
- Molecule 2: Splicing factor U2AF 59 kDa subunit



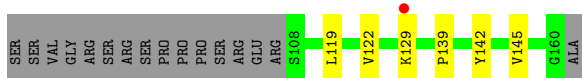
- Molecule 2: Splicing factor U2AF 59 kDa subunit



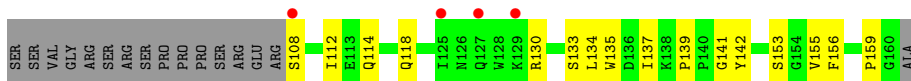
- Molecule 2: Splicing factor U2AF 59 kDa subunit



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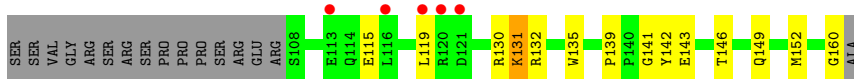


- Molecule 2: Splicing factor U2AF 59 kDa subunit



- Molecule 2: Splicing factor U2AF 59 kDa subunit





- Molecule 2: Splicing factor U2AF 59 kDa subunit



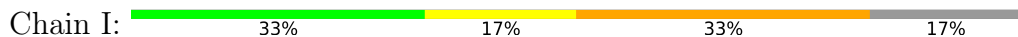
- Molecule 3: RNA (5'-R(*U*UP*AP*GP*GP*U)-3')



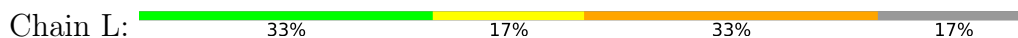
- Molecule 3: RNA (5'-R(*U*UP*AP*GP*GP*U)-3')



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



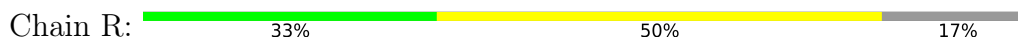
- Molecule 3: RNA (5'-R(*U*UP*AP*GP*GP*U)-3')



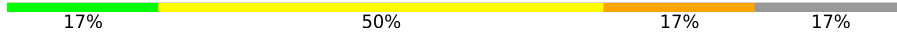
- Molecule 3: RNA (5'-R(*U*UP*AP*GP*GP*U)-3')



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



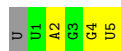
- Molecule 3: RNA (5'-R(*U*UP*AP*GP*GP*U)-3')

Chain U:  17% 50% 17% 17%



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

Chain X:  33% 50% 17%



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

Chain 1:  33% 33% 17% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.51Å 259.00Å 94.82Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	46.59 – 3.35 48.40 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.59-3.35) 100.0 (48.40-3.35)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.214 , 0.252 0.213 , 0.251	Depositor DCC
R_{free} test set	3250 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtrriage
Anisotropy	0.811	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for l,-k,h	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18449	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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

5.1 Standard geometry

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	0.25	0/1602	0.42	0/2161
1	D	0.24	0/1567	0.40	0/2113
1	G	0.24	0/1611	0.41	0/2173
1	J	0.25	0/1611	0.42	0/2173
1	M	0.24	0/1485	0.41	0/2003
1	P	0.24	0/1602	0.40	0/2161
1	S	0.24	0/1574	0.43	0/2123
1	V	0.24	0/1459	0.40	0/1965
1	Y	0.24	0/1494	0.41	0/2015
2	B	0.24	0/465	0.40	0/629
2	E	0.24	0/416	0.40	0/564
2	H	0.24	0/440	0.41	0/596
2	K	0.24	0/445	0.43	0/603
2	N	0.24	0/440	0.40	0/596
2	Q	0.26	0/440	0.40	0/596
2	T	0.24	0/416	0.43	0/564
2	W	0.24	0/440	0.46	0/596
2	Z	0.23	0/402	0.44	0/545
3	1	0.14	0/117	0.68	0/181
3	C	0.14	0/117	0.64	0/181
3	F	0.14	0/117	0.61	0/181
3	I	0.16	0/117	0.69	0/181
3	L	0.12	0/117	0.64	0/181
3	O	0.16	0/117	0.68	0/181
3	R	0.11	0/117	0.60	0/181
3	U	0.13	0/117	0.63	0/181
3	X	0.15	0/117	0.68	0/181
All	All	0.24	0/18962	0.43	0/25805

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	1564	0	1486	9	0
1	D	1530	0	1452	12	0
1	G	1573	0	1491	18	0
1	J	1573	0	1491	8	0
1	M	1449	0	1380	14	0
1	P	1564	0	1485	14	0
1	S	1536	0	1457	15	0
1	V	1425	0	1361	12	0
1	Y	1458	0	1387	18	0
2	B	455	0	460	2	0
2	E	406	0	409	9	0
2	H	430	0	436	8	0
2	K	435	0	441	3	0
2	N	430	0	436	6	0
2	Q	430	0	436	11	0
2	T	406	0	409	6	0
2	W	430	0	436	15	0
2	Z	392	0	393	8	0
3	1	105	0	55	2	0
3	C	105	0	55	2	0
3	F	105	0	55	1	0
3	I	105	0	55	2	0
3	L	105	0	55	2	0
3	O	105	0	55	1	0
3	R	105	0	55	0	0
3	U	105	0	55	2	0
3	X	105	0	55	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	18449	0	17341	149	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 4.

All (149) 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:Y:23:LYS:NZ	3:1:4:G:O2'	2.27	0.67
2:W:146:THR:HG23	2:W:149:GLN:OE1	1.97	0.65
1:D:23:LYS:NZ	3:F:4:G:O2'	2.30	0.65
1:D:28:ARG:NH1	2:H:153:SER:O	2.30	0.65
1:G:58:GLU:HG3	1:G:59:PRO:HD2	1.79	0.65
1:A:14:ASP:O	1:A:35:ARG:NH2	2.29	0.64
2:E:141:GLY:HA2	1:P:57:HIS:HB3	1.79	0.63
1:J:150:ARG:NH1	3:L:5:U:O4	2.33	0.62
1:P:50:ASN:HD22	2:Q:159:PRO:HD3	1.64	0.61
1:D:153:GLU:OE1	1:D:153:GLU:N	2.35	0.60
1:Y:185:LYS:NZ	2:Z:122:VAL:O	2.35	0.59
1:A:11:THR:HB	3:C:5:U:H5'	1.85	0.58
2:W:149:GLN:NE2	1:Y:160:GLY:HA3	2.18	0.57
2:E:153:SER:O	1:P:28:ARG:NH1	2.39	0.56
1:D:60:ASN:HB2	1:D:63:LYS:HE2	1.87	0.56
1:A:56:ILE:O	1:A:62:LYS:NZ	2.28	0.55
1:P:144:PHE:HD1	1:P:166:MET:HE1	1.71	0.55
2:H:139:PRO:HG2	2:H:142:TYR:CD1	2.43	0.55
2:Q:130:ARG:NH1	2:Q:133:SER:OG	2.38	0.55
1:G:144:PHE:HD1	1:G:166:MET:HE1	1.72	0.54
1:G:150:ARG:NH1	3:I:5:U:O4	2.40	0.54
1:P:93:LEU:HD13	1:P:109:VAL:HG22	1.89	0.54
1:J:130:SER:HB2	2:K:134:LEU:HD13	1.90	0.54
1:V:83:GLU:OE1	2:W:130:ARG:NH1	2.29	0.54
1:V:23:LYS:NZ	1:V:146:GLU:O	2.37	0.54
1:M:19:SER:HB2	1:M:23:LYS:HE2	1.91	0.52
1:P:54:ASN:HD21	1:P:56:ILE:HD12	1.73	0.52
1:S:47:LEU:HB2	1:S:139:SER:HB2	1.91	0.52
1:G:149:CYS:SG	1:G:151:GLN:HG2	2.49	0.52
1:G:23:LYS:HG3	1:G:24:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:23:LYS:NZ	3:O:4:G:O2'	2.42	0.52
2:Q:139:PRO:HG2	2:Q:142:TYR:CG	2.45	0.51
1:Y:54:ASN:HB3	1:Y:57:HIS:CE1	2.45	0.51
1:A:121:ILE:HD13	1:A:138:LEU:HG	1.93	0.51
1:A:8:ILE:O	1:A:14:ASP:HB2	2.12	0.50
2:W:143:GLU:OE2	1:Y:57:HIS:HA	2.11	0.50
1:S:29:HIS:O	1:S:32:ARG:HG2	2.12	0.50
1:S:83:GLU:O	1:S:86:LYS:HG2	2.11	0.50
1:V:184:ARG:HB3	2:W:119:LEU:HD11	1.92	0.50
1:Y:58:GLU:HG3	1:Y:59:PRO:HD2	1.94	0.50
1:Y:150:ARG:HG3	3:1:4:G:N1	2.27	0.49
1:G:19:SER:O	1:G:23:LYS:HG2	2.11	0.49
1:A:29:HIS:HB2	1:A:33:CYS:HB2	1.94	0.49
1:A:149:CYS:SG	1:A:151:GLN:HG2	2.53	0.49
1:J:58:GLU:HB3	1:J:59:PRO:HD2	1.95	0.49
2:Q:114:GLN:O	2:Q:118:GLN:NE2	2.45	0.49
1:Y:181:LEU:HA	1:Y:184:ARG:HG2	1.93	0.49
3:C:5:U:O2'	1:G:174:GLN:HG3	2.13	0.49
2:N:119:LEU:O	2:N:122:VAL:HG22	2.13	0.49
1:G:154:THR:HB	1:G:156:GLU:HG2	1.94	0.48
2:W:149:GLN:HA	2:W:152:MET:HG2	1.95	0.48
1:V:184:ARG:HH21	2:W:115:GLU:HG3	1.77	0.48
1:M:34:TYR:HB2	1:V:61:GLY:HA3	1.96	0.48
1:S:33:CYS:HA	3:U:1:U:H3	1.79	0.48
1:S:82:CYS:HB3	2:T:130:ARG:HH21	1.79	0.48
1:J:54:ASN:HD21	1:J:56:ILE:HD12	1.79	0.48
2:T:115:GLU:O	2:T:119:LEU:HG	2.13	0.47
2:W:131:LYS:HG2	2:W:132:ARG:HG3	1.95	0.47
2:Z:139:PRO:HG2	2:Z:142:TYR:CD1	2.49	0.47
2:E:139:PRO:HG2	2:E:142:TYR:CG	2.49	0.47
2:E:155:VAL:HG23	2:E:156:PHE:CD2	2.49	0.47
2:E:123:THR:HG22	2:E:127:GLN:HB3	1.96	0.47
2:T:139:PRO:HG2	2:T:142:TYR:CG	2.48	0.47
2:N:139:PRO:HG2	2:N:142:TYR:CG	2.50	0.47
2:W:139:PRO:HG2	2:W:142:TYR:CG	2.49	0.47
1:Y:82:CYS:O	1:Y:85:SER:OG	2.33	0.47
1:M:54:ASN:HD21	1:M:56:ILE:HD12	1.80	0.46
2:W:141:GLY:HA2	1:Y:57:HIS:HB2	1.97	0.46
2:Z:120:ARG:O	2:Z:122:VAL:HG23	2.15	0.46
1:P:131:GLN:HA	2:Q:139:PRO:HD3	1.95	0.46
1:D:16:VAL:O	1:D:36:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLU:OE1	2:E:131:LYS:NZ	2.35	0.46
1:S:83:GLU:HG2	2:T:135:TRP:CE2	2.50	0.46
1:G:55:PRO:O	1:G:61:GLY:HA3	2.16	0.46
2:W:141:GLY:HA2	1:Y:57:HIS:CB	2.45	0.46
2:Q:155:VAL:HG23	2:Q:156:PHE:CD2	2.50	0.46
1:G:115:GLU:OE1	1:G:115:GLU:N	2.49	0.45
1:Y:55:PRO:O	1:Y:61:GLY:HA3	2.16	0.45
1:D:121:ILE:HD13	1:D:138:LEU:HG	1.99	0.45
2:Q:134:LEU:HA	2:Q:137:ILE:HD12	1.99	0.45
1:S:83:GLU:OE1	2:T:130:ARG:NH1	2.49	0.45
1:S:121:ILE:HD13	1:S:138:LEU:HG	1.98	0.45
2:Z:139:PRO:HG2	2:Z:142:TYR:CG	2.52	0.45
1:M:47:LEU:HD13	1:M:108:TYR:CE2	2.52	0.45
1:M:47:LEU:HB2	1:M:139:SER:HB2	1.99	0.44
1:M:50:ASN:O	1:M:132:ARG:NH2	2.41	0.44
1:Y:185:LYS:HD3	2:Z:119:LEU:HB3	1.99	0.44
1:A:184:ARG:HD2	2:B:115:GLU:OE2	2.18	0.44
1:P:83:GLU:O	1:P:86:LYS:HG2	2.16	0.44
1:G:121:ILE:HD13	1:G:138:LEU:HG	1.99	0.44
1:M:185:LYS:HD3	2:N:119:LEU:HB3	1.99	0.44
1:P:121:ILE:HD13	1:P:138:LEU:HG	1.99	0.44
1:D:83:GLU:O	1:D:86:LYS:HG2	2.17	0.44
2:H:139:PRO:HG2	2:H:142:TYR:CG	2.52	0.44
1:M:131:GLN:HA	2:N:139:PRO:HD3	1.99	0.44
1:G:77:TYR:CE1	1:G:93:LEU:HD22	2.52	0.44
1:D:47:LEU:HD13	1:D:108:TYR:CE2	2.53	0.44
1:D:93:LEU:HD13	1:D:109:VAL:HG23	2.00	0.43
1:J:23:LYS:NZ	3:L:4:G:O2'	2.51	0.43
1:A:53:LYS:HE2	1:A:132:ARG:NH1	2.34	0.43
2:H:120:ARG:O	2:H:122:VAL:HG23	2.19	0.43
1:Y:121:ILE:HD13	1:Y:138:LEU:HG	2.01	0.43
1:S:11:THR:HG22	3:U:5:U:H5'	2.01	0.43
1:G:99:VAL:HG21	2:N:145:VAL:HG21	2.01	0.43
1:P:8:ILE:O	1:P:14:ASP:HB2	2.19	0.43
1:P:83:GLU:HG2	2:Q:135:TRP:CE2	2.54	0.42
2:E:142:TYR:HE2	1:P:162:LEU:HD11	1.84	0.42
2:Q:153:SER:O	1:S:28:ARG:NH2	2.50	0.42
1:V:90:VAL:HG13	1:V:109:VAL:HG23	2.01	0.42
1:G:47:LEU:HB2	1:G:139:SER:HB2	2.01	0.42
1:G:128:TRP:CD1	2:H:138:LYS:HE2	2.55	0.42
1:J:83:GLU:O	1:J:86:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:131:GLN:HA	2:W:139:PRO:HD3	2.02	0.42
2:B:129:LYS:HE3	1:G:2:ALA:O	2.18	0.42
2:H:155:VAL:HG23	2:H:156:PHE:CD2	2.54	0.42
1:S:29:HIS:HB2	1:S:33:CYS:HB2	2.00	0.42
1:Y:99:VAL:HB	1:Y:162:LEU:HD12	2.01	0.42
1:M:162:LEU:HD11	2:Z:142:TYR:CE2	2.55	0.42
1:S:47:LEU:HD22	1:S:49:PRO:HG3	2.00	0.42
2:H:150:ALA:HB1	2:H:156:PHE:CD2	2.54	0.42
1:M:102:HIS:CD2	1:M:103:LEU:HG	2.55	0.42
2:Q:108:SER:O	2:Q:112:ILE:HG13	2.20	0.42
2:Q:141:GLY:HA2	1:S:57:HIS:HB3	2.01	0.42
2:K:139:PRO:HG2	2:K:142:TYR:HB2	2.02	0.42
1:V:83:GLU:HG2	2:W:135:TRP:CE2	2.54	0.42
1:D:56:ILE:HD11	1:D:69:LEU:HD13	2.02	0.41
1:G:150:ARG:HD3	3:I:4:G:N1	2.35	0.41
1:V:47:LEU:HD13	1:V:108:TYR:CE2	2.55	0.41
1:Y:47:LEU:HD13	1:Y:108:TYR:CE2	2.55	0.41
1:S:128:TRP:CD1	2:T:138:LYS:HE2	2.54	0.41
1:Y:101:ASP:O	2:Z:159:PRO:HB2	2.20	0.41
1:G:56:ILE:HG23	1:G:57:HIS:ND1	2.36	0.41
1:P:55:PRO:HA	1:P:58:GLU:HG2	2.02	0.41
1:D:83:GLU:HG2	2:E:135:TRP:CE2	2.55	0.41
1:M:29:HIS:HB2	1:M:33:CYS:HB2	2.03	0.41
1:S:185:LYS:O	1:S:189:LEU:HD13	2.20	0.41
1:J:19:SER:HB2	1:J:23:LYS:HE2	2.03	0.41
1:V:56:ILE:HG13	1:V:57:HIS:ND1	2.36	0.41
1:M:28:ARG:HA	1:M:102:HIS:CG	2.56	0.41
1:M:162:LEU:HD11	2:Z:142:TYR:HE2	1.85	0.41
1:P:47:LEU:HD13	1:P:108:TYR:CE2	2.56	0.41
1:V:189:LEU:O	1:V:189:LEU:HD23	2.21	0.41
2:E:153:SER:OG	2:E:155:VAL:HG22	2.20	0.41
2:H:114:GLN:O	2:H:118:GLN:HG2	2.21	0.41
2:W:142:TYR:HE2	1:Y:162:LEU:HD21	1.85	0.41
2:K:150:ALA:HB1	2:K:156:PHE:CD2	2.56	0.40
1:V:102:HIS:NE2	2:W:160:GLY:HA3	2.35	0.40
1:J:93:LEU:HD13	1:J:109:VAL:HG23	2.02	0.40
2:N:139:PRO:HG2	2:N:142:TYR:CD1	2.56	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	190/216 (88%)	184 (97%)	6 (3%)	0	100	100
1	D	185/216 (86%)	179 (97%)	6 (3%)	0	100	100
1	G	191/216 (88%)	186 (97%)	5 (3%)	0	100	100
1	J	191/216 (88%)	186 (97%)	5 (3%)	0	100	100
1	M	175/216 (81%)	169 (97%)	6 (3%)	0	100	100
1	P	190/216 (88%)	182 (96%)	8 (4%)	0	100	100
1	S	186/216 (86%)	179 (96%)	7 (4%)	0	100	100
1	V	170/216 (79%)	166 (98%)	4 (2%)	0	100	100
1	Y	176/216 (82%)	169 (96%)	7 (4%)	0	100	100
2	B	54/69 (78%)	52 (96%)	2 (4%)	0	100	100
2	E	48/69 (70%)	44 (92%)	4 (8%)	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	51/69 (74%)	48 (94%)	3 (6%)	0	100	100
2	Q	51/69 (74%)	46 (90%)	5 (10%)	0	100	100
2	T	48/69 (70%)	44 (92%)	4 (8%)	0	100	100
2	W	51/69 (74%)	47 (92%)	4 (8%)	0	100	100
2	Z	46/69 (67%)	42 (91%)	4 (9%)	0	100	100
All	All	2106/2565 (82%)	2019 (96%)	87 (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	169/192 (88%)	167 (99%)	2 (1%)	71	85
1	D	166/192 (86%)	165 (99%)	1 (1%)	86	93
1	G	170/192 (88%)	169 (99%)	1 (1%)	86	93
1	J	170/192 (88%)	169 (99%)	1 (1%)	86	93
1	M	157/192 (82%)	155 (99%)	2 (1%)	69	84
1	P	169/192 (88%)	169 (100%)	0	100	100
1	S	166/192 (86%)	164 (99%)	2 (1%)	71	85
1	V	154/192 (80%)	152 (99%)	2 (1%)	69	84
1	Y	158/192 (82%)	156 (99%)	2 (1%)	69	84
2	B	50/62 (81%)	50 (100%)	0	100	100
2	E	45/62 (73%)	44 (98%)	1 (2%)	52	76
2	H	48/62 (77%)	48 (100%)	0	100	100
2	K	48/62 (77%)	48 (100%)	0	100	100
2	N	48/62 (77%)	47 (98%)	1 (2%)	53	77
2	Q	48/62 (77%)	48 (100%)	0	100	100
2	T	45/62 (73%)	44 (98%)	1 (2%)	52	76
2	W	48/62 (77%)	47 (98%)	1 (2%)	53	77
2	Z	43/62 (69%)	41 (95%)	2 (5%)	26	58
All	All	1902/2286 (83%)	1883 (99%)	19 (1%)	76	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	TYR
1	A	193	GLU
1	D	77	TYR
2	E	131	LYS
1	G	77	TYR
1	J	77	TYR
1	M	74	ASP
1	M	77	TYR
2	N	129	LYS
1	S	77	TYR
1	S	157	CYS

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Mol	Chain	Res	Type
2	T	117	GLU
1	V	39	LYS
1	V	183	GLN
2	W	131	LYS
1	Y	157	CYS
1	Y	183	GLN
2	Z	128	TRP
2	Z	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	4/6 (66%)	3 (75%)	0
3	C	4/6 (66%)	3 (75%)	0
3	F	4/6 (66%)	2 (50%)	0
3	I	4/6 (66%)	3 (75%)	0
3	L	4/6 (66%)	3 (75%)	0
3	O	4/6 (66%)	3 (75%)	0
3	R	4/6 (66%)	3 (75%)	0
3	U	4/6 (66%)	3 (75%)	0
3	X	4/6 (66%)	3 (75%)	0
All	All	36/54 (66%)	26 (72%)	0

All (26) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
3	O	4	G
3	O	5	U
3	R	2	A
3	R	4	G
3	R	5	U
3	U	2	A
3	U	4	G
3	U	5	U
3	X	2	A
3	X	4	G
3	X	5	U
3	1	2	A
3	1	4	G
3	1	5	U

There are no RNA pucker outliers to report.

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	192/216 (88%)	-0.02	0 100 100	39, 57, 94, 125	0
1	D	187/216 (86%)	-0.08	0 100 100	34, 53, 91, 104	0
1	G	193/216 (89%)	0.06	1 (0%) 91 93	29, 51, 91, 120	0
1	J	193/216 (89%)	0.06	1 (0%) 91 93	40, 69, 103, 117	0
1	M	177/216 (81%)	0.07	2 (1%) 80 84	41, 71, 103, 125	0
1	P	192/216 (88%)	-0.00	1 (0%) 91 93	41, 65, 98, 114	0
1	S	187/216 (86%)	0.22	3 (1%) 72 74	44, 73, 112, 127	0
1	V	174/216 (80%)	0.23	2 (1%) 80 84	58, 79, 108, 132	0
1	Y	178/216 (82%)	0.13	2 (1%) 80 84	35, 79, 112, 127	0
2	B	56/69 (81%)	-0.00	0 100 100	45, 65, 125, 141	0
2	E	50/69 (72%)	0.09	0 100 100	39, 66, 130, 134	0
2	H	53/69 (76%)	0.02	0 100 100	28, 55, 110, 120	0
2	K	54/69 (78%)	0.22	2 (3%) 41 43	44, 74, 123, 145	0
2	N	53/69 (76%)	-0.13	1 (1%) 66 70	45, 77, 134, 141	0
2	Q	53/69 (76%)	0.28	4 (7%) 14 16	43, 68, 122, 137	0
2	T	50/69 (72%)	0.17	4 (8%) 12 14	55, 86, 140, 153	0
2	W	53/69 (76%)	0.34	5 (9%) 8 10	52, 84, 141, 145	0
2	Z	48/69 (69%)	0.13	2 (4%) 36 38	35, 64, 136, 150	0
3	I	5/6 (83%)	-0.12	0 100 100	87, 91, 105, 128	0
3	C	5/6 (83%)	0.02	0 100 100	52, 59, 64, 90	0
3	F	5/6 (83%)	0.04	0 100 100	60, 60, 74, 121	0
3	I	5/6 (83%)	0.03	0 100 100	57, 62, 84, 88	0
3	L	5/6 (83%)	-0.13	0 100 100	67, 74, 78, 95	0
3	O	5/6 (83%)	-0.00	0 100 100	86, 91, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	R	5/6 (83%)	0.13	0 100 100	54, 64, 84, 100	0
3	U	5/6 (83%)	-0.40	0 100 100	65, 65, 72, 121	0
3	X	5/6 (83%)	-0.20	0 100 100	88, 92, 93, 96	0
All	All	2188/2619 (83%)	0.08	30 (1%) 75 78	28, 68, 115, 153	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	62	LYS	5.3
1	P	2	ALA	4.3
1	S	61	GLY	3.9
2	W	119	LEU	3.5
2	W	121	ASP	3.4
2	W	113	GLU	3.4
2	T	132	ARG	3.3
2	Z	129	LYS	3.3
2	W	120	ARG	3.2
1	V	189	LEU	2.8
2	K	131	LYS	2.6
2	T	130	ARG	2.6
1	Y	38	VAL	2.6
2	T	131	LYS	2.5
1	V	138	LEU	2.5
2	Q	127	GLN	2.5
2	K	127	GLN	2.4
2	N	129	LYS	2.4
2	Q	125	ILE	2.4
1	S	60	ASN	2.3
2	T	129	LYS	2.3
2	Z	128	TRP	2.3
1	M	24	ILE	2.3
2	W	116	LEU	2.2
1	J	4	HIS	2.1
1	M	146	GLU	2.1
2	Q	108	SER	2.1
2	Q	129	LYS	2.0
1	G	2	ALA	2.0
1	Y	192	ALA	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](#)

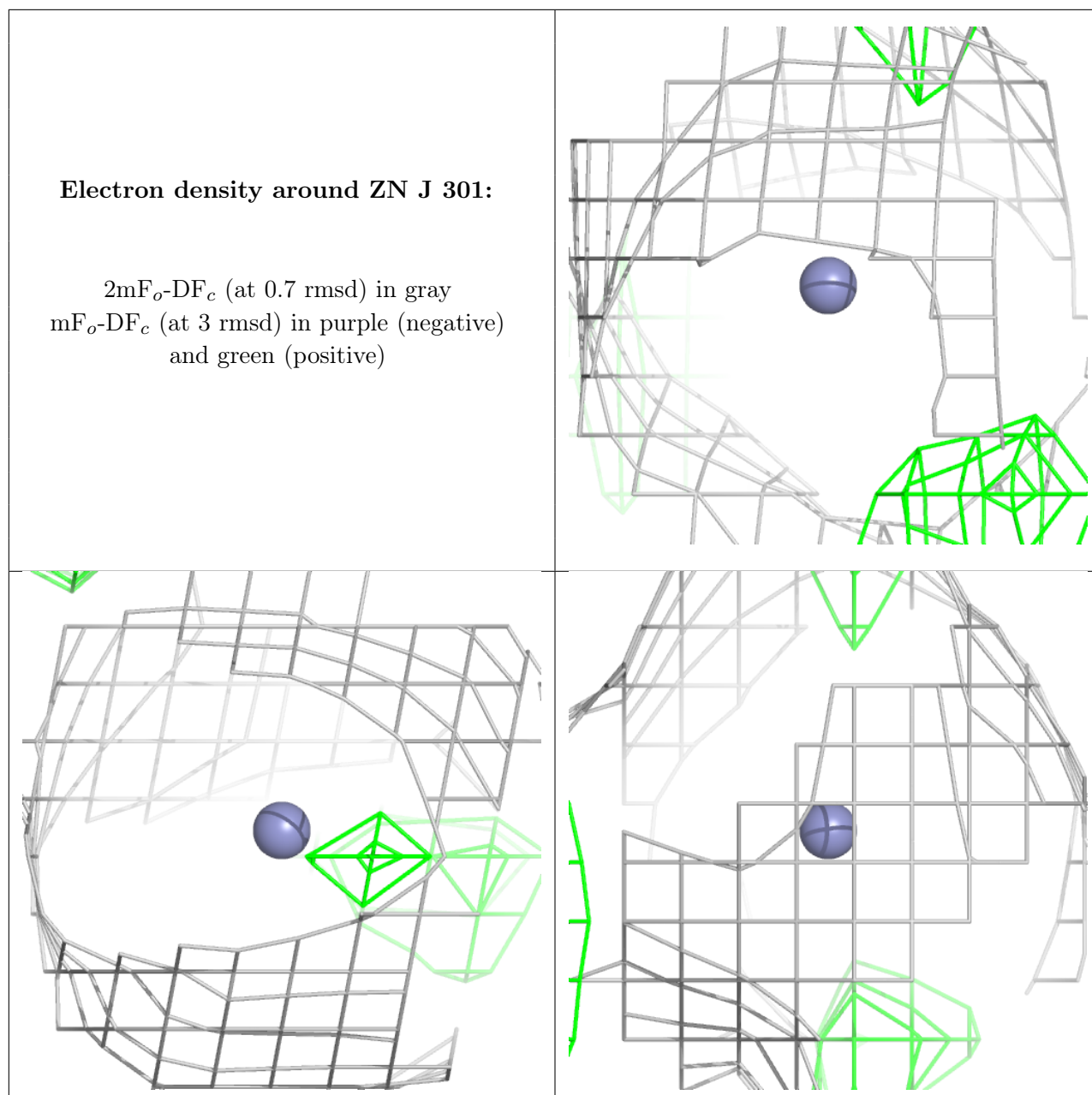
There are no monosaccharides in this entry.

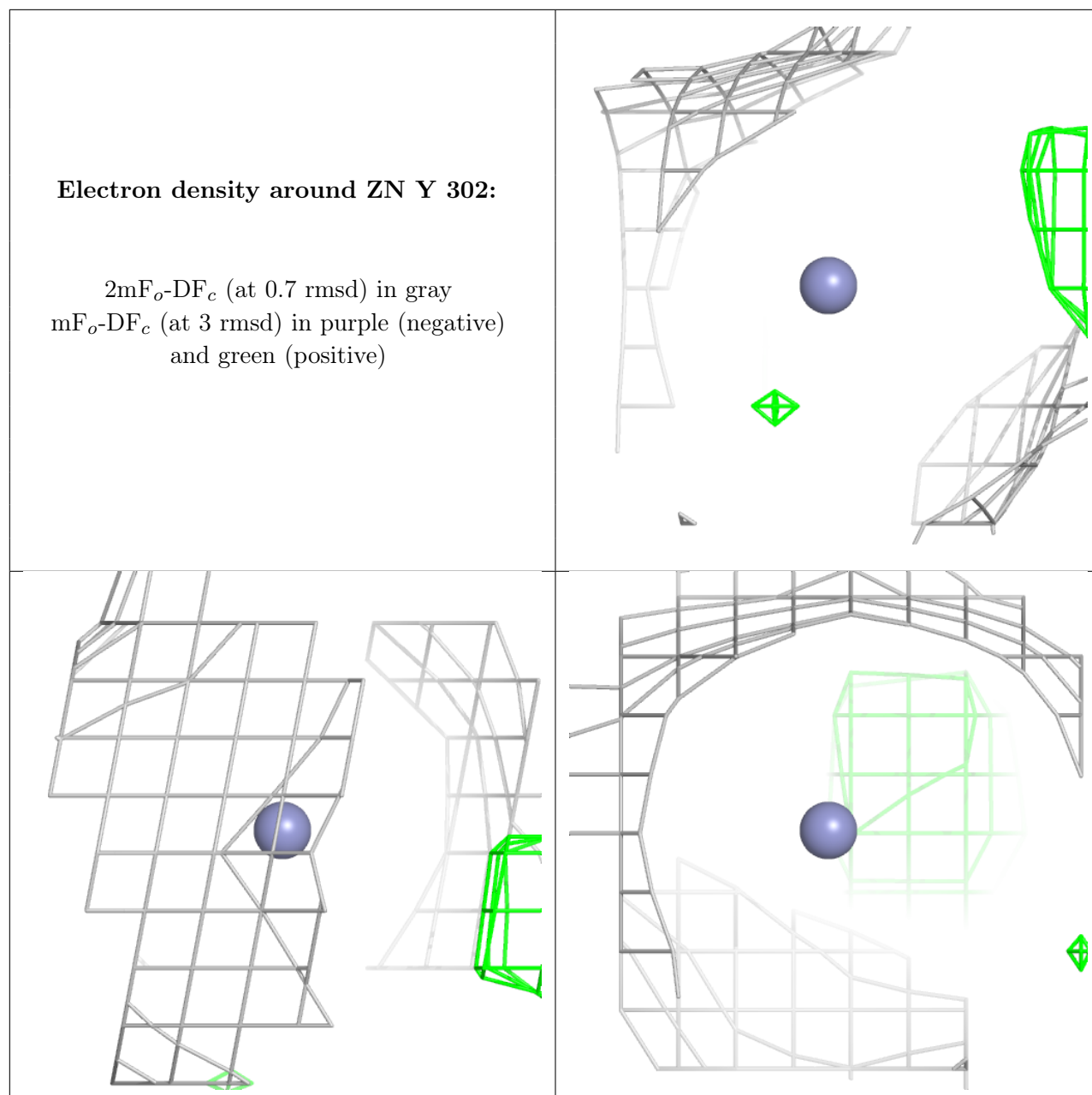
6.4 Ligands [i](#)

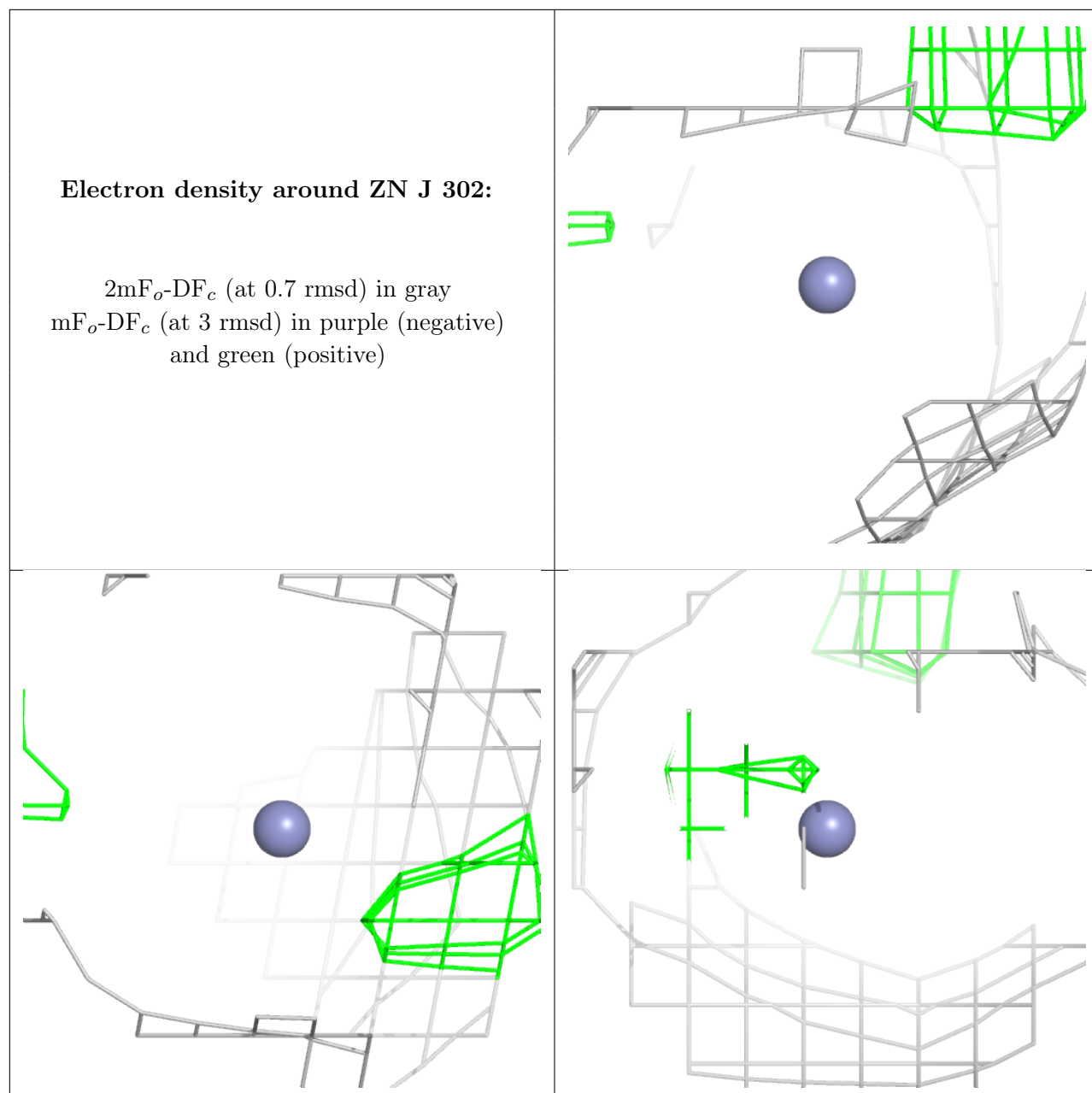
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	J	301	1/1	0.96	0.20	52,52,52,52	0
4	ZN	Y	302	1/1	0.96	0.13	52,52,52,52	0
4	ZN	J	302	1/1	0.98	0.17	56,56,56,56	0
4	ZN	M	302	1/1	0.98	0.13	47,47,47,47	0
4	ZN	P	302	1/1	0.98	0.17	33,33,33,33	0
4	ZN	S	302	1/1	0.98	0.14	47,47,47,47	0
4	ZN	V	301	1/1	0.98	0.14	58,58,58,58	0
4	ZN	A	302	1/1	0.98	0.14	43,43,43,43	0
4	ZN	P	301	1/1	0.99	0.20	43,43,43,43	0
4	ZN	D	301	1/1	0.99	0.18	45,45,45,45	0
4	ZN	S	301	1/1	0.99	0.17	51,51,51,51	0
4	ZN	D	302	1/1	0.99	0.18	35,35,35,35	0
4	ZN	M	301	1/1	0.99	0.17	75,75,75,75	0
4	ZN	V	302	1/1	0.99	0.13	51,51,51,51	0
4	ZN	Y	301	1/1	0.99	0.10	68,68,68,68	0
4	ZN	G	302	1/1	0.99	0.20	33,33,33,33	0
4	ZN	G	301	1/1	1.00	0.17	41,41,41,41	0
4	ZN	A	301	1/1	1.00	0.16	43,43,43,43	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.

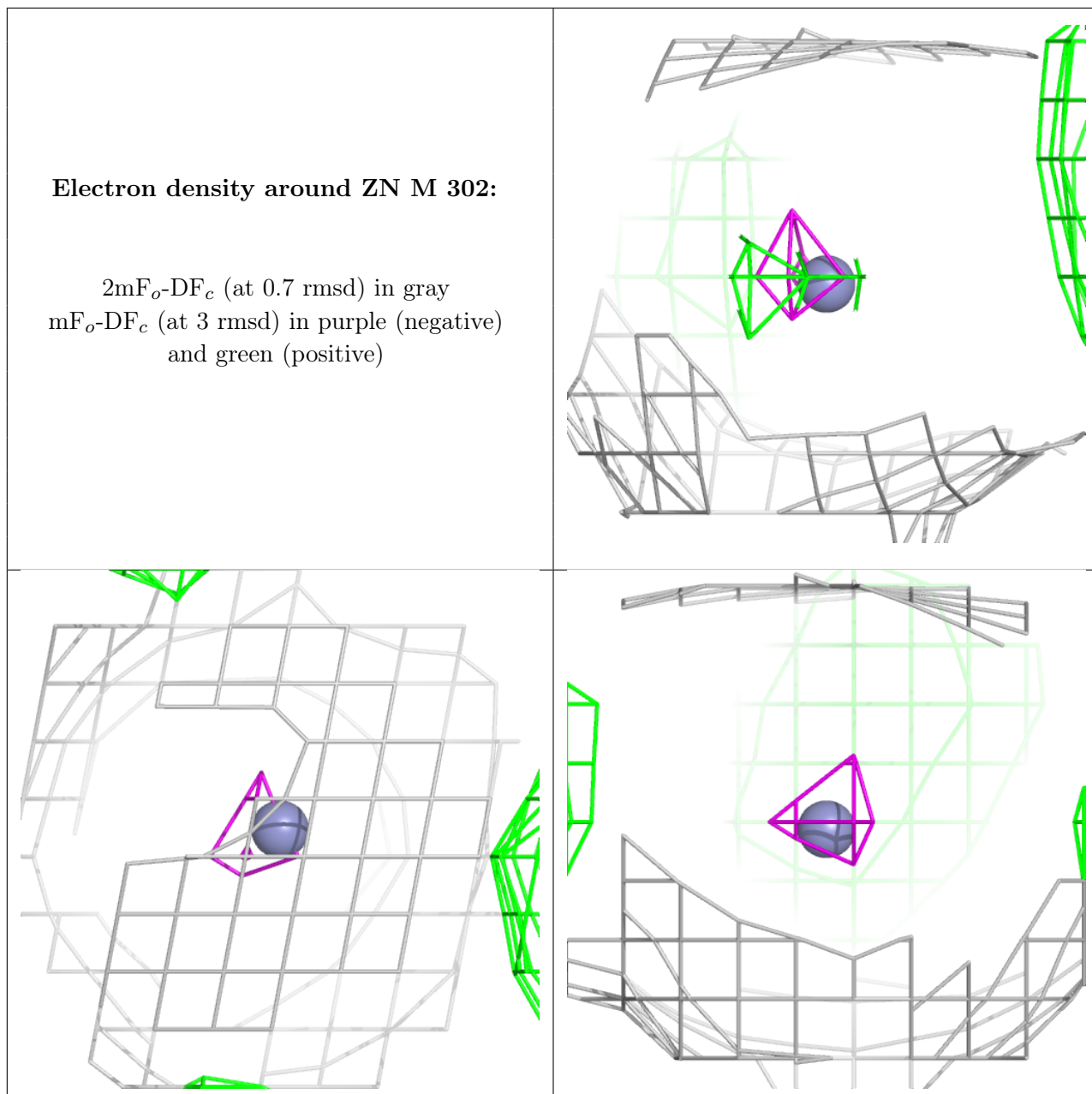






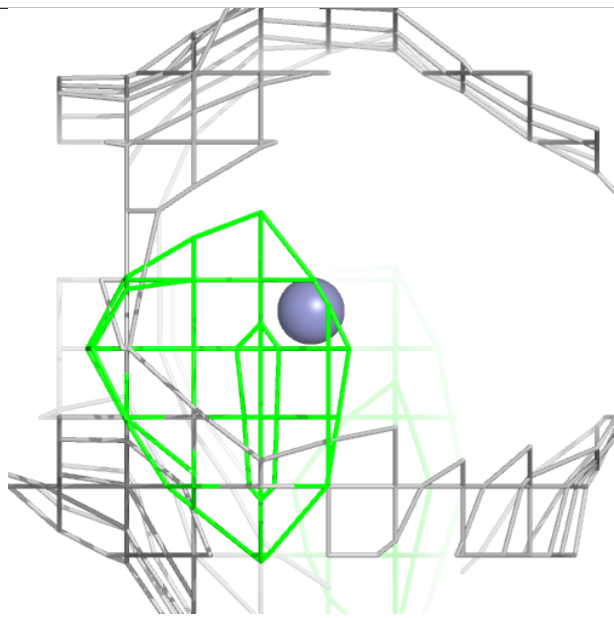
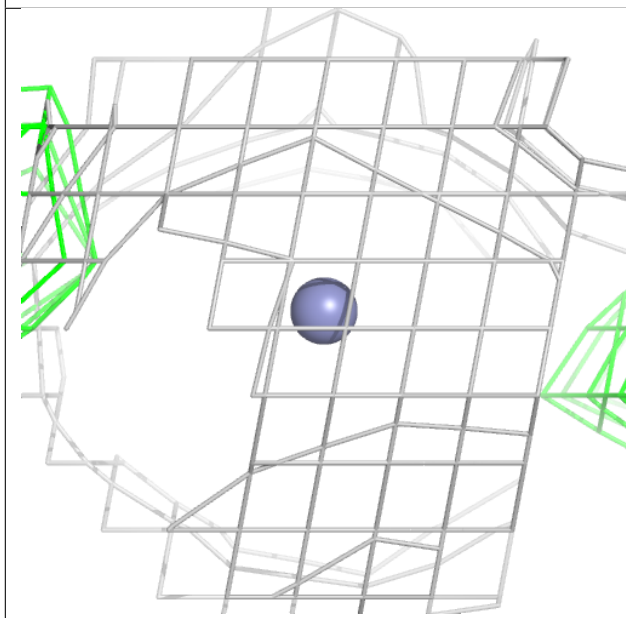
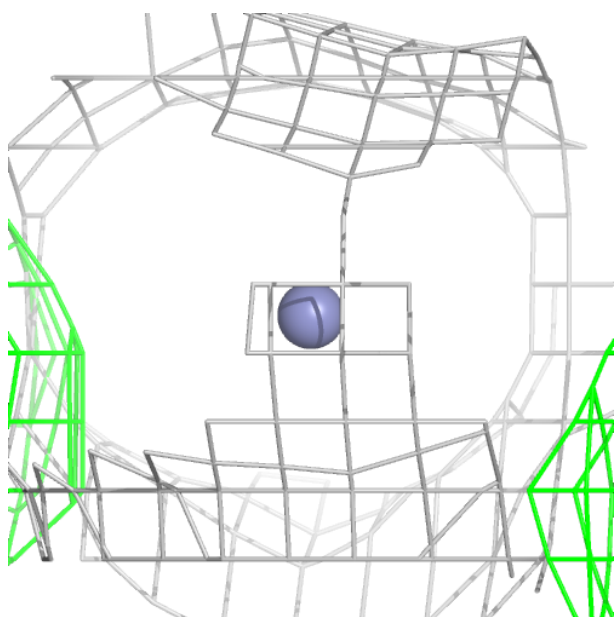
Electron density around ZN M 302:

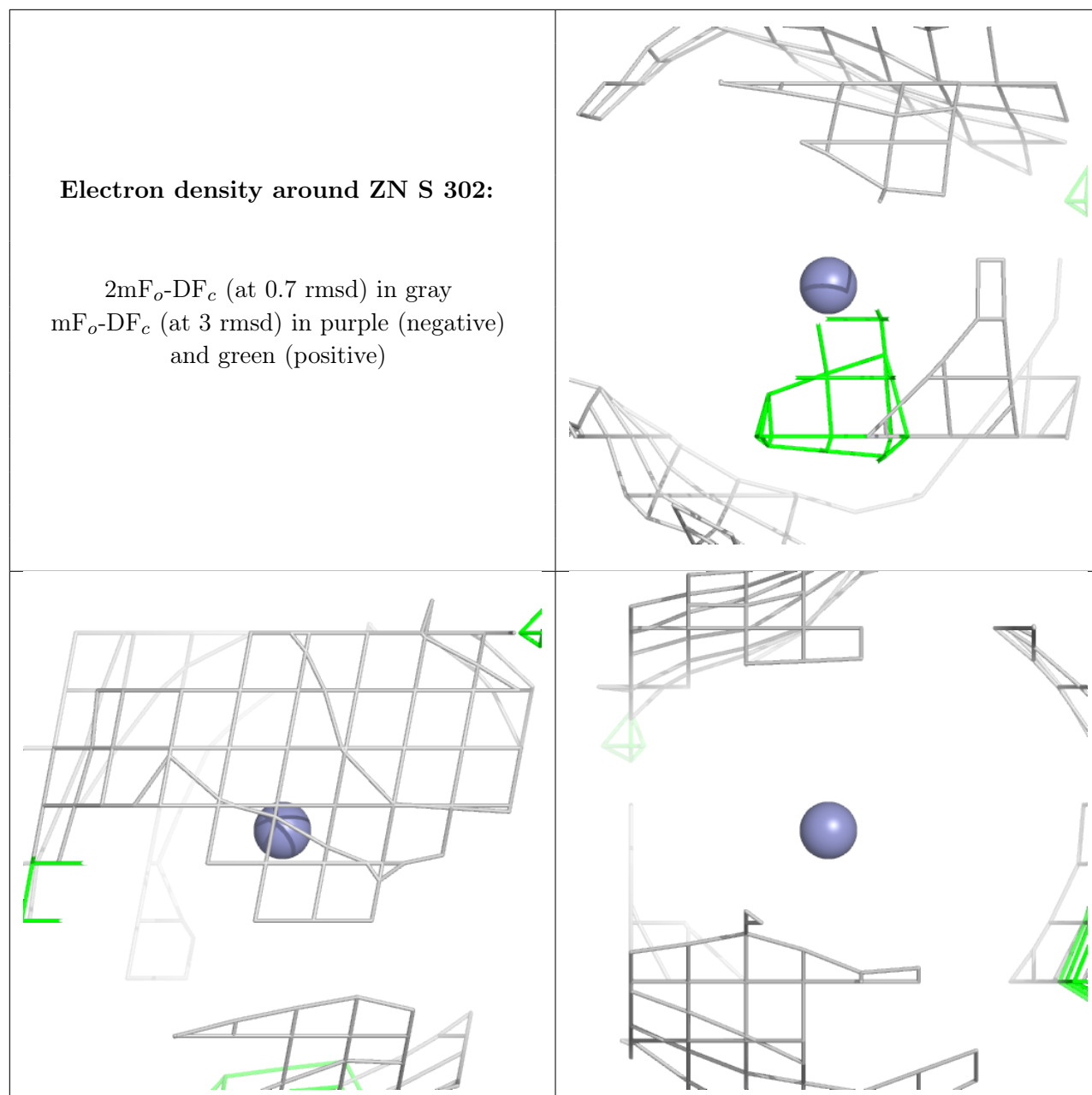
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN P 302:

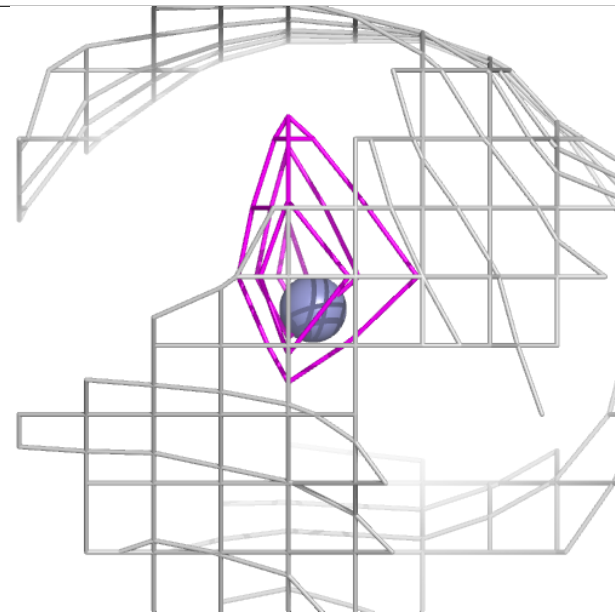
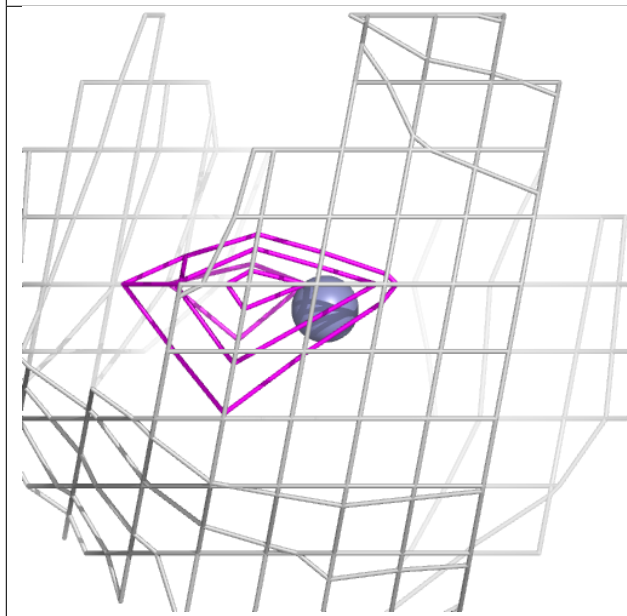
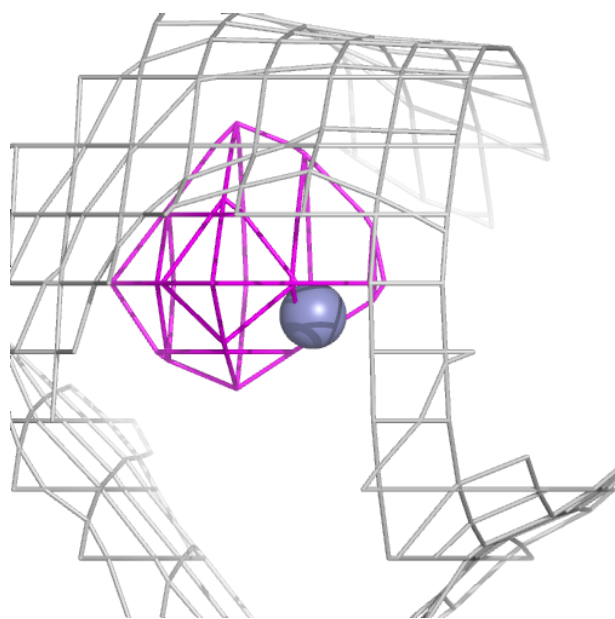
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





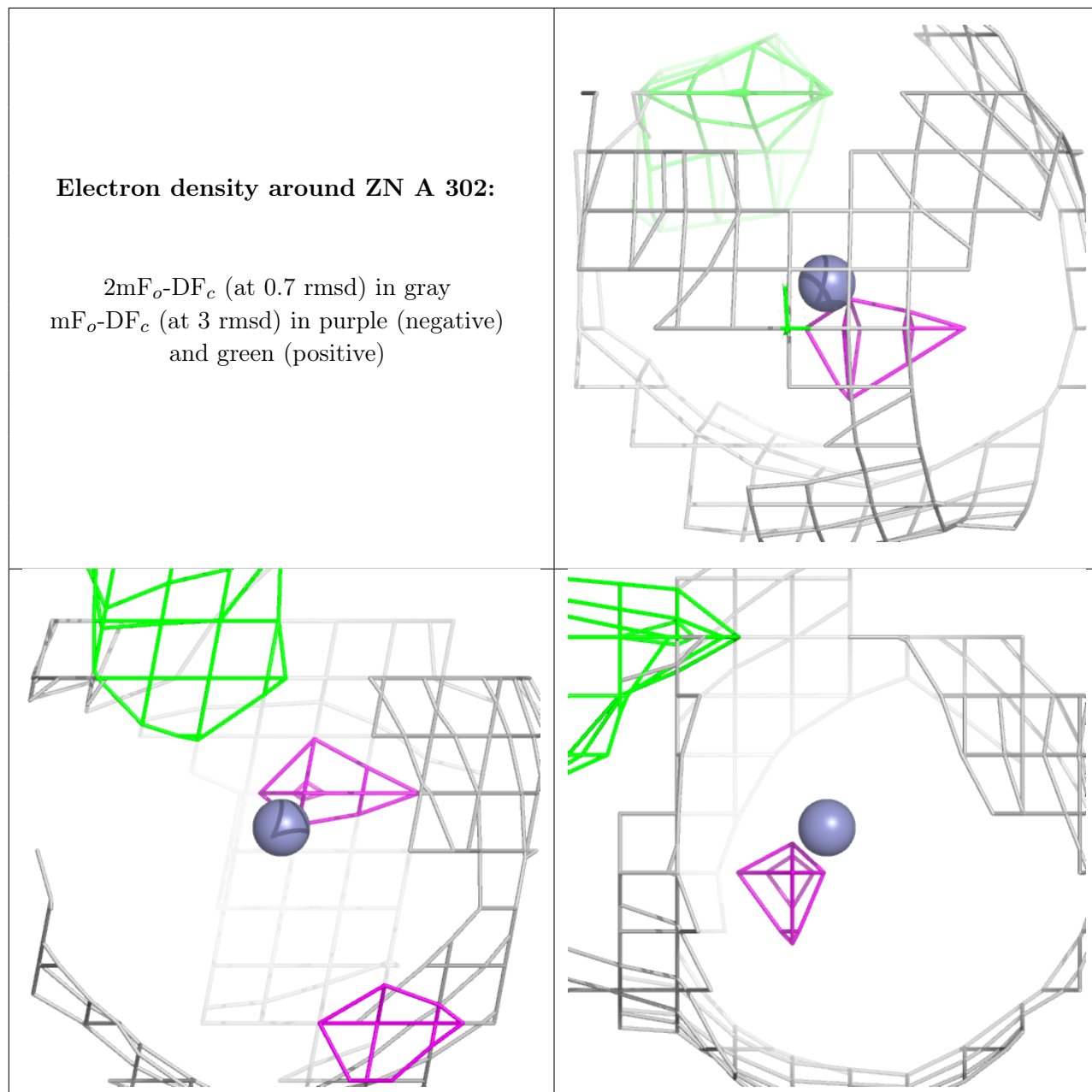
Electron density around ZN V 301:

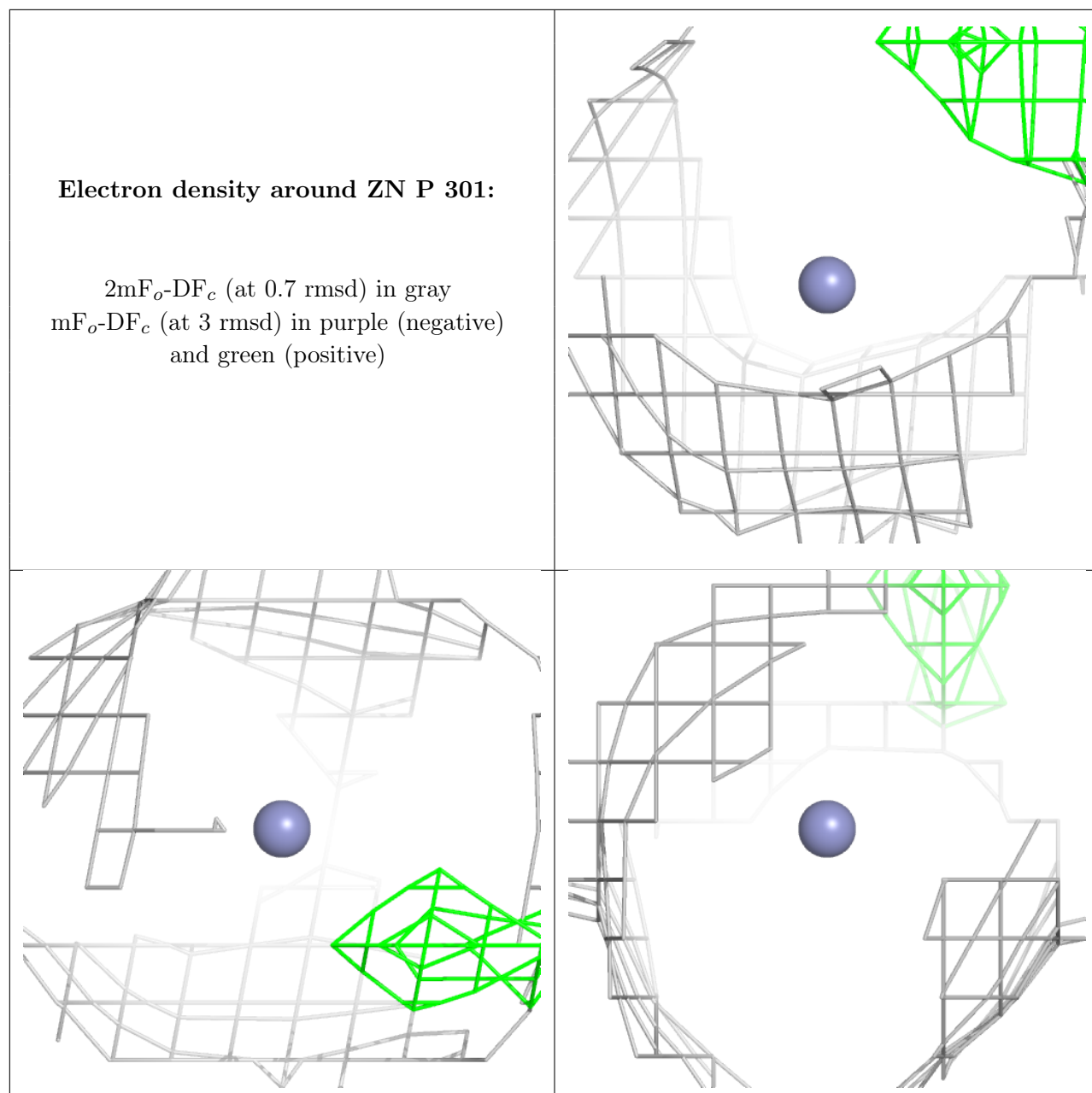
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 302:

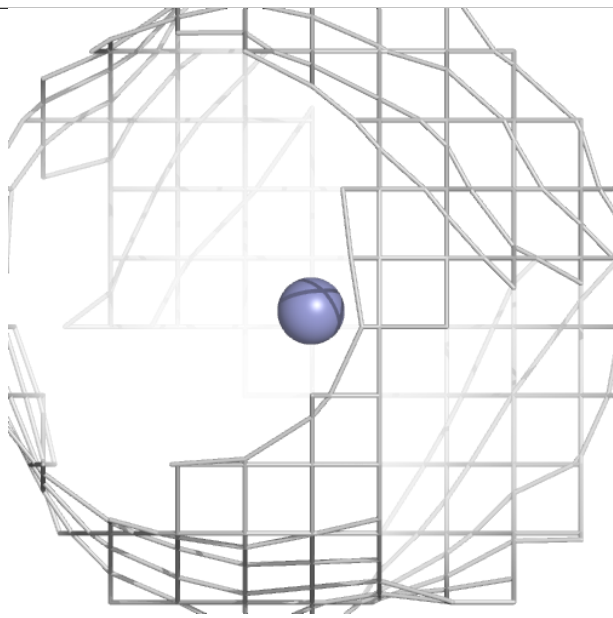
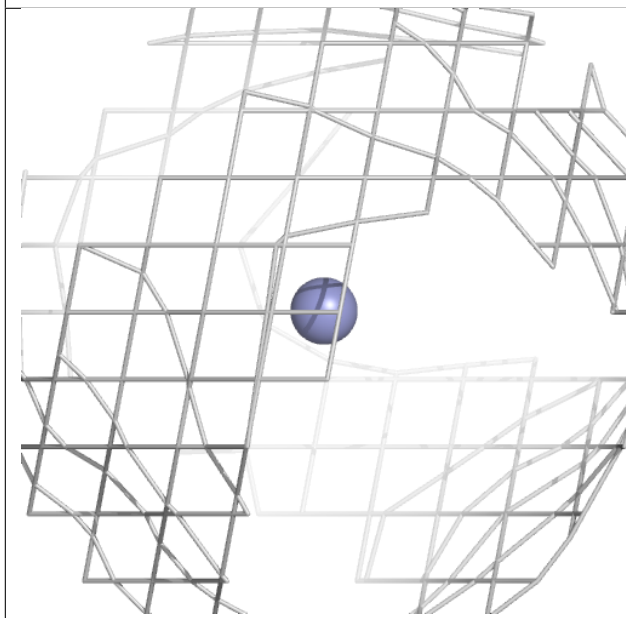
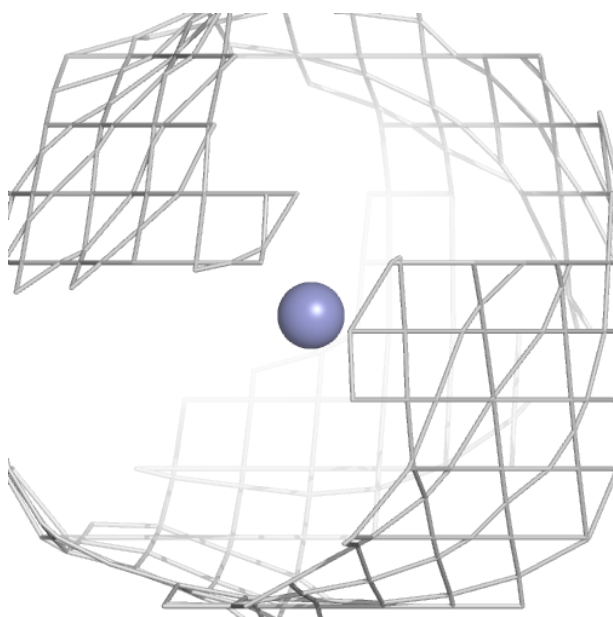
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

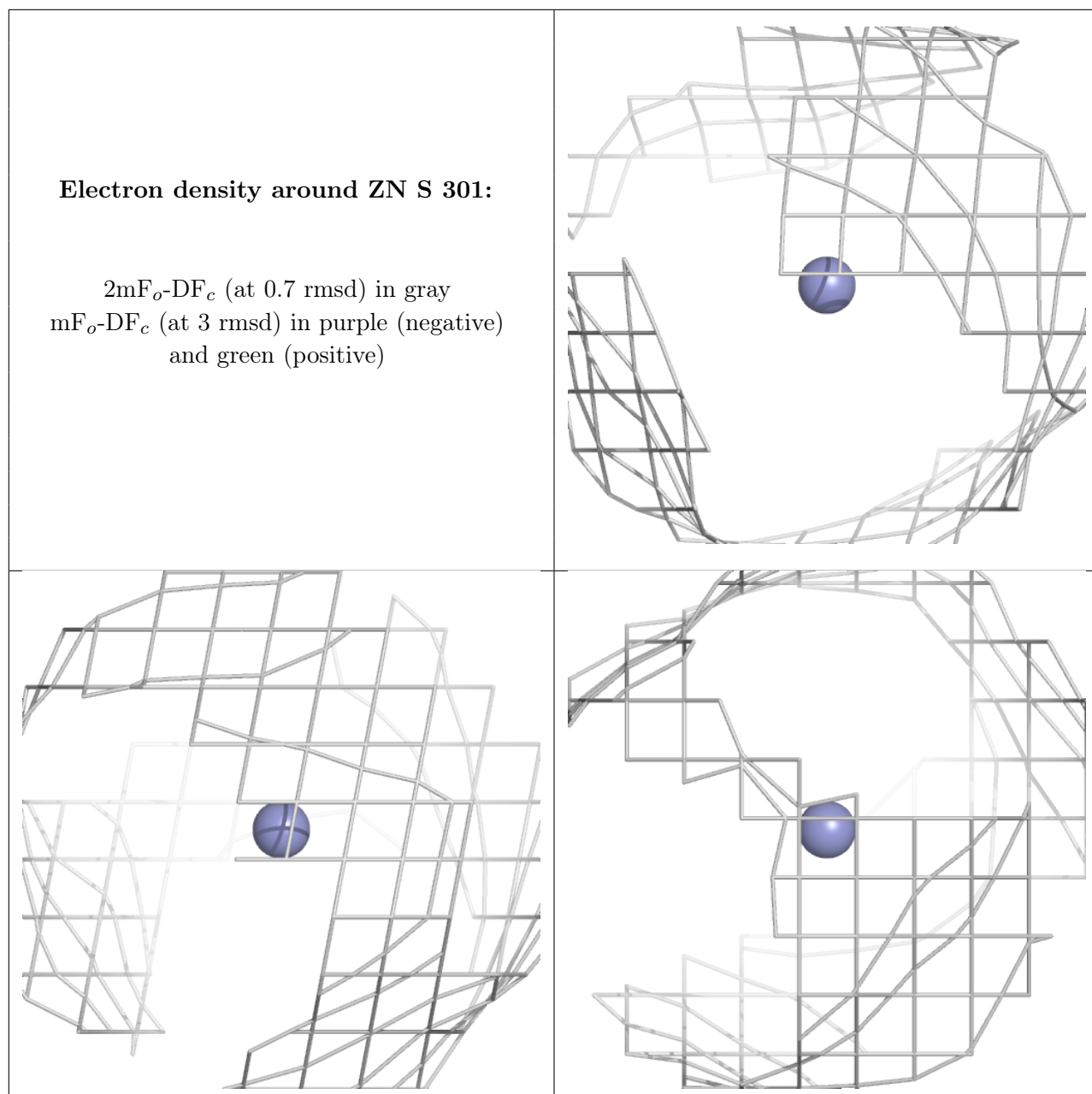


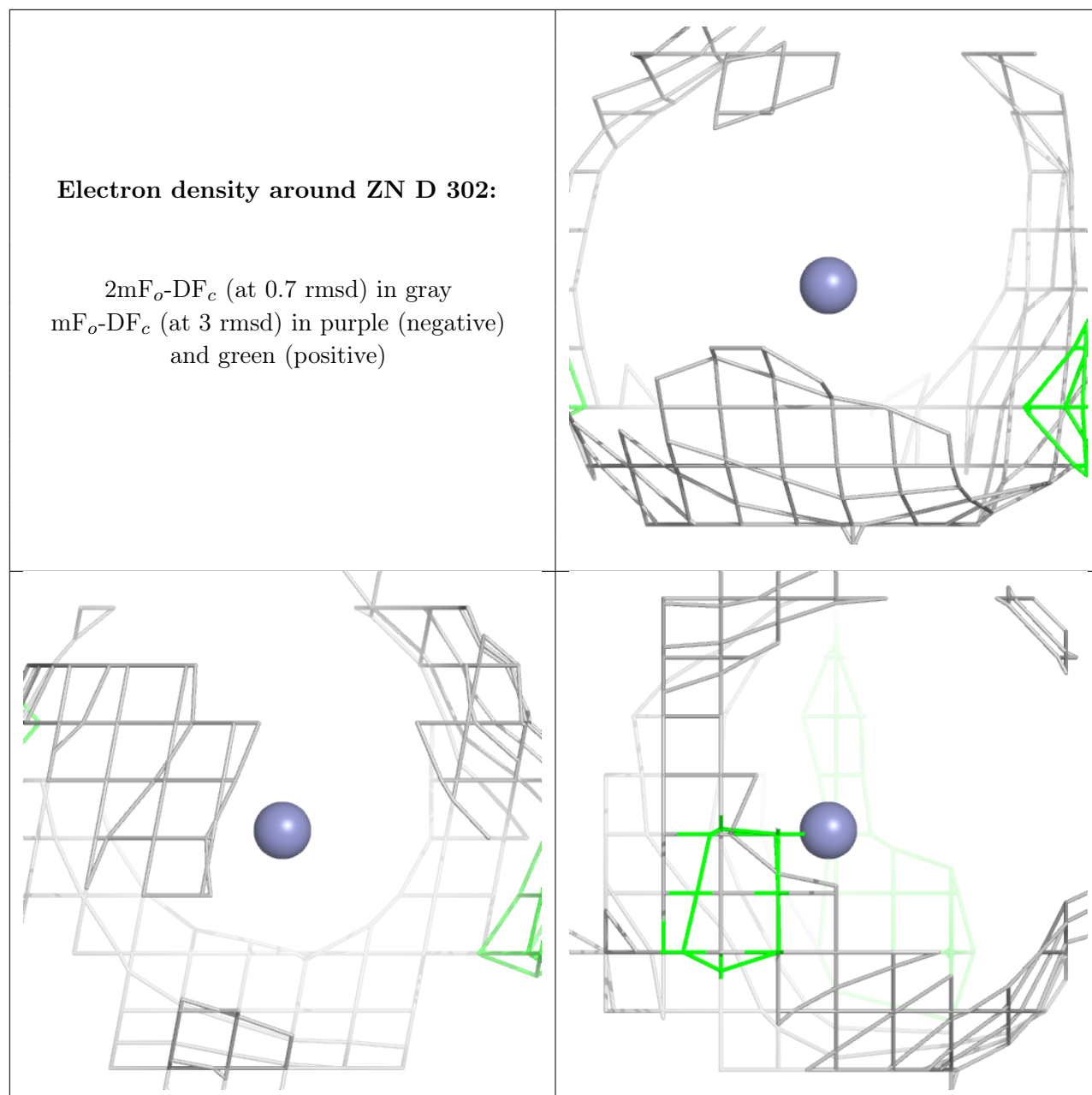


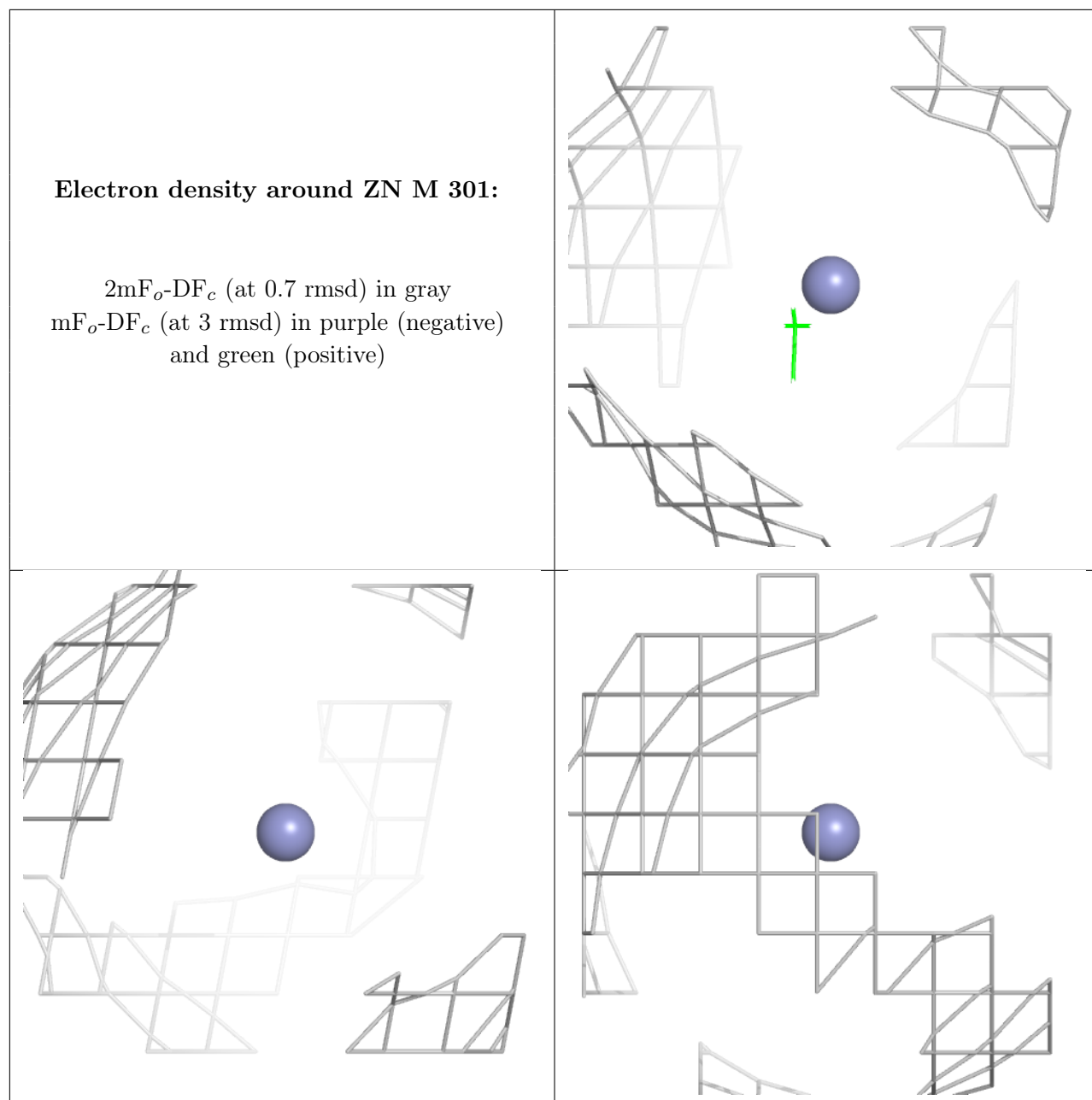
Electron density around ZN D 301:

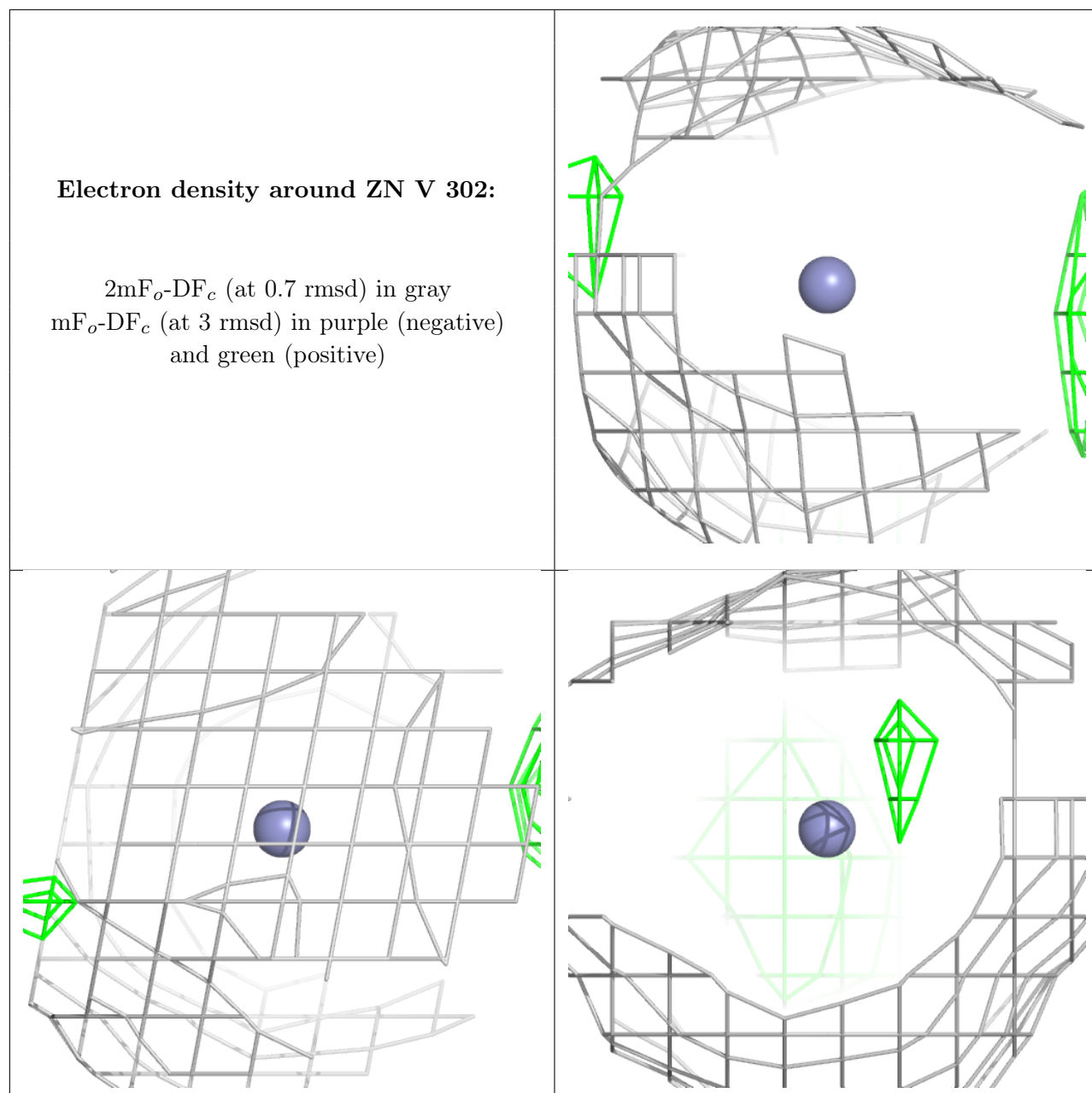
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

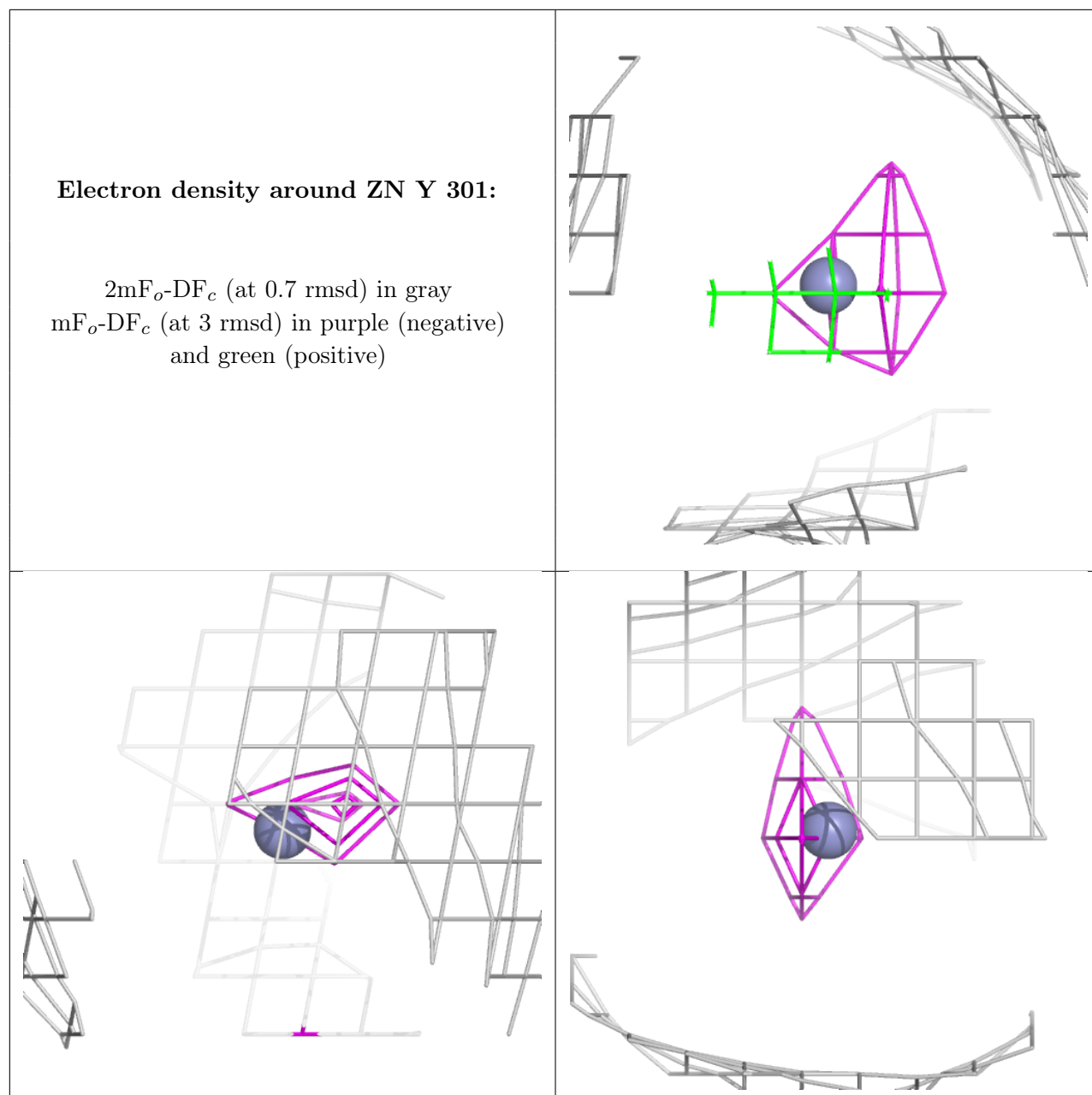


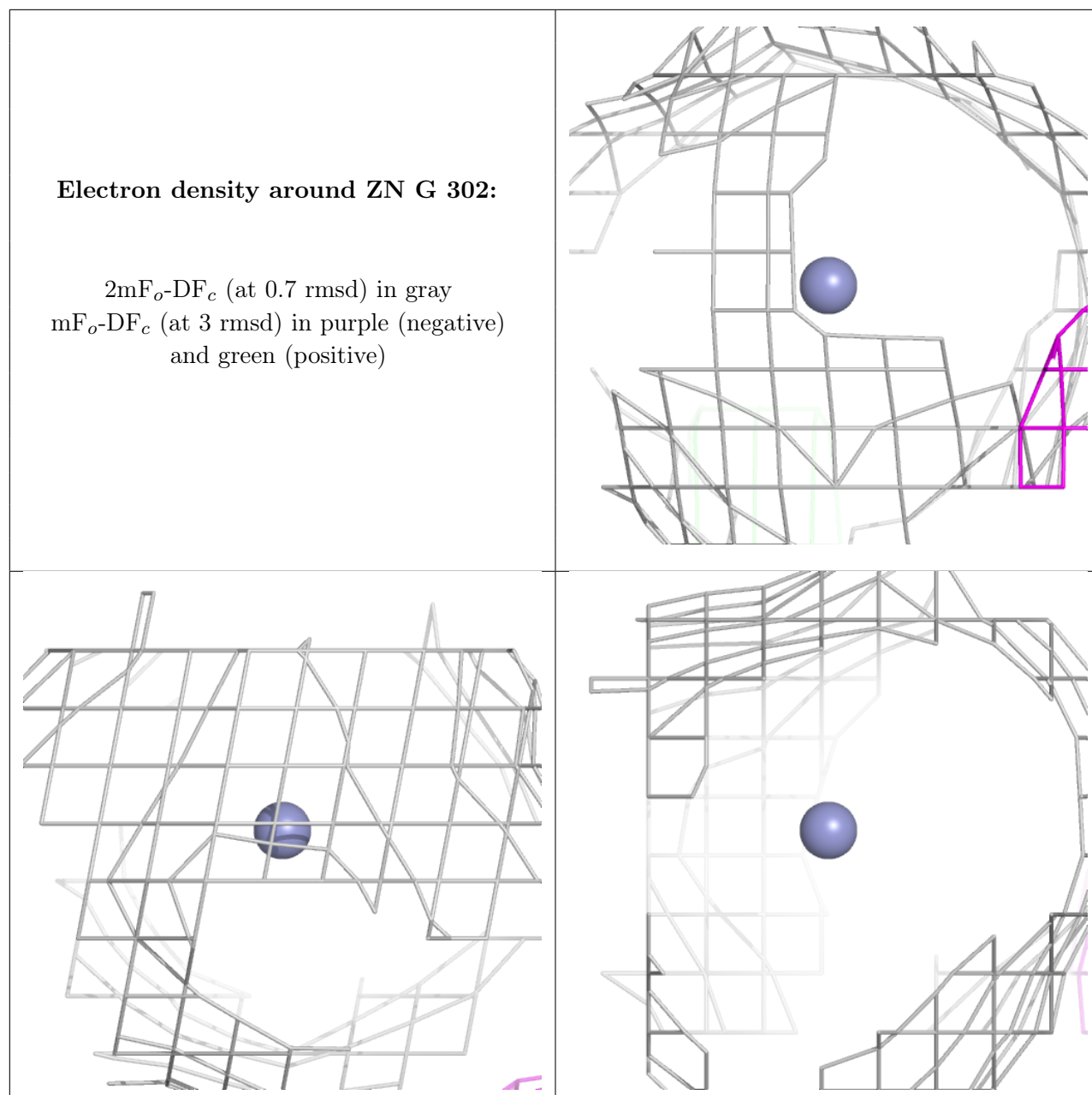






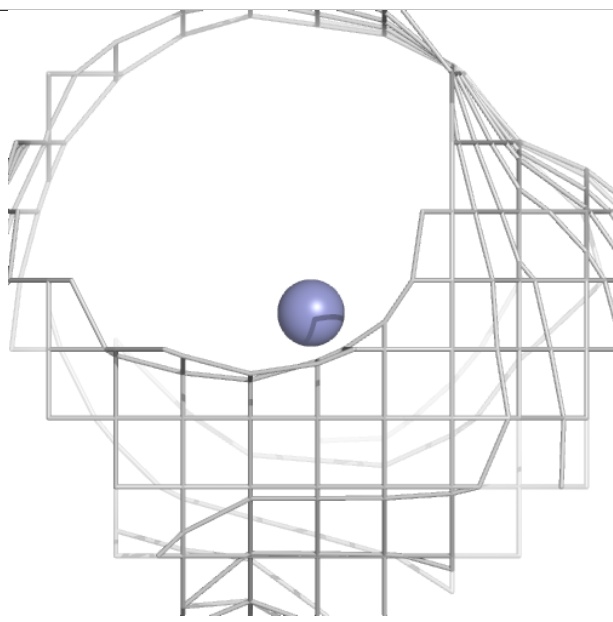
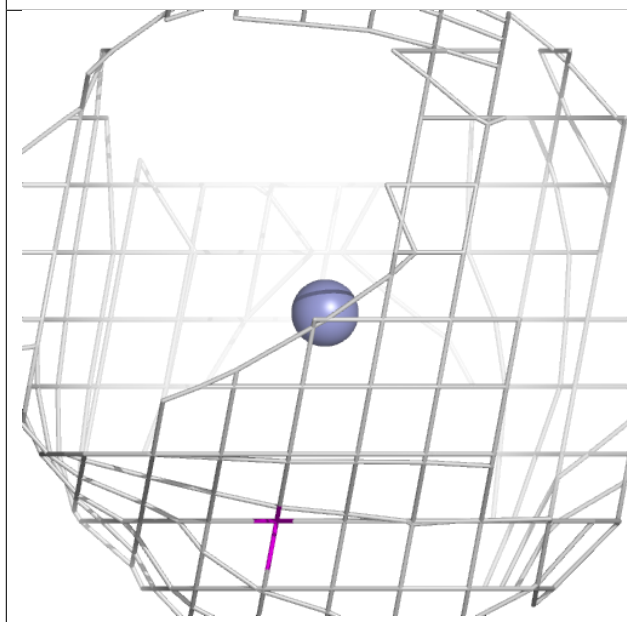
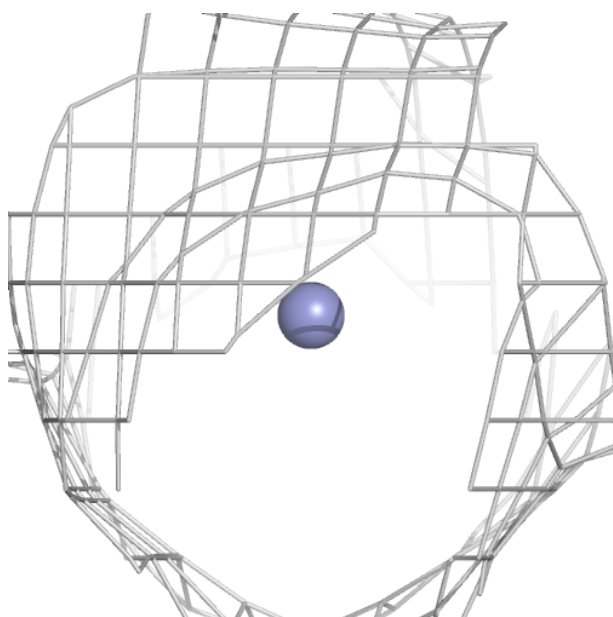


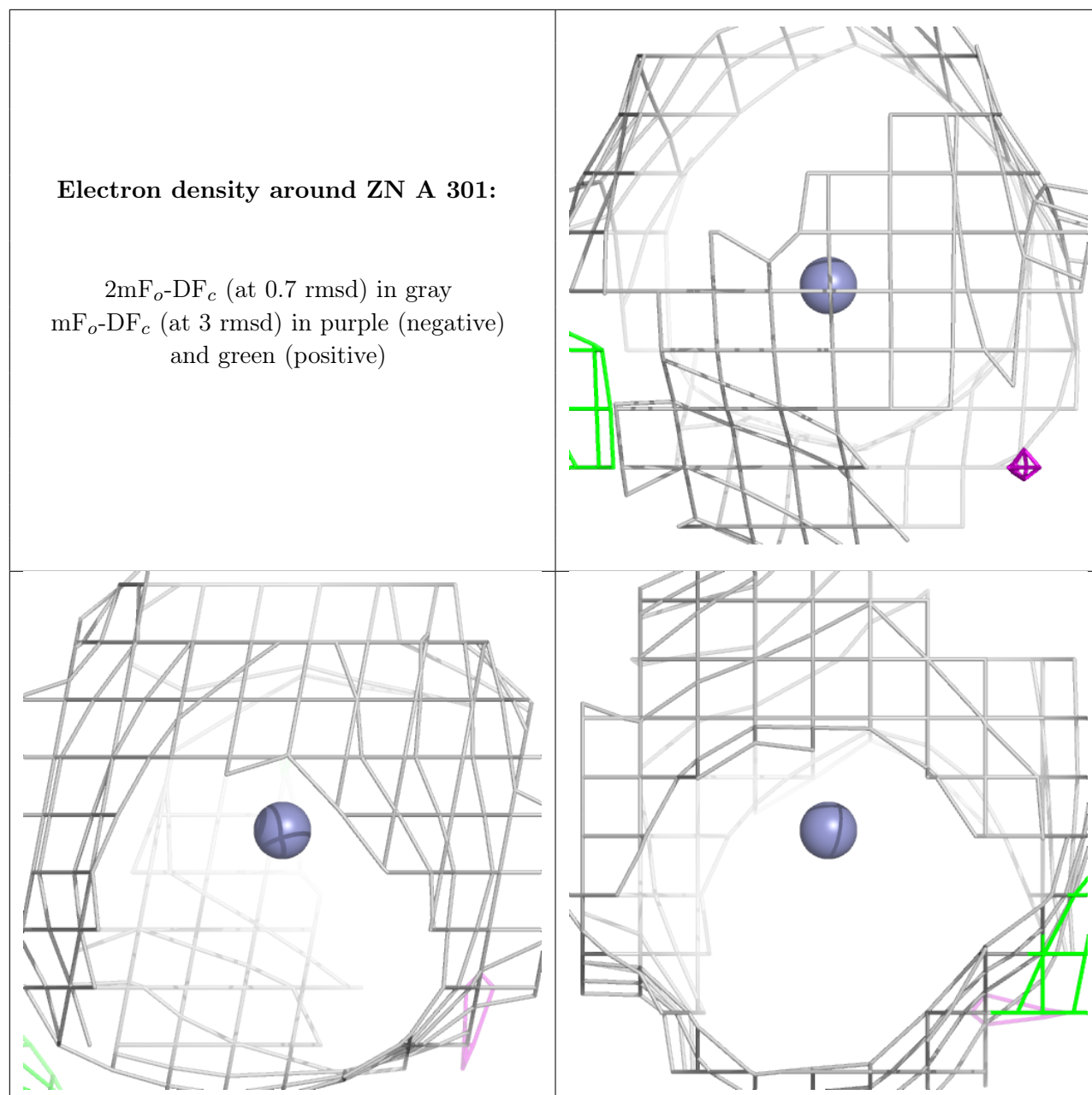




Electron density around ZN G 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.