wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2024 – 04:36 pm BST

PDB ID	:	8RXB
Title	:	Human UPF1 CH domain in complex with SMG6 peptide
Authors	:	Langer, L.; Basquin, J.; Conti, E.
Deposited on	:	2024-02-06
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

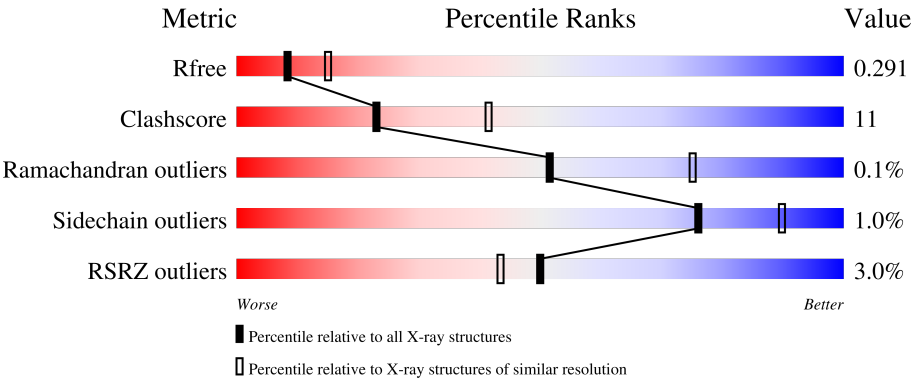
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	173	2% 71% 14% 15%
1	D	173	3% 64% 20% • 16%
1	E	173	% 66% 19% • 14%
1	I	173	2% 70% 15% 15%
1	L	173	2% 75% 9% 16%

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Mol	Chain	Length	Quality of chain
1	P	173	4% 67% 17% 16%
2	B	15	13% 40% 13% 47%
2	F	15	27% 27% 47%
2	G	15	27% 27% 47%
2	J	15	13% 40% 47%
2	N	15	7% 27% 27% 47%
2	Q	15	13% 33% 20% 47%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14051 atoms, of which 6856 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 Regulator of nonsense transcripts 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	148	Total	C	H	N	O	S	0	0	0
			2234	726	1083	207	206	12			
1	A	147	Total	C	H	N	O	S	0	0	0
			2239	725	1089	207	206	12			
1	D	146	Total	C	H	N	O	S	0	0	0
			2225	721	1082	206	204	12			
1	I	147	Total	C	H	N	O	S	0	0	0
			2224	722	1078	206	206	12			
1	L	145	Total	C	H	N	O	S	0	0	0
			2199	715	1069	202	201	12			
1	P	146	Total	C	H	N	O	S	0	0	0
			2233	722	1089	206	204	12			

- Molecule 2 is a protein called Telomerase-binding protein EST1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			
2	B	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			
2	G	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			
2	J	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			
2	N	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			
2	Q	8	Total	C	H	N	O	0	0	0
			114	37	61	8	8			

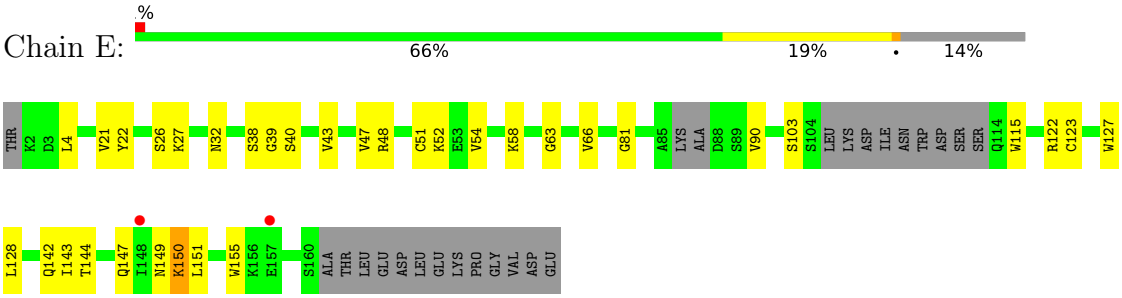
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total Zn 3 3	0	0
3	A	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	L	2	Total Zn 2 2	0	0
3	P	2	Total Zn 2 2	0	0

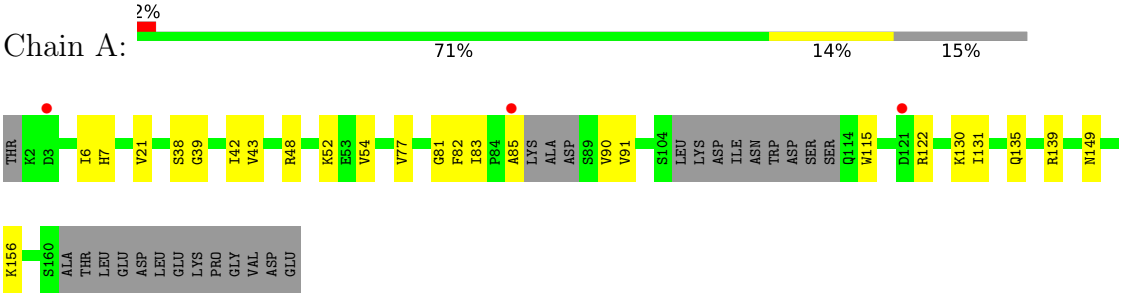
3 Residue-property plots (i)

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.

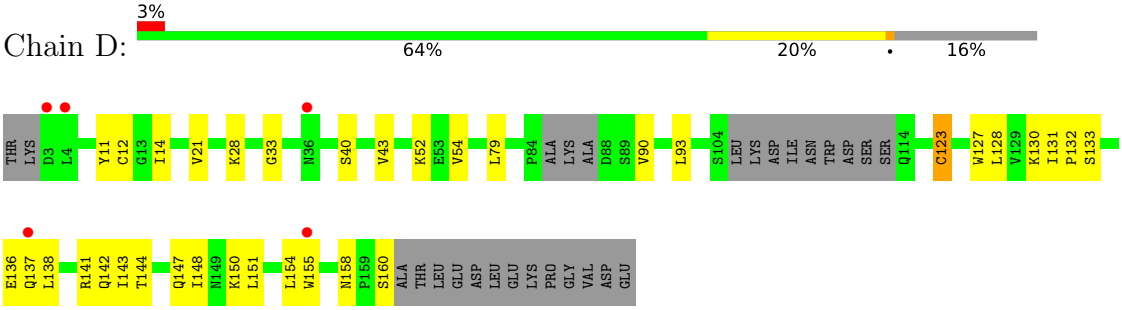
• Molecule 1: Regulator of nonsense transcripts 1



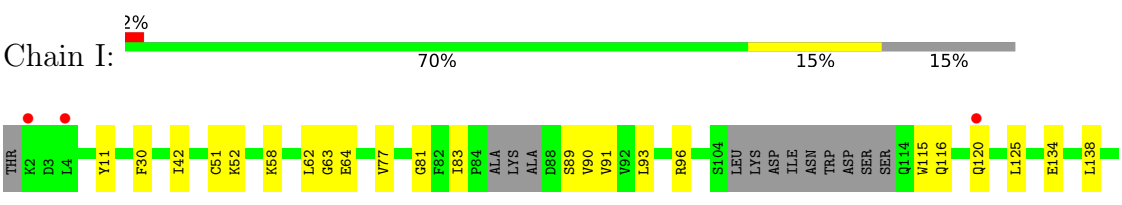
• Molecule 1: Regulator of nonsense transcripts 1

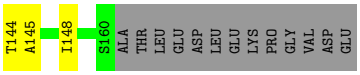


• Molecule 1: Regulator of nonsense transcripts 1



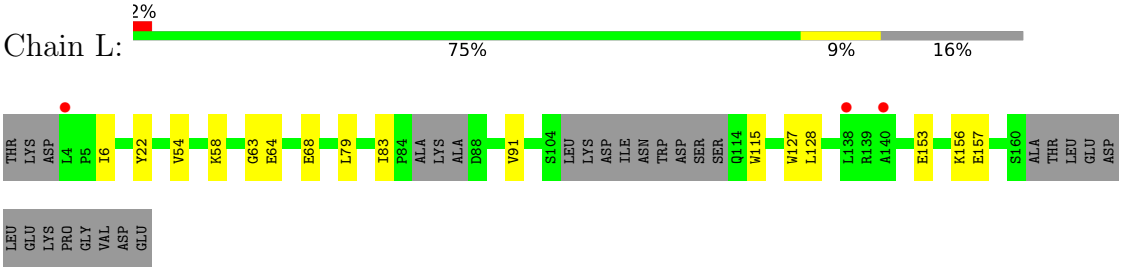
• Molecule 1: Regulator of nonsense transcripts 1





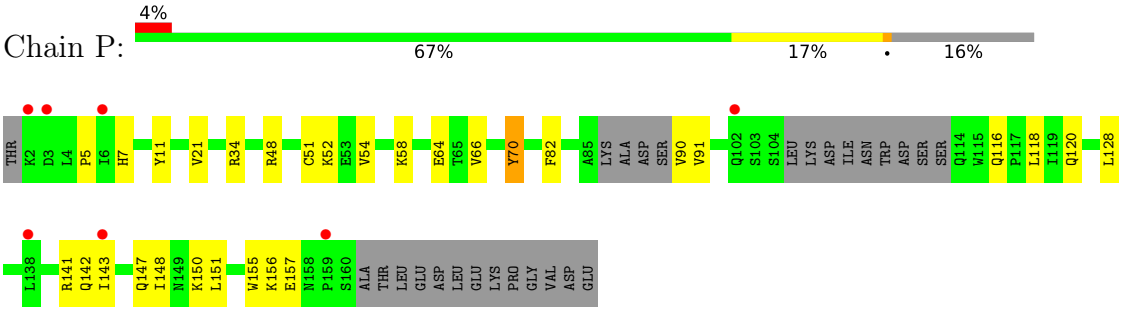
• Molecule 1: Regulator of nonsense transcripts 1

Chain L:



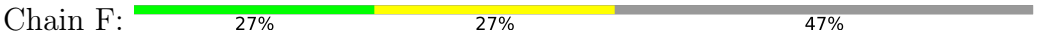
• Molecule 1: Regulator of nonsense transcripts 1

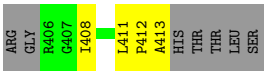
Chain P:



• Molecule 2: Telomerase-binding protein EST1A

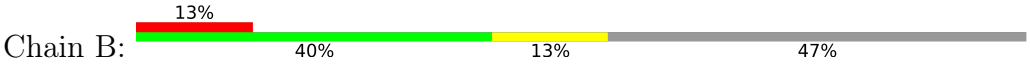
Chain F:

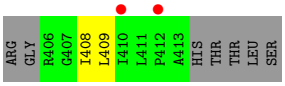




• Molecule 2: Telomerase-binding protein EST1A

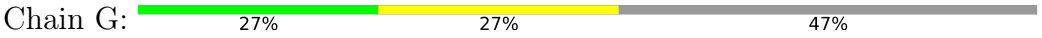
Chain B:

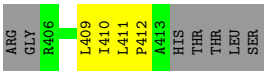




• Molecule 2: Telomerase-binding protein EST1A

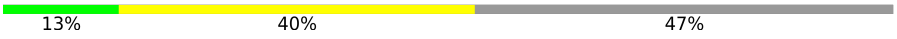
Chain G:

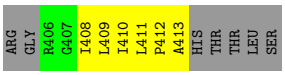




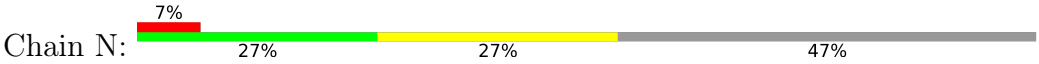
• Molecule 2: Telomerase-binding protein EST1A

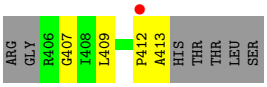
Chain J:



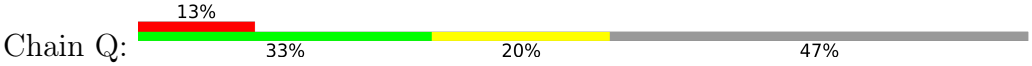


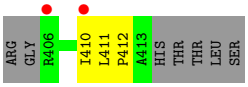
• Molecule 2: Telomerase-binding protein EST1A





• Molecule 2: Telomerase-binding protein EST1A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.17Å 90.68Å 92.29Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	43.44 – 2.60 43.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (43.44-2.60) 97.8 (43.44-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5109	Depositor
R, R_{free}	0.281 , 0.295 0.280 , 0.291	Depositor DCC
R_{free} test set	2001 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14051	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/1175	0.64	0/1593
1	D	0.36	0/1168	0.64	0/1583
1	E	0.36	0/1176	0.65	0/1595
1	I	0.39	0/1171	0.64	0/1589
1	L	0.34	0/1155	0.67	0/1567
1	P	0.38	0/1169	0.69	0/1585
2	B	0.45	0/53	0.81	0/72
2	F	0.37	0/53	0.75	0/72
2	G	0.38	0/53	0.74	0/72
2	J	0.46	0/53	0.76	0/72
2	N	0.46	0/53	1.06	0/72
2	Q	0.31	0/53	0.71	0/72
All	All	0.37	0/7332	0.66	0/9944

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	1150	1089	1125	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1143	1082	1115	35	0
1	E	1151	1083	1121	34	0
1	I	1146	1078	1111	22	0
1	L	1130	1069	1102	15	0
1	P	1144	1089	1120	27	0
2	B	53	61	60	3	0
2	F	53	61	60	3	0
2	G	53	61	60	3	0
2	J	53	61	60	10	0
2	N	53	61	60	4	0
2	Q	53	61	60	4	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	I	2	0	0	0	0
3	L	2	0	0	0	0
3	P	2	0	0	0	0
All	All	7195	6856	7054	163	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 11.

The worst 5 of 163 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:144:THR:HG22	1:D:147:GLN:HG3	1.51	0.93
1:I:62:LEU:HD21	2:J:411:LEU:HD12	1.55	0.89
1:I:62:LEU:HD11	2:J:411:LEU:HD11	1.55	0.87
1:P:151:LEU:HD21	1:P:155:TRP:CZ2	2.15	0.82
1:E:144:THR:HG22	1:E:147:GLN:CD	2.04	0.78

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	141/173 (82%)	140 (99%)	1 (1%)	0	100 100
1	D	140/173 (81%)	138 (99%)	2 (1%)	0	100 100
1	E	142/173 (82%)	140 (99%)	2 (1%)	0	100 100
1	I	141/173 (82%)	138 (98%)	2 (1%)	1 (1%)	22 43
1	L	139/173 (80%)	137 (99%)	2 (1%)	0	100 100
1	P	140/173 (81%)	137 (98%)	3 (2%)	0	100 100
2	B	6/15 (40%)	6 (100%)	0	0	100 100
2	F	6/15 (40%)	6 (100%)	0	0	100 100
2	G	6/15 (40%)	6 (100%)	0	0	100 100
2	J	6/15 (40%)	6 (100%)	0	0	100 100
2	N	6/15 (40%)	6 (100%)	0	0	100 100
2	Q	6/15 (40%)	6 (100%)	0	0	100 100
All	All	879/1128 (78%)	866 (98%)	12 (1%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	89	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	129/155 (83%)	129 (100%)	0	100 100
1	D	128/155 (83%)	126 (98%)	2 (2%)	62 82
1	E	128/155 (83%)	126 (98%)	2 (2%)	62 82
1	I	128/155 (83%)	127 (99%)	1 (1%)	81 92
1	L	126/155 (81%)	126 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	128/155 (83%)	125 (98%)	3 (2%)	50 75
2	B	5/12 (42%)	5 (100%)	0	100 100
2	F	5/12 (42%)	5 (100%)	0	100 100
2	G	5/12 (42%)	5 (100%)	0	100 100
2	J	5/12 (42%)	5 (100%)	0	100 100
2	N	5/12 (42%)	5 (100%)	0	100 100
2	Q	5/12 (42%)	5 (100%)	0	100 100
All	All	797/1002 (80%)	789 (99%)	8 (1%)	76 90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	70	TYR
1	P	48	ARG
1	I	96	ARG
1	D	123	CYS
1	P	34	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	D	135	GLN
1	D	137	GLN
1	I	120	GLN
1	I	158	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 13 ligands modelled in this entry, 13 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	147/173 (84%)	0.02	3 (2%) 65 60	38, 55, 79, 110	0
1	D	146/173 (84%)	0.21	5 (3%) 45 38	42, 65, 94, 107	0
1	E	148/173 (85%)	0.01	2 (1%) 75 71	36, 52, 84, 107	0
1	I	147/173 (84%)	-0.01	3 (2%) 65 60	39, 55, 80, 115	0
1	L	145/173 (83%)	0.08	3 (2%) 63 58	40, 58, 83, 95	0
1	P	146/173 (84%)	0.19	7 (4%) 30 24	45, 65, 100, 119	0
2	B	8/15 (53%)	1.01	2 (25%) 0 0	58, 76, 88, 94	0
2	F	8/15 (53%)	0.06	0 100 100	42, 51, 77, 85	0
2	G	8/15 (53%)	0.36	0 100 100	49, 58, 72, 73	0
2	J	8/15 (53%)	0.03	0 100 100	45, 51, 73, 81	0
2	N	8/15 (53%)	0.04	1 (12%) 3 2	44, 53, 93, 94	0
2	Q	8/15 (53%)	1.24	2 (25%) 0 0	59, 75, 83, 88	0
All	All	927/1128 (82%)	0.10	28 (3%) 50 43	36, 58, 90, 119	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	4	LEU	4.2
2	Q	410	ILE	3.7
1	D	4	LEU	3.6
1	P	3	ASP	3.4
1	A	3	ASP	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

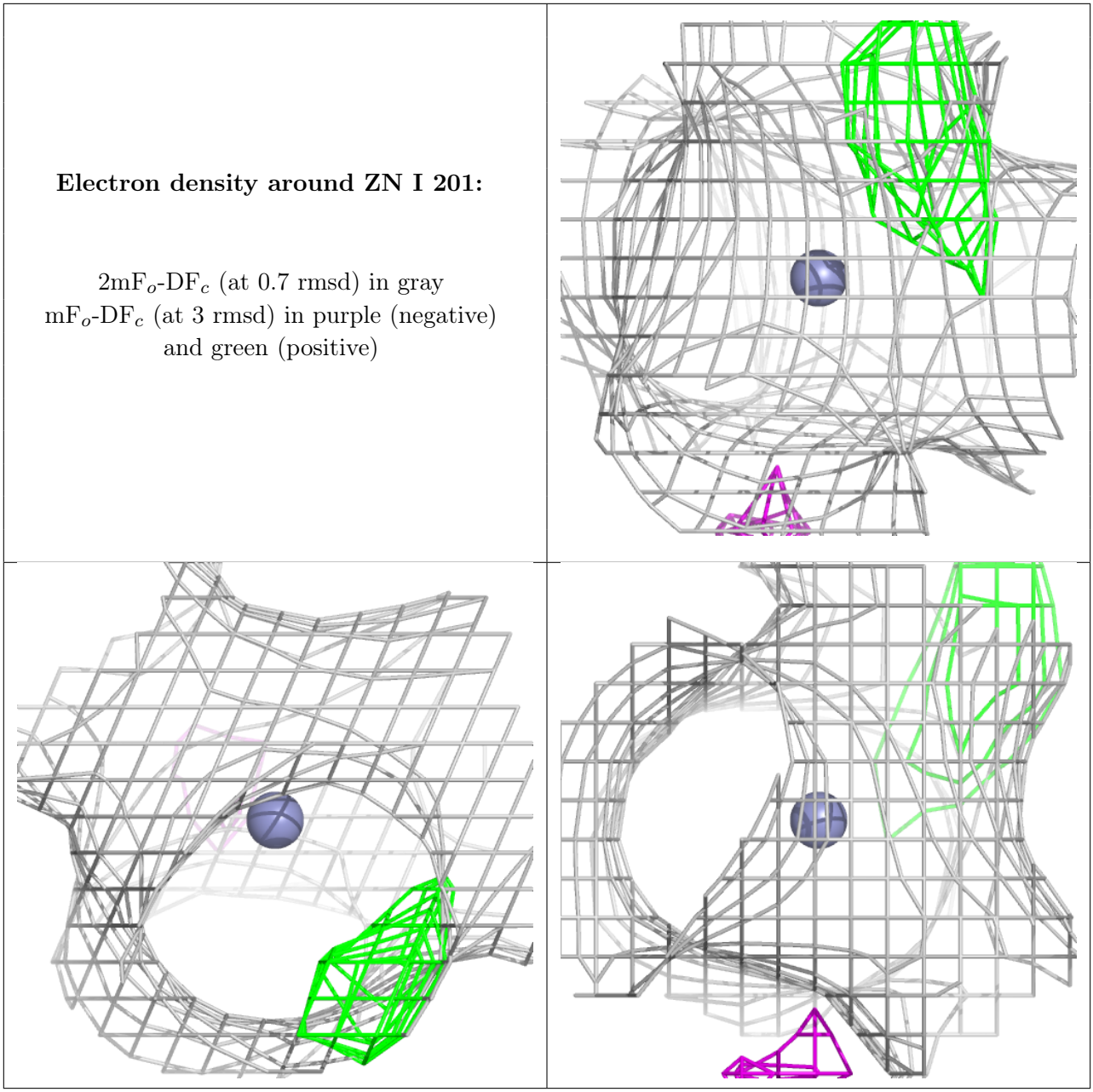
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ZN	I	201	1/1	0.95	0.17	50,50,50,50	0
3	ZN	I	202	1/1	0.96	0.17	47,47,47,47	0
3	ZN	D	202	1/1	0.97	0.17	44,44,44,44	0
3	ZN	L	201	1/1	0.97	0.10	62,62,62,62	0
3	ZN	P	201	1/1	0.97	0.21	53,53,53,53	0
3	ZN	E	203	1/1	0.98	0.12	76,76,76,76	0
3	ZN	A	202	1/1	0.98	0.19	52,52,52,52	0
3	ZN	D	201	1/1	0.98	0.17	61,61,61,61	0
3	ZN	E	202	1/1	0.98	0.20	49,49,49,49	0
3	ZN	P	202	1/1	0.98	0.15	45,45,45,45	0
3	ZN	L	202	1/1	0.99	0.16	52,52,52,52	0
3	ZN	E	201	1/1	0.99	0.23	45,45,45,45	0
3	ZN	A	201	1/1	0.99	0.18	42,42,42,42	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.

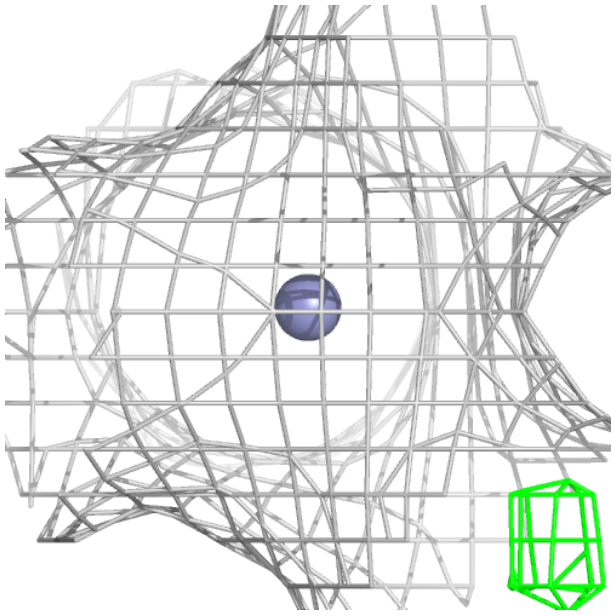
Electron density around ZN I 201:

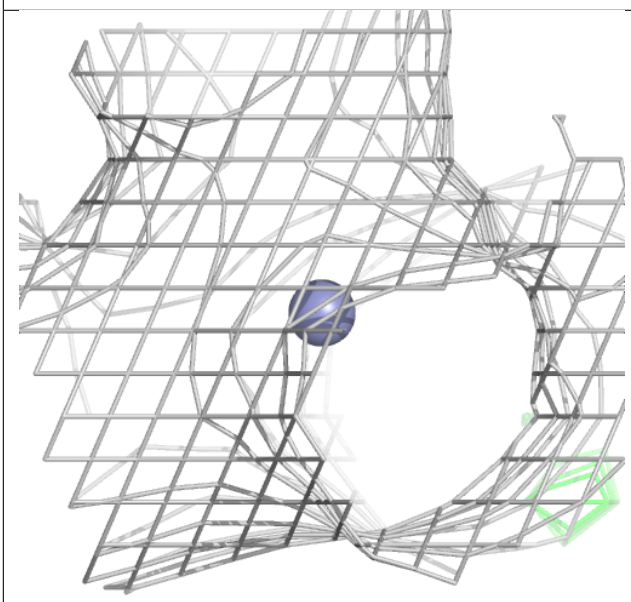
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

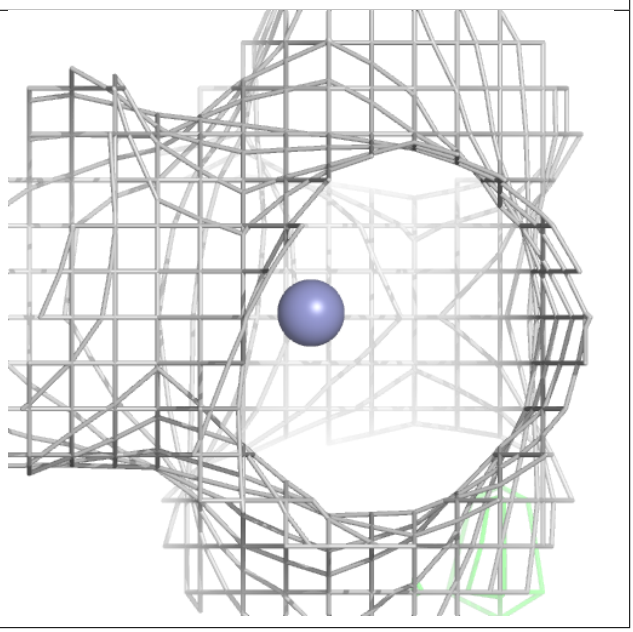


Electron density around ZN I 202:

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

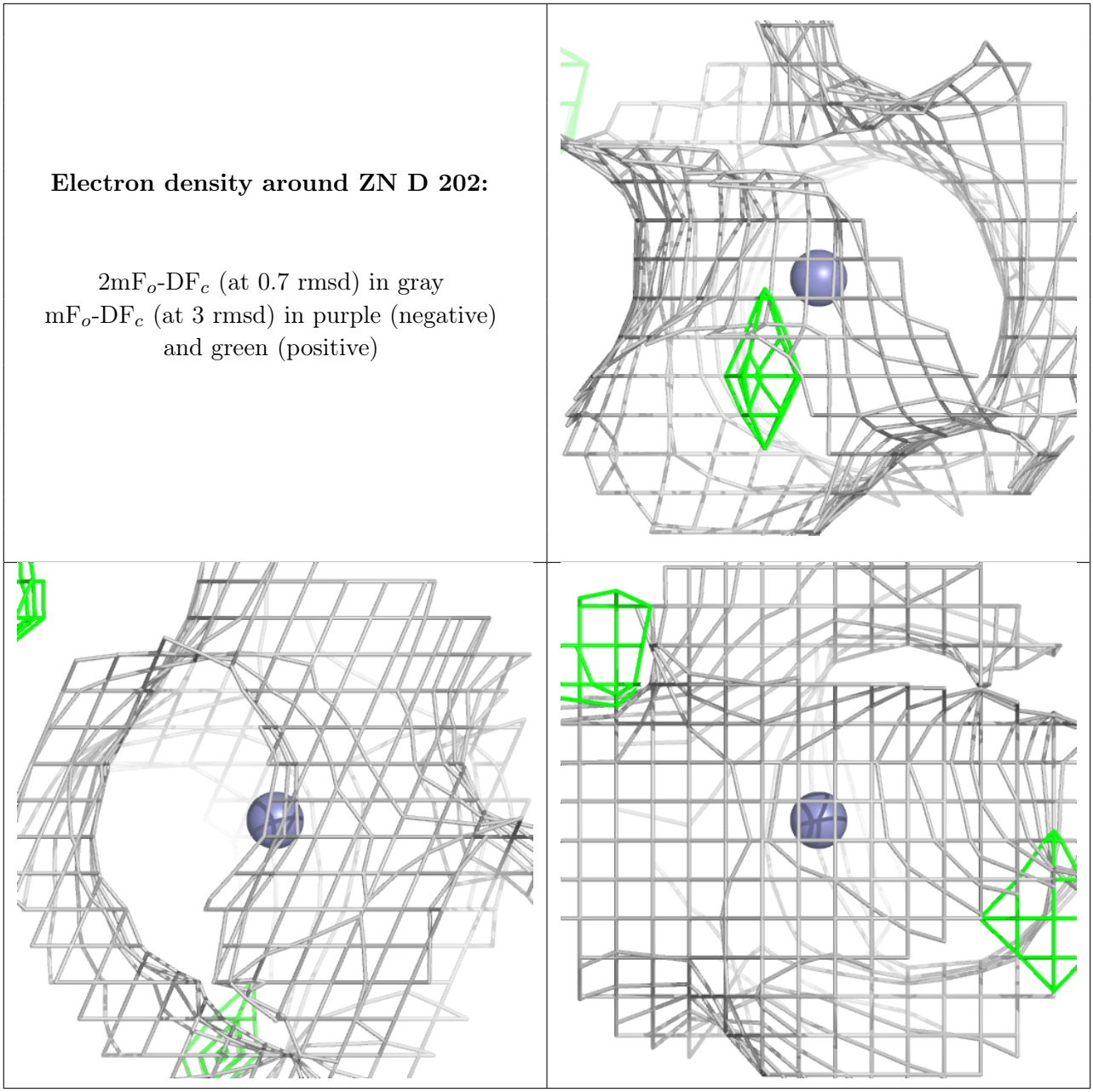






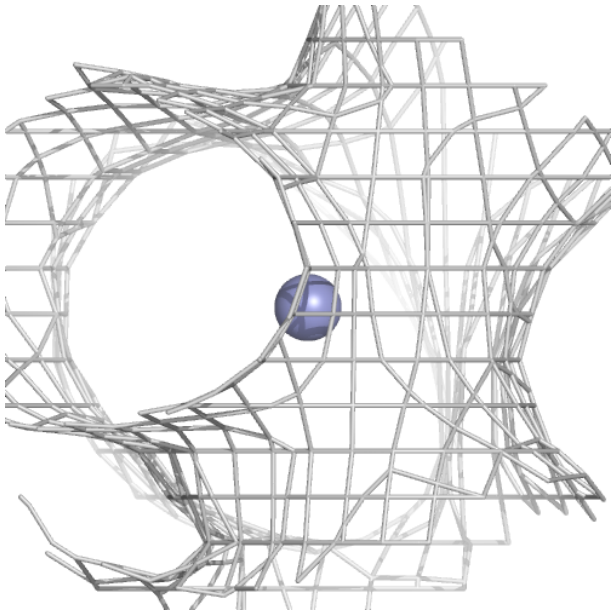
Electron density around ZN D 202:

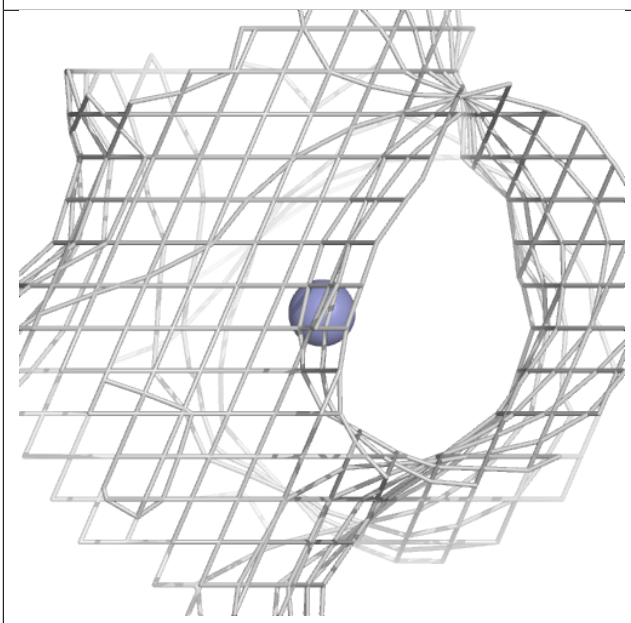
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

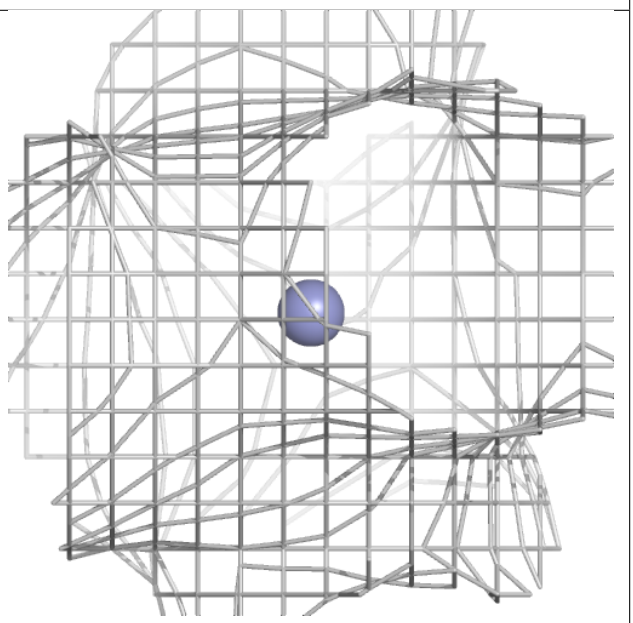


Electron density around ZN L 201:

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

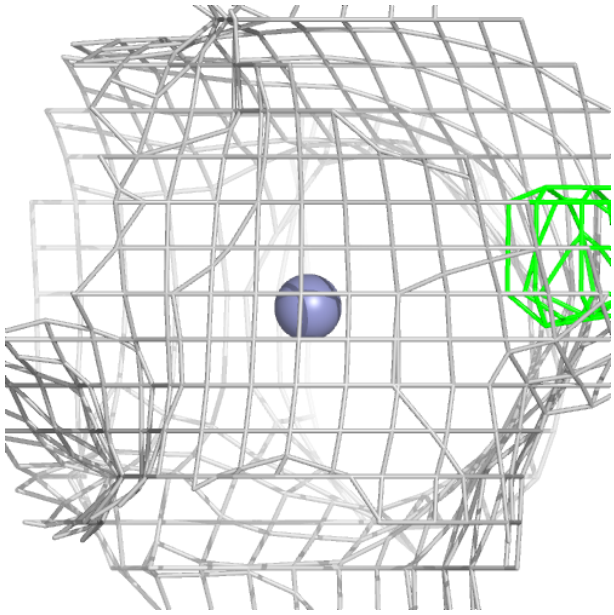


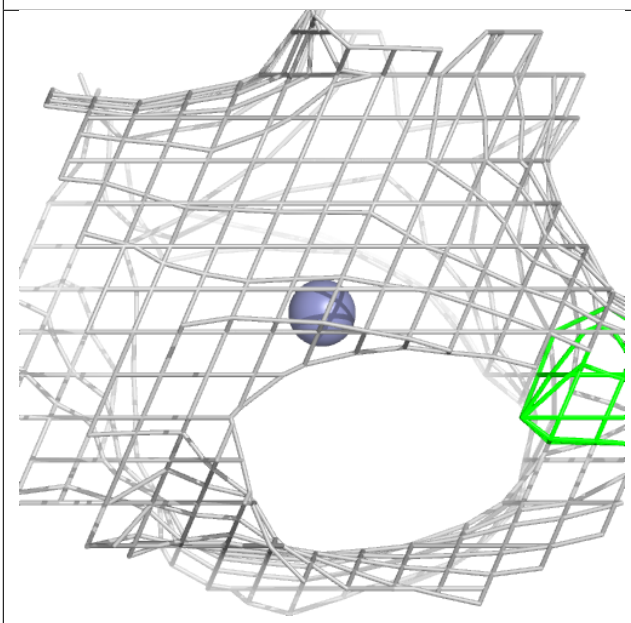


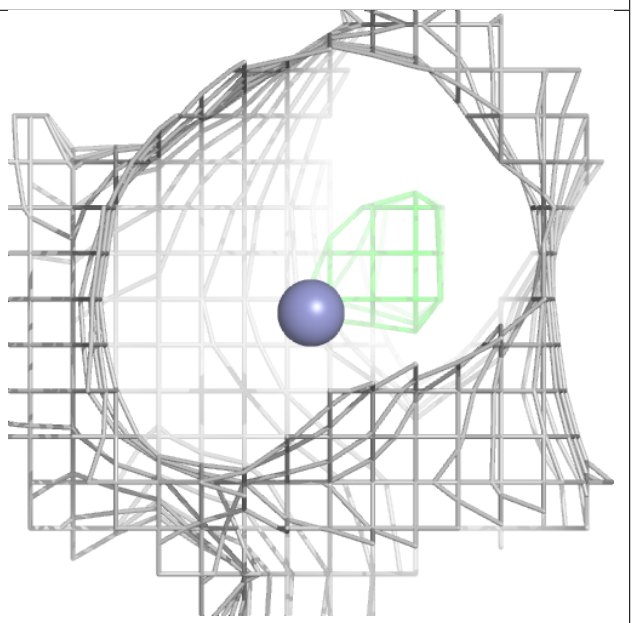


Electron density around ZN P 201:

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

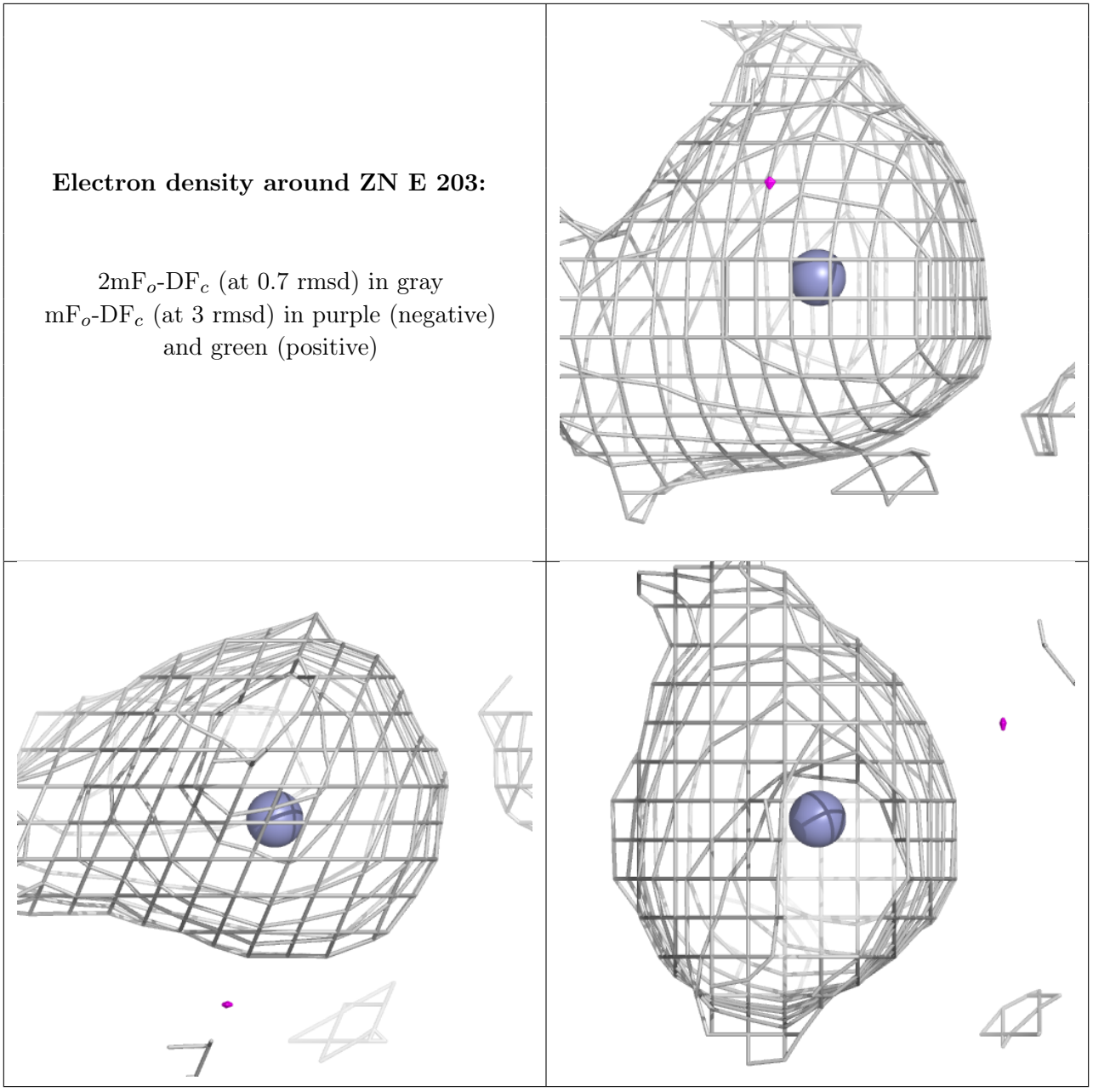






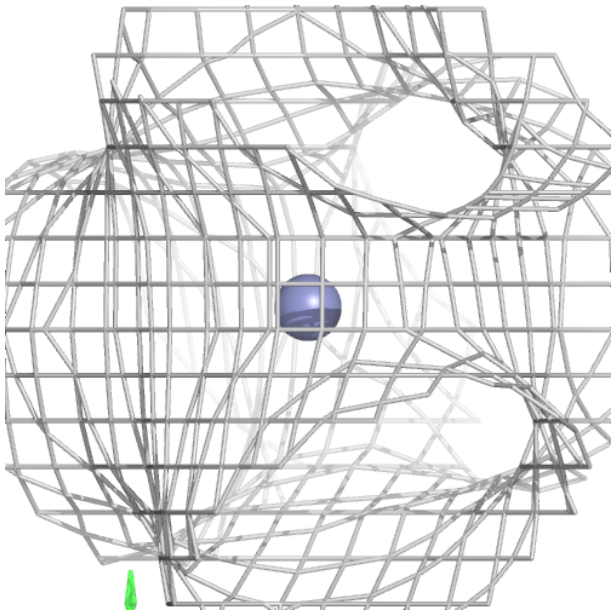
Electron density around ZN E 203:

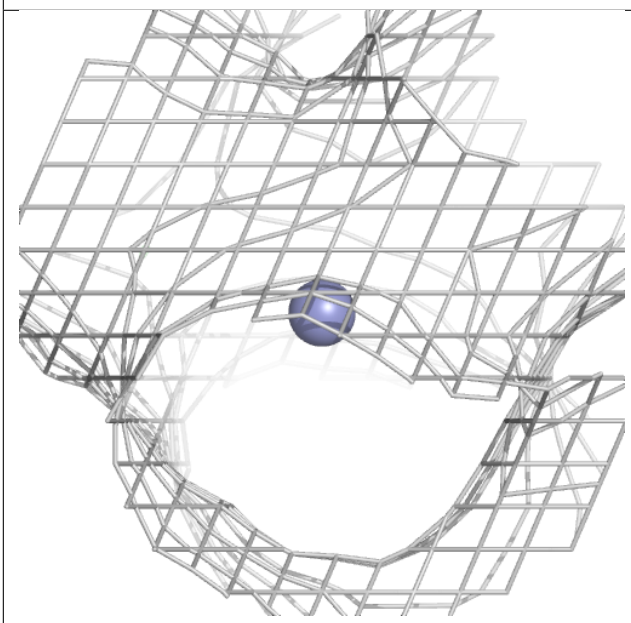
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

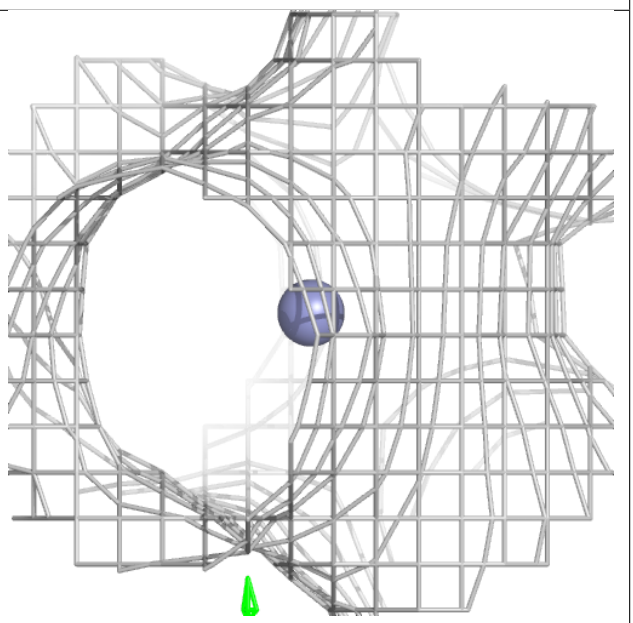


Electron density around ZN A 202:

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

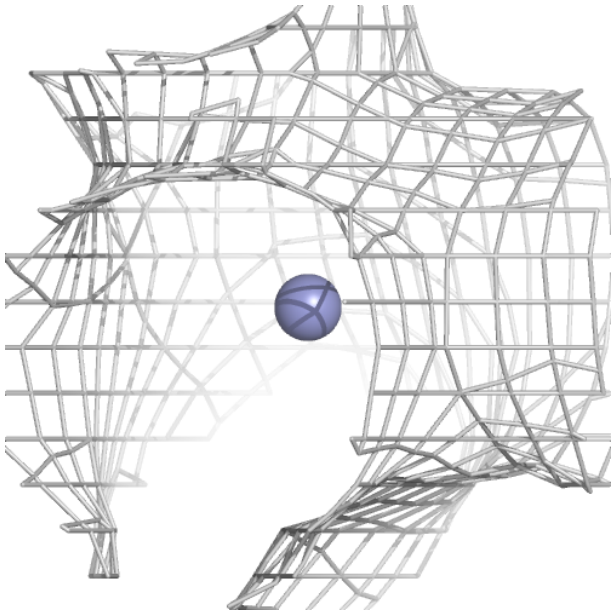


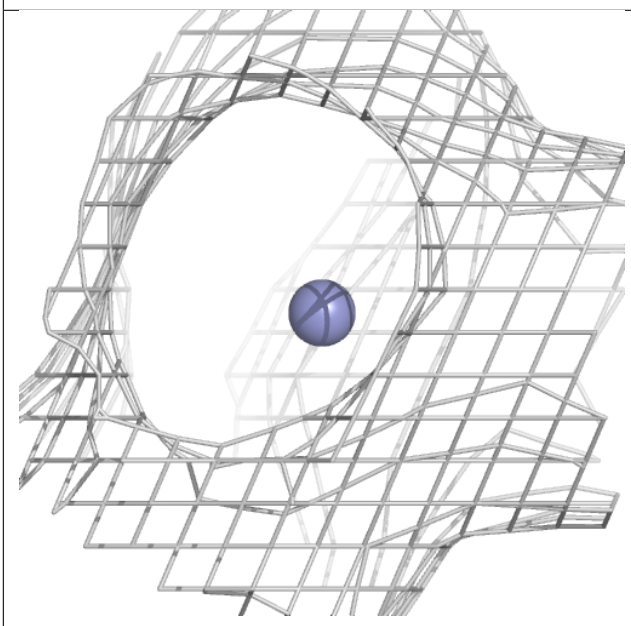


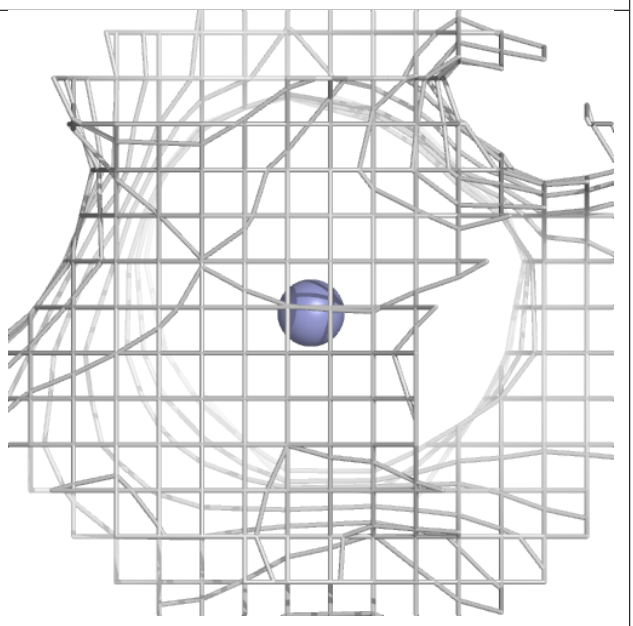


Electron density around ZN D 201:

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

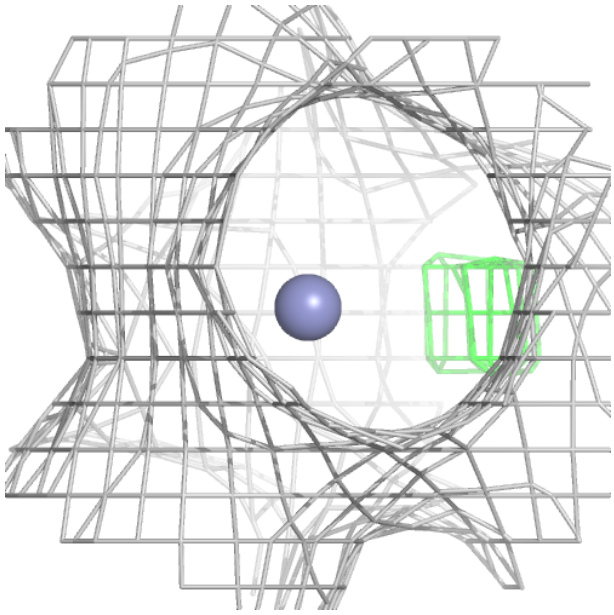


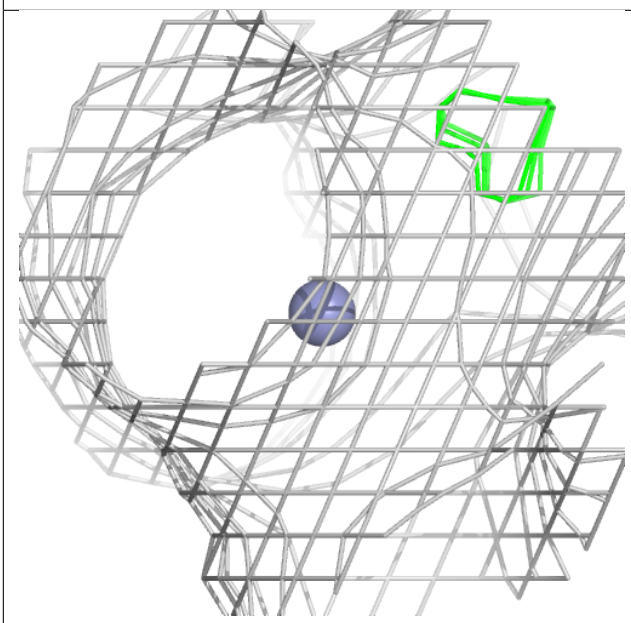


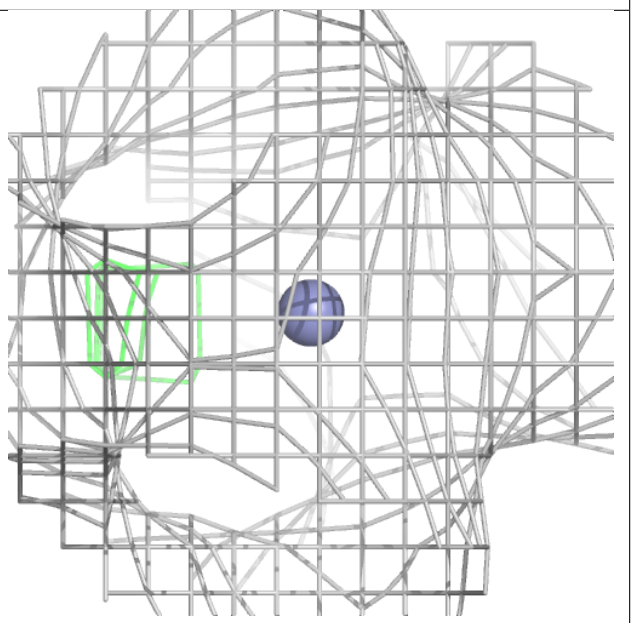


Electron density around ZN E 202:

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

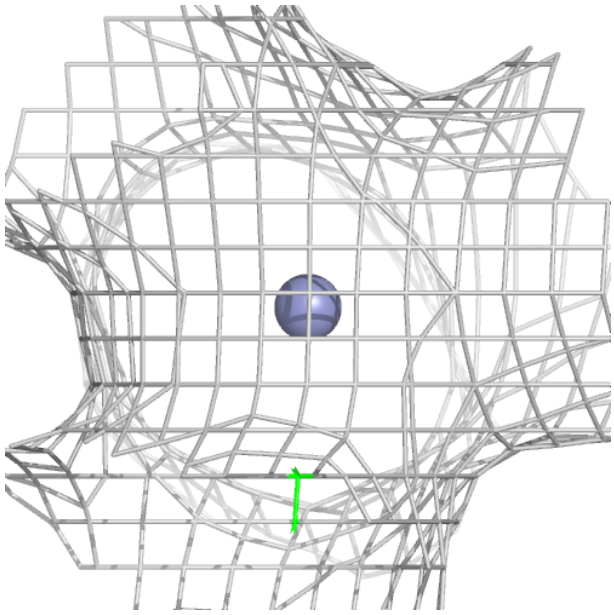


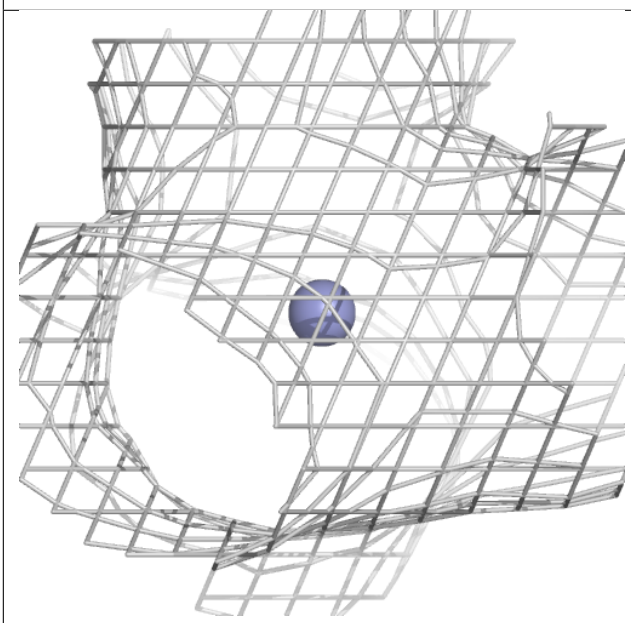


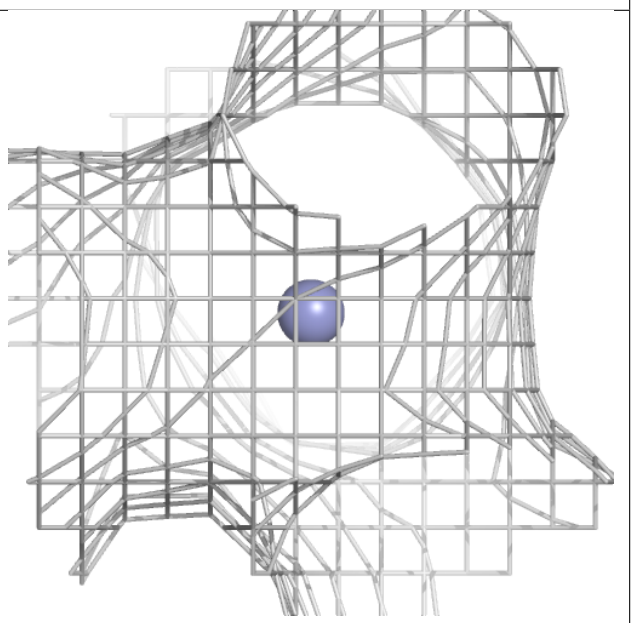


Electron density around ZN P 202:

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

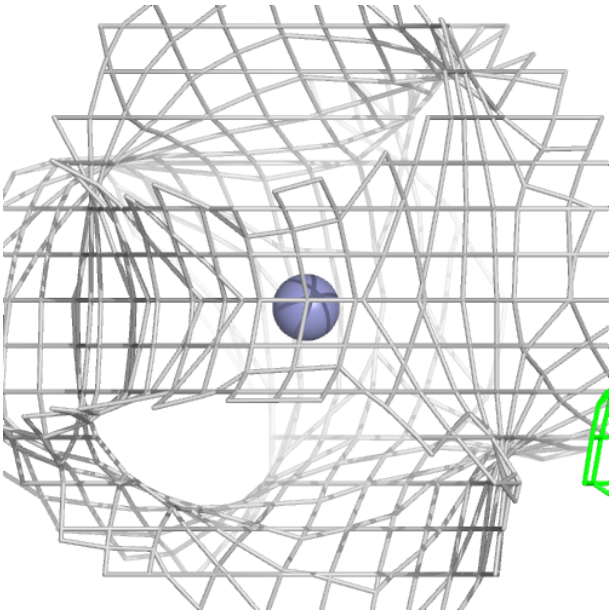


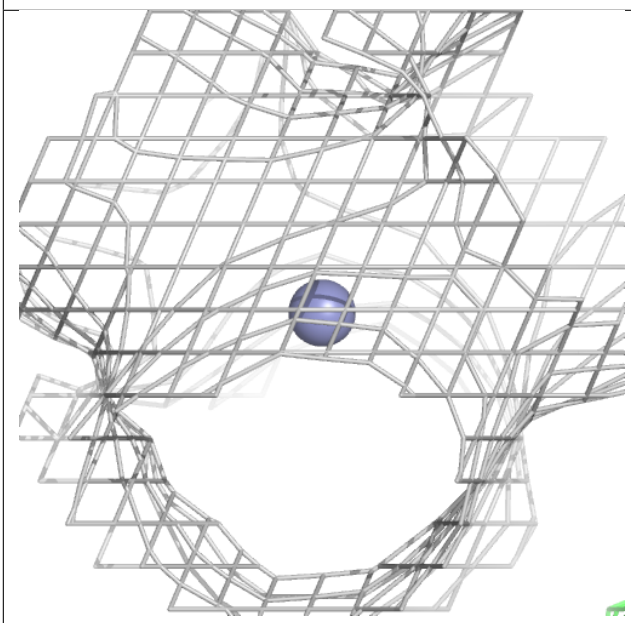


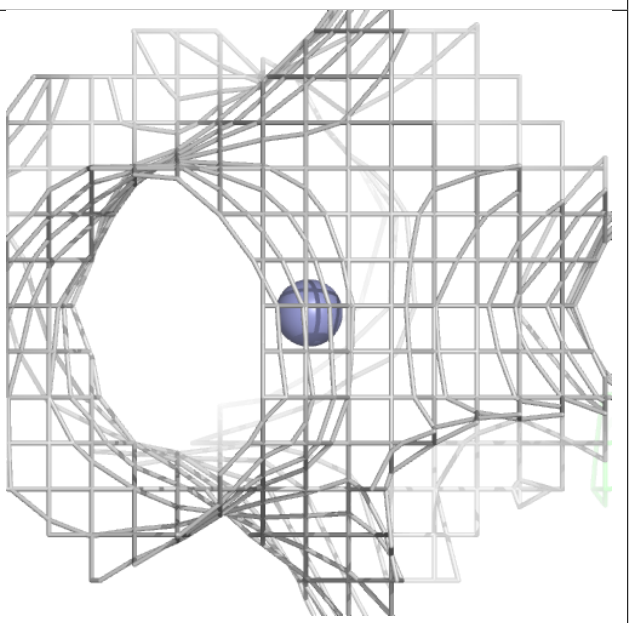


Electron density around ZN L 202:

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

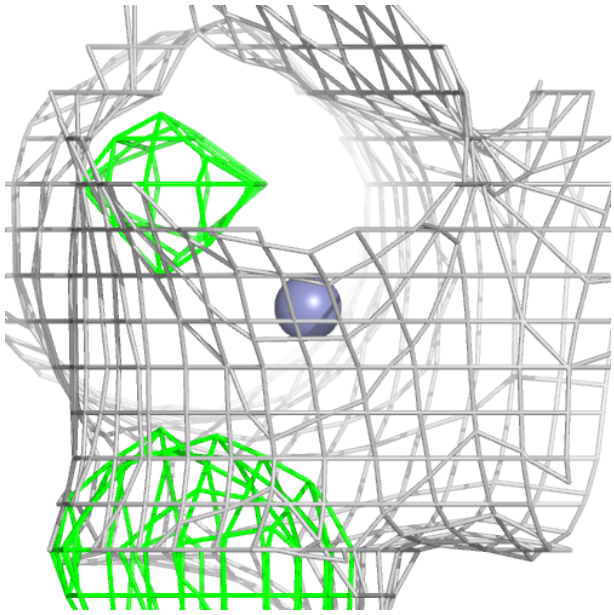


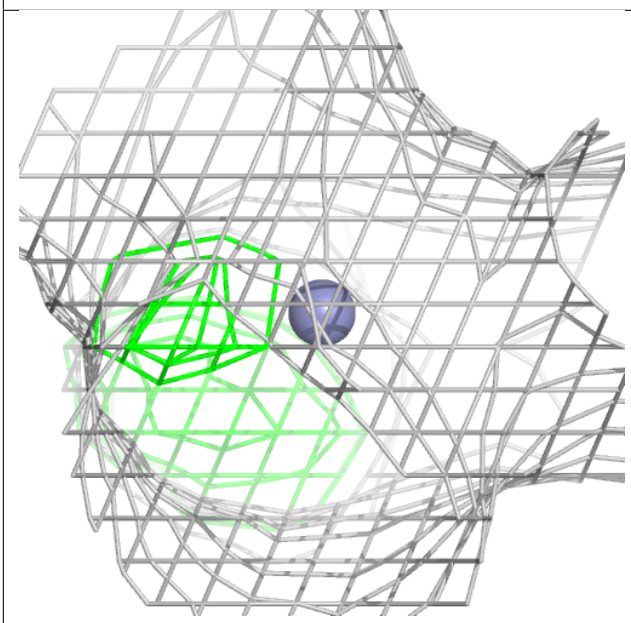


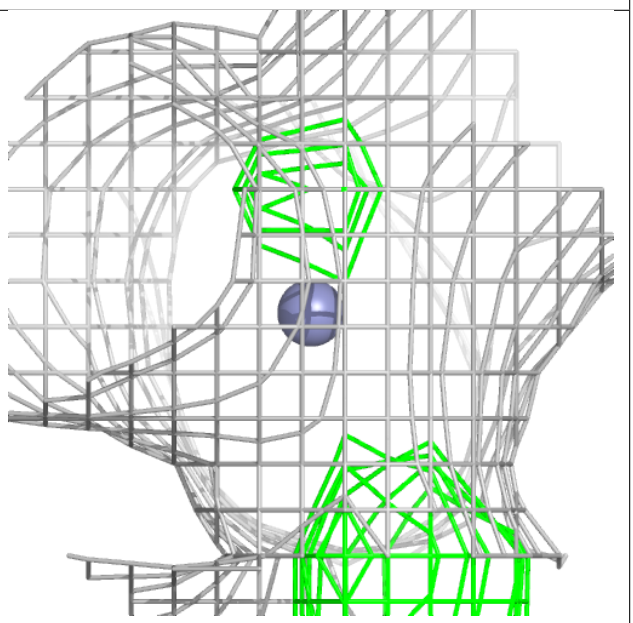


Electron density around ZN E 201:

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

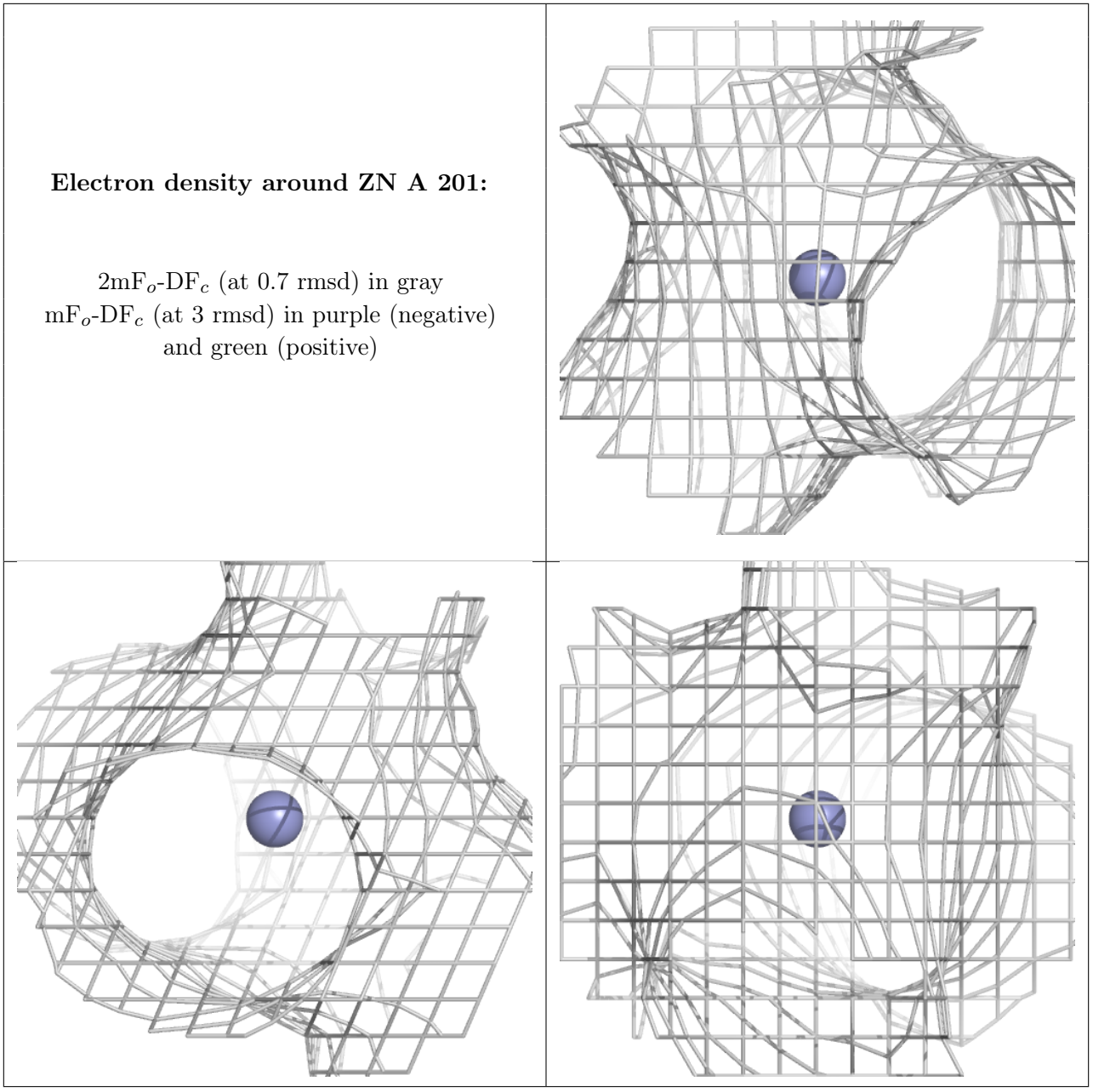






Electron density around ZN A 201:

$2mF_o$-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.