



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:34 PM UTC

PDB ID : 8AMN / pdb\_00008amn  
Title : Crystal structure of AUGUGGCAU duplex with strontium ions  
Authors : Kiliszek, A.; Rypniewski, W.  
Deposited on : 2022-08-03  
Resolution : 2.46 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

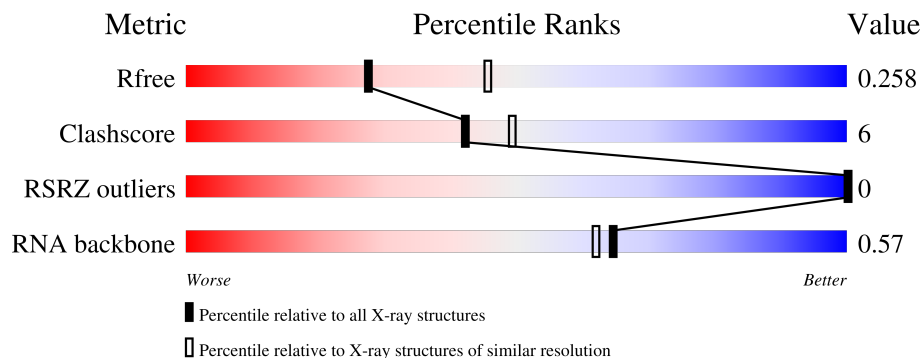
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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.














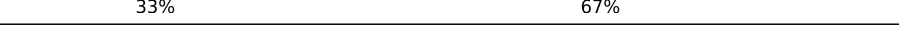







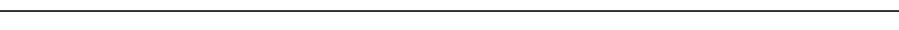

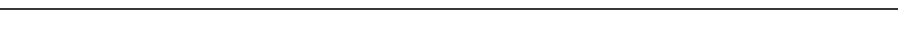
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	9	78% (green), 22% (yellow)
1	B	9	78% (green), 22% (yellow)
1	C	9	67% (green), 33% (yellow)
1	D	9	56% (green), 44% (yellow)
1	E	9	89% (green), 11% (yellow)
1	F	9	89% (green), 11% (yellow)

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Mol	Chain	Length	Quality of chain
1	G	9	 78% 22%
1	H	9	 33% 67%
1	I	9	 78% 22%
1	J	9	 78% 22%
1	K	9	 56% 44%
1	L	9	 89% 11%
1	M	9	 67% 22% 11%
1	N	9	 44% 44% 11%
1	O	9	 78% 22%
1	P	9	 78% 22%
1	Q	9	 89% 11%
1	R	9	 33% 67%
1	S	9	 56% 22% 22%
1	T	9	 56% 33% 11%
1	U	9	 33% 67%
1	V	9	 44% 56%
1	Y	9	 56% 44%
1	Z	9	 67% 33%
1	a	9	 22% 44% 33%
1	b	9	 56% 22% 22%
1	c	9	 78% 22%
1	d	9	 33% 67%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5400 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 RNA chain called RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	9	Total 213	C 96	N 39	O 69	P 9	0	1	0
1	B	9	Total 213	C 96	N 39	O 69	P 9	0	1	0
1	C	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	D	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	E	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	F	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	G	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	H	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	I	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	J	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	K	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	L	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	M	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	N	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	O	9	Total 190	C 86	N 34	O 62	P 8	0	0	0
1	P	9	Total 190	C 86	N 34	O 62	P 8	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Q	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	R	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	S	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	T	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	U	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	V	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	Y	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	Z	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	a	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	b	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	c	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			
1	d	9	Total	C	N	O	P	0	0	0
			190	86	34	62	8			

- Molecule 2 is STRONTIUM ION (CCD ID: SR) (formula: Sr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Sr	0	0
			1	1		
2	C	2	Total	Sr	0	0
			2	2		
2	E	1	Total	Sr	0	0
			1	1		
2	G	1	Total	Sr	0	0
			1	1		
2	H	1	Total	Sr	0	0
			1	1		
2	I	1	Total	Sr	0	0
			1	1		
2	L	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	2	Total 2	Sr 2	0	0
2	O	1	Total 1	Sr 1	0	0
2	Q	2	Total 2	Sr 2	0	0
2	S	2	Total 2	Sr 2	0	0
2	U	1	Total 1	Sr 1	0	0
2	Y	2	Total 2	Sr 2	0	0
2	a	1	Total 1	Sr 1	0	0
2	b	1	Total 1	Sr 1	0	0
2	d	1	Total 2	Sr 2	0	1


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	2	Total 2	O 2	0	0
3	E	2	Total 2	O 2	0	0
3	F	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0
3	M	1	Total 1	O 1	0	0
3	O	1	Total 1	O 1	0	0
3	U	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain A:  78% 22%



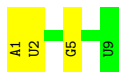
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain B:  78% 22%



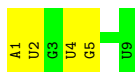
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain C:  67% 33%




- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain D:  56% 44%




- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain E:  89% 11%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain F:  89% 11%



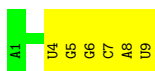
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain G: 78% 22%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain H: 33% 67%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain I: 78% 22%



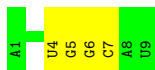
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain J: 78% 22%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain K: 56% 44%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain L: 89% 11%



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

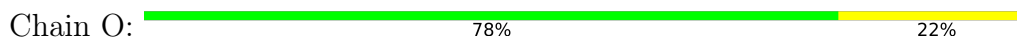
Chain M: 67% 22% 11%



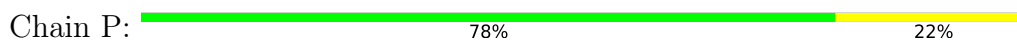
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



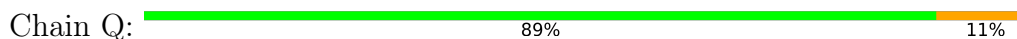
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



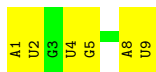
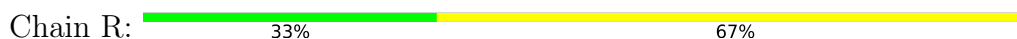
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

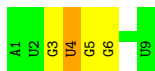


- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

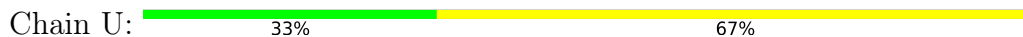


- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')





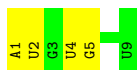
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



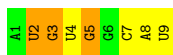
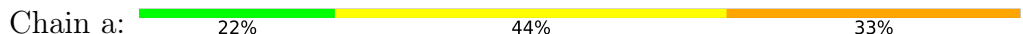
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



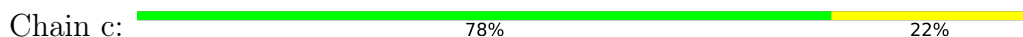
- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

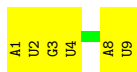


- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')



- Molecule 1: RNA (5'-R(\*AP\*UP\*GP\*UP\*GP\*GP\*CP\*AP\*U)-3')

Chain d:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	28.10Å 90.13Å 138.18Å 90.00° 91.39° 90.00°	Depositor
Resolution (Å)	46.05 – 2.46 46.05 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.05-2.46) 91.8 (46.05-2.46)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.199 , 0.248 0.218 , 0.258	Depositor DCC
$R_{free}$ test set	1979 reflections (7.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/238	0.55	0/370
1	B	0.45	0/238	0.55	0/370
1	C	0.45	0/212	0.53	0/329
1	D	0.39	0/212	0.50	0/329
1	E	0.39	0/212	0.49	0/329
1	F	0.38	0/212	0.62	0/329
1	G	0.45	0/212	0.57	0/329
1	H	0.37	0/212	0.51	0/329
1	I	0.39	0/212	0.57	0/329
1	J	0.39	0/212	0.61	0/329
1	K	0.39	0/212	0.47	0/329
1	L	0.42	0/212	0.51	0/329
1	M	0.39	0/212	0.51	0/329
1	N	0.42	0/212	0.55	0/329
1	O	0.21	0/212	0.29	0/329
1	P	0.26	0/212	0.40	0/329
1	Q	0.27	0/212	0.41	0/329
1	R	0.36	0/212	0.50	0/329
1	S	0.32	0/212	0.46	0/329
1	T	0.35	0/212	0.48	0/329
1	U	0.22	0/212	0.35	0/329
1	V	0.22	0/212	0.31	0/329
1	Y	0.26	0/212	0.42	0/329
1	Z	0.30	0/212	0.41	0/329
1	a	0.25	0/212	0.41	0/329
1	b	0.26	0/212	0.42	0/329
1	c	0.18	0/212	0.35	0/329
1	d	0.22	0/212	0.35	0/329
All	All	0.35	0/5988	0.48	0/9294

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	213	0	107	1	0
1	B	213	0	106	1	0
1	C	190	0	98	1	0
1	D	190	0	98	2	0
1	E	190	0	98	0	0
1	F	190	0	98	0	0
1	G	190	0	98	1	0
1	H	190	0	98	3	0
1	I	190	0	98	0	0
1	J	190	0	98	1	0
1	K	190	0	98	2	0
1	L	190	0	98	1	0
1	M	190	0	98	2	0
1	N	190	0	98	3	0
1	O	190	0	98	1	0
1	P	190	0	98	1	0
1	Q	190	0	98	1	0
1	R	190	0	98	3	0
1	S	190	0	98	2	0
1	T	190	0	98	3	1
1	U	190	0	98	3	0
1	V	190	0	98	3	0
1	Y	190	0	98	3	0
1	Z	190	0	98	1	0
1	a	190	0	98	5	1
1	b	190	0	98	3	0
1	c	190	0	98	1	0
1	d	190	0	98	4	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	L	1	0	0	0	0
2	M	2	0	0	0	0
2	O	1	0	0	0	0
2	Q	2	0	0	0	0
2	S	2	0	0	0	0
2	U	1	0	0	0	0
2	Y	2	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	d	2	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	U	1	0	0	1	0
All	All	5400	0	2761	49	1

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 6.

All (49) 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:U:6:G:O6	3:U:201:HOH:O	2.03	0.75
1:T:4:U:H2'	1:T:5:G:C8	2.29	0.68
1:a:2:U:H5'	1:a:3:G:OP2	1.96	0.66
1:a:4:U:H2'	1:a:5:G:C8	2.37	0.59
1:Y:4:U:H2'	1:Y:5:G:C8	2.39	0.58
1:D:4:U:H2'	1:D:5:G:C8	2.39	0.58
1:R:4:U:H2'	1:R:5:G:C8	2.40	0.57
1:c:4:U:H2'	1:c:5:G:C8	2.40	0.56
1:N:4:U:H2'	1:N:5:G:C8	2.42	0.55
1:V:4:U:H2'	1:V:5:G:C8	2.44	0.53
1:J:4:U:H2'	1:J:5:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:G:H5''	1:L:5:G:N3	2.25	0.51
1:U:8:A:H61	1:V:2:U:H3	1.60	0.50
1:b:4:U:H2'	1:b:5:G:N3	2.28	0.48
1:H:4:U:H2'	1:H:5:G:C8	2.48	0.48
1:K:4:U:H2'	1:K:5:G:C8	2.49	0.47
1:B:5[B]:G:O2'	1:B:6:G:H5'	2.13	0.47
1:a:7:C:H2'	1:a:8:A:H8	1.79	0.47
1:C:1:A:H2'	1:C:2:U:C6	2.50	0.47
1:U:1:A:H2'	1:U:2:U:C6	2.50	0.47
1:N:1:A:O5'	1:N:2:U:OP2	2.27	0.46
1:D:1:A:H2'	1:D:2:U:C6	2.51	0.46
1:T:3:G:O2'	1:T:4:U:H5'	2.16	0.46
1:d:3:G:C6	1:d:4:U:C4	3.04	0.45
1:M:1:A:H2'	1:M:2:U:C6	2.52	0.45
1:Y:1:A:H2'	1:Y:2:U:C6	2.51	0.45
1:b:5:G:H5''	1:b:6:G:OP2	2.17	0.45
1:a:2:U:H6	1:a:2:U:H5''	1.83	0.44
1:Y:5:G:H8	1:Y:5:G:O5'	2.00	0.44
1:V:7:C:H2'	1:V:8:A:H8	1.81	0.44
1:d:1:A:H2'	1:d:2:U:H6	1.82	0.44
1:M:5:G:H5''	1:M:5:G:N3	2.33	0.44
1:d:8:A:H2'	1:d:9:U:C6	2.53	0.43
1:H:8:A:C6	1:H:9:U:C4	3.06	0.43
1:Q:5:G:N3	1:Q:5:G:H5''	2.33	0.43
1:P:3:G:H2'	1:P:4:U:O4'	2.18	0.43
1:G:1:A:H1'	1:O:9:U:C2	2.54	0.43
1:R:8:A:C5	1:R:9:U:C4	3.06	0.43
1:T:3:G:C2'	1:T:4:U:H5'	2.49	0.43
1:a:9:U:H3	1:b:1:A:H61	1.66	0.43
1:d:1:A:H2'	1:d:2:U:C6	2.53	0.43
1:R:1:A:H2'	1:R:2:U:C6	2.55	0.42
1:S:4:U:H2'	1:S:5:G:N3	2.35	0.42
1:A:1:A:H2'	1:A:2:U:C6	2.55	0.42
1:Z:8:A:H2'	1:Z:9:U:C6	2.56	0.41
1:K:6:G:H2'	1:K:7:C:O4'	2.21	0.41
1:S:3:G:H2'	1:S:4:U:C6	2.55	0.41
1:N:5:G:OP2	1:N:5:G:H8	2.03	0.40
1:H:6:G:C6	1:H:7:C:C4	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:6:G:O2'	1:a:2:U:OP1[1_655]	2.18	0.02

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

#### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	7/9 (77%)	0	0
1	B	7/9 (77%)	0	0
1	C	8/9 (88%)	1 (12%)	0
1	D	8/9 (88%)	0	0
1	E	8/9 (88%)	1 (12%)	0
1	F	8/9 (88%)	1 (12%)	0
1	G	8/9 (88%)	1 (12%)	0
1	H	8/9 (88%)	0	0
1	I	8/9 (88%)	2 (25%)	0
1	J	8/9 (88%)	0	0
1	K	8/9 (88%)	0	0
1	L	8/9 (88%)	1 (12%)	0
1	M	8/9 (88%)	1 (12%)	0
1	N	8/9 (88%)	2 (25%)	0
1	O	8/9 (88%)	1 (12%)	0
1	P	8/9 (88%)	0	0
1	Q	8/9 (88%)	1 (12%)	0
1	R	8/9 (88%)	0	0
1	S	8/9 (88%)	3 (37%)	0
1	T	8/9 (88%)	1 (12%)	0
1	U	8/9 (88%)	2 (25%)	0
1	V	8/9 (88%)	0	0
1	Y	8/9 (88%)	0	0
1	Z	8/9 (88%)	1 (12%)	0
1	a	8/9 (88%)	3 (37%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	b	8/9 (88%)	2 (25%)	0
1	c	8/9 (88%)	0	0
1	d	8/9 (88%)	0	0
All	All	222/252 (88%)	24 (10%)	0

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	5	G
1	E	5	G
1	F	3	G
1	G	5	G
1	I	4	U
1	I	5	G
1	L	5	G
1	M	5	G
1	N	5	G
1	N	6	G
1	O	5	G
1	Q	5	G
1	S	3	G
1	S	5	G
1	S	6	G
1	T	4	U
1	U	5	G
1	U	9	U
1	Z	5	G
1	a	2	U
1	a	3	G
1	a	5	G
1	b	5	G
1	b	6	G

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 22 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	9/9 (100%)	-0.86	0 100 100	32, 56, 66, 71	1 (11%)
1	B	9/9 (100%)	-0.87	0 100 100	28, 60, 65, 68	1 (11%)
1	C	9/9 (100%)	-0.47	0 100 100	67, 71, 85, 100	0
1	D	9/9 (100%)	-0.70	0 100 100	64, 74, 83, 86	0
1	E	9/9 (100%)	-0.65	0 100 100	69, 76, 80, 81	0
1	F	9/9 (100%)	-0.64	0 100 100	66, 72, 83, 84	0
1	G	9/9 (100%)	-0.55	0 100 100	55, 70, 115, 116	0
1	H	9/9 (100%)	-0.79	0 100 100	59, 68, 88, 102	0
1	I	9/9 (100%)	-0.68	0 100 100	75, 81, 83, 88	0
1	J	9/9 (100%)	-0.67	0 100 100	71, 75, 86, 88	0
1	K	9/9 (100%)	-0.85	0 100 100	59, 64, 78, 82	0
1	L	9/9 (100%)	-0.78	0 100 100	60, 62, 88, 91	0
1	M	9/9 (100%)	-0.54	0 100 100	59, 67, 80, 93	0
1	N	9/9 (100%)	-0.41	0 100 100	63, 77, 101, 101	0
1	O	9/9 (100%)	-0.31	0 100 100	106, 112, 119, 128	0
1	P	9/9 (100%)	-0.40	0 100 100	80, 96, 120, 122	0
1	Q	9/9 (100%)	-0.40	0 100 100	77, 87, 117, 123	0
1	R	9/9 (100%)	-0.34	0 100 100	67, 83, 103, 114	0
1	S	9/9 (100%)	0.03	0 100 100	93, 101, 119, 123	0
1	T	9/9 (100%)	-0.08	0 100 100	82, 103, 150, 153	0
1	U	9/9 (100%)	-0.19	0 100 100	121, 132, 148, 149	0
1	V	9/9 (100%)	-0.20	0 100 100	94, 126, 160, 164	0
1	Y	9/9 (100%)	-0.13	0 100 100	84, 116, 152, 153	0
1	Z	9/9 (100%)	-0.24	0 100 100	70, 94, 152, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
1	a	9/9 (100%)	-0.07	0	100 100	98, 121, 151, 155	0
1	b	9/9 (100%)	-0.03	0	100 100	110, 121, 160, 170	0
1	c	9/9 (100%)	-0.09	0	100 100	125, 133, 147, 159	0
1	d	9/9 (100%)	0.06	0	100 100	119, 133, 159, 160	0
All	All	252/252 (100%)	-0.42	0	100 100	28, 87, 153, 170	2 (0%)

There are no RSRZ outliers to report.

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SR	d	101[A]	1/1	0.75	0.27	176,176,176,176	1
2	SR	d	101[B]	1/1	0.75	0.27	189,189,189,189	1
2	SR	S	102	1/1	0.84	0.25	115,115,115,115	1
2	SR	H	101	1/1	0.85	0.26	92,92,92,92	1
2	SR	Y	102	1/1	0.87	0.24	202,202,202,202	1
2	SR	M	102	1/1	0.88	0.23	125,125,125,125	1
2	SR	a	101	1/1	0.89	0.21	206,206,206,206	0
2	SR	b	101	1/1	0.89	0.22	229,229,229,229	0
2	SR	G	101	1/1	0.89	0.27	153,153,153,153	0
2	SR	O	101	1/1	0.89	0.24	187,187,187,187	0
2	SR	S	101	1/1	0.91	0.23	191,191,191,191	0
2	SR	C	101	1/1	0.92	0.19	175,175,175,175	0
2	SR	Y	101	1/1	0.93	0.21	222,222,222,222	0
2	SR	C	102	1/1	0.93	0.21	172,172,172,172	0

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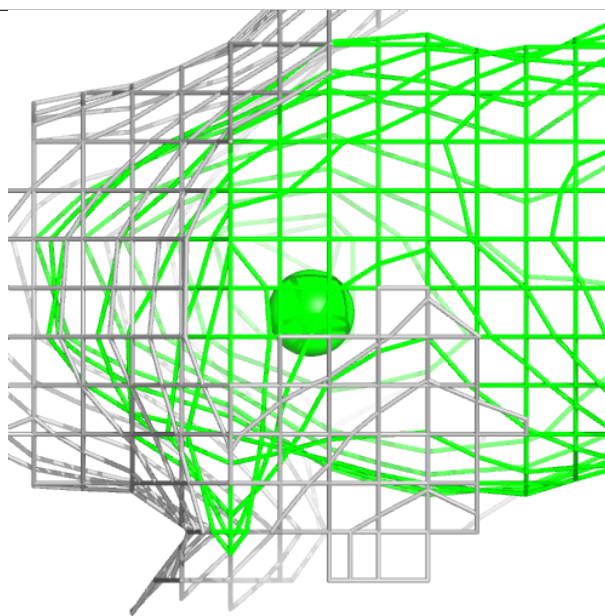
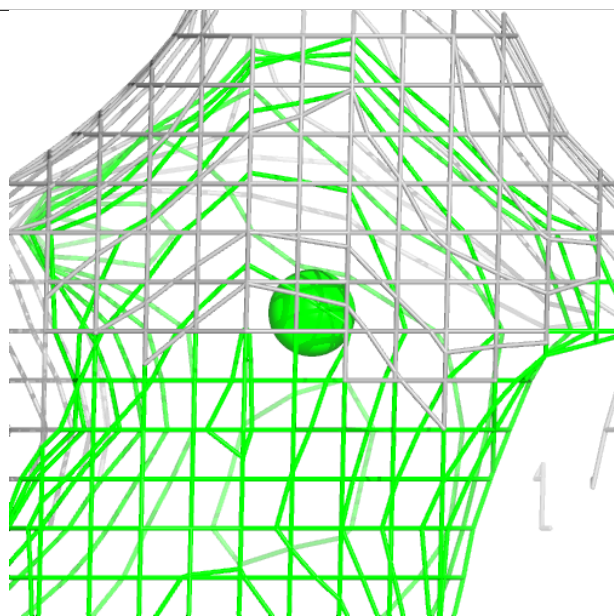
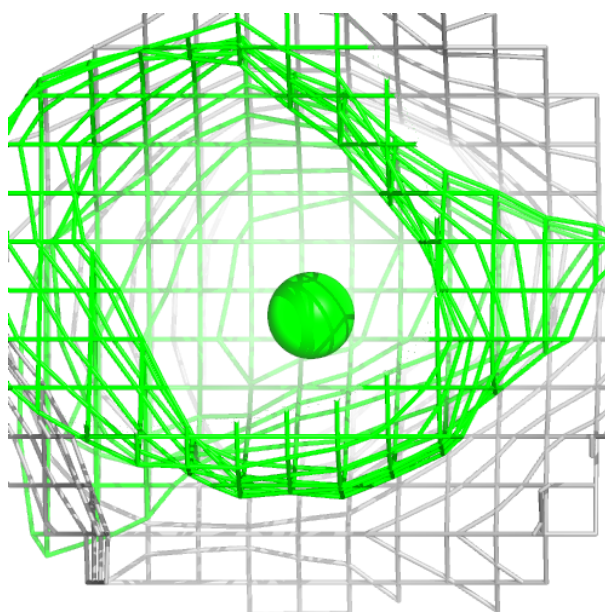
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SR	Q	102	1/1	0.94	0.21	180,180,180,180	0
2	SR	U	101	1/1	0.94	0.18	219,219,219,219	0
2	SR	L	101	1/1	0.95	0.24	140,140,140,140	0
2	SR	Q	101	1/1	0.95	0.17	188,188,188,188	0
2	SR	I	101	1/1	0.96	0.26	131,131,131,131	0
2	SR	B	101	1/1	0.96	0.25	134,134,134,134	0
2	SR	M	101	1/1	0.96	0.19	152,152,152,152	0
2	SR	E	101	1/1	0.96	0.25	125,125,125,125	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.

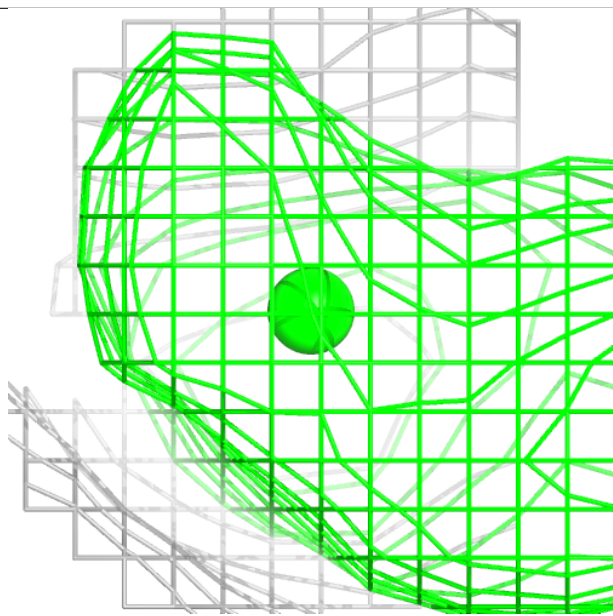
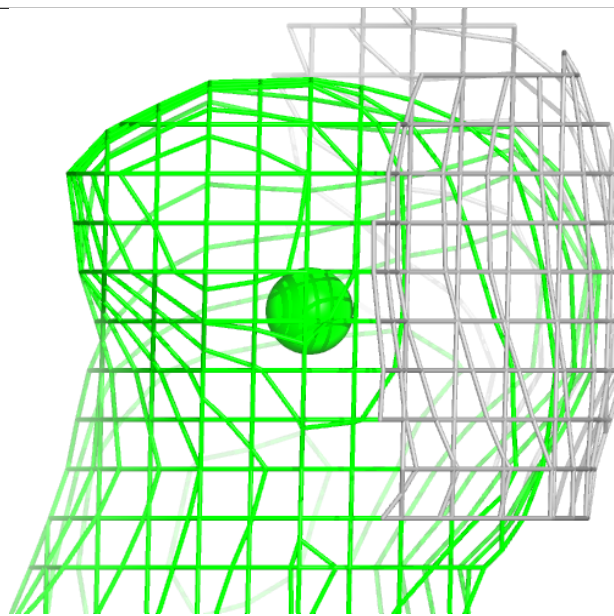
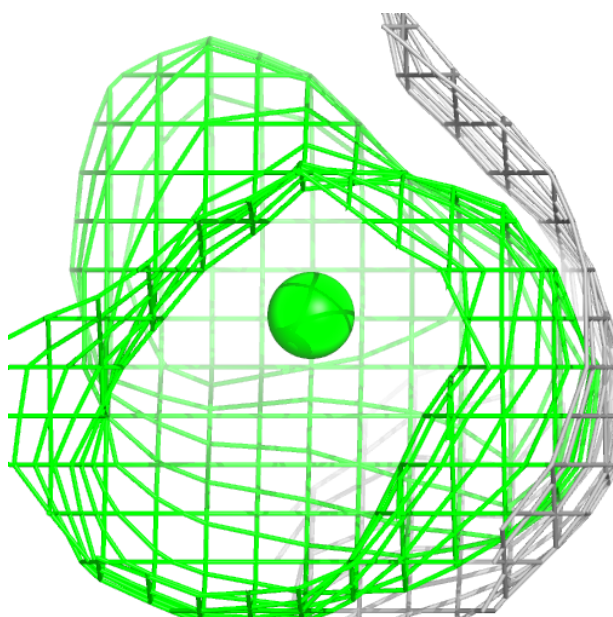
**Electron density around SR d 101 (A):**

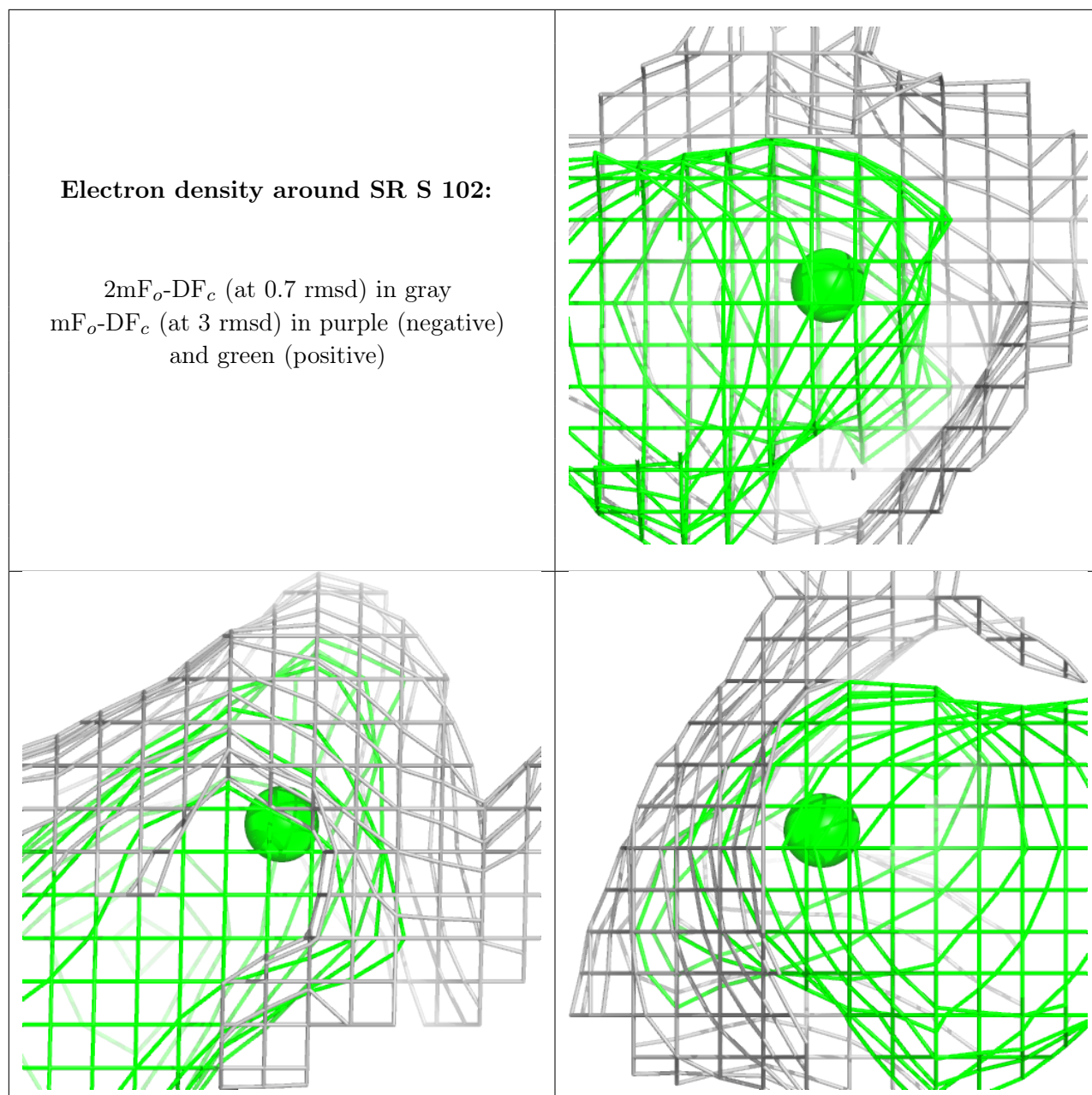
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SR d 101 (B):**

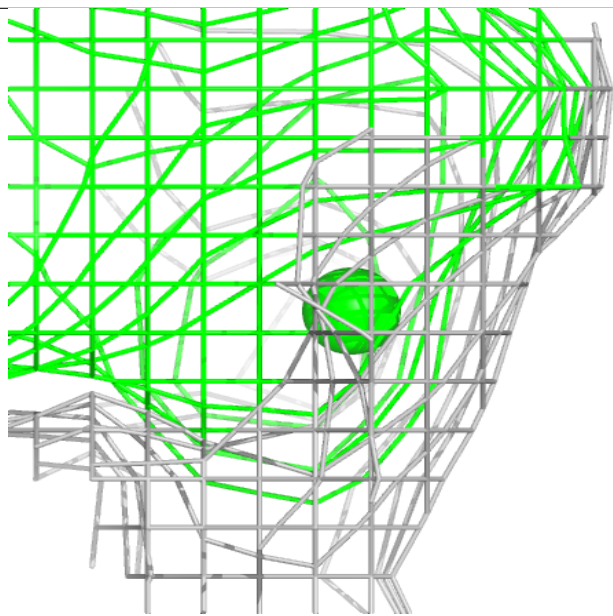
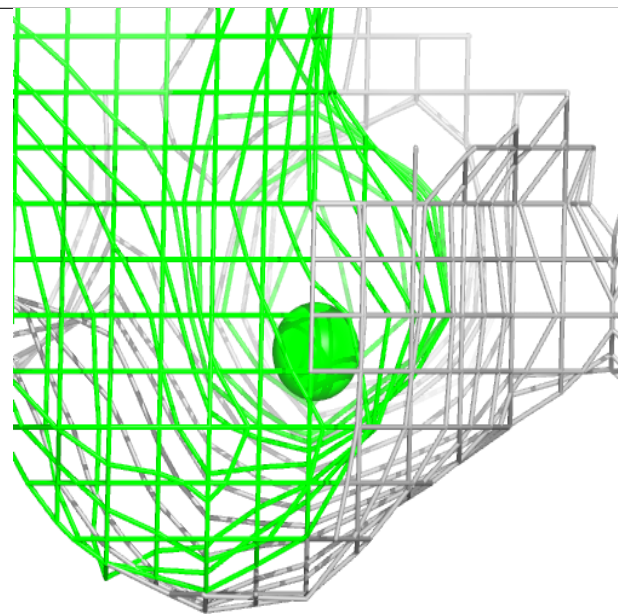
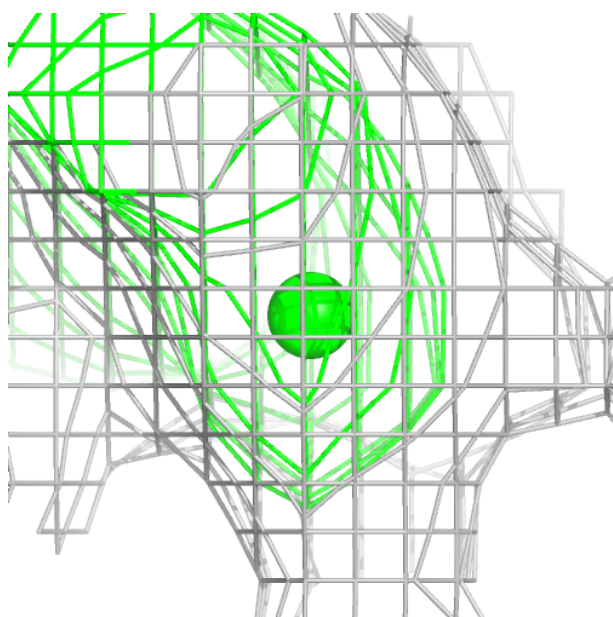
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





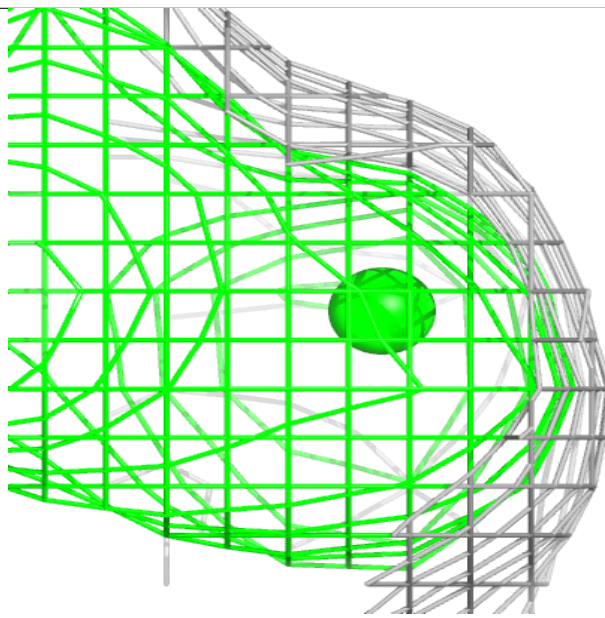
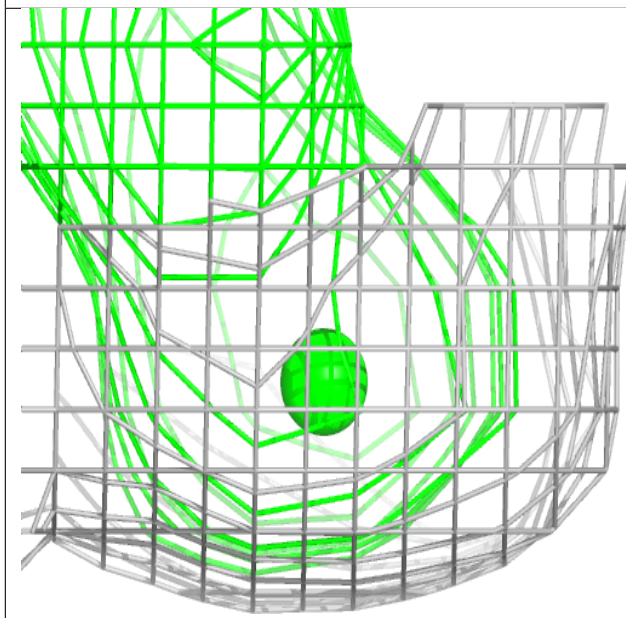
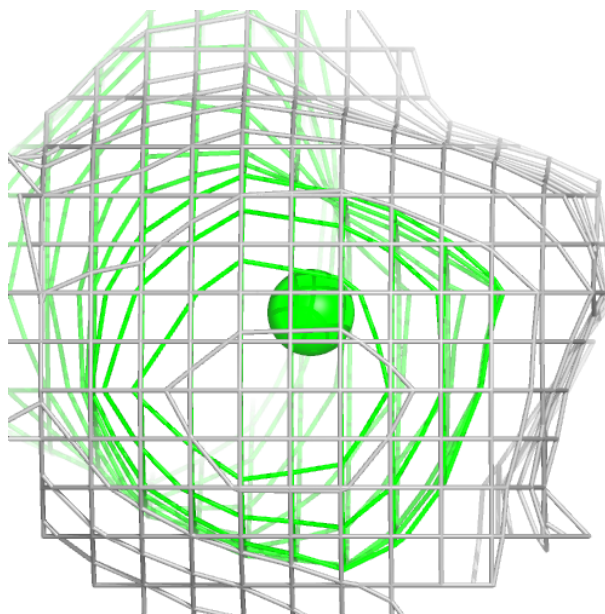
**Electron density around SR H 101:**

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



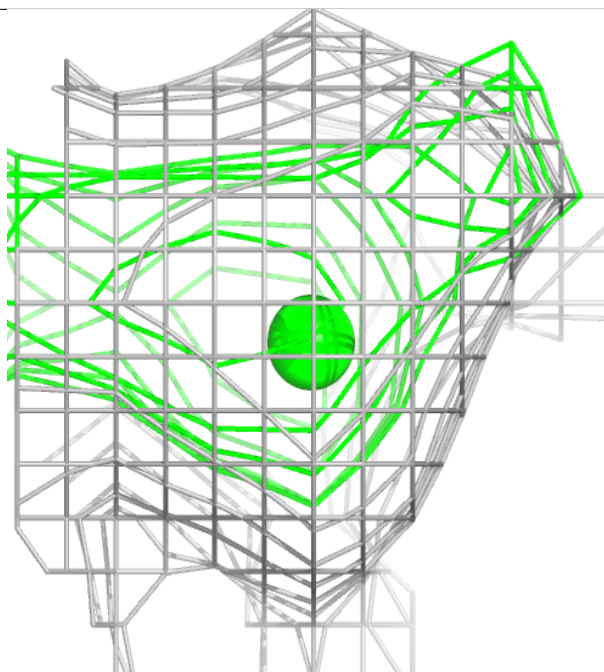
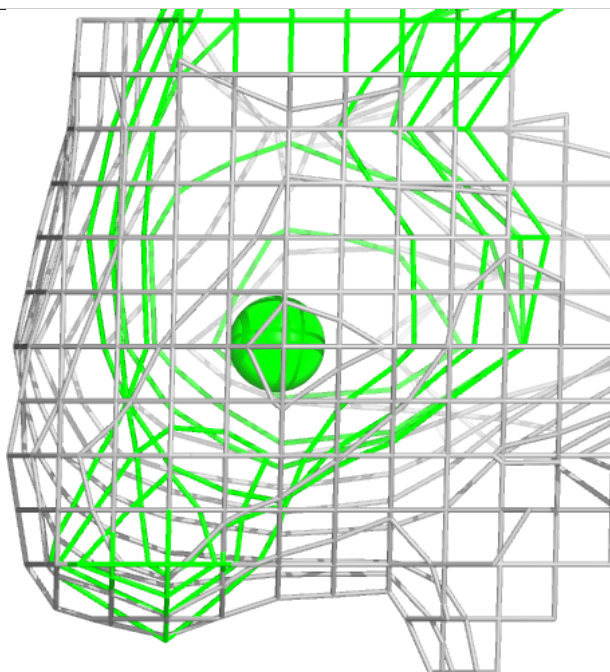
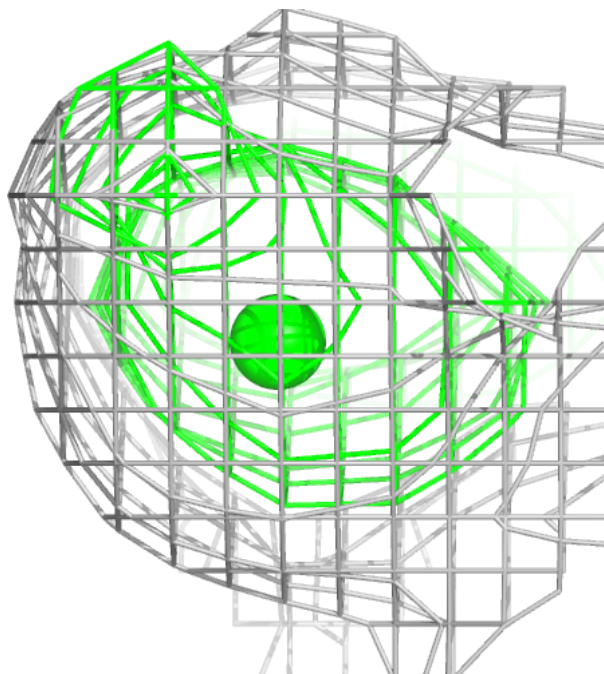
**Electron density around SR Y 102:**

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and green (positive)



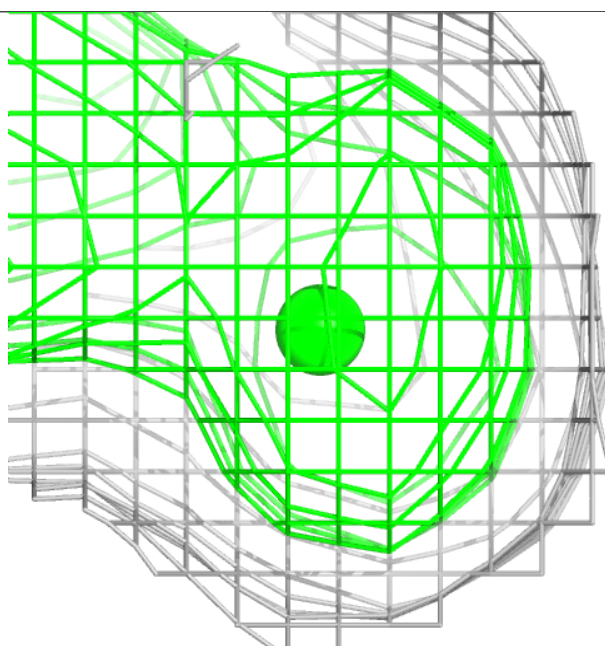
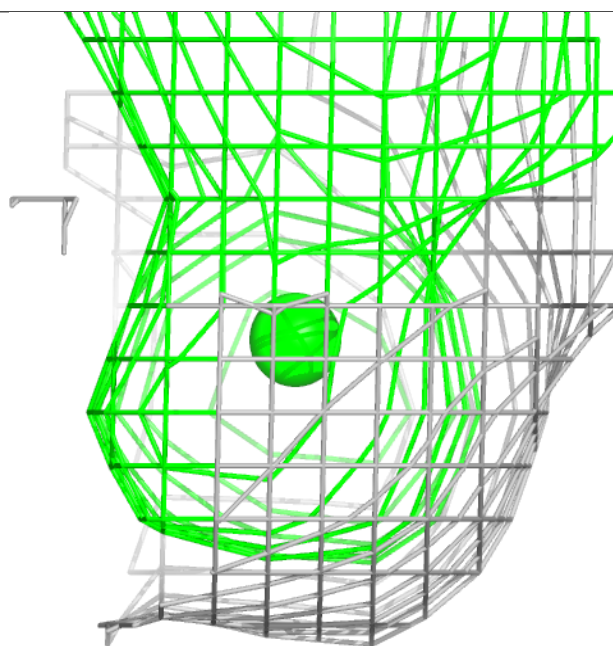
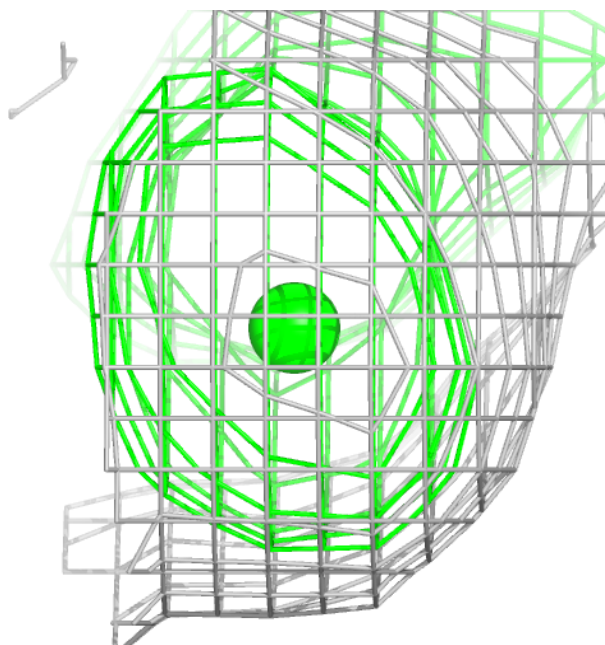
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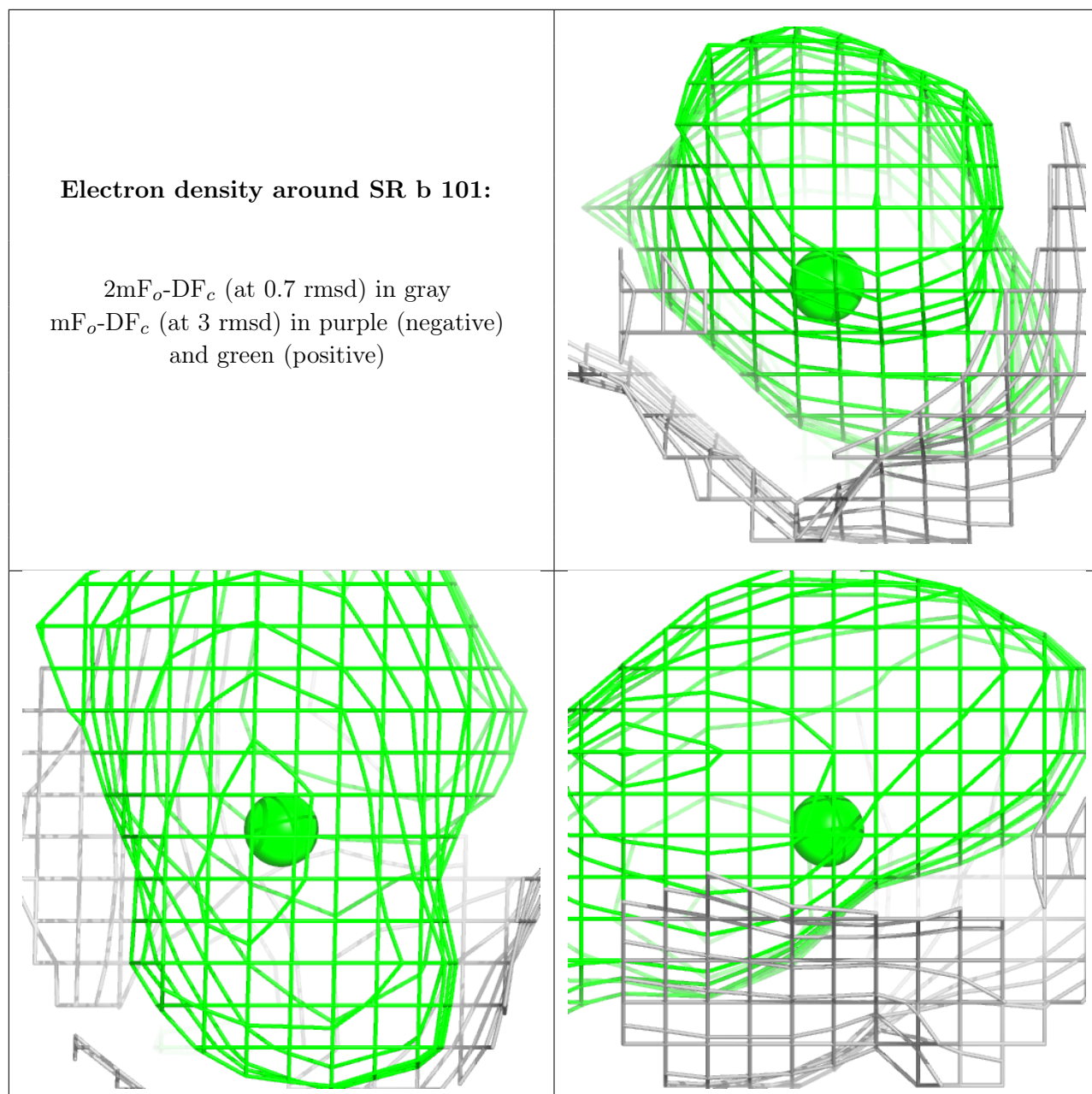
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SR a 101:**

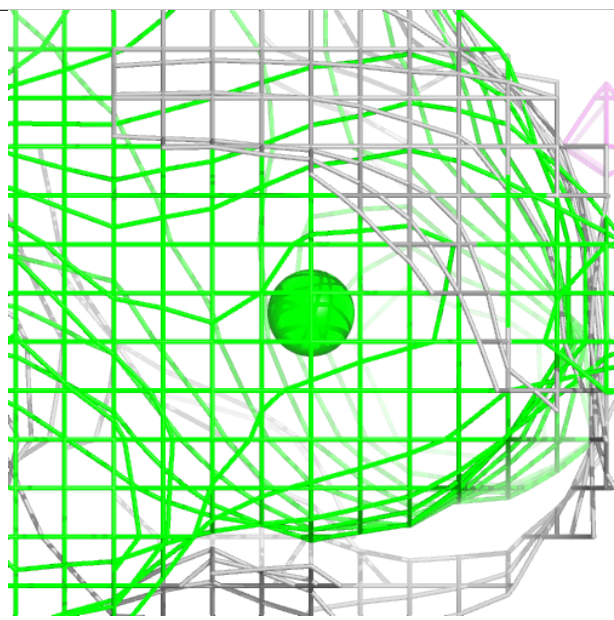
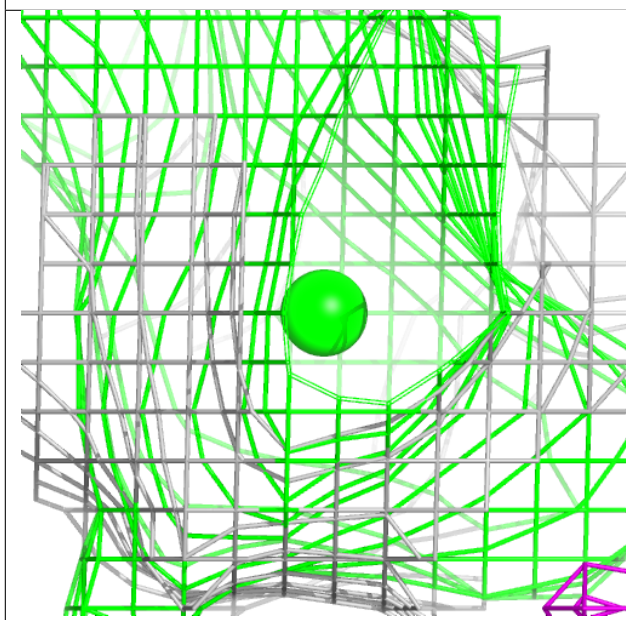
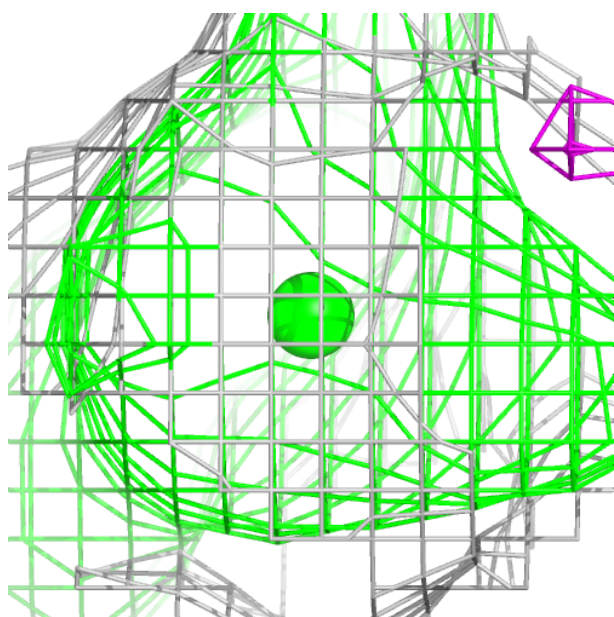
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





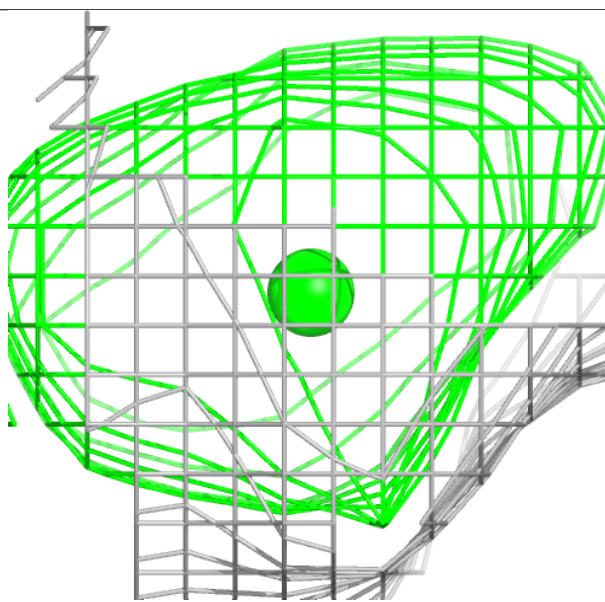
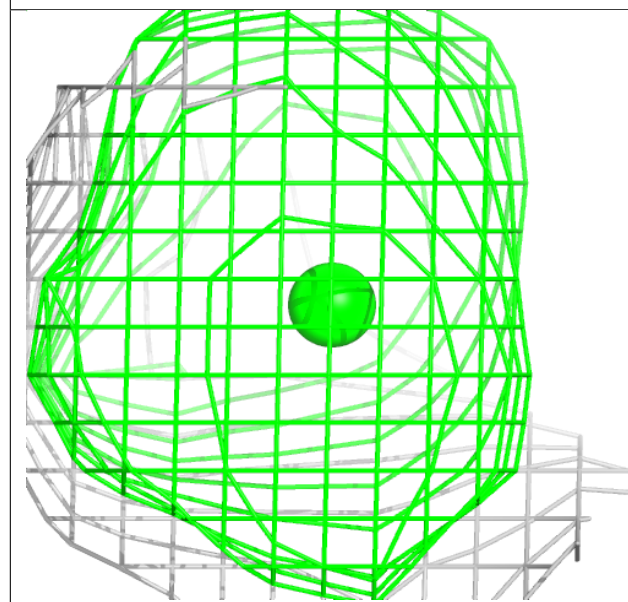
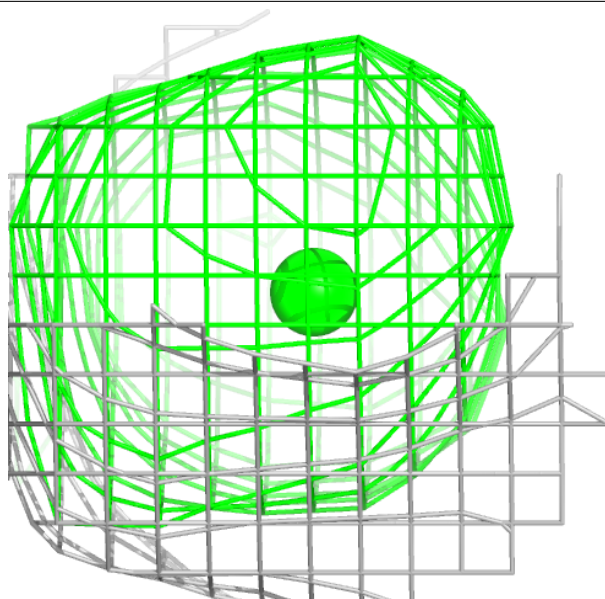
**Electron density around SR G 101:**

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and green (positive)



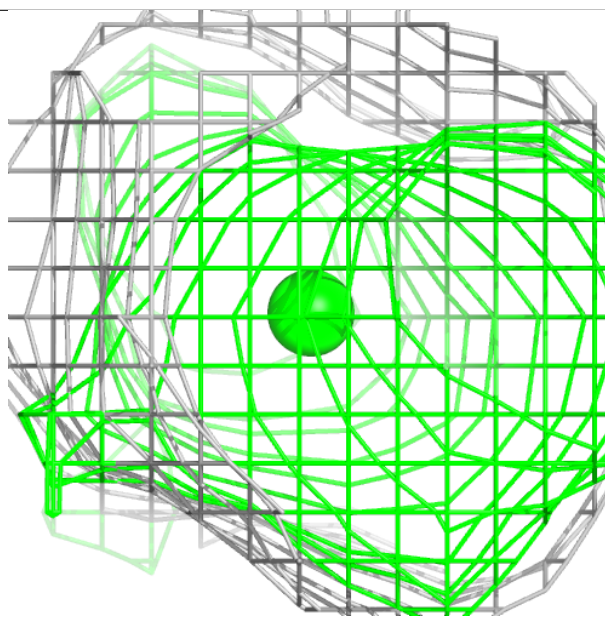
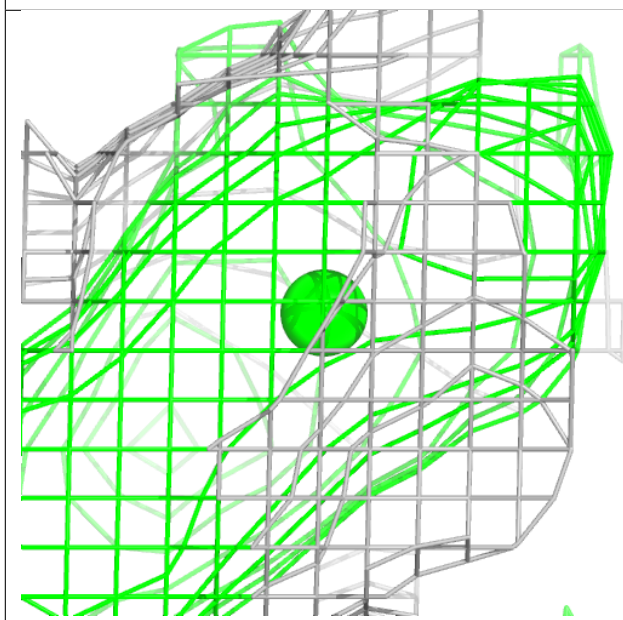
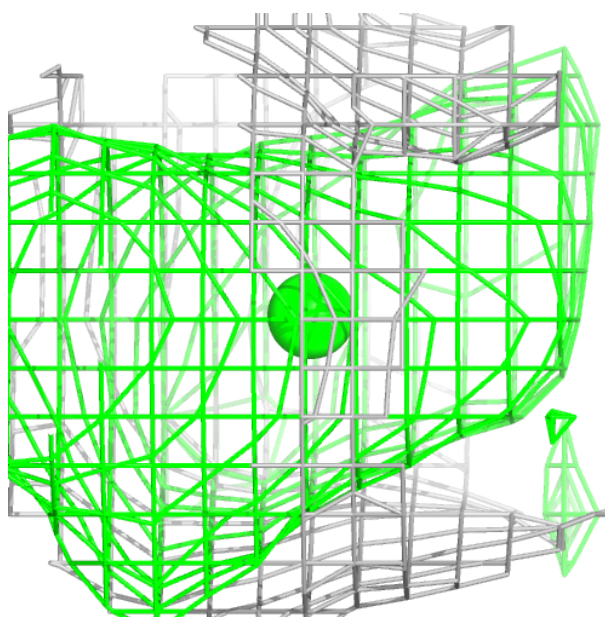
**Electron density around SR O 101:**

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



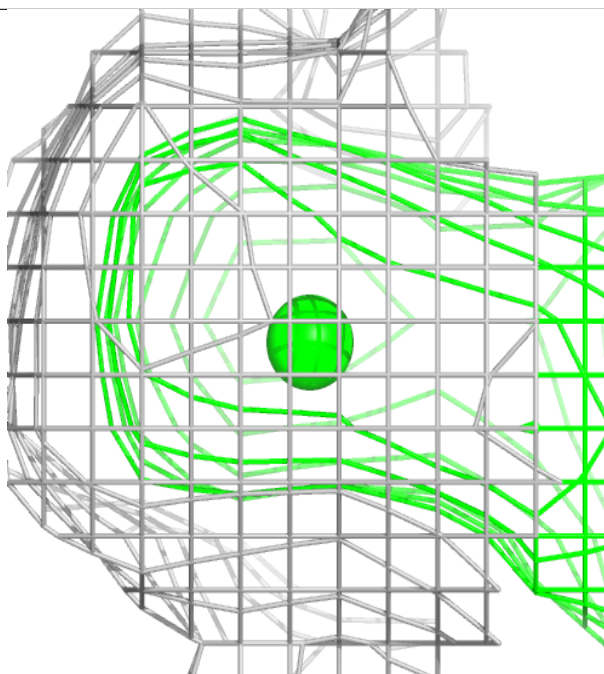
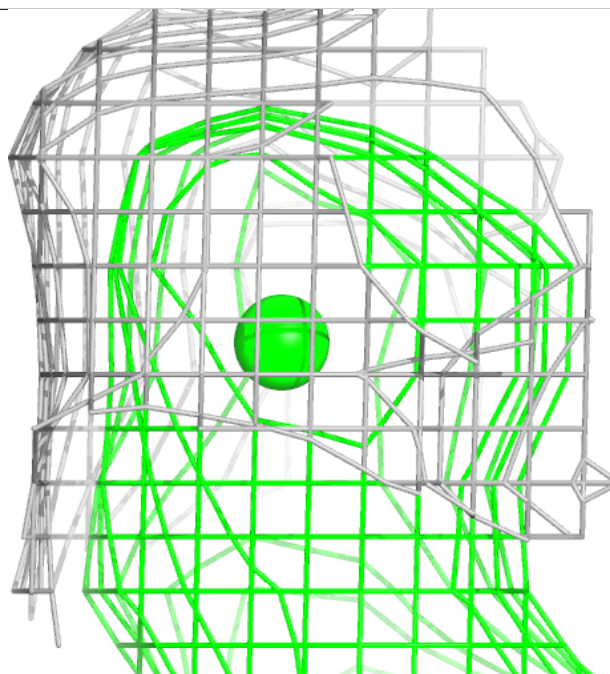
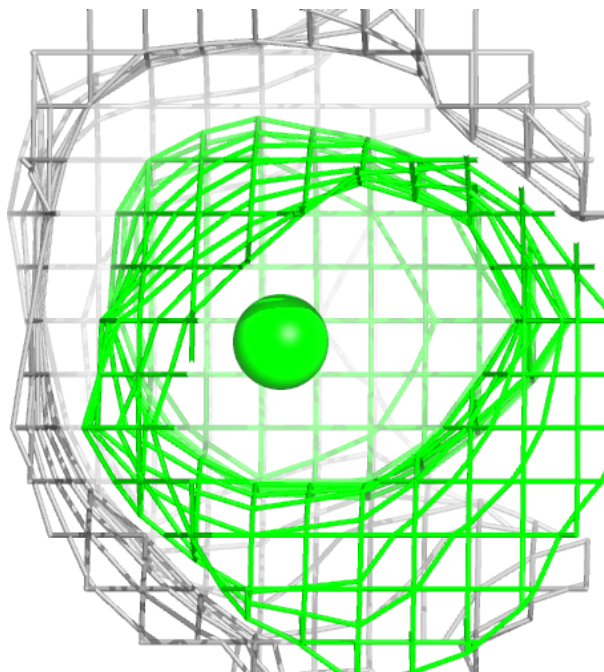
**Electron density around SR S 101:**

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



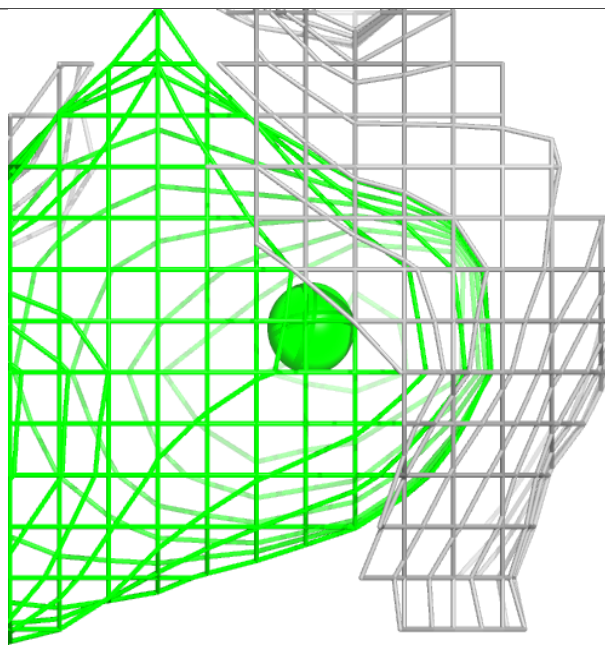
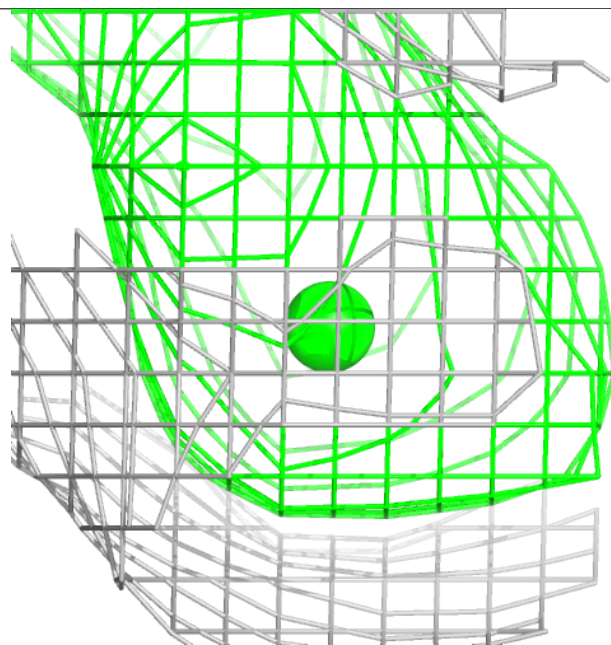
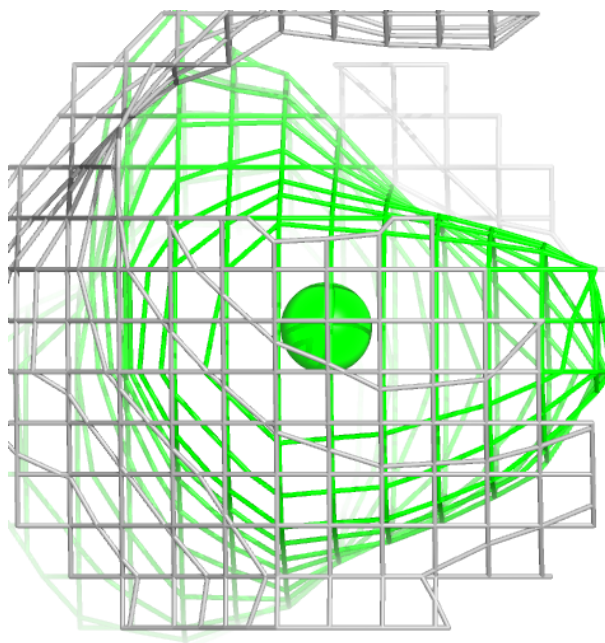
**Electron density around SR C 101:**

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



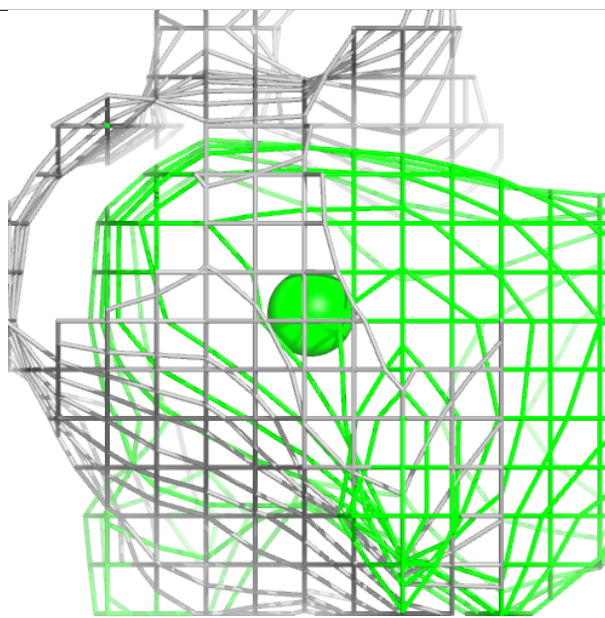
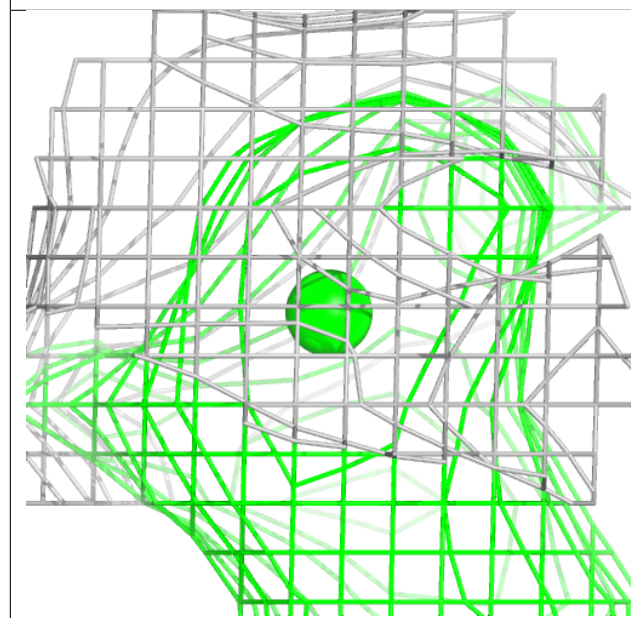
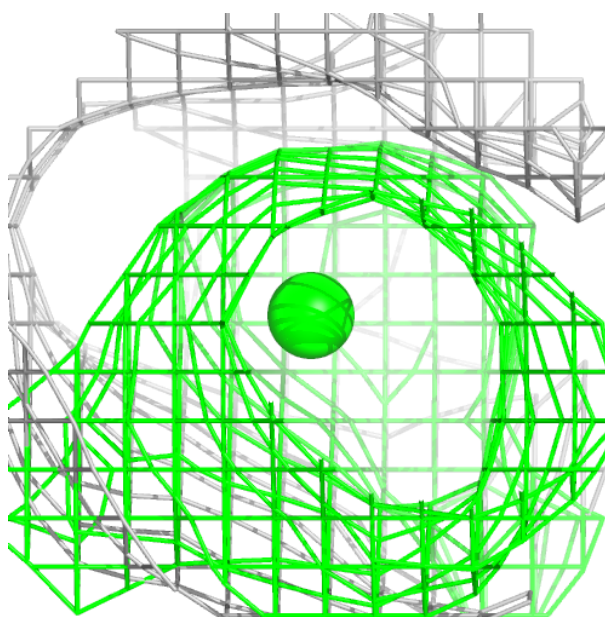
**Electron density around SR Y 101:**

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



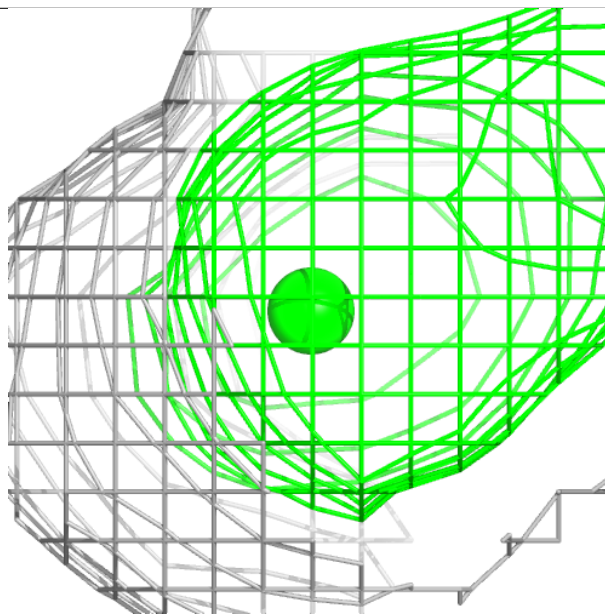
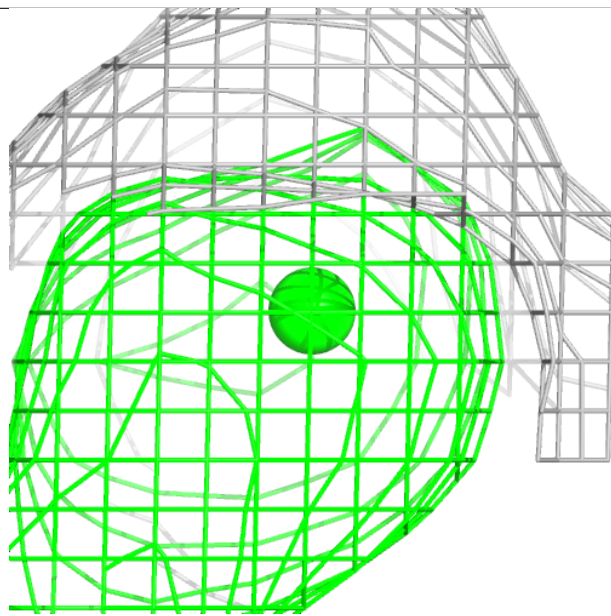
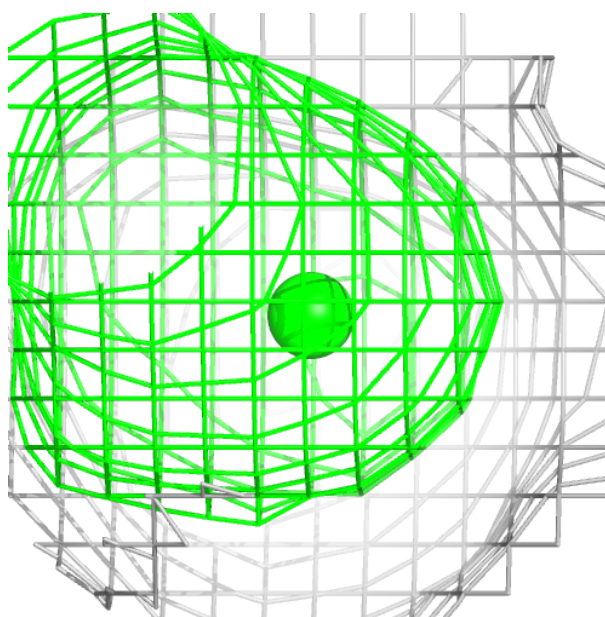
**Electron density around SR C 102:**

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



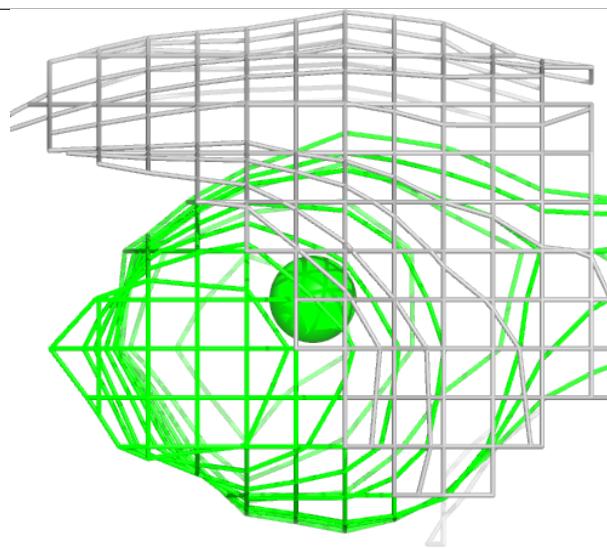
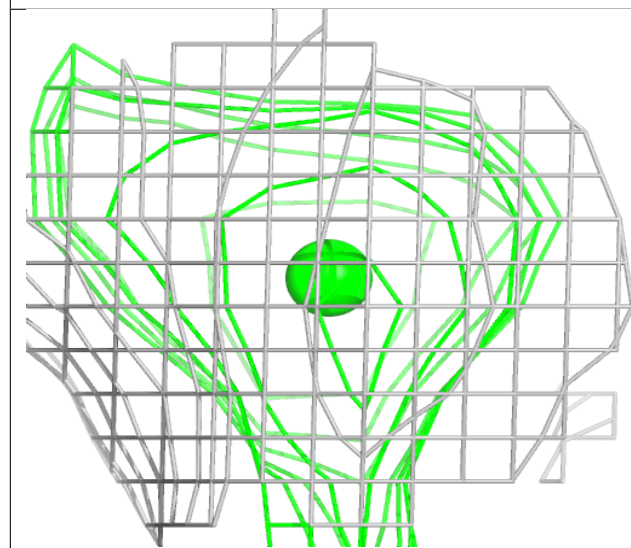
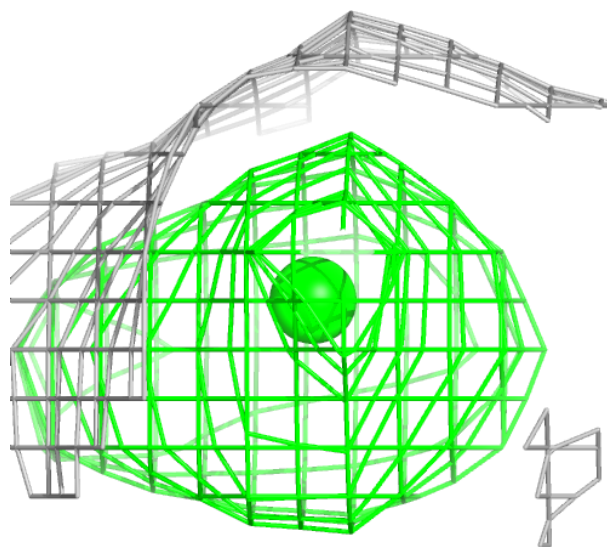
**Electron density around SR Q 102:**

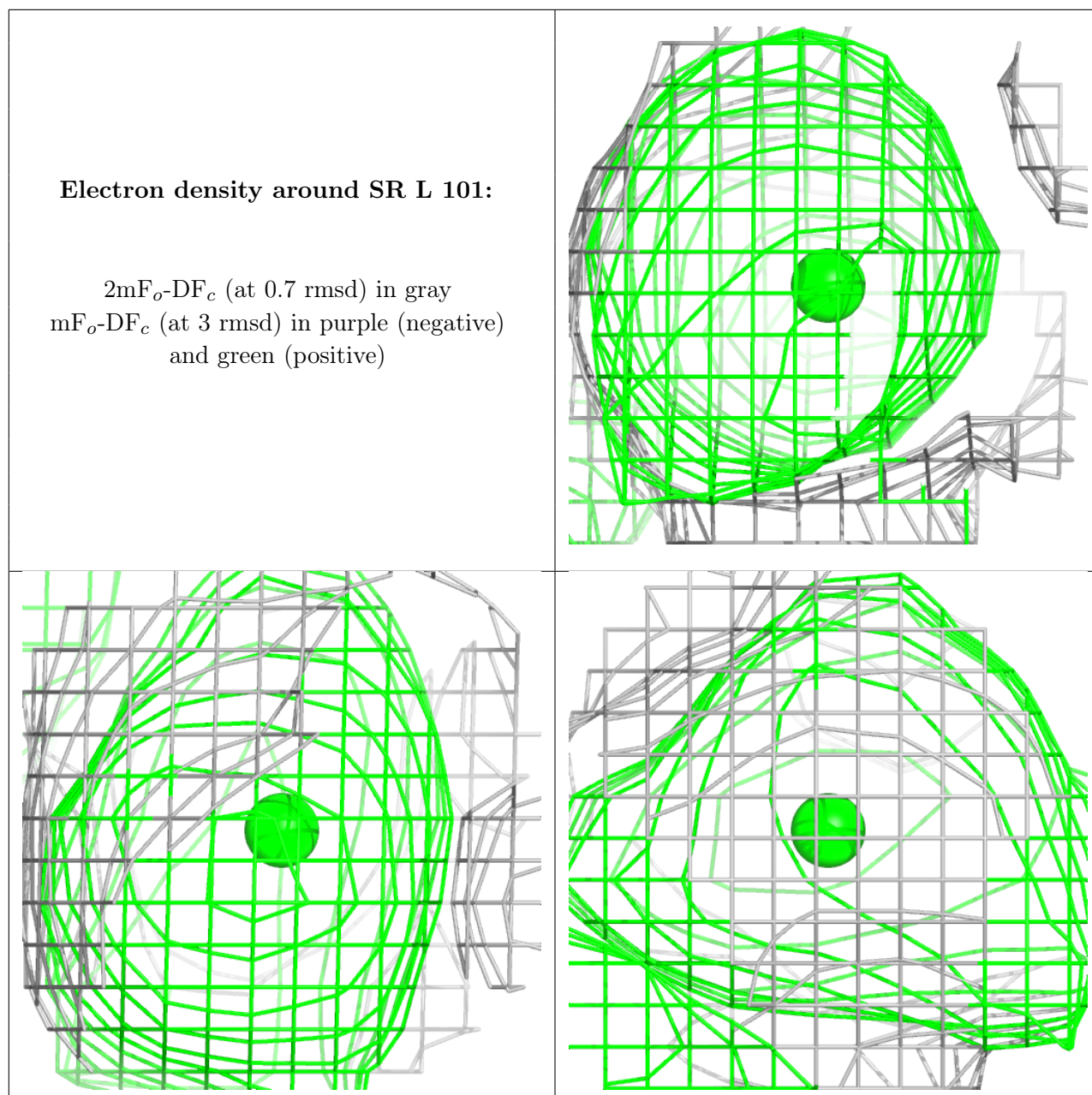
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SR U 101:**

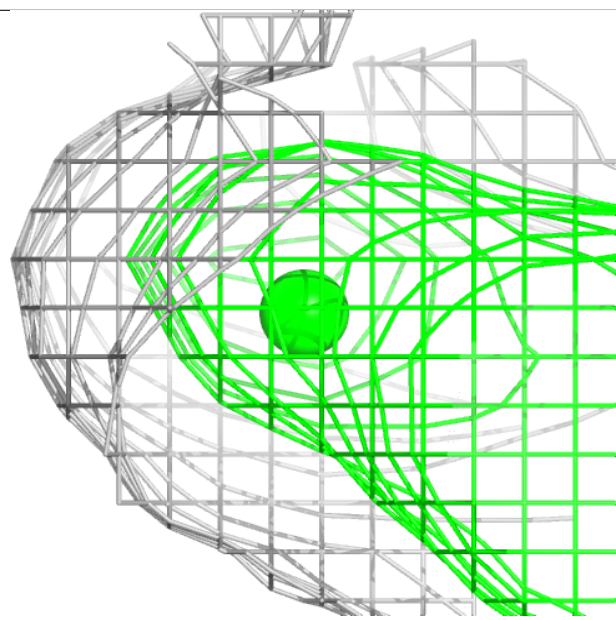
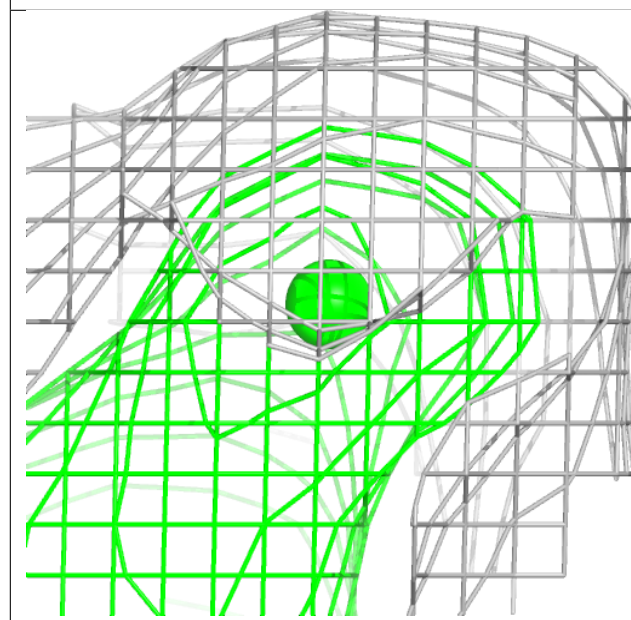
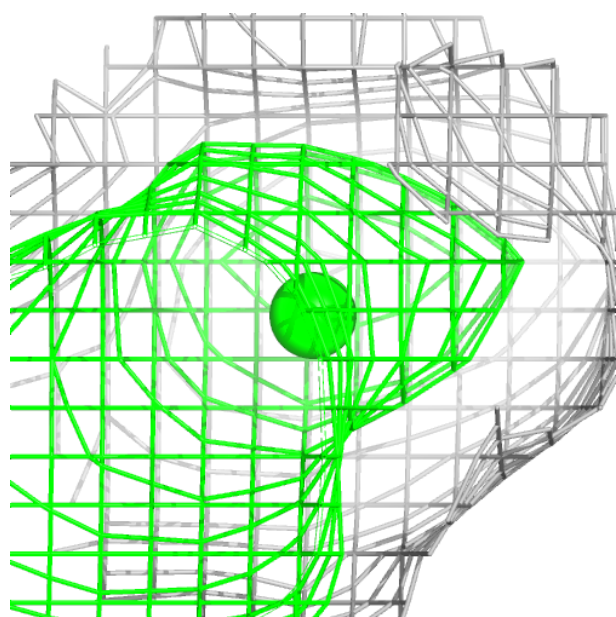
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





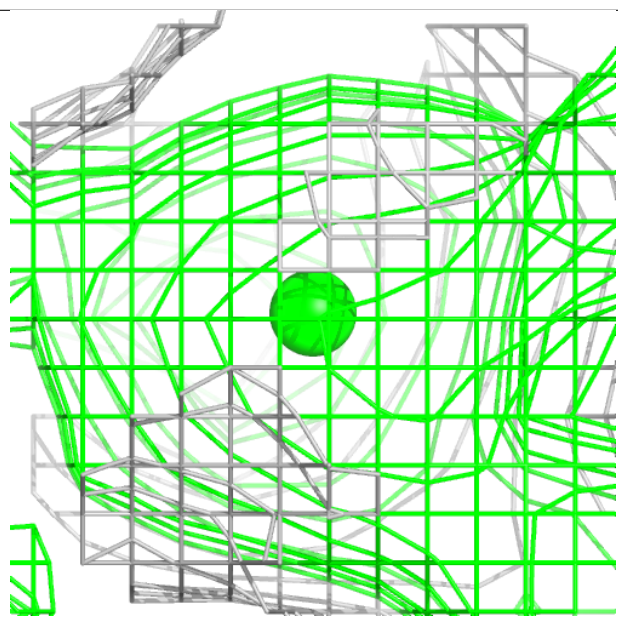
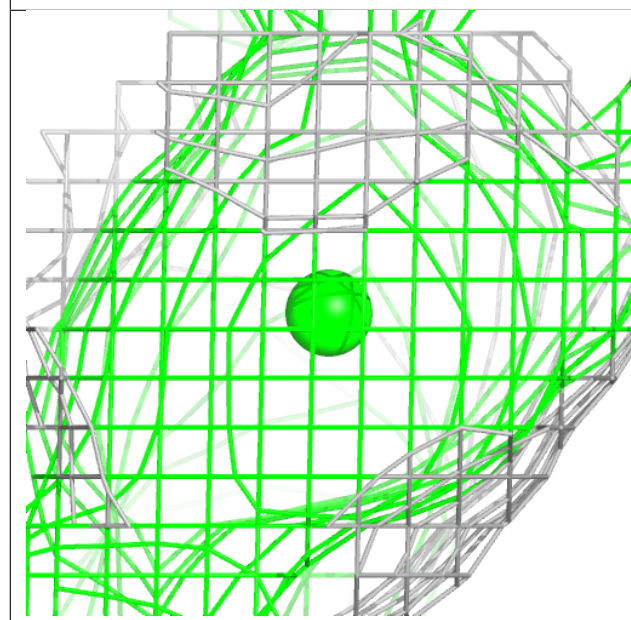
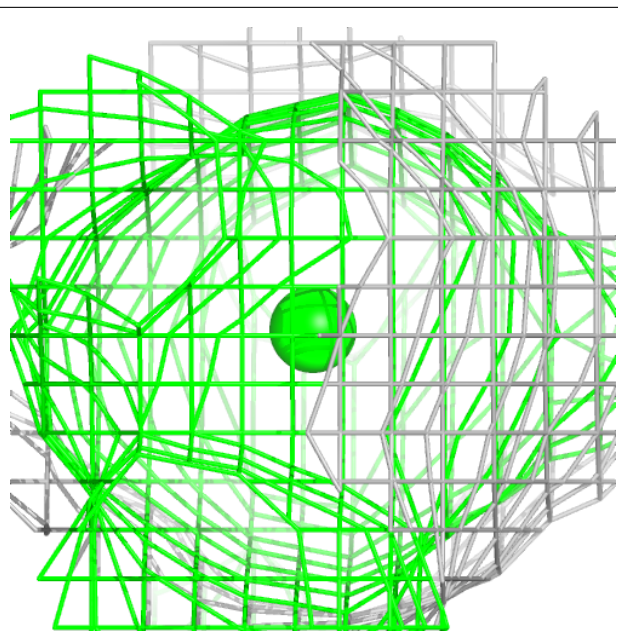
**Electron density around SR Q 101:**

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



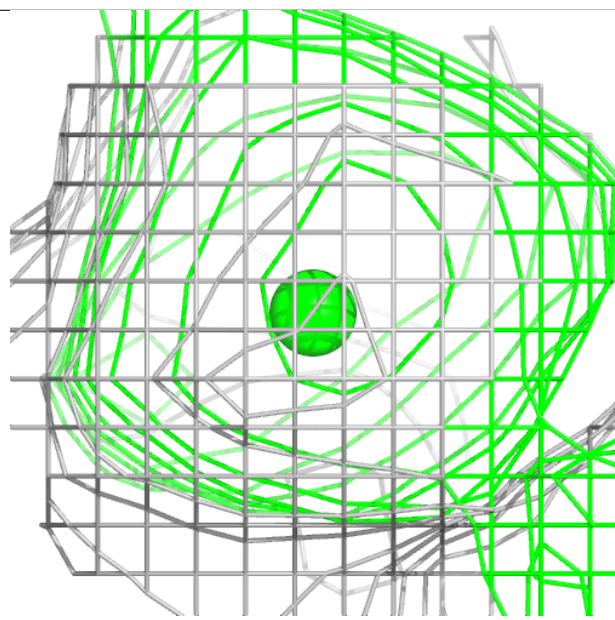
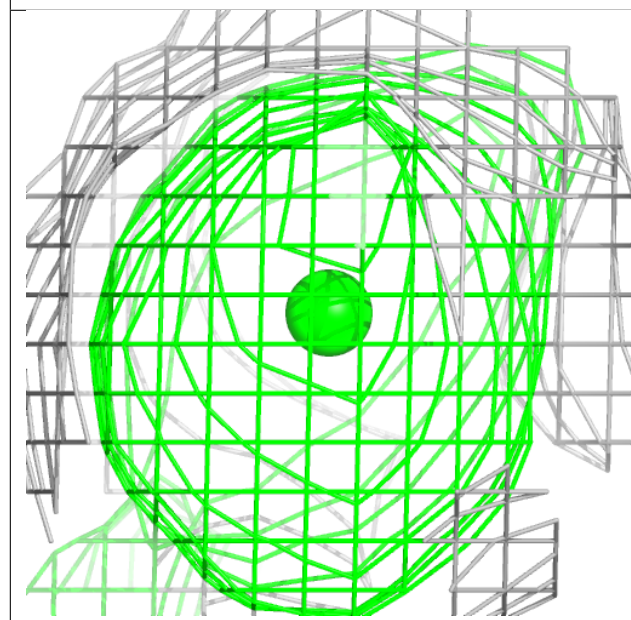
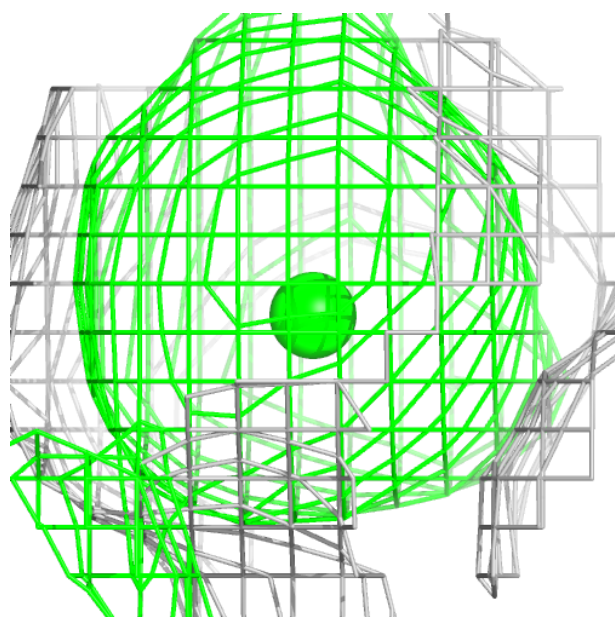
**Electron density around SR I 101:**

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



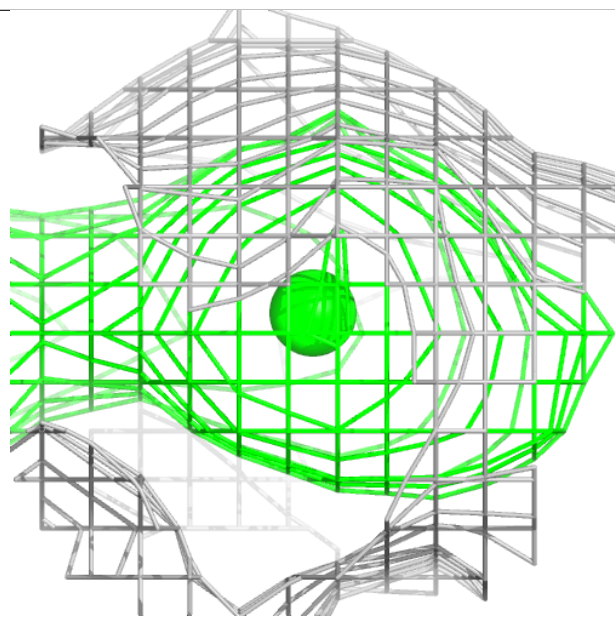
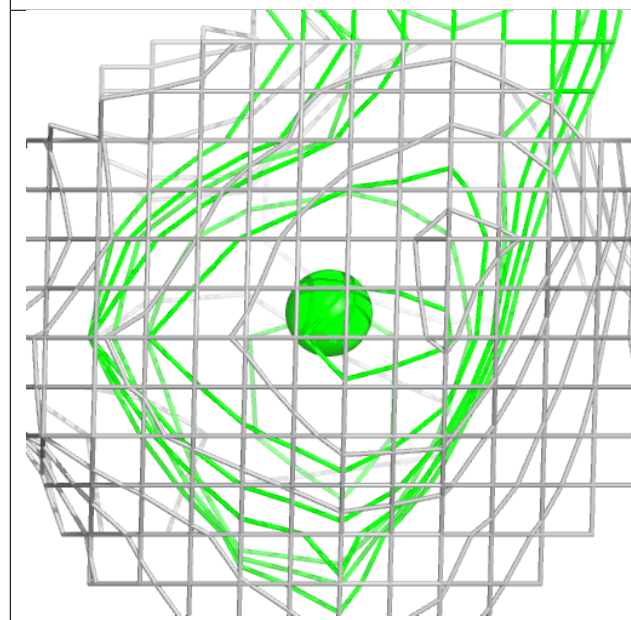
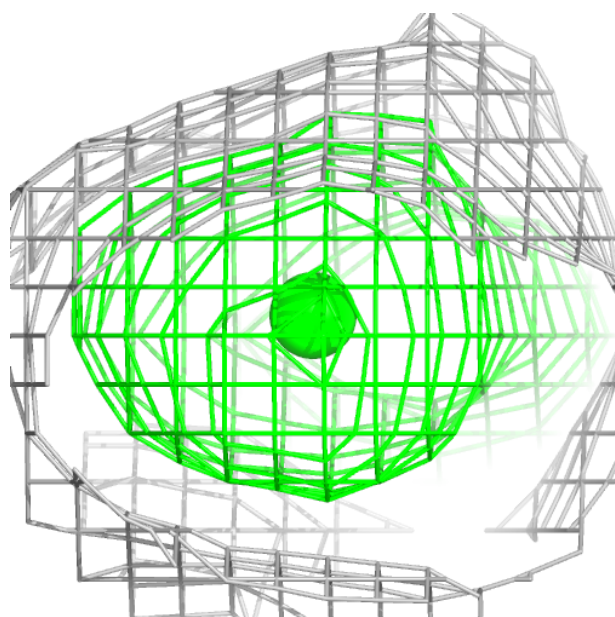
**Electron density around SR B 101:**

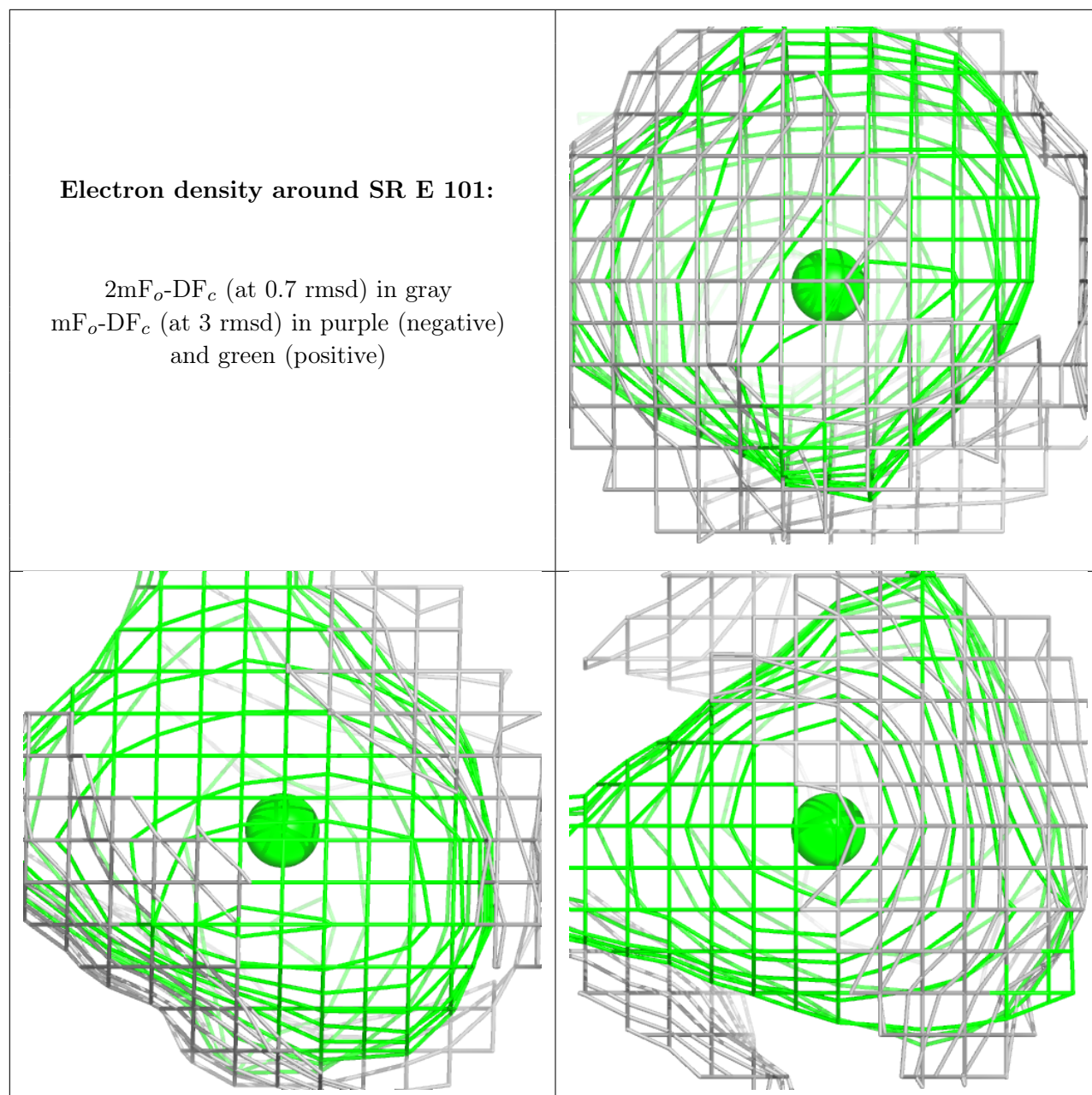
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SR M 101:**

$2mF_o-DF_c$  (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.