wwPDB X-ray Structure Validation Summary Report (i)

Nov 11, 2023 – 07:16 pm GMT

PDB ID	:	8BHU
Title	:	Crystal Structure of SilF (Ag(I) form
Authors	:	Lithgo, R.M.; Carr, S.B.; Quigley, A.M.; Scott, D.J.
Deposited on	:	2022-11-01
Resolution	:	1.70 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 (i)) were used in the production of this report:

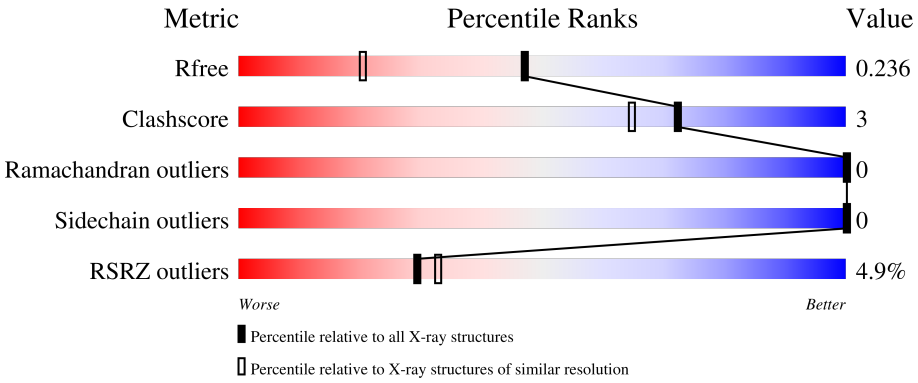
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	120	5% 60% · 36%
1	BBB	120	2% 62% 5% 33%
1	CCC	120	3% 60% 5% 35%
1	DDD	120	4% 62% · 34%
1	EEE	120	4% 58% 7% 36%

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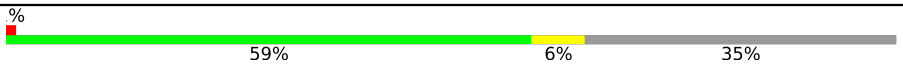
Mol	Chain	Length	Quality of chain
1	FFF	120	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7457 atoms, of which 3667 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.

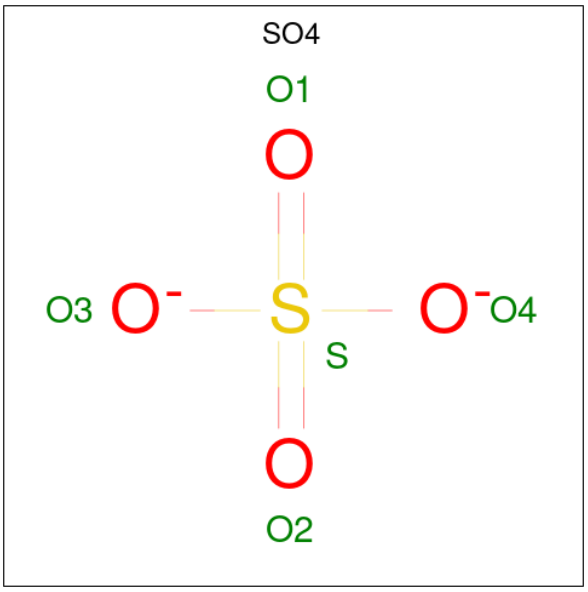
- Molecule 1 is a protein called SilF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	77	Total	C	H	N	O	S	14	0	0
			1183	371	599	102	108	3			
1	BBB	80	Total	C	H	N	O	S	15	0	0
			1231	385	622	107	114	3			
1	CCC	78	Total	C	H	N	O	S	14	0	0
			1200	376	607	104	110	3			
1	DDD	79	Total	C	H	N	O	S	15	0	0
			1214	380	614	105	112	3			
1	EEE	77	Total	C	H	N	O	S	14	0	0
			1183	371	599	102	108	3			
1	FFF	78	Total	C	H	N	O	S	14	0	0
			1200	376	607	104	110	3			

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

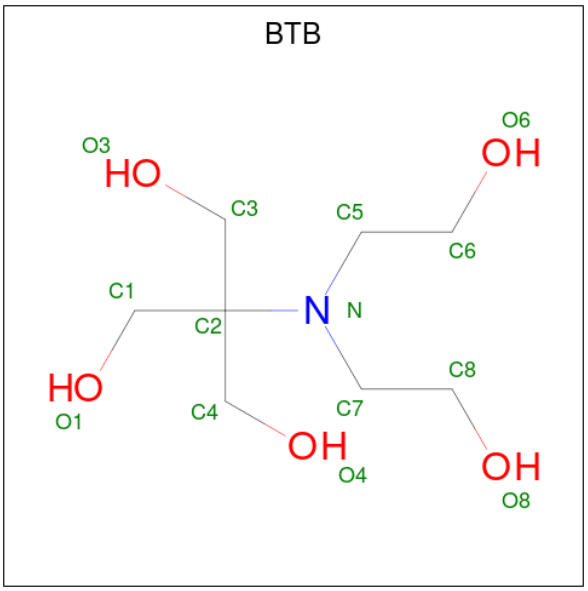
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Ag	0	0
			1	1		
2	BBB	1	Total	Ag	0	0
			1	1		
2	CCC	1	Total	Ag	0	0
			1	1		
2	DDD	1	Total	Ag	0	0
			1	1		
2	EEE	1	Total	Ag	0	0
			1	1		
2	FFF	1	Total	Ag	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0
3	CCC	1	Total O S 5 4 1	0	0
3	DDD	1	Total O S 5 4 1	0	0
3	DDD	1	Total O S 5 4 1	0	0
3	EEE	1	Total O S 5 4 1	0	0
3	FFF	1	Total O S 5 4 1	0	0
3	FFF	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C H N O 33 8 19 1 5	4	0

- Molecule 5 is water.

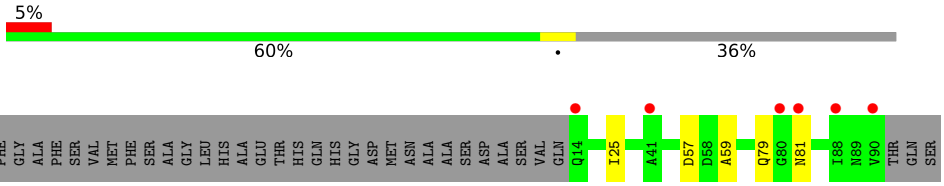
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	30	Total O 30 30	0	0
5	BBB	30	Total O 30 30	0	0
5	CCC	22	Total O 22 22	0	0
5	DDD	30	Total O 30 30	0	0
5	EEE	27	Total O 27 27	0	0
5	FFF	28	Total O 28 28	0	0

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.

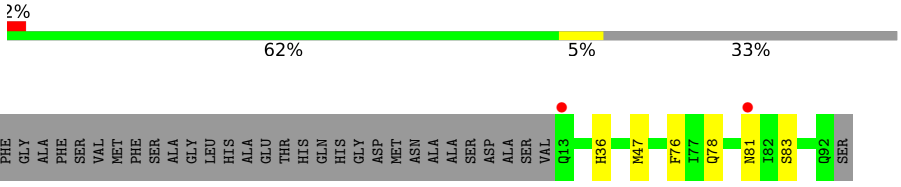
- Molecule 1: SilF

Chain AAA:



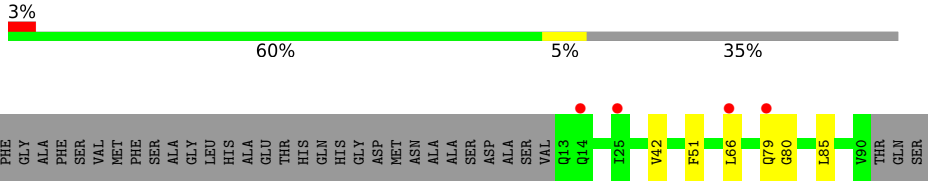
- Molecule 1: SilF

Chain BBB:



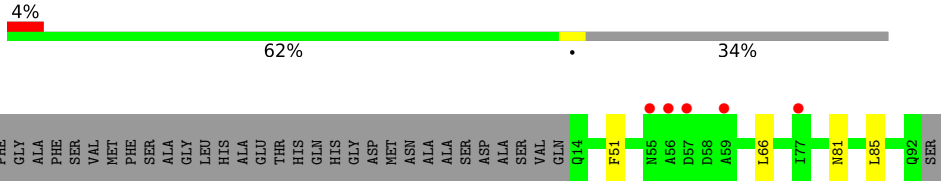
- Molecule 1: SilF

Chain CCC:



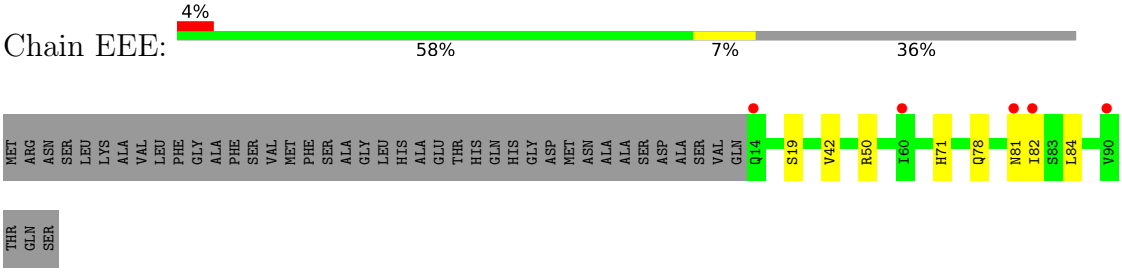
- Molecule 1: SilF

Chain DDD:



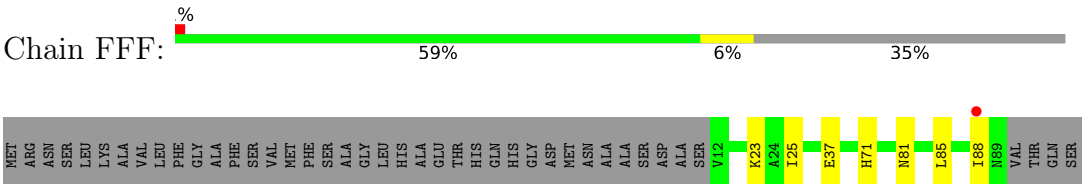
- Molecule 1: SilF

Chain EEE:



• Molecule 1: SilF

Chain FFF:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.94Å 81.59Å 95.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.11 – 1.70 62.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.11-1.70) 100.0 (62.11-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.230 0.206 , 0.236	Depositor DCC
R_{free} test set	2620 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: SO4, BTB, AG

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	AAA	0.78	0/593	0.88	1/802 (0.1%)
1	BBB	0.75	0/618	0.81	0/836
1	CCC	0.69	0/602	0.84	0/814
1	DDD	0.72	0/609	0.88	0/824
1	EEE	0.71	0/593	0.85	0/802
1	FFF	0.70	0/602	0.88	0/814
All	All	0.73	0/3617	0.86	1/4892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	57	ASP	CB-CG-OD1	-5.28	113.55	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	584	599	596	5	0
1	BBB	609	622	619	6	0
1	CCC	593	607	604	8	0
1	DDD	600	614	611	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EEE	584	599	596	7	0
1	FFF	593	607	604	6	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	1	0	0	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	5	0	0	0	0
3	DDD	10	0	0	0	0
3	EEE	5	0	0	1	0
3	FFF	10	0	0	1	0
4	BBB	14	19	19	0	0
5	AAA	30	0	0	1	0
5	BBB	30	0	0	0	0
5	CCC	22	0	0	0	0
5	DDD	30	0	0	0	0
5	EEE	27	0	0	0	0
5	FFF	28	0	0	0	0
All	All	3790	3667	3649	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 25 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:CCC:79:GLN:HG2	1:EEE:42:VAL:O	1.67	0.93
1:BBB:76:PHE:HE2	1:BBB:78:GLN:HE21	1.19	0.87
1:BBB:78:GLN:NE2	1:BBB:83:SER:OG	2.25	0.68
1:FFF:23:LYS:HE3	3:FFF:103:SO4:O2	2.00	0.62
1:CCC:79:GLN:NE2	1:EEE:78:GLN:HE22	2.05	0.55

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	AAA	75/120 (62%)	75 (100%)	0	0	100	100
1	BBB	78/120 (65%)	77 (99%)	1 (1%)	0	100	100
1	CCC	76/120 (63%)	76 (100%)	0	0	100	100
1	DDD	77/120 (64%)	77 (100%)	0	0	100	100
1	EEE	75/120 (62%)	75 (100%)	0	0	100	100
1	FFF	76/120 (63%)	76 (100%)	0	0	100	100
All	All	457/720 (64%)	456 (100%)	1 (0%)	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	AAA	64/97 (66%)	64 (100%)	0	100	100
1	BBB	67/97 (69%)	67 (100%)	0	100	100
1	CCC	65/97 (67%)	65 (100%)	0	100	100
1	DDD	66/97 (68%)	66 (100%)	0	100	100
1	EEE	64/97 (66%)	64 (100%)	0	100	100
1	FFF	65/97 (67%)	65 (100%)	0	100	100
All	All	391/582 (67%)	391 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	EEE	102	-	4,4,4	0.52	0	6,6,6	0.10	0
3	SO4	DDD	103	-	4,4,4	0.40	0	6,6,6	0.17	0
3	SO4	CCC	102	-	4,4,4	0.51	0	6,6,6	0.08	0
3	SO4	FFF	102	-	4,4,4	0.57	0	6,6,6	0.14	0
3	SO4	FFF	103	-	4,4,4	0.41	0	6,6,6	0.19	0
3	SO4	AAA	102	-	4,4,4	0.62	0	6,6,6	0.19	0
3	SO4	BBB	103	-	4,4,4	0.63	0	6,6,6	0.13	0
4	BTB	BBB	101	-	13,13,13	1.48	3 (23%)	7,16,16	0.60	0
3	SO4	DDD	102	-	4,4,4	0.52	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	BBB	101	-	-	1/21/21/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	101	BTB	C2-N	3.38	1.55	1.48
4	BBB	101	BTB	C5-N	3.24	1.52	1.48
4	BBB	101	BTB	C7-N	2.20	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	101	BTB	N-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EEE	102	SO4	1	0
3	FFF	103	SO4	1	0

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	AAA	77/120 (64%)	0.45	6 (7%)	13	15	20, 30, 62, 82	0
1	BBB	80/120 (66%)	0.26	2 (2%)	57	61	21, 28, 45, 67	0
1	CCC	78/120 (65%)	0.49	4 (5%)	28	31	21, 34, 58, 68	0
1	DDD	79/120 (65%)	0.44	5 (6%)	20	22	20, 30, 47, 60	0
1	EEE	77/120 (64%)	0.49	5 (6%)	18	21	22, 30, 51, 60	0
1	FFF	78/120 (65%)	0.30	1 (1%)	77	81	21, 30, 47, 54	0
All	All	469/720 (65%)	0.40	23 (4%)	29	33	20, 30, 52, 82	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	77	ILE	3.9
1	EEE	90	VAL	3.4
1	AAA	88	ILE	3.3
1	BBB	13	GLN	3.2
1	AAA	90	VAL	3.2

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

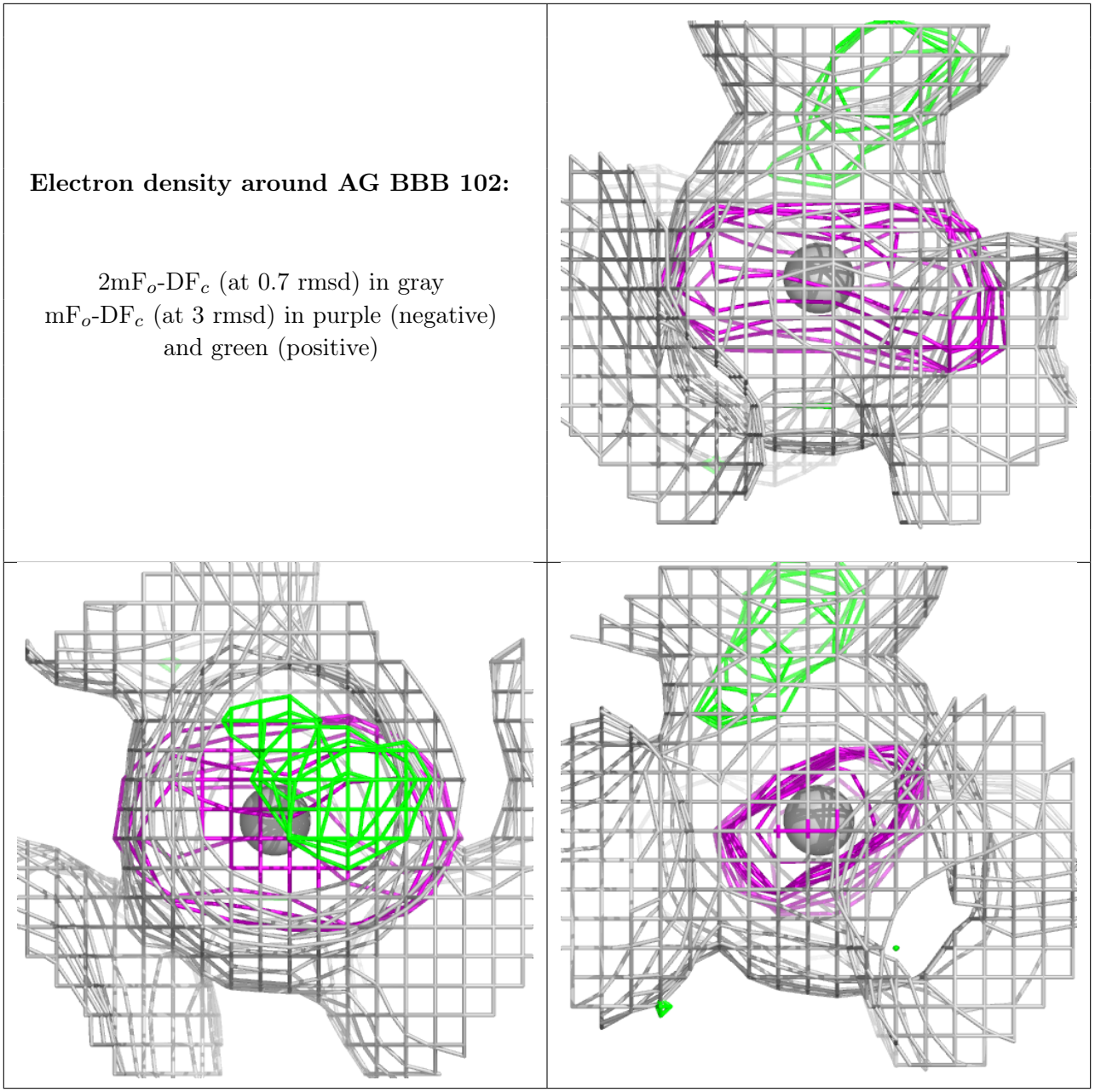
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BTB	BBB	101	14/14	0.87	0.17	34,40,49,49	4
3	SO4	FFF	103	5/5	0.91	0.13	63,64,71,78	0
3	SO4	DDD	103	5/5	0.95	0.13	60,61,67,73	0
3	SO4	EEE	102	5/5	0.96	0.10	48,50,56,57	0
3	SO4	BBB	103	5/5	0.97	0.13	49,53,57,58	0
3	SO4	CCC	102	5/5	0.97	0.10	47,49,55,56	0
3	SO4	DDD	102	5/5	0.98	0.09	42,45,47,51	0
3	SO4	FFF	102	5/5	0.98	0.11	42,44,48,57	0
2	AG	BBB	102	1/1	0.99	0.12	27,27,27,27	0
2	AG	DDD	101	1/1	0.99	0.11	26,26,26,26	0
2	AG	EEE	101	1/1	0.99	0.11	26,26,26,26	0
3	SO4	AAA	102	5/5	0.99	0.11	44,48,48,51	0
2	AG	AAA	101	1/1	1.00	0.12	23,23,23,23	0
2	AG	CCC	101	1/1	1.00	0.12	26,26,26,26	0
2	AG	FFF	101	1/1	1.00	0.11	25,25,25,25	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.

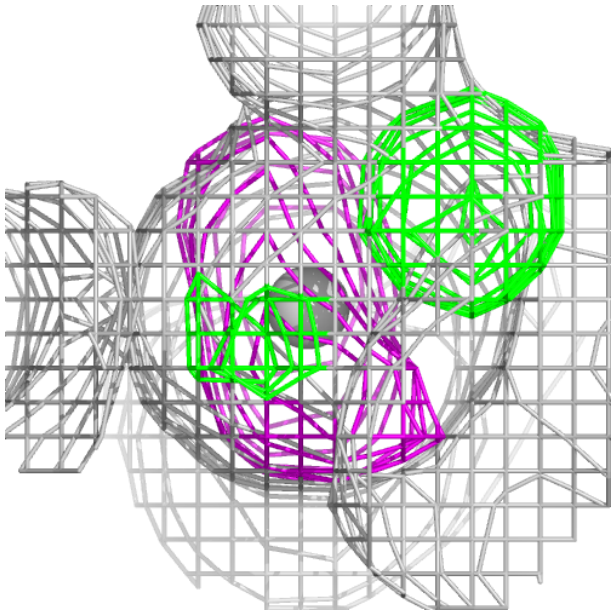
Electron density around AG BBB 102:

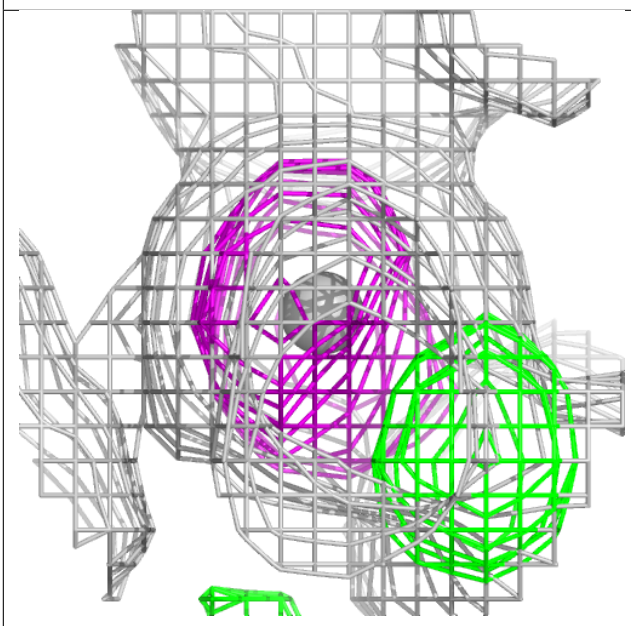
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

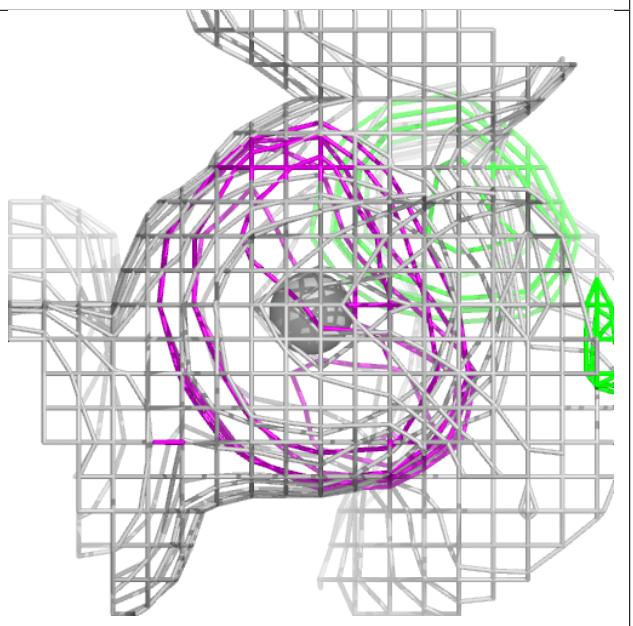


Electron density around AG DDD 101:

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

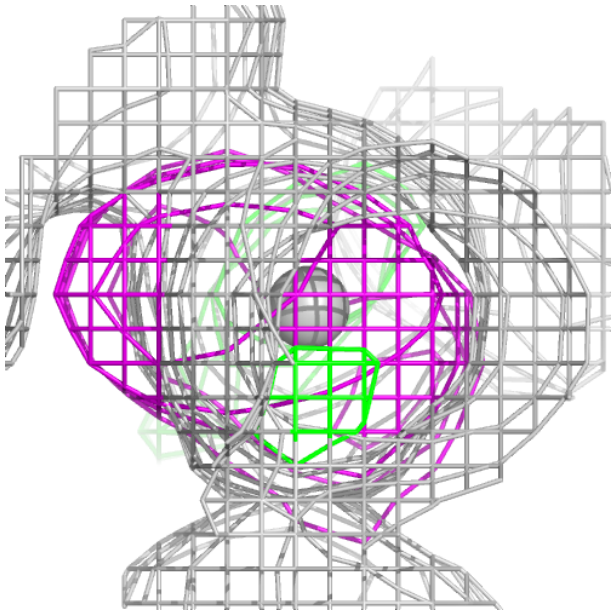


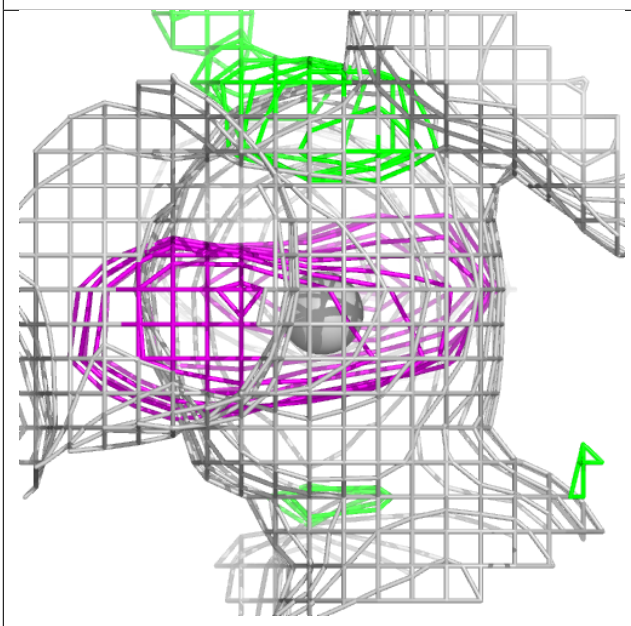


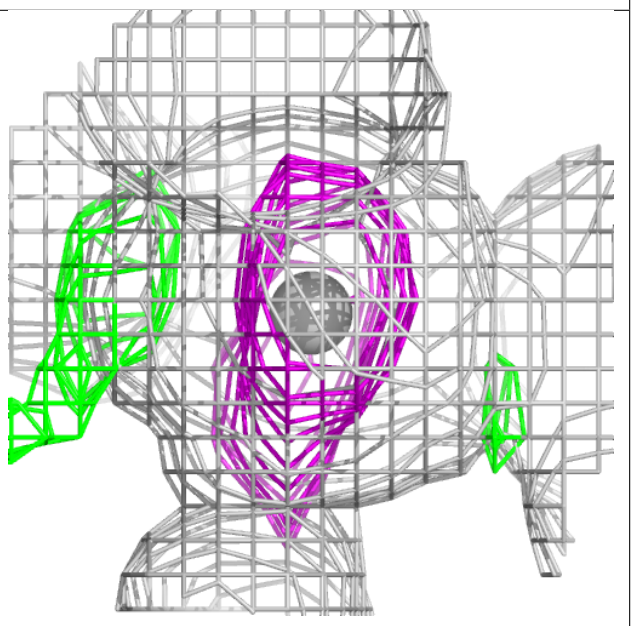


Electron density around AG EEE 101:

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

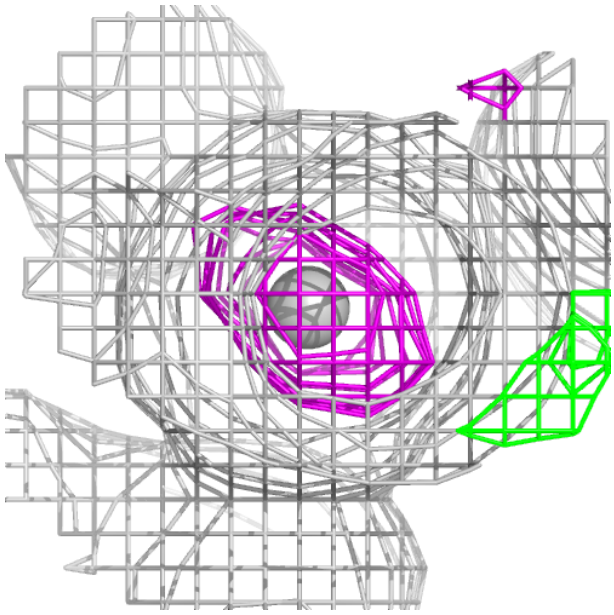


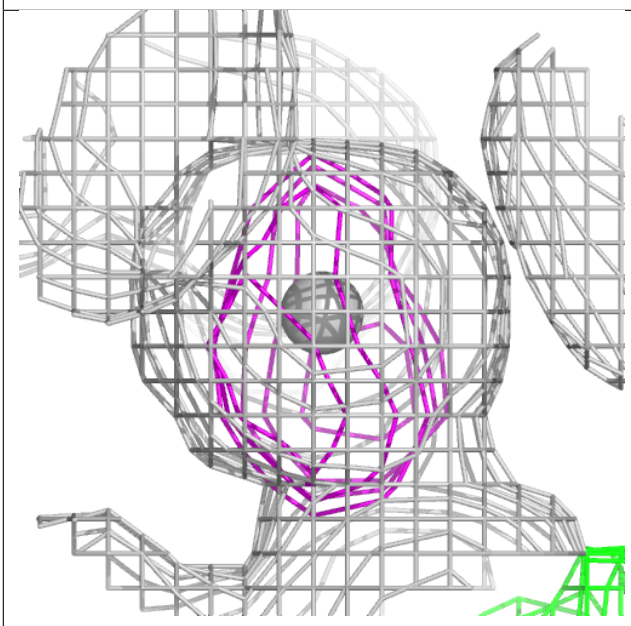


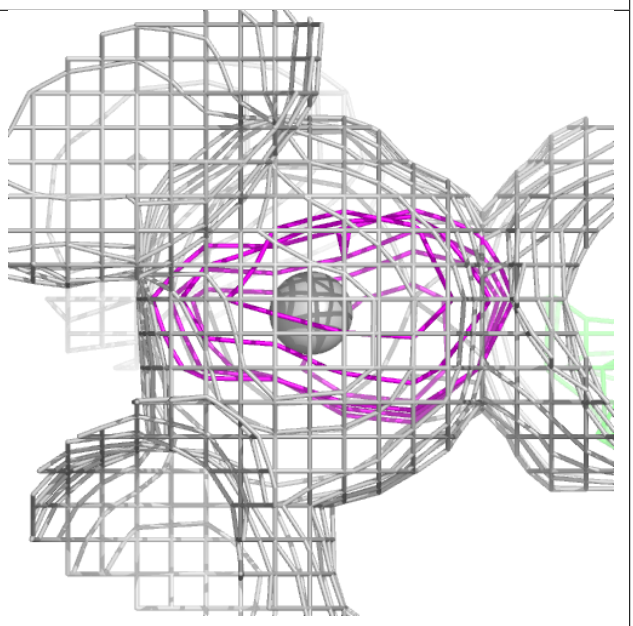


Electron density around AG AAA 101:

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

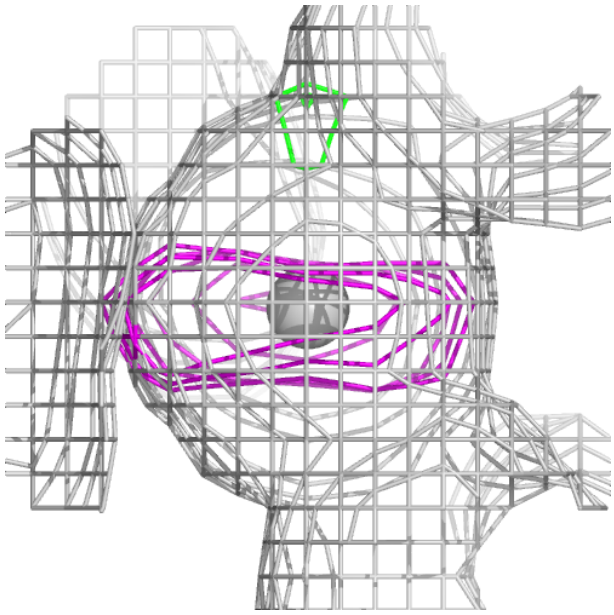


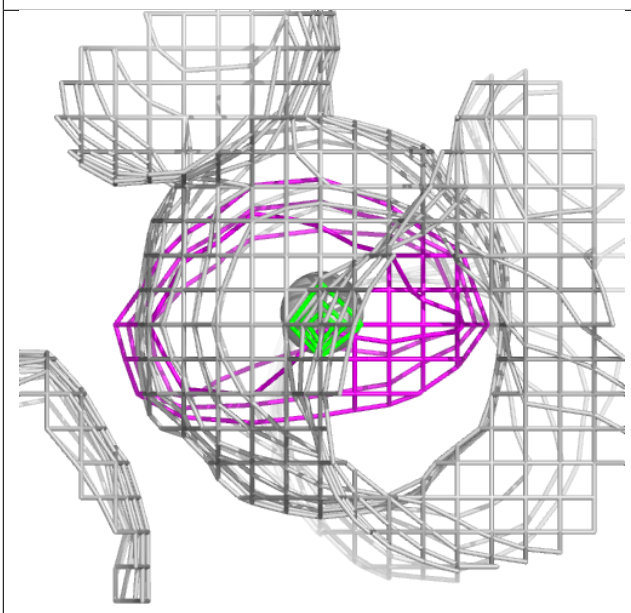


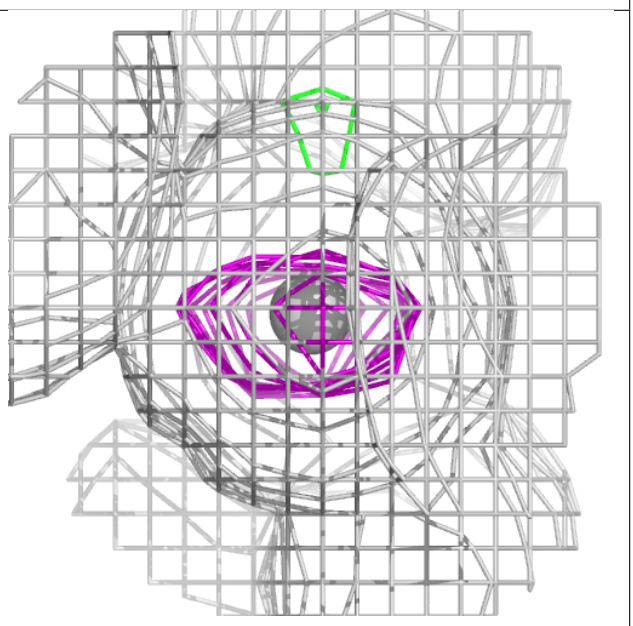


Electron density around AG CCC 101:

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

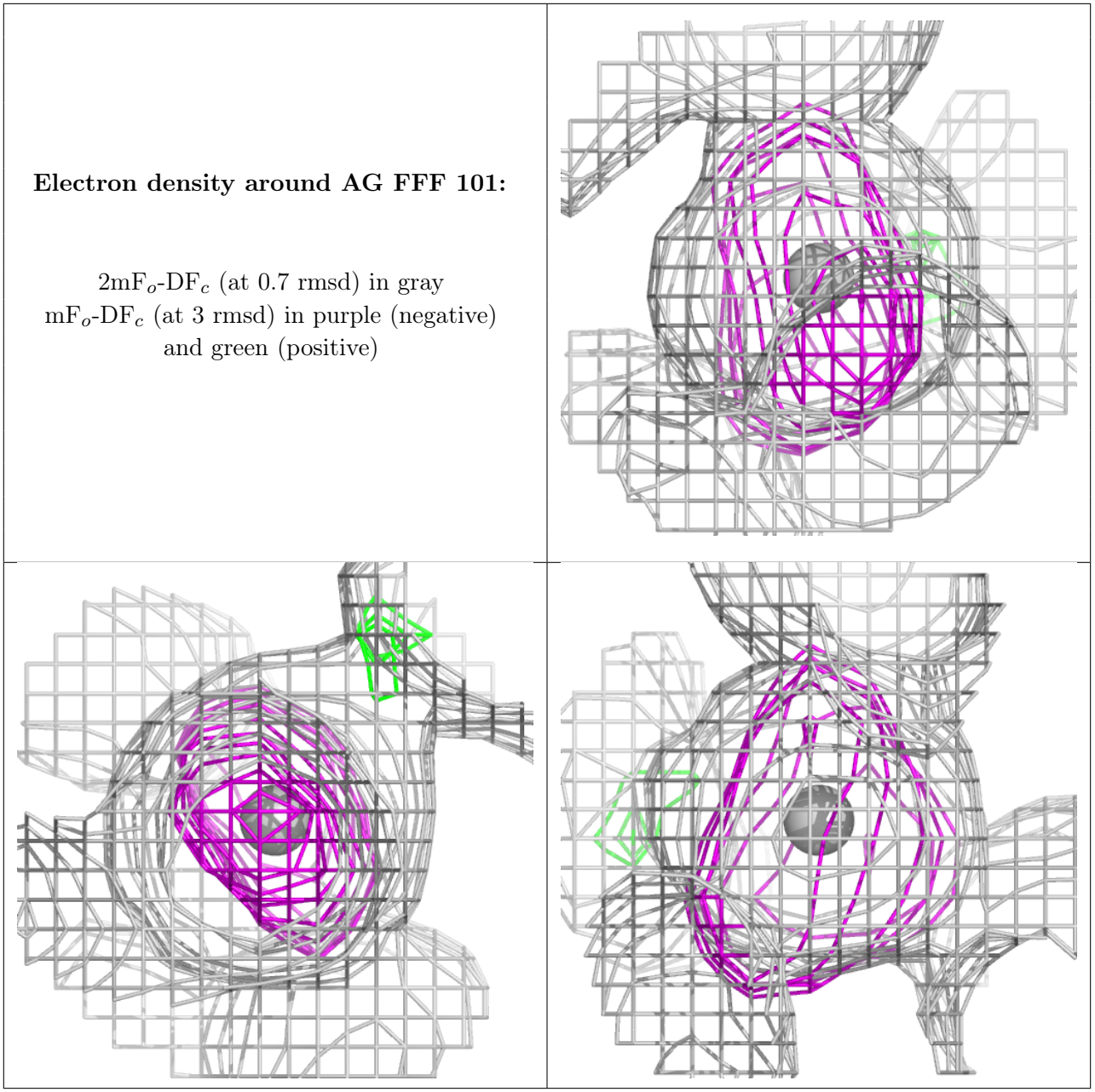






Electron density around AG FFF 101:

$2mF_o$-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

There are no such residues in this entry.