wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2026 – 04:53 PM JST

PDB ID	:	9XP9 / pdb_00009xp9
Title	:	Crystal structure of Acinetobacter baumannii phage AbP20 tail fiber protein gp44
Authors	:	Hu, F.
Deposited on	:	2025-11-16
Resolution	:	2.47 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:

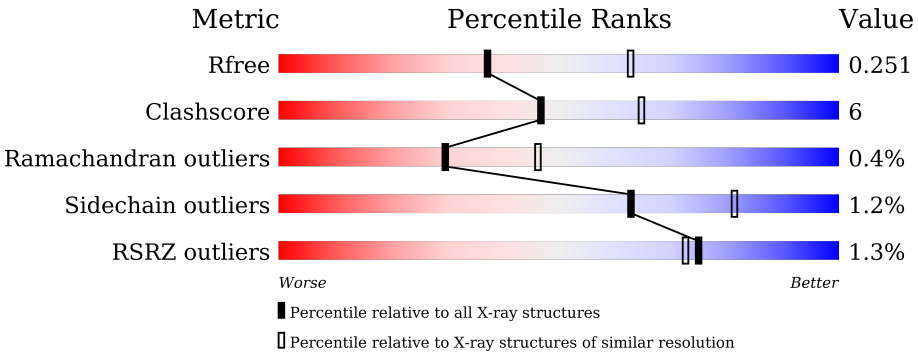
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	627	83% 12% •
1	B	627	83% 13% •
1	C	627	82% 13% • •
1	D	627	81% 14% 5%
1	E	627	78% 14% 8%
1	F	627	78% 16% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28093 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gp44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4537	2837	788	892	20			
1	B	601	Total	C	N	O	S	0	0	0
			4537	2837	788	892	20			
1	C	601	Total	C	N	O	S	0	0	0
			4537	2837	788	892	20			
1	D	596	Total	C	N	O	S	0	0	0
			4504	2819	782	883	20			
1	E	579	Total	C	N	O	S	0	0	0
			4379	2746	759	854	20			
1	F	595	Total	C	N	O	S	0	0	0
			4495	2813	780	882	20			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	196	Total	O	0	0
			196	196		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	180	Total O 180 180	0	0
3	D	180	Total O 180 180	0	0
3	E	186	Total O 186 186	0	0
3	F	161	Total O 161 161	0	0

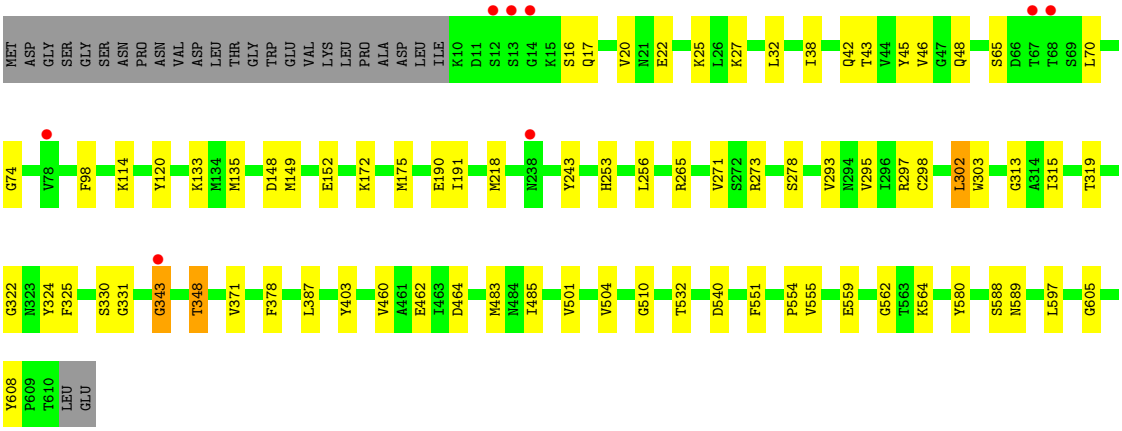
3 Residue-property plots (i)

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: gp44

Chain A:

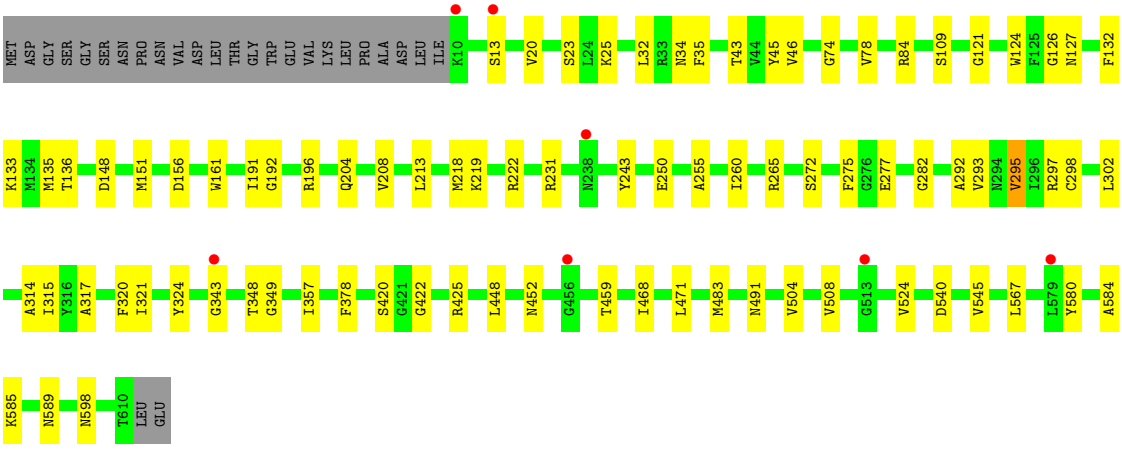




• Molecule 1: gp44

Chain B:

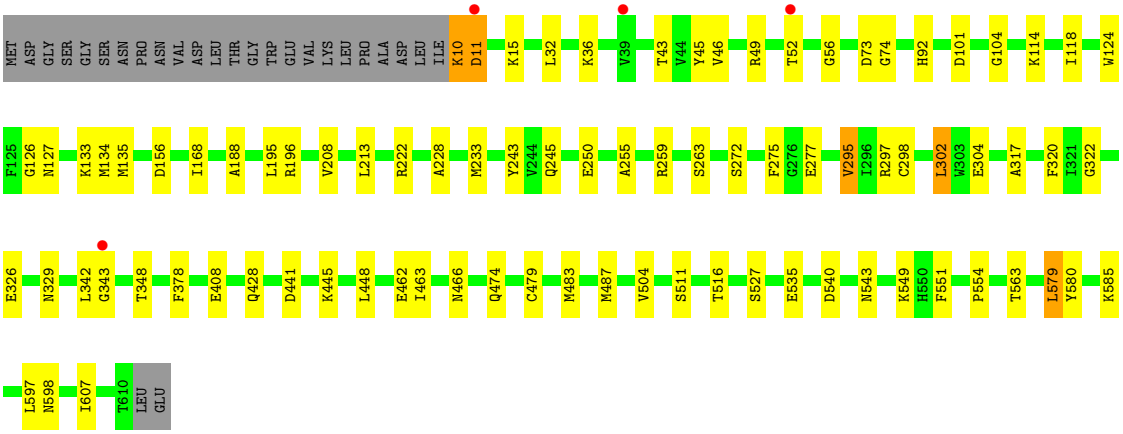




• Molecule 1: gp44

Chain C:

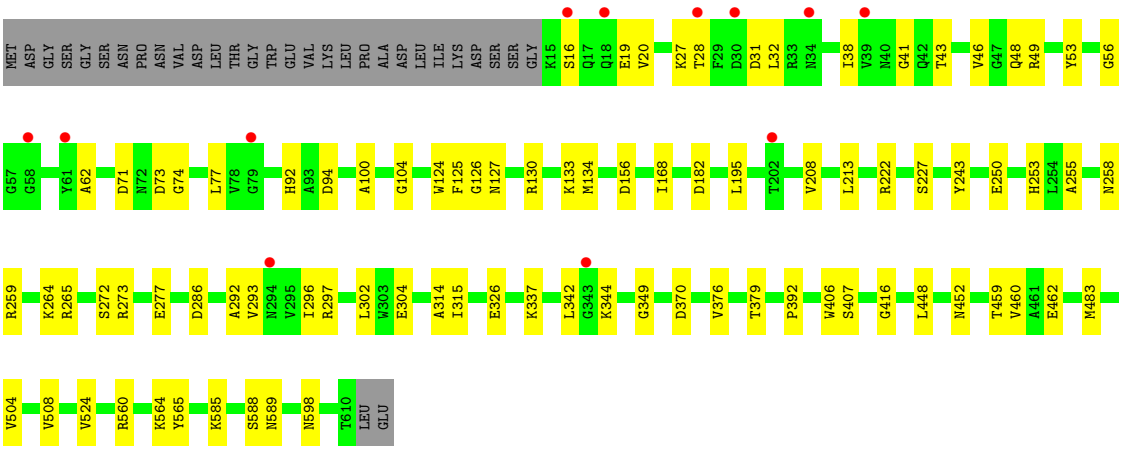




• Molecule 1: gp44

Chain D:

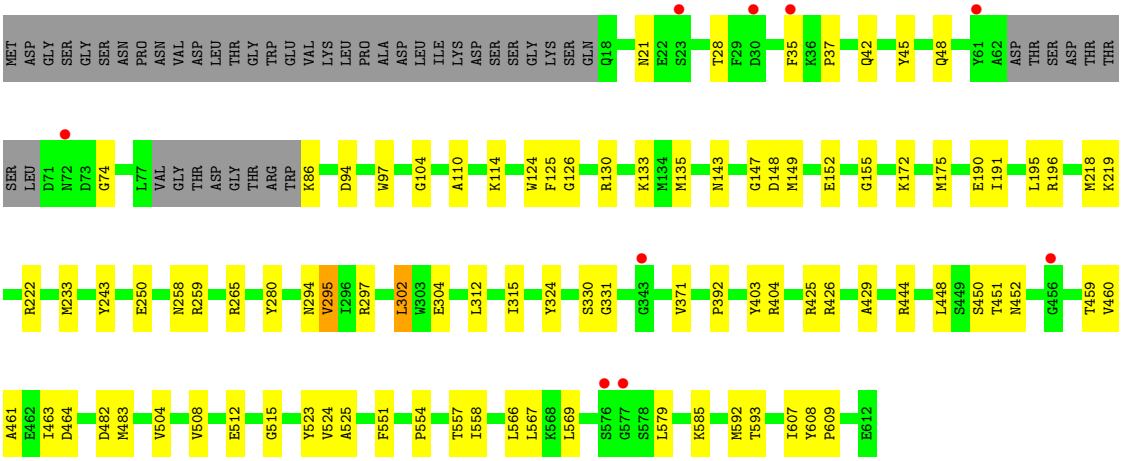




• Molecule 1: gp44

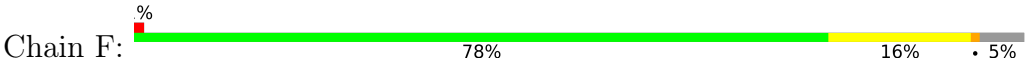
Chain E:

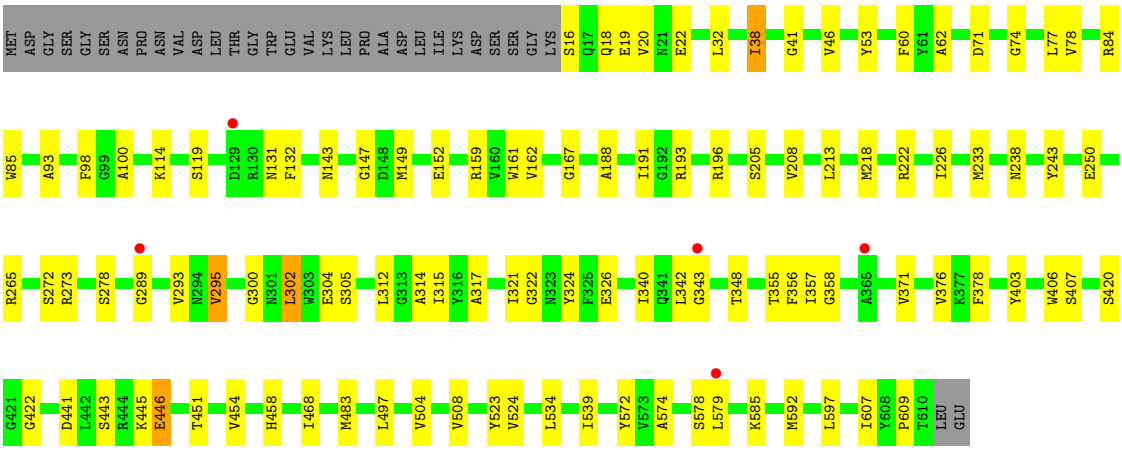




• Molecule 1: gp44

Chain F:


%
78%
16%
• 5%


MET ASP GLY SER GLY SER ASN PRO ASN VAL ASP LEU THR GLY TRP GLU VAL LYS LEU PRO ALA ASP LEU ILE LYS ASP SER SER GLY LYS S16 Q17 Q18 E19 V20 N21 E22 L32 I38 G41 V46 Y53 F60 Y61 A62 D71 G74 L77 V78 R84
W85 A93 F98 G99 A100 K114 S119 D129 R130 N131 F132 N143 G147 D148 M149 E152 R159 V160 W161 V162 G167 A188 I191 G192 R193 R196 S205 V208 L213 M218 R222 I226 M233 N238 Y243 E250
R265 S272 R273 S278 G289 V293 N294 V295 G300 N301 L302 W303 E304 S305 L312 G313 A314 I315 Y316 A317 I321 G322 N323 Y324 F325 E326 I340 Q341 L342 G343 T348 T355 F356 I357 G358 A365 V371 V376 K377 F378 Y403 W406 S407 S420
G421 G422 D441 L442 S443 R444 K445 E446 T451 V454 H458 I468 M483 L497 V504 V508 Y523 V524 L534 I539 Y572 V573 A574 S578 L579 K585 M592 L597 I607 Y608 P609 T610 LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.80Å 104.97Å 139.88Å 103.92° 97.82° 91.21°	Depositor
Resolution (Å)	67.16 – 2.47 67.16 – 2.47	Depositor EDS
% Data completeness (in resolution range)	93.6 (67.16-2.47) 93.6 (67.16-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.249 0.207 , 0.251	Depositor DCC
R_{free} test set	5936 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28093	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: MG

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	0.35	1/4620 (0.0%)	0.48	0/6266
1	B	0.21	0/4620	0.43	0/6266
1	C	0.27	0/4620	0.46	0/6266
1	D	0.18	0/4587	0.38	0/6223
1	E	0.24	0/4458	0.43	0/6042
1	F	0.26	0/4578	0.47	1/6212 (0.0%)
All	All	0.26	1/27483 (0.0%)	0.44	1/37275 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLY	CA-C	-8.23	1.40	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	289	GLY	N-CA-C	11.12	126.09	112.64

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	4537	0	4432	47	0
1	B	4537	0	4432	53	0
1	C	4537	0	4432	51	0
1	D	4504	0	4402	56	0
1	E	4379	0	4285	58	0
1	F	4495	0	4389	67	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	2	0	0	0	0
3	A	196	0	0	9	0
3	B	196	0	0	4	0
3	C	180	0	0	6	0
3	D	180	0	0	5	0
3	E	186	0	0	7	0
3	F	161	0	0	7	0
All	All	28093	0	26372	306	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 6.

The worst 5 of 306 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:F:143:ASN:HB2	1:F:149:MET:HE2	1.52	0.90
1:A:133:LYS:HD3	1:A:135:MET:HE3	1.61	0.81
1:C:551:PHE:HB3	1:C:554:PRO:HG3	1.65	0.77
1:A:551:PHE:HB3	1:A:554:PRO:HG3	1.67	0.76
1:B:204:GLN:HE21	1:B:231:ARG:HH12	1.34	0.76

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	599/627 (96%)	569 (95%)	28 (5%)	2 (0%)	36	53
1	B	599/627 (96%)	569 (95%)	27 (4%)	3 (0%)	24	40
1	C	599/627 (96%)	568 (95%)	28 (5%)	3 (0%)	24	40
1	D	594/627 (95%)	569 (96%)	24 (4%)	1 (0%)	43	61
1	E	573/627 (91%)	547 (96%)	23 (4%)	3 (0%)	24	40
1	F	593/627 (95%)	559 (94%)	32 (5%)	2 (0%)	36	53
All	All	3557/3762 (95%)	3381 (95%)	162 (5%)	14 (0%)	30	46

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	SER
1	A	74	GLY
1	C	74	GLY
1	E	295	VAL
1	A	295	VAL

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	488/510 (96%)	481 (99%)	7 (1%)	59	79
1	B	488/510 (96%)	487 (100%)	1 (0%)	87	94
1	C	488/510 (96%)	478 (98%)	10 (2%)	48	72
1	D	484/510 (95%)	481 (99%)	3 (1%)	78	90
1	E	469/510 (92%)	464 (99%)	5 (1%)	65	83
1	F	483/510 (95%)	475 (98%)	8 (2%)	53	75
All	All	2900/3060 (95%)	2866 (99%)	34 (1%)	63	81

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	348	THR

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Mol	Chain	Res	Type
1	F	445	LYS
1	F	454	VAL
1	C	118	ILE
1	C	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	21	ASN
1	F	341	GLN
1	C	245	GLN
1	E	428	GLN
1	C	234	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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	601/627 (95%)	-0.02	8 (1%)	75	72	7, 17, 32, 58	0
1	B	601/627 (95%)	0.04	7 (1%)	76	74	8, 17, 31, 53	0
1	C	601/627 (95%)	0.01	4 (0%)	84	82	7, 18, 29, 47	0
1	D	596/627 (95%)	0.13	12 (2%)	65	62	8, 19, 36, 50	0
1	E	579/627 (92%)	0.20	9 (1%)	70	68	9, 20, 35, 61	0
1	F	595/627 (94%)	0.22	5 (0%)	82	80	9, 21, 34, 42	0
All	All	3573/3762 (94%)	0.10	45 (1%)	75	72	7, 19, 33, 61	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	ASN	4.2
1	A	343	GLY	3.6
1	D	343	GLY	3.5
1	C	11	ASP	3.4
1	C	343	GLY	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 oligosaccharides in this entry.

6.4 Ligands (i)

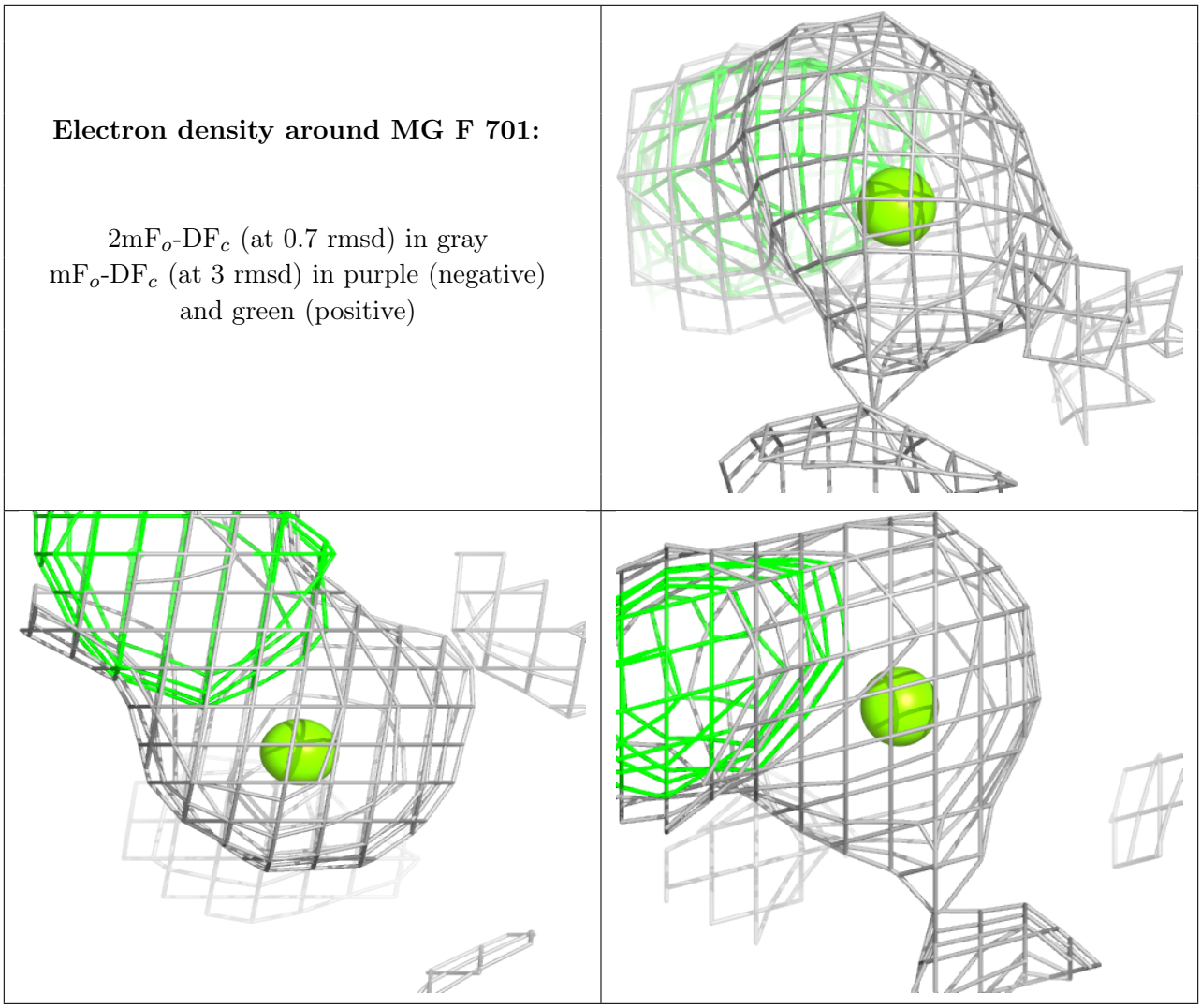
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	F	701	1/1	0.84	0.10	16,16,16,16	0
2	MG	D	701	1/1	0.85	0.13	19,19,19,19	0
2	MG	F	702	1/1	0.90	0.11	30,30,30,30	0
2	MG	B	701	1/1	0.96	0.03	16,16,16,16	0
2	MG	C	701	1/1	0.97	0.04	18,18,18,18	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.

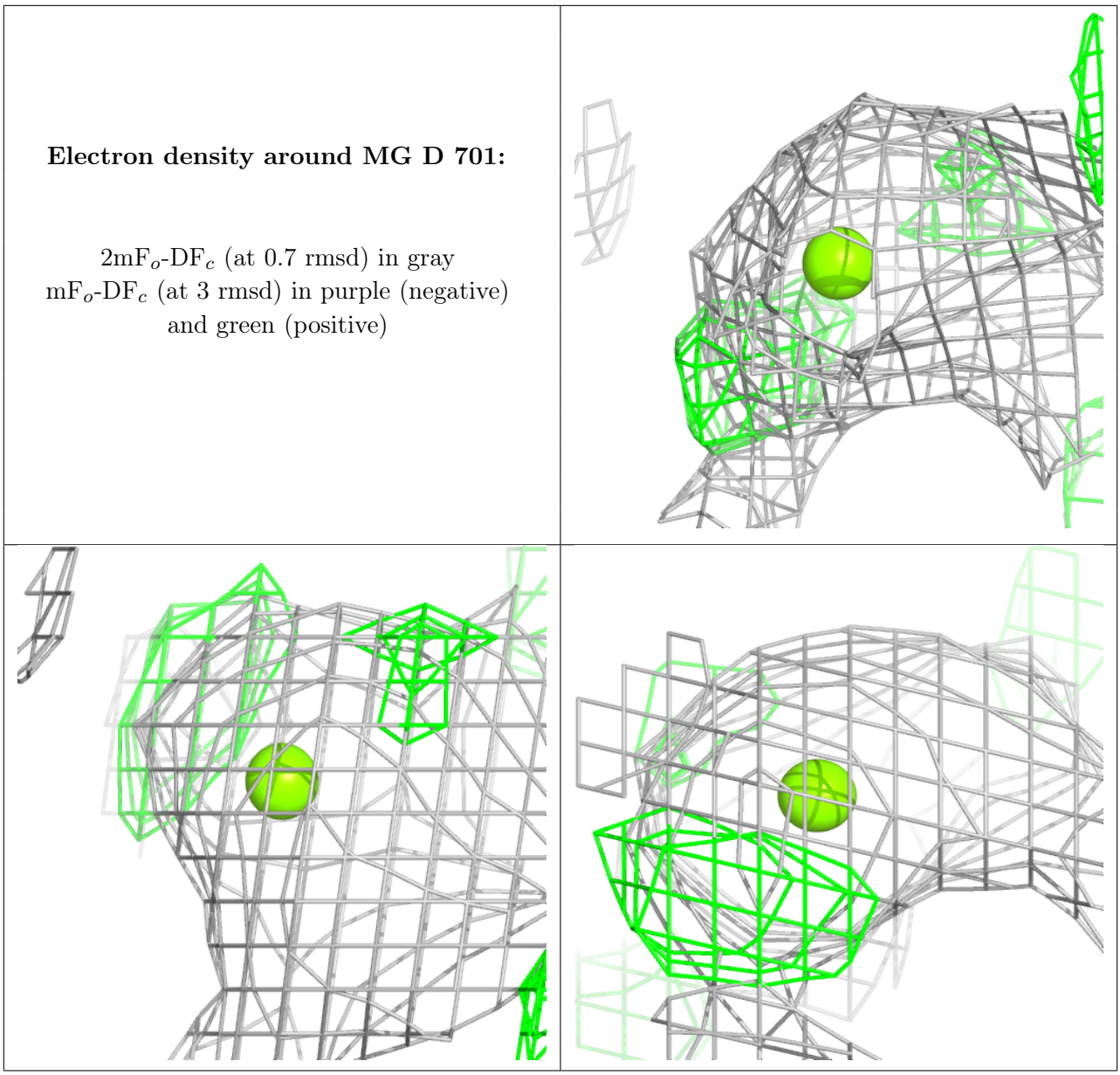
Electron density around MG F 701:

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



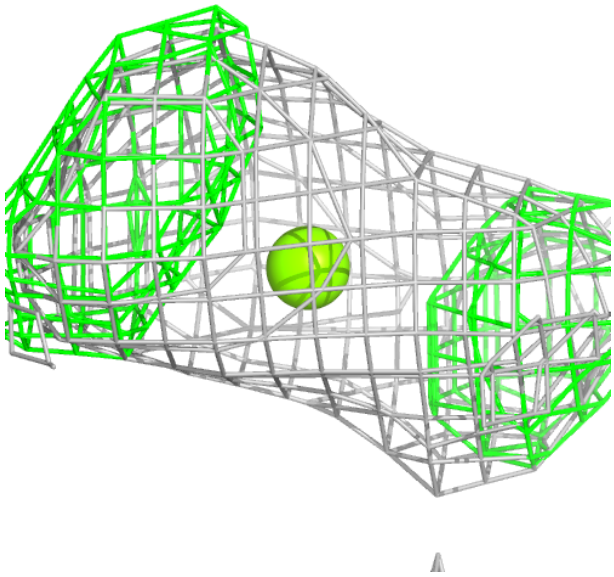
Electron density around MG D 701:

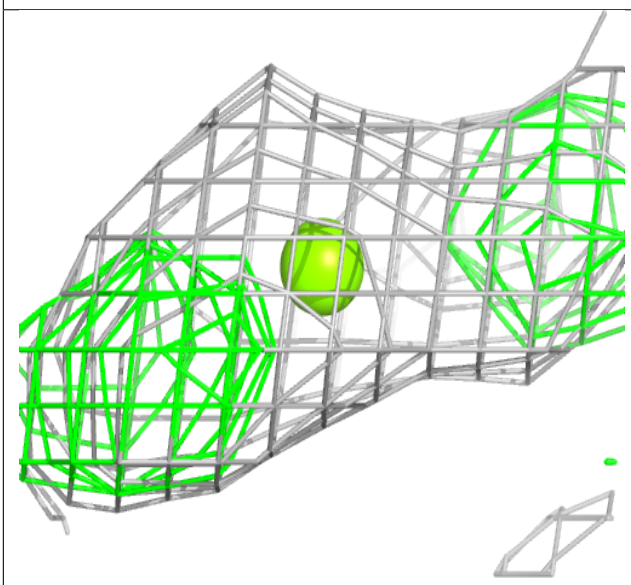
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

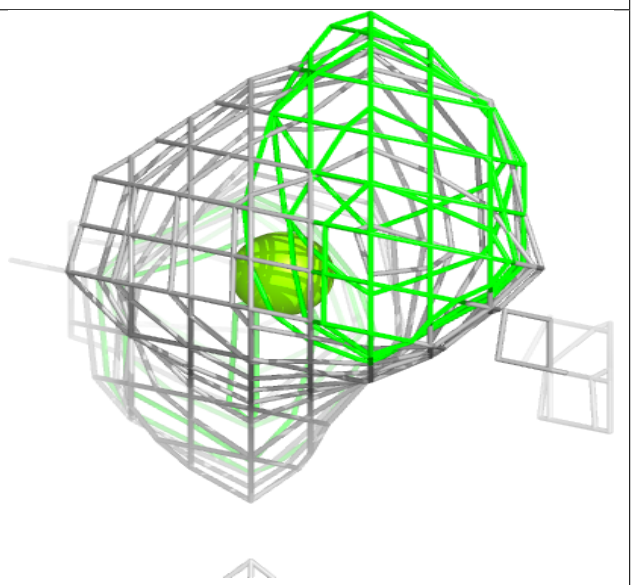


Electron density around MG F 702:

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

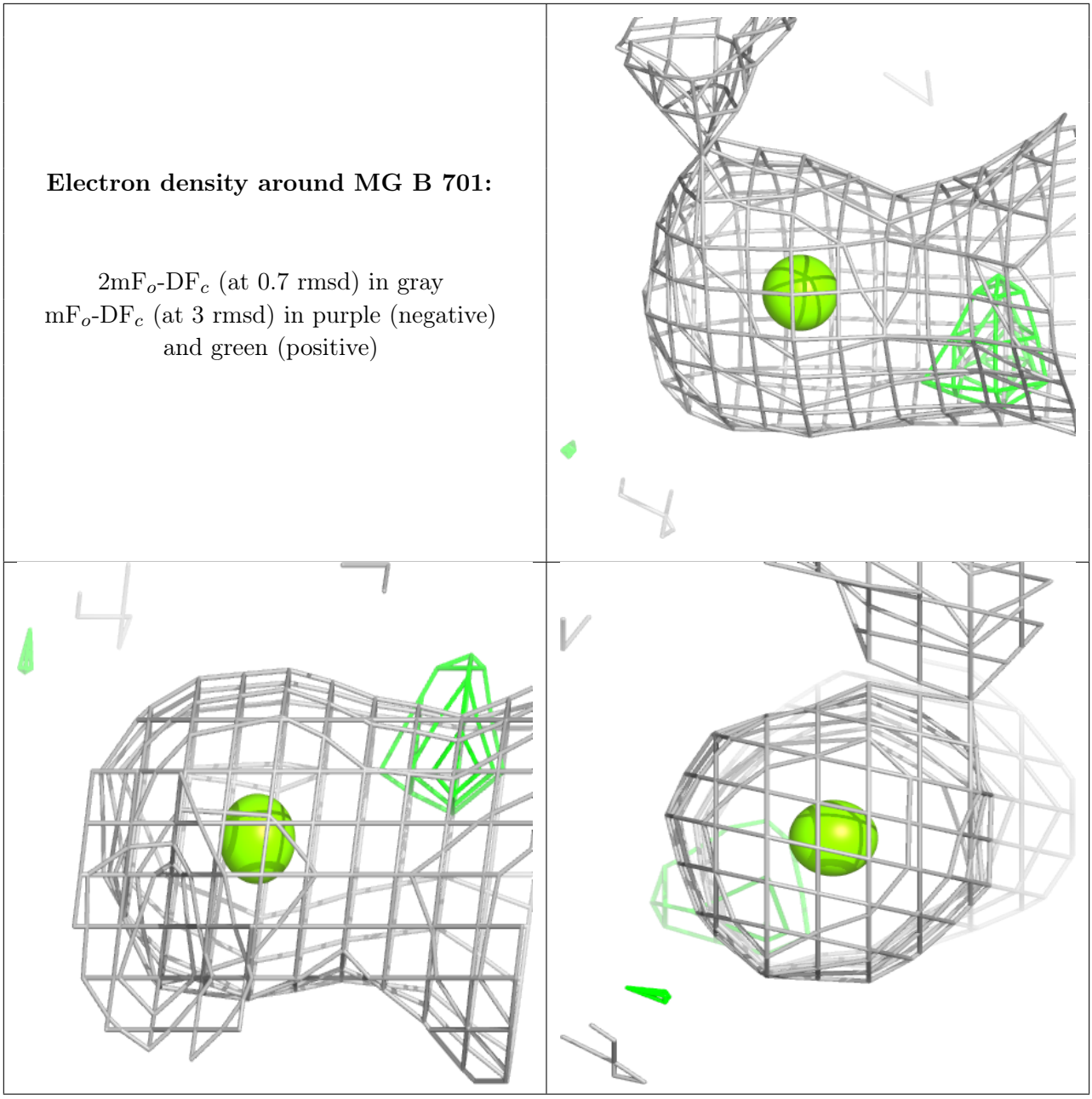






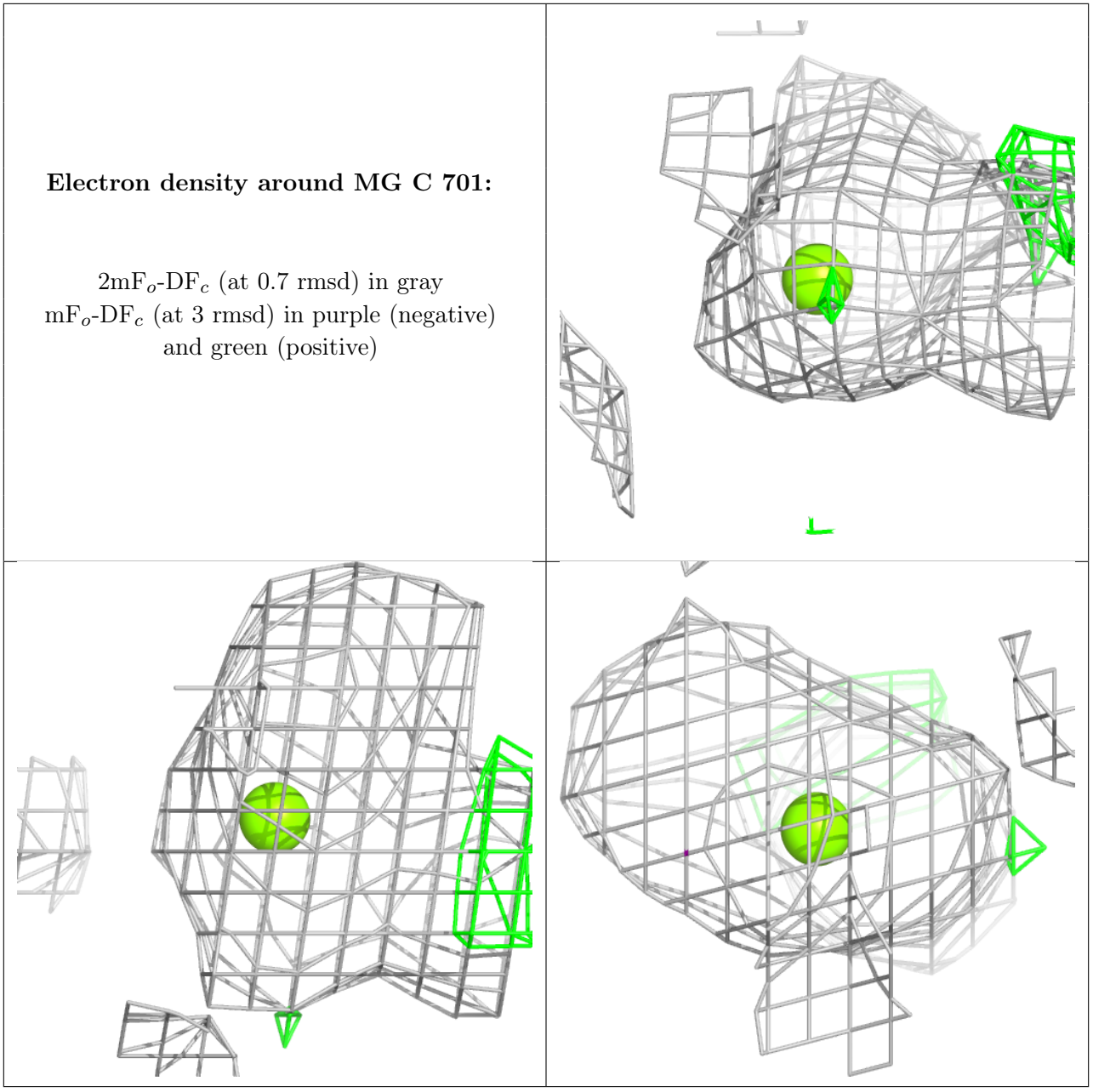
Electron density around MG B 701:

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



Electron density around MG C 701:

$2mF_o$-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.