wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 09:12 AM EDT

PDB ID	:	7V03
Title	:	Crystal structure of cytoplasmic triosephosphate isomerase from Cuscuta australis
Authors	:	Jones, G.; Vickers, C.; Patrick, W.; Jameson, G.
Deposited on	:	2022-05-09
Resolution	:	1.78 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:

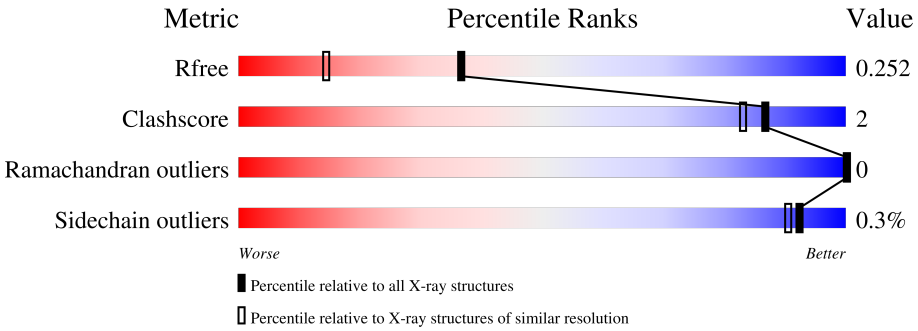
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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%

Mol	Chain	Length	Quality of chain
1	A	274	88% · 10%
1	B	274	82% 6% 12%
1	C	274	85% 5% 9%
1	D	274	84% · 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8246 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 triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1816	1161	309	340	6			
1	B	241	Total	C	N	O	S	0	0	0
			1745	1118	297	324	6			
1	C	248	Total	C	N	O	S	0	0	0
			1829	1171	310	342	6			
1	D	241	Total	C	N	O	S	0	0	0
			1739	1110	298	325	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A328CVN3
A	-18	GLY	-	expression tag	UNP A0A328CVN3
A	-17	SER	-	expression tag	UNP A0A328CVN3
A	-16	SER	-	expression tag	UNP A0A328CVN3
A	-15	HIS	-	expression tag	UNP A0A328CVN3
A	-14	HIS	-	expression tag	UNP A0A328CVN3
A	-13	HIS	-	expression tag	UNP A0A328CVN3
A	-12	HIS	-	expression tag	UNP A0A328CVN3
A	-11	HIS	-	expression tag	UNP A0A328CVN3
A	-10	HIS	-	expression tag	UNP A0A328CVN3
A	-9	SER	-	expression tag	UNP A0A328CVN3
A	-8	SER	-	expression tag	UNP A0A328CVN3
A	-7	GLY	-	expression tag	UNP A0A328CVN3
A	-6	LEU	-	expression tag	UNP A0A328CVN3
A	-5	VAL	-	expression tag	UNP A0A328CVN3
A	-4	PRO	-	expression tag	UNP A0A328CVN3
A	-3	ARG	-	expression tag	UNP A0A328CVN3
A	-2	GLY	-	expression tag	UNP A0A328CVN3
A	-1	SER	-	expression tag	UNP A0A328CVN3
A	0	HIS	-	expression tag	UNP A0A328CVN3
B	-19	MET	-	initiating methionine	UNP A0A328CVN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A328CVN3
B	-17	SER	-	expression tag	UNP A0A328CVN3
B	-16	SER	-	expression tag	UNP A0A328CVN3
B	-15	HIS	-	expression tag	UNP A0A328CVN3
B	-14	HIS	-	expression tag	UNP A0A328CVN3
B	-13	HIS	-	expression tag	UNP A0A328CVN3
B	-12	HIS	-	expression tag	UNP A0A328CVN3
B	-11	HIS	-	expression tag	UNP A0A328CVN3
B	-10	HIS	-	expression tag	UNP A0A328CVN3
B	-9	SER	-	expression tag	UNP A0A328CVN3
B	-8	SER	-	expression tag	UNP A0A328CVN3
B	-7	GLY	-	expression tag	UNP A0A328CVN3
B	-6	LEU	-	expression tag	UNP A0A328CVN3
B	-5	VAL	-	expression tag	UNP A0A328CVN3
B	-4	PRO	-	expression tag	UNP A0A328CVN3
B	-3	ARG	-	expression tag	UNP A0A328CVN3
B	-2	GLY	-	expression tag	UNP A0A328CVN3
B	-1	SER	-	expression tag	UNP A0A328CVN3
B	0	HIS	-	expression tag	UNP A0A328CVN3
C	-19	MET	-	initiating methionine	UNP A0A328CVN3
C	-18	GLY	-	expression tag	UNP A0A328CVN3
C	-17	SER	-	expression tag	UNP A0A328CVN3
C	-16	SER	-	expression tag	UNP A0A328CVN3
C	-15	HIS	-	expression tag	UNP A0A328CVN3
C	-14	HIS	-	expression tag	UNP A0A328CVN3
C	-13	HIS	-	expression tag	UNP A0A328CVN3
C	-12	HIS	-	expression tag	UNP A0A328CVN3
C	-11	HIS	-	expression tag	UNP A0A328CVN3
C	-10	HIS	-	expression tag	UNP A0A328CVN3
C	-9	SER	-	expression tag	UNP A0A328CVN3
C	-8	SER	-	expression tag	UNP A0A328CVN3
C	-7	GLY	-	expression tag	UNP A0A328CVN3
C	-6	LEU	-	expression tag	UNP A0A328CVN3
C	-5	VAL	-	expression tag	UNP A0A328CVN3
C	-4	PRO	-	expression tag	UNP A0A328CVN3
C	-3	ARG	-	expression tag	UNP A0A328CVN3
C	-2	GLY	-	expression tag	UNP A0A328CVN3
C	-1	SER	-	expression tag	UNP A0A328CVN3
C	0	HIS	-	expression tag	UNP A0A328CVN3
D	-19	MET	-	initiating methionine	UNP A0A328CVN3
D	-18	GLY	-	expression tag	UNP A0A328CVN3
D	-17	SER	-	expression tag	UNP A0A328CVN3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A328CVN3
D	-15	HIS	-	expression tag	UNP A0A328CVN3
D	-14	HIS	-	expression tag	UNP A0A328CVN3
D	-13	HIS	-	expression tag	UNP A0A328CVN3
D	-12	HIS	-	expression tag	UNP A0A328CVN3
D	-11	HIS	-	expression tag	UNP A0A328CVN3
D	-10	HIS	-	expression tag	UNP A0A328CVN3
D	-9	SER	-	expression tag	UNP A0A328CVN3
D	-8	SER	-	expression tag	UNP A0A328CVN3
D	-7	GLY	-	expression tag	UNP A0A328CVN3
D	-6	LEU	-	expression tag	UNP A0A328CVN3
D	-5	VAL	-	expression tag	UNP A0A328CVN3
D	-4	PRO	-	expression tag	UNP A0A328CVN3
D	-3	ARG	-	expression tag	UNP A0A328CVN3
D	-2	GLY	-	expression tag	UNP A0A328CVN3
D	-1	SER	-	expression tag	UNP A0A328CVN3
D	0	HIS	-	expression tag	UNP A0A328CVN3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	1	Total Cl 1 1	0	0
2	C	2	Total Cl 2 2	0	0

- Molecule 3 is water.

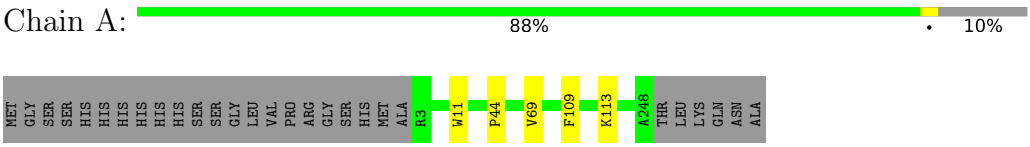
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	307	Total O 307 307	0	0
3	B	235	Total O 235 235	0	0
3	C	322	Total O 322 322	0	0
3	D	247	Total O 247 247	0	0

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. 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. 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.

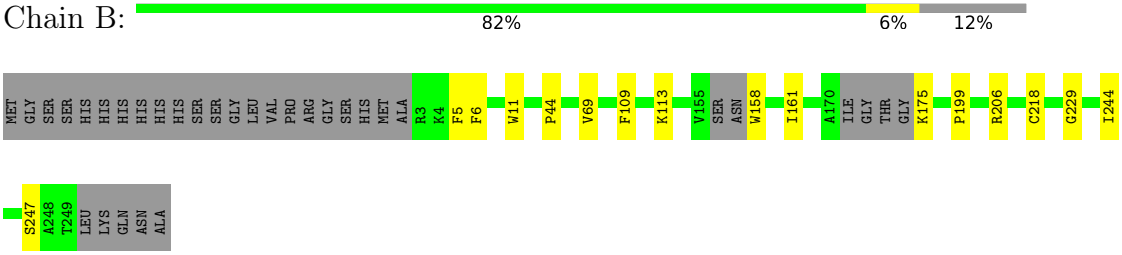
• Molecule 1: triosephosphate isomerase

Chain A:



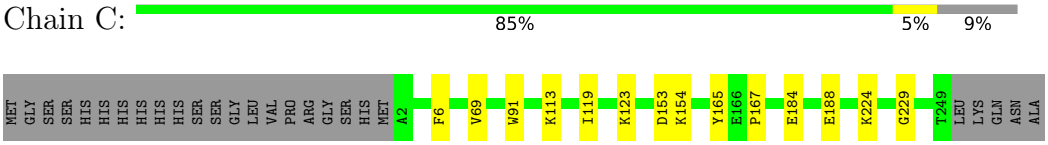
• Molecule 1: triosephosphate isomerase

Chain B:



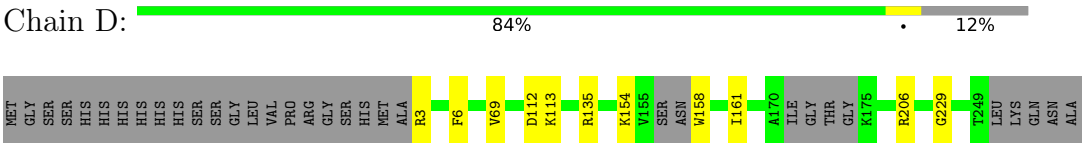
• Molecule 1: triosephosphate isomerase

Chain C:



• Molecule 1: triosephosphate isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.10Å 130.13Å 75.00Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	45.94 – 1.78 45.94 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.94-1.78) 99.6 (45.94-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.31 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.211 , 0.253 0.210 , 0.252	Depositor DCC
R_{free} test set	4533 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8246	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: CL

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	0.38	0/1853	0.59	0/2529
1	B	0.36	0/1778	0.58	0/2426
1	C	0.40	0/1866	0.60	0/2546
1	D	0.36	0/1771	0.57	0/2412
All	All	0.38	0/7268	0.59	0/9913

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	1816	0	1775	3	0
1	B	1745	0	1672	11	0
1	C	1829	0	1789	8	0
1	D	1739	0	1655	7	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	307	0	0	0	0
3	B	235	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	322	0	0	0	0
3	D	247	0	0	1	0
All	All	8246	0	6891	29	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 2.

The worst 5 of 29 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:C:69:VAL:HA	1:C:113:LYS:HG2	1.76	0.65
1:A:69:VAL:HA	1:A:113:LYS:HG2	1.82	0.62
1:B:175:LYS:N	3:B:405:HOH:O	2.34	0.60
1:B:158:TRP:O	1:B:161:ILE:HG22	2.05	0.56
1:D:135:ARG:HH11	1:D:135:ARG:HG3	1.73	0.53

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	244/274 (89%)	238 (98%)	6 (2%)	0	100	100
1	B	235/274 (86%)	229 (97%)	6 (3%)	0	100	100
1	C	246/274 (90%)	239 (97%)	7 (3%)	0	100	100
1	D	235/274 (86%)	228 (97%)	7 (3%)	0	100	100
All	All	960/1096 (88%)	934 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	185/224 (83%)	185 (100%)	0	100	100
1	B	170/224 (76%)	169 (99%)	1 (1%)	86	82
1	C	185/224 (83%)	185 (100%)	0	100	100
1	D	168/224 (75%)	167 (99%)	1 (1%)	86	82
All	All	708/896 (79%)	706 (100%)	2 (0%)	92	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	206	ARG
1	D	206	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

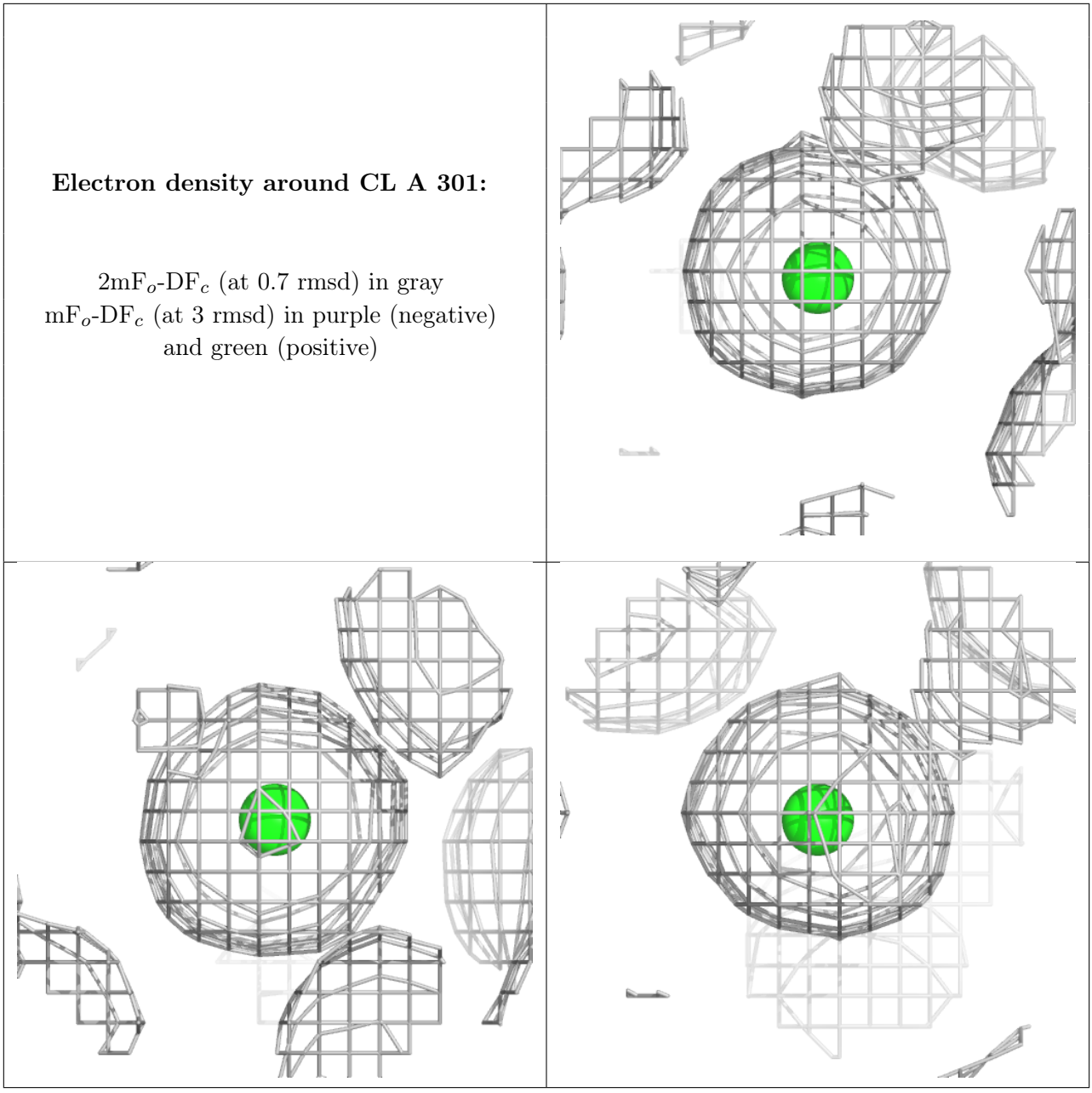
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

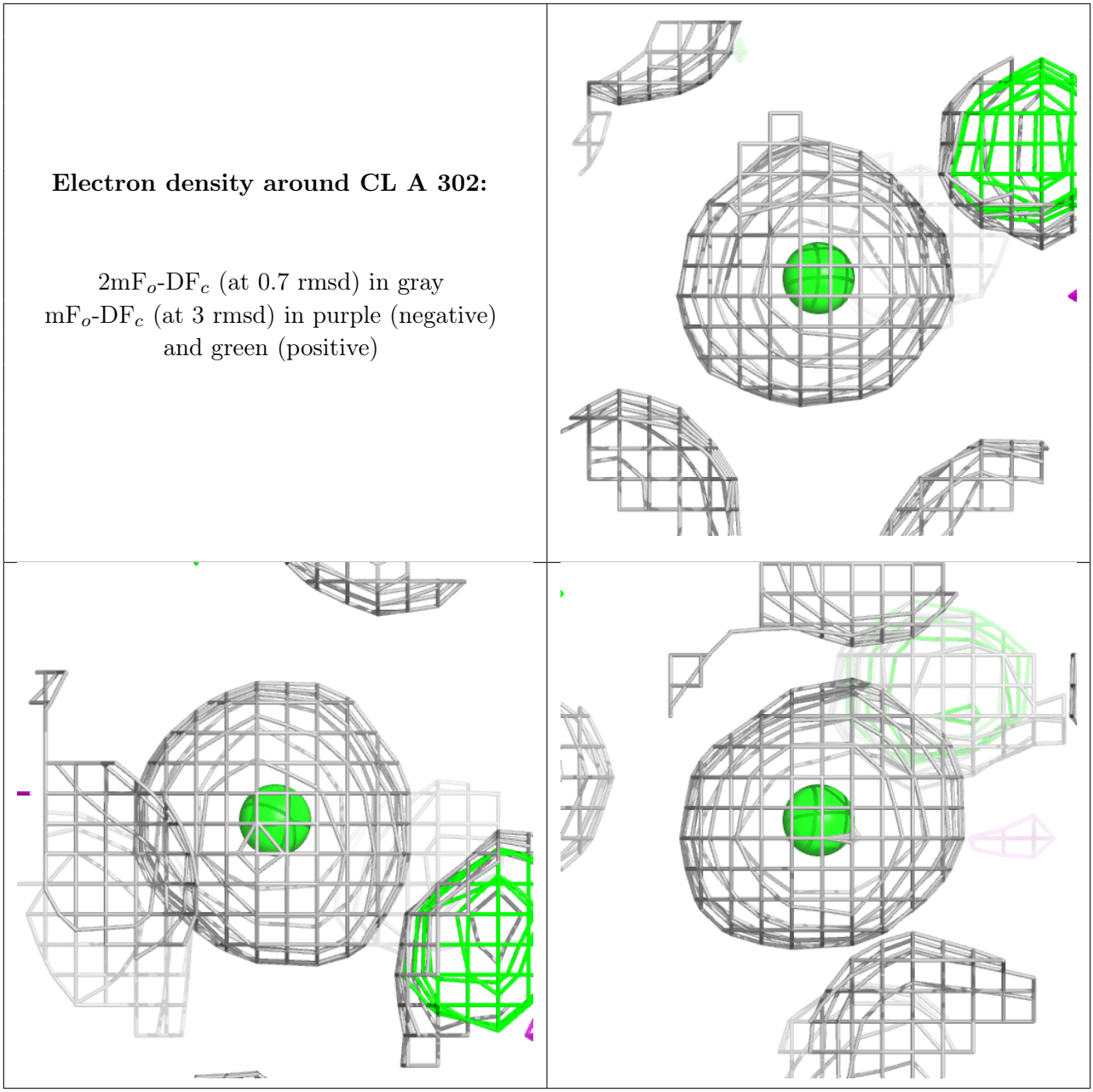
Electron density around CL A 301:

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



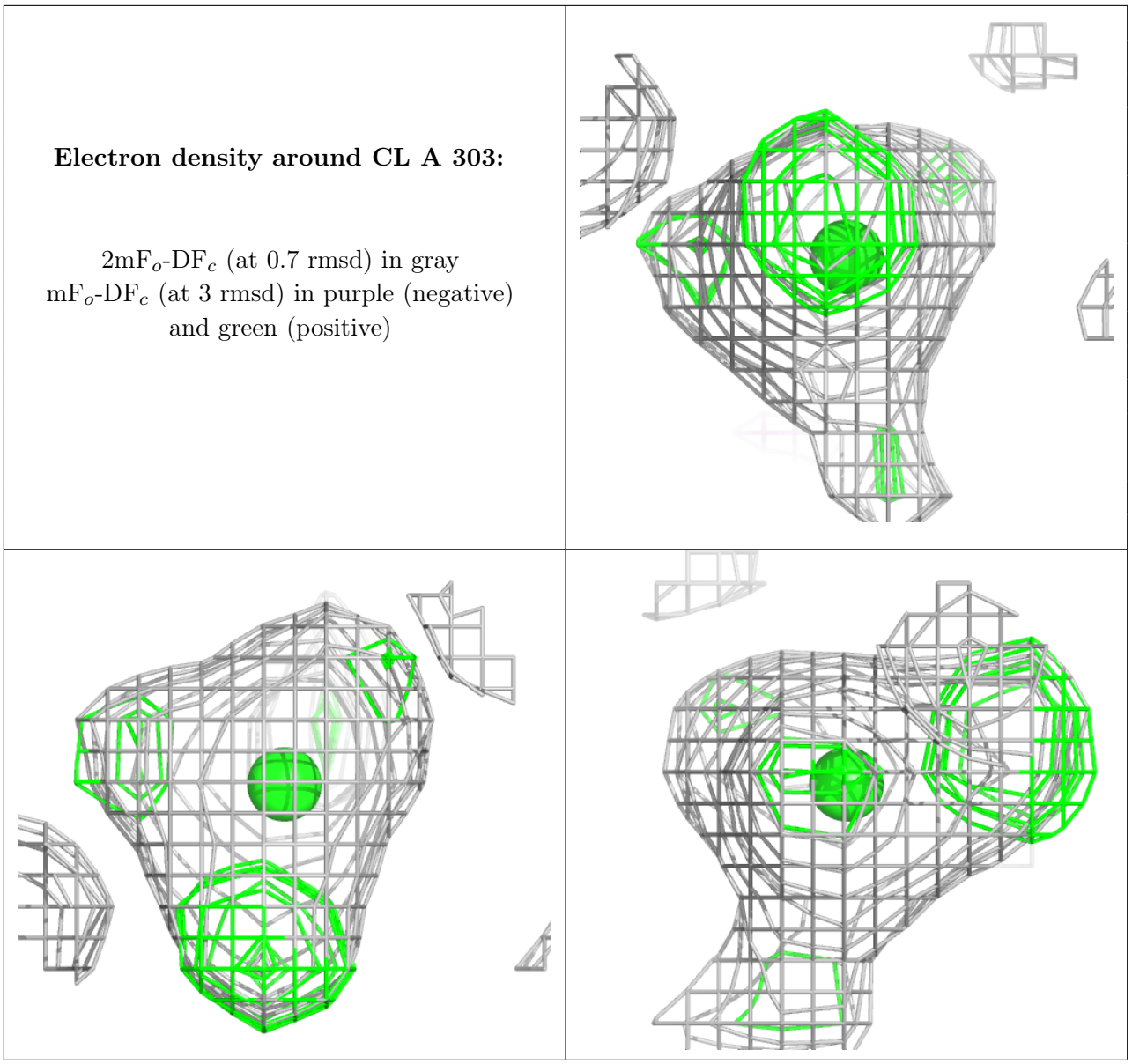
Electron density around CL A 302:

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



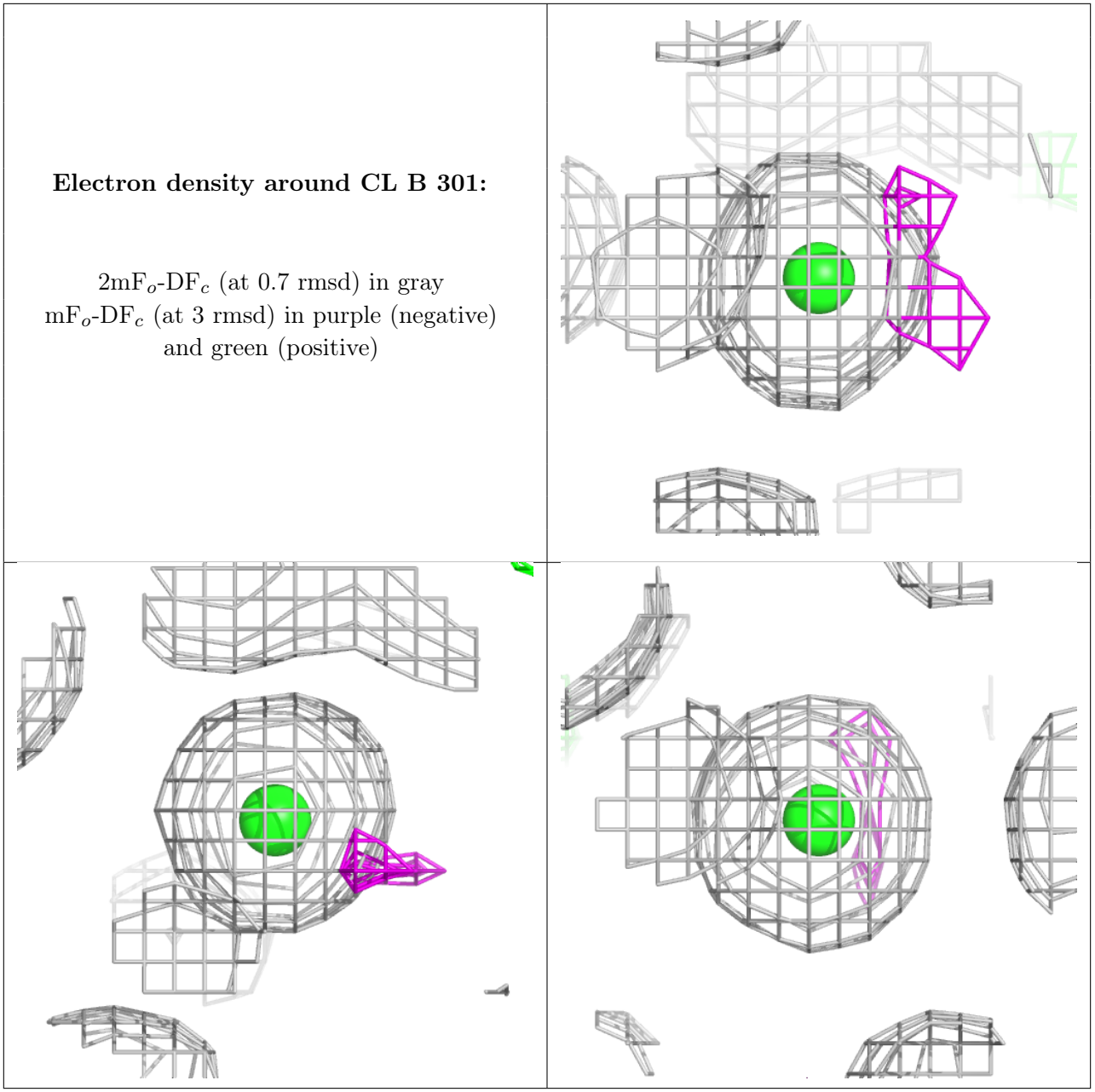
Electron density around CL A 303:

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



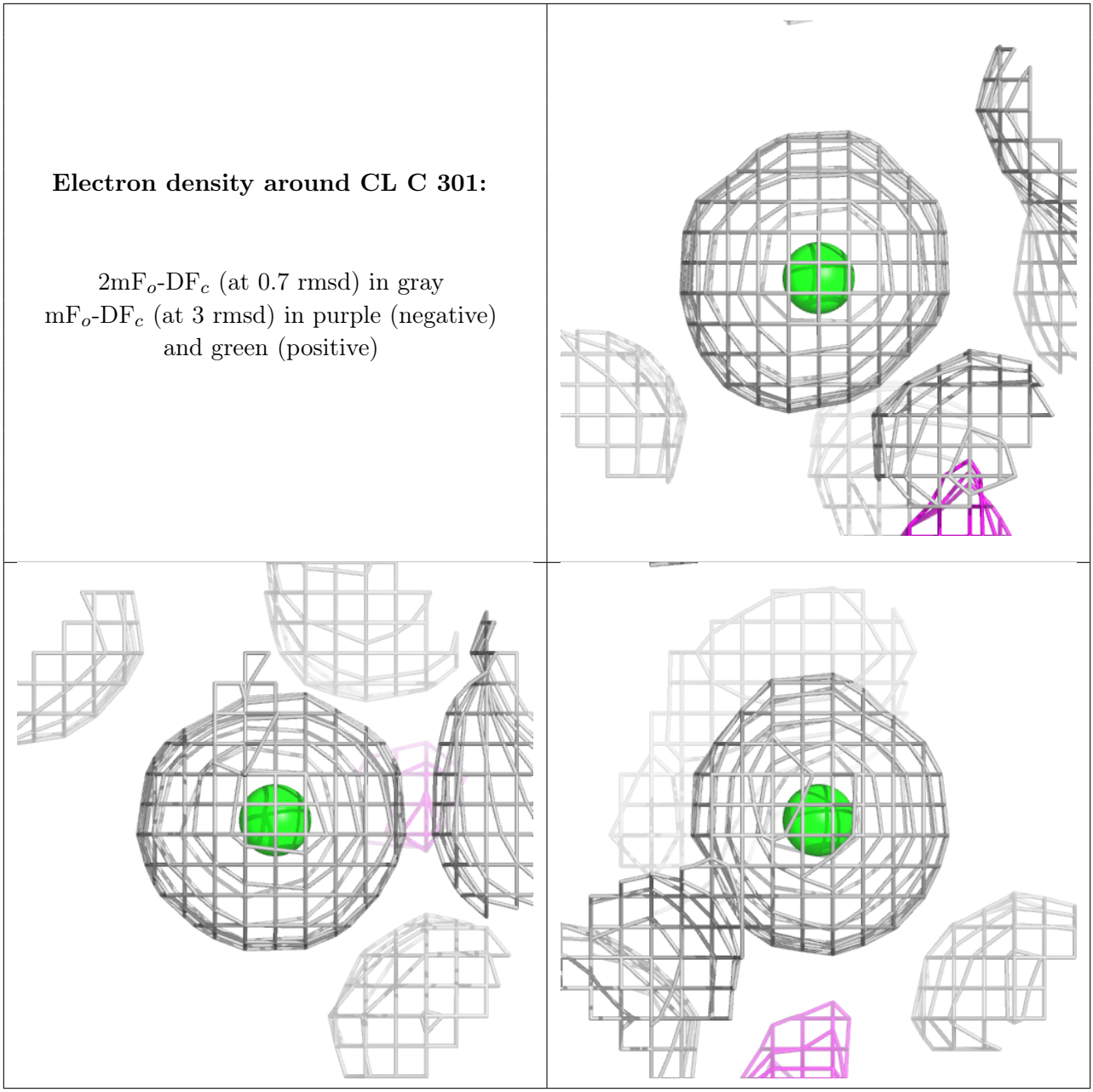
Electron density around CL B 301:

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



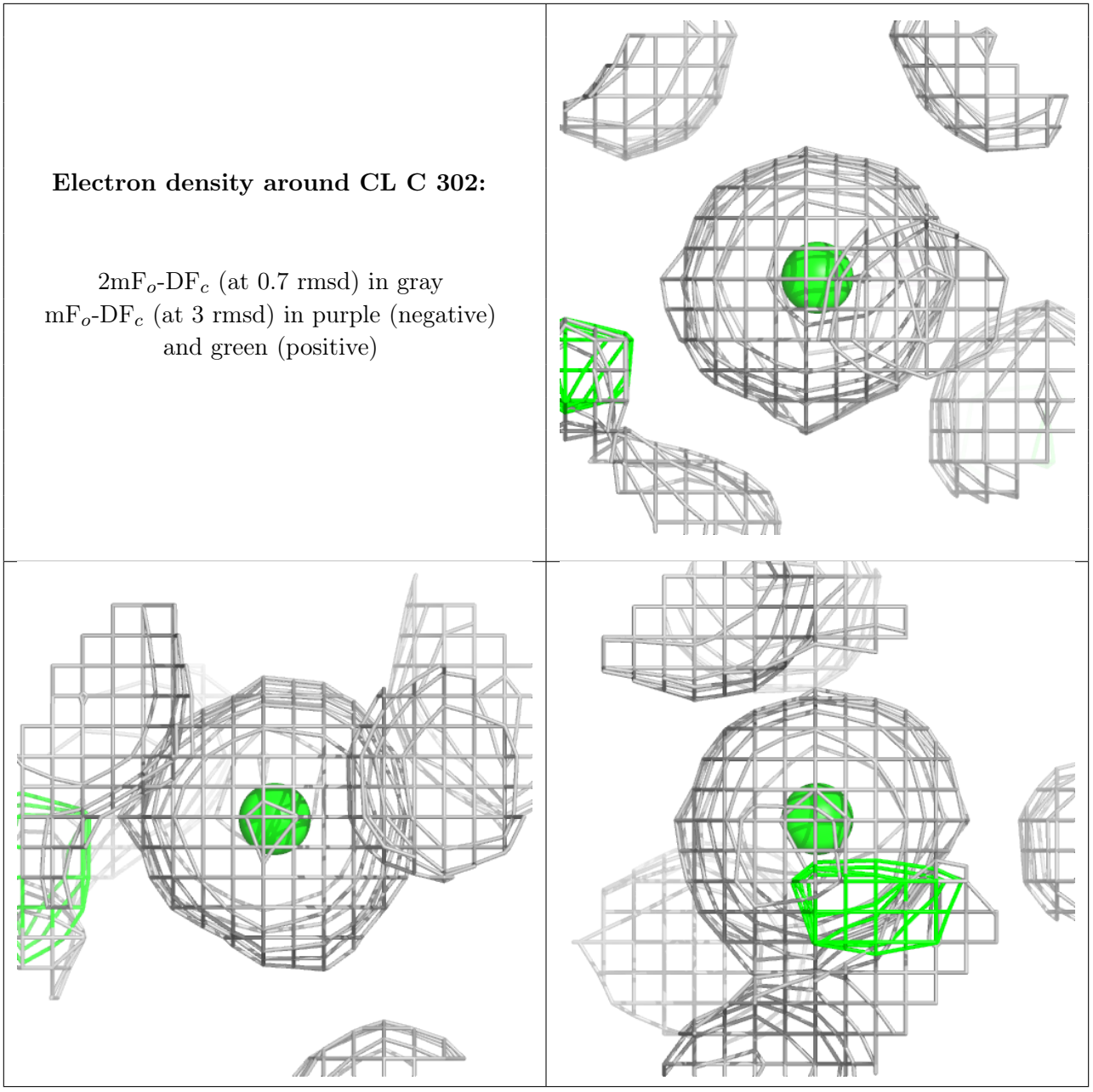
Electron density around CL C 301:

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



Electron density around CL C 302:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.