wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2024 – 02:36 am BST

PDB ID	:	8QND
Title	:	Crystal structure of the ribonucleoside hydrolase C from Lactobacillus reuteri
Authors	:	Matyuta, I.O.; Minyaev, M.E.; Shaposhnikov, L.A.; Pometun, A.A.; Tishkov, V.I.; Popov, V.O.; Boyko, K.M.
Deposited on	:	2023-09-26
Resolution	:	1.90 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:

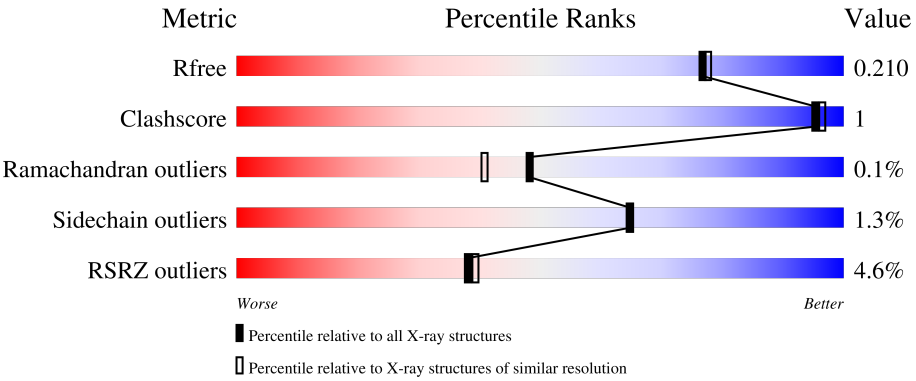
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	308	4% 92% . .
1	B	308	4% 92% . .
1	C	308	5% 90% 6% .
1	D	308	6% 91% . 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9654 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 Inosine-uridine nucleoside N-ribohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	2	0
			2239	1430	359	437	13			
1	B	296	Total	C	N	O	S	0	2	0
			2212	1415	354	430	13			
1	C	297	Total	C	N	O	S	0	2	0
			2236	1431	360	432	13			
1	D	294	Total	C	N	O	S	0	2	0
			2194	1408	349	423	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A5JJT3
A	2	HIS	-	expression tag	UNP A5JJT3
A	3	HIS	-	expression tag	UNP A5JJT3
A	4	HIS	-	expression tag	UNP A5JJT3
A	5	HIS	-	expression tag	UNP A5JJT3
A	6	HIS	-	expression tag	UNP A5JJT3
A	7	HIS	-	expression tag	UNP A5JJT3
B	1	MET	-	initiating methionine	UNP A5JJT3
B	2	HIS	-	expression tag	UNP A5JJT3
B	3	HIS	-	expression tag	UNP A5JJT3
B	4	HIS	-	expression tag	UNP A5JJT3
B	5	HIS	-	expression tag	UNP A5JJT3
B	6	HIS	-	expression tag	UNP A5JJT3
B	7	HIS	-	expression tag	UNP A5JJT3
C	1	MET	-	initiating methionine	UNP A5JJT3
C	2	HIS	-	expression tag	UNP A5JJT3
C	3	HIS	-	expression tag	UNP A5JJT3
C	4	HIS	-	expression tag	UNP A5JJT3
C	5	HIS	-	expression tag	UNP A5JJT3
C	6	HIS	-	expression tag	UNP A5JJT3
C	7	HIS	-	expression tag	UNP A5JJT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A5JJT3
D	2	HIS	-	expression tag	UNP A5JJT3
D	3	HIS	-	expression tag	UNP A5JJT3
D	4	HIS	-	expression tag	UNP A5JJT3
D	5	HIS	-	expression tag	UNP A5JJT3
D	6	HIS	-	expression tag	UNP A5JJT3
D	7	HIS	-	expression tag	UNP A5JJT3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

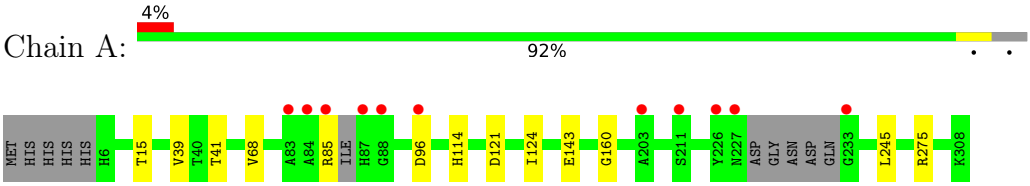
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	226	Total O 226 226	0	0
3	B	211	Total O 211 211	0	0
3	C	183	Total O 183 183	0	0
3	D	146	Total O 147 147	0	1

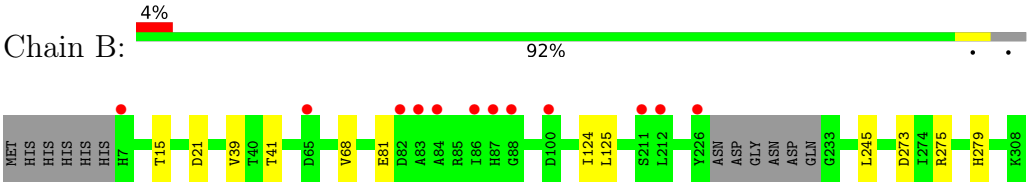
3 Residue-property plots (i)

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.

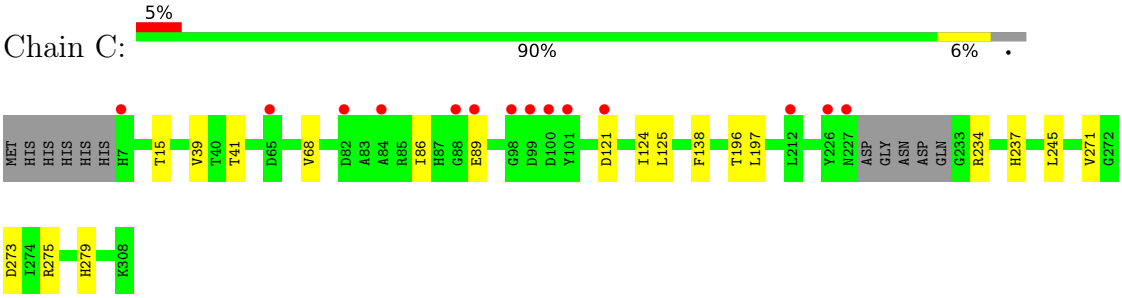
• Molecule 1: Inosine-uridine nucleoside N-ribohydrolase



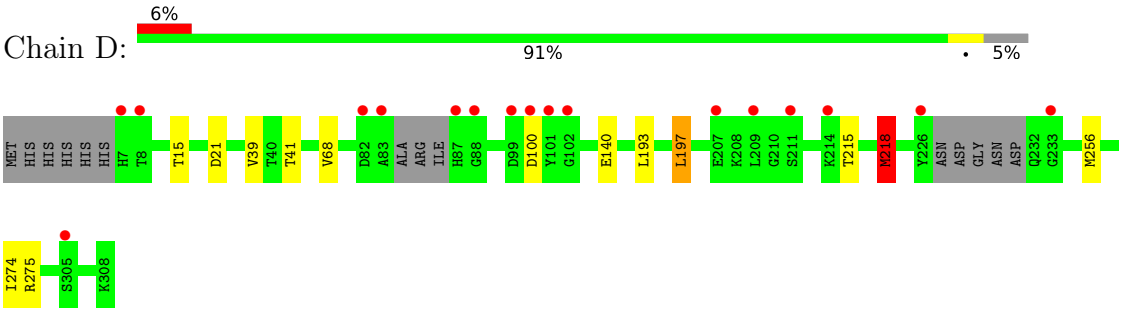
• Molecule 1: Inosine-uridine nucleoside N-ribohydrolase



• Molecule 1: Inosine-uridine nucleoside N-ribohydrolase



• Molecule 1: Inosine-uridine nucleoside N-ribohydrolase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.11Å 81.53Å 86.85Å 90.00° 95.76° 90.00°	Depositor
Resolution (Å)	63.38 – 1.90 63.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.38-1.90) 99.6 (63.38-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.95 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.201 0.178 , 0.210	Depositor DCC
R_{free} test set	4557 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9654	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: CA

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	0.87	1/2292 (0.0%)	0.98	3/3115 (0.1%)
1	B	0.87	2/2266 (0.1%)	1.00	2/3084 (0.1%)
1	C	0.87	0/2290	1.04	8/3113 (0.3%)
1	D	0.83	1/2244 (0.0%)	0.98	4/3051 (0.1%)
All	All	0.86	4/9092 (0.0%)	1.00	17/12363 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE2	6.66	1.32	1.25
1	B	81	GLU	CD-OE1	6.38	1.32	1.25
1	A	160	GLY	C-O	5.72	1.32	1.23
1	D	140	GLU	CD-OE1	5.37	1.31	1.25

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	275	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	C	275	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	A	275	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	271	VAL	CG1-CB-CG2	7.20	122.42	110.90
1	A	275	ARG	NE-CZ-NH2	-7.15	116.72	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2239	0	2184	4	0
1	B	2212	0	2148	5	0
1	C	2236	0	2198	6	0
1	D	2194	0	2148	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	226	0	0	0	0
3	B	211	0	0	1	0
3	C	183	0	0	1	0
3	D	147	0	0	0	0
All	All	9654	0	8678	20	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 1.

The worst 5 of 20 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:273:ASP:OD1	1:C:279:HIS:HD2	1.93	0.51
1:A:114:HIS:HE1	1:A:143:GLU:OE1	1.96	0.48
1:C:15:THR:O	1:C:41:THR:HA	2.14	0.47
1:C:279:HIS:HE1	3:C:578:HOH:O	1.98	0.47
1:B:273:ASP:OD1	1:B:279:HIS:HD2	1.98	0.47

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	293/308 (95%)	285 (97%)	8 (3%)	0	100	100
1	B	294/308 (96%)	285 (97%)	9 (3%)	0	100	100
1	C	295/308 (96%)	285 (97%)	10 (3%)	0	100	100
1	D	290/308 (94%)	279 (96%)	10 (3%)	1 (0%)	37	29
All	All	1172/1232 (95%)	1134 (97%)	37 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	100	ASP

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	234/250 (94%)	231 (99%)	3 (1%)	65	65
1	B	228/250 (91%)	226 (99%)	2 (1%)	75	77
1	C	234/250 (94%)	229 (98%)	5 (2%)	48	45
1	D	226/250 (90%)	222 (98%)	4 (2%)	54	52
All	All	922/1000 (92%)	908 (98%)	14 (2%)	65	59

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	ASP
1	C	125	LEU
1	D	218[B]	MET
1	D	197	LEU
1	D	218[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	183	ASN
1	C	240	ASN
1	D	232	GLN
1	D	150	GLN
1	D	183	ASN

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 oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	297/308 (96%)	-0.03	11 (3%)	45	47	8, 18, 40, 64	2 (0%)
1	B	296/308 (96%)	0.03	12 (4%)	42	43	11, 20, 44, 82	2 (0%)
1	C	297/308 (96%)	0.05	14 (4%)	37	38	10, 20, 43, 82	2 (0%)
1	D	294/308 (95%)	0.33	17 (5%)	30	31	11, 25, 49, 82	2 (0%)
All	All	1184/1232 (96%)	0.09	54 (4%)	38	39	8, 21, 45, 82	8 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	7.6
1	D	83	ALA	6.3
1	C	88	GLY	5.2
1	A	84	ALA	5.0
1	C	101	TYR	4.8

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

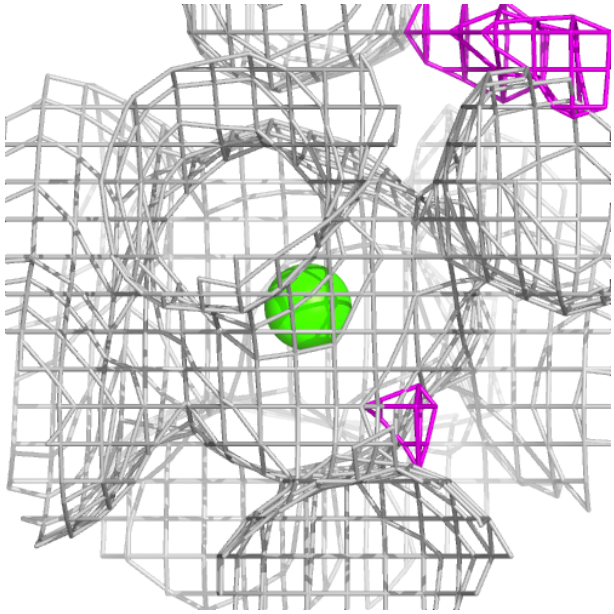
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

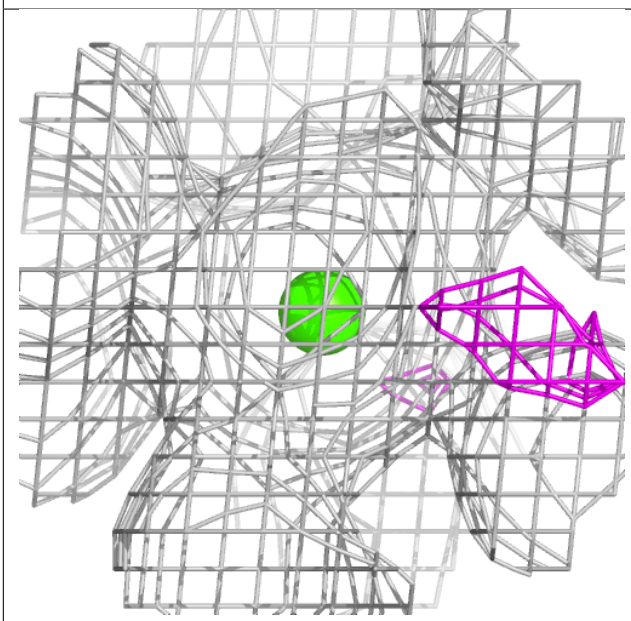
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	401	1/1	0.99	0.03	14,14,14,14	0
2	CA	C	401	1/1	0.99	0.04	16,16,16,16	0
2	CA	D	401	1/1	0.99	0.06	18,18,18,18	0
2	CA	B	402	1/1	1.00	0.04	17,17,17,17	0
2	CA	A	402	1/1	1.00	0.02	16,16,16,16	0
2	CA	B	401	1/1	1.00	0.03	15,15,15,15	0

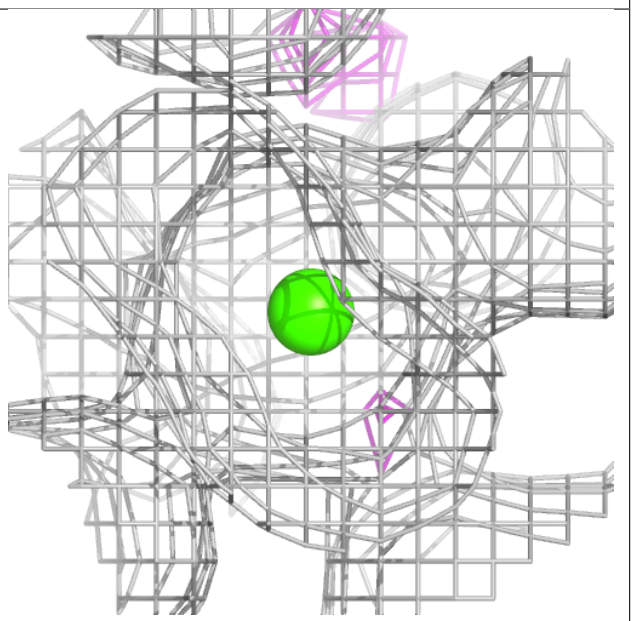
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CA A 401:

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

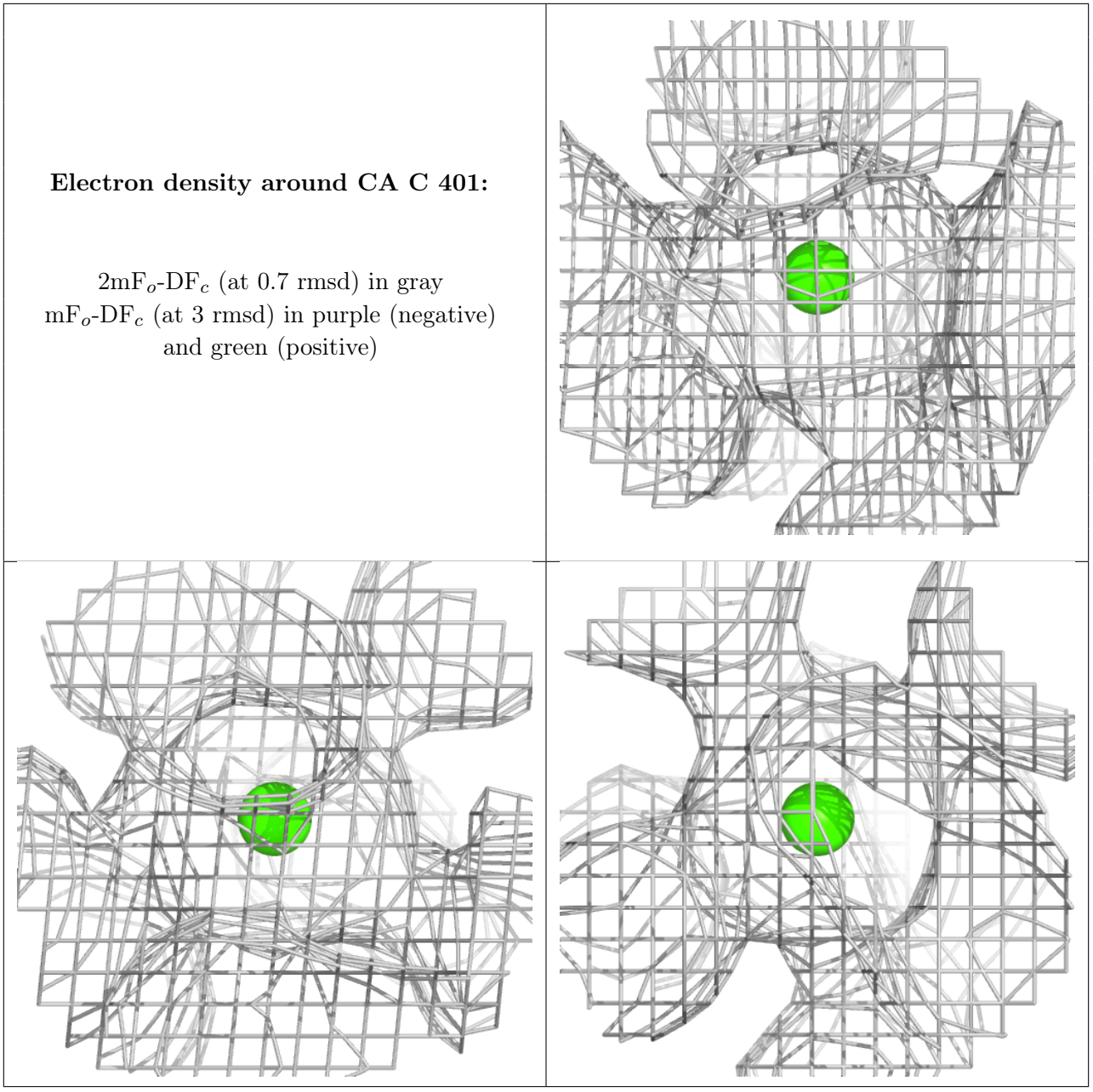






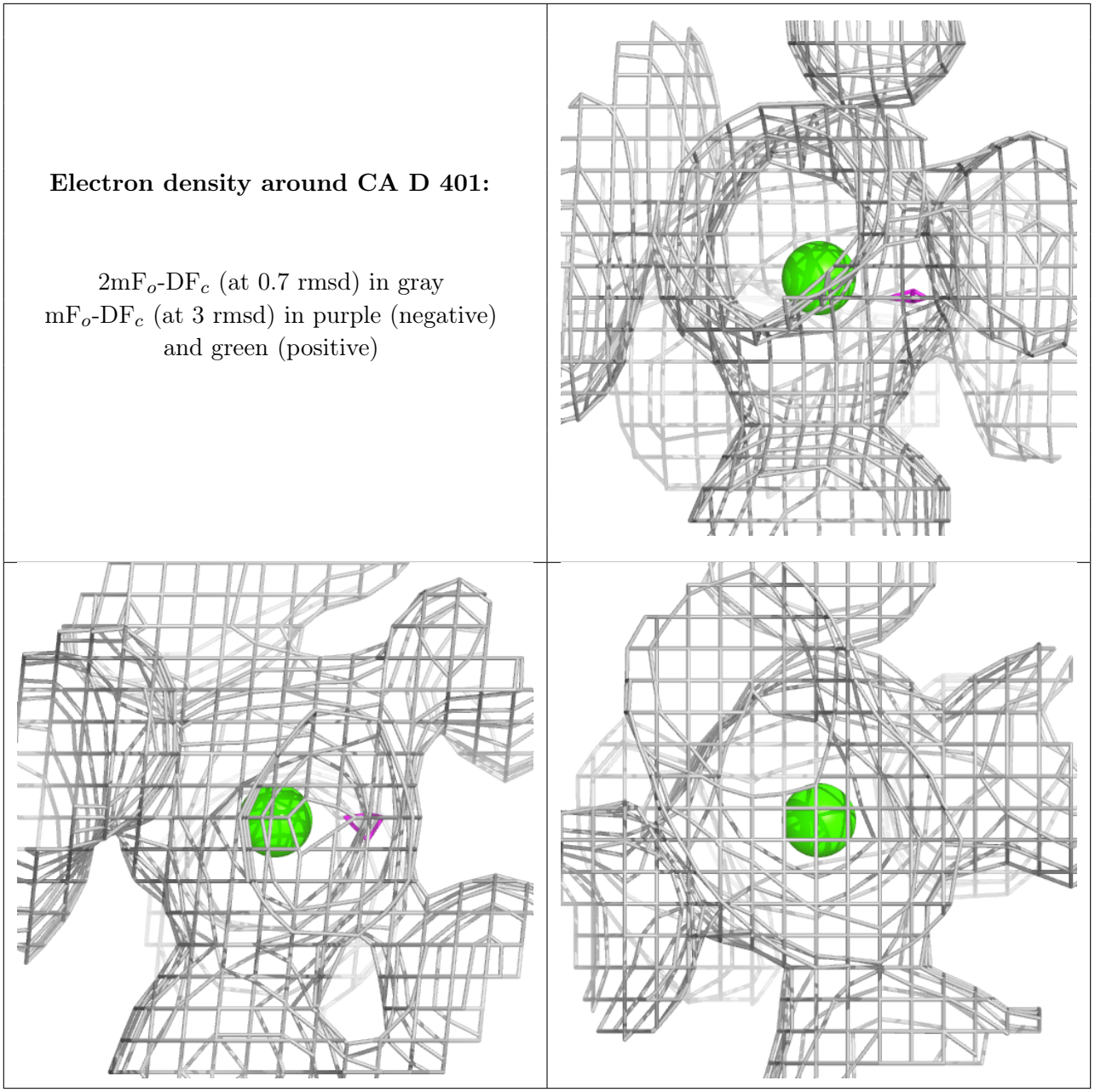
Electron density around CA C 401:

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



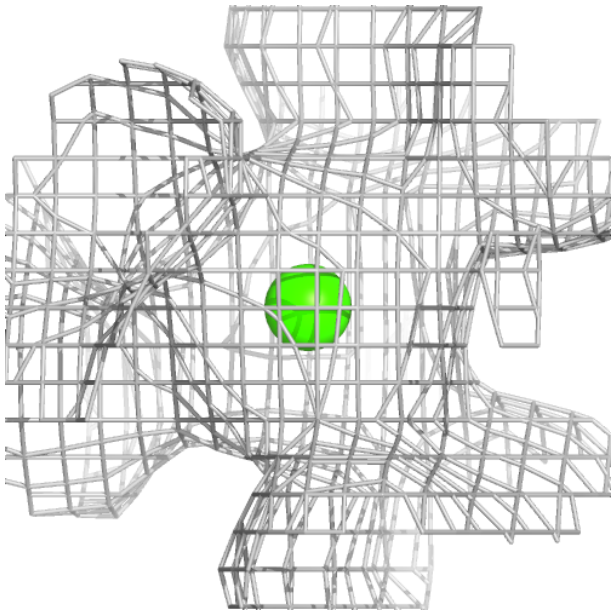
Electron density around CA D 401:

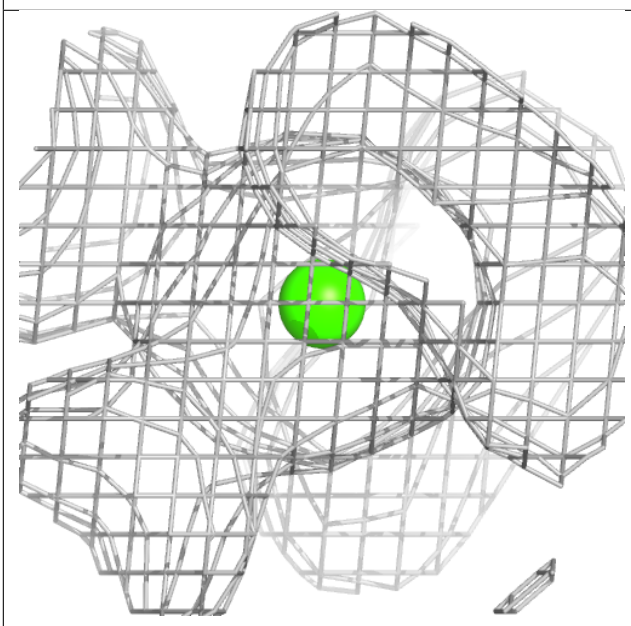
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

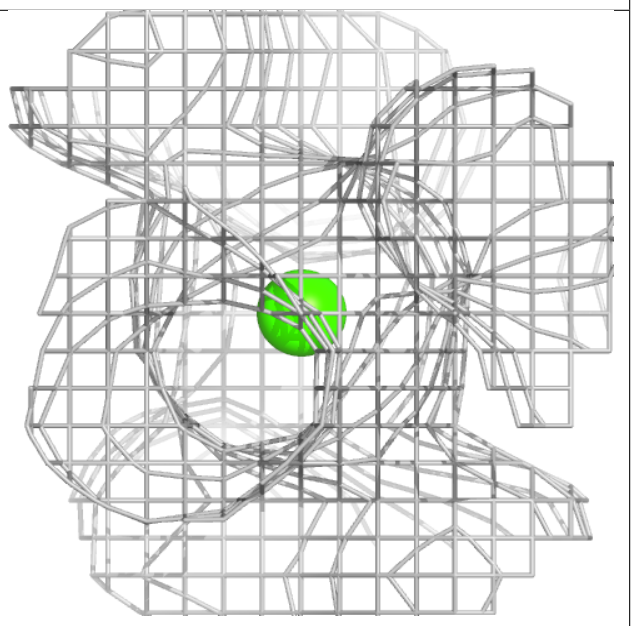


Electron density around CA B 402:

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

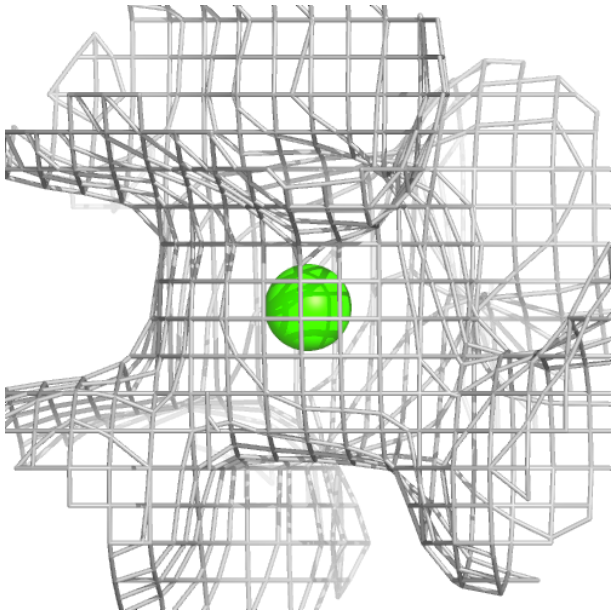


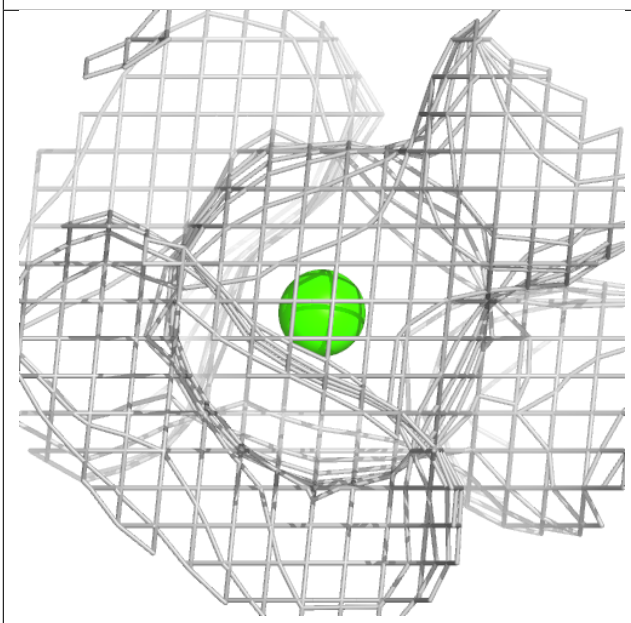


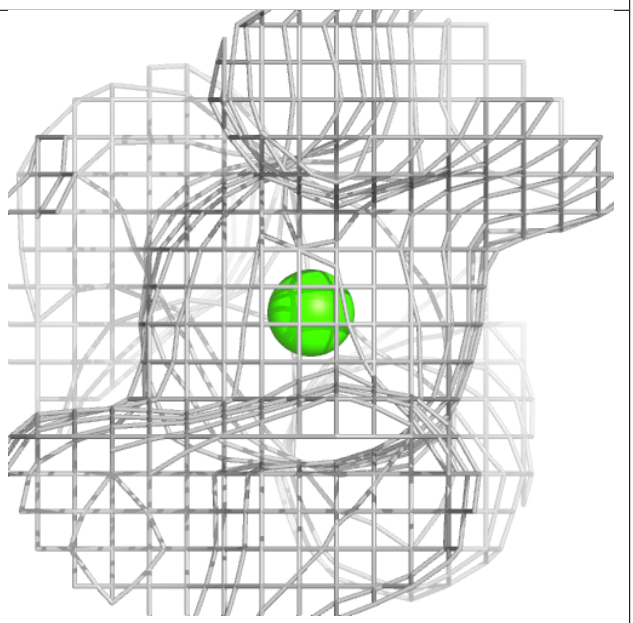


Electron density around CA A 402:

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

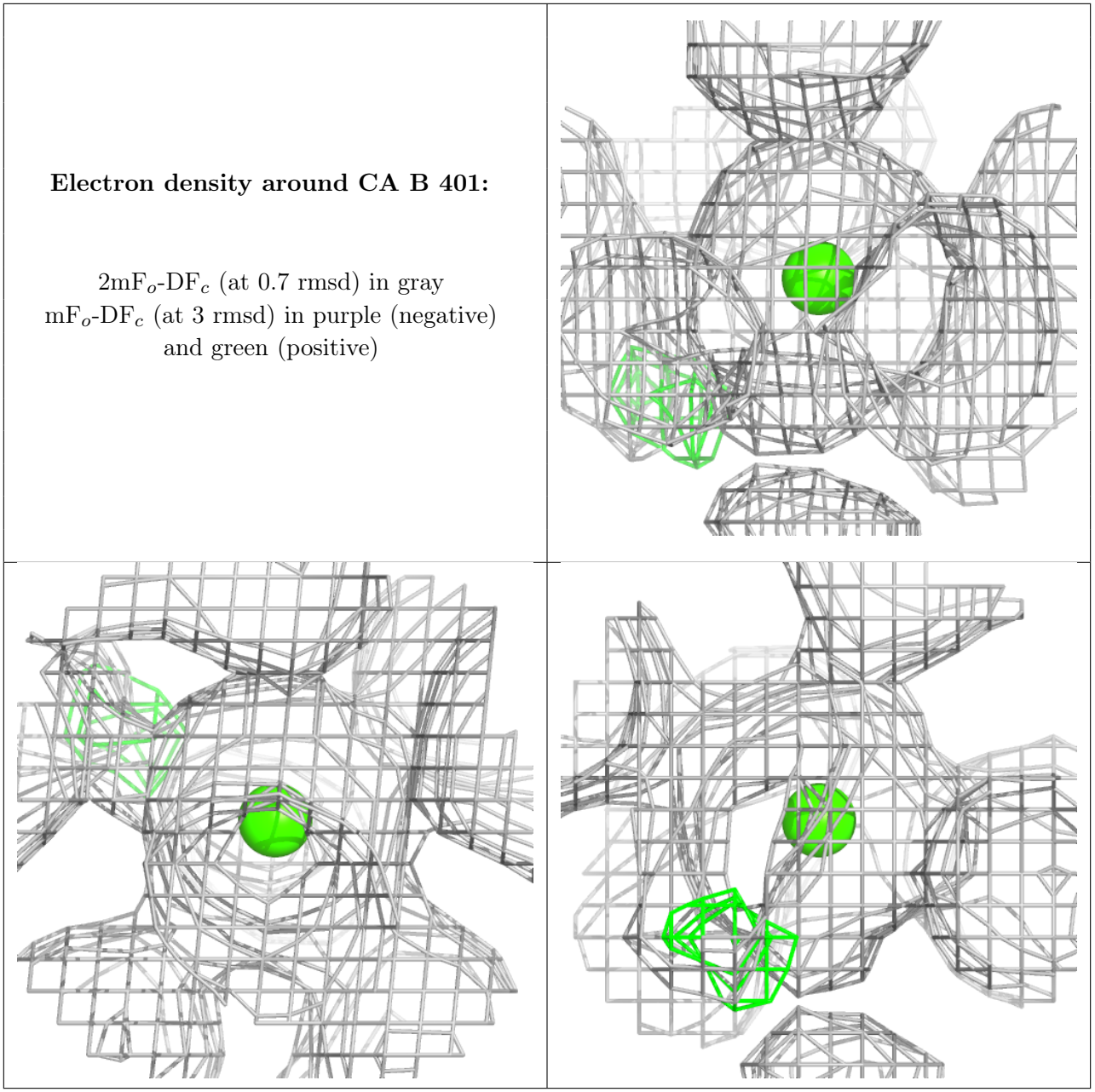






Electron density around CA B 401:

$2mF_o$-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.