



# Full wwPDB X-ray Structure Validation Report

Feb 23, 2023 – 06:32 pm GMT

PDB ID : 8AXT  
Title : Sialidases and Fucosidases of Akkermansia muciniphila are key for rapid growth on colonic mucin and nutrient sharing amongst mucin-associated human gut microbiota  
Authors : Sakanaka, H.; Nielsen, T.S.; Pichler, M.J.; Nordberg Karlsson, E.; Abou Hachem, M.; Morth, J.P.  
Deposited on : 2022-08-31  
Resolution : 1.59 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
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) : 2.32.1

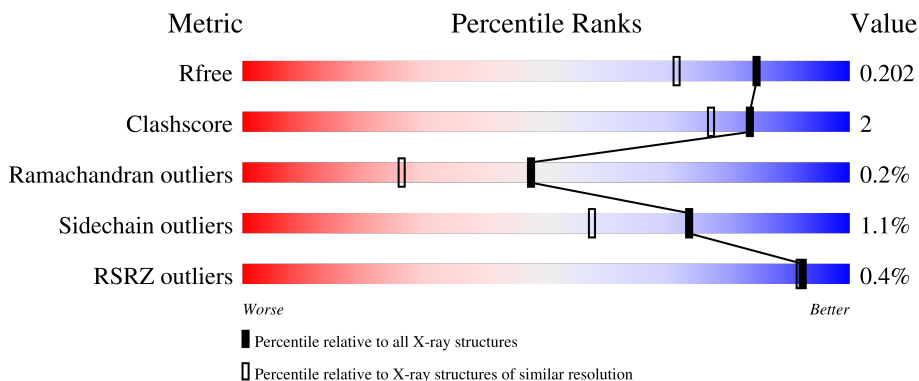
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	582	
1	B	582	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19227 atoms, of which 8878 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 Sialidase domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	571	8966	2840	4449	830	835	12	0	2	0
1	B	571	8926	2829	4429	825	831	12	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP B2ULI1
A	596	LEU	-	expression tag	UNP B2ULI1
A	597	GLU	-	expression tag	UNP B2ULI1
A	598	HIS	-	expression tag	UNP B2ULI1
A	599	HIS	-	expression tag	UNP B2ULI1
A	600	HIS	-	expression tag	UNP B2ULI1
A	601	HIS	-	expression tag	UNP B2ULI1
A	602	HIS	-	expression tag	UNP B2ULI1
A	603	HIS	-	expression tag	UNP B2ULI1
B	22	MET	-	initiating methionine	UNP B2ULI1
B	596	LEU	-	expression tag	UNP B2ULI1
B	597	GLU	-	expression tag	UNP B2ULI1
B	598	HIS	-	expression tag	UNP B2ULI1
B	599	HIS	-	expression tag	UNP B2ULI1
B	600	HIS	-	expression tag	UNP B2ULI1
B	601	HIS	-	expression tag	UNP B2ULI1
B	602	HIS	-	expression tag	UNP B2ULI1
B	603	HIS	-	expression tag	UNP B2ULI1

- 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	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	4	Total Cl 4 4	0	0

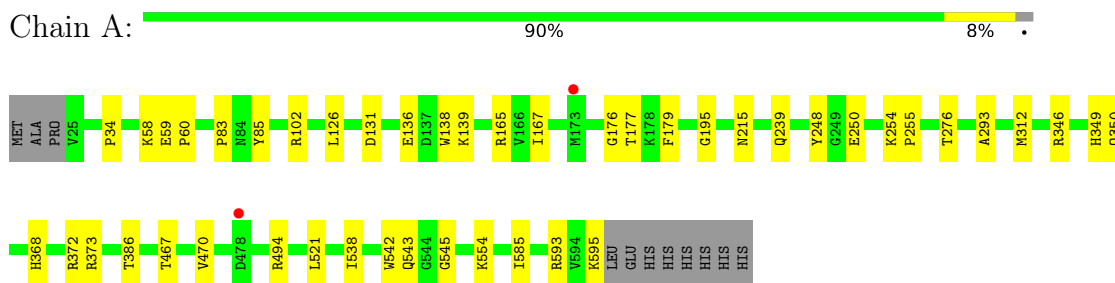
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	683	Total O 683 683	0	0
4	B	645	Total O 645 645	0	0

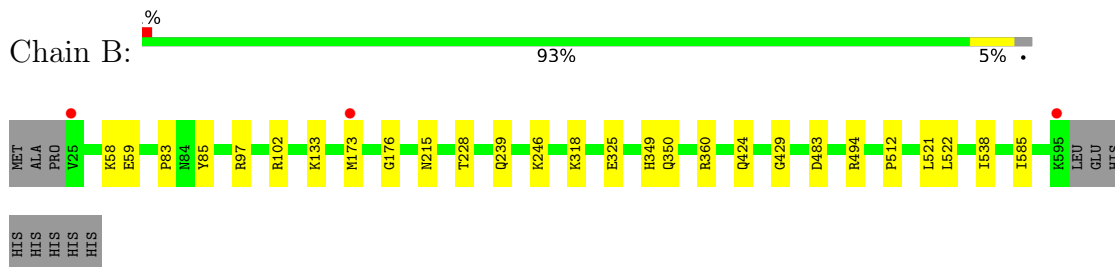
### 3 Residue-property plots [i](#)

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: Sialidase domain-containing protein



- Molecule 1: Sialidase domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.96Å 56.79Å 146.72Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	72.73 – 1.59 146.26 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.73-1.59) 99.8 (146.26-1.59)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.59Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.168 , 0.202 0.167 , 0.202	Depositor DCC
$R_{free}$ test set	8032 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19227	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: CA, 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	0.49	0/4633	0.72	0/6280
1	B	0.47	1/4613 (0.0%)	0.69	0/6254
All	All	0.48	1/9246 (0.0%)	0.70	0/12534

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	GLU	CB-CG	-5.31	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	ARG	Sidechain

### 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	4517	4449	4444	29	0
1	B	4497	4429	4427	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
4	A	683	0	0	5	1
4	B	645	0	0	2	0
All	All	10349	8878	8871	42	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 2.

All (42) 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:A:293:ALA:O	4:A:801:HOH:O	2.01	0.77
1:B:483:ASP:OD2	4:B:801:HOH:O	2.07	0.72
1:B:424:GLN:NE2	1:B:429:GLY:O	2.28	0.65
1:B:228:THR:HG22	1:B:246:LYS:HD2	1.80	0.64
1:A:368:HIS:O	1:A:372[B]:ARG:HG3	2.00	0.61
1:A:102:ARG:NH1	4:A:804:HOH:O	2.33	0.60
1:A:167:ILE:HG23	1:A:179:PHE:HB3	1.85	0.58
1:A:373:ARG:NH1	4:A:807:HOH:O	2.38	0.56
1:B:228:THR:HG22	1:B:246:LYS:CD	2.35	0.56
1:A:254:LYS:HD3	1:A:255:PRO:O	2.07	0.54
1:A:60:PRO:HG3	1:A:83:PRO:HA	1.90	0.53
1:B:176:GLY:HA2	1:B:215:ASN:O	2.09	0.53
1:A:126:LEU:CD2	1:A:136:GLU:HG2	2.40	0.52
1:A:176:GLY:HA2	1:A:215:ASN:O	2.10	0.51
1:A:386:THR:HG21	1:A:593:ARG:NH1	2.26	0.51
1:A:126:LEU:HD21	1:A:136:GLU:HG2	1.92	0.50
1:A:521:LEU:HD21	1:A:538:ILE:HD11	1.94	0.50
1:A:167:ILE:HD11	1:A:248:TYR:O	2.12	0.49
1:A:34:PRO:HG2	1:A:372[A]:ARG:HD3	1.95	0.48
1:B:521:LEU:HD21	1:B:538:ILE:HD11	1.96	0.48
1:A:372[A]:ARG:O	1:A:372[A]:ARG:HG3	2.15	0.47
1:A:59:GLU:H	1:A:59:GLU:CD	2.18	0.47
1:B:585:ILE:HD12	1:B:585:ILE:C	2.36	0.46
1:B:360:ARG:NH2	4:B:809:HOH:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:HD3	1:A:254:LYS:C	2.37	0.45
1:A:545:GLY:N	4:A:802:HOH:O	2.19	0.45
1:A:138:TRP:CZ3	1:A:139:LYS:HG2	2.53	0.44
1:B:97:ARG:HD2	1:B:102:ARG:NH1	2.32	0.44
1:A:83:PRO:HG2	1:A:85:TYR:CZ	2.53	0.43
1:B:512:PRO:HG2	1:B:522:LEU:HB3	2.01	0.43
1:A:470:VAL:HG23	1:A:542:TRP:CZ3	2.54	0.43
1:A:177:THR:O	1:A:195:GLY:HA3	2.18	0.42
1:B:58:LYS:HD3	1:B:58:LYS:H	1.84	0.42
1:A:239:GLN:NE2	4:A:825:HOH:O	2.51	0.42
1:A:467:THR:HG22	1:A:543:GLN:HG3	2.01	0.42
1:A:276:THR:HG21	1:A:312:MET:HE2	2.02	0.41
1:B:83:PRO:HG2	1:B:85:TYR:CZ	2.56	0.41
1:A:585:ILE:C	1:A:585:ILE:HD12	2.41	0.41
1:A:165:ARG:HH12	1:A:250:GLU:HG2	1.85	0.41
1:B:318:LYS:HB2	1:B:318:LYS:HE2	1.94	0.41
1:A:470:VAL:HG23	1:A:542:TRP:HZ3	1.85	0.40
1:A:595:LYS:HD3	1:A:595:LYS:HA	1.96	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)
4:A:959:HOH:O	4:A:1322:HOH:O[2_655]	2.12	0.08

## 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	571/582 (98%)	552 (97%)	18 (3%)	1 (0%)	47 26
1	B	569/582 (98%)	547 (96%)	21 (4%)	1 (0%)	47 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1140/1164 (98%)	1099 (96%)	39 (3%)	2 (0%)	47 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	GLN
1	A	350	GLN

### 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	481/489 (98%)	476 (99%)	5 (1%)	76 61
1	B	479/489 (98%)	473 (99%)	6 (1%)	69 50
All	All	960/978 (98%)	949 (99%)	11 (1%)	73 57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	131	ASP
1	A	349	HIS
1	A	494	ARG
1	A	554	LYS
1	B	59	GLU
1	B	133	LYS
1	B	173	MET
1	B	239	GLN
1	B	349	HIS
1	B	494	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	407	GLN
1	B	146	ASN

### 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 7 ligands modelled in this entry, 7 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	571/582 (98%)	-0.31	2 (0%) 92 92	8, 15, 32, 66	0
1	B	571/582 (98%)	-0.29	3 (0%) 91 90	9, 18, 35, 58	0
All	All	1142/1164 (98%)	-0.30	5 (0%) 92 92	8, 16, 33, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	MET	4.5
1	B	173	MET	3.5
1	B	595	LYS	3.0
1	A	478	ASP	2.1
1	B	25	VAL	2.0

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

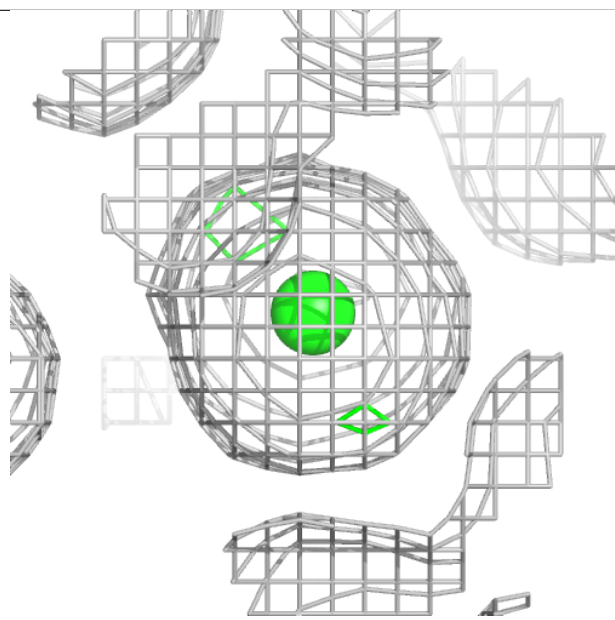
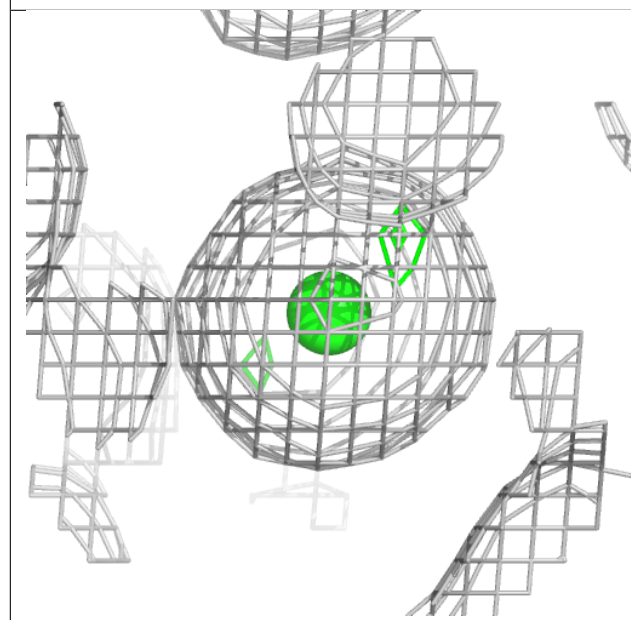
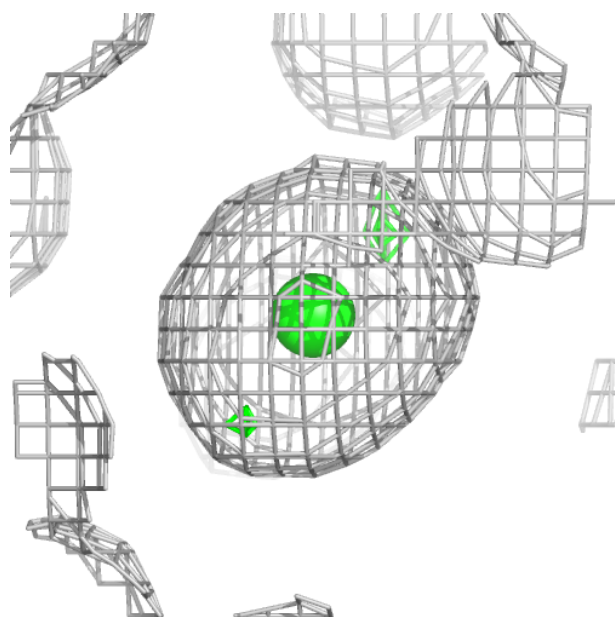
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	B	704	1/1	0.97	0.07	19,19,19,19	0
3	CL	B	702	1/1	0.98	0.04	24,24,24,24	0
3	CL	B	703	1/1	0.98	0.06	24,24,24,24	0
2	CA	B	701	1/1	0.98	0.07	20,20,20,20	0
2	CA	A	701	1/1	0.99	0.07	21,21,21,21	0
3	CL	A	702	1/1	1.00	0.05	19,19,19,19	0
3	CL	B	705	1/1	1.00	0.03	21,21,21,21	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.

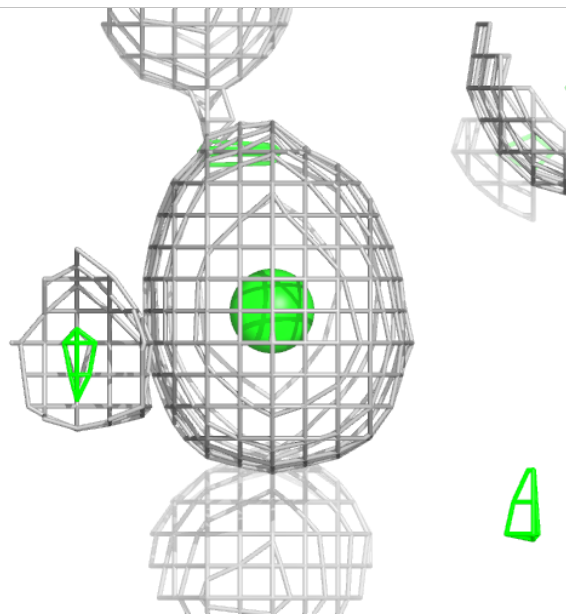
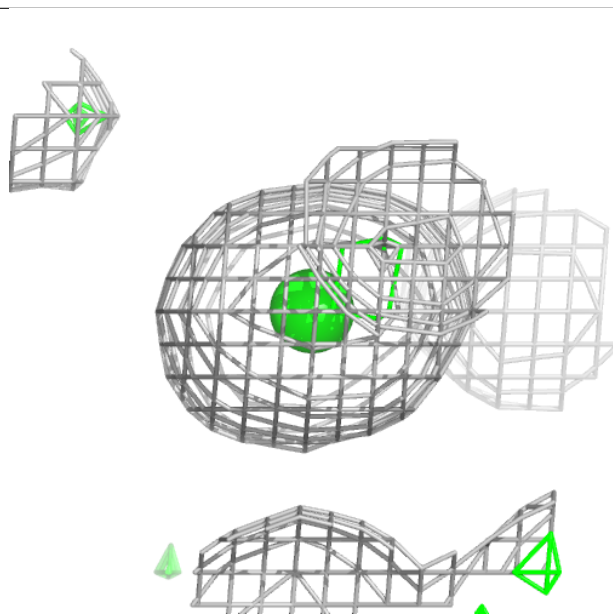
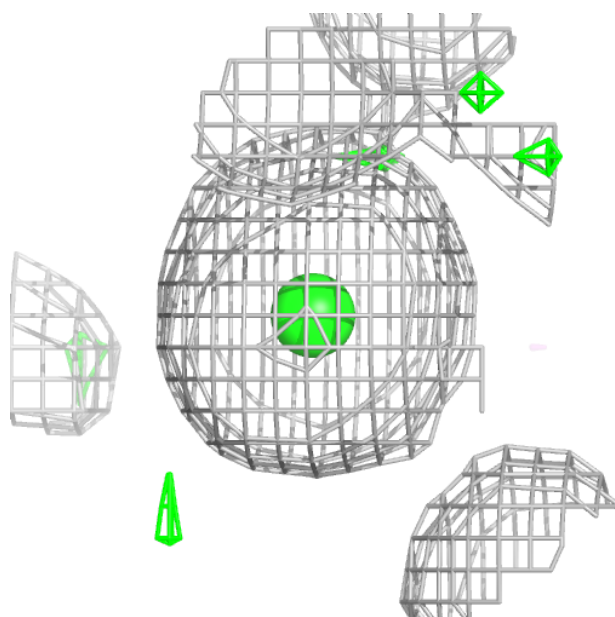
**Electron density around CL B 704:**

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



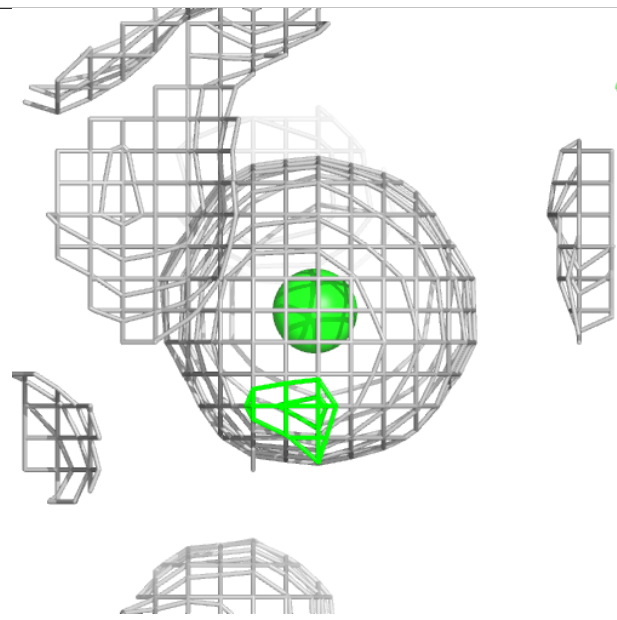
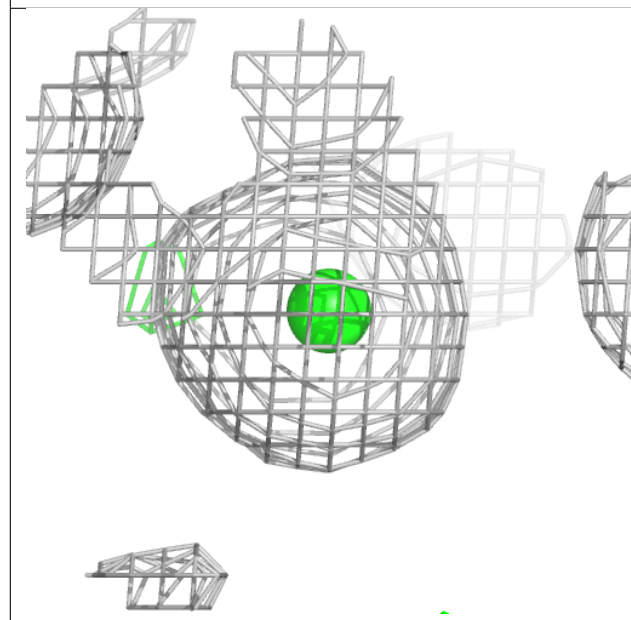
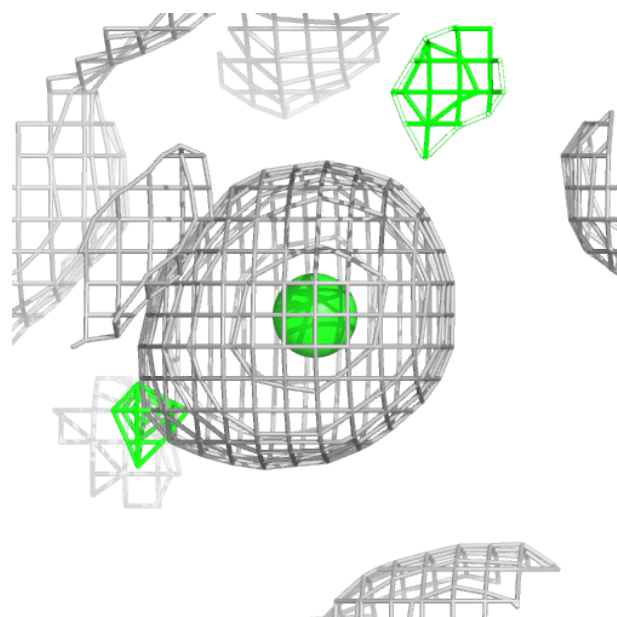
**Electron density around CL B 702:**

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



**Electron density around CL B 703:**

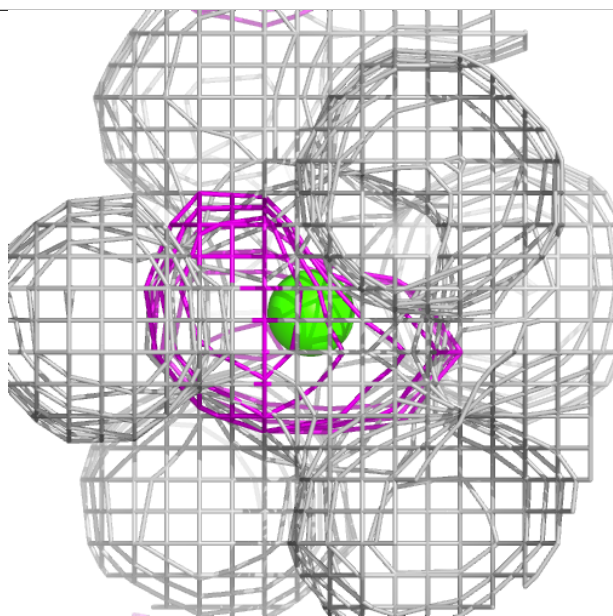
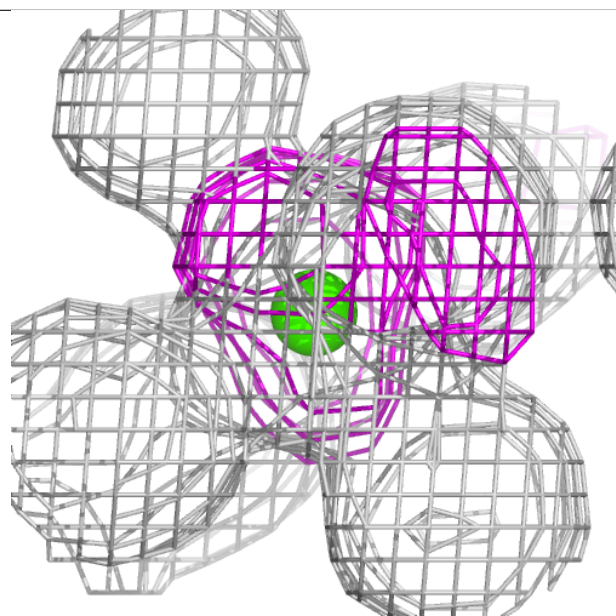
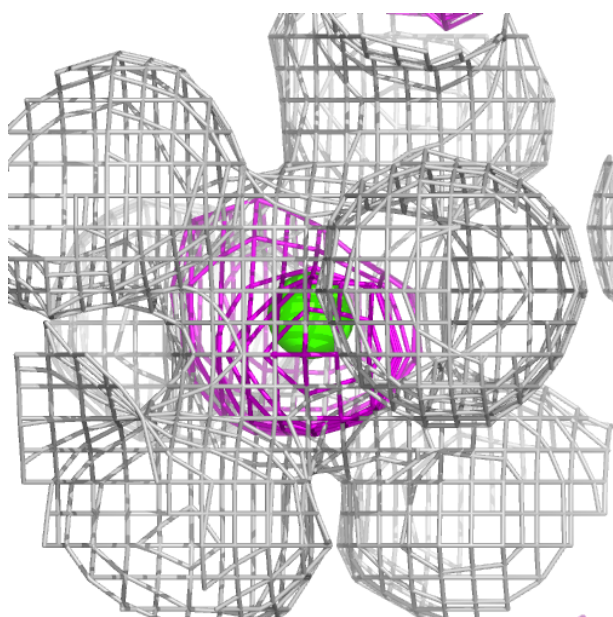
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





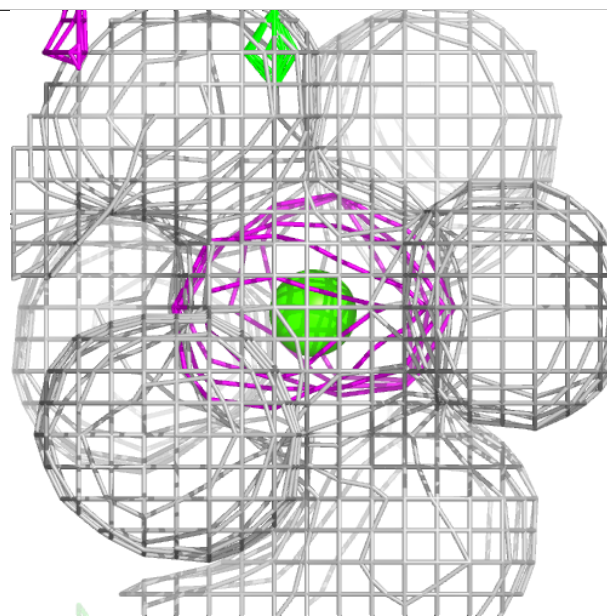
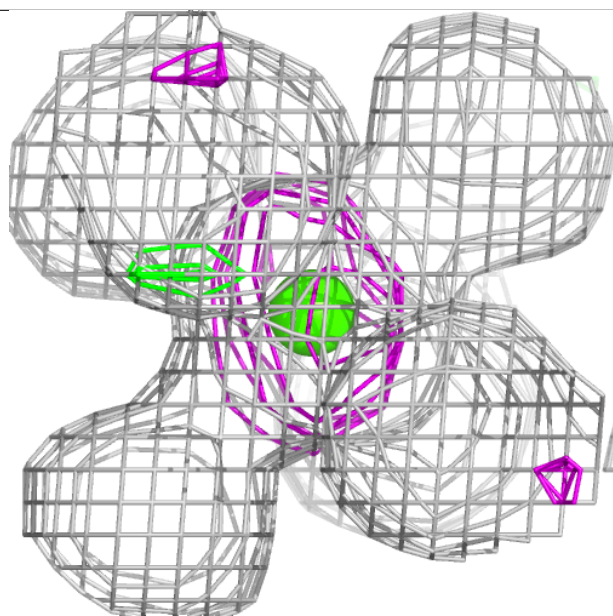
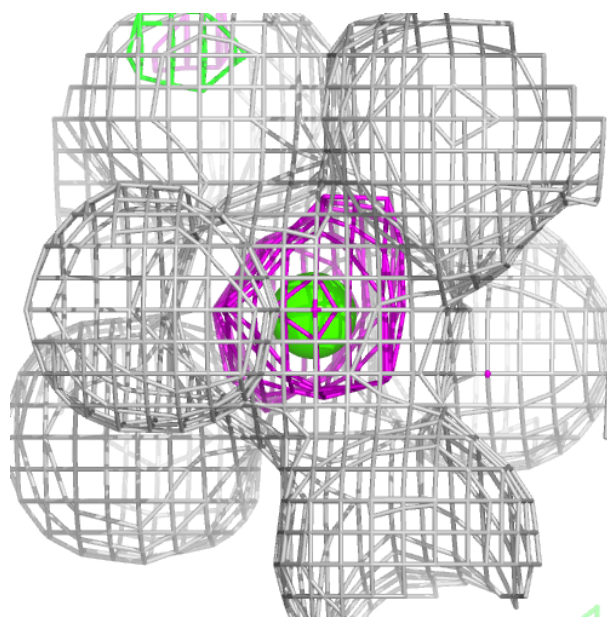
**Electron density around CA B 701:**

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



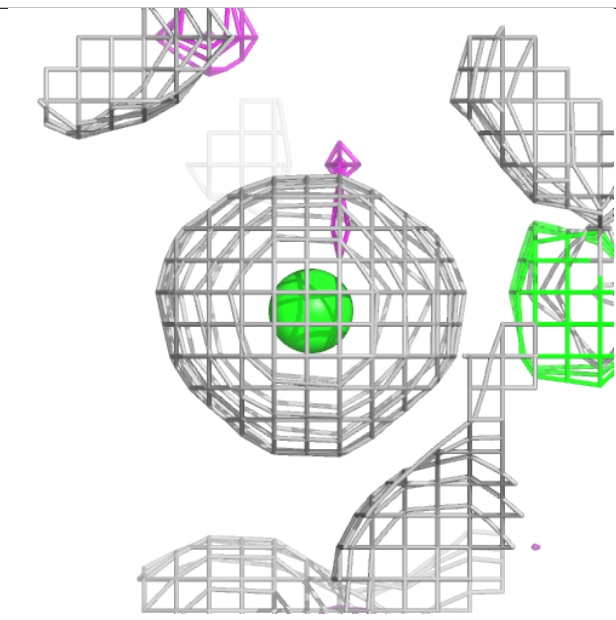
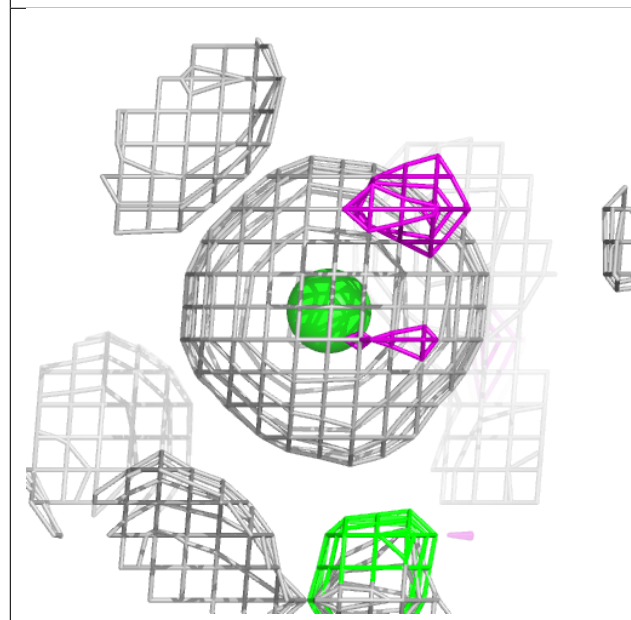
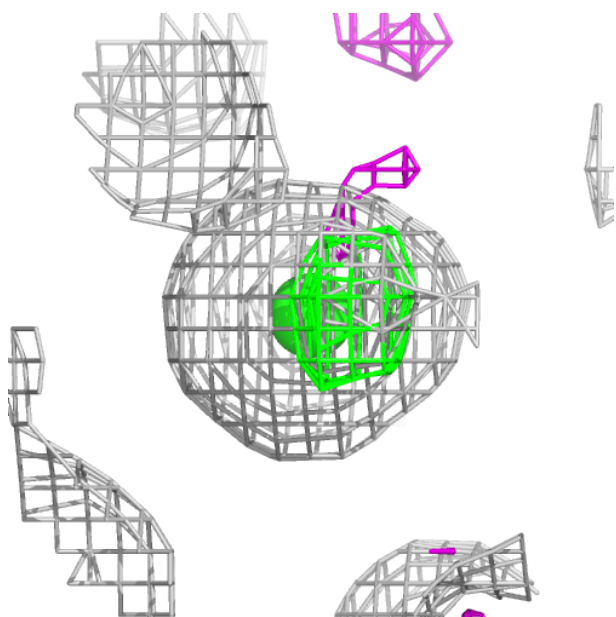
**Electron density around CA A 701:**

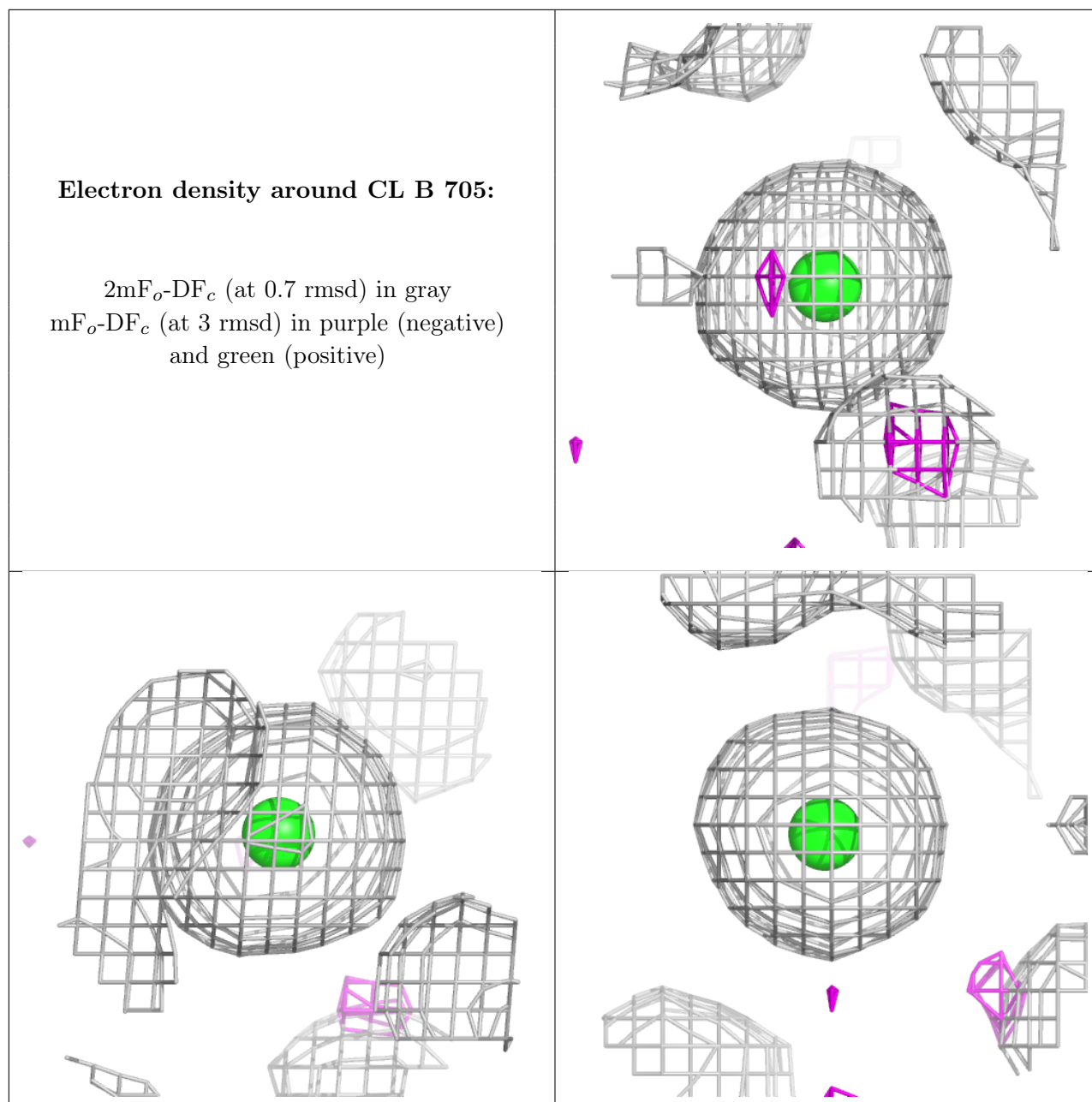
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CL A 702:**

$2mF_o-DF_c$  (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.