



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 03:36 pm GMT

PDB ID : 7BF2  
Title : Ca<sup>2+</sup>-Calmodulin in complex with human muscle form creatine kinase peptide in extended 1:2 binding mode  
Authors : Sprenger, J.; Akerfeldt, K.S.; Bredfelt, J.; Patel, N.; Rowlett, R.; Trifan, A.; Vanderbeck, A.; Lo Leggio, L.; Snogerup Linse, S.  
Deposited on : 2020-12-31  
Resolution : 1.43 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 : 2.36  
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

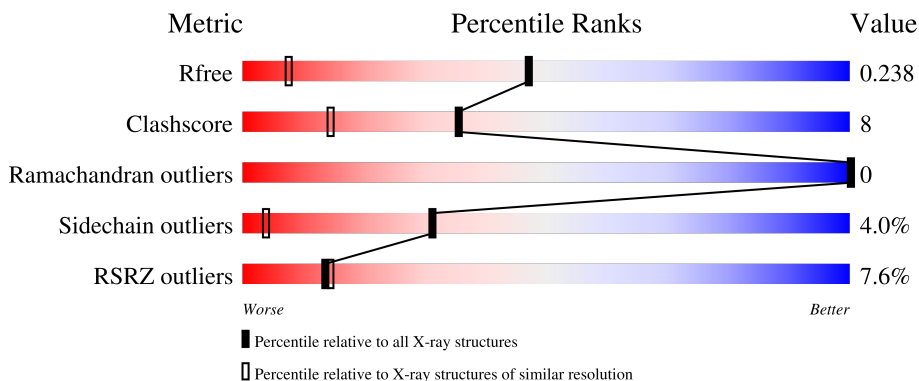
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	AAA	149	
2	CCC	18	
2	DDD	18	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2917 atoms, of which 1394 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 Calmodulin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	143	2283	722	1110	188	252	11	45	6	0

- Molecule 2 is a protein called Creatine kinase M-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	CCC	15	282	87	147	26	22	5	0	0
2	DDD	13	261	81	137	22	21	3	1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	4	Total	Ca	0	0
			4	4		

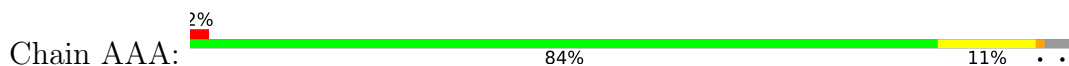
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	84	Total	O	0	0
			84	84		
4	CCC	2	Total	O	0	0
			2	2		
4	DDD	1	Total	O	0	0
			1	1		

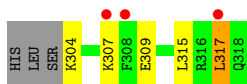
### 3 Residue-property plots [i](#)

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.

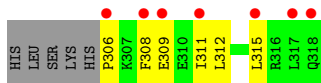
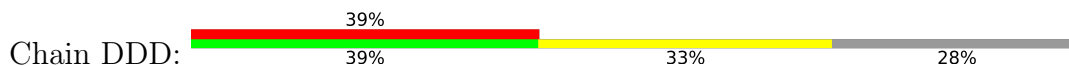
- Molecule 1: Calmodulin-1



- Molecule 2: Creatine kinase M-type



- Molecule 2: Creatine kinase M-type



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.69Å 24.53Å 60.35Å 90.00° 104.84° 90.00°	Depositor
Resolution (Å)	34.35 – 1.43 34.32 – 1.43	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.35-1.43) 97.5 (34.32-1.43)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.43Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.201 , 0.228 0.206 , 0.238	Depositor DCC
$R_{free}$ test set	1334 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.364	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 40.8	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	0.97	EDS
Total number of atoms	2917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.43% 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

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	0.55	0/1189	0.85	0/1596
2	CCC	2.15	1/137 (0.7%)	0.97	1/180 (0.6%)
2	DDD	0.82	1/125 (0.8%)	1.30	2/164 (1.2%)
All	All	0.86	2/1451 (0.1%)	0.91	3/1940 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	309	GLU	CD-OE1	-24.41	0.98	1.25
2	DDD	309	GLU	CD-OE2	6.85	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	309	GLU	OE1-CD-OE2	-10.06	111.22	123.30
2	CCC	309	GLU	OE1-CD-OE2	-6.47	115.53	123.30
2	DDD	309	GLU	CG-CD-OE2	6.46	131.22	118.30

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	AAA	1173	1110	1104	21	0
2	CCC	135	147	145	2	1
2	DDD	124	137	136	7	0
3	AAA	4	0	0	0	0
4	AAA	84	0	0	5	0
4	CCC	2	0	0	0	0
4	DDD	1	0	0	0	0
All	All	1523	1394	1385	23	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 8.

All (23) 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:AAA:5:LEU:HD23	1:AAA:9:GLN:HE21	1.48	0.78
1:AAA:5:LEU:HD23	1:AAA:9:GLN:NE2	2.04	0.72
1:AAA:19:LEU:HB3	2:CCC:315:LEU:HD13	1.74	0.70
1:AAA:123:ASP:OD2	4:AAA:401:HOH:O	2.10	0.69
1:AAA:136:GLN:NE2	4:AAA:402:HOH:O	2.18	0.66
1:AAA:19:LEU:HB3	2:CCC:315:LEU:CD1	2.36	0.55
1:AAA:103:ALA:HA	1:AAA:126[B]:ILE:HD11	1.89	0.55
2:DDD:308:PHE:O	2:DDD:311[B]:ILE:HG12	2.08	0.52
1:AAA:110:MET:SD	2:DDD:311[A]:ILE:HD13	2.50	0.51
1:AAA:145[B]:MET:HE3	4:AAA:434:HOH:O	2.11	0.50
1:AAA:92:VAL:HG11	2:DDD:315:LEU:HD11	1.94	0.48
1:AAA:129:ALA:HA	1:AAA:145[B]:MET:CE	2.43	0.47
1:AAA:146:MET:SD	2:DDD:308:PHE:HB3	2.54	0.47
1:AAA:129:ALA:HA	1:AAA:145[B]:MET:HE3	1.95	0.47
1:AAA:37[B]:MET:SD	1:AAA:52:MET:SD	3.13	0.47
2:DDD:308:PHE:HA	2:DDD:311[B]:ILE:HG12	1.97	0.47
1:AAA:129:ALA:CB	1:AAA:145[A]:MET:HG3	2.46	0.46
1:AAA:5:LEU:CD2	1:AAA:9:GLN:NE2	2.77	0.46
1:AAA:145[A]:MET:HE3	1:AAA:145[A]:MET:HA	1.98	0.45
1:AAA:146:MET:HE1	2:DDD:312:LEU:HB2	1.99	0.44
1:AAA:145[B]:MET:CE	4:AAA:434:HOH:O	2.67	0.41
1:AAA:125:MET:SD	2:DDD:306:PRO:HG2	2.60	0.41
1:AAA:96:ASP:OD2	4:AAA:403:HOH:O	2.22	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)
2:CCC:317:LEU:HD11	2:CCC:317:LEU:HD11[2_655]	1.16	0.44

### 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	147/149 (99%)	147 (100%)	0	0	100	100
2	CCC	13/18 (72%)	13 (100%)	0	0	100	100
2	DDD	12/18 (67%)	12 (100%)	0	0	100	100
All	All	172/185 (93%)	172 (100%)	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	129/127 (102%)	126 (98%)	3 (2%)	50	16
2	CCC	15/18 (83%)	12 (80%)	3 (20%)	1	0
2	DDD	14/18 (78%)	14 (100%)	0	100	100
All	All	158/163 (97%)	152 (96%)	6 (4%)	31	4

All (6) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	AAA	5	LEU
1	AAA	70	LEU
1	AAA	124	GLU
2	CCC	304	LYS
2	CCC	307	LYS
2	CCC	317	LEU

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 4 ligands modelled in this entry, 4 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

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	AAA	143/149 (95%)	0.14	3 (2%) 63 64	19, 28, 47, 70	0
2	CCC	15/18 (83%)	1.45	3 (20%) 1 1	37, 54, 73, 74	0
2	DDD	13/18 (72%)	1.96	7 (53%) 0 0	33, 54, 78, 87	0
All	All	171/185 (92%)	0.39	13 (7%) 13 14	19, 29, 67, 87	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DDD	306	PRO	4.7
2	CCC	317	LEU	4.6
1	AAA	5	LEU	4.4
2	CCC	307	LYS	4.0
2	DDD	309	GLU	3.0
2	DDD	318	GLN	2.9
1	AAA	147	THR	2.6
2	DDD	308	PHE	2.6
1	AAA	6	THR	2.6
2	CCC	308	PHE	2.3
2	DDD	311[A]	ILE	2.2
2	DDD	317	LEU	2.2
2	DDD	315	LEU	2.2

### 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

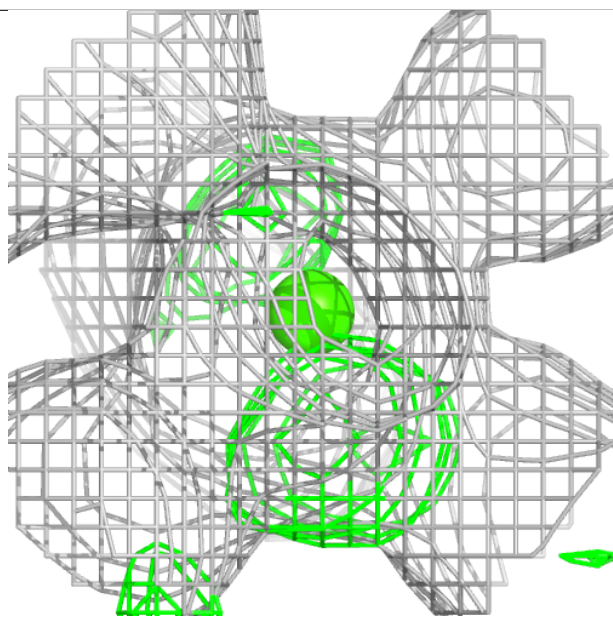
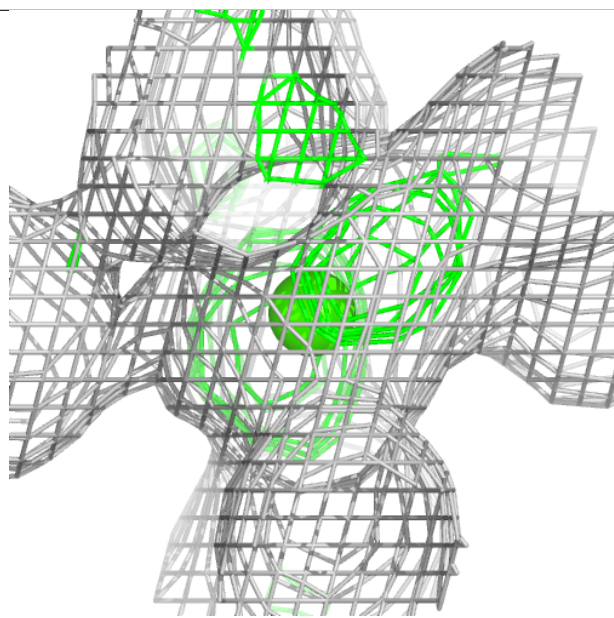
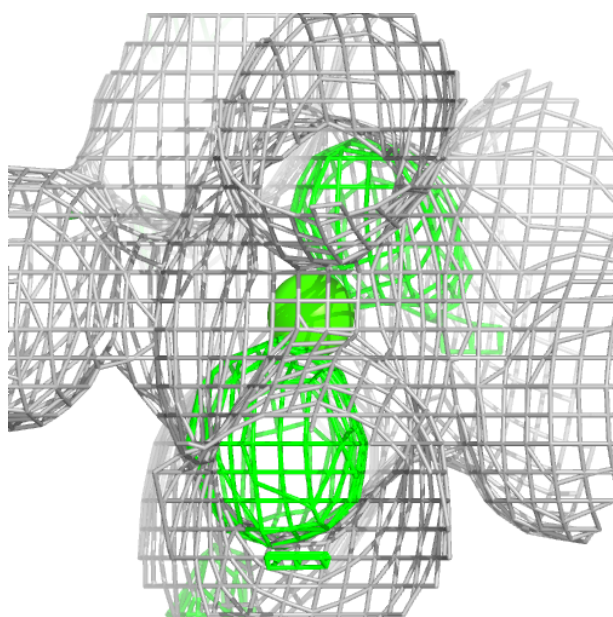
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	AAA	304	1/1	0.95	0.13	25,25,25,25	0
3	CA	AAA	301	1/1	0.96	0.10	30,30,30,30	0
3	CA	AAA	302	1/1	0.99	0.09	19,19,19,19	0
3	CA	AAA	303	1/1	1.00	0.07	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.

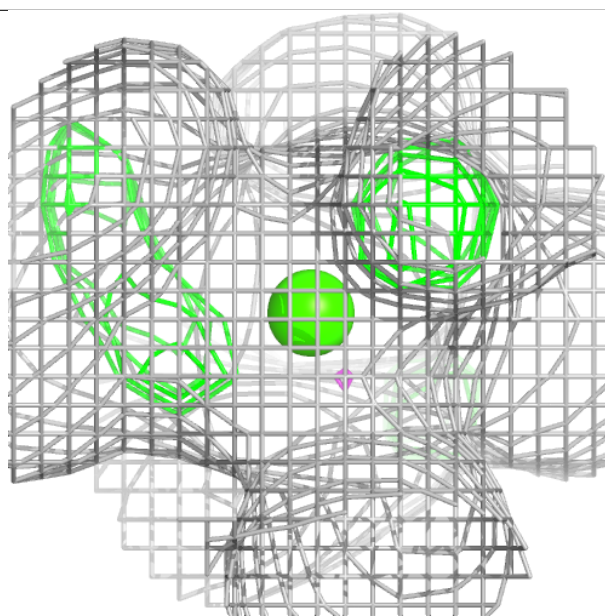
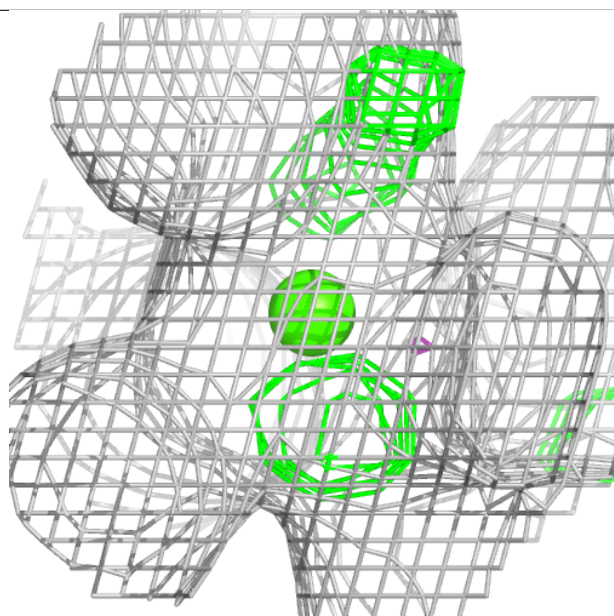
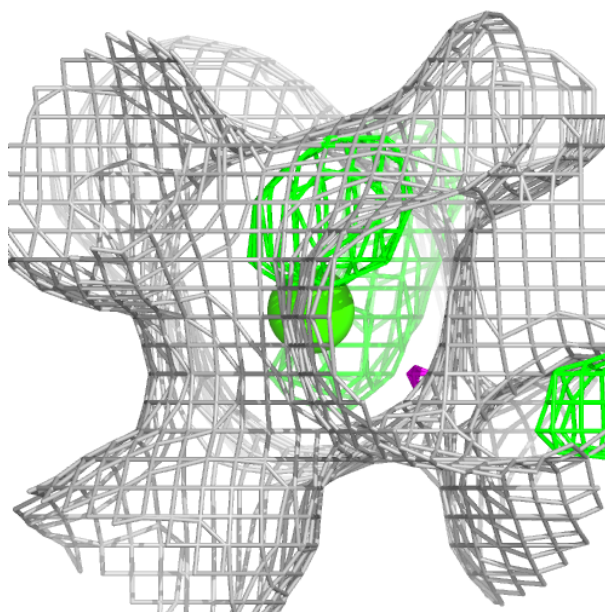
**Electron density around CA AAA 304:**

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



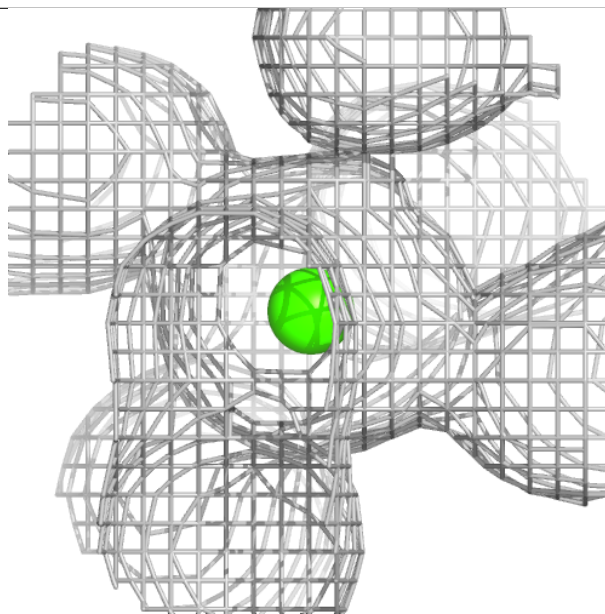
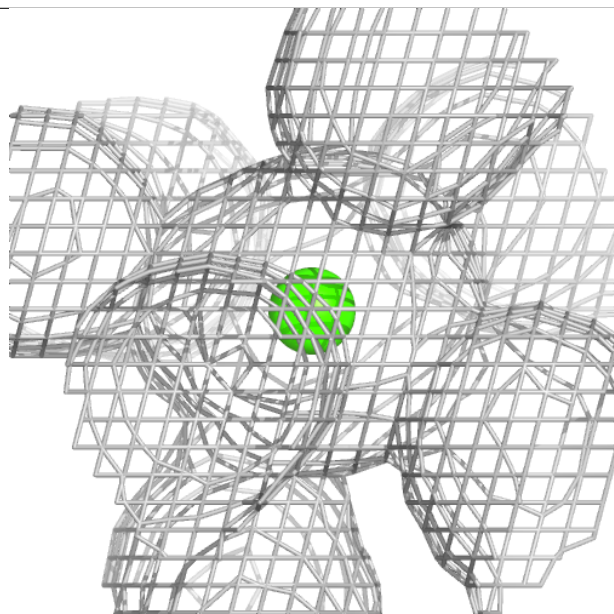
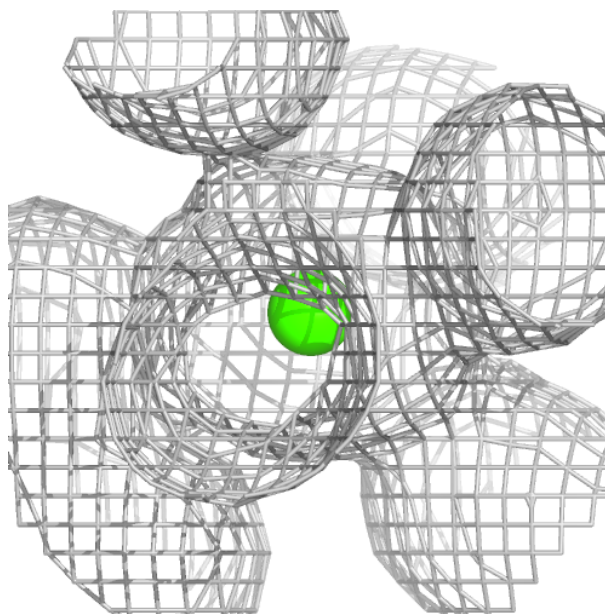
**Electron density around CA AAA 301:**

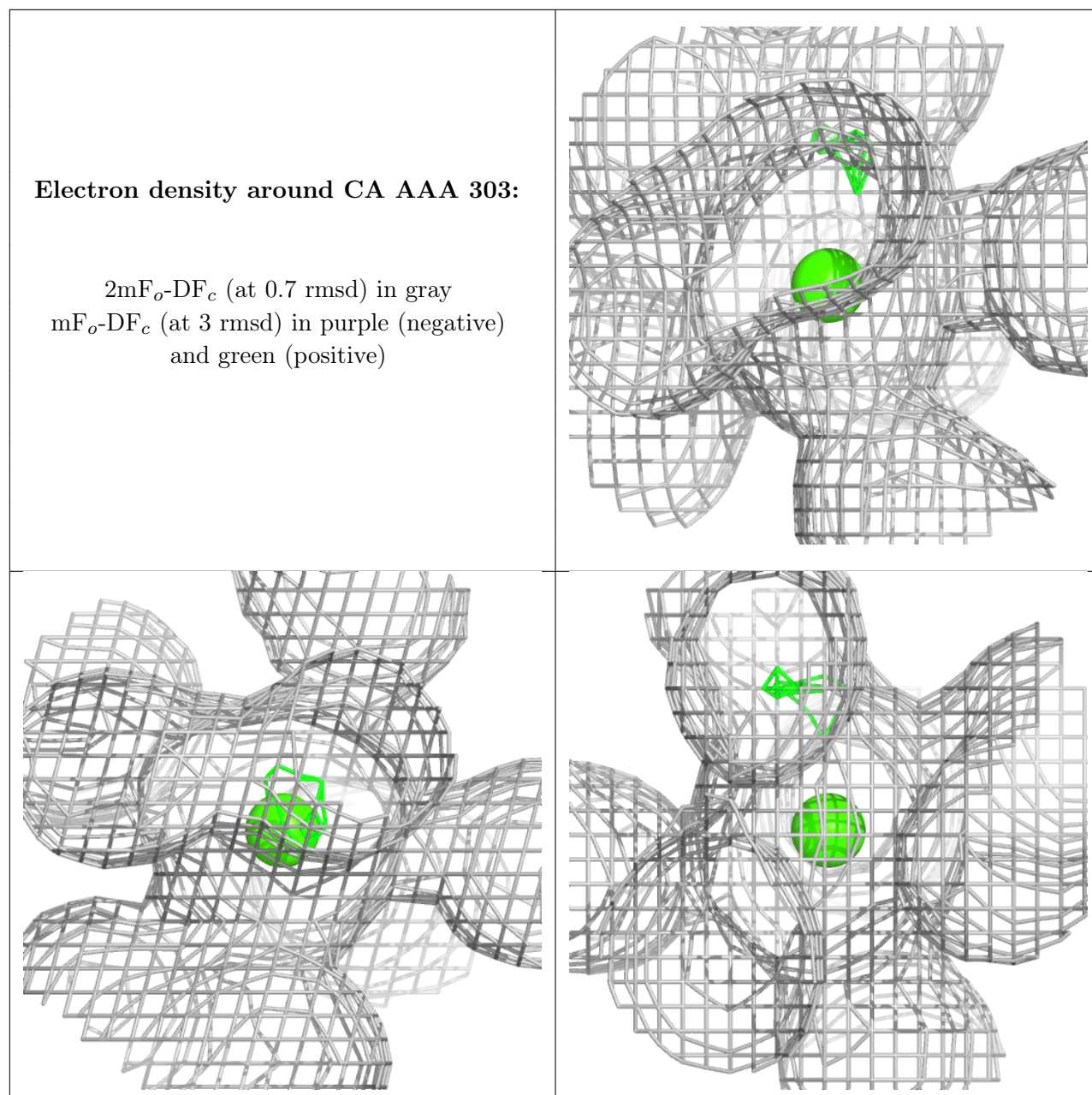
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA AAA 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](#)

There are no such residues in this entry.