

# wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 09:19 AM JST

PDB ID : 6LGA

Title : Bombyx mori GH13 sucrose hydrolase

Authors : Miyazaki, T. Deposited on : 2019-12-05

Resolution : 1.85 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

Mogul : 1.8.5 (274361), CSD as541be (2020)

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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

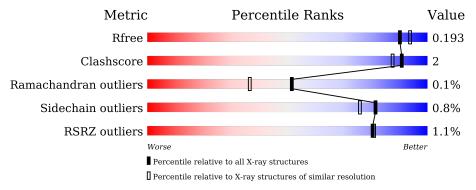
Validation Pipeline (wwPDB-VP) : 2.36

# 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 1.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	598	90%	6%	5%
1	В	598	90%	5%	6%



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10595 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 Sucrose hydrolase.

	Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
	1	Λ	570	Total	С	N	О	S	0	6	0
	1	А	310	4684	3006	773	891	14	0	0	U
ĺ	1	D	565	Total C N O		S	0	6	0		
	1	Ъ	303	4643	2984	763	883	13	0		U

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP A0A077JI83
A	10	GLY	-	expression tag	UNP A0A077JI83
A	11	SER	-	expression tag	UNP A0A077JI83
A	12	SER	-	expression tag	UNP A0A077JI83
A	13	HIS	-	expression tag	UNP A0A077JI83
A	14	HIS	-	expression tag	UNP A0A077JI83
A	15	HIS	-	expression tag	UNP A0A077JI83
A	16	HIS	-	expression tag	UNP A0A077JI83
A	17	HIS	-	expression tag	UNP A0A077JI83
A	18	HIS	-	expression tag	UNP A0A077JI83
A	19	SER	-	expression tag	UNP A0A077JI83
A	20	SER	-	expression tag	UNP A0A077JI83
A	21	GLY	-	expression tag	UNP A0A077JI83
A	22	LEU	-	expression tag	UNP A0A077JI83
A	23	VAL	-	expression tag	UNP A0A077JI83
A	24	PRO	-	expression tag	UNP A0A077JI83
A	25	ARG	-	expression tag	UNP A0A077JI83
A	26	GLY	-	expression tag	UNP A0A077JI83
A	27	SER	-	expression tag	UNP A0A077JI83
A	28	HIS	-	expression tag	UNP A0A077JI83
A	29	MET	-	expression tag	UNP A0A077JI83
В	9	MET	-	expression tag	UNP A0A077JI83
В	10	GLY	-	expression tag	UNP A0A077JI83
В	11	SER	-	expression tag	UNP A0A077JI83
В	12	SER		expression tag	UNP A0A077JI83

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Chain	Residue	Modelled	Actual	Comment	Reference
В	13	HIS	-	expression tag	UNP A0A077JI83
В	14	HIS	-	expression tag	UNP A0A077JI83
В	15	HIS	-	expression tag	UNP A0A077JI83
В	16	HIS	-	expression tag	UNP A0A077JI83
В	17	HIS	-	expression tag	UNP A0A077JI83
В	18	HIS	-	expression tag	UNP A0A077JI83
В	19	SER	-	expression tag	UNP A0A077JI83
В	20	SER	-	expression tag	UNP A0A077JI83
В	21	GLY	-	expression tag	UNP A0A077JI83
В	22	LEU	-	expression tag	UNP A0A077JI83
В	23	VAL	-	expression tag	UNP A0A077JI83
В	24	PRO	-	expression tag	UNP A0A077JI83
В	25	ARG	-	expression tag	UNP A0A077JI83
В	26	GLY	-	expression tag	UNP A0A077JI83
В	27	SER	-	expression tag	UNP A0A077JI83
В	28	HIS	=	expression tag	UNP A0A077JI83
В	29	MET	-	expression tag	UNP A0A077JI83

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

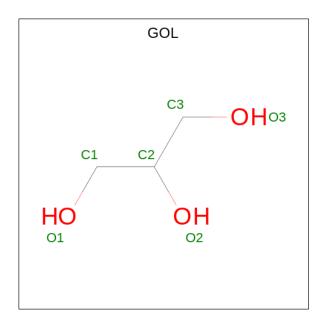
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	В	1	Total Mg 1 1	0	0

• 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	A	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0

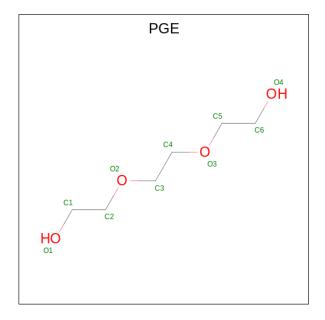
• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O	0	0
			6 3 3		
4	A	1	Total C O	0	0
			6 3 3		
4	A	1	Total C O	0	0
	11	_	6 3 3	Ŭ	
1	В	1	Total C O	0	0
	D	1	6 3 3	0	
1	D	1	Total C O	0	0
4	Б	1	6 3 3	U	0

 $\bullet$  Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $\mathrm{C_6H_{14}O_4}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0

#### $\bullet\,$ Molecule 6 is water.

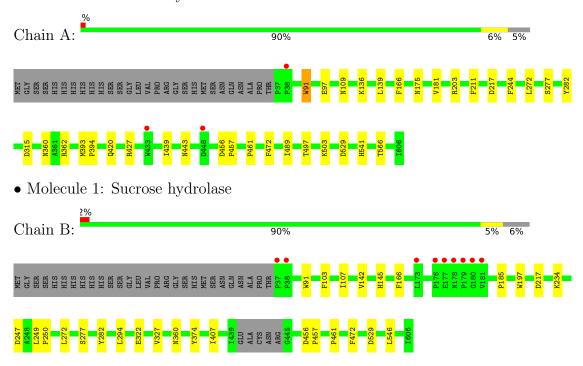
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	614	Total O 614 614	0	0
6	В	609	Total O 609 609	0	0



# 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: Sucrose hydrolase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.88Å 145.68Å 153.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 - 1.85	Depositor
rtesolution (A)	48.86 - 1.85	EDS
% Data completeness	99.7 (48.91-1.85)	Depositor
(in resolution range)	99.7 (48.86-1.85)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.157 , 0.185	Depositor
$R, R_{free}$	0.167 , $0.193$	DCC
$R_{free}$ test set	6257 reflections $(4.95%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 42.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10595	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 3.31% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: GOL, PGE, CA, 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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.66	0/4846	0.75	1/6597~(0.0%)
1	В	0.66	0/4804	0.75	0/6541
All	All	0.66	0/9650	0.75	1/13138 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	A	211	PHE	CB-CA-C	5.33	121.06	110.40

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	4684	0	4423	17	0
1	В	4643	0	4383	16	0
2	A	2	0	0	0	0
2	В	1	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	18	0	24	0	0
4	В	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
5	A	10	0	14	0	0
6	A	614	0	0	2	0
6	В	609	0	0	3	0
All	All	10595	0	8860	31	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 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:B:234:LYS:HE3	6:B:1279:HOH:O	1.85	0.73
1:A:541:HIS:HD2	6:A:1303:HOH:O	1.79	0.65
1:A:393:MET:HB3	1:A:394:PRO:HD3	1.83	0.59
1:A:566:THR:HG23	6:A:1265:HOH:O	2.06	0.55
1:A:136:LYS:HE3	1:A:315:ASP:OD2	2.08	0.54

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	Analysed Favoured Allowed		Outliers	Perce	ntiles
1	A	574/598 (96%)	562 (98%)	11 (2%)	1 (0%)	47	33
1	В	567/598 (95%)	559 (99%)	8 (1%)	0	100	100
All	All	1141/1196 (95%)	1121 (98%)	19 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type
1	A	420	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	506/524 (97%)	502 (99%)	4 (1%)	81 76
1	В	502/524 (96%)	498 (99%)	4 (1%)	81 76
All	All	1008/1048 (96%)	1000 (99%)	8 (1%)	81 76

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	217	ASP
1	В	166	PHE
1	В	91	TRP
1	A	217	ASP
1	В	103	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	GLN
1	A	541	HIS
1	В	391	ASN
1	В	204	GLN
1	A	443	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trmo	Chain	Dag	T inle	В	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	704	-	5,5,5	0.15	0	5,5,5	0.23	0
4	GOL	A	705	-	5,5,5	0.08	0	5,5,5	0.27	0
5	PGE	A	707	-	9,9,9	0.30	0	8,8,8	0.27	0
4	GOL	A	706	-	5,5,5	0.13	0	5,5,5	0.25	0
4	GOL	В	703	-	5,5,5	0.15	0	5,5,5	0.40	0
4	GOL	В	704	-	5,5,5	0.11	0	5,5,5	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	704	-	-	2/4/4/4	-
4	GOL	A	705	-	-	0/4/4/4	-
5	PGE	A	707	-	-	7/7/7/7	_
4	GOL	A	706	-	-	2/4/4/4	-
4	GOL	В	703	-	-	3/4/4/4	-
4	GOL	В	704	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	A	706	GOL	O1-C1-C2-C3
4	В	703	GOL	C1-C2-C3-O3
4	В	704	GOL	O1-C1-C2-C3
5	A	707	PGE	O2-C3-C4-O3
5	A	707	PGE	O3-C5-C6-O4

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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	570/598~(95%)	-0.48	3 (0%) 91 91	15, 21, 38, 68	0
1	В	565/598~(94%)	-0.33	9 (1%) 72 72	14, 21, 41, 92	0
All	All	1135/1196~(94%)	-0.41	12 (1%) 80 81	14, 21, 39, 92	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	176	PRO	5.4
1	В	177	GLU	5.3
1	В	181	VAL	3.9
1	В	37	PRO	3.8
1	В	180	GLY	3.3

#### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	A	706	6/6	0.71	0.22	39,45,48,51	0
5	PGE	A	707	10/10	0.78	0.22	51,55,58,58	0
4	GOL	В	703	6/6	0.86	0.14	36,41,42,43	0
4	GOL	A	705	6/6	0.90	0.19	34,43,47,49	0
4	GOL	В	704	6/6	0.91	0.13	27,41,42,51	0
4	GOL	A	704	6/6	0.95	0.10	21,24,25,27	0
2	MG	A	701	1/1	0.99	0.07	18,18,18,18	0
2	MG	A	703	1/1	0.99	0.04	18,18,18,18	0
2	MG	В	701	1/1	0.99	0.05	20,20,20,20	0
3	CA	A	702	1/1	1.00	0.06	16,16,16,16	0
3	CA	В	702	1/1	1.00	0.08	17,17,17,17	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.

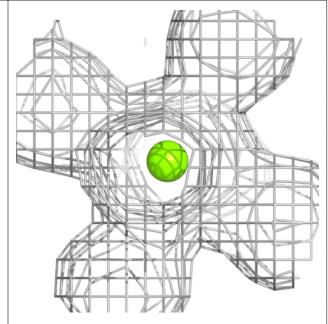


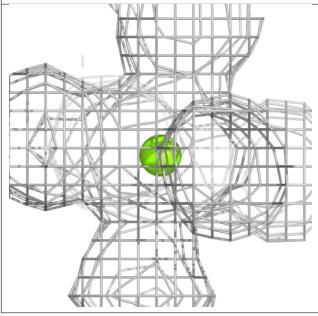
# Electron density around MG A 701: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)

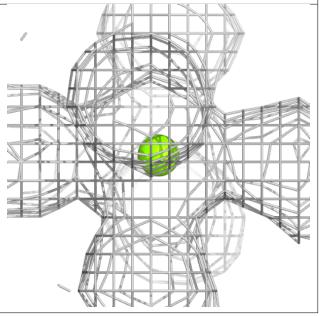


#### Electron density around MG A 703:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



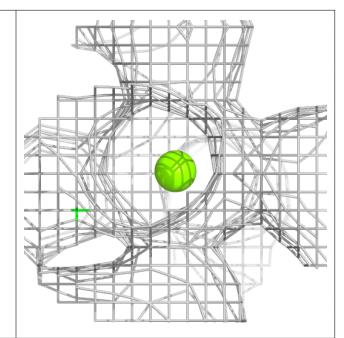


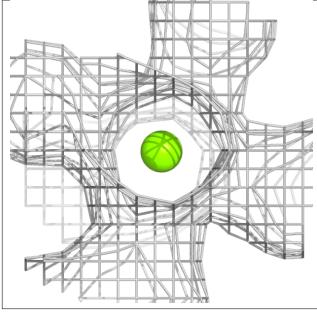


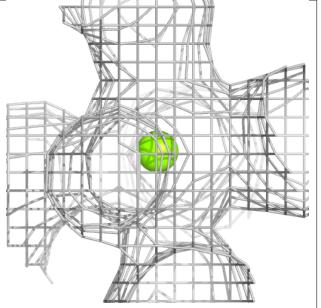


#### Electron density around MG B 701:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

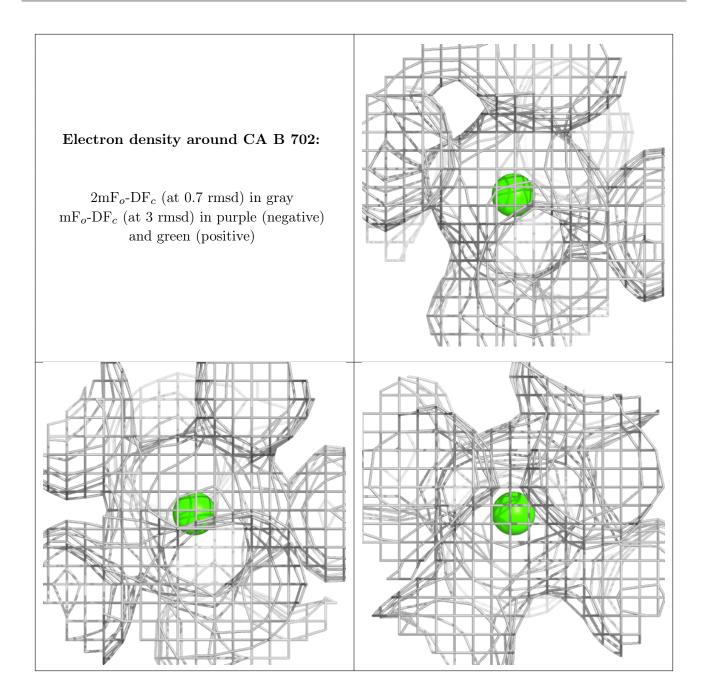






# Electron density around CA A 702: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

