



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:27 AM UTC

PDB ID : 7CBS / pdb_00007cbs
Title : Crystal structure of SpaB basal pilin from *Lactobacillus rhamnosus* GG
Authors : Megta, A.K.; Pratap, S.; Kant, A.; Krishnan, V.
Deposited on : 2020-06-13
Resolution : 2.39 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

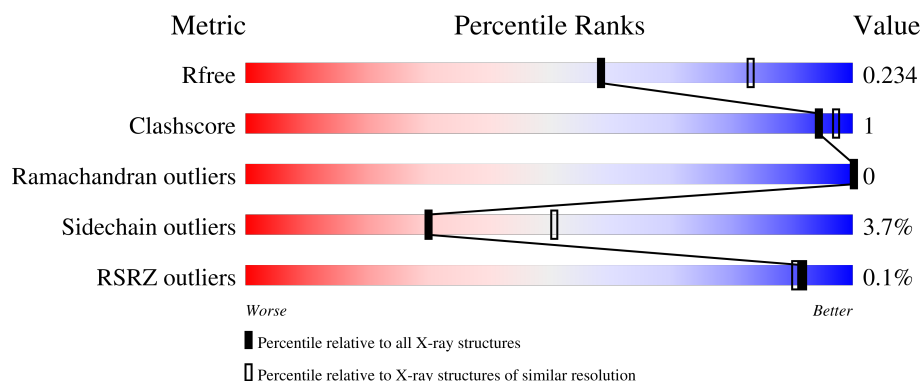
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	175	
1	B	175	
1	C	175	
1	D	175	
1	E	175	

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Mol	Chain	Length	Quality of chain
1	F	175	56% 41%
1	G	175	70% 27%
1	L	175	65% 31%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7270 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 LPXTG cell wall anchor domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			968	613	161	193	1			
1	B	131	Total	C	N	O	S	0	0	0
			969	613	165	190	1			
1	C	130	Total	C	N	O	S	0	0	0
			957	605	163	188	1			
1	D	126	Total	C	N	O	S	0	0	0
			949	604	158	186	1			
1	E	121	Total	C	N	O	S	0	0	0
			877	554	148	174	1			
1	G	127	Total	C	N	O	S	0	0	0
			921	579	158	183	1			
1	F	104	Total	C	N	O	S	0	0	0
			662	419	112	130	1			
1	L	120	Total	C	N	O	S	0	0	0
			885	559	148	177	1			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
A	11	GLY	-	expression tag	UNP A0A5P5Z9C8
A	12	SER	-	expression tag	UNP A0A5P5Z9C8
A	13	SER	-	expression tag	UNP A0A5P5Z9C8
A	14	HIS	-	expression tag	UNP A0A5P5Z9C8
A	15	HIS	-	expression tag	UNP A0A5P5Z9C8
A	16	HIS	-	expression tag	UNP A0A5P5Z9C8
A	17	HIS	-	expression tag	UNP A0A5P5Z9C8
A	18	HIS	-	expression tag	UNP A0A5P5Z9C8
A	19	HIS	-	expression tag	UNP A0A5P5Z9C8
A	20	SER	-	expression tag	UNP A0A5P5Z9C8
A	21	SER	-	expression tag	UNP A0A5P5Z9C8
A	22	GLY	-	expression tag	UNP A0A5P5Z9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP A0A5P5Z9C8
A	24	VAL	-	expression tag	UNP A0A5P5Z9C8
A	25	PRO	-	expression tag	UNP A0A5P5Z9C8
A	26	ARG	-	expression tag	UNP A0A5P5Z9C8
A	27	GLY	-	expression tag	UNP A0A5P5Z9C8
A	28	SER	-	expression tag	UNP A0A5P5Z9C8
A	29	HIS	-	expression tag	UNP A0A5P5Z9C8
A	30	MET	-	expression tag	UNP A0A5P5Z9C8
B	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
B	11	GLY	-	expression tag	UNP A0A5P5Z9C8
B	12	SER	-	expression tag	UNP A0A5P5Z9C8
B	13	SER	-	expression tag	UNP A0A5P5Z9C8
B	14	HIS	-	expression tag	UNP A0A5P5Z9C8
B	15	HIS	-	expression tag	UNP A0A5P5Z9C8
B	16	HIS	-	expression tag	UNP A0A5P5Z9C8
B	17	HIS	-	expression tag	UNP A0A5P5Z9C8
B	18	HIS	-	expression tag	UNP A0A5P5Z9C8
B	19	HIS	-	expression tag	UNP A0A5P5Z9C8
B	20	SER	-	expression tag	UNP A0A5P5Z9C8
B	21	SER	-	expression tag	UNP A0A5P5Z9C8
B	22	GLY	-	expression tag	UNP A0A5P5Z9C8
B	23	LEU	-	expression tag	UNP A0A5P5Z9C8
B	24	VAL	-	expression tag	UNP A0A5P5Z9C8
B	25	PRO	-	expression tag	UNP A0A5P5Z9C8
B	26	ARG	-	expression tag	UNP A0A5P5Z9C8
B	27	GLY	-	expression tag	UNP A0A5P5Z9C8
B	28	SER	-	expression tag	UNP A0A5P5Z9C8
B	29	HIS	-	expression tag	UNP A0A5P5Z9C8
B	30	MET	-	expression tag	UNP A0A5P5Z9C8
C	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
C	11	GLY	-	expression tag	UNP A0A5P5Z9C8
C	12	SER	-	expression tag	UNP A0A5P5Z9C8
C	13	SER	-	expression tag	UNP A0A5P5Z9C8
C	14	HIS	-	expression tag	UNP A0A5P5Z9C8
C	15	HIS	-	expression tag	UNP A0A5P5Z9C8
C	16	HIS	-	expression tag	UNP A0A5P5Z9C8
C	17	HIS	-	expression tag	UNP A0A5P5Z9C8
C	18	HIS	-	expression tag	UNP A0A5P5Z9C8
C	19	HIS	-	expression tag	UNP A0A5P5Z9C8
C	20	SER	-	expression tag	UNP A0A5P5Z9C8
C	21	SER	-	expression tag	UNP A0A5P5Z9C8
C	22	GLY	-	expression tag	UNP A0A5P5Z9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	LEU	-	expression tag	UNP A0A5P5Z9C8
C	24	VAL	-	expression tag	UNP A0A5P5Z9C8
C	25	PRO	-	expression tag	UNP A0A5P5Z9C8
C	26	ARG	-	expression tag	UNP A0A5P5Z9C8
C	27	GLY	-	expression tag	UNP A0A5P5Z9C8
C	28	SER	-	expression tag	UNP A0A5P5Z9C8
C	29	HIS	-	expression tag	UNP A0A5P5Z9C8
C	30	MET	-	expression tag	UNP A0A5P5Z9C8
D	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
D	11	GLY	-	expression tag	UNP A0A5P5Z9C8
D	12	SER	-	expression tag	UNP A0A5P5Z9C8
D	13	SER	-	expression tag	UNP A0A5P5Z9C8
D	14	HIS	-	expression tag	UNP A0A5P5Z9C8
D	15	HIS	-	expression tag	UNP A0A5P5Z9C8
D	16	HIS	-	expression tag	UNP A0A5P5Z9C8
D	17	HIS	-	expression tag	UNP A0A5P5Z9C8
D	18	HIS	-	expression tag	UNP A0A5P5Z9C8
D	19	HIS	-	expression tag	UNP A0A5P5Z9C8
D	20	SER	-	expression tag	UNP A0A5P5Z9C8
D	21	SER	-	expression tag	UNP A0A5P5Z9C8
D	22	GLY	-	expression tag	UNP A0A5P5Z9C8
D	23	LEU	-	expression tag	UNP A0A5P5Z9C8
D	24	VAL	-	expression tag	UNP A0A5P5Z9C8
D	25	PRO	-	expression tag	UNP A0A5P5Z9C8
D	26	ARG	-	expression tag	UNP A0A5P5Z9C8
D	27	GLY	-	expression tag	UNP A0A5P5Z9C8
D	28	SER	-	expression tag	UNP A0A5P5Z9C8
D	29	HIS	-	expression tag	UNP A0A5P5Z9C8
D	30	MET	-	expression tag	UNP A0A5P5Z9C8
E	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
E	11	GLY	-	expression tag	UNP A0A5P5Z9C8
E	12	SER	-	expression tag	UNP A0A5P5Z9C8
E	13	SER	-	expression tag	UNP A0A5P5Z9C8
E	14	HIS	-	expression tag	UNP A0A5P5Z9C8
E	15	HIS	-	expression tag	UNP A0A5P5Z9C8
E	16	HIS	-	expression tag	UNP A0A5P5Z9C8
E	17	HIS	-	expression tag	UNP A0A5P5Z9C8
E	18	HIS	-	expression tag	UNP A0A5P5Z9C8
E	19	HIS	-	expression tag	UNP A0A5P5Z9C8
E	20	SER	-	expression tag	UNP A0A5P5Z9C8
E	21	SER	-	expression tag	UNP A0A5P5Z9C8
E	22	GLY	-	expression tag	UNP A0A5P5Z9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	23	LEU	-	expression tag	UNP A0A5P5Z9C8
E	24	VAL	-	expression tag	UNP A0A5P5Z9C8
E	25	PRO	-	expression tag	UNP A0A5P5Z9C8
E	26	ARG	-	expression tag	UNP A0A5P5Z9C8
E	27	GLY	-	expression tag	UNP A0A5P5Z9C8
E	28	SER	-	expression tag	UNP A0A5P5Z9C8
E	29	HIS	-	expression tag	UNP A0A5P5Z9C8
E	30	MET	-	expression tag	UNP A0A5P5Z9C8
G	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
G	11	GLY	-	expression tag	UNP A0A5P5Z9C8
G	12	SER	-	expression tag	UNP A0A5P5Z9C8
G	13	SER	-	expression tag	UNP A0A5P5Z9C8
G	14	HIS	-	expression tag	UNP A0A5P5Z9C8
G	15	HIS	-	expression tag	UNP A0A5P5Z9C8
G	16	HIS	-	expression tag	UNP A0A5P5Z9C8
G	17	HIS	-	expression tag	UNP A0A5P5Z9C8
G	18	HIS	-	expression tag	UNP A0A5P5Z9C8
G	19	HIS	-	expression tag	UNP A0A5P5Z9C8
G	20	SER	-	expression tag	UNP A0A5P5Z9C8
G	21	SER	-	expression tag	UNP A0A5P5Z9C8
G	22	GLY	-	expression tag	UNP A0A5P5Z9C8
G	23	LEU	-	expression tag	UNP A0A5P5Z9C8
G	24	VAL	-	expression tag	UNP A0A5P5Z9C8
G	25	PRO	-	expression tag	UNP A0A5P5Z9C8
G	26	ARG	-	expression tag	UNP A0A5P5Z9C8
G	27	GLY	-	expression tag	UNP A0A5P5Z9C8
G	28	SER	-	expression tag	UNP A0A5P5Z9C8
G	29	HIS	-	expression tag	UNP A0A5P5Z9C8
G	30	MET	-	expression tag	UNP A0A5P5Z9C8
F	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
F	11	GLY	-	expression tag	UNP A0A5P5Z9C8
F	12	SER	-	expression tag	UNP A0A5P5Z9C8
F	13	SER	-	expression tag	UNP A0A5P5Z9C8
F	14	HIS	-	expression tag	UNP A0A5P5Z9C8
F	15	HIS	-	expression tag	UNP A0A5P5Z9C8
F	16	HIS	-	expression tag	UNP A0A5P5Z9C8
F	17	HIS	-	expression tag	UNP A0A5P5Z9C8
F	18	HIS	-	expression tag	UNP A0A5P5Z9C8
F	19	HIS	-	expression tag	UNP A0A5P5Z9C8
F	20	SER	-	expression tag	UNP A0A5P5Z9C8
F	21	SER	-	expression tag	UNP A0A5P5Z9C8
F	22	GLY	-	expression tag	UNP A0A5P5Z9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	23	LEU	-	expression tag	UNP A0A5P5Z9C8
F	24	VAL	-	expression tag	UNP A0A5P5Z9C8
F	25	PRO	-	expression tag	UNP A0A5P5Z9C8
F	26	ARG	-	expression tag	UNP A0A5P5Z9C8
F	27	GLY	-	expression tag	UNP A0A5P5Z9C8
F	28	SER	-	expression tag	UNP A0A5P5Z9C8
F	29	HIS	-	expression tag	UNP A0A5P5Z9C8
F	30	MET	-	expression tag	UNP A0A5P5Z9C8
L	10	MET	-	initiating methionine	UNP A0A5P5Z9C8
L	11	GLY	-	expression tag	UNP A0A5P5Z9C8
L	12	SER	-	expression tag	UNP A0A5P5Z9C8
L	13	SER	-	expression tag	UNP A0A5P5Z9C8
L	14	HIS	-	expression tag	UNP A0A5P5Z9C8
L	15	HIS	-	expression tag	UNP A0A5P5Z9C8
L	16	HIS	-	expression tag	UNP A0A5P5Z9C8
L	17	HIS	-	expression tag	UNP A0A5P5Z9C8
L	18	HIS	-	expression tag	UNP A0A5P5Z9C8
L	19	HIS	-	expression tag	UNP A0A5P5Z9C8
L	20	SER	-	expression tag	UNP A0A5P5Z9C8
L	21	SER	-	expression tag	UNP A0A5P5Z9C8
L	22	GLY	-	expression tag	UNP A0A5P5Z9C8
L	23	LEU	-	expression tag	UNP A0A5P5Z9C8
L	24	VAL	-	expression tag	UNP A0A5P5Z9C8
L	25	PRO	-	expression tag	UNP A0A5P5Z9C8
L	26	ARG	-	expression tag	UNP A0A5P5Z9C8
L	27	GLY	-	expression tag	UNP A0A5P5Z9C8
L	28	SER	-	expression tag	UNP A0A5P5Z9C8
L	29	HIS	-	expression tag	UNP A0A5P5Z9C8
L	30	MET	-	expression tag	UNP A0A5P5Z9C8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

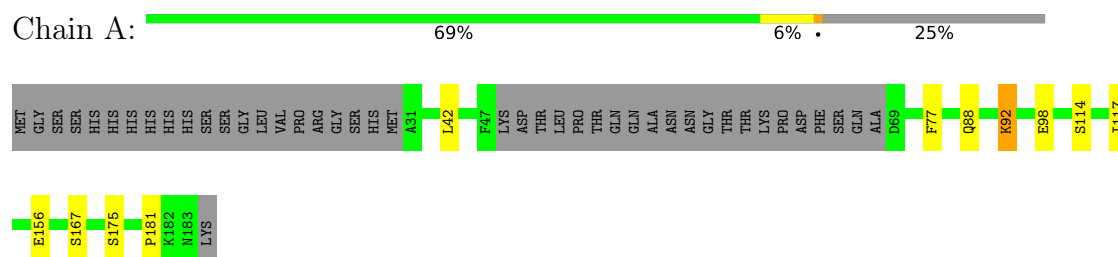
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	12	Total O 12 12	0	0
4	C	8	Total O 8 8	0	0
4	D	6	Total O 6 6	0	0
4	E	6	Total O 6 6	0	0
4	G	10	Total O 10 10	0	0
4	F	15	Total O 15 15	0	0
4	L	6	Total O 6 6	0	0

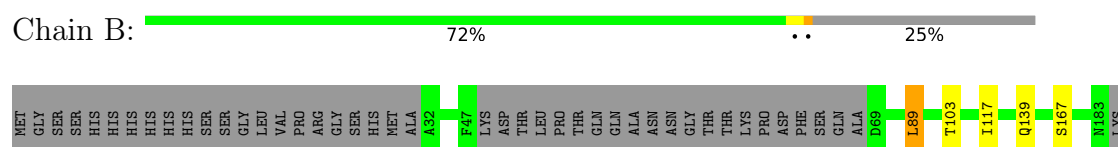
3 Residue-property plots [i](#)

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.

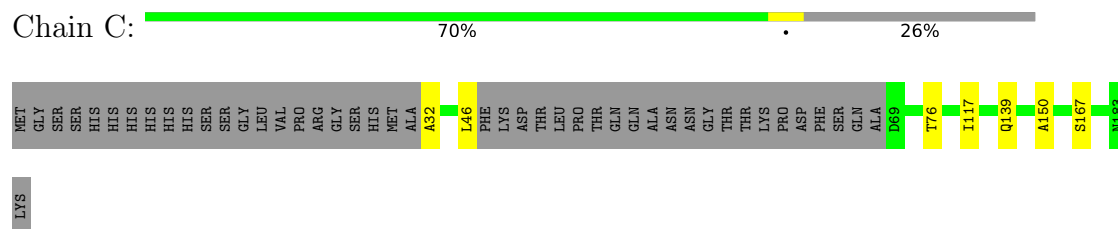
- Molecule 1: LPXTG cell wall anchor domain-containing protein



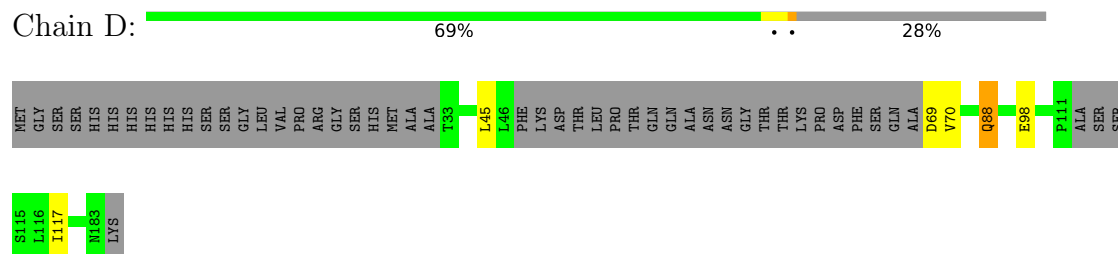
- Molecule 1: LPXTG cell wall anchor domain-containing protein



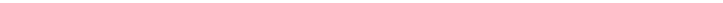
- Molecule 1: LPXTG cell wall anchor domain-containing protein

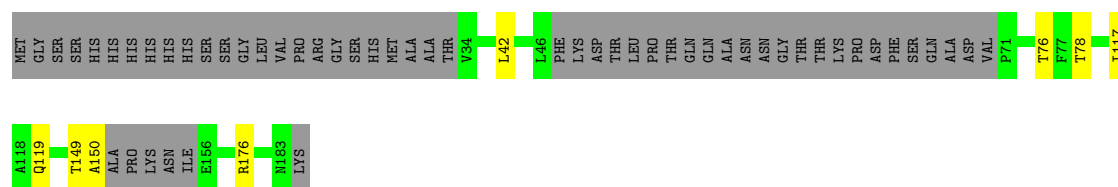


- Molecule 1: LPXTG cell wall anchor domain-containing protein

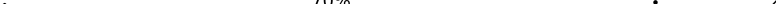


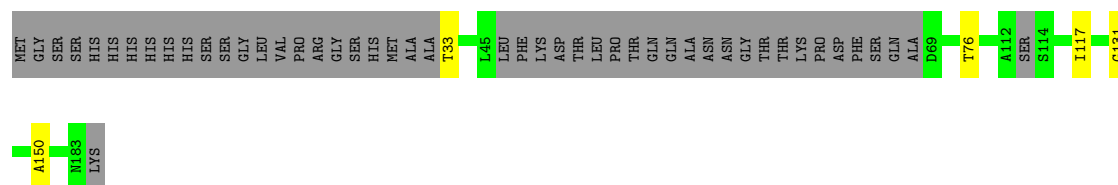
- Molecule 1: LPXTG cell wall anchor domain-containing protein

Chain E:  65% 5% 31%



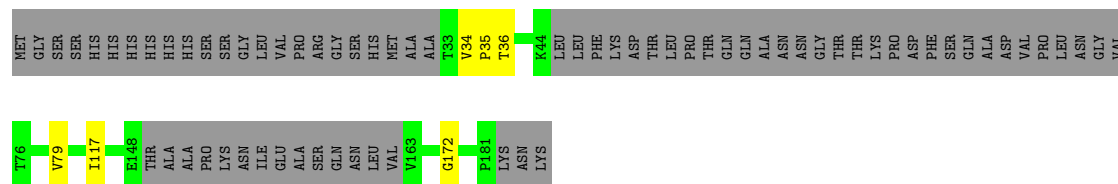
- Molecule 1: LPXTG cell wall anchor domain-containing protein.

Chain G:  70% 3% 27%

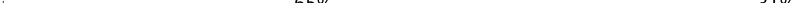


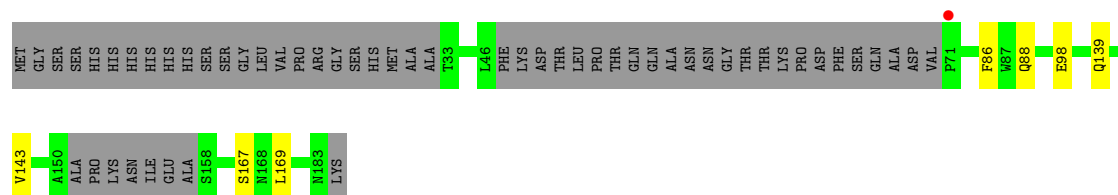
- Molecule 1: LPXTG cell wall anchor domain-containing protein

Chain F: 56% . 41%



- Molecule 1: LPXTG cell wall anchor domain-containing protein.

Chain L:  65% 31% 4%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	51.53Å 51.53Å 408.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.59 – 2.39 43.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.2 (43.59-2.39) 86.2 (43.59-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.228 0.196 , 0.234	Depositor DCC
R_{free} test set	2145 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l 0.488 for h,-h-k,-l 0.478 for -k,-h,-l	Xtriage
Reported twinning fraction	0.259 for H, K, L 0.250 for K, H, -L 0.246 for -K, -H, -L 0.245 for -h,-k,l	Depositor
Outliers	0 of 41160 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	0/986	1.38	0/1351
1	B	1.04	0/987	1.38	0/1349
1	C	1.03	0/975	1.38	0/1334
1	D	1.03	1/966 (0.1%)	1.37	0/1319
1	E	1.05	0/892	1.39	0/1219
1	F	1.12	0/673	1.52	0/927
1	G	1.04	0/937	1.37	0/1283
1	L	1.03	0/900	1.41	0/1229
All	All	1.05	1/7316 (0.0%)	1.40	0/10011

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	VAL	N-CA	5.05	1.50	1.46

There are no bond angle outliers.

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	968	0	922	5	0
1	B	969	0	930	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	957	0	912	2	0
1	D	949	0	922	2	0
1	E	877	0	816	3	0
1	F	662	0	511	3	0
1	G	921	0	858	2	0
1	L	885	0	840	2	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	F	1	0	0	0	0
2	L	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	15	0	0	0	0
4	G	10	0	0	0	0
4	L	6	0	0	0	0
All	All	7270	0	6711	18	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.

All (18) 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:42:LEU:HD21	1:A:181:PRO:HG3	1.73	0.71
1:A:42:LEU:HD21	1:A:181:PRO:CG	2.36	0.53
1:F:35:PRO:HG2	1:F:172:GLY:HA3	1.93	0.51
1:F:36:THR:O	1:F:36:THR:HG22	2.14	0.48
1:C:32:ALA:N	1:G:131:GLY:O	2.47	0.47
1:D:88:GLN:HA	1:D:88:GLN:HE21	1.79	0.47
1:A:42:LEU:HD13	1:A:77:PHE:CD2	2.50	0.47
1:L:86:PHE:CD2	1:L:143:VAL:HG11	2.53	0.44
1:A:88:GLN:O	1:A:92:LYS:HD3	2.18	0.44
1:D:45:LEU:HD22	1:D:69:ASP:C	2.43	0.43
1:F:79:VAL:HG13	1:F:117:ILE:HB	2.01	0.42
1:A:175:SER:OG	1:E:176:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD21	1:B:103:THR:HG21	2.01	0.41
1:L:169:LEU:CD1	1:L:169:LEU:N	2.83	0.41
1:G:76:THR:HB	1:G:150:ALA:HB3	2.02	0.41
1:E:119:GLN:HE21	1:E:149:THR:HG21	1.85	0.41
1:E:76:THR:HB	1:E:150:ALA:HB3	2.03	0.41
1:C:76:THR:HB	1:C:150:ALA:HB3	2.03	0.40

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	128/175 (73%)	125 (98%)	3 (2%)	0	100	100
1	B	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
1	C	126/175 (72%)	121 (96%)	5 (4%)	0	100	100
1	D	120/175 (69%)	115 (96%)	5 (4%)	0	100	100
1	E	115/175 (66%)	113 (98%)	2 (2%)	0	100	100
1	F	98/175 (56%)	92 (94%)	6 (6%)	0	100	100
1	G	121/175 (69%)	118 (98%)	3 (2%)	0	100	100
1	L	114/175 (65%)	111 (97%)	3 (3%)	0	100	100
All	All	949/1400 (68%)	919 (97%)	30 (3%)	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	A	102/147 (69%)	96 (94%)	6 (6%)	18	31
1	B	102/147 (69%)	98 (96%)	4 (4%)	28	48
1	C	100/147 (68%)	96 (96%)	4 (4%)	28	47
1	D	103/147 (70%)	100 (97%)	3 (3%)	37	60
1	E	89/147 (60%)	86 (97%)	3 (3%)	32	54
1	F	46/147 (31%)	45 (98%)	1 (2%)	45	67
1	G	94/147 (64%)	92 (98%)	2 (2%)	47	69
1	L	94/147 (64%)	90 (96%)	4 (4%)	26	44
All	All	730/1176 (62%)	703 (96%)	27 (4%)	30	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	98	GLU
1	A	114	SER
1	A	117	ILE
1	A	156	GLU
1	A	167	SER
1	B	89	LEU
1	B	117	ILE
1	B	139	GLN
1	B	167	SER
1	C	46	LEU
1	C	117	ILE
1	C	139	GLN
1	C	167	SER
1	D	88	GLN
1	D	98	GLU
1	D	117	ILE
1	E	42	LEU
1	E	78	THR
1	E	117	ILE
1	G	33	THR
1	G	117	ILE
1	F	34	VAL
1	L	88	GLN

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Mol	Chain	Res	Type
1	L	98	GLU
1	L	139	GLN
1	L	167	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	106	GLN
1	A	160	ASN
1	A	168	ASN
1	A	173	ASN
1	A	174	GLN
1	B	88	GLN
1	B	160	ASN
1	B	170	GLN
1	B	171	HIS
1	C	88	GLN
1	C	101	GLN
1	C	160	ASN
1	C	168	ASN
1	C	171	HIS
1	C	173	ASN
1	C	174	GLN
1	D	88	GLN
1	D	159	GLN
1	D	160	ASN
1	D	171	HIS
1	E	88	GLN
1	E	101	GLN
1	E	106	GLN
1	E	119	GLN
1	E	160	ASN
1	E	168	ASN
1	E	170	GLN
1	E	171	HIS
1	E	173	ASN
1	G	88	GLN
1	G	101	GLN
1	G	106	GLN
1	G	119	GLN
1	G	160	ASN

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Mol	Chain	Res	Type
1	G	171	HIS
1	G	174	GLN
1	L	101	GLN
1	L	106	GLN
1	L	137	GLN
1	L	159	GLN
1	L	160	ASN
1	L	171	HIS

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 oligosaccharides 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 ⓘ

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, 95th 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	132/175 (75%)	-0.60	0 100 100	47, 68, 97, 102	0
1	B	131/175 (74%)	-0.64	0 100 100	44, 66, 95, 108	0
1	C	130/175 (74%)	-0.70	0 100 100	38, 65, 87, 98	0
1	D	126/175 (72%)	-0.69	0 100 100	43, 66, 88, 105	0
1	E	121/175 (69%)	-0.42	0 100 100	41, 71, 126, 153	0
1	F	104/175 (59%)	-0.45	0 100 100	40, 70, 107, 131	0
1	G	127/175 (72%)	-0.43	0 100 100	38, 74, 138, 164	0
1	L	120/175 (68%)	-0.31	1 (0%) 82 80	47, 79, 129, 147	0
All	All	991/1400 (70%)	-0.54	1 (0%) 92 90	38, 69, 119, 164	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	71	PRO	2.4

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 oligosaccharides 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,

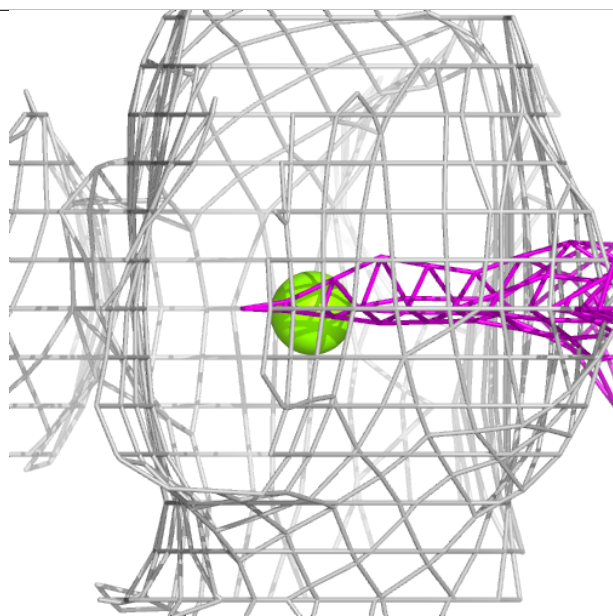
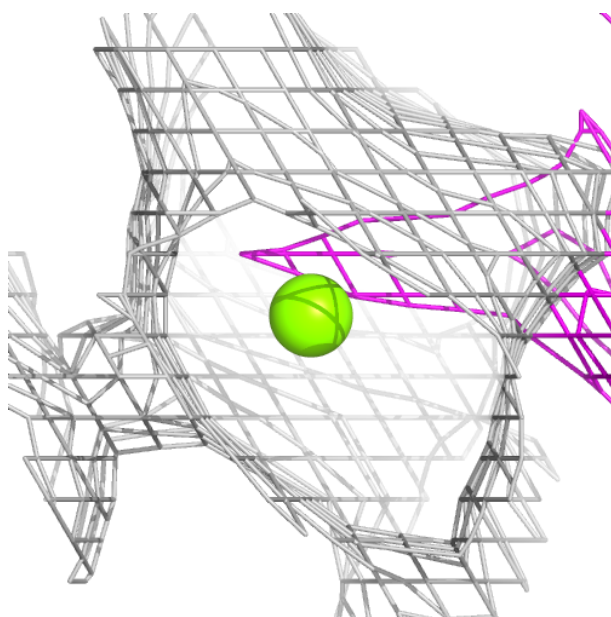
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	201	1/1	0.99	0.04	27,27,27,27	0
2	MG	C	201	1/1	0.99	0.07	29,29,29,29	0
2	MG	F	201	1/1	0.99	0.07	33,33,33,33	0
3	CL	B	201	1/1	0.99	0.04	60,60,60,60	0
3	CL	C	202	1/1	0.99	0.03	48,48,48,48	0
3	CL	D	201	1/1	0.99	0.02	55,55,55,55	0
2	MG	L	201	1/1	1.00	0.06	41,41,41,41	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.

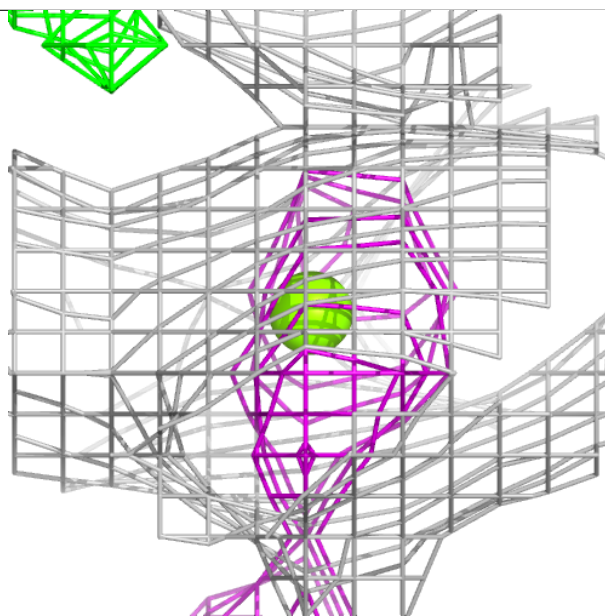
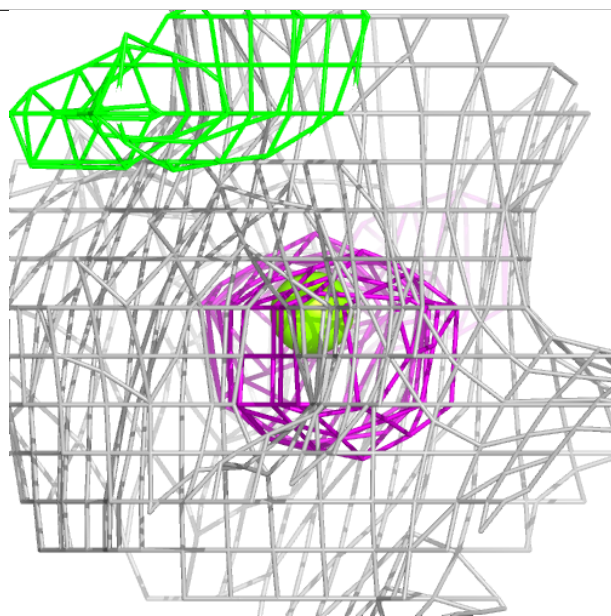
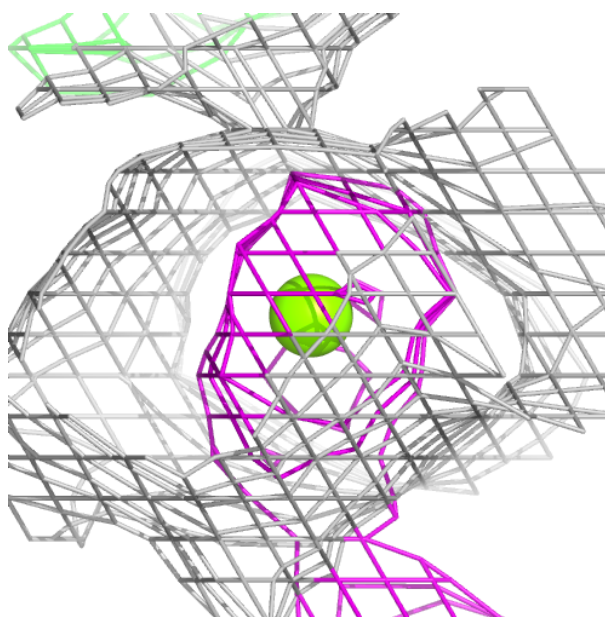
Electron density around MG A 201:

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



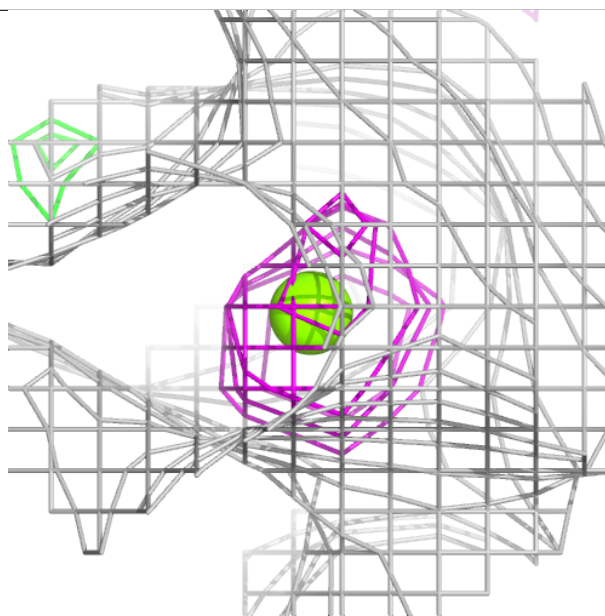
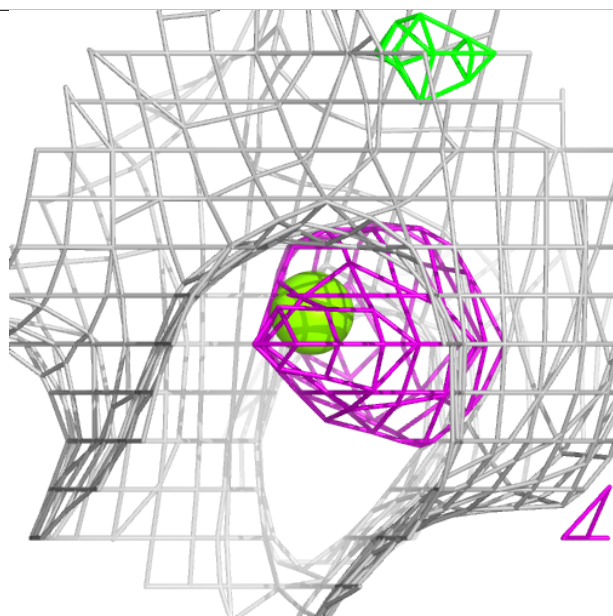
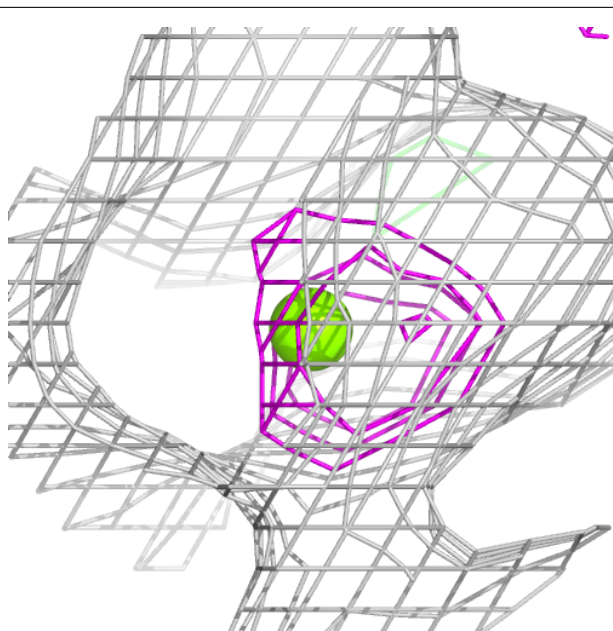
Electron density around MG C 201:

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



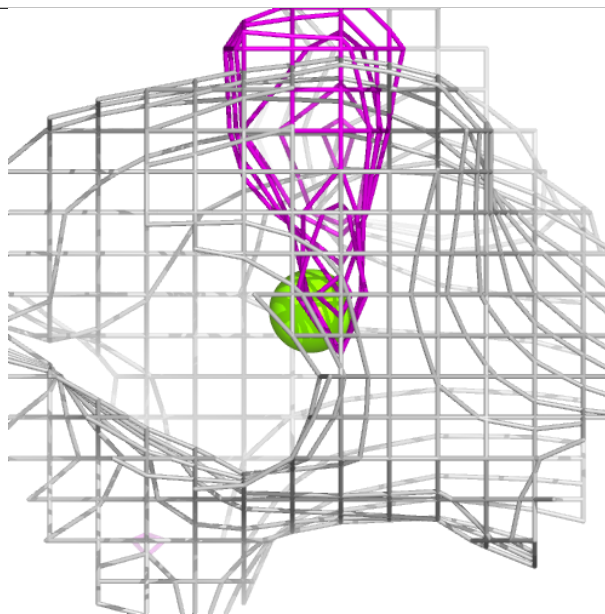
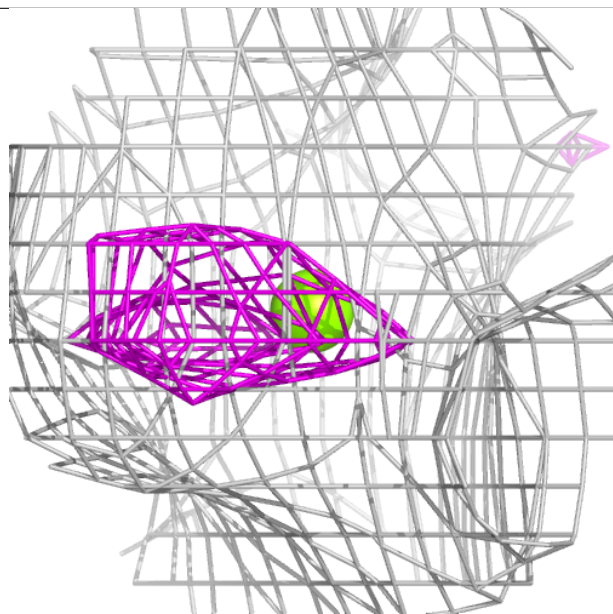
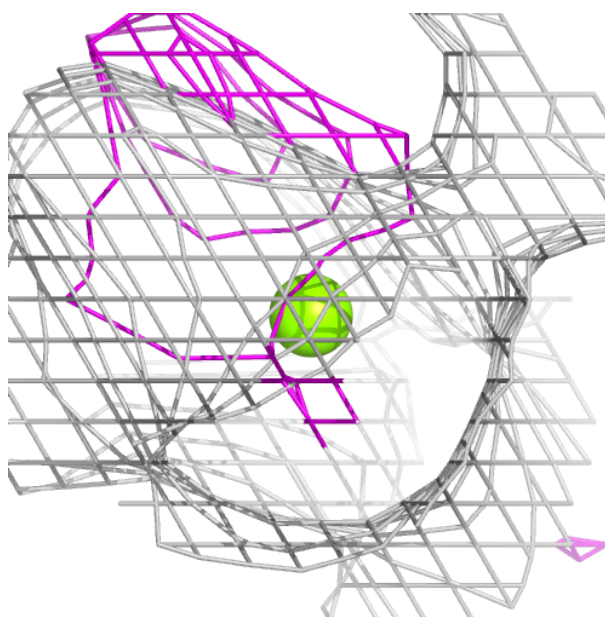
Electron density around MG F 201:

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



Electron density around MG L 201:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.