



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:19 AM UTC

PDB ID : 6RIA / pdb_00006ria
Title : Bactofilin from Thermus thermophilus, F105R mutant crystal structure
Authors : Lowe, J.; Gonzalez Llamazares, A.
Deposited on : 2019-04-23
Resolution : 3.50 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 ⓘ 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

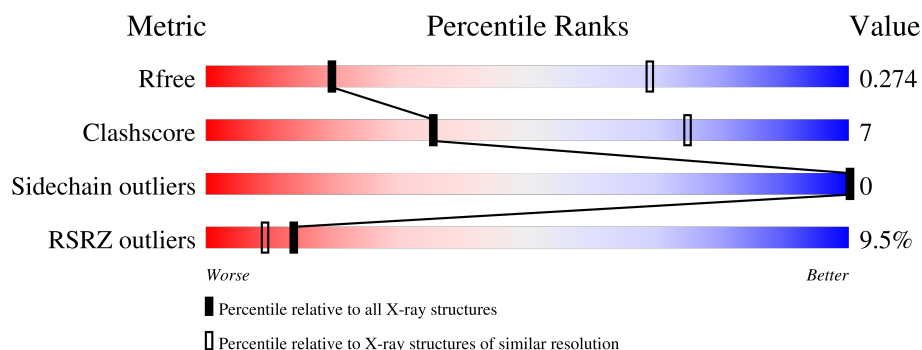
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1	123	21% 63% 11% 27%
1	2	123	20% 56% 17% 27%
1	3	123	7% 54% 20% 27%
1	4	123	11% 56% 17% 27%
1	5	123	28% 61% 12% 27%
1	6	123	26% 53% 20% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	A	123	4% 55% 18% 27%
1	B	123	4% 59% 14% 27%
1	C	123	3% 67% 6% 27%
1	D	123	2% 66% 7% 27%
1	E	123	4% 67% 6% 27%
1	F	123	2% 59% 14% 27%
1	G	123	2% 59% 14% 27%
1	H	123	2% 62% 11% 27%
1	I	123	3% 56% 17% 27%
1	J	123	5% 63% 10% 27%
1	K	123	2% 54% 19% 27%
1	L	123	3% 55% 18% 27%
1	M	123	6% 59% 15% 27%
1	N	123	7% 60% 13% 27%
1	O	123	7% 61% 12% 27%
1	P	123	7% 59% 14% 27%
1	Q	123	2% 59% 14% 27%
1	R	123	7% 59% 14% 27%
1	S	123	2% 61% 12% 27%
1	T	123	2% 63% 11% 27%
1	U	123	2% 63% 11% 27%
1	V	123	4% 55% 18% 27%
1	W	123	2% 62% 11% 27%
1	X	123	2% 61% 12% 27%
1	Y	123	12% 47% 26% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Z	123	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21663 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 bactofilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			676	421	120	134	1			
1	B	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	C	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	D	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	E	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	F	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	G	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	H	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	I	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	J	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	K	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	L	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	M	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	N	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	O	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	P	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			

Continued on next page...

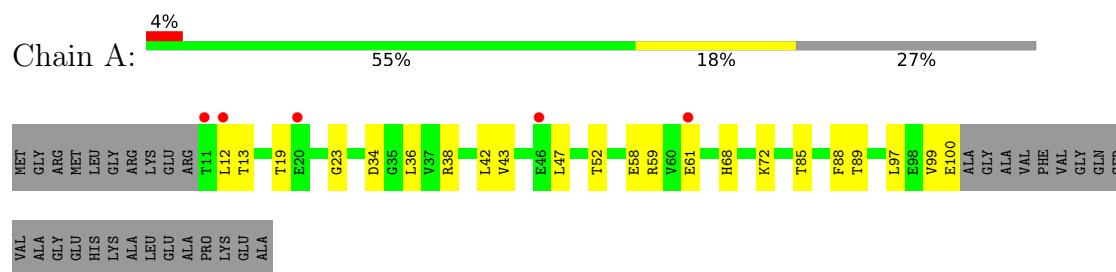
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	R	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	S	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	T	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	U	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	V	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	W	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	X	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	Y	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	Z	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	1	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	2	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	3	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	4	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	5	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	6	90	Total 677	C 421	N 121	O 134	S 1	0	0	0

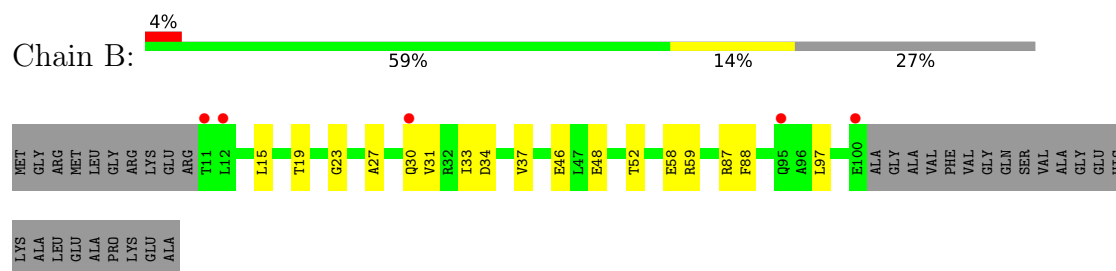
3 Residue-property plots [i](#)

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.

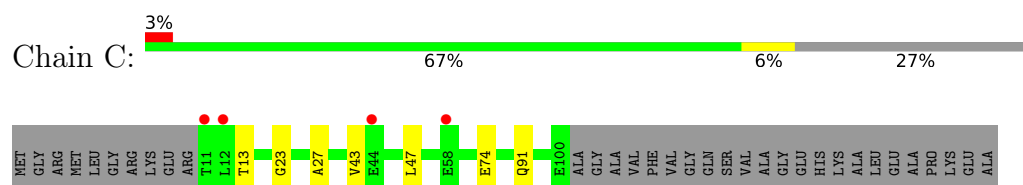
- Molecule 1: bactofilin



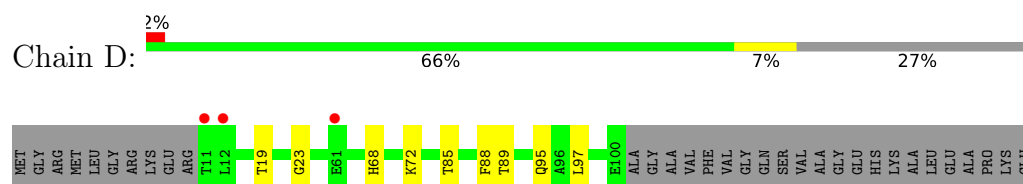
- Molecule 1: bactofilin



- Molecule 1: bactofilin

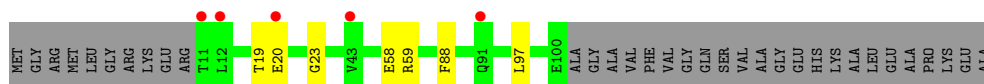


- Molecule 1: bactofilin

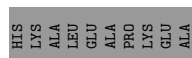
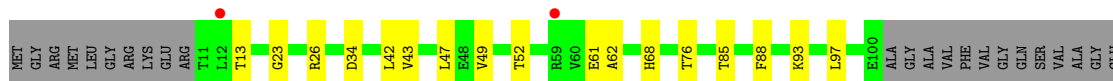


- Molecule 1: bactofilin

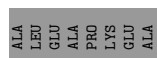




● Molecule 1: bactofilin



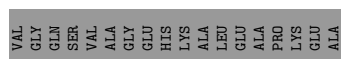
● Molecule 1: bactofilin



● Molecule 1: bactofilin



● Molecule 1: bactofilin



● Molecule 1: bactofilin



GLU
ALA
PRO
LYS
GLU
ALA

● Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13
T19 G23 R26 R27 K28 I33 D34 V37 L42 V43 E44 L47 T52 G53 R54 E58 R59 R63 R68 G69 E70 A77 T85 F88 A94 L97 E100
ALA GLY ALA

VAL PHE VAL GLY MET LEU GLN SER VAL ALA GLU HIS GLU ARG LYS GLU

● Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13 L14 L15 D18 T19 E20 V21 L22 G23 D24 D34 G35 L36 V37 R38 L42 T52 E56 G57 E58 R59 V60 E61 K72 R87 F88 T89 L92 L97 E100
ALA GLY ALA VAL PHE VAL GLY GLN

SER VAL ALA GLY MET LEU GLY HIS LYS ALA LEU GLU ARG LYS GLU ALA

● Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13 T19 G23 R26 D34 G39 T52 E58 R59 A62 R63 H68 K72 A73 E74 L75 T76 A77 T85 T89 K93 A94 L97 E100
ALA GLY ALA VAL PHE VAL GLY SER

VAL ALA GLY MET LEU GLY HIS LYS ALA LEU GLU ARG LYS GLU ALA

● Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13 L14 L15 T19 E20 V21 L22 G23 D34 G35 R38 T52 G53 R54 V55 E56 G57 H68 G69 E70 V71 K72 A73 E74 T85 A86 R87 F88 T89 L97 E100
ALA GLY ALA VAL PHE VAL GLY SER

VAL ALA GLY MET LEU GLY HIS LYS ALA LEU GLU ARG LYS GLU ALA

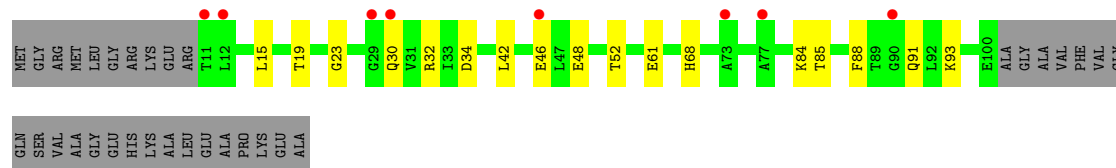
● Molecule 1: bactofilin



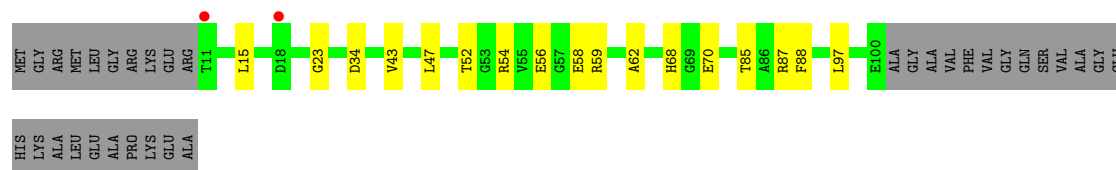
MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13 L14 G23 A27 R32 I33 D34 G45 T52 A62 L66 L67 H68 T76 A77 V81 T85 A86 R87 K93 A94 Q95 A96 L97 E98 V99 E100
ALA GLY ALA VAL PHE VAL GLY GLN SER VAL

ALA GLY GLU HIS LYS ALA LEU GLU ALA PRO LYS GLU ALA

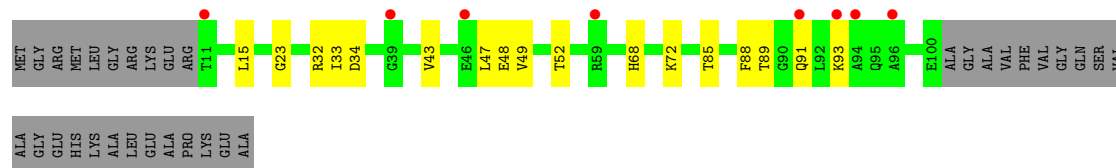
● Molecule 1: bactofilin



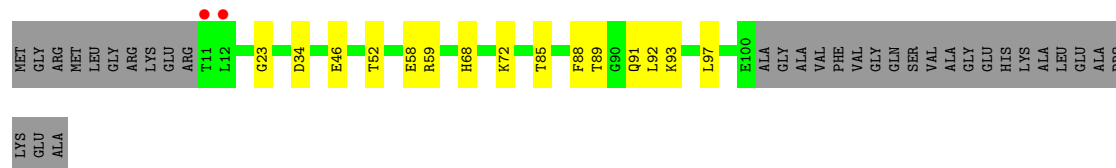
● Molecule 1: bactofilin



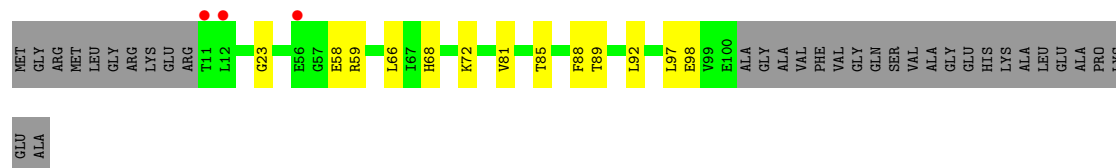
● Molecule 1: bactofilin



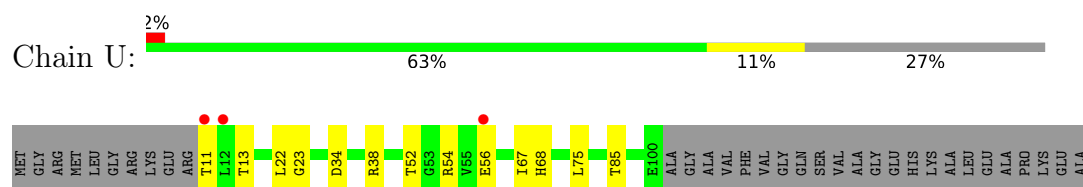
● Molecule 1: bactofilin



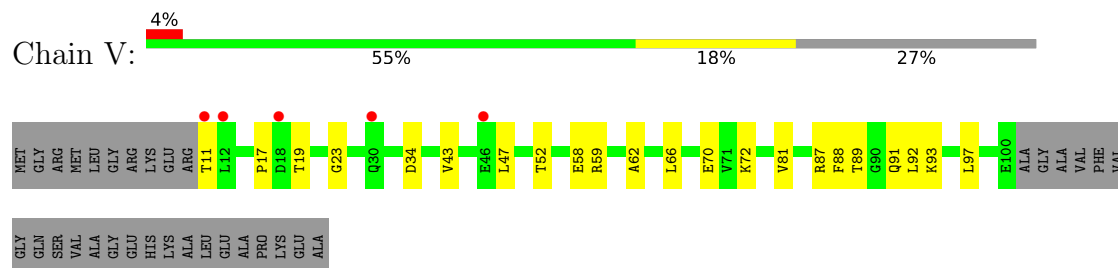
● Molecule 1: bactofilin



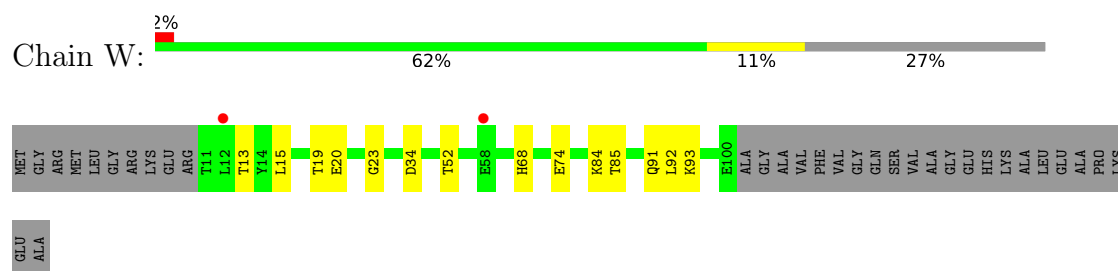
● Molecule 1: bactofilin



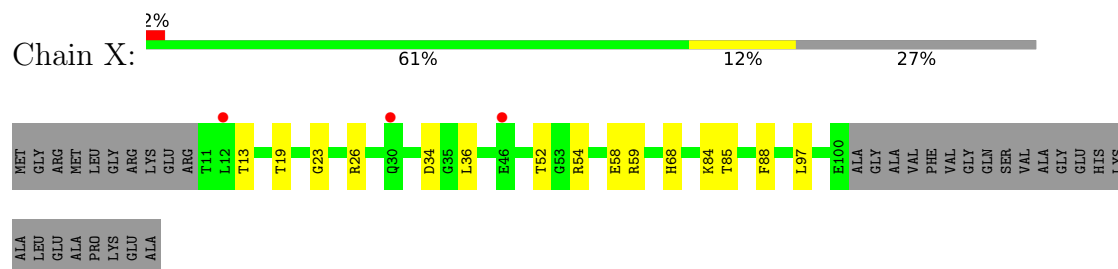
- Molecule 1: bactofilin



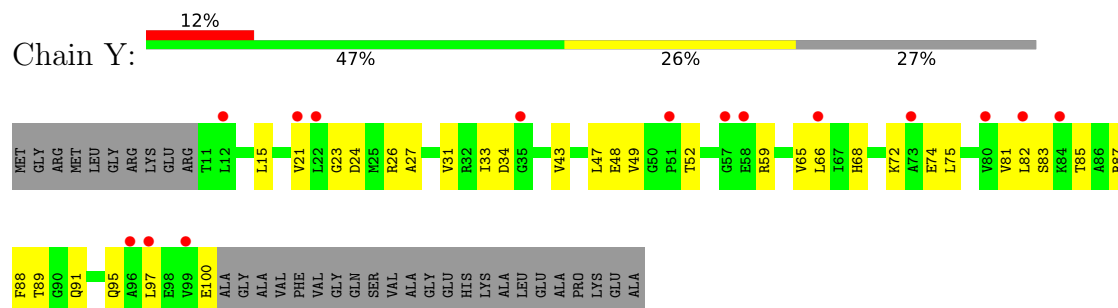
- Molecule 1: bactofilin



- Molecule 1: bactofilin

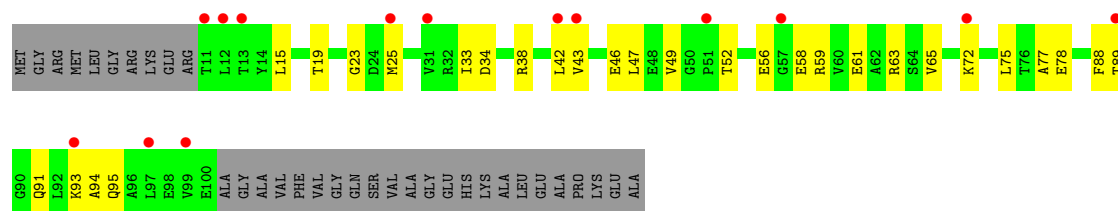


- Molecule 1: bactofilin

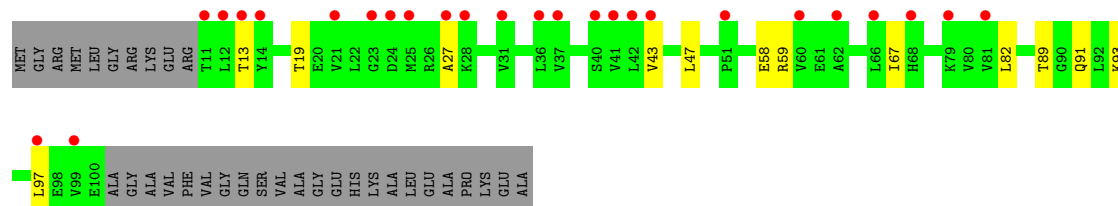


- Molecule 1: bactofilin

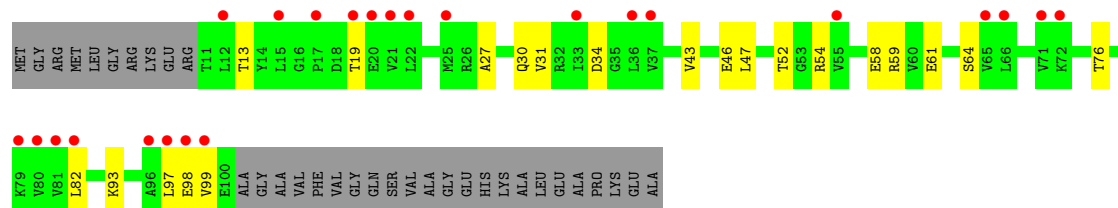




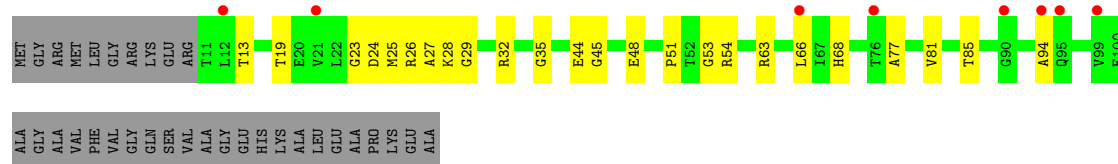
• Molecule 1: bactofilin



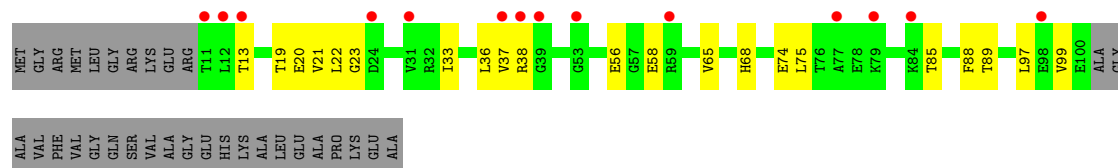
• Molecule 1: bactofilin



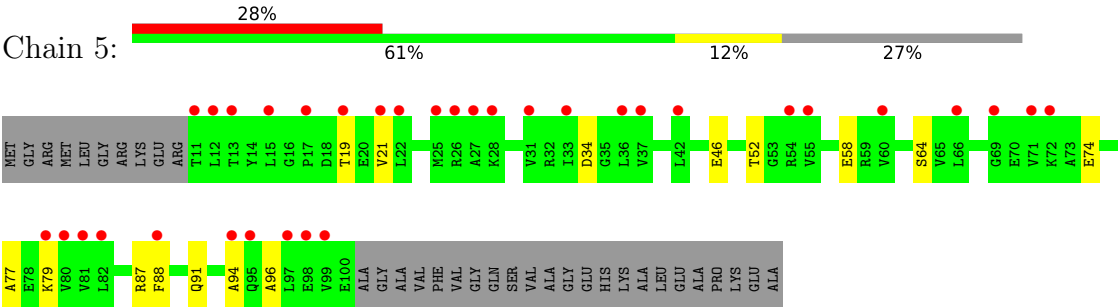
• Molecule 1: bactofilin



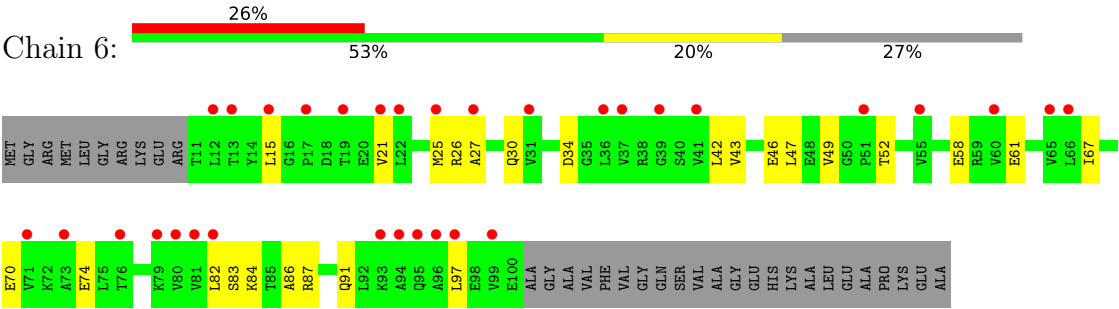
• Molecule 1: bactofilin



• Molecule 1: bactofilin



• Molecule 1: bactofilin



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	191.87Å 244.90Å 505.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.50 49.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.89-3.50) 99.0 (49.89-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.283 , 0.307 (Not available) , 0.274	Depositor DCC
R_{free} test set	7389 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	1.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21663	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

5.1 Standard geometry

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	1	0.11	0/681	0.38	0/917
1	2	0.12	0/681	0.38	0/917
1	3	0.12	0/681	0.40	0/917
1	4	0.18	0/681	0.42	0/917
1	5	0.12	0/681	0.40	0/917
1	6	0.13	0/681	0.43	0/917
1	A	0.12	0/680	0.39	0/915
1	B	0.13	0/681	0.39	0/917
1	C	0.14	0/681	0.43	0/917
1	D	0.14	0/681	0.43	0/917
1	E	0.13	0/681	0.36	0/917
1	F	0.14	0/681	0.43	0/917
1	G	0.15	0/681	0.47	0/917
1	H	0.12	0/681	0.40	0/917
1	I	0.16	0/681	0.44	0/917
1	J	0.19	0/681	0.44	0/917
1	K	0.14	0/681	0.40	0/917
1	L	0.13	0/681	0.41	0/917
1	M	0.13	0/681	0.38	0/917
1	N	0.12	0/681	0.38	0/917
1	O	0.13	0/681	0.40	0/917
1	P	0.13	0/681	0.40	0/917
1	Q	0.12	0/681	0.38	0/917
1	R	0.13	0/681	0.41	0/917
1	S	0.12	0/681	0.36	0/917
1	T	0.11	0/681	0.39	0/917
1	U	0.15	0/681	0.42	0/917
1	V	0.13	0/681	0.41	0/917
1	W	0.14	0/681	0.45	0/917
1	X	0.13	0/681	0.44	0/917
1	Y	0.13	0/681	0.40	0/917
1	Z	0.12	0/681	0.37	0/917
All	All	0.14	0/21791	0.41	0/29342

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	677	0	703	11	0
1	2	677	0	703	17	0
1	3	677	0	703	17	2
1	4	677	0	703	18	0
1	5	677	0	703	11	0
1	6	677	0	703	16	0
1	A	676	0	702	15	0
1	B	677	0	703	14	0
1	C	677	0	703	5	0
1	D	677	0	703	8	0
1	E	677	0	703	5	2
1	F	677	0	703	13	0
1	G	677	0	703	12	0
1	H	677	0	703	9	0
1	I	677	0	703	18	0
1	J	677	0	703	11	0
1	K	677	0	703	17	0
1	L	677	0	703	17	0
1	M	677	0	703	13	0
1	N	677	0	703	12	0
1	O	677	0	703	10	0
1	P	677	0	703	11	0
1	Q	677	0	703	13	0
1	R	677	0	703	12	0
1	S	677	0	703	12	0
1	T	677	0	703	9	0
1	U	677	0	703	10	0
1	V	677	0	703	19	0
1	W	677	0	703	13	0
1	X	677	0	703	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	677	0	703	23	0
1	Z	677	0	703	21	0
All	All	21663	0	22495	328	2

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 7.

The worst 5 of 328 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:R:91:GLN:HE22	1:R:93:LYS:HG3	1.35	0.90
1:2:46:GLU:HG3	1:2:64:SER:HB2	1.65	0.79
1:V:91:GLN:HE22	1:V:93:LYS:HG3	1.46	0.79
1:J:68:HIS:O	1:J:85:THR:OG1	2.05	0.75
1:K:23:GLY:HA3	1:L:23:GLY:HA3	1.69	0.74

All (2) 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)
1:E:20:GLU:OE2	1:3:26:ARG:NH1[7_656]	1.37	0.83
1:E:20:GLU:CD	1:3:26:ARG:NH1[7_656]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	1	72/94 (77%)	72 (100%)	0	100	100
1	2	72/94 (77%)	72 (100%)	0	100	100
1	3	60/94 (64%)	60 (100%)	0	100	100
1	4	44/94 (47%)	44 (100%)	0	100	100
1	5	67/94 (71%)	67 (100%)	0	100	100
1	6	72/94 (77%)	72 (100%)	0	100	100
1	A	71/94 (76%)	71 (100%)	0	100	100
1	B	72/94 (77%)	72 (100%)	0	100	100
1	C	72/94 (77%)	72 (100%)	0	100	100
1	D	72/94 (77%)	72 (100%)	0	100	100
1	E	72/94 (77%)	72 (100%)	0	100	100
1	F	72/94 (77%)	72 (100%)	0	100	100
1	G	72/94 (77%)	72 (100%)	0	100	100
1	H	72/94 (77%)	72 (100%)	0	100	100
1	I	72/94 (77%)	72 (100%)	0	100	100
1	J	72/94 (77%)	72 (100%)	0	100	100
1	K	72/94 (77%)	72 (100%)	0	100	100
1	L	72/94 (77%)	72 (100%)	0	100	100
1	M	72/94 (77%)	72 (100%)	0	100	100
1	N	72/94 (77%)	72 (100%)	0	100	100
1	O	72/94 (77%)	72 (100%)	0	100	100
1	P	72/94 (77%)	72 (100%)	0	100	100
1	Q	72/94 (77%)	72 (100%)	0	100	100
1	R	72/94 (77%)	72 (100%)	0	100	100
1	S	72/94 (77%)	72 (100%)	0	100	100
1	T	72/94 (77%)	72 (100%)	0	100	100
1	U	72/94 (77%)	72 (100%)	0	100	100
1	V	72/94 (77%)	72 (100%)	0	100	100
1	W	72/94 (77%)	72 (100%)	0	100	100
1	X	72/94 (77%)	72 (100%)	0	100	100
1	Y	72/94 (77%)	72 (100%)	0	100	100
1	Z	72/94 (77%)	72 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2258/3008 (75%)	2258 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	N	91	GLN
1	R	91	GLN
1	V	91	GLN

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](#)

There are no ligands in this entry.

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 ⓘ

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, 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	1	90/123 (73%)	1.58	26 (28%)	1 1	146, 167, 182, 193	0
1	2	90/123 (73%)	1.56	24 (26%)	1 2	161, 184, 197, 204	0
1	3	90/123 (73%)	0.93	8 (8%)	15 10	131, 151, 164, 170	0
1	4	90/123 (73%)	1.08	14 (15%)	5 5	127, 141, 157, 186	0
1	5	90/123 (73%)	1.84	34 (37%)	1 1	179, 194, 206, 222	0
1	6	90/123 (73%)	1.71	32 (35%)	1 1	183, 202, 215, 223	0
1	A	90/123 (73%)	0.55	5 (5%)	30 17	66, 90, 115, 140	0
1	B	90/123 (73%)	0.60	5 (5%)	30 17	69, 100, 122, 156	0
1	C	90/123 (73%)	0.54	4 (4%)	39 21	59, 86, 114, 165	0
1	D	90/123 (73%)	0.61	3 (3%)	49 28	52, 84, 116, 147	0
1	E	90/123 (73%)	0.51	5 (5%)	30 17	59, 90, 119, 131	0
1	F	90/123 (73%)	0.64	2 (2%)	62 37	64, 89, 119, 131	0
1	G	90/123 (73%)	0.57	2 (2%)	62 37	58, 84, 107, 140	0
1	H	90/123 (73%)	0.54	2 (2%)	62 37	65, 89, 110, 155	0
1	I	90/123 (73%)	0.63	4 (4%)	39 21	54, 75, 109, 119	0
1	J	90/123 (73%)	0.59	6 (6%)	24 15	57, 83, 109, 119	0
1	K	90/123 (73%)	0.68	3 (3%)	49 28	60, 90, 117, 149	0
1	L	90/123 (73%)	0.79	4 (4%)	39 21	66, 94, 120, 131	0
1	M	90/123 (73%)	0.95	7 (7%)	19 12	86, 110, 137, 141	0
1	N	90/123 (73%)	0.97	9 (10%)	12 8	74, 106, 135, 149	0
1	O	90/123 (73%)	1.13	9 (10%)	12 8	99, 124, 145, 155	0
1	P	90/123 (73%)	1.08	8 (8%)	15 10	89, 121, 142, 158	0
1	Q	90/123 (73%)	0.73	2 (2%)	62 37	56, 102, 126, 154	0
1	R	90/123 (73%)	1.04	8 (8%)	15 10	92, 118, 140, 151	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	S	90/123 (73%)	0.56	2 (2%) 62 37	58, 85, 116, 151	0
1	T	90/123 (73%)	0.56	3 (3%) 49 28	65, 97, 120, 143	0
1	U	90/123 (73%)	0.57	3 (3%) 49 28	54, 76, 108, 119	0
1	V	90/123 (73%)	0.58	5 (5%) 30 17	56, 81, 111, 131	0
1	W	90/123 (73%)	0.51	2 (2%) 62 37	54, 80, 106, 122	0
1	X	90/123 (73%)	0.71	3 (3%) 49 28	58, 84, 110, 122	0
1	Y	90/123 (73%)	1.26	15 (16%) 4 4	119, 148, 165, 175	0
1	Z	90/123 (73%)	1.26	14 (15%) 5 5	127, 153, 167, 172	0
All	All	2880/3936 (73%)	0.87	273 (9%) 14 9	52, 103, 193, 223	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	6	97	LEU	6.4
1	V	11	THR	6.1
1	6	12	LEU	6.1
1	5	37	VAL	5.5
1	1	12	LEU	5.5

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.