wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 01:50 AM EDT

PDB ID	:	6RIA
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 (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 (i)) were used in the production of this report:

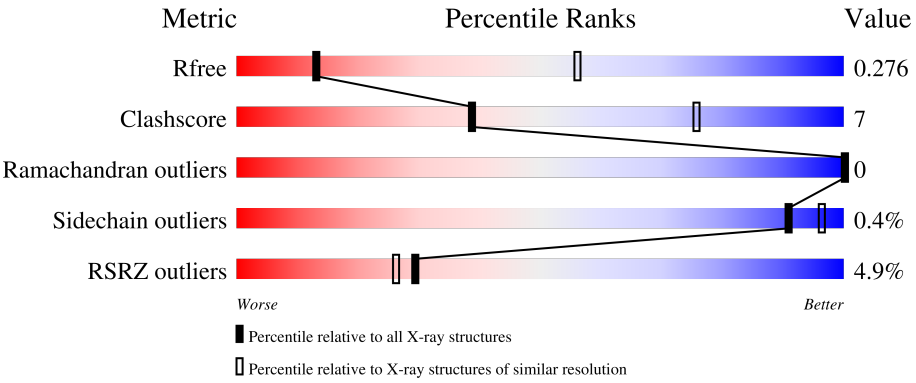
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	11% 63% 11% 27%
1	2	123	17% 56% 17% 27%
1	3	123	8% 54% 19% 27%
1	4	123	6% 56% 17% 27%
1	5	123	28% 61% 12% 27%

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Mol	Chain	Length	Quality of chain
1	6	123	28% 54% 18% 27%
1	A	123	55% 18% 27%
1	B	123	58% 15% 27%
1	C	123	63% 10% 27%
1	D	123	66% 7% 27%
1	E	123	67% 6% 27%
1	F	123	59% 14% 27%
1	G	123	59% 14% 27%
1	H	123	% 62% 11% 27%
1	I	123	55% 18% 27%
1	J	123	63% 11% 27%
1	K	123	54% 19% 27%
1	L	123	55% 18% 27%
1	M	123	% 60% 12% 27%
1	N	123	60% 12% 27%
1	O	123	% 61% 12% 27%
1	P	123	% 59% 13% 27%
1	Q	123	59% 14% 27%
1	R	123	% 59% 14% 27%
1	S	123	61% 12% 27%
1	T	123	% 63% 11% 27%
1	U	123	63% 11% 27%
1	V	123	% 55% 18% 27%
1	W	123	62% 11% 27%
1	X	123	61% 12% 27%

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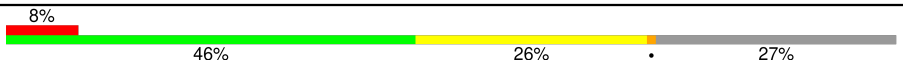
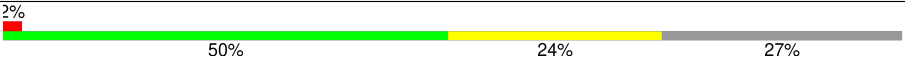
Mol	Chain	Length	Quality of chain
1	Y	123	
1	Z	123	

2 Entry composition (i)

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			

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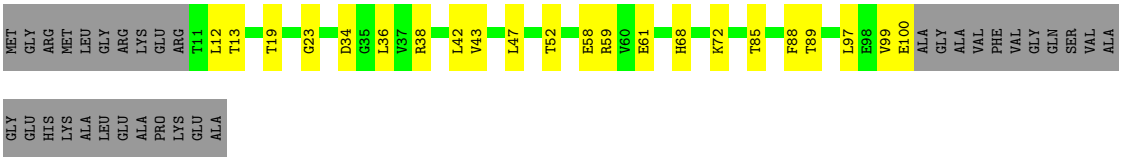
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	R	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	S	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	T	90	Total	C	N	O	S	0	0	0
			677	421	121	134	1			
1	U	90	Total	C	N	O	S	0	0	0
			677	421	121	134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

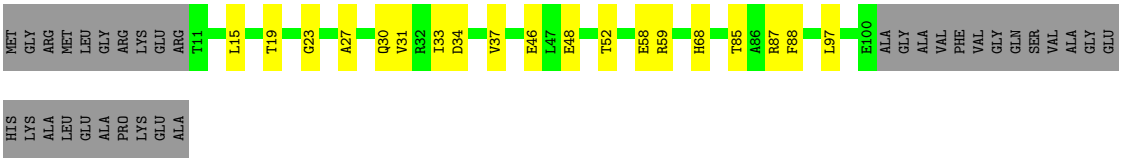
- Molecule 1: bactofilin

Chain A:



- Molecule 1: bactofilin

Chain B:

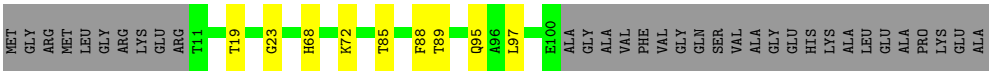


- Molecule 1: bactofilin

Chain C:

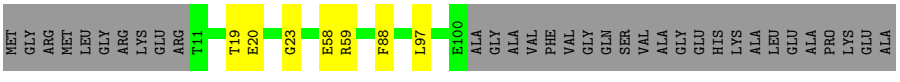
- Molecule 1: bactofilin

Chain D:



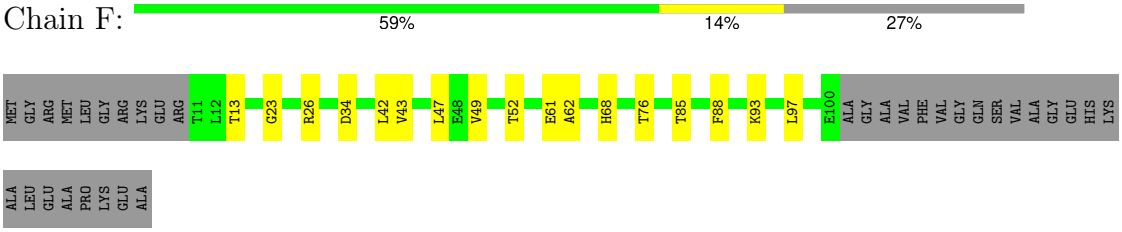
- Molecule 1: bactofilin

Chain E:



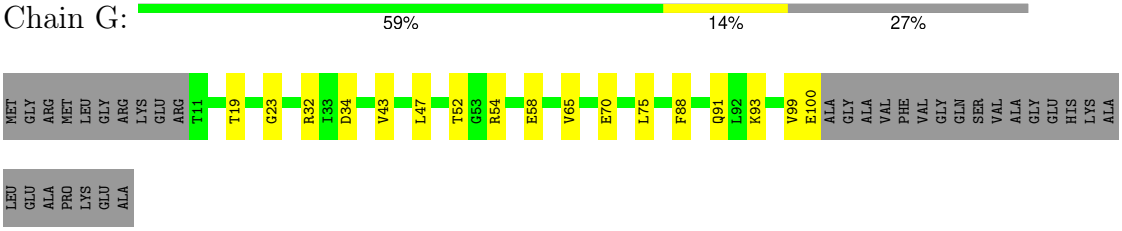
• Molecule 1: bactofilin

Chain F:



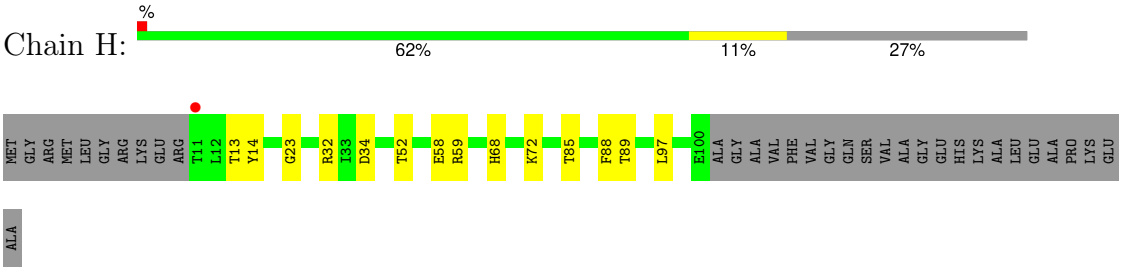
• Molecule 1: bactofilin

Chain G:



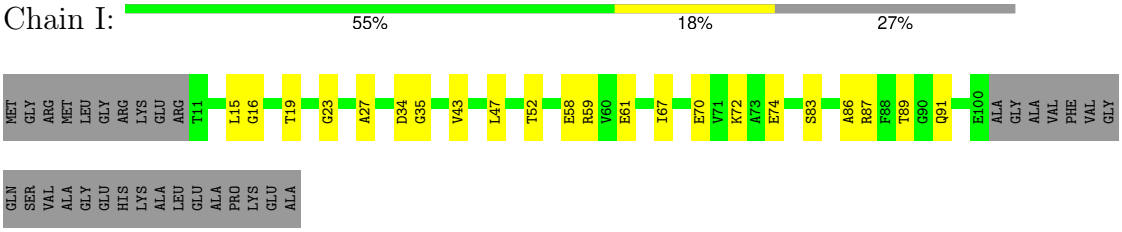
• Molecule 1: bactofilin

Chain H:



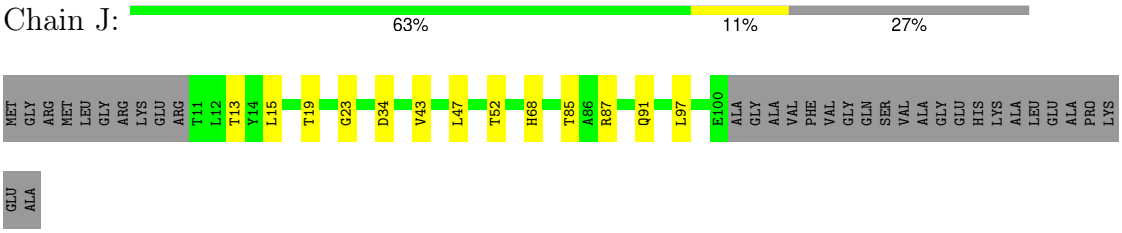
• Molecule 1: bactofilin

Chain I:



• Molecule 1: bactofilin

Chain J:

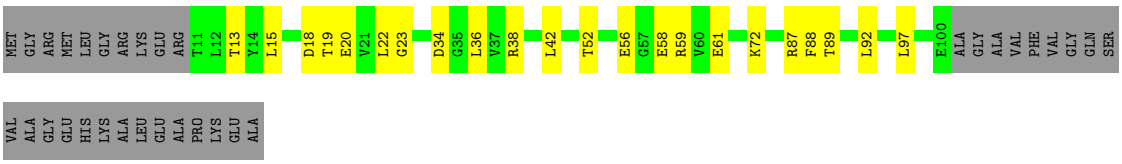


• Molecule 1: bactofilin

Chain K:

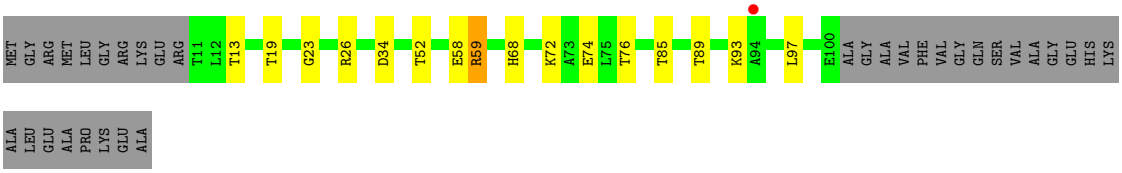
• Molecule 1: bactofilin

Chain L:



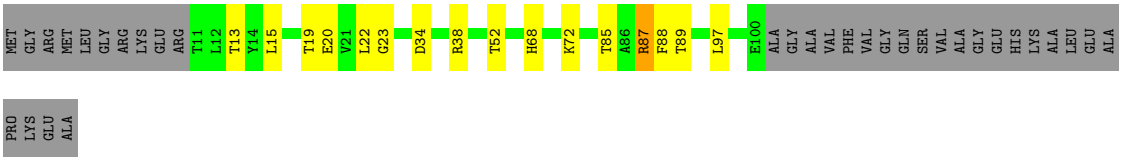
• Molecule 1: bactofilin

Chain M:



• Molecule 1: bactofilin

Chain N:

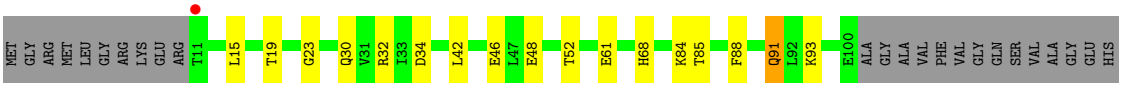


• Molecule 1: bactofilin

Chain O:

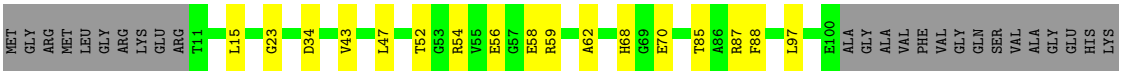
• Molecule 1: bactofilin

Chain P:



• Molecule 1: bactofilin

Chain Q:

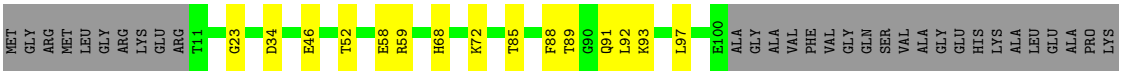


• Molecule 1: bactofilin

Chain R:

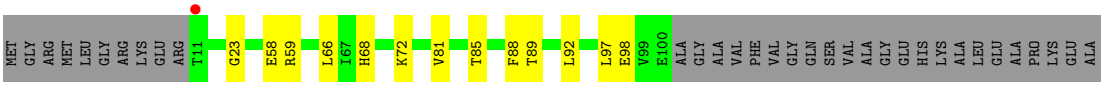
• Molecule 1: bactofilin

Chain S:



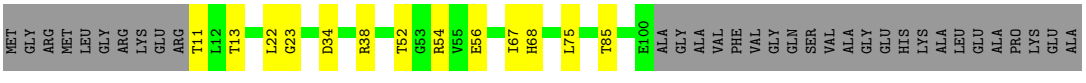
• Molecule 1: bactofilin

Chain T:



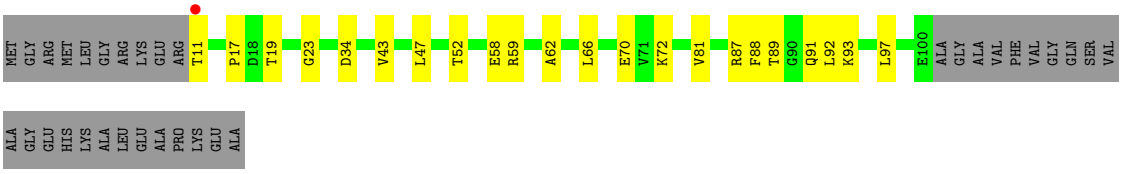
• Molecule 1: bactofilin

Chain U:



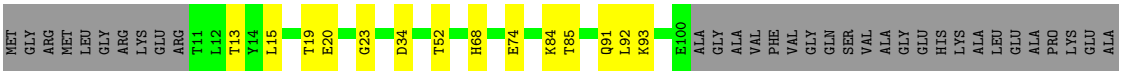
• Molecule 1: bactofilin

Chain V:



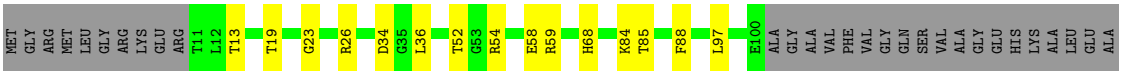
• Molecule 1: bactofilin

Chain W:



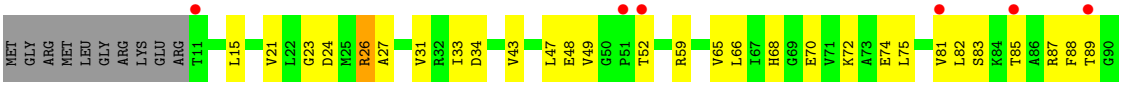
• Molecule 1: bactofilin

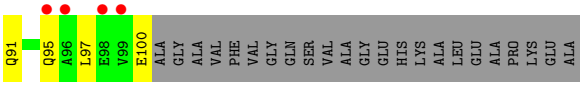
Chain X:



• Molecule 1: bactofilin

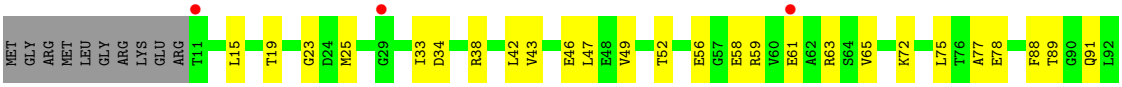
Chain Y:

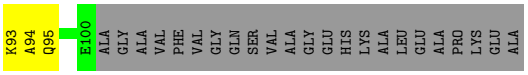




• Molecule 1: bactofilin

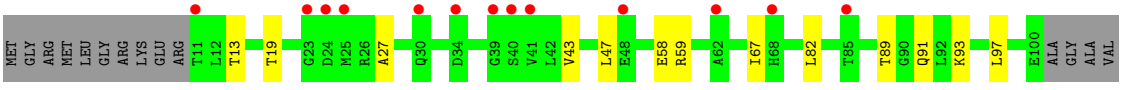
Chain Z:





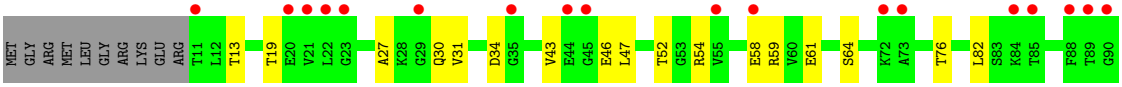
• Molecule 1: bactofilin

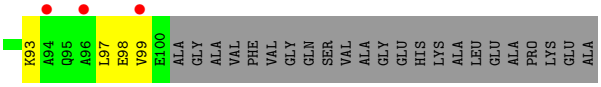
Chain 1:



• Molecule 1: bactofilin

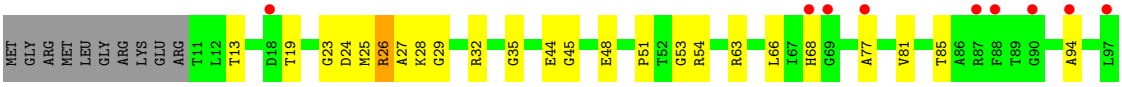
Chain 2:

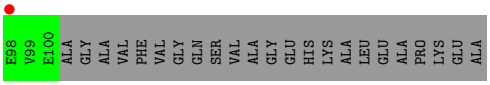




• Molecule 1: bactofilin

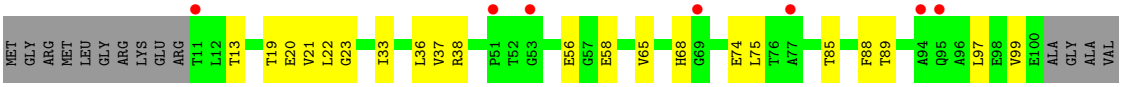
Chain 3:





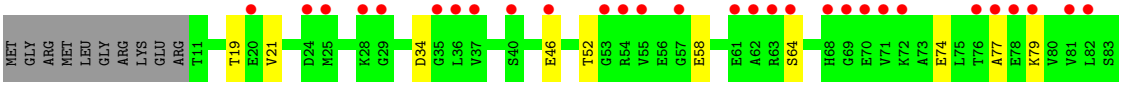
• Molecule 1: bactofilin

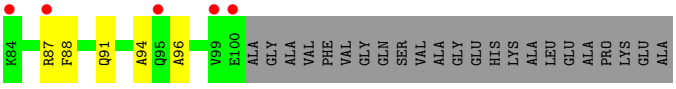
Chain 4:



• Molecule 1: bactofilin

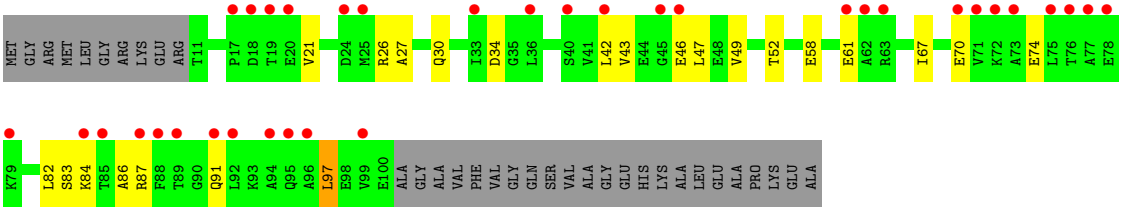
Chain 5:





• Molecule 1: bactofilin

Chain 6:


MET GLY ARG MET LEU GLY ARG LYS GLU ARG T11 P17 D18 T19 E20 V21 D24 M25 R26 A27 Q30 I33 D34 G35 L36 S40 V41 L42 V43 E44 G45 E46 L47 E48 V49 T52 E58 E61 A62 R63 I67 E70 V71 K72 A73 E74 L75 T76 A77 E78
K79 L82 S83 K84 T85 A86 R87 F88 T89 G90 Q91 L92 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

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.46 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.283 , 0.307 0.279 , 0.276	Depositor DCC
R_{free} test set	7389 reflections (5.00%)	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)	0.30 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	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.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.24	0/681	0.52	0/917
1	2	0.24	0/681	0.53	0/917
1	3	0.24	0/681	0.54	0/917
1	4	0.30	0/681	0.56	0/917
1	5	0.24	0/681	0.54	0/917
1	6	0.25	0/681	0.55	0/917
1	A	0.25	0/680	0.52	0/915
1	B	0.25	0/681	0.54	0/917
1	C	0.26	0/681	0.55	0/917
1	D	0.26	0/681	0.56	0/917
1	E	0.26	0/681	0.53	0/917
1	F	0.27	0/681	0.58	0/917
1	G	0.26	0/681	0.57	0/917
1	H	0.25	0/681	0.53	0/917
1	I	0.28	0/681	0.56	0/917
1	J	0.32	0/681	0.58	0/917
1	K	0.26	0/681	0.55	0/917
1	L	0.26	0/681	0.54	0/917
1	M	0.25	0/681	0.53	0/917
1	N	0.25	0/681	0.53	0/917
1	O	0.25	0/681	0.54	0/917
1	P	0.24	0/681	0.56	0/917
1	Q	0.25	0/681	0.53	0/917
1	R	0.25	0/681	0.55	0/917
1	S	0.26	0/681	0.52	0/917
1	T	0.25	0/681	0.54	0/917
1	U	0.27	0/681	0.56	0/917
1	V	0.26	0/681	0.55	0/917
1	W	0.27	0/681	0.57	0/917
1	X	0.26	0/681	0.56	0/917
1	Y	0.26	0/681	0.54	0/917
1	Z	0.24	0/681	0.54	0/917
All	All	0.26	0/21791	0.55	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 (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	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	15	0
1	A	676	0	702	15	0
1	B	677	0	703	15	0
1	C	677	0	703	7	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	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	677	0	703	24	0
1	Z	677	0	703	21	0
All	All	21663	0	22495	330	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 330 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)

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	1	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	2	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	3	88/123 (72%)	83 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	5	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	6	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	A	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	B	88/123 (72%)	83 (94%)	5 (6%)	0	100	100
1	C	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	D	88/123 (72%)	83 (94%)	5 (6%)	0	100	100
1	E	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	F	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	G	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	H	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	I	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	J	88/123 (72%)	83 (94%)	5 (6%)	0	100	100
1	K	88/123 (72%)	79 (90%)	9 (10%)	0	100	100
1	L	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	M	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	N	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	O	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	P	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	Q	88/123 (72%)	80 (91%)	8 (9%)	0	100	100
1	R	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	S	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	T	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	U	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
1	V	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	W	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	X	88/123 (72%)	81 (92%)	7 (8%)	0	100	100
1	Y	88/123 (72%)	83 (94%)	5 (6%)	0	100	100
1	Z	88/123 (72%)	82 (93%)	6 (7%)	0	100	100
All	All	2816/3936 (72%)	2606 (92%)	210 (8%)	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	1	72/94 (77%)	72 (100%)	0	100 100
1	2	72/94 (77%)	72 (100%)	0	100 100
1	3	72/94 (77%)	71 (99%)	1 (1%)	67 85
1	4	72/94 (77%)	72 (100%)	0	100 100
1	5	72/94 (77%)	72 (100%)	0	100 100
1	6	72/94 (77%)	71 (99%)	1 (1%)	67 85
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%)	71 (99%)	1 (1%)	67 85
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%)	71 (99%)	1 (1%)	67 85
1	J	72/94 (77%)	71 (99%)	1 (1%)	67 85
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%)	71 (99%)	1 (1%)	67 85
1	N	72/94 (77%)	71 (99%)	1 (1%)	67 85
1	O	72/94 (77%)	72 (100%)	0	100 100
1	P	72/94 (77%)	71 (99%)	1 (1%)	67 85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	71 (99%)	1 (1%)	67 85
1	Z	72/94 (77%)	72 (100%)	0	100 100
All	All	2303/3008 (77%)	2294 (100%)	9 (0%)	91 96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	26	ARG
1	6	97	LEU
1	M	59	ARG
1	N	87	ARG
1	P	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
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 monosaccharides 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, 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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	90/123 (73%)	1.33	13 (14%) 2 3	146, 167, 182, 193	0
1	2	90/123 (73%)	1.33	21 (23%) 0 0	161, 184, 197, 204	0
1	3	90/123 (73%)	1.03	10 (11%) 5 6	131, 151, 164, 170	0
1	4	90/123 (73%)	0.86	7 (7%) 13 13	127, 141, 157, 186	0
1	5	90/123 (73%)	1.79	34 (37%) 0 0	179, 194, 206, 222	0
1	6	90/123 (73%)	1.80	35 (38%) 0 0	183, 202, 215, 223	0
1	A	90/123 (73%)	0.14	0 100 100	66, 90, 115, 140	0
1	B	90/123 (73%)	0.15	0 100 100	69, 100, 122, 156	0
1	C	90/123 (73%)	0.08	0 100 100	59, 86, 114, 165	0
1	D	90/123 (73%)	0.19	0 100 100	52, 84, 116, 147	0
1	E	90/123 (73%)	0.18	0 100 100	59, 90, 119, 131	0
1	F	90/123 (73%)	0.18	0 100 100	64, 89, 119, 131	0
1	G	90/123 (73%)	0.23	0 100 100	58, 84, 107, 140	0
1	H	90/123 (73%)	0.19	1 (1%) 80 75	65, 89, 110, 155	0
1	I	90/123 (73%)	0.11	0 100 100	54, 75, 109, 119	0
1	J	90/123 (73%)	0.19	0 100 100	57, 83, 109, 119	0
1	K	90/123 (73%)	0.21	0 100 100	60, 90, 117, 149	0
1	L	90/123 (73%)	0.29	0 100 100	66, 94, 120, 131	0
1	M	90/123 (73%)	0.43	1 (1%) 80 75	86, 110, 137, 141	0
1	N	90/123 (73%)	0.24	0 100 100	74, 106, 135, 149	0
1	O	90/123 (73%)	0.49	1 (1%) 80 75	99, 124, 145, 155	0
1	P	90/123 (73%)	0.48	1 (1%) 80 75	89, 121, 142, 158	0
1	Q	90/123 (73%)	0.17	0 100 100	56, 102, 126, 154	0
1	R	90/123 (73%)	0.27	1 (1%) 80 75	92, 118, 140, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	S	90/123 (73%)	0.21	0 100 100	58, 85, 116, 151	0
1	T	90/123 (73%)	0.27	1 (1%) 80 75	65, 97, 120, 143	0
1	U	90/123 (73%)	0.16	0 100 100	54, 76, 108, 119	0
1	V	90/123 (73%)	0.11	1 (1%) 80 75	56, 81, 111, 131	0
1	W	90/123 (73%)	0.17	0 100 100	54, 80, 106, 122	0
1	X	90/123 (73%)	0.09	0 100 100	58, 84, 110, 122	0
1	Y	90/123 (73%)	0.88	10 (11%) 5 6	119, 148, 165, 175	0
1	Z	90/123 (73%)	0.76	3 (3%) 46 41	127, 153, 167, 172	0
All	All	2880/3936 (73%)	0.47	140 (4%) 29 26	52, 103, 193, 223	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	24	ASP	6.8
1	6	95	GLN	5.3
1	R	11	THR	4.7
1	Y	11	THR	4.6
1	1	40	SER	4.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.