



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:21 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 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

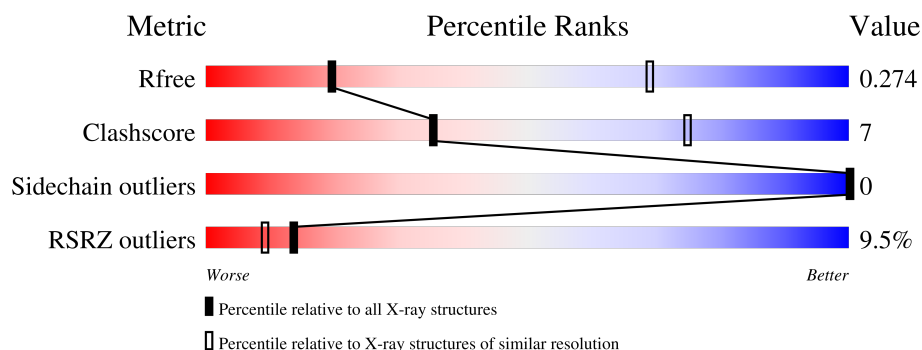
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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%

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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%

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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			

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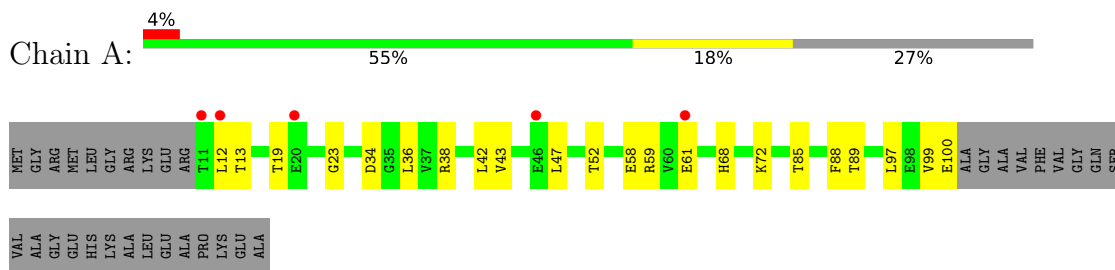
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	R	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	S	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	T	90	Total 677	C 421	N 121	O 134	S 1	0	0	0
1	U	90	Total 677	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

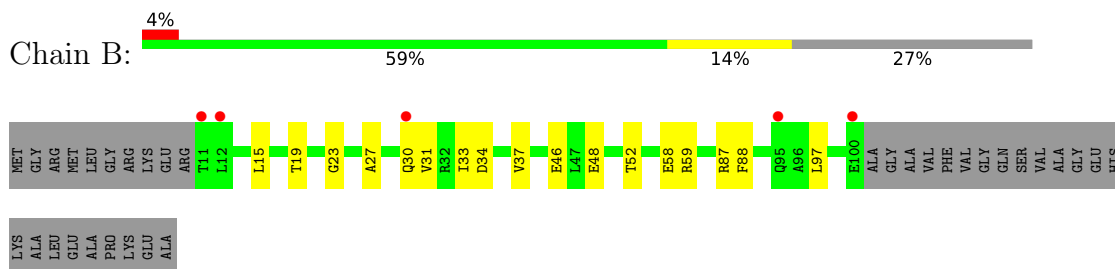
3 Residue-property plots [i](#)

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.

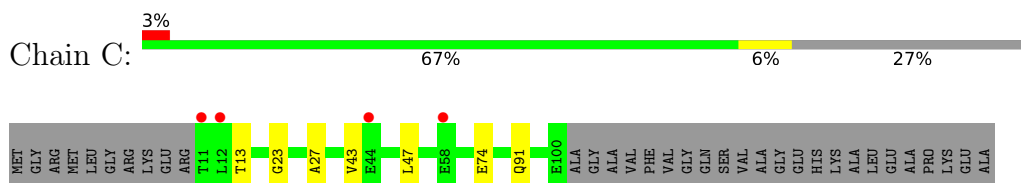
- Molecule 1: bactofilin



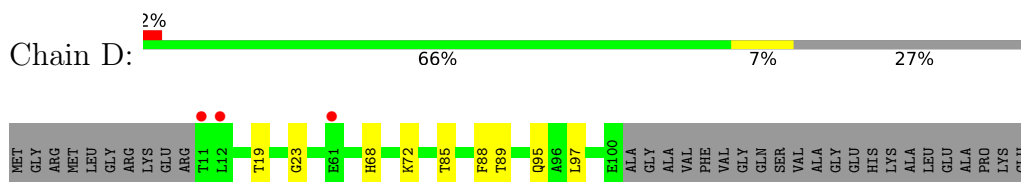
- Molecule 1: bactofilin



- Molecule 1: bactofilin

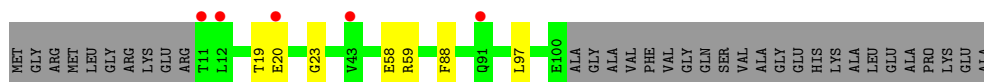


- Molecule 1: bactofilin

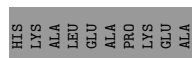


- Molecule 1: bactofilin

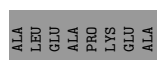




• Molecule 1: bactofilin



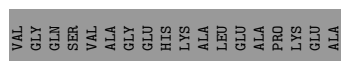
• Molecule 1: bactofilin



• 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 R28
I33 D34 V37
L42 V43 E44
L47 T52 G53 R54
E58 R59 R63
H68 G69 E70
A77 T85 F88
A94 L97
E100
ALA GLY GLN ALA

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

• Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13
T14 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 VAL PHE
VAL GLY GLN SER

SER VAL ALA GLY HIS LYS ALA LEU GLU ARG
T11 L12 L13
T14 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 VAL PHE
VAL GLY GLN SER

• 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 VAL PHE
VAL GLY GLN SER

VAL ALA GLY HIS LYS ALA LEU GLU ARG
T11 L12 L13
T14 L15
D18 T19 E20
V21 L22 G23
D24 D34 G35
L36 V37 R38
L42 T52 E56
G57 E58
R59 A62
R63 H68
K72 A73
E74 L75
T76 A77
T85 T89
K93 A94
L97
E100
ALA GLY VAL PHE
VAL GLY GLN SER

• Molecule 1: bactofilin



MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13
T14 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 VAL PHE
VAL GLY GLN SER

VAL ALA GLY HIS LYS ALA LEU GLU ARG
T11 L12 L13
T14 L15
D18 T19 E20
V21 L22 G23
D24 D34 G35
L36 V37 R38
L42 T52 E56
G57 E58
R59 A62
R63 H68
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E74 L75
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K93 A94
L97
E100
ALA GLY VAL PHE
VAL GLY GLN SER

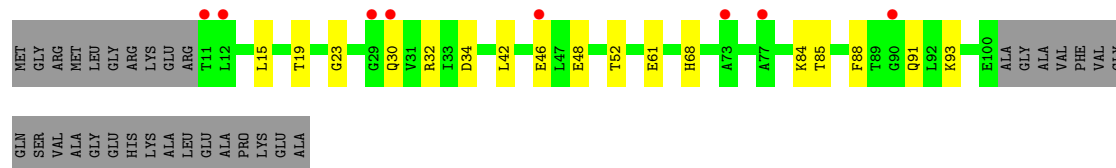
• Molecule 1: bactofilin



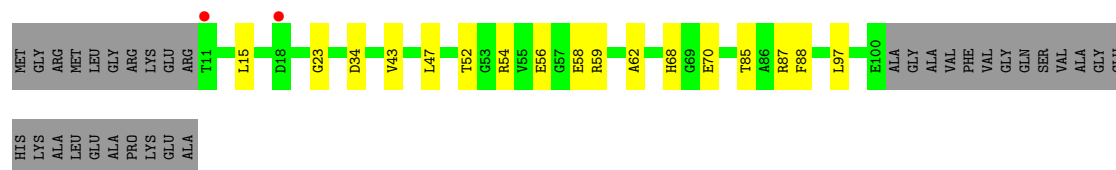
MET GLY ARG MET LEU GLY ARG LYS GLU ARG
T11 L12 L13
T14 L15
G23 A27
R32 I33
D34 G45
T52 A62
L66 I67
H68 T76
A77 V81
T85 A86
R87 K93
A94 Q95
A96 L97
E98 V99
E100
ALA GLY VAL PHE
VAL GLY GLN SER
VAL

ALA GLY GLU HIS LYS ALA LEU GLU ARG
T11 L12 L13
T14 L15
D18 T19 E20
V21 L22 G23
D24 D34 G35
L36 V37 R38
L42 T52 E56
G57 E58
R59 A62
R63 H68
K72 A73
E74 L75
T76 A77
T85 T89
K93 A94
L97
E100
ALA GLY VAL PHE
VAL GLY GLN SER

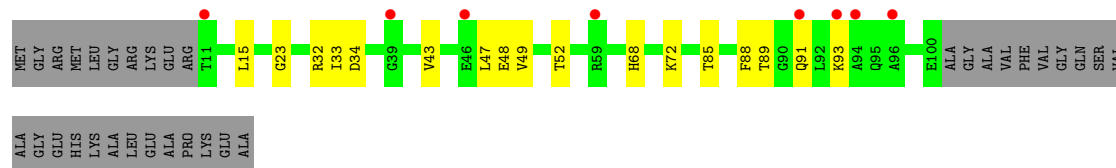
● Molecule 1: bactofilin



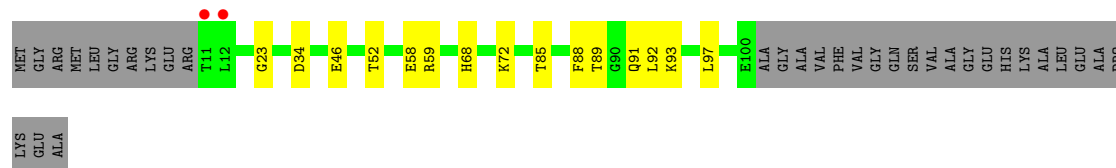
● Molecule 1: bactofilin



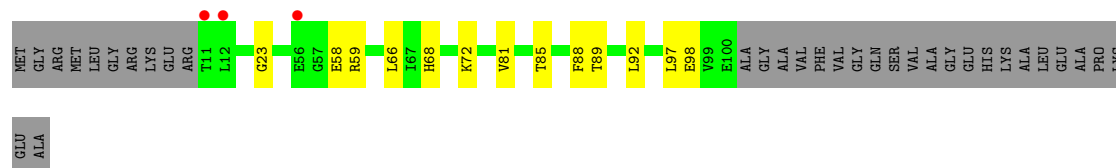
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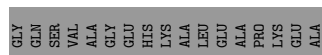
● Molecule 1: bactofilin



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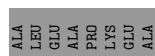
• Molecule 1: bactofilin



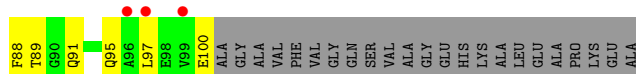
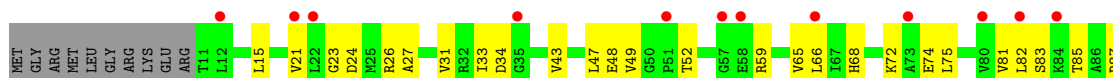
• Molecule 1: bactofilin



• Molecule 1: bactofilin

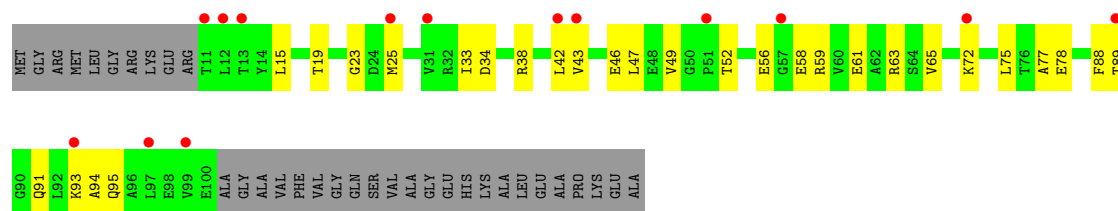


• Molecule 1: bactofilin

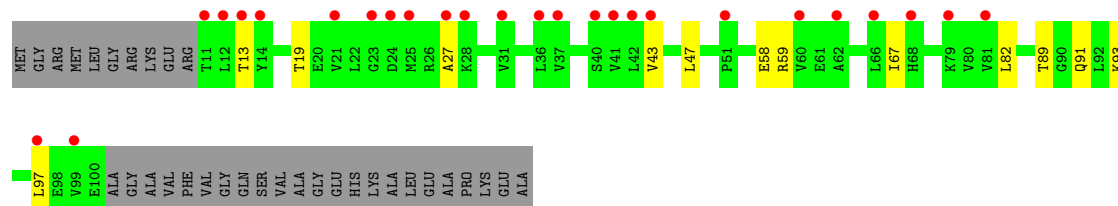


• Molecule 1: bactofilin

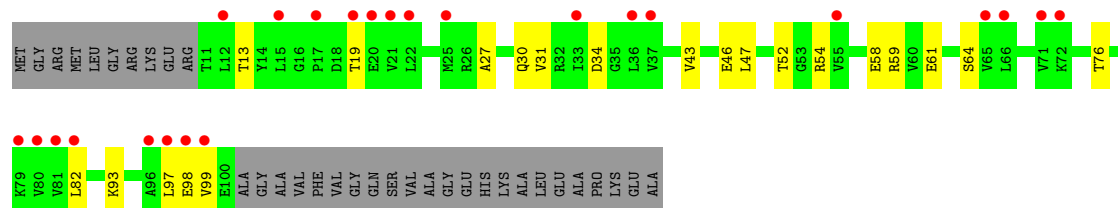




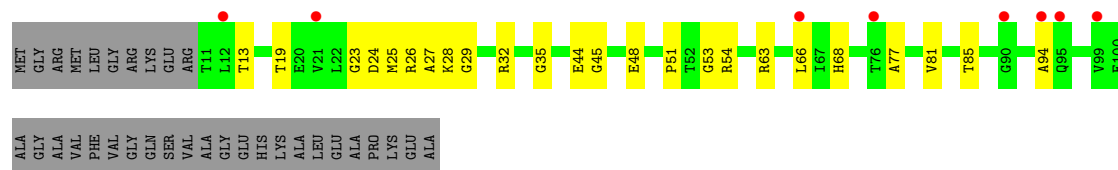
• Molecule 1: bactofilin



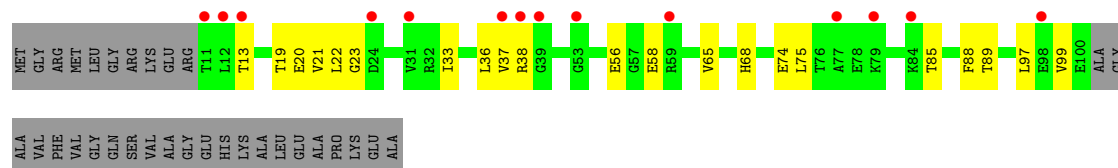
• Molecule 1: bactofilin



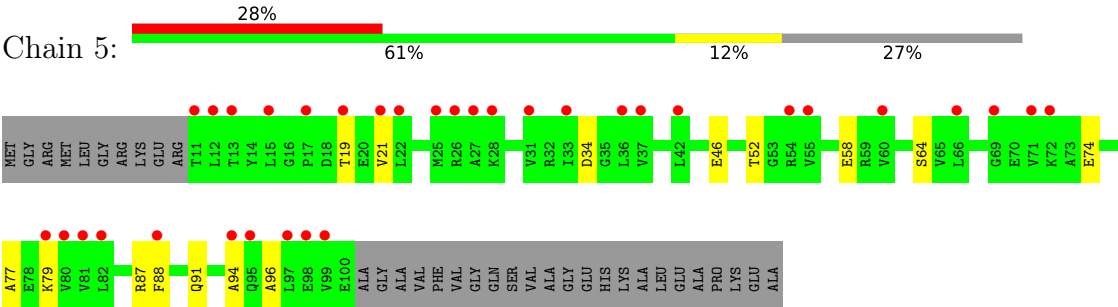
• Molecule 1: bactofilin



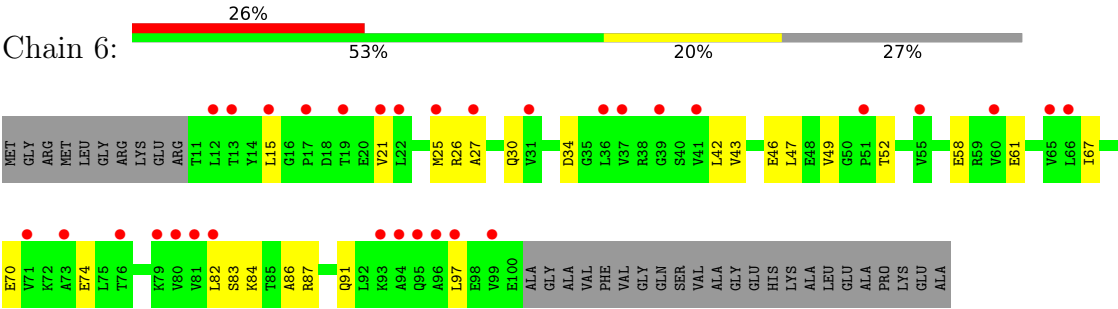
• Molecule 1: bactofilin



• 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

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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.

All (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
1:2:58:GLU:HG2	1:2:59:ARG:HG3	1.70	0.72
1:M:13:THR:HG21	1:N:19:THR:HG21	1.72	0.71
1:Z:93:LYS:HG3	1:1:91:GLN:HG3	1.73	0.71
1:Q:56:GLU:OE2	1:U:54:ARG:NH1	2.24	0.70
1:3:23:GLY:HA3	1:4:23:GLY:HA3	1.72	0.70
1:M:58:GLU:HG3	1:M:59:ARG:HG3	1.73	0.69
1:J:34:ASP:O	1:J:52:THR:OG1	2.10	0.68
1:Y:88:PHE:HB3	1:4:97:LEU:HB3	1.77	0.67
1:O:13:THR:HG21	1:P:19:THR:HG21	1.76	0.67
1:6:15:LEU:HD21	1:6:25:MET:HE1	1.76	0.67
1:Q:97:LEU:HB3	1:X:88:PHE:HB3	1.77	0.67
1:G:91:GLN:NE2	1:J:91:GLN:OE1	2.29	0.66
1:Y:26:ARG:NH2	1:Y:27:ALA:O	2.27	0.66
1:1:58:GLU:HG2	1:1:59:ARG:HG3	1.78	0.66
1:C:23:GLY:HA3	1:D:23:GLY:HA3	1.78	0.65
1:1:13:THR:HG21	1:2:19:THR:HG21	1.77	0.65
1:Q:58:GLU:HG2	1:Q:59:ARG:HG3	1.78	0.65
1:6:86:ALA:O	1:6:87:ARG:NH2	2.29	0.65
1:S:91:GLN:HG3	1:V:91:GLN:HE21	1.60	0.64
1:I:19:THR:HG21	1:J:13:THR:HG21	1.79	0.64
1:U:11:THR:HG23	1:V:17:PRO:HD2	1.78	0.64
1:Z:72:LYS:HG2	1:Z:89:THR:HB	1.80	0.64
1:A:13:THR:HG21	1:B:19:THR:HG21	1.79	0.64
1:W:23:GLY:HA3	1:X:23:GLY:HA3	1.80	0.64
1:L:18:ASP:OD2	1:Z:38:ARG:NH2	2.30	0.64
1:S:23:GLY:HA3	1:T:23:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ASP:O	1:F:52:THR:OG1	2.17	0.63
1:N:68:HIS:O	1:N:85:THR:OG1	2.15	0.63
1:G:93:LYS:HG2	1:J:91:GLN:HG2	1.79	0.63
1:5:19:THR:HA	1:6:27:ALA:HA	1.81	0.63
1:B:46:GLU:N	1:B:46:GLU:OE1	2.32	0.63
1:A:88:PHE:HB3	1:D:97:LEU:HB3	1.81	0.62
1:L:59:ARG:NH1	1:L:61:GLU:OE2	2.26	0.62
1:U:68:HIS:O	1:U:85:THR:OG1	2.17	0.62
1:3:13:THR:HG21	1:4:19:THR:HG21	1.82	0.61
1:N:34:ASP:O	1:N:52:THR:OG1	2.15	0.61
1:K:13:THR:HG21	1:L:19:THR:HG21	1.83	0.60
1:F:88:PHE:HB3	1:K:97:LEU:HB3	1.82	0.60
1:I:58:GLU:HG2	1:I:59:ARG:HG3	1.82	0.60
1:2:34:ASP:O	1:2:52:THR:OG1	2.15	0.60
1:Q:23:GLY:HA3	1:R:23:GLY:HA3	1.83	0.60
1:E:23:GLY:HA3	1:F:23:GLY:HA3	1.84	0.60
1:Z:63:ARG:NH1	1:Z:78:GLU:OE2	2.34	0.60
1:O:97:LEU:HB3	1:R:88:PHE:HB3	1.83	0.60
1:Z:88:PHE:HB3	1:1:97:LEU:HB3	1.82	0.60
1:P:68:HIS:O	1:P:85:THR:OG1	2.17	0.60
1:Q:88:PHE:HB3	1:X:97:LEU:HB3	1.84	0.60
1:I:34:ASP:O	1:I:52:THR:OG1	2.14	0.60
1:X:84:LYS:H	1:X:84:LYS:HD2	1.67	0.60
1:3:51:PRO:O	1:3:54:ARG:NH1	2.35	0.60
1:4:38:ARG:HD3	1:4:56:GLU:HB2	1.83	0.60
1:F:26:ARG:HH11	1:F:42:LEU:HG	1.66	0.60
1:4:58:GLU:O	1:4:74:GLU:N	2.32	0.60
1:B:34:ASP:O	1:B:52:THR:OG1	2.20	0.59
1:P:34:ASP:O	1:P:52:THR:OG1	2.20	0.59
1:V:58:GLU:HG2	1:V:59:ARG:HG3	1.83	0.59
1:W:34:ASP:O	1:W:52:THR:OG1	2.19	0.59
1:O:13:THR:HG23	1:P:15:LEU:HA	1.83	0.59
1:3:66:LEU:HG	1:3:81:VAL:HB	1.85	0.59
1:I:72:LYS:HG2	1:I:89:THR:HB	1.84	0.59
1:K:26:ARG:NH2	1:Y:24:ASP:OD1	2.35	0.59
1:L:87:ARG:NH1	1:T:98:GLU:OE1	2.36	0.59
1:X:34:ASP:O	1:X:52:THR:OG1	2.19	0.59
1:K:68:HIS:O	1:K:85:THR:OG1	2.18	0.59
1:6:82:LEU:HD23	1:6:83:SER:O	2.03	0.59
1:A:58:GLU:HG2	1:A:59:ARG:HG3	1.83	0.58
1:S:97:LEU:HB3	1:V:88:PHE:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:GLU:HG2	1:L:59:ARG:HG3	1.84	0.58
1:Z:58:GLU:HG2	1:Z:59:ARG:HG3	1.85	0.58
1:M:97:LEU:HB3	1:P:88:PHE:HB3	1.85	0.58
1:W:19:THR:HG21	1:X:13:THR:HG21	1.86	0.58
1:S:58:GLU:HG2	1:S:59:ARG:HG3	1.84	0.58
1:U:23:GLY:HA3	1:V:23:GLY:HA3	1.85	0.58
1:D:68:HIS:O	1:D:85:THR:OG1	2.20	0.58
1:Y:72:LYS:HG2	1:Y:89:THR:HB	1.85	0.58
1:3:53:GLY:O	1:3:54:ARG:NE	2.36	0.58
1:T:68:HIS:O	1:T:85:THR:OG1	2.20	0.57
1:O:23:GLY:HA3	1:P:23:GLY:HA3	1.86	0.57
1:V:70:GLU:HG3	1:V:87:ARG:HB2	1.87	0.57
1:M:76:THR:HG23	1:M:93:LYS:HD2	1.86	0.57
1:Q:70:GLU:HG2	1:Q:87:ARG:HB3	1.85	0.57
1:G:34:ASP:O	1:G:52:THR:OG1	2.17	0.57
1:R:32:ARG:HG3	1:R:48:GLU:OE2	2.05	0.57
1:W:84:LYS:H	1:W:84:LYS:HD2	1.69	0.57
1:G:88:PHE:HB3	1:J:97:LEU:HB3	1.87	0.56
1:Y:72:LYS:HE3	1:Y:87:ARG:HH22	1.70	0.56
1:P:42:LEU:HD13	1:P:61:GLU:HB2	1.87	0.56
1:S:46:GLU:OE2	1:S:46:GLU:N	2.37	0.56
1:E:58:GLU:HG2	1:E:59:ARG:HG3	1.88	0.56
1:Y:23:GLY:HA3	1:Z:23:GLY:HA3	1.88	0.56
1:F:68:HIS:O	1:F:85:THR:OG1	2.20	0.56
1:G:23:GLY:HA3	1:H:23:GLY:HA3	1.88	0.56
1:J:43:VAL:HG11	1:J:47:LEU:HB2	1.88	0.56
1:K:34:ASP:O	1:K:52:THR:OG1	2.16	0.56
1:Q:68:HIS:O	1:Q:85:THR:OG1	2.22	0.56
1:V:91:GLN:NE2	1:V:93:LYS:HG3	2.19	0.56
1:W:20:GLU:OE1	1:X:26:ARG:NH2	2.38	0.56
1:3:27:ALA:HB2	1:4:19:THR:HG23	1.88	0.56
1:A:97:LEU:HB3	1:D:88:PHE:HB3	1.88	0.55
1:P:84:LYS:H	1:P:84:LYS:HD2	1.71	0.55
1:K:54:ARG:HG3	1:K:70:GLU:HB2	1.88	0.55
1:N:72:LYS:HG2	1:N:89:THR:HB	1.88	0.55
1:K:58:GLU:HG2	1:K:59:ARG:HG3	1.89	0.55
1:M:26:ARG:HD3	1:N:20:GLU:OE2	2.07	0.55
1:P:91:GLN:OE1	1:P:93:LYS:HG3	2.07	0.55
1:6:49:VAL:HB	1:6:67:ILE:HA	1.89	0.55
1:G:19:THR:HG21	1:H:13:THR:HG21	1.89	0.55
1:Z:34:ASP:O	1:Z:52:THR:OG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:46:GLU:HG3	1:5:64:SER:HB3	1.89	0.54
1:1:91:GLN:N	1:1:91:GLN:OE1	2.40	0.54
1:2:30:GLN:HE22	1:2:46:GLU:HB2	1.72	0.54
1:L:34:ASP:O	1:L:52:THR:OG1	2.20	0.54
1:O:34:ASP:O	1:O:52:THR:OG1	2.21	0.54
1:B:88:PHE:HB3	1:N:97:LEU:HB3	1.90	0.54
1:E:88:PHE:HB3	1:H:97:LEU:HB3	1.89	0.54
1:K:33:ILE:HD13	1:K:37:VAL:HG21	1.89	0.54
1:2:82:LEU:HB2	1:2:99:VAL:HG22	1.88	0.54
1:5:46:GLU:N	1:5:46:GLU:OE1	2.41	0.54
1:W:91:GLN:HG3	1:W:93:LYS:CE	2.38	0.54
1:3:68:HIS:O	1:3:85:THR:OG1	2.24	0.53
1:3:25:MET:HA	1:4:21:VAL:HA	1.90	0.53
1:H:34:ASP:O	1:H:52:THR:OG1	2.23	0.53
1:A:34:ASP:O	1:A:52:THR:OG1	2.23	0.53
1:W:74:GLU:HG2	1:W:91:GLN:HB3	1.91	0.53
1:F:76:THR:HG23	1:F:93:LYS:HB3	1.91	0.52
1:Y:47:LEU:HD22	1:Y:65:VAL:HG23	1.91	0.52
1:6:91:GLN:N	1:6:91:GLN:OE1	2.43	0.52
1:I:87:ARG:HA	1:I:87:ARG:NE	2.25	0.52
1:Q:34:ASP:O	1:Q:52:THR:OG1	2.20	0.52
1:S:91:GLN:HG3	1:V:91:GLN:NE2	2.25	0.51
1:Y:68:HIS:O	1:Y:85:THR:OG1	2.22	0.51
1:A:23:GLY:HA3	1:B:23:GLY:HA3	1.91	0.51
1:V:91:GLN:HE22	1:V:93:LYS:CG	2.22	0.51
1:O:68:HIS:O	1:O:85:THR:OG1	2.28	0.51
1:Z:91:GLN:OE1	1:Z:91:GLN:N	2.43	0.51
1:6:26:ARG:HG3	1:6:42:LEU:HB3	1.93	0.51
1:A:13:THR:HG23	1:B:15:LEU:HA	1.92	0.51
1:W:92:LEU:C	1:W:93:LYS:HE2	2.36	0.51
1:1:27:ALA:HA	1:2:19:THR:HA	1.93	0.51
1:S:34:ASP:O	1:S:52:THR:OG1	2.24	0.50
1:C:27:ALA:HB2	1:D:19:THR:HG23	1.93	0.50
1:H:58:GLU:HG2	1:H:59:ARG:HG3	1.93	0.50
1:V:72:LYS:HG2	1:V:89:THR:HB	1.92	0.50
1:Y:97:LEU:HB3	1:4:88:PHE:HB3	1.92	0.50
1:Q:54:ARG:NH2	1:U:56:GLU:OE2	2.41	0.50
1:6:97:LEU:H	1:6:97:LEU:HD23	1.75	0.50
1:L:88:PHE:HB3	1:T:97:LEU:HB3	1.93	0.50
1:R:68:HIS:O	1:R:85:THR:OG1	2.23	0.50
1:B:33:ILE:HD13	1:B:37:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:21:VAL:HG12	1:Z:25:MET:HG3	1.92	0.50
1:R:43:VAL:HG11	1:R:47:LEU:HD12	1.94	0.50
1:Y:65:VAL:HG11	1:Y:75:LEU:HD21	1.94	0.50
1:B:87:ARG:NH2	1:B:88:PHE:O	2.45	0.50
1:E:19:THR:HG21	1:F:13:THR:HG21	1.93	0.49
1:F:97:LEU:HB3	1:K:88:PHE:HB3	1.93	0.49
1:I:43:VAL:HG11	1:I:47:LEU:HB2	1.94	0.49
1:A:99:VAL:HG12	1:A:100:GLU:H	1.75	0.49
1:A:42:LEU:HD13	1:A:61:GLU:HB2	1.95	0.49
1:C:74:GLU:HG2	1:C:91:GLN:HB3	1.94	0.49
1:Z:91:GLN:HG3	1:1:93:LYS:HG3	1.93	0.49
1:4:68:HIS:O	1:4:85:THR:OG1	2.28	0.49
1:M:72:LYS:HG2	1:M:89:THR:HB	1.94	0.49
1:B:97:LEU:HB3	1:N:88:PHE:HB3	1.94	0.49
1:U:13:THR:HG21	1:V:19:THR:HG21	1.94	0.49
1:B:97:LEU:O	1:N:87:ARG:HA	2.13	0.49
1:W:13:THR:HG21	1:X:19:THR:HG21	1.94	0.49
1:X:36:LEU:HD12	1:X:54:ARG:HH21	1.78	0.49
1:B:58:GLU:HG2	1:B:59:ARG:HG3	1.95	0.48
1:M:68:HIS:O	1:M:85:THR:OG1	2.23	0.48
1:I:59:ARG:NH1	1:I:61:GLU:OE2	2.28	0.48
1:Y:74:GLU:HG3	1:Y:91:GLN:HB3	1.94	0.48
1:6:30:GLN:HE22	1:6:46:GLU:HB3	1.78	0.48
1:Z:43:VAL:HG11	1:Z:47:LEU:HD12	1.95	0.48
1:6:34:ASP:HB3	1:6:52:THR:HG23	1.94	0.48
1:Z:38:ARG:HD3	1:Z:56:GLU:HB2	1.95	0.48
1:F:43:VAL:HG11	1:F:47:LEU:HD12	1.95	0.48
1:I:70:GLU:HG2	1:I:87:ARG:HB2	1.95	0.48
1:F:47:LEU:HD21	1:F:49:VAL:HG23	1.96	0.48
1:Y:82:LEU:O	1:Y:100:GLU:N	2.27	0.48
1:1:67:ILE:HB	1:1:82:LEU:HD13	1.95	0.47
1:F:42:LEU:HD13	1:F:61:GLU:HB2	1.96	0.47
1:U:22:LEU:HD23	1:U:38:ARG:HB2	1.95	0.47
1:H:68:HIS:O	1:H:85:THR:OG1	2.26	0.47
1:N:22:LEU:HD13	1:N:38:ARG:HB3	1.97	0.47
1:Y:66:LEU:HG	1:Y:81:VAL:HG23	1.96	0.47
1:C:13:THR:HG21	1:D:19:THR:HG21	1.97	0.47
1:M:13:THR:HG23	1:N:15:LEU:HA	1.96	0.47
1:E:97:LEU:HB3	1:H:88:PHE:HB3	1.97	0.47
1:H:72:LYS:HG2	1:H:89:THR:HB	1.96	0.47
1:R:72:LYS:HG2	1:R:89:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:34:ASP:O	1:V:52:THR:OG1	2.24	0.47
1:3:26:ARG:NE	1:4:20:GLU:OE2	2.40	0.47
1:Q:15:LEU:HD11	1:R:15:LEU:HD21	1.97	0.47
1:O:86:ALA:O	1:O:87:ARG:NH2	2.45	0.47
1:Q:54:ARG:CZ	1:U:54:ARG:HD3	2.45	0.47
1:X:68:HIS:O	1:X:85:THR:OG1	2.26	0.47
1:2:97:LEU:O	1:5:87:ARG:HA	2.15	0.47
1:I:74:GLU:HG2	1:I:91:GLN:HB3	1.97	0.47
1:R:34:ASP:O	1:R:52:THR:OG1	2.27	0.46
1:Y:83:SER:O	1:4:99:VAL:HG11	2.15	0.46
1:Z:46:GLU:N	1:Z:46:GLU:OE1	2.48	0.46
1:L:72:LYS:HG2	1:L:89:THR:HB	1.97	0.46
1:2:97:LEU:HD23	1:5:88:PHE:HB3	1.96	0.46
1:G:43:VAL:HG11	1:G:47:LEU:HB2	1.97	0.46
1:I:27:ALA:HB2	1:J:19:THR:HG23	1.97	0.46
1:6:58:GLU:O	1:6:74:GLU:N	2.44	0.46
1:G:99:VAL:O	1:G:100:GLU:HB2	2.15	0.46
1:2:52:THR:O	1:2:54:ARG:NH2	2.49	0.46
1:O:66:LEU:HG	1:O:81:VAL:HB	1.97	0.46
1:A:68:HIS:O	1:A:85:THR:OG1	2.26	0.46
1:I:15:LEU:HD11	1:J:15:LEU:HD21	1.98	0.46
1:K:43:VAL:HG11	1:K:47:LEU:HB2	1.97	0.46
1:I:86:ALA:O	1:I:87:ARG:CZ	2.64	0.46
1:B:31:VAL:O	1:B:48:GLU:N	2.47	0.45
1:M:19:THR:HG21	1:N:13:THR:HG21	1.98	0.45
1:X:58:GLU:HG2	1:X:59:ARG:HG3	1.99	0.45
1:S:88:PHE:HB3	1:V:97:LEU:HB3	1.97	0.45
1:A:72:LYS:HG2	1:A:89:THR:HB	1.98	0.45
1:I:23:GLY:HA3	1:J:23:GLY:HA3	1.99	0.45
1:W:15:LEU:HA	1:X:13:THR:HG23	1.97	0.45
1:L:20:GLU:HA	1:L:36:LEU:O	2.16	0.45
1:U:34:ASP:O	1:U:52:THR:OG1	2.26	0.45
1:T:66:LEU:HG	1:T:81:VAL:HB	1.99	0.45
1:2:46:GLU:N	1:2:46:GLU:OE2	2.49	0.45
1:F:26:ARG:HE	1:F:26:ARG:HB2	1.62	0.45
1:Y:43:VAL:HG11	1:Y:47:LEU:HD12	1.98	0.45
1:G:32:ARG:NE	1:G:34:ASP:OD1	2.50	0.45
1:I:16:GLY:HA3	1:I:35:GLY:N	2.32	0.45
1:A:43:VAL:HG11	1:A:47:LEU:HB2	1.99	0.45
1:3:24:ASP:O	1:4:22:LEU:N	2.35	0.45
1:G:65:VAL:HG11	1:G:75:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:15:LEU:HB2	1:R:33:ILE:HD13	1.98	0.44
1:S:92:LEU:HB3	1:V:92:LEU:HB3	1.99	0.44
1:S:91:GLN:NE2	1:S:93:LYS:HE2	2.32	0.44
1:W:74:GLU:HA	1:W:91:GLN:HB3	1.98	0.44
1:Z:95:GLN:HA	1:1:89:THR:HG23	2.00	0.44
1:5:21:VAL:HG21	1:6:21:VAL:HG21	2.00	0.44
1:P:32:ARG:HA	1:P:48:GLU:HB3	1.99	0.44
1:1:19:THR:HG23	1:2:27:ALA:HB2	1.99	0.44
1:T:58:GLU:HG2	1:T:59:ARG:HG3	1.99	0.44
1:3:19:THR:HG21	1:4:13:THR:HG21	2.00	0.44
1:6:70:GLU:HA	1:6:87:ARG:O	2.17	0.44
1:Y:34:ASP:O	1:Y:52:THR:OG1	2.33	0.44
1:Q:43:VAL:HG11	1:Q:47:LEU:HD12	1.99	0.44
1:S:68:HIS:O	1:S:85:THR:OG1	2.30	0.44
1:3:28:LYS:HE3	1:3:44:GLU:OE1	2.18	0.44
1:5:34:ASP:HB3	1:5:52:THR:HG23	2.00	0.43
1:I:70:GLU:HA	1:I:87:ARG:O	2.18	0.43
1:6:42:LEU:HD12	1:6:61:GLU:HB3	2.00	0.43
1:I:86:ALA:O	1:I:87:ARG:NH2	2.51	0.43
1:S:72:LYS:HG2	1:S:89:THR:HB	2.00	0.43
1:6:84:LYS:HE2	1:6:84:LYS:HB3	1.86	0.43
1:A:12:LEU:H	1:A:12:LEU:HD23	1.83	0.43
1:M:23:GLY:HA3	1:N:23:GLY:HA3	2.00	0.43
1:M:34:ASP:O	1:M:52:THR:OG1	2.33	0.43
1:M:62:ALA:C	1:M:63:ARG:HH21	2.27	0.43
1:Y:27:ALA:HA	1:Z:19:THR:HA	2.01	0.43
1:2:61:GLU:HA	1:2:76:THR:O	2.18	0.43
1:Y:31:VAL:O	1:Y:48:GLU:N	2.52	0.43
1:3:29:GLY:O	1:3:45:GLY:HA3	2.19	0.43
1:D:95:GLN:O	1:D:95:GLN:HG3	2.19	0.43
1:G:54:ARG:HG2	1:G:70:GLU:HB2	2.00	0.43
1:M:58:GLU:O	1:M:74:GLU:N	2.47	0.43
1:4:36:LEU:HD21	1:4:38:ARG:HE	1.83	0.43
1:O:14:TYR:HD1	1:O:32:ARG:HB3	1.84	0.43
1:B:30:GLN:HG3	1:B:46:GLU:HB2	2.01	0.42
1:K:26:ARG:CZ	1:K:42:LEU:HD22	2.49	0.42
1:K:26:ARG:HG3	1:K:42:LEU:HB2	2.00	0.42
1:3:32:ARG:HH21	1:3:48:GLU:HG2	1.84	0.42
1:P:30:GLN:HG3	1:P:46:GLU:HB3	2.00	0.42
1:4:36:LEU:HD21	1:4:38:ARG:NE	2.34	0.42
1:5:77:ALA:O	1:5:94:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LYS:HG2	1:D:89:THR:HB	2.01	0.42
1:I:15:LEU:HA	1:J:13:THR:HG23	2.01	0.42
1:Z:77:ALA:O	1:Z:94:ALA:HA	2.20	0.42
1:T:72:LYS:HG2	1:T:89:THR:HB	2.01	0.42
1:I:43:VAL:HG11	1:I:47:LEU:HD12	2.01	0.42
1:U:67:ILE:HD11	1:U:75:LEU:HD11	2.02	0.42
1:4:33:ILE:HD13	1:4:37:VAL:HG21	2.01	0.42
1:R:47:LEU:HD21	1:R:49:VAL:HG23	2.01	0.42
1:Z:15:LEU:HB2	1:Z:33:ILE:HD13	2.00	0.42
1:K:13:THR:HG23	1:L:15:LEU:HA	2.02	0.42
1:L:22:LEU:HD23	1:Y:59:ARG:HE	1.85	0.42
1:L:38:ARG:HD3	1:L:56:GLU:HB2	2.01	0.42
1:R:91:GLN:NE2	1:R:93:LYS:HG3	2.18	0.42
1:Y:47:LEU:HD21	1:Y:49:VAL:HG23	2.01	0.42
1:3:35:GLY:O	1:3:54:ARG:N	2.49	0.42
1:A:36:LEU:HD21	1:A:38:ARG:HE	1.84	0.42
1:O:77:ALA:O	1:O:94:ALA:HA	2.19	0.42
1:V:11:THR:O	1:V:11:THR:OG1	2.36	0.42
1:K:19:THR:HG21	1:L:13:THR:HG21	2.01	0.42
1:L:97:LEU:HB3	1:T:88:PHE:HB3	2.01	0.42
1:C:43:VAL:HG11	1:C:47:LEU:HB2	2.00	0.41
1:I:67:ILE:HG22	1:I:86:ALA:HB1	2.02	0.41
1:Q:43:VAL:HG13	1:Q:62:ALA:HB2	2.01	0.41
1:W:68:HIS:O	1:W:85:THR:OG1	2.34	0.41
1:Y:95:GLN:HA	1:4:89:THR:HG23	2.01	0.41
1:W:91:GLN:HG3	1:W:93:LYS:HE3	2.02	0.41
1:3:44:GLU:HG3	1:3:63:ARG:CZ	2.51	0.41
1:3:77:ALA:O	1:3:94:ALA:HA	2.20	0.41
1:Z:42:LEU:HD12	1:Z:61:GLU:HB2	2.03	0.41
1:2:93:LYS:HE2	1:5:91:GLN:OE1	2.20	0.41
1:K:28:LYS:NZ	1:K:44:GLU:OE1	2.45	0.41
1:Z:65:VAL:HG21	1:Z:75:LEU:HD11	2.03	0.41
1:2:13:THR:HB	1:2:31:VAL:HG12	2.01	0.41
1:4:65:VAL:HG11	1:4:75:LEU:HD11	2.02	0.41
1:V:43:VAL:HG13	1:V:62:ALA:HB2	2.03	0.41
1:V:66:LEU:HG	1:V:81:VAL:HB	2.02	0.41
1:Y:15:LEU:HB2	1:Y:33:ILE:HD13	2.01	0.41
1:V:43:VAL:HG11	1:V:47:LEU:HD12	2.03	0.41
1:2:43:VAL:HG11	1:2:47:LEU:HD12	2.03	0.41
1:5:79:LYS:HG3	1:5:96:ALA:HB3	2.03	0.41
1:Z:33:ILE:O	1:Z:49:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLU:N	1:G:58:GLU:OE1	2.54	0.40
1:6:43:VAL:HG11	1:6:47:LEU:HD12	2.02	0.40
1:2:98:GLU:OE1	1:2:98:GLU:N	2.54	0.40
1:A:19:THR:HG23	1:B:27:ALA:HB2	2.04	0.40
1:F:43:VAL:HG13	1:F:62:ALA:HB2	2.04	0.40
1:H:14:TYR:HD1	1:H:32:ARG:HB3	1.87	0.40
1:K:77:ALA:O	1:K:94:ALA:HA	2.22	0.40
1:L:42:LEU:HD23	1:L:42:LEU:O	2.22	0.40
1:L:92:LEU:HB3	1:T:92:LEU:HB3	2.04	0.40
1:5:58:GLU:O	1:5:74:GLU:N	2.48	0.40

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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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

All (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
1	5	12	LEU	5.4
1	5	25	MET	5.3
1	1	24	ASP	5.0
1	5	36	LEU	4.9
1	D	11	THR	4.8
1	2	37	VAL	4.7
1	6	25	MET	4.7
1	6	19	THR	4.7
1	U	11	THR	4.6
1	2	97	LEU	4.6
1	2	36	LEU	4.5
1	6	36	LEU	4.5
1	N	12	LEU	4.5
1	6	81	VAL	4.3
1	H	12	LEU	4.3
1	6	22	LEU	4.3
1	3	12	LEU	4.3
1	2	81	VAL	4.3
1	Y	22	LEU	4.3
1	5	55	VAL	4.3
1	1	13	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	6	60	VAL	4.1
1	H	11	THR	4.1
1	2	82	LEU	4.1
1	A	11	THR	4.1
1	D	12	LEU	4.0
1	5	99	VAL	4.0
1	5	13	THR	4.0
1	Y	12	LEU	4.0
1	1	25	MET	3.9
1	Z	12	LEU	3.8
1	5	31	VAL	3.8
1	C	11	THR	3.7
1	1	31	VAL	3.7
1	5	21	VAL	3.6
1	B	11	THR	3.6
1	2	12	LEU	3.6
1	2	19	THR	3.6
1	3	90	GLY	3.6
1	5	81	VAL	3.6
1	N	54	ARG	3.6
1	5	11	THR	3.5
1	P	12	LEU	3.5
1	1	42	LEU	3.5
1	I	11	THR	3.4
1	4	12	LEU	3.4
1	5	42	LEU	3.4
1	5	97	LEU	3.4
1	2	21	VAL	3.3
1	U	12	LEU	3.3
1	2	65	VAL	3.3
1	2	71	VAL	3.3
1	2	99	VAL	3.2
1	2	66	LEU	3.2
1	Y	99	VAL	3.2
1	Q	11	THR	3.2
1	5	19	THR	3.2
1	P	30	GLN	3.2
1	2	55	VAL	3.2
1	2	79	LYS	3.2
1	6	99	VAL	3.1
1	E	12	LEU	3.1
1	O	12	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	12	LEU	3.1
1	1	41	VAL	3.1
1	6	13	THR	3.1
1	A	12	LEU	3.1
1	V	18	ASP	3.1
1	X	12	LEU	3.1
1	2	22	LEU	3.1
1	1	21	VAL	3.1
1	5	27	ALA	3.0
1	5	28	LYS	3.0
1	M	12	LEU	3.0
1	1	97	LEU	3.0
1	5	72	LYS	3.0
1	2	17	PRO	3.0
1	V	12	LEU	3.0
1	5	98	GLU	3.0
1	5	17	PRO	2.9
1	O	96	ALA	2.9
1	Y	73	ALA	2.9
1	Y	66	LEU	2.9
1	6	15	LEU	2.9
1	1	40	SER	2.9
1	L	12	LEU	2.9
1	4	53	GLY	2.9
1	J	11	THR	2.9
1	5	15	LEU	2.9
1	6	66	LEU	2.9
1	1	51	PRO	2.9
1	O	45	GLY	2.9
1	Y	21	VAL	2.9
1	6	41	VAL	2.8
1	M	94	ALA	2.8
1	6	96	ALA	2.8
1	L	61	GLU	2.8
1	2	80	VAL	2.8
1	C	12	LEU	2.8
1	P	11	THR	2.8
1	Z	31	VAL	2.8
1	Z	11	THR	2.8
1	B	12	LEU	2.8
1	G	12	LEU	2.8
1	P	46	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	90	GLY	2.8
1	Z	13	THR	2.8
1	5	82	LEU	2.7
1	W	58	GLU	2.7
1	5	66	LEU	2.7
1	I	12	LEU	2.7
1	Z	89	THR	2.7
1	M	77	ALA	2.7
1	O	98	GLU	2.7
1	T	12	LEU	2.7
1	1	66	LEU	2.7
1	5	33	ILE	2.7
1	6	95	GLN	2.7
1	M	39	GLY	2.7
1	O	62	ALA	2.7
1	T	11	THR	2.7
1	Y	58	GLU	2.7
1	6	31	VAL	2.6
1	6	65	VAL	2.6
1	Z	93	LYS	2.6
1	S	11	THR	2.6
1	Y	97	LEU	2.6
1	5	22	LEU	2.6
1	1	43	VAL	2.6
1	6	71	VAL	2.6
1	6	39	GLY	2.6
1	G	100	GLU	2.6
1	U	56	GLU	2.6
1	Z	99	VAL	2.6
1	1	28	LYS	2.6
1	6	17	PRO	2.6
1	2	72	LYS	2.5
1	S	12	LEU	2.5
1	Z	42	LEU	2.5
1	1	23	GLY	2.5
1	5	26	ARG	2.5
1	J	70	GLU	2.5
1	R	39	GLY	2.5
1	R	59	ARG	2.5
1	M	11	THR	2.5
1	6	82	LEU	2.5
1	Y	80	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	5	71	VAL	2.5
1	J	100	GLU	2.4
1	E	91	GLN	2.4
1	4	38	ARG	2.4
1	5	60	VAL	2.4
1	5	80	VAL	2.4
1	V	30	GLN	2.4
1	6	94	ALA	2.4
1	P	29	GLY	2.4
1	2	98	GLU	2.4
1	Y	84	LYS	2.4
1	1	11	THR	2.4
1	6	76	THR	2.4
1	L	59	ARG	2.4
1	J	38	ARG	2.4
1	A	61	GLU	2.4
1	I	30	GLN	2.3
1	Y	57	GLY	2.3
1	4	59	ARG	2.3
1	1	27	ALA	2.3
1	E	43	VAL	2.3
1	1	79	LYS	2.3
1	X	46	GLU	2.3
1	Y	82	LEU	2.3
1	4	31	VAL	2.3
1	6	37	VAL	2.3
1	O	27	ALA	2.3
1	A	20	GLU	2.3
1	N	56	GLU	2.3
1	2	20	GLU	2.3
1	2	33	ILE	2.3
1	N	53	GLY	2.3
1	5	54	ARG	2.3
1	6	79	LYS	2.3
1	1	36	LEU	2.3
1	P	73	ALA	2.3
1	R	94	ALA	2.3
1	3	94	ALA	2.3
1	6	27	ALA	2.3
1	X	30	GLN	2.3
1	R	93	LYS	2.3
1	K	63	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	Y	96	ALA	2.3
1	A	46	GLU	2.3
1	D	61	GLU	2.3
1	6	55	VAL	2.3
1	6	80	VAL	2.3
1	3	76	THR	2.2
1	C	58	GLU	2.2
1	N	70	GLU	2.2
1	N	35	GLY	2.2
1	4	11	THR	2.2
1	4	24	ASP	2.2
1	4	39	GLY	2.2
1	O	93	LYS	2.2
1	J	12	LEU	2.2
1	4	84	LYS	2.2
1	5	94	ALA	2.2
1	Z	25	MET	2.2
1	Z	43	VAL	2.2
1	B	100	GLU	2.2
1	E	20	GLU	2.2
1	V	46	GLU	2.2
1	4	98	GLU	2.2
1	4	13	THR	2.2
1	5	79	LYS	2.2
1	2	25	MET	2.2
1	W	12	LEU	2.2
1	3	66	LEU	2.2
1	5	88	PHE	2.2
1	4	79	LYS	2.2
1	6	93	LYS	2.2
1	K	12	LEU	2.2
1	R	91	GLN	2.1
1	Y	35	GLY	2.1
1	C	44	GLU	2.1
1	M	62	ALA	2.1
1	2	96	ALA	2.1
1	1	37	VAL	2.1
1	1	81	VAL	2.1
1	N	74	GLU	2.1
1	T	56	GLU	2.1
1	Y	51	PRO	2.1
1	6	51	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	1	99	VAL	2.1
1	4	37	VAL	2.1
1	Q	18	ASP	2.1
1	I	46	GLU	2.1
1	Z	97	LEU	2.1
1	M	76	THR	2.1
1	1	60	VAL	2.1
1	Z	57	GLY	2.1
1	1	14	TYR	2.1
1	Z	51	PRO	2.1
1	E	11	THR	2.1
1	K	11	THR	2.1
1	N	87	ARG	2.1
1	O	94	ALA	2.1
1	B	95	GLN	2.1
1	5	69	GLY	2.1
1	F	59	ARG	2.1
1	3	95	GLN	2.1
1	5	95	GLN	2.1
1	O	76	THR	2.0
1	R	11	THR	2.0
1	R	46	GLU	2.0
1	R	96	ALA	2.0
1	6	73	ALA	2.0
1	2	15	LEU	2.0
1	6	21	VAL	2.0
1	L	24	ASP	2.0
1	B	30	GLN	2.0
1	3	21	VAL	2.0
1	3	99	VAL	2.0
1	N	57	GLY	2.0
1	Z	72	LYS	2.0
1	1	68	HIS	2.0
1	J	56	GLU	2.0
1	P	77	ALA	2.0
1	1	62	ALA	2.0
1	4	77	ALA	2.0

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 [i](#)

There are no oligosaccharides 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.