



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:14 PM GMT

PDB ID : 3T5P  
Title : Crystal structure of a putative diacylglycerol kinase from *Bacillus anthracis* str. Sterne  
Authors : Hou, J.; Zheng, H.; Chruszcz, M.; Cooper, D.R.; Onopriyenko, O.; Grimshaw, S.; Savchenko, A.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-07-27  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

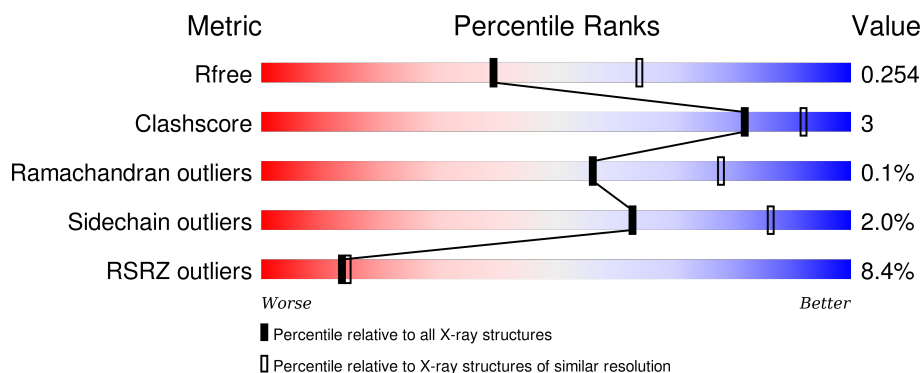
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	<div> <div>9%</div> <div>82% 11% 6%</div> </div>
1	B	306	<div> <div>7%</div> <div>90% 8%</div> </div>
1	C	306	<div> <div>7%</div> <div>90% 5% 5%</div> </div>
1	D	306	<div> <div>6%</div> <div>85% 10%</div> </div>
1	E	306	<div> <div>4%</div> <div>91% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	306	<div><div></div><div>10%</div><div>82%</div><div>7%</div><div>11%</div></div>
1	G	306	<div><div></div><div>5%</div><div>87%</div><div>8%</div><div>5%</div></div>
1	H	306	<div><div></div><div>10%</div><div>84%</div><div>5%</div><div>11%</div></div>
1	I	306	<div><div></div><div>9%</div><div>82%</div><div>8%</div><div>9%</div></div>
1	J	306	<div><div></div><div>13%</div><div>85%</div><div>6%</div><div>9%</div></div>
1	K	306	<div><div></div><div>7%</div><div>89%</div><div>5%</div><div>6%</div></div>
1	L	306	<div><div></div><div>8%</div><div>92%</div><div>7%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26322 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 BmrU protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	Se	0	0	0
			2159	1389	353	410	5	2			
1	B	299	Total	C	N	O	S	Se	0	0	0
			2267	1453	368	439	5	2			
1	C	292	Total	C	N	O	S	Se	0	0	0
			2173	1397	355	413	5	3			
1	D	293	Total	C	N	O	S	Se	0	0	0
			2216	1425	359	425	5	2			
1	E	295	Total	C	N	O	S	Se	0	0	0
			2202	1411	362	422	5	2			
1	F	273	Total	C	N	O	S	Se	0	0	0
			2036	1315	330	384	5	2			
1	G	291	Total	C	N	O	S	Se	0	0	0
			2179	1403	354	415	5	2			
1	H	272	Total	C	N	O	S	Se	0	0	0
			1970	1267	323	373	5	2			
1	I	277	Total	C	N	O	S	Se	0	0	0
			2078	1338	338	395	5	2			
1	J	278	Total	C	N	O	S	Se	0	0	0
			2070	1336	336	391	5	2			
1	K	289	Total	C	N	O	S	Se	0	0	0
			2169	1393	349	420	5	2			
1	L	302	Total	C	N	O	S	Se	0	0	0
			2286	1469	371	439	5	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
A	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
A	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
A	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
A	-1	SER	-	EXPRESSION TAG	UNP Q81KC6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
B	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
B	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
B	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
B	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
B	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
B	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
C	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
C	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
C	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
C	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
C	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
C	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
D	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
D	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
D	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
D	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
D	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
D	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
E	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
E	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
E	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
E	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
E	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
E	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
F	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
F	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
F	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
F	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
F	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
F	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
G	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
G	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
G	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
G	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
G	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
G	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
H	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
H	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
H	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
H	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
H	-1	SER	-	EXPRESSION TAG	UNP Q81KC6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
I	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
I	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
I	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
I	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
I	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
I	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
J	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
J	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
J	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
J	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
J	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
J	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
K	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
K	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
K	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
K	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
K	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
K	0	ALA	-	EXPRESSION TAG	UNP Q81KC6
L	-5	TYR	-	EXPRESSION TAG	UNP Q81KC6
L	-4	PHE	-	EXPRESSION TAG	UNP Q81KC6
L	-3	GLN	-	EXPRESSION TAG	UNP Q81KC6
L	-2	ASN	-	EXPRESSION TAG	UNP Q81KC6
L	-1	SER	-	EXPRESSION TAG	UNP Q81KC6
L	0	ALA	-	EXPRESSION TAG	UNP Q81KC6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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

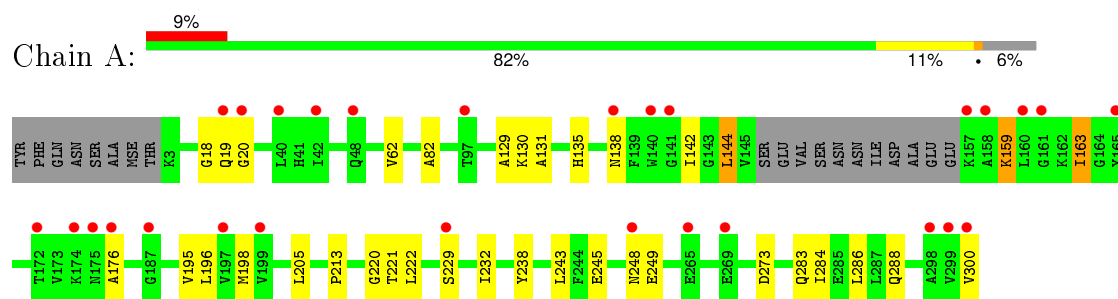
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	66	Total 66	O 66	0	0
3	C	43	Total 43	O 43	0	0
3	D	61	Total 61	O 61	0	0
3	E	32	Total 32	O 32	0	0
3	F	36	Total 36	O 36	0	0
3	G	45	Total 45	O 45	0	0
3	H	10	Total 10	O 10	0	0
3	I	38	Total 38	O 38	0	0
3	J	35	Total 35	O 35	0	0
3	K	49	Total 49	O 49	0	0
3	L	62	Total 62	O 62	0	0

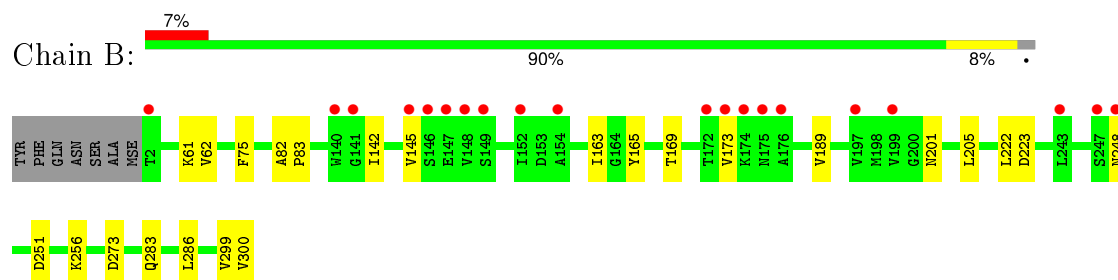
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

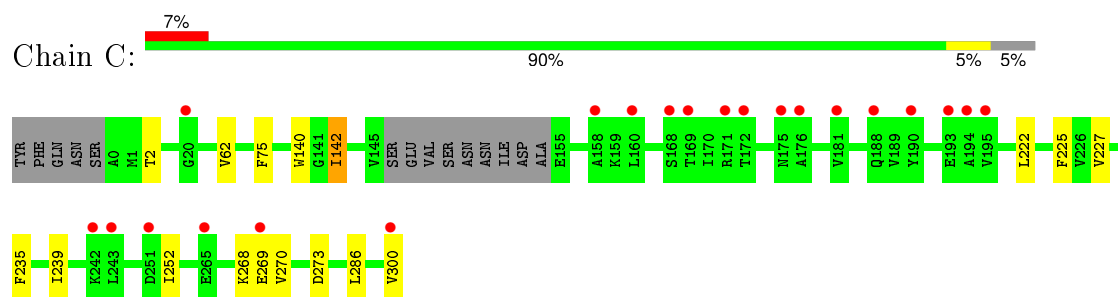
#### • Molecule 1: BmrU protein



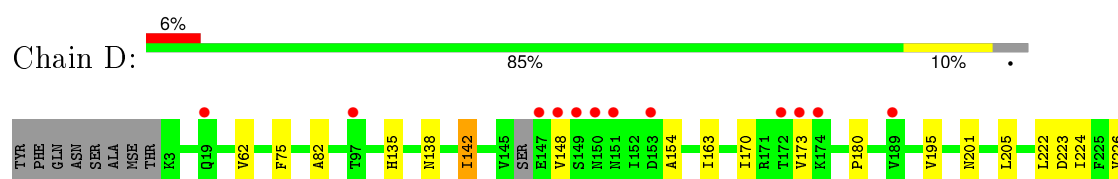
#### • Molecule 1: BmrU protein



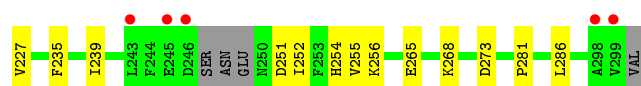
#### • Molecule 1: BmrU protein



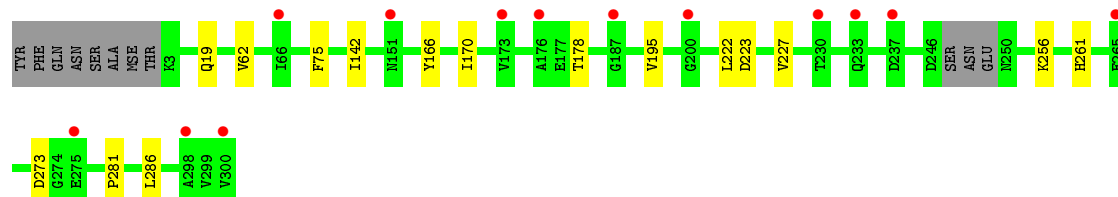
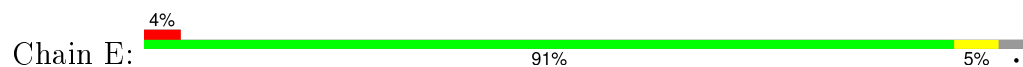
#### • Molecule 1: BmrU protein



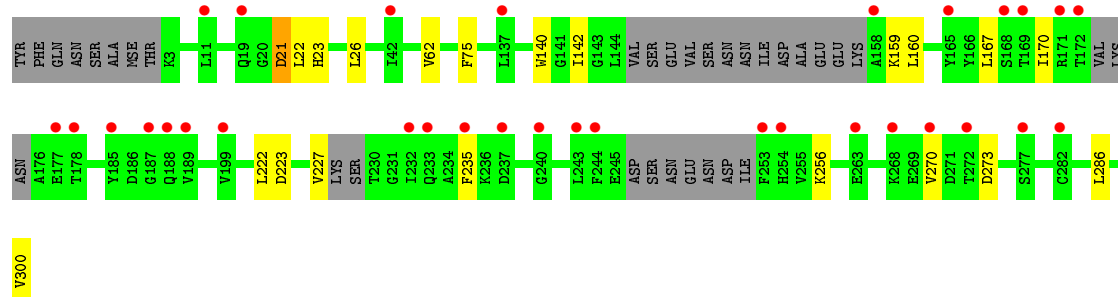
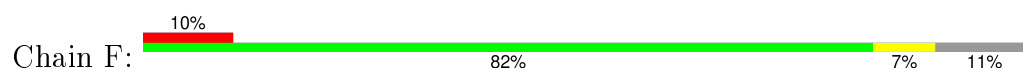




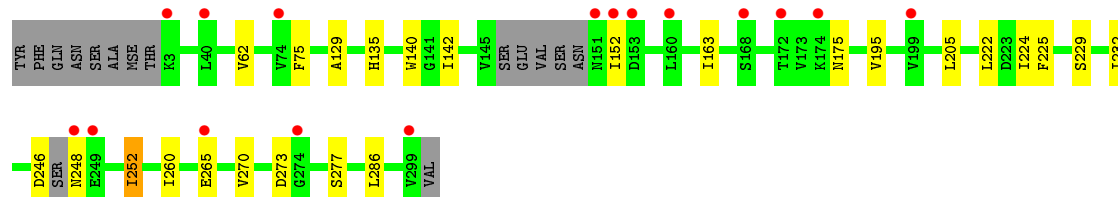
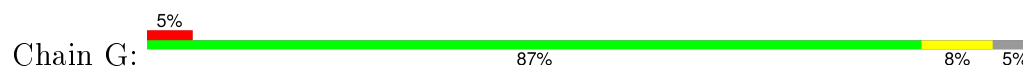
- Molecule 1: BmrU protein



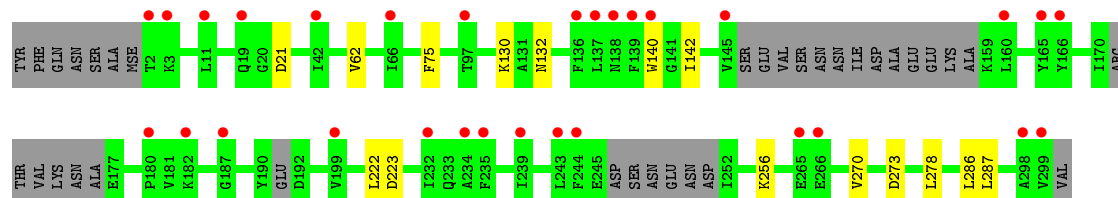
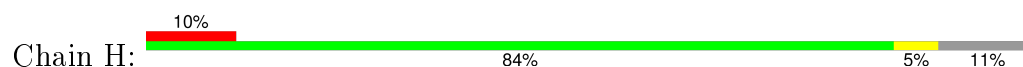
- Molecule 1: BmrU protein



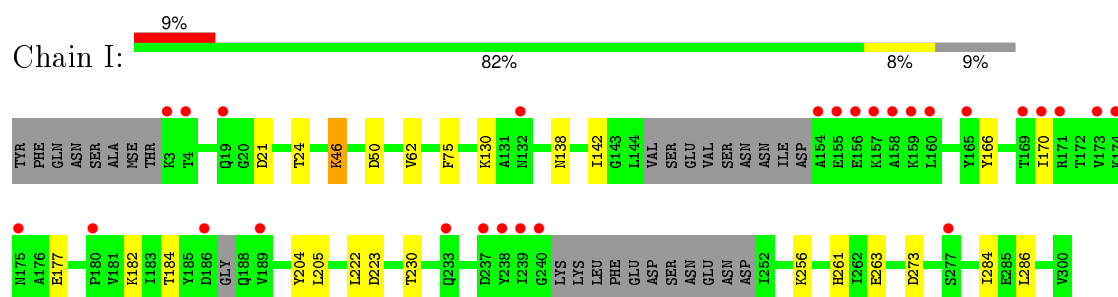
- Molecule 1: BmrU protein



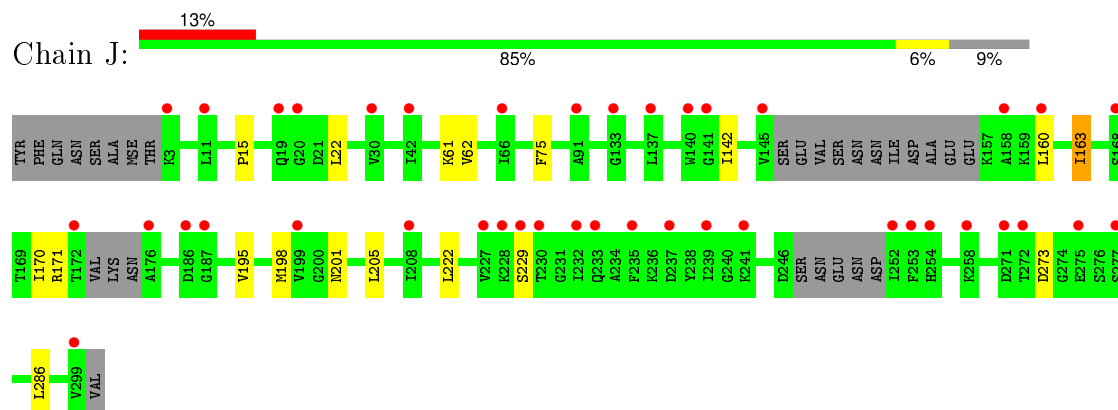
- Molecule 1: BmrU protein



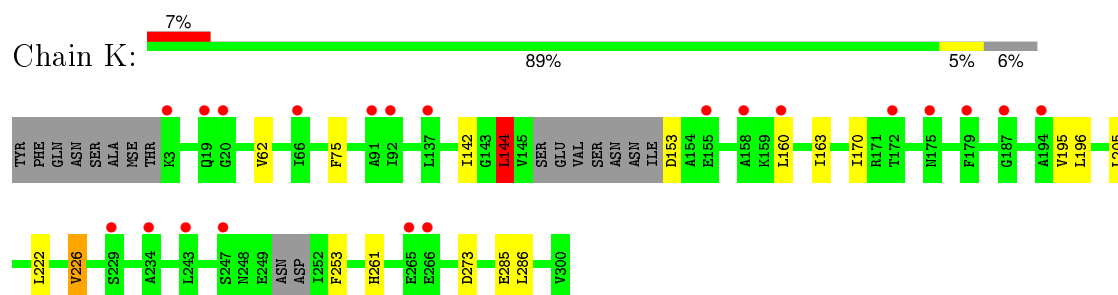
- Molecule 1: BmrU protein



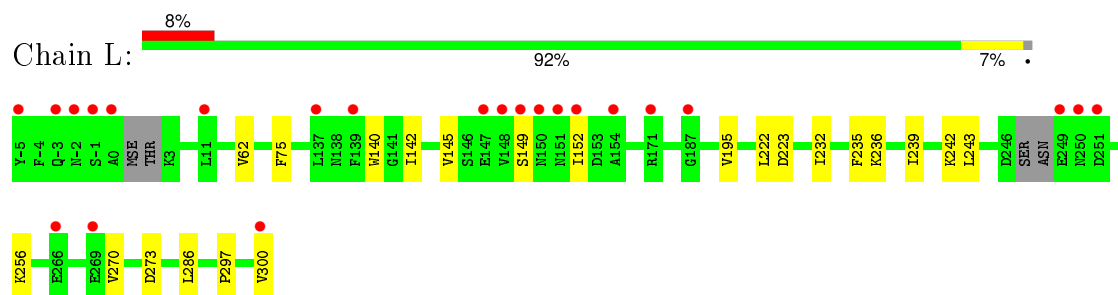
• Molecule 1: BmrU protein



• Molecule 1: BmrU protein



• Molecule 1: BmrU protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.02Å 115.10Å 208.02Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	29.56 – 2.50 29.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.56-2.50) 98.6 (29.56-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.205 , 0.241 0.216 , 0.254	Depositor DCC
$R_{free}$ test set	6264 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.2	EDS
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 124704 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	0/2203	0.67	2/2994 (0.1%)
1	B	0.63	0/2312	0.65	0/3142
1	C	0.56	0/2215	0.62	0/3011
1	D	0.60	0/2259	0.63	0/3066
1	E	0.56	0/2246	0.60	0/3056
1	F	0.55	0/2077	0.61	0/2823
1	G	0.59	0/2222	0.65	0/3021
1	H	0.48	0/2008	0.60	0/2736
1	I	0.55	0/2119	0.62	0/2878
1	J	0.54	0/2111	0.60	0/2869
1	K	0.57	0/2212	0.63	1/3007 (0.0%)
1	L	0.59	0/2331	0.62	0/3166
All	All	0.57	0/26315	0.63	3/35769 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LYS	C-N-CA	5.70	135.94	121.70
1	A	144	LEU	CB-CG-CD1	5.68	120.66	111.00
1	K	144	LEU	CB-CG-CD1	5.35	120.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LYS	Peptide

## 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	A	2159	0	2094	24	0
1	B	2267	0	2226	14	0
1	C	2173	0	2110	12	0
1	D	2216	0	2171	28	0
1	E	2202	0	2122	9	0
1	F	2036	0	1966	12	0
1	G	2179	0	2114	12	0
1	H	1970	0	1841	7	0
1	I	2078	0	2022	12	0
1	J	2070	0	2011	10	0
1	K	2169	0	2087	11	0
1	L	2286	0	2228	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	28	0	0	2	0
3	B	66	0	0	1	0
3	C	43	0	0	0	0
3	D	61	0	0	4	0
3	E	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	36	0	0	0	0
3	G	45	0	0	0	0
3	H	10	0	0	0	0
3	I	38	0	0	0	0
3	J	35	0	0	1	0
3	K	49	0	0	1	0
3	L	62	0	0	0	0
All	All	26322	0	24992	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 163 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:I:222:LEU:HG	1:I:286:LEU:HD13	1.49	0.94
1:L:297:PRO:HA	1:L:300:VAL:HG23	1.57	0.86
1:D:222:LEU:HG	1:D:286:LEU:HD13	1.56	0.85
1:H:222:LEU:HG	1:H:286:LEU:HD13	1.62	0.82
1:D:226:VAL:O	1:D:252:ILE:HG22	1.84	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/306 (92%)	270 (95%)	12 (4%)	1 (0%)	39	61
1	B	297/306 (97%)	288 (97%)	9 (3%)	0	100	100
1	C	288/306 (94%)	277 (96%)	11 (4%)	0	100	100
1	D	287/306 (94%)	278 (97%)	8 (3%)	1 (0%)	46	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	291/306 (95%)	280 (96%)	11 (4%)	0	100	100
1	F	263/306 (86%)	257 (98%)	6 (2%)	0	100	100
1	G	285/306 (93%)	276 (97%)	8 (3%)	1 (0%)	39	61
1	H	262/306 (86%)	256 (98%)	6 (2%)	0	100	100
1	I	269/306 (88%)	259 (96%)	10 (4%)	0	100	100
1	J	270/306 (88%)	262 (97%)	8 (3%)	0	100	100
1	K	283/306 (92%)	274 (97%)	9 (3%)	0	100	100
1	L	296/306 (97%)	284 (96%)	12 (4%)	0	100	100
All	All	3374/3672 (92%)	3261 (97%)	110 (3%)	3 (0%)	56	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	G	152	ILE
1	D	173	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/257 (87%)	218 (97%)	6 (3%)	52	79
1	B	244/257 (95%)	241 (99%)	3 (1%)	78	93
1	C	225/257 (88%)	220 (98%)	5 (2%)	60	84
1	D	235/257 (91%)	232 (99%)	3 (1%)	76	92
1	E	229/257 (89%)	225 (98%)	4 (2%)	68	89
1	F	210/257 (82%)	206 (98%)	4 (2%)	65	87
1	G	227/257 (88%)	222 (98%)	5 (2%)	60	84
1	H	194/257 (76%)	191 (98%)	3 (2%)	72	91
1	I	217/257 (84%)	212 (98%)	5 (2%)	58	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	215/257 (84%)	211 (98%)	4 (2%)	65	87
1	K	226/257 (88%)	218 (96%)	8 (4%)	43	70
1	L	242/257 (94%)	238 (98%)	4 (2%)	68	89
All	All	2688/3084 (87%)	2634 (98%)	54 (2%)	63	86

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	300	VAL
1	H	21	ASP
1	K	285	GLU
1	G	62	VAL
1	G	252	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	135	HIS
1	K	135	HIS
1	G	135	HIS
1	D	175	ASN
1	G	23	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/306 (93%)	0.40	28 (9%) 10 10	38, 63, 97, 125	0
1	B	297/306 (97%)	0.31	20 (6%) 21 23	30, 53, 98, 109	0
1	C	289/306 (94%)	0.25	21 (7%) 18 20	38, 64, 111, 126	0
1	D	291/306 (95%)	0.34	17 (5%) 26 30	33, 57, 109, 130	0
1	E	293/306 (95%)	0.15	13 (4%) 38 43	37, 62, 103, 112	0
1	F	271/306 (88%)	0.55	32 (11%) 6 6	35, 66, 133, 166	0
1	G	289/306 (94%)	0.38	16 (5%) 29 32	34, 59, 102, 139	0
1	H	270/306 (88%)	0.55	30 (11%) 7 7	44, 78, 127, 139	0
1	I	275/306 (89%)	0.41	27 (9%) 10 10	36, 62, 109, 130	0
1	J	276/306 (90%)	0.70	41 (14%) 3 3	36, 73, 115, 141	2 (0%)
1	K	287/306 (93%)	0.12	21 (7%) 18 20	33, 56, 106, 124	0
1	L	300/306 (98%)	0.33	23 (7%) 16 18	34, 58, 100, 111	0
All	All	3423/3672 (93%)	0.37	289 (8%) 14 14	30, 63, 110, 166	2 (0%)

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	154	ALA	8.2
1	H	299	VAL	7.3
1	F	232	ILE	6.8
1	L	-5	TYR	5.9
1	J	253	PHE	5.8

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	H	301	1/1	0.80	0.16	-0.32	73,73,73,73	0
2	MG	F	301	1/1	0.80	0.12	-0.76	58,58,58,58	0
2	MG	D	301	1/1	0.94	0.12	-0.96	39,39,39,39	0
2	MG	B	301	1/1	0.98	0.09	-1.33	36,36,36,36	0
2	MG	L	301	1/1	0.90	0.08	-1.39	44,44,44,44	0
2	MG	J	301	1/1	0.72	0.08	-1.49	69,69,69,69	0
2	MG	G	301	1/1	0.82	0.10	-1.63	43,43,43,43	0
2	MG	K	301	1/1	0.97	0.07	-1.64	53,53,53,53	0
2	MG	C	301	1/1	0.94	0.07	-2.01	56,56,56,56	0
2	MG	A	301	1/1	0.92	0.07	-2.18	48,48,48,48	0
2	MG	I	301	1/1	0.88	0.05	-3.01	59,59,59,59	0
2	MG	E	301	1/1	0.86	0.04	-3.87	59,59,59,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.