



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 04:11 AM EDT

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 : unknown  
Resolution : 2.50 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](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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

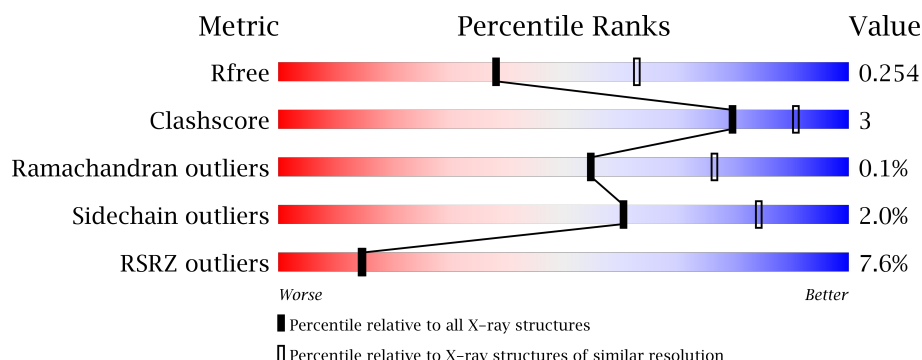
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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%</div> <div>11%</div> <div>6%</div> </div>
1	B	306	<div> <div>6%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	C	306	<div> <div>7%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	306	<div> <div>5%</div> <div>85%</div> <div>10%</div> <div>.</div> </div>
1	E	306	<div> <div>3%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	306	<div><div></div><div>9%</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>8%</div><div>84%</div><div>5%</div><div>11%</div></div>
1	I	306	<div><div></div><div>8%</div><div>82%</div><div>8%</div><div>9%</div></div>
1	J	306	<div><div></div><div>12%</div><div>85%</div><div>6%</div><div>9%</div></div>
1	K	306	<div><div></div><div>6%</div><div>89%</div><div>5%</div><div>6%</div></div>
1	L	306	<div><div></div><div>7%</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

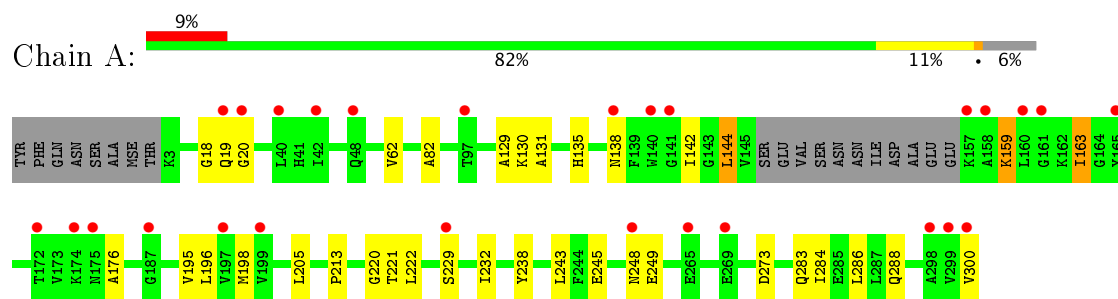
- Molecule 3 is water.

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

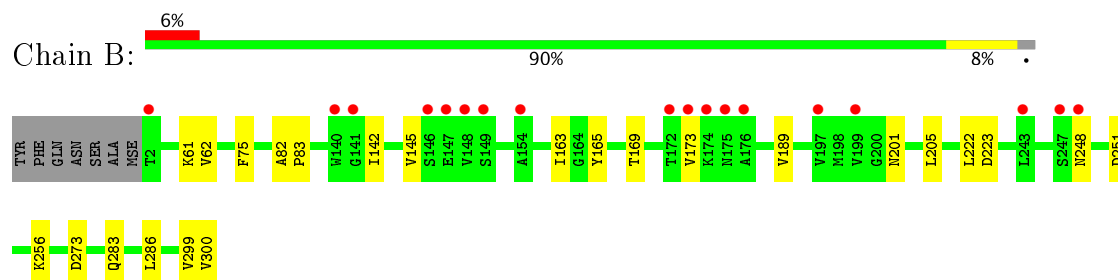
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

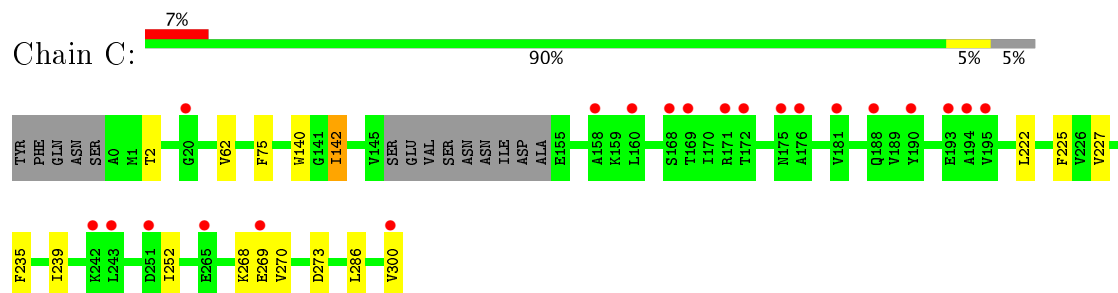
- Molecule 1: BmrU protein



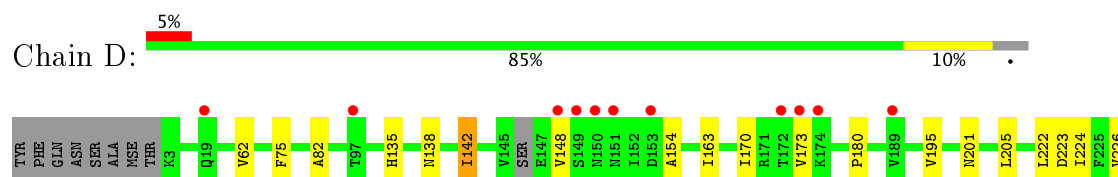
- Molecule 1: BmrU protein



- Molecule 1: BmrU protein



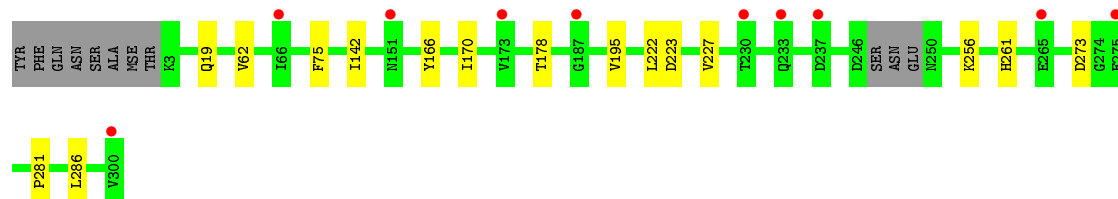
- Molecule 1: BmrU protein



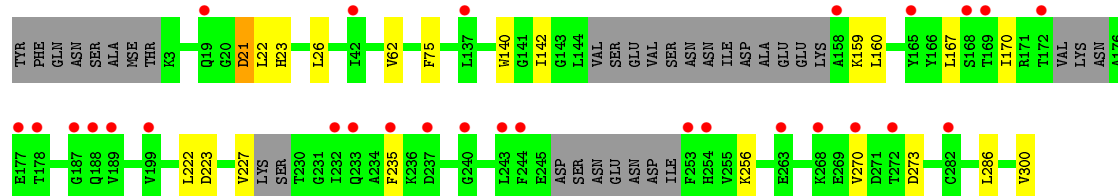
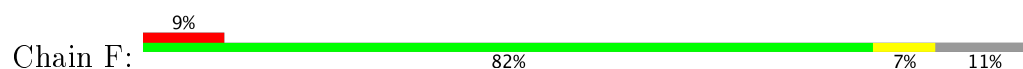




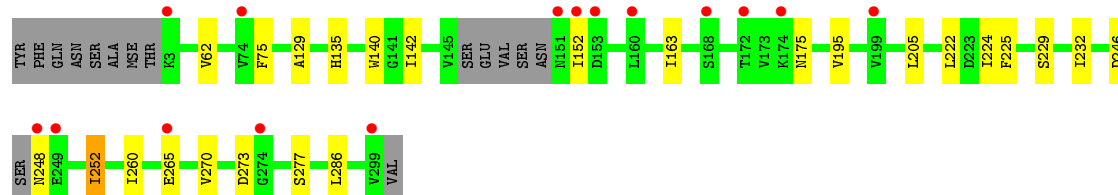
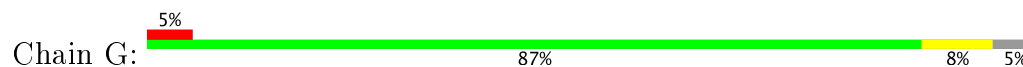
• Molecule 1: BmrU protein



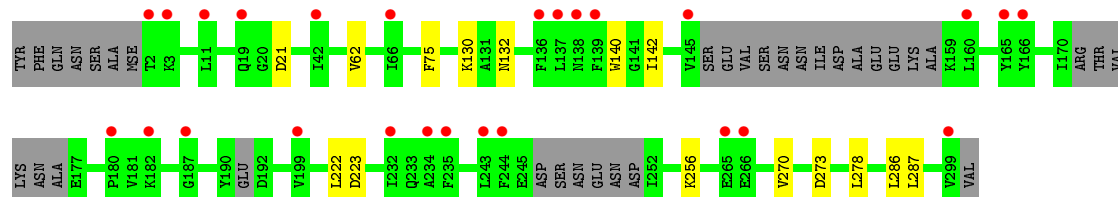
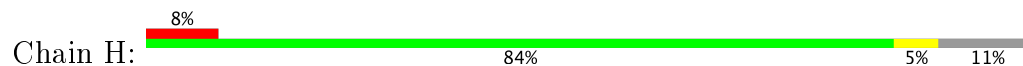
• Molecule 1: BmrU protein



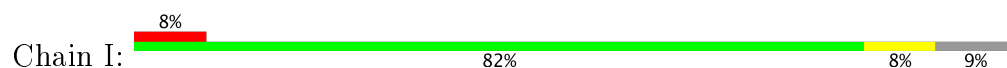
• Molecule 1: BmrU protein

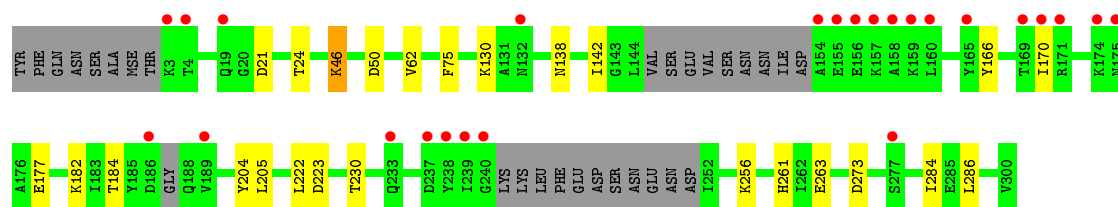


• Molecule 1: BmrU protein

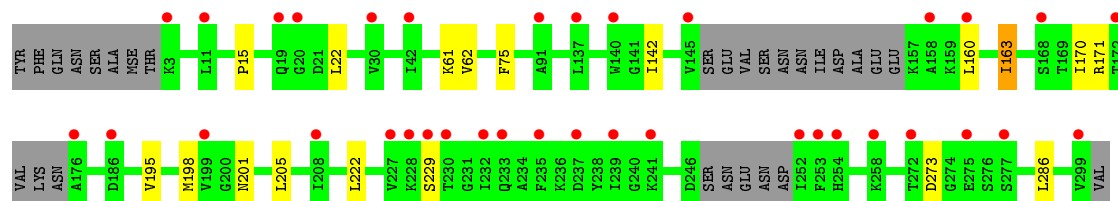
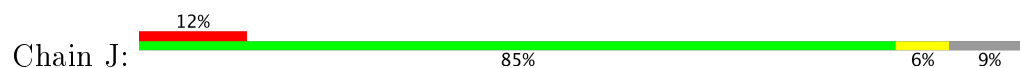


• Molecule 1: BmrU protein

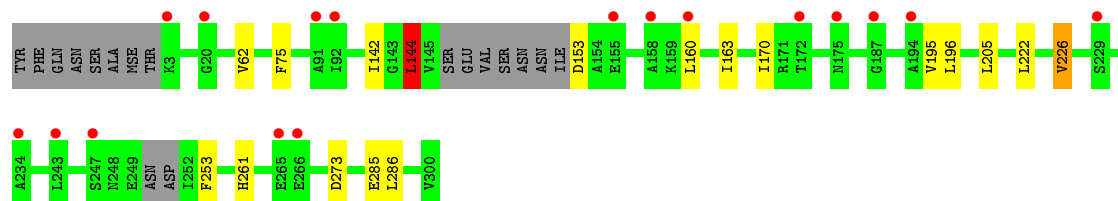
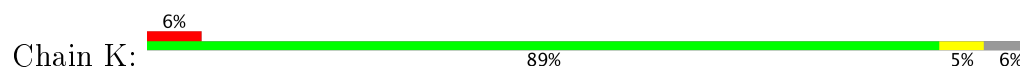




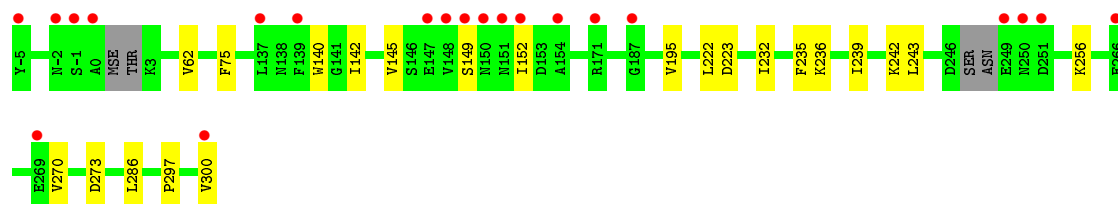
• Molecule 1: BmrU protein



• 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	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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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.

All (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
1:A:222:LEU:HG	1:A:286:LEU:HD13	1.67	0.76
1:E:222:LEU:HG	1:E:286:LEU:HD13	1.68	0.75
1:K:226:VAL:HG22	1:K:253:PHE:HB3	1.68	0.75
1:D:148:VAL:HG21	1:D:154:ALA:HB2	1.69	0.74
1:K:222:LEU:HG	1:K:286:LEU:HD13	1.69	0.74
1:L:222:LEU:HG	1:L:286:LEU:HD13	1.71	0.72
1:A:163:ILE:HD11	1:A:198:MSE:HE1	1.72	0.70
1:A:176:ALA:HB3	1:A:232:ILE:HD11	1.74	0.68
1:B:222:LEU:HG	1:B:286:LEU:HD13	1.76	0.68
1:C:222:LEU:HG	1:C:286:LEU:HD13	1.77	0.67
1:I:222:LEU:CG	1:I:286:LEU:HD13	2.24	0.66
1:G:163:ILE:HD13	1:G:205:LEU:HB3	1.78	0.66
1:D:226:VAL:O	1:D:252:ILE:CG2	2.44	0.65
1:J:163:ILE:HD11	1:J:198:MSE:HE1	1.79	0.65
1:J:222:LEU:HG	1:J:286:LEU:HD13	1.78	0.65
1:C:235:PHE:CE1	1:C:239:ILE:HD11	2.32	0.65
1:F:222:LEU:HG	1:F:286:LEU:HD13	1.78	0.65
1:G:222:LEU:HG	1:G:286:LEU:HD13	1.79	0.64
1:J:163:ILE:HD12	1:J:205:LEU:HB3	1.79	0.63
1:B:299:VAL:HG12	1:B:300:VAL:HG13	1.78	0.63
1:I:21:ASP:HB3	1:I:24:THR:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:ASP:O	1:G:248:ASN:N	2.32	0.63
1:F:21:ASP:OD1	1:F:23:HIS:N	2.32	0.62
1:A:144:LEU:HD13	1:A:196:LEU:HD11	1.81	0.62
1:C:235:PHE:CE1	1:C:239:ILE:CD1	2.82	0.62
1:F:159:LYS:O	1:F:160:LEU:CB	2.48	0.61
1:D:75:PHE:CD1	1:D:273:ASP:HB2	2.37	0.60
1:L:75:PHE:CD1	1:L:273:ASP:HB2	2.36	0.59
1:A:144:LEU:HD13	1:A:196:LEU:CD1	2.33	0.59
1:L:235:PHE:CZ	1:L:239:ILE:HD11	2.37	0.59
1:F:75:PHE:CD1	1:F:273:ASP:HB2	2.38	0.58
1:C:75:PHE:CD1	1:C:273:ASP:HB2	2.39	0.57
1:A:243:LEU:O	1:A:245:GLU:N	2.37	0.57
1:K:75:PHE:CD1	1:K:273:ASP:HB2	2.38	0.57
1:F:21:ASP:C	1:F:21:ASP:OD1	2.43	0.56
1:L:300:VAL:O	1:L:300:VAL:CG1	2.53	0.56
1:I:75:PHE:CD1	1:I:273:ASP:HB2	2.40	0.56
1:K:153:ASP:N	3:K:565:HOH:O	2.38	0.55
1:E:75:PHE:CD1	1:E:273:ASP:HB2	2.41	0.55
1:H:75:PHE:CD1	1:H:273:ASP:HB2	2.41	0.55
1:A:18:GLY:C	1:A:20:GLY:N	2.58	0.55
1:B:169:THR:O	1:B:173:VAL:HG23	2.07	0.55
1:B:248:ASN:O	1:B:251:ASP:N	2.39	0.55
1:K:144:LEU:HD13	1:K:196:LEU:HD11	1.88	0.55
1:A:213:PRO:HG3	1:A:238:TYR:OH	2.07	0.54
1:H:140:TRP:NE1	1:H:270:VAL:HG11	2.23	0.54
1:D:163:ILE:HG21	1:D:205:LEU:HB3	1.90	0.53
1:L:145:VAL:O	1:L:145:VAL:HG13	2.08	0.53
1:A:138:ASN:HB2	1:A:273:ASP:OD1	2.07	0.53
1:A:82:ALA:HB1	1:A:135:HIS:ND1	2.23	0.53
1:D:222:LEU:CG	1:D:286:LEU:HD13	2.33	0.53
1:D:180:PRO:HG2	1:D:265:GLU:CG	2.39	0.53
1:F:167:LEU:O	1:F:170:ILE:HG22	2.08	0.53
1:L:297:PRO:HA	1:L:300:VAL:CG2	2.35	0.52
1:D:223:ASP:OD1	1:D:256:LYS:NZ	2.41	0.52
1:A:195:VAL:HG23	1:A:229:SER:HA	1.91	0.52
1:L:300:VAL:O	1:L:300:VAL:HG12	2.10	0.51
1:B:283:GLN:OE1	1:D:281:PRO:HG2	2.10	0.51
1:A:18:GLY:C	1:A:20:GLY:H	2.13	0.51
1:C:142:ILE:HG21	1:C:268:LYS:HG2	1.92	0.51
1:J:75:PHE:CD1	1:J:273:ASP:HB2	2.45	0.51
1:K:144:LEU:HD13	1:K:196:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:CZ	1:C:252:ILE:HG21	2.46	0.50
1:G:75:PHE:CD1	1:G:273:ASP:HB2	2.48	0.49
1:K:222:LEU:CG	1:K:286:LEU:HD13	2.39	0.49
1:L:232:ILE:HG22	1:L:236:LYS:HE3	1.94	0.49
1:B:75:PHE:CD1	1:B:273:ASP:HB2	2.48	0.48
1:A:220:GLY:C	1:A:286:LEU:CD2	2.81	0.48
1:H:222:LEU:CG	1:H:286:LEU:HD13	2.38	0.48
1:E:222:LEU:CG	1:E:286:LEU:HD13	2.42	0.47
1:L:222:LEU:CG	1:L:286:LEU:HD13	2.43	0.47
1:B:61:LYS:HG2	3:D:515:HOH:O	2.15	0.47
1:B:165:TYR:CZ	1:B:169:THR:HG21	2.49	0.47
1:C:227:VAL:HG21	1:C:235:PHE:CD2	2.50	0.47
1:D:135:HIS:HD2	3:D:467:HOH:O	1.98	0.47
1:J:195:VAL:HG23	1:J:229:SER:HA	1.97	0.47
1:A:288:GLN:HG3	3:A:345:HOH:O	2.14	0.47
1:I:130:LYS:O	1:I:284:ILE:HA	2.15	0.47
1:D:235:PHE:CE1	1:D:239:ILE:HD11	2.50	0.47
1:I:184:THR:HB	1:I:261:HIS:HB3	1.97	0.46
1:A:82:ALA:CB	1:A:135:HIS:CG	2.99	0.46
1:A:144:LEU:CD1	1:A:196:LEU:HD11	2.44	0.46
1:G:175:ASN:HD21	1:G:232:ILE:HD12	1.80	0.46
1:F:22:LEU:HD11	1:F:26:LEU:HD11	1.98	0.46
1:D:82:ALA:HB1	1:D:135:HIS:CG	2.50	0.46
1:G:75:PHE:CE1	1:G:273:ASP:HB2	2.51	0.46
1:G:224:ILE:CG1	1:G:260:ILE:HD13	2.46	0.46
1:A:131:ALA:HA	1:A:283:GLN:O	2.16	0.45
1:G:163:ILE:HG21	1:G:205:LEU:HB3	1.97	0.45
1:D:82:ALA:CB	1:D:135:HIS:CG	2.99	0.45
1:D:170:ILE:CD1	1:D:235:PHE:CE2	2.98	0.45
1:A:130:LYS:O	1:A:284:ILE:HA	2.16	0.45
1:A:129:ALA:HB2	1:A:222:LEU:HD21	1.99	0.45
1:E:223:ASP:OD1	1:E:256:LYS:NZ	2.46	0.45
1:I:223:ASP:OD1	1:I:256:LYS:NZ	2.47	0.45
1:D:148:VAL:HG11	1:D:154:ALA:HA	1.99	0.45
1:G:195:VAL:HG23	1:G:229:SER:HA	1.99	0.45
1:I:182:LYS:HB3	1:I:263:GLU:HB2	1.99	0.45
1:I:46:LYS:HG3	1:I:50:ASP:OD2	2.17	0.45
1:L:235:PHE:O	1:L:239:ILE:HD12	2.16	0.45
1:A:163:ILE:HD13	1:A:205:LEU:HB3	1.98	0.45
1:E:195:VAL:HG12	1:E:227:VAL:O	2.17	0.45
1:J:170:ILE:HD12	1:J:171:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:CE1	1:C:252:ILE:HG21	2.51	0.45
1:C:142:ILE:CG2	1:C:268:LYS:HG2	2.47	0.44
1:A:82:ALA:HB1	1:A:135:HIS:CE1	2.53	0.44
1:D:170:ILE:HD11	1:D:235:PHE:CD2	2.51	0.44
1:B:163:ILE:HG21	1:B:205:LEU:HB3	2.00	0.44
1:D:195:VAL:HG12	1:D:227:VAL:O	2.17	0.44
1:I:166:TYR:CZ	1:I:170:ILE:HD13	2.52	0.44
1:I:204:TYR:O	1:I:205:LEU:HD23	2.18	0.44
1:C:222:LEU:CG	1:C:286:LEU:HD13	2.47	0.44
1:J:201:ASN:HA	3:J:324:HOH:O	2.17	0.44
1:D:201:ASN:HA	3:D:303:HOH:O	2.17	0.44
1:G:129:ALA:O	1:G:135:HIS:HA	2.18	0.44
1:H:223:ASP:OD1	1:H:256:LYS:NZ	2.50	0.44
1:D:82:ALA:HB1	1:D:135:HIS:ND1	2.33	0.44
1:H:130:LYS:HE3	1:H:287:LEU:HD11	2.00	0.43
1:H:132:ASN:HB2	1:H:278:LEU:HD11	1.99	0.43
1:A:18:GLY:O	1:A:20:GLY:N	2.52	0.43
1:J:170:ILE:HD12	1:J:171:ARG:H	1.82	0.43
1:E:281:PRO:HG2	1:K:261:HIS:CD2	2.54	0.43
1:F:21:ASP:OD1	1:F:22:LEU:N	2.52	0.43
1:B:201:ASN:HA	3:B:302:HOH:O	2.18	0.43
1:L:243:LEU:HA	1:L:243:LEU:HD12	1.83	0.42
1:D:180:PRO:HG2	1:D:265:GLU:HG2	2.01	0.42
1:L:140:TRP:NE1	1:L:270:VAL:HG11	2.34	0.42
1:D:135:HIS:HE1	3:D:315:HOH:O	2.01	0.42
1:D:170:ILE:HD11	1:D:235:PHE:CE2	2.54	0.42
1:D:235:PHE:CZ	1:D:239:ILE:HD11	2.55	0.42
1:C:227:VAL:HG21	1:C:235:PHE:CE2	2.55	0.42
1:E:166:TYR:CZ	1:E:170:ILE:CD1	3.02	0.42
1:B:223:ASP:OD1	1:B:256:LYS:NZ	2.52	0.42
1:F:227:VAL:HG21	1:F:235:PHE:CD1	2.55	0.42
1:B:82:ALA:N	1:B:83:PRO:CD	2.83	0.42
1:D:138:ASN:HB2	1:D:273:ASP:OD1	2.19	0.42
1:D:224:ILE:O	1:D:254:HIS:HD2	2.03	0.42
1:B:145:VAL:O	1:B:145:VAL:HG12	2.19	0.41
1:I:138:ASN:HB2	1:I:273:ASP:OD1	2.20	0.41
1:K:144:LEU:CD1	1:K:196:LEU:HD11	2.50	0.41
1:K:163:ILE:HG21	1:K:205:LEU:HB3	2.03	0.41
1:F:223:ASP:OD1	1:F:256:LYS:NZ	2.52	0.41
1:G:140:TRP:NE1	1:G:270:VAL:HG11	2.35	0.41
1:J:15:PRO:HA	1:J:22:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ILE:HA	1:E:170:ILE:HD12	1.95	0.41
1:A:221:THR:N	1:A:286:LEU:HD22	2.35	0.41
1:C:140:TRP:NE1	1:C:270:VAL:HG11	2.34	0.41
1:F:140:TRP:NE1	1:F:270:VAL:HG11	2.35	0.41
1:G:225:PHE:CE1	1:G:252:ILE:HG21	2.55	0.41
1:L:223:ASP:OD1	1:L:256:LYS:NZ	2.51	0.41
1:A:163:ILE:HG21	1:A:205:LEU:HB3	2.02	0.41
1:B:222:LEU:CG	1:B:286:LEU:HD13	2.49	0.41
1:D:224:ILE:HD12	1:D:255:VAL:HG13	2.03	0.41
3:A:311:HOH:O	1:J:61:LYS:HG2	2.21	0.41
1:L:149:SER:HA	1:L:152:ILE:HD11	2.03	0.40
1:F:140:TRP:CD1	1:F:270:VAL:HG11	2.55	0.40
1:D:142:ILE:HG21	1:D:268:LYS:HD3	2.03	0.40
1:E:261:HIS:HE2	1:K:261:HIS:CE1	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	38	59
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%)	44	66
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%)	38	59
1	H	262/306 (86%)	256 (98%)	6 (2%)	0	100	100
1	I	269/306 (88%)	259 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	55	76

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%)	50	77
1	B	244/257 (95%)	241 (99%)	3 (1%)	75	91
1	C	225/257 (88%)	220 (98%)	5 (2%)	57	82
1	D	235/257 (91%)	232 (99%)	3 (1%)	73	90
1	E	229/257 (89%)	225 (98%)	4 (2%)	66	87
1	F	210/257 (82%)	206 (98%)	4 (2%)	62	85
1	G	227/257 (88%)	222 (98%)	5 (2%)	57	82
1	H	194/257 (76%)	191 (98%)	3 (2%)	70	89
1	I	217/257 (84%)	212 (98%)	5 (2%)	56	81
1	J	215/257 (84%)	211 (98%)	4 (2%)	62	85
1	K	226/257 (88%)	218 (96%)	8 (4%)	41	68
1	L	242/257 (94%)	238 (98%)	4 (2%)	66	87
All	All	2688/3084 (87%)	2634 (98%)	54 (2%)	60	84

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	142	ILE
1	A	163	ILE
1	A	248	ASN
1	A	249	GLU
1	A	300	VAL
1	B	62	VAL
1	B	142	ILE
1	B	189	VAL
1	C	2	THR
1	C	62	VAL
1	C	142	ILE
1	C	269	GLU
1	C	300	VAL
1	D	62	VAL
1	D	142	ILE
1	D	251	ASP
1	E	19	GLN
1	E	62	VAL
1	E	142	ILE
1	E	178	THR
1	F	21	ASP
1	F	62	VAL
1	F	142	ILE
1	F	300	VAL
1	G	62	VAL
1	G	142	ILE
1	G	252	ILE
1	G	265	GLU
1	G	277	SER
1	H	21	ASP
1	H	62	VAL
1	H	142	ILE
1	I	46	LYS
1	I	62	VAL
1	I	142	ILE
1	I	177	GLU
1	I	230	THR
1	J	62	VAL
1	J	142	ILE
1	J	160	LEU
1	J	163	ILE

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Mol	Chain	Res	Type
1	K	62	VAL
1	K	142	ILE
1	K	144	LEU
1	K	160	LEU
1	K	170	ILE
1	K	195	VAL
1	K	226	VAL
1	K	285	GLU
1	L	62	VAL
1	L	142	ILE
1	L	195	VAL
1	L	242	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	D	135	HIS
1	D	175	ASN
1	D	188	GLN
1	F	135	HIS
1	G	23	HIS
1	G	135	HIS
1	G	261	HIS
1	K	135	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 ⓘ

### 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<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%)	0.34	27 (9%) 9 8	38, 63, 97, 125	0
1	B	297/306 (97%)	0.24	18 (6%) 22 22	30, 53, 98, 109	0
1	C	289/306 (94%)	0.19	21 (7%) 16 16	38, 64, 111, 126	0
1	D	291/306 (95%)	0.27	15 (5%) 28 29	33, 57, 109, 130	0
1	E	293/306 (95%)	0.10	10 (3%) 46 48	37, 62, 103, 112	0
1	F	271/306 (88%)	0.48	28 (10%) 7 6	35, 66, 133, 166	0
1	G	289/306 (94%)	0.31	15 (5%) 28 29	34, 59, 102, 139	0
1	H	270/306 (88%)	0.48	26 (9%) 9 8	44, 78, 127, 139	0
1	I	275/306 (89%)	0.34	25 (9%) 10 10	36, 62, 109, 130	0
1	J	276/306 (90%)	0.63	36 (13%) 4 3	36, 73, 115, 141	2 (0%)
1	K	287/306 (93%)	0.07	17 (5%) 23 24	33, 56, 106, 124	0
1	L	300/306 (98%)	0.27	21 (7%) 17 17	34, 58, 100, 111	0
All	All	3423/3672 (93%)	0.31	259 (7%) 15 14	30, 63, 110, 166	2 (0%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	154	ALA	7.9
1	H	299	VAL	7.0
1	F	232	ILE	6.6
1	L	-5	TYR	5.7
1	J	253	PHE	5.6
1	I	169	THR	5.5
1	G	153	ASP	5.5
1	F	169	THR	5.2
1	I	171	ARG	5.2
1	H	165	TYR	5.2
1	B	148	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	299	VAL	5.1
1	C	172	THR	5.1
1	G	151	ASN	4.9
1	H	2	THR	4.7
1	D	149	SER	4.7
1	L	187	GLY	4.6
1	F	235	PHE	4.6
1	F	172	THR	4.5
1	H	160	LEU	4.5
1	L	0	ALA	4.4
1	A	160	LEU	4.4
1	J	145	VAL	4.4
1	L	148	VAL	4.4
1	G	299	VAL	4.4
1	J	252	ILE	4.3
1	H	234	ALA	4.3
1	G	152	ILE	4.3
1	F	237	ASP	4.3
1	F	168	SER	4.2
1	I	165	TYR	4.1
1	B	2	THR	4.1
1	F	165	TYR	4.1
1	I	170	ILE	4.0
1	A	172	THR	4.0
1	F	178	THR	4.0
1	J	176	ALA	4.0
1	J	254	HIS	3.9
1	C	158	ALA	3.8
1	B	149	SER	3.8
1	H	235	PHE	3.7
1	D	148	VAL	3.7
1	F	233	GLN	3.7
1	I	174	LYS	3.7
1	E	173	VAL	3.7
1	A	248	ASN	3.6
1	D	174	LYS	3.6
1	A	199	VAL	3.6
1	J	199	VAL	3.5
1	B	197	VAL	3.5
1	H	145	VAL	3.5
1	I	240	GLY	3.5
1	I	238	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	299	VAL	3.5
1	B	199	VAL	3.4
1	G	265	GLU	3.4
1	E	151	ASN	3.3
1	F	240	GLY	3.3
1	F	177	GLU	3.3
1	D	173	VAL	3.3
1	A	299	VAL	3.3
1	J	229	SER	3.3
1	I	237	ASP	3.3
1	G	168	SER	3.3
1	K	160	LEU	3.2
1	J	237	ASP	3.2
1	A	19	GLN	3.2
1	A	229	SER	3.2
1	K	194	ALA	3.2
1	L	171	ARG	3.2
1	K	3	LYS	3.2
1	H	11	LEU	3.2
1	B	147	GLU	3.2
1	I	3	LYS	3.2
1	A	300	VAL	3.2
1	I	158	ALA	3.1
1	C	181	VAL	3.1
1	A	174	LYS	3.1
1	C	171	ARG	3.1
1	H	243	LEU	3.1
1	H	139	PHE	3.1
1	C	169	THR	3.1
1	D	153	ASP	3.1
1	E	187	GLY	3.1
1	F	187	GLY	3.1
1	F	158	ALA	3.1
1	I	160	LEU	3.1
1	J	158	ALA	3.1
1	L	147	GLU	3.0
1	E	230	THR	3.0
1	K	243	LEU	3.0
1	L	300	VAL	3.0
1	I	155	GLU	3.0
1	D	172	THR	3.0
1	I	175	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	235	PHE	3.0
1	J	228	LYS	3.0
1	L	151	ASN	3.0
1	C	243	LEU	2.9
1	L	154	ALA	2.9
1	C	175	ASN	2.9
1	L	269	GLU	2.9
1	F	244	PHE	2.9
1	J	208	ILE	2.9
1	J	160	LEU	2.9
1	H	19	GLN	2.9
1	L	150	ASN	2.9
1	A	265	GLU	2.9
1	H	187	GLY	2.9
1	B	146	SER	2.9
1	I	157	LYS	2.9
1	F	199	VAL	2.8
1	I	189	VAL	2.8
1	A	157	LYS	2.8
1	B	175	ASN	2.8
1	D	97	THR	2.8
1	J	277	SER	2.8
1	I	239	ILE	2.8
1	L	-2	ASN	2.8
1	I	159	LYS	2.8
1	F	189	VAL	2.7
1	J	275	GLU	2.7
1	D	151	ASN	2.7
1	B	154	ALA	2.7
1	D	150	ASN	2.7
1	E	300	VAL	2.7
1	C	194	ALA	2.7
1	I	277	SER	2.6
1	G	172	THR	2.6
1	I	4	THR	2.6
1	B	140	TRP	2.6
1	C	168	SER	2.6
1	K	172	THR	2.6
1	L	250	ASN	2.6
1	B	174	LYS	2.6
1	H	182	LYS	2.6
1	A	187	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	188	GLN	2.6
1	H	265	GLU	2.6
1	D	189	VAL	2.6
1	J	137	LEU	2.6
1	A	140	TRP	2.6
1	A	197	VAL	2.6
1	A	175	ASN	2.6
1	J	3	LYS	2.5
1	F	42	ILE	2.5
1	J	140	TRP	2.5
1	H	137	LEU	2.5
1	C	160	LEU	2.5
1	L	266	GLU	2.5
1	J	239	ILE	2.5
1	K	266	GLU	2.5
1	D	298	ALA	2.5
1	J	20	GLY	2.5
1	G	3	LYS	2.5
1	H	138	ASN	2.5
1	J	230	THR	2.4
1	A	20	GLY	2.4
1	B	172	THR	2.4
1	A	269	GLU	2.4
1	B	173	VAL	2.4
1	A	165	TYR	2.4
1	A	158	ALA	2.4
1	A	298	ALA	2.4
1	J	30	VAL	2.4
1	F	19	GLN	2.4
1	B	176	ALA	2.4
1	F	272	THR	2.4
1	A	48	GLN	2.4
1	E	265	GLU	2.4
1	F	270	VAL	2.4
1	C	176	ALA	2.4
1	I	186	ASP	2.3
1	H	166	TYR	2.3
1	H	199	VAL	2.3
1	H	180	PRO	2.3
1	C	190	TYR	2.3
1	J	91	ALA	2.3
1	A	97	THR	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	186	ASP	2.3
1	F	282	CYS	2.3
1	A	42	ILE	2.3
1	K	175	ASN	2.3
1	J	272	THR	2.3
1	J	241	LYS	2.3
1	L	251	ASP	2.3
1	G	248	ASN	2.3
1	J	168	SER	2.3
1	K	187	GLY	2.3
1	K	158	ALA	2.3
1	C	242	LYS	2.3
1	K	234	ALA	2.3
1	J	172	THR	2.3
1	I	132	ASN	2.2
1	D	246	ASP	2.2
1	D	19	GLN	2.2
1	H	66	ILE	2.2
1	F	268	LYS	2.2
1	K	229	SER	2.2
1	G	160	LEU	2.2
1	C	195	VAL	2.2
1	G	74	VAL	2.2
1	J	227	VAL	2.2
1	C	251	ASP	2.2
1	C	300	VAL	2.2
1	K	265	GLU	2.2
1	B	248	ASN	2.2
1	C	265	GLU	2.2
1	F	263	GLU	2.2
1	E	237	ASP	2.2
1	L	152	ILE	2.2
1	A	141	GLY	2.2
1	H	136	PHE	2.2
1	F	137	LEU	2.2
1	J	11	LEU	2.2
1	L	249	GLU	2.2
1	I	19	GLN	2.1
1	L	-1	SER	2.2
1	A	161	GLY	2.1
1	I	156	GLU	2.1
1	A	40	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	3	LYS	2.1
1	I	233	GLN	2.1
1	H	232	ILE	2.1
1	J	232	ILE	2.1
1	H	244	PHE	2.1
1	B	243	LEU	2.1
1	C	193	GLU	2.1
1	F	188	GLN	2.1
1	J	42	ILE	2.1
1	B	247	SER	2.1
1	H	266	GLU	2.1
1	G	274	GLY	2.1
1	L	139	PHE	2.1
1	K	91	ALA	2.1
1	G	249	GLU	2.1
1	F	254	HIS	2.1
1	K	20	GLY	2.1
1	C	269	GLU	2.1
1	E	66	ILE	2.1
1	K	92	ILE	2.1
1	L	149	SER	2.1
1	J	258	LYS	2.1
1	D	245	GLU	2.0
1	E	233	GLN	2.0
1	J	19	GLN	2.0
1	J	233	GLN	2.0
1	E	275	GLU	2.0
1	G	199	VAL	2.0
1	A	138	ASN	2.0
1	G	174	LYS	2.0
1	B	141	GLY	2.0
1	C	20	GLY	2.0
1	H	42	ILE	2.0
1	K	155	GLU	2.0
1	K	247	SER	2.0
1	F	243	LEU	2.0
1	L	137	LEU	2.0
1	F	253	PHE	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 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( $\text{\AA}^2$ )	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.