



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 04:35 PM JST

PDB ID : 6JOH  
Title : The crystal of nucleoside diphosphate kinase from *Aspergillus flavus*  
Authors : Wang, Y.; Wang, S.; Wang, S.H.  
Deposited on : 2019-03-21  
Resolution : 2.40 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

<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>.

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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) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

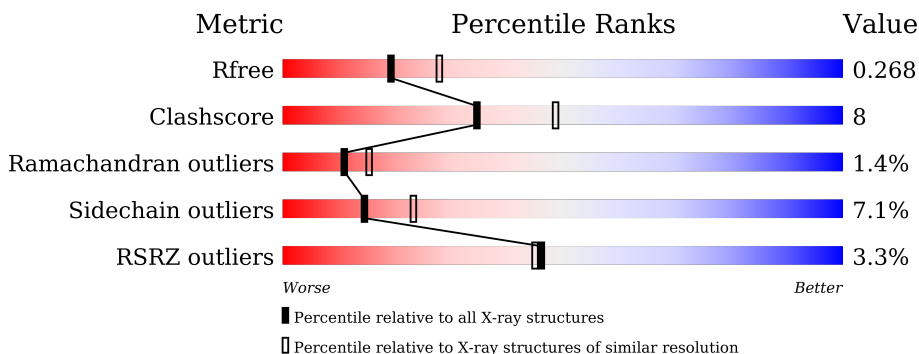
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	155	
1	B	155	
1	C	155	
1	D	155	
1	E	155	
1	F	155	

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Mol	Chain	Length	Quality of chain
1	G	155	3% 68% 23% 5%
1	H	155	8% 77% 15% 5%
1	I	155	83% 14%
1	J	155	2% 88% 8%
1	K	155	82% 13% 5%
1	L	155	6% 72% 21% 5%
1	M	155	82% 13%
1	N	155	12% 74% 17% 5%
1	O	155	78% 15%
1	P	155	3% 79% 16% 2%
1	Q	155	85% 10%
1	R	155	81% 13%
1	S	155	73% 21%
1	T	155	2% 84% 12%
1	U	155	3% 78% 14% 5%
1	V	155	3% 78% 16% 3%
1	W	155	14% 66% 24% 5%
1	X	155	10% 58% 32% 5%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28040 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1162	748	200	210	4	0	0	0
1	B	149	1169	750	201	214	4	0	0	0
1	C	149	1171	752	201	214	4	0	0	0
1	D	149	1171	752	201	214	4	0	0	0
1	E	149	1171	752	201	214	4	0	0	0
1	F	149	1171	752	201	214	4	0	0	0
1	G	148	1159	745	200	210	4	0	0	0
1	H	148	1162	748	200	210	4	0	0	0
1	I	149	1171	752	201	214	4	0	0	0
1	J	149	1171	752	201	214	4	0	0	0
1	K	148	1159	745	200	210	4	0	0	0
1	L	148	1162	748	200	210	4	0	0	0
1	M	149	1171	752	201	214	4	0	0	0
1	N	149	1171	752	201	214	4	0	0	0
1	Q	149	1171	752	201	214	4	0	0	0
1	R	149	1171	752	201	214	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	148	Total	C	N	O	S	0	0	0
			1162	748	200	210	4			
1	V	149	Total	C	N	O	S	0	0	0
			1169	750	201	214	4			
1	W	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	X	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	O	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	P	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	S	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	T	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B8NQF0
A	0	PRO	-	expression tag	UNP B8NQF0
B	-1	GLY	-	expression tag	UNP B8NQF0
B	0	PRO	-	expression tag	UNP B8NQF0
C	-1	GLY	-	expression tag	UNP B8NQF0
C	0	PRO	-	expression tag	UNP B8NQF0
D	-1	GLY	-	expression tag	UNP B8NQF0
D	0	PRO	-	expression tag	UNP B8NQF0
E	-1	GLY	-	expression tag	UNP B8NQF0
E	0	PRO	-	expression tag	UNP B8NQF0
F	-1	GLY	-	expression tag	UNP B8NQF0
F	0	PRO	-	expression tag	UNP B8NQF0
G	-1	GLY	-	expression tag	UNP B8NQF0
G	0	PRO	-	expression tag	UNP B8NQF0
H	-1	GLY	-	expression tag	UNP B8NQF0
H	0	PRO	-	expression tag	UNP B8NQF0
I	-1	GLY	-	expression tag	UNP B8NQF0
I	0	PRO	-	expression tag	UNP B8NQF0
J	-1	GLY	-	expression tag	UNP B8NQF0
J	0	PRO	-	expression tag	UNP B8NQF0
K	-1	GLY	-	expression tag	UNP B8NQF0
K	0	PRO	-	expression tag	UNP B8NQF0
L	-1	GLY	-	expression tag	UNP B8NQF0

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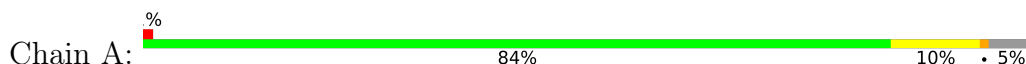
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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	PRO	-	expression tag	UNP B8NQF0
M	-1	GLY	-	expression tag	UNP B8NQF0
M	0	PRO	-	expression tag	UNP B8NQF0
N	-1	GLY	-	expression tag	UNP B8NQF0
N	0	PRO	-	expression tag	UNP B8NQF0
Q	-1	GLY	-	expression tag	UNP B8NQF0
Q	0	PRO	-	expression tag	UNP B8NQF0
R	-1	GLY	-	expression tag	UNP B8NQF0
R	0	PRO	-	expression tag	UNP B8NQF0
U	-1	GLY	-	expression tag	UNP B8NQF0
U	0	PRO	-	expression tag	UNP B8NQF0
V	-1	GLY	-	expression tag	UNP B8NQF0
V	0	PRO	-	expression tag	UNP B8NQF0
W	-1	GLY	-	expression tag	UNP B8NQF0
W	0	PRO	-	expression tag	UNP B8NQF0
X	-1	GLY	-	expression tag	UNP B8NQF0
X	0	PRO	-	expression tag	UNP B8NQF0
O	-1	GLY	-	expression tag	UNP B8NQF0
O	0	PRO	-	expression tag	UNP B8NQF0
P	-1	GLY	-	expression tag	UNP B8NQF0
P	0	PRO	-	expression tag	UNP B8NQF0
S	-1	GLY	-	expression tag	UNP B8NQF0
S	0	PRO	-	expression tag	UNP B8NQF0
T	-1	GLY	-	expression tag	UNP B8NQF0
T	0	PRO	-	expression tag	UNP B8NQF0

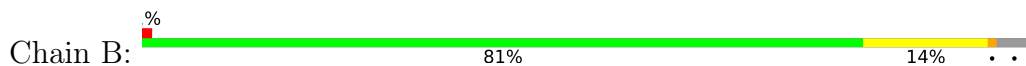
### 3 Residue-property plots [i](#)

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.

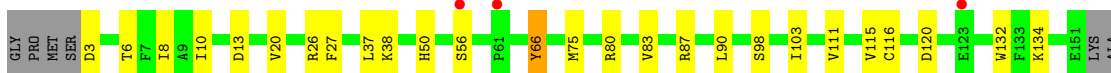
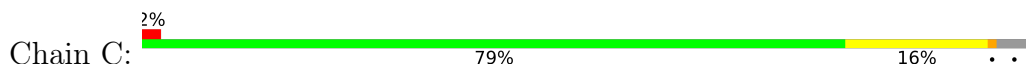
- Molecule 1: Nucleoside diphosphate kinase



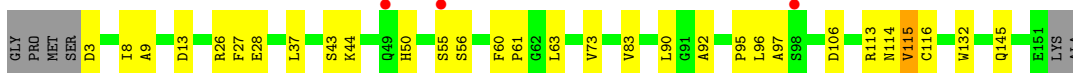
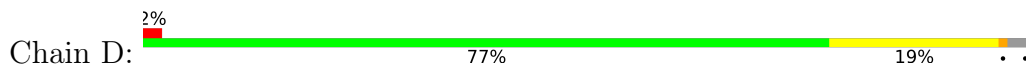
- Molecule 1: Nucleoside diphosphate kinase



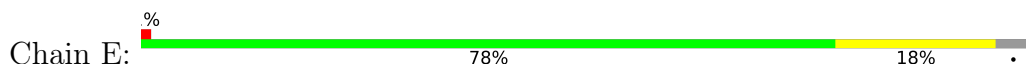
- Molecule 1: Nucleoside diphosphate kinase




- Molecule 1: Nucleoside diphosphate kinase

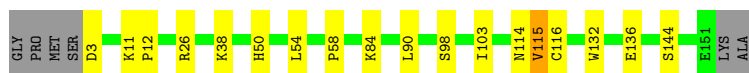


- Molecule 1: Nucleoside diphosphate kinase



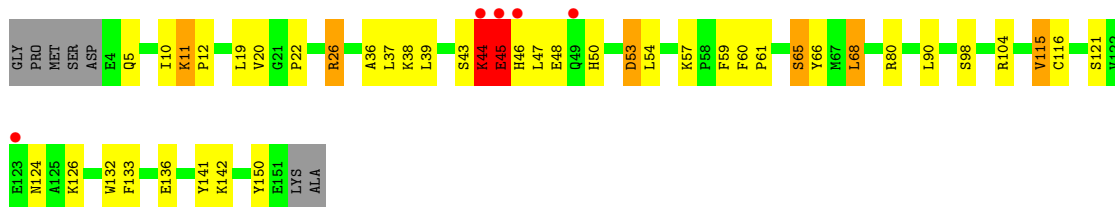
- Molecule 1: Nucleoside diphosphate kinase

Chain F:  85% 11% . .




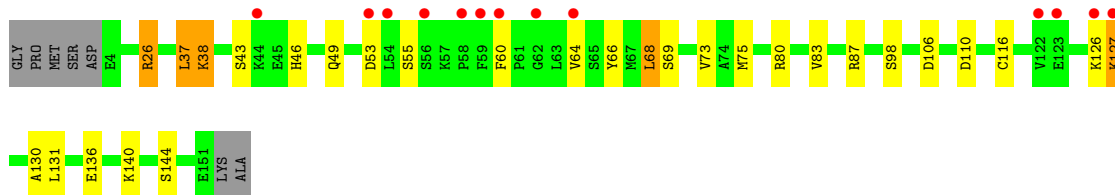
• Molecule 1: Nucleoside diphosphate kinase

Chain G:  3% 68% 23% . . 5%




• Molecule 1: Nucleoside diphosphate kinase

Chain H:  8% 77% 15% . 5%




• Molecule 1: Nucleoside diphosphate kinase

Chain I:  83% 14% .




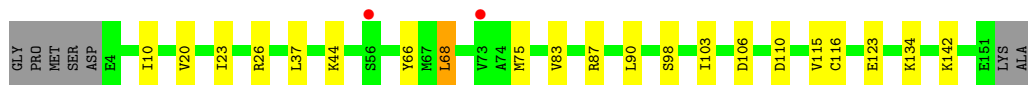
• Molecule 1: Nucleoside diphosphate kinase

Chain J:  2% 88% 8% .



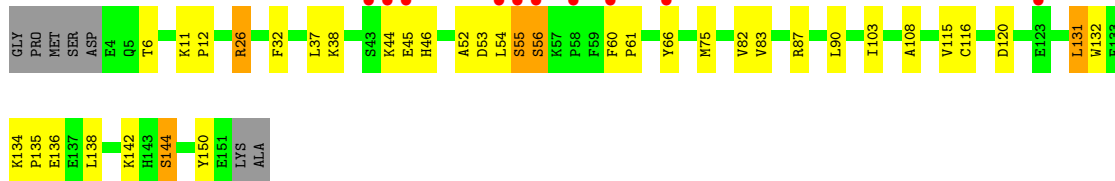
• Molecule 1: Nucleoside diphosphate kinase

Chain K:  % 82% 13% . 5%

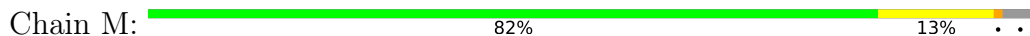


• Molecule 1: Nucleoside diphosphate kinase

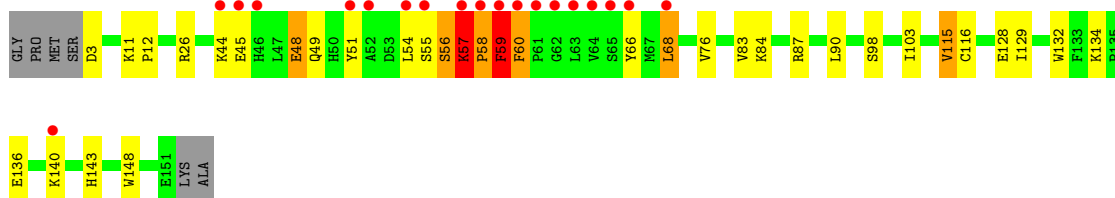
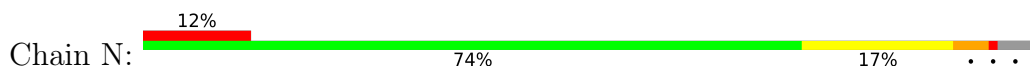




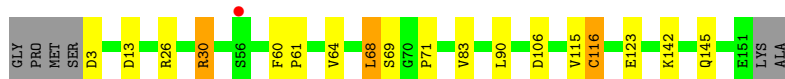
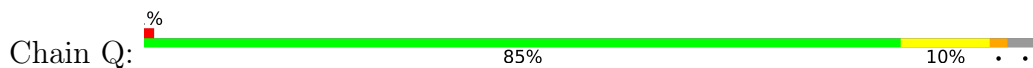
- Molecule 1: Nucleoside diphosphate kinase



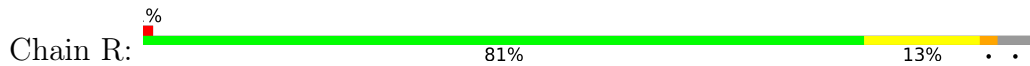
- Molecule 1: Nucleoside diphosphate kinase



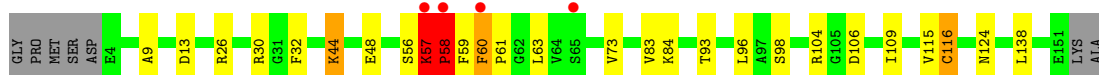
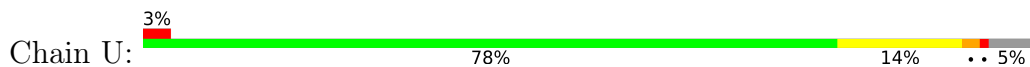
- Molecule 1: Nucleoside diphosphate kinase



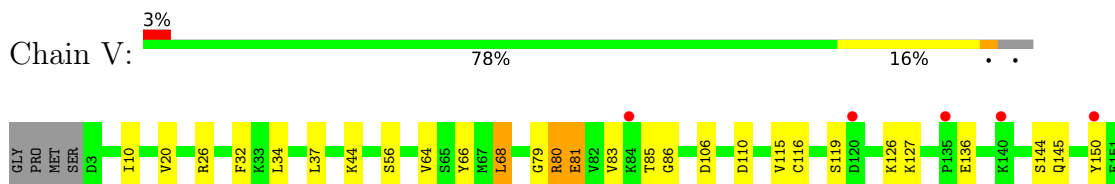
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

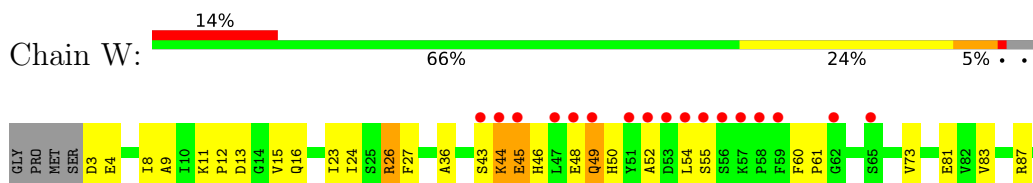


- Molecule 1: Nucleoside diphosphate kinase



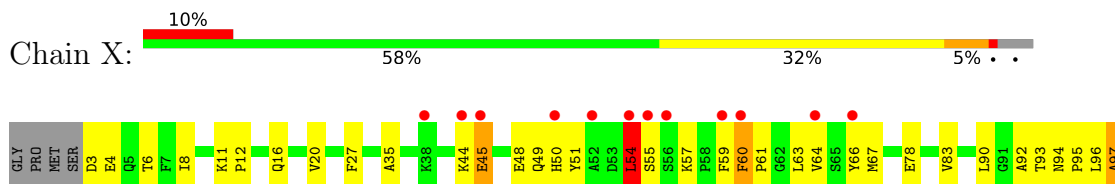
LYS  
ALA

- Molecule 1: Nucleoside diphosphate kinase



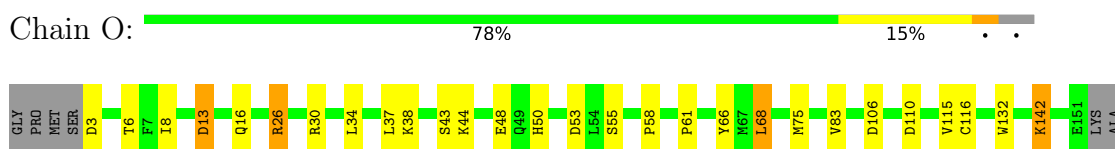
A87 S88 R104 G105 D106 F107 A108 I109 V115 C116 E123 N124 E128 W132 F133 Y141 S144 E151 LYS ALA

- Molecule 1: Nucleoside diphosphate kinase

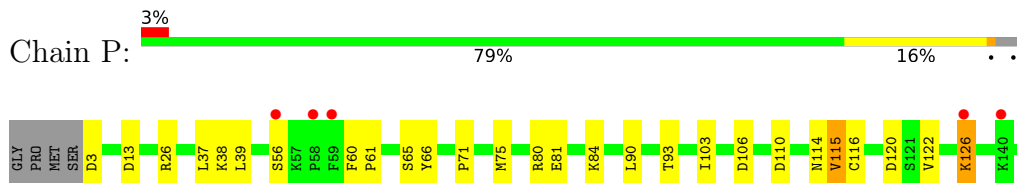


S88 A99 I103 R104 D110 V111 G112 R113 N114 V115 C116 S119 E123 N124 A125 K126 I129 W132 F133 K134 P135 E136 L138 Q139 K140 Y141 S144 Q145 E151 LYS ALA

- Molecule 1: Nucleoside diphosphate kinase

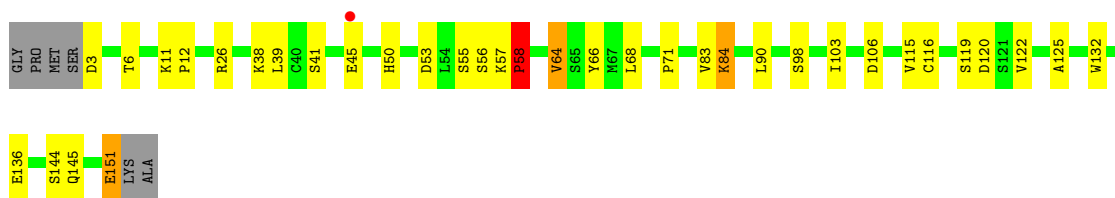


- Molecule 1: Nucleoside diphosphate kinase

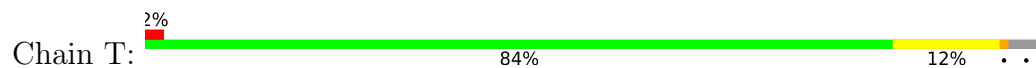


- Molecule 1: Nucleoside diphosphate kinase





- Molecule 1: Nucleoside diphosphate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.84Å 169.47Å 146.94Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	33.69 – 2.40 33.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (33.69-2.40) 98.9 (33.67-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.222 , 0.268 0.225 , 0.268	Depositor DCC
$R_{free}$ test set	8979 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtrriage
Anisotropy	0.441	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	0/1192	0.87	0/1612
1	B	0.69	0/1198	0.84	0/1619
1	C	0.74	0/1201	0.84	0/1624
1	D	0.71	0/1201	0.85	0/1624
1	E	0.74	0/1201	0.87	0/1624
1	F	0.71	0/1201	0.85	0/1624
1	G	0.74	0/1189	0.90	0/1608
1	H	0.70	0/1192	0.87	0/1612
1	I	0.73	0/1201	0.88	0/1624
1	J	0.72	0/1201	0.85	0/1624
1	K	0.71	0/1189	0.87	0/1608
1	L	0.73	0/1192	0.88	0/1612
1	M	0.73	0/1201	0.86	0/1624
1	N	0.71	0/1201	0.87	0/1624
1	O	0.74	0/1201	0.90	0/1624
1	P	0.69	0/1201	0.86	0/1624
1	Q	0.70	0/1201	0.89	0/1624
1	R	0.69	0/1201	0.84	0/1624
1	S	0.69	0/1201	0.85	0/1624
1	T	0.71	0/1201	0.89	1/1624 (0.1%)
1	U	0.76	0/1192	0.93	1/1612 (0.1%)
1	V	0.72	0/1198	0.86	0/1619
1	W	0.74	0/1201	0.87	0/1624
1	X	0.75	0/1201	0.93	0/1624
All	All	0.72	0/28758	0.87	2/38886 (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	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	H	0	2
1	L	0	2
1	N	0	2
1	S	0	1
1	U	0	2
1	W	0	2
1	X	0	6
All	All	0	20

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	58	PRO	CA-N-CD	-5.77	103.42	111.50
1	T	140	LYS	CB-CA-C	5.71	121.82	110.40

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	56	SER	Peptide
1	G	44	LYS	Peptide
1	G	45	GLU	Peptide
1	H	127	LYS	Peptide
1	H	37	LEU	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1162	0	1157	9	0
1	B	1169	0	1158	15	0
1	C	1171	0	1164	11	0
1	D	1171	0	1164	17	0
1	E	1171	0	1164	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1171	0	1164	10	0
1	G	1159	0	1148	54	0
1	H	1162	0	1157	60	0
1	I	1171	0	1164	12	0
1	J	1171	0	1164	6	0
1	K	1159	0	1148	9	0
1	L	1162	0	1157	21	0
1	M	1171	0	1164	9	0
1	N	1171	0	1163	86	0
1	O	1171	0	1164	18	0
1	P	1171	0	1164	16	0
1	Q	1171	0	1164	7	0
1	R	1171	0	1164	12	0
1	S	1171	0	1164	18	0
1	T	1171	0	1164	11	0
1	U	1162	0	1157	81	0
1	V	1169	0	1158	21	0
1	W	1171	0	1164	31	0
1	X	1171	0	1164	42	0
All	All	28040	0	27863	464	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 8.

The worst 5 of 464 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:N:56:SER:N	1:U:58:PRO:HA	1.30	1.45
1:G:38:LYS:HA	1:H:38:LYS:CG	1.50	1.41
1:N:57:LYS:CB	1:U:58:PRO:CD	1.98	1.40
1:N:57:LYS:CG	1:U:58:PRO:HD3	1.58	1.33
1:N:56:SER:OG	1:U:59:PHE:C	1.86	1.15

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	146/155 (94%)	142 (97%)	3 (2%)	1 (1%)	22	32
1	B	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	22	32
1	C	147/155 (95%)	140 (95%)	6 (4%)	1 (1%)	22	32
1	D	147/155 (95%)	134 (91%)	11 (8%)	2 (1%)	11	15
1	E	147/155 (95%)	143 (97%)	3 (2%)	1 (1%)	22	32
1	F	147/155 (95%)	140 (95%)	5 (3%)	2 (1%)	11	15
1	G	146/155 (94%)	131 (90%)	11 (8%)	4 (3%)	5	5
1	H	146/155 (94%)	136 (93%)	9 (6%)	1 (1%)	22	32
1	I	147/155 (95%)	142 (97%)	3 (2%)	2 (1%)	11	15
1	J	147/155 (95%)	142 (97%)	4 (3%)	1 (1%)	22	32
1	K	146/155 (94%)	140 (96%)	5 (3%)	1 (1%)	22	32
1	L	146/155 (94%)	133 (91%)	9 (6%)	4 (3%)	5	5
1	M	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	22	32
1	N	147/155 (95%)	132 (90%)	9 (6%)	6 (4%)	3	2
1	O	147/155 (95%)	141 (96%)	5 (3%)	1 (1%)	22	32
1	P	147/155 (95%)	135 (92%)	11 (8%)	1 (1%)	22	32
1	Q	147/155 (95%)	140 (95%)	6 (4%)	1 (1%)	22	32
1	R	147/155 (95%)	143 (97%)	3 (2%)	1 (1%)	22	32
1	S	147/155 (95%)	139 (95%)	6 (4%)	2 (1%)	11	15
1	T	147/155 (95%)	136 (92%)	9 (6%)	2 (1%)	11	15
1	U	146/155 (94%)	136 (93%)	7 (5%)	3 (2%)	7	8
1	V	147/155 (95%)	138 (94%)	7 (5%)	2 (1%)	11	15
1	W	147/155 (95%)	130 (88%)	13 (9%)	4 (3%)	5	5
1	X	147/155 (95%)	126 (86%)	15 (10%)	6 (4%)	3	2
All	All	3522/3720 (95%)	3301 (94%)	170 (5%)	51 (1%)	11	15



5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	VAL
1	C	115	VAL
1	G	45	GLU
1	G	115	VAL
1	I	115	VAL

### 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	A	123/129 (95%)	116 (94%)	7 (6%)	20 33
1	B	124/129 (96%)	117 (94%)	7 (6%)	21 34
1	C	125/129 (97%)	117 (94%)	8 (6%)	17 28
1	D	125/129 (97%)	118 (94%)	7 (6%)	21 34
1	E	125/129 (97%)	118 (94%)	7 (6%)	21 34
1	F	125/129 (97%)	120 (96%)	5 (4%)	31 49
1	G	122/129 (95%)	108 (88%)	14 (12%)	5 7
1	H	123/129 (95%)	113 (92%)	10 (8%)	11 18
1	I	125/129 (97%)	117 (94%)	8 (6%)	17 28
1	J	125/129 (97%)	123 (98%)	2 (2%)	62 79
1	K	122/129 (95%)	115 (94%)	7 (6%)	20 33
1	L	123/129 (95%)	114 (93%)	9 (7%)	14 22
1	M	125/129 (97%)	118 (94%)	7 (6%)	21 34
1	N	125/129 (97%)	110 (88%)	15 (12%)	5 6
1	O	125/129 (97%)	115 (92%)	10 (8%)	12 18
1	P	125/129 (97%)	118 (94%)	7 (6%)	21 34
1	Q	125/129 (97%)	116 (93%)	9 (7%)	14 23
1	R	125/129 (97%)	118 (94%)	7 (6%)	21 34
1	S	125/129 (97%)	112 (90%)	13 (10%)	7 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	125/129 (97%)	118 (94%)	7 (6%)	21	34
1	U	123/129 (95%)	114 (93%)	9 (7%)	14	22
1	V	124/129 (96%)	113 (91%)	11 (9%)	9	14
1	W	125/129 (97%)	113 (90%)	12 (10%)	8	12
1	X	125/129 (97%)	111 (89%)	14 (11%)	6	8
All	All	2984/3096 (96%)	2772 (93%)	212 (7%)	14	23

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	30	ARG
1	V	83	VAL
1	S	84	LYS
1	Q	116	CYS
1	U	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	145	GLN
1	O	50	HIS
1	T	117	HIS
1	I	29	ASN
1	H	145	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	148/155 (95%)	-0.19	1 (0%) 87 86	37, 49, 66, 84	0
1	B	149/155 (96%)	-0.17	1 (0%) 87 86	34, 49, 80, 96	0
1	C	149/155 (96%)	-0.18	3 (2%) 65 63	38, 53, 79, 93	0
1	D	149/155 (96%)	-0.07	3 (2%) 65 63	39, 55, 97, 131	0
1	E	149/155 (96%)	-0.21	1 (0%) 87 86	33, 49, 67, 90	0
1	F	149/155 (96%)	-0.25	0 100 100	31, 48, 70, 84	0
1	G	148/155 (95%)	0.10	5 (3%) 45 44	41, 63, 96, 131	0
1	H	148/155 (95%)	0.41	13 (8%) 10 9	47, 66, 108, 127	0
1	I	149/155 (96%)	-0.39	0 100 100	37, 52, 68, 79	0
1	J	149/155 (96%)	-0.15	3 (2%) 65 63	37, 52, 79, 118	0
1	K	148/155 (95%)	-0.16	2 (1%) 75 73	36, 51, 69, 85	0
1	L	148/155 (95%)	0.16	10 (6%) 17 15	36, 56, 99, 155	0
1	M	149/155 (96%)	-0.23	0 100 100	36, 48, 65, 79	0
1	N	149/155 (96%)	0.74	19 (12%) 3 3	38, 58, 148, 247	0
1	O	149/155 (96%)	-0.24	0 100 100	36, 53, 83, 98	0
1	P	149/155 (96%)	0.26	5 (3%) 45 44	34, 62, 92, 115	0
1	Q	149/155 (96%)	-0.18	1 (0%) 87 86	33, 47, 66, 86	0
1	R	149/155 (96%)	-0.20	1 (0%) 87 86	35, 52, 75, 102	0
1	S	149/155 (96%)	-0.15	1 (0%) 87 86	36, 53, 77, 96	0
1	T	149/155 (96%)	-0.06	3 (2%) 65 63	36, 53, 75, 114	0
1	U	148/155 (95%)	-0.11	4 (2%) 54 52	36, 53, 79, 176	0
1	V	149/155 (96%)	0.16	5 (3%) 45 44	41, 63, 90, 114	0
1	W	149/155 (96%)	0.74	21 (14%) 2 2	50, 71, 122, 156	0
1	X	149/155 (96%)	0.71	16 (10%) 6 5	50, 72, 117, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3570/3720 (95%)	0.01	118 (3%) 46 45	31, 55, 92, 247	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	58	PRO	18.7
1	N	61	PRO	13.0
1	N	55	SER	11.9
1	X	98	SER	11.5
1	N	59	PHE	10.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.