

wwPDB X-ray Structure Validation Summary Report (i)

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This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R _{free}	130704	$1000 \ (9.00-3.90)$
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain			
1	Е	26	100%			
1	0	26	96%			•
1	s	26	100%			
1	u	26	100%			
2	F	26	100%			
2	Р	26	100%			
2	t	26	100%			
2	v	26	96%			•
3	А	105	79%	9%	•	11%



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Chain Length Quality of chain Mol С 3 10582% 7% 11% 3 \mathbf{G} 10510% 78% 11% 3 Ι 10590% 9% • J 3 10579% 10% 11% Κ 3 10592% 7% • Q 3 10591% 7% • R 3 10580% 9% 11% \mathbf{S} 3 10579% 9% 11% . Т 1053 90% 10% Υ 3 10582% 7% 11% 3 105 \mathbf{a} 84% 5% 11% 1053 \mathbf{c} 82% 7% 11% 3 105е 91% 9% 3 f 10582% 7% 11% 3 10591% g 9% 3 k 10591% 8% • $\mathbf{3}$ l 10577% 11% 11% 1053 \mathbf{m} 81% 8% 11% 3 105n 92% 8% В 744 95% 5% D 4 74• • 95% Η 4 7493% 7% \mathbf{L} 4 74• 96% М 4 749% 91% Ν 4 7412% 88%



Mol	Chain	Length	Quality of chain	
4	U	74	95%	
4	V	74	93%	7%
4	W	74	96%	•
4	Х	74	91%	9%
4	Ζ	74	95%	5%
4	b	74	95%	5%
4	d	74	95%	5%
4	h	74	95%	5%
4	i	74	89%	11%
4	i	74	93%	7%
4	0	74	93%	7%
4	D	74	93%	7%
4	r n	74	96%	
4	r	74	99%	





2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31827 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.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
1	Г	26	Total	С	Ν	Ο	Р	0	0	0
	Ľ	20	546	260	130	130	26	0	0	0
1	0	26	Total	С	Ν	Ο	Р	0	0	0
1	0	20	546	260	130	130	26		0	0
1		26	Total	С	Ν	Ο	Р	0	0	0
	S	20	546	260	130	130	26	0	0	0
1	1 u	26	Total	С	Ν	Ο	Р	0	0	0
		20	546	260	130	130	26	U	0	U

• Molecule 1 is a DNA chain called DNA (26-MER).

• Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
0	Б	26	Total	С	Ν	0	Р	0	0	0	0
	Г	20	520	260	52	182	26	0	0	0	
0	D	26	Total	С	Ν	0	Р	0	0	0	
	P	20	520	260	52	182	26			0	
0	t	26	Total	С	Ν	0	Р	0	0	0	
		20	520	260	52	182	26	0	0	0	
0		26	Total	С	Ν	0	Р	0	0	0	
	20	520	260	52	182	26	U	U	U		

• Molecule 3 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	0.2	Total	С	Ν	Ο	S	0	0	0
J J	U	90	743	464	132	142	5	0	0	0
2	C	0.2	Total	С	Ν	Ο	S	0	0	0
J J	G	90	743	464	132	142	5	0		0
9	Δ	0.2	Total	С	Ν	Ο	S	0	0	0
	A	90	743	464	132	142	5	0	0	0
2	т	I 105	Total	С	Ν	Ο	S	0	0	0
3 1	105	844	526	154	159	5	U	0	U	



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Communea from	previous	puyc

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	т	0.2	Total	С	Ν	Ο	S	0	0	0
0	J	90	743	464	132	142	5	0	0	0
2	K	105	Total	С	Ν	Ο	S	0	0	0
0		105	844	526	154	159	5	0	0	0
3	0	105	Total	С	Ν	Ο	S	0	0	0
0	Q Q	100	844	526	154	159	5	0	0	0
3	B	93	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	10	50	743	464	132	142	5	0	0	0
3	S	93	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			743	464	132	142	5	0	0	0
3	Т	105	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-	100	844	526	154	159	5	0	0	0
3	Y	93	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-		743	464	132	142	5	0		Ŭ
3	a	93	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			743	464	132	142	5	_		
3	с	93	Total	С	N	0	S	0	0	0
			743	464	132	142	5	_	_	_
3	е	105	Total	С	Ν	0	S	0	0	0
			844	526	154	159	5	_	_	_
3	f	93	Total	C	N	0	S	0	0	0
			743	464	132	142	$\frac{5}{c}$			
3	g	105	lotal	C	N	0	S	0	0	0
			844	526	154	159	<u>b</u>			
3	k	105	lotal	C	N	0	S	0	0	0
			844	<u>526</u>	154 	159	$\frac{b}{c}$			
3	1	93	Total	C	N 100	140	S	0	0	0
			743	464	132	142	<u>b</u>			
3	m	93	l Iotal	U AC A	N 199	U 149	S	0	0	0
			743	404	132 	142	0 0			
3	n	105	lotal	C	N 1F4	150	S	0	0	0
			844	526	154	159	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	39	ALA	GLU	$\operatorname{conflict}$	UNP Q8N2Z9
С	106	ALA	ILE	$\operatorname{conflict}$	UNP Q8N2Z9
G	39	ALA	GLU	$\operatorname{conflict}$	UNP Q8N2Z9
G	106	ALA	ILE	$\operatorname{conflict}$	UNP Q8N2Z9
А	39	ALA	GLU	$\operatorname{conflict}$	UNP Q8N2Z9
А	106	ALA	ILE	conflict	UNP Q8N2Z9
Ι	39	ALA	GLU	$\operatorname{conflict}$	UNP Q8N2Z9



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	106	ALA	ILE	conflict	UNP Q8N2Z9
J	39	ALA	GLU	conflict	UNP Q8N2Z9
J	106	ALA	ILE	conflict	UNP Q8N2Z9
K	39	ALA	GLU	conflict	UNP Q8N2Z9
K	106	ALA	ILE	conflict	UNP Q8N2Z9
Q	39	ALA	GLU	conflict	UNP Q8N2Z9
Q	106	ALA	ILE	conflict	UNP Q8N2Z9
R	39	ALA	GLU	conflict	UNP Q8N2Z9
R	106	ALA	ILE	conflict	UNP Q8N2Z9
S	39	ALA	GLU	conflict	UNP Q8N2Z9
S	106	ALA	ILE	conflict	UNP Q8N2Z9
Т	39	ALA	GLU	conflict	UNP Q8N2Z9
Т	106	ALA	ILE	conflict	UNP Q8N2Z9
Y	39	ALA	GLU	conflict	UNP Q8N2Z9
Y	106	ALA	ILE	conflict	UNP Q8N2Z9
a	39	ALA	GLU	conflict	UNP Q8N2Z9
a	106	ALA	ILE	conflict	UNP Q8N2Z9
с	39	ALA	GLU	conflict	UNP Q8N2Z9
с	106	ALA	ILE	conflict	UNP Q8N2Z9
е	39	ALA	GLU	conflict	UNP Q8N2Z9
e	106	ALA	ILE	conflict	UNP Q8N2Z9
f	39	ALA	GLU	conflict	UNP Q8N2Z9
f	106	ALA	ILE	conflict	UNP Q8N2Z9
g	39	ALA	GLU	conflict	UNP Q8N2Z9
g	106	ALA	ILE	conflict	UNP Q8N2Z9
k	39	ALA	GLU	conflict	UNP Q8N2Z9
k	106	ALA	ILE	conflict	UNP Q8N2Z9
1	39	ALA	GLU	conflict	UNP Q8N2Z9
1	106	ALA	ILE	conflict	UNP Q8N2Z9
m	39	ALA	GLU	conflict	UNP Q8N2Z9
m	106	ALA	ILE	conflict	UNP Q8N2Z9
n	39	ALA	GLU	conflict	UNP Q8N2Z9
n	106	ALA	ILE	conflict	UNP Q8N2Z9

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• Molecule 4 is a protein called Centromere protein X.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	D	74	Total	С	Ν	Ο	S	0	0	0
			590	378	104	107	1			
4	Н	74	Total	С	Ν	0	S	0	0	0
			590	378	104	107	1			
4	В	2 74	Total	С	Ν	Ο	\mathbf{S}	0	1	0
		D ((4	596	382	105	108	1	0	L



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Continued	from	previous	page
		1	1 0

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace			
4	т	74	Total	С	Ν	Ο	S	0	1	0			
	L	14	596	382	105	108	1	0		0			
	м	74	Total	С	Ν	Ο	S	0	1	0			
4	IVI	(4	596	382	105	108	1	0	1	0			
4	N	74	Total	С	Ν	Ο	S	0	1	0			
4		14	596	382	105	108	1	0		0			
4	T	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	U	14	596	382	105	108	1	0	T	0			
4	V	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	v	14	596	382	105	108	1	0	T	0			
4	W	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	**	14	596	382	105	108	1	0	L				
4	v	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	Λ	14	596	382	105	108	1	0	1	0			
4	7	74	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0			
			590	378	104	107	1		0				
4	h	b 74	Total	С	Ν	Ο	\mathbf{S}	0	0	0			
	U U	14	590	378	104	107	1	0	0	0			
4	4 d	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	u	14	596	382	105	108	1	0	T	0			
1	h	n 74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	11	14	596	382	105	108	1	0	0 1	U			
1	i	i 74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	1	1	14	596	382	105	108	1	0	T	0		
4	i	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4	J	J (4	596	382	105	108	1	0	T	0			
4	0	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
	U	U	0	0		596	382	105	108	1	0	T	0
4	4 p	74	Total	С	Ν	Ο	\mathbf{S}	0	1	0			
4		14	596	382	105	108	1	0	T	0			
		74	Total	С	Ν	0	S	0	1	0			
<u>+</u>	Ч		596	382	105	108	1			0			
	r	74	Total	С	Ν	0	S	0	1	0			
4	r	r	r	1'4	595	382	105	107	1			U	



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. 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. 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: DNA (26-MER)	
Chain E: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 1: DNA (26-MER)	
Chain O: 96%	·
A24 A25 A26	
• Molecule 1: DNA (26-MER)	
Chain s: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 1: DNA (26-MER)	
Chain u: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 2: DNA (26-MER)	
Chain F: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 2: DNA (26-MER)	
Chain P: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 2: DNA (26-MER)	
Chain t: 100%	
There are no outlier residues recorded for this chain.	

• Molecule 2: DNA (26	G-MER)		
Chain v:	96%		•
• Molecule 3: Centrom	ere protein S		
Chain C:	82%	7%	11%
S14 136 136 140 140 141 192 193 193 193 193 193 193 193 193 193 193	GLU ARG ALA ALA ALA ALA SIN SIN SIN SIN SIN		
• Molecule 3: Centrom	ere protein S		
Chain G:	78%	10%	11%
S 14 126 126 126 126 126 141 126 188 188 192 192 192	K94 Y95 ASW ALA GLU GLU GLU CYS LYS LYS SER SER		
• Molecule 3: Centrom	ere protein S		
Chain A:	79%	9% •	11%
814 115 1236 136 136 136 153 153 153 153 153 153 153 153 153 153	Least Allowed Start Allowed Start Allowed Start		
• Molecule 3: Centrom	ere protein S		
Chain I:	90%		9% •
S14 R18 126 C31 C31 C31 C31 C31 C31 C31 C31 C31 C31	192 K115 K116 X117 S118 S118		
• Molecule 3: Centrom	ere protein S		
Chain J:	79%	10%	11%
314 M40 Q41 Q45 P55 R70 R70 R87 R87 R88 R88 R88 R88	L93 K94 K94 A106 A106 A106 A106 A106 A106 A106 A106		
• Molecule 3: Centrom	ere protein S		
Chain K:	92%		7% •
S14 M40 Q41 Q41 R44 R44 H71 H71 H71 H71 H71 H71 K12 K115 K115 S118			
• Molecule 3: Centrom	ere protein S		



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Chain Q:	91%		7%
L36 M40 Q41 176 L84 L92 L92	2 1113 2 1113 1 11111 1 11111 1 11111 1 11111111		
Molecule 3: Centro	mere protein S		
Chain R:	- 80%	9%	11%
9 9 1 9 1 9 1 9 5 2 9	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		
N 1 7 0 C 1	S1 E1 AS AS AS AS AS AS AS AS AS AS		
Molecule 3: Centro	mere protein S		
hain S:	79%	9% •	11%
Y15 Q16 136 41 41 41 41 41 41 88 88 88 88 88 88 88 88 88 88 88 88 88	R99 ASI 06 ASI 06 ALA ALA ALA ALA CLN CLN CLN SER CSS SER SER		
Molecule 3: Centro	mere protein S		
hain T:	90%		10%
L30 L36 L36 M40 Q41 C41 L53 F55 F55	R87 R87 K115 S118		
Molecule 3: Centro	mere protein S		
hain Y:	82%	7%	11%
L36 M40 741 R40 R40 R41 L92 L92 L92 L92	A LUC A RL A RL A RL A RL A RL C VS C LVS SER SER SER		
Molecule 3: Centro	mere protein S		
hain a:	84%	5%	11%
M40 K44 R88 R88 A106 A106 CLU C92 CLU C10 CLU	LYS ALA GLN CYS LYS LYS SER SER SER		
Molecule 3: Centro	mere protein S		
bain c:	82%	7%	11%
Y 15 M40 Q41 K44 L53 R87 L92 L92 L92	L ASJA C LU C ARG C LU ALA ALA L VS SER SER SER		

• Molecule 3: Centromere protein S



Chain e:	91%		9%
514 0 17 0 40 1 40 1 40	192 111 111 111 111 111 111 111		
• Molecule 3: Cen	ntromere protein S		
Chain f:	82%	7%	11%
S14 1440 041 1440 1441 1442 184 184 187 187 192	A106 ASIN ASIN ARIC ARIC ARIC ARIC ARIC CLIYS LLYS LLYS SER SER SER		
• Molecule 3: Cen	ntromere protein S		
Chain g:	91%		9%
S14 136 136 136 136 136 136 171 1 171 187	192 193 114 115 118 118		
• Molecule 3: Cen	ntromere protein S		
Chain k:	91%		8% •
514 M40 K44 R70 R87 L92 L92 L92 K94	R110 K1116 K1117 S118 S118		
• Molecule 3: Cen	ntromere protein S		
Chain l:	77%	11%	11%
<mark>S 14</mark> Y 15 R 18 R 18 R 40 R 40 F 42 F 42 F 42 F 42 F 42 F 42 F 42 F 42	REG R70 R70 R87 R87 R87 A106 A106 A11A C192 C192 C192 C192 C192 C193 C193 C193 C193 C193 C193 C193 C193		
• Molecule 3: Cen	ntromere protein S		
Chain m:	81%	8%	11%
514 715 136 140 140 140 170 188 188	192 192 A106 A10 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12		
• Molecule 3: Cen	ntromere protein S		
Chain n:	92%		8%
S14 M40 Q41 K44 R70 R87 L92 L93	K94 K115 S118		

• Molecule 4: Centromere protein X



Chain D:	95%	•••
B8 100 100 100 100 100 100 100 100 100 10		
• Molecule 4: Centromere protein X		
Chain H:	93%	7%
S8 F13 1178 1179 1177 1178 117		
• Molecule 4: Centromere protein X		
Chain B:	95%	5%
288 1179 1179 1179 1180 1180 1179		
• Molecule 4: Centromere protein X		
Chain L:	96%	•
• Molecule 4: Centromere protein X		
Chain M:	91%	9%
88 84 86 86 81 81 81 81 81 81 81 81 81 81 81 81 81		
• Molecule 4: Centromere protein X		
Chain N:	88%	12%
88 81 86 86 86 86 86 86 86 86 86 86 86 86 86		
• Molecule 4: Centromere protein X		
Chain U:	95%	
E E E E E E E E		

• Molecule 4: Centromere protein X



T T T T T T T T T T

Chain V:	93%	7%
R 29 R 46 R 65 R 64 R 70 R 70		
• Molecule 4: Centromere protein X		
Chain W:	96%	·
88 H112 193 193 193 193 193 193 193 193 193 193		
• Molecule 4: Centromere protein X		
Chain X:	91%	9%
S8 137 137 137 143 166 166 166 166 181		
• Molecule 4: Centromere protein X		
Chain Z:	95%	5%
E 13 E 63 P 66 F 81 F 81 F 81 F 81 F 81 F 81 F 81 F 81		
• Molecule 4: Centromere protein X		
Chain b:	95%	5%
88 86 86 86 86 87 8 8 8 8 8 8 8 8 8 8 8		
• Molecule 4: Centromere protein X		
Chain d:	95%	5%
88 167 167 167 167 167 167 167 167 167 167		
• Molecule 4: Centromere protein X		
Chain h:	95%	5%
F 8 8 F 8 1 F 8 1 F 8 1		

• Molecule 4: Centromere protein X



Chain i:	89%	11%
S8 E13 L21 L21 K29 K64 V65 V65 V65 V65 V65 V65		
• Molecule 4: Centrom	nere protein X	
Chain j:	93%	7%
58 E13 H20 L21 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 765 776 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 77 777 77 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777 777777 777 777 777777 777 777777 		
• Molecule 4: Centrom	nere protein X	
Chain o:	93%	7%
88 69 121 121 121 138 180 80 80		
• Molecule 4: Centrom	nere protein X	
Chain p:	93%	7%
88 E13 K29 K65 K66 K66 K66 K66 K66 K66 K66 K66 K66		
• Molecule 4: Centrom	nere protein X	
Chain q:	96%	
58 K12 F13 F66 F81		
• Molecule 4: Centrom	nere protein X	
Chain r:	99%	



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 3	Depositor	
Cell constants	252.39Å 252.39 Å 131.36 Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{\hat{A}})$	112.59 - 6.50	Depositor	
Resolution (A)	112.59 - 6.50	EDS	
% Data completeness	$99.7\ (112.59\text{-}6.50)$	Depositor	
(in resolution range)	$99.9\ (112.59\text{-}6.50)$	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.02 (at 6.73 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.7.0029	Depositor	
D D	0.266 , 0.295	Depositor	
κ, κ_{free}	0.286 , 0.320	DCC	
R_{free} test set	826 reflections (4.48%)	wwPDB-VP	
Wilson B-factor $(Å^2)$	433.4	Xtriage	
Anisotropy	0.287	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37 , 446.5	EDS	
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.24$	Xtriage	
	0.029 for -h,-k,l		
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage	
	0.027 for -k,-h,-l		
	0.452 for H, K, L		
Penerted twinning fraction	0.032 for -K, -H, -L	Depositor	
Reported twinning fraction	0.022 for -h,-k,l	Depositor	
	0.495 for K, H, -L		
Outliers	0 of 18426 reflections	Xtriage	
F_o, F_c correlation	0.83	EDS	
Total number of atoms	31827	wwPDB-VP	
Average B, all atoms $(Å^2)$	363.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 52.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5016e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Mol Chain		nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Ε	0.38	0/623	0.88	0/958	
1	0	0.46	1/623~(0.2%)	0.90	0/958	
1	s	0.31	0/623	0.83	0/958	
1	u	0.33	0/623	0.81	0/958	
2	F	0.42	0/571	0.73	0/880	
2	Р	0.40	0/571	0.71	0/880	
2	t	0.30	0/571	0.71	0/880	
2	V	0.31	0/571	0.74	0/880	
3	А	0.63	0/751	0.87	1/1007~(0.1%)	
3	С	0.66	0/751	0.81	1/1007~(0.1%)	
3	G	0.65	0/751	0.84	2/1007~(0.2%)	
3	Ι	0.72	0/852	0.93	3/1137~(0.3%)	
3	J	0.68	0/751	0.88	0/1007	
3	Κ	0.63	0/852	0.82	1/1137~(0.1%)	
3	Q	0.62	0/852	0.88	2/1137~(0.2%)	
3	R	0.65	0/751	0.84	0/1007	
3	S	0.65	0/751	0.85	1/1007~(0.1%)	
3	Т	0.56	0/852	0.77	2/1137~(0.2%)	
3	Y	0.45	0/751	0.65	0/1007	
3	a	0.42	0/751	0.64	0/1007	
3	с	0.43	0/751	0.71	0/1007	
3	е	0.42	0/852	0.70	0/1137	
3	f	0.45	0/751	0.68	0/1007	
3	g	0.44	0/852	0.63	0/1137	
3	k	0.38	0/852	0.65	1/1137~(0.1%)	
3	1	0.44	0/751	0.60	0/1007	
3	m	0.43	0/751	0.63	0/1007	
3	n	0.39	0/852	0.61	0/1137	
4	В	0.62	$0/\overline{605}$	0.85	$1/813$ $\overline{(0.1\%)}$	
4	D	0.67	0/596	0.88	0/801	
4	Н	0.68	0/596	0.88	2/801~(0.2%)	
4	L	0.62	$0/\overline{605}$	0.79	$0/\overline{813}$	
4	М	0.68	0/605	0.81	0/813	
4	N	0.71	$0/\overline{605}$	0.95	0/813	



		Bo	nd longths	Bond angles		
Mol	Chain					
		RMSZ	# Z > 5	RMSZ	# Z > 5	
4	U	0.51	0/605	0.83	3/813~(0.4%)	
4	V	0.63	0/605	0.93	1/813~(0.1%)	
4	W	0.60	0/605	0.84	0/813	
4	Х	0.63	0/605	0.94	1/813~(0.1%)	
4	Z	0.42	0/596	0.70	0/801	
4	b	0.39	0/596	0.63	0/801	
4	d	0.39	0/605	0.69	1/813~(0.1%)	
4	h	0.39	0/605	0.65	0/813	
4	i	0.42	0/605	0.71	0/813	
4	j	0.39	0/605	0.62	0/813	
4	0	0.37	0/605	0.68	1/813~(0.1%)	
4	р	0.40	0/605	0.70	0/813	
4	q	0.37	0/605	0.64	0/813	
4	r	0.40	0/604	0.63	0/812	
All	All	0.52	$1/32667 \ (0.0\%)$	0.77	$24/44743 \ (0.1\%)$	

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
4	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	0	24	DA	O3'-P	5.08	1.67	1.61

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	В	79	LEU	CA-CB-CG	7.28	132.03	115.30
3	Т	53	LEU	CA-CB-CG	6.64	130.58	115.30
3	G	36	LEU	CA-CB-CG	6.51	130.28	115.30
4	Н	79	LEU	CA-CB-CG	6.49	130.23	115.30
4	U	74	LEU	CA-CB-CG	6.37	129.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	\mathbf{Res}	Type	Group
4	D	63	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Perce	entiles
3	А	91/105~(87%)	88~(97%)	3~(3%)	0	100	100
3	С	91/105~(87%)	88 (97%)	3~(3%)	0	100	100
3	G	91/105~(87%)	88 (97%)	3~(3%)	0	100	100
3	Ι	103/105~(98%)	99~(96%)	3~(3%)	1 (1%)	15	54
3	J	91/105~(87%)	89~(98%)	2(2%)	0	100	100
3	K	103/105~(98%)	101~(98%)	2(2%)	0	100	100
3	Q	103/105~(98%)	102 (99%)	1 (1%)	0	100	100
3	R	91/105~(87%)	90~(99%)	1 (1%)	0	100	100
3	S	91/105~(87%)	90 (99%)	1 (1%)	0	100	100
3	Т	103/105~(98%)	102 (99%)	1 (1%)	0	100	100
3	Y	91/105~(87%)	89 (98%)	2(2%)	0	100	100
3	a	91/105~(87%)	90~(99%)	1 (1%)	0	100	100
3	с	91/105~(87%)	91 (100%)	0	0	100	100
3	е	103/105~(98%)	101 (98%)	2(2%)	0	100	100
3	f	91/105~(87%)	90 (99%)	1 (1%)	0	100	100
3	g	103/105~(98%)	103~(100%)	0	0	100	100
3	k	103/105~(98%)	102 (99%)	1 (1%)	0	100	100
3	1	91/105~(87%)	91 (100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	m	91/105~(87%)	91 (100%)	0	0	100	100
3	n	103/105~(98%)	103~(100%)	0	0	100	100
4	В	73/74~(99%)	70 (96%)	3(4%)	0	100	100
4	D	72/74~(97%)	65~(90%)	7 (10%)	0	100	100
4	Н	72/74~(97%)	69~(96%)	3(4%)	0	100	100
4	L	73/74~(99%)	72 (99%)	1 (1%)	0	100	100
4	М	73/74~(99%)	71 (97%)	2(3%)	0	100	100
4	Ν	73/74~(99%)	70~(96%)	3(4%)	0	100	100
4	U	73/74~(99%)	72 (99%)	1 (1%)	0	100	100
4	V	73/74~(99%)	72 (99%)	1 (1%)	0	100	100
4	W	73/74~(99%)	72 (99%)	1 (1%)	0	100	100
4	Х	73/74~(99%)	73 (100%)	0	0	100	100
4	Z	72/74~(97%)	72 (100%)	0	0	100	100
4	b	72/74~(97%)	72 (100%)	0	0	100	100
4	d	73/74~(99%)	72 (99%)	1 (1%)	0	100	100
4	h	73/74~(99%)	73 (100%)	0	0	100	100
4	i	73/74~(99%)	73 (100%)	0	0	100	100
4	j	73/74~(99%)	73 (100%)	0	0	100	100
4	О	73/74~(99%)	73 (100%)	0	0	100	100
4	р	73/74~(99%)	73 (100%)	0	0	100	100
4	q	73/74~(99%)	73 (100%)	0	0	100	100
4	r	73/74~(99%)	73 (100%)	0	0	100	100
All	All	3372/3580~(94%)	3321 (98%)	50 (2%)	1 (0%)	100	100

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All (1) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
3	Ι	117	LYS

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.



Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
3	А	80/91~(88%)	71 (89%)	9 (11%)	6	21
3	С	80/91~(88%)	74 (92%)	6 (8%)	13	38
3	G	80/91~(88%)	71 (89%)	9 (11%)	6	21
3	Ι	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	J	80/91~(88%)	70 (88%)	10 (12%)	4	19
3	K	91/91~(100%)	83 (91%)	8 (9%)	10	31
3	Q	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	R	80/91~(88%)	71 (89%)	9 (11%)	6	21
3	S	80/91~(88%)	70 (88%)	10 (12%)	4	19
3	Т	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	Y	80/91~(88%)	73 (91%)	7 (9%)	10	31
3	а	80/91~(88%)	75 (94%)	5 (6%)	18	43
3	с	80/91~(88%)	73 (91%)	7 (9%)	10	31
3	е	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	f	80/91~(88%)	73 (91%)	7 (9%)	10	31
3	g	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	k	91/91~(100%)	82 (90%)	9 (10%)	8	26
3	1	80/91~(88%)	68 (85%)	12 (15%)	3	15
3	m	80/91~(88%)	72 (90%)	8 (10%)	7	26
3	n	91/91~(100%)	83 (91%)	8 (9%)	10	31
4	В	66/65~(102%)	63~(96%)	3 (4%)	27	52
4	D	65/65~(100%)	61 (94%)	4 (6%)	18	43
4	Н	65/65~(100%)	62 (95%)	3(5%)	27	52
4	L	66/65~(102%)	63~(96%)	3 (4%)	27	52
4	М	66/65~(102%)	59 (89%)	7 (11%)	6	24
4	Ν	66/65~(102%)	57 (86%)	9 (14%)	3	17
4	U	66/65~(102%)	64 (97%)	2 (3%)	41	63
4	V	66/65~(102%)	62 (94%)	4 (6%)	18	44
4	W	66/65~(102%)	63~(96%)	3 (4%)	27	52
4	Х	66/65~(102%)	60 (91%)	6 (9%)	9	30

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	Perce	entiles
4	Z	65/65~(100%)	61~(94%)	4(6%)	18	43
4	b	65/65~(100%)	61 (94%)	4(6%)	18	43
4	d	66/65~(102%)	63~(96%)	3 (4%)	27	52
4	h	66/65~(102%)	62 (94%)	4 (6%)	18	44
4	i	66/65~(102%)	58 (88%)	8 (12%)	5	20
4	j	66/65~(102%)	61 (92%)	5 (8%)	13	37
4	О	66/65~(102%)	62 (94%)	4 (6%)	18	44
4	р	66/65~(102%)	61 (92%)	5 (8%)	13	37
4	q	66/65~(102%)	63~(96%)	3 (4%)	27	52
4	r	66/65~(102%)	65~(98%)	1 (2%)	65	80
All	All	3004/3120~(96%)	2750 (92%)	254 (8%)	10	33

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5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
3	Т	87	ARG
4	Ζ	66	ASP
3	n	41	GLN
4	U	66	ASP
4	Х	61	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	71	HIS
4	W	58	GLN
3	m	60	ASN
4	V	20	HIS
3	Ι	17	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

