

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	7XX6
Title	:	Crystal Structure of Nucleosome-H1.0 Linker Histone Assembly (sticky-169a
		DNA fragment)
Authors	:	Adhireksan, Z.; Qiuye, B.; Lee, P.L.; Sharma, D.; Padavattan, S.; Davey, C.A.
Deposited on	:	2022-05-28
Resolution	:	3.39 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.39 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1026 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 ch	ain	
1	А	138	^{2%} 70%	•	28%
1	Е	138	% • 67%	••	28%
1	K	138	4% 67%	6%	28%
1	О	138	<u>4%</u> 67%	•	28%
1	U	138	2% 7 0%	•	28%
1	Y	138	% 67%		28%
1	е	138	<u>4%</u> 69%	·	28%



Mol	Chain	Length	Quality of chain		
1		190	4%		
	1	138	68%	•	28%
2	В	105	74%	•	24%
2	F	105	76%	•••	20%
			5%		
2	L	105	75% 5%		24%
2	Р	105	73%	•	24%
2	V	105	75%		24%
2	Z	105	75%	5%	20%
2	f	105	<u>75%</u>	·	24%
2	j	105	3% 73%	·	24%
3	С	132	% • 77%	· ·	19%
3	G	132	2% 77%	9%	14%
3	М	132	6% 77%	••	20%
3	Q	132	5%		20%
3	W	132	.% ■ 77%		19%
3	a	132	5%	50	4 . 14%
	a	102	5%		·0 • 1470
3	g	132	<u>80%</u>	<u> </u>	20%
3	k	132	76%	· .	20%
4	D	128	70%	8%	23%
4	Н	128	67%	10%	23%
4	Ν	128	<u>2%</u> 74%	•	23%
4	R	128	5% 71%	5% •	23%
4	X	128	4%	8%	22%
4	h	128	4% 73%	5%	22%
-		120	4%		22,3
4	h	128	72%	5%	23%
4	1	128	70%	6% ·	23%



Mal	Chain	Longth	page	Quality	of aboin	
WIOI	Chain	Length		Quanty		
_	-	1.0.0	.% •			
5	1	169		99%	0	•
_	~		.% ■			
5	S	169		98%		•
_			.% ■			
5	С	169		100	%	
			2%			
5	m	169		99%	Ď	•
	_		2%			
6	J	169		98%		•
	-		2%			
6	Т	169		98%		•
			.% ■			
6	d	169		99%	0	•
			2%			
6	n	169		98%		•
			33%			
7	0	195	33%	6% •	61%	
			34%			
7	р	195	33%	5%	62%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CA	G	201	-	-	-	Х
8	CA	d	104	-	-	-	Х



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 53518 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	00	Total	С	Ν	0	S	0	0	0
	A	99	816	514	158	140	4	0	0	0
1	F	00	Total	С	Ν	0	S	0	0	0
		99	816	514	158	140	4	0	0	0
1	K	100	Total	С	Ν	0	S	0	0	0
1	Γ	100	825	520	160	141	4	0	0	0
1	0	00	Total	С	Ν	0	S	0	0	0
1	0	99	816	514	158	140	4	0	0	0
1	I	00	Total	С	Ν	0	S	0	0	0
1	U	99	816	514	158	140	4	0	0	0
1	V	00	Total	С	Ν	0	S	0	0	0
	I	99	816	514	158	140	4	0	0	0
1	0	100	Total	С	Ν	0	S	0	0	0
	е	100	825	520	160	141	4	0	0	0
1	;	00	Total	С	Ν	Ο	S	0	0	0
	1	99	816	514	158	140	4			U

• Molecule 1 is a protein called Histone H3.1.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	GLY	-	expression tag	UNP P68431
А	-1	SER	-	expression tag	UNP P68431
Е	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
K	-2	GLY	-	expression tag	UNP P68431
K	-1	SER	-	expression tag	UNP P68431
0	-2	GLY	-	expression tag	UNP P68431
0	-1	SER	-	expression tag	UNP P68431
U	-2	GLY	-	expression tag	UNP P68431
U	-1	SER	-	expression tag	UNP P68431
Y	-2	GLY	-	expression tag	UNP P68431
Y	-1	SER	-	expression tag	UNP P68431
е	-2	GLY	-	expression tag	UNP P68431



Chain	Residue	Modelled	Actual	Comment	Reference
е	-1	SER	-	expression tag	UNP P68431
i	-2	GLY	-	expression tag	UNP P68431
i	-1	SER	-	expression tag	UNP P68431

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• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	80	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	80	638	401	125	111	1	0	0	0
9	Б	84	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Г	04	673	424	133	115	1	0	0	0
0	т	80	Total	С	Ν	0	S	0	0	0
		80	638	401	125	111	1	0	0	0
0	D	80	Total	С	Ν	0	S	0	0	0
	1	80	638	401	125	111	1			0
2	V	80	Total	С	Ν	Ο	S	0	0	0
	v	80	638	401	125	111	1	0	0	0
2	7	84	Total	С	Ν	0	S	0	0	0
		04	673	424	133	115	1	0	0	0
2	f	80	Total	С	Ν	Ο	S	0	0	0
	1	80	638	401	125	111	1	0	0	0
2	i	80	Total	С	Ν	Ο	S	0	0	0
	J		638	401	125	111	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-2	GLY	-	expression tag	UNP P62805
В	-1	SER	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
L	-2	GLY	-	expression tag	UNP P62805
L	-1	SER	-	expression tag	UNP P62805
Р	-2	GLY	-	expression tag	UNP P62805
Р	-1	SER	-	expression tag	UNP P62805
V	-2	GLY	-	expression tag	UNP P62805
V	-1	SER	-	expression tag	UNP P62805
Z	-2	GLY	-	expression tag	UNP P62805
Z	-1	SER	-	expression tag	UNP P62805
f	-2	GLY	-	expression tag	UNP P62805
f	-1	SER	-	expression tag	UNP P62805
j	-2	GLY	-	expression tag	UNP P62805



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Chain	Residue	Modelled	Actual	Comment	Reference
j	-1	SER	-	expression tag	UNP P62805

• Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
9	C	107	Total	С	Ν	Ο	0	0	0
5	U	107	826	521	161	144	0	0	0
2	C	114	Total	С	Ν	Ο	0	0	0
0	G	114	873	549	173	151	0	0	0
9	м	106	Total	С	Ν	Ο	0	0	0
5	111	100	821	518	160	143	0	0	0
9	0	105	Total	С	Ν	Ο	0	0	0
0	Q	105	810	511	158	141	0	0	0
2	W/	107	Total	С	Ν	Ο	0	0	0
0	vv	107	826	521	161	144	0	0	0
2	0	114	Total	С	Ν	Ο	0	0	0
0	a	114	873	549	173	151	0	0	0
2	a cr	106	Total	С	Ν	Ο	0	0	0
0	g	100	821	518	160	143	0	0	0
3	Ŀ	105	Total	С	Ν	Ο	0	0	0
5	ĸ	105	810	511	158	141		U	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-2	GLY	-	expression tag	UNP P04908
С	-1	SER	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
М	-2	GLY	-	expression tag	UNP P04908
M	-1	SER	-	expression tag	UNP P04908
Q	-2	GLY	-	expression tag	UNP P04908
Q	-1	SER	-	expression tag	UNP P04908
W	-2	GLY	-	expression tag	UNP P04908
W	-1	SER	-	expression tag	UNP P04908
a	-2	GLY	-	expression tag	UNP P04908
a	-1	SER	-	expression tag	UNP P04908
g	-2	GLY	-	expression tag	UNP P04908
g	-1	SER	-	expression tag	UNP P04908
k	-2	GLY	-	expression tag	UNP P04908
k	-1	SER	_	expression tag	UNP P04908



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	р	00	Total	С	Ν	0	S	0	0	0
4	D	99	784	492	146	144	2	0	0	0
4	ц	00	Total	С	Ν	0	S	0	0	0
4	11	99	784	492	146	144	2	0	0	0
4	N	08	Total	С	Ν	0	S	0	0	0
4	IN	90	775	486	144	143	2	0	0	0
4	В	08	Total	С	Ν	0	S	0	0	0
4	п	90	775	486	144	143	2	0	0	0
4	v	100	Total	С	Ν	0	S	0	0	0
4	Λ	100	788	494	147	145	2	0	0	0
4	h	100	Total	С	Ν	0	S	0	0	0
4	D	100	788	494	147	145	2	0	0	0
4	h	08	Total	С	Ν	0	S	0	0	0
4	11	90	775	486	144	143	2	0	0	0
4	1	08	Total	С	Ν	0	S	0	0	0
4	1	90	775	486	144	143	2			U

• Molecule 4 is a protein called Histone H2B type 1-J.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
Н	-2	GLY	-	expression tag	UNP P06899
Н	-1	SER	-	expression tag	UNP P06899
N	-2	GLY	-	expression tag	UNP P06899
N	-1	SER	-	expression tag	UNP P06899
R	-2	GLY	-	expression tag	UNP P06899
R	-1	SER	-	expression tag	UNP P06899
Х	-2	GLY	-	expression tag	UNP P06899
Х	-1	SER	-	expression tag	UNP P06899
b	-2	GLY	-	expression tag	UNP P06899
b	-1	SER	-	expression tag	UNP P06899
h	-2	GLY	-	expression tag	UNP P06899
h	-1	SER	-	expression tag	UNP P06899
1	-2	GLY	-	expression tag	UNP P06899
1	-1	SER	-	expression tag	UNP P06899

 $\bullet\,$ Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
5	Ι	169	Total 3462	C 1646	N 637	O 1011	Р 168	0	0	0



Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
5	q	160	Total	С	Ν	Ο	Р	0	0	0
5	U U	109	3462	1646	637	1011	168	0	0	0
F	0	160	Total	С	Ν	Ο	Р	0	0	0
5	C	109	3462	1646	637	1011	168	0	0	0
F	m	160	Total	С	Ν	Ο	Р	0	0	0
5	111	109	3462	1646	637	1011	168	0	0	0

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• Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues		Atoms					AltConf	Trace
6	Т	160	Total	С	Ν	Ο	Р	0	0	0
0	J	109	3461	1646	634	1013	168	0	0	0
6	т	160	Total	С	Ν	Ο	Р	0	0	0
0	1	109	3461	1646	634	1013	168	0	0	0
6	d	160	Total	С	Ν	Ο	Р	0	0	0
0	u	109	3461	1646	634	1013	168	0	0	0
6	n	160	Total	С	Ν	Ο	Р	0	0	0
0	11	109	3461	1646	634	1013	168	0	0	0

• Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7		76	Total	С	Ν	0	S	0	0	0
1	0	70	583	362	109	111	1	0	0	U
7	n	74	Total	С	Ν	0	S	0	0	0
(h	14	566	353	107	105	1		0	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	0	GLY	-	expression tag	UNP P07305
0	1	PRO	-	expression tag	UNP P07305
р	0	GLY	-	expression tag	UNP P07305
р	1	PRO	-	expression tag	UNP P07305

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Ι	8	Total Ca 8 8	0	0
8	J	4	Total Ca 4 4	0	0
8	0	2	Total Ca 2 2	0	0
8	S	1	Total Ca 1 1	0	0
8	Т	3	Total Ca 3 3	0	0
8	W	1	Total Ca 1 1	0	0
8	Y	1	Total Ca 1 1	0	0
8	a	2	Total Ca 2 2	0	0
8	С	7	Total Ca 7 7	0	0
8	d	8	Total Ca 8 8	0	0
8	i	1	Total Ca 1 1	0	0
8	j	1	Total Ca 1 1	0	0
8	m	2	Total Ca 2 2	0	0
8	n	2	Total Ca 2 2	0	0
8	0	1	Total Ca 1 1	0	0
8	р	1	Total Ca 1 1	0	0

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• Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Ι	1	Total K 1 1	0	0
9	Т	3	Total K 3 3	0	0
9	с	1	Total K 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	d	1	Total K 1 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Histone H3.1

7	X	Х	76	;
	∡ x	~	rc	,

• Molecule 1:	Histone H3.1				
Chain Y:		67%		28%	-
GLY SER MET ALA ARG THR LYS GLN THR ALA	ARG LYS SER THR GLY CLY GLY PRO PRO CLYS CLYS	LEU LEU THR LYS LYS ALA ALA ALA ALA ALA ALA ALA THR CIY	GLY VAL LYS LYS H39 H39 P43 P43 L48	D77 P121 R129 R134	A135
• Molecule 1:	Histone H3.1				
Chain e:		69%	·	28%	-
GLY SER MET ALA ARG THR LYS GLN THR THR ALA	ARG LYS SER THR GLY GLY CLYS ARG ARG CLYS GLM	LEU LEU THR LYS LYS ALA ALA ALA ALA ALA PRO PRO PRO CIV	GLY VAL K36 F38 H39 R63 R63 Q76	T100 S86 N108	A135
• Molecule 1:	Histone H3.1				
Chain i:		68%	·	28%	
GLY SER MET ALA ARG THR LYS GLN THR ALA	ARG LYS SER THR GLY GLY ARG ARG LYS GLN CGLN	LEU LYS LYS LYS ALA ALA ALA SER SER PRO PRO PRO CGLY	GLY VAL LYS LYS R37 P38 H39 R40 Y41 Y41 Y42 P43	L48 Q76 R83 N108	R129 A135
• Molecule 2:	Histone H4				
Chain B:		74%	•	24%	-
GLY SER MET SER GLY GLY GLY GLY GLY	LYS GLY LEU GLY CLYS GLY GLY ALA LYS ALA ARG ARG	LYS VAL LEU LEU RJS R95 G102			
• Molecule 2:	Histone H4				
Chain F:		76%	• •	20%	-
GLY SER MET SER GLY GLY GLY GLY GLY	LYS GLY LEU GLY GLY CLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA	K20 K23 Q27 G102			
• Molecule 2:	Histone H4				
Chain L:		75%	·	24%	-
GLY SER MET SER GLY GLY GLY CLY GLY GLY GLY	LYS GLY LEU GLY GLY GLY GLY ALA ARG ARG	LYN VAL LEU REU R23 C28 C28 C28 C28 C28 C28 C28 C28 C28 C28			
• Molecule 2:	Histone H4				
Chain P:		73%	·	24%	-
GLY MET MET SER SER GLY GLY GLY GLY	LYS CLU CLU CLY CLY CLY CLY CLY CLY ALA ARG ARG ARG	L V. L V.A.L. V.A.L. L.E.U. L.E.U. L.E.U. R.25 1.25 1.25 1.26 1.26 1.26 1.26 1.26 1.26 1.26 1.26	173 6102		



• Molecule 2: Histone H4		
Chain V:	75%	• 24%
0.17 SER NET NET NET NET 0.17 0.17 0.17 0.17 0.17 0.17 0.17 0.17	HIS ANG VAL LEU RC3 RC3 RC3 RC3 RC3 RC3 RC3 RC3 RC3 RC3	
• Molecule 2: Histone H4		
Chain Z:	75%	5% 20%
GLY SER MET SER SER SER SER SER SER GLY GLY GLY GLY GLY GLY GLY ARA ALA	HIS K19 K20 R23 D68 D68 D102	
• Molecule 2: Histone H4		
Chain f:	75%	• 24%
617 MET MET SER SER SER G17 C175 C175 C17 C175 C17 C175 C17 C175 C17 C175 C17 C175 C177 C177	HIS ARG LYS VAL LEU RZ3 T54 T 54 G 102	
• Molecule 2: Histone H4		
Chain j:	73%	• 24%
GLY MET MET SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ALA ALA ARG GLY ALA	HIS ARG LYS VAL LVAL LEU R23 D24 I26 I26 G102 G102	
• Molecule 3: Histone H2A	type $1-B/E$	
Chain C:	77%	• 19%
GLY SER MET MET SER GLY GLY GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	D72 N73 R119 C1120 C1120 C1120 C120 C120 C127 C120 C127 C127 C127 C127 C127 C127 C127 C127	
• Molecule 3: Histone H2A	type $1-B/E$	
Chain G:	77%	9% 14%
GLY SER MET SER GLY GLY ARG GLY GLN M10 M10 M13 A114 A114 A113 A114 A113 A114 A113 A114 A113 A114 A113 A114 A110 A113 A114 A113 A114 A113 A114 A113 A114 A113 A113	R32 R71 R71 R71 R73 K74 R81 R81 R119 D90 C112 C1120 C112 C1120 C112 C112 C112 C	SAT A TB
• Molecule 3: Histone H2A	type $1-B/E$	
Chain M:	77%	•• 20%
GLY BER MET SER SER SER SER SER ARG GLY GLY GLY CLYS GLY LYS CLY KIS CL3 CL3 CL3 CL3 CL3 CL3 CL3 CL3 CL3 CL3	A45 A45 D72 D72 D72 M73 A115 A116 P116 A116 A116 G110 G110 G110 G110 A114 A114 A114 A114 A114 A114 A114 A	SAT CTA
	WORLDWIDE PROTEIN DATA BANK	









• Molecule 5: DNA (169-MER)



$1 \Lambda \Lambda 0$	7XX6	
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Chain I:	99% .
G-82 G10 C58 A86 A86 A86 A86 A86 A86 A86 A8	
• Molecule 5: DNA (169-MER)	
Chain S:	98% •
G-82 A-66 C-10 C84 A86 A86	
• Molecule 5: DNA (169-MER)	
Chain c:	100%
G = 82 C 88 A8 66	
• Molecule 5: DNA (169-MER)	
Chain m:	99% .
0 0 0 0 0 0 0 0 0 0 0 0 0 0	
• Molecule 6: DNA (169-MER)	
Chain J:	98% •
A 83 A 84 A 84 A 85 A 8	
• Molecule 6: DNA (169-MER)	
Chain T:	98% .
0 -82 7 -1 7 -1 6 -6 6 -6 7 -6 7 -6 8 -1 10 -1 10 -1 10 -1 10 -1 10 -1 10 -1 10 -1 10 -1 10 -1	
• Molecule 6: DNA (169-MER)	
Chain d:	99% .
G-82 - 77 - 77 - 57 - 183 - 886 - 886	



• Molecule 6:	DNA (169-ME	ER)			
Chain n:		98	3%	.	
G-82 1-77 1-77 1-77 10 11 11 11 11 12 12	T33 G84 A86 A86				
• Molecule 7:	Histone H1.0				
Chain o:	33% 33%	6% •	61%		I
GLY PRO GLU GLU ASN SER SER ALLA PRO	ALA ALA LYS LYS PRO LYS ALA ALA ALA SER LYS SER LYS	LYS SER THR ASP P26 Y28 Y28 S29 S29	D30 131 132 133 434 434 434 435 136 136 136 833 840 841 841 841 841 841	A43 644 845 846 846 846 848 848 150 051 851 851 854 851	K55 S56 H57 Y58 K59
V60 N63 A64 D65 S66 C67 C67 K69 K69	571 172 172 173 174 175 177 178 178 178 178 178 178 178 181	K82 1933 1184 K85 636 638 638 839 839 839	593 193 194 195 195 195 195 195 195 195 195 195 195	SER VAL ALA ALA PHE LYS THR LYS GLU TLE TLE	LYS VAL ALA THR PRO
LYS LYS ALA SER SER LYS LYS LYS ALA ALA	SER LYS ALA PRO PRO LYS LYS PRO LYS PRO LYS THR	PRO VAL LYS LYS LYS LYS LEU	ALA ALA THR PRO LYS LYS LYS LYS LYS LYS VAL	LYS ALA LYS PRO PRO VAL LYS ALA SER LYS PRO LYS LYS	ALA LYS PRO VAL LYS
PRO LYS ALA LYS SER SER ALA LYS ALA	LYS LYS GLY GLY				
• Molecule 7:	Histone H1.0 34%				
Chain p:	33%	5%	62%		
GLY PRO GLU GLU ASN SER SER ALA PRO	ALA ALA LYS PRO LYS LYS ALA ALA ALA SER LYS SER	LYS SER THR ASP P26 P26 Y28 S29 S29 S29	D30 131 132 133 434 434 436 136 136 637 637 838 840 841 841 841	A43 644 845 846 846 846 849 849 150 150 150 150 153	S56 H57 Y58 K59 V60
G61 E62 A64 A64 D65 S66 C65 C65 C65 C65 C65 C65 C65 C65 C65 C	271 172 172 172 174 174 177 177 177 178 178 178 178 178 178 178	X 82 Q 83 T 84 C 86 Q 86 Q 86 Q 88 Q 88 Q 88 Q 88 Q 89 Q 89 Q 89 Q 89	691 693 894 894 894 896 896 896 8396 8396 610 010 0110 11YS 11YS	SER VAL ALA PHLE LYS LYS LYS LYS GLU IILE LYS	LYS VAL ALA THR PRO
LYS LYS ALA SER LYS PRO LYS ALA ALA	SER LYS ALA PRO THR LYS LYS PRO LYS ALA ALA	PRO VAL LYS LYS ALA LYS LYS LYS LYS	ALA THR PRO LYS LYS LYS ALA LYS LYS LYS THR VAL	LYS ALA LYS PRO VAL LYS ALA SER LYS PRO LYS LYS LYS	ALA LYS PRO VAL LYS
PRO LYS ALA LYS SER SER ALA ALA ALA	GLY LYS LYS				



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	208.78Å 102.37 Å 212.71 Å	Deperitor	
a, b, c, α , β , γ	90.00° 101.12° 90.00°	Depositor	
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.83 - 3.39	Depositor	
Resolution (A)	48.83 - 3.39	EDS	
% Data completeness	98.9 (48.83-3.39)	Depositor	
(in resolution range)	98.9(48.83-3.39)	EDS	
R _{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.51 (at 3.40 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0189	Depositor	
D D	0.227 , 0.296	Depositor	
Λ, Λ_{free}	0.230 , 0.290	DCC	
R_{free} test set	2430 reflections $(1.99%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	135.9	Xtriage	
Anisotropy	0.057	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 121.5	EDS	
L-test for twinning ²	$< L > = 0.40, < L^2 > = 0.23$	Xtriage	
Estimated twinning fraction	0.000 for l,-k,h	Xtriage	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	53518	wwPDB-VP	
Average B, all atoms $(Å^2)$	177.0	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 70.83 % 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 2.9170e-06. 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)

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

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	Chain	Bond lengths		Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.56	0/828	0.83	1/1109~(0.1%)
1	Ε	0.56	0/828	0.92	3/1109~(0.3%)
1	Κ	0.51	0/837	0.76	0/1120
1	0	0.52	0/828	0.74	0/1109
1	U	0.59	0/828	0.85	0/1109
1	Y	0.57	0/828	0.93	1/1109~(0.1%)
1	е	0.50	0/837	0.74	0/1120
1	i	0.52	0/828	0.76	0/1109
2	В	0.56	0/645	0.92	2/862~(0.2%)
2	F	0.59	0/680	0.92	1/908~(0.1%)
2	L	0.51	0/645	0.83	0/862
2	Р	0.52	0/645	0.86	0/862
2	V	0.61	0/645	0.91	0/862
2	Ζ	0.59	0/680	0.94	1/908~(0.1%)
2	f	0.51	0/645	0.85	0/862
2	j	0.55	0/645	0.85	0/862
3	С	0.52	0/836	0.83	0/1128
3	G	0.57	0/883	0.85	2/1188~(0.2%)
3	М	0.51	0/831	0.78	0/1121
3	Q	0.47	0/820	0.69	0/1107
3	W	0.52	0/836	0.86	1/1128~(0.1%)
3	a	0.57	0/883	0.82	0/1188
3	g	0.47	0/831	0.76	1/1121~(0.1%)
3	k	0.46	0/820	0.70	0/1107
4	D	0.54	0/795	0.81	0/1062
4	Н	0.54	0/795	0.86	0/1062
4	Ν	0.46	0/786	0.69	0/1051
4	R	0.47	0/786	0.73	0/1051
4	Х	0.57	0/799	0.81	0/1067
4	b	0.55	0/799	0.85	0/1067
4	h	0.50	0/786	0.73	1/1051~(0.1%)
4	l	0.48	0/786	0.74	0/1051



Mal	Chain	Bo	nd lengths	В	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
5	Ι	0.45	0/3884	0.86	2/5993~(0.0%)
5	S	0.35	0/3884	0.86	3/5993~(0.1%)
5	с	0.47	0/3884	0.85	0/5993
5	m	0.36	0/3884	0.85	1/5993~(0.0%)
6	J	0.46	0/3882	0.85	4/5990~(0.1%)
6	Т	0.35	0/3882	0.85	3/5990~(0.1%)
6	d	0.46	1/3882~(0.0%)	0.85	1/5990~(0.0%)
6	n	0.35	0/3882	0.84	3/5990~(0.1%)
7	0	0.64	0/589	0.75	0/785
7	р	0.72	0/572	0.79	0/762
All	All	0.47	1/57169~(0.0%)	0.84	31/82911~(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
4	R	0	1
4	b	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
6	d	-57	DC	O3'-P	-5.24	1.54	1.61

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
5	Ι	10	DG	O5'-P-OP2	-7.60	98.86	105.70
3	W	81	ARG	NE-CZ-NH1	7.15	123.87	120.30
6	n	-10	DC	C1'-O4'-C4'	-6.12	103.98	110.10
1	Е	134	ARG	NE-CZ-NH1	6.11	123.35	120.30
6	Т	-10	DC	C1'-O4'-C4'	-6.08	104.02	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group		
4	R	51	ASP	Peptide		
Continued on next nage						



Continued from previous page...

Mol	Chain	Res	Type	Group
4	b	31	ARG	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
1	А	97/138~(70%)	95~(98%)	2(2%)	0	100	100
1	Е	97/138~(70%)	89 (92%)	8 (8%)	0	100	100
1	K	98/138~(71%)	86 (88%)	9 (9%)	3(3%)	4	23
1	Ο	97/138~(70%)	88 (91%)	8 (8%)	1 (1%)	15	46
1	U	97/138~(70%)	92~(95%)	5 (5%)	0	100	100
1	Y	97/138~(70%)	92~(95%)	3 (3%)	2(2%)	7	30
1	е	98/138~(71%)	92~(94%)	5 (5%)	1 (1%)	15	46
1	i	97/138~(70%)	83~(86%)	12 (12%)	2(2%)	7	30
2	В	78/105~(74%)	74~(95%)	4 (5%)	0	100	100
2	F	82/105~(78%)	76~(93%)	6 (7%)	0	100	100
2	L	78/105~(74%)	72 (92%)	6 (8%)	0	100	100
2	Р	78/105~(74%)	66~(85%)	10 (13%)	2(3%)	5	26
2	V	78/105~(74%)	75~(96%)	3 (4%)	0	100	100
2	Z	82/105~(78%)	78~(95%)	4 (5%)	0	100	100
2	f	78/105~(74%)	70 (90%)	8 (10%)	0	100	100
2	j	78/105~(74%)	$70 \ (90\%)$	6 (8%)	2(3%)	5	26
3	С	$10\overline{5/132}\ (80\%)$	99(94%)	6 (6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
3	G	112/132~(85%)	102 (91%)	9~(8%)	1 (1%)	17	49
3	М	104/132~(79%)	90~(86%)	13~(12%)	1 (1%)	15	46
3	\mathbf{Q}	103/132~(78%)	97~(94%)	6~(6%)	0	100	100
3	W	105/132~(80%)	100~(95%)	5 (5%)	0	100	100
3	a	112/132~(85%)	97~(87%)	12 (11%)	3~(3%)	5	26
3	g	104/132~(79%)	97~(93%)	7~(7%)	0	100	100
3	k	103/132~(78%)	97~(94%)	5 (5%)	1 (1%)	15	46
4	D	97/128~(76%)	89~(92%)	7~(7%)	1 (1%)	15	46
4	Н	97/128~(76%)	86~(89%)	7~(7%)	4 (4%)	3	18
4	Ν	96/128~(75%)	85~(88%)	11 (12%)	0	100	100
4	R	96/128~(75%)	88~(92%)	6~(6%)	2(2%)	7	30
4	Х	98/128~(77%)	89 (91%)	7~(7%)	2(2%)	7	30
4	b	98/128~(77%)	84 (86%)	13~(13%)	1 (1%)	15	46
4	h	96/128~(75%)	88 (92%)	8 (8%)	0	100	100
4	1	96/128~(75%)	84 (88%)	10 (10%)	2(2%)	7	30
7	О	74/195~(38%)	64 (86%)	8 (11%)	2(3%)	5	26
7	р	72/195~(37%)	66~(92%)	3 (4%)	3 (4%)	3	18
All	All	3178/4414 (72%)	2900 (91%)	242 (8%)	36~(1%)	14	44

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
3	G	14	ALA
4	Н	32	SER
4	Х	104	GLY
3	a	13	LYS
3	a	14	ALA

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.



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	86/112~(77%)	84 (98%)	2(2%)	50	74
1	Ε	86/112~(77%)	81 (94%)	5~(6%)	20	50
1	Κ	87/112~(78%)	82 (94%)	5~(6%)	20	50
1	Ο	86/112~(77%)	81 (94%)	5~(6%)	20	50
1	U	86/112~(77%)	84 (98%)	2(2%)	50	74
1	Y	86/112~(77%)	81 (94%)	5 (6%)	20	50
1	е	87/112 (78%)	83 (95%)	4 (5%)	27	57
1	i	86/112~(77%)	83 (96%)	3 (4%)	36	65
2	В	65/80~(81%)	65 (100%)	0	100	100
2	F	69/80~(86%)	65 (94%)	4 (6%)	20	50
2	L	65/80~(81%)	64 (98%)	1 (2%)	65	82
2	Р	65/80~(81%)	64 (98%)	1 (2%)	65	82
2	V	65/80~(81%)	64 (98%)	1 (2%)	65	82
2	Z	69/80~(86%)	65 (94%)	4 (6%)	20	50
2	f	65/80~(81%)	64 (98%)	1 (2%)	65	82
2	j	65/80~(81%)	64 (98%)	1 (2%)	65	82
3	С	85/101 (84%)	80 (94%)	5 (6%)	19	49
3	G	88/101 (87%)	79 (90%)	9 (10%)	7	26
3	М	85/101 (84%)	81 (95%)	4 (5%)	26	57
3	Q	83/101 (82%)	78 (94%)	5 (6%)	19	49
3	W	85/101 (84%)	80 (94%)	5 (6%)	19	49
3	a	88/101 (87%)	80 (91%)	8 (9%)	9	32
3	g	85/101 (84%)	84 (99%)	1 (1%)	71	85
3	k	83/101 (82%)	79 (95%)	4 (5%)	25	56
4	D	85/106~(80%)	76 (89%)	9 (11%)	6	24
4	Н	85/106~(80%)	76 (89%)	9 (11%)	6	24
4	Ν	84/106~(79%)	81 (96%)	3 (4%)	35	63
4	R	84/106~(79%)	79 (94%)	5 (6%)	19	49
4	Х	85/106 (80%)	77 (91%)	8 (9%)	8	30
4	b	85/106 (80%)	81 (95%)	4 (5%)	26	57
4	h	84/106~(79%)	79 (94%)	5 (6%)	19	49
4	1	84/106~(79%)	76 (90%)	8 (10%)	8	29



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
7	О	63/158~(40%)	52 (82%)	11 (18%)	2	7	
7	р	61/158~(39%)	54 (88%)	7 (12%)	5	20	
All	All	2700/3508~(77%)	2546~(94%)	154 (6%)	20	50	

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
4	h	28	LYS
7	0	77	THR
4	h	63	ASN
4	1	32	SER
7	р	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	е	93	GLN
1	i	93	GLN
1	е	108	ASN
4	h	49	HIS
3	k	104	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)

Of 53 ligands modelled in this entry, 53 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 (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^{th} 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	99/138~(71%)	0.17	3 (3%) 50 49	79, 108, 157, 189	0
1	Е	99/138~(71%)	0.05	1 (1%) 82 81	84, 109, 153, 193	0
1	K	100/138~(72%)	0.37	6 (6%) 21 23	131, 173, 218, 250	0
1	Ο	99/138~(71%)	0.43	6 (6%) 21 22	118, 170, 224, 260	0
1	U	99/138~(71%)	0.23	3 (3%) 50 49	78, 107, 154, 203	0
1	Y	99/138 (71%)	0.09	1 (1%) 82 81	81, 110, 151, 194	0
1	e	100/138 (72%)	0.39	6 (6%) 21 23	133, 180, 228, 269	0
1	i	99/138~(71%)	0.42	6 (6%) 21 22	130, 170, 218, 246	0
2	В	80/105~(76%)	0.19	0 100 100	84, 108, 136, 192	0
2	F	84/105 (80%)	0.10	0 100 100	87, 109, 162, 192	0
2	L	80/105~(76%)	0.32	5 (6%) 20 21	133, 169, 216, 236	0
2	Р	80/105~(76%)	0.27	5 (6%) 20 21	120, 156, 198, 206	0
2	V	80/105~(76%)	0.17	0 100 100	81, 106, 134, 185	0
2	Z	84/105 (80%)	0.08	0 100 100	88, 110, 160, 201	0
2	f	80/105~(76%)	0.39	2 (2%) 57 55	141, 176, 231, 244	0
2	j	80/105~(76%)	0.24	3 (3%) 40 39	125, 166, 198, 212	0
3	С	107/132~(81%)	0.13	1 (0%) 84 83	92, 115, 162, 200	0
3	G	114/132~(86%)	0.35	3 (2%) 56 54	87, 117, 195, 228	0
3	М	106/132~(80%)	0.45	8 (7%) 14 16	137, 172, 206, 250	0
3	Q	105/132~(79%)	0.42	6 (5%) 23 24	136, 178, 213, 231	0
3	W	107/132~(81%)	0.12	1 (0%) 84 83	90, 110, 163, 197	0
3	a	114/132 (86%)	0.56	7 (6%) 21 22	87, 112, 197, 240	0
3	g	106/132~(80%)	0.42	6 (5%) 23 24	137, 178, 208, 233	0
3	k	$10\overline{5}/132~(79\%)$	0.40	3 (2%) 51 50	139, 187, 218, 244	0



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Mol	Chain	Analysed	$<$ RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
4	D	99/128~(77%)	0.33	5 (5%) 28 28	94, 117, 177, 229	0
4	Н	99/128~(77%)	0.28	3 (3%) 50 49	93, 117, 191, 225	0
4	Ν	98/128~(76%)	0.31	3 (3%) 49 48	122, 176, 214, 235	0
4	R	98/128~(76%)	0.28	6 (6%) 21 22	126, 167, 222, 258	0
4	Х	100/128~(78%)	0.34	5 (5%) 28 29	91, 114, 191, 247	0
4	b	100/128 (78%)	0.34	5 (5%) 28 29	91, 114, 197, 256	0
4	h	98/128~(76%)	0.36	5 (5%) 28 28	133, 176, 214, 239	0
4	1	98/128~(76%)	0.33	5 (5%) 28 28	139, 181, 235, 261	0
5	Ι	169/169~(100%)	-0.59	2 (1%) 79 77	121, 160, 275, 354	0
5	S	169/169~(100%)	-0.34	1 (0%) 89 89	170, 217, 295, 343	0
5	с	169/169~(100%)	-0.58	2 (1%) 79 77	121, 156, 271, 324	0
5	m	169/169~(100%)	-0.35	3 (1%) 68 67	169, 226, 287, 362	0
6	J	169/169~(100%)	-0.61	3 (1%) 68 67	119, 162, 262, 356	0
6	Т	169/169~(100%)	-0.32	4 (2%) 59 57	165, 221, 295, 341	0
6	d	169/169~(100%)	-0.63	1 (0%) 89 89	117, 159, 270, 370	0
6	n	169/169~(100%)	-0.32	3 (1%) 68 67	167, 224, 294, 317	0
7	0	76/195~(38%)	4.45	65 (85%) 0 0	206, 239, 263, 285	1 (1%)
7	р	74/195~(37%)	4.47	67 (90%) 0 0	201, 237, 264, 273	1 (1%)
All	All	4598/5766 (79%)	0.21	270 (5%) 22 23	78, 164, 252, 370	2 (0%)

Continued from previous page...

The worst 5 of 270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	р	90	SER	13.1
7	0	87	VAL	12.8
7	0	90	SER	10.0
3	a	120	THR	9.8
7	р	56	SER	9.8

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

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



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6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(A^2)$	Q<0.9
8	CA	Ι	105	1/1	0.24	0.18	163,163,163,163	0
8	CA	d	104	1/1	0.49	0.51	160,160,160,160	0
8	CA	i	201	1/1	0.56	0.13	170,170,170,170	0
8	CA	0	202	1/1	0.62	0.12	175,175,175,175	0
8	CA	с	105	1/1	0.66	0.11	145,145,145,145	0
8	CA	G	201	1/1	0.67	0.80	164,164,164,164	0
8	CA	0	201	1/1	0.68	0.22	157,157,157,157	0
9	K	Т	105	1/1	0.71	0.15	172,172,172,172	0
8	CA	a	202	1/1	0.73	0.30	$157,\!157,\!157,\!157$	0
8	CA	р	201	1/1	0.73	0.27	$155,\!155,\!155,\!155$	0
8	CA	Ι	107	1/1	0.73	0.10	160,160,160,160	0
8	CA	J	101	1/1	0.74	0.23	$133,\!133,\!133,\!133$	0
8	CA	Ι	103	1/1	0.76	0.19	130,130,130,130	0
8	CA	0	201	1/1	0.77	0.17	$157,\!157,\!157,\!157$	0
8	CA	m	102	1/1	0.80	0.12	185,185,185,185	0
8	CA	Т	102	1/1	0.80	0.32	163,163,163,163	0
8	CA	Т	103	1/1	0.81	0.84	174,174,174,174	0
8	CA	с	106	1/1	0.81	0.17	$153,\!153,\!153,\!153$	0
8	CA	d	106	1/1	0.82	0.23	$157,\!157,\!157,\!157$	0
8	CA	J	103	1/1	0.82	0.16	158,158,158,158	0
8	CA	Ι	108	1/1	0.83	0.39	137,137,137,137	0
9	K	d	109	1/1	0.83	0.12	161,161,161,161	0
8	CA	С	201	1/1	0.85	0.28	145,145,145,145	0
9	K	Ι	109	1/1	0.85	0.09	141,141,141,141	0
8	CA	d	101	1/1	0.86	0.45	150,150,150,150	0
8	CA	d	107	1/1	0.86	0.16	152,152,152,152	0
8	CA	I	101	1/1	0.86	0.34	147,147,147,147	0
8	CA	d	105	1/1	0.86	0.48	144,144,144,144	0
8	CA	n	101	1/1	0.86	0.27	150,150,150,150	0
8	CA	с	107	1/1	0.87	0.40	149,149,149,149	0
8	CA	a	201	1/1	0.87	0.49	147,147,147,147	0
8	CA	J	104	1/1	0.87	0.15	130,130,130,130	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	d	108	1/1	0.87	0.15	162,162,162,162	0
8	CA	W	201	1/1	0.88	0.36	146,146,146,146	0
8	CA	m	101	1/1	0.90	0.27	$159,\!159,\!159,\!159,\!159$	0
8	CA	с	103	1/1	0.91	0.10	$135,\!135,\!135,\!135$	0
8	CA	d	102	1/1	0.91	0.24	128,128,128,128	0
9	K	Т	104	1/1	0.92	0.15	157, 157, 157, 157, 157	0
8	CA	Y	201	1/1	0.92	0.31	$125,\!125,\!125,\!125,\!125$	0
9	K	Т	106	1/1	0.92	0.41	$153,\!153,\!153,\!153$	0
8	CA	j	201	1/1	0.92	0.11	156, 156, 156, 156, 156	0
8	CA	d	103	1/1	0.93	0.31	139,139,139,139	0
8	CA	n	102	1/1	0.94	0.28	166, 166, 166, 166	0
9	K	с	108	1/1	0.94	0.11	143,143,143,143	0
8	CA	Ι	106	1/1	0.94	0.37	$134,\!134,\!134,\!134$	0
8	CA	J	102	1/1	0.95	0.60	165, 165, 165, 165, 165	0
8	CA	с	104	1/1	0.95	0.05	$159,\!159,\!159,\!159,\!159$	0
8	CA	S	101	1/1	0.95	0.38	$159,\!159,\!159,\!159,\!159$	0
8	CA	с	102	1/1	0.96	0.40	$131,\!131,\!131,\!131$	0
8	CA	Т	101	1/1	0.96	0.10	160,160,160,160	0
8	CA	Ι	102	1/1	0.97	0.33	$117,\!117,\!117,\!117$	0
8	CA	Ι	104	1/1	0.97	0.12	148,148,148,148	0
8	CA	с	101	1/1	0.98	0.41	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.

