

Full wwPDB X-ray Structure Validation Report (i)

Mar 26, 2024 – 10:14 AM JST

PDB ID	:	7XVL
Title	:	Crystal Structure of Nucleosome-H1.0 Linker Histone Assembly (sticky-169an
		DNA fragment)
Authors	:	Adhireksan, Z.; Qiuye, B.; Lee, P.L.; Sharma, D.; Padavattan, S.; Davey, C.A.
Deposited on	:	2022-05-24
Resolution	:	3.51 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 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 3.51 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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 >=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 chain		
1	А	138	69%	•	29%
1	Е	138	.% 67%	•	29%
1	K	138	69%	•	29%
1	0	138	67%	•	29%
1	U	138	% 	•	29%
1	Y	138	70%	•	29%
1	е	138	66%	5%	29%



Chain Length Quality of chain Mol .% 1 i 13867% 29% . 2В 10574% 25% • 2F 10581% 17% 2L 10571% 25% • Р 210574% 21% • • 4% \mathbf{V} 210570% 6% 25% .% 2Ζ 10575% 6%• 17% 2f 10525% 71% • .% 2j 10573% 24% • .% С 3 13280% 18% .% \mathbf{G} 3 13276% • 20% 2% М 3 13277% 5% 18% .% 3 Q 13273% 6% 20% W 3 13277% 5% 18% 11% 3 132 \mathbf{a} 75% 21% • • 3 132g 77% • 20% 3 k 13271% 7% • 21% D 4 12867% 8% 25% Η 1284 65% 9% • 25% .% Ν 1284 71% 25% • 4 R 12825% 65% 9% • Х 1284 66% 9% 25% 14% \mathbf{b} 1284 66% 25% 9% 2% 1284 h 68% 7% 25% 1 128 4 69% 6% 25%

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Mol	Chain	Length		Quality of chain		
5	Ι	169		96%		•
5	S	169		97%		•
5	с	169	% 	98%		•
5	m	169		99%		·
6	J	169		95%		5%
6	Т	169		96%		•
6	d	169	% 	98%		•
6	n	169	.% •	96%		•
7	О	195	28% 32% 8	3%	60%	



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 52574 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	08	Total	С	Ν	0	S	0	0	0
	A	90	807	508	156	139	4	0	0	0
1	F	08	Total	С	Ν	0	S	0	0	0
		90	807	508	156	139	4	0	0	0
1	K	08	Total	С	Ν	0	S	0	0	0
	Γ	98	807	508	156	139	4	0	0	0
1	0	08	Total	С	Ν	0	S	0	0	0
		90	807	508	156	139	4	0	0	0
1	II	08	Total	С	Ν	0	S	0	0	0
	U	90	807	508	156	139	4	0	0	0
1	V	08	Total	С	Ν	0	S	0	0	0
	I	90	807	508	156	139	4	0	0	0
1	0	08	Total	С	Ν	0	S	0	0	0
	е	90	807	508	156	139	4	0	0	0
1	;	08	Total	С	Ν	Ο	S	0	0	0
	1	90	807	508	156	139	4		U	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
E	-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
Ý	-1	SER	-	expression tag	UNP P68431
e	-2	GLY	-	expression tag	UNP P68431



00.000.00	ea ji ente pi e	ere as pagem			
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
9	В	70	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	19	627	395	121	110	1	0	0	0
9	Б	87	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Г	01	703	442	142	118	1	0	0	0
2	т	70	Total	С	Ν	0	S	0	0	0
		79	627	395	121	110	1	0	0	0
2	D	83	Total	С	Ν	Ο	S	0	0	0
	1	00	662	418	129	114	1	0	0	0
2	V	70	Total	С	Ν	Ο	S	0	0	0
2	v	19	627	395	121	110	1			0
2	7	87	Total	С	Ν	Ο	S	0	0	0
2		01	703	442	142	118	1	0	0	0
2	f	70	Total	С	Ν	Ο	\mathbf{S}	0	0	0
2	L	13	627	395	121	110	1	0	0	0
2	i	80	Total	С	Ν	Ο	S	0	0	0
	J	00	638	401	125	111	1	U		U

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



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
3 C	109	Total	С	Ν	Ο	0	0	0	
5	U	108	835	526	165	144	0	0	0
2	3 C	105	Total	С	Ν	Ο	0	0	0
0	G	105	810	511	158	141	0	0	0
9	м	109	Total	С	Ν	Ο	0	0	0
5	3 M	108	835	526	165	144	0	0	0
9	3 Q	105	Total	С	Ν	Ο	0	0	0
5			810	511	158	141			0
2	W/	108	Total	С	Ν	Ο	0	0	0
0	vv	108	835	526	165	144	0		
2		104	Total	С	Ν	Ο	0	0	0
0	a	104	805	508	157	140	0	0	0
3	ď	105	Total	С	Ν	Ο	0	0	0
0	g	105	810	511	158	141	0	0	0
3	Ŀ	104	Total	С	Ν	Ο	0	0	0
5	ĸ	104	805	508	157	140	0	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		Total	С	Ν	0	S	0	0	0
4	D	90	755	474	138	141	2	0	0	0
4	Ц	06	Total	С	Ν	0	S	0	0	0
4	11	90	755	474	138	141	2	0	0	0
4	N	06	Total	С	Ν	0	S	0	0	0
4	11	90	755	474	138	141	2	0	0	0
4	D	06	Total	С	Ν	0	S	0	0	0
4	n	90	755	474	138	141	2	0	0	0
4	v	V 06	Total	С	Ν	0	S	0	0	0
4	Λ	90	755	474	138	141	2	0		
4	h	06	Total	С	Ν	0	S	0	0	0
4	D	90	755	474	138	141	2	0	0	0
4	h	06	Total	С	Ν	0	S	0	0	0
4 n	90	755	474	138	141	2	0	0	0	
4	4 l	1 96	Total	С	Ν	0	S	0	0	0
4			755	474	138	141	2	0	0	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

• Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
5	Ι	169	Total 3457	C 1639	N 656	O 993	Р 169	0	0	0



Mol	Chain	Residues		At	toms			ZeroOcc	AltConf	Trace
5 S	C	160	Total	С	Ν	0	Р	0	0	0
	109	3457	1639	656	993	169	0	0	0	
н	F .	160	Total	С	Ν	0	Р	0	0	0
o c	109	3457	1639	656	993	169	0	0	0	
5 m	169	Total	С	Ν	0	Р	0	0	0	
		3457	1639	656	993	169				

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

Mol	Chain	Residues		Atoms					AltConf	Trace
6	C I	160	Total	С	Ν	Ο	Р	0	0	0
0	J	109	3474	1652	616	1037	169	0	0	
6	т	169	Total	С	Ν	Ο	Р	0	0	0
0	0 1		3474	1652	616	1037	169	0		
6	d	160	Total	С	Ν	Ο	Р	0	0	0
0	0 0	109	3474	1652	616	1037	169			0
6 n	169	Total	С	Ν	Ο	Р	0	0	0	
		3474	1652	616	1037	169			0	

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	О	78	Total 595	C 368	N 111	0 115	S 1	0	0	0

There are 2 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



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

GLY SER MET MET ARG LIYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS CL	LEU THLA LYS LYS ALA ALA ALA ALA ALA ALA ALA CLY VAL CLY VAL CLY	A135
• Molecule 1: Histone H3.1		
Chain e: 6	6% 5%	29%
GLY SER MET ARE ARC LYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	LEU THR LYS LYS ALA ALA ALA ALA ALA ALA ALA CYS CLY VAL LYS CLY	151 151 857 857 857 865 864 863 864 863 866 866 866 866 866 866 866 866 866
• Molecule 1: Histone H3.1		
Chain i: 6	7% ·	29%
GLY SER MET ALA ALA ARA CLYS GLN CLYS GLY CLYS CLY PRO CLN	LEU THR LYS LYS ALA ALA ALA ALA ALA ALA CLY GLY CLYS CLY CLYS	H39 L48 R83 R129 A135 A135
• Molecule 2: Histone H4		
Chain B:	74%	• 25%
CLY SER SER SER SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	LYS VAL LEU LEU LEU D24 D24 C102 C102	
• Molecule 2: Histone H4		
Chain F:	81%	• 17%
GLY SER MET SER SER SER GLY GLY GLY CLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	000 000	
• Molecule 2: Histone H4		
Chain L:	71%	• 25%
GLY SER SER SER SER GLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	VAL VAL LEU ARG ARG ARG ARG ARG R92 R92 R95 R95 R95	
• Molecule 2: Histone H4		
Chain P:	74%	•• 21%
CLY SER SER SER SER CLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	K20 122 122 122 125 126 126 126 126 126	
• Molecule 2: Histone H4		
Chain V:	70%	6% 25%





• Molecule 3: Histone H2A type 1-B/E



Chain Q:		73%	6%	20%
ELY EET EET LLY KG CV CV	24 10 11 44	29 101 101 118 118 118 118 118 118	HR LLU IS IS YS YS YS YS	
• Molecule 3:	Histone H2A type	≝ ≝ ≝ ⊨ ≥ ≝ ⊒ e 1-B/E	LGCFFLHW0H	
Chain W:		77%	5%	18%
X H H H X G X S N X		<mark>오</mark>	^{δ0} × δ0	
• Molecule 3:	[©] Histone H2A type .%	е 1- Б /Е		
Chain a:		75%	••	21%
GLY SER MET SER SER GLY GLY GLN GLN	C C C C C C C C C C C C C C C C C C C	C22 C22 C22 C23 C23 C23 C23 C23 C23 C23	K74 T76 R77 I78 I78 R81 H81 H82 104	LYS LYS GLU GLU HIS HIS LYS ALA ALA GLY LYS CLY
• Molecule 3:	Histone H2A type	e 1-B/E		
Chain g:		77%		20%
GLY SER MET MET SER GLY GLY GLY GLN GLN	CLYS CLYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	VI14 K18 LYS LYS CLU GLU GLU HIS HIS HIS LYS LYS LYS	CLY CLYS	
• Molecule 3:	Histone H2A type	e 1-B/E		
Chain k:	7	71%	7% •	21%
GLY SER MET SER GLY ARG GLY CJN GLN	GLY GLY LYS ALA ALA ALA ALA T16 716 716 729 729 729	R42 A47 L65 D72 N73 K74 K74 K81	K118 LYS THR GLU GLU HIS HIS HIS LYS GLY GLY	217
• Molecule 4:	Histone H2B type	e 1-J		
Chain D:	67	%	8%	25%
GLY SER MET MET PRO GLU PRO ALA LYS SER SER	PRO PRO ALA ALA CLYS CLYS GLY GLY SER LYS ALA ALA ALA ALA THR THR	ALA GLN LYS LYS ASP CLY LYS LYS ASD K30 K31 K31 S32	R33 S36 V48 N63 S56 N63 S64 S64 S64	60 6104 K125
• Molecule 4:	Histone H2B type	e 1-J		
Chain H:	659	%	9% •	25%
GLY SER MET PRO GLU PRO ALA LYS SER	PRO ALA ALA ALA LYS CLYS GLY GLYS CLYS ALA ALA ALA ALA ALA CLYS CLYS	ALA GLN LYS LYS LYS ASP CLYS LYS LYS ASP K30 K30 K30 K30 K31 S32	R33 836 836 838 838 838 838 838 858 856 856 856	L80 K85 K85 S91 K125
• Molecule 4:	Histone H2B type	e 1-J		



Chain N:	71%		25%
GLY SER MET PRO GLU PRO PRO LYS SER ALA	PR0 ALA ALA ALA ALA ALA CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	<mark>8123 A124</mark> K125	
• Molecule 4:	: Histone H2B type 1-J		
Chain R:	65% 9%	% •	25%
GLY SER MET PRO GLU PRO PRO ALA LYS SER ALA	PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	S55 S64 L80	N85 188 6104 119 119 124 124 K125
• Molecule 4:	: Histone H2B type 1-J		
Chain X:	66% 9	%	25%
GLY SER MET PRO GLU PRO ALA LYS SER ALA	PRO ALA ALA ALA ALA PRO LYS CLY CLYS CLYS CLYS CLYS CLYS CLYS C	N63 K85 R86	591 (104 8112 8112 1115 1115 1115 1115
• Molecule 4:	Histone H2B type 1-J		
Chain b:	66% 9 [.]	% •	25%
GLY SER MET PRO GLU PRO PRO ALA ALA ALA	PRO ALA ALA PRO LYS CLY CLY CLY CLY SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	Y40 V41 Y42 L45 K46	D51 152 154 154 154 855 855 855 855 855 862 862 862
L80 K85 F196 G104 A124 K125			
• Molecule 4:	Histone H2B type 1-J		
Chain h:	68%	7%	25%
GLY SER MET PRO GLU PRO PRO ALA ALA ALA	PR0 ALA ALA ALA ALA ALA LLYS GLY LLYS LLYS LLYS LLYS LLYS LLYS	K85 891 E93	T115 T122 K126
• Molecule 4:	: Histone H2B type 1-J		
Chain l:	69% 6	5%	25%
GLY SER MET PRO GLU PRO ALA SER SER	PRD ALA ALA ALA CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	R99 G104 V118	K 125
• Molecule 5:	: DNA (169-MER)		
Chain I:	96%		·



C-82 T-47 C-2 G9 A39 G9 A39 G58 G58 C58

• Molecule 5: DNA (169-MER)

Chain S:	97%
C-82 A-76 G63 G63 A67 T366	
• Molecule 5: DNA (169-MER)	
Chain c:	98%
• Molecule 5: DNA (169-MER)	
Chain m:	99%
C-82 C45 B8	
• Molecule 6: DNA (169-MER)	
Chain J:	95% 5%
C-82 G-64 G-64 C-47 C-47 C-47 C-47 C-47 C-47 C-47 C-4	
• Molecule 6: DNA (169-MER)	
Chain T:	96% •
C-82 G-64 G-64 A-34 A-34 A-34 C-86 C-88 C-88 C-82	
• Molecule 6: DNA (169-MER)	
Chain d:	98% •
0 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	
• Molecule 6: DNA (169-MER)	
Chain n:	96% .
	WORLDWIDE PROTEIN DATA BANK



• Molecule 7: Histone H1.0





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	213.85Å 102.46Å 218.29Å	Deperitor
a, b, c, α , β , γ	90.00° 100.49° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	88.44 - 3.51	Depositor
Resolution (A)	88.28 - 3.51	EDS
% Data completeness	95.9 (88.44-3.51)	Depositor
(in resolution range)	$95.9 \ (88.28 - 3.51)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.11 (at 3.49 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.206 , 0.280	Depositor
Λ, Λ_{free}	0.209 , 0.276	DCC
R_{free} test set	2266 reflections $(2.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	116.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 100.2	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52574	wwPDB-VP
Average B, all atoms $(Å^2)$	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.

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).

Mol Chain		Bo	ond lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.68	0/819	0.90	0/1097	
1	Е	0.68	0/819	0.92	0/1097	
1	Κ	0.65	0/819	0.85	0/1097	
1	0	0.66	0/819	0.84	0/1097	
1	U	0.67	0/819	0.81	0/1097	
1	Y	0.66	0/819	0.82	0/1097	
1	е	0.67	0/819	0.88	0/1097	
1	i	0.66	0/819	0.84	0/1097	
2	В	0.71	0/634	0.98	0/848	
2	F	0.69	0/711	0.95	0/948	
2	L	0.69	0/634	0.86	0/848	
2	Р	0.68	0/669	0.91	1/894~(0.1%)	
2	V	0.68	0/634	0.85	0/848	
2	Ζ	0.73	0/711	0.94	0/948	
2	f	0.70	0/634	0.95	0/848	
2	j	0.66	0/645	0.91	0/862	
3	С	0.67	0/845	0.92	0/1139	
3	G	0.71	0/820	0.90	0/1107	
3	М	0.68	0/845	0.85	0/1139	
3	\mathbf{Q}	0.68	0/820	0.84	0/1107	
3	W	0.68	0/845	0.83	0/1139	
3	a	0.69	0/815	0.84	0/1100	
3	g	0.68	0/820	0.86	0/1107	
3	k	0.66	0/815	0.84	0/1100	
4	D	0.69	0/766	0.89	0/1026	
4	Н	0.70	0/766	0.89	0/1026	
4	Ν	0.69	0/766	0.85	0/1026	
4	R	0.69	0/766	0.85	0/1026	
4	Х	0.70	0/766	0.82	0/1026	
4	b	0.70	0/766	0.81	0/1026	
4	h	0.69	0/766	0.86	0/1026	
4	1	0.68	$0/\overline{766}$	0.84	0/1026	
5	Ι	0.55	3/3883~(0.1%)	0.87	3/5983~(0.1%)	
5	S	0.48	2/3883~(0.1%)	0.85	3/5983~(0.1%)	



Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
5	с	0.41	1/3883~(0.0%)	0.83	1/5983~(0.0%)
5	m	0.46	2/3883~(0.1%)	0.86	0/5983
6	J	0.55	5/3891~(0.1%)	0.88	4/6008~(0.1%)
6	Т	0.52	4/3891~(0.1%)	0.84	2/6008~(0.0%)
6	d	0.40	1/3891~(0.0%)	0.84	1/6008~(0.0%)
6	n	0.48	2/3891~(0.1%)	0.86	6/6008~(0.1%)
7	0	0.74	0/601	0.88	0/802
All	All	0.58	20/56274~(0.0%)	0.86	21/81732~(0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	Ι	-82	DC	OP3-P	-10.36	1.48	1.61
6	d	-82	DC	OP3-P	-10.30	1.48	1.61
6	J	-82	DC	OP3-P	-10.17	1.49	1.61
6	Т	-82	DC	OP3-P	-10.05	1.49	1.61
5	S	-82	DC	OP3-P	-10.03	1.49	1.61
5	с	-82	DC	OP3-P	-9.95	1.49	1.61
5	m	-82	DC	OP3-P	-9.91	1.49	1.61
6	n	-82	DC	OP3-P	-9.82	1.49	1.61
6	Т	-46	DT	O3'-P	-6.20	1.53	1.61
5	Ι	-47	DT	O3'-P	-6.06	1.53	1.61
6	J	-38	DA	O3'-P	-5.89	1.54	1.61
6	J	-47	DC	O3'-P	-5.78	1.54	1.61
6	J	-57	DT	O3'-P	-5.70	1.54	1.61
6	Т	-34	DA	O3'-P	-5.61	1.54	1.61
6	n	56	DG	O3'-P	-5.56	1.54	1.61
5	m	45	DC	O3'-P	5.51	1.67	1.61
6	Т	-60	DG	O3'-P	-5.50	1.54	1.61
5	Ι	58	DG	O3'-P	-5.36	1.54	1.61
6	J	-16	DT	O3'-P	-5.31	1.54	1.61
5	S	-7	DG	O3'-P	-5.17	1.54	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
6	J	-68	DA	O5'-P-OP1	-8.23	98.29	105.70
6	n	29	DG	O5'-P-OP1	-7.27	99.16	105.70
6	J	-64	DG	C1'-O4'-C4'	-6.66	103.44	110.10
6	n	-60	DG	O4'-C4'-C3'	-6.22	102.01	104.50
6	J	-5	DA	O5'-P-OP2	-5.95	100.34	105.70
6	J	29	DG	O5'-P-OP2	-5.84	100.44	105.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	S	67	DA	C1'-O4'-C4'	-5.73	104.37	110.10
5	Ι	9	DG	O5'-P-OP2	-5.58	100.67	105.70
6	n	39	DA	O5'-P-OP2	5.53	117.34	110.70
5	с	63	DG	C1'-O4'-C4'	-5.47	104.63	110.10
6	n	-54	DC	O5'-P-OP2	-5.44	100.80	105.70
6	Т	-64	DG	C1'-O4'-C4'	-5.42	104.68	110.10
6	Т	75	DT	C1'-O4'-C4'	-5.41	104.69	110.10
2	Р	25	ASN	CB-CA-C	-5.32	99.76	110.40
5	S	-76	DA	C1'-O4'-C4'	-5.25	104.86	110.10
6	n	-60	DG	C1'-O4'-C4'	-5.25	104.86	110.10
6	d	-60	DG	C1'-O4'-C4'	-5.16	104.94	110.10
5	Ι	-2	DC	O5'-P-OP2	-5.12	101.09	105.70
5	Ι	39	DA	O5'-P-OP2	5.12	116.84	110.70
5	S	63	DG	C1'-O4'-C4'	-5.07	105.03	110.10
6	n	-80	DT	O5'-P-OP1	-5.03	101.17	105.70

There are no chirality outliers.

There are no planarity outliers.

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	96/138~(70%)	88 (92%)	8 (8%)	0	100	100
1	Е	96/138~(70%)	91 (95%)	5 (5%)	0	100	100
1	K	96/138 (70%)	86 (90%)	10 (10%)	0	100	100
1	Ο	96/138~(70%)	92 (96%)	4 (4%)	0	100	100

7XVL



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	U	96/138~(70%)	87 (91%)	7~(7%)	2(2%)	7	38
1	Y	96/138~(70%)	88~(92%)	8 (8%)	0	100	100
1	е	96/138~(70%)	89~(93%)	6~(6%)	1 (1%)	15	54
1	i	96/138~(70%)	88 (92%)	8 (8%)	0	100	100
2	В	77/105~(73%)	66~(86%)	11 (14%)	0	100	100
2	F	85/105~(81%)	71 (84%)	13~(15%)	1 (1%)	13	50
2	L	77/105~(73%)	66~(86%)	11 (14%)	0	100	100
2	Р	81/105~(77%)	72~(89%)	8 (10%)	1 (1%)	13	50
2	V	77/105~(73%)	68~(88%)	7~(9%)	2(3%)	5	33
2	Z	85/105 (81%)	72 (85%)	10 (12%)	3 (4%)	3	27
2	f	77/105~(73%)	67 (87%)	10 (13%)	0	100	100
2	j	78/105~(74%)	69~(88%)	9~(12%)	0	100	100
3	С	106/132~(80%)	94 (89%)	12 (11%)	0	100	100
3	G	103/132~(78%)	92 (89%)	11 (11%)	0	100	100
3	М	106/132~(80%)	94 (89%)	11 (10%)	1 (1%)	17	56
3	Q	103/132~(78%)	95~(92%)	7 (7%)	1 (1%)	15	54
3	W	106/132~(80%)	92 (87%)	13 (12%)	1 (1%)	17	56
3	a	102/132~(77%)	88 (86%)	12 (12%)	2 (2%)	7	39
3	g	103/132~(78%)	87 (84%)	16 (16%)	0	100	100
3	k	102/132~(77%)	89~(87%)	11 (11%)	2 (2%)	7	39
4	D	94/128~(73%)	84 (89%)	8 (8%)	2 (2%)	7	38
4	Н	94/128~(73%)	86 (92%)	6 (6%)	2 (2%)	7	38
4	N	94/128~(73%)	86 (92%)	7 (7%)	1 (1%)	14	52
4	R	94/128~(73%)	78 (83%)	12 (13%)	4 (4%)	2	22
4	Х	94/128~(73%)	79 (84%)	13 (14%)	2 (2%)	7	38
4	b	94/128~(73%)	81 (86%)	11 (12%)	2 (2%)	7	38
4	h	94/128~(73%)	83 (88%)	10 (11%)	1 (1%)	14	52
4	1	94/128~(73%)	84 (89%)	8 (8%)	2 (2%)	7	38
7	0	76/195~(39%)	64 (84%)	10 (13%)	2 (3%)	5	33
All	All	3064/4219 (73%)	2716 (89%)	313 (10%)	35 (1%)	14	52

All (35) Ramachandran outliers are listed below:



\mathbf{Mol}	Chain	\mathbf{Res}	Type
4	Ν	104	GLY
2	Р	21	VAL
4	R	33	ARG
2	V	28	GLY
2	Ζ	22	LEU
3	a	16	THR
4	b	33	ARG
4	D	31	ARG
4	D	104	GLY
4	Н	33	ARG
4	R	104	GLY
4	R	124	ALA
1	U	43	PRO
2	V	96	THR
2	Ζ	20	LYS
4	b	104	GLY
4	1	104	GLY
7	0	26	PRO
4	Н	31	ARG
2	Ζ	23	ARG
3	a	45	ALA
3	k	16	THR
4	1	70	PHE
4	R	85	LYS
2	F	23	ARG
7	0	98	SER
1	U	51	ILE
4	Х	112	SER
1	е	51	ILE
3	М	109	PRO
4	Х	104	GLY
3	Q	47	ALA
3	W	109	PRO
4	h	54	ILE
3	k	47	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.



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	85/112~(76%)	82 (96%)	3~(4%)	36	67
1	Ε	85/112~(76%)	80 (94%)	5~(6%)	19	53
1	К	85/112~(76%)	82 (96%)	3 (4%)	36	67
1	Ο	85/112~(76%)	80 (94%)	5~(6%)	19	53
1	U	85/112~(76%)	83 (98%)	2(2%)	49	76
1	Y	85/112~(76%)	84 (99%)	1 (1%)	71	87
1	е	85/112~(76%)	79 (93%)	6 (7%)	14	46
1	i	85/112 (76%)	80 (94%)	5 (6%)	19	53
2	В	64/80~(80%)	63 (98%)	1 (2%)	62	83
2	F	72/80~(90%)	71 (99%)	1 (1%)	67	85
2	L	64/80~(80%)	60 (94%)	4 (6%)	18	51
2	Р	68/80~(85%)	63 (93%)	5 (7%)	13	44
2	V	64/80~(80%)	61 (95%)	3 (5%)	26	60
2	Ζ	72/80~(90%)	66 (92%)	6 (8%)	11	40
2	f	64/80~(80%)	60 (94%)	4 (6%)	18	51
2	j	65/80~(81%)	62 (95%)	3~(5%)	27	61
3	С	85/101~(84%)	83 (98%)	2(2%)	49	76
3	G	83/101~(82%)	78 (94%)	5~(6%)	19	52
3	М	85/101 (84%)	80 (94%)	5~(6%)	19	53
3	Q	83/101~(82%)	76 (92%)	7 (8%)	11	40
3	W	85/101~(84%)	80 (94%)	5~(6%)	19	53
3	a	83/101~(82%)	79~(95%)	4(5%)	25	60
3	g	83/101~(82%)	79 (95%)	4(5%)	25	60
3	k	83/101 (82%)	74 (89%)	9(11%)	6	30
4	D	82/106~(77%)	74 (90%)	8 (10%)	8	33
4	Н	82/106~(77%)	70 (85%)	12 (15%)	3	18
4	Ν	82/106~(77%)	$78 \ (95\%)$	4(5%)	25	59
4	R	$82/106~(\overline{77\%})$	72 (88%)	10 (12%)	5	23
4	X	82/106~(77%)	72 (88%)	10 (12%)	5	23
4	b	82/106~(77%)	72 (88%)	10 (12%)	5	23
4	h	82/106~(77%)	74 (90%)	8 (10%)	8	33
4	1	$82/106~(\overline{77\%})$	76 (93%)	6(7%)	14	45



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	0	65/158~(41%)	52 (80%)	13 (20%)	1 7
All	All	2604/3350~(78%)	2425 (93%)	179 (7%)	15 47

All (179) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	58	THR
1	А	63	ARG
1	А	129	ARG
2	В	95	ARG
3	С	74	LYS
3	С	101	THR
4	D	33	ARG
4	D	36	SER
4	D	48	VAL
4	D	56	SER
4	D	63	ASN
4	D	64	SER
4	D	85	LYS
4	D	86	ARG
1	Е	45	THR
1	Е	65	LEU
1	Е	68	GLN
1	Е	129	ARG
1	Е	134	ARG
2	F	16	LYS
3	G	15	LYS
3	G	29	ARG
3	G	74	LYS
3	G	79	ILE
3	G	81	ARG
4	Н	31	ARG
4	Н	36	SER
4	Н	38	SER
4	Н	52	THR
4	Н	55	SER
4	Н	56	SER
4	Н	64	SER
4	Н	80	LEU
4	Н	85	LYS
4	Н	86	ARG
4	Н	91	SER



Mol	Chain	Res	Type
4	Н	125	LYS
1	К	63	ARG
1	K	86	SER
1	K	129	ARG
2	L	24	ASP
2	L	50	ILE
2	L	92	ARG
2	L	95	ARG
3	М	36	LYS
3	М	42	ARG
3	М	74	LYS
3	М	81	ARG
3	М	118	LYS
4	N	85	LYS
4	N	86	ARG
4	Ν	87	SER
4	Ν	123	SER
1	Ο	48	LEU
1	0	59	GLU
1	0	77	ASP
1	0	87	SER
1	0	129	ARG
2	Р	21	VAL
2	Р	23	ARG
2	Р	24	ASP
2	Р	25	ASN
2	Р	27	GLN
3	Q	15	LYS
3	Q	19	SER
3	Q	24	GLN
3	Q	29	ARG
3	Q	81	ARG
3	Q	101	THR
3	Q	107	VAL
4	R	31	ARG
4	R	42	TYR
4	R	52	THR
4	R	55	SER
4	R	64	SER
4	R	80	LEU
4	R	85	LYS
4	R	88	THR



Mol	Chain	Res	Type
4	R	119	THR
4	R	125	LYS
1	U	63	ARG
1	U	134	ARG
2	V	26	ILE
2	V	92	ARG
2	V	95	ARG
3	W	24	GLN
3	W	74	LYS
3	W	81	ARG
3	W	100	VAL
3	W	101	THR
4	Х	32	SER
4	Х	36	SER
4	Х	42	TYR
4	Х	55	SER
4	Х	63	ASN
4	Х	85	LYS
4	Х	86	ARG
4	Х	91	SER
4	Х	95	GLN
4	Х	115	THR
1	Y	58	THR
2	Ζ	16	LYS
2	Ζ	17	ARG
2	Z	18	HIS
2	Ζ	19	ARG
2	Z	20	LYS
2	Ζ	92	ARG
3	a	15	LYS
3	a	16	THR
3	a	74	LYS
3	a	81	ARG
4	b	31	ARG
4	b	33	ARG
4	b	42	TYR
4	b	46	LYS
4	b	52	THR
4	b	63	ASN
4	b	80	LEU
4	b	85	LYS
4	b	96	THR



Mol	Chain	Res	Type
4	b	125	LYS
1	е	56	LYS
1	е	58	THR
1	е	63	ARG
1	е	65	LEU
1	е	86	SER
1	е	129	ARG
2	f	24	ASP
2	f	50	ILE
2	f	95	ARG
2	f	96	THR
3	g	24	GLN
3	g	73	ASN
3	g	74	LYS
3	g	114	VAL
4	h	31	ARG
4	h	55	SER
4	h	64	SER
4	h	85	LYS
4	h	91	SER
4	h	93	GLU
4	h	115	THR
4	h	122	THR
1	i	48	LEU
1	i	83	ARG
1	i	87	SER
1	i	129	ARG
1	i	134	ARG
2	j	23	ARG
2	j	26	ILE
2	j	27	GLN
3	k	15	LYS
3	k	16	THR
3	k	24	GLN
3	k	29	ARG
3	k	42	ARG
3	k	65	LEU
3	k	72	ASP
3	k	74	LYS
3	k	81	ARG
4	1	33	ARG
4	1	80	LEU



Mol	Chain	Res	Type
4	1	85	LYS
4	1	99	ARG
4	l	118	VAL
4	l	125	LYS
7	0	29	SER
7	0	37	GLN
7	0	39	GLU
7	0	41	ASN
7	0	47	ARG
7	0	52	LYS
7	0	59	LYS
7	0	75	LEU
7	0	81	LEU
7	0	84	THR
7	0	92	SER
7	0	95	LEU
7	0	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	76	GLN
1	А	93	GLN
3	С	31	HIS
3	С	73	ASN
4	D	95	GLN
2	F	18	HIS
2	F	27	GLN
2	F	64	ASN
3	G	31	HIS
4	Н	47	GLN
4	Н	95	GLN
1	K	68	GLN
1	K	108	ASN
4	N	84	ASN
4	N	95	GLN
2	Р	27	GLN
3	Q	24	GLN
3	Q	110	ASN
4	R	95	GLN
4	Х	67	ASN
4	Х	95	GLN



Mol	Chain	Res	Type
1	Y	76	GLN
1	Y	108	ASN
2	Ζ	27	GLN
1	е	108	ASN
2	f	25	ASN
3	g	24	GLN
4	h	95	GLN
4	h	109	HIS
1	i	76	GLN
1	i	108	ASN
2	j	27	GLN
2	j	64	ASN
3	k	24	GLN
3	k	73	ASN
4	1	95	GLN
7	0	41	ASN
7	0	67	GLN
7	0	83	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^{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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	98/138~(71%)	-0.17	0 100 100	63, 88, 132, 174	0
1	Е	98/138~(71%)	-0.26	1 (1%) 82 77	59,84,123,147	0
1	K	98/138~(71%)	-0.38	0 100 100	90, 115, 155, 190	0
1	Ο	98/138~(71%)	-0.07	0 100 100	84, 116, 149, 189	0
1	U	98/138~(71%)	0.05	1 (1%) 82 77	101, 149, 191, 202	0
1	Y	98/138 (71%)	-0.25	0 100 100	118, 162, 210, 227	0
1	е	98/138~(71%)	-0.41	0 100 100	78, 108, 152, 185	0
1	i	98/138~(71%)	-0.04	1 (1%) 82 77	84, 109, 155, 185	0
2	В	79/105~(75%)	-0.22	0 100 100	60, 82, 114, 156	0
2	F	87/105~(82%)	-0.20	0 100 100	64, 82, 187, 217	0
2	L	79/105~(75%)	-0.24	0 100 100	84, 111, 137, 147	0
2	Р	83/105 (79%)	-0.09	0 100 100	88, 115, 156, 224	0
2	V	79/105~(75%)	0.14	4 (5%) 28 25	104, 141, 172, 185	0
2	Z	87/105~(82%)	-0.18	1 (1%) 80 75	106, 159, 221, 253	0
2	f	79/105~(75%)	-0.36	0 100 100	84, 106, 138, 145	0
2	j	80/105~(76%)	-0.01	1 (1%) 77 71	80, 105, 150, 179	0
3	С	108/132 (81%)	-0.29	1 (0%) 84 79	63, 89, 127, 190	0
3	G	105/132~(79%)	-0.16	1 (0%) 82 77	59, 85, 136, 184	0
3	М	108/132 (81%)	0.00	3 (2%) 53 47	90, 124, 178, 226	0
3	Q	105/132~(79%)	-0.27	1 (0%) 82 77	91, 116, 159, 195	0
3	W	108/132~(81%)	-0.20	0 100 100	108, 152, 197, 250	0
3	a	104/132~(78%)	0.73	15 (14%) 2 3	119, 156, 208, 245	0
3	g	105/132~(79%)	0.23	0 100 100	86, 109, 159, 186	0
3	k	$10\overline{4/132}~(78\%)$	-0.32	0 100 100	84, 112, 150, 185	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
4	D	96/128~(75%)	-0.29	0 100 100	64, 90, 145, 216	0
4	Н	96/128~(75%)	-0.26	0 100 100	54, 88, 160, 183	0
4	Ν	96/128~(75%)	-0.15	1 (1%) 82 77	92, 124, 179, 228	0
4	R	96/128~(75%)	-0.21	0 100 100	100, 127, 177, 200	0
4	Х	96/128~(75%)	-0.22	0 100 100	121, 157, 206, 212	0
4	b	96/128~(75%)	0.50	18 (18%) 1 1	121, 166, 207, 222	0
4	h	96/128~(75%)	0.18	3 (3%) 49 43	77, 115, 174, 212	0
4	1	96/128~(75%)	-0.26	0 100 100	80, 113, 168, 231	0
5	Ι	169/169~(100%)	-0.67	0 100 100	89, 145, 240, 312	0
5	S	169/169~(100%)	-0.62	0 100 100	121, 186, 251, 316	0
5	с	169/169~(100%)	-0.45	1 (0%) 89 86	158, 221, 301, 363	0
5	m	169/169~(100%)	-0.60	0 100 100	118, 178, 244, 290	0
6	J	169/169~(100%)	-0.73	0 100 100	99, 142, 254, 339	0
6	Т	169/169~(100%)	-0.67	0 100 100	127, 186, 258, 295	0
6	d	169/169~(100%)	-0.33	2 (1%) 79 73	162, 228, 285, 342	0
6	n	169/169~(100%)	-0.41	1 (0%) 89 86	130, 183, 265, 338	0
7	0	78/195~(40%)	3.39	55~(70%) 0 0	152, 196, 239, 272	1 (1%)
All	All	$448\overline{2}/5571~(80\%)$	-0.19	111 (2%) 57 51	54, 135, 236, 363	1 (0%)

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All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	0	22	SER	10.3
7	0	60	VAL	8.8
7	0	25	HIS	8.3
7	0	83	GLN	7.7
7	0	80	VAL	7.3
7	0	79	GLY	6.8
7	0	94	ARG	6.6
7	0	93	PHE	6.6
4	b	52	THR	6.5
7	0	23	THR	6.4
7	0	24	ASP	6.3
7	0	65	ASP	5.8
3	a	26	PRO	5.6
7	0	61	GLY	5.5



Mol	Chain	Res	Type	RSRZ
7	0	84	THR	5.5
2	V	102	GLY	5.3
7	0	82	LYS	5.3
7	0	26	PRO	5.3
7	0	81	LEU	5.2
3	a	22	GLY	5.1
7	0	57	HIS	5.0
7	0	28	TYR	5.0
3	a	76	THR	4.6
7	0	54	ILE	4.5
7	0	33	VAL	4.5
7	0	55	LYS	4.4
7	0	43	ALA	4.3
4	b	41	VAL	4.3
7	0	45	SER	4.3
7	0	76	VAL	4.3
7	0	78	THR	4.3
2	V	101	GLY	4.1
7	0	99	ASP	4.0
7	0	77	THR	4.0
7	0	66	SER	3.9
4	b	40	TYR	3.9
4	b	31	ARG	3.8
7	0	64	ALA	3.6
3	a	78	ILE	3.5
7	0	62	GLU	3.5
4	b	53	GLY	3.5
4	b	54	ILE	3.4
3	М	13	LYS	3.4
7	0	32	ILE	3.3
7	0	37	GLN	3.3
2	V	100	PHE	3.3
7	0	68	ILE	3.3
7	0	53	TYR	3.3
7	0	89	ALA	3.2
7	0	92	SER	3.2
3	Q	14	ALA	3.2
7	0	59	LYS	3.2
7	0	29	SER	3.1
6	d	-63	DC	3.1
4	b	62	MET	3.0
4	b	35	GLU	3.0



Mol	Chain	Res	Type	RSRZ
7	0	67	GLN	3.0
7	0	34	ALA	3.0
7	0	50	ILE	2.9
4	b	32	SER	2.9
7	0	70	LEU	2.9
3	a	20	ARG	2.9
7	0	72	ILE	2.8
6	d	-62	DC	2.8
7	0	95	LEU	2.8
2	V	99	GLY	2.8
3	G	14	ALA	2.7
3	a	82	HIS	2.7
3	a	21	ALA	2.7
4	b	42	TYR	2.7
7	0	51	GLN	2.6
7	0	75	LEU	2.6
4	b	61	ILE	2.6
3	a	118	LYS	2.6
4	b	30	LYS	2.6
3	a	25	PHE	2.5
4	h	31	ARG	2.5
3	a	18	SER	2.5
4	b	45	LEU	2.5
2	Z	44	LYS	2.5
7	0	85	LYS	2.4
4	b	55	SER	2.4
1	U	84	PHE	2.4
7	0	52	LYS	2.4
4	b	36	SER	2.4
3	a	34	LEU	2.3
4	b	57	LYS	2.3
7	0	86	GLY	2.3
3	a	30	VAL	2.3
1	i	39	HIS	2.2
3	С	12	ALA	2.2
3	М	104	GLN	2.2
5	с	-62	DC	2.2
7	0	71	SER	2.2
3	a	23	LEU	2.2
7	0	88	GLY	2.2
2	j	102	GLY	2.1
3	М	115	LEU	2.1



		1	1 0	
Mol	Chain	Res	Type	RSRZ
4	b	37	TYR	2.1
7	0	58	TYR	2.1
7	0	39	GLU	2.1
1	Е	39	HIS	2.1
3	a	104	GLN	2.1
4	h	54	ILE	2.1
7	0	56	SER	2.1
4	Ν	51	ASP	2.1
3	a	77	ARG	2.1
4	h	43	LYS	2.0
4	b	124	ALA	2.0
7	0	36	ILE	2.0
6	n	86	DC	2.0

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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.

