

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 08:17 AM JST

PDB ID	:	6LA2
Title	:	343 bp di-nucleosome harboring cohesive DNA termini assembled with linker
		histone H1.0
Authors	:	Adhireksan, Z.; Sharma, D.; Lee, P.L.; Davey, C.A.
Deposited on	:	2019-11-11
Resolution	:	3.89 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 3.89 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	1002 (4.14-3.66)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	136	71%	•	26%					
1	Е	136	^{3%} 70%	•	26%					
1	Κ	136	69%	•	27%					
1	Ο	136	% 6 9%	•	27%					
1	U	136	^{2%} 70%	·	27%					
1	Y	136	70%	•	26%					
1	е	136	^{2%} 69%	•	27%					



Mol	Chain	Length	Quality of chain		
1	i	136	70%	•	26%
2	В	103	76%	5%	19%
2	F	103	80%	•	18%
2	L	103	2% 7 6%	•	20%
2	Р	103	6% 78%	5%	• 17%
2	V	103	6% 79%	·	18%
2	Z	103	4% 79%	•	17%
2	f	103	^{3%} 76%	•	20%
2	j	103	% 	•	21%
3	С	130	80%	•	16%
3	G	130	75%	5%	20%
3	М	130	81%	<u> </u>	16%
3	Q	130	76%	5%	18%
3	W	130	80%	<u> </u>	16%
3	a	130	75%	•	21%
3	g	130	80%	•	16%
3	k	130	79%	•	17%
4	D	126	68%	9%	23%
4	Н	126	% 67%	10%	24%
4	N	126	68%	9%	23%
4	R	126	⁷⁰ 67%	10%	24%
4	Х	126	64% 8%		28%
4	b	126	66% 1	.0%	24%
4	h	126	67%	9% •	24%
4	1	126	66% 1	.0%	24%



Mol	Chain	Length		Quali	ty of chain	
5	Ι	343			98%	•
5	с	343			99%	
6	J	343			99%	
6	d	343			98%	•
7	S	194	16% 33%	6%	61%	
7	Т	194	21%	5%•	61%	



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 53828 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	0	00	Total	С	Ν	0	\mathbf{S}	0	0	0
1	е	99	816	514	158	140	4	0	0	0
1	;	100	Total	С	Ν	0	S	0	0	0
1	1	100	825	520	160	141	4	0	0	0
1	Δ	100	Total	С	Ν	0	S	0	0	0
1	A	100	825	520	160	141	4	0	0	0
1	F	100	Total	С	Ν	0	S	0	0	0
1	Ľ	100	825	520	160	141	4	0	0	0
1	K	00	Total	С	Ν	0	S	0	0	0
1	Γ	99	816	514	158	140	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	TT	00	Total	С	Ν	0	S	0	0	0
	U	99	816	514	158	140	4	0	0	0
1	V	100	Total	С	Ν	0	S	0	0	0
	I	100	825	520	160	141	4			U

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

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	f	82	Total	С	Ν	Ο	S	0	0	0
2	I	02	653	412	127	113	1	0	0	0
2	i	81	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	J	81	646	407	126	112	1	0	0	0
0	Р	\$3	Total	С	Ν	0	S	0	0	0
	D	00	662	418	129	114	1	0	0	0
0	Б	84	Total	С	Ν	0	S	0	0	0
	Г	04	673	424	133	115	1	0	0	U
0	т	80	Total	С	Ν	0	S	0	0	0
		82	653	412	127	113	1	0	0	0
9	D 86	86	Total	С	Ν	0	S	0	0	0
	1		694	436	140	117	1		0	U



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	V	81	Total	С	Ν	Ο	\mathbf{S}	0	0	0
Z V	04	673	424	133	115	1	0	0	0	
9	0 7	7 95	Total	С	Ν	0	S	0	0	0
Z	L	00	683	430	136	116	1	0	0	0

Continued from previous page...

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

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace										
2	G	100	Total	С	Ν	Ο	0	0	0										
0	g	109	844	532	167	145	0	0	0										
3	Ŀ	108	Total	С	Ν	Ο	0	0	0										
0	ĸ	100	835	526	165	144	0	0	0										
3	С	100	Total	С	Ν	Ο	0	0	0										
0		109	844	532	167	145	0	0	0										
3	С	104	Total	С	Ν	Ο	0	0	0										
0	G	104	805	508	157	140	0	0	0										
3	М	100	Total	С	Ν	Ο	0	0	0										
0	111	109	844	532	167	145	0		U										
3	0	106	Total	С	Ν	Ο	0	0	0										
0	Q	106	819	517	160	142	0	0	0										
3	W	100	Total	С	Ν	Ο	0	0	0										
0	W	W 109	844	532	167	145	0	0	0										
3	3 a	103	Total	С	Ν	0	0	0	0										
0		a	a	a	a	a	a	a	a	a	a	a	103	796	502	155	139	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	h	06	Total	С	Ν	0	S	0	0	0
4	11	90	755	474	138	141	2	0	0	0
1	1	96	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	1	30	755	474	138	141	2		0	0
4	Л	97	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	D		766	480	142	142	2	0	0	0
4	п	06	Total	С	Ν	0	\mathbf{S}	0	0	0
4	11	90	755	474	138	141	2	0	0	0
4	N	07	Total	С	Ν	0	\mathbf{S}	0	0	0
4	11	91	766	480	142	142	2	0	0	0
4	В	06	Total	С	Ν	0	S	0	0	0
4	4 R	96	755	474	138	141	2	0	0	0
4	4 X	91	Total	С	Ν	0	S	0	0	0
<u>+</u>			709	447	125	135	2		0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	b	96	Total 755	С 474	N 138	0 141	${ m S} { m 2}$	0	0	0

• Molecule 5 is a DNA chain called DNA (343-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	Ι	343	Total 7024	C 3330	N 1329	O 2022	Р 343	0	0	0
5	С	343	Total 7024	C 3330	N 1329	O 2022	Р 343	0	0	0

• Molecule 6 is a DNA chain called DNA (343-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
6	J	343	Total 7041	C 3348	N 1254	O 2096	Р 343	0	0	0
6	d	343	Total 7041	C 3348	N 1254	O 2096	Р 343	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
7	q	75	Total	С	Ν	0	\mathbf{S}	0	0	0
(10	575	358	108	108	1	0		
7	Т	75	Total	С	Ν	0	S	0	0	0
1	75	575	358	108	108	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.

2%			
Chain e:	69%	•	27%
MET ALA ARG ARG CLYS CLYS GLN THR ARG CLY GLY CLYS CLY CLY CLY CLY CLY ALA ALA ALA ALA ARG CLN CLN	THR LIYS ALA ALA ALA ALA ALA ALA PAG CLY GLY GLY GLY GLY GLY GLY	F67 V89	C96 R129 A135
• Molecule 1: Histone H3.1			
Chain i:	70%	•	26%
MET ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLN CLN ALA ALA	THR LLYS ALA ALA ALA ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLA CLY CLY	C96 C96 R129 R134	A135
• Molecule 1: Histone H3.1			
Chain A:	71%		26%
MET ALA ALA ALA ALA ALA CLY GLN CLY CLY CLY CLY CLY CLY CLY CLN CLN ALA ALA	THR LLYS ALA ALA ALA ALA ALA ALA ALA ALA ARG GLY GLY GLY GLY GLY GLY CLA	C96 R129 A135	
• Molecule 1: Histone H3.1			
Chain E:	70%	•	26%
MET ARG ARG THR THR CLN GLN GLN GLY GLY GLY GLY GLN CLS CLN CLU ALA	THR LIYS ALA ALA ALA ALA ALA ALA PRO PLA GLY GLY GLY GLY GLY GLY GLY H39 A35 H39	L48 V89 C96	R129 R134 A135
• Molecule 1: Histone H3.1			
Chain K:	69%	•	27%
MET ALA ALA ALA ALA LYS CLY ALA ALA PLO CLY CLY CLY CLY CLY CLY ALA	THR LYS ALA ALA ALA ALA ALA ALA CYS GLY CAL CYS CS CS CS CS CS CS CS CS CS CS CS CS CS	D77 V89 C96	A135
• Molecule 1: Histone H3.1			
Chain O:	69%	·	27%

• Molecule 1: Histone H3.1









• Molecule 3: Histone H2A type 1-B/E



Chain G:	75%	5%	20%
MET SER GLY GLY GLY GLY GLY GLY GLY ALA ALA ALA ALA ALA	KALA KALA Q24 Q24 Q24 V29 V29 V29 V29 V29 K118 K118 K118 K118 K118 K118 K118 K11		
• Molecule 3: Histor	ne H2A type $1-B/E$		
Chain M:	81%	•	16%
MET SER GLY ARG GLY GLY GLY GLY ALA ALA PL1 ALA 224 C24	V49 K74 K74 B1 B1 B1 F115 F116 F117 F116 F117 F118 F117 F118 F118 F118 F118 F118		
• Molecule 3: Histor	ne H2A type $1-B/E$		
Chain Q:	76%	5%	18%
MET SER GLY GLY GLY CLN CLN CLY CLY CLY ALA ARG ALA ARA ARA	A14 M15 M15 M15 M15 M29 M29 M19 M119 M119 M119 M119 M119 M1		
• Molecule 3: Histor	ne H2A type $1-B/E$		
Chain W:	80%	•	16%
MET ARG GLY GLY GLY GLY GLY GLY GLY ALL ALL ALL ALL ALL ALL	Q24 V49 E64 K74 K74 K119 K81 H81 H115 H115 H115 H115 H115 H115 H11		
• Molecule 3: Histor	ne H2A type $1-B/E$		
Chain a:	75%		21%
MET SER GLY GLY GLY GLY GLY CLY ALA ARG ARG ARG ARG	Auk 116 116 224 624 128 132 143 143 144 143 144 144 144 144 144 144	SER HIS HIS LYS LYS LYS LYS LYS	
• Molecule 4: Histor	ne H2B type 1-J		
Chain h:	67%	9% •	24%
MET PRO CIU PRO PRO LYS SER ALA ALA ALA PRO PRO PRO CIY SFR	LYS LYS ALA VALA VALA THAL THAL THAL ALA GLN GLN GLN GLN ARG GLY CLYS LYS CLY S33 S36 S32 S36 S32 S32 S32 S36 S32 S32 S32 S32 S32 S32 S32 S32 S32 S32	S55 N63 E71 K85 K85	R125
• Molecule 4: Histor	ne H2B type 1-J		
Chain l:	66%	10%	24%
MET PRO GLU PRO PRO LYS SER ALA ALA ALA ALA PRO PRO CLY SER CLY SRO	LYS LYS LYS ALA ALA ALA THR THR THR ALA ALA GLN GLN GLN AR3 AR3 R33 R33 R33 R33 R33 R33 R33 R33	T52 S55 L80 R85 R86	891 6104 8123 8123 8123 8124
• Molecule 4: Histor	ne H2B type 1-J		



2%			
Chain D:	68%	9%	23%
MET PRO PRO PRO ALA LYS SER ALA ALA	PR0 LYS LYS GLY GLY SER LYS LYS LYS LYS CLN GLA GLA GLA GLA GLA CLA S32 S32 S32 S32 S32 S32 S32 S32 S32 S32	T52 S55 N63 K85	R86 391 6104 125
• Molecule 4:	Histone H2B type 1-J		
Chain H:	67%	10%	24%
	<u> </u>		
MET PRO GLU PRO ALA LYS SER ALA PRO ALA	PR0 LVS LVS LVS LVS LVS LVS LVS LVS LVS CLN CVS CLN CVS CLN CVS CLN CVS CLN CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	T52 S55 L80 K85	R86 S91 G104 S123 A124 K125
• Molecule 4:	Histone H2B type 1-J		
Chain N:	68%	9%	23%
MET PRO GLU GLU ALA CYS SER ALA PRO ALA	PR0 LYSS LYSS CLY SFR LYSS LYSS LYSS LYSS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	Q47 T52 S55 N63	K85 S91 G10 K12
• Molecule 4:	Histone H2B type 1-J		
Chain R:	67%	10%	24%
HODOdwedd			
A PRUS A		T5 S5 L8 K8	R S S S S S S S S S S S S S S S S S S S
• Molecule 4:	Histone H2B type 1-J		
Chain X:	64%	8%	28%
MET PRO GLU PRO ALA LYS SER ALA ALA ALA	PRO LYS GLY SER SER SER LYS LYS LYS CLYS GLA GLN CLYS CLYS ARG GLN ARG CLYS SER ARG CLYS SER ARG CLYS SER ARG CLYS SER ARG CLYS SER ARG CLY SER CLYS SER SER SER SER SER SER SER SER SER SE	Y42 T52 S55 N63	E71 K85 S91 G104 K125
• Molecule 4:	Histone H2B type 1-J		
Chain b:	66%	10%	24%
MET PRO GLU PRO ALA LYS SER ALA ALA	PR0 LVS CLY SER CLY SER LVS CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	T52 S55 L80	K85 R86 S91 G104 G104 S123 K125 K125
• Molecule 5:	DNA (343-MER)		
Chain I:	98%		•
C1 C149 A158 A158 C188 C188 C246	139 138 138		
• Molecule 5:	DNA (343-MER)		
	W O R L D W I	DE	
	PROTEIN DATA	BANK	

Chain c:	99%
C1 A179 C246 C343 C343	
• Molecule 6: DNA (343-MER)	
Chain J:	99%
C1 C5 C5 C1 C5 C1 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	
• Molecule 6: DNA (343-MER)	
Chain d:	98% .
C1 116 0176 0197 C230 C343 C343	
• Molecule 7: Histone H1.0	
Chain S: 33% 6%	61%
MET THR ASN ASN ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	VZ 7 VZ 7 VZ 8 VZ 8 V2 8 V3 3 V3 4 V3 3 V3 4 V3 4 V3 4 V3 6 V4 0 V5 6 V5 6 V5 6 V5 6 V5 6 V5 6 V5 6 V5 6
T77 T78 679 679 679 679 679 679 738 739 739 739 739 739 739 739 739 739 739	LLE LYS LYS ALA ALA ALA LYS LYS LYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LYS LYS LYS ALA ALA ALA THR PRO LYS LYS LYS LYS THR VAL LYS FRO CYS CYS SR CYS SR CYS SR CYS SR CYS SR CYS SR CYS SR CYS SR CYS SC CYS SC CYS CYS CYS CYS CYS CYS C	LYS LYS PRO VAL VAL VAL LYS SER ALA LYS SER ALA CYS LYS LYS LYS LYS LYS LYS
• Molecule 7: Histone H1.0	
Chain T: 33% 5%.	61%
MET THR CIU ASN ASR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	229 230 232 132 133 135 135 135 135 135 135 135 135 135
178 178 759 759 781 789 783 788 784 788 785 788 786 788 787 788 788 788 788 788 796 788 796 788 832 88 832 88 832 88 832 88 832 88 832 88 849 88 85 88 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 85 <tr< td=""><td>PALA PALA LIYS LIYS LIYS CLU CIYS CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV</td></tr<>	PALA PALA LIYS LIYS LIYS CLU CIYS CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV
ALA THR THR VAL LYS LYS LYS LYS LYS LYS LYS LYS LYS LY	PRO VAL ALYS ALYS SER PRO PRO PRO PRO PRO PRO PRO PRO PRO PR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	107.75Å 205.90Å 237.68Å	Depositor
a, b, c, α , β , γ	90.00° 97.19° 90.00°	Depositor
Bosolution(A)	49.35 - 3.89	Depositor
Resolution (A)	49.30 - 3.89	EDS
% Data completeness	99.3 (49.35-3.89)	Depositor
(in resolution range)	99.4 (49.30-3.89)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 3.88 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
B B.	0.199 , 0.267	Depositor
II, II free	0.202 , 0.262	DCC
R_{free} test set	1885 reflections (2.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	185.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.23, 165.8	EDS
L-test for $twinning^2$	$ < L >=0.38, < L^2>=0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53828	wwPDB-VP
Average B, all atoms $(Å^2)$	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.17% 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	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.67	0/837	0.81	0/1120	
1	Е	0.67	0/837	0.82	0/1120	
1	Κ	0.66	0/828	0.81	0/1109	
1	0	0.65	0/828	0.81	0/1109	
1	U	0.67	0/828	0.82	0/1109	
1	Y	0.66	0/837	0.82	0/1120	
1	е	0.66	0/828	0.79	0/1109	
1	i	0.67	0/837	0.82	0/1120	
2	В	0.68	0/669	0.85	0/894	
2	F	0.69	0/680	0.87	0/908	
2	L	0.68	0/660	0.85	0/883	
2	Р	0.69	0/702	0.84	0/937	
2	V	0.68	0/680	0.86	0/908	
2	Ζ	0.67	0/691	0.85	0/923	
2	f	0.68	0/660	0.83	0/883	
2	j	0.68	0/653	0.84	0/873	
3	С	0.70	0/854	0.81	0/1150	
3	G	0.68	0/815	0.77	0/1100	
3	М	0.69	0/854	0.81	0/1150	
3	Q	0.67	0/829	0.80	0/1118	
3	W	0.69	0/854	0.80	0/1150	
3	a	0.68	0/806	0.77	0/1089	
3	g	0.69	0/854	0.81	0/1150	
3	k	0.67	0/845	0.77	0/1139	
4	D	0.70	0/777	0.80	0/1040	
4	Н	0.68	0/766	0.79	0/1026	
4	Ν	0.71	0/777	0.79	0/1040	
4	R	0.69	0/766	0.79	0/1026	
4	Х	0.70	0/720	0.79	0/968	
4	b	0.71	0/766	0.80	0/1026	
4	h	0.77	0/766	1.20	4/1026~(0.4%)	
4	1	0.70	0/766	0.78	0/1026	
5	Ι	0.39	2/7890~(0.0%)	0.83	5/12165~(0.0%)	
5	с	0.38	1/7890~(0.0%)	0.81	3/12165~(0.0%)	



Mal	Chain	Bo	nd lengths	Bond angles		
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
6	J	0.40	1/7888~(0.0%)	0.83	5/12180~(0.0%)	
6	d	0.38	1/7888~(0.0%)	0.81	5/12180~(0.0%)	
7	S	0.75	0/581	0.82	0/775	
7	Т	0.73	0/581	0.81	0/775	
All	All	0.54	5/57588~(0.0%)	0.82	22/83589~(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
2	Р	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	DC	OP3-P	-10.56	1.48	1.61
5	с	1	DC	OP3-P	-10.51	1.48	1.61
6	d	1	DC	OP3-P	-10.31	1.48	1.61
5	Ι	1	DC	OP3-P	-9.59	1.49	1.61
5	Ι	149	DC	O3'-P	-5.20	1.54	1.61

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	h	31	ARG	NE-CZ-NH2	-20.69	109.95	120.30
4	h	31	ARG	NE-CZ-NH1	17.92	129.26	120.30
6	J	176	DG	C1'-O4'-C4'	-8.98	101.12	110.10
5	Ι	158	DA	C1'-O4'-C4'	-7.55	102.55	110.10
5	Ι	159	DA	C1'-O4'-C4'	-7.25	102.86	110.10
6	J	184	DT	C1'-O4'-C4'	-6.23	103.87	110.10
4	h	31	ARG	CG-CD-NE	6.20	124.81	111.80
6	J	152	DG	C1'-O4'-C4'	-5.84	104.26	110.10
4	h	31	ARG	CD-NE-CZ	-5.64	115.70	123.60
6	J	176	DG	N9-C1'-C2'	5.55	123.15	112.60
6	d	176	DG	C1'-O4'-C4'	-5.38	104.72	110.10
5	Ι	246	DG	C1'-O4'-C4'	-5.37	104.73	110.10
6	d	343	DC	C1'-O4'-C4'	-5.34	104.76	110.10
5	с	246	DG	C1'-O4'-C4'	-5.32	104.78	110.10
6	d	197	DG	C1'-O4'-C4'	-5.29	104.81	110.10
5	с	292	DT	C1'-O4'-C4'	-5.26	104.84	110.10

All (22) bond angle outliers are listed below:





Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	J	51	DC	C1'-O4'-C4'	-5.24	104.86	110.10
5	с	179	DA	C1'-O4'-C4'	-5.20	104.90	110.10
5	Ι	292	DT	C1'-O4'-C4'	-5.18	104.92	110.10
5	Ι	188	DC	C1'-O4'-C4'	-5.16	104.94	110.10
6	d	230	DC	C1'-O4'-C4'	-5.04	105.06	110.10
6	d	16	DT	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Р	18	HIS	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	P	erce	entiles
1	А	98/136~(72%)	83~(85%)	13 (13%)	2 (2%)		7	40
1	Е	98/136~(72%)	84 (86%)	12 (12%)	2 (2%)		7	40
1	K	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)		7	39
1	Ο	97/136~(71%)	83 (86%)	12 (12%)	2 (2%)		7	39
1	U	97/136 (71%)	83 (86%)	12 (12%)	2 (2%)		7	39
1	Y	98/136~(72%)	84 (86%)	12 (12%)	2 (2%)		7	40
1	e	97/136 (71%)	82 (84%)	12 (12%)	3 (3%)		4	32
1	i	98/136~(72%)	83 (85%)	13 (13%)	2 (2%)		7	40
2	В	81/103 (79%)	62 (76%)	19 (24%)	0]	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	F	82/103~(80%)	65~(79%)	17 (21%)	0	100	100
2	L	80/103~(78%)	64 (80%)	16 (20%)	0	100	100
2	Р	84/103 (82%)	65 (77%)	18 (21%)	1 (1%)	13	49
2	V	82/103 (80%)	64 (78%)	18 (22%)	0	100	100
2	Z	83/103 (81%)	64 (77%)	19 (23%)	0	100	100
2	f	80/103~(78%)	63~(79%)	17 (21%)	0	100	100
2	j	79/103~(77%)	61 (77%)	18 (23%)	0	100	100
3	С	107/130 (82%)	93~(87%)	13 (12%)	1 (1%)	17	54
3	G	102/130~(78%)	90 (88%)	11 (11%)	1 (1%)	15	52
3	М	107/130 (82%)	95~(89%)	11 (10%)	1 (1%)	17	54
3	Q	104/130 (80%)	92 (88%)	11 (11%)	1 (1%)	15	52
3	W	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	17	54
3	a	101/130 (78%)	89~(88%)	11 (11%)	1 (1%)	15	52
3	g	107/130 (82%)	94 (88%)	12 (11%)	1 (1%)	17	54
3	k	106/130 (82%)	93~(88%)	12 (11%)	1 (1%)	17	54
4	D	95/126~(75%)	73 (77%)	21 (22%)	1 (1%)	14	51
4	Н	94/126~(75%)	71 (76%)	21 (22%)	2 (2%)	7	39
4	Ν	95/126~(75%)	73 (77%)	21 (22%)	1 (1%)	14	51
4	R	94/126~(75%)	71 (76%)	21 (22%)	2 (2%)	7	39
4	Х	89/126 (71%)	70 (79%)	18 (20%)	1 (1%)	14	51
4	b	94/126~(75%)	70 (74%)	22 (23%)	2 (2%)	7	39
4	h	94/126~(75%)	72 (77%)	20 (21%)	2 (2%)	7	39
4	1	94/126~(75%)	70 (74%)	22 (23%)	2 (2%)	7	39
7	S	73/194~(38%)	59 (81%)	10 (14%)	4 (6%)	2	22
7	Т	73/194~(38%)	59 (81%)	10 (14%)	4 (6%)	2	22
All	All	3167/4348 (73%)	2601 (82%)	519 (16%)	47 (2%)	10	45

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All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1	33	ARG
4	Н	33	ARG
7	S	87	VAL



Mol	Chain	Res	Type
7	Т	87	VAL
2	Р	18	HIS
4	R	33	ARG
4	b	33	ARG
4	h	104	GLY
4	1	104	GLY
4	D	104	GLY
4	Н	104	GLY
7	Т	39	GLU
7	Т	40	LYS
4	N	104	GLY
4	R	104	GLY
4	Х	104	GLY
4	b	104	GLY
7	S	39	GLU
7	S	40	LYS
1	А	96	CYS
1	Е	96	CYS
1	е	96	CYS
1	i	96	CYS
1	Κ	96	CYS
1	0	96	CYS
1	U	96	CYS
1	Y	96	CYS
1	е	38	PRO
4	h	31	ARG
7	S	96	ALA
7	Т	96	ALA
1	i	89	VAL
1	е	89	VAL
3	g	49	VAL
3	k	49	VAL
1	А	89	VAL
3	С	49	VAL
1	Е	89	VAL
3	G	49	VAL
1	Κ	89	VAL
3	Μ	49	VAL
1	0	89	VAL
3	Q	49	VAL
1	U	89	VAL
3	W	49	VAL



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Mol	Chain	Res	Type
1	Y	89	VAL
3	a	49	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	87/111 (78%)	85~(98%)	2(2%)	50 71
1	Е	87/111~(78%)	84 (97%)	3~(3%)	37 62
1	Κ	86/111 (78%)	84 (98%)	2(2%)	50 71
1	Ο	86/111~(78%)	83~(96%)	3~(4%)	36 62
1	U	86/111 (78%)	84 (98%)	2(2%)	50 71
1	Y	87/111~(78%)	84 (97%)	3~(3%)	37 62
1	е	86/111~(78%)	84 (98%)	2(2%)	50 71
1	i	87/111 (78%)	84 (97%)	3(3%)	37 62
2	В	68/79~(86%)	63~(93%)	5 (7%)	13 43
2	F	69/79~(87%)	67~(97%)	2(3%)	42 65
2	L	67/79~(85%)	63 (94%)	4 (6%)	19 49
2	Р	71/79~(90%)	65~(92%)	6 (8%)	10 39
2	V	69/79~(87%)	66~(96%)	3~(4%)	29 57
2	Z	70/79~(89%)	66 (94%)	4 (6%)	20 50
2	f	67/79~(85%)	63~(94%)	4 (6%)	19 49
2	j	66/79~(84%)	63~(96%)	3 (4%)	27 56
3	С	86/100~(86%)	82 (95%)	4(5%)	26 55
3	G	83/100 (83%)	79~(95%)	4 (5%)	25 54
3	М	86/100~(86%)	83~(96%)	3 (4%)	36 62
3	Q	84/100~(84%)	78~(93%)	6(7%)	14 44
3	W	86/100~(86%)	83~(96%)	3 (4%)	36 62
3	a	82/100~(82%)	78 (95%)	4 (5%)	25 54



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Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
3	g	86/100~(86%)	82 (95%)	4 (5%)	26	55
3	k	85/100 (85%)	81 (95%)	4(5%)	26	55
4	D	83/105~(79%)	73~(88%)	10 (12%)	5	25
4	Н	82/105 (78%)	72 (88%)	10 (12%)	5	24
4	Ν	83/105~(79%)	73~(88%)	10 (12%)	5	25
4	R	82/105 (78%)	72 (88%)	10 (12%)	5	24
4	Х	77/105~(73%)	68 (88%)	9 (12%)	5	26
4	b	82/105 (78%)	71 (87%)	11 (13%)	4	22
4	h	82/105 (78%)	72 (88%)	10 (12%)	5	24
4	1	82/105~(78%)	71 (87%)	11 (13%)	4	22
7	S	62/158~(39%)	55 (89%)	7 (11%)	6	27
7	Т	62/158~(39%)	54 (87%)	8 (13%)	4	23
All	All	2694/3476 (78%)	2515 (93%)	179 (7%)	16	46

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

Mol	Chain	Res	Type
1	е	63	ARG
1	е	129	ARG
2	f	30	THR
2	f	50	ILE
2	f	92	ARG
2	f	95	ARG
3	g	24	GLN
3	g	71	ARG
3	g	74	LYS
3	g	81	ARG
4	h	32	SER
4	h	36	SER
4	h	42	TYR
4	h	52	THR
4	h	55	SER
4	h	63	ASN
4	h	71	GLU
4	h	85	LYS
4	h	86	ARG
4	h	91	SER
1	i	48	LEU



1 i 129 ARG 1 i 134 ARG 2 j 30 THR 2 j 50 ILE 2 j 92 ARG 3 k 11 ARG	
1 i 134 ARG 2 j 30 THR 2 j 50 ILE 2 j 92 ARG 3 k 11 ARG	
2 j 30 THR 2 j 50 ILE 2 j 92 ARG 3 k 11 ARG	
2 j 50 ILE 2 j 92 ARG 3 k 11 ARG	
2 j 92 ARG 3 k 11 ARG	
3 k 11 ARG	
$3 \mid k \mid 15 \mid LYS$	
3 k 24 GLN	
3 k 81 ARG	
4 l 31 ARG	
4 1 36 SER	
4 1 42 TYR	
4 1 52 THR	
4 1 55 SER	
4 1 80 LEU	
4 1 85 LYS	
4 1 86 ARG	
4 1 91 SER	
4 l 123 SER	
4 l 125 LYS	
1 A 63 ARG	
1 A 129 ARG	
2 B 20 LYS	
2 B 23 ARG	
2 B 30 THR	
2 B 92 ARG	
2 B 95 ARG	
3 C 24 GLN	
3 C 74 LYS	
3 C 81 ARG	
3 C 91 GLU	
4 D 31 ARG	
4 D 32 SER	
4 D 36 SER	
4 D 42 TYR	
4 D 52 THR	
4 D 55 SER	
4 D 63 ASN	
4 D 85 LYS	
4 D 86 ARG	
4 D 91 SER	
1 E 48 LEU	



Mol	Chain	Res	Type
1	Е	129	ARG
1	Е	134	ARG
2	F	30	THR
2	F	92	ARG
3	G	15	LYS
3	G	24	GLN
3	G	29	ARG
3	G	81	ARG
4	Н	36	SER
4	Н	42	TYR
4	Н	52	THR
4	Н	55	SER
4	Н	80	LEU
4	Н	85	LYS
4	Н	86	ARG
4	Н	91	SER
4	Н	123	SER
4	Н	125	LYS
7	S	25	HIS
7	S	31	MET
7	S	45	SER
7	S	49	SER
7	S	60	VAL
7	S	93	PHE
7	S	97	LYS
7	Т	25	HIS
7	Т	31	MET
7	Т	40	LYS
7	Т	45	SER
7	Т	49	SER
7	Т	60	VAL
7	Т	93	PHE
7	Т	97	LYS
1	K	63	ARG
1	Κ	129	ARG
2	L	22	LEU
2	L	30	THR
2	L	92	ARG
2	L	95	ARG
3	М	24	GLN
3	М	74	LYS
3	М	81	ARG



Mol	Chain	Res	Type
4	N	31	ARG
4	N	32	SER
4	N	36	SER
4	N	42	TYR
4	N	47	GLN
4	N	52	THR
4	N	55	SER
4	N	63	ASN
4	N	85	LYS
4	N	91	SER
1	0	48	LEU
1	0	129	ARG
1	0	134	ARG
2	 P	17	ARG
2	P	18	HIS
2	 P	30	THR
2	P	50	ILE
2	Р	92	ARG
2	 P	95	ARG
3	0	15	LYS
3	Q	24	GLN
3	$\overline{\mathbf{Q}}$	29	ARG
3	Q	81	ARG
3	Q	118	LYS
3	Q	119	LYS
4	R	36	SER
4	R	42	TYR
4	R	52	THR
4	R	55	SER
4	R	80	LEU
4	R	85	LYS
4	R	86	ARG
4	R	91	SER
4	R	123	SER
4	R	125	LYS
1	U	63	ARG
1	U	129	ARG
2	V	30	THR
2	V	92	ARG
2	V	95	ARG
3	W	24	GLN
~	117	74	IVC



Mol	Chain	Res	Type
3	W	81	ARG
4	Х	36	SER
4	Х	42	TYR
4	Х	52	THR
4	Х	55	SER
4	Х	63	ASN
4	Х	71	GLU
4	Х	85	LYS
4	Х	86	ARG
4	Х	91	SER
1	Y	48	LEU
1	Y	129	ARG
1	Y	134	ARG
2	Ζ	18	HIS
2	Ζ	19	ARG
2	Ζ	30	THR
2	Ζ	92	ARG
3	a	24	GLN
3	a	29	ARG
3	a	74	LYS
3	a	81	ARG
4	b	31	ARG
4	b	36	SER
4	b	42	TYR
4	b	52	THR
4	b	55	SER
4	b	80	LEU
4	b	85	LYS
4	b	86	ARG
4	b	91	SER
4	b	123	SER
4	b	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	g	24	GLN
4	h	47	GLN
4	h	63	ASN
4	h	67	ASN
4	h	95	GLN
1	i	76	GLN



Mol	Chain	Res	Type
2	j	64	ASN
4	1	95	GLN
3	С	24	GLN
4	D	63	ASN
4	D	67	ASN
4	D	95	GLN
1	Е	76	GLN
2	F	64	ASN
4	N	49	HIS
4	Ν	63	ASN
4	N	67	ASN
4	N	95	GLN
1	0	76	GLN
2	Р	64	ASN
3	Q	24	GLN
3	Q	38	ASN
4	R	95	GLN
4	R	109	HIS
3	W	24	GLN
4	Х	47	GLN
4	Х	49	HIS
4	Х	63	ASN
4	Х	67	ASN
4	Х	95	GLN
1	Y	76	GLN
2	Z	64	ASN
3	a	24	GLN
3	a	68	ASN
4	b	95	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	100/136~(73%)	-0.45	0 100 100	122, 175, 243, 313	0
1	E	100/136~(73%)	-0.40	4 (4%) 38 30	89, 163, 240, 277	0
1	K	99/136~(72%)	-0.40	0 100 100	125, 168, 232, 344	0
1	0	99/136~(72%)	-0.16	2 (2%) 65 55	133, 192, 258, 309	0
1	U	99/136~(72%)	-0.26	3 (3%) 50 38	112, 166, 226, 290	0
1	Y	100/136~(73%)	-0.29	1 (1%) 82 75	146, 211, 270, 310	0
1	е	99/136~(72%)	-0.27	3 (3%) 50 38	122, 191, 265, 313	0
1	i	100/136~(73%)	-0.44	0 100 100	123, 173, 259, 297	0
2	В	83/103 (80%)	-0.30	0 100 100	112, 162, 226, 452	0
2	F	84/103 (81%)	-0.17	4 (4%) 30 25	112, 162, 280, 391	0
2	L	82/103~(79%)	-0.19	2 (2%) 59 48	125, 161, 208, 255	0
2	Р	86/103~(83%)	0.38	6 (6%) 16 12	140, 202, 306, 364	0
2	V	84/103 (81%)	-0.04	6 (7%) 16 11	118, 159, 249, 399	0
2	Z	85/103 (82%)	-0.11	4 (4%) 31 25	143, 204, 283, 336	0
2	f	82/103~(79%)	-0.24	3 (3%) 41 32	144, 190, 231, 423	0
2	j	81/103 (78%)	-0.20	1 (1%) 79 70	116, 162, 219, 338	0
3	С	109/130~(83%)	-0.35	0 100 100	103, 167, 239, 270	0
3	G	104/130~(80%)	-0.21	0 100 100	128, 183, 243, 285	0
3	М	109/130 (83%)	-0.15	6 (5%) 25 20	162, 220, 297, 357	0
3	Q	106/130~(81%)	-0.12	4 (3%) 40 31	125, 196, 262, 323	0
3	W	109/130~(83%)	-0.14	5 (4%) 32 26	116, 185, 264, 298	0
3	a	103/130~(79%)	-0.22	4 (3%) 39 30	126, 197, 273, 365	0
3	g	109/130~(83%)	-0.18	3 (2%) 53 41	109, 175, 267, 308	0
3	k	108/130 (83%)	-0.27	2 (1%) 66 57	163, 213, 278, 360	0



Mol	Chain	Analysed	$<$ RSRZ $>$	#RSRZ>2	$OWAB(A^2)$	Q < 0.9
4	D	97/126~(76%)	-0.25	2 (2%) 63 53	110, 169, 252, 326	0
4	Н	96/126~(76%)	-0.43	1 (1%) 82 75	109, 180, 245, 282	0
4	Ν	97/126~(76%)	-0.40	1 (1%) 82 75	155, 220, 301, 328	0
4	R	96/126~(76%)	-0.35	1 (1%) 82 75	145, 201, 264, 298	0
4	Х	91/126~(72%)	-0.35	0 100 100	125, 178, 240, 296	0
4	b	96/126~(76%)	-0.40	0 100 100	127, 209, 267, 330	0
4	h	96/126~(76%)	-0.43	0 100 100	122, 181, 250, 298	0
4	1	96/126~(76%)	-0.41	0 100 100	154, 213, 286, 318	0
5	Ι	343/343~(100%)	-0.97	0 100 100	151, 264, 394, 469	0
5	С	343/343~(100%)	-0.99	0 100 100	155, 266, 391, 518	0
6	J	343/343~(100%)	-0.97	0 100 100	112, 266, 386, 446	0
6	d	343/343~(100%)	-0.95	0 100 100	159, 274, 404, 479	0
7	S	75/194~(38%)	2.00	31 (41%) 0 0	234, 312, 398, 432	1 (1%)
7	Т	75/194~(38%)	2.97	40 (53%) 0 0	273, 348, 409, 437	1 (1%)
All	All	4607/5720 (80%)	-0.38	139 (3%) 50 38	89, 209, 350, 518	2(0%)

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All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Р	18	HIS	13.5
7	Т	86	GLY	13.1
2	Р	17	ARG	11.3
7	Т	96	ALA	9.9
7	S	61	GLY	9.1
7	Т	85	LYS	8.5
2	F	19	ARG	8.2
2	Р	21	VAL	8.0
7	Т	95	LEU	7.8
7	Т	42	ARG	7.7
2	Р	19	ARG	7.6
1	U	37	LYS	7.5
7	Т	40	LYS	7.5
7	Т	83	GLN	7.5
7	S	60	VAL	7.1
2	Р	20	LYS	7.1
7	S	62	GLU	7.1
7	Т	77	THR	6.9



7

5.9	
5.8	
5.8	
5.8	
5.6	
5.5	
5.4	
5 4	1

Continued from previous page					
\mathbf{Mol}	Chain	\mathbf{Res}	Type	RSRZ	

Т

84

THR

6.7

7T41ASN 6.0 7T43ALA 6.0 7T59LYS 5.9 1U38PRO 5.8 7S 54 ILE 5.8 7T76VAL 5.8 7T57HIS 5.6 7T79GLY 5.5 7S 55 LYS 5.4 7T94ARG 5.4 7S37GLN 5.3 7S65ASP 5.3 7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7S76VAL 5.2 7S77THR 5.2 7S78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 7S33VAL 4.5 7T88GLY 4.5 7T38ALA 4.3 7T38ALA 4.3 7T78VAL 4.2 7T72ILE 4.1 7T38ALA 4.3 7T87VAL 4.2 7T72ILE 4.1 7T56SER 4.0 1E38PRO 4	2	Р	22	LEU	6.4
7T43ALA 6.0 7T59LYS 5.9 1U38PRO 5.8 7S 54 ILE 5.8 7T76VAL 5.8 7T57HIS 5.6 7T79GLY 5.5 7S 55 LYS 5.4 7T94ARG 5.4 7T94ARG 5.4 7S37GLN 5.3 7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7S76VAL 5.2 7S77THR 5.2 7T78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 7S33VAL 4.5 7T37GLN 4.5 7T88GLY 4.5 7T38ALA 4.3 7S38ALA 4.3 7T72ILE 4.1 7T56SER 4.0 2V22LEU 4.4 2V22LEU 4.4 7S38ALA 4.3 7T87VAL 4.2 7T72ILE 4	7	Т	41	ASN	6.0
7T59LYS 5.9 1U38PRO 5.8 7S 54 ILE 5.8 7T 76 VAL 5.8 7T 57 HIS 5.6 7T 79 GLY 5.5 7S 55 LYS 5.4 7T 94 ARG 5.4 7S 37 GLN 5.3 7S 65 ASP 5.3 7S 29 SER 5.2 7S 56 SER 5.2 7S 56 SER 5.2 7S 77 THR 5.2 7S 76 VAL 5.2 7T 78 THR 5.0 1E 36 LYS 4.8 2Z18HIS 4.8 7S 33 VAL 4.5 7T 88 GLY 4.5 7T 37 GLN 4.5 7T 38 ALA 4.3 7S 38 ALA 4.3 7T 87 VAL 4.2 7T 72 ILE 4.1 7T 38 ALA 4.3 7T 87 VAL 4.2 7T 72 ILE 4.1 7T 56 SER 4.0 2V 22 LEU 4.4 <tr< td=""><td>7</td><td>Т</td><td>43</td><td>ALA</td><td>6.0</td></tr<>	7	Т	43	ALA	6.0
1 U 38 PRO 5.8 7 S 54 ILE 5.8 7 T 76 VAL 5.8 7 T 57 HIS 5.6 7 T 79 GLY 5.5 7 S 55 LYS 5.4 7 T 94 ARG 5.4 7 S 37 GLN 5.3 7 S 32 ILE 5.3 7 S 29 SER 5.2 7 S 56 SER 5.2 7 S 56 SER 5.2 7 T 60 VAL 5.2 7 T 60 VAL 5.2 7 T 60 VAL 5.2 7 T 78 THR 5.0 1 E 36 LYS 4.8 2 Z IEU 4.8 7<	7	Т	59	LYS	5.9
7 S 54 ILE 5.8 7 T 57 HIS 5.6 7 T 79 GLY 5.5 7 S 55 LYS 5.4 7 T 94 ARG 5.4 7 S 37 GLN 5.3 7 S 32 ILE 5.3 7 S 32 ILE 5.3 7 S 29 SER 5.2 7 S 56 SER 5.2 7 S 77 THR 5.2 7 S 76 VAL 5.2 7 T 60 VAL 5.2 7 T 78 THR 5.0 1 E 36 LYS 4.8 2 Z 18 HIS 4.8 7 S 33 VAL 4.5 7 T 37 GLN 4.5	1	U	38	PRO	5.8
7 T 76 VAL 5.8 7 T 57 HIS 5.6 7 S 55 LYS 5.4 7 T 94 ARG 5.4 7 T 94 ARG 5.4 7 S 37 GLN 5.3 7 S 65 ASP 5.3 7 S 29 SER 5.2 7 S 56 SER 5.2 7 S 56 SER 5.2 7 T 60 VAL 5.2 7 T 60 VAL 5.2 7 T 78 71 78 71 7 T 78 71 78 71 8.2 7 T 78 71 78 71 8.8 2 Z 18 118 4.8 7 7 T 33 VAL 4.5	7	S	54	ILE	5.8
7 T 57 HIS 5.6 7 T 79 GLY 5.5 7 S 55 LYS 5.4 7 T 94 ARG 5.4 7 S 37 GLN 5.3 7 S 65 ASP 5.3 7 S 29 SER 5.2 7 S 56 SER 5.2 7 S 56 SER 5.2 7 S 77 THR 5.2 7 S 77 THR 5.2 7 T 60 VAL 5.2 7 T 78 THR 5.0 1 E 36 LYS 4.8 2 Z 18 HIS 4.8 7 S 33 VAL 4.5 7 T 37 GLN 4.5 7 T 37 GLN 4.5 <	7	Т	76	VAL	5.8
7T79GLY 5.5 7S55LYS 5.4 7T94ARG 5.4 7S37GLN 5.3 7S65ASP 5.3 7S29SER 5.2 7S56SER 5.2 7S7T7S777S77S7777777777777777777777777877777879149491411411511511611717181811191819141011116121713161416151716141717181419171014101411161217131614161517161617	7	Т	57	HIS	5.6
7S55LYS 5.4 7T94ARG 5.4 7S37GLN 5.3 7S65ASP 5.3 7S29SER 5.2 7S56SER 5.2 7S7THR 5.2 7S777S777787777777777777777777777778797879791494.81777779791418914.511114.522114.522114.4214.411114.5114.5115.5114.4115.5114.4115.5114.4115.5114.4115.5114.4115.5114.41<	7	Т	79	GLY	5.5
7T94ARG 5.4 7S37GLN 5.3 7S65ASP 5.3 7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7T60VAL 5.2 7T60VAL 5.2 7T78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 2F22LEU 4.8 7S33VAL 4.5 7T88GLY 4.5 7T37GLN 4.5 7T38ALA 4.3 7S38ALA 4.3 7T72ILE 4.1 7T56SER 4.0 1E38PRO 4.0 2V22LEU 4.4 7S38ALA 4.3 7T38ALA 4.3 7T56SER 4.0 1E38PRO 4.0 2V94GLY 3.9 7S28TYR 3.9 2Z19ARG 3.8	7	S	55	LYS	5.4
7S37GLN 5.3 7S65ASP 5.3 7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7T60VAL 5.2 7S77THR 5.2 7S77THR 5.2 7T78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 7S79GLY 4.8 2F22LEU 4.8 7S33VAL 4.5 7T88GLY 4.5 7T37GLN 4.5 2Z22LEU 4.4 2V22LEU 4.4 7S38ALA 4.3 7T38ALA 4.3 7T87VAL 4.2 7T72ILE 4.1 7T56SER 4.0 1E38PRO 4.0 2V94GLY 3.9 7S28TYR 3.9 2Z19ARG 3.8	7	Т	94	ARG	5.4
7S65ASP 5.3 7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7T60VAL 5.2 7T78THR 5.2 7T78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 7S79GLY 4.8 2F22LEU 4.8 7S33VAL 4.5 7T88GLY 4.5 7T37GLN 4.5 2Z22LEU 4.4 2V22LEU 4.4 7S38ALA 4.3 7T38ALA 4.3 7T72ILE 4.1 7T56SER 4.0 1E38PRO 4.0 2V94GLY 3.9 7S28TYR 3.9 7S28TYR 3.9 2V19ARG 3.8	7	S	37	GLN	5.3
7S32ILE 5.3 7S29SER 5.2 7S56SER 5.2 7T60VAL 5.2 7T78THR 5.0 1E36LYS 4.8 2Z18HIS 4.8 7S79GLY 4.8 7S79GLY 4.8 7S33VAL 4.5 7T88GLY 4.5 7T88GLY 4.5 7T37GLN 4.5 2Z22LEU 4.4 2V22LEU 4.4 2V22LEU 4.4 7S38ALA 4.3 7T87VAL 4.2 7T72ILE 4.1 7T56SER 4.0 1E38PRO 4.0 2F21VAL 4.0 2F21VAL 4.0 2F21VAL 4.0 2V94GLY 3.9 7T97LYS 3.9 2Z19ARG 3.8	7	S	65	ASP	5.3
7S29SER 5.2 7S 56 SER 5.2 7T 60 VAL 5.2 7T 78 THR 5.0 1E 36 LYS 4.8 2Z18HIS 4.8 7S 79 GLY 4.8 2F 22 LEU 4.8 7S 33 VAL 4.5 7T 88 GLY 4.5 7T 37 GLN 4.5 7T 37 GLN 4.5 7T 37 GLN 4.5 2Z 22 LEU 4.4 2V 22 LEU 4.4 7S 38 ALA 4.3 7T 87 VAL 4.2 7T 72 ILE 4.1 7T 56 SER 4.0 1E 38 PRO 4.0 2F 21 VAL 4.0 2F 21 VAL 4.0 2F 21 VAL 4.0 2V 94 GLY 3.9 7S 28 TYR 3.9 2Z19ARG 3.8	7	S	32	ILE	5.3
7S56SER 5.2 7T 60 VAL 5.2 7S 77 THR 5.2 7T78THR 5.0 1E 36 LYS 4.8 2Z18HIS 4.8 7S 79 GLY 4.8 2F 22 LEU 4.8 7S 33 VAL 4.5 7T88GLY 4.5 7T 37 GLN 4.5 7T 37 GLN 4.5 7T 37 GLN 4.5 2Z 22 LEU 4.4 2V 22 LEU 4.4 7S 38 ALA 4.3 7T 38 ALA 4.3 7T 87 VAL 4.2 7T 72 ILE 4.1 7T 56 SER 4.0 1E 38 PRO 4.0 2F 21 VAL 4.0 2V 94 GLY 3.9 7S 28 TYR 3.9 2V19ARG 3.8	7	S	29	SER	5.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	S	56	SER	5.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	60	VAL	5.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	S	77	THR	5.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	78	THR	5.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	36	LYS	4.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Ζ	18	HIS	4.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	S	79	GLY	4.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	F	22	LEU	4.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	S	33	VAL	4.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	88	GLY	4.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	37	GLN	4.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Ζ	22	LEU	4.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	V	22	LEU	4.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	S	38	ALA	4.3
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	38	ALA	4.3
7 T 87 VAL 4.2 7 T 72 ILE 4.1 7 T 56 SER 4.0 1 E 38 PRO 4.0 2 F 21 VAL 4.0 2 V 94 GLY 3.9 7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.8	7	S	40	LYS	4.3
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Т	87	VAL	4.2
7 T 56 SER 4.0 1 E 38 PRO 4.0 2 F 21 VAL 4.0 2 F 21 VAL 4.0 2 V 94 GLY 3.9 7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.8	7	Т	72	ILE	4.1
1 E 38 PRO 4.0 2 F 21 VAL 4.0 2 V 94 GLY 3.9 7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.9 2 Z 19 ARG 3.8	7	Т	56	SER	4.0
2 F 21 VAL 4.0 2 V 94 GLY 3.9 7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.8	1	Е	38	PRO	4.0
2 V 94 GLY 3.9 7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.9 3 3.9 3.9 3.9 3.9 3 3.9 3.9 3.9 3.9 3 3.9 3.9 3.9 3.9 3 Y Y Y 3.9 3 Y Y Y 3.9 3 Y Y Y Y 3 Y Y Y Y	2	F	21	VAL	4.0
7 S 28 TYR 3.9 2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.9	2	V	94	GLY	3.9
2 V 19 ARG 3.9 7 T 97 LYS 3.9 2 Z 19 ARG 3.8	7	S	28	TYR	3.9
7 T 97 LYS 3.9 2 Z 19 ARG 3.8	2	V	19	ARG	3.9
2 Z 19 ARG 3.8	7	Т	97	LYS	3.9
	2	Ζ	19	ARG	3.8



Mol

3

7

7

1

7

2

3

7

1

7

7 1

7 7

7

27

7

3

7 2

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3

7

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7

3

4

4

7

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1

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2

3

1

$\overline{39}$	HIS	3.5
36	ILE	3.4
30	ASP	3.3
37	LYS	3.3
92	SER	3.3
57	HIS	3.3
58	TYR	3.2
20	LYS	3.2
58	TYR	3.2
39	GLU	3.2
31	HIS	3.2
53	TYR	3.2
21	VAL	3.1
29	SER	3.1
82	LYS	3.1
99	ARG	3.0

3.0

3.0

3.0

3.0

3.0

3.0

3.0

3.0

2.9

2.9

2.9

2.9

2.8

2.7

2.7

2.7

2.7

2.7

Continued from previous page...

 Res

11

78

69

37

80

23

99

45

Type

ARG

THR

LYS

LYS

VAL

ARG

ARG

SER

RSRZ

3.8

3.7

3.6

3.6

3.6

3.5

3.5

3.5

Chain

W

 \mathbf{S}

Т

0

Т

j Q

 \mathbf{S}

Е

Т S

Е Т

S

 \mathbf{S} V

Т

S

k \mathbf{S}

f

Т

Т

g

Т

g

k

 \mathbf{S}

a

D

D

S

 \mathbf{S}

 \mathbf{a}

W

Q

е

L

F

V

М

е

23

119

99

64

99

30

125

96

34

31

119

14

67

94

20

23

119

37

THR

LYS

ARG

ALA

ARG

LYS

LYS

ALA

ALA

HIS

LYS

ALA

PHE

GLY

LYS

ARG

LYS



6LA	$\lambda 2$
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Mol	Chain	Res	Type	RSRZ
3	Q	118	LYS	2.7
7	S	50	ILE	2.6
3	Q	119	LYS	2.6
7	Т	32	ILE	2.6
1	е	62	ILE	2.6
3	М	117	PRO	2.6
7	S	63	ASN	2.5
2	V	21	VAL	2.5
7	Т	44	GLY	2.5
7	Т	65	ASP	2.5
7	Т	81	LEU	2.4
3	М	118	LYS	2.4
2	Z	21	VAL	2.4
3	W	99	ARG	2.4
2	f	22	LEU	2.4
7	S	76	VAL	2.4
4	Н	30	LYS	2.4
3	a	45	ALA	2.3
7	S	25	HIS	2.3
3	М	115	LEU	2.2
7	Т	33	VAL	2.2
3	W	13	LYS	2.2
7	S	26	PRO	2.1
1	0	69	ARG	2.1
3	М	11	ARG	2.1
3	М	99	ARG	2.1
4	R	124	ALA	2.1
7	Т	70	LEU	2.1
4	Ν	125	LYS	2.1
2	L	99	GLY	2.1
7	Т	93	PHE	2.1
3	g	118	LYS	2.1
2	f	28	GLY	2.1
3	a	25	PHE	2.0
3	W	12	ALA	2.0
1	Y	81	ASP	2.0
1	U	132	GLY	2.0

Continued from previous page...

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.

