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PDB ID	:	9GMK
EMDB ID	:	EMD-51449
Title	:	SIRT7:H3K18DTU nucleosome complex
Authors	:	Moreno-Yruela, C.; Ekundayo, B.; Foteva, P.; Calvino-Sanles, E.; Ni, D.;
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Deposited on	:	2024-08-29
Resolution	:	3.50 Å(reported)
This is	s a l	Full wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.50 Å.

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



Motria	Whole archive	EM structures
Metric	$(\# { m Entries})$	(# Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Qı	uality of chain	
1	А	136	35%	35% ·	30%
1	Е	136	42%	29%	29%
2	В	103	38%	43%	19%
2	F	103	42%	34%	24%
3	С	129	44%	36%	19%
3	G	129	52%	29%	• 19%
4	D	126	38%	33% •	27%
4	Н	126	36%	38%	26%
5	K	401	41%	41%	• 17%



Mol	Chain	Length	Quality of chain					
6	L	148	45%	55%				
7	М	148	28%	72%				



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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	Atoms					AltConf	Trace
1	А	95	Total 784	C 494	N 151	O 136	${ m S} { m 3}$	0	0
1	Е	97	Total 800	C 503	N 155	0 139	${ m S} { m 3}$	0	0

• Molecule 1 is a protein called Histone H3.2.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	47	CYS	ALA	conflict	UNP Q71DI3
А	110	ALA	CYS	conflict	UNP Q71DI3
Е	47	CYS	ALA	conflict	UNP Q71DI3
Е	110	ALA	CYS	conflict	UNP Q71DI3

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	В	83	Total	С	Ν	0	S	0	0
	D	00	662	418	129	114	1	0	0
9	Б	79	Total	С	Ν	0	S	0	0
	Г	10	619	391	120	107	1	0	0

• Molecule 3 is a protein called Histone H2A type 2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	104	Total	С	Ν	0	S	0	0
່ <u>ບ</u>	3 0	104	801	506	155	139	1		
2	C	105	Total	С	Ν	0	S	0	0
່ <u>ບ</u>	G	105	806	509	156	140	1	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
4	П	02	Total	С	Ν	0	S	0	0
4	D	92	717	453	127	135	2	0	0
4	ц	03	Total	С	Ν	0	S	0	0
4	11	90	724	456	130	136	2	0	0

• Molecule 5 is a protein called NAD-dependent protein deacetylase sirtuin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	334	Total 2662	C 1642	N 516	0 489	S 15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Residue Modelled		Comment	Reference
Κ	0	GLY	-	expression tag	UNP Q9NRC8

• Molecule 6 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms			AltConf	Trace		
6	L	148	Total 3014	C 1436	N 535	O 895	Р 148	0	0

• Molecule 7 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms			AltConf	Trace		
7	М	148	Total 3054	C 1447	N 578	0 881	Р 148	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Histone H3.2



• Molecule 3: Hi	istone H2A type 2-A		
Chain C:	44%	36%	19%
SER GLY GLY GLY CLN CLN GLN GLY ARA ALA	LYS LYS K1LA K1LA R17 R17 R20 R20 C28 C28 C28 C28 C28 C28 C28 C28 C28 C28	H 30 H 31 H 32 H 33 H 32 H 33 H 33 H 33 H 33 H 33	159 162 162 162 162 178 178 178 178 178 178 178 178 178 178
187 187 187 188 189 193 193 193 193 193 193 193	0104 0105 0106 0106 0112 0113 0113 1115 1115 1115 1118 1118 1118 1118 1	HIS HIS LIYS ALA LIYS GLY LIYS	
• Molecule 3: H	istone H2A type 2-A		
Chain G:	52%	29%	• 19%
SER CLY ARG CLY GLY CLN GLN GLY CLY ALA ALA	LYS A14 A14 K15 K15 R17 R29 R30 R32 R32 R35 R35 R35 R35 R35 R35 R35	A47 P48 V50 M51 M51 E64 E64 A69 A69 A71 A71	T76 T78 178 178 183 187 187 187 187 187 187 187 187 187 187
L96 L97 698 K99 V100 110 111 111 111	LITE RITE LYS THR LYS CLYS CLY LYS LYS CLY CLY		
• Molecule 4: H	istone H2B type 1-J		
Chain D:	38%	33% •	27%
MET PRO PRO PRO PRO ALA SER ALA PRO PRO LYS	LYS SGLY SGLY SGLY LYS LYS THR THR LYS GLA CYS CYS CLY SGLY	LVS LVS ARG ARG SER SER SER X43 V41 V42 V43 V43	L45 K46 K46 V43 P50 P50 P50 P50 R53 R55 R55 R55 R55 R55 R55 R55 R55 R55
NG3 564 765 765 765 765 166 169 169 169 170 871 871 871	R79 189 189 194 194 194 194 198 198 198 198 198	P103 A107 A107 A106 A110 A110 C111 C111 C114 A112 C114 C114 C114 C114 C114 C114 C114 C	
• Molecule 4: H	istone H2B type 1-J		
Chain H:	36%	38%	26%
MET PRO GLU PRO LVS ALA SER ALA ALA ALA PRO PRO LVS	LYS GLY SER LYS LYS LYS ALA VAL LYS GLN LYS CLN CLY CLY	LYS LYS ARG ARG ARG ARG 832 832 832 832 832 832 832 832 832 832	V48 H49 KK57 K67 A58 A58 A58 M63 N63 N63 N63 N63 N63 N63 F51 F57
173 474 675 676 876 879 180 180 883 885 885	190 891 892 892 893 897 196 1100 1100 1100 1100 1100 1100 1100	E106 1106 1106 1107 1108 1110 1111 1115 11115 11115 11115 11115 11115 11115 11115 11115 11115 11115	2
• Molecule 5: N.	AD-dependent protei	n deacetylase sirtuin-7	,
Chain K:	41%	41%	• 17%
GLY MET MET ALA ALA GLY GLY LEU SER SER SER E10 E10	A14 A14 A15 A15 A16 A15 A15 A15 A18 A18 A26 A26 A26 A26 A26 A26 A26 A26 A26 A26	129 129 130 135 136 136 136 136 136 136 136 136 136 136	L61 663 663 664 865 865 865 865 865 870 670 877 877 877 877 877 877 877 875
E77 D81 D81 E84 E84 E85 R90 R90 A93	V96 R97 N98 N99 V101 V102 V102 V102 V102 C107 G107 S111 S111	1116 1118 1118 1118 1118 1118 1118 1118	LI'S GLI'S ARG SER VAL VAL ALA ALA ALA ALA ALA ALA ALA ALA
		PROTEIN DATA BANK	

MRG L322 C222 T153 ARG L322 R223 T155 ARG R331 R233 T156 LYS R333 T234 L155 VAL N331 R233 L156 VAL N335 T236 H156 VAL N336 T236 H166 NA40 R233 T236 H166 R341 R233 T236 H166 R343 R243 R244 H16 R344 R243 L245 H166 R344 R243 L347 H16 R345 R246 L346 H166 R345 R246 L347 H166 R355 R271 R726 H176 R355 R271 R177 H178 R355 R271 R177 H187 R355 R271 R177 H187 R356 R271 R276 H187 <td

• Molecule 6: DNA (148-MER)





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Agnification Not provided		
Image detector	FEI FALCON IV (4k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.29	0/794	0.66	0/1064	
1	Е	0.29	0/811	0.63	0/1086	
2	В	0.29	0/669	0.64	0/894	
2	F	0.30	0/626	0.65	0/837	
3	С	0.30	0/811	0.58	0/1093	
3	G	0.26	0/816	0.58	0/1100	
4	D	0.31	0/728	0.65	2/978~(0.2%)	
4	Н	0.32	0/735	0.62	0/989	
5	K	0.26	0/2706	0.59	0/3648	
6	L	0.50	0/3374	0.93	0/5201	
7	М	0.48	0/3432	0.87	0/5299	
All	All	0.39	0/15502	0.76	2/22189~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	45	LEU	CA-CB-CG	5.38	127.66	115.30
4	D	45	LEU	CB-CG-CD2	-5.05	102.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	784	0	824	45	0
1	Е	800	0	836	39	0
2	В	662	0	709	43	0
2	F	619	0	659	35	0
3	С	801	0	857	50	0
3	G	806	0	862	33	0
4	D	717	0	737	46	0
4	Н	724	0	742	44	0
5	K	2662	0	2694	136	0
6	L	3014	0	1668	72	0
7	М	3054	0	1661	102	0
All	All	14643	0	12249	564	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:130:ILE:HD12	1:E:130:ILE:HD13	1.57	0.86
5:K:274:LEU:HB3	5:K:281:TRP:HE1	1.42	0.82
6:L:26:DG:N2	7:M:172:DC:O2	2.13	0.81
6:L:26:DG:N1	7:M:172:DC:N3	2.29	0.80
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.16	0.79
2:B:94:GLY:O	3:G:99:LYS:NZ	2.17	0.78
4:H:80:LEU:HD11	4:H:93:GLU:HB2	1.66	0.78
4:H:102:LEU:HD12	4:H:103:PRO:HD2	1.67	0.77
6:L:157:DA:H2"	6:L:158:DT:H5"	1.67	0.76
2:F:45:ARG:HE	6:L:101:DC:H4'	1.52	0.74
4:H:73:ILE:HG22	4:H:101:LEU:HD21	1.68	0.74
5:K:32:VAL:HG12	5:K:50:LEU:HD21	1.70	0.74
2:B:35:ARG:HH21	2:B:39:ARG:HH12	1.34	0.74
1:E:50:GLU:HA	1:E:53:ARG:HG2	1.70	0.72
2:B:88:TYR:HD2	2:B:91:LYS:HZ3	1.38	0.71
4:D:45:LEU:HD21	4:D:54:ILE:HG13	1.72	0.71
5:K:207:VAL:HB	5:K:360:LEU:HB2	1.74	0.70
1:E:51:ILE:O	1:E:55:GLN:NE2	2.25	0.70
2:F:74:GLU:O	4:H:92:ARG:NH2	2.24	0.69
6:L:120:DG:N2	7:M:79:DC:O2	2.26	0.69
5:K:205:VAL:HB	5:K:344:ALA:HA	1.74	0.69
1:E:79:LYS:HG3	1:E:82:LEU:HD21	1.73	0.69
5:K:106:THR:HB	5:K:166:SER:HA	1.73	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:K:173:HIS:HB2	5:K:178:LEU:HD12	1.75	0.68
3:C:87:ILE:HD12	3:C:93:LEU:HB3	1.74	0.68
3:C:25:PHE:HD2	3:C:56:GLU:HG2	1.58	0.67
3:C:42:ARG:NH2	4:D:88:THR:OG1	2.28	0.67
3:C:104:GLN:N	1:E:94:GLU:OE2	2.25	0.66
5:K:159:LYS:O	5:K:162:GLN:NE2	2.29	0.66
3:C:112:GLN:HE22	3:C:114:VAL:HG22	1.61	0.65
1:E:79:LYS:NZ	1:E:80:THR:O	2.24	0.65
3:G:93:LEU:HA	3:G:96:LEU:HD23	1.78	0.65
3:C:90:ASP:O	3:C:94:ASN:ND2	2.30	0.65
4:H:33:ARG:NH2	7:M:59:DG:OP1	2.29	0.65
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.29	0.64
3:C:17:ARG:HA	3:C:20:ARG:HG2	1.79	0.64
6:L:120:DG:H2"	6:L:121:DG:C8	2.33	0.64
3:C:25:PHE:CD2	3:C:56:GLU:HG2	2.31	0.64
4:D:46:LYS:HE3	4:D:46:LYS:HA	1.79	0.64
6:L:59:DA:H2"	6:L:60:DG:C8	2.34	0.63
7:M:125:DG:H2'	7:M:126:DT:H71	1.79	0.63
2:B:82:THR:HG22	2:B:84:MET:H	1.64	0.63
5:K:297:ASN:ND2	5:K:299:GLN:O	2.31	0.63
3:G:68:ASN:ND2	5:K:19:ARG:HE	1.97	0.63
1:A:47:CYS:O	1:A:51:ILE:HG12	1.99	0.62
5:K:342:SER:H	5:K:362:ARG:HH21	1.46	0.62
1:E:129:ARG:HH21	1:E:134:ARG:HG3	1.65	0.62
5:K:110:ILE:HD11	5:K:267:LEU:HG	1.80	0.62
5:K:212:GLU:HG2	5:K:356:SER:HB3	1.82	0.62
4:D:61:ILE:HG23	2:F:98:TYR:HD2	1.64	0.62
5:K:208:PHE:HB3	5:K:359:SER:HA	1.81	0.62
3:C:97:LEU:HD21	4:D:65:PHE:HE1	1.64	0.62
5:K:71:LEU:O	5:K:75:GLN:NE2	2.32	0.61
4:H:104:GLY:O	4:H:108:LYS:HG3	2.00	0.61
4:H:115:THR:O	4:H:119:THR:HG23	2.00	0.61
5:K:189:ASN:HD22	5:K:192:ILE:HD12	1.65	0.61
2:B:87:VAL:HG12	2:B:91:LYS:NZ	2.16	0.61
3:C:27:VAL:HG13	3:C:48:PRO:HB2	1.82	0.61
3:G:70:ALA:HA	3:G:82:HIS:CE1	2.35	0.61
4:H:85:LYS:HE3	4:H:85:LYS:HA	1.81	0.61
5:K:147:LEU:HD11	5:K:330:ILE:HD12	1.83	0.61
5:K:27:GLU:HA	5:K:30:ARG:HG2	1.83	0.60
7:M:97:DG:H2"	7:M:98:DG:C8	2.36	0.60
3:C:55:LEU:HD11	4:D:66:VAL:HG23	1.83	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:K:14:ALA:HA	5:K:17:VAL:HG22	1.83	0.60
5:K:268:GLY:N	5:K:296:VAL:O	2.34	0.60
1:E:130:ILE:HG13	1:E:131:ARG:N	2.16	0.60
4:H:80:LEU:HA	4:H:83:TYR:HB2	1.82	0.60
7:M:119:DT:H2"	7:M:120:DA:C8	2.35	0.60
1:A:126:LEU:O	1:A:130:ILE:HG12	2.00	0.60
2:B:75:HIS:O	4:D:92:ARG:NH1	2.33	0.60
2:F:89:ALA:O	2:F:93:GLN:NE2	2.35	0.60
5:K:223:ARG:HG3	5:K:351:GLU:HG3	1.84	0.60
5:K:355:HIS:ND1	5:K:357:ARG:O	2.35	0.59
7:M:112:DG:H2'	7:M:113:DT:H71	1.84	0.59
5:K:111:SER:HB3	5:K:116:ILE:HB	1.84	0.59
3:G:110:ASN:O	3:G:110:ASN:ND2	2.32	0.59
5:K:36:LEU:HD11	5:K:57:LEU:HD13	1.84	0.59
3:C:79:ILE:HG22	3:C:82:HIS:CD2	2.37	0.59
4:H:103:PRO:HG2	4:H:106:LEU:HD12	1.83	0.59
5:K:342:SER:N	5:K:362:ARG:HH21	2.00	0.59
2:B:29:ILE:HD11	2:B:55:ARG:HG2	1.84	0.59
3:G:90:ASP:O	3:G:94:ASN:ND2	2.35	0.59
5:K:189:ASN:O	5:K:235:THR:OG1	2.21	0.59
3:C:41:GLU:HG2	3:C:42:ARG:HG3	1.84	0.59
5:K:104:VAL:HB	5:K:164:VAL:HG22	1.85	0.59
2:B:60:VAL:O	2:B:63:GLU:HG2	2.02	0.59
3:C:24:GLN:N	3:C:56:GLU:OE2	2.21	0.58
6:L:102:DC:H2"	6:L:103:DG:C8	2.38	0.58
4:D:68:ASP:O	4:D:72:ARG:HG3	2.02	0.58
7:M:139:DT:H2"	7:M:140:DA:C8	2.39	0.58
5:K:283:MET:O	5:K:290:ARG:NH2	2.37	0.58
1:A:100:LEU:HD11	2:B:37:LEU:HD22	1.86	0.58
1:A:118:THR:HG22	2:B:45:ARG:HG2	1.86	0.58
3:C:15:LYS:O	3:C:20:ARG:NH2	2.37	0.57
3:C:96:LEU:HD21	4:D:103:PRO:HD3	1.86	0.57
4:D:57:LYS:O	4:D:61:ILE:HD12	2.05	0.57
7:M:32:DA:H2"	7:M:33:DA:C8	2.40	0.57
7:M:124:DG:H2"	7:M:125:DG:H5"	1.85	0.57
3:G:29:ARG:HH12	6:L:142:DG:H5"	1.69	0.57
6:L:58:DT:H2"	6:L:59:DA:N7	2.19	0.57
5:K:71:LEU:HD23	5:K:74:ARG:HE	1.69	0.56
4:D:102:LEU:HD23	4:D:107:ALA:HA	1.85	0.56
1:E:105:GLU:O	1:E:109:LEU:HG	2.05	0.56
6:L:26:DG:O6	7:M:172:DC:N4	2.36	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:76:ALA:HB3	2:F:78:ARG:NH1	2.21	0.56
3:C:84:GLN:NE2	3:C:106:GLY:O	2.34	0.56
2:F:63:GLU:HA	2:F:66:ILE:HG12	1.86	0.56
1:E:107:THR:HG21	1:E:124:ILE:HG13	1.88	0.56
4:H:41:VAL:HA	4:H:44:VAL:HG22	1.88	0.56
4:H:90:THR:HG23	4:H:92:ARG:H	1.71	0.56
6:L:164:DT:H2"	6:L:165:DT:H71	1.88	0.56
3:C:77:ARG:HA	4:D:53:GLY:O	2.06	0.55
5:K:68:ARG:HA	5:K:71:LEU:HD12	1.88	0.55
5:K:86:ARG:HG3	5:K:90:ARG:HH12	1.71	0.55
3:C:75:LYS:HG3	3:C:77:ARG:H	1.71	0.55
5:K:166:SER:HB3	5:K:183:ILE:HD11	1.87	0.55
6:L:149:DT:H2"	6:L:150:DC:C5	2.41	0.55
1:A:71:VAL:HA	1:A:74:ILE:HG12	1.87	0.55
2:B:29:ILE:O	2:B:55:ARG:NH2	2.38	0.55
2:F:60:VAL:O	2:F:63:GLU:HG3	2.06	0.55
6:L:139:DC:H2"	6:L:140:DA:N7	2.21	0.55
2:B:64:ASN:O	2:B:67:ARG:HG2	2.06	0.55
6:L:80:DA:H2"	6:L:81:DA:C8	2.42	0.55
6:L:158:DT:H2"	6:L:159:DA:C8	2.41	0.55
6:L:139:DC:H2"	6:L:140:DA:C8	2.41	0.55
1:A:52:ARG:NE	7:M:39:DT:OP2	2.35	0.55
1:E:108:ASN:O	1:E:112:ILE:HG12	2.06	0.55
3:G:15:LYS:HG3	7:M:61:DA:H4'	1.89	0.55
3:C:42:ARG:HH22	6:L:59:DA:H4'	1.72	0.55
2:F:50:ILE:O	2:F:53:GLU:HG2	2.07	0.55
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.34	0.55
6:L:118:DA:H2"	6:L:119:DG:C8	2.42	0.55
4:D:76:GLU:HA	4:D:79:ARG:NE	2.21	0.54
3:C:112:GLN:HB3	3:C:115:LEU:HD12	1.90	0.54
5:K:70:GLY:O	5:K:74:ARG:HG3	2.07	0.54
3:C:29:ARG:HH12	3:C:32:ARG:HD2	1.72	0.54
5:K:271:LEU:O	5:K:275:LYS:N	2.33	0.54
6:L:37:DC:H2"	6:L:38:DC:C5	2.42	0.54
4:H:113:GLU:HA	4:H:116:LYS:NZ	2.22	0.54
6:L:86:DC:H2"	6:L:87:DG:C8	2.41	0.54
5:K:269:SER:O	5:K:297:ASN:ND2	2.40	0.54
1:A:53:ARG:HA	1:A:56:LYS:HE3	1.89	0.54
1:E:107:THR:HB	1:E:119:ILE:HD11	1.90	0.54
6:L:143:DC:H2"	6:L:144:DA:C8	2.43	0.54
5:K:185:GLU:OE2	5:K:189:ASN:ND2	2.41	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:M:70:DA:H2"	7:M:71:DG:C8	2.43	0.54
7:M:157:DC:H2"	7:M:158:DT:C5	2.43	0.54
5:K:21:ARG:HA	5:K:24:GLN:HG2	1.89	0.54
3:C:50:TYR:CE1	4:D:114:GLY:HA3	2.43	0.54
4:H:33:ARG:HH22	7:M:59:DG:P	2.32	0.53
6:L:31:DC:N3	7:M:168:DG:N2	2.56	0.53
7:M:167:DG:H2"	7:M:168:DG:C8	2.44	0.53
2:B:88:TYR:HA	2:B:91:LYS:HZ3	1.72	0.53
6:L:61:DA:H61	7:M:137:DT:H3	1.57	0.53
7:M:33:DA:H2"	7:M:34:DA:C8	2.44	0.53
5:K:18:ARG:O	5:K:21:ARG:HG3	2.09	0.53
6:L:90:DC:H2"	6:L:91:DG:C8	2.44	0.53
3:C:26:PRO:HD3	4:D:40:TYR:CG	2.44	0.53
7:M:159:DC:H2"	7:M:160:DG:C8	2.44	0.53
3:G:50:TYR:CE2	4:H:114:GLY:HA3	2.44	0.53
3:G:68:ASN:ND2	3:G:71:ARG:HH21	2.07	0.53
1:A:84:PHE:HA	2:B:81:VAL:HG22	1.91	0.52
1:E:86:SER:O	1:E:90:MET:HG2	2.09	0.52
4:H:96:THR:O	4:H:100:LEU:HG	2.09	0.52
5:K:146:THR:HG23	5:K:149:HIS:H	1.75	0.52
6:L:35:DT:H2"	6:L:36:DG:C8	2.44	0.52
6:L:82:DC:H2"	6:L:83:DG:C8	2.44	0.52
5:K:271:LEU:O	5:K:275:LYS:HG2	2.09	0.52
6:L:56:DC:H2"	6:L:57:DG:C8	2.44	0.52
7:M:100:DG:H2"	7:M:101:DA:C8	2.43	0.52
3:G:32:ARG:HA	3:G:35:ARG:HG2	1.92	0.52
4:H:36:SER:OG	4:H:37:TYR:N	2.42	0.52
7:M:65:DT:H2"	7:M:66:DA:N7	2.24	0.52
5:K:15:GLU:O	5:K:18:ARG:HD3	2.09	0.52
3:G:75:LYS:NZ	3:G:77:ARG:HB2	2.24	0.52
3:G:84:GLN:NE2	3:G:88:ARG:HG3	2.24	0.52
5:K:170:ASP:HB2	5:K:172:LEU:HG	1.91	0.52
2:F:29:ILE:HG23	2:F:55:ARG:HE	1.74	0.52
5:K:40:ALA:HA	5:K:43:ARG:HH21	1.74	0.52
3:C:80:PRO:HA	3:C:83:LEU:HG	1.92	0.52
2:F:36:ARG:NH1	7:M:91:DA:OP2	2.43	0.52
5:K:64:ARG:O	5:K:68:ARG:NE	2.39	0.52
5:K:77:GLU:HG3	5:K:298:LEU:HD12	1.91	0.52
3:C:21:ALA:HB2	4:D:121:TYR:HD2	1.75	0.52
3:G:70:ALA:HB2	3:G:78:ILE:HG22	1.92	0.52
5:K:90:ARG:HG2	5:K:325:GLU:HG2	1.92	0.52



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance $(Å)$		
6:L:26:DG:H2"	6:L:27:DA:C8	2.45	0.52	
2:F:92:ARG:HH22	4:H:101:LEU:HB3	1.75	0.51	
5:K:340:ILE:HG13	5:K:341:PHE:N	2.24	0.51	
2:B:26:ILE:HG22	2:B:55:ARG:HD3	1.93	0.51	
1:E:68:GLN:HG3	1:E:89:VAL:HG11	1.92	0.51	
1:E:133:GLU:HG3	2:F:61:PHE:HZ	1.75	0.51	
5:K:173:HIS:ND1	5:K:183:ILE:HG12	2.26	0.51	
7:M:47:DT:H2"	7:M:48:DG:C8	2.44	0.51	
7:M:150:DG:H2"	7:M:151:DA:N7	2.25	0.51	
4:D:95:GLN:O	4:D:99:ARG:HG3	2.11	0.51	
4:H:79:ARG:NH2	4:H:83:TYR:OH	2.44	0.51	
7:M:31:DA:H2"	7:M:32:DA:C8	2.44	0.51	
5:K:71:LEU:HA	5:K:74:ARG:HE	1.75	0.51	
5:K:104:VAL:O	5:K:164:VAL:HA	2.09	0.51	
6:L:47:DT:H2"	6:L:48:DC:C5	2.45	0.51	
1:A:121:PRO:O	1:A:124:ILE:HG22	2.11	0.51	
5:K:221:THR:HG22	5:K:223:ARG:HD3	1.92	0.51	
5:K:341:PHE:HE2	5:K:360:LEU:HB3	1.75	0.51	
1:A:94:GLU:OE2	3:G:104:GLN:N	2.33	0.51	
2:B:35:ARG:NH2	2:B:39:ARG:HH12	2.04	0.51	
5:K:235:THR:HG22	5:K:248:PRO:HB3	1.93	0.51	
1:E:129:ARG:NH2	1:E:134:ARG:HG3	2.26	0.50	
3:G:30:VAL:HG13	3:G:48:PRO:HB3	1.92	0.50	
5:K:107:GLY:H	5:K:110:ILE:HD12	1.75	0.50	
7:M:66:DA:H4'	7:M:67:DG:OP1	2.11	0.50	
3:C:70:ALA:HA	3:C:82:HIS:CE1	2.45	0.50	
7:M:30:DA:H2"	7:M:31:DA:C8	2.47	0.50	
5:K:26:ARG:O	5:K:29:LEU:HG	2.12	0.50	
7:M:56:DC:H2"	7:M:57:DC:C5	2.46	0.50	
7:M:141:DC:H2"	7:M:142:DG:C8	2.46	0.50	
5:K:24:GLN:HA	5:K:27:GLU:HG3	1.94	0.50	
5:K:196:THR:HA	5:K:245:LEU:HD21	1.94	0.50	
5:K:204:TYR:HE2	5:K:226:HIS:HD2	1.59	0.50	
2:B:45:ARG:HD3	2:B:46:ILE:H	1.77	0.50	
6:L:49:DA:H2"	6:L:50:DA:C8	2.47	0.50	
2:B:87:VAL:HA	2:B:90:LEU:HG	1.93	0.50	
5:K:303:LYS:HA	5:K:306:TRP:HB2	1.94	0.50	
7:M:91:DA:H2"	7:M:92:DA:H8	1.75	0.50	
4:H:58:ALA:O	4:H:62:MET:HG2	2.11	0.49	
1:A:99:TYR:CE1	1:A:103:LEU:HD23	2.46	0.49	
3:C:42:ARG:NH2	6:L:59:DA:H4'	2.26	0.49	



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
7:M:72:DT:C2	7:M:73:DA:N7	2.80	0.49	
3:C:17:ARG:HD2	3:C:28:GLY:N	2.28	0.49	
3:C:55:LEU:CD1	4:D:66:VAL:HG23	2.42	0.49	
3:C:89:ASN:OD1	3:C:90:ASP:N	2.45	0.49	
3:G:63:LEU:HD22	4:H:45:LEU:HD23	1.93	0.49	
5:K:274:LEU:HB3	5:K:281:TRP:NE1	2.20	0.49	
7:M:115:DC:H2"	7:M:116:DG:C8	2.47	0.49	
7:M:34:DA:H2"	7:M:35:DA:C8	2.47	0.49	
7:M:142:DG:H2"	7:M:143:DA:H8	1.77	0.49	
7:M:157:DC:H2"	7:M:158:DT:C6	2.47	0.49	
1:A:128:ARG:HD3	1:A:134:ARG:HH21	1.76	0.49	
7:M:109:DT:H2"	7:M:110:DA:N7	2.27	0.49	
5:K:273:VAL:HA	5:K:276:LYS:HZ3	1.78	0.49	
1:A:54:TYR:HB3	2:B:40:ARG:HG2	1.93	0.49	
3:G:75:LYS:HZ2	3:G:77:ARG:HB2	1.76	0.49	
4:H:57:LYS:HD3	4:H:57:LYS:N	2.27	0.49	
1:A:86:SER:HB2	1:A:90:MET:HE3	1.94	0.49	
2:F:42:GLY:O	2:F:44:LYS:NZ	2.32	0.48	
7:M:60:DG:H2"	7:M:61:DA:H8	1.78	0.48	
1:A:49:ARG:HA	1:A:52:ARG:CZ	2.43	0.48	
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.13	0.48	
3:C:112:GLN:NE2	3:C:114:VAL:HG22	2.27	0.48	
7:M:75:DT:H2"	7:M:76:DC:C5	2.48	0.48	
3:G:41:GLU:OE1	3:G:41:GLU:N	2.41	0.48	
5:K:194:VAL:HG13	5:K:245:LEU:HD22	1.94	0.48	
5:K:294:TYR:HE1	5:K:308:ALA:HB3	1.78	0.48	
6:L:66:DT:H2"	6:L:67:DC:C6	2.49	0.48	
7:M:107:DC:H2"	7:M:108:DG:C8	2.49	0.48	
1:A:65:LEU:HD12	7:M:121:DA:H2'	1.96	0.48	
2:B:88:TYR:HA	2:B:91:LYS:NZ	2.28	0.48	
5:K:43:ARG:HH12	5:K:51:LEU:HD13	1.78	0.48	
5:K:74:ARG:O	5:K:299:GLN:NE2	2.43	0.48	
6:L:97:DT:H2"	6:L:98:DC:C6	2.48	0.48	
2:B:77:LYS:HG3	4:D:92:ARG:NH1	2.29	0.48	
4:D:108:LYS:HA	4:D:111:VAL:HG22	1.95	0.48	
3:G:97:LEU:O	3:G:100:VAL:HG22	2.13	0.48	
5:K:301:THR:O	5:K:304:ASP:HB2	2.13	0.48	
7:M:135:DT:H2"	7:M:136:DG:C8	2.48	0.48	
1:A:112:ILE:HD13	3:G:112:GLN:HG3	1.95	0.48	
1:E:127:ALA:HA	1:E:130:ILE:HG12	1.96	0.48	
7:M:124:DG:H2"	7:M:125:DG:H8	1.77	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:62:ILE:HD11	1:E:93:GLN:HE22	1.78	0.48	
5:K:154:ARG:O	5:K:158:GLN:HG2	2.13	0.48	
5:K:219:HIS:CE1	5:K:233:ARG:HD3	2.49	0.48	
7:M:37:DT:H2"	7:M:38:DG:C8	2.49	0.48	
5:K:295:ILE:HD13	5:K:303:LYS:HB3	1.95	0.48	
7:M:65:DT:H2"	7:M:66:DA:C8	2.49	0.48	
4:H:113:GLU:HA	4:H:116:LYS:HZ2	1.78	0.48	
5:K:35:ILE:HG22	5:K:51:LEU:HB2	1.96	0.48	
6:L:88:DT:H2"	6:L:89:DA:N7	2.29	0.48	
1:A:73:GLU:O	1:A:76:GLN:HG2	2.14	0.47	
5:K:163:HIS:NE2	5:K:184:SER:OG	2.44	0.47	
7:M:109:DT:H2"	7:M:110:DA:C8	2.49	0.47	
1:E:61:LEU:HD21	2:F:36:ARG:HB2	1.96	0.47	
7:M:59:DG:H2"	7:M:60:DG:C8	2.49	0.47	
2:B:27:GLN:HA	2:B:55:ARG:CZ	2.43	0.47	
5:K:195:CYS:SG	5:K:230:THR:OG1	2.71	0.47	
2:B:87:VAL:HG12	2:B:91:LYS:HZ1	1.77	0.47	
3:C:88:ARG:C	3:C:94:ASN:HD21	2.14	0.47	
1:E:63:ARG:NH2	7:M:90:DA:H5"	2.28	0.47	
7:M:149:DT:H2"	7:M:150:DG:C8	2.50	0.47	
1:E:61:LEU:HD22	2:F:37:LEU:HB3	1.95	0.47	
1:E:133:GLU:HG3	2:F:61:PHE:CZ	2.50	0.47	
5:K:296:VAL:HG22	5:K:311:LEU:HD13	1.96	0.47	
7:M:29:DA:H2"	7:M:30:DA:C8	2.50	0.47	
5:K:25:GLN:O	5:K:28:ARG:HG2	2.15	0.47	
4:D:44:VAL:O	4:D:47:GLN:HG2	2.15	0.47	
2:F:85:ASP:HA	2:F:88:TYR:CD2	2.50	0.47	
4:H:111:VAL:O	4:H:115:THR:HG23	2.15	0.47	
3:G:71:ARG:HH22	4:H:49:HIS:CE1	2.33	0.47	
7:M:76:DC:H2"	7:M:77:DC:C6	2.50	0.47	
6:L:67:DC:O2	7:M:131:DG:N2	2.39	0.47	
6:L:92:DC:H2"	6:L:93:DG:C8	2.50	0.47	
7:M:105:DC:H2"	7:M:106:DG:C8	2.50	0.47	
5:K:61:LEU:HD23	5:K:64:ARG:HH21	1.79	0.47	
3:C:57:TYR:HB2	4:D:113:GLU:OE2	2.15	0.46	
6:L:163:DT:H2"	6:L:164:DT:C6	2.50	0.46	
4:D:92:ARG:O	4:D:95:GLN:HG2	2.14	0.46	
6:L:48:DC:H2"	6:L:49:DA:C8	2.50	0.46	
6:L:109:DT:H2"	6:L:110:DA:N7	2.31	0.46	
3:G:83:LEU:HD13	4:H:61:ILE:HD12	1.97	0.46	
5:K:285:LYS:O	5:K:290:ARG:NH2	2.47	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:54:TYR:HE1	2:B:36:ARG:HD2	1.80	0.46	
1:A:67:PHE:CD2	1:A:93:GLN:NE2	2.84	0.46	
4:H:33:ARG:HH12	7:M:59:DG:H5'	1.81	0.46	
5:K:73:ARG:HA	5:K:76:GLU:HG3	1.96	0.46	
1:A:72:ARG:HG2	1:A:84:PHE:CE2	2.50	0.46	
1:A:82:LEU:HB3	1:A:84:PHE:CE1	2.51	0.46	
4:H:96:THR:O	4:H:99:ARG:HG2	2.16	0.46	
1:A:70:LEU:HD11	2:B:26:ILE:HG13	1.97	0.46	
6:L:111:DA:C8	6:L:111:DA:H5'	2.51	0.46	
2:B:62:LEU:O	2:B:66:ILE:HG12	2.16	0.46	
3:C:78:ILE:CG2	4:D:54:ILE:HG23	2.46	0.46	
4:D:42:TYR:CE1	4:D:46:LYS:HD3	2.51	0.46	
1:A:67:PHE:HD2	1:A:93:GLN:NE2	2.13	0.46	
2:F:70:VAL:O	2:F:74:GLU:OE1	2.34	0.46	
1:A:126:LEU:HD11	1:E:110:ALA:HA	1.98	0.46	
3:C:79:ILE:HD12	3:C:80:PRO:HD2	1.98	0.46	
4:D:103:PRO:HD2	4:D:106:LEU:HD12	1.98	0.46	
4:H:34:LYS:HD2	4:H:34:LYS:HA	1.76	0.46	
5:K:74:ARG:HD2	5:K:300:TRP:CZ3	2.51	0.46	
3:C:26:PRO:HD3	4:D:40:TYR:CD2	2.51	0.46	
4:D:44:VAL:O	4:D:48:VAL:HG12	2.16	0.46	
7:M:86:DG:C8	7:M:86:DG:H5'	2.51	0.46	
7:M:142:DG:H2"	7:M:143:DA:C8	2.50	0.46	
4:D:67:ASN:O	4:D:71:GLU:OE1	2.33	0.45	
5:K:31:GLN:O	5:K:35:ILE:HG12	2.16	0.45	
6:L:129:DC:H2"	6:L:130:DC:C6	2.51	0.45	
5:K:43:ARG:HH22	5:K:51:LEU:HD13	1.81	0.45	
6:L:68:DT:H2"	6:L:69:DA:N7	2.31	0.45	
6:L:162:DA:H1'	6:L:163:DT:H5'	1.98	0.45	
2:F:88:TYR:HA	2:F:91:LYS:HE3	1.98	0.45	
5:K:111:SER:O	5:K:116:ILE:N	2.49	0.45	
5:K:319:MET:HE1	5:K:322:LEU:HD23	1.97	0.45	
6:L:39:DG:H2"	6:L:40:DA:C8	2.52	0.45	
6:L:78:DT:H2"	6:L:79:DA:N7	2.32	0.45	
3:C:112:GLN:HG3	1:E:112:ILE:HD12	1.98	0.45	
5:K:204:TYR:HE2	5:K:226:HIS:CD2	2.33	0.45	
7:M:27:DA:H2"	7:M:28:DA:C8	2.52	0.45	
1:E:130:ILE:HG13	1:E:131:ARG:HG2	1.97	0.45	
5:K:25:GLN:HA	5:K:28:ARG:NE	2.32	0.45	
5:K:28:ARG:HA	5:K:31:GLN:HG3	1.99	0.45	
5:K:69:GLU:OE1	5:K:73:ARG:NH1	2.49	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:K:179:PRO:O	5:K:183:ILE:HG22	2.15	0.45	
1:E:102:GLY:HA2	1:E:105:GLU:OE1	2.17	0.45	
4:H:58:ALA:HA	4:H:61:ILE:HG12	1.99	0.45	
7:M:58:DT:H2"	7:M:59:DG:C8	2.52	0.45	
2:B:70:VAL:O	2:B:74:GLU:OE1	2.34	0.45	
1:E:102:GLY:HA2	1:E:105:GLU:CD	2.37	0.45	
6:L:140:DA:H2"	6:L:141:DG:N7	2.32	0.45	
1:A:116:ARG:NH1	1:A:118:THR:O	2.50	0.45	
2:F:34:ILE:HA	2:F:37:LEU:HG	1.99	0.45	
7:M:113:DT:H2"	7:M:114:DG:C8	2.52	0.45	
1:A:68:GLN:O	1:A:72:ARG:HG3	2.16	0.45	
7:M:93:DC:C2	7:M:94:DG:N7	2.85	0.45	
2:B:52:GLU:HG2	2:B:53:GLU:N	2.32	0.44	
5:K:173:HIS:O	5:K:176:SER:OG	2.23	0.44	
1:A:68:GLN:HA	1:A:71:VAL:HG22	1.99	0.44	
4:H:41:VAL:O	4:H:45:LEU:HG	2.17	0.44	
4:H:97:ALA:HA	4:H:100:LEU:HD12	1.99	0.44	
7:M:151:DA:H2"	7:M:152:DG:C8	2.52	0.44	
5:K:336:TRP:NE1	5:K:337:GLN:NE2	2.65	0.44	
6:L:60:DG:H1'	6:L:61:DA:C8	2.52	0.44	
6:L:98:DC:H4'	6:L:99:DC:OP1	2.17	0.44	
7:M:131:DG:H2"	7:M:132:DA:C8	2.53	0.44	
7:M:162:DC:H2"	7:M:163:DA:C8	2.52	0.44	
2:F:84:MET:HG3	2:F:88:TYR:CZ	2.53	0.44	
2:B:63:GLU:HA	2:B:66:ILE:HG12	2.00	0.44	
5:K:271:LEU:HD12	5:K:301:THR:CB	2.48	0.44	
7:M:66:DA:H2'	7:M:67:DG:C8	2.52	0.44	
3:C:88:ARG:O	3:C:94:ASN:ND2	2.37	0.44	
1:E:126:LEU:O	1:E:130:ILE:HG23	2.18	0.44	
5:K:96:VAL:HG23	5:K:102:LEU:HD13	1.99	0.44	
5:K:209:ASP:OD1	5:K:209:ASP:N	2.51	0.44	
6:L:74:DC:H2"	6:L:75:DG:C8	2.53	0.44	
6:L:148:DG:H2"	6:L:149:DT:C6	2.53	0.44	
7:M:128:DC:H2"	7:M:129:DT:C6	2.53	0.44	
3:C:97:LEU:HD21	4:D:65:PHE:CE1	2.50	0.44	
5:K:24:GLN:O	5:K:27:GLU:HG3	2.18	0.44	
5:K:107:GLY:HA3	5:K:269:SER:HA	2.00	0.44	
5:K:170:ASP:OD1	5:K:171:GLY:N	2.51	0.44	
5:K:281:TRP:HB2	5:K:283:MET:HG2	1.98	0.44	
6:L:66:DT:H2"	6:L:67:DC:C5	2.52	0.44	
6:L:110:DA:H1'	6:L:111:DA:N7	2.33	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:87:ILE:CD1	3:C:93:LEU:HB3	2.45	0.44	
3:G:112:GLN:HB2	3:G:115:LEU:HG	1.99	0.44	
5:K:101:TYR:OH	5:K:260:ARG:NH2	2.51	0.44	
2:B:27:GLN:HG3	2:B:55:ARG:NH1	2.33	0.43	
2:B:79:LYS:NZ	7:M:131:DG:OP2	2.50	0.43	
3:G:84:GLN:HA	3:G:87:ILE:HG12	2.00	0.43	
4:H:110:ALA:O	4:H:113:GLU:HG2	2.18	0.43	
5:K:93:ALA:HA	5:K:96:VAL:HG12	1.99	0.43	
5:K:190:MET:HE2	5:K:210:VAL:H	1.81	0.43	
5:K:305:ASP:OD1	5:K:306:TRP:N	2.50	0.43	
6:L:98:DC:H2"	6:L:99:DC:C6	2.53	0.43	
2:F:63:GLU:O	2:F:67:ARG:HG3	2.18	0.43	
3:G:41:GLU:OE2	3:G:42:ARG:HG2	2.18	0.43	
5:K:96:VAL:HG22	5:K:160:LEU:HB3	2.00	0.43	
3:C:59:THR:HA	3:C:62:ILE:HG12	2.00	0.43	
4:D:94:ILE:O	4:D:98:VAL:HG23	2.18	0.43	
2:F:70:VAL:O	2:F:73:THR:HB	2.18	0.43	
6:L:119:DG:H2"	6:L:120:DG:C8	2.53	0.43	
7:M:49:DA:H2"	7:M:50:DC:C5	2.53	0.43	
7:M:143:DA:H2"	7:M:144:DC:H5'	2.00	0.43	
3:C:92:GLU:HB3	4:D:103:PRO:HG2	1.99	0.43	
7:M:59:DG:H2"	7:M:60:DG:H8	1.83	0.43	
7:M:102:DC:H2"	7:M:103:DA:H8	1.83	0.43	
1:A:114:ALA:O	1:A:115:LYS:HG3	2.18	0.43	
5:K:210:VAL:HG12	5:K:214:THR:HG23	2.00	0.43	
5:K:285:LYS:HZ3	5:K:289:ARG:HG2	1.81	0.43	
5:K:187:HIS:O	5:K:236:ILE:HD12	2.19	0.43	
6:L:164:DT:H2"	6:L:165:DT:C7	2.48	0.43	
2:F:50:ILE:HA	2:F:53:GLU:OE2	2.19	0.43	
1:A:90:MET:O	1:A:93:GLN:HB2	2.18	0.43	
3:C:43:VAL:HA	4:D:89:ILE:HD11	2.00	0.43	
4:D:63:ASN:HA	4:D:66:VAL:HG12	2.01	0.43	
6:L:104:DC:H2"	6:L:105:DG:C8	2.54	0.43	
7:M:87:DT:H2"	7:M:88:DT:C6	2.54	0.43	
7:M:153:DC:H2"	7:M:154:DG:C8	2.54	0.43	
4:D:76:GLU:O	4:D:79:ARG:HG2	2.19	0.43	
3:G:62:ILE:HG22	3:G:93:LEU:HD11	2.01	0.43	
5:K:11:ARG:O	5:K:15:GLU:HG2	2.18	0.43	
5:K:105:TYR:OH	5:K:281:TRP:HA	2.19	0.43	
1:A:104:PHE:CD2	2:B:38:ALA:HA	2.54	0.42	
4:H:86:ARG:NH2	7:M:71:DG:OP2	2.51	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap(Å)	
5·K·341·PHE·CE2	5·K·360·LEU·HB3	2.54	0.42	
3:C:30:VAL:HA	3:C:33:LEU:HG	2.01	0.42	
5:K:26:ABG:HE	5:K:30:ARG:HH22	1.67	0.42	
5:K:96:VAL:HG13	5:K:160:LEU:HD23	2.00	0.42	
5:K:103:VAL:HA	5:K:163:HIS:O	2.19	0.42	
2:B:30:THR:HG23	2:B:33:ALA:H	1.84	0.42	
2:B:50:ILE:O	2:B:54:THR:HG23	2.19	0.42	
2:F:60:VAL:HA	2:F:63:GLU:HG3	2.01	0.42	
5:K:285:LYS:NZ	5:K:289:ARG:HG2	2.33	0.42	
7:M:28:DA:H2"	7:M:29:DA:C8	2.54	0.42	
4:D:110:ALA:O	4:D:113:GLU:HG2	2.20	0.42	
1:E:101:VAL:O	1:E:105:GLU:OE1	2.37	0.42	
1:E:124:ILE:HD12	1:E:124:ILE:H	1.84	0.42	
3:C:84:GLN:HA	3:C:87:ILE:HG22	2.02	0.42	
4:D:34:LYS:HA	4:D:34:LYS:HD2	1.76	0.42	
3:G:87:ILE:HB	3:G:97:LEU:HD11	2.00	0.42	
4:H:67:ASN:O	4:H:71:GLU:OE1	2.37	0.42	
5:K:213:ARG:HG3	5:K:223:ARG:HH12	1.85	0.42	
7:M:46:DC:H2"	7:M:47:DT:C5	2.54	0.42	
7:M:148:DT:H2"	7:M:149:DT:C6	2.55	0.42	
3:G:94:ASN:O	3:G:98:GLY:N	2.52	0.42	
4:H:102:LEU:HD23	4:H:107:ALA:HA	2.01	0.42	
5:K:63:GLY:HA2	5:K:66:ARG:HG2	2.02	0.42	
6:L:70:DG:N2	7:M:129:DT:O2	2.53	0.42	
6:L:134:DG:H2'	6:L:135:DT:H71	2.01	0.42	
7:M:46:DC:H2"	7:M:47:DT:C6	2.55	0.42	
7:M:57:DC:H2"	7:M:58:DT:C5	2.55	0.42	
4:D:38:SER:HA	4:D:59:MET:HE1	2.02	0.42	
2:F:92:ARG:HH12	4:H:100:LEU:HB3	1.84	0.42	
2:F:31:LYS:N	2:F:32:PRO:HD2	2.35	0.42	
2:F:47:SER:OG	2:F:48:GLY:N	2.52	0.42	
5:K:348:ARG:HB2	5:K:351:GLU:HG2	2.01	0.42	
6:L:78:DT:H2"	6:L:79:DA:C8	2.54	0.42	
6:L:104:DC:H2"	6:L:105:DG:H8	1.85	0.42	
7:M:69:DG:H2"	7:M:70:DA:C8	2.55	0.42	
1:A:62:ILE:HD11	2:B:37:LEU:HD11	2.02	0.42	
1:E:116:ARG:NH1	1:E:118:THR:O	2.53	0.42	
2:F:25:ASN:N	2:F:27:GLN:OE1	2.53	0.42	
4:H:69:ILE:O	4:H:73:ILE:HG12	2.19	0.42	
4:H:80:LEU:CD1	4:H:93:GLU:HB2	2.44	0.42	
6:L:147:DT:H2"	6:L:148:DG:C8	2.54	0.42	



	ious page	International	Clash
Atom-1	Atom-2	distance $(Å)$	α overlap (Å)
1·A·63·ABG·HD2	$7 \cdot M \cdot 121 \cdot DA \cdot O3'$	2.20	$\frac{0.42}{0.42}$
4.D.38.SEB.HA	4·D:59·MET·CE	$\frac{2.20}{2.50}$	0.42
4·H·72·ABG·O	4·H·76·GLU·OE1	2.38	0.42
5·K·98·ASN·OD1	$5 \cdot K \cdot 99 \cdot ALA \cdot N$	2.58	0.42
6:L:63:DA:C8	6:L:63:DA:H5'	2.55	0.42
7:M:52:DC:H2"	7:M:53:DG:C8	2.55	0.42
7:M:82:DG:H2"	7:M:83:DG:H8	1.84	0.42
1·A·101·VAL:O	1·A·105·GLU·OE1	2.38	0.41
5:K:105:TYB:CD2	5:K:165:VAL:HB	2.55	0.41
5:K:274:LEU:HD13	5:K:281:TRP:CZ2	2.55	0.41
7:M:69:DG:H2"	7:M:70:DA:H8	1.85	0.41
7:M:123:DC:C2	7:M:124:DG:N7	2.88	0.41
2:B:87:VAL:HG12	2:B:91:LYS:HZ2	1.85	0.41
5:K:81:ASP:HB3	5:K:84:GLU:HG2	2.02	0.41
7:M:107:DC:H2"	7:M:108:DG:N7	2.35	0.41
5:K:208:PHE:HE1	5:K:347:LEU:HD13	1.84	0.41
5:K:247:GLN:N	5:K:248:PRO:HD2	2.35	0.41
4:D:65:PHE:O	4:D:69:ILE:HD12	2.20	0.41
1:E:65:LEU:HG	6:L:112:DC:OP2	2.20	0.41
5:K:150:MET:HB3	5:K:331:PRO:HD2	2.02	0.41
5:K:154:ARG:CZ	5:K:331:PRO:HG3	2.51	0.41
7:M:76:DC:H6	7:M:76:DC:H2'	1.70	0.41
1:A:86:SER:O	1:A:89:VAL:HG12	2.20	0.41
1:A:130:ILE:O	1:E:131:ARG:NE	2.48	0.41
2:B:29:ILE:HG13	2:B:55:ARG:HE	1.85	0.41
2:F:92:ARG:NH1	4:H:100:LEU:HB3	2.35	0.41
7:M:82:DG:C2	7:M:83:DG:C5	3.08	0.41
7:M:122:DG:C4	7:M:123:DC:C5	3.09	0.41
3:C:78:ILE:HG21	4:D:54:ILE:HG23	2.02	0.41
4:D:34:LYS:NZ	4:D:35:GLU:O	2.51	0.41
4:D:103:PRO:O	4:D:107:ALA:N	2.37	0.41
1:E:119:ILE:HG22	2:F:45:ARG:O	2.21	0.41
4:H:68:ASP:HA	4:H:71:GLU:OE2	2.20	0.41
5:K:15:GLU:HA	5:K:18:ARG:CD	2.50	0.41
5:K:16:ARG:O	5:K:20:LEU:HG	2.20	0.41
5:K:199:VAL:HB	5:K:200:PRO:HD3	2.02	0.41
6:L:158:DT:H2"	6:L:159:DA:H8	1.84	0.41
7:M:93:DC:H2"	7:M:94:DG:H8	1.85	0.41
7:M:102:DC:H2"	7:M:103:DA:C8	2.55	0.41
7:M:111:DC:H2"	7:M:112:DG:C8	2.56	0.41
1:A:60:LEU:HD21	1:A:93:GLN:OE1	2.20	0.41



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap(Å)	
1:A:109:LEU:HA	1:A:112:ILE:HG12	2.03	0.41	
4:D:46:LYS:HE3	4:D:50:PRO:HA	2.03	0.41	
1:A:65:LEU:HB2	1:A:66:PRO:HD3	2.02	0.41	
1:A:102:GLY:HA2	1:A:105:GLU:OE2	2.21	0.41	
2:B:67:ARG:O	2:B:71:THR:HG23	2.20	0.41	
3:C:29:ARG:NH1	3:C:32:ARG:HD2	2.35	0.41	
2:F:57:VAL:O	2:F:61:PHE:HD2	2.04	0.41	
5:K:186:LEU:HB2	5:K:277:TYR:HD2	1.85	0.41	
5:K:273:VAL:HG22	5:K:276:LYS:HZ1	1.85	0.41	
7:M:52:DC:H2"	7:M:53:DG:H8	1.84	0.41	
1:A:99:TYR:CE2	2:B:61:PHE:CD1	3.09	0.41	
1:A:110:ALA:HA	1:E:126:LEU:HD21	2.03	0.41	
1:E:46:VAL:HB	6:L:103:DG:OP1	2.20	0.41	
1:E:70:LEU:O	1:E:74:ILE:HG12	2.21	0.41	
2:F:32:PRO:HG3	7:M:91:DA:H3'	2.02	0.41	
5:K:118:ASP:OD1	5:K:119:TYR:N	2.54	0.41	
5:K:154:ARG:NH2	5:K:329:GLU:OE1	2.54	0.41	
7:M:95:DC:H2"	7:M:96:DG:C8	2.56	0.41	
7:M:129:DT:H2"	7:M:130:DA:N7	2.36	0.41	
1:A:126:LEU:HD21	1:A:130:ILE:HD13	2.02	0.41	
2:B:89:ALA:O	2:B:92:ARG:HB3	2.21	0.41	
4:D:111:VAL:O	4:D:115:THR:HG23	2.20	0.41	
5:K:36:LEU:HA	5:K:51:LEU:HD12	2.03	0.41	
5:K:154:ARG:HA	5:K:154:ARG:HD3	1.95	0.41	
6:L:132:DT:H2"	6:L:133:DA:C8	2.56	0.41	
7:M:66:DA:H2"	7:M:67:DG:O5'	2.21	0.41	
2:F:27:GLN:HA	2:F:55:ARG:CZ	2.50	0.40	
3:G:64:GLU:HG2	4:H:48:VAL:HG11	2.03	0.40	
6:L:87:DG:H2"	6:L:88:DT:C6	2.56	0.40	
3:C:50:TYR:CD1	4:D:114:GLY:HA3	2.56	0.40	
4:H:73:ILE:HG13	4:H:74:ALA:N	2.35	0.40	
5:K:165:VAL:HA	5:K:184:SER:O	2.21	0.40	
5:K:169:CYS:HB2	5:K:236:ILE:HD13	2.03	0.40	
5:K:341:PHE:HB2	5:K:362:ARG:NH2	2.36	0.40	
6:L:141:DG:H2"	6:L:142:DG:C8	2.56	0.40	
7:M:148:DT:H2"	7:M:149:DT:C5	2.56	0.40	
3:C:27:VAL:O	3:C:31:HIS:N	2.52	0.40	
5:K:86:ARG:HG3	5:K:90:ARG:NH1	2.36	0.40	
5:K:152:ILE:HA	5:K:155:LEU:HD12	2.02	0.40	
6:L:34:DG:C8	6:L:35:DT:H72	2.57	0.40	
6:L:40:DA:C8	6:L:40:DA:H5'	2.57	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:M:61:DA:H2"	7:M:62:DG:H8	1.86	0.40
2:B:35:ARG:HH12	2:B:46:ILE:HB	1.86	0.40
3:G:17:ARG:NH2	7:M:61:DA:OP2	2.55	0.40
3:G:47:ALA:O	3:G:51:MET:HG2	2.21	0.40
3:G:110:ASN:HD22	3:G:110:ASN:C	2.14	0.40
6:L:38:DC:H2"	6:L:39:DG:N7	2.36	0.40
1:E:102:GLY:HA2	1:E:105:GLU:OE2	2.22	0.40
5:K:153:THR:O	5:K:157:GLU:OE1	2.40	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	93/136~(68%)	90~(97%)	3~(3%)	0	100	100
1	Ε	95/136~(70%)	93~(98%)	2(2%)	0	100	100
2	В	81/103~(79%)	80~(99%)	1 (1%)	0	100	100
2	F	76/103~(74%)	75~(99%)	1 (1%)	0	100	100
3	С	102/129~(79%)	100 (98%)	2(2%)	0	100	100
3	G	103/129~(80%)	100~(97%)	3~(3%)	0	100	100
4	D	90/126~(71%)	88~(98%)	2(2%)	0	100	100
4	Η	91/126~(72%)	87~(96%)	4 (4%)	0	100	100
5	Κ	330/401~(82%)	327~(99%)	3(1%)	0	100	100
All	All	1061/1389~(76%)	1040 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.



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 PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	А	83/111 (75%)	82~(99%)	1 (1%)	67	82
1	Ε	84/111~(76%)	84 (100%)	0	100	100
2	В	68/79~(86%)	68~(100%)	0	100	100
2	\mathbf{F}	63/79~(80%)	63~(100%)	0	100	100
3	С	82/98~(84%)	82 (100%)	0	100	100
3	G	82/98~(84%)	81~(99%)	1 (1%)	67	82
4	D	77/105~(73%)	76~(99%)	1 (1%)	65	81
4	Н	78/105~(74%)	77~(99%)	1 (1%)	65	81
5	Κ	286/335~(85%)	281 (98%)	5 (2%)	56	75
All	All	903/1121~(81%)	894 (99%)	9 (1%)	71	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	115	LYS
4	D	108	LYS
3	G	110	ASN
4	Н	63	ASN
5	Κ	18	ARG
5	Κ	19	ARG
5	Κ	31	GLN
5	Κ	97	ARG
5	Κ	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	С	82	HIS
1	Ε	93	GLN
1	Е	108	ASN
3	G	68	ASN



Continued from previous page...

Mol	Chain	Res	Type
5	Κ	173	HIS
5	Κ	189	ASN

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 oligosaccharides 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.

