

May 1, 2025 – 11:43 am BST

PD	)B ID	:	$9\mathrm{G1Z} \ / \ \mathrm{pdb} \ 00009\mathrm{g1z}$
EMD	)B ID	:	EMD-50957
	Title	:	Structure of Candida albicans 80S ribosome in complex with mefloquine (non-
			rotated state)
Au	ithors	:	Kolosova, O.; Zgadzay, Y.; Stetsenko, A.; Atamas, A.; Jenner, L.B.; Guskov,
			A.; Yusupov, M.
Deposit	ed on	:	2024-07-10
Resol	lution	:	3.10 Å(reported)
r	This is	a F	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	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

# 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 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	210492	15764		
Ramachandran outliers	207382	16835		
Sidechain outliers	206894	16415		
RNA backbone	6643	2191		

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  $\geq=3, 2, 1$  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  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chai	in
1	0	172	77%	22% •
2	2	160	85%	14% •
3	3	121	• 70%	28% •
4	4	158	<b>•</b> 59%	37% ••
5	5	124	56% 44%	40% 17%
6	6	137	82%	13% •
7	7	155	32% 8%	60%

Continued on next page...



 $Continued \ from \ previous \ page...$ 

Chain Length Quality of chain Mol i 8 8 14215% 68% 17% i 9 912780% 19% 24% 10 А 1787 41% 39% 9% 11% 51% В 11 26156% 24% 20% 37% С 1225659% 25% 16% 27% 13D 24967% 20% 13% 77% Е 1425161% 28% 11% 54% . F 2621565% 34% 88% G 2251654% 37% 8% 61% Η 1723667% 28% • 41% Ι 18 18638% 14% 48% 24% J 1920650% 24% 26% 54% 20Κ 18965% 6% 30% 75% L 2111841% 37% 21% • 44% 22М 15580% 11% 9% 81% 23Ν 143 32% 49% 19% 42% Ο 2415172% 28% 34% Р 2513267% 30% 80% Q 2614229% 54% 17% 75% . 27R 14264% 35% 34%  $\mathbf{S}$ 2813729% 14% 57% 86% Т 29•• 14563% 34% 87% 30 U 14572% • 26% 74% V 11931 54% 30% 16% 57% 32W 87 55% 45%

Continued on next page...



Continue contraction contrac	nued from	n previous	page		
Mol	Chain	Length	Quality of chain		
33	Х	130	67%	32	% •
34	Y	145	29%		22% •
35	Ζ	135	61% 75%		23% •
36	a	105	67% 47% 22%	3	1%
37	b	119	73%	11%	16%
38	с	82	83%		16% •
39	d	67	58%	34%	7%
40	е	56	54% 71%	2	7% •
41	f	63	62%	27%	11%
42	g	193	27% 9% 64%		
43	h	317	58%	40%	·
44	j	254	87%		11% •
45	k	389	84%		15% •
46	l	363	88%		12% •
47	m	298	80%		18% •
48	0	241	83%		11% 7%
49	q	191	<b>•</b> 79%		20% •
50	S	174	76%		21% •
51	t	202	83%		15% ••
52	u	131	83%		16% •
53	v	204	77%		23%
54	W	200	87%		12%
55	У	186	86%		13% •
56	Z	190	72%	14%	14%
57	1	3359	58%	30%	5% 6%

Continued on next page...



Mol	Chain	Length	Quality of chain		
58	10	76	• 97%		
59	n	176	<b>▲</b> 76%	13%	12%
60	р	262	80%	12%	8%
61	r	220	73%	21%	5%
62	х	185		15%	7%
63	AA	136	<b></b> 79%	21	% •
64	AB	149	<b>●</b> 85%		14% •
65	AC	63	86%		14%
66	AD	106	68%	23%	9%
67	AE	112	8%		8% •
68	AF	131	83%	11%	6 • 5%
69	AG	107	92%		7% •
70	AH	121	7%	16%	7%
71	AI	120	<b>-</b> 86%		13% •
72	AJ	99	88%		11% •
73	AK	90	79%	17%	·
74	AL	78	86%		13% •
75	AM	51	<b>6</b> 5%	33%	·
76	AN	52	88%		12%
77	AO	25	76%	24%	,
78	AP	106	87%		10% •
79	AQ	92		1	7% •

Continued from previous page...



# 2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 194174 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.

• Molecule 1 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues		At	oms		AltConf	Trace	
1	0	171	Total 1442	C 933	N 262	0 244	${ m S} { m 3}$	2	0

• Molecule 2 is a protein called Ribosomal 60S subunit protein L21A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
2	2	159	Total 1276	C 807	N 244	0 223	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	2	0

• Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
3	3	121	Total 2579	C 1153	N 463	0 842	Р 121	0	0

• Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues		Α	AltConf	Trace			
4	4	156	Total 3313	C 1482	N 581	O 1094	Р 156	0	0

• Molecule 5 is a protein called Ribosomal 60S subunit protein L22B.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
5	5	103	Total 848	C 553	N 139	O 156	2	0

• Molecule 6 is a protein called Ribosomal 60S subunit protein L23B.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
6	6	131	Total 986	C 621	N 186	0 171	S 8	1	0



• Molecule 7 is a protein called Ribosomal 60S subunit protein L24A.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
7	7	62	Total 516	C 328	N 102	0 85	S 1	0	0
			010	328	102	80	T		

• Molecule 8 is a protein called Ribosomal 60S subunit protein L25.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	8	121	Total 974	C 622	N 175	0 176	S 1	0	0

• Molecule 9 is a protein called Ribosomal 60S subunit protein L26B.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
9	9	126	Total 989	C 618	N 190	0 181	0	0

• Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues		I	Atoms			AltConf	Trace
10	А	1635	Total 34879	C 15594	N 6210	O 11440	Р 1635	0	0

• Molecule 11 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
11	В	208	Total 1627	C 1041	N 284	O 297	${ m S}{ m 5}$	0	0

• Molecule 12 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
12	С	214	Total 1724	C 1094	N 313	0 313	${S \atop 4}$	0	0

• Molecule 13 is a protein called Ribosomal 40S subunit protein S2.

Mol	Chain	Residues		At	AltConf	Trace			
13	D	216	Total 1620	C 1033	N 287	O 295	${ m S}{ m 5}$	0	0

• Molecule 14 is a protein called Ribosomal 40S subunit protein S3.



Mol	Chain	Residues		At	AltConf	Trace			
14	Е	223	Total 1707	C 1087	N 311	O 305	$\frac{S}{4}$	0	0

• Molecule 15 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues		Ate	AltConf	Trace			
15	F	260	Total 2055	C 1306	N 386	O 358	${ m S}{ m 5}$	0	0

• Molecule 16 is a protein called Ribosomal 40S subunit protein S5.

Mol	Chain	Residues		Ate	AltConf	Trace			
16	G	206	Total 1614	C 1008	N 301	O 301	$\frac{S}{4}$	0	0

• Molecule 17 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	Н	226	Total 1820	C 1133	N 351	O 330	S 6	0	0

• Molecule 18 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
18	Ι	96	Total 780	C 500	N 144	O 136	0	0

• Molecule 19 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	J	152	Total 1216	C 752	N 248	0 215	S 1	0	0

• Molecule 20 is a protein called Ribosomal 40S subunit protein S9B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	K	178	Total 1453	C 918	N 286	0 248	S 1	0	0

• Molecule 21 is a protein called Ribosomal 40S subunit protein S10A.



Mol	Chain	Residues		At	oms	AltConf	Trace		
21	L	93	Total 783	C 511	N 129	0 142	S 1	0	0

• Molecule 22 is a protein called Ribosomal 40S subunit protein S11A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	М	141	Total 1129	С 722	N 212	0 192	${ m S} { m 3}$	0	0

• Molecule 23 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	N	116	Total 885	C 550	N 158	0 172	${f S}{5}$	0	0

• Molecule 24 is a protein called Ribosomal 40S subunit protein S13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	О	150	Total 1187	C 757	N 219	O 210	S 1	0	0

• Molecule 25 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	Р	127	Total 942	C 579	N 186	0 174	${ m S} { m 3}$	0	0

• Molecule 26 is a protein called Ribosomal 40S subunit protein S15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	Q	118	Total 935	C 598	N 169	0 162	S 6	0	0

• Molecule 27 is a protein called Ribosomal 40S subunit protein S16A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	R	140	Total 1091	C 700	N 198	0 192	S 1	0	0

• Molecule 28 is a protein called Ribosomal 40S subunit protein S17B.



Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
28	S	59	Total 489	C 310	N 96	O 82	S 1	0	0

• Molecule 29 is a protein called Ribosomal 40S subunit protein S18B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	Т	142	Total 1169	C 733	N 228	O 205	${ m S} { m 3}$	0	0

• Molecule 30 is a protein called Ribosomal 40S subunit protein S19A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	U	141	Total 1100	C 689	N 210	O 200	S 1	0	0

• Molecule 31 is a protein called Ribosomal 40S subunit protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	V	100	Total 790	C 499	N 146	0 143	S 2	0	0

• Molecule 32 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues		At	AltConf	Trace			
32	W	87	Total 676	C 415	N 126	0 133	S 2	0	0

• Molecule 33 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	Х	129	Total 1032	$\begin{array}{c} \mathrm{C} \\ 655 \end{array}$	N 191	0 183	${ m S} { m 3}$	0	0

• Molecule 34 is a protein called Ribosomal 40S subunit protein S23B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	Y	143	Total 1110	C 701	N 219	0 188	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 35 is a protein called 40S ribosomal protein S24.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
35	Z	132	Total 1072	C 670	N 216	O 186	0	0

• Molecule 36 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
36	a	72	Total 578	C 369	N 103	O 106	0	0

• Molecule 37 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	b	100	Total 799	C 494	N 169	0 130	S 6	0	0

• Molecule 38 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues		At	oms	AltConf	Trace		
38	С	81	Total 614	C 383	N 110	0 114	${f S}7$	0	0

• Molecule 39 is a protein called Ribosomal 40S subunit protein S28B.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
39	d	62	Total	C 200	N 08	0	S 2	0	0
			407	299	98	00	$\boldsymbol{Z}$		

• Molecule 40 is a protein called Ribosomal 40S subunit protein S29A.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
40	0	55	Total	С	Ν	Ο	$\mathbf{S}$	0	0
40	е	- 55	454	281	94	75	4	0	0

• Molecule 41 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
41	f	56	Total 444	C 278	N 89	O 75	${S \over 2}$	0	0

• Molecule 42 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.



Mol	Chain	Residues		Ate	oms	AltConf	Trace		
42	g	70	Total 574	C 362	N 113	O 93	S 6	0	0

• Molecule 43 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues		Ate	AltConf	Trace			
43	h	311	Total 2398	C 1519	N 412	0 462	${ m S}{ m 5}$	0	0

• Molecule 44 is a protein called Ribosomal 60S subunit protein L2A.

Mol	Chain	Residues		At		AltConf	Trace		
44	j	249	Total 1894	C 1185	N 377	O 330	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	1	0

• Molecule 45 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	k	386	Total 3084	$\begin{array}{c} \mathrm{C} \\ 1955 \end{array}$	N 584	O 538	S 7	1	0

• Molecule 46 is a protein called Ribosomal 60S subunit protein L4B.

Mol	Chain	Residues		At	oms			AltConf	Trace
46	1	361	Total 2751	C 1729	N 529	0 490	$\frac{S}{3}$	0	0

• Molecule 47 is a protein called Ribosomal 60S subunit protein L5.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	m	292	Total 2394	C 1526	N 416	O 450	${S \over 2}$	0	0

• Molecule 48 is a protein called Ribosomal 60S subunit protein L7A.

Mol	Chain	Residues		Ate			AltConf	Trace	
48	О	225	Total 1819	C 1167	N 335	0 316	S 1	1	0

• Molecule 49 is a protein called Ribosomal 60S subunit protein L9B.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	q	188	Total 1501	C 948	N 274	O 275	$\frac{S}{4}$	0	0

• Molecule 50 is a protein called Ribosomal 60S subunit protein L11B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	s	170	Total 1371	C 857	N 260	O 250	$\frac{S}{4}$	1	0

• Molecule 51 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues		Ator	AltConf	Trace		
51	t	200	Total 1610	C 1009	N 318	O 283	0	0

• Molecule 52 is a protein called Ribosomal 60S subunit protein L14B.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	u	130	Total 1029	C 660	N 193	0 175	S 1	0	0

• Molecule 53 is a protein called Ribosomal protein L15.

Mol	Chain	Residues		Ate		AltConf	Trace		
53	v	203	Total 1713	C 1075	N 356	O 280	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 54 is a protein called Ribosomal 60S subunit protein L16A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
54	W	199	Total 1590	C 1025	N 294	O 269	${S \over 2}$	0	0

• Molecule 55 is a protein called Ribosomal 60S subunit protein L18A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
55	У	185	Total 1478	C 930	N 302	O 246	3	0

• Molecule 56 is a protein called Ribosomal protein L19.



Mol	Chain	Residues		At	oms	AltConf	Trace		
56	Z	164	Total 1331	C 829	N 277	O 222	${ m S} { m 3}$	1	0

• Molecule 57 is a RNA chain called 25S rRNA.

Mol	Chain	Residues				AltConf	Trace		
57	1	3147	Total 67271	C 30053	N 12088	O 21983	Р 3147	0	0

• Molecule 58 is a RNA chain called Endogenous tRNA.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
58	10	2	Total 42	C 19	N 8	0 13	Р 2	0	0

• Molecule 59 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
59	n	155	Total 1237	C 794	N 226	O 217	1	0

• Molecule 60 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues		At		AltConf	Trace		
60	р	242	Total 1875	C 1204	N 333	0 334	$\frac{S}{4}$	0	0

• Molecule 61 is a protein called Ribosomal 60S subunit protein L10.

Mol	Chain	Residues		At	AltConf	Trace			
61	r	208	Total 1689	C 1069	N 322	0 291	${f S}{7}$	0	0

• Molecule 62 is a protein called Ribosomal 60S subunit protein L17B.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
62	x	172	Total 1375	C 850	N 279	O 246	0	0

• Molecule 63 is a protein called 60S ribosomal protein L27.



Mol	Chain	Residues		At	oms	AltConf	Trace		
63	AA	135	Total 1087	C 705	N 197	O 183	${ m S} { m 2}$	0	0

• Molecule 64 is a protein called Ribosomal 60S subunit protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
64	AB	148	Total 1170	C 741	N 231	O 197	S 1	0	0

• Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		Ate	$\mathbf{oms}$	AltConf	Trace		
65	AC	63	Total 509	C 317	N 109	O 82	S 1	1	0

• Molecule 66 is a protein called Ribosomal 60S subunit protein L30.

Mol	Chain	Residues		At	oms		AltConf	Trace	
66	AD	96	Total 729	C 469	N 121	0 137	${ m S} { m 2}$	0	0

• Molecule 67 is a protein called Ribosomal 60S subunit protein L31B.

Mol	Chain	Residues		At	oms			AltConf	Trace
67	AE	109	Total 889	C 562	N 167	0 158	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 68 is a protein called Ribosomal 60S subunit protein L32.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
68	AF	125	Total 1015	C 649	N 197	0 168	S 1	1	0

• Molecule 69 is a protein called Ribosomal 60S subunit protein L33A.

Mol	Chain	Residues		At	AltConf	Trace			
69	AG	106	Total 867	C 558	N 166	0 142	S 1	3	0

• Molecule 70 is a protein called Large ribosomal subunit protein eL34.



Mol	Chain	Residues		At	AltConf	Trace			
70	AH	112	Total 913	C 567	N 188	0 154	$\frac{S}{4}$	4	0

• Molecule 71 is a protein called Ribosomal 60S subunit protein L35A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
71	AI	119	Total 990	C 629	N 195	O 166	1	0

• Molecule 72 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues		At	oms	AltConf	Trace		
72	AJ	98	Total 772	C 481	N 158	0 131	${S \over 2}$	1	0

• Molecule 73 is a protein called Ribosomal protein L37.

Mol	Chain	Residues		At	oms			AltConf	Trace
73	AK	86	Total	C	N	0	S	0	0
			677	413	148	110	6		

• Molecule 74 is a protein called Ribosomal 60S subunit protein L38.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
74	AL	77	Total 623	C 398	N 116	O 109	1	0

• Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
75	AM	50	Total 446	C 280	N 100	O 66	1	0

• Molecule 76 is a protein called Rpl40bp.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
76	AN	52	Total 427	C 265	N 89	O 67	S 6	1	0

• Molecule 77 is a protein called 60S ribosomal protein L41.



Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
77	AO	25	Total 236	C 144	N 63	O 28	S 1	0	0

• Molecule 78 is a protein called Ribosomal 60S subunit protein L42A.

Mol	Chain	Residues		At	AltConf	Trace			
78	AP	103	Total 843	C 533	N 168	0 137	${ m S}{ m 5}$	2	0

• Molecule 79 is a protein called Ribosomal 60S subunit protein L43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AQ	91	Total 698	C 430	N 140	0 124	$\frac{S}{4}$	0	0

• Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
80	b	1	Total Zn 1 1	0
80	g	1	Total Zn 1 1	0
80	AH	1	Total Zn 1 1	0
80	AK	1	Total Zn 1 1	0
80	AN	1	Total Zn 1 1	0
80	AP	1	Total Zn 1 1	0
80	AQ	1	Total Zn 1 1	0

• Molecule 81 is (11R,12S)- Mefloquine (CCD ID: YMZ) (formula:  $C_{17}H_{16}F_6N_2O$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
81	j	1	Total	С	F	Ν	0	0
			26	17	6	2	1	
81	1	1	Total	С	F	Ν	0	0
		1	26	17	6	2	1	0

- Molecule 82 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula:  $\rm C_{10}H_{30}N_4).$ 



Mol	Chain	Residues	Atoms	AltConf
82	1	1	Total         C         N           14         10         4	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 60S ribosomal protein L20



• Molecule 2: Ribosomal 60S subunit protein L21A

















 $\bullet$  Molecule 14: Ribosomal 40S subunit protein S3

















• Molecule 27: Ribosomal 40S subunit protein S16A











### 











• Molecule 39: Ribosomal 40S subunit protein S28B









• Molecule 46: Ribosomal 60S subunit protein L4B







 $\bullet$  Molecule 47: Ribosomal 60S subunit protein L5



• Molecule 51: 60S ribosomal protein L13





### ALA ARG GLU ARG GLN GLN GLN CLLEU CLYS GLU LYS GLU LYS GLU LYS GLU ALA ALA ALA ALA ALA ALA ALA

 $\bullet$  Molecule 57: 25S rRNA






U2624   U2627   U2627   U2627   A2628   Q2633   Q2633   Q2633   Q2633   Q2633   Q2633   Q2634   Q2633   Q2634   Q2635   Q2634   Q2645   Q2646   Q2665   Q2666   Q2666   Q2666   Q2666   Q2666   Q2666   Q2666   Q2667   Q2668   Q2668   Q2668   Q2668   Q2668   Q2668   Q2668   Q2668   Q2668   Q2668 </th
A2720 C2725 C2725 C2725 C2725 C2735 C2735 C2735 C2735 C2735 C2735 C2735 C2735 C2735 C2735 C2749 C2749 C2749 C2760
C2839 C2844 C2844 C2847 C2855 C2855 C2855 C2855 C2855 C2855 C2855 C2855 C2855 C2855 C2855 C2856 C2856 C2866 C2866 C2866 C2866 C2866 C2867 C2867 C2867 C2867 C2867 C2867 C2869 C2873 C2895 C2873 C2873 C2895 C2895 C2873 C2895 C2895 C2873 C2895 C2855 C2895 C28555 C28555 C28555 C285555 C285555 C285555555555
C2924   U2925   U2925   U2933   U2934   U2933   U2934   U2933   U2934   U2933   U2934   U2933   U2934   U2947   U2943   C2944   U2945   U2944   U2944   U2944   U2945   U2946   U2946 </td
A30.42   C30.45   C30.45   C30.45   C30.45   C30.45   C30.45   C30.45   C30.55   C31.15   C31.14   C31.15   C31.45   C31.45   C31.46   C
A3159 C3160 U3161 U3165 U3165 U3165 C3167 U3166 C3171 U3166 C3171 U3175 C3167 C3167 C3167 C3167 C3167 C3167 C3199 C3219 C3219 C3219 C3226 C3229 C
C3252 C3255 C3315 C3325 C3315 C3315 C3325 C3315 C3325 C325 C
A 3335 (33336 A 3337 A 3335 (33351 13358 135588 13558 13558 13558 13558 13558 13558 13558
• Molecule 58: Endogenous tRNA
Chain 10: • 97%
90 90 90 90 90 90 90 90 90 90 90 90 90 9
N U V P C U C A V U P C U C A V U P C U C C C C C C C C C C C C C C C C
$\bullet$ Molecule 59: 60S ribosomal protein L6
Chain n: 76% 13% 12%
MET MET RER RER RER RES RER RES RES RES RES RES

 $\bullet$  Molecule 60: 60S ribosomal protein L8

L146 K150 L159 L159 R170 P171 H172 F176







• Molecule 72: 60S ribosomal protein L36



Chain AJ:	88%	11% •
M1 125 125 125 826 828 833 833 833 136 136 136 136 136 136 136 136 136 1	157 R81 193 193 R97 H1S	
• Molecule 73: Riboso	mal protein L37	
Chain AK:	79%	17% •
MET 62 118 118 826 826 826 826 826 826 826 826 826 82	M44 M49 M49 M69 H69 H69 M85 M13 M16 M16 M16 M16 M16 M16 M11 M11	
• Molecule 74: Riboso	mal 60S subunit protein L38	
Chain AL:	86%	13% •
MET A.2 I.5 I.5 K26 N32 A.3 A.3 A.3 A.3 A.3 A.3 A.3 C.35 K26 K36 K36 K36	K44 K444 R465 R465 R46 C47 C47 C47 C47 C47 C47 C47 C47	
• Molecule 75: 60S rib	oosomal protein L39	
Chain AM:	65%	33% •
MET MET R8 R8 R12 L13 P24 P24 P24 P23 P23 P23 P24 R30 R30	1-31 1-31 1-32 1-33 1-33 1-33 1-33 1-33	
• Molecule 76: Rpl40b	op	
Chain AN:	88%	12%
M1 K22 C23 V24 P28 K38 K38 K38 K38 K38 K52		
• Molecule 77: 60S rib	oosomal protein L41	
Chain AO:	% 76%	24%
M1 R2 R3 W5 W5 W5 M1 R1 R1 R1 R2 M22 M23 M23	K28	
• Molecule 78: Riboso	mal 60S subunit protein L42A	
6% CI. : A.D.	-	
Chain AP:	87%	10% •
MET V2 K9 K9 T10 T21 Q22 Q25 C39 C39 C39 C39 C39 C39 C39 C39 C39 C39	L72 q99 d101 d102 d102 d102 gL10 PHE	

• Molecule 79: Ribosomal 60S subunit protein L43A





## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	47.3	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.318	Depositor
Minimum map value	-1.278	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.022, 1.022, 1.022	Depositor



## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, OMC, YMZ, OMG, SPK, ZN

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		
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	0	0.32	0/1483	0.44	0/1997	
2	2	0.30	0/1305	0.42	0/1749	
3	3	0.29	0/2884	0.31	0/4492	
4	4	0.31	0/3702	0.35	0/5764	
5	5	0.20	0/871	0.57	0/1175	
6	6	0.28	0/994	0.40	0/1339	
7	7	0.31	0/528	0.50	0/701	
8	8	0.28	0/990	0.41	0/1337	
9	9	0.27	0/999	0.44	0/1334	
10	А	0.18	0/39022	0.40	0/60803	
11	В	0.19	0/1666	0.53	0/2273	
12	С	0.20	0/1750	0.48	0/2354	
13	D	0.19	0/1648	0.44	0/2237	
14	Ε	0.19	0/1731	0.55	0/2324	
15	F	0.16	0/2096	0.44	0/2822	
16	G	0.20	0/1631	0.58	0/2199	
17	Н	0.16	0/1845	0.56	2/2464~(0.1%)	
18	Ι	0.14	0/792	0.33	0/1062	
19	J	0.16	0/1238	0.34	0/1658	
20	Κ	0.19	0/1478	0.50	0/1978	
21	L	0.20	0/801	0.64	0/1081	
22	М	0.15	0/1154	0.35	0/1553	
23	Ν	0.22	0/892	0.64	0/1203	
24	Ο	0.21	0/1210	0.52	0/1631	
25	Р	0.22	0/953	0.58	0/1279	
26	Q	0.22	0/954	0.67	0/1282	
27	R	0.17	0/1109	0.50	0/1486	
28	S	0.15	0/494	0.34	0/658	
29	Т	0.20	0/1186	0.61	1/1590~(0.1%)	
30	U	0.20	0/1120	0.54	0/1508	
31	V	0.19	0/800	0.53	0/1082	
32	W	0.16	0/683	0.42	0/918	



Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	Х	0.20	0/1049	0.49	0/1412	
34	Y	0.18	0/1128	0.49	0/1505	
35	Ζ	0.15	0/1086	0.43	0/1447	
36	a	0.16	0/585	0.45	0/789	
37	b	0.19	0/811	0.47	0/1085	
38	с	0.16	0/624	0.45	0/843	
39	d	0.15	0/489	0.45	0/654	
40	е	0.16	0/466	0.44	0/620	
41	f	0.17	0/451	0.50	0/601	
42	g	0.16	0/585	0.48	0/778	
43	h	0.15	0/2451	0.48	0/3337	
44	j	0.31	0/1931	0.42	0/2592	
45	k	0.31	0/3156	0.41	0/4246	
46	1	0.31	0/2799	0.42	0/3777	
47	m	0.25	0/2447	0.46	0/3294	
48	0	0.32	0/1855	0.41	0/2492	
49	q	0.26	0/1519	0.40	0/2043	
50	s	0.21	0/1390	0.48	0/1861	
51	t	0.31	0/1637	0.51	0/2195	
52	u	0.28	0/1044	0.43	0/1407	
53	V	0.34	0/1753	0.43	0/2347	
54	W	0.32	0/1620	0.47	0/2167	
55	У	0.32	0/1511	0.46	0/2022	
56	Z	0.30	0/1352	0.53	0/1800	
57	1	0.32	0/75238	0.37	0/117289	
58	10	0.19	0/46	0.16	0/69	
59	n	0.24	0/1258	0.41	0/1696	
60	р	0.26	0/1907	0.44	0/2567	
61	r	0.29	0/1724	0.46	0/2314	
62	Х	0.31	0/1398	0.46	0/1879	
63	AA	0.22	0/1112	0.36	0/1488	
64	AB	0.32	0/1199	0.38	0/1607	
65	AC	0.28	0/522	0.46	0/692	
66	AD	0.24	0/738	0.44	0/994	
67	AE	0.27	0/902	0.39	0/1212	
68	AF	0.31	0/1039	0.43	0/1390	
69	AG	0.32	0/895	0.38	0/1201	
70	AH	0.29	0/934	0.43	0/1242	
71	AI	0.26	0/1004	0.44	0/1337	
72	AJ	0.23	0/780	0.37	0/1033	
73	AK	0.32	0/690	0.44	0/916	
74	AL	0.23	0/632	0.40	0/842	
75	AM	0.30	0/458	0.36	0/609	



Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
76	AN	0.27	0/436	0.38	0/577	
77	AO	0.18	0/237	0.57	0/304	
78	AP	0.26	0/840	0.38	0/1108	
79	AQ	0.27	0/705	0.50	0/940	
All	All	0.27	0/208442	0.41	3/305953~(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
25	Р	0	1
61	r	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	Н	144	PHE	CA-C-N	-9.35	108.17	123.04
17	Н	144	PHE	C-N-CA	-9.35	108.17	123.04
29	Т	116	LEU	CA-CB-CG	6.88	140.40	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	Р	118	SER	Peptide
61	r	178	ARG	Mainchain

## 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	0	1442	0	1500	30	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1276	0	1333	17	0
3	3	2579	0	1304	25	0
4	4	3313	0	1674	43	0
5	5	848	0	864	39	0
6	6	986	0	1040	12	0
7	7	516	0	534	10	0
8	8	974	0	1032	17	0
9	9	989	0	1064	19	0
10	А	34879	0	17538	720	0
11	В	1627	0	1644	52	0
12	С	1724	0	1805	47	0
13	D	1620	0	1715	33	0
14	Е	1707	0	1807	58	0
15	F	2055	0	2137	73	0
16	G	1614	0	1688	73	0
17	Н	1820	0	1896	60	0
18	Ι	780	0	838	22	0
19	J	1216	0	1230	39	0
20	K	1453	0	1532	48	0
21	L	783	0	799	37	0
22	М	1129	0	1183	12	0
23	Ν	885	0	915	36	0
24	0	1187	0	1249	37	0
25	Р	942	0	981	34	0
26	Q	935	0	970	34	0
27	R	1091	0	1155	44	0
28	S	489	0	539	16	0
29	Т	1169	0	1216	45	0
30	U	1100	0	1114	35	0
31	V	790	0	855	32	0
32	W	676	0	677	34	0
33	X	1032	0	1066	32	0
34	Y	1110	0	1182	27	0
35	Z	1072	0	1123	25	0
36	a	578	0	613	15	0
37	b	799	0	858	12	0
38	С	614	0	630		0
39	d	487	0	523	17	0
40	e	454	0	434	12	0
41	t	444	0	483	22	0
42	g	574	0	607	14	0
43	h	2398	0	2374	95	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	j	1894	0	1975	22	0
45	k	3084	0	3173	43	0
46	1	2751	0	2879	40	0
47	m	2394	0	2362	39	0
48	0	1819	0	1908	15	0
49	q	1501	0	1576	24	0
50	s	1371	0	1409	30	0
51	t	1610	0	1686	29	0
52	u	1029	0	1116	20	0
53	V	1713	0	1764	34	0
54	W	1590	0	1705	21	0
55	у	1478	0	1590	21	0
56	Z	1331	0	1432	24	0
57	1	67271	0	33817	699	0
58	10	42	0	23	1	0
59	n	1237	0	1316	16	0
60	р	1875	0	2014	25	0
61	r	1689	0	1731	31	0
62	X	1375	0	1403	15	0
63	AA	1087	0	1154	18	0
64	AB	1170	0	1203	19	0
65	AC	509	0	545	7	0
66	AD	729	0	775	14	0
67	AE	889	0	936	7	0
68	AF	1015	0	1095	11	0
69	AG	867	0	932	6	0
70	AH	913	0	998	15	0
71	AI	990	0	1094	13	0
72	AJ	772	0	863	10	0
73	AK	677	0	697	14	0
74	AL	623	0	688	11	0
75	AM	446	0	488	13	0
76	AN	427	0	473	5	0
77	AO	236	0	285	6	0
78	AP	843	0	914	9	0
79	AQ	698	0	734	12	0
80	AH	1	0	0	0	0
80	AK	1	0	0	0	0
80	AN	1	0	0	0	0
80	AP	1	0	0	0	0
80	AQ	1	0	0	0	0
80	b	1	0	0	0	0



	f = f = f = f = f = f = f = f = f = f =					
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	g	1	0	0	0	0
81	1	26	0	0	1	0
81	j	26	0	0	2	0
82	1	14	0	30	0	0
All	All	194174	0	144504	2932	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 9.

All (2932) 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)
10:A:485:G:H1	10:A:499:U:H3	1.04	0.98
10:A:898:G:H21	57:1:2185:A:H62	1.11	0.97
47:m:197:LYS:HG2	47:m:202:GLY:HA3	1.49	0.94
74:AL:46:ARG:NH1	74:AL:47:GLY:O	2.02	0.93
57:1:1014:G:H1	57:1:1030:U:H3	0.95	0.90
57:1:538:G:H1	57:1:547:U:H3	1.17	0.89
10:A:588:C:H5"	41:f:43:ARG:HH22	1.39	0.88
23:N:95:LYS:HE3	23:N:117:GLY:HA3	1.57	0.87
57:1:437:G:H22	57:1:620:A:H61	1.23	0.86
10:A:1670:U:H3	10:A:1705:G:H1	1.23	0.86
13:D:34:THR:HG23	13:D:37:GLY:H	1.40	0.86
10:A:1575:G:H1	10:A:1595:U:H3	1.23	0.85
8:8:68:ALA:HA	8:8:73:MET:HE3	1.56	0.85
43:h:240:LEU:HD12	43:h:249:LEU:HD11	1.59	0.83
10:A:1367:U:H4'	31:V:58:PRO:HG3	1.59	0.83
49:q:54:LYS:NZ	49:q:56:THR:OG1	2.10	0.83
10:A:1597:G:H5"	16:G:107:LYS:HD2	1.61	0.83
11:B:63:ILE:HG12	32:W:36:ILE:HG12	1.59	0.83
14:E:63:GLN:HB3	21:L:93:LYS:HE2	1.61	0.83
10:A:477:C:H4'	20:K:120:ARG:HG3	1.61	0.82
57:1:3199:G:H1	57:1:3218:U:H3	1.27	0.82
46:1:290:LEU:HD22	55:y:129:LEU:HD11	1.60	0.82
57:1:935:U:OP2	64:AB:26:ARG:NH2	2.12	0.82
10:A:921:G:OP1	10:A:1059:G:N2	2.14	0.81
3:3:28:C:OP1	50:s:137:ARG:NH1	2.14	0.81
23:N:34:THR:O	23:N:37:VAL:HG12	1.81	0.81
42:g:142:LEU:HD13	42:g:145:LEU:HD12	1.63	0.81
15:F:57:ASN:HD21	15:F:59:ARG:HE	1.29	0.80
12:C:149:GLN:NE2	12:C:151:LYS:O	2.14	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
26:Q:81:ARG:NH2	26:Q:120:SER:O	2.14	0.80
46:l:68:THR:HG21	57:1:2380:A:H2'	1.63	0.80
4:4:155:G:H22	57:1:3:U:H3	1.30	0.79
45:k:266:ARG:NH2	57:1:2370:C:O2'	2.15	0.79
17:H:145:PHE:HZ	17:H:156:PHE:HB3	1.45	0.79
10:A:485:G:N2	10:A:499:U:O2	2.15	0.79
10:A:1529:G:N2	10:A:1556:A:OP2	2.14	0.79
34:Y:102:VAL:HG12	34:Y:127:VAL:HG12	1.65	0.79
23:N:59:LEU:HD22	23:N:133:ARG:HH12	1.48	0.79
65:AC:8:THR:HG22	65:AC:10:HIS:H	1.47	0.78
10:A:850:A:N6	10:A:950:U:O4	2.17	0.77
51:t:4:SER:O	64:AB:44:ASN:ND2	2.17	0.77
53:v:4:TYR:OH	57:1:147:G:OP2	2.01	0.77
10:A:78:A:H8	17:H:154:ARG:HG3	1.49	0.77
53:v:143:ARG:O	53:v:149:ASN:ND2	2.18	0.77
57:1:437:G:N2	57:1:620:A:H61	1.82	0.77
57:1:1238:G:N2	57:1:1266:A:O2'	2.17	0.77
10:A:1214:G:N2	10:A:1240:G:O2'	2.17	0.77
43:h:42:LEU:HB2	43:h:62:PHE:HB2	1.67	0.77
10:A:110:U:OP1	10:A:738:A:O2'	2.03	0.76
19:J:57:ALA:HB2	19:J:183:GLY:HA2	1.66	0.76
57:1:1550:U:O2'	57:1:1551:U:OP1	2.02	0.76
24:O:62:GLN:HB2	24:O:65:VAL:HG22	1.68	0.76
30:U:16:ASN:OD1	30:U:56:LYS:NZ	2.18	0.76
33:X:53:ILE:HD13	38:c:24:LEU:HD11	1.68	0.76
59:n:101:ASN:ND2	59:n:103:GLU:OE2	2.19	0.76
74:AL:36:LYS:HG3	74:AL:37:LYS:H	1.51	0.76
16:G:108:LEU:HD22	27:R:43:LEU:HD11	1.68	0.75
17:H:71:THR:HG22	17:H:72:ARG:H	1.51	0.75
43:h:236:GLU:OE2	43:h:238:HIS:NE2	2.19	0.75
57:1:1225:G:H2'	57:1:1226:G:C8	2.21	0.75
57:1:1269:A:H3'	57:1:1270:A:H8	1.50	0.75
15:F:253:ARG:HD2	15:F:257:ARG:HH21	1.51	0.75
43:h:186:ASN:OD1	43:h:187:ALA:N	2.18	0.75
43:h:90:LEU:HB2	43:h:104:PHE:HB2	1.67	0.75
46:1:4:ARG:NH1	46:1:23:LEU:O	2.19	0.75
5:5:84:LYS:HE3	5:5:93:ARG:HH21	1.50	0.75
21:L:40:LEU:HA	21:L:43:ILE:HG12	1.69	0.75
44:j:27:ALA:O	44:j:128:ARG:NH2	2.19	0.75
17:H:1:MET:HE2	17:H:106:LEU:HB2	1.69	0.74
29:T:134:ARG:HB2	29:T:136:GLN:HE22	1.53	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
50:s:65:ILE:HD11	57:1:2653:U:H5'	1.70	0.74
10:A:945:U:H5'	24:O:55:ARG:HD3	1.68	0.74
47:m:148:ILE:O	47:m:151:GLN:NE2	2.21	0.74
56:z:62:ARG:NH2	57:1:3040:U:OP2	2.20	0.74
10:A:822:G:O2'	10:A:823:G:N3	2.19	0.74
15:F:45:VAL:HG23	15:F:61:VAL:HG11	1.69	0.74
29:T:114:GLU:OE1	29:T:118:LYS:NZ	2.21	0.73
44:j:69:TYR:OH	57:1:2535:A:OP1	2.05	0.73
10:A:215:A:H62	10:A:830:G:H1'	1.53	0.73
10:A:1479:A:H4'	10:A:1480:G:O4'	1.88	0.73
23:N:57:ALA:HB3	23:N:124:LYS:HA	1.71	0.73
10:A:1475:U:O2'	10:A:1501:A:N6	2.21	0.73
10:A:1669:U:O4	10:A:1707:G:N2	2.21	0.73
46:1:99:ARG:NH2	57:1:800:C:OP1	2.19	0.73
66:AD:16:LEU:HD22	66:AD:82:VAL:HG12	1.71	0.73
10:A:1042:U:H3'	10:A:1043:U:H2'	1.71	0.73
12:C:190:PRO:HG2	12:C:192:VAL:HG23	1.70	0.73
43:h:75:SER:HB2	43:h:120:LEU:HD11	1.71	0.73
10:A:1159:C:H42	10:A:1451:C:H42	1.37	0.73
16:G:222:LYS:HD2	16:G:225:ARG:HH21	1.53	0.73
43:h:26:THR:HG22	43:h:28:ALA:H	1.52	0.72
56:z:46:LYS:NZ	57:1:1762:G:N7	2.36	0.72
10:A:799:G:H5'	56:z:163:ARG:HG3	1.68	0.72
10:A:1368:A:H5"	31:V:59:THR:HG23	1.71	0.72
15:F:139:VAL:HG11	15:F:154:ILE:HD13	1.69	0.72
10:A:552:C:N4	10:A:569:G:O6	2.21	0.72
32:W:64:GLU:HG2	38:c:3:LEU:HG	1.70	0.72
51:t:132:ALA:HA	51:t:135:VAL:HG12	1.71	0.72
57:1:564:G:H2'	57:1:565:A:C8	2.25	0.72
59:n:71:ASN:ND2	59:n:159:LEU:O	2.19	0.72
56:z:98:ARG:NH2	56:z:130:ASN:OD1	2.23	0.72
11:B:157:ASP:OD1	11:B:158:VAL:N	2.23	0.71
11:B:148:ASP:OD1	11:B:151:SER:OG	2.04	0.71
57:1:2184:G:O2'	57:1:2187:U:O4	2.08	0.71
16:G:62:ILE:O	16:G:65:ARG:NH1	2.24	0.71
25:P:80:ALA:H	25:P:114:THR:HG22	1.54	0.71
25:P:86:THR:HG22	25:P:88:THR:H	1.55	0.71
43:h:19:TRP:HB2	43:h:38:ARG:HD2	1.72	0.71
10:A:737:A:OP1	15:F:187:ARG:NH1	2.21	0.71
16:G:130:ILE:HA	16:G:133:VAL:HG12	1.71	0.71
13:D:126:ILE:HA	13:D:129:LEU:HG	1.72	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
32:W:15:ARG:NH1	32:W:33:GLN:OE1	2.23	0.71
10:A:1148:A:N3	10:A:1600:U:O2'	2.23	0.71
10:A:1387:A:OP1	28:S:56:HIS:NE2	2.24	0.71
62:x:56:ARG:NH2	62:x:75:GLU:OE2	2.24	0.71
5:5:107:LYS:HZ2	5:5:109:GLN:HG2	1.56	0.70
17:H:159:ARG:NH1	17:H:170:THR:OG1	2.23	0.70
27:R:22:LYS:HE2	27:R:65:ARG:HH22	1.56	0.70
15:F:31:PRO:HG3	15:F:43:PRO:HG3	1.73	0.70
47:m:289:LYS:HD2	61:r:206:LEU:HD23	1.73	0.70
10:A:908:A:H2'	10:A:909:A:C8	2.26	0.70
30:U:76:LEU:HB2	30:U:101:ASN:HD21	1.56	0.70
44:j:128:ARG:NH1	57:1:2155:G:OP2	2.24	0.70
10:A:1535:G:H1'	29:T:89:GLN:HE21	1.53	0.70
31:V:68:LYS:O	40:e:44:ARG:NH1	2.24	0.70
19:J:78:ILE:HG22	19:J:104:ILE:HG22	1.72	0.70
57:1:1043:A:N3	57:1:2605:U:O2'	2.24	0.70
5:5:102:LYS:HG3	5:5:103:GLN:H	1.56	0.70
10:A:774:U:H2'	10:A:775:A:H8	1.55	0.70
10:A:217:A:N1	10:A:828:U:O2'	2.23	0.70
33:X:15:ASN:ND2	33:X:72:CYS:O	2.24	0.70
36:a:78:VAL:HG22	36:a:81:ARG:HH21	1.56	0.70
10:A:747:A:OP1	20:K:79:ARG:NH2	2.25	0.70
57:1:2867:G:O2'	76:AN:24:TYR:O	2.09	0.70
27:R:100:SER:HA	27:R:103:GLU:HG3	1.74	0.69
10:A:1019:C:HO2'	33:X:2:THR:N	1.90	0.69
10:A:1236:U:O2'	10:A:1237:C:O2	2.07	0.69
13:D:40:VAL:HG21	13:D:63:ILE:HG12	1.74	0.69
10:A:1575:G:O6	10:A:1595:U:O4	2.10	0.69
30:U:12:GLN:O	30:U:16:ASN:ND2	2.25	0.69
57:1:2932:C:H2'	57:1:2933:G:H8	1.58	0.69
68:AF:84:ASP:OD1	68:AF:112:LYS:NZ	2.25	0.69
10:A:1026:G:H2'	10:A:1027:G:C8	2.26	0.69
10:A:1334:G:N3	10:A:1365:C:N4	2.39	0.69
10:A:1668:A:H1'	17:H:66:GLY:HA2	1.74	0.69
43:h:177:SER:OG	43:h:186:ASN:OD1	2.10	0.69
10:A:766:U:H4'	10:A:767:G:H5"	1.74	0.69
51:t:18:TRP:NE1	57:1:795:G:O2'	2.25	0.69
53:v:183:THR:HG22	53:v:187:ARG:HB2	1.75	0.69
11:B:41:ARG:NH2	11:B:43:ASP:OD2	2.25	0.69
23:N:41:LEU:HD11	23:N:121:VAL:HB	1.74	0.69
57:1:1774:G:O2'	57:1:1776:G:OP2	2.11	0.69



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
61:r:30:LYS:HG3	61:r:63:GLU:HG3	1.75	0.69
1:0:71:LYS:O	1:0:73:LYS:NZ	2.24	0.69
10:A:784:U:H2'	10:A:785:G:H8	1.57	0.69
39:d:8:THR:OG1	39:d:59:SER:OG	2.10	0.69
57:1:716:G:OP1	64:AB:117:ARG:NH2	2.25	0.69
57:1:2334:A:N3	62:x:131:ARG:NH2	2.41	0.69
30:U:135:ILE:O	30:U:139:THR:OG1	2.06	0.69
46:l:188:LEU:HD11	46:1:199:ARG:HE	1.58	0.69
11:B:92:HIS:HD1	11:B:202:TYR:HH	1.39	0.68
19:J:174:VAL:HG23	19:J:190:LEU:HD11	1.75	0.68
32:W:71:ARG:HD3	38:c:4:VAL:HG21	1.75	0.68
57:1:2163:G:O2'	57:1:2292:U:OP2	2.09	0.68
10:A:396:G:OP2	19:J:47:ARG:NH2	2.26	0.68
10:A:1316:A:H61	14:E:162:GLY:HA3	1.57	0.68
51:t:62:THR:HG22	51:t:64:LYS:H	1.58	0.68
57:1:1261:U:H2'	57:1:1262:G:C8	2.27	0.68
10:A:898:G:H21	57:1:2185:A:N6	1.89	0.68
20:K:132:ARG:HB3	20:K:140:ILE:HD11	1.74	0.68
57:1:1575:A:OP1	57:1:2500:G:N2	2.24	0.68
10:A:856:G:H2'	10:A:857:G:C8	2.29	0.68
26:Q:73:PRO:HG3	26:Q:92:SER:HA	1.75	0.68
10:A:821:U:H2'	10:A:822:G:C8	2.28	0.68
10:A:1335:U:H2'	10:A:1336:G:C8	2.29	0.68
10:A:211:A:H62	10:A:250:U:H3	1.40	0.68
10:A:78:A:C8	17:H:154:ARG:HG3	2.28	0.67
10:A:1080:U:O2'	33:X:19:LYS:NZ	2.23	0.67
66:AD:42:LYS:HB3	66:AD:103:LEU:HD21	1.76	0.67
46:l:194:LYS:HB2	46:l:199:ARG:HD2	1.76	0.67
57:1:1611:U:O3'	70:AH:64:GLN:NE2	2.26	0.67
53:v:68:ARG:NH1	53:v:124:ASP:O	2.25	0.67
57:1:545:G:N2	57:1:546:C:O2'	2.27	0.67
57:1:2869:A:H2'	57:1:2871:C:H5"	1.75	0.67
57:1:3014:U:OP2	57:1:3064:C:N4	2.27	0.67
17:H:12:THR:OG1	17:H:124:LEU:O	2.11	0.67
43:h:12:THR:OG1	43:h:53:ASN:OD1	2.07	0.67
43:h:102:GLN:NE2	43:h:103:ARG:O	2.28	0.67
49:q:8:GLN:HB3	49:q:72:LYS:HD2	1.76	0.67
57:1:2171:U:H5'	57:1:2172:G:H5'	1.77	0.67
14:E:91:ARG:HD2	14:E:95:ARG:HH21	1.59	0.67
56:z:43:LYS:NZ	57:1:1760:U:OP1	2.18	0.67
4:4:155:G:H5'	60:p:186:ARG:HD2	1.75	0.67



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
10:A:1579:A:H2	10:A:1580:A:H8	1.59	0.67
56:z:62:ARG:NH1	57:1:3042:A:OP1	2.28	0.67
57:1:2183:U:O2'	57:1:2184:G:O5'	2.12	0.67
10:A:1156:A:H2'	10:A:1157:G:C8	2.30	0.67
10:A:1474:G:O2'	10:A:1481:C:O2	2.12	0.67
10:A:1486:G:H5"	30:U:122:ARG:HH12	1.59	0.67
10:A:1491:G:N3	10:A:1550:C:O2'	2.26	0.67
43:h:12:THR:HG22	43:h:308:ARG:HG2	1.76	0.67
53:v:155:VAL:O	53:v:162:ARG:NH2	2.28	0.67
6:6:40:LYS:HD3	6:6:59:MET:HE2	1.76	0.67
39:d:44:VAL:HG11	39:d:48:VAL:HG21	1.76	0.67
51:t:73:ARG:NH1	57:1:76:A:OP2	2.28	0.67
57:1:1657:G:H2'	57:1:1658:G:C8	2.30	0.67
26:Q:56:LEU:HD12	26:Q:83:MET:HE1	1.77	0.67
57:1:2932:C:H2'	57:1:2933:G:C8	2.29	0.67
10:A:1511:A:N3	10:A:1577:G:O2'	2.22	0.66
32:W:74:GLN:NE2	32:W:83:TRP:O	2.26	0.66
57:1:437:G:H22	57:1:620:A:N6	1.91	0.66
43:h:202:SER:HB2	43:h:207:LEU:HB3	1.76	0.66
43:h:207:LEU:HG	43:h:219:LEU:HD12	1.76	0.66
45:k:313:ARG:NH1	57:1:3060:G:OP1	2.27	0.66
10:A:1478:A:O2'	10:A:1479:A:O4'	2.11	0.66
20:K:148:VAL:HG11	20:K:156:ILE:HD11	1.77	0.66
57:1:62:A:N3	57:1:77:U:O2'	2.23	0.66
33:X:36:LYS:HB3	33:X:110:ILE:HG21	1.78	0.66
15:F:58:GLY:HA2	15:F:61:VAL:HG12	1.77	0.66
57:1:1936:G:H21	57:1:3327:A:H8	1.43	0.66
4:4:100:U:O2'	8:8:89:LYS:NZ	2.23	0.66
10:A:903:U:H2'	10:A:904:A:C8	2.31	0.66
51:t:90:ALA:HB1	51:t:95:ILE:HB	1.78	0.66
10:A:1470:G:H21	10:A:1593:C:H1'	1.60	0.66
24:O:55:ARG:NH2	38:c:51:GLN:OE1	2.22	0.66
5:5:59:GLU:HG3	5:5:60:SER:H	1.60	0.66
4:4:103:G:OP2	4:4:105:A:O2'	2.13	0.66
10:A:787:A:N3	18:I:100:ARG:NH1	2.43	0.66
16:G:124:LEU:O	16:G:125:THR:HG22	1.96	0.66
25:P:66:CYS:HB2	25:P:71:ILE:HG13	1.78	0.66
26:Q:32:GLU:OE1	26:Q:32:GLU:N	2.29	0.66
30:U:27:LYS:NZ	30:U:111:ILE:HB	2.10	0.66
61:r:99:ILE:HG21	61:r:102:MET:HE2	1.77	0.66
10:A:774:U:H2'	10:A:775:A:C8	2.31	0.65



	A t arra 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
15:F:40:GLU:OE1	15:F:103:TYR:OH	2.12	0.65
43:h:198:CYS:SG	43:h:199:ILE:N	2.69	0.65
47:m:205:ALA:HB2	47:m:236:VAL:HG11	1.78	0.65
55:y:90:ASP:O	55:y:113[A]:ARG:NH1	2.28	0.65
58:10:75:C:O2'	78:AP:56:GLN:O	2.14	0.65
41:f:55:LYS:HB2	41:f:58:PRO:HG3	1.77	0.65
57:1:339:C:OP1	57:1:1376:G:O2'	2.14	0.65
10:A:1275:U:H2'	10:A:1276:G:C8	2.31	0.65
57:1:3287:A:H2'	57:1:3288:A:C8	2.30	0.65
44:j:54:ARG:NH2	57:1:2154:U:OP1	2.27	0.65
5:5:89:LYS:NZ	57:1:1680:U:OP1	2.28	0.65
10:A:509:A:OP2	20:K:176:ASN:ND2	2.27	0.65
11:B:197:VAL:HG13	11:B:201:LEU:HD23	1.78	0.65
51:t:163:VAL:HG12	64:AB:144:VAL:HG22	1.79	0.65
57:1:2200:A:H2'	57:1:2201:A:C8	2.31	0.65
57:1:2988:A:H2'	57:1:2989:A:H8	1.61	0.65
10:A:880:G:H1	10:A:902:U:H3	1.43	0.65
30:U:108:LEU:HA	30:U:111:ILE:HG12	1.78	0.65
53:v:46:ASP:OD2	53:v:50:ARG:NH2	2.29	0.65
6:6:9:ASN:ND2	57:1:3010:U:O2	2.30	0.65
10:A:458:A:O2'	15:F:27:TYR:OH	2.15	0.65
14:E:106:LEU:HD21	14:E:123:VAL:HB	1.78	0.65
11:B:30:GLN:NE2	11:B:151:SER:O	2.30	0.65
13:D:218:SER:HB2	32:W:25:LYS:HZ3	1.61	0.65
16:G:122:HIS:HB2	16:G:129:PRO:HG3	1.79	0.65
35:Z:7:ILE:HD11	35:Z:47:ILE:HD12	1.77	0.65
61:r:178:ARG:O	61:r:182:ILE:HG13	1.97	0.65
57:1:2183:U:H2'	57:1:2184:G:C8	2.32	0.65
10:A:1052:G:H5"	12:C:150:ILE:HG22	1.78	0.64
33:X:94:LEU:HD11	33:X:102:VAL:HG23	1.78	0.64
1:0:2:SER:HA	57:1:1319:G:H4'	1.78	0.64
2:2:84:TYR:HB2	65:AC:24:PRO:HD3	1.78	0.64
4:4:65:A:H5"	71:AI:6:THR:HG21	1.79	0.64
5:5:92:ILE:HD12	5:5:96:ILE:HD12	1.79	0.64
57:1:637:G:OP1	68:AF:41:SER:OG	2.15	0.64
57:1:2873:G:O2'	57:1:2996:A:N1	2.30	0.64
10:A:854:A:H61	10:A:943:U:H5	1.45	0.64
10:A:1765:G:O6	77:AO:12:ARG:NH2	2.30	0.64
52:u:129:VAL:HG11	57:1:3194:G:H4'	1.80	0.64
63:AA:101:LEU:O	63:AA:107:ARG:NH2	2.30	0.64
78:AP:25:VAL:HG22	78:AP:72:LEU:HD22	1.80	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
4:4:21:C:OP1	46:1:194:LYS:NZ	2.25	0.64
10:A:1276:G:H22	10:A:1309:G:H22	1.46	0.64
16:G:25:LEU:HD12	27:R:26:GLY:HA3	1.79	0.64
28:S:29:GLU:OE1	28:S:29:GLU:N	2.29	0.64
57:1:1269:A:H3'	57:1:1270:A:C8	2.33	0.64
5:5:107:LYS:NZ	5:5:109:GLN:HG2	2.11	0.64
10:A:1156:A:H2'	10:A:1157:G:H8	1.61	0.64
10:A:1460:G:H2'	10:A:1461:A:H8	1.60	0.64
10:A:1546:G:H5"	29:T:135:GLY:HA3	1.79	0.64
12:C:109:LYS:HE3	12:C:113:LEU:HD11	1.80	0.64
14:E:29:GLU:HG2	14:E:70:LEU:HD11	1.78	0.64
30:U:127:ASN:HB2	30:U:130:ARG:HH21	1.60	0.64
46:1:36:VAL:HG21	46:l:245:LEU:HD21	1.79	0.64
47:m:50:ARG:NH2	47:m:72:ASP:OD2	2.31	0.64
57:1:186:A:N3	57:1:207:C:O2'	2.29	0.64
57:1:833:A:OP2	79:AQ:4:ARG:NH1	2.30	0.64
10:A:530:U:OP1	35:Z:64:PHE:HA	1.98	0.64
27:R:12:LYS:HG3	27:R:13:LYS:H	1.63	0.64
27:R:45:PHE:HA	27:R:48:TYR:HB2	1.79	0.64
30:U:42:GLY:HA2	30:U:84:LYS:HG3	1.79	0.64
57:1:3287:A:H2'	57:1:3288:A:H8	1.63	0.64
68:AF:60:SER:OG	68:AF:65:LYS:HG3	1.97	0.64
34:Y:54:LEU:HD11	34:Y:75:GLN:HB2	1.79	0.63
10:A:168:U:H3	10:A:287:U:H1'	1.63	0.63
10:A:1511:A:H2'	10:A:1512:A:C8	2.32	0.63
16:G:109:LYS:HG3	16:G:112:ARG:HH21	1.61	0.63
39:d:11:LYS:N	39:d:31:GLU:O	2.30	0.63
47:m:119:TYR:OH	47:m:139:PRO:O	2.15	0.63
10:A:556:U:OP1	41:f:55:LYS:NZ	2.29	0.63
10:A:1276:G:H22	10:A:1309:G:N2	1.97	0.63
15:F:129:VAL:HG22	15:F:139:VAL:HG12	1.79	0.63
16:G:45:LYS:NZ	16:G:119:GLU:OE2	2.31	0.63
20:K:77:ILE:HG12	20:K:91:MET:HG3	1.79	0.63
10:A:122:U:H2'	10:A:123:G:H5"	1.80	0.63
15:F:31:PRO:HD2	15:F:38:LEU:HD11	1.79	0.63
39:d:12:VAL:HG12	39:d:30:VAL:HG12	1.81	0.63
48:0:182:LEU:HD21	48:0:200:LEU:HD11	1.79	0.63
57:1:1720:U:H1'	57:1:1721:C:C6	2.33	0.63
10:A:17:C:O2'	10:A:1122:A:N1	2.27	0.63
10:A:1043:U:O2'	10:A:1045:U:OP2	2.17	0.63
10:A:1143:C:H42	10:A:1148:A:H61	1.46	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:315:C:OP2	72:AJ:27:TYR:OH	2.13	0.63
10:A:1445:C:OP2	29:T:138:THR:OG1	2.17	0.63
50:s:126:ASP:OD1	57:1:2645:A:O2'	2.14	0.63
57:1:307:A:H2'	57:1:308:A:C8	2.33	0.63
57:1:480:G:H5"	57:1:481:G:N7	2.13	0.63
10:A:336:C:H5"	19:J:10:LYS:HD2	1.81	0.63
24:O:35:GLU:C	24:O:39:LYS:HZ2	2.07	0.63
25:P:15:PHE:HB3	25:P:22:PHE:HB2	1.80	0.63
10:A:1086:G:H4'	33:X:76:GLN:HG3	1.80	0.63
17:H:159:ARG:HB2	17:H:170:THR:HB	1.80	0.63
29:T:28:ILE:HD11	29:T:54:LEU:HA	1.80	0.63
45:k:308:MET:HE2	57:1:3294:U:H5"	1.80	0.63
53:v:159:ARG:HB2	53:v:164:LEU:HB2	1.81	0.63
57:1:925:A:O2'	73:AK:49:TRP:O	2.15	0.63
57:1:3079:U:OP1	76:AN:38:LYS:NZ	2.32	0.63
19:J:87:ASN:HB3	19:J:90:LEU:HD13	1.80	0.62
27:R:3:THR:HG22	27:R:4:GLN:H	1.64	0.62
54:w:76:ALA:HB3	54:w:79:ARG:HG2	1.81	0.62
10:A:1600:U:OP1	16:G:169:ASN:HB2	1.98	0.62
12:C:145:ARG:NH2	12:C:152:LYS:O	2.32	0.62
57:1:2191:A:H2'	57:1:2192:A:C8	2.34	0.62
57:1:3313:G:H1	57:1:3322:U:H3	1.47	0.62
10:A:1399:U:OP2	28:S:3:ARG:NH2	2.32	0.62
14:E:60:LEU:HD21	14:E:67:ILE:HD12	1.81	0.62
7:7:56:ARG:HG3	7:7:61:LYS:HB2	1.82	0.62
10:A:870:G:H2'	10:A:871:U:C6	2.34	0.62
12:C:137:VAL:HG12	12:C:215:VAL:HG12	1.81	0.62
27:R:124:GLU:HG2	27:R:133:ALA:HB1	1.81	0.62
57:1:1713:U:H2'	57:1:1714:G:C8	2.35	0.62
19:J:62:THR:HG22	19:J:77:ARG:HA	1.81	0.62
31:V:25:LEU:HB3	31:V:33:LEU:HD11	1.82	0.62
57:1:545:G:H5'	57:1:546:C:H4'	1.80	0.62
10:A:91:G:OP1	10:A:395:A:N6	2.31	0.62
21:L:76:LEU:O	21:L:80:LEU:HB2	1.99	0.62
24:O:110:ASP:OD1	24:O:111:SER:N	2.33	0.62
43:h:297:ASN:ND2	43:h:311:GLN:OE1	2.26	0.62
51:t:63:VAL:HA	51:t:66:ASN:ND2	2.15	0.62
57:1:2079:C:HO2'	57:1:2080:U:H6	1.48	0.62
57:1:208:A:H4'	57:1:210:A:N7	2.15	0.62
10:A:1489:G:N2	10:A:1492:A:OP2	2.33	0.62
15:F:126:VAL:HG21	15:F:154:ILE:HD11	1.80	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
26:Q:24:ASP:O	26:Q:28:MET:HG3	2.00	0.62
41:f:43:ARG:NH2	41:f:56:MET:SD	2.73	0.62
45:k:372:THR:HG22	45:k:374:ALA:H	1.64	0.62
57:1:1110:U:OP1	64:AB:23:GLY:N	2.29	0.62
19:J:77:ARG:NH1	57:1:3319:U:O2'	2.33	0.62
21:L:89:LEU:HD12	21:L:92:LEU:HD21	1.82	0.62
46:l:345:VAL:HG12	57:1:512:A:H5"	1.82	0.62
57:1:1014:G:O6	57:1:1030:U:O4	2.17	0.62
1:0:150:PHE:O	52:u:13:VAL:HG12	2.00	0.62
10:A:149:G:N2	17:H:13:GLN:OE1	2.28	0.62
43:h:10:ARG:NE	43:h:51:GLU:OE1	2.29	0.62
47:m:233:SER:O	47:m:236:VAL:HG12	2.00	0.62
57:1:636:C:N4	57:1:637:G:O6	2.32	0.62
66:AD:59:GLU:OE1	66:AD:71:TYR:OH	2.16	0.62
10:A:1533:G:N2	29:T:87:ASN:OD1	2.33	0.61
29:T:29:MET:HE2	29:T:44:ASN:HB3	1.80	0.61
39:d:19:THR:HG23	39:d:25:VAL:HG23	1.82	0.61
44:j:37:ARG:NH2	57:1:2504:C:OP1	2.31	0.61
10:A:1578:C:H2'	10:A:1579:A:H8	1.65	0.61
20:K:110:GLN:HE21	20:K:122:ILE:HG13	1.65	0.61
24:O:49:GLN:HA	24:O:52:VAL:HG12	1.80	0.61
5:5:10:LYS:HD2	5:5:11:SER:H	1.64	0.61
10:A:345:G:H5"	22:M:85:ILE:HD11	1.82	0.61
10:A:589:A:H2'	10:A:590:A:C8	2.36	0.61
10:A:748:G:H5"	20:K:78:ARG:HH22	1.65	0.61
10:A:142:G:O2'	10:A:143:A:O5'	2.17	0.61
10:A:304:U:OP2	22:M:105:LYS:NZ	2.27	0.61
10:A:1131:G:H2'	10:A:1132:A:C8	2.35	0.61
10:A:908:A:H2'	10:A:909:A:H8	1.64	0.61
11:B:62:ARG:HH22	32:W:78:LEU:HB3	1.63	0.61
19:J:38:ILE:HG12	19:J:96:LEU:HD11	1.82	0.61
10:A:78:A:H2	17:H:174:LYS:HG3	1.64	0.61
10:A:551:G:N2	10:A:569:G:N7	2.48	0.61
10:A:1024:A:O2'	10:A:1025:G:O5'	2.19	0.61
10:A:1579:A:H2'	10:A:1580:A:C8	2.35	0.61
24:O:37:ILE:HG21	24:O:74:ILE:HD11	1.82	0.61
43:h:92:LEU:HB2	43:h:104:PHE:HE1	1.63	0.61
63:AA:33:THR:HG22	63:AA:34:LYS:H	1.66	0.61
29:T:43:ALA:HA	29:T:46:VAL:HG22	1.83	0.61
10:A:1226:G:H4'	26:Q:78:THR:HA	1.82	0.61
10:A:1659:G:H2'	10:A:1660:G:C8	2.36	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
17:H:57:ASP:HA	17:H:106:LEU:HA	1.82	0.61
21:L:8:ARG:HG2	21:L:12:HIS:CE1	2.35	0.61
49:q:33:GLU:OE1	49:q:33:GLU:N	2.34	0.61
57:1:316:U:O2'	72:AJ:29:LYS:NZ	2.33	0.61
57:1:653:C:H2'	57:1:654:A:H8	1.65	0.61
1:0:96:ASP:OD1	1:0:97:VAL:N	2.30	0.61
10:A:485:G:O6	10:A:499:U:O4	2.19	0.61
10:A:501:G:H2'	10:A:502:U:C6	2.35	0.61
15:F:89:VAL:HG22	15:F:100:ARG:HE	1.63	0.61
16:G:218:GLU:O	16:G:222:LYS:HG2	2.00	0.61
7:7:1:MET:N	45:k:71:GLU:OE2	2.34	0.61
10:A:1398:G:H4'	10:A:1399:U:O5'	2.01	0.61
26:Q:85:VAL:HG23	26:Q:112:VAL:HA	1.83	0.61
43:h:41:THR:OG1	43:h:61:SER:HB3	2.01	0.61
10:A:79:C:OP1	17:H:159:ARG:NH2	2.33	0.60
10:A:609:U:OP2	34:Y:5:LYS:NZ	2.32	0.60
10:A:784:U:H2'	10:A:785:G:C8	2.36	0.60
10:A:1097:G:OP1	77:AO:6:ARG:NH2	2.34	0.60
27:R:99:ALA:HA	27:R:102:ASN:HD21	1.65	0.60
32:W:73:ALA:HB1	32:W:78:LEU:HB2	1.83	0.60
43:h:169:ALA:HB2	43:h:199:ILE:HD12	1.82	0.60
57:1:3256:G:H2'	57:1:3257:A:C8	2.35	0.60
62:x:177:ALA:O	62:x:181:ARG:HG3	2.01	0.60
10:A:261:C:O2'	10:A:262:G:N2	2.31	0.60
10:A:405:A:H2'	10:A:406:C:H6	1.65	0.60
10:A:898:G:N2	57:1:2185:A:H62	1.93	0.60
11:B:56:LYS:NZ	32:W:70:ASN:OD1	2.34	0.60
48:0:87:ILE:HD11	48:0:226:THR:HG22	1.82	0.60
10:A:970:G:H2'	10:A:971:G:C8	2.36	0.60
13:D:124:ILE:HG22	13:D:128:LYS:HE2	1.83	0.60
13:D:234:PRO:HA	13:D:237:VAL:HG12	1.83	0.60
26:Q:25:LEU:HA	26:Q:28:MET:HE2	1.84	0.60
57:1:547:U:H2'	57:1:548:G:C8	2.37	0.60
64:AB:36:GLY:HA3	64:AB:40:HIS:CE1	2.37	0.60
57:1:1617:A:H2'	57:1:1618:U:C6	2.36	0.60
57:1:2669:A:H2'	57:1:2670:G:C8	2.37	0.60
57:1:2988:A:H2'	57:1:2989:A:C8	2.37	0.60
19:J:34:ALA:HB2	19:J:56:ARG:HD2	1.84	0.60
55:y:69:ARG:NH2	57:1:780:A:OP2	2.34	0.60
57:1:2925:U:H2'	57:1:2926:U:H2'	1.83	0.60
5:5:102:LYS:HG3	5:5:103:GLN:N	2.16	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
63:AA:42:ILE:HD11	63:AA:98:SER:HB2	1.83	0.60
16:G:23:VAL:N	16:G:34:GLN:OE1	2.32	0.60
57:1:2273:A:N3	57:1:2901:C:O2'	2.34	0.60
53:v:49:ARG:NH2	57:1:148:U:OP2	2.33	0.60
10:A:1629:G:H2'	10:A:1630:U:H6	1.66	0.60
20:K:85:VAL:HG22	20:K:99:LEU:HD11	1.84	0.60
40:e:2:ALA:HB1	40:e:5:ASN:HB2	1.84	0.60
45:k:95:THR:OG1	45:k:98:GLY:O	2.18	0.60
1:0:60:SER:OG	1:0:62:ASN:ND2	2.33	0.59
10:A:588:C:H5"	41:f:43:ARG:NH2	2.12	0.59
18:I:150:LEU:HB2	18:I:181:ILE:HG13	1.83	0.59
16:G:162:VAL:HG13	16:G:166:ARG:HD3	1.84	0.59
57:1:169:G:N2	57:1:250:U:OP2	2.35	0.59
57:1:706:G:N2	57:1:709:A:OP2	2.28	0.59
57:1:3256:G:H2'	57:1:3257:A:H8	1.67	0.59
10:A:873:U:O2	10:A:973:A:O2'	2.18	0.59
10:A:1245:U:H2'	10:A:1246:G:H8	1.67	0.59
10:A:1473:A:OP2	14:E:9:LYS:NZ	2.34	0.59
21:L:8:ARG:O	21:L:12:HIS:ND1	2.32	0.59
30:U:127:ASN:HB2	30:U:130:ARG:NH2	2.18	0.59
32:W:55:LEU:HD11	32:W:69:LEU:HD11	1.84	0.59
14:E:43:THR:OG1	14:E:48:GLU:OE1	2.20	0.59
47:m:275:GLN:OE1	47:m:275:GLN:N	2.35	0.59
52:u:120:ARG:NH1	54:w:192:ALA:HB2	2.17	0.59
57:1:547:U:H2'	57:1:548:G:H8	1.66	0.59
75:AM:27:ILE:O	75:AM:33:ASN:ND2	2.34	0.59
10:A:1188:A:H61	10:A:1540:G:H1'	1.67	0.59
23:N:89:ILE:HD11	23:N:136:LEU:HD11	1.83	0.59
26:Q:77:LYS:HB2	26:Q:102:PHE:CD2	2.38	0.59
33:X:9:ASP:OD1	33:X:10:ALA:N	2.35	0.59
9:9:3:LYS:HD3	9:9:8:VAL:HG23	1.83	0.59
15:F:192:VAL:HG12	15:F:244:GLY:HA3	1.84	0.59
19:J:81:VAL:HG12	19:J:94:ASN:HA	1.84	0.59
27:R:92:HIS:HA	27:R:96:VAL:HG22	1.84	0.59
32:W:30:ALA:O	32:W:60:ARG:NE	2.32	0.59
43:h:126:ALA:HB1	43:h:152:VAL:HG23	1.84	0.59
56:z:40:ALA:HA	56:z:43:LYS:HE2	1.84	0.59
10:A:829:A:H2'	10:A:830:G:C8	2.37	0.59
10:A:1218:G:H1	10:A:1237:C:H5	1.48	0.59
16:G:48:PHE:O	16:G:51:VAL:HG12	2.03	0.59
43:h:39:ASP:OD1	43:h:41:THR:HG22	2.02	0.59



A + 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:2655:U:H2'	57:1:2656:C:C6	2.37	0.59
57:1:2862:A:O2'	57:1:2905:A:N3	2.32	0.59
2:2:49:GLN:HA	2:2:52:MET:HE3	1.84	0.59
10:A:545:U:H1'	10:A:594:C:H1'	1.83	0.59
10:A:913:U:H4'	25:P:119:ASP:OD2	2.03	0.59
10:A:1372:G:OP2	28:S:44:LYS:NZ	2.31	0.59
14:E:50:ILE:HD11	14:E:90:GLU:HG3	1.84	0.59
17:H:98:ARG:NH2	17:H:105:ASP:OD1	2.35	0.59
48:0:185:GLU:HG2	48:0:196:VAL:HG21	1.85	0.59
52:u:107:ASP:OD2	59:n:50:ARG:NH2	2.36	0.59
57:1:1091:U:H4'	57:1:1092:U:H5'	1.84	0.59
57:1:3309:A:H2	57:1:3326:G:H21	1.51	0.59
10:A:938:G:H2'	10:A:939:G:C8	2.38	0.59
10:A:1399:U:N3	10:A:1570:A:OP2	2.23	0.59
25:P:59:ALA:HB3	25:P:99:ALA:HB3	1.85	0.59
44:j:36:GLU:OE1	44:j:163:ARG:NH1	2.36	0.59
13:D:44:LYS:HE2	13:D:241:GLU:HG3	1.85	0.59
19:J:70:GLU:OE1	19:J:70:GLU:N	2.35	0.59
57:1:2239:G:O2'	57:1:2241:C:N4	2.35	0.59
57:1:2669:A:H2'	57:1:2670:G:H8	1.68	0.59
10:A:1597:G:N7	27:R:13:LYS:NZ	2.51	0.58
57:1:1473:A:OP1	57:1:3047:G:O2'	2.20	0.58
17:H:142:ARG:HH12	17:H:149:LYS:HE2	1.67	0.58
25:P:14:ILE:HD11	25:P:96:ALA:HB3	1.85	0.58
60:p:1:MET:HG2	60:p:3:PRO:HD2	1.84	0.58
10:A:1160:U:H2'	10:A:1161:G:H8	1.68	0.58
32:W:53:TYR:OH	32:W:76:ASP:OD2	2.15	0.58
35:Z:46:GLU:O	35:Z:49:LYS:NZ	2.35	0.58
46:l:109:ARG:HG2	53:v:203:ARG:HD2	1.84	0.58
57:1:361:A:OP1	73:AK:24:ARG:NH1	2.37	0.58
4:4:150:G:OP1	8:8:27:ARG:NH2	2.37	0.58
7:7:16:GLY:O	57:1:3022:U:O2'	2.20	0.58
10:A:249:A:C2	15:F:131:LEU:HD12	2.38	0.58
10:A:829:A:H2'	10:A:830:G:H8	1.68	0.58
26:Q:107:ILE:HG22	26:Q:111:MET:HE1	1.86	0.58
33:X:20:THR:HG23	33:X:22:LYS:HG3	1.86	0.58
45:k:240:ARG:NH2	57:1:1903:C:O2	2.35	0.58
51:t:5:LYS:H	51:t:5:LYS:HD3	1.68	0.58
55:y:90:ASP:O	55:y:113[B]:ARG:NH1	2.28	0.58
57:1:662:U:H2'	57:1:663:A:C8	2.39	0.58
75:AM:49:LEU:HB3	75:AM:51:ILE:HG12	1.86	0.58



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:5:14:LYS:HG2	5:5:67:VAL:HG22	1.85	0.58
10:A:422:C:O2'	10:A:424:G:OP1	2.18	0.58
10:A:871:U:O2'	25:P:116:VAL:O	2.20	0.58
10:A:1533:G:OP1	29:T:123:ARG:NH1	2.35	0.58
11:B:122:VAL:HG22	11:B:144:ILE:HB	1.85	0.58
17:H:135:PRO:HB2	17:H:141:ILE:HG12	1.85	0.58
49:q:80:THR:HA	49:q:83:THR:HG22	1.85	0.58
51:t:134:GLU:OE1	51:t:134:GLU:N	2.34	0.58
57:1:976:A:H2'	57:1:977:U:H5'	1.85	0.58
5:5:22:PRO:HB2	5:5:28:PHE:HB2	1.86	0.58
10:A:1538:U:O4	26:Q:40:ARG:NH1	2.37	0.58
43:h:50:GLY:H	43:h:55:TYR:HA	1.68	0.58
49:q:92:PHE:HB2	49:q:142:ASP:HB3	1.84	0.58
57:1:412:G:OP1	62:x:62:ARG:NH1	2.35	0.58
57:1:843:A:H2'	57:1:844:A:C8	2.38	0.58
57:1:3260:A:H2'	57:1:3261:A:C8	2.39	0.58
10:A:1533:G:OP2	29:T:134:ARG:NH2	2.31	0.58
22:M:111:VAL:HG23	22:M:139:VAL:HG11	1.86	0.58
34:Y:69:ARG:HG3	34:Y:117:ILE:HG12	1.85	0.58
57:1:1231:U:H4'	57:1:1232:G:H5'	1.84	0.58
13:D:53:LEU:O	32:W:15:ARG:NE	2.36	0.58
13:D:135:ARG:H	13:D:216:THR:HG21	1.68	0.58
57:1:827:G:O2'	57:1:1860:A:N3	2.36	0.58
57:1:2740:U:H2'	57:1:2741:A:H8	1.69	0.58
10:A:800:G:N3	18:I:106:GLN:NE2	2.52	0.58
10:A:1145:A:H2'	10:A:1146:C:H6	1.69	0.58
30:U:113:VAL:HG23	30:U:114:LEU:HD13	1.85	0.58
37:b:45:VAL:HG23	37:b:50:VAL:HG12	1.85	0.58
57:1:429:U:H2'	57:1:430:G:H8	1.68	0.58
57:1:486:C:H2'	57:1:487:C:C6	2.39	0.58
57:1:538:G:H2'	57:1:539:G:C8	2.39	0.58
16:G:197:GLU:OE2	16:G:198:LEU:HG	2.04	0.58
74:AL:5:ILE:HD11	74:AL:52:TYR:HB3	1.86	0.58
10:A:871:U:H2'	10:A:872:A:H8	1.67	0.57
10:A:948:A:N7	24:O:70:LYS:NZ	2.52	0.57
10:A:1007:C:O2'	10:A:1110:A:N1	2.37	0.57
10:A:1491:G:H5'	30:U:97:SER:HA	1.86	0.57
10:A:1629:G:H2'	10:A:1630:U:C6	2.38	0.57
22:M:66:ILE:HG13	22:M:140:LEU:HD21	1.85	0.57
44:j:129:THR:OG1	44:j:132:ASN:ND2	2.32	0.57
10:A:52:U:H2'	10:A:53:G:H8	1.69	0.57



Atom-1	Atom-2	Interatomic	Clash
	10 4 001 4 00	distance (A)	overlap (A)
10:A:317:U:H4	10:A:321:A:C8	2.40	0.57
32:W:79:LEU:HD13	32:W:82:VAL:HG11	1.86	0.57
34:Y:126:LYS:HG2	34:Y:131:SER:HA	1.86	0.57
42:g:162:GLU:HA	42:g:173:PHE:HA	1.84	0.57
57:1:2191:A:H2'	57:1:2192:A:H8	1.69	0.57
2:2:68:THR:HG1	2:2:71:SER:HG	1.48	0.57
10:A:1219:A:HO2'	42:g:182:TYR:HH	1.50	0.57
41:f:50:THR:OG1	41:f:53:LYS:HB2	2.04	0.57
57:1:628:A:H2'	57:1:629:A:C8	2.38	0.57
59:n:129:GLU:OE1	59:n:129:GLU:N	2.37	0.57
61:r:208:ALA:HA	61:r:211:GLN:HG2	1.86	0.57
10:A:1463:G:H2'	10:A:1464:G:H8	1.69	0.57
43:h:71:ASP:OD1	43:h:72:VAL:N	2.37	0.57
49:q:23:ARG:NH1	57:1:3157:A:OP1	2.37	0.57
10:A:154:A:N6	10:A:416:G:O6	2.38	0.57
10:A:759:A:H61	10:A:770:C:N4	2.02	0.57
57:1:120:A:N6	60:p:127:SER:OG	2.37	0.57
10:A:1187:A:H1'	10:A:1192:C:N4	2.20	0.57
36:a:71:ILE:HB	36:a:75:LEU:HD23	1.85	0.57
57:1:600:U:C2	57:1:602:A:H1'	2.39	0.57
57:1:896:G:H1'	57:1:1585:A:N6	2.19	0.57
57:1:1559:C:O2'	57:1:1560:U:OP1	2.23	0.57
57:1:1592:C:H2'	57:1:1593:C:C6	2.39	0.57
1:0:8:GLN:HB2	1:0:64:ILE:HD11	1.87	0.57
2:2:40:VAL:HB	2:2:96:VAL:HG13	1.86	0.57
9:9:80:ILE:HG23	9:9:101:PRO:HG3	1.86	0.57
10:A:52:U:H2'	10:A:53:G:C8	2.39	0.57
10:A:1198:G:H1	10:A:1436:U:H3	1.53	0.57
20:K:113:VAL:HG23	20:K:118:LEU:HD12	1.86	0.57
10:A:290:U:H2'	10:A:291:U:C6	2.40	0.57
13:D:111:LYS:HG2	13:D:122:ALA:HB3	1.87	0.57
57:1:1260:G:N2	57:1:1273:C:N3	2.52	0.57
57:1:1530:A:H2'	57:1:1531:A:C8	2.39	0.57
57:1:1795:A:H2'	57:1:1796:A:C8	2.39	0.57
63:AA:70:PRO:HG3	63:AA:115:LYS:HB2	1.86	0.57
29:T:134:ARG:HB2	29:T:136:GLN:NE2	2.19	0.57
47:m:83:LEU:HD13	47:m:88:ILE:HD12	1.87	0.57
13:D:53:LEU:HA	32:W:12:TYR:HE1	1.70	0.57
17:H:58:LYS:HA	17:H:107:SER:HB2	1.86	0.57
22:M:7:VAL:HG23	22:M:8:GLN:HG2	1.85	0.57
51:t:61:PRO:O	51:t:62:THR:HB	2.05	0.57



	A t arra 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
64:AB:24:LYS:O	64:AB:26:ARG:HG2	2.05	0.57
10:A:974:U:H1'	25:P:121:THR:HB	1.86	0.56
15:F:63:ALA:O	15:F:67:GLN:HG3	2.04	0.56
16:G:58:LEU:O	16:G:62:ILE:HG12	2.05	0.56
24:O:100:LYS:HG2	24:O:104:LYS:NZ	2.20	0.56
24:O:119:GLU:O	24:O:123:HIS:ND1	2.38	0.56
43:h:211:ALA:HB3	43:h:240:LEU:HD21	1.87	0.56
1:0:79:LEU:HD13	1:0:110:LEU:HD21	1.87	0.56
10:A:332:G:O6	19:J:5:ARG:NH2	2.37	0.56
10:A:1182:C:O2'	31:V:67:ARG:NH1	2.28	0.56
11:B:48:ILE:HD12	11:B:149:MET:HE3	1.87	0.56
45:k:360:ASP:OD2	45:k:364:ARG:NH2	2.38	0.56
51:t:155:GLU:OE1	64:AB:126:LYS:NZ	2.35	0.56
57:1:679:U:O2'	57:1:695:G:O6	2.18	0.56
61:r:43:VAL:HG21	61:r:197:VAL:HG13	1.87	0.56
66:AD:17:ALA:O	66:AD:20:ILE:HG12	2.04	0.56
72:AJ:57:ILE:HB	72:AJ:93:ILE:HD11	1.87	0.56
10:A:15:U:H2'	10:A:16:G:O4'	2.05	0.56
10:A:38:C:O3'	20:K:6:ARG:NE	2.39	0.56
10:A:511:U:H2'	10:A:512:G:C8	2.39	0.56
15:F:36:HIS:CG	15:F:85:GLY:HA3	2.41	0.56
23:N:81:GLU:OE1	42:g:155:ASN:HB3	2.06	0.56
28:S:13:SER:HB2	28:S:53:TYR:HD2	1.70	0.56
30:U:28:LEU:HD12	30:U:111:ILE:HG21	1.87	0.56
53:v:126:THR:HG23	53:v:127:TYR:CD2	2.40	0.56
57:1:1014:G:N2	57:1:1030:U:O2	2.31	0.56
57:1:1400:G:N2	57:1:1403:A:OP2	2.35	0.56
57:1:1692:A:H2'	57:1:1693:A:C8	2.39	0.56
57:1:2244:U:H2'	57:1:2245:C:H6	1.71	0.56
4:4:51:G:O6	75:AM:30:ARG:NH2	2.32	0.56
9:9:11:SER:HB2	9:9:14:LYS:HB2	1.87	0.56
10:A:512:G:H1	10:A:541:C:H5	1.52	0.56
10:A:898:G:C2	57:1:2186:A:N6	2.73	0.56
10:A:1265:C:H2'	10:A:1266:G:H8	1.71	0.56
10:A:1637:U:H2'	10:A:1638:A:C8	2.40	0.56
11:B:140:ASN:ND2	32:W:31:SER:O	2.32	0.56
21:L:7:ASP:O	21:L:11:ILE:HG13	2.06	0.56
49:q:84:LYS:HB3	49:q:186:THR:HG21	1.87	0.56
57:1:1302:G:O6	57:1:2344:C:O2'	2.23	0.56
10:A:518:A:H2'	10:A:519:A:C8	2.40	0.56
11:B:62:ARG:HG2	11:B:184:LEU:HD21	1.88	0.56



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
14:E:78:PHE:O	14:E:79:LYS:HG2	2.06	0.56
16:G:156:ARG:O	16:G:157:ARG:NE	2.39	0.56
43:h:200:THR:N	43:h:209:ALA:O	2.39	0.56
10:A:249:A:H2	15:F:131:LEU:HD12	1.71	0.56
10:A:1301:G:OP1	28:S:7:LYS:N	2.28	0.56
10:A:1306:A:H61	11:B:108:THR:HG21	1.70	0.56
11:B:34:LYS:O	11:B:37:VAL:HG22	2.06	0.56
47:m:48:LYS:HG2	47:m:145:PHE:HE2	1.71	0.56
53:v:68:ARG:NH2	57:1:292:U:OP2	2.37	0.56
63:AA:103:GLU:HG3	63:AA:106:GLN:H	1.69	0.56
70:AH:41:ARG:HE	70:AH:50:ALA:HB1	1.70	0.56
14:E:141:GLY:HA3	14:E:183:LEU:HD23	1.87	0.56
22:M:123:VAL:HG12	22:M:142:VAL:HG13	1.88	0.56
47:m:85:ARG:NH2	47:m:250:ASP:OD2	2.39	0.56
50:s:99:THR:HG21	57:1:2656:C:O2'	2.06	0.56
74:AL:5:ILE:CD1	74:AL:52:TYR:HB3	2.35	0.56
74:AL:36:LYS:HG3	74:AL:37:LYS:HG2	1.88	0.56
10:A:778:U:O2'	10:A:779:U:O2	2.23	0.56
10:A:1366:U:O2'	10:A:1503:A:N1	2.33	0.56
57:1:539:G:H2'	57:1:540:C:C6	2.40	0.56
57:1:1230:G:N2	57:1:1259:A:OP1	2.38	0.56
57:1:1632:C:H1'	63:AA:76:ASN:HB2	1.88	0.56
57:1:1663:A:H2'	57:1:1664:G:C8	2.41	0.56
5:5:34:VAL:HG21	5:5:58:ALA:HB2	1.87	0.56
10:A:1602:C:P	16:G:81:ARG:HE	2.29	0.56
16:G:110:ALA:HA	16:G:113:ILE:HG12	1.87	0.56
25:P:66:CYS:HB2	25:P:71:ILE:CG1	2.36	0.56
43:h:107:HIS:HD2	43:h:127:SER:HB2	1.71	0.56
10:A:768:C:H2'	10:A:769:U:O4'	2.06	0.56
11:B:105:GLY:N	11:B:135:GLU:OE2	2.34	0.56
35:Z:57:VAL:HB	35:Z:60:PHE:HE2	1.69	0.56
50:s:108:GLU:OE1	50:s:122:ILE:HG21	2.06	0.56
57:1:1386:A:N6	57:1:1414:A:O2'	2.39	0.56
30:U:76:LEU:CB	30:U:101:ASN:HD21	2.18	0.55
57:1:437:G:O2'	57:1:438:A:OP1	2.23	0.55
57:1:653:C:H2'	57:1:654:A:C8	2.41	0.55
57:1:2244:U:H2'	57:1:2245:C:C6	2.42	0.55
3:3:23:A:H2'	3:3:24:A:C8	2.41	0.55
10:A:116:U:H2'	10:A:117:U:C6	2.41	0.55
10:A·538·G·N2	41:f:25·GLU·OE2	2.22	0.55
17:H:206:ALA:O	17:H:210:GLN·HG2	2.07	0.55



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
33:X:31:SER:O	33:X:34:ILE:HG22	2.05	0.55
57:1:1174:G:N3	57:1:1324:U:O2'	2.38	0.55
57:1:2527:G:N2	57:1:2527:G:OP2	2.39	0.55
10:A:405:A:H2'	10:A:406:C:C6	2.41	0.55
10:A:446:C:OP2	15:F:49:ARG:NH1	2.35	0.55
10:A:457:G:OP1	35:Z:109:LYS:NZ	2.33	0.55
10:A:1145:A:H2'	10:A:1146:C:C6	2.42	0.55
10:A:1265:C:H5'	40:e:44:ARG:HH12	1.70	0.55
41:f:54:ARG:HH12	41:f:56:MET:HE3	1.71	0.55
10:A:739:A:H5"	10:A:740:A:H5'	1.88	0.55
10:A:1258:G:N7	10:A:1416:U:H3'	2.21	0.55
10:A:1716:C:HO2'	19:J:2:GLY:N	2.04	0.55
12:C:88:VAL:HG21	12:C:96:LEU:HD23	1.89	0.55
43:h:200:THR:O	43:h:209:ALA:N	2.39	0.55
57:1:438:A:N1	57:1:489:G:O2'	2.30	0.55
57:1:2334:A:H61	57:1:2955:C:H5	1.54	0.55
10:A:1232:U:H2'	10:A:1233:C:H6	1.72	0.55
10:A:1240:G:N7	23:N:46:ARG:NH2	2.55	0.55
10:A:1383:U:O2'	10:A:1386:A:N6	2.28	0.55
13:D:122:ALA:O	13:D:125:VAL:HG22	2.06	0.55
21:L:54:TYR:HD1	21:L:72:GLY:HA2	1.71	0.55
57:1:1242:G:H22	57:1:1262:G:P	2.29	0.55
57:1:1268:C:H3'	57:1:1269:A:H4'	1.88	0.55
57:1:1275:C:H2'	57:1:1276:C:C6	2.42	0.55
10:A:1072:A:H2'	10:A:1073:A:C8	2.42	0.55
10:A:1395:G:N2	10:A:1398:G:OP2	2.39	0.55
10:A:1566:U:H2'	10:A:1567:C:C6	2.41	0.55
10:A:1669:U:H4'	17:H:65:GLN:NE2	2.22	0.55
14:E:210:ALA:O	28:S:19:ARG:NH1	2.40	0.55
15:F:151:ASP:OD2	17:H:215:ARG:NH2	2.40	0.55
57:1:252:U:H5'	57:1:253:A:C8	2.42	0.55
57:1:2808:OMC:H5	57:1:2824:C:H42	1.52	0.55
62:x:126:ARG:HD3	62:x:140:GLN:HG2	1.88	0.55
10:A:822:G:O2'	10:A:823:G:H5"	2.06	0.55
10:A:1431:G:N2	42:g:129:THR:O	2.29	0.55
10:A:1469:A:H2'	10:A:1470:G:C8	2.41	0.55
26:Q:25:LEU:HG	26:Q:87:PRO:HB3	1.89	0.55
29:T:33:THR:HA	29:T:38:VAL:O	2.07	0.55
38:c:14:THR:O	38:c:18:GLN:HG3	2.06	0.55
57:1:1735:U:O2'	70:AH:41:ARG:NH1	2.40	0.55
10:A:1339:G:O6	10:A:1354:U:O2	2.25	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
11:B:21:ASN:HB2	11:B:24:LEU:HD12	1.87	0.55
12:C:111:ARG:NH2	12:C:114:VAL:HG11	2.21	0.55
15:F:54:TYR:OH	15:F:97:GLU:OE2	2.25	0.55
16:G:97:LEU:HD23	16:G:176:THR:OG1	2.06	0.55
29:T:113:LEU:HA	29:T:116:LEU:HD23	1.88	0.55
54:w:122:PRO:HA	54:w:125:LEU:HD12	1.89	0.55
57:1:1550:U:H3'	57:1:1551:U:H6	1.72	0.55
57:1:1782:G:H2'	57:1:1783:A:C8	2.41	0.55
57:1:2335:A:H2'	57:1:2336:A:H8	1.72	0.55
9:9:51:ARG:HG2	9:9:52:GLN:H	1.71	0.55
10:A:1399:U:O2'	10:A:1400:U:OP1	2.24	0.55
10:A:1503:A:H5"	31:V:57:MET:SD	2.46	0.55
19:J:3:ILE:O	19:J:30:GLY:N	2.40	0.55
37:b:91:ASP:O	37:b:94:ILE:HG12	2.07	0.55
57:1:730:A:H4'	57:1:730:A:OP1	2.05	0.55
10:A:932:U:H2'	10:A:933:A:H8	1.71	0.55
17:H:37:GLU:N	17:H:37:GLU:OE1	2.40	0.55
33:X:80:ASN:OD1	33:X:124:LYS:NZ	2.29	0.55
50:s:29:ARG:HH11	50:s:32:ARG:HH12	1.52	0.55
54:w:11:ASP:HB2	54:w:118:ARG:HB3	1.88	0.55
57:1:2558:G:O2'	60:p:49:ARG:NH2	2.40	0.55
57:1:3166:A:H2'	57:1:3167:G:C8	2.41	0.55
60:p:83:LEU:HD12	60:p:181:VAL:HG12	1.88	0.55
3:3:11:A:N6	47:m:16:PHE:O	2.40	0.54
14:E:214:ASP:CG	14:E:215:GLU:H	2.13	0.54
17:H:145:PHE:CZ	17:H:156:PHE:HB3	2.36	0.54
55:y:76:ALA:HA	55:y:79:LYS:HG3	1.89	0.54
57:1:2232:U:H2'	57:1:2239:G:N2	2.21	0.54
73:AK:24:ARG:HG2	73:AK:24:ARG:HH11	1.71	0.54
10:A:1396:A:O2'	10:A:1397:A:OP1	2.25	0.54
10:A:1784:A:H5'	37:b:95:ARG:NE	2.22	0.54
49:q:168:ARG:NH1	57:1:2866:C:OP2	2.41	0.54
57:1:218:A:O2'	57:1:219:G:N2	2.27	0.54
79:AQ:86:LEU:HD12	79:AQ:87:ARG:HG3	1.88	0.54
7:7:50:SER:OG	57:1:3298:G:O2'	2.25	0.54
12:C:30:PHE:HB3	12:C:96:LEU:HD11	1.89	0.54
24:O:100:LYS:O	24:O:103:GLU:HG3	2.07	0.54
57:1:1623:U:H2'	57:1:1810:A:H62	1.71	0.54
57:1:2126:U:H2'	57:1:2127:A:C8	2.43	0.54
1:0:158:LYS:NZ	1:0:159:SER:O	2.32	0.54
14:E:50:ILE:HD12	14:E:88:TYR:HB2	1.89	0.54



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
26:Q:75:VAL:HG22	26:Q:93:VAL:HB	1.89	0.54
45:k:123:TYR:CZ	45:k:124:LYS:HG3	2.42	0.54
50:s:110:ILE:HG21	50:s:116:TYR:HD2	1.72	0.54
52:u:19:VAL:HG11	52:u:55:ILE:HD12	1.88	0.54
57:1:2090:U:H4'	57:1:2091:A:O5'	2.06	0.54
10:A:1160:U:OP2	29:T:137:HIS:ND1	2.41	0.54
10:A:1783:C:O2'	37:b:95:ARG:NH1	2.41	0.54
26:Q:73:PRO:CG	26:Q:92:SER:HA	2.36	0.54
35:Z:83:LYS:HE3	35:Z:96:LEU:HB3	1.90	0.54
47:m:19:PRO:HG2	47:m:24:GLN:HB3	1.89	0.54
57:1:1199:A:H2'	57:1:1200:A:C8	2.42	0.54
57:1:1225:G:H2'	57:1:1226:G:H8	1.72	0.54
57:1:2546:U:H5'	57:1:2547:G:O4'	2.08	0.54
81:1:3401:YMZ:NAP	81:1:3401:YMZ:FAF	2.31	0.54
10:A:211:A:N6	10:A:250:U:H3	2.05	0.54
10:A:1237:C:O2'	42:g:184:GLY:N	2.41	0.54
11:B:8:ASP:OD1	11:B:9:LEU:N	2.41	0.54
11:B:66:ALA:HB2	32:W:37:ALA:N	2.22	0.54
39:d:18:ARG:HD2	39:d:26:THR:HG22	1.89	0.54
46:1:296:VAL:O	46:1:300:VAL:HG13	2.07	0.54
52:u:121:ARG:NH2	57:1:3179:U:OP2	2.40	0.54
57:1:1837:A:H1'	75:AM:45:ARG:HH22	1.72	0.54
10:A:17:C:H2'	10:A:18:C:C6	2.42	0.54
10:A:600:U:H2'	10:A:601:U:C6	2.43	0.54
10:A:815:U:O2'	10:A:816:U:O5'	2.26	0.54
12:C:90:GLU:OE2	12:C:92:GLN:HG3	2.08	0.54
25:P:74:VAL:HG13	25:P:105:LEU:HD11	1.88	0.54
46:l:289:ARG:O	46:1:293:SER:OG	2.14	0.54
47:m:235:ASP:OD1	47:m:235:ASP:N	2.41	0.54
50:s:133:ARG:NH2	50:s:158:ASP:OD2	2.35	0.54
53:v:91:GLN:O	53:v:93:LYS:NZ	2.40	0.54
53:v:113:LEU:HB2	53:v:134:LEU:HD23	1.90	0.54
57:1:498:C:H5"	59:n:25:ARG:NH2	2.23	0.54
57:1:1611:U:H2'	57:1:1612:U:C6	2.43	0.54
57:1:1617:A:H2'	57:1:1618:U:H6	1.73	0.54
59:n:12:GLU:OE2	68:AF:91:LYS:HB2	2.08	0.54
78:AP:8:ARG:HG2	78:AP:10:THR:HG23	1.89	0.54
5:5:106:TYR:OH	57:1:1673:G:OP2	2.21	0.54
10:A:824:U:H4'	10:A:825:U:OP2	2.07	0.54
12:C:36:THR:HA	12:C:41:ARG:HD2	1.90	0.54
20:K:41:GLU:HG2	20:K:44:ARG:NH2	2.22	0.54



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
21:L:70:ASP:OD1	21:L:91:ARG:NH2	2.40	0.54
25:P:14:ILE:HG23	25:P:78:LEU:HA	1.88	0.54
51:t:138:PHE:HE1	71:AI:120:ALA:HB2	1.73	0.54
31:V:101:ARG:O	31:V:105:ILE:HG23	2.07	0.54
57:1:264:G:OP1	72:AJ:33:SER:OG	2.16	0.54
1:0:115:ARG:NH1	57:1:1316:C:O2'	2.32	0.54
10:A:1776:G:OP2	25:P:127:ARG:NH2	2.41	0.54
16:G:194:LEU:HD12	16:G:197:GLU:OE2	2.08	0.54
34:Y:88:PRO:O	34:Y:89:ASN:HB2	2.08	0.54
57:1:248:U:H2'	57:1:249:G:H4'	1.89	0.54
10:A:1160:U:H2'	10:A:1161:G:C8	2.43	0.53
10:A:1668:A:H8	17:H:65:GLN:HG3	1.73	0.53
10:A:1719:A:H2'	10:A:1720:C:C6	2.43	0.53
27:R:47:VAL:HG22	27:R:81:ARG:HB3	1.90	0.53
40:e:3:HIS:HA	40:e:6:VAL:HG12	1.89	0.53
57:1:649:G:O2'	57:1:1431:A:OP1	2.26	0.53
24:O:98:VAL:HG13	24:O:115:LEU:HD13	1.90	0.53
30:U:27:LYS:HZ3	30:U:111:ILE:HB	1.71	0.53
43:h:69:VAL:HA	43:h:85:SER:HA	1.90	0.53
43:h:107:HIS:CD2	43:h:127:SER:HB2	2.44	0.53
53:v:5:LYS:NZ	57:1:266:C:OP1	2.32	0.53
57:1:2632:G:OP1	57:1:2722:U:O2'	2.27	0.53
75:AM:28:ARG:HA	75:AM:33:ASN:ND2	2.23	0.53
10:A:970:G:H2'	10:A:971:G:H8	1.71	0.53
10:A:1011:A:N7	10:A:1759:C:O2'	2.34	0.53
17:H:43:ASP:O	17:H:46:LYS:NZ	2.30	0.53
34:Y:3:LYS:HD2	34:Y:7:ARG:HH21	1.74	0.53
49:q:167:VAL:HG23	49:q:172:ILE:HG22	1.90	0.53
57:1:2544:U:H1'	57:1:2545:C:H2'	1.91	0.53
10:A:403:C:O2'	17:H:92:ARG:O	2.25	0.53
10:A:1573:A:H2'	10:A:1574:A:O4'	2.08	0.53
11:B:184:LEU:HB3	32:W:45:ALA:HB2	1.90	0.53
14:E:124:LEU:HD22	14:E:155:ASP:HB2	1.89	0.53
16:G:33:VAL:HG12	27:R:45:PHE:CZ	2.43	0.53
16:G:116:HIS:O	16:G:120:ILE:HG13	2.09	0.53
35:Z:86:GLU:OE2	35:Z:90:ARG:HD2	2.08	0.53
43:h:148:HIS:CD2	43:h:178:TRP:HZ2	2.26	0.53
52:u:129:VAL:HG21	57:1:3194:G:H5'	1.91	0.53
57:1:158:A:H2'	57:1:159:A:C8	2.43	0.53
57:1:1550:U:HO2'	57:1:1551:U:P	2.30	0.53
57:1:2634:G:H2'	57:1:2635:A:C8	2.42	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:99:C:OP2	10:A:376:A:O2'	2.21	0.53
10:A:1154:G:N1	10:A:1562:G:OP2	2.39	0.53
14:E:73:LEU:HD21	21:L:67:THR:HG22	1.90	0.53
22:M:66:ILE:HG21	22:M:140:LEU:HD11	1.89	0.53
46:l:85:ARG:NH1	57:1:365:A:OP1	2.41	0.53
52:u:124:THR:OG1	54:w:186:THR:HG21	2.09	0.53
57:1:3082:C:H2'	57:1:3083:U:C6	2.44	0.53
72:AJ:36:THR:HA	72:AJ:39:VAL:HG12	1.90	0.53
79:AQ:10:ILE:HD13	79:AQ:30:GLU:HG2	1.91	0.53
1:0:12:ARG:HB3	1:0:24:LEU:HD23	1.91	0.53
10:A:835:A:H5'	56:z:165:ARG:HD2	1.90	0.53
13:D:121:LYS:O	13:D:125:VAL:HG13	2.08	0.53
14:E:9:LYS:HE3	31:V:60:LYS:HD3	1.90	0.53
16:G:161:ASP:OD1	16:G:162:VAL:N	2.40	0.53
21:L:15:LEU:O	21:L:19:GLY:HA2	2.08	0.53
29:T:113:LEU:HA	29:T:116:LEU:CD2	2.39	0.53
59:n:39:LEU:HD13	59:n:83:VAL:HG11	1.90	0.53
68:AF:106:ARG:NH2	68:AF:122:ASN:O	2.42	0.53
10:A:12:U:H2'	10:A:13:C:C6	2.43	0.53
10:A:39:A:OP1	20:K:3:ARG:NH2	2.42	0.53
10:A:898:G:H8	10:A:898:G:OP1	1.91	0.53
11:B:112:THR:HG22	11:B:115:PHE:HB2	1.89	0.53
14:E:171:ILE:HG12	14:E:188:LYS:HG3	1.90	0.53
15:F:127:LYS:HB2	15:F:140:VAL:HG13	1.91	0.53
36:a:65:LEU:HD23	36:a:69:LEU:HD13	1.91	0.53
56:z:98:ARG:HD2	56:z:133:LYS:O	2.09	0.53
57:1:1810:A:H4'	57:1:1811:U:O4'	2.09	0.53
66:AD:45:ILE:HD12	66:AD:92:LEU:HD11	1.90	0.53
72:AJ:54:ARG:O	72:AJ:57:ILE:HG12	2.08	0.53
1:0:172:TYR:OH	52:u:57:LEU:HG	2.08	0.53
2:2:158:THR:OG1	61:r:169:LYS:NZ	2.29	0.53
10:A:1282:G:N2	10:A:1285:A:OP2	2.28	0.53
12:C:69:CYS:HA	12:C:83:LYS:HA	1.90	0.53
15:F:41:SER:OG	15:F:84:ALA:O	2.21	0.53
15:F:85:GLY:N	15:F:88:ASP:OD2	2.42	0.53
20:K:86:LEU:HD23	20:K:87:SER:O	2.08	0.53
29:T:44:ASN:OD1	29:T:45:LEU:N	2.42	0.53
31:V:102:ILE:HA	31:V:105:ILE:HG12	1.89	0.53
54:w:190:GLU:OE1	54:w:190:GLU:N	2.40	0.53
55:y:66:ARG:HH21	55:y:143:PRO:HD3	1.74	0.53
57:1:716:G:H3'	57:1:717:A:H5"	1.91	0.53



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
61:r:75:TYR:O	61:r:79:VAL:HG22	2.09	0.53
2:2:68:THR:O	47:m:41:LYS:HB2	2.08	0.53
10:A:1245:U:H2'	10:A:1246:G:C8	2.44	0.53
10:A:1659:G:H2'	10:A:1660:G:H8	1.72	0.53
53:v:178:HIS:ND1	57:1:68:C:OP1	2.28	0.53
57:1:353:G:O6	73:AK:55:ARG:NH2	2.42	0.53
57:1:1943:G:O2'	57:1:1944:G:OP1	2.24	0.53
4:4:8:C:H2'	4:4:9:A:H8	1.74	0.53
5:5:97:ARG:NH1	57:1:1675:A:OP1	2.30	0.53
10:A:881:U:H5'	12:C:23:PRO:HG2	1.90	0.53
10:A:1478:A:OP2	10:A:1479:A:N6	2.42	0.53
11:B:187:ILE:HG13	11:B:188:ILE:N	2.24	0.53
14:E:165:THR:HA	14:E:169:ILE:HD12	1.91	0.53
27:R:98:GLU:O	27:R:102:ASN:ND2	2.41	0.53
30:U:117:SER:HB3	30:U:123:ARG:HB2	1.90	0.53
39:d:12:VAL:HG22	39:d:52:ASP:H	1.74	0.53
57:1:487:C:H2'	57:1:488:G:O4'	2.09	0.53
57:1:2130:A:H2'	57:1:2131:U:H6	1.74	0.53
57:1:3196:U:H2'	57:1:3197:G:H8	1.74	0.53
61:r:44:ASP:OD1	61:r:181:TYR:OH	2.18	0.53
68:AF:35:LYS:HB3	68:AF:37:LYS:NZ	2.24	0.53
15:F:98:HIS:HB2	15:F:114:ILE:O	2.09	0.52
17:H:72:ARG:HD3	17:H:96:SER:HB2	1.91	0.52
21:L:82:ILE:HG13	21:L:83:PRO:HD2	1.90	0.52
57:1:716:G:O2'	57:1:717:A:OP1	2.24	0.52
57:1:1795:A:H2'	57:1:1796:A:H8	1.74	0.52
76:AN:23:CYS:HB2	76:AN:38:LYS:HD2	1.91	0.52
3:3:112:G:H2'	3:3:113:C:C6	2.44	0.52
5:5:29:ASP:OD2	5:5:32:SER:OG	2.25	0.52
10:A:167:A:OP1	17:H:137:ARG:NE	2.36	0.52
10:A:283:G:H2'	10:A:284:C:C6	2.44	0.52
10:A:352:C:H5"	19:J:16:ALA:HB2	1.90	0.52
10:A:1699:G:N1	10:A:1700:G:N3	2.57	0.52
12:C:26:ARG:O	12:C:50:ARG:N	2.39	0.52
17:H:64:LYS:HB2	17:H:97:VAL:HG21	1.91	0.52
20:K:110:GLN:NE2	20:K:122:ILE:HG13	2.25	0.52
27:R:64:ILE:HG21	27:R:84:ILE:HD13	1.91	0.52
10:A:78:A:H2'	10:A:79:C:H6	1.75	0.52
10:A:1486:G:H1	10:A:1495:U:H3	1.57	0.52
45:k:25:GLN:NE2	57:1:3269:C:O2	2.42	0.52
57:1:1653:C:O2'	57:1:1793:A:OP2	2.24	0.52



Atom-1	Atom-2	Interatomic	Clash
		distance $(\text{\AA})$	overlap (Å)
10:A:1064:U:H2'	10:A:1065:U:C6	2.44	0.52
12:C:131:ASP:CG	12:C:180:THR:HG1	2.18	0.52
18:I:159:ASP:OD1	18:I:160:TYR:N	2.42	0.52
43:h:112:LEU:N	43:h:126:ALA:O	2.32	0.52
47:m:238:GLU:OE1	47:m:238:GLU:N	2.26	0.52
57:1:482:U:H2'	57:1:483:U:C4	2.44	0.52
57:1:1190:G:H2'	57:1:1191:A:C8	2.44	0.52
57:1:2525:A:H2'	57:1:2526:C:O4'	2.09	0.52
60:p:140:VAL:HG11	60:p:198:VAL:HG11	1.91	0.52
75:AM:23:LEU:HD12	75:AM:24:PRO:HD2	1.90	0.52
10:A:853:G:H22	10:A:945:U:H3	1.57	0.52
10:A:1772:U:P	25:P:128:ARG:HH22	2.33	0.52
21:L:14:TYR:CE2	21:L:35:ILE:HD11	2.45	0.52
23:N:97:LEU:HD23	23:N:100:TRP:CZ2	2.44	0.52
57:1:1059:G:N7	57:1:1093:G:O2'	2.35	0.52
57:1:1153:G:O2'	57:1:1165:A:N3	2.40	0.52
4:4:75:G:OP2	9:9:74:TYR:OH	2.28	0.52
6:6:10:LYS:NZ	6:6:54:ALA:O	2.41	0.52
10:A:903:U:H2'	10:A:904:A:H8	1.73	0.52
10:A:1324:C:O2'	10:A:1326:A:N7	2.38	0.52
10:A:1460:G:H2'	10:A:1461:A:C8	2.42	0.52
13:D:139:TRP:CE2	33:X:97:ARG:HD2	2.45	0.52
29:T:52:VAL:HG12	29:T:65:GLU:HG2	1.91	0.52
30:U:70:GLN:HB2	30:U:121:GLY:HA3	1.91	0.52
43:h:155:VAL:O	43:h:156:ARG:NH1	2.37	0.52
57:1:172:C:O2'	57:1:173:C:OP1	2.24	0.52
10:A:1152:G:N2	27:R:138:GLN:OE1	2.42	0.52
10:A:1602:C:OP1	16:G:81:ARG:NH2	2.38	0.52
10:A:1670:U:O2'	10:A:1671:G:O5'	2.28	0.52
14:E:23:ASN:O	14:E:27:THR:HG23	2.10	0.52
50:s:20:ASN:HB3	50:s:126:ASP:HB3	1.90	0.52
57:1:358:G:N2	57:1:361:A:OP2	2.42	0.52
57:1:654:A:H2'	57:1:655:A:C8	2.44	0.52
57:1:1080:A:H2'	57:1:1081:A:C8	2.44	0.52
57:1:2335:A:H2'	57:1:2336:A:C8	2.45	0.52
63:AA:33:THR:HG22	63:AA:34:LYS:N	2.24	0.52
4:4:29:U:H5"	51:t:27:ASP:HB3	1.92	0.52
24:O:124:ARG:HG2	24:O:127:ARG:HH22	1.75	0.52
42:g:187:HIS:O	42:g:187:HIS:ND1	2.43	0.52
43:h:70:GLN:HB2	43:h:86:TRP:HE1	1.74	0.52
47:m:290:ILE:HG21	61:r:218:TYR:CD2	2.45	0.52



Atom-1	Atom-2	Interatomic	Clash
		distance $(\text{\AA})$	overlap (Å)
53:v:6:TYR:OH	60:p:145:GLU:OE2	2.22	0.52
57:1:1060:A:H4'	57:1:1061:A:O5'	2.10	0.52
57:1:2384:C:H2'	57:1:2385:C:C6	2.45	0.52
10:A:10:G:O2'	13:D:82:GLN:OE1	2.26	0.52
47:m:286:VAL:HG23	61:r:206:LEU:HD22	1.92	0.52
53:v:65:ARG:HG3	53:v:129:TYR:CE1	2.45	0.52
57:1:108:A:N1	57:1:322:U:O2'	2.42	0.52
57:1:995:G:N3	57:1:998:A:N6	2.57	0.52
57:1:1124:U:OP1	61:r:4:ARG:NH1	2.36	0.52
59:n:39:LEU:HD11	59:n:53:TYR:HB2	1.90	0.52
60:p:102:THR:HG22	60:p:103:SER:H	1.75	0.52
2:2:106:LEU:O	2:2:110:LYS:HG2	2.09	0.52
10:A:189:G:H1'	10:A:193:G:N2	2.25	0.52
10:A:1168:A:N3	10:A:1195:C:O2'	2.36	0.52
18:I:162:LEU:O	18:I:166:GLN:HG3	2.09	0.52
21:L:8:ARG:HG2	21:L:12:HIS:HE1	1.73	0.52
29:T:63:GLN:O	29:T:67:GLU:HG3	2.10	0.52
43:h:132:VAL:O	43:h:145:LEU:N	2.29	0.52
57:1:1264:G:O5'	57:1:1264:G:H8	1.92	0.52
57:1:2933:G:H2'	57:1:2934:U:C6	2.45	0.52
62:x:27:LYS:O	62:x:31:GLU:HG2	2.09	0.52
10:A:151:G:H2'	10:A:152:G:C8	2.46	0.51
10:A:1486:G:H5"	30:U:122:ARG:NH1	2.26	0.51
10:A:1783:C:O2'	37:b:95:ARG:HD3	2.10	0.51
14:E:102:GLN:O	14:E:106:LEU:HD23	2.11	0.51
16:G:32:ASP:OD1	16:G:33:VAL:N	2.42	0.51
24:O:26:PHE:HZ	24:O:60:VAL:HG22	1.74	0.51
63:AA:115:LYS:NZ	63:AA:119:GLU:OE2	2.42	0.51
5:5:53:ASP:HA	5:5:69:SER:HB3	1.91	0.51
19:J:98:LYS:HE2	19:J:178:ARG:HG2	1.91	0.51
20:K:58:ASP:O	20:K:61:THR:HG22	2.09	0.51
32:W:66:ASP:OD1	32:W:67:ASP:N	2.42	0.51
54:w:183:LYS:HA	54:w:186:THR:HG22	1.92	0.51
57:1:3261:A:H2'	57:1:3262:U:H6	1.74	0.51
4:4:8:C:H2'	4:4:9:A:C8	2.45	0.51
10:A:876:A:H2'	10:A:877:G:H8	1.75	0.51
10:A:1524:C:O4'	10:A:1559:G:N2	2.43	0.51
10:A:1578:C:H2'	10:A:1579:A:C8	2.46	0.51
26:Q:29:PRO:HG2	26:Q:32:GLU:CD	2.35	0.51
57:1:1079:G:H2'	57:1:1080:A:C8	2.45	0.51
57:1:1451:U:H1'	67:AE:25:LYS:HE3	1.92	0.51


		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:2583:U:H2'	57:1:2584:U:C6	2.45	0.51
63:AA:83:THR:HG22	70:AH:93:PHE:CZ	2.45	0.51
4:4:52:A:H62	75:AM:27:ILE:HD13	1.75	0.51
10:A:165:U:H2'	10:A:166:A:H5"	1.92	0.51
10:A:560:G:H2'	10:A:561:U:O2	2.11	0.51
10:A:748:G:H4'	15:F:256:ARG:NH1	2.26	0.51
10:A:961:G:H1	10:A:1008:A:HO2'	1.55	0.51
17:H:216:LEU:O	17:H:220:LYS:HG2	2.11	0.51
18:I:92:ARG:HH12	18:I:120:LYS:HB3	1.76	0.51
25:P:73:ALA:HB2	25:P:106:ARG:HB2	1.93	0.51
47:m:94:ASN:HB2	47:m:97:ALA:H	1.75	0.51
57:1:1218:G:O2'	57:1:1219:A:OP2	2.24	0.51
57:1:1762:G:O2'	57:1:1763:C:OP1	2.26	0.51
64:AB:19:LYS:HB3	64:AB:25:HIS:HB2	1.93	0.51
10:A:103:A:H4'	10:A:105:A:N7	2.26	0.51
10:A:338:U:H2'	10:A:339:A:H8	1.76	0.51
10:A:433:C:H5"	34:Y:50:LYS:HE3	1.92	0.51
10:A:1661:C:OP1	17:H:92:ARG:NH1	2.41	0.51
13:D:163:ARG:HD3	13:D:165:ILE:HD11	1.93	0.51
15:F:199:GLU:OE2	15:F:201:HIS:NE2	2.31	0.51
31:V:112:ASP:OD1	31:V:113:VAL:N	2.43	0.51
34:Y:92:CYS:HG	34:Y:136:TRP:CD1	2.29	0.51
6:6:36:VAL:HG22	6:6:58:VAL:HG11	1.93	0.51
13:D:75:VAL:HG21	13:D:120:ILE:HD13	1.92	0.51
16:G:58:LEU:HD21	16:G:167:ARG:HH11	1.76	0.51
20:K:119:ALA:HB2	20:K:128:LEU:HD12	1.91	0.51
21:L:38:ARG:O	21:L:42:VAL:HG23	2.10	0.51
35:Z:88:ALA:O	35:Z:92:VAL:HG23	2.10	0.51
46:l:299:VAL:HG21	55:y:133:LYS:HG3	1.91	0.51
50:s:65:ILE:HG13	50:s:66:ALA:N	2.26	0.51
51:t:57:VAL:HG22	51:t:69:VAL:HG22	1.91	0.51
56:z:62:ARG:HH22	57:1:3039:C:H3'	1.75	0.51
57:1:628:A:H2'	57:1:629:A:H8	1.76	0.51
57:1:1029:U:O2'	57:1:1030:U:OP1	2.26	0.51
57:1:1241:A:N6	57:1:1268:C:O2'	2.42	0.51
61:r:187:ASN:ND2	61:r:189:GLU:OE2	2.43	0.51
75:AM:24:PRO:HG2	75:AM:27:ILE:HD12	1.92	0.51
10:A:1131:G:H2'	10:A:1132:A:H8	1.76	0.51
10:A:1205:C:H2'	10:A:1206:A:C8	2.46	0.51
10:A:1302:C:H2'	10:A:1303:G:O4'	2.09	0.51
10:A:1593:C:H2'	10:A:1594:G:C8	2.46	0.51



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
15:F:71:GLN:OE1	15:F:74:GLY:HA2	2.10	0.51
43:h:70:GLN:HB2	43:h:86:TRP:NE1	2.26	0.51
57:1:617:A:H5'	57:1:619:A:H1'	1.92	0.51
57:1:619:A:H2'	57:1:620:A:C8	2.45	0.51
57:1:729:C:H3'	57:1:730:A:H5"	1.93	0.51
10:A:119:A:H1'	10:A:395:A:C5	2.46	0.51
10:A:188:U:H2'	10:A:189:G:C8	2.45	0.51
10:A:415:A:H5'	10:A:416:G:C5	2.46	0.51
10:A:1276:G:H1	10:A:1309:G:H22	1.59	0.51
10:A:1672:G:H2'	10:A:1674:U:C2	2.46	0.51
28:S:37:GLU:OE1	43:h:151:TRP:NE1	2.41	0.51
29:T:62:THR:OG1	29:T:65:GLU:OE1	2.29	0.51
47:m:283:GLN:O	47:m:286:VAL:HG12	2.10	0.51
57:1:1637:U:O2'	57:1:1638:A:H3'	2.11	0.51
57:1:3136:C:H2'	57:1:3137:A:C8	2.46	0.51
66:AD:16:LEU:O	66:AD:19:THR:HG22	2.10	0.51
4:4:9:A:H2'	4:4:10:A:C8	2.46	0.51
10:A:1580:A:H2'	10:A:1581:G:C8	2.46	0.51
10:A:1635:A:H2'	10:A:1636:C:C6	2.45	0.51
14:E:69:GLU:O	14:E:73:LEU:HD23	2.11	0.51
43:h:153:SER:HB3	43:h:171:TRP:CD1	2.46	0.51
44:j:9:ARG:HD2	57:1:907:C:OP2	2.10	0.51
51:t:129:LYS:O	51:t:131:LYS:NZ	2.43	0.51
51:t:168:ALA:N	64:AB:135:GLU:OE2	2.35	0.51
54:w:59:LEU:HD21	54:w:75:ARG:HH22	1.76	0.51
57:1:85:G:O2'	57:1:97:G:O6	2.20	0.51
57:1:1493:C:H2'	57:1:1494:A:C8	2.46	0.51
61:r:179:ASP:OD1	61:r:180:GLU:N	2.44	0.51
12:C:180:THR:HG23	12:C:183:GLN:H	1.76	0.51
51:t:2:ALA:HB1	64:AB:33:GLY:O	2.11	0.51
57:1:374:A:N3	57:1:376:G:H5"	2.26	0.51
57:1:1476:G:O2'	57:1:1867:U:O4	2.26	0.51
57:1:1787:U:H2'	57:1:1788:C:C6	2.46	0.51
3:3:27:A:H2'	3:3:28:C:C6	2.45	0.50
4:4:142:C:H2'	4:4:143:U:C6	2.47	0.50
10:A:103:A:H4'	10:A:105:A:C8	2.46	0.50
11:B:118:PRO:HG2	11:B:141:ILE:HD13	1.93	0.50
16:G:160:VAL:HG23	39:d:43:ASN:CG	2.36	0.50
27:R:98:GLU:HG3	27:R:101:LYS:HE3	1.93	0.50
39:d:10:ALA:HA	39:d:32:PHE:HA	1.93	0.50
43:h:81:ALA:O	43:h:93:TRP:N	2.30	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
43:h:201:LEU:H	43:h:201:LEU:HD23	1.75	0.50
57:1:496:A:H2'	57:1:497:U:C6	2.46	0.50
57:1:3308:G:H21	57:1:3327:A:H2	1.58	0.50
59:n:65:SER:HB2	59:n:75:LEU:HD23	1.93	0.50
3:3:121:U:OP2	47:m:265:TYR:OH	2.28	0.50
10:A:510:A:O2'	20:K:133:HIS:NE2	2.42	0.50
10:A:740:A:O2'	10:A:741:A:OP1	2.29	0.50
10:A:1469:A:N3	10:A:1594:G:O2'	2.38	0.50
10:A:1774:C:H2'	10:A:1775:G:C8	2.46	0.50
21:L:32:HIS:HE1	21:L:35:ILE:HD13	1.75	0.50
26:Q:26:VAL:HG21	26:Q:90:ILE:HD13	1.93	0.50
27:R:49:GLU:OE1	27:R:81:ARG:NH2	2.39	0.50
34:Y:70:LYS:O	34:Y:87:VAL:HG22	2.10	0.50
43:h:214:ASP:N	43:h:214:ASP:OD1	2.41	0.50
52:u:34:ASP:OD1	52:u:35:GLN:N	2.40	0.50
73:AK:69:HIS:O	73:AK:73:ARG:HG3	2.11	0.50
2:2:133:ALA:HB3	48:0:119:LYS:HB2	1.94	0.50
10:A:1143:C:O2'	10:A:1568:C:OP2	2.25	0.50
11:B:20:ALA:O	11:B:21:ASN:ND2	2.45	0.50
15:F:11:ARG:HH12	15:F:24:SER:HB2	1.76	0.50
17:H:43:ASP:HA	17:H:46:LYS:HG3	1.93	0.50
30:U:107:ALA:O	30:U:111:ILE:HG23	2.12	0.50
57:1:486:C:H2'	57:1:487:C:H6	1.74	0.50
59:n:170:ARG:HB3	59:n:172:HIS:CE1	2.47	0.50
61:r:4:ARG:NH1	61:r:99:ILE:HG13	2.26	0.50
10:A:108:A:H2'	10:A:109:G:C8	2.46	0.50
10:A:268:C:H41	17:H:182:GLN:HE22	1.58	0.50
10:A:291:U:H2'	10:A:292:C:H6	1.75	0.50
10:A:1498:G:H2'	10:A:1499:G:H8	1.76	0.50
10:A:1602:C:N4	16:G:80:LYS:O	2.44	0.50
28:S:31:ASN:O	28:S:35:THR:HG23	2.11	0.50
29:T:110:ARG:NH2	29:T:114:GLU:HG3	2.26	0.50
48:0:147:TYR:OH	48:0:180:GLU:OE2	2.25	0.50
49:q:85:GLY:O	49:q:186:THR:HG23	2.11	0.50
57:1:1116:A:H2'	57:1:1117:U:C6	2.46	0.50
10:A:878:U:H5'	10:A:879:U:OP2	2.10	0.50
10:A:1092:G:O2'	10:A:1093:G:H5'	2.11	0.50
10:A:1463:G:H2'	10:A:1464:G:C8	2.46	0.50
13:D:133:PRO:HB2	13:D:217:TYR:HE2	1.77	0.50
15:F:57:ASN:HD21	15:F:59:ARG:NE	2.03	0.50
17:H:71:THR:HG22	17:H:72:ARG:N	2.24	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
17:H:151:ASP:OD1	17:H:152:ASP:N	2.44	0.50
21:L:17:GLN:H	21:L:88:PRO:HB3	1.76	0.50
21:L:43:ILE:HG13	21:L:44:LYS:N	2.27	0.50
25:P:11:VAL:HG12	25:P:13:ARG:HG3	1.94	0.50
29:T:33:THR:HG23	29:T:39:GLY:HA2	1.94	0.50
45:k:315:GLY:HA2	57:1:3344:U:H4'	1.94	0.50
55:y:43:PRO:HB2	57:1:726:G:H5"	1.93	0.50
59:n:39:LEU:HB3	59:n:83:VAL:HG13	1.92	0.50
8:8:48:ARG:HH22	57:1:16:G:P	2.33	0.50
8:8:67:ILE:HD12	8:8:121:LYS:HG3	1.94	0.50
8:8:96:LYS:HG3	8:8:107:ALA:HB3	1.94	0.50
9:9:12:ARG:NH1	57:1:214:G:OP1	2.41	0.50
10:A:372:U:O2'	10:A:601:U:OP1	2.29	0.50
10:A:944:U:H5'	24:O:15:ALA:O	2.12	0.50
10:A:1238:U:H2'	10:A:1239:U:H6	1.76	0.50
11:B:135:GLU:O	11:B:139:VAL:HG22	2.12	0.50
14:E:203:LEU:HD13	14:E:205:ASP:OD1	2.11	0.50
15:F:18:TRP:C	15:F:51:ARG:HH22	2.20	0.50
27:R:82:GLN:HE22	27:R:118:ALA:HA	1.76	0.50
56:z:62:ARG:NH2	57:1:3039:C:H3'	2.26	0.50
57:1:362:U:O4	73:AK:24:ARG:NH2	2.44	0.50
57:1:602:A:H2'	57:1:603:C:C6	2.46	0.50
57:1:1273:C:O2'	57:1:1274:A:H2'	2.11	0.50
60:p:102:THR:HG22	60:p:103:SER:N	2.26	0.50
60:p:206:SER:HA	60:p:209:GLU:HG3	1.93	0.50
1:0:130:GLU:HG2	1:0:131:LYS:HG2	1.94	0.50
4:4:26:U:H2'	4:4:27:U:C6	2.46	0.50
10:A:188:U:H2'	10:A:189:G:H8	1.77	0.50
10:A:839:U:O4	10:A:840:A:N6	2.44	0.50
11:B:59:LEU:HD22	32:W:79:LEU:HD11	1.94	0.50
14:E:135:VAL:HG23	14:E:189:ILE:HG12	1.93	0.50
15:F:147:ILE:HG21	15:F:169:ILE:HG13	1.94	0.50
17:H:74:ARG:HA	17:H:96:SER:HA	1.94	0.50
20:K:113:VAL:HG13	20:K:125:ALA:HB1	1.94	0.50
33:X:106:THR:HG21	33:X:121:VAL:HB	1.93	0.50
40:e:46:LYS:O	40:e:50:ILE:HG12	2.12	0.50
43:h:257:ILE:O	43:h:271:LEU:N	2.44	0.50
57:1:158:A:H2'	57:1:159:A:H8	1.77	0.50
57:1:200:A:H2'	57:1:201:G:H8	1.77	0.50
57:1:2655:U:H2'	57:1:2656:C:H6	1.75	0.50
57:1:3093:U:H1'	57:1:3094:A:H5"	1.93	0.50



	A t and 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:3261:A:H2'	57:1:3262:U:C6	2.46	0.50
10:A:55:A:OP1	35:Z:112:LYS:NZ	2.36	0.50
10:A:924:A:H2'	10:A:925:A:C8	2.47	0.50
10:A:1512:A:N3	10:A:1576:C:O2'	2.34	0.50
21:L:37:THR:HG22	21:L:38:ARG:H	1.77	0.50
21:L:55:VAL:HG12	21:L:68:LEU:HA	1.94	0.50
24:O:26:PHE:CZ	24:O:60:VAL:HG22	2.47	0.50
46:1:68:THR:HG22	57:1:2380:A:H5"	1.94	0.50
46:l:120:ARG:NH2	57:1:694:C:OP2	2.44	0.50
53:v:7:LEU:HD21	60:p:163:LEU:HA	1.94	0.50
57:1:173:C:H2'	57:1:174:C:C6	2.47	0.50
57:1:1264:G:N2	57:1:1265:U:O4	2.40	0.50
57:1:1919:C:H5"	77:AO:25:LYS:HD2	1.94	0.50
73:AK:18:LEU:HD23	73:AK:25:ARG:HB2	1.94	0.50
6:6:7:SER:HA	57:1:2989:A:H4'	1.94	0.50
10:A:74:U:O2'	10:A:76:A:OP1	2.23	0.50
10:A:291:U:H2'	10:A:292:C:C6	2.47	0.50
10:A:622:G:H2'	10:A:623:C:C6	2.47	0.50
10:A:988:A:H2'	10:A:990:A:N7	2.27	0.50
12:C:127:VAL:HG13	12:C:176:VAL:HG11	1.93	0.50
57:1:627:U:H2'	57:1:628:A:C8	2.45	0.50
57:1:999:A:N1	57:1:1045:C:O2'	2.42	0.50
57:1:1116:A:H2'	57:1:1117:U:H6	1.76	0.50
64:AB:94:SER:HB2	64:AB:121:VAL:HG13	1.94	0.50
66:AD:26:THR:OG1	66:AD:93:SER:OG	2.30	0.50
67:AE:78:ARG:HA	67:AE:88:LEU:HD23	1.94	0.50
10:A:4:C:O2'	20:K:17:ARG:NH2	2.44	0.49
19:J:52:ASN:OD1	19:J:53:GLN:N	2.45	0.49
21:L:69:THR:O	21:L:73:VAL:HG23	2.12	0.49
24:O:52:VAL:HG23	24:O:55:ARG:NH2	2.27	0.49
46:1:3:SER:OG	46:1:4:ARG:N	2.33	0.49
52:u:65:LEU:HD12	52:u:77:LYS:HD2	1.94	0.49
57:1:1106:U:H2'	57:1:1107:U:C6	2.47	0.49
60:p:160:PRO:HB2	60:p:162:GLU:OE1	2.12	0.49
79:AQ:32:GLN:O	79:AQ:37:TYR:OH	2.22	0.49
10:A:366:U:H2'	10:A:367:A:O4'	2.12	0.49
10:A:904:A:H2'	10:A:905:C:C6	2.47	0.49
10:A:1341:U:H2'	10:A:1342:A:C8	2.48	0.49
10:A:1472:G:N2	10:A:1580:A:OP1	2.41	0.49
14:E:214:ASP:OD1	14:E:215:GLU:N	2.44	0.49
15:F:100:ARG:HB2	15:F:114:ILE:HD13	1.92	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
16:G:133:VAL:O	16:G:137:ILE:HG23	2.12	0.49
21:L:1:MET:HE2	21:L:41:PHE:HE1	1.76	0.49
27:R:21:VAL:HG22	27:R:64:ILE:HG12	1.94	0.49
56:z:38:ARG:O	56:z:42:ARG:HG3	2.12	0.49
57:1:1493:C:H2'	57:1:1494:A:H8	1.77	0.49
57:1:2978:A:H2'	57:1:2979:U:O4'	2.12	0.49
10:A:78:A:H2'	10:A:79:C:C6	2.47	0.49
10:A:803:G:H2'	10:A:806:A:C8	2.47	0.49
10:A:1026:G:H2'	10:A:1027:G:H8	1.72	0.49
10:A:1239:U:H2'	10:A:1240:G:C8	2.47	0.49
10:A:1242:U:H2'	10:A:1242:U:O2	2.11	0.49
11:B:107:PHE:HB3	11:B:139:VAL:HG21	1.94	0.49
14:E:121:TYR:O	14:E:125:ARG:HG2	2.12	0.49
47:m:187:ALA:O	47:m:189:GLU:N	2.45	0.49
49:q:134:MET:SD	49:q:146:VAL:HG22	2.53	0.49
57:1:156:A:N7	72:AJ:25:ILE:HG12	2.27	0.49
57:1:1007:A:H2'	57:1:1008:A:C8	2.47	0.49
78:AP:21:THR:HG22	78:AP:22:GLN:N	2.26	0.49
1:0:10:ILE:HG12	1:0:26:ARG:HG3	1.94	0.49
8:8:43:SER:O	8:8:43:SER:OG	2.28	0.49
10:A:961:G:N1	10:A:1008:A:O2'	2.33	0.49
10:A:1325:U:O4'	10:A:1364:U:H5"	2.12	0.49
10:A:1615:U:H2'	10:A:1616:G:C8	2.48	0.49
22:M:26:LYS:HE2	22:M:28:ASN:ND2	2.27	0.49
23:N:67:THR:O	23:N:68:GLU:HG3	2.12	0.49
43:h:116:ILE:HG22	43:h:123:ILE:HG12	1.94	0.49
45:k:117:ARG:HD2	45:k:176:ALA:O	2.12	0.49
51:t:110:ASP:OD1	51:t:111:ALA:N	2.46	0.49
53:v:14:LYS:HE2	57:1:269:G:H5"	1.95	0.49
57:1:1218:G:N2	57:1:1281:G:O2'	2.45	0.49
57:1:1228:C:H41	57:1:1257:G:H22	1.58	0.49
57:1:1556:G:O2'	57:1:1557:U:H5'	2.12	0.49
5:5:16:VAL:HG13	5:5:105:GLN:HG2	1.93	0.49
10:A:1393:U:H2'	10:A:1394:G:C8	2.47	0.49
13:D:30:TRP:NE1	13:D:60:GLU:OE1	2.31	0.49
45:k:58:ARG:HD2	45:k:354:VAL:HG13	1.93	0.49
57:1:1007:A:H2'	57:1:1008:A:H8	1.77	0.49
57:1:1199:A:H2'	57:1:1200:A:H8	1.77	0.49
57:1:2347:G:H2'	57:1:2348:G:C8	2.47	0.49
1:0:48:LEU:O	1:0:49[A]:HIS:ND1	2.46	0.49
4:4:145:U:H2'	4:4:146:U:C6	2.48	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:840:A:C2	10:A:842:U:H1'	2.47	0.49
10:A:1334:G:H2'	10:A:1335:U:C6	2.47	0.49
10:A:1481:C:H2'	10:A:1482:C:C6	2.47	0.49
10:A:1523:G:O2'	10:A:1524:C:OP1	2.27	0.49
24:O:70:LYS:O	24:O:74:ILE:HG23	2.13	0.49
57:1:1239:G:N2	57:1:1240:A:H62	2.11	0.49
57:1:2696:U:OP2	57:1:2698:C:N4	2.46	0.49
57:1:3318:G:H5"	57:1:3319:U:H4'	1.93	0.49
62:x:29:THR:HA	62:x:32:THR:HG22	1.94	0.49
66:AD:29:TYR:OH	66:AD:57:GLU:OE2	2.30	0.49
5:5:19:VAL:O	5:5:21:ALA:N	2.46	0.49
7:7:56:ARG:NH2	57:1:3334:G:C4	2.80	0.49
10:A:1187:A:N6	10:A:1443:C:O5'	2.46	0.49
10:A:1205:C:H5'	21:L:51:SER:OG	2.12	0.49
17:H:121:ILE:HB	17:H:124:LEU:HB3	1.94	0.49
25:P:56:MET:HG2	25:P:99:ALA:HB2	1.94	0.49
34:Y:37:ALA:O	34:Y:41:SER:HB2	2.12	0.49
43:h:67:HIS:CG	43:h:68:ILE:H	2.29	0.49
51:t:16:LYS:HG2	57:1:46:C:H5"	1.93	0.49
54:w:86:ARG:HG3	54:w:100:LEU:HD11	1.93	0.49
57:1:2717:G:N2	57:1:2720:A:OP2	2.38	0.49
57:1:3244:A:O2'	57:1:3245:A:H5'	2.13	0.49
5:5:59:GLU:HG3	5:5:60:SER:N	2.27	0.49
10:A:86:A:H5'	35:Z:119:PHE:CE1	2.48	0.49
10:A:479:A:H2'	10:A:480:U:C6	2.47	0.49
10:A:767:G:N7	35:Z:12:VAL:N	2.57	0.49
10:A:1472:G:N2	10:A:1509:U:O4	2.45	0.49
27:R:40:PRO:HG2	27:R:43:LEU:HD13	1.94	0.49
29:T:122:HIS:CE1	29:T:126:ARG:HD2	2.47	0.49
30:U:108:LEU:HB3	30:U:113:VAL:CG2	2.42	0.49
54:w:22:SER:OG	57:1:1177:U:O4	2.28	0.49
57:1:536:A:H2'	57:1:537:C:H6	1.78	0.49
57:1:783:G:H2'	57:1:784:C:C6	2.47	0.49
57:1:1079:G:H2'	57:1:1080:A:H8	1.78	0.49
8:8:73:MET:HE1	8:8:141:TYR:HE2	1.78	0.49
10:A:327:G:H2'	10:A:328:G:H8	1.78	0.49
16:G:172:ILE:O	16:G:176:THR:HG22	2.12	0.49
17:H:161:GLU:HB3	17:H:170:THR:HG22	1.95	0.49
17:H:180:THR:HG22	17:H:183:THR:HG23	1.94	0.49
21:L:37:THR:HG22	21:L:38:ARG:N	2.28	0.49
29:T:24:GLY:O	29:T:59:GLY:N	2.40	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
33:X:31:SER:H	33:X:34:ILE:HG22	1.76	0.49
45:k:92:TYR:HB2	45:k:157:VAL:HB	1.95	0.49
56:z:105:LEU:HD12	56:z:135:LYS:HE2	1.94	0.49
57:1:2186:A:O2'	57:1:2187:U:H5'	2.13	0.49
10:A:256:C:O2	19:J:184:ARG:NH1	2.44	0.49
10:A:331:A:N6	19:J:27:PHE:O	2.46	0.49
10:A:863:G:O2'	24:O:108:ASP:OD1	2.30	0.49
10:A:1739:U:H2'	10:A:1740:A:H8	1.78	0.49
15:F:160:VAL:HG12	15:F:172:PHE:HB3	1.94	0.49
16:G:58:LEU:HD11	16:G:167:ARG:HH12	1.76	0.49
19:J:92:ARG:HH21	57:1:1940:U:H4'	1.78	0.49
30:U:19:ALA:O	30:U:23:GLN:HG3	2.13	0.49
31:V:40:ILE:HD11	31:V:90:ILE:HD12	1.95	0.49
57:1:99:A:H3'	57:1:100:G:H21	1.78	0.49
57:1:371:G:N1	57:1:374:A:OP2	2.39	0.49
66:AD:101:ASP:OD1	66:AD:101:ASP:N	2.46	0.49
2:2:93:VAL:HG11	47:m:41:LYS:HE2	1.95	0.48
10:A:518:A:H2'	10:A:519:A:H8	1.77	0.48
10:A:871:U:C2	10:A:872:A:C8	3.01	0.48
10:A:1548:U:H2'	10:A:1549:G:H8	1.77	0.48
16:G:134:VAL:O	16:G:137:ILE:HG12	2.13	0.48
17:H:29:GLU:HG3	17:H:29:GLU:O	2.12	0.48
36:a:42:LEU:HD21	36:a:47:TYR:HD1	1.78	0.48
46:1:8:SER:OG	46:l:148:GLU:OE2	2.31	0.48
52:u:120:ARG:HH11	52:u:120:ARG:HG3	1.77	0.48
56:z:60:ARG:NH1	57:1:1856:G:O3'	2.46	0.48
57:1:1482:G:H21	70:AH:6:THR:HG22	1.77	0.48
57:1:2167:U:O3'	79:AQ:21:SER:OG	2.22	0.48
57:1:2322:U:H2'	57:1:2323:A:C8	2.47	0.48
57:1:3193:C:H4'	57:1:3194:G:O5'	2.13	0.48
8:8:99:VAL:HG11	8:8:124:ILE:HD13	1.96	0.48
10:A:150:U:O2	17:H:4:ASN:ND2	2.36	0.48
10:A:261:C:O2'	10:A:262:G:H5'	2.13	0.48
10:A:1188:A:N6	10:A:1540:G:H1'	2.27	0.48
11:B:62:ARG:NH2	32:W:78:LEU:HB3	2.27	0.48
11:B:144:ILE:HG12	11:B:158:VAL:CG1	2.43	0.48
14:E:59:VAL:HG12	14:E:60:LEU:HD23	1.93	0.48
36:a:59:TYR:CE1	36:a:100:ILE:HG23	2.48	0.48
41:f:13:LYS:O	41:f:17:GLN:HG2	2.13	0.48
43:h:156:ARG:HB3	43:h:201:LEU:HD22	1.95	0.48
44:j:79:ASN:ND2	44:j:165:VAL:HG12	2.27	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
45:k:25:GLN:OE1	57:1:3277:U:H4'	2.13	0.48
47:m:178:ASN:HA	47:m:183:TRP:CD2	2.48	0.48
48:0:141:THR:HG23	48:0:237:VAL:HG11	1.94	0.48
54:w:90:PRO:HD3	57:1:1172:C:H4'	1.95	0.48
57:1:25:A:H2'	57:1:26:C:H6	1.78	0.48
57:1:496:A:H4'	59:n:27:GLN:HG3	1.94	0.48
57:1:1655:U:H2'	57:1:1656:C:C6	2.48	0.48
57:1:2084:A:H2'	57:1:2085:A:C8	2.48	0.48
57:1:2740:U:H2'	57:1:2741:A:C8	2.48	0.48
10:A:1344:C:OP1	30:U:130:ARG:HG3	2.13	0.48
10:A:1715:U:H2'	10:A:1716:C:C6	2.48	0.48
10:A:1719:A:H2'	10:A:1720:C:H6	1.78	0.48
13:D:149:LEU:HG	13:D:191:VAL:HG12	1.94	0.48
21:L:32:HIS:CE1	21:L:35:ILE:HD13	2.48	0.48
26:Q:43:ARG:NH1	26:Q:47:ARG:HH11	2.10	0.48
39:d:11:LYS:O	39:d:31:GLU:N	2.31	0.48
43:h:291:TRP:CE2	43:h:298:LEU:HD13	2.48	0.48
47:m:201:GLY:O	47:m:204:VAL:HG12	2.13	0.48
49:q:27:VAL:HG12	49:q:82:VAL:HG21	1.95	0.48
53:v:19:MET:HE1	60:p:162:GLU:HG2	1.95	0.48
79:AQ:82:THR:HG22	79:AQ:86:LEU:HD23	1.94	0.48
5:5:42:LYS:NZ	57:1:1683:U:OP1	2.43	0.48
6:6:129:ILE:O	6:6:133:SER:HB3	2.13	0.48
9:9:9:SER:HB3	57:1:335:G:OP1	2.14	0.48
13:D:71:LEU:HD23	13:D:101:ASP:HB3	1.94	0.48
21:L:38:ARG:HB2	21:L:41:PHE:CD2	2.48	0.48
32:W:59:VAL:HG13	32:W:64:GLU:HB3	1.96	0.48
49:q:84:LYS:HB3	49:q:186:THR:CG2	2.44	0.48
57:1:782:A:H4'	57:1:783:G:H5'	1.95	0.48
57:1:3256:G:C2	57:1:3257:A:C5	3.01	0.48
1:0:130:GLU:OE1	1:0:130:GLU:N	2.33	0.48
10:A:1772:U:H2'	10:A:1773:G:H8	1.79	0.48
12:C:103:LEU:HB3	12:C:215:VAL:HG22	1.95	0.48
12:C:103:LEU:CB	12:C:215:VAL:HG22	2.44	0.48
14:E:159:ILE:HG13	14:E:169:ILE:HD11	1.94	0.48
18:I:163:ASP:O	18:I:167:GLN:HG3	2.14	0.48
22:M:122:VAL:HG23	22:M:143:SER:HB3	1.94	0.48
24:O:71:ILE:O	24:O:74:ILE:HG12	2.14	0.48
29:T:109:LEU:O	29:T:113:LEU:HD12	2.13	0.48
43:h:70:GLN:HB2	43:h:86:TRP:CD1	2.49	0.48
45:k:250:ALA:HB1	57:1:2919:G:C2	2.49	0.48



	A + ama - D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
46:1:82:GLY:HA3	57:1:357:A:O4'	2.14	0.48
46:1:89:ALA:HB3	57:1:1434:U:H4'	1.96	0.48
57:1:480:G:H2'	57:1:480:G:N3	2.29	0.48
57:1:2634:G:H2'	57:1:2635:A:H8	1.76	0.48
57:1:3019:U:O2'	57:1:3020:A:H5'	2.13	0.48
57:1:3064:C:O2'	57:1:3066:A:OP2	2.28	0.48
63:AA:5:ILE:O	63:AA:6:LYS:HE2	2.13	0.48
10:A:444:A:N6	10:A:459:G:H21	2.12	0.48
10:A:996:G:H2'	10:A:997:U:C5	2.48	0.48
10:A:1123:A:H2'	10:A:1124:A:H8	1.78	0.48
10:A:1668:A:H2'	10:A:1669:U:H5'	1.96	0.48
50:s:99:THR:O	50:s:99:THR:HG22	2.13	0.48
57:1:660:U:H2'	57:1:661:C:C6	2.48	0.48
57:1:1115:C:H2'	57:1:1116:A:H8	1.77	0.48
57:1:1258:G:H1'	57:1:1274:A:N6	2.28	0.48
57:1:2385:C:H2'	57:1:2386:U:H6	1.79	0.48
71:AI:118:ILE:HG22	71:AI:119:LYS:N	2.28	0.48
10:A:16:G:H2'	10:A:17:C:C6	2.48	0.48
10:A:217:A:H8	10:A:217:A:H5"	1.78	0.48
10:A:335:G:H3'	22:M:133:LYS:HB2	1.95	0.48
10:A:772:A:OP1	15:F:106:LYS:NZ	2.44	0.48
10:A:1513:A:N1	10:A:1595:U:O2'	2.40	0.48
10:A:1706:A:H2'	10:A:1707:G:O4'	2.14	0.48
12:C:131:ASP:OD2	12:C:180:THR:OG1	2.31	0.48
15:F:257:ARG:HH12	20:K:78:ARG:NH2	2.12	0.48
20:K:74:ASN:HA	20:K:77:ILE:HG22	1.96	0.48
20:K:80:LEU:HD22	20:K:85:VAL:HG11	1.94	0.48
25:P:87:LYS:HZ3	25:P:116:VAL:HG13	1.79	0.48
31:V:43:ASN:HD22	31:V:43:ASN:C	2.20	0.48
32:W:70:ASN:HB3	32:W:83:TRP:HB2	1.95	0.48
48:0:143[B]:ARG:NH1	48:0:180:GLU:OE2	2.46	0.48
57:1:2130:A:H2'	57:1:2131:U:C6	2.48	0.48
1:0:119:ARG:HB2	3:3:96:U:H4'	1.94	0.48
10:A:299:A:H2'	10:A:300:U:C6	2.49	0.48
10:A:1127:A:H5"	37:b:2:PRO:HB3	1.94	0.48
10:A:1335:U:H2'	10:A:1336:G:H8	1.75	0.48
10:A:1740:A:H2'	10:A:1741:A:H8	1.79	0.48
28:S:7:LYS:HD2	28:S:11:ARG:HH12	1.79	0.48
29:T:64:GLU:OE1	29:T:64:GLU:N	2.42	0.48
53:v:44:ARG:NH1	53:v:120:TRP:O	2.47	0.48
57:1:1148:G:OP2	57:1:1148:G:N2	2.47	0.48



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
10:A:470:U:O2'	10:A:754:A:N3	2.42	0.48
10:A:759:A:N6	10:A:770:C:H42	2.11	0.48
10:A:841:A:N1	18:I:111:SER:OG	2.47	0.48
10:A:932:U:H2'	10:A:933:A:C8	2.48	0.48
16:G:165:LEU:HD22	39:d:47:PRO:HG2	1.95	0.48
26:Q:68:GLU:N	26:Q:69:PRO:HD3	2.29	0.48
30:U:14:PHE:CD2	30:U:63:ARG:HD2	2.49	0.48
31:V:21:ILE:HD13	31:V:99:VAL:HG11	1.96	0.48
43:h:33:LEU:HB3	43:h:45:TRP:HB2	1.95	0.48
43:h:239:ALA:HB3	43:h:289:LEU:HD23	1.96	0.48
57:1:2260:U:OP1	57:1:2945:G:O2'	2.31	0.48
61:r:140:THR:HG21	61:r:148:VAL:HG21	1.96	0.48
1:0:42:TRP:O	1:0:46:GLN:HG3	2.14	0.48
4:4:21:C:H5"	46:1:195:LEU:HD21	1.96	0.48
9:9:58:VAL:HA	9:9:104:VAL:HG12	1.96	0.48
10:A:1123:A:H2'	10:A:1124:A:C8	2.49	0.48
10:A:1514:C:OP1	16:G:106:LYS:HE2	2.14	0.48
10:A:1610:C:H2'	10:A:1611:C:H6	1.79	0.48
12:C:71:ALA:HB2	12:C:80:SER:HA	1.96	0.48
16:G:159:ALA:HB3	16:G:225:ARG:HB3	1.96	0.48
17:H:180:THR:O	17:H:183:THR:OG1	2.24	0.48
21:L:5:LYS:O	21:L:9:LYS:HG2	2.14	0.48
46:1:11:SER:OG	46:l:15:GLU:HG2	2.14	0.48
6:6:30:GLY:HA3	6:6:66:LYS:HE2	1.96	0.47
7:7:23:ARG:NE	7:7:25:ASP:OD2	2.44	0.47
10:A:265:U:H2'	10:A:266:C:H6	1.79	0.47
10:A:1141:C:H2'	10:A:1142:A:C8	2.49	0.47
13:D:135:ARG:HB3	13:D:216:THR:OG1	2.13	0.47
17:H:28:TYR:CZ	17:H:104:GLN:HG3	2.49	0.47
17:H:136:LYS:HG3	17:H:173:PRO:HB2	1.96	0.47
27:R:9:PHE:CE2	27:R:11:LYS:HE3	2.49	0.47
29:T:61:LEU:HD23	29:T:62:THR:O	2.14	0.47
33:X:37:PHE:O	33:X:40:VAL:HG22	2.13	0.47
33:X:115:GLU:O	33:X:119:LYS:HG2	2.13	0.47
81:j:301:YMZ:FAE	81:j:301:YMZ:NAP	2.37	0.47
56:z:81:ARG:NH2	57:1:2082:A:OP2	2.33	0.47
57:1:157:G:H2'	57:1:158:A:H8	1.79	0.47
57:1:1807:G:H2'	57:1:1808:G:O4'	2.13	0.47
66:AD:18:LEU:O	66:AD:21:LYS:HG2	2.14	0.47
3:3:7:G:OP1	47:m:33:ARG:HD2	2.13	0.47
10:A:30:G:H2'	10:A:31:C:C6	2.48	0.47



	A t a ma 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:519:A:N3	35:Z:34:ASN:ND2	2.53	0.47
10:A:882:C:O2'	10:A:899:G:N2	2.47	0.47
10:A:1762:U:OP1	77:AO:11:ARG:NH2	2.39	0.47
11:B:23:HIS:HA	11:B:48:ILE:HB	1.96	0.47
12:C:198:GLU:O	12:C:202:GLN:HG2	2.14	0.47
14:E:28:ARG:HD2	21:L:60:SER:OG	2.14	0.47
14:E:107:LYS:HD2	14:E:174:ARG:HB3	1.95	0.47
16:G:99:MET:HB2	16:G:180:ARG:CZ	2.44	0.47
22:M:73:GLY:HA3	22:M:86:ILE:HD12	1.95	0.47
24:O:46:THR:OG1	24:O:49:GLN:HG3	2.13	0.47
30:U:130:ARG:HG2	30:U:134:ARG:HH12	1.78	0.47
46:1:17:GLY:O	46:1:18:SER:OG	2.27	0.47
50:s:4:LYS:HG3	50:s:6:GLN:H	1.78	0.47
57:1:296:A:N3	57:1:299:G:O2'	2.43	0.47
57:1:1396:U:H2'	57:1:1397:G:O4'	2.14	0.47
57:1:2239:G:H21	57:1:2240:A:N6	2.12	0.47
78:AP:21:THR:HG22	78:AP:22:GLN:H	1.79	0.47
10:A:299:A:H5"	19:J:27:PHE:CZ	2.49	0.47
10:A:325:U:H2'	10:A:326:A:C8	2.49	0.47
10:A:1016:U:H4'	10:A:1017:G:OP2	2.13	0.47
11:B:134:LYS:HG3	11:B:138:TYR:CE2	2.49	0.47
11:B:136:SER:HB2	11:B:141:ILE:HB	1.96	0.47
45:k:250:ALA:HB1	57:1:2919:G:N3	2.29	0.47
57:1:476:C:H2'	57:1:477:U:C6	2.49	0.47
57:1:623:A:H2'	57:1:624:U:C6	2.49	0.47
57:1:1099:A:N6	57:1:1359:A:H1'	2.29	0.47
57:1:1482:G:N2	70:AH:6:THR:HG22	2.29	0.47
57:1:1909:A:N3	57:1:2098:A:H2'	2.29	0.47
57:1:2085:A:H2	57:1:3309:A:C8	2.32	0.47
57:1:2709:C:O2'	65:AC:36:ASP:OD1	2.31	0.47
57:1:2814:U:O2	57:1:2814:U:H2'	2.12	0.47
57:1:2876:U:H2'	57:1:2877:U:C6	2.50	0.47
2:2:129:LYS:HE2	57:1:1093:G:H5'	1.96	0.47
10:A:66:U:O2	17:H:160:ARG:NE	2.36	0.47
10:A:1535:G:O2'	29:T:89:GLN:NE2	2.47	0.47
10:A:1540:G:O6	26:Q:43:ARG:NH2	2.41	0.47
11:B:182:LEU:HD22	11:B:187:ILE:HD13	1.96	0.47
12:C:46:THR:HG22	12:C:47:LEU:N	2.29	0.47
21:L:17:GLN:N	21:L:88:PRO:HB3	2.29	0.47
27:R:131:ARG:HG3	27:R:137:PHE:HE1	1.79	0.47
44:j:101:ILE:HG13	44:j:165:VAL:HG22	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
46:1:305:GLU:O	57:1:1342:G:O2'	2.29	0.47
64:AB:83:ASP:OD1	64:AB:86:LYS:HB2	2.14	0.47
65:AC:14[B]:ARG:HE	65:AC:18:ARG:HH21	1.61	0.47
10:A:569:G:H5"	34:Y:114:LYS:HE2	1.97	0.47
10:A:1457:A:H2	10:A:1460:G:N3	2.12	0.47
10:A:1475:U:H6	10:A:1476:A:C2	2.33	0.47
24:O:110:ASP:O	24:O:114:ARG:HG2	2.14	0.47
29:T:7:GLU:OE1	29:T:10:SER:OG	2.26	0.47
35:Z:83:LYS:NZ	35:Z:96:LEU:HD13	2.28	0.47
36:a:39:ILE:HG21	36:a:46:LYS:HE2	1.97	0.47
50:s:53:THR:HG23	50:s:60:ARG:HA	1.95	0.47
57:1:629:A:H2'	57:1:630:G:C8	2.50	0.47
57:1:1199:A:N3	57:1:2827:U:O2'	2.36	0.47
57:1:2855:U:H2'	57:1:2856:C:C6	2.49	0.47
5:5:84:LYS:HE3	5:5:93:ARG:NH2	2.26	0.47
10:A:748:G:H4'	15:F:256:ARG:HH12	1.80	0.47
10:A:787:A:C4	18:I:100:ARG:HD2	2.50	0.47
10:A:869:A:N6	10:A:870:G:O6	2.48	0.47
10:A:1143:C:N4	10:A:1148:A:H61	2.12	0.47
10:A:1709:A:N3	17:H:68:MET:HE1	2.30	0.47
15:F:11:ARG:HA	15:F:28:ALA:HB2	1.96	0.47
26:Q:43:ARG:HH12	26:Q:47:ARG:HH11	1.63	0.47
39:d:10:ALA:HB1	39:d:30:VAL:HB	1.97	0.47
43:h:75:SER:HB3	43:h:80:TYR:HB2	1.97	0.47
43:h:149:ASN:HB2	43:h:172:ASP:OD2	2.13	0.47
46:1:140:GLY:O	46:l:142:ARG:NH1	2.47	0.47
47:m:184:ASP:HB3	47:m:187:ALA:O	2.15	0.47
57:1:179:C:H2'	57:1:180:U:H6	1.78	0.47
57:1:1662:G:H2'	57:1:1663:A:H8	1.79	0.47
57:1:3245:A:O2'	57:1:3246:C:H6	1.97	0.47
62:x:40:LYS:HD2	62:x:113:VAL:HG22	1.97	0.47
74:AL:44:LYS:HB3	74:AL:51:GLN:HE21	1.79	0.47
79:AQ:38:ASP:HA	79:AQ:45:ARG:HA	1.97	0.47
5:5:78:TYR:CE1	5:5:82:LEU:HD21	2.50	0.47
10:A:383:A:H2'	10:A:384:G:C8	2.50	0.47
10:A:1265:C:H2'	10:A:1266:G:C8	2.49	0.47
10:A:1436:U:H2'	10:A:1437:C:H6	1.80	0.47
10:A:1584:A:C8	40:e:14:PHE:HD1	2.32	0.47
10:A:1595:U:O3'	27:R:72:GLY:HA3	2.15	0.47
17:H:21:GLU:OE1	17:H:28:TYR:OH	2.32	0.47
19:J:39:GLY:O	19:J:61:GLU:HG3	2.15	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
27:R:48:TYR:O	27:R:51:LEU:HG	2.15	0.47
27:R:89:VAL:HG21	27:R:116:LEU:HD11	1.97	0.47
28:S:10:LYS:HG2	28:S:53:TYR:CZ	2.50	0.47
29:T:91:ASP:OD1	29:T:92:GLN:N	2.47	0.47
40:e:53:ASN:HB2	40:e:55:TYR:CZ	2.49	0.47
43:h:113:SER:HB3	43:h:154:ALA:HA	1.97	0.47
43:h:132:VAL:HB	43:h:145:LEU:HB2	1.96	0.47
44:j:117:GLU:HB2	44:j:162:ALA:HB1	1.96	0.47
45:k:25:GLN:HE21	45:k:334:ARG:HD3	1.79	0.47
49:q:110:ASP:HB3	49:q:128:ILE:HD12	1.95	0.47
57:1:246:U:H2'	57:1:247:C:C6	2.49	0.47
57:1:428:U:H2'	57:1:429:U:C6	2.50	0.47
57:1:757:A:C2	57:1:767:A:H1'	2.50	0.47
57:1:961:A:O2'	64:AB:44:ASN:HB2	2.15	0.47
57:1:2206:A:H2'	57:1:2207:A:C8	2.49	0.47
57:1:2557:G:H2'	57:1:2557:G:N3	2.29	0.47
57:1:2836:A:H5"	61:r:114:GLY:HA2	1.97	0.47
70:AH:109:GLN:OE1	70:AH:113:LYS:HD2	2.15	0.47
75:AM:9:THR:O	75:AM:13:LEU:HG	2.13	0.47
1:0:8:GLN:HE21	1:0:26:ARG:HD2	1.79	0.47
4:4:36:G:C5	71:AI:86:ARG:HD3	2.50	0.47
5:5:86:TYR:O	5:5:90:ASN:ND2	2.42	0.47
10:A:1206:A:H2'	10:A:1207:C:O4'	2.14	0.47
12:C:64:ARG:NH2	25:P:32:GLU:OE2	2.41	0.47
12:C:145:ARG:HB2	12:C:154:THR:HG21	1.97	0.47
12:C:185:THR:O	12:C:189:ILE:HG12	2.14	0.47
16:G:103:ASN:HA	16:G:106:LYS:HD2	1.97	0.47
19:J:107:THR:OG1	19:J:108:PRO:HD3	2.14	0.47
43:h:75:SER:OG	43:h:77:ASP:OD1	2.29	0.47
57:1:2587:G:H2'	57:1:2588:C:H6	1.80	0.47
62:x:25:SER:OG	62:x:28:ASN:HB2	2.14	0.47
10:A:583:A:H2'	10:A:584:G:H8	1.80	0.47
10:A:1582:U:H5'	10:A:1583:C:OP2	2.14	0.47
15:F:65:MET:HG2	15:F:70:VAL:HG11	1.96	0.47
16:G:146:SER:HA	16:G:159:ALA:HA	1.96	0.47
17:H:87:ARG:HB2	17:H:91:GLU:OE1	2.15	0.47
27:R:3:THR:HG22	27:R:4:GLN:N	2.30	0.47
31:V:98:THR:O	31:V:102:ILE:HG13	2.15	0.47
46:1:68:THR:CG2	57:1:2380:A:H5"	2.45	0.47
57:1:1115:C:H2'	57:1:1116:A:C8	2.50	0.47
57:1:1298:A:N7	57:1:2829:C:O2'	2.47	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:0:64:ILE:HG12	46:1:360:VAL:HG22	1.97	0.47
10:A:443:A:H1'	10:A:523:A:H5'	1.95	0.47
10:A:444:A:OP1	15:F:59:ARG:HD3	2.15	0.47
10:A:1323:C:H1'	10:A:1396:A:C5	2.50	0.47
18:I:125:LEU:HD11	18:I:169:TYR:HB2	1.96	0.47
43:h:173:LYS:HG3	43:h:194:GLY:O	2.15	0.47
57:1:941:C:H2'	57:1:942:U:C6	2.50	0.47
62:x:178:SER:O	62:x:182:LEU:HG	2.14	0.47
67:AE:71:ARG:HH11	67:AE:103:LEU:HD13	1.80	0.47
69:AG:43:PHE:HZ	69:AG:107:ILE:HD11	1.80	0.47
6:6:13:MET:HE1	6:6:54:ALA:HB3	1.97	0.46
10:A:933:A:H2'	10:A:934:C:C6	2.50	0.46
10:A:1540:G:N7	26:Q:43:ARG:NH2	2.63	0.46
10:A:1597:G:OP1	16:G:72:HIS:NE2	2.44	0.46
17:H:7:TYR:O	17:H:11:GLY:N	2.47	0.46
20:K:112:GLN:OE1	20:K:153:GLN:NE2	2.48	0.46
23:N:63:CYS:SG	23:N:66:VAL:HG23	2.55	0.46
24:O:102:LEU:HD11	24:O:112:LYS:HA	1.96	0.46
26:Q:125:PRO:HB3	29:T:129:TRP:CH2	2.50	0.46
27:R:93:GLN:NE2	43:h:63:LYS:HD3	2.30	0.46
29:T:118:LYS:HD3	29:T:118:LYS:HA	1.63	0.46
33:X:17:ALA:HA	33:X:20:THR:HG22	1.96	0.46
42:g:178:LYS:O	42:g:180:ARG:HG2	2.15	0.46
45:k:250:ALA:HB3	57:1:2852:U:H1'	1.98	0.46
52:u:40:ILE:HD11	52:u:48:GLN:HE21	1.80	0.46
57:1:164:U:H2'	57:1:165:C:H6	1.80	0.46
57:1:429:U:H5"	69:AG:87:LYS:HE3	1.98	0.46
57:1:1050:A:H5"	57:1:2609:A:H61	1.80	0.46
4:4:135:G:OP1	8:8:49:LYS:NZ	2.31	0.46
7:7:53:VAL:O	7:7:57:ARG:HG3	2.15	0.46
10:A:30:G:H4'	34:Y:131:SER:HB3	1.96	0.46
10:A:107:C:H2'	10:A:108:A:H8	1.80	0.46
10:A:334:G:O6	19:J:5:ARG:NH1	2.38	0.46
10:A:512:G:O2'	10:A:513:A:H8	1.98	0.46
13:D:138:TYR:OH	13:D:144:GLY:O	2.31	0.46
15:F:57:ASN:OD1	15:F:59:ARG:HG2	2.15	0.46
24:O:95:ALA:HA	24:O:98:VAL:HG12	1.97	0.46
27:R:99:ALA:HA	27:R:102:ASN:ND2	2.28	0.46
48:0:149:ARG:HD2	48:0:205:LEU:HD23	1.97	0.46
50:s:28:ASP:N	50:s:28:ASP:OD1	2.47	0.46
50:s:32:ARG:HB2	50:s:123:TYR:OH	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
52:u:19:VAL:HG12	52:u:57:LEU:HD23	1.97	0.46
55:y:66:ARG:NH2	55:y:143:PRO:HD3	2.30	0.46
57:1:536:A:H2'	57:1:537:C:C6	2.50	0.46
57:1:1588:G:OP2	70:AH:37:LYS:NZ	2.39	0.46
60:p:11:ALA:N	60:p:12:PRO:HD3	2.30	0.46
1:0:171:PHE:O	1:0:172:TYR:HB2	2.15	0.46
10:A:593:G:H2'	10:A:594:C:C6	2.50	0.46
10:A:856:G:H5'	38:c:51:GLN:HB3	1.98	0.46
10:A:903:U:H4'	25:P:13:ARG:HD3	1.95	0.46
10:A:1149:G:H2'	10:A:1150:G:C8	2.50	0.46
10:A:1219:A:OP2	10:A:1230:G:O2'	2.30	0.46
10:A:1380:G:OP1	43:h:281:ALA:N	2.48	0.46
30:U:23:GLN:HG2	30:U:55:TYR:CD2	2.51	0.46
47:m:60:ILE:HB	47:m:80:ALA:HB2	1.96	0.46
55:y:31[B]:LYS:NZ	57:1:1344:U:O4	2.46	0.46
57:1:1104:U:H2'	57:1:1105:U:C6	2.50	0.46
57:1:1561:U:H2'	57:1:1562:G:C8	2.49	0.46
57:1:1632:C:O2'	63:AA:79:HIS:ND1	2.45	0.46
57:1:2210:A:H2'	57:1:2211:A:C8	2.51	0.46
3:3:84:A:H2'	3:3:85:G:C8	2.51	0.46
9:9:12:ARG:NH1	46:1:199:ARG:HH12	2.12	0.46
10:A:504:A:O2'	10:A:505:U:OP1	2.31	0.46
10:A:530:U:OP2	20:K:132:ARG:NH2	2.48	0.46
10:A:834:C:OP1	56:z:162:ARG:NH1	2.49	0.46
16:G:48:PHE:CD1	16:G:67:PRO:HB3	2.51	0.46
16:G:194:LEU:HA	16:G:197:GLU:HG3	1.96	0.46
51:t:131:LYS:HB2	51:t:134:GLU:OE1	2.15	0.46
57:1:638:U:H2'	57:1:639:C:C6	2.50	0.46
57:1:2418:A:H2'	57:1:2419:A:H8	1.80	0.46
3:3:19:C:H2'	3:3:20:A:H8	1.81	0.46
10:A:161:G:O2'	17:H:110:ALA:HB1	2.15	0.46
10:A:393:U:H2'	10:A:394:G:O4'	2.15	0.46
10:A:748:G:H5"	20:K:78:ARG:NH2	2.28	0.46
10:A:813:U:O2'	10:A:814:A:O5'	2.34	0.46
10:A:1270:U:O2'	10:A:1407:A:N1	2.32	0.46
10:A:1512:A:H2'	10:A:1513:A:C8	2.50	0.46
10:A:1664:C:H42	10:A:1711:C:H42	1.63	0.46
11:B:182:LEU:HD22	11:B:187:ILE:CD1	2.45	0.46
16:G:100:ASN:ND2	16:G:180:ARG:HD3	2.30	0.46
32:W:58:TYR:O	32:W:62:ARG:HG2	2.16	0.46
36:a:80:LEU:HD13	36:a:101:TYR:CD2	2.50	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
43:h:45:TRP:CZ3	43:h:58:PRO:HG3	2.50	0.46
55:y:96:PHE:CD1	55:y:97:PRO:HD2	2.50	0.46
57:1:662:U:H2'	57:1:663:A:H8	1.81	0.46
57:1:792:U:H2'	57:1:793:U:C6	2.51	0.46
57:1:1286:A:H2'	57:1:1287:A:C8	2.51	0.46
57:1:3135:A:H2'	57:1:3136:C:C6	2.51	0.46
9:9:51:ARG:HG2	9:9:52:GLN:N	2.31	0.46
10:A:325:U:H2'	10:A:326:A:H8	1.81	0.46
10:A:929:A:OP2	37:b:19:LYS:NZ	2.48	0.46
10:A:1469:A:C2	10:A:1594:G:H1'	2.51	0.46
11:B:29:VAL:HG23	11:B:149:MET:HB3	1.96	0.46
30:U:117:SER:OG	30:U:120:GLY:O	2.32	0.46
53:v:174:ILE:HG21	57:1:62:A:H5"	1.97	0.46
54:w:9:VAL:HG12	54:w:118:ARG:HG3	1.97	0.46
57:1:451:C:H2'	57:1:452:A:C5	2.50	0.46
57:1:638:U:OP1	64:AB:21:ARG:NH1	2.46	0.46
57:1:1227:A:H1'	57:1:1257:G:C8	2.50	0.46
57:1:3171:C:H5"	57:1:3172:U:O5'	2.16	0.46
69:AG:43:PHE:CZ	69:AG:107:ILE:HD11	2.50	0.46
69:AG:49:ILE:HG12	69:AG:100:ILE:HD13	1.97	0.46
8:8:84:PHE:HD2	8:8:124:ILE:HD12	1.81	0.46
10:A:17:C:H2'	10:A:18:C:H6	1.78	0.46
10:A:149:G:N1	10:A:162:A:C6	2.83	0.46
10:A:874:U:H2'	10:A:875:C:C6	2.51	0.46
10:A:1105:U:H2'	10:A:1106:C:C6	2.50	0.46
10:A:1635:A:H2'	10:A:1636:C:H6	1.80	0.46
10:A:1741:A:H2'	10:A:1742:A:C8	2.50	0.46
11:B:17:LEU:HD23	11:B:22:VAL:HG21	1.97	0.46
13:D:36:LEU:HD11	13:D:51:ILE:HD12	1.97	0.46
15:F:127:LYS:HE2	15:F:142:HIS:HA	1.97	0.46
20:K:86:LEU:HD21	20:K:90:LYS:O	2.16	0.46
25:P:12:ALA:N	25:P:75:HIS:O	2.42	0.46
55:y:83:VAL:O	55:y:103:ALA:HA	2.15	0.46
56:z:128:LYS:NZ	57:1:1720:U:OP2	2.45	0.46
57:1:527:G:H2'	57:1:528:A:C8	2.50	0.46
57:1:569:U:H2'	57:1:570:A:H8	1.81	0.46
57:1:2138:G:H2'	57:1:2139:G:H8	1.81	0.46
57:1:2196:G:H2'	57:1:2197:A:H8	1.81	0.46
76:AN:22:LYS:HG3	76:AN:42:THR:HG21	1.98	0.46
3:3:19:C:H2'	3:3:20:A:C8	2.51	0.46
5:5:101:VAL:HG23	5:5:102:LYS:H	1.81	0.46



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:759:A:H61	10:A:770:C:H42	1.62	0.46
10:A:871:U:OP2	12:C:216:LYS:NZ	2.49	0.46
10:A:1774:C:H2'	10:A:1775:G:H8	1.80	0.46
11:B:157:ASP:O	32:W:66:ASP:HA	2.16	0.46
14:E:208:LYS:HA	14:E:208:LYS:HD2	1.73	0.46
16:G:100:ASN:HD22	16:G:180:ARG:HD3	1.80	0.46
17:H:180:THR:HG23	17:H:183:THR:H	1.81	0.46
20:K:68:LYS:HG2	20:K:72:GLU:OE2	2.16	0.46
38:c:54:VAL:HG13	38:c:63:LEU:HB2	1.98	0.46
43:h:246:ARG:HB3	43:h:248:TRP:CD1	2.51	0.46
49:q:94:TYR:HA	49:q:177:ASP:OD1	2.15	0.46
57:1:252:U:H5'	57:1:253:A:H8	1.80	0.46
57:1:431:A:H2'	57:1:432:G:C8	2.49	0.46
57:1:1801:C:H2'	57:1:1802:A:H8	1.80	0.46
10:A:123:G:H21	15:F:146:THR:HG21	1.80	0.46
10:A:327:G:H5"	19:J:98:LYS:HB3	1.98	0.46
10:A:933:A:H2'	10:A:934:C:H6	1.79	0.46
11:B:90:ALA:HB2	11:B:97:ALA:HB2	1.98	0.46
15:F:256:ARG:HG3	15:F:257:ARG:N	2.30	0.46
23:N:80:ASN:OD1	23:N:85:LYS:HE3	2.16	0.46
28:S:11:ARG:HA	28:S:14:LYS:HG2	1.97	0.46
29:T:40:ARG:HD3	29:T:40:ARG:H	1.80	0.46
43:h:207:LEU:CG	43:h:219:LEU:HD12	2.45	0.46
55:y:102:ALA:HA	55:y:122:ILE:O	2.16	0.46
57:1:119:G:N2	60:p:127:SER:O	2.49	0.46
57:1:179:C:H2'	57:1:180:U:C6	2.50	0.46
60:p:114:ALA:HA	60:p:117:ILE:HG22	1.97	0.46
10:A:25:C:H4'	10:A:26:A:O5'	2.14	0.46
10:A:176:U:O2'	10:A:177:A:OP2	2.32	0.46
10:A:739:A:H5"	10:A:740:A:C5'	2.46	0.46
10:A:1107:G:N2	10:A:1110:A:OP2	2.43	0.46
10:A:1303:G:H2'	10:A:1304:A:C8	2.51	0.46
13:D:134:ILE:HD13	13:D:186:ALA:HB1	1.97	0.46
14:E:44:PRO:HG2	31:V:104:GLN:OE1	2.16	0.46
14:E:107:LYS:HG2	14:E:176:VAL:HG22	1.97	0.46
14:E:121:TYR:CD1	14:E:124:LEU:HD12	2.51	0.46
15:F:211:LYS:HD2	15:F:215:GLU:CD	2.41	0.46
23:N:62:LEU:HG	23:N:90:LYS:NZ	2.31	0.46
29:T:6:GLN:OE1	29:T:6:GLN:N	2.49	0.46
48:0:174:PHE:CZ	48:0:195:GLN:HG2	2.51	0.46
53:v:27:CYS:HB2	53:v:122:ASN:HD21	1.81	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
56:z:159:ALA:O	56:z:163:ARG:HD2	2.16	0.46
57:1:1841:G:H5"	57:1:1842:C:H5'	1.98	0.46
60:p:9:ALA:HB3	60:p:10:PRO:HD3	1.97	0.46
73:AK:39:TYR:CD1	73:AK:40:PRO:HA	2.51	0.46
3:3:113:C:H2'	3:3:114:U:O4'	2.16	0.45
10:A:168:U:N3	10:A:287:U:H1'	2.29	0.45
10:A:191:U:H4'	10:A:192:U:H5'	1.97	0.45
10:A:555:G:H1'	41:f:59:SER:OG	2.16	0.45
10:A:938:G:H2'	10:A:939:G:H8	1.81	0.45
10:A:1472:G:H2'	10:A:1473:A:C8	2.51	0.45
10:A:1648:U:H2'	10:A:1649:G:H8	1.81	0.45
16:G:149:ILE:HD11	16:G:156:ARG:NH2	2.31	0.45
23:N:136:LEU:O	23:N:136:LEU:HD23	2.16	0.45
24:O:87:ASP:OD1	24:O:87:ASP:N	2.48	0.45
31:V:36:VAL:O	31:V:40:ILE:HG12	2.16	0.45
35:Z:12:VAL:HA	35:Z:23:PHE:HB3	1.98	0.45
81:j:301:YMZ:FAF	79:AQ:83:ILE:HG12	2.06	0.45
47:m:127:GLY:O	47:m:195:LEU:HD23	2.17	0.45
49:q:45:PHE:CD2	49:q:55:ILE:HG12	2.50	0.45
57:1:117:U:O2	57:1:120:A:H5"	2.16	0.45
57:1:1576:A:H5"	57:1:1576:A:C8	2.51	0.45
5:5:83:THR:O	5:5:87:LEU:HG	2.17	0.45
9:9:31:LEU:HB3	9:9:101:PRO:HG2	1.98	0.45
10:A:165:U:C2'	10:A:166:A:H5"	2.46	0.45
10:A:260:U:C2'	10:A:261:C:H5'	2.46	0.45
10:A:260:U:O2'	10:A:261:C:H5'	2.15	0.45
10:A:871:U:H2'	10:A:872:A:C8	2.51	0.45
12:C:121:VAL:HG13	12:C:168:MET:HE1	1.98	0.45
12:C:184:LEU:O	12:C:188:LEU:HG	2.15	0.45
13:D:147:HIS:HB2	13:D:190:ASP:OD2	2.16	0.45
45:k:217:VAL:HG11	45:k:328:ILE:HB	1.97	0.45
52:u:98:ASN:C	52:u:98:ASN:HD22	2.22	0.45
57:1:196:G:N2	57:1:372:A:C8	2.83	0.45
57:1:561:U:H2'	57:1:562:C:C6	2.52	0.45
57:1:3323:U:H2'	57:1:3324:A:H8	1.81	0.45
62:x:122:ALA:HB3	62:x:143:PRO:HB2	1.98	0.45
66:AD:44:VAL:CG1	66:AD:69:VAL:HG12	2.47	0.45
70:AH:98:GLN:HA	70:AH:101:VAL:HG22	1.98	0.45
10:A:558:U:H2'	10:A:559:G:H8	1.81	0.45
10:A:565:A:OP1	34:Y:68:ILE:HG22	2.16	0.45
10:A:964:A:H4'	10:A:1773:G:N2	2.31	0.45



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:1212:A:C8	23:N:116:VAL:HG11	2.51	0.45
10:A:1220:C:H3'	10:A:1221:A:H8	1.80	0.45
10:A:1276:G:N2	10:A:1309:G:H22	2.10	0.45
10:A:1469:A:H2	10:A:1594:G:H1'	1.82	0.45
21:L:52:LYS:HG3	21:L:52:LYS:O	2.16	0.45
25:P:63:ALA:HA	25:P:66:CYS:SG	2.56	0.45
43:h:199:ILE:HG13	43:h:210:SER:HB2	1.99	0.45
45:k:218:ILE:HB	45:k:337:THR:HB	1.99	0.45
50:s:52:TYR:HH	57:1:2651:A:HO2'	1.60	0.45
54:w:66:ASN:HB3	54:w:69:LYS:HG3	1.99	0.45
57:1:99:A:H2'	57:1:100:G:N3	2.32	0.45
57:1:437:G:O2'	57:1:438:A:H5"	2.17	0.45
57:1:1660:G:H2'	57:1:1661:U:C6	2.51	0.45
57:1:1762:G:HO2'	57:1:1763:C:P	2.39	0.45
73:AK:84:LYS:HE3	73:AK:84:LYS:HB3	1.81	0.45
3:3:3:U:H2'	3:3:4:U:C6	2.52	0.45
3:3:4:U:H2'	3:3:5:G:H8	1.82	0.45
10:A:824:U:O2'	10:A:825:U:N3	2.40	0.45
10:A:1086:G:O2'	33:X:4:THR:OG1	2.26	0.45
10:A:1168:A:C6	26:Q:100:LYS:HB2	2.51	0.45
10:A:1512:A:N1	10:A:1595:U:H1'	2.32	0.45
10:A:1555:C:H4'	10:A:1556:A:O5'	2.16	0.45
10:A:1727:A:H2'	10:A:1728:U:C6	2.52	0.45
12:C:66:PHE:CE1	25:P:29:SER:HB3	2.51	0.45
16:G:29:ILE:HG22	16:G:33:VAL:HG23	1.98	0.45
19:J:196:ALA:O	19:J:200:ARG:HG3	2.16	0.45
25:P:12:ALA:HA	25:P:25:VAL:HG22	1.97	0.45
43:h:91:ARG:NH1	43:h:103:ARG:HH11	2.14	0.45
52:u:109:GLU:OE1	54:w:198:PHE:CE1	2.69	0.45
55:y:69:ARG:HH21	57:1:780:A:H2'	1.81	0.45
57:1:1442:A:H61	57:1:2334:A:H5"	1.81	0.45
57:1:1481:G:N2	70:AH:4:ARG:HD2	2.32	0.45
57:1:3196:U:H2'	57:1:3197:G:C8	2.52	0.45
57:1:3322:U:H2'	57:1:3323:U:C6	2.52	0.45
10:A:1302:C:O2'	10:A:1386:A:N3	2.45	0.45
10:A:1486:G:O6	10:A:1496:C:N4	2.50	0.45
12:C:134:VAL:HG23	12:C:219:LYS:HE3	1.99	0.45
12:C:136:ARG:HG3	12:C:218:LEU:HD11	1.97	0.45
15:F:184:THR:O	15:F:184:THR:HG22	2.17	0.45
46:l:361:LEU:HD11	57:1:515:A:N7	2.32	0.45
50:s:55:ARG:HA	50:s:55:ARG:HD3	1.62	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:122:A:C6	57:1:149:A:C5	3.05	0.45
57:1:654:A:H2'	57:1:655:A:H8	1.82	0.45
57:1:948:A:H4'	57:1:964:G:N2	2.31	0.45
57:1:983:U:H2'	57:1:984:U:C6	2.52	0.45
59:n:146:LEU:O	59:n:150:LYS:HG2	2.16	0.45
4:4:4:C:H2'	4:4:5:U:C6	2.52	0.45
5:5:16:VAL:HG23	5:5:65:VAL:HG22	1.98	0.45
10:A:1219:A:H5"	10:A:1230:G:H2'	1.99	0.45
15:F:60:GLU:CD	35:Z:20:ARG:HH22	2.23	0.45
15:F:130:GLN:HG3	15:F:131:LEU:H	1.82	0.45
15:F:183:VAL:HA	15:F:224:ASN:O	2.16	0.45
17:H:161:GLU:HA	17:H:170:THR:HA	1.99	0.45
20:K:11:THR:O	20:K:11:THR:HG22	2.16	0.45
20:K:112:GLN:HB3	20:K:153:GLN:HE22	1.81	0.45
24:O:99:ARG:NH2	24:O:119:GLU:OE2	2.49	0.45
36:a:54:VAL:HG13	36:a:60:VAL:HG11	1.99	0.45
44:j:60:LYS:HB3	44:j:73:GLU:OE2	2.17	0.45
57:1:482:U:H2'	57:1:483:U:C5	2.52	0.45
57:1:1616:U:H2'	57:1:1617:A:C8	2.52	0.45
57:1:2181:U:H2'	57:1:2182:C:C6	2.52	0.45
57:1:2404:U:H2'	57:1:2405:U:C6	2.51	0.45
57:1:2515:G:H1'	57:1:2516:U:O4'	2.17	0.45
57:1:2603:U:OP1	57:1:2729:U:O2'	2.27	0.45
4:4:71:A:N1	4:4:82:U:O2'	2.44	0.45
4:4:142:C:H2'	4:4:143:U:H6	1.82	0.45
8:8:24:LEU:HD21	57:1:2557:G:C6	2.52	0.45
10:A:876:A:H2'	10:A:877:G:C8	2.51	0.45
10:A:1219:A:H3'	10:A:1230:G:C8	2.52	0.45
10:A:1238:U:H2'	10:A:1239:U:C6	2.52	0.45
10:A:1502:A:O2'	10:A:1504:U:OP2	2.27	0.45
14:E:49:VAL:CG1	14:E:87:ILE:HG12	2.46	0.45
16:G:207:THR:O	16:G:212:LYS:HE2	2.16	0.45
20:K:46:GLY:HA2	20:K:49:LEU:HG	1.97	0.45
23:N:97:LEU:HA	23:N:100:TRP:CE2	2.51	0.45
29:T:49:LYS:HA	29:T:49:LYS:HD3	1.69	0.45
30:U:14:PHE:HE2	30:U:63:ARG:HB2	1.80	0.45
43:h:297:ASN:HD21	43:h:311:GLN:CD	2.20	0.45
57:1:67:C:OP2	57:1:301:G:N2	2.49	0.45
57:1:163:A:H2'	57:1:164:U:O4'	2.17	0.45
57:1:619:A:H2'	57:1:620:A:N7	2.32	0.45
57:1:844:A:C5	57:1:845:C:H1'	2.52	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
67:AE:71:ARG:NH1	67:AE:103:LEU:HD13	2.32	0.45
77:AO:2:ARG:C	77:AO:4:LYS:H	2.25	0.45
4:4:23:U:OP1	9:9:16:ARG:NH1	2.50	0.45
5:5:42:LYS:HD3	5:5:45:GLY:HA2	1.98	0.45
10:A:626:G:OP1	24:O:124:ARG:NH1	2.42	0.45
10:A:795:A:H62	18:I:109:PRO:HD3	1.82	0.45
10:A:1140:G:H2'	10:A:1141:C:C6	2.51	0.45
10:A:1235:U:O2'	42:g:177:MET:SD	2.62	0.45
11:B:21:ASN:HA	11:B:23:HIS:CE1	2.52	0.45
11:B:134:LYS:HE3	11:B:138:TYR:CZ	2.52	0.45
14:E:143:LEU:HD12	14:E:143:LEU:O	2.17	0.45
20:K:63:ASP:OD1	20:K:64:GLU:N	2.50	0.45
25:P:8:VAL:HG23	25:P:71:ILE:HA	1.99	0.45
34:Y:50:LYS:HD3	34:Y:101:GLU:OE2	2.17	0.45
57:1:65:A:N6	57:1:75:G:H1'	2.32	0.45
57:1:359:U:H4'	57:1:813:A:H62	1.82	0.45
57:1:3284:U:O2'	57:1:3285:A:OP1	2.33	0.45
73:AK:24:ARG:NH1	73:AK:24:ARG:HG2	2.32	0.45
75:AM:33:ASN:OD1	75:AM:34:LYS:N	2.50	0.45
1:0:27:MET:HE2	1:0:27:MET:HB3	1.90	0.45
4:4:17:A:H1'	57:1:407:A:C2	2.52	0.45
5:5:77:LYS:NZ	57:1:1674:G:N7	2.64	0.45
10:A:65:A:H2	10:A:84:A:H62	1.65	0.45
10:A:733:U:O2'	33:X:122:SER:O	2.33	0.45
10:A:1148:A:H2'	10:A:1149:G:O4'	2.16	0.45
15:F:257:ARG:HH22	20:K:78:ARG:HH21	1.63	0.45
19:J:60:VAL:HG21	19:J:185:CYS:SG	2.56	0.45
25:P:79:ARG:HA	25:P:114:THR:HG22	1.99	0.45
40:e:53:ASN:HB2	40:e:55:TYR:CE2	2.51	0.45
45:k:67:MET:SD	45:k:70:ARG:NH1	2.90	0.45
57:1:538:G:O2'	57:1:539:G:OP1	2.32	0.45
57:1:1358:C:H2'	57:1:1359:A:C8	2.52	0.45
57:1:1456:A:H2'	57:1:1457:A:C8	2.52	0.45
57:1:2084:A:H2'	57:1:2085:A:H8	1.82	0.45
57:1:2683:C:O2'	57:1:2716:U:OP1	2.32	0.45
57:1:3166:A:H2'	57:1:3167:G:H8	1.82	0.45
4:4:6:U:H2'	4:4:7:U:C6	2.52	0.45
9:9:109:LEU:HD22	9:9:115:ARG:NH2	2.32	0.45
10:A:254:A:H2'	10:A:255:A:O4'	2.17	0.45
10:A:897:U:H4'	10:A:898:G:H5"	1.99	0.45
10:A:1783:C:O2	37:b:92:ARG:HB3	2.17	0.45



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
15:F:44:LEU:HD12	15:F:82:TYR:HB3	1.99	0.45
18:I:146:GLN:HB2	18:I:177:VAL:HG22	1.99	0.45
29:T:63:GLN:HA	29:T:66:LEU:HG	1.99	0.45
36:a:78:VAL:HG22	36:a:81:ARG:NH2	2.28	0.45
57:1:1218:G:HO2'	57:1:1219:A:P	2.37	0.45
57:1:1911:A:H2'	57:1:1912:U:C6	2.51	0.45
57:1:3247:A:H2'	57:1:3248:U:C6	2.52	0.45
61:r:31:ILE:HA	61:r:66:GLU:OE1	2.17	0.45
67:AE:96:ILE:O	67:AE:96:ILE:HG13	2.16	0.45
68:AF:35:LYS:HB3	68:AF:37:LYS:HZ1	1.82	0.45
2:2:136:ARG:HD3	2:2:139:ARG:NH2	2.31	0.44
9:9:2:ALA:N	57:1:212:A:OP1	2.50	0.44
10:A:339:A:H2'	10:A:340:C:C6	2.52	0.44
10:A:502:U:O2'	10:A:503:A:OP1	2.29	0.44
10:A:997:U:H2'	10:A:998:A:H8	1.81	0.44
10:A:1157:G:N2	10:A:1588:G:H22	2.15	0.44
10:A:1213:G:OP1	23:N:119:SER:N	2.47	0.44
10:A:1436:U:H2'	10:A:1437:C:C6	2.52	0.44
23:N:76:GLU:O	23:N:80:ASN:ND2	2.50	0.44
23:N:79:CYS:SG	23:N:86:ILE:HB	2.57	0.44
26:Q:96:VAL:N	26:Q:103:ASN:O	2.43	0.44
33:X:8:ALA:HB2	33:X:74:VAL:HG21	2.00	0.44
33:X:90:THR:HA	33:X:94:LEU:HD13	1.99	0.44
36:a:89:ILE:CG2	36:a:101:TYR:HB3	2.47	0.44
42:g:129:THR:HG23	42:g:130:PRO:HD2	2.00	0.44
43:h:130:LYS:HZ2	43:h:150:ASP:HA	1.82	0.44
44:j:117:GLU:OE2	44:j:163:ARG:NH2	2.49	0.44
44:j:183:GLY:HA2	57:1:892:A:H5'	1.98	0.44
45:k:94:GLU:OE1	54:w:156:LYS:NZ	2.41	0.44
46:l:68:THR:HG23	57:1:1432:U:O4	2.17	0.44
57:1:602:A:H2'	57:1:603:C:H6	1.82	0.44
57:1:1322:A:H2'	57:1:1323:C:O4'	2.17	0.44
57:1:2808:OMC:HN42	57:1:2824:C:N4	2.14	0.44
57:1:2882:A:O2'	57:1:3102:A:N1	2.42	0.44
57:1:3300:A:H2'	57:1:3301:A:C8	2.52	0.44
70:AH:23:VAL:HG21	70:AH:33:GLN:OE1	2.17	0.44
2:2:56:TYR:CZ	2:2:78:LYS:HG3	2.53	0.44
10:A:382:G:H2'	10:A:383:A:C8	2.52	0.44
10:A:1206:A:H5'	21:L:52:LYS:NZ	2.33	0.44
10:A:1227:A:O2'	10:A:1229:A:OP1	2.29	0.44
10:A:1670:U:O2'	10:A:1671:G:H8	1.99	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
28:S:13:SER:O	28:S:17:ILE:HG12	2.16	0.44
41:f:54:ARG:HH22	41:f:56:MET:HE2	1.81	0.44
43:h:84:ALA:HA	43:h:90:LEU:HD23	1.99	0.44
43:h:199:ILE:HA	43:h:210:SER:HA	1.99	0.44
53:v:48:ALA:HB1	53:v:53:TYR:HB3	1.98	0.44
55:y:94:LEU:HD22	64:AB:119:PRO:HG3	1.99	0.44
57:1:229:C:H2'	57:1:230:G:O4'	2.17	0.44
57:1:1291:G:H2'	57:1:1292:C:C6	2.52	0.44
70:AH:67:LYS:O	70:AH:71:THR:HG22	2.17	0.44
10:A:1489:G:O6	30:U:102:ARG:NH1	2.50	0.44
29:T:116:LEU:HD11	29:T:123:ARG:HG2	1.99	0.44
33:X:16:ASN:HA	33:X:19:LYS:HG2	1.99	0.44
43:h:126:ALA:HB2	43:h:155:VAL:HG23	1.99	0.44
51:t:60:ALA:HB3	51:t:65:TYR:O	2.18	0.44
53:v:158:HIS:HB3	53:v:161:ALA:HB3	1.98	0.44
57:1:3197:G:H2'	57:1:3198:C:C6	2.52	0.44
61:r:82:ARG:NH1	61:r:83:ASP:OD1	2.51	0.44
2:2:129:LYS:HG2	57:1:1093:G:H4'	1.99	0.44
4:4:9:A:H2'	4:4:10:A:H8	1.80	0.44
4:4:75:G:H2'	4:4:76:C:C6	2.53	0.44
10:A:1604:U:H2'	10:A:1605:C:C6	2.52	0.44
14:E:56:THR:O	14:E:56:THR:HG22	2.17	0.44
16:G:91:GLU:HA	16:G:94:THR:HG22	2.00	0.44
17:H:3:LEU:HD13	17:H:18:ILE:HG12	1.99	0.44
24:O:3:ARG:HB3	24:O:6:SER:HB3	1.98	0.44
26:Q:107:ILE:O	26:Q:107:ILE:HG13	2.16	0.44
31:V:47:TYR:O	31:V:49:ILE:N	2.48	0.44
33:X:31:SER:H	33:X:34:ILE:CG2	2.30	0.44
38:c:54:VAL:HG12	38:c:64:CYS:SG	2.58	0.44
43:h:218:ILE:HG23	43:h:230:THR:HG22	1.99	0.44
46:l:35:LEU:HD22	46:l:121:TYR:HD2	1.82	0.44
48:0:82:VAL:HG21	48:0:134:TYR:HD2	1.82	0.44
57:1:989:G:N3	57:1:2609:A:H2'	2.33	0.44
57:1:1157:G:O2'	68:AF:55:ASN:OD1	2.34	0.44
57:1:1230:G:H3'	57:1:1230:G:OP2	2.17	0.44
57:1:1338:G:H2'	57:1:1339:A:O4'	2.18	0.44
1:0:2:SER:O	1:0:104:GLU:HG2	2.17	0.44
4:4:126:A:O2'	4:4:128:U:OP2	2.28	0.44
10:A:512:G:N3	10:A:513:A:C8	2.86	0.44
10:A:810:U:H2'	10:A:811:U:O4'	2.18	0.44
10:A:904:A:H2'	10:A:905:C:H6	1.83	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:948:A:OP2	10:A:948:A:H8	2.01	0.44
10:A:1375:C:H6	28:S:28:PHE:CZ	2.36	0.44
10:A:1672:G:H2'	10:A:1674:U:N3	2.33	0.44
11:B:43:ASP:OD1	11:B:44:GLY:N	2.51	0.44
11:B:78:SER:OG	11:B:129:ASP:OD1	2.26	0.44
18:I:162:LEU:HD22	18:I:179:PHE:HB2	1.99	0.44
19:J:84:HIS:NE2	19:J:97:THR:OG1	2.36	0.44
27:R:51:LEU:HD12	27:R:52:THR:N	2.33	0.44
29:T:63:GLN:O	29:T:66:LEU:HG	2.18	0.44
31:V:96:ALA:HA	31:V:99:VAL:HG12	1.99	0.44
46:1:68:THR:HG22	46:1:69:GLY:N	2.33	0.44
56:z:17:VAL:HG11	56:z:52:LYS:HG3	1.99	0.44
56:z:67:LYS:HE3	56:z:71:ARG:HH22	1.82	0.44
57:1:1221:A:H2'	57:1:1222:G:H8	1.82	0.44
57:1:2158:A:H2'	57:1:2159:C:C6	2.52	0.44
57:1:2876:U:H2'	57:1:2877:U:H6	1.81	0.44
60:p:153:LEU:HD13	60:p:181:VAL:HG11	2.00	0.44
61:r:169:LYS:HD2	61:r:169:LYS:N	2.33	0.44
63:AA:104:PRO:O	63:AA:108:GLU:HG2	2.18	0.44
4:4:141:C:O3'	53:v:62:TYR:OH	2.34	0.44
10:A:327:G:H2'	10:A:328:G:C8	2.53	0.44
10:A:485:G:N3	10:A:485:G:H2'	2.32	0.44
10:A:1425:C:H2'	10:A:1426:C:H6	1.82	0.44
15:F:134:LYS:HE3	15:F:134:LYS:HB2	1.85	0.44
16:G:63:GLN:HA	16:G:65:ARG:CZ	2.47	0.44
32:W:51:ILE:HD12	32:W:78:LEU:HD21	1.99	0.44
33:X:119:LYS:HG3	33:X:121:VAL:HG22	2.00	0.44
43:h:33:LEU:HD22	43:h:45:TRP:CD1	2.53	0.44
44:j:44:VAL:HG13	44:j:46:LYS:HE3	1.99	0.44
46:1:106:THR:HG22	51:t:26:PHE:CE2	2.52	0.44
50:s:158:ASP:OD1	50:s:159:THR:N	2.50	0.44
55:y:98:LYS:HE3	55:y:98:LYS:HB2	1.63	0.44
57:1:1684:U:H2'	57:1:1685:U:C6	2.52	0.44
57:1:2408:A:H2'	57:1:2409:C:C6	2.53	0.44
57:1:2739:U:H2'	57:1:2740:U:C6	2.52	0.44
57:1:2854:U:H2'	57:1:2855:U:C6	2.52	0.44
74:AL:36:LYS:HG3	74:AL:37:LYS:N	2.26	0.44
10:A:476:A:OP1	41:f:37:ARG:NH1	2.50	0.44
10:A:588:C:H2'	10:A:589:A:C8	2.53	0.44
10:A:800:G:H21	18:I:106:GLN:HE22	1.65	0.44
10:A:872:A:H2'	10:A:873:U:H6	1.82	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:1344:C:H2'	10:A:1345:A:C8	2.53	0.44
11:B:76:CYS:SG	11:B:98:ILE:HD12	2.58	0.44
54:w:69:LYS:HB3	54:w:69:LYS:HE2	1.69	0.44
57:1:981:U:H2'	57:1:982:U:H6	1.83	0.44
57:1:2086:C:H1'	57:1:3309:A:C8	2.53	0.44
57:1:2232:U:H2'	57:1:2239:G:H22	1.82	0.44
57:1:3044:C:H2'	57:1:3045:A:O4'	2.17	0.44
62:x:4:TYR:OH	62:x:18:ARG:HG3	2.17	0.44
1:0:168:PRO:HG3	54:w:125:LEU:HD13	2.00	0.44
3:3:45:A:H2'	3:3:46:A:C8	2.52	0.44
4:4:61:A:OP1	71:AI:49:LYS:NZ	2.40	0.44
9:9:106:ILE:HG21	9:9:109:LEU:HD23	1.98	0.44
10:A:63:G:O4'	10:A:168:U:H5	2.01	0.44
10:A:138:C:H5"	10:A:139:U:C6	2.52	0.44
10:A:286:A:H2'	10:A:287:U:O4'	2.18	0.44
14:E:72:SER:HA	14:E:75:VAL:HG22	1.99	0.44
15:F:128:LYS:HA	15:F:128:LYS:HD2	1.85	0.44
19:J:67:TRP:NE1	19:J:191:GLU:OE2	2.46	0.44
24:O:18:TYR:O	33:X:56:HIS:ND1	2.50	0.44
26:Q:34:THR:HA	26:Q:37:CYS:SG	2.57	0.44
33:X:6:VAL:O	33:X:9:ASP:OD1	2.36	0.44
34:Y:107:PHE:CD1	34:Y:114:LYS:HD3	2.53	0.44
35:Z:63:GLN:OE1	35:Z:68:LYS:HD3	2.17	0.44
38:c:13:ALA:O	38:c:17:LYS:HG3	2.17	0.44
57:1:671:U:H2'	57:1:672:G:C8	2.53	0.44
57:1:817:U:H2'	57:1:818:G:H8	1.82	0.44
57:1:1277:G:N3	57:1:1277:G:H2'	2.33	0.44
57:1:1491:U:H5	57:1:1831:A:N1	2.16	0.44
57:1:2352:C:OP1	57:1:2795:G:O2'	2.34	0.44
57:1:3285:A:H2'	57:1:3286:C:C6	2.52	0.44
75:AM:43:HIS:HB3	75:AM:46:ARG:HD3	2.00	0.44
10:A:874:U:H2'	10:A:875:C:H6	1.82	0.44
10:A:1345:A:H8	10:A:1345:A:OP2	2.01	0.44
10:A:1369:G:O2'	10:A:1370:A:H8	2.01	0.44
12:C:46:THR:HG22	12:C:47:LEU:H	1.83	0.44
12:C:114:VAL:O	12:C:114:VAL:HG13	2.18	0.44
16:G:43:PHE:CZ	16:G:115:LYS:HB2	2.53	0.44
20:K:68:LYS:O	20:K:72:GLU:HG2	2.18	0.44
36:a:99:ALA:HB1	36:a:101:TYR:CE2	2.53	0.44
40:e:19:ARG:NE	40:e:32:ARG:HD3	2.33	0.44
45:k:29:VAL:HG22	45:k:218:ILE:HD12	2.00	0.44



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
45:k:274:HIS:ND1	57:1:3110:U:OP1	2.47	0.44
57:1:563:U:H2'	57:1:564:G:C8	2.52	0.44
57:1:3336:G:H2'	57:1:3337:A:C8	2.53	0.44
60:p:65:ILE:O	60:p:69:ARG:HG2	2.18	0.44
60:p:125:ASP:OD1	60:p:126:VAL:HG23	2.18	0.44
6:6:77:ILE:HD12	6:6:103:VAL:HG11	2.00	0.43
10:A:38:C:O2'	20:K:6:ARG:HD2	2.18	0.43
10:A:85:A:N3	10:A:146:A:O2'	2.45	0.43
10:A:279:G:H2'	10:A:280:C:C6	2.53	0.43
10:A:553:A:H2'	10:A:554:A:C8	2.53	0.43
10:A:857:G:H2'	10:A:858:U:O4'	2.18	0.43
10:A:885:A:H2'	10:A:886:G:H8	1.83	0.43
15:F:104:ASP:O	15:F:190:GLY:HA3	2.17	0.43
16:G:209:TYR:C	16:G:211:ILE:H	2.26	0.43
21:L:82:ILE:CG1	21:L:83:PRO:HD2	2.48	0.43
23:N:31:VAL:HB	23:N:133:ARG:NH2	2.33	0.43
27:R:35:ILE:HD12	27:R:38:VAL:HG21	2.00	0.43
34:Y:95:PHE:O	34:Y:142:LYS:NZ	2.48	0.43
43:h:49:GLY:HA2	43:h:55:TYR:CE1	2.51	0.43
47:m:113:LEU:HD22	57:1:1075:A:C2	2.53	0.43
47:m:164:LYS:NZ	47:m:168:ASP:OD1	2.50	0.43
47:m:205:ALA:HA	47:m:208:MET:HE3	1.99	0.43
57:1:1631:G:N2	57:1:1634:A:OP2	2.42	0.43
57:1:1689:C:O2'	57:1:1768:U:O2'	2.29	0.43
57:1:3260:A:H2'	57:1:3261:A:H8	1.82	0.43
69:AG:38:PRO:HD3	69:AG:77:ASN:O	2.18	0.43
1:0:8:GLN:HG3	1:0:26:ARG:HD2	1.99	0.43
10:A:346:U:H4'	19:J:14:THR:HG22	2.00	0.43
10:A:457:G:OP2	35:Z:105:ARG:NH2	2.45	0.43
10:A:605:G:H5'	10:A:611:G:N2	2.32	0.43
10:A:1102:U:H2'	10:A:1103:G:C8	2.53	0.43
10:A:1238:U:H5"	42:g:172:ILE:HG23	1.99	0.43
10:A:1423:U:H2'	10:A:1424:G:C8	2.53	0.43
10:A:1580:A:O2'	10:A:1581:G:H5'	2.18	0.43
13:D:44:LYS:HB3	13:D:238:TYR:CD2	2.53	0.43
14:E:121:TYR:HD1	14:E:124:LEU:HD12	1.83	0.43
20:K:11:THR:HG22	20:K:44:ARG:HG3	2.00	0.43
37:b:37:LYS:O	37:b:38:ARG:NH1	2.50	0.43
43:h:62:PHE:HB3	43:h:93:TRP:CZ3	2.53	0.43
45:k:284:ARG:HH11	45:k:356:LEU:HD12	1.84	0.43
50:s:158:ASP:O	50:s:161:GLN:HG3	2.18	0.43



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:385:A:H2'	57:1:386:A:C8	2.53	0.43
57:1:1077:U:H5'	57:1:1078:U:H5	1.82	0.43
57:1:1562:G:C2	57:1:1563:A:H1'	2.53	0.43
57:1:2516:U:O2'	57:1:2519:A:N6	2.50	0.43
57:1:3358:U:H2'	57:1:3359:U:C6	2.53	0.43
68:AF:33:TRP:CH2	68:AF:53:GLN:HG2	2.53	0.43
2:2:26:PRO:HB2	3:3:9:C:OP1	2.18	0.43
5:5:61:ASP:OD1	5:5:61:ASP:N	2.43	0.43
9:9:69:LYS:HE2	9:9:69:LYS:HB3	1.79	0.43
10:A:267:G:N7	17:H:186:ARG:NH2	2.66	0.43
10:A:457:G:P	35:Z:105:ARG:HH22	2.40	0.43
10:A:484:G:H2'	10:A:485:G:C8	2.53	0.43
10:A:561:U:H4'	41:f:17:GLN:NE2	2.33	0.43
10:A:985:C:H5	10:A:988:A:H5"	1.82	0.43
10:A:1664:C:H2'	10:A:1665:C:C6	2.53	0.43
11:B:55:GLU:OE1	32:W:82:VAL:HB	2.18	0.43
12:C:34:ALA:HB3	12:C:41:ARG:HA	2.00	0.43
14:E:44:PRO:HD3	31:V:107:ILE:HG12	2.00	0.43
31:V:66:THR:HG22	31:V:67:ARG:N	2.33	0.43
50:s:132:GLY:HA2	50:s:154:THR:HG21	2.01	0.43
57:1:830:U:H2'	57:1:831:G:O4'	2.18	0.43
57:1:1069:U:H2'	57:1:1070:U:C6	2.52	0.43
57:1:1163:U:H2'	57:1:1164:U:O4'	2.17	0.43
75:AM:8:ARG:O	75:AM:12:LYS:HG2	2.17	0.43
5:5:97:ARG:HD2	57:1:1675:A:OP1	2.18	0.43
10:A:1275:U:H2'	10:A:1276:G:H8	1.78	0.43
10:A:1495:U:H2'	10:A:1496:C:C6	2.53	0.43
14:E:79:LYS:HE2	14:E:79:LYS:HB3	1.73	0.43
14:E:105:ALA:O	14:E:109:LYS:HG2	2.18	0.43
15:F:11:ARG:HD2	15:F:20:LEU:HB3	2.00	0.43
16:G:32:ASP:O	16:G:44:ASN:ND2	2.48	0.43
16:G:128:ASN:OD1	16:G:130:ILE:HG22	2.18	0.43
23:N:71:ILE:HA	23:N:74:LEU:HB3	2.00	0.43
23:N:97:LEU:HD23	23:N:100:TRP:HZ2	1.82	0.43
31:V:49:ILE:HD13	31:V:94:ALA:HB2	2.00	0.43
33:X:18:GLU:OE2	33:X:67:GLY:HA2	2.18	0.43
43:h:7:LEU:HD11	43:h:248:TRP:CZ3	2.53	0.43
43:h:92:LEU:HB2	43:h:104:PHE:CE1	2.49	0.43
43:h:104:PHE:CD2	43:h:139:GLY:HA2	2.53	0.43
43:h:242:PHE:CE1	43:h:249:LEU:HD13	2.53	0.43
55:y:139:ILE:HB	57:1:725:G:H22	1.84	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:1852:C:H2'	57:1:1853:C:C6	2.53	0.43
57:1:2855:U:H2'	57:1:2856:C:H6	1.84	0.43
57:1:3309:A:N3	57:1:3309:A:H2'	2.33	0.43
78:AP:99:GLN:HB3	78:AP:102:GLN:OE1	2.18	0.43
10:A:29:U:H2'	10:A:30:G:H8	1.83	0.43
10:A:349:C:H5	10:A:629:G:H5"	1.84	0.43
10:A:585:C:OP1	41:f:23:LYS:HG2	2.18	0.43
10:A:873:U:H2'	10:A:874:U:C6	2.54	0.43
10:A:944:U:O2	24:O:61:SER:HB2	2.18	0.43
10:A:1403:A:H2	40:e:56:ARG:HD2	1.84	0.43
10:A:1529:G:H22	10:A:1555:C:H1'	1.84	0.43
10:A:1542:A:H8	10:A:1542:A:OP2	2.02	0.43
10:A:1609:G:H2'	10:A:1610:C:C6	2.53	0.43
12:C:108:ASP:N	12:C:108:ASP:OD1	2.49	0.43
12:C:135:LEU:HD23	12:C:217:LEU:HD23	2.01	0.43
22:M:111:VAL:HA	22:M:139:VAL:HG12	2.01	0.43
31:V:25:LEU:O	31:V:87:LYS:HA	2.19	0.43
49:q:37:ASP:OD1	49:q:39:LYS:HG2	2.17	0.43
50:s:35:LYS:O	50:s:39:GLN:HG2	2.17	0.43
51:t:66:ASN:OD1	57:1:71:C:O2'	2.30	0.43
55:y:151:ARG:HD2	57:1:777:G:OP1	2.18	0.43
57:1:200:A:H2'	57:1:201:G:C8	2.53	0.43
57:1:1077:U:H5'	57:1:1078:U:C5	2.54	0.43
57:1:2492:U:OP2	57:1:2558:G:N2	2.51	0.43
57:1:2995:U:H2'	57:1:2996:A:H8	1.84	0.43
61:r:38:ARG:NH2	61:r:45:GLU:OE1	2.52	0.43
61:r:73:ASN:O	61:r:77:THR:HG23	2.18	0.43
5:5:19:VAL:HG12	5:5:22:PRO:HD2	2.00	0.43
10:A:82:U:H2'	10:A:83:G:O4'	2.19	0.43
10:A:1238:U:C2	10:A:1239:U:C5	3.06	0.43
11:B:197:VAL:HG11	11:B:202:TYR:HE1	1.83	0.43
14:E:109:LYS:HA	14:E:112:SER:OG	2.18	0.43
14:E:128:MET:HE2	14:E:135:VAL:HG12	1.99	0.43
43:h:215:GLY:O	43:h:232:GLU:HA	2.19	0.43
45:k:236:LYS:HE2	45:k:236:LYS:HB2	1.80	0.43
48:0:92:LYS:NZ	57:1:1152:C:OP2	2.45	0.43
57:1:277:G:H2'	57:1:278:U:C6	2.54	0.43
57:1:629:A:H2'	57:1:630:G:H8	1.84	0.43
57:1:849:G:OP2	79:AQ:2:THR:HG21	2.19	0.43
57:1:2085:A:C2	57:1:3309:A:H8	2.36	0.43
57:1:2236:U:C2	57:1:2237:A:C8	3.06	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:2385:C:H2'	57:1:2386:U:C6	2.53	0.43
57:1:2687:A:HO2'	78:AP:8:ARG:HH22	1.66	0.43
57:1:3318:G:H3'	57:1:3319:U:O3'	2.19	0.43
59:n:58:GLU:H	59:n:58:GLU:CD	2.27	0.43
4:4:4:C:H2'	4:4:5:U:H6	1.82	0.43
10:A:151:G:H2'	10:A:152:G:H8	1.82	0.43
10:A:415:A:H4'	10:A:416:G:O5'	2.18	0.43
10:A:578:A:O2'	10:A:580:U:OP1	2.36	0.43
10:A:600:U:H2'	10:A:601:U:H6	1.81	0.43
10:A:935:C:H2'	10:A:936:A:C8	2.54	0.43
10:A:1674:U:H2'	10:A:1675:U:C5	2.53	0.43
14:E:9:LYS:CE	31:V:60:LYS:HD3	2.48	0.43
23:N:35:SER:O	23:N:40:GLY:N	2.33	0.43
34:Y:92:CYS:HA	34:Y:95:PHE:CD2	2.54	0.43
35:Z:63:GLN:CD	35:Z:68:LYS:HD3	2.43	0.43
35:Z:87:PRO:HD2	35:Z:90:ARG:NH1	2.33	0.43
41:f:54:ARG:HH12	41:f:56:MET:CE	2.31	0.43
46:l:136:VAL:HG12	46:1:141:HIS:HB2	2.01	0.43
47:m:7:PHE:CE2	57:1:2659:G:H4'	2.53	0.43
50:s:91:LEU:O	50:s:171:VAL:HA	2.19	0.43
57:1:912:G:H5'	57:1:913:A:OP1	2.18	0.43
57:1:1923:G:C8	79:AQ:16:VAL:HG12	2.54	0.43
57:1:2183:U:O2'	57:1:2184:G:O4'	2.37	0.43
57:1:2899:C:H2'	57:1:2900:C:C6	2.53	0.43
57:1:3199:G:C6	57:1:3219:G:C6	3.06	0.43
60:p:198:VAL:HG12	60:p:199:ALA:N	2.34	0.43
69:AG:9:VAL:HB	69:AG:100:ILE:HB	2.00	0.43
1:0:164:GLN:OE1	57:1:3172:U:N3	2.47	0.43
3:3:45:A:H2'	3:3:46:A:H8	1.84	0.43
4:4:5:U:H2'	4:4:6:U:C6	2.54	0.43
10:A:626:G:H21	10:A:956:A:H62	1.67	0.43
10:A:1575:G:H5'	10:A:1576:C:OP2	2.19	0.43
14:E:107:LYS:HD2	14:E:174:ARG:CB	2.49	0.43
16:G:222:LYS:HD2	16:G:225:ARG:NH2	2.28	0.43
18:I:134:LYS:C	18:I:135:ARG:HD2	2.44	0.43
27:R:48:TYR:CD1	27:R:51:LEU:HD21	2.54	0.43
33:X:23:ARG:HG3	38:c:4:VAL:HG12	2.01	0.43
44:j:7:ASN:OD1	57:1:2161:A:H5"	2.18	0.43
44:j:200:ARG:HD2	57:1:2164:U:OP2	2.19	0.43
45:k:7:GLU:HG3	57:1:2887:U:C5	2.52	0.43
46:1:37:HIS:NE2	57:1:1421:U:O2'	2.47	0.43



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:445:A:N6	57:1:485:A:N1	2.67	0.43
57:1:1714:G:H2'	57:1:1715:G:C8	2.54	0.43
57:1:1852:C:H2'	57:1:1853:C:H6	1.82	0.43
57:1:2079:C:O2'	57:1:2080:U:H6	2.00	0.43
57:1:3224:U:H5"	57:1:3226:C:H5	1.83	0.43
67:AE:82:GLU:HA	67:AE:83:ASP:HA	1.55	0.43
3:3:39:U:O2'	50:s:43:GLN:HB3	2.19	0.43
10:A:598:U:H2'	10:A:599:A:C8	2.54	0.43
10:A:1413:A:O2'	10:A:1414:G:OP1	2.29	0.43
10:A:1589:C:H2'	10:A:1590:U:C6	2.53	0.43
10:A:1625:G:O6	10:A:1754:G:N2	2.51	0.43
12:C:136:ARG:O	12:C:215:VAL:HA	2.19	0.43
15:F:136:VAL:HB	15:F:148:ARG:NH2	2.34	0.43
15:F:210:ILE:HB	15:F:218:PHE:CE1	2.54	0.43
16:G:58:LEU:HD22	16:G:168:VAL:HG23	2.01	0.43
57:1:2915:G:H2'	57:1:2916:U:O4'	2.19	0.43
57:1:3005:A:H2'	57:1:3006:C:H6	1.84	0.43
7:7:3:ILE:HG21	7:7:12:LYS:HG2	2.01	0.43
10:A:265:U:H2'	10:A:266:C:C6	2.54	0.43
10:A:477:C:P	41:f:37:ARG:HH22	2.41	0.43
10:A:947:C:OP1	24:O:70:LYS:HB3	2.19	0.43
10:A:1132:A:H2'	10:A:1133:C:C6	2.54	0.43
10:A:1209:A:OP2	23:N:114:LYS:HD3	2.19	0.43
10:A:1241:A:H5'	10:A:1242:U:C5	2.54	0.43
10:A:1335:U:O2'	10:A:1336:G:OP1	2.30	0.43
10:A:1532:A:OP1	29:T:133:VAL:HG22	2.19	0.43
10:A:1575:G:O6	10:A:1595:U:C4	2.71	0.43
10:A:1648:U:H2'	10:A:1649:G:C8	2.54	0.43
14:E:66:ARG:O	14:E:70:LEU:HD23	2.19	0.43
15:F:89:VAL:HG22	15:F:100:ARG:NE	2.31	0.43
20:K:17:ARG:O	20:K:23:ARG:NH2	2.52	0.43
24:0:128:TYR:0	24:O:132:VAL:HG22	2.19	0.43
57:1:445:A:C6	57:1:446:U:C4	3.07	0.43
57:1:1456:A:H2'	57:1:1457:A:H8	1.84	0.43
57:1:1663:A:H2'	57:1:1664:G:H8	1.81	0.43
57:1:2394:U:H2'	57:1:2395:U:C6	2.53	0.43
57:1:2485:U:H2'	57:1:2486:U:C6	2.53	0.43
57:1:2808:OMC:HM23	57:1:2808:OMC:H1'	1.77	0.43
57:1:3271:U:H2'	57:1:3272:A:H5"	2.01	0.43
63:AA:41:ALA:HB2	63:AA:77:TYR:HE1	1.84	0.43
4:4:85:G:H4'	4:4:86:U:OP1	2.19	0.42



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
5:5:68:VAL:HG11	5:5:74:PHE:HB3	2.01	0.42
10:A:331:A:N6	19:J:27:PHE:HB2	2.34	0.42
10:A:1029:U:H2'	10:A:1030:C:C6	2.54	0.42
15:F:153:LEU:HD12	15:F:153:LEU:HA	1.85	0.42
21:L:14:TYR:CD2	21:L:35:ILE:HD11	2.53	0.42
31:V:19:HIS:HB3	31:V:94:ALA:O	2.19	0.42
31:V:108:GLU:CD	31:V:109:PRO:HD2	2.44	0.42
39:d:33:LEU:HD21	39:d:53:ILE:HG23	2.01	0.42
43:h:21:THR:OG1	43:h:69:VAL:O	2.34	0.42
46:1:345:VAL:CG1	57:1:512:A:H5"	2.48	0.42
47:m:36:LEU:HD23	57:1:2720:A:H1'	2.00	0.42
48:0:201:TRP:CD1	48:0:202:PRO:HD2	2.53	0.42
50:s:65:ILE:HG13	50:s:66:ALA:H	1.83	0.42
51:t:83:VAL:O	51:t:83:VAL:HG12	2.19	0.42
57:1:208:A:H4'	57:1:210:A:C8	2.54	0.42
57:1:1662:G:H2'	57:1:1663:A:C8	2.53	0.42
57:1:2587:G:H2'	57:1:2588:C:C6	2.54	0.42
61:r:56:GLU:OE1	61:r:161:GLY:HA3	2.19	0.42
10:A:112:A:O2'	10:A:113:U:H5'	2.19	0.42
10:A:334:G:N2	19:J:5:ARG:O	2.47	0.42
10:A:339:A:H2'	10:A:340:C:H6	1.83	0.42
10:A:415:A:H5'	10:A:416:G:C4	2.54	0.42
10:A:451:C:O2	10:A:451:C:H2'	2.19	0.42
10:A:518:A:O2'	10:A:519:A:OP1	2.29	0.42
10:A:824:U:O2	10:A:824:U:H2'	2.19	0.42
10:A:1234:U:C4	10:A:1235:U:C4	3.07	0.42
10:A:1293:G:H2'	10:A:1294:C:C6	2.54	0.42
27:R:17:ALA:HA	27:R:68:VAL:HA	2.00	0.42
43:h:247:TYR:O	43:h:261:LYS:HA	2.18	0.42
45:k:211:GLN:NE2	45:k:283:TYR:O	2.52	0.42
57:1:266:C:N4	72:AJ:29:LYS:HA	2.33	0.42
57:1:546:C:H2'	57:1:547:U:O4'	2.19	0.42
57:1:2418:A:H2'	57:1:2419:A:C8	2.54	0.42
57:1:3165:U:H2'	57:1:3166:A:O4'	2.18	0.42
61:r:150:GLU:O	61:r:154:ARG:HG3	2.19	0.42
64:AB:24:LYS:O	64:AB:25:HIS:C	2.61	0.42
2:2:88:ARG:O	57:1:2694:U:O2'	2.32	0.42
3:3:12:U:OP2	3:3:68:C:O2'	2.37	0.42
10:A:214:U:O2'	10:A:215:A:OP1	2.33	0.42
10:A:598:U:H2'	10:A:599:A:H8	1.84	0.42
10:A:1040:U:H3	10:A:1049:G:H1	1.66	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:1155:G:C2	10:A:1156:A:C8	3.07	0.42
14:E:116:ILE:HD13	14:E:143:LEU:HD22	2.00	0.42
15:F:141:THR:OG1	15:F:143:ASP:OD1	2.36	0.42
27:R:48:TYR:O	27:R:52:THR:HG22	2.19	0.42
34:Y:92:CYS:HA	34:Y:95:PHE:HD2	1.84	0.42
36:a:54:VAL:N	36:a:55:PRO:HD2	2.33	0.42
42:g:161:ARG:HH12	42:g:164:PRO:HG3	1.84	0.42
44:j:195:SER:O	44:j:198:LYS:NZ	2.48	0.42
47:m:205:ALA:HA	47:m:208:MET:CE	2.48	0.42
49:q:57:VAL:HG23	49:q:68:LEU:HD13	2.00	0.42
57:1:79:G:H2'	57:1:80:C:H6	1.85	0.42
57:1:834:G:O6	79:AQ:4:ARG:NH2	2.52	0.42
57:1:1821:G:H5"	74:AL:48:SER:HB3	2.00	0.42
57:1:2196:G:H2'	57:1:2197:A:C8	2.54	0.42
57:1:2647:C:OP2	57:1:2648:A:O2'	2.32	0.42
71:AI:8:GLU:O	71:AI:11:THR:HG22	2.19	0.42
71:AI:22:VAL:O	71:AI:26:GLN:HG3	2.19	0.42
73:AK:21:ARG:HD3	73:AK:44:MET:SD	2.58	0.42
4:4:16:G:N2	57:1:406:G:H1'	2.34	0.42
10:A:1566:U:H2'	10:A:1567:C:H6	1.85	0.42
10:A:1579:A:O2'	10:A:1580:A:OP1	2.35	0.42
16:G:200:ASN:HB3	16:G:208:SER:HB3	2.01	0.42
18:I:146:GLN:HB2	18:I:177:VAL:HA	2.02	0.42
25:P:12:ALA:HB3	25:P:76:ILE:HD13	2.01	0.42
27:R:46:LYS:HD2	27:R:46:LYS:HA	1.74	0.42
27:R:97:ASP:OD1	43:h:59:LYS:HA	2.19	0.42
29:T:116:LEU:HG	29:T:124:GLY:CA	2.49	0.42
30:U:130:ARG:HH11	30:U:134:ARG:NH1	2.17	0.42
43:h:287:ILE:O	43:h:287:ILE:HG22	2.20	0.42
44:j:30:ARG:NH1	44:j:36:GLU:HG3	2.34	0.42
48:0:39:ARG:HA	48:0:42:ILE:HG12	2.01	0.42
49:q:137:SER:HB3	49:q:143:GLU:HB3	2.01	0.42
57:1:2184:G:H1'	57:1:2186:A:N6	2.35	0.42
57:1:2345:A:H2'	57:1:2346:A:C8	2.54	0.42
57:1:2405:U:H2'	57:1:2406:U:C6	2.54	0.42
57:1:2486:U:H2'	57:1:2487:U:H6	1.85	0.42
57:1:3264:C:C2	57:1:3265:U:C5	3.07	0.42
3:3:1:G:C4	47:m:266:LYS:HA	2.54	0.42
5:5:90:ASN:O	5:5:92:ILE:HG23	2.19	0.42
10:A:298:A:H2'	10:A:299:A:C8	2.55	0.42
10:A:520:U:H2'	10:A:521:G:O4'	2.20	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:A:565:A:O2'	41:f:14:VAL:HG12	2.20	0.42
10:A:872:A:H5"	25:P:115:PRO:HB2	2.01	0.42
10:A:974:U:H2'	10:A:975:C:C6	2.53	0.42
10:A:1144:C:H4'	10:A:1567:C:OP1	2.19	0.42
10:A:1163:G:H2'	10:A:1164:G:O4'	2.20	0.42
10:A:1245:U:C2	10:A:1246:G:N7	2.87	0.42
10:A:1502:A:OP2	14:E:8:LYS:HG2	2.20	0.42
10:A:1636:C:H2'	10:A:1637:U:C6	2.55	0.42
12:C:128:LYS:CG	12:C:132:ASP:HA	2.50	0.42
15:F:131:LEU:HD22	15:F:135:GLY:C	2.44	0.42
17:H:155:ASP:OD1	17:H:155:ASP:N	2.51	0.42
18:I:137:ARG:HG2	33:X:51:GLU:OE1	2.20	0.42
20:K:154:LYS:HG3	20:K:155:HIS:CD2	2.53	0.42
21:L:59:PHE:CZ	21:L:62:GLN:HA	2.54	0.42
30:U:34:VAL:HG23	30:U:53:TRP:CZ2	2.54	0.42
57:1:1639:A:H2'	57:1:1640:C:C2	2.54	0.42
57:1:1755:U:H2'	57:1:1756:A:H5"	2.00	0.42
61:r:48:LEU:HD21	61:r:145:LYS:HG3	2.01	0.42
71:AI:20:GLN:O	71:AI:23:GLU:HG2	2.20	0.42
73:AK:27:PHE:HA	73:AK:34:CYS:HA	2.01	0.42
75:AM:41:ARG:HA	75:AM:41:ARG:HD2	1.82	0.42
4:4:49:G:OP1	71:AI:45:HIS:HB2	2.20	0.42
9:9:85:LEU:HA	9:9:85:LEU:HD23	1.78	0.42
10:A:338:U:H2'	10:A:339:A:C8	2.53	0.42
10:A:410:A:H2	10:A:419:A:N1	2.17	0.42
10:A:761:G:N2	10:A:769:U:H1'	2.35	0.42
10:A:1248:G:H2'	10:A:1249:G:O4'	2.19	0.42
10:A:1334:G:H2'	10:A:1335:U:H6	1.82	0.42
10:A:1360:C:H2'	10:A:1361:A:C8	2.55	0.42
11:B:12:GLU:O	11:B:16:LEU:HD12	2.20	0.42
14:E:71:THR:O	14:E:74:ILE:HG12	2.20	0.42
15:F:180:LEU:HD12	15:F:193:GLY:O	2.20	0.42
20:K:113:VAL:HG21	20:K:134:ILE:HD13	2.01	0.42
24:O:5:HIS:HB2	24:O:121:ARG:HH21	1.85	0.42
25:P:66:CYS:HB2	25:P:71:ILE:CD1	2.48	0.42
30:U:14:PHE:HD2	30:U:63:ARG:HD2	1.84	0.42
32:W:3:ASN:CG	32:W:4:ASP:H	2.28	0.42
32:W:65:ALA:O	32:W:69:LEU:HD13	2.20	0.42
56:z:134:HIS:CE1	56:z:136:ARG:HB3	2.55	0.42
57:1:1149:A:O2'	57:1:1150:A:H5'	2.20	0.42
57:1:1714:G:H2'	57:1:1715:G:H8	1.85	0.42



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
57:1:3159:A:H2'	57:1:3160:C:C6	2.55	0.42
57:1:3161:U:H2'	57:1:3162:U:C6	2.55	0.42
67:AE:109:GLU:H	67:AE:109:GLU:CD	2.26	0.42
71:AI:114:ARG:HD3	71:AI:114:ARG:HA	1.81	0.42
73:AK:25:ARG:O	73:AK:25:ARG:HG2	2.18	0.42
1:0:60:SER:HG	1:0:62:ASN:HD21	1.67	0.42
3:3:56:A:H4'	50:s:152:HIS:HB2	2.02	0.42
7:7:11:SER:HB3	45:k:369:ARG:HH11	1.84	0.42
7:7:44:LYS:HD2	57:1:2089:G:H1'	2.02	0.42
8:8:36:LYS:HE2	57:1:1556:G:N7	2.34	0.42
10:A:1021:A:H2'	10:A:1022:C:H6	1.84	0.42
10:A:1105:U:H2'	10:A:1106:C:H6	1.84	0.42
10:A:1566:U:H1'	27:R:138:GLN:HG3	2.02	0.42
12:C:108:ASP:OD2	37:b:65:PRO:HB3	2.20	0.42
12:C:168:MET:O	12:C:172:MET:HG3	2.18	0.42
13:D:135:ARG:H	13:D:216:THR:CG2	2.32	0.42
14:E:22:LEU:HD12	14:E:23:ASN:N	2.34	0.42
17:H:74:ARG:HG2	17:H:96:SER:HB3	2.01	0.42
26:Q:118:GLU:HG2	29:T:122:HIS:H	1.84	0.42
31:V:68:LYS:HE2	31:V:79:ASP:OD1	2.19	0.42
47:m:261:THR:HG23	47:m:264:GLN:H	1.85	0.42
53:v:64:ILE:HG21	53:v:102:ALA:HB1	2.01	0.42
53:v:146:ALA:HA	53:v:149:ASN:OD1	2.18	0.42
57:1:972:U:H2'	57:1:973:C:O4'	2.20	0.42
57:1:1832:C:O2'	57:1:1838:A:N1	2.49	0.42
57:1:2796:G:H2'	57:1:2797:C:H6	1.84	0.42
57:1:3056:C:H2'	57:1:3057:G:O4'	2.20	0.42
57:1:3318:G:C4	57:1:3318:G:OP2	2.73	0.42
63:AA:97:THR:HG23	63:AA:100:ALA:H	1.85	0.42
73:AK:84:LYS:HD2	73:AK:85:ALA:O	2.19	0.42
10:A:584:G:H2'	10:A:585:C:H6	1.84	0.42
10:A:803:G:H2'	10:A:806:A:H8	1.84	0.42
10:A:869:A:H62	10:A:913:U:H3	1.66	0.42
10:A:974:U:O2'	25:P:122:ARG:O	2.35	0.42
10:A:1226:G:H5'	26:Q:77:LYS:HG3	2.02	0.42
10:A:1239:U:H5'	42:g:185:LYS:HE2	2.01	0.42
10:A:1369:G:C8	10:A:1370:A:C8	3.08	0.42
10:A:1489:G:C2	10:A:1493:G:C6	3.08	0.42
10:A:1543:A:H1'	10:A:1547:U:OP2	2.20	0.42
11:B:164:ASN:O	11:B:170:ILE:HD11	2.20	0.42
23:N:71:ILE:H	23:N:71:ILE:HD12	1.84	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
23:N:81:GLU:CD	42:g:156:VAL:HG12	2.44	0.42
35:Z:37:LYS:NZ	35:Z:93:ARG:HD3	2.34	0.42
44:j:49:ILE:HD11	44:j:60:LYS:HE2	2.01	0.42
45:k:213:GLU:OE2	45:k:340:LYS:NZ	2.51	0.42
49:q:166:ARG:HA	49:q:166:ARG:HD2	1.85	0.42
51:t:173:ARG:HA	51:t:173:ARG:HD2	1.90	0.42
57:1:37:U:H2'	57:1:38:A:O4'	2.20	0.42
57:1:269:G:N2	57:1:295:A:OP2	2.32	0.42
57:1:1198:A:C2	57:1:2829:C:H5'	2.55	0.42
57:1:1287:A:H2'	57:1:1288:C:O4'	2.20	0.42
57:1:1937:C:O2'	57:1:3309:A:N6	2.53	0.42
57:1:2734:A:H2'	57:1:2735:U:H6	1.85	0.42
57:1:2853:C:H2'	57:1:2854:U:C6	2.55	0.42
61:r:5:PRO:HB2	61:r:7:ARG:HG2	2.01	0.42
68:AF:17[A]:LYS:HE3	68:AF:17[A]:LYS:HB3	1.79	0.42
4:4:66:A:OP1	71:AI:10:ARG:NH2	2.53	0.42
10:A:557:C:O2'	41:f:60:PRO:HG2	2.19	0.42
10:A:770:C:OP1	10:A:770:C:H6	2.03	0.42
10:A:800:G:N2	18:I:106:GLN:HE22	2.18	0.42
10:A:1333:A:H2'	10:A:1334:G:C8	2.55	0.42
13:D:52:TYR:CZ	13:D:133:PRO:HD3	2.55	0.42
17:H:140:HIS:HA	17:H:143:LYS:HG2	2.01	0.42
20:K:123:HIS:O	20:K:127:VAL:HG23	2.20	0.42
20:K:150:LEU:HD23	20:K:151:ASP:H	1.85	0.42
23:N:67:THR:C	23:N:69:GLU:H	2.28	0.42
27:R:113:LYS:O	27:R:117:VAL:HG22	2.20	0.42
29:T:31:ALA:O	29:T:34:LYS:HB2	2.20	0.42
46:l:108:ARG:HG2	46:l:109:ARG:N	2.35	0.42
49:q:129:HIS:H	49:q:157:ASN:HD21	1.67	0.42
53:v:193:LYS:HE2	53:v:193:LYS:HB3	1.71	0.42
57:1:209:C:C2	57:1:229:C:H4'	2.55	0.42
57:1:307:A:H2'	57:1:308:A:H8	1.79	0.42
57:1:502:U:H2'	57:1:503:U:C6	2.54	0.42
57:1:627:U:H2'	57:1:628:A:H8	1.85	0.42
57:1:1502:A:H1'	57:1:1844:G:O6	2.20	0.42
57:1:1690:U:O2'	57:1:1691:U:H5'	2.19	0.42
57:1:1765:G:H2'	57:1:1766:C:H6	1.85	0.42
57:1:2111:U:O4	57:1:2125:A:H2	2.02	0.42
57:1:2627:U:H4'	57:1:2628:A:O4'	2.20	0.42
57:1:3195:G:H2'	57:1:3196:U:C6	2.55	0.42
63:AA:126:LYS:O	63:AA:126:LYS:HG3	2.20	0.42


		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
70:AH:8:ARG:HD2	70:AH:32:ALA:O	2.20	0.42	
1:0:50:LYS:HD3	3:3:77:G:C8	2.55	$0.\overline{42}$	
10:A:267:G:H2'	10:A:268:C:C6	2.55	0.42	
10:A:391:C:H2'	10:A:392:C:C6	2.54	0.42	
10:A:472:A:H5"	20:K:144:PRO:HD2	2.01	0.42	
10:A:1218:G:N1	10:A:1237:C:H5	2.15	0.42	
10:A:1308:C:H2'	10:A:1309:G:C8	2.55	0.42	
10:A:1580:A:H2'	10:A:1581:G:H8	1.84	0.42	
14:E:137:VAL:O	14:E:153:TYR:N	2.39	0.42	
19:J:78:ILE:HA	19:J:104:ILE:HA	2.01	0.42	
20:K:28:LEU:HD22	41:f:44:PHE:HE2	1.85	0.42	
26:Q:49:LEU:HD12	26:Q:54:MET:HE3	2.02	0.42	
31:V:57:MET:HB3	31:V:87:LYS:HB3	2.01	0.42	
36:a:74:SER:O	36:a:78:VAL:HG23	2.19	0.42	
43:h:156:ARG:HD3	43:h:156:ARG:HA	1.88	0.42	
45:k:35:ASP:OD2	45:k:191:LYS:NZ	2.36	0.42	
49:q:11:ASP:OD1	49:q:11:ASP:N	2.52	0.42	
53:v:44:ARG:NH2	57:1:269:G:OP2	2.52	0.42	
57:1:2107:U:H2'	57:1:2108:G:C8	2.55	0.42	
57:1:2807:U:H2'	57:1:2808:OMC:O2	2.19	0.42	
61:r:101:LYS:HE3	61:r:101:LYS:HB3	1.85	0.42	
62:x:128:ARG:NE	62:x:130:TYR:OH	2.38	0.42	
4:4:114:G:OP1	57:1:1827:U:O2'	2.23	0.41	
4:4:149:A:H2'	4:4:150:G:C8	2.55	0.41	
10:A:161:G:O3'	17:H:53:THR:HG21	2.19	0.41	
10:A:399:A:O2'	10:A:400:C:H4'	2.20	0.41	
10:A:588:C:H2'	10:A:589:A:H8	1.84	0.41	
10:A:1442:C:OP1	10:A:1443:C:H2'	2.20	0.41	
10:A:1609:G:H2'	10:A:1610:C:H6	1.85	0.41	
10:A:1709:A:H2'	10:A:1710:G:O4'	2.21	0.41	
10:A:1712:U:H2'	10:A:1713:G:C8	2.54	0.41	
11:B:56:LYS:HE2	11:B:159:ALA:O	2.20	0.41	
24:O:100:LYS:HG2	24:O:104:LYS:HZ2	1.85	0.41	
26:Q:20:VAL:HG11	26:Q:28:MET:HE2	2.02	0.41	
43:h:252:ALA:HB2	43:h:289:LEU:HD21	2.02	0.41	
55:y:165:ILE:HD11	55:y:172:PHE:HB3	2.02	0.41	
57:1:779:A:H5"	57:1:780:A:H5"	2.02	0.41	
57:1:2737:C:O3'	78:AP:39:GLY:HA3	2.21	0.41	
4:4:13:A:O2'	62:x:121:HIS:O	2.35	0.41	
10:A:182:C:H2'	10:A:183:C:H6	1.85	0.41	
10:A:577:A:C6	14:E:144:ARG:HG2	2.55	0.41	



A + a 1	At ama 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
10:A:1187:A:N7	10:A:1442:C:H2'	2.35	0.41	
10:A:1536:C:OP1	29:T:90:LYS:NZ	2.41	0.41	
10:A:1569:U:H5"	27:R:134:ARG:HH11	1.85	0.41	
10:A:1590:U:H5'	27:R:137:PHE:CZ	2.55	0.41	
17:H:137:ARG:O	17:H:141:ILE:HG13	2.19	0.41	
17:H:140:HIS:O	17:H:143:LYS:HG2	2.19	0.41	
19:J:5:ARG:HH21	19:J:28:GLU:HA	1.86	0.41	
23:N:33:ARG:HD2	23:N:33:ARG:C	2.45	0.41	
46:l:188:LEU:HD11	46:l:199:ARG:NE	2.32	0.41	
56:z:160:GLU:O	56:z:164:VAL:HG22	2.19	0.41	
57:1:1756:A:C6	57:1:1762:G:C5	3.08	0.41	
57:1:1762:G:H2'	57:1:1763:C:H6	1.85	0.41	
57:1:2484:U:H2'	57:1:2485:U:C6	2.55	0.41	
57:1:2486:U:H2'	57:1:2487:U:C6	2.55	0.41	
57:1:3318:G:C4	57:1:3321:G:C8	3.09	0.41	
72:AJ:74:LYS:HA	72:AJ:74:LYS:HD2	1.93	0.41	
74:AL:5:ILE:N	74:AL:5:ILE:HD12	2.35	0.41	
1:0:78:TRP:HZ3	1:0:127:VAL:HG12	1.85	0.41	
8:8:72:ALA:O	8:8:76:VAL:HG23	2.20	0.41	
10:A:449:G:H2'	10:A:451:C:C5	2.56	0.41	
10:A:913:U:H3'	10:A:929:A:O2'	2.20	0.41	
10:A:1129:U:H2'	10:A:1130:U:C6	2.55	0.41	
10:A:1423:U:O2'	14:E:182:VAL:HG23	2.20	0.41	
10:A:1491:G:H21	10:A:1550:C:H1'	1.85	0.41	
12:C:115:ARG:HD3	12:C:115:ARG:HA	1.75	0.41	
13:D:117:ALA:O	13:D:121:LYS:HG2	2.21	0.41	
15:F:181:VAL:HG22	15:F:193:GLY:O	2.20	0.41	
16:G:41:LYS:HD3	16:G:47:SER:HB3	2.02	0.41	
23:N:42:ALA:HB3	23:N:122:VAL:HG12	2.01	0.41	
43:h:44:LYS:HD3	43:h:62:PHE:CZ	2.55	0.41	
43:h:59:LYS:HA	43:h:59:LYS:HD3	1.71	0.41	
44:j:4:VAL:HG13	44:j:8:GLN:HB2	2.02	0.41	
54:w:62:ALA:HA	54:w:71:PRO:HD2	2.02	0.41	
57:1:19:A:H2'	57:1:20:G:C8	2.55	0.41	
57:1:1273:C:C5'	57:1:1275:C:H41	2.33	0.41	
57:1:1814:U:O2'	57:1:1815:U:O5'	2.39	0.41	
57:1:1852:C:C2	57:1:1853:C:C5	3.08	0.41	
57:1:2946:U:H2'	57:1:2947:U:C6	2.55	0.41	
57:1:2967:A:H2'	57:1:2968:U:O4'	2.20	0.41	
59:n:59:ASP:HB2	59:n:102:VAL:CG2	2.50	0.41	
68:AF:77:VAL:HG13	68:AF:82:ASP:HB2	2.01	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
74:AL:36:LYS:CG	74:AL:37:LYS:H	2.26	0.41	
10:A:107:C:H2'	10:A:108:A:C8	2.55	0.41	
10:A:433:C:OP2	34:Y:50:LYS:HB2	2.20	0.41	
10:A:1149:G:H2'	10:A:1150:G:H8	1.84	0.41	
10:A:1545:U:O4	26:Q:121:ILE:HA	2.20	0.41	
12:C:171:ILE:HD13	12:C:196:GLU:OE1	2.20	0.41	
15:F:87:MET:O	15:F:122:LYS:HE3	2.21	0.41	
20:K:110:GLN:OE1	20:K:126:ARG:NH2	2.53	0.41	
26:Q:48:GLY:O	26:Q:49:LEU:HD22	2.20	0.41	
45:k:57:VAL:HG12	45:k:357:LYS:HB3	2.02	0.41	
53:v:54:LYS:NZ	57:1:113:A:OP1	2.53	0.41	
57:1:172:C:HO2'	57:1:173:C:P	2.41	0.41	
57:1:1142:C:H4'	57:1:1327:U:C4	2.56	0.41	
57:1:1655:U:H2'	57:1:1656:C:H6	1.86	0.41	
57:1:1794:A:H2'	57:1:1795:A:C8	2.55	0.41	
57:1:2354:G:H2'	57:1:2355:G:C8	2.55	0.41	
3:3:4:U:H2'	3:3:5:G:C8	2.55	0.41	
5:5:35:LYS:HA	5:5:38:VAL:HG12	2.02	0.41	
10:A:583:A:H2'	10:A:584:G:C8	2.55	0.41	
10:A:767:G:O2'	10:A:768:C:H6	2.04	0.41	
10:A:788:A:C8	33:X:107:SER:HA	2.56	0.41	
10:A:1520:C:H5"	29:T:27:LYS:HD2	2.02	0.41	
10:A:1669:U:HO2'	10:A:1670:U:H6	1.69	0.41	
15:F:111:VAL:HG13	15:F:111:VAL:O	2.20	0.41	
15:F:151:ASP:O	15:F:154:ILE:HG22	2.21	0.41	
16:G:112:ARG:HH11	36:a:95:HIS:CE1	2.38	0.41	
18:I:110:ARG:HA	18:I:113:THR:HG23	2.01	0.41	
30:U:117:SER:HB3	30:U:123:ARG:H	1.85	0.41	
34:Y:19:ARG:O	34:Y:23:ARG:HG2	2.20	0.41	
35:Z:83:LYS:HZ2	35:Z:96:LEU:HD13	1.85	0.41	
43:h:273:PRO:HG3	43:h:302:TYR:CE2	2.55	0.41	
45:k:257:PRO:C	45:k:259:ASN:H	2.29	0.41	
57:1:745:C:H5"	65:AC:32:LEU:HD12	2.02	0.41	
57:1:788:G:H2'	57:1:789:C:C6	2.55	0.41	
57:1:1218:G:H1'	57:1:1282:A:N6	2.36	0.41	
57:1:1478:A:H4'	57:1:1479:G:OP2	2.19	0.41	
57:1:1612:U:P	70:AH:64:GLN:HE21	2.43	0.41	
57:1:3264:C:H2'	57:1:3265:U:C6	2.55	0.41	
61:r:50:ILE:HD13	61:r:149:ILE:HG13	2.02	0.41	
4:4:66:A:H2'	4:4:67:U:C6	2.56	0.41	
8:8:127:THR:HG22	8:8:128:SER:N	2.35	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
9:9:82:VAL:HG12	9:9:83:ASP:H	1.86	0.41	
10:A:151:G:C6	10:A:160:A:C6	3.09	0.41	
10:A:158:C:H2'	10:A:159:U:O4'	2.21	0.41	
10:A:397:A:H4'	15:F:3:ARG:HG2	2.03	0.41	
10:A:584:G:H2'	10:A:585:C:C6	2.56	0.41	
10:A:1453:C:OP1	27:R:131:ARG:NH1	2.54	0.41	
10:A:1463:G:O4'	30:U:48:GLN:HG3	2.21	0.41	
10:A:1503:A:O2'	10:A:1504:U:H5'	2.20	0.41	
10:A:1757:U:H2'	10:A:1758:U:C6	2.56	0.41	
10:A:1763:A:H2'	10:A:1764:G:H8	1.86	0.41	
12:C:66:PHE:HD1	25:P:28:LEU:HB3	1.84	0.41	
12:C:129:THR:OG1	12:C:133:TYR:HB2	2.21	0.41	
12:C:129:THR:OG1	12:C:131:ASP:OD1	2.34	0.41	
16:G:97:LEU:HD23	16:G:97:LEU:HA	1.86	0.41	
23:N:24:ILE:HG13	23:N:25:GLU:N	2.36	0.41	
23:N:58:GLN:HG2	23:N:86:ILE:HD12	2.03	0.41	
29:T:113:LEU:O	29:T:116:LEU:HD23	2.21	0.41	
31:V:36:VAL:HG13	31:V:106:THR:HG22	2.03	0.41	
31:V:49:ILE:HG23	31:V:93:GLN:O	2.20	0.41	
32:W:34:ILE:HD11	32:W:53:TYR:HB2	2.02	0.41	
37:b:94:ILE:O	37:b:94:ILE:HG13	2.20	0.41	
43:h:253:THR:OG1	43:h:256:GLY:O	2.24	0.41	
46:l:61:THR:HG23	57:1:364:G:OP1	2.20	0.41	
46:1:82:GLY:O	57:1:356:C:O2'	2.30	0.41	
51:t:163:VAL:HG23	51:t:163:VAL:O	2.21	0.41	
53:v:122:ASN:OD1	53:v:123:GLN:N	2.44	0.41	
57:1:422:A:C2	57:1:2341:A:H4'	2.54	0.41	
57:1:976:A:C2'	57:1:977:U:H5'	2.50	0.41	
57:1:1622:U:H3	57:1:1813:G:H1	1.69	0.41	
57:1:3101:A:H2'	57:1:3102:A:H5"	2.03	0.41	
57:1:3264:C:H2'	57:1:3265:U:H6	1.84	0.41	
60:p:99:ARG:NH2	60:p:189:THR:O	2.53	0.41	
64:AB:89:GLU:OE1	64:AB:89:GLU:N	2.51	0.41	
65:AC:14[B]:ARG:NE	65:AC:18:ARG:HH21	2.19	0.41	
66:AD:19:THR:N	66:AD:100:SER:OG	2.54	0.41	
4:4:27:U:H2'	4:4:28:C:H6	1.86	0.41	
10:A:584:G:C6	10:A:585:C:C4	3.09	0.41	
10:A:740:A:H2'	10:A:741:A:H8	1.84	0.41	
10:A:1518:G:H2'	10:A:1519:U:C6	2.56	0.41	
11:B:23:HIS:O	11:B:48:ILE:HG12	2.21	0.41	
13:D:155:GLY:N	13:D:212:ALA:HB2	2.36	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
14:E:223:THR:HG21	43:h:225:ASN:O	2.20	0.41	
15:F:139:VAL:HG13	15:F:150:PRO:HG3	2.01	0.41	
16:G:33:VAL:HG11	27:R:48:TYR:CE2	2.56	0.41	
23:N:41:LEU:HD12	23:N:122:VAL:O	2.21	0.41	
34:Y:43:PHE:CE1	34:Y:49:ALA:HB3	2.56	0.41	
43:h:110:ASP:HB2	43:h:128:ARG:HD2	2.01	0.41	
45:k:30:LYS:HG3	57:1:3110:U:OP2	2.21	0.41	
54:w:75:ARG:HG3	57:1:2979:U:OP1	2.20	0.41	
57:1:164:U:H2'	57:1:165:C:C6	2.55	0.41	
57:1:314:U:H2'	57:1:315:C:C6	2.55	0.41	
57:1:377:A:H1'	57:1:392:G:N2	2.36	0.41	
57:1:755:U:H2'	57:1:756:G:O4'	2.19	0.41	
57:1:757:A:H2'	57:1:758:U:C6	2.56	0.41	
57:1:859:C:H2'	57:1:860:G:O4'	2.21	0.41	
57:1:1240:A:N6	57:1:1267:A:OP1	2.54	0.41	
57:1:1256:A:O2'	57:1:1257:G:O4'	2.34	0.41	
57:1:2888:U:H5	57:1:2907:U:HO2'	1.68	0.41	
63:AA:50:PRO:HD3	63:AA:68:VAL:HG22	2.02	0.41	
71:AI:49:LYS:HD3	71:AI:49:LYS:HA	1.82	0.41	
2:2:44:ALA:HB2	2:2:53:PRO:HG2	2.03	0.41	
5:5:16:VAL:CG1	5:5:105:GLN:HG2	2.50	0.41	
10:A:71:A:H2'	10:A:72:A:C8	2.56	0.41	
10:A:173:G:H1	10:A:264:A:P	2.43	0.41	
10:A:378:U:H4'	20:K:2:PRO:HD2	2.02	0.41	
10:A:504:A:O2'	10:A:505:U:P	2.79	0.41	
10:A:583:A:OP1	41:f:15:LYS:NZ	2.53	0.41	
10:A:748:G:H4'	15:F:256:ARG:NH2	2.36	0.41	
10:A:1087:G:OP2	34:Y:7:ARG:NH1	2.49	0.41	
10:A:1093:G:H2'	34:Y:25:ALA:HB1	2.02	0.41	
10:A:1199:U:O2'	40:e:3:HIS:ND1	2.50	0.41	
10:A:1500:G:H1'	10:A:1505:C:O2	2.20	0.41	
10:A:1749:A:H1'	10:A:1770:C:H5'	2.03	0.41	
16:G:114:VAL:O	16:G:118:LEU:HD12	2.21	0.41	
16:G:156:ARG:HE	39:d:67:ARG:NH2	2.18	0.41	
20:K:80:LEU:HA	20:K:83:ILE:HG22	2.03	0.41	
20:K:113:VAL:CG1	20:K:125:ALA:HB1	2.51	0.41	
30:U:14:PHE:HZ	30:U:132:LEU:HD22	1.84	0.41	
32:W:5:LYS:HB2	32:W:7:GLN:OE1	2.20	0.41	
33:X:77:PRO:HD2	33:X:79:PHE:CZ	2.56	0.41	
35:Z:6:THR:CG2	35:Z:28:LEU:HB2	2.50	0.41	
39:d:38:ARG:O	39:d:40:ILE:HG13	2.21	0.41	



	At ama 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
45:k:81:THR:OG1	45:k:205:VAL:HG21	2.21	0.41	
45:k:288:GLY:N	45:k:320:ASP:OD1	2.37	0.41	
45:k:294:GLY:N	45:k:303:LYS:O	2.53	0.41	
48:0:143[B]:ARG:HG2	48:0:183:ILE:HD13	2.02	0.41	
49:q:167:VAL:CG2	49:q:172:ILE:HG22	2.50	0.41	
50:s:29:ARG:NH1	50:s:32:ARG:HH12	2.18	0.41	
51:t:107:GLU:O	51:t:110:ASP:OD1	2.39	0.41	
52:u:12:PHE:H	52:u:17:ARG:NH2	2.19	0.41	
53:v:187:ARG:HD2	57:1:48:A:N7	2.35	0.41	
54:w:77:PRO:HB3	54:w:139:VAL:HG12	2.03	0.41	
56:z:159:ALA:O	56:z:163:ARG:CD	2.69	0.41	
57:1:643:A:C2	57:1:645:A:H2'	2.56	0.41	
57:1:1224:C:O2	57:1:1224:C:H2'	2.20	0.41	
57:1:2081:U:H2'	57:1:2082:A:C8	2.56	0.41	
57:1:2656:C:H2'	57:1:2657:C:C6	2.56	0.41	
57:1:2959:A:H2'	57:1:2960:C:C6	2.56	0.41	
66:AD:36:LEU:HD13	66:AD:61:TYR:HB3	2.03	0.41	
5:5:51:GLY:C	5:5:53:ASP:H	2.29	0.41	
10:A:30:G:H2'	10:A:31:C:H6	1.86	0.41	
10:A:58:U:OP1	10:A:454:G:O2'	2.34	0.41	
10:A:154:A:N6	10:A:416:G:C6	2.89	0.41	
10:A:327:G:H5'	19:J:99:SER:HB3	2.02	0.41	
10:A:553:A:N3	10:A:588:C:O2'	2.46	0.41	
10:A:608:G:H21	34:Y:19:ARG:NH2	2.19	0.41	
10:A:1083:U:OP1	13:D:154:THR:OG1	2.35	0.41	
10:A:1152:G:OP1	16:G:101:GLY:HA3	2.21	0.41	
10:A:1157:G:H2'	10:A:1158:C:C6	2.56	0.41	
10:A:1200:C:H2'	10:A:1201:C:C6	2.56	0.41	
10:A:1375:C:O2'	28:S:52:GLY:HA3	2.21	0.41	
10:A:1474:G:H3'	10:A:1502:A:H61	1.84	0.41	
11:B:52:LYS:HD3	32:W:82:VAL:HG23	2.03	0.41	
11:B:201:LEU:O	11:B:202:TYR:HB2	2.21	0.41	
12:C:192:VAL:HG13	12:C:195:ARG:NH1	2.35	0.41	
14:E:71:THR:HB	14:E:87:ILE:HD12	2.02	0.41	
16:G:58:LEU:HD21	16:G:167:ARG:NH1	2.35	0.41	
16:G:106:LYS:HD3	16:G:109:LYS:HE3	2.02	0.41	
16:G:130:ILE:CA	16:G:133:VAL:HG12	2.47	0.41	
16:G:143:ARG:HG3	16:G:167:ARG:HH21	1.86	0.41	
16:G:170:GLN:HE21	16:G:170:GLN:HB3	1.71	0.41	
19:J:106:ALA:HB2	19:J:171:LEU:HG	2.03	0.41	
24:O:86:GLU:OE1	24:O:86:GLU:N	2.42	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
32:W:72:LEU:O	32:W:75:GLN:HG2	2.20	0.41	
34:Y:59:ILE:O	34:Y:69:ARG:N	2.54	0.41	
36:a:79:ALA:O	36:a:82:GLN:HG3	2.21	0.41	
37:b:18:VAL:HG21	37:b:33:ASP:OD2	2.21	0.41	
43:h:208:CYS:O	43:h:220:TRP:HD1	2.04	0.41	
43:h:244:PRO:HD3	43:h:291:TRP:HB3	2.03	0.41	
43:h:258:LYS:HB3	43:h:267:LEU:HD11	2.02	0.41	
47:m:85:ARG:NH1	47:m:86:TYR:OH	2.53	0.41	
47:m:271:LYS:HB2	47:m:271:LYS:HE3	1.88	0.41	
50:s:155:ASN:O	50:s:158:ASP:OD1	2.38	0.41	
51:t:66:ASN:HB3	57:1:72:A:N7	2.36	0.41	
52:u:17:ARG:HG2	52:u:57:LEU:HD22	2.03	0.41	
57:1:445:A:N6	57:1:485:A:C6	2.88	0.41	
57:1:624:U:H2'	57:1:625:C:C6	2.56	0.41	
57:1:1186:A:N3	57:1:1186:A:H2'	2.36	0.41	
57:1:1229:G:H2'	57:1:1229:G:N3	2.35	0.41	
57:1:1231:U:H1'	57:1:1233:G:OP2	2.21	0.41	
57:1:1493:C:O2'	57:1:1598:A:N3	2.52	0.41	
57:1:1600:A:H4'	57:1:1831:A:H4'	2.03	0.41	
57:1:1618:U:H2'	57:1:1619:G:H8	1.86	0.41	
57:1:1720:U:H1'	57:1:1721:C:C5	2.56	0.41	
57:1:1949:G:O6	57:1:2070:A:H2'	2.21	0.41	
57:1:2183:U:H2'	57:1:2184:G:H8	1.84	0.41	
57:1:2339:A:H2'	57:1:2340:C:H6	1.85	0.41	
57:1:2401:U:H2'	57:1:2402:A:C8	2.56	0.41	
57:1:2628:A:C5	57:1:2630:G:C8	3.09	0.41	
57:1:2656:C:H2'	57:1:2657:C:H6	1.86	0.41	
57:1:2902:A:H2'	57:1:2903:C:C6	2.56	0.41	
57:1:3218:U:H2'	57:1:3219:G:C8	2.56	0.41	
59:n:29:LEU:HD23	59:n:29:LEU:HA	1.84	0.41	
61:r:48:LEU:O	61:r:139:ARG:HA	2.21	0.41	
62:x:60:PHE:HB3	62:x:64:ASN:HB3	2.03	0.41	
63:AA:78:ASN:OD1	66:AD:37:ARG:NH2	2.54	0.41	
72:AJ:61:ARG:CZ	72:AJ:93:ILE:HD12	2.51	0.41	
2:2:89:VAL:HG23	2:2:91:LEU:HD11	2.03	0.41	
3:3:13:A:OP2	3:3:67:G:N2	2.50	0.41	
6:6:15:LEU:HD13	6:6:51:ALA:HB3	2.02	0.41	
10:A:335:G:O2'	19:J:10:LYS:NZ	2.54	0.41	
10:A:574:G:H4'	10:A:578:A:C4	2.56	0.41	
10:A:815:U:O2'	10:A:816:U:H6	2.03	0.41	
10:A:1508:G:O2'	10:A:1510:G:OP2	2.34	0.41	



	A targe 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
10:A:1572:U:OP1	27:R:124:GLU:N	2.33	0.41	
10:A:1577:G:C2	10:A:1594:G:C2	3.09	0.41	
10:A:1611:C:H2'	10:A:1612:C:H6	1.86	0.41	
13:D:181:ARG:HD2	13:D:181:ARG:HA	1.90	0.41	
19:J:26:LYS:HG2	19:J:29:LEU:HD23	2.03	0.41	
21:L:44:LYS:HA	21:L:44:LYS:HD3	1.92	0.41	
24:O:49:GLN:O	24:O:52:VAL:HG12	2.20	0.41	
31:V:65:THR:HA	31:V:79:ASP:O	2.21	0.41	
38:c:74:THR:HG22	38:c:75:GLU:N	2.36	0.41	
43:h:107:HIS:HD2	43:h:127:SER:CB	2.33	0.41	
55:y:170:ARG:NH1	64:AB:56:VAL:O	2.51	0.41	
55:y:178:ARG:HD2	55:y:178:ARG:HA	1.91	0.41	
56:z:10:LEU:HD23	56:z:10:LEU:HA	1.89	0.41	
57:1:152:U:O2'	57:1:153:U:H5'	2.21	0.41	
57:1:1330:U:H2'	57:1:1331:U:C6	2.56	0.41	
57:1:1713:U:H2'	57:1:1714:G:H8	1.84	0.41	
57:1:1747:G:H5'	74:AL:26:LYS:HE2	2.02	0.41	
57:1:2560:U:OP1	60:p:49:ARG:NH2	2.33	0.41	
57:1:2942:C:H4'	57:1:2943:A:C6	2.55	0.41	
60:p:125:ASP:OD1	60:p:126:VAL:N	2.54	0.41	
79:AQ:81:SER:HA	79:AQ:84:ARG:HG2	2.02	0.41	
1:0:109:ASP:OD1	1:0:113:ARG:HD2	2.20	0.40	
10:A:180:A:H2'	10:A:181:U:C6	2.57	0.40	
10:A:549:G:H2'	10:A:550:G:H8	1.86	0.40	
10:A:554:A:H5'	41:f:56:MET:SD	2.61	0.40	
10:A:863:G:H1'	24:O:110:ASP:OD2	2.22	0.40	
10:A:997:U:H2'	10:A:998:A:C8	2.56	0.40	
10:A:1196:A:H4'	26:Q:100:LYS:HG3	2.02	0.40	
10:A:1218:G:N2	10:A:1238:U:H1'	2.36	0.40	
10:A:1298:A:N3	10:A:1300:U:H5'	2.36	0.40	
10:A:1370:A:H2'	10:A:1371:G:O4'	2.21	0.40	
10:A:1396:A:HO2'	10:A:1397:A:P	2.44	0.40	
10:A:1415:G:H1'	31:V:71:ASN:HD21	1.85	0.40	
10:A:1488:C:N4	10:A:1494:G:O6	2.54	0.40	
10:A:1491:G:OP1	30:U:99:SER:N	2.25	0.40	
10:A:1656:U:H2'	10:A:1657:G:O4'	2.20	0.40	
15:F:18:TRP:O	15:F:51:ARG:NH1	2.42	0.40	
15:F:151:ASP:CG	17:H:215:ARG:HH21	2.28	0.40	
16:G:82:PHE:CZ	39:d:49:ARG:HG3	2.55	0.40	
20:K:92:LYS:C	20:K:94:ASP:H	2.29	0.40	
23:N:36:LEU:HD11	23:N:43:ARG:HH21	1.85	0.40	



A + a 1		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance $(\text{\AA})$		
23:N:36:LEU:HD11	23:N:43:ARG:NH2	2.36	0.40	
28:S:24:LEU:HD23	28:S:34:LEU:HD23	2.03	0.40	
31:V:106:THR:HG22	31:V:106:THR:O	2.21	0.40	
43:h:162:GLN:C	43:h:164:SER:H	2.29	0.40	
45:k:34:LYS:HE2	45:k:34:LYS:HB3	1.88	0.40	
45:k:48:GLY:HA3	45:k:81:THR:HG22	2.03	0.40	
45:k:215:ILE:HD12	45:k:338:LEU:HB3	2.02	0.40	
48:0:108:GLN:HG3	48:0:111:ALA:HB2	2.03	0.40	
50:s:37:LEU:HD23	50:s:37:LEU:HA	1.91	0.40	
57:1:120:A:C2	60:p:130:PRO:HB3	2.56	0.40	
57:1:480:G:H5"	57:1:481:G:C5	2.56	0.40	
57:1:624:U:H2'	57:1:625:C:H6	1.85	0.40	
57:1:1035:U:H2'	57:1:1036:A:C8	2.56	0.40	
57:1:1612:U:H2'	57:1:1613:G:C8	2.56	0.40	
57:1:2391:A:H2'	57:1:2392:G:H8	1.86	0.40	
57:1:2938:G:H2'	57:1:2939:A:C8	2.56	0.40	
6:6:88:ARG:HA	6:6:88:ARG:HD2	1.95	0.40	
8:8:133:LEU:O	8:8:137:ASN:ND2	2.54	0.40	
8:8:142:ILE:HD12	8:8:142:ILE:HA	1.89	0.40	
9:9:83:ASP:O	9:9:84:LYS:HD2	2.21	0.40	
10:A:189:G:H1'	10:A:193:G:C2	2.57	0.40	
10:A:787:A:H62	18:I:101:LYS:HE2	1.86	0.40	
10:A:1021:A:H2'	10:A:1022:C:C6	2.56	0.40	
10:A:1219:A:H3'	10:A:1230:G:H8	1.86	0.40	
10:A:1259:C:H5	10:A:1413:A:C8	2.39	0.40	
10:A:1569:U:H5"	27:R:134:ARG:NH1	2.36	0.40	
10:A:1571:G:H22	10:A:1598:A:P	2.44	0.40	
15:F:34:GLY:HA3	15:F:83:PRO:HG2	2.03	0.40	
23:N:64:ASP:HA	23:N:72:ILE:HD12	2.04	0.40	
25:P:14:ILE:CD1	25:P:96:ALA:HB3	2.51	0.40	
33:X:10:ALA:HB1	33:X:27:ILE:HD13	2.02	0.40	
35:Z:11:LYS:HD2	35:Z:24:VAL:HG21	2.01	0.40	
40:e:22:ARG:HG3	40:e:37:ASP:O	2.22	0.40	
57:1:194:U:H2'	57:1:195:G:O4'	2.22	0.40	
57:1:498:C:H2'	57:1:499:G:H8	1.85	0.40	
57:1:564:G:H2'	57:1:565:A:H8	1.79	0.40	
57:1:1221:A:H2'	57:1:1222:G:C8	2.56	0.40	
57:1:1516:G:O2'	57:1:1599:A:N1	2.49	0.40	
57:1:2514:G:C4	57:1:2515:G:N2	2.90	0.40	
57:1:2649:G:H2'	57:1:2649:G:N3	2.37	0.40	
57:1:2987:G:H2'	57:1:2988:A:H8	1.86	0.40	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
61:r:79:VAL:HG21	61:r:147:VAL:HG13	2.02	0.40	
1:0:23:LYS:HD3	1:0:23:LYS:HA	1.82	0.40	
5:5:101:VAL:HG23	5:5:102:LYS:N	2.37	0.40	
10:A:122:U:C2'	10:A:123:G:H5"	2.48	0.40	
10:A:828:U:H2'	10:A:829:A:C8	2.57	0.40	
10:A:1306:A:H4'	10:A:1307:A:O5'	2.22	0.40	
10:A:1506:U:H2'	10:A:1507:U:C5	2.56	0.40	
26:Q:50:ASP:OD1	26:Q:50:ASP:N	2.54	0.40	
43:h:48:THR:HG22	43:h:48:THR:O	2.20	0.40	
43:h:231:LEU:H	43:h:231:LEU:HD23	1.86	0.40	
44:j:14:SER:OG	57:1:907:C:OP1	2.39	0.40	
45:k:256:HIS:HA	45:k:257:PRO:C	2.46	0.40	
49:q:34:LEU:HB3	49:q:78:LEU:HD22	2.03	0.40	
50:s:96:PHE:CD2	50:s:102:PHE:HB3	2.57	0.40	
50:s:109:HIS:HD2	50:s:123:TYR:H	1.69	0.40	
52:u:13:VAL:HG23	52:u:29:ILE:HD13	2.02	0.40	
57:1:296:A:O2'	57:1:297:G:H5'	2.21	0.40	
57:1:2857:C:O2'	57:1:2858:U:H5'	2.22	0.40	
57:1:3216:U:H2'	7:1:3216:U:H2' 57:1:3217:G:C8		0.40	
57:1:3270:A:H2'	57:1:3271:U:O4'	2.21	0.40	
65:AC:47:LEU:HA	65:AC:50:THR:HG22	2.02	0.40	
70:AH:57:LEU:HB3	70:AH:61:GLN:HB2	2.03	0.40	
5:5:96:ILE:HG21	5:5:108:LEU:HD13	2.04	0.40	
6:6:88:ARG:HB2	45:k:67:MET:HE2	2.04	0.40	
10:A:795:A:N6	18:I:109:PRO:HD3	2.37	0.40	
10:A:1088:U:P	34:Y:7:ARG:H	2.43	0.40	
10:A:1131:G:C6	10:A:1132:A:C6	3.10	0.40	
10:A:1142:A:H2'	10:A:1145:A:N7	2.36	0.40	
10:A:1181:A:H4'	10:A:1182:C:H5"	2.03	0.40	
10:A:1424:G:H2'	10:A:1425:C:O4'	2.22	0.40	
10:A:1602:C:C4	16:G:81:ARG:HA	2.56	0.40	
10:A:1760:C:OP2	77:AO:4:LYS:HB2	2.21	0.40	
11:B:111:ILE:O	11:B:111:ILE:HG22	2.22	0.40	
14:E:160:HIS:C	14:E:165:THR:HG21	2.47	0.40	
21:L:46:LEU:HD23	21:L:66:TYR:CG	2.56	0.40	
25:P:66:CYS:HB2	25:P:71:ILE:HD11	2.03	0.40	
25:P:73:ALA:CB	25:P:106:ARG:HB2	2.50	0.40	
32:W:17:CYS:HB2	32:W:56:SER:HB3	2.04	0.40	
39:d:53:ILE:HG22	39:d:53:ILE:O	2.21	0.40	
52:u:92:TRP:CZ2	57:1:3171:C:H2'	2.57	0.40	
54:w:59:LEU:HD21	54:w:75:ARG:HH12	1.86	0.40	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
57:1:15:A:H2'	57:1:16:G:O4'	2.22	0.40	
57:1:785:A:H2'	57:1:786:U:C6	2.57	0.40	
57:1:1093:G:H2'	57:1:1093:G:N3	2.37	0.40	
57:1:1220:C:C2	57:1:1221:A:C8	3.09	0.40	
57:1:1239:G:H21	57:1:1240:A:H62	1.67	0.40	
57:1:2296:U:H2'	57:1:2297:U:O4'	2.22	0.40	
57:1:2959:A:H2'	57:1:2960:C:H6	1.87	0.40	
3:3:3:U:H2'	3:3:4:U:H6	1.84	0.40	
4:4:81:A:H2'	4:4:82:U:C6	2.56	0.40	
5:5:18:ASP:O	5:5:107:LYS:HA	2.22	0.40	
10:A:93:A:N7	10:A:397:A:C4	2.89	0.40	
10:A:184:C:H2'	10:A:185:G:O4'	2.22	0.40	
10:A:588:C:OP1	41:f:43:ARG:NH2	2.54	0.40	
10:A:741:A:O2'	0:A:741:A:O2' 15:F:12:LEU:O		0.40	
10:A:1213:G:P	23:N:119:SER:H	2.44	0.40	
10:A:1486:G:N1	10:A:1496:C:N3	2.70	0.40	
10:A:1716:C:H2'	10:A:1717:A:O4'	2.21	0.40	
14:E:18:PHE:HD1	14:E:78:PHE:CE1	2.40	0.40	
16:G:83:ARG:HD3	16:G:83:ARG:HA	1.85	0.40	
16:G:147:THR:N	16:G:158:GLN:O	2.54	0.40	
18:I:132:ILE:HD12	18:I:132:ILE:HA	1.94	0.40	
21:L:50:THR:HB	21:L:55:VAL:HG23	2.02	0.40	
35:Z:118:ILE:HD12	35:Z:118:ILE:HA	1.89	0.40	
53:v:188:ARG:HH12	57:1:29:G:H5"	1.87	0.40	
57:1:498:C:H2'	57:1:499:G:C8	2.56	0.40	
57:1:757:A:O5'	57:1:757:A:H8	2.05	0.40	
57:1:1491:U:C5	57:1:1831:A:N1	2.89	0.40	
57:1:2415:G:C6	57:1:2489:A:C5	3.09	0.40	
57:1:2687:A:O2'	78:AP:8:ARG:NH2	2.45	0.40	
57:1:3091:U:H4'	76:AN:28:PRO:HG2	2.04	0.40	
61:r:19:LYS:HD2	61:r:26:VAL:HB	2.03	0.40	
63:AA:93:LYS:HG3	63:AA:94:SER:N	2.36	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	0	171/172~(99%)	169 (99%)	2 (1%)	0	100	100
2	2	159/160~(99%)	157~(99%)	2 (1%)	0	100	100
5	5	103/124~(83%)	95~(92%)	7 (7%)	1 (1%)	13	42
6	6	129/137~(94%)	126 (98%)	3 (2%)	0	100	100
7	7	60/155~(39%)	60 (100%)	0	0	100	100
8	8	119/142~(84%)	118 (99%)	1 (1%)	0	100	100
9	9	124/127~(98%)	123 (99%)	1 (1%)	0	100	100
11	В	206/261~(79%)	201 (98%)	5 (2%)	0	100	100
12	С	212/256~(83%)	207 (98%)	5 (2%)	0	100	100
13	D	214/249~(86%)	209 (98%)	5 (2%)	0	100	100
14	Е	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
15	F	258/262~(98%)	255 (99%)	3 (1%)	0	100	100
16	G	204/225~(91%)	196 (96%)	8 (4%)	0	100	100
17	Н	224/236~(95%)	220 (98%)	4 (2%)	0	100	100
18	Ι	94/186~(50%)	92 (98%)	2 (2%)	0	100	100
19	J	148/206~(72%)	141 (95%)	7 (5%)	0	100	100
20	K	176/189~(93%)	175 (99%)	1 (1%)	0	100	100
21	L	91/118~(77%)	84 (92%)	6 (7%)	1 (1%)	12	39
22	М	139/155~(90%)	136 (98%)	3 (2%)	0	100	100
23	N	114/143~(80%)	98 (86%)	16 (14%)	0	100	100
24	Ο	148/151~(98%)	145 (98%)	3 (2%)	0	100	100
25	Р	125/132~(95%)	122 (98%)	3 (2%)	0	100	100
26	Q	116/142~(82%)	106 (91%)	10 (9%)	0	100	100
27	R	138/142~(97%)	134 (97%)	4 (3%)	0	100	100
28	S	57/137 (42%)	56 (98%)	1 (2%)	0	100	100
29	Т	$\overline{140/145}~(97\%)$	136 (97%)	4 (3%)	0	100	100
30	U	139/145~(96%)	137 (99%)	2 (1%)	0	100	100
31	V	98/119~(82%)	96 (98%)	2 (2%)	0	100	100
32	W	85/87~(98%)	83 (98%)	2 (2%)	0	100	100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Continued	from	previous	page
Contracta	110110	proceeduo	pagem

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
33	Х	127/130~(98%)	126 (99%)	1 (1%)	0	100	100
34	Y	141/145~(97%)	138 (98%)	3 (2%)	0	100	100
35	Z	130/135~(96%)	130 (100%)	0	0	100	100
36	a	70/105~(67%)	69 (99%)	1 (1%)	0	100	100
37	b	98/119~(82%)	96 (98%)	2 (2%)	0	100	100
38	с	79/82~(96%)	75 (95%)	4 (5%)	0	100	100
39	d	60/67~(90%)	55 (92%)	5 (8%)	0	100	100
40	e	53/56~(95%)	51 (96%)	2 (4%)	0	100	100
41	f	54/63~(86%)	53 (98%)	1 (2%)	0	100	100
42	g	68/193~(35%)	61 (90%)	7 (10%)	0	100	100
43	h	309/317~(98%)	292 (94%)	17 (6%)	0	100	100
44	j	248/254~(98%)	240 (97%)	8 (3%)	0	100	100
45	k	385/389~(99%)	373 (97%)	12 (3%)	0	100	100
46	1	359/363~(99%)	349 (97%)	10 (3%)	0	100	100
47	m	290/298~(97%)	279 (96%)	11 (4%)	0	100	100
48	О	224/241~(93%)	218 (97%)	6 (3%)	0	100	100
49	q	186/191~(97%)	182 (98%)	4 (2%)	0	100	100
50	s	169/174~(97%)	164 (97%)	5 (3%)	0	100	100
51	t	198/202~(98%)	195 (98%)	1 (0%)	2(1%)	13	42
52	u	128/131~(98%)	125 (98%)	3 (2%)	0	100	100
53	v	201/204~(98%)	198 (98%)	3 (2%)	0	100	100
54	W	197/200~(98%)	195 (99%)	2 (1%)	0	100	100
55	У	186/186~(100%)	183 (98%)	3 (2%)	0	100	100
56	Z	163/190~(86%)	161 (99%)	2 (1%)	0	100	100
59	n	152/176~(86%)	150 (99%)	2 (1%)	0	100	100
60	р	238/262~(91%)	229 (96%)	9 (4%)	0	100	100
61	r	$\overline{204/220} \; (93\%)$	201 (98%)	3 (2%)	0	100	100
62	х	168/185~(91%)	165 (98%)	3 (2%)	0	100	100
63	AA	$\overline{133/136}~(98\%)$	132 (99%)	1 (1%)	0	100	100
64	AB	146/149~(98%)	138 (94%)	8 (6%)	0	100	100
65	AC	$62/63~(9\overline{8\%})$	62 (100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
66	AD	94/106~(89%)	93~(99%)	1 (1%)	0	100	100
67	AE	107/112~(96%)	106 (99%)	1 (1%)	0	100	100
68	AF	124/131~(95%)	123~(99%)	1 (1%)	0	100	100
69	AG	107/107~(100%)	104 (97%)	3 (3%)	0	100	100
70	AH	114/121~(94%)	112 (98%)	2 (2%)	0	100	100
71	AI	118/120~(98%)	114 (97%)	4 (3%)	0	100	100
72	AJ	97/99~(98%)	96~(99%)	1 (1%)	0	100	100
73	AK	84/90~(93%)	81 (96%)	3 (4%)	0	100	100
74	AL	76/78~(97%)	73~(96%)	3 (4%)	0	100	100
75	AM	49/51~(96%)	48 (98%)	1 (2%)	0	100	100
76	AN	51/52~(98%)	51 (100%)	0	0	100	100
77	AO	23/25~(92%)	22~(96%)	1 (4%)	0	100	100
78	AP	101/106~(95%)	100 (99%)	1 (1%)	0	100	100
79	AQ	89/92~(97%)	85 (96%)	4 (4%)	0	100	100
All	All	10672/11870~(90%)	10385 (97%)	283 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	t	5	LYS
5	5	20	ALA
21	L	88	PRO
51	t	62	THR

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

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	Percentiles
1	0	158/157~(101%)	158 (100%)	0	100 100
2	2	135/134~(101%)	135~(100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Percentile	
5	5	95/112~(85%)	95~(100%)	0	100	100
6	6	101/103~(98%)	101 (100%)	0	100	100
7	7	56/127~(44%)	56~(100%)	0	100	100
8	8	108/121~(89%)	108 (100%)	0	100	100
9	9	111/112~(99%)	111 (100%)	0	100	100
11	В	176/215~(82%)	176 (100%)	0	100	100
12	С	194/229~(85%)	194 (100%)	0	100	100
13	D	174/198~(88%)	174 (100%)	0	100	100
14	Е	174/196~(89%)	174 (100%)	0	100	100
15	F	218/220~(99%)	218 (100%)	0	100	100
16	G	178/197~(90%)	178 (100%)	0	100	100
17	Н	195/204~(96%)	195 (100%)	0	100	100
18	Ι	86/167~(52%)	86 (100%)	0	100	100
19	J	126/160~(79%)	126 (100%)	0	100	100
20	К	153/160~(96%)	153 (100%)	0	100	100
21	L	87/104 (84%)	87 (100%)	0	100	100
22	М	122/134~(91%)	122 (100%)	0	100	100
23	Ν	98/123~(80%)	98 (100%)	0	100	100
24	О	129/130~(99%)	129 (100%)	0	100	100
25	Р	97/102~(95%)	97 (100%)	0	100	100
26	Q	102/121 (84%)	102 (100%)	0	100	100
27	R	114/116~(98%)	114 (100%)	0	100	100
28	S	54/122~(44%)	54 (100%)	0	100	100
29	Т	126/129~(98%)	126 (100%)	0	100	100
30	U	113/117~(97%)	113 (100%)	0	100	100
31	V	90/105~(86%)	90 (100%)	0	100	100
32	W	71/71~(100%)	71 (100%)	0	100	100
33	Х	112/113~(99%)	112 (100%)	0	100	100
34	Y	116/118~(98%)	116 (100%)	0	100	100
35	Ζ	109/112~(97%)	109 (100%)	0	100	100
36	a	64/85~(75%)	64 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	b	86/102~(84%)	86 (100%)	0	100	100
38	с	72/73~(99%)	72~(100%)	0	100	100
39	d	54/58~(93%)	54 (100%)	0	100	100
40	е	47/48~(98%)	47 (100%)	0	100	100
41	f	48/54~(89%)	48 (100%)	0	100	100
42	g	62/175~(35%)	62 (100%)	0	100	100
43	h	259/263~(98%)	259 (100%)	0	100	100
44	j	191/194 (98%)	191 (100%)	0	100	100
45	k	326/328~(99%)	326 (100%)	0	100	100
46	1	290/292~(99%)	290 (100%)	0	100	100
47	m	247/252~(98%)	247 (100%)	0	100	100
48	0	191/204~(94%)	191 (100%)	0	100	100
49	q	167/170~(98%)	167 (100%)	0	100	100
50	s	146/149~(98%)	146 (100%)	0	100	100
51	t	166/168~(99%)	166 (100%)	0	100	100
52	u	108/109~(99%)	108 (100%)	0	100	100
53	V	177/178~(99%)	177 (100%)	0	100	100
54	W	166/167~(99%)	166 (100%)	0	100	100
55	У	156/154~(101%)	156 (100%)	0	100	100
56	Z	135/153~(88%)	135 (100%)	0	100	100
59	n	135/154~(88%)	135 (100%)	0	100	100
60	р	202/216~(94%)	202 (100%)	0	100	100
61	r	178/186~(96%)	178 (100%)	0	100	100
62	х	142/154~(92%)	142 (100%)	0	100	100
63	AA	117/118 (99%)	117 (100%)	0	100	100
64	AB	120/121~(99%)	120 (100%)	0	100	100
65	AC	50/49~(102%)	50 (100%)	0	100	100
66	AD	81/90 (90%)	81 (100%)	0	100	100
67	AE	98/100~(98%)	98 (100%)	0	100	100
68	AF	111/115~(96%)	109 (98%)	2 (2%)	54	76
69	AG	94/92~(102%)	94 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
70	AH	99/101~(98%)	99~(100%)	0	100	100
71	AI	106/106~(100%)	106 (100%)	0	100	100
72	AJ	79/79~(100%)	79~(100%)	0	100	100
73	AK	70/73~(96%)	70 (100%)	0	100	100
74	AL	69/69~(100%)	69~(100%)	0	100	100
75	AM	47/47~(100%)	47 (100%)	0	100	100
76	AN	48/47~(102%)	48 (100%)	0	100	100
77	AO	24/24~(100%)	24 (100%)	0	100	100
78	AP	88/89~(99%)	88 (100%)	0	100	100
79	AQ	72/73~(99%)	72 (100%)	0	100	100
All	All	9166/10008~(92%)	9164 (100%)	2(0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	AF	17[A]	LYS
68	AF	17[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	8	GLN
1	0	62	ASN
2	2	122	ASN
5	5	91	GLN
11	В	21	ASN
11	В	30	GLN
12	С	173	GLN
13	D	84	GLN
14	Е	68	HIS
14	Е	160	HIS
15	F	36	HIS
15	F	57	ASN
15	F	197	HIS
15	F	216	ASN
17	Н	59	GLN
17	Н	182	GLN



Mol	Chain	Res	Type
17	Н	197	ASN
18	Ι	146	GLN
19	J	116	HIS
22	М	81	HIS
22	М	92	HIS
22	М	127	GLN
24	0	5	HIS
27	R	102	ASN
29	Т	12	GLN
29	Т	89	GLN
29	Т	104	ASN
30	U	25	GLN
30	U	101	ASN
33	Х	42	GLN
34	Y	27	GLN
37	b	8	ASN
43	h	17	ASN
43	h	107	HIS
43	h	305	ASN
44	j	132	ASN
45	k	25	GLN
45	k	165	GLN
45	k	182	GLN
45	k	259	ASN
45	k	316	ASN
46	1	222	ASN
46	1	312	HIS
46	1	323	GLN
47	m	151	GLN
47	m	242	ASN
48	0	91	ASN
49	q	46	ASN
49	q	157	ASN
50	S	109	HIS
50	S	150	ASN
51	t	19	GLN
52	u	98	ASN
53	v	156	HIS
55	У	5	HIS
60	р	42	GLN
62	x	34	GLN
62	x	50	GLN



Mol	Chain	$\mathbf{Res}$	Type
62	Х	97	ASN
62	Х	121	HIS
63	AA	122	HIS
65	AC	12	GLN
67	AE	68	ASN
68	AF	36	GLN
68	AF	89	HIS
70	AH	3	GLN
71	AI	16	GLN
71	AI	99	GLN
72	AJ	91	GLN
78	AP	22	GLN
78	AP	23	HIS
79	AQ	33	GLN
79	AQ	56	ASN

## 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	А	1629/1787~(91%)	371 (22%)	42 (2%)
3	3	120/121~(99%)	9~(7%)	0
4	4	155/158~(98%)	22~(14%)	2(1%)
57	1	3142/3359~(93%)	540 (17%)	31~(0%)
58	10	1/76~(1%)	1 (100%)	0
All	All	5047/5501~(91%)	943 (18%)	75 (1%)

All (943) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	3	7	G
3	3	22	А
3	3	54	U
3	3	55	А
3	3	65	G
3	3	73	С
3	3	76	А
3	3	102	А
3	3	112	G
4	4	23	U
4	4	34	U
4	4	35	Ċ



Mol	Chain	Res	Type
4	4	59	А
4	4	62	С
4	4	63	G
4	4	81	А
4	4	84	С
4	4	85	G
4	4	86	U
4	4	87	G
4	4	92	А
4	4	95	G
4	4	102	U
4	4	104	А
4	4	106	С
4	4	111	A
4	4	113	U
4	4	125	U
4	4	126	A
4	4	148	G
4	4	152	G
10	А	17	С
10	А	25	С
10	А	26	А
10	А	27	U
10	А	34	G
10	А	47	А
10	А	57	G
10	А	66	U
10	А	74	U
10	А	75	U
10	А	76	A
10	A	78	A
10	A	79	С
10	A	81	G
10	А	84	A
10	A	104	A
10	A	114	С
10	А	115	G
10	A	123	G
10	А	126	А
10	А	127	G
10	А	128	U
10	А	129	А



Mol	Chain	Res	Type
10	А	138	С
10	А	139	U
10	А	142	G
10	А	143	А
10	А	150	U
10	А	151	G
10	А	152	G
10	А	154	А
10	А	159	U
10	А	166	А
10	А	168	U
10	А	173	G
10	А	176	U
10	A	177	A
10	А	179	А
10	A	190	U
10	А	191	U
10	А	193	G
10	А	199	G
10	А	200	А
10	А	202	G
10	А	206	U
10	А	211	А
10	А	214	U
10	А	215	А
10	А	216	А
10	А	217	А
10	А	218	А
10	А	247	U
10	А	255	А
10	A	259	U
10	A	260	U
10	A	261	С
10	A	262	G
10	А	266	С
10	A	269	A
10	А	270	U
10	А	274	С
10	A	276	U
10	A	277	G
10	A	278	U
10	А	279	G



Mol	Chain	Res	Type
10	А	283	G
10	А	285	G
10	А	297	А
10	А	312	С
10	А	314	А
10	А	318	U
10	А	319	С
10	А	320	G
10	А	335	G
10	А	336	С
10	А	350	А
10	А	357	А
10	А	358	А
10	A	359	С
10	A	388	G
10	A	398	A
10	A	400	С
10	А	402	G
10	А	414	А
10	А	421	G
10	А	422	С
10	А	423	А
10	А	424	G
10	А	432	G
10	А	437	U
10	А	442	C
10	А	446	С
10	А	452	A
10	А	458	А
10	A	466	А
10	A	475	A
10	A	480	U
10	A	482	C
10	A	483	A
10	A	485	G
10	A	501	G
10	A	502	U
10	A	503	A
10	A	504	А
10	A	505	U
10	A	506	U
10	A	509	А



Mol	Chain	Res	Type
10	А	512	G
10	А	513	А
10	А	515	U
10	А	518	A
10	А	519	А
10	А	525	А
10	А	530	U
10	А	534	С
10	А	536	А
10	А	537	G
10	А	539	А
10	А	540	А
10	А	547	G
10	А	553	А
10	A	554	A
10	А	555	G
10	А	556	U
10	А	557	C
10	А	563	С
10	А	566	G
10	А	575	G
10	А	576	U
10	А	580	U
10	А	592	А
10	А	593	G
10	А	604	А
10	А	609	U
10	А	617	А
10	А	618	А
10	А	620	А
10	A	621	A
10	А	633	А
10	A	730	U
10	A	739	А
10	A	740	A
10	A	741	A
10	A	750	G
10	A	751	U
10	A	756	А
10	A	759	A
10	A	760	G
10	А	762	С



Mol	Chain	Res	Type
10	А	764	U
10	А	765	U
10	А	766	U
10	А	767	G
10	А	768	С
10	А	770	С
10	А	771	G
10	А	773	А
10	А	778	U
10	А	779	U
10	А	796	А
10	А	798	А
10	А	799	G
10	A	802	С
10	А	803	G
10	A	804	U
10	А	805	U
10	А	807	U
10	А	808	G
10	А	814	А
10	А	815	U
10	А	816	U
10	А	818	U
10	А	819	G
10	А	820	U
10	А	821	U
10	А	823	G
10	А	824	U
10	А	825	U
10	A	826	U
10	A	828	U
10	A	831	G
10	A	840	A
10	A	842	U
10	A	848	A
10	A	856	G
10	А	857	G
10	A	869	A
10	A	871	U
10	A	875	С
10	A	877	G
10	А	878	U



Mol	Chain	Res	Type
10	А	879	U
10	А	881	U
10	А	891	А
10	А	898	G
10	А	909	А
10	А	910	G
10	А	911	А
10	А	918	А
10	А	920	U
10	А	945	U
10	А	951	А
10	А	973	А
10	А	975	С
10	А	977	A
10	Α	988	A
10	А	989	U
10	А	997	U
10	А	998	А
10	А	1004	А
10	А	1005	А
10	А	1011	А
10	А	1013	С
10	А	1017	G
10	А	1024	А
10	А	1025	G
10	А	1039	U
10	А	1042	U
10	А	1043	U
10	А	1044	U
10	А	1047	U
10	А	1055	А
10	А	1056	U
10	А	1057	С
10	А	1058	G
10	А	1059	G
10	A	1060	С
10	А	1061	A
10	А	1067	С
10	А	1077	A
10	А	1081	С
10	А	1085	G
10	А	1123	А



Mol	Chain	Res	Type
10	А	1135	G
10	А	1143	С
10	А	1145	А
10	А	1152	G
10	А	1168	А
10	А	1169	А
10	А	1170	U
10	А	1179	А
10	А	1181	А
10	А	1184	G
10	А	1185	G
10	А	1186	G
10	А	1187	А
10	A	1193	A
10	А	1202	А
10	A	1203	G
10	А	1206	А
10	А	1207	С
10	А	1212	А
10	А	1215	А
10	А	1219	А
10	А	1220	С
10	А	1221	А
10	А	1229	А
10	А	1230	G
10	А	1231	С
10	А	1236	U
10	А	1243	U
10	А	1250	G
10	А	1270	U
10	A	1284	G
10	А	1299	U
10	А	1300	U
10	A	1301	G
10	А	1306	A
10	A	1325	U
10	А	1330	A
10	A	1336	G
10	А	1339	G
10	A	1342	A
10	А	1343	G
10	А	1345	А



Mol	Chain	Res	Type
10	А	1346	U
10	А	1348	U
10	А	1349	G
10	А	1352	G
10	А	1355	А
10	А	1356	U
10	А	1357	А
10	А	1359	U
10	А	1360	С
10	А	1364	U
10	А	1365	С
10	А	1369	G
10	А	1370	А
10	А	1376	U
10	А	1380	G
10	А	1381	А
10	А	1382	U
10	А	1384	U
10	А	1385	С
10	А	1392	А
10	А	1397	А
10	А	1398	G
10	А	1399	U
10	А	1400	U
10	А	1401	U
10	А	1410	А
10	А	1413	А
10	А	1414	G
10	А	1415	G
10	А	1422	А
10	А	1431	G
10	А	1433	С
10	А	1445	С
10	А	1446	А
10	А	1455	А
10	А	1457	А
10	А	1458	С
10	А	1461	А
10	А	1462	С
10	А	1463	G
10	А	1468	С
10	А	1476	А



Mol	Chain	Res	Type
10	А	1477	U
10	А	1483	U
10	А	1491	G
10	А	1503	А
10	А	1508	G
10	А	1510	G
10	А	1511	А
10	А	1523	G
10	А	1524	С
10	А	1529	G
10	А	1530	А
10	А	1542	А
10	А	1544	U
10	А	1546	G
10	А	1547	U
10	A	1556	A
10	А	1560	А
10	А	1561	G
10	А	1569	U
10	А	1571	G
10	А	1574	А
10	А	1575	G
10	А	1577	G
10	А	1580	А
10	А	1582	U
10	А	1584	А
10	А	1588	G
10	А	1621	С
10	А	1644	U
10	А	1645	G
10	A	1665	C
10	А	1667	G
10	A	1670	U
10	A	1671	G
10	A	$1\overline{672}$	G
10	A	1673	U
10	A	1674	U
10	A	1677	G
10	A	1700	G
10	A	1704	С
10	А	1737	A
10	А	1743	А



Mol	Chain	Res	Type
10	А	1747	G
10	А	1749	А
10	А	1753	А
10	А	1756	U
10	А	1767	G
10	А	1769	А
10	А	1770	С
10	А	1779	G
10	А	1780	G
10	А	1781	А
10	А	1782	U
10	А	1783	С
57	1	24	U
57	1	25	A
57	1	29	G
57	1	39	A
57	1	42	А
57	1	48	А
57	1	56	А
57	1	58	G
57	1	59	А
57	1	64	А
57	1	65	А
57	1	91	G
57	1	98	А
57	1	104	С
57	1	108	А
57	1	109	G
57	1	110	С
57	1	121	A
57	1	135	G
57	1	155	A
57	1	156	A
57	1	164	U
57	1	169	G
57	1	172	C
57	1	173	C
57	1	175	G
57	1	186	A
57	1	189	U
57	1	190	U
57	1	199	С



Mol	Chain	Res	Type
57	1	205	G
57	1	209	С
57	1	212	А
57	1	217	G
57	1	218	А
57	1	219	G
57	1	230	G
57	1	236	А
57	1	239	А
57	1	240	С
57	1	243	G
57	1	245	G
57	1	249	G
57	1	250	U
57	1	251	G
57	1	269	G
57	1	286	U
57	1	295	А
57	1	305	U
57	1	311	С
57	1	323	А
57	1	329	U
57	1	337	G
57	1	338	А
57	1	339	С
57	1	349	А
57	1	350	С
57	1	376	G
57	1	377	A
57	1	395	A
57	1	398	А
57	1	402	A
57	1	403	С
57	1	$40\overline{4}$	G
57	1	420	G
57	1	421	G
57	1	422	A
57	1	438	A
57	1	439	C
57	1	452	A
57	1	453	U
57	1	454	G



Mol	Chain	Res	Type
57	1	479	С
57	1	481	G
57	1	482	U
57	1	506	А
57	1	517	А
57	1	519	U
57	1	531	G
57	1	532	U
57	1	538	G
57	1	539	G
57	1	540	С
57	1	541	U
57	1	542	U
57	1	543	С
57	1	544	U
57	1	545	G
57	1	546	С
57	1	555	А
57	1	556	U
57	1	557	А
57	1	564	G
57	1	577	G
57	1	589	G
57	1	590	А
57	1	598	U
57	1	600	U
57	1	601	U
57	1	602	А
57	1	609	А
57	1	618	U
57	1	619	A
57	1	620	А
57	1	635	C
57	1	647	А
57	1	658	A
57	1	675	A
57	1	679	U
57	1	688	A
57	1	703	А
57	1	710	G
57	1	713	А
57	1	717	А



Mol	Chain	Res	Type
57	1	723	G
57	1	730	А
57	1	732	U
57	1	760	U
57	1	763	U
57	1	772	U
57	1	773	U
57	1	776	А
57	1	777	G
57	1	780	А
57	1	781	G
57	1	802	А
57	1	813	А
57	1	826	A
57	1	845	С
57	1	857	С
57	1	861	U
57	1	870	U
57	1	875	U
57	1	892	А
57	1	903	G
57	1	904	G
57	1	910	А
57	1	912	G
57	1	913	А
57	1	917	А
57	1	919	С
57	1	921	А
57	1	933	G
57	1	940	С
57	1	949	G
57	1	955	C
57	1	956	U
57	1	$95\overline{9}$	G
57	1	976	А
57	1	$97\overline{7}$	U
57	1	990	G
57	1	991	U
57	1	996	C
57	1	997	G
57	1	998	A
57	1	1006	G



Mol	Chain	Res	Type
57	1	1011	С
57	1	1012	U
57	1	1014	G
57	1	1030	U
57	1	1033	С
57	1	1043	А
57	1	1045	С
57	1	1060	А
57	1	1061	А
57	1	1068	G
57	1	1077	U
57	1	1078	U
57	1	1090	А
57	1	1091	U
57	1	1092	U
57	1	1094	А
57	1	1099	A
57	1	1100	G
57	1	1113	G
57	1	1127	G
57	1	1140	U
57	1	1149	А
57	1	1150	А
57	1	1151	С
57	1	1155	А
57	1	1156	С
57	1	1164	U
57	1	1174	G
57	1	1176	А
57	1	1177	U
57	1	1178	G
57	1	1188	С
57	1	1189	A
57	1	1192	С
57	1	1197	С
57	1	1204	U
57	1	1205	G
57	1	1215	С
57	1	1218	G
57	1	1223	С
57	1	1224	С
57	1	1225	G



Mol	Chain	Res	Type
57	1	1228	С
57	1	1229	G
57	1	1230	G
57	1	1231	U
57	1	1232	G
57	1	1234	С
57	1	1238	G
57	1	1239	G
57	1	1241	А
57	1	1242	G
57	1	1243	U
57	1	1244	С
57	1	1245	G
57	1	1247	А
57	1	1249	U
57	1	1251	C
57	1	1252	G
57	1	1253	С
57	1	1255	А
57	1	1258	G
57	1	1259	А
57	1	1262	G
57	1	1263	U
57	1	1264	G
57	1	1265	U
57	1	1266	А
57	1	1267	А
57	1	1268	С
57	1	1269	A
57	1	1270	A
57	1	1273	С
57	1	1278	G
57	1	1280	С
57	1	1282	A
57	1	1283	A
57	1	1303	G
57	1	1304	A
57	1	1305	U
57	1	1309	G
57	1	1326	A
57	1	1345	G
57	1	1346	U



Mol	Chain	Res	Type
57	1	1347	U
57	1	1348	U
57	1	1349	U
57	1	1382	А
57	1	1395	U
57	1	1415	А
57	1	1417	G
57	1	1421	U
57	1	1427	G
57	1	1430	G
57	1	1433	С
57	1	1442	А
57	1	1446	G
57	1	1465	С
57	1	1471	А
57	1	1477	A
57	1	1484	G
57	1	1498	С
57	1	1504	С
57	1	1520	А
57	1	1523	С
57	1	1532	G
57	1	1535	А
57	1	1551	U
57	1	1552	С
57	1	1556	G
57	1	1558	G
57	1	1559	С
57	1	1560	U
57	1	1561	U
57	1	1562	G
57	1	1563	A
57	1	1565	U
57	1	1566	U
57	1	1567	U
57	1	1568	U
57	1	1569	С
57	1	1571	G
57	1	1572	G
57	1	1574	С
57	1	1576	A
57	1	1577	С



Mol	Chain	Res	Type
57	1	1585	А
57	1	1589	А
57	1	1601	А
57	1	1603	U
57	1	1624	С
57	1	1625	U
57	1	1635	С
57	1	1638	А
57	1	1639	А
57	1	1641	U
57	1	1648	G
57	1	1654	G
57	1	1679	А
57	1	1720	U
57	1	1721	С
57	1	1732	G
57	1	1746	А
57	1	1747	G
57	1	1755	U
57	1	1756	А
57	1	1757	А
57	1	1758	U
57	1	1760	U
57	1	1761	U
57	1	1762	G
57	1	1763	С
57	1	1776	G
57	1	1793	A
57	1	1804	G
57	1	1809	A
57	1	1810	A
57	1	1811	U
57	1	1812	A
57	1	1815	U
57	1	1816	U
57	1	1817	U
57	1	1835	A
57	1	1838	A
57	1	1842	C
57	1	1845	C
57	1	1862	C
57	1	1874	G


Mol	Chain	Res	Type
57	1	1877	А
57	1	1882	A
57	1	1889	А
57	1	1902	G
57	1	1944	G
57	1	1949	G
57	1	2070	А
57	1	2071	А
57	1	2078	А
57	1	2088	G
57	1	2089	G
57	1	2090	U
57	1	2091	А
57	1	2092	C
57	1	2099	G
57	1	2100	G
57	1	2109	А
57	1	2118	U
57	1	2122	А
57	1	2136	А
57	1	2147	G
57	1	2149	G
57	1	2183	U
57	1	2184	G
57	1	2185	А
57	1	2186	A
57	1	2187	U
57	1	2188	G
57	1	2222	A
57	1	2227	G
57	1	2233	A
57	1	2234	A
57	1	2235	С
57	1	2250	G
57	1	2251	G
57	1	2257	A
57	1	2259	A
57	1	2260	U
57	1	2276	U
57	1	2285	G
57	1	2286	С
57	1	2288	U



Mol	Chain	Res	Type
57	1	2291	А
57	1	2292	U
57	1	2293	G
57	1	2312	U
57	1	2313	G
57	1	2314	U
57	1	2341	А
57	1	2351	А
57	1	2352	С
57	1	2353	G
57	1	2363	G
57	1	2366	U
57	1	2371	G
57	1	2372	G
57	1	2375	A
57	1	2380	A
57	1	2381	G
57	1	2382	А
57	1	2389	U
57	1	2413	G
57	1	2420	G
57	1	2489	А
57	1	2492	U
57	1	2493	А
57	1	2511	G
57	1	2513	А
57	1	2515	G
57	1	2516	U
57	1	2517	С
57	1	2518	А
57	1	2519	A
$5\overline{7}$	1	2520	А
57	1	2521	C
$5\overline{7}$	1	2529	U
57	1	2530	С
57	1	2533	G
57	1	2536	U
57	1	2538	A
57	1	2545	С
57	1	2546	U
57	1	2554	С
57	1	2557	G



Mol	Chain	Res	Type	
57	1	2565	А	
57	1	2566	С	
57	1	2578	G	
57	1	2579	G	
57	1	2586	G	
57	1	2598	А	
57	1	2623	G	
57	1	2624	U	
57	1	2628	А	
57	1	2644	G	
57	1	2646	А	
57	1	2649	G	
57	1	2661	А	
57	1	2662	G	
57	1	2663	A	
57	1	2666	A	
57	1	2676	А	
57	1	2677	A	
57	1	2686	G	
57	1	2699	А	
57	1	2700	G	
57	1	2701	U	
57	1	2725	G	
57	1	2734	А	
57	1	2745	С	
57	1	2749	G	
57	1	2750	G	
57	1	2768	G	
57	1	2771	A	
57	1	2772	G	
57	1	2773	A	
57	1	2774	A	
57	1	2782	С	
57	1	2786	G	
57	1	2789	A	
57	1	2790	U	
57	1	2814	U	
57	1	2815	U	
57	1	2817	A	
57	1	2833	U	
57	1	2839	C	
57	1	2843	G	



Mol	Chain	Res	Type
57	1	2844	А
57	1	2847	U
57	1	2859	А
57	1	2861	С
57	1	2866	С
57	1	2870	G
57	1	2871	С
57	1	2886	G
57	1	2895	U
57	1	2907	U
57	1	2908	А
57	1	2911	G
57	1	2914	С
57	1	2919	G
57	1	2920	С
57	1	2923	G
57	1	2926	U
57	1	2943	А
57	1	2955	С
57	1	2960	С
57	1	2962	G
57	1	2969	G
57	1	2984	А
57	1	3021	А
57	1	3028	U
57	1	3031	G
57	1	3050	А
57	1	3051	С
57	1	3052	G
57	1	3058	А
57	1	3064	С
57	1	3076	U
57	1	3094	A
57	1	3101	A
57	1	3102	А
57	1	3103	U
57	1	3114	А
57	1	3115	С
57	1	3134	С
57	1	3143	G
57	1	3144	A
57	1	3146	G



Mol	Chain	Res	Type
57	1	3149	U
57	1	3151	С
57	1	3157	А
57	1	3160	С
57	1	3161	U
57	1	3163	U
57	1	3164	U
57	1	3165	U
57	1	3171	С
57	1	3172	U
57	1	3182	С
57	1	3183	А
57	1	3184	G
57	1	3194	G
57	1	3208	A
57	1	3210	A
57	1	3212	G
57	1	3214	U
57	1	3221	G
57	1	3224	U
57	1	3228	G
57	1	3235	А
57	1	3241	G
57	1	3246	С
57	1	3252	С
57	1	3259	А
57	1	3260	A
57	1	3268	G
57	1	3269	С
57	1	3272	А
57	1	3278	U
57	1	3281	A
57	1	3284	U
57	1	3285	A
57	1	3306	U
57	1	3307	A
57	1	3309	A
57	1	3310	G
57	1	3316	U
57	1	3317	U
57	1	3318	G
57	1	3319	U



Continued from previous page...

Mol	Chain	Res	Type
57	1	3320	U
57	1	3321	G
57	1	3334	G
57	1	3343	С
57	1	3351	G
57	1	3361	U
58	10	76	А

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	4	85	G
4	4	125	U
10	А	25	С
10	А	78	А
10	А	137	А
10	А	151	G
10	А	176	U
10	А	214	U
10	А	259	U
10	A	265	U
10	А	278	U
10	А	451	С
10	А	502	U
10	А	504	А
10	А	505	U
10	А	514	G
10	А	518	А
10	А	529	С
10	А	533	А
10	А	553	А
10	А	556	U
10	А	740	А
10	А	763	С
10	A	769	U
10	А	817	U
10	А	820	U
10	А	824	U
10	А	855	С
10	А	874	U
10	А	876	А
10	А	1168	А



Mol	Chain	Res	Type	
10	А	1335	U	
10	А	1355	А	
10	А	1359	U	
10	А	1369	G	
10	А	1396	А	
10	А	1398	G	
10	А	1457	А	
10	А	1467	С	
10	А	1523	G	
10	А	1555	С	
10	А	1573	А	
10	А	1579	А	
10	А	1581	G	
57	1	172	C	
57	1	403	С	
57	1	538	G	
57	1	563	U	
57	1	601	U	
57	1	759	G	
57	1	912	G	
57	1	1029	U	
57	1	1060	А	
57	1	1099	А	
57	1	1346	U	
57	1	1347	U	
57	1	1559	С	
57	1	1561	U	
57	1	1576	A	
57	1	1762	G	
57	1	1815	U	
57	1	1943	G	
57	1	2090	U	
57	1	2515	G	
57	1	2519	A	
57	1	2789	A	
57	1	2790	U	
57	1	3093	U	
57	1	3193	С	
57	1	3234	U	
57	1	3240	U	
57	1	3284	U	
57	1	3309	A	



Continued from previous page...

Mol	Chain	Res	Type
57	1	3315	С
57	1	3317	U

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	OMG	1	2765	57	18,26,27	2.40	8 (44%)	19,38,41	1.52	4 (21%)
78	MLZ	AP	40	78	8,9,10	0.72	0	4,9,11	0.92	0
57	OMC	1	2808	57	19,22,23	2.86	8 (42%)	26,31,34	1.01	2 (7%)
6	MLZ	6	110	6	8,9,10	0.72	0	4,9,11	1.09	0
78	MLZ	AP	55	78	8,9,10	0.84	0	4,9,11	2.17	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	OMG	1	2765	57	-	0/5/27/28	0/3/3/3
78	MLZ	AP	40	78	-	0/7/8/10	-
57	OMC	1	2808	57	-	3/9/27/28	0/2/2/2
6	MLZ	6	110	6	-	3/7/8/10	-
78	MLZ	AP	55	78	-	3/7/8/10	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1	2808	OMC	C2-N3	5.97	1.48	1.36
57	1	2808	OMC	C6-C5	5.77	1.48	1.35
57	1	2765	OMG	C2-N3	5.21	1.45	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1	2808	OMC	C4-N4	4.83	1.45	1.33
57	1	2765	OMG	C4-N3	4.65	1.48	1.37
57	1	2808	OMC	C4-N3	4.45	1.43	1.34
57	1	2808	OMC	C2-N1	4.08	1.48	1.40
57	1	2765	OMG	C2-N2	3.75	1.43	1.34
57	1	2765	OMG	C6-N1	3.71	1.43	1.37
57	1	2808	OMC	O2-C2	-3.33	1.17	1.23
57	1	2765	OMG	C5-C4	-2.84	1.35	1.43
57	1	2808	OMC	C6-N1	2.81	1.44	1.38
57	1	2765	OMG	C5-C6	2.53	1.52	1.47
57	1	2765	OMG	06-C6	-2.53	1.18	1.23
57	1	2808	OMC	C5-C4	2.21	1.48	1.42
57	1	2765	OMG	C2-N1	2.20	1.43	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
78	AP	55	MLZ	CD-CG-CB	-3.59	100.92	113.62
57	1	2765	OMG	C5-C6-N1	3.51	120.14	113.95
57	1	2765	OMG	C2-N1-C6	-2.95	119.67	125.10
57	1	2808	OMC	O2-C2-N3	-2.64	118.04	122.33
57	1	2765	OMG	C8-N7-C5	2.59	107.93	102.99
57	1	2765	OMG	O6-C6-C5	-2.47	119.55	124.37
57	1	2808	OMC	C1'-N1-C2	2.25	123.44	118.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	6	110	MLZ	N-CA-CB-CG
6	6	110	MLZ	C-CA-CB-CG
57	1	2808	OMC	O4'-C1'-N1-C2
57	1	2808	OMC	O4'-C1'-N1-C6
57	1	2808	OMC	C1'-C2'-O2'-CM2
78	AP	55	MLZ	CG-CD-CE-NZ
78	AP	55	MLZ	CA-CB-CG-CD
78	AP	55	MLZ	CE-CD-CG-CB
6	6	110	MLZ	CD-CE-NZ-CM

There are no ring outliers.

1 monomer is involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1	2808	OMC	4	0

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec Link		Their Dec		Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
82	SPK	1	3402	-	13,13,13	0.33	0	$12,\!12,\!12$	0.91	0		
81	YMZ	j	301	-	28,28,28	0.45	0	41,43,43	0.65	2 (4%)		
81	YMZ	1	3401	-	28,28,28	0.44	0	41,43,43	0.57	2 (4%)		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SPK	1	3402	-	-	3/11/11/11	-
81	YMZ	j	301	-	-	15/20/28/28	0/3/3/3
81	YMZ	1	3401	-	-	8/20/28/28	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
81	j	301	YMZ	CAN-NAQ-CAX	3.21	113.62	111.62
81	1	3401	YMZ	CAN-NAQ-CAX	2.67	113.29	111.62
81	1	3401	YMZ	CAO-CAX-NAQ	-2.10	108.82	111.90



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
81	j	301	YMZ	CAO-CAX-NAQ	-2.02	108.93	111.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	j	301	YMZ	CAV-CAT-CAZ-FAE
81	j	301	YMZ	CAV-CAT-CAZ-FAF
81	j	301	YMZ	CAV-CAT-CAZ-FAG
81	1	3401	YMZ	CAV-CAT-CAZ-FAE
81	1	3401	YMZ	CAV-CAT-CAZ-FAF
81	1	3401	YMZ	CAV-CAT-CAZ-FAG
82	1	3402	SPK	C2-C3-C4-N5
81	1	3401	YMZ	CAI-CAT-CAZ-FAF
81	1	3401	YMZ	CAI-CAT-CAZ-FAG
81	1	3401	YMZ	CAI-CAT-CAZ-FAE
81	j	301	YMZ	CAK-CAS-CAW-OAA
81	j	301	YMZ	CAU-CAS-CAW-OAA
81	1	3401	YMZ	CAS-CAW-CAX-CAO
81	j	301	YMZ	CAI-CAT-CAZ-FAE
81	j	301	YMZ	CAI-CAT-CAZ-FAF
81	j	301	YMZ	CAI-CAT-CAZ-FAG
82	1	3402	SPK	C12-C11-N10-C9
81	j	301	YMZ	NAP-CAR-CAY-FAB
81	j	301	YMZ	CAK-CAR-CAY-FAB
82	1	3402	SPK	N10-C11-C12-C13
81	j	301	YMZ	NAP-CAR-CAY-FAC
81	j	301	YMZ	CAK-CAR-CAY-FAD
81	j	301	YMZ	NAP-CAR-CAY-FAD
81	j	301	YMZ	CAK-CAR-CAY-FAC
81	j	301	YMZ	OAA-CAW-CAX-CAO
81	1	3401	YMZ	CAS-CAW-CAX-NAQ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	j	301	YMZ	2	0
81	1	3401	YMZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







# 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50957. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

# 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



## 6.2 Central slices (i)

## 6.2.1 Primary map



X Index: 210





Z Index: 210

### 6.2.2 Raw map



X Index: 210

Y Index: 210



The images above show central slices of the map in three orthogonal directions.



## 6.3 Largest variance slices (i)

## 6.3.1 Primary map



X Index: 227





Z Index: 173

### 6.3.2 Raw map



X Index: 227

Y Index: 216



The images above show the largest variance slices of the map in three orthogonal directions.



# 6.4 Orthogonal standard-deviation projections (False-color) (i)

## 6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

# 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1201 \text{ nm}^3$ ; this corresponds to an approximate mass of 1085 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$ 



# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$ 



## 8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estim	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	3.10	-	-			
Author-provided FSC curve	3.91	6.55	4.04			
Unmasked-calculated*	3.89	6.50	4.02			

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.1 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50957 and PDB model 9G1Z. Per-residue inclusion information can be found in section 3 on page 19.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



## 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).



## 9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7180	0.4380
0	0.8650	0.5590
1	0.9000	0.5270
10	0.5710	0.4990
2	0.8370	0.5390
3	0.9500	0.5450
4	0.9520	0.5560
5	0.2950	0.3590
6	0.8780	0.5590
7	0.8590	0.5360
8	0.8590	0.5440
9	0.8460	0.5520
А	0.5970	0.3130
AA	0.7740	0.5090
AB	0.9030	0.5760
AC	0.8030	0.5090
AD	0.7640	0.4990
AE	0.7970	0.5320
$\operatorname{AF}$	0.9000	0.5630
AG	0.9010	0.5740
AH	0.8080	0.5310
AI	0.8550	0.5440
AJ	0.8280	0.5290
AK	0.9280	0.5770
AL	0.6430	0.4880
AM	0.9090	0.5690
AN	0.8350	0.5480
AO	0.5440	0.4280
AP	0.8230	0.5470
AQ	0.8360	0.5310
В	0.3380	0.2680
С	0.4590	0.3470
D	0.5170	0.3570
E	0.2000	0.1490
F	0.3790	0.2860



Chain	Atom inclusion	Q-score
G	0.1170	0.1170
Н	0.3490	0.2410
Ι	0.2160	0.2690
J	0.5220	0.4090
К	0.3840	0.2730
L	0.1090	0.0910
М	0.4290	0.3730
N	0.0130	0.0890
0	0.4840	0.3640
Р	0.5020	0.3960
Q	0.0970	0.0980
R	0.2380	0.1400
S	0.2740	0.2310
Т	0.1340	0.1380
U	0.1680	0.1390
V	0.1590	0.1110
W	0.3740	0.2770
X	0.5170	0.3720
Y	0.5370	0.3650
Z	0.3530	0.2410
a	0.0780	0.0880
b	0.5780	0.4140
с	0.2980	0.2970
d	0.0840	0.1310
e	0.3360	0.1890
f	0.3280	0.2130
g	0.0230	0.0690
h	0.0470	0.1020
j	0.8780	0.5690
k	0.8790	0.5580
<u> </u>	0.8720	0.5530
m	0.7860	0.5030
n	0.8020	0.5130
0	0.8560	0.5510
р	0.7760	0.5170
q	0.8160	0.5320
r	0.8260	0.5470
S	0.7100	0.4680
t	0.8390	0.5330
u	0.8030	0.5220
V	0.9260	0.5780
W	0.8600	0.5510



Continued from previous page...

Chain	Atom inclusion	Q-score
x	0.8700	0.5490
У	0.8820	0.5660
Z	0.8150	0.5160

