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PDB ID EMDB ID	:	8RDV EMD-19076	
Title	:	Cryo-EM structure of P. urativorans 70S ribosome in complex with hibernat factor Balon mBNA and P-site tBNA (structure 2)	ion
Authors Deposited on Resolution	: : :	Helena-Bueno, K.; Rybak, M.Y.; Gagnon, M.G.; Hill, C.H.; Melnikov, S.V. 2023-12-08 2.60 Å(reported)	
This is	a I	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	
h	ittp	os://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.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 cha				
1	В	369	15%			21%	
	Б	100	55%				
2	F	128	70%		2	27%	••
_			38%				
3	H	396	34% 11% ·	5	3%		
4	Z2	2882	60%		30%		• 6%
5	R3	76	61%	12%	•	26%	
			57%				
6	A4	269	67%		19%		13%
7	E5	171	73%		1	9%	9%



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
8	L6	124	6% 77%	21% •
9	F7	178	57%	39% ••
10	D8	115	72%	25% ·
11	E9	200	78%	20% •
12	aA	60	88%	12%
13	MB	119	88%	11% •
14	UC	219	37% 7%	56%
15	WD	78	69%	27% ••
16	XE	65	75%	20% 5%
17	RF	109	72%	27% ·
18	FG	134	37% 56% 19%	• 24%
19	VH	85	84%	12% ••
20	TI	105	80%	16% · ·
21	fJ	93	56%	34%
22	HK	101	76%	22% ••
23	OL	88	81%	16% ••
24	MM	118	44% 28%	6% 22%
25	РО	118	86%	12% •••
26	SP	91	58% 2	5% • 12%
27	BQ	132	74%	24% •••
28	GR	177	72%	25% ••
29	GS	157	69%	27% ••
30	CT	241	<u>43%</u> 56% 26 ⁶	% • 15%
31	KU	129	71%	17% • 11%
32	NV	71	58% 23	% 20%



Mol	Chain	Length	Quality of chain	
33	YW	59	• 85%	8% • 5%
34	IX	142	• 81%	18% •
35	JY	103	64% 71%	26% ·
36	QZ	91	18%	13% • 13%
37	Ba	44	100%	
38	Qb	103	98%	•
39	Nc	116	95%	
40	Kd	146	5% 99%	•
41	Je	122	93%	7%
42	Af	212	- 96%	·
43	Lg	137	• 96%	·
44	dh	65	92%	6% ·
45	Oi	130	83%	5% 12%
46	Pi	89	16%	• 9%
47	bk	51	• 88%	8% •
48	Cl	274	• 97%	
49	Dm	213	44%	
50	Sn	116		. 24%
51	То	88	22%	
52	en	38	97%	
53	V	76	25%	12%
54	v	6	33% 50%	1704
55	C1	166	16% 28%	L / /0
56	iN	1590	13%	17% 5%



2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 142063 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 Methyl-accepting chemotaxis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	В	362	Total 2829	C 1759	N 501	O 560	S 9	0	0

• Molecule 2 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	126	Total 985	C 613	N 194	0 177	S 1	0	0

• Molecule 3 is a protein called Elongation factor Tu.

		Atoms						
3 H	185	Total	C 870	N 252	0 270	S 8	0	0

• Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues			AltConf	Trace			
4	Z2	2710	Total	C	N 10675	0	P 2710	0	0
			58145	25950	10075	18804	2710		

• Molecule 5 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues		Atom	ıs	AltConf	Trace	
5	R3	56	Total 457	C 290	N 80	O 87	0	0

• Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	233	Total 1816	C 1147	N 327	O 335	${ m S} 7$	0	0



• Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	E5	156	Total 1151	C 716	N 218	0 211	S 6	0	0

• Molecule 8 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	L6	122	Total 946	C 583	N 193	0 165	${f S}{5}$	0	0

• Molecule 9 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	F7	177	Total 1362	C 873	N 237	0 246	S 6	0	0

• Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
10	D8	115	Total 2446	C 1093	N 436	O 802	Р 115	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D8	85	U	-	insertion	GB 930356181
D8	88	А	С	variant	GB 930356181

• Molecule 11 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues		At	AltConf	Trace			
11	E9	199	Total 1537	C 966	N 282	0 284	${ m S}{ m 5}$	0	0

• Molecule 12 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues		Ate	\mathbf{oms}			AltConf	Trace
12	aA	53	Total 442	C 264	N 100	O 75	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called Large ribosomal subunit protein bL17.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	MB	119	Total 947	C 587	N 188	O 164	S 8	0	0

• Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	UC	97	Total 760	C 485	N 138	0 136	S 1	0	0

• Molecule 15 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues		At	AltConf	Trace			
15	WD	76	Total 618	C 383	N 131	0 101	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
16	XE	62	Total	C	N	0	S	0	0
			502	307	99	95	T		

• Molecule 17 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues		At	AltConf	Trace			
17	RF	109	Total 834	C 521	N 159	0 151	${ m S} { m 3}$	0	0

• Molecule 18 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	FG	102	Total 849	C 535	N 154	0 158	${ m S} { m 2}$	0	0

• Molecule 19 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	VH	84	Total 626	C 389	N 124	0 110	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called Large ribosomal subunit protein uL24.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
20	TI	102	Total 784	C 487	N 149	0 148	0	0

• Molecule 21 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
21	fJ	61	Total 493	C 313	N 85	0 94	S 1	0	0

• Molecule 22 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	HK	100	Total 811	C 498	N 162	0 144	${f S}{7}$	0	0

• Molecule 23 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues		Atoms					Trace
23	OL	86	Total 694	C 427	N 137	0 128	${ m S} { m 2}$	0	0

• Molecule 24 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	MM	92	Total 717	C 446	N 138	0 130	${ m S} { m 3}$	0	0

• Molecule 25 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	РО	116	Total 935	C 586	N 199	0 148	${ m S} { m 2}$	0	0

• Molecule 26 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	SP	80	Total 637	C 405	N 121	0 108	${ m S} { m 3}$	0	0

• Molecule 27 is a protein called Small ribosomal subunit protein uS8.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	BQ	131	Total 974	C 602	N 179	O 187	S 6	0	0

• Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
28	GR	175	Total 1357	C 848	N 248	O 259	${S \over 2}$	0	0

• Molecule 29 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues		At	oms			AltConf	Trace
29	GS	153	Total 1200	C 744	N 233	0 216	S 7	0	0

• Molecule 30 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CT	205	Total 1613	C 1013	N 302	0 291	${ m S} 7$	0	0

• Molecule 31 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	KU	115	Total 842	C 521	N 163	0 157	S 1	0	0

• Molecule 32 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
32	NV	57	Total 472	C 299	N 95	O 77	S 1	0	0

• Molecule 33 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
33	YW	56	Total 438	С 272	N 88	O 76	${S \over 2}$	0	0

• Molecule 34 is a protein called Large ribosomal subunit protein uL13.



Mol	Chain	Residues		At	oms	AltConf	Trace		
34	IX	142	Total 1108	C 710	N 198	O 197	${ m S} { m 3}$	0	0

• Molecule 35 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
35	JY	100	Total 793	C 492	N 151	0 147	${ m S} { m 3}$	0	0

• Molecule 36 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	QZ	79	Total 632	C 395	N 119	0 116	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 37 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
27	Bo	4.4	Total	С	Ν	Ο	S	0	0
51	Da	44	369	227	89	51	2	0	0

• Molecule 38 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	Qb	103	Total 827	C 524	N 153	0 148	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
39	Nc	113	Total 852	C 530	N 170	O 152	0	0

• Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	Kd	144	Total 1062	C 656	N 206	0 197	${ m S} { m 3}$	1	0

• Molecule 41 is a protein called Large ribosomal subunit protein uL14.



Mol	Chain	Residues		At	oms	AltConf	Trace		
41	Je	122	Total 937	$\begin{array}{c} \mathrm{C} \\ 585 \end{array}$	N 181	O 166	${ m S}{ m 5}$	0	0

• Molecule 42 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
42	Af	211	Total 1548	C 954	N 292	O 296	S 6	0	0

• Molecule 43 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	Lg	137	Total 1093	C 697	N 210	0 179	S 7	0	0

• Molecule 44 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
44	dh	64	Total 519	C 326	N 107	O 82	${S \atop 4}$	0	0

• Molecule 45 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
45	Oi	115	Total 917	C 572	N 184	O 161	0	0

• Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues		At	oms			AltConf	Trace
46	Рj	81	Total 648	C 409	N 126	0 111	${S \over 2}$	0	0

• Molecule 47 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
47	bk	49	Total 394	C 254	N 68	O 69	${ m S} { m 3}$	0	0

• Molecule 48 is a protein called Large ribosomal subunit protein uL2.



Mol	Chain	Residues		At	oms			AltConf	Trace
48	Cl	272	Total 2107	C 1305	N 432	O 364	S 6	0	0

• Molecule 49 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues		Ate	AltConf	Trace			
49	Dm	212	Total 1688	C 1058	N 318	O 309	${ m S} { m 3}$	0	0

• Molecule 50 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	Sn	88	Total 698	C 446	N 126	0 124	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 51 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
51	То	87	Total 684	C 415	N 146	0 121	${ m S} { m 2}$	0	0

• Molecule 52 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
52	ер	38	Total 298	C 182	N 66	O 46	$\frac{S}{4}$	0	0

• Molecule 53 is a RNA chain called Heterogenous tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
53	V	76	Total 1521	C 686	N 160	O 600	Р 75	0	0

• Molecule 54 is a RNA chain called Heterogenous mRNA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
54	Y	6	Total 120	C 54	N 12	0 48	Р 6	0	0

• Molecule 55 is a protein called Large ribosomal subunit protein bL9.



Mol	Chain	Residues	Atoms				AltConf	Trace	
55	C1	49	Total 374	C 244	N 64	O 65	S 1	0	0

 $\bullet\,$ Molecule 56 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		A	Atoms			AltConf	Trace
56	iN	1503	Total 32246	C 14388	N 5917	O 10438	Р 1503	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Methyl-accepting chemotaxis protein











 \bullet Molecule 7: Small ribosomal subunit protein uS5













Chain OL:	81%			16% ••	
MI B6 B1 B3 B3 C1 111 A12 A12 A12 A12 A12 A12 A12 A12 A1	617 E18 N19 D20 D20 C22 C22 C22 C22 C22 C22 C22 C22 C22 C	L55 M58 R63 S82 S82 L86	ARG ARG		
• Molecule 24: Smal	l ribosomal subunit	protein uS13			
Chain MM:	58% 44%	28%	6%	22%	
MET A2 I4 A5 A5 A5 A5 A5 A14 P10 P10 P10 N12	K13 H14 A16 A16 S18 F23 C24 C25 C25 C26 C26 C26 C26 C26 C26 C26 C26 C26 C26	T29 A30 (31 (32 (33 (33 (33 (33) (33) (33)	139 A40 T41 T42 T43	V45 V45 Q47 L48 D49 D50	151 652 153 156 855 855 858 958 958 958 958 958 958 958
M64 T65 E66 G67 G67 D68 L69 R70 R71 E72 C73 S74 M75	K78 R79 R79 L80 V81 D82 C85 C85 C85 C85	I 89 R90 R92 ASN ASN VAL VAL PRD CIV CIV	GLN ASN LYS ASN ASN ALA	ARG THR ARG LYS GLY PRO ARG	PR0 LEU LVS ARG
• Molecule 25: Large	e ribosomal subunit	protein bL20			
Chain PO:	86	%		12% ••	I
MET A2 R3 K6 K6 K6 K22 V31 V31 V34 V34 R83 R83 R83 R83	R58 R59 N61 V61 V61 V61 K112 K112	ALA ALA			
• Molecule 26: Smal	l ribosomal subunit	protein uS19			
Chain SP:	58%	2	5%	• 12%	
MET P2 R3 R3 R3 R4 K6 K7 K7 F10 F10 T11	H14 F15 F15 A17 V19 F20 F20 A22 A22	E24 125 827 827 828 829 930 731 832 833	W34 835 R36 R37 838 M39 ♠	140 141 P42 Q43 M44 V45	646 147 148 148 850 850 850 850 853 855 855 855 855 855 855 855 855 855
161 V62 863 664 066 066 066 067 068 068 068 171 672	E73 F74 A75 P76 P76 R81 K81 GLY H12 GLY ASP ASP	ARG LYS ALA LYS ARG			
• Molecule 27: Smal	l ribosomal subunit	protein uS8			
Chain BQ:	74%			24% ••	
MET 82 83 83 83 83 83 84 84 81 81 81 81 81 81 81 81 81 81 81 81 81	K34 L39 L40 E43 V46 N152 A33	E54	177 177 879 881 881 882	L85 H88 K98 K98	M101 V103 A104 1105 I105
D115 R116 A120 E126 A132					
• Molecule 28: Large	e ribosomal subunit 35%	protein uL6			
Chain GR:	72%		2	5% ••	
		WORLDWIDE PPDB PROTEIN DATA BANK			

MET ALA LYS ASP ASP ARG SER ARG SER LYS LYS LYS VAL YAR 77 77 78 78











• Molecule 38: Large ribosomal subunit protein bL21

Chain Qb: 98% .
M1 E28 E31 T33 E31 T33 C44 C44 C44 C44 C44 C44 C44 C44 C44 C
• Molecule 39: Large ribosomal subunit protein uL18
Chain Nc: 95% · ·
PHE ASP R4 R5 C57 S58 C57 S58 C57 C57 C52 C52 C52 C52 C52 C52 C52 C52 C52 C52
• Molecule 40: Large ribosomal subunit protein uL15
Chain Kd: 99%
MET 13 13 1117 1119 1117 1119 1117 010 010 010
• Molecule 41: Large ribosomal subunit protein uL14
Unain Je: 93% 7%
C nam Je: 93% 7% Image: Image: 93% 7%
• Molecule 42: Large ribosomal subunit protein uL3
Imain Je: 93% 7% Imain Je: Imain Je: 93% 7% Imain Je: Imain Je: Imain Je: 1main Je: Imain Je: Imain Je: 1main Je: 1main Je:
Onain Je: 93% 7% • Molecule 42: Large ribosomal subunit protein uL3 Chain Af: 96% • • • • • • • • • • • • • • • • • • •
Molecule 42: Large ribosomal subunit protein uL3 Chain Af: 96% • Molecule 43: Large ribosomal subunit protein uL16
Chain Je: 93% 7% • Molecule 42: Large ribosomal subunit protein uL3 Chain Af: 96% • Molecule 43: Large ribosomal subunit protein uL16 Chain Lg: 96% • Molecule 43: Large ribosomal subunit protein uL16
Chain Je: 93% 7% • Molecule 42: Large ribosomal subunit protein uL3 Chain Af: 96% • Molecule 43: Large ribosomal subunit protein uL16 Chain Lg: 96% • Molecule 43: Large ribosomal subunit protein uL16
Chain Je: 93% Molecule 42: Large ribosomal subunit protein uL3 Chain Af: 96% Molecule 43: Large ribosomal subunit protein uL16 Chain Lg: 96% Molecule 44: Large ribosomal subunit protein bL35



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MET K2 K17 132 K52 K52 K52 K52 K52			
• Molecule 45: Large ribo	somal subunit protein bL19		
Chain Oi:	83%	5% 12%	
MET 82 82 82 82 83 83 83 85 85 85 85 85 85 85 85 85 85 85 85 85	K108 L116 ALM ALM ALM ALM ALM ALM ALM ALM ALM ALM		
• Molecule 46: Small ribo	somal subunit protein $bS16$		
Chain Pj:	88%	• 9%	
M1 V10 V20 E45 E45 E48 E48 E47 E55 E47 E55 E47 E55	A62 D69 A77 A77 A77 A77 A77 A77 K80 A81 A81 A81 A1A A1A A1A ALA ALA		
• Molecule 47: Large ribo	somal subunit protein bL33		
Chain bk:	88%	8% •	
MET R2 R2 R3 M26 M26 A48 K38 K49 K49 K49 K49 LYS			
• Molecule 48: Large ribo	somal subunit protein uL2		
Chain Cl:	97%	•••	
MET P2 K5 K5 0110 0147 0168 0168 0188 17 1245	K272 K273		
• Molecule 49: Small ribo	somal subunit protein uS4		
Chain Dm:	98%	·	
MET A2 L9 E15 E15 C19 C19 C24 C24 C24 C26 C24 C26 C24 C26 C24 C26 C26 C26 C26 C26 C26 C26 C26 C26 C26	D29 V30 K31 K33 K34 A35 A36 A36 A36 A36 A36 A36 A36 A36 A36 A36	R84 E89 E89 E96 H106 G107 F108 G109 G109 G117 K127	K128 A129 G130 R131 B132 E133 F134 V135
q145 q145 d147 d147 d148 d149 d149 d145 d147 d148 d148 d149 d147 d148 d148 d148 d148 d148 d155 g155 g155 g155 g155 g156 g157 g158 g158 g158 g158 g158 g158 g158 g158 g158 g158	L160 L162 R161 R162 K163 A165 L165 E165 L168 A169 A169 A169 A169 A169 A169 A169 A169	L1/6 D179 V180 D181 H182 S183 S183 C185 Q186 Q186 Q186 A192 P193 P194 D194	R195 1196 1196 L198 P199 A200 E201 1202 K213
• Molecule 50: Large ribo	somal subunit protein uL23		

Chain Sn: 72% · 24%









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV $(4k \ge 4k)$	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.41998, 390.41998, 390.41998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mal	Chain	Bond	lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	В	0.33	0/2870	0.56	1/3890~(0.0%)	
2	F	0.30	0/998	0.65	0/1336	
3	Н	0.29	0/1429	0.57	0/1925	
4	Z2	0.85	0/65123	0.86	27/101564~(0.0%)	
5	R3	0.34	0/465	0.52	0/629	
6	A4	0.30	0/1848	0.51	0/2494	
7	E5	0.35	0/1163	0.58	0/1564	
8	L6	0.37	0/959	0.60	0/1282	
9	F7	0.30	0/1383	0.53	0/1858	
10	D8	0.60	0/2733	0.81	1/4256~(0.0%)	
11	E9	0.38	0/1559	0.58	0/2103	
12	aA	0.36	0/450	0.63	0/596	
13	MB	0.39	0/961	0.62	0/1282	
14	UC	0.34	0/774	0.54	0/1043	
15	WD	0.36	0/628	0.60	0/841	
16	XE	0.27	0/503	0.57	0/670	
17	RF	0.38	0/840	0.59	0/1125	
18	FG	0.30	0/864	0.53	0/1169	
19	VH	0.38	0/635	0.58	0/847	
20	TI	0.33	0/790	0.51	0/1057	
21	fJ	0.28	0/508	0.52	0/690	
22	HK	0.27	0/821	0.53	0/1091	
23	OL	0.33	0/702	0.53	0/941	
24	MM	0.26	0/724	0.54	0/976	
25	PO	0.43	0/947	0.65	0/1261	
26	SP	0.27	0/652	0.58	0/879	
27	BQ	0.32	0/982	0.55	0/1318	
28	GR	0.32	0/1377	0.58	1/1861~(0.1%)	
29	GS	0.30	$0/1\overline{219}$	0.57	$0/1\overline{634}$	
30	CT	0.29	0/1637	0.59	0/2200	
31	KU	0.30	0/857	0.55	0/1158	
32	NV	0.33	0/478	0.55	0/632	
33	YW	0.35	0/442	0.62	0/590	
34	IX	0.39	0/1134	0.53	0/1529	



Mal	Chain	Bond	lengths	E	Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
35	JY	0.29	0/803	0.59	0/1084
36	QZ	0.31	0/638	0.63	0/858
37	Ba	0.38	0/373	0.75	0/489
38	Qb	0.37	0/839	0.58	0/1127
39	Nc	0.33	0/863	0.60	0/1158
40	Kd	0.37	0/1073	0.64	0/1429
41	Je	0.38	0/946	0.65	0/1271
42	Af	0.39	0/1566	0.58	0/2103
43	Lg	0.43	0/1112	0.63	0/1483
44	dh	0.40	0/524	0.63	0/686
45	Oi	0.38	0/927	0.64	0/1239
46	Pj	0.37	0/660	0.60	0/887
47	bk	0.40	0/401	0.58	0/534
48	Cl	0.39	0/2147	0.61	0/2883
49	Dm	0.31	0/1712	0.57	0/2296
50	Sn	0.38	0/705	0.57	0/939
51	То	0.30	0/688	0.57	0/916
52	ep	0.37	0/300	0.65	0/395
53	V	0.36	0/1674	0.95	0/2586
54	Y	0.39	0/131	0.87	0/200
55	C1	0.31	0/379	0.53	0/511
56	iN	0.59	0/36108	0.79	$6/\overline{56315}~(0.0\%)$
All	All	0.66	0/154024	0.77	$36/\overline{229680\ (0.0\%)}$

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
19	VH	0	1
29	GS	0	1
All	All	0	2

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Z2	942	U	C2-N1-C1'	8.60	128.02	117.70
4	Z2	495	G	O4'-C1'-N9	7.98	114.58	108.20
1	В	99	PRO	CA-N-CD	-7.37	101.18	111.50
4	Z2	942	U	N1-C2-O2	7.33	127.93	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Z2	1297	U	C2-N1-C1'	6.83	125.89	117.70
56	iN	607	С	N3-C2-O2	-6.61	117.27	121.90
4	Z2	638	С	C2-N1-C1'	6.47	125.92	118.80
4	Z2	775	U	C2-N1-C1'	6.46	125.45	117.70
56	iN	607	С	N1-C2-O2	6.44	122.76	118.90
56	iN	798	С	C2-N1-C1'	6.19	125.61	118.80
4	Z2	689	G	O4'-C1'-N9	5.96	112.97	108.20
4	Z2	942	U	C6-N1-C1'	-5.93	112.89	121.20
4	Z2	733	G	O4'-C1'-N9	5.87	112.89	108.20
4	Z2	638	С	N1-C2-O2	5.86	122.42	118.90
56	iN	607	С	C2-N1-C1'	5.78	125.16	118.80
28	GR	154	PRO	C-N-CA	5.76	136.11	121.70
56	iN	1203	С	C2-N1-C1'	5.57	124.92	118.80
4	Z2	942	U	N3-C2-O2	-5.44	118.39	122.20
4	Z2	1885	А	N7-C8-N9	5.43	116.52	113.80
4	Z2	2767	U	N3-C2-O2	-5.43	118.40	122.20
4	Z2	942	U	C5-C6-N1	5.43	125.41	122.70
4	Z2	189	G	C8-N9-C1'	-5.40	119.98	127.00
56	iN	1203	С	N1-C2-O2	5.31	122.08	118.90
4	Z2	638	C	C6-N1-C2	-5.30	118.18	120.30
4	Z2	464	G	O4'-C1'-N9	5.24	112.39	108.20
10	D8	86	С	N1-C2-O2	5.20	122.02	118.90
4	Z2	958	G	O4'-C1'-N9	5.17	112.34	108.20
4	Z2	775	U	N1-C2-O2	5.17	126.42	122.80
4	Z2	916	А	OP2-P-O3'	5.13	116.48	105.20
4	Z2	34	G	O4'-C1'-N9	5.11	112.29	108.20
4	Z2	702	С	C2-N1-C1'	5.11	124.42	118.80
4	Z2	1297	U	N1-C2-O2	5.10	126.37	122.80
4	Z2	1113	A	O4'-C1'-N9	5.07	112.26	108.20
4	Z2	968	A	O4'-C1'-N9	5.04	112.23	108.20
4	Z2	702	С	N1-C2-O2	5.03	121.92	118.90
4	Z2	2814	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	GS	112	ARG	Sidechain
19	VH	2	ALA	Peptide



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	В	2829	0	2781	55	0
2	F	985	0	1035	22	0
3	Н	1409	0	1416	25	0
4	Z2	58145	0	29231	503	0
5	R3	457	0	466	8	0
6	A4	1816	0	1843	37	0
7	E5	1151	0	1205	19	0
8	L6	946	0	1008	15	0
9	F7	1362	0	1402	45	0
10	D8	2446	0	1241	17	0
11	E9	1537	0	1590	26	0
12	aA	442	0	432	0	0
13	MB	947	0	988	10	0
14	UC	760	0	774	7	0
15	WD	618	0	637	18	0
16	XE	502	0	527	8	0
17	RF	834	0	898	18	0
18	FG	849	0	838	19	0
19	VH	626	0	629	8	0
20	ΤI	784	0	820	12	0
21	fJ	493	0	441	0	0
22	HK	811	0	845	15	0
23	OL	694	0	710	8	0
24	MM	717	0	748	23	0
25	PO	935	0	999	16	0
26	SP	637	0	665	14	0
27	BQ	974	0	1009	21	0
28	GR	1357	0	1397	28	0
29	GS	1200	0	1231	28	0
30	CT	1613	0	1677	34	0
31	KU	842	0	850	16	0
32	NV	472	0	520	10	0
33	YW	438	0	476	4	0
34	IX	1108	0	1145	16	0
35	JY	793	0	821	18	0
36	QZ	632	0	676	12	0
37	Ba	369	0	418	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Qb	827	0	862	0	0
39	Nc	852	0	880	0	0
40	Kd	1062	0	1123	0	0
41	Je	937	0	1003	0	0
42	Af	1548	0	1574	0	0
43	Lg	1093	0	1188	0	0
44	dh	519	0	581	0	0
45	Oi	917	0	969	0	0
46	Рj	648	0	661	0	0
47	bk	394	0	412	0	0
48	Cl	2107	0	2195	0	0
49	Dm	1688	0	1745	0	0
50	Sn	698	0	750	0	0
51	То	684	0	727	0	0
52	ep	298	0	334	0	0
53	V	1521	0	766	19	0
54	Y	120	0	61	1	0
55	C1	374	0	406	1	0
56	iN	32246	0	16224	0	0
All	All	142063	0	96850	1071	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 8.

All (1071) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z2:281:A:N7	4:Z2:331:G:N2	2.12	0.96
4:Z2:2083:U:H3	4:Z2:2178:G:H1	0.94	0.93
4:Z2:655:A:H4'	4:Z2:656:C:H5'	1.58	0.84
29:GS:112:ARG:HH22	29:GS:123:GLY:HA3	1.48	0.79
16:XE:16:GLN:NE2	16:XE:20:GLU:OE1	2.16	0.79
7:E5:39:THR:HG22	7:E5:57:LYS:HG2	1.64	0.79
4:Z2:68:A:OP2	16:XE:47:ARG:NH2	2.16	0.79
4:Z2:570:G:N7	25:PO:6:ARG:NH2	2.31	0.79
25:PO:86:ALA:HB2	25:PO:116:GLU:HG3	1.65	0.79
4:Z2:2288:U:H5"	9:F7:131:GLY:HA3	1.67	0.77
4:Z2:52:G:H5"	4:Z2:53:G:H5'	1.67	0.76
24:MM:23:PHE:HB3	24:MM:66:GLU:HB3	1.67	0.76
1:B:129:THR:HG22	1:B:131:ASP:H	1.50	0.76
4:Z2:2053:G:H1	4:Z2:2426:U:H3	1.30	0.76



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:Z2:1885:A:H8	4:Z2:1888:C:H41	1.33	0.75
31:KU:93:ARG:NH2	31:KU:112:ASP:OD2	2.19	0.75
20:TI:92:GLN:HG3	20:TI:101:VAL:HG13	1.69	0.74
4:Z2:219:C:H5	4:Z2:229:G:H21	1.34	0.73
4:Z2:1417:A:H2'	4:Z2:1418:A:C8	2.23	0.73
24:MM:64:MET:HG3	24:MM:68:ASP:HB2	1.71	0.73
28:GR:164:TYR:HB2	28:GR:167:GLU:HB2	1.70	0.72
4:Z2:2311:A:H2'	4:Z2:2312:A:C8	2.25	0.72
4:Z2:272:U:H3	4:Z2:342:G:H1	1.34	0.71
30:CT:19:ASN:O	30:CT:40:ARG:NH2	2.24	0.71
30:CT:51:MET:HG3	30:CT:71:ALA:HB3	1.73	0.71
11:E9:3:LEU:HD23	11:E9:13:LEU:HD12	1.72	0.71
2:F:112:LYS:NZ	2:F:116:LEU:O	2.23	0.71
4:Z2:1707:G:O2'	4:Z2:1725:A:N6	2.24	0.70
7:E5:111:ILE:O	7:E5:130:THR:OG1	2.09	0.70
4:Z2:197:U:H4'	15:WD:22:ASN:HB3	1.72	0.70
30:CT:11:ARG:HB3	30:CT:16:LYS:HG3	1.74	0.70
4:Z2:194:A:N6	4:Z2:2413:A:O2'	2.25	0.69
4:Z2:2083:U:O2	4:Z2:2178:G:N2	2.25	0.69
4:Z2:281:A:H62	4:Z2:331:G:H21	1.38	0.69
4:Z2:1453:A:H2'	4:Z2:1454:A:C8	2.27	0.69
2:F:82:THR:HG23	2:F:96:LEU:HD13	1.74	0.69
9:F7:8:TYR:HA	9:F7:12:LEU:HB2	1.73	0.69
17:RF:1:MET:SD	17:RF:62:HIS:ND1	2.66	0.69
7:E5:162:ARG:NH1	27:BQ:101:MET:O	2.26	0.69
15:WD:6:GLN:HB3	15:WD:71:LEU:HD11	1.75	0.68
4:Z2:562:G:O2'	4:Z2:1238:A:OP1	2.12	0.68
8:L6:99:ARG:HD2	8:L6:104:CYS:SG	2.34	0.68
1:B:277:ARG:O	3:H:384:ARG:NH1	2.27	0.68
4:Z2:2009:C:H5'	4:Z2:2600:U:H4'	1.75	0.68
30:CT:124:LEU:HD21	30:CT:153:LEU:HD11	1.74	0.68
31:KU:30:THR:HG21	31:KU:63:ALA:HB2	1.76	0.67
1:B:34:PRO:HG3	1:B:73:HIS:HD2	1.59	0.67
4:Z2:185:G:H5'	15:WD:14:VAL:HG11	1.75	0.67
9:F7:134:GLU:HB3	9:F7:136:ILE:HD13	1.77	0.67
3:H:252:ASP:OD1	3:H:252:ASP:N	2.27	0.66
1:B:19:ILE:HG12	1:B:44:VAL:HG21	1.77	0.66
1:B:63:LYS:NZ	1:B:85:SER:O	2.24	0.66
4:Z2:1020:G:H1	4:Z2:1103:U:H3	1.42	0.66
18:FG:25:TYR:OH	18:FG:81:ASN:ND2	2.28	0.66
2:F:26:ILE:HG12	2:F:61:LEU:HD12	1.77	0.66



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:CT:51:MET:HB2	30:CT:115:LEU:HD22	1.76	0.66
4:Z2:327:A:O2'	11:E9:161:ARG:NH2	2.29	0.66
7:E5:16:LEU:HD21	7:E5:44:VAL:HB	1.78	0.66
4:Z2:2196:A:H2'	4:Z2:2197:C:C6	2.31	0.66
1:B:212:ILE:HB	1:B:235:THR:HG22	1.76	0.66
22:HK:34:MET:SD	22:HK:34:MET:N	2.62	0.66
31:KU:22:HIS:HB2	31:KU:33:THR:HG22	1.79	0.65
4:Z2:2274:U:H2'	4:Z2:2275:G:C8	2.31	0.65
17:RF:12:ILE:HD12	17:RF:42:LYS:HE2	1.77	0.65
34:IX:114:LEU:O	34:IX:118:MET:HG3	1.95	0.65
4:Z2:2083:U:O4	4:Z2:2178:G:O6	2.14	0.65
35:JY:46:ILE:HG12	35:JY:68:ARG:HG2	1.78	0.65
24:MM:39:ILE:HD11	24:MM:52:GLN:HB2	1.79	0.65
16:XE:24:ASP:OD1	16:XE:27:ARG:NH1	2.29	0.64
2:F:50:LEU:HD21	2:F:61:LEU:HD11	1.79	0.64
16:XE:5:GLU:O	16:XE:9:LYS:NZ	2.30	0.64
1:B:304:ARG:NH1	1:B:357:MET:O	2.29	0.64
35:JY:66:GLU:OE2	35:JY:68:ARG:NH1	2.30	0.64
4:Z2:1089:U:H2'	4:Z2:1090:A:H8	1.62	0.64
23:OL:20:ASP:OD1	23:OL:21:THR:N	2.29	0.64
1:B:298:GLY:HA2	1:B:367:THR:HA	1.79	0.64
6:A4:20:HIS:HB3	6:A4:48:LEU:HD21	1.79	0.64
4:Z2:1160:G:H4'	4:Z2:1161:U:H3'	1.79	0.64
4:Z2:1788:A:H2'	4:Z2:1789:A:C8	2.32	0.64
14:UC:35:ILE:HD11	14:UC:43:PRO:HB2	1.80	0.64
6:A4:168:VAL:HG21	6:A4:178:ILE:HD11	1.78	0.63
30:CT:97:VAL:HB	30:CT:98:PRO:HD2	1.79	0.63
1:B:134:ARG:NH2	1:B:245:GLY:O	2.31	0.63
30:CT:52:ILE:HG22	30:CT:70:THR:HB	1.81	0.63
4:Z2:836:C:H2'	4:Z2:837:A:H8	1.63	0.63
4:Z2:2282:G:OP2	9:F7:71:ARG:NH2	2.31	0.63
9:F7:24:ASN:HB3	9:F7:27:GLN:HG3	1.80	0.63
4:Z2:578:U:H2'	4:Z2:579:U:C6	2.33	0.62
4:Z2:397:C:H2'	4:Z2:398:A:C8	2.35	0.62
36:QZ:71:ARG:HH11	36:QZ:71:ARG:HG3	1.62	0.62
4:Z2:2050:C:H2'	4:Z2:2051:C:C6	2.35	0.62
4:Z2:644:G:H4'	11:E9:94:LYS:HG2	1.80	0.62
4:Z2:836:C:H2'	4:Z2:837:A:C8	2.35	0.62
4:Z2:2617:A:N1	4:Z2:2767:U:H5	1.98	0.62
4:Z2:2226:U:H2'	4:Z2:2227:U:C6	2.35	0.62
16:XE:39:ASN:ND2	16:XE:42:GLU:OE2	2.32	0.62



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:10:ARG:HG3	2:F:11:LYS:HG2	1.80	0.62
4:Z2:345:A:HO2'	4:Z2:346:A:H8	1.46	0.62
4:Z2:527:A:H2'	4:Z2:528:A:C8	2.34	0.62
4:Z2:1580:A:O2'	4:Z2:1581:A:OP1	2.18	0.62
3:H:336:ARG:NH2	3:H:370:ALA:O	2.32	0.61
18:FG:18:VAL:HG11	18:FG:58:HIS:CE1	2.35	0.61
4:Z2:688:U:H2'	4:Z2:689:G:O4'	2.00	0.61
6:A4:171:VAL:HG13	6:A4:178:ILE:HG13	1.83	0.61
8:L6:8:ILE:HG21	36:QZ:44:LEU:HD21	1.82	0.61
31:KU:112:ASP:HB3	32:NV:2:PRO:HB2	1.83	0.61
36:QZ:64:LEU:HB3	36:QZ:85:VAL:HG23	1.81	0.61
6:A4:86:ALA:O	6:A4:90:THR:HG23	2.01	0.61
18:FG:2:ARG:HH21	18:FG:91:ARG:HE	1.46	0.60
27:BQ:104:ALA:HB3	27:BQ:115:ASP:HB3	1.82	0.60
4:Z2:1795:A:H2'	4:Z2:1796:A:C8	2.36	0.60
7:E5:43:VAL:HG12	7:E5:122:VAL:HG11	1.81	0.60
4:Z2:2216:U:H2'	4:Z2:2217:G:C8	2.37	0.60
9:F7:7:LEU:HD12	9:F7:11:GLU:HG3	1.82	0.60
34:IX:45:THR:HG23	34:IX:48:VAL:HB	1.84	0.60
18:FG:51:ILE:O	18:FG:54:ILE:HG12	2.02	0.60
4:Z2:169:C:O2'	4:Z2:170:A:OP1	2.18	0.60
18:FG:9:LEU:HB2	18:FG:86:ARG:HB3	1.84	0.60
8:L6:54:ARG:NH1	8:L6:62:GLU:O	2.34	0.60
24:MM:25:VAL:HG13	24:MM:29:THR:HG22	1.83	0.60
13:MB:37:THR:HG23	13:MB:39:PRO:HD2	1.83	0.59
30:CT:14:VAL:HG22	30:CT:15:VAL:HG13	1.84	0.59
4:Z2:2574:C:H2'	4:Z2:2575:G:C8	2.37	0.59
4:Z2:2328:A:N3	4:Z2:2364:A:H2'	2.17	0.59
4:Z2:2060:U:H2'	4:Z2:2061:U:C6	2.37	0.59
20:TI:92:GLN:OE1	20:TI:92:GLN:N	2.33	0.59
4:Z2:724:A:H1'	4:Z2:725:C:H5	1.68	0.59
30:CT:11:ARG:NH2	30:CT:177:THR:O	2.33	0.59
35:JY:57:VAL:HG22	35:JY:58:ASN:H	1.67	0.59
6:A4:122:LEU:HD23	6:A4:146:MET:HG3	1.83	0.59
18:FG:41:ASP:OD1	18:FG:58:HIS:NE2	2.36	0.59
4:Z2:1356:U:O2'	4:Z2:2196:A:N3	2.29	0.59
5:R3:25:ASP:OD1	18:FG:101:GLN:NE2	2.35	0.59
4:Z2:2310:A:H2'	4:Z2:2311:A:C8	2.36	0.59
18:FG:18:VAL:HG11	18:FG:58:HIS:HE1	1.68	0.58
20:TI:94:VAL:HG12	20:TI:101:VAL:HA	1.85	0.58
28:GR:139:GLN:OE1	28:GR:140:GLN:NE2	2.36	0.58


Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
53:V:13:U:H2'	53:V:14:U:H5"	1.84	0.58
7:E5:99:VAL:HB	7:E5:116:MET:HE3	1.85	0.58
7:E5:112:ALA:HB1	7:E5:116:MET:HB3	1.85	0.58
1:B:23:THR:OG1	1:B:77:LEU:O	2.15	0.58
4:Z2:1413:G:H2'	4:Z2:1414:G:H8	1.69	0.58
4:Z2:2622:A:O2'	34:IX:96:LYS:NZ	2.34	0.58
6:A4:141:GLU:O	6:A4:144:ARG:HG3	2.04	0.58
27:BQ:43:GLU:HG3	27:BQ:103:VAL:HG21	1.86	0.58
4:Z2:1341:C:H2'	4:Z2:1342:G:O4'	2.03	0.58
4:Z2:1585:A:H5"	4:Z2:1586:A:H5'	1.83	0.58
4:Z2:2537:U:H2'	4:Z2:2538:U:C6	2.39	0.58
4:Z2:1447:A:H2'	4:Z2:1448:G:C8	2.39	0.58
17:RF:92:ARG:NH1	17:RF:92:ARG:HB3	2.19	0.58
4:Z2:642:U:H2'	4:Z2:643:U:C6	2.39	0.58
4:Z2:1012:A:N6	4:Z2:1109:G:H2'	2.19	0.58
4:Z2:2256:A:H2'	4:Z2:2257:A:C8	2.39	0.58
4:Z2:1782:U:H2'	4:Z2:1783:C:C6	2.39	0.58
4:Z2:2288:U:C2	9:F7:151:GLY:HA3	2.39	0.58
6:A4:166:ILE:HG13	6:A4:186:ILE:HD11	1.86	0.58
2:F:10:ARG:HG3	2:F:11:LYS:H	1.69	0.58
4:Z2:1343:A:H2	4:Z2:1356:U:H3	1.52	0.58
5:R3:63:ARG:HD3	5:R3:70:TYR:HA	1.85	0.58
24:MM:31:GLN:O	24:MM:35:GLU:HG2	2.04	0.58
1:B:44:VAL:HG12	1:B:61:LEU:HD21	1.84	0.57
8:L6:4:THR:HG21	27:BQ:85:LEU:HD13	1.86	0.57
18:FG:8:LEU:HD13	18:FG:84:ILE:HD13	1.86	0.57
2:F:32:PRO:HG2	2:F:35:GLU:HB3	1.86	0.57
4:Z2:12:A:H2'	4:Z2:13:A:C8	2.40	0.57
1:B:304:ARG:HG3	1:B:357:MET:HB3	1.87	0.57
4:Z2:380:U:OP2	15:WD:10:LYS:NZ	2.34	0.57
5:R3:34:SER:OG	5:R3:36:ASN:OD1	2.21	0.57
4:Z2:2011:C:H2'	4:Z2:2012:A:C8	2.39	0.57
4:Z2:798:U:H2'	4:Z2:799:C:C6	2.39	0.57
29:GS:46:ALA:HA	29:GS:122:ALA:HB2	1.86	0.57
4:Z2:1089:U:H2'	4:Z2:1090:A:C8	2.39	0.57
4:Z2:1639:G:OP1	13:MB:37:THR:HG21	2.05	0.57
4:Z2:2076:A:O2'	15:WD:53:THR:HG21	2.05	0.57
4:Z2:281:A:H62	4:Z2:331:G:N2	2.02	0.57
7:E5:99:VAL:HB	7:E5:116:MET:CE	2.35	0.57
18:FG:63:ASN:HD22	18:FG:96:ILE:HB	1.69	0.57
6:A4:84:ILE:HG21	6:A4:216:SER:HA	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:132:LYS:HE3	1:B:163:PRO:HB2	1.86	0.56
4:Z2:1453:A:H2'	4:Z2:1454:A:H8	1.70	0.56
4:Z2:2771:C:H2'	4:Z2:2772:C:C6	2.40	0.56
28:GR:84:GLU:OE2	28:GR:86:ARG:NH1	2.38	0.56
28:GR:107:VAL:HG23	28:GR:108:GLY:H	1.70	0.56
4:Z2:1480:A:N3	4:Z2:1565:C:O2'	2.34	0.56
4:Z2:1855:G:H3'	4:Z2:1856:U:H5"	1.87	0.56
9:F7:119:PRO:O	9:F7:167:ARG:NH2	2.37	0.56
4:Z2:1780:A:H2'	4:Z2:1781:C:C6	2.41	0.56
4:Z2:2413:A:H2'	4:Z2:2413:A:N3	2.19	0.56
18:FG:26:ILE:HG23	18:FG:36:ILE:HG13	1.87	0.56
4:Z2:579:U:H2'	4:Z2:580:C:C6	2.40	0.56
4:Z2:727:G:H2'	4:Z2:728:U:C6	2.40	0.56
4:Z2:1875:A:H2'	4:Z2:1876:A:C8	2.40	0.56
53:V:5:U:H3	53:V:68:U:H3	1.52	0.56
4:Z2:617:A:H2'	4:Z2:618:A:C8	2.41	0.56
32:NV:40:LYS:O	32:NV:44:VAL:HG23	2.06	0.56
1:B:287:GLN:NE2	1:B:319:THR:HA	2.21	0.56
6:A4:167:PHE:HA	6:A4:189:ILE:HG23	1.88	0.56
9:F7:14:GLN:OE1	9:F7:14:GLN:N	2.34	0.56
36:QZ:23:MET:HE3	36:QZ:26:SER:HB3	1.87	0.56
3:H:287:GLU:OE1	3:H:287:GLU:N	2.34	0.56
4:Z2:1681:U:H5"	4:Z2:1682:C:H5	1.70	0.56
9:F7:108:ILE:HG22	9:F7:109:PRO:HD3	1.88	0.56
22:HK:4:LYS:HA	22:HK:7:ILE:HD12	1.87	0.56
1:B:174:ASP:HB3	53:V:74:C:H41	1.71	0.56
6:A4:83:GLY:O	6:A4:87:GLU:HG2	2.06	0.56
9:F7:6:ALA:O	9:F7:10:ASN:ND2	2.38	0.56
4:Z2:462:A:H4'	4:Z2:463:A:H5'	1.88	0.56
4:Z2:1782:U:H2'	4:Z2:1783:C:H6	1.71	0.56
1:B:179:ARG:HD3	4:Z2:2567:U:H4'	1.88	0.55
4:Z2:2196:A:O2'	4:Z2:2197:C:OP1	2.21	0.55
18:FG:9:LEU:HD11	18:FG:59:TYR:CZ	2.41	0.55
4:Z2:1459:G:O2'	4:Z2:1500:G:O6	2.24	0.55
4:Z2:2661:A:H2'	4:Z2:2662:A:C8	2.41	0.55
28:GR:155:GLU:HG2	28:GR:157:TYR:H	1.71	0.55
2:F:63:ILE:HG21	2:F:77:ILE:HG12	1.88	0.55
4:Z2:397:C:H2'	4:Z2:398:A:H8	1.72	0.55
4:Z2:1031:G:O2'	4:Z2:1094:G:N1	2.39	0.55
4:Z2:2573:A:H2'	4:Z2:2574:C:C6	2.41	0.55
22:HK:83:MET:HA	22:HK:86:GLU:HG3	1.89	0.55



Atom-1	Atom-2	Interatomic	Clash
	1100m =	distance (Å)	overlap (Å)
1:B:220:SER:OG	4:Z2:2541:C:H5'	2.06	0.55
4:Z2:2295:U:H5'	9:F7:85:ILE:HD11	1.89	0.55
35:JY:7:ARG:NH1	35:JY:73:MET:SD	2.77	0.55
3:H:216:PRO:HA	3:H:294:VAL:HG12	1.88	0.55
3:H:216:PRO:HG3	3:H:336:ARG:HD2	1.88	0.55
4:Z2:818:A:H2'	4:Z2:819:G:C8	2.41	0.55
4:Z2:984:A:H2'	4:Z2:985:A:C8	2.42	0.55
2:F:26:ILE:HG21	2:F:33:LEU:HD12	1.89	0.55
4:Z2:2194:U:H3	4:Z2:2199:A:H61	1.54	0.55
4:Z2:993:A:H5'	25:PO:59:ARG:HG3	1.89	0.55
6:A4:95:PRO:HG3	6:A4:159:MET:HG3	1.89	0.55
27:BQ:79:ARG:NH1	27:BQ:81:SER:O	2.40	0.55
4:Z2:275:U:H2'	4:Z2:276:A:C8	2.42	0.54
6:A4:125:GLN:OE1	6:A4:130:THR:OG1	2.25	0.54
18:FG:42:TRP:CD2	18:FG:102:LEU:HD22	2.43	0.54
15:WD:31:PRO:HB2	15:WD:33:LEU:HG	1.90	0.54
28:GR:135:SER:HB3	28:GR:141:LEU:HB2	1.88	0.54
53:V:5:U:H2'	53:V:6:U:O4'	2.07	0.54
18:FG:22:VAL:O	18:FG:26:ILE:HG12	2.08	0.54
30:CT:43:LEU:HD12	30:CT:55:ILE:HD13	1.88	0.54
4:Z2:71:G:H2'	4:Z2:72:C:C6	2.42	0.54
4:Z2:2632:C:H2'	4:Z2:2633:U:H6	1.73	0.54
4:Z2:2644:G:O6	28:GR:175:LYS:NZ	2.40	0.54
24:MM:49:ASP:HB3	24:MM:52:GLN:HG2	1.90	0.54
29:GS:26:PHE:HE2	29:GS:121:LEU:HD21	1.71	0.54
36:QZ:17:ARG:HD2	36:QZ:64:LEU:HD13	1.87	0.54
30:CT:88:GLN:NE2	30:CT:100:GLN:HA	2.22	0.54
4:Z2:1580:A:H2'	4:Z2:1581:A:C8	2.43	0.54
31:KU:31:ILE:HG12	31:KU:46:THR:HG22	1.90	0.54
4:Z2:788:C:O5'	4:Z2:788:C:H6	1.91	0.54
4:Z2:1833:A:H1'	4:Z2:1834:A:N7	2.23	0.54
10:D8:111:C:H2'	10:D8:112:A:H8	1.73	0.54
23:OL:11:ILE:HG21	23:OL:21:THR:HG22	1.89	0.54
34:IX:88:ASN:HB2	34:IX:91:LYS:HE2	1.88	0.54
6:A4:167:PHE:HA	6:A4:189:ILE:O	2.08	0.53
4:Z2:982:C:OP2	25:PO:58:ARG:NH2	2.38	0.53
4:Z2:1370:U:H2'	4:Z2:1371:U:C6	2.43	0.53
13:MB:24:MET:HE1	13:MB:40:LYS:HD2	1.90	0.53
26:SP:3:ARG:NH1	26:SP:7:LYS:HB3	2.23	0.53
4:Z2:380:U:H5"	15:WD:32:ASN:HB2	1.89	0.53
4:Z2:2057:A:H2'	4:Z2:2058:C:C6	2.43	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
11:E9:82:ARG:HB2	11:E9:85:ALA:HB2	1.90	0.53
7:E5:86:LEU:HB2	7:E5:103:PRO:HG3	1.90	0.53
4:Z2:932:C:H1'	4:Z2:968:A:C8	2.43	0.53
29:GS:67:LEU:HB3	29:GS:71:ARG:HH21	1.73	0.53
4:Z2:734:A:H4'	4:Z2:1255:G:N3	2.23	0.53
4:Z2:463:A:O2'	20:TI:41:THR:O	2.27	0.53
4:Z2:1413:G:H2'	4:Z2:1414:G:C8	2.44	0.53
53:V:8:U:H3	53:V:14:U:H5	1.57	0.53
4:Z2:1489:G:H2'	4:Z2:1490:U:C6	2.44	0.53
4:Z2:2286:G:O2'	9:F7:121:ALA:O	2.22	0.53
4:Z2:2444:A:H2'	4:Z2:2445:C:C6	2.44	0.53
4:Z2:2683:A:H2'	4:Z2:2684:C:C6	2.44	0.53
26:SP:24:GLU:OE1	26:SP:24:GLU:N	2.40	0.53
30:CT:134:MET:HG3	30:CT:153:LEU:HG	1.90	0.53
4:Z2:2573:A:H2'	4:Z2:2574:C:H6	1.73	0.53
5:R3:73:ASN:ND2	5:R3:73:ASN:O	2.37	0.53
6:A4:84:ILE:H	6:A4:84:ILE:HD12	1.73	0.53
3:H:221:PHE:HA	3:H:286:ARG:HE	1.72	0.52
4:Z2:477:G:H4'	17:RF:6:LYS:HB2	1.91	0.52
4:Z2:799:C:H2'	4:Z2:800:C:H6	1.74	0.52
4:Z2:1918:A:H2'	4:Z2:1919:G:O4'	2.09	0.52
4:Z2:2805:G:O2'	13:MB:49:GLU:OE2	2.27	0.52
30:CT:72:ARG:HH11	30:CT:72:ARG:HG3	1.75	0.52
36:QZ:27:ILE:HG21	36:QZ:59:CYS:SG	2.49	0.52
4:Z2:2024:G:H2'	4:Z2:2025:U:O4'	2.09	0.52
27:BQ:75:GLU:HG2	27:BQ:76:THR:HG23	1.91	0.52
4:Z2:124:A:H5'	4:Z2:125:A:H8	1.75	0.52
4:Z2:288:C:OP2	20:TI:80:ARG:NH2	2.37	0.52
4:Z2:593:A:H2'	4:Z2:594:A:C8	2.44	0.52
4:Z2:2550:G:H2'	4:Z2:2551:A:C8	2.44	0.52
2:F:13:SER:HB3	2:F:68:GLY:HA3	1.91	0.52
4:Z2:85:U:H2'	4:Z2:86:C:C6	2.45	0.52
4:Z2:1166:A:H2'	4:Z2:1167:A:C8	2.45	0.52
30:CT:47:LEU:HB2	30:CT:52:ILE:HD13	1.91	0.52
3:H:339:ASP:N	3:H:339:ASP:OD1	2.43	0.52
4:Z2:169:C:HO2'	4:Z2:170:A:P	2.31	0.52
4:Z2:293:U:H2'	4:Z2:294:G:O4'	2.10	0.52
4:Z2:931:A:H2'	4:Z2:932:C:C6	2.44	0.52
4:Z2:1986:C:OP1	13:MB:5:LYS:NZ	2.39	0.52
6:A4:47:ASN:O	6:A4:51:THR:HG23	2.10	0.52
4:Z2:156:U:H2'	4:Z2:157:C:C6	2.44	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:F7:4:LEU:HG	9:F7:101:ASP:HB2	1.92	0.52
10:D8:18:G:H2'	10:D8:19:A:C8	2.45	0.52
10:D8:111:C:H2'	10:D8:112:A:C8	2.44	0.52
2:F:48:GLN:HA	2:F:51:GLU:HG2	1.92	0.52
10:D8:18:G:H2'	10:D8:19:A:H8	1.73	0.52
3:H:310:GLU:HB3	3:H:390:VAL:HG13	1.91	0.52
4:Z2:37:G:H2'	4:Z2:38:C:C6	2.45	0.52
8:L6:107:VAL:HG23	8:L6:117:TYR:HB3	1.91	0.52
27:BQ:34:LYS:HD3	27:BQ:51:VAL:HG23	1.92	0.52
3:H:230:VAL:HG11	3:H:289:VAL:HG11	1.91	0.52
4:Z2:841:G:H2'	4:Z2:842:G:C8	2.44	0.52
4:Z2:1468:C:H2'	4:Z2:1469:A:H8	1.74	0.52
35:JY:10:LEU:HD22	35:JY:98:VAL:HG12	1.92	0.52
4:Z2:1062:U:H4'	4:Z2:1063:C:H5'	1.90	0.52
8:L6:67:ILE:HG12	8:L6:74:LEU:HD12	1.92	0.52
32:NV:4:VAL:HG21	32:NV:19:PHE:HA	1.91	0.52
4:Z2:46:G:H2'	4:Z2:47:U:C6	2.45	0.51
4:Z2:532:A:HO2'	4:Z2:533:U:H6	1.57	0.51
4:Z2:583:U:H2'	4:Z2:584:A:C8	2.44	0.51
4:Z2:2073:U:H2'	4:Z2:2074:A:H8	1.75	0.51
4:Z2:2580:G:H2'	4:Z2:2581:A:C8	2.45	0.51
35:JY:85:ASP:OD1	35:JY:86:ALA:N	2.43	0.51
4:Z2:275:U:H2'	4:Z2:276:A:H8	1.75	0.51
4:Z2:1633:G:H5"	4:Z2:1634:C:H5'	1.92	0.51
9:F7:63:GLN:HE22	10:D8:41:C:H4'	1.76	0.51
24:MM:16:VAL:HB	24:MM:41:PRO:HB3	1.92	0.51
7:E5:101:MET:HG2	7:E5:130:THR:HG22	1.91	0.51
4:Z2:1426:U:H2'	4:Z2:1427:C:C6	2.45	0.51
17:RF:81:THR:HG21	17:RF:97:SER:HB2	1.92	0.51
4:Z2:1839:A:H2'	4:Z2:1840:A:C8	2.45	0.51
18:FG:49:TYR:OH	18:FG:86:ARG:NH1	2.44	0.51
27:BQ:116:ARG:HG2	27:BQ:116:ARG:HH11	1.74	0.51
32:NV:29:LEU:HA	32:NV:32:VAL:HG12	1.92	0.51
4:Z2:1182:U:H2'	4:Z2:1183:U:C6	2.46	0.51
4:Z2:1996:G:H5"	17:RF:42:LYS:HB2	1.93	0.51
4:Z2:2316:A:OP1	19:VH:77:ARG:NH2	2.43	0.51
7:E5:77:ILE:HD13	7:E5:150:ARG:HB2	1.92	0.51
11:E9:129:LYS:HB3	11:E9:132:GLU:HG3	1.91	0.51
1:B:132:LYS:HD2	1:B:165:ASP:HA	1.92	0.51
11:E9:128:PRO:HB3	11:E9:155:ASN:HB2	1.92	0.51
28:GR:35:LEU:HD21	28:GR:72:LEU:HD13	1.93	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:Z2:27:C:OP1	25:PO:22:LYS:HE3	2.11	0.51
15:WD:39:TRP:HE1	15:WD:41:GLU:HG2	1.76	0.51
4:Z2:334:A:H2'	4:Z2:335:C:C6	2.46	0.51
4:Z2:655:A:H4'	4:Z2:656:C:C5'	2.36	0.51
4:Z2:1012:A:H2'	4:Z2:1013:A:C8	2.46	0.51
27:BQ:22:LYS:O	27:BQ:67:TYR:OH	2.22	0.51
3:H:357:ASP:OD1	3:H:357:ASP:N	2.42	0.50
4:Z2:1581:A:H2'	4:Z2:1582:A:C8	2.46	0.50
22:HK:81:ARG:HD2	35:JY:52:LEU:HB2	1.93	0.50
29:GS:26:PHE:CE2	29:GS:121:LEU:HD21	2.46	0.50
4:Z2:2240:U:H5"	19:VH:11:ARG:CZ	2.41	0.50
24:MM:9:ILE:HD12	24:MM:18:SER:HB3	1.93	0.50
4:Z2:566:C:OP1	25:PO:33:ARG:HB2	2.11	0.50
15:WD:61:LYS:HG2	15:WD:62:LEU:HD23	1.92	0.50
4:Z2:565:U:H2'	4:Z2:566:C:C6	2.46	0.50
4:Z2:2754:C:H2'	4:Z2:2755:C:C6	2.46	0.50
26:SP:3:ARG:HG2	26:SP:4:SER:H	1.76	0.50
4:Z2:2297:G:H1'	9:F7:155:THR:HG21	1.93	0.50
6:A4:25:THR:HG23	6:A4:44:HIS:NE2	2.27	0.50
28:GR:47:ASP:N	28:GR:47:ASP:OD1	2.44	0.50
30:CT:11:ARG:NH2	30:CT:175:LEU:O	2.39	0.50
4:Z2:624:U:H2'	4:Z2:625:C:C6	2.47	0.50
4:Z2:2540:G:H2'	4:Z2:2541:C:C6	2.47	0.50
9:F7:24:ASN:ND2	10:D8:55:A:C8	2.80	0.50
29:GS:50:VAL:HG13	29:GS:122:ALA:HB1	1.94	0.50
3:H:218:GLU:HG2	3:H:291:ARG:HH21	1.77	0.50
4:Z2:9:G:H2'	4:Z2:10:U:C6	2.47	0.50
4:Z2:566:C:H2'	4:Z2:567:A:C8	2.46	0.50
4:Z2:977:G:OP1	25:PO:50:ARG:NH1	2.36	0.50
8:L6:57:LEU:HD11	8:L6:63:VAL:HG22	1.92	0.50
4:Z2:244:G:H4'	4:Z2:369:G:C5	2.46	0.50
4:Z2:1392:U:H2'	4:Z2:1393:U:C6	2.46	0.50
4:Z2:1418:A:H2'	4:Z2:1419:G:O4'	2.12	0.50
4:Z2:2037:U:O2	4:Z2:2038:A:N6	2.42	0.50
10:D8:3:U:OP1	10:D8:59:A:O2'	2.28	0.50
24:MM:10:PRO:HB2	24:MM:13:LYS:HG3	1.94	0.50
27:BQ:10:MET:HG3	27:BQ:27:MET:SD	2.51	0.50
28:GR:128:GLN:HG3	28:GR:129:THR:HG23	1.94	0.50
29:GS:87:GLN:O	29:GS:149:ASN:ND2	2.45	0.50
1:B:169:LEU:HD13	1:B:175:GLY:HA3	1.92	0.50
4:Z2:741:A:H2'	4:Z2:742:G:O4'	2.12	0.50



A + a 1	At and 9	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
19:VH:75:PHE:HB2	19:VH:77:ARG:HD2	1.93	0.50
4:Z2:781:U:H2'	4:Z2:782:C:C6	2.47	0.49
28:GR:17:VAL:HG21	28:GR:50:VAL:HG21	1.94	0.49
28:GR:73:ASN:O	28:GR:77:ILE:HG22	2.12	0.49
4:Z2:561:U:H2'	4:Z2:562:G:C8	2.47	0.49
4:Z2:1513:A:H2'	4:Z2:1514:A:H8	1.76	0.49
4:Z2:2356:A:H2'	4:Z2:2357:C:C6	2.47	0.49
4:Z2:2452:A:H2'	4:Z2:2453:G:O4'	2.12	0.49
2:F:10:ARG:CG	2:F:11:LYS:H	2.25	0.49
5:R3:32:TYR:CG	5:R3:55:LEU:HD21	2.47	0.49
6:A4:58:ALA:HB1	6:A4:189:ILE:HD12	1.94	0.49
7:E5:120:LEU:HD13	7:E5:128:VAL:HG11	1.95	0.49
23:OL:11:ILE:O	23:OL:15:GLN:HG2	2.12	0.49
28:GR:17:VAL:HG12	28:GR:26:VAL:HG22	1.93	0.49
30:CT:53:SER:HB2	30:CT:114:ARG:HB3	1.94	0.49
53:V:54:U:H3	53:V:58:U:H5	1.60	0.49
4:Z2:379:G:H1'	15:WD:29:PHE:HB3	1.93	0.49
31:KU:56:ARG:HG3	31:KU:56:ARG:HH11	1.76	0.49
3:H:218:GLU:HB2	3:H:232:GLY:HA2	1.93	0.49
4:Z2:842:G:H2'	4:Z2:843:G:O4'	2.12	0.49
4:Z2:1479:A:H2'	4:Z2:1480:A:C8	2.47	0.49
4:Z2:2073:U:H2'	4:Z2:2074:A:C8	2.46	0.49
4:Z2:2823:G:N2	4:Z2:2826:A:OP2	2.32	0.49
36:QZ:17:ARG:HH11	36:QZ:64:LEU:HD13	1.78	0.49
3:H:341:THR:HB	3:H:366:ILE:HD13	1.95	0.49
4:Z2:709:C:H2'	4:Z2:710:G:C8	2.48	0.49
4:Z2:2081:A:H2'	4:Z2:2082:C:C6	2.47	0.49
4:Z2:2081:A:H2'	4:Z2:2082:C:H6	1.77	0.49
4:Z2:2814:G:N2	4:Z2:2833:U:O2	2.45	0.49
22:HK:64:CYS:HB2	22:HK:80:SER:HB3	1.94	0.49
24:MM:65:THR:OG1	24:MM:66:GLU:OE1	2.23	0.49
29:GS:70:VAL:HG21	29:GS:105:LEU:HD21	1.95	0.49
4:Z2:1776:C:H2'	4:Z2:1777:A:C5	2.47	0.49
4:Z2:2294:A:C2	9:F7:77:PHE:HB3	2.48	0.49
11:E9:193:LYS:O	11:E9:197:GLU:HG2	2.12	0.49
28:GR:62:MET:HA	28:GR:65:THR:HG22	1.94	0.49
4:Z2:695:G:H2'	4:Z2:696:C:C6	2.48	0.49
4:Z2:916:A:N1	4:Z2:1152:U:O2'	2.43	0.49
4:Z2:1286:A:OP2	4:Z2:1595:U:O2'	2.30	0.49
4:Z2:1706:U:H2'	4:Z2:1707:G:O4'	2.13	0.49
4:Z2:1869:U:H2'	4:Z2:1870:G:O4'	2.13	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
14:UC:13:ARG:O	14:UC:45:SER:OG	2.31	0.49
16:XE:42:GLU:HA	16:XE:45:VAL:HG12	1.95	0.49
4:Z2:1514:A:N6	4:Z2:1515:G:O2'	2.46	0.48
4:Z2:2000:A:H2'	4:Z2:2001:A:C8	2.47	0.48
24:MM:86:TYR:CE1	24:MM:90:ARG:HD3	2.48	0.48
27:BQ:43:GLU:OE1	27:BQ:116:ARG:NH2	2.32	0.48
3:H:266:LYS:HE2	3:H:266:LYS:HB2	1.59	0.48
4:Z2:732:U:O2	4:Z2:2000:A:H1'	2.13	0.48
4:Z2:1668:U:H2'	4:Z2:1669:G:O4'	2.13	0.48
27:BQ:11:LEU:HD22	27:BQ:77:ILE:HD11	1.93	0.48
2:F:25:SER:OG	2:F:60:ASP:OD1	2.31	0.48
2:F:47:ARG:HA	2:F:50:LEU:HD12	1.95	0.48
4:Z2:10:U:H2'	4:Z2:11:C:C6	2.48	0.48
4:Z2:262:A:N1	4:Z2:410:U:O2'	2.41	0.48
4:Z2:779:A:H2'	4:Z2:780:C:C6	2.49	0.48
7:E5:17:VAL:HG12	7:E5:122:VAL:HG23	1.95	0.48
9:F7:96:MET:HG3	9:F7:97:TYR:N	2.27	0.48
4:Z2:2457:U:HO2'	4:Z2:2458:C:P	2.35	0.48
4:Z2:2632:C:H2'	4:Z2:2633:U:C6	2.48	0.48
6:A4:112:LEU:HD22	6:A4:153:LEU:HD21	1.95	0.48
9:F7:29:PRO:HB3	9:F7:160:ALA:HB2	1.94	0.48
29:GS:137:LYS:N	29:GS:137:LYS:HD2	2.28	0.48
53:V:17:U:H3'	53:V:18:U:H5"	1.96	0.48
4:Z2:1431:C:H2'	4:Z2:1432:U:C6	2.49	0.48
4:Z2:2497:U:H2'	4:Z2:2498:C:C6	2.48	0.48
8:L6:71:GLY:O	8:L6:99:ARG:NH2	2.37	0.48
11:E9:170:ASP:OD1	11:E9:171:THR:N	2.45	0.48
22:HK:27:LEU:CD2	22:HK:48:LEU:HB2	2.42	0.48
4:Z2:625:C:H2'	4:Z2:626:U:C6	2.49	0.48
4:Z2:1558:A:H2'	4:Z2:1559:A:C8	2.48	0.48
4:Z2:1866:U:H2'	4:Z2:1867:C:C6	2.49	0.48
4:Z2:2274:U:OP1	4:Z2:2363:U:O2'	2.29	0.48
4:Z2:2620:U:H2'	4:Z2:2621:G:O4'	2.13	0.48
9:F7:36:LEU:HD22	9:F7:154:VAL:HG22	1.95	0.48
25:PO:74:LEU:HD23	25:PO:74:LEU:H	1.78	0.48
4:Z2:178:A:H2'	4:Z2:179:A:C8	2.48	0.48
4:Z2:205:C:H2'	4:Z2:206:C:C6	2.48	0.48
4:Z2:1427:C:H2'	4:Z2:1428:A:O4'	2.13	0.48
11:E9:97:ARG:O	11:E9:101:ARG:HG3	2.14	0.48
19:VH:70:ALA:HB3	19:VH:81:MET:HE1	1.96	0.48
1:B:26:GLU:HG2	4:Z2:1900:C:C4	2.49	0.48



Atom-1	Atom-2	Interatomic	Clash
	2100m 2	distance (Å)	overlap (Å)
2:F:104:ARG:NH1	2:F:105:ASP:O	2.44	0.48
4:Z2:834:A:H2'	4:Z2:835:C:C6	2.49	0.48
4:Z2:2435:C:H2'	4:Z2:2436:A:C8	2.49	0.48
11:E9:21:GLU:HG3	11:E9:22:PHE:H	1.79	0.48
11:E9:46:LYS:HB3	11:E9:50:GLU:HB2	1.95	0.48
19:VH:12:ASN:O	19:VH:12:ASN:ND2	2.43	0.48
4:Z2:943:A:H2'	4:Z2:944:A:C8	2.48	0.48
4:Z2:1378:U:H2'	4:Z2:1379:A:O4'	2.14	0.48
9:F7:66:VAL:HG22	10:D8:39:C:C5	2.49	0.48
30:CT:191:THR:HG21	30:CT:196:ILE:HD12	1.94	0.48
31:KU:121:CYS:O	32:NV:35:ARG:NH2	2.33	0.48
4:Z2:1672:A:H2'	4:Z2:1673:C:C6	2.49	0.48
4:Z2:2311:A:H2'	4:Z2:2312:A:H8	1.74	0.48
4:Z2:2853:C:H2'	4:Z2:2854:U:C6	2.49	0.48
6:A4:75:VAL:HB	6:A4:168:VAL:HG12	1.95	0.48
9:F7:135:GLN:HE22	9:F7:146:ILE:HD11	1.79	0.48
34:IX:98:GLU:HB3	34:IX:124:LEU:HG	1.95	0.48
4:Z2:134:C:H2'	4:Z2:135:C:C6	2.49	0.47
4:Z2:205:C:H2'	4:Z2:206:C:H6	1.79	0.47
4:Z2:1932:U:H2'	4:Z2:1933:C:C6	2.49	0.47
5:R3:26:VAL:O	5:R3:30:LYS:HG2	2.14	0.47
9:F7:135:GLN:HG2	9:F7:150:ARG:HB2	1.95	0.47
27:BQ:40:LEU:HB3	27:BQ:46:VAL:HG22	1.96	0.47
4:Z2:459:G:H4'	4:Z2:485:A:N1	2.29	0.47
11:E9:116:ARG:HG2	11:E9:183:ASP:O	2.14	0.47
16:XE:32:LYS:HB2	16:XE:37:LEU:HD23	1.96	0.47
25:PO:58:ARG:HA	25:PO:61:TRP:CE3	2.49	0.47
34:IX:55:VAL:HA	34:IX:123:LYS:O	2.14	0.47
35:JY:53:THR:HG23	35:JY:62:ARG:HA	1.97	0.47
4:Z2:1480:A:H2'	4:Z2:1482:C:C5	2.49	0.47
4:Z2:2216:U:H2'	4:Z2:2217:G:H8	1.77	0.47
9:F7:10:ASN:O	9:F7:14:GLN:NE2	2.48	0.47
9:F7:135:GLN:HE21	9:F7:150:ARG:H	1.62	0.47
17:RF:37:THR:HG23	17:RF:38:TYR:CD2	2.48	0.47
1:B:97:ASP:O	1:B:115:ARG:NH2	2.48	0.47
4:Z2:1764:U:H2'	4:Z2:1770:A:N6	2.29	0.47
30:CT:175:LEU:HD21	30:CT:201:TRP:CD1	2.49	0.47
4:Z2:833:U:H2'	4:Z2:834:A:H8	1.77	0.47
4:Z2:1064:C:H2'	4:Z2:1065:U:H6	1.79	0.47
15:WD:39:TRP:NE1	15:WD:41:GLU:HG2	2.29	0.47
35:JY:59:LYS:HE3	35:JY:62:ARG:HH22	1.80	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:H:303:PRO:HA	3:H:370:ALA:HA	1.96	0.47
4:Z2:140:U:H2'	4:Z2:141:A:C8	2.50	0.47
4:Z2:1338:A:H2'	4:Z2:1339:G:O4'	2.14	0.47
4:Z2:1552:C:H2'	4:Z2:1553:C:C6	2.49	0.47
6:A4:13:ASP:OD1	6:A4:14:LEU:N	2.47	0.47
1:B:17:VAL:HG21	1:B:48:LEU:HD11	1.97	0.47
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.78	0.47
1:B:213:VAL:HG11	1:B:239:LEU:HD22	1.95	0.47
4:Z2:346:A:H2'	4:Z2:347:C:C6	2.50	0.47
4:Z2:824:U:H2'	4:Z2:825:C:C6	2.49	0.47
4:Z2:1582:A:H2'	4:Z2:1583:C:O4'	2.15	0.47
4:Z2:2670:U:H2'	4:Z2:2671:G:O4'	2.15	0.47
26:SP:52:HIS:HB2	26:SP:57:HIS:CE1	2.50	0.47
27:BQ:75:GLU:OE1	27:BQ:98:LYS:NZ	2.36	0.47
1:B:10:GLU:CD	1:B:10:GLU:N	2.68	0.47
1:B:174:ASP:HB3	53:V:74:C:N4	2.29	0.47
4:Z2:633:G:H4'	4:Z2:2334:G:H5'	1.97	0.47
4:Z2:2530:A:H2'	4:Z2:2531:U:C6	2.50	0.47
31:KU:46:THR:O	31:KU:50:GLN:HG2	2.15	0.47
35:JY:28:THR:HG21	35:JY:90:LEU:HD22	1.96	0.47
4:Z2:728:U:O2'	4:Z2:1647:U:OP1	2.29	0.47
4:Z2:1255:G:N7	4:Z2:1309:U:H5	2.13	0.47
6:A4:230:LYS:O	6:A4:234:GLN:HG2	2.15	0.47
26:SP:44:MET:HB2	26:SP:47:LEU:HD21	1.97	0.47
27:BQ:7:VAL:O	27:BQ:11:LEU:HG	2.15	0.47
2:F:28:VAL:HG22	2:F:63:ILE:HB	1.97	0.47
4:Z2:1253:A:H2'	4:Z2:1254:C:C6	2.50	0.47
17:RF:14:ALA:O	17:RF:18:ARG:HG3	2.15	0.47
26:SP:12:ASP:OD2	26:SP:14:HIS:ND1	2.40	0.47
31:KU:64:GLN:HG2	31:KU:99:ALA:HB2	1.97	0.47
1:B:220:SER:HB3	4:Z2:2540:G:H4'	1.96	0.46
4:Z2:247:G:H2'	4:Z2:248:A:C8	2.50	0.46
4:Z2:295:G:H2'	4:Z2:296:G:C8	2.50	0.46
4:Z2:527:A:H2'	4:Z2:528:A:H8	1.80	0.46
4:Z2:1780:A:H2'	4:Z2:1781:C:H6	1.79	0.46
4:Z2:2283:A:H2'	4:Z2:2284:A:C8	2.50	0.46
4:Z2:2457:U:O2'	4:Z2:2458:C:OP1	2.30	0.46
4:Z2:2714:G:H2'	4:Z2:2715:G:C8	2.50	0.46
30:CT:60:PRO:HB3	35:JY:94:ALA:N	2.30	0.46
34:IX:19:ASP:OD1	34:IX:58:ASN:ND2	2.36	0.46
5:R3:73:ASN:C	5:R3:73:ASN:HD22	2.15	0.46



Atom-1	Atom-2	Interatomic	Clash
	7100m 2	distance (Å)	overlap (Å)
6:A4:46:ILE:HD11	6:A4:194:THR:HB	1.97	0.46
11:E9:144:ARG:HB3	11:E9:165:HIS:HB2	1.97	0.46
24:MM:34:LEU:HD12	24:MM:39:ILE:HB	1.97	0.46
28:GR:77:ILE:HA	28:GR:80:THR:HG22	1.97	0.46
4:Z2:644:G:O2'	11:E9:94:LYS:O	2.31	0.46
4:Z2:2628:U:H4'	4:Z2:2715:G:O2'	2.15	0.46
8:L6:67:ILE:HG22	8:L6:99:ARG:HH11	1.80	0.46
9:F7:162:THR:HB	9:F7:165:GLU:HG3	1.98	0.46
29:GS:66:VAL:O	29:GS:70:VAL:HG23	2.14	0.46
53:V:24:U:H2'	53:V:25:U:C6	2.50	0.46
1:B:239:LEU:HD12	1:B:253:GLY:HA3	1.97	0.46
1:B:246:ASN:O	1:B:250:ILE:HG12	2.16	0.46
4:Z2:1181:G:H2'	4:Z2:1182:U:H6	1.80	0.46
4:Z2:1671:U:H2'	4:Z2:1672:A:C8	2.51	0.46
4:Z2:1843:G:H1'	4:Z2:1871:A:H61	1.80	0.46
23:OL:16:ARG:HA	23:OL:16:ARG:HD2	1.61	0.46
4:Z2:402:U:H2'	4:Z2:403:C:C6	2.51	0.46
26:SP:14:HIS:O	26:SP:18:LYS:HG3	2.16	0.46
34:IX:120:LYS:O	34:IX:123:LYS:NZ	2.46	0.46
1:B:99:PRO:HD2	1:B:99:PRO:O	2.16	0.46
4:Z2:1012:A:H61	4:Z2:1109:G:H2'	1.80	0.46
6:A4:84:ILE:HD11	6:A4:212:ILE:HD11	1.98	0.46
6:A4:122:LEU:O	6:A4:125:GLN:HG3	2.16	0.46
8:L6:72:HIS:HB3	8:L6:99:ARG:NH1	2.31	0.46
24:MM:86:TYR:O	24:MM:90:ARG:HG2	2.15	0.46
27:BQ:88:HIS:CE1	27:BQ:126:GLU:HB2	2.51	0.46
4:Z2:1139:G:OP2	25:PO:58:ARG:NH1	2.48	0.46
4:Z2:1349:A:OP2	15:WD:2:SER:OG	2.33	0.46
8:L6:8:ILE:HD11	36:QZ:42:LYS:HB3	1.97	0.46
1:B:214:GLY:O	1:B:237:SER:HA	2.15	0.46
4:Z2:1602:A:C2	17:RF:93:ALA:HB2	2.51	0.46
4:Z2:2072:U:H2'	4:Z2:2073:U:C6	2.51	0.46
4:Z2:2274:U:H2'	4:Z2:2275:G:H8	1.78	0.46
14:UC:41:GLU:N	14:UC:41:GLU:OE1	2.48	0.46
17:RF:20:VAL:HG11	17:RF:44:ALA:HA	1.97	0.46
28:GR:84:GLU:HG3	28:GR:134:LYS:HZ3	1.81	0.46
4:Z2:140:U:H2'	4:Z2:141:A:H8	1.80	0.46
4:Z2:191:G:H2'	4:Z2:192:A:O4'	2.16	0.46
4:Z2:942:U:O2	4:Z2:942:U:H2'	2.15	0.46
4:Z2:2355:U:O2'	4:Z2:2356:A:OP1	2.30	0.46
4:Z2:2629:C:H2'	4:Z2:2630:U:O4'	2.15	0.46



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:D8:46:U:H2'	10:D8:47:C:C6	2.50	0.46
11:E9:1:MET:O	11:E9:12:GLU:HA	2.16	0.46
24:MM:88:GLY:O	24:MM:92:ARG:HG2	2.16	0.46
1:B:249:ARG:NH1	1:B:249:ARG:HG2	2.31	0.46
4:Z2:1163:U:H2'	4:Z2:1164:U:O4'	2.16	0.46
4:Z2:1300:A:H2'	4:Z2:1301:G:C8	2.51	0.46
6:A4:166:ILE:HG22	6:A4:168:VAL:HG13	1.98	0.46
53:V:25:U:H2'	53:V:26:U:O4'	2.16	0.46
4:Z2:448:G:H2'	4:Z2:449:A:C8	2.51	0.45
4:Z2:932:C:H2'	4:Z2:933:G:C8	2.51	0.45
4:Z2:1266:U:H2'	4:Z2:1267:G:O4'	2.17	0.45
6:A4:153:LEU:HD23	6:A4:156:ILE:HD11	1.98	0.45
4:Z2:272:U:H2'	4:Z2:273:G:H8	1.81	0.45
4:Z2:1468:C:H2'	4:Z2:1469:A:C8	2.51	0.45
4:Z2:1698:G:H4'	4:Z2:2824:C:O2	2.16	0.45
4:Z2:2287:G:H22	4:Z2:2295:U:H3	1.65	0.45
4:Z2:2654:G:H2'	4:Z2:2655:U:C6	2.51	0.45
26:SP:46:GLY:H	26:SP:62:VAL:HG23	1.80	0.45
28:GR:143:GLN:O	28:GR:147:LYS:HG2	2.17	0.45
30:CT:39:VAL:HG21	30:CT:95:MET:SD	2.56	0.45
31:KU:97:VAL:HB	32:NV:16:ILE:HD12	1.97	0.45
33:YW:9:LEU:HD21	33:YW:55:LYS:HG2	1.98	0.45
2:F:88:LEU:HD12	2:F:89:ASP:HB2	1.98	0.45
4:Z2:476:G:H2'	4:Z2:477:G:O4'	2.16	0.45
4:Z2:2800:G:H2'	4:Z2:2845:A:H61	1.81	0.45
28:GR:154:PRO:HD3	28:GR:162:ILE:O	2.15	0.45
35:JY:15:HIS:HB3	35:JY:70:HIS:CE1	2.52	0.45
53:V:31:U:H2'	53:V:32:U:H6	1.81	0.45
53:V:53:U:H2'	53:V:54:U:C6	2.51	0.45
4:Z2:1644:C:H2'	4:Z2:1645:U:H6	1.82	0.45
4:Z2:2200:U:H2'	4:Z2:2201:A:C8	2.51	0.45
7:E5:18:GLU:HG2	7:E5:44:VAL:HG12	1.96	0.45
10:D8:19:A:H2'	10:D8:20:U:C6	2.52	0.45
11:E9:96:ASN:HB2	11:E9:99:MET:HB2	1.97	0.45
4:Z2:564:G:O2'	4:Z2:2005:A:OP1	2.35	0.45
9:F7:4:LEU:HD23	9:F7:4:LEU:HA	1.78	0.45
11:E9:147:ILE:HB	11:E9:168:VAL:HG22	1.99	0.45
18:FG:20:GLY:HA2	18:FG:23:GLU:HG3	1.98	0.45
4:Z2:533:U:H2'	4:Z2:534:U:C6	2.52	0.45
4:Z2:2610:G:N2	4:Z2:2760:G:OP2	2.48	0.45
30:CT:190:GLU:OE1	30:CT:195:THR:OG1	2.33	0.45



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
33:YW:9:LEU:HD11	33:YW:55:LYS:NZ	2.32	0.45	
34:IX:8:PRO:O	34:IX:11:VAL:HG12	2.17	0.45	
4:Z2:188:A:H2'	4:Z2:189:G:N3	2.32	0.45	
4:Z2:199:U:H2'	4:Z2:200:C:O4'	2.17	0.45	
4:Z2:1707:G:HO2'	4:Z2:1725:A:N6	2.14	0.45	
4:Z2:2178:G:H2'	4:Z2:2179:G:C8	2.51	0.45	
8:L6:37:VAL:HG11	8:L6:72:HIS:HE1	1.81	0.45	
24:MM:68:ASP:OD1	24:MM:68:ASP:N	2.49	0.45	
4:Z2:1470:G:H2'	4:Z2:1471:U:H6	1.81	0.45	
4:Z2:1856:U:O2'	4:Z2:1857:A:OP1	2.32	0.45	
17:RF:55:ILE:HG23	17:RF:66:ILE:HG13	1.99	0.45	
22:HK:99:ALA:HB2	35:JY:66:GLU:HB3	1.98	0.45	
29:GS:109:ALA:O	29:GS:120:ARG:HD2	2.17	0.45	
29:GS:115:LYS:HD3	29:GS:115:LYS:HA	1.83	0.45	
30:CT:116:VAL:O	30:CT:120:ILE:HG13	2.17	0.45	
3:H:220:VAL:HG12	3:H:286:ARG:HG2	1.99	0.45	
4:Z2:341:C:H2'	4:Z2:342:G:C8	2.51	0.45	
4:Z2:525:U:H2'	4:Z2:526:C:C6	2.52	0.45	
4:Z2:672:C:H2'	4:Z2:673:U:O4'	2.17	0.45	
4:Z2:708:C:H2'	4:Z2:709:C:O4'	2.17	0.45	
29:GS:130:GLU:HB2	29:GS:132:LYS:NZ	2.31	0.45	
1:B:170:TYR:CE1	1:B:187:TYR:HB3	2.53	0.44	
4:Z2:374:A:H1'	4:Z2:394:G:O4'	2.16	0.44	
4:Z2:517:U:H2'	4:Z2:518:A:C8	2.52	0.44	
6:A4:102:LEU:HG	6:A4:105:MET:HE2	1.98	0.44	
9:F7:63:GLN:NE2	10:D8:41:C:H4'	2.32	0.44	
9:F7:67:VAL:HG11	9:F7:84:PRO:HB3	1.98	0.44	
30:CT:183:ASP:HB2	30:CT:204:ARG:NH2	2.32	0.44	
31:KU:82:ILE:O	31:KU:108:ASN:N	2.45	0.44	
2:F:42:SER:O	2:F:46:VAL:HG23	2.17	0.44	
4:Z2:59:A:H2'	4:Z2:60:A:C8	2.51	0.44	
4:Z2:817:U:H2'	4:Z2:818:A:C8	2.52	0.44	
4:Z2:1116:U:H5"	34:IX:84:ILE:HG12	1.97	0.44	
4:Z2:2196:A:H2'	4:Z2:2197:C:H6	1.79	0.44	
11:E9:150:LYS:HG3	11:E9:194:GLN:OE1	2.17	0.44	
15:WD:3:ARG:HG3	15:WD:33:LEU:HD12	1.99	0.44	
1:B:83:PHE:HE2	1:B:92:ILE:HD11	1.81	0.44	
1:B:239:LEU:HD21	1:B:250:ILE:HD13	1.99	0.44	
2:F:10:ARG:HA	2:F:10:ARG:HD3	1.88	0.44	
4:Z2:47:U:H2'	4:Z2:48:C:C6	2.52	0.44	
4:Z2:82:G:H22	4:Z2:117:A:H2	1.63	0.44	



Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:Z2:272:U:H2'	4:Z2:273:G:C8	2.52	0.44	
29:GS:130:GLU:HB2	29:GS:132:LYS:HZ2	1.82	0.44	
1:B:369:TYR:HB3	4:Z2:1079:A:C8	2.52	0.44	
4:Z2:221:U:O4	4:Z2:403:C:H5'	2.17	0.44	
4:Z2:1997:U:H2'	4:Z2:1998:G:O4'	2.18	0.44	
4:Z2:2265:G:H4'	4:Z2:2372:G:O2'	2.17	0.44	
4:Z2:2288:U:O2	9:F7:151:GLY:HA3	2.17	0.44	
26:SP:3:ARG:NH2	26:SP:10:PHE:HB2	2.32	0.44	
34:IX:99:ASP:O	34:IX:103:LYS:HB2	2.18	0.44	
4:Z2:609:C:O2'	4:Z2:642:U:OP1	2.30	0.44	
4:Z2:707:A:H2'	4:Z2:708:C:O4'	2.18	0.44	
4:Z2:1099:G:H2'	4:Z2:1100:G:H8	1.82	0.44	
4:Z2:1421:U:H2'	4:Z2:1422:U:C6	2.52	0.44	
4:Z2:1551:U:H2'	4:Z2:1552:C:C6	2.52	0.44	
6:A4:194:THR:HG23	6:A4:194:THR:O	2.16	0.44	
22:HK:27:LEU:HD22	22:HK:48:LEU:HB2	2.00	0.44	
26:SP:44:MET:O	26:SP:47:LEU:HG	2.17	0.44	
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.83	0.44	
4:Z2:624:U:H2'	4:Z2:625:C:H6	1.83	0.44	
4:Z2:721:C:H2'	4:Z2:722:C:C6	2.53	0.44	
4:Z2:2229:G:H2'	4:Z2:2230:A:C8	2.53	0.44	
7:E5:102:GLN:HE21	7:E5:129:LEU:HD12	1.82	0.44	
13:MB:35:LYS:HB2	13:MB:112:TYR:CE1	2.53	0.44	
19:VH:51:VAL:HG12	19:VH:82:VAL:HG23	2.00	0.44	
24:MM:72:GLU:O	24:MM:75:MET:HG3	2.17	0.44	
28:GR:147:LYS:HD2	28:GR:147:LYS:HA	1.83	0.44	
29:GS:63:PHE:HA	29:GS:66:VAL:HG12	1.99	0.44	
53:V:53:U:H2'	53:V:54:U:H6	1.82	0.44	
4:Z2:12:A:H2'	4:Z2:13:A:H8	1.80	0.44	
4:Z2:1276:G:H2'	4:Z2:1277:C:C6	2.53	0.44	
4:Z2:1416:G:H2'	4:Z2:1417:A:C8	2.52	0.44	
16:XE:39:ASN:OD1	16:XE:39:ASN:N	2.41	0.44	
17:RF:92:ARG:HB3	17:RF:92:ARG:CZ	2.48	0.44	
23:OL:13:GLN:HG2	23:OL:14:TYR:CD2	2.53	0.44	
30:CT:130:PHE:HB2	30:CT:153:LEU:HD12	1.99	0.44	
1:B:249:ARG:HH11	1:B:249:ARG:CG	2.31	0.44	
4:Z2:91:A:C2	4:Z2:109:A:C5	3.06	0.44	
4:Z2:194:A:H4'	4:Z2:2055:G:OP2	2.18	0.44	
4:Z2:465:A:H1'	4:Z2:481:G:N2	2.33	0.44	
4:Z2:516:G:H2'	4:Z2:517:U:C6	2.53	0.44	
4:Z2:583:U:H2'	4:Z2:584:A:H8	1.82	0.44	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
4:Z2:849:G:H2'	4:Z2:850:C:C6	2.53	0.44	
4:Z2:1593:C:H2'	4:Z2:1594:C:O4'	2.17	0.44	
4:Z2:2450:C:H2'	4:Z2:2451:A:O4'	2.17	0.44	
34:IX:93:ILE:HG12	34:IX:100:VAL:HG21	2.00	0.44	
4:Z2:157:C:H2'	4:Z2:158:U:H6	1.83	0.44	
4:Z2:221:U:O4	4:Z2:402:U:O2'	2.34	0.44	
4:Z2:1447:A:H2'	4:Z2:1448:G:H8	1.82	0.44	
13:MB:37:THR:CG2	13:MB:39:PRO:HD2	2.48	0.44	
35:JY:42:LEU:HD12	35:JY:71:LYS:HE2	2.00	0.44	
1:B:239:LEU:HD11	1:B:250:ILE:HA	1.99	0.43	
4:Z2:204:A:H2'	4:Z2:205:C:O4'	2.18	0.43	
4:Z2:2681:U:H2'	4:Z2:2682:C:C6	2.53	0.43	
6:A4:144:ARG:HA	6:A4:147:GLN:HG3	2.00	0.43	
9:F7:121:ALA:HB3	9:F7:128:TYR:CE1	2.53	0.43	
30:CT:59:ARG:HA	30:CT:64:ALA:HA	1.99	0.43	
4:Z2:555:G:H2'	4:Z2:2016:A:N7	2.33	0.43	
4:Z2:1914:A:H2'	4:Z2:1915:G:O4'	2.19	0.43	
4:Z2:2537:U:H2'	4:Z2:2538:U:H6	1.82	0.43	
4:Z2:2786:A:O2'	4:Z2:2787:A:OP1	2.35	0.43	
11:E9:4:LYS:HA	11:E9:4:LYS:HD3	1.74	0.43	
24:MM:30:ALA:O	24:MM:34:LEU:HD23	2.18	0.43	
24:MM:39:ILE:HD12	24:MM:56:ILE:HD11	1.99	0.43	
29:GS:15:ASP:OD2	29:GS:18:PHE:HB2	2.18	0.43	
29:GS:104:TRP:HA	29:GS:107:GLU:HG2	2.00	0.43	
30:CT:73:PRO:HG3	30:CT:105:GLU:HG3	1.99	0.43	
3:H:250:ILE:H	3:H:250:ILE:HG12	1.28	0.43	
4:Z2:173:A:O2'	4:Z2:174:A:H5'	2.18	0.43	
4:Z2:1162:U:C4	4:Z2:1163:U:N3	2.85	0.43	
4:Z2:1280:G:OP1	4:Z2:2692:G:O2'	2.27	0.43	
4:Z2:1394:U:H2'	4:Z2:1395:A:C8	2.53	0.43	
4:Z2:1629:A:H2'	4:Z2:1630:G:O4'	2.17	0.43	
4:Z2:2360:A:H2'	4:Z2:2361:A:C8	2.52	0.43	
4:Z2:2598:U:H2'	4:Z2:2599:C:H6	1.83	0.43	
22:HK:6:MET:HG2	22:HK:63:ARG:NH2	2.34	0.43	
22:HK:45:MET:O	22:HK:49:GLN:HG3	2.17	0.43	
30:CT:38:GLN:HA	30:CT:41:GLU:OE1	2.18	0.43	
4:Z2:769:G:H5'	4:Z2:770:G:OP1	2.17	0.43	
4:Z2:1183:U:H1'	25:PO:4:VAL:HG22	2.00	0.43	
4:Z2:1312:A:H2'	4:Z2:1314:C:C4	2.54	0.43	
4:Z2:1842:U:H2'	4:Z2:1843:G:O4'	2.18	0.43	
4:Z2:2207:G:H4'	4:Z2:2209:C:C2	2.54	0.43	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:Z2:2230:A:H2'	4:Z2:2231:C:H6	1.84	0.43
4:Z2:2731:A:H5"	28:GR:4:VAL:HG21	1.99	0.43
13:MB:106:ASP:N	13:MB:106:ASP:OD1	2.51	0.43
24:MM:37:VAL:HG11	24:MM:56:ILE:HG13	2.00	0.43
28:GR:46:GLU:HB2	28:GR:49:VAL:HG12	2.00	0.43
4:Z2:482:U:H2'	4:Z2:483:G:O4'	2.18	0.43
4:Z2:656:C:H2'	4:Z2:657:C:C6	2.53	0.43
4:Z2:799:C:H2'	4:Z2:800:C:C6	2.52	0.43
4:Z2:898:U:H1'	4:Z2:899:C:H5	1.83	0.43
4:Z2:1138:C:H2'	4:Z2:1139:G:O4'	2.18	0.43
4:Z2:1161:U:H4'	4:Z2:1162:U:H5'	2.01	0.43
4:Z2:1226:U:H2'	4:Z2:1227:C:C6	2.53	0.43
4:Z2:1384:A:H2'	4:Z2:1385:A:C8	2.54	0.43
4:Z2:1425:G:H2'	4:Z2:1426:U:C6	2.53	0.43
4:Z2:2391:U:H2'	4:Z2:2392:G:C8	2.53	0.43
6:A4:47:ASN:HD22	6:A4:50:HIS:CE1	2.37	0.43
7:E5:77:ILE:HG12	7:E5:146:PHE:CZ	2.54	0.43
17:RF:86:LEU:HD23	17:RF:88:ARG:HD3	2.00	0.43
23:OL:35:ILE:O	23:OL:39:GLN:HG2	2.18	0.43
24:MM:11:ASP:HA	24:MM:45:VAL:HG12	2.01	0.43
29:GS:26:PHE:HZ	29:GS:121:LEU:HD11	1.83	0.43
1:B:2:LYS:HB2	1:B:2:LYS:HE2	1.75	0.43
4:Z2:341:C:H2'	4:Z2:342:G:H8	1.82	0.43
4:Z2:627:U:O2'	4:Z2:629:A:N7	2.45	0.43
4:Z2:2082:C:H2'	4:Z2:2083:U:H6	1.84	0.43
4:Z2:2213:G:H5"	15:WD:30:LEU:HD12	2.01	0.43
4:Z2:2574:C:H2'	4:Z2:2575:G:H8	1.84	0.43
4:Z2:2815:G:C6	4:Z2:2833:U:C2	3.06	0.43
9:F7:31:ILE:HA	9:F7:158:THR:HA	2.01	0.43
15:WD:59:ILE:HD12	15:WD:64:ILE:HD13	1.99	0.43
27:BQ:2:SER:OG	27:BQ:3:MET:N	2.48	0.43
30:CT:178:LEU:HD12	30:CT:178:LEU:HA	1.86	0.43
4:Z2:2812:G:H2'	4:Z2:2813:U:C6	2.53	0.43
11:E9:144:ARG:CB	11:E9:165:HIS:HB2	2.48	0.43
18:FG:9:LEU:O	18:FG:85:ILE:N	2.51	0.43
26:SP:3:ARG:HH11	26:SP:7:LYS:HB3	1.83	0.43
29:GS:80:ARG:HD2	29:GS:83:GLY:H	1.84	0.43
2:F:65:VAL:HG11	2:F:77:ILE:HD11	2.00	0.43
3:H:306:LYS:NZ	3:H:364:GLU:OE2	2.32	0.43
4:Z2:1072:A:N3	4:Z2:1072:A:H2'	2.34	0.43
4:Z2:1312:A:H2'	4:Z2:1314:C:C5	2.54	0.43



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
6:A4:125:GLN:HE22	6:A4:131:PHE:HE1	1.67	0.43	
8:L6:44:LYS:HE2	8:L6:44:LYS:HB2	1.61	0.43	
10:D8:66:C:H2'	10:D8:67:G:O4'	2.18	0.43	
10:D8:109:G:H2'	10:D8:110:U:C6	2.53	0.43	
28:GR:170:ILE:H	28:GR:170:ILE:HD12	1.82	0.43	
30:CT:139:GLN:HB3	30:CT:143:ARG:HH21	1.84	0.43	
1:B:53:ASP:OD1	1:B:53:ASP:N	2.50	0.43	
3:H:336:ARG:HE	3:H:336:ARG:HB2	1.50	0.43	
4:Z2:91:A:P	20:TI:5:ARG:HD2	2.59	0.43	
4:Z2:574:U:H2'	4:Z2:575:A:C8	2.54	0.43	
4:Z2:745:G:H2'	4:Z2:746:A:O4'	2.19	0.43	
4:Z2:1389:U:H2'	4:Z2:1390:U:C6	2.53	0.43	
4:Z2:1567:A:H2'	4:Z2:1568:A:C8	2.54	0.43	
14:UC:38:GLY:O	14:UC:99:ARG:NH1	2.52	0.43	
20:TI:90:LYS:HE2	20:TI:92:GLN:HB3	2.00	0.43	
31:KU:19:GLY:O	31:KU:82:ILE:HA	2.19	0.43	
33:YW:15:ARG:HG3	33:YW:53:LEU:HD11	2.00	0.43	
4:Z2:856:U:H2'	4:Z2:857:U:C6	2.54	0.43	
9:F7:90:THR:HG23	10:D8:41:C:H1'	2.01	0.43	
15:WD:10:LYS:HE3	15:WD:54:LYS:HD2	2.01	0.43	
20:TI:39:ILE:HG12	20:TI:60:GLU:HG3	2.01	0.43	
22:HK:23:LYS:HB2	22:HK:23:LYS:HE3	1.86	0.43	
53:V:66:U:H2'	53:V:67:U:C6	2.53	0.43	
4:Z2:1271:A:O2'	4:Z2:1272:G:H5'	2.19	0.42	
4:Z2:2014:U:H2'	4:Z2:2015:G:C8	2.54	0.42	
11:E9:110:GLU:O	11:E9:114:GLN:HG3	2.19	0.42	
20:TI:79:ASP:OD2	20:TI:95:TYR:HB3	2.19	0.42	
20:TI:92:GLN:HE21	20:TI:101:VAL:HG22	1.82	0.42	
4:Z2:567:A:H2'	4:Z2:568:G:C8	2.55	0.42	
4:Z2:2754:C:H2'	4:Z2:2755:C:H6	1.84	0.42	
18:FG:25:TYR:HH	18:FG:81:ASN:ND2	2.16	0.42	
30:CT:46:LYS:HE2	30:CT:46:LYS:HB2	1.69	0.42	
1:B:167:ASN:OD1	19:VH:3:HIS:HA	2.19	0.42	
4:Z2:720:A:H3'	4:Z2:721:C:H6	1.84	0.42	
4:Z2:1074:A:C2	4:Z2:1086:C:H1'	2.53	0.42	
4:Z2:1391:G:H2'	4:Z2:1392:U:C6	2.54	0.42	
4:Z2:2288:U:H2'	4:Z2:2289:C:C6	2.54	0.42	
9:F7:93:GLY:N	9:F7:96:MET:HG2	2.34	0.42	
13:MB:37:THR:HG22	13:MB:40:LYS:H	1.84	0.42	
22:HK:28:LYS:HA	22:HK:31:ILE:HG12	2.02	0.42	
1:B:220:SER:HB3	4:Z2:2540:G:O3'	2.19	0.42	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:287:GLN:HE22	1:B:319:THR:HA	1.83	0.42	
1:B:314:ASP:OD1	1:B:319:THR:OG1	2.31	0.42	
4:Z2:629:A:H2'	4:Z2:631:A:N7	2.34	0.42	
4:Z2:2813:U:H2'	4:Z2:2814:G:O4'	2.19	0.42	
7:E5:161:LYS:HG2	27:BQ:73:VAL:HG22	2.00	0.42	
9:F7:5:LYS:HB2	9:F7:97:TYR:CD2	2.54	0.42	
9:F7:54:VAL:HG22	9:F7:87:CYS:SG	2.59	0.42	
53:V:11:U:H2'	53:V:12:U:C6	2.55	0.42	
4:Z2:286:A:N3	4:Z2:306:C:O2'	2.48	0.42	
4:Z2:678:A:H2'	4:Z2:679:U:C6	2.54	0.42	
4:Z2:895:A:H2'	4:Z2:896:A:C8	2.55	0.42	
4:Z2:2197:C:H2'	4:Z2:2198:A:O4'	2.20	0.42	
6:A4:157:LYS:HG3	6:A4:158:ASP:OD2	2.20	0.42	
24:MM:66:GLU:HG2	24:MM:67:GLY:N	2.35	0.42	
27:BQ:9:ASP:O	27:BQ:13:ARG:HG3	2.19	0.42	
32:NV:34:LYS:N	32:NV:34:LYS:HD2	2.33	0.42	
34:IX:141:ASP:N	34:IX:141:ASP:OD1	2.38	0.42	
36:QZ:64:LEU:HD12	36:QZ:64:LEU:HA	1.92	0.42	
1:B:203:TRP:CH2	1:B:207:LYS:HD3	2.55	0.42	
4:Z2:9:G:O2'	4:Z2:10:U:OP1	2.34	0.42	
4:Z2:355:G:OP2	15:WD:62:LEU:HD21	2.20	0.42	
4:Z2:847:G:H2'	4:Z2:848:A:O4'	2.19	0.42	
4:Z2:1273:C:H2'	4:Z2:1274:U:C6	2.54	0.42	
4:Z2:1299:C:H2'	4:Z2:1300:A:H8	1.85	0.42	
4:Z2:2082:C:H2'	4:Z2:2083:U:C6	2.55	0.42	
6:A4:105:MET:HA	6:A4:112:LEU:HD12	2.01	0.42	
26:SP:65:GLN:OE1	26:SP:65:GLN:N	2.47	0.42	
28:GR:160:LYS:HB3	28:GR:160:LYS:HE2	1.87	0.42	
4:Z2:36:U:H2'	4:Z2:37:G:C8	2.54	0.42	
4:Z2:558:U:O2'	4:Z2:560:A:OP1	2.20	0.42	
4:Z2:658:C:OP1	11:E9:48:ARG:HD2	2.19	0.42	
4:Z2:1003:U:OP1	4:Z2:1019:U:O2'	2.23	0.42	
4:Z2:1299:C:H2'	4:Z2:1300:A:C8	2.54	0.42	
4:Z2:1824:C:N4	4:Z2:1884:U:H2'	2.35	0.42	
4:Z2:2637:A:N1	4:Z2:2648:A:H5"	2.35	0.42	
27:BQ:39:LEU:HD23	27:BQ:105:ILE:HG12	2.02	0.42	
1:B:263:THR:HG23	1:B:356:MET:HE2	2.01	0.42	
1:B:301:LEU:HD12	1:B:364:ALA:O	2.20	0.42	
3:H:324:PRO:HB3	3:H:354:MET:HA	2.02	0.42	
4:Z2:554:U:H5"	4:Z2:806:A:C2	2.54	0.42	
4:Z2:629:A:H2'	4:Z2:631:A:C8	2.54	0.42	



Atom-1	Atom-2 Interatomic		Clash	
		distance (A)	overlap (A)	
4:Z2:833:U:H2 ⁷	4:Z2:834:A:C8	2.54	0.42	
4:Z2:895:A:N3	4:Z2:2247:C:O2	2.50	0.42	
4:Z2:1232:G:C2	25:PO:3:ARG:HD2	2.55	0.42	
4:Z2:1417:A:H2'	4:Z2:1418:A:H8	1.78	0.42	
4:Z2:2296:C:H5"	9:F7:88:LYS:HD2	2.01	0.42	
4:Z2:2791:U:H2'	4:Z2:2792:A:O4'	2.19	0.42	
4:Z2:2863:U:H2'	4:Z2:2864:U:C6	2.55	0.42	
6:A4:74:PHE:HB3	6:A4:85:ILE:HG23	2.01	0.42	
9:F7:7:LEU:HG	9:F7:12:LEU:HD13	2.01	0.42	
14:UC:81:LYS:HG3	14:UC:98:GLN:HB2	2.01	0.42	
17:RF:13:SER:HB2	17:RF:16:LYS:HG3	2.02	0.42	
1:B:263:THR:HG23	1:B:356:MET:CE	2.50	0.42	
4:Z2:134:C:H2'	4:Z2:135:C:H6	1.83	0.42	
4:Z2:1653:A:H2'	4:Z2:1654:G:O4'	2.20	0.42	
4:Z2:2312:A:H2'	4:Z2:2313:G:C8	2.54	0.42	
5:R3:25:ASP:CG	18:FG:101:GLN:HE21	2.21	0.42	
11:E9:121:GLU:O	11:E9:122:GLU:HG2	2.20	0.42	
26:SP:40:ILE:HG22	26:SP:67:VAL:HA	2.01	0.42	
3:H:241:VAL:HG22	3:H:260:GLY:HA2	2.01	0.42	
4:Z2:720:A:H3'	4:Z2:721:C:C6	2.55	0.42	
4:Z2:761:G:O2'	4:Z2:2224:A:OP2	2.25	0.42	
4:Z2:1031:G:O2'	4:Z2:1094:G:N2	2.53	0.42	
4:Z2:1044:U:C2	4:Z2:1046:G:H5'	2.55	0.42	
4:Z2:1052:G:N2	4:Z2:1079:A:O2'	2.52	0.42	
4:Z2:1664:A:H2'	4:Z2:1665:A:O4'	2.19	0.42	
4:Z2:2348:G:H4'	19:VH:60:PHE:CZ	2.55	0.42	
6:A4:167:PHE:HD1	6:A4:189:ILE:HG12	1.85	0.42	
29:GS:103:ARG:O	29:GS:107:GLU:HG2	2.20	0.42	
29:GS:114:GLU:O	29:GS:120:ARG:NH1	2.53	0.42	
31:KU:68:GLU:HG2	31:KU:103:LEU:HD12	2.01	0.42	
53:V:64:U:H2'	53:V:65:U:C6	2.54	0.42	
4:Z2:302:U:H2'	4:Z2:303:G:O4'	2.20	0.41	
4:Z2:1064:C:H2'	4:Z2:1065:U:C6	2.55	0.41	
4:Z2:1616:G:H2'	4:Z2:1617:U:C6	2.55	0.41	
4:Z2:2196:A:HO2'	4:Z2:2197:C:P	2.42	0.41	
53:V:18:U:O4	53:V:55:U:H1'	2.20	0.41	
3:H:310:GLU:HG3	3:H:310:GLU:O	2.20	0.41	
4:Z2:24:G:H2'	4:Z2:25:C:C6	2.54	0.41	
4:Z2:71:G:H2'	4:Z2:72:C:H6	1.84	0.41	
4:Z2:1125:U:H4'	4:Z2:1127:A:O4'	2.20	0.41	
4:Z2:1401:C:O2'	4:Z2:1575:G:O2'	2.36	0.41	
5:R3:25:ASP:CG 11:E9:121:GLU:O 26:SP:40:ILE:HG22 3:H:241:VAL:HG22 4:Z2:720:A:H3' 4:Z2:761:G:O2' 4:Z2:1031:G:O2' 4:Z2:1031:G:O2' 4:Z2:1052:G:N2 4:Z2:1064:A:H2' 4:Z2:348:G:H4' 6:A4:167:PHE:HD1 29:GS:103:ARG:O 29:GS:114:GLU:O 31:KU:68:GLU:HG2 53:V:64:U:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:1064:C:H2' 4:Z2:106:G:H2' 4:Z2:106:G:H2' 4:Z2:106:G:H2' 4:Z2:10:G:H2' 4:Z2:1125:U:H4' 4:Z2:1125:U:H4' 4:Z2:1401:C:O2'	18:FG:101:GLN:HE21 11:E9:122:GLU:HG2 26:SP:67:VAL:HA 3:H:260:GLY:HA2 4:Z2:721:C:C6 4:Z2:1094:G:N2 4:Z2:1094:G:N2 4:Z2:1079:A:O2' 4:Z2:1065:A:O4' 19:VH:60:PHE:CZ 6:A4:189:ILE:HG12 29:GS:107:GLU:HG2 29:GS:107:GLU:HG2 29:GS:107:GLU:HG2 29:GS:107:GLU:HD12 53:V:65:U:C6 4:Z2:1065:U:C6 4:Z2:1617:U:C6 4:Z2:1617:U:C6 4:Z2:1617:U:C6 4:Z2:25:C:C6 4:Z2:127:C:H6 4:Z2:1127:A:O4' 4:Z2:1575:G:O2'	$\begin{array}{c} 2.21 \\ 2.20 \\ 2.01 \\ 2.01 \\ 2.55 \\ 2.25 \\ 2.53 \\ 2.55 \\ 2.52 \\ 2.52 \\ 2.19 \\ 2.55 \\ 1.85 \\ 2.20 \\ 2.53 \\ 2.01 \\ 2.53 \\ 2.01 \\ 2.54 \\ 2.20 \\ 2.55 \\ 2.55 \\ 2.55 \\ 2.42 \\ 2.20 \\ 2.55 \\ 2.42 \\ 2.20 \\ 2.54 \\ 1.84 \\ 2.20 \\ 2.36 \end{array}$	$\begin{array}{c} 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.42 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.41 \\ 0.$	



Atom 1	Atom 1 Atom 2		Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:Z2:1630:G:H2'	4:Z2:1631:G:O4'	2.20	0.41	
4:Z2:1669:G:N3	4:Z2:1748:A:H2'	2.35	0.41	
4:Z2:2056:A:H2'	4:Z2:2057:A:O4'	2.19	0.41	
4:Z2:2804:G:H2'	4:Z2:2805:G:O4'	2.20	0.41	
9:F7:36:LEU:HD12	9:F7:61:ALA:HB2	2.02	0.41	
15:WD:8:THR:HG21	15:WD:54:LYS:HD3	2.01	0.41	
25:PO:74:LEU:H	25:PO:74:LEU:CD2	2.33	0.41	
34:IX:110:PRO:HG2	34:IX:118:MET:HE2	2.01	0.41	
34:IX:125:TYR:OH	34:IX:132:HIS:NE2	2.33	0.41	
3:H:267:LEU:HD12	3:H:267:LEU:HA	1.88	0.41	
4:Z2:289:A:H2'	4:Z2:290:G:H8	1.85	0.41	
4:Z2:1708:A:N6	4:Z2:1724:G:O2'	2.48	0.41	
4:Z2:2390:A:H2'	4:Z2:2391:U:C6	2.56	0.41	
6:A4:76:GLY:O	6:A4:98:ASP:HA	2.20	0.41	
22:HK:69:ARG:NH2	22:HK:71:HIS:O	2.53	0.41	
35:JY:8:ILE:HB	35:JY:74:VAL:HG22	2.02	0.41	
36:QZ:71:ARG:HG3	36:QZ:71:ARG:NH1	2.31	0.41	
3:H:307:PHE:CZ	3:H:335:PHE:HZ	2.39	0.41	
4:Z2:273:G:H2'	4:Z2:274:C:C6	2.55	0.41	
4:Z2:521:A:H2'	4:Z2:522:G:O4'	2.19	0.41	
4:Z2:564:G:H2'	4:Z2:565:U:C6	2.55	0.41	
4:Z2:1381:U:OP2	4:Z2:1382:C:N4	2.45	0.41	
4:Z2:1414:G:H2'	4:Z2:1415:A:O4'	2.20	0.41	
7:E5:165:SER:HB3	7:E5:168:GLU:HG3	2.02	0.41	
10:D8:109:G:H2'	10:D8:110:U:H6	1.84	0.41	
13:MB:103:ARG:HD2	13:MB:106:ASP:OD1	2.19	0.41	
26:SP:48:THR:OG1	26:SP:61:ILE:HG22	2.21	0.41	
29:GS:67:LEU:HD12	29:GS:67:LEU:HA	1.84	0.41	
2:F:114:LEU:HD21	35:JY:62:ARG:NE	2.35	0.41	
4:Z2:90:G:OP1	20:TI:91:LYS:NZ	2.39	0.41	
4:Z2:2229:G:H2'	4:Z2:2230:A:H8	1.86	0.41	
8:L6:33:VAL:HG12	8:L6:79:VAL:HG22	2.03	0.41	
9:F7:54:VAL:HG13	9:F7:65:PRO:HG2	2.02	0.41	
22:HK:16:GLU:OE1	22:HK:54:ASN:HB2	2.20	0.41	
30:CT:157:LEU:HD12	30:CT:164:ARG:HG2	2.02	0.41	
4:Z2:46:G:H2'	4:Z2:47:U:H6	1.85	0.41	
4:Z2:241:A:H2'	4:Z2:242:G:O4'	2.21	0.41	
4:Z2:562:G:H2'	4:Z2:563:G:C8	2.55	0.41	
4:Z2:2608:G:H2'	4:Z2:2609:C:O4'	2.21	0.41	
4:Z2:2683:A:H2'	4:Z2:2684:C:H6	1.83	0.41	
4:Z2:2717:U:H4'	4:Z2:2718:G:H5"	2.02	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
6:A4:58:ALA:HB1	6:A4:189:ILE:CD1	2.51	0.41	
8:L6:4:THR:OG1	27:BQ:82:ARG:NH2	2.52	0.41	
11:E9:5:THR:HG23	11:E9:8:GLY:H	1.86	0.41	
22:HK:27:LEU:O	22:HK:31:ILE:HG23	2.21	0.41	
24:MM:45:VAL:O	24:MM:48:LEU:HB2	2.20	0.41	
28:GR:154:PRO:HA	28:GR:160:LYS:O	2.21	0.41	
35:JY:49:PHE:HE2	35:JY:67:ILE:HG22	1.85	0.41	
1:B:217:ARG:NH2	4:Z2:2538:U:O4	2.46	0.41	
4:Z2:533:U:O2'	4:Z2:534:U:O4'	2.37	0.41	
4:Z2:2347:C:H2'	4:Z2:2348:G:O4'	2.21	0.41	
4:Z2:2785:G:H2'	4:Z2:2787:A:N7	2.35	0.41	
17:RF:13:SER:O	17:RF:17:VAL:HG23	2.21	0.41	
31:KU:56:ARG:HG3	31:KU:56:ARG:NH1	2.34	0.41	
32:NV:44:VAL:HG13	32:NV:47:ARG:HH21	1.85	0.41	
36:QZ:70:THR:OG1	36:QZ:71:ARG:N	2.54	0.41	
54:Y:16:U:H2'	54:Y:17:U:O4'	2.21	0.41	
1:B:39:ASN:O	1:B:43:ILE:HG22	2.19	0.41	
2:F:61:LEU:HB3	2:F:63:ILE:HD11	2.03	0.41	
4:Z2:307:G:H4'	4:Z2:309:A:C8	2.55	0.41	
4:Z2:566:C:H2'	4:Z2:567:A:H8	1.86	0.41	
4:Z2:834:A:H2'	4:Z2:835:C:H6	1.86	0.41	
4:Z2:1156:A:N3	4:Z2:1156:A:H2'	2.35	0.41	
4:Z2:1510:A:H8	4:Z2:1510:A:OP2	2.03	0.41	
4:Z2:2633:U:H2'	4:Z2:2634:C:H6	1.83	0.41	
4:Z2:2730:G:O6	4:Z2:2738:C:H5"	2.21	0.41	
23:OL:42:PHE:CE2	23:OL:55:LEU:HD22	2.56	0.41	
32:NV:39:GLU:CD	32:NV:44:VAL:HG22	2.41	0.41	
53:V:52:U:C4	53:V:53:U:C5	3.09	0.41	
1:B:132:LYS:HG3	1:B:164:ILE:O	2.21	0.41	
4:Z2:13:A:H4'	34:IX:131:PRO:O	2.21	0.41	
4:Z2:63:A:H2'	4:Z2:64:C:O4'	2.21	0.41	
4:Z2:176:C:H2'	4:Z2:177:G:O4'	2.21	0.41	
4:Z2:189:G:O2'	4:Z2:662:A:N1	2.48	0.41	
4:Z2:224:A:C2	4:Z2:2390:A:H1'	2.55	0.41	
4:Z2:259:A:H2'	4:Z2:260:G:O4'	2.21	0.41	
4:Z2:674:A:H2'	4:Z2:675:U:C6	2.56	0.41	
4:Z2:957:A:H5'	4:Z2:1172:U:H1'	2.01	0.41	
4:Z2:1224:U:O2'	4:Z2:1225:A:O5'	2.34	0.41	
4:Z2:1299:C:O2'	4:Z2:1376:A:N3	2.47	0.41	
4:Z2:1335:C:H2'	4:Z2:1336:U:O4'	2.21	0.41	
4:Z2:1580:A:HO2'	4:Z2:1581:A:P	2.39	0.41	



A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
4:Z2:1670:G:H2'	4:Z2:1671:U:C6	2.56	0.41	
4:Z2:1772:A:H1'	4:Z2:1924:A:N6	2.36	0.41	
4:Z2:2644:G:H2'	4:Z2:2645:A:C8	2.55	0.41	
4:Z2:2825:G:H2'	4:Z2:2826:A:C8	2.56	0.41	
4:Z2:2864:U:H2'	4:Z2:2865:G:C8	2.56	0.41	
9:F7:120:LYS:HB2	9:F7:120:LYS:HE2	1.73	0.41	
9:F7:134:GLU:O	9:F7:137:VAL:HG13	2.21	0.41	
14:UC:36:ILE:O	14:UC:43:PRO:HA	2.21	0.41	
24:MM:27:ARG:HE	24:MM:27:ARG:HB2	1.59	0.41	
28:GR:77:ILE:HG23	28:GR:83:PHE:CZ	2.55	0.41	
29:GS:71:ARG:NH1	29:GS:98:THR:HG22	2.36	0.41	
32:NV:2:PRO:HG2	32:NV:28:VAL:HG21	2.03	0.41	
4:Z2:396:C:H2'	4:Z2:397:C:C6	2.56	0.41	
4:Z2:1717:U:H4'	4:Z2:1718:C:OP2	2.21	0.41	
4:Z2:2058:C:H2'	4:Z2:2059:C:H6	1.86	0.41	
4:Z2:2586:G:H2'	4:Z2:2587:U:O4'	2.21	0.41	
11:E9:2:ASP:OD1	11:E9:2:ASP:N	2.46	0.41	
14:UC:33:PRO:HB2	14:UC:94:HIS:HD2	1.86	0.41	
17:RF:74:ILE:HG13	17:RF:105:ILE:HG12	2.03	0.41	
29:GS:108:ALA:HB1	29:GS:134:ASN:HB2	2.02	0.41	
30:CT:28:GLN:O	30:CT:31:GLU:HG2	2.21	0.41	
30:CT:79:LYS:HB3	30:CT:79:LYS:HE2	1.89	0.41	
4:Z2:814:A:N7	4:Z2:2230:A:O2'	2.47	0.40	
4:Z2:1635:U:P	4:Z2:1635:U:H3'	2.61	0.40	
4:Z2:1985:G:H5"	4:Z2:2706:C:O2'	2.21	0.40	
20:TI:98:ASN:HB2	20:TI:100:GLU:OE1	2.20	0.40	
25:PO:22:LYS:HB3	25:PO:22:LYS:HE2	1.85	0.40	
28:GR:109:TYR:C	28:GR:111:HIS:H	2.24	0.40	
29:GS:15:ASP:HB2	29:GS:44:TYR:OH	2.22	0.40	
1:B:9:ARG:HB2	1:B:10:GLU:OE1	2.22	0.40	
4:Z2:971:C:H2'	4:Z2:972:A:O4'	2.21	0.40	
10:D8:38:U:N3	10:D8:42:G:OP2	2.44	0.40	
17:RF:17:VAL:HG21	17:RF:101:CYS:SG	2.61	0.40	
23:OL:20:ASP:OD2	23:OL:23:SER:OG	2.34	0.40	
29:GS:22:THR:O	29:GS:102:MET:HE1	2.21	0.40	
31:KU:81:ASN:OD1	31:KU:106:LYS:HD2	2.21	0.40	
33:YW:55:LYS:HD2	33:YW:57:GLU:OE2	2.21	0.40	
1:B:332:ASP:OD1	1:B:332:ASP:N	2.43	0.40	
4:Z2:335:C:H2'	4:Z2:336:A:N3	2.36	0.40	
4:Z2:978:C:OP2	25:PO:50:ARG:HG2	2.21	0.40	
4:Z2:1470:G:H2'	4:Z2:1471:U:C6	2.54	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:Z2:1721:C:H2'	4:Z2:1722:U:C6	2.56	0.40
4:Z2:2528:G:H2'	4:Z2:2529:U:O4'	2.21	0.40
4:Z2:2773:U:OP2	4:Z2:2858:U:O2'	2.35	0.40
10:D8:76:A:H2'	10:D8:77:G:O4'	2.22	0.40
28:GR:54:PRO:HB2	28:GR:56:VAL:O	2.21	0.40
31:KU:53:ARG:HD2	31:KU:53:ARG:HA	1.78	0.40
1:B:251:ILE:HA	1:B:254:VAL:HG22	2.03	0.40
4:Z2:497:A:N3	4:Z2:566:C:O2'	2.49	0.40
4:Z2:632:G:H2'	4:Z2:633:G:O4'	2.22	0.40
4:Z2:727:G:H2'	4:Z2:728:U:H6	1.85	0.40
4:Z2:787:A:H2'	4:Z2:788:C:C6	2.57	0.40
4:Z2:1532:A:O2'	4:Z2:1533:A:O4'	2.37	0.40
4:Z2:1660:A:C2	4:Z2:2565:G:H5'	2.56	0.40
4:Z2:2005:A:H4'	25:PO:34:VAL:HG21	2.02	0.40
4:Z2:2438:G:H2'	4:Z2:2439:C:C6	2.57	0.40
4:Z2:2598:U:H2'	4:Z2:2599:C:C6	2.57	0.40
4:Z2:2711:U:H2'	4:Z2:2712:U:C6	2.57	0.40
7:E5:94:HIS:CE1	7:E5:143:ARG:HD2	2.56	0.40
9:F7:115:ARG:HA	9:F7:115:ARG:HD2	1.91	0.40
30:CT:132:ARG:HH11	30:CT:132:ARG:HG2	1.86	0.40
35:JY:10:LEU:O	35:JY:71:LYS:HA	2.21	0.40
36:QZ:44:LEU:HD13	36:QZ:46:ARG:NH2	2.37	0.40
53:V:16:U:H5"	53:V:17:U:H5	1.85	0.40
4:Z2:39:C:O2'	4:Z2:40:U:H5'	2.21	0.40
4:Z2:1999:A:H4'	17:RF:96:ILE:HD13	2.02	0.40
4:Z2:2564:G:OP2	4:Z2:2564:G:N2	2.54	0.40
4:Z2:2728:C:O2	28:GR:139:GLN:NE2	2.47	0.40
9:F7:8:TYR:OH	9:F7:29:PRO:O	2.30	0.40
11:E9:21:GLU:HG3	11:E9:22:PHE:N	2.36	0.40
29:GS:31:MET:SD	29:GS:34:GLY:HA2	2.62	0.40
29:GS:38:THR:O	29:GS:42:ILE:HG12	2.21	0.40
55:C1:41:ALA:HA	55:C1:44:ILE:HG12	2.02	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	entiles
1	В	358/369~(97%)	344 (96%)	13~(4%)	1 (0%)	41	64
2	F	124/128~(97%)	117 (94%)	7 (6%)	0	100	100
3	Н	183/396~(46%)	175 (96%)	8 (4%)	0	100	100
5	R3	54/76~(71%)	53 (98%)	1 (2%)	0	100	100
6	A4	231/269~(86%)	220 (95%)	11 (5%)	0	100	100
7	E5	154/171~(90%)	147 (96%)	7 (4%)	0	100	100
8	L6	120/124~(97%)	111 (92%)	9 (8%)	0	100	100
9	F7	175/178~(98%)	166 (95%)	9 (5%)	0	100	100
11	E9	197/200~(98%)	191 (97%)	6 (3%)	0	100	100
12	aA	51/60~(85%)	51 (100%)	0	0	100	100
13	MB	117/119~(98%)	112 (96%)	5 (4%)	0	100	100
14	UC	95/219~(43%)	92 (97%)	3 (3%)	0	100	100
15	WD	74/78~(95%)	72 (97%)	2 (3%)	0	100	100
16	XE	60/65~(92%)	58 (97%)	2 (3%)	0	100	100
17	RF	107/109~(98%)	104 (97%)	3 (3%)	0	100	100
18	FG	100/134~(75%)	98 (98%)	2 (2%)	0	100	100
19	VH	82/85~(96%)	78 (95%)	4 (5%)	0	100	100
20	TI	100/105~(95%)	96 (96%)	4 (4%)	0	100	100
21	fJ	57/93~(61%)	56 (98%)	1 (2%)	0	100	100
22	HK	98/101~(97%)	97 (99%)	1 (1%)	0	100	100
23	OL	84/88~(96%)	81 (96%)	3 (4%)	0	100	100
24	MM	90/118~(76%)	87 (97%)	3 (3%)	0	100	100
25	PO	114/118~(97%)	111 (97%)	3 (3%)	0	100	100
26	SP	78/91~(86%)	75 (96%)	3 (4%)	0	100	100
27	BQ	129/132~(98%)	127 (98%)	2 (2%)	0	100	100
28	GR	173/177~(98%)	163 (94%)	10 (6%)	0	100	100
29	GS	151/157~(96%)	148 (98%)	3 (2%)	0	100	100
30	CT	203/241~(84%)	185 (91%)	18 (9%)	0	100	100
31	KU	113/129~(88%)	106 (94%)	7 (6%)	0	100	100

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
32	NV	55/71~(78%)	55 (100%)	0	0	100	100
33	YW	54/59~(92%)	54 (100%)	0	0	100	100
34	IX	140/142~(99%)	136 (97%)	4 (3%)	0	100	100
35	JY	98/103~(95%)	87 (89%)	11 (11%)	0	100	100
36	QZ	77/91~(85%)	75 (97%)	2 (3%)	0	100	100
37	Ba	42/44~(96%)	40 (95%)	2 (5%)	0	100	100
38	Qb	101/103~(98%)	99~(98%)	2 (2%)	0	100	100
39	Nc	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
40	Kd	143/146~(98%)	133 (93%)	10 (7%)	0	100	100
41	Je	120/122~(98%)	117 (98%)	3 (2%)	0	100	100
42	Af	209/212~(99%)	199 (95%)	9 (4%)	1 (0%)	29	52
43	Lg	135/137~(98%)	128 (95%)	7 (5%)	0	100	100
44	dh	62/65~(95%)	61 (98%)	0	1 (2%)	9	19
45	Oi	113/130 (87%)	105 (93%)	8 (7%)	0	100	100
46	Рj	79/89~(89%)	78~(99%)	1 (1%)	0	100	100
47	bk	47/51~(92%)	45 (96%)	2 (4%)	0	100	100
48	Cl	270/274~(98%)	258 (96%)	12 (4%)	0	100	100
49	Dm	210/213~(99%)	195 (93%)	15 (7%)	0	100	100
50	Sn	86/116 (74%)	85 (99%)	1 (1%)	0	100	100
51	То	85/88~(97%)	82 (96%)	3 (4%)	0	100	100
52	ер	36/38~(95%)	36 (100%)	0	0	100	100
55	C1	47/166~(28%)	44 (94%)	3 (6%)	0	100	100
All	All	5992/6906~(87%)	5742 (96%)	247 (4%)	3 (0%)	54	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	140	ASN
42	Af	141	VAL
44	dh	32	ILE



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	В	303/310~(98%)	285~(94%)	18~(6%)	19	39
2	F	103/105~(98%)	94 (91%)	9~(9%)	10	20
3	Н	151/327~(46%)	128 (85%)	23~(15%)	3	4
5	R3	51/67~(76%)	50 (98%)	1 (2%)	55	78
6	A4	188/211 (89%)	185 (98%)	3 (2%)	62	82
7	E5	118/131 (90%)	115 (98%)	3 (2%)	47	73
8	L6	102/103~(99%)	94 (92%)	8 (8%)	12	25
9	F7	139/146~(95%)	112 (81%)	27 (19%)	1	2
11	E9	159/159~(100%)	155 (98%)	4 (2%)	47	73
12	aA	46/53~(87%)	46 (100%)	0	100	100
13	MB	101/102~(99%)	96~(95%)	5 (5%)	24	47
14	UC	79/184~(43%)	76~(96%)	3 (4%)	33	59
15	WD	67/71~(94%)	65~(97%)	2(3%)	41	67
16	XE	54/57~(95%)	53~(98%)	1 (2%)	57	79
17	RF	88/88~(100%)	81 (92%)	7 (8%)	12	24
18	FG	92/121~(76%)	90 (98%)	2(2%)	52	76
19	VH	60/62~(97%)	55 (92%)	5 (8%)	11	22
20	TI	83/85~(98%)	78 (94%)	5 (6%)	19	39
21	fJ	52/81~(64%)	41 (79%)	11 (21%)	1	1
22	HK	87/88~(99%)	85 (98%)	2(2%)	50	75
23	OL	75/77~(97%)	71 (95%)	4(5%)	22	45
24	MM	76/99~(77%)	62 (82%)	14 (18%)	1	2
25	РО	88/90 (98%)	85~(97%)	3~(3%)	37	63
26	SP	$\overline{71/79}\ (90\%)$	59 (83%)	12 (17%)	2	3
27	BQ	103/104~(99%)	102 (99%)	1 (1%)	76	90
28	GR	149/151~(99%)	140 (94%)	9 (6%)	19	39



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
29	GS	124/128~(97%)	119~(96%)	5(4%)	31	57
30	CT	168/198~(85%)	146 (87%)	22 (13%)	4	7
31	KU	85/98~(87%)	83 (98%)	2(2%)	49	74
32	NV	49/63~(78%)	46 (94%)	3 (6%)	18	38
33	YW	50/52~(96%)	48 (96%)	2 (4%)	31	57
34	IX	116/117~(99%)	114 (98%)	2 (2%)	60	81
35	JY	88/90~(98%)	87 (99%)	1 (1%)	73	88
36	QZ	73/84 (87%)	69 (94%)	4 (6%)	21	43
37	Ba	37/37~(100%)	37 (100%)	0	100	100
38	Qb	89/89~(100%)	87 (98%)	2 (2%)	52	76
39	Nc	81/85~(95%)	78~(96%)	3 (4%)	34	60
40	Kd	108/110 (98%)	108 (100%)	0	100	100
41	Je	102/102~(100%)	94 (92%)	8 (8%)	12	25
42	Af	161/162~(99%)	154 (96%)	7 (4%)	29	54
43	Lg	114/114 (100%)	108 (95%)	6~(5%)	22	45
44	dh	55/56~(98%)	52 (94%)	3 (6%)	21	43
45	Oi	97/108~(90%)	90~(93%)	7 (7%)	14	29
46	Рj	63/68~(93%)	60 (95%)	3(5%)	25	49
47	bk	42/46~(91%)	38 (90%)	4 (10%)	8	16
48	Cl	$219/221 \ (99\%)$	212 (97%)	7(3%)	39	65
49	Dm	177/181 (98%)	173 (98%)	4 (2%)	50	75
50	Sn	76/97~(78%)	71 (93%)	5 (7%)	16	33
51	То	67/69~(97%)	65~(97%)	2 (3%)	41	67
52	ер	33/33~(100%)	32 (97%)	1 (3%)	41	67
55	C1	39/135~(29%)	39 (100%)	0	100	100
All	All	4998/5694 (88%)	4713 (94%)	285 (6%)	24	41

All (285) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	2	LYS
1	В	42	LYS
1	В	56	THR



Mol	Chain	Res	Type
1	В	91	LEU
1	В	94	MET
1	В	98	THR
1	В	106	ASN
1	В	143	VAL
1	В	151	ASN
1	В	188	LEU
1	В	210	LEU
1	В	217	ARG
1	В	225	VAL
1	В	249	ARG
1	В	259	GLU
1	В	275	LYS
1	В	332	ASP
1	В	358	SER
2	F	10	ARG
2	F	16	ARG
2	F	53	LEU
2	F	103	THR
2	F	104	ARG
2	F	110	GLU
2	F	121	LYS
2	F	127	LYS
2	F	128	ARG
3	Н	222	SER
3	Н	235	GLU
3	Н	250	ILE
3	Н	252	ASP
3	Н	269	ASP
3	Н	270	GLU
3	Н	277	CYS
3	Н	279	VAL
3	Η	286	ARG
3	H	293	GLN
3	H	300	SER
3	Н	305	THR
3	Н	308	ASP
3	Н	314	LEU
3	Н	316	LYS
3	Н	336	ARG
3	Н	339	ASP
3	Н	348	ASP



Mol	Chain	Res	Type
3	Н	357	ASP
3	Н	379	ILE
3	Н	380	ARG
3	Н	381	GLU
3	Н	390	VAL
5	R3	73	ASN
6	A4	28	TRP
6	A4	124	LYS
6	A4	144	ARG
7	E5	70	GLU
7	E5	91	LYS
7	E5	152	MET
8	L6	18	LYS
8	L6	30	ARG
8	L6	41	THR
8	L6	51	LYS
8	L6	59	SER
8	L6	75	GLN
8	L6	94	ARG
8	L6	123	LYS
9	F7	5	LYS
9	F7	11	GLU
9	F7	19	GLU
9	F7	23	ASP
9	F7	25	VAL
9	F7	28	VAL
9	F7	47	LYS
9	F7	48	LYS
9	F7	49	LEU
9	F7	50	LEU
9	F7	64	LYS
9	F7	66	VAL
9	F7	72	LYS
9	F7	73	SER
9	F7	74	ILE
9	F7	83	TRP
9	F7	100	LEU
9	F7	103	LEU
9	F7	120	LYS
9	F7	127	ASN
9	F7	130	LEU
9	F7	136	ILE



Mol	Chain	Res	Type
9	F7	141	VAL
9	F7	145	LYS
9	F7	147	ASP
9	F7	159	SER
9	F7	163	ASP
11	E9	61	GLN
11	E9	151	GLU
11	E9	171	THR
11	E9	193	LYS
13	MB	6	SER
13	MB	37	THR
13	MB	54	MET
13	MB	57	GLU
13	MB	95	LEU
14	UC	17	LEU
14	UC	65	HIS
14	UC	77	GLN
15	WD	7	VAL
15	WD	22	ASN
16	XE	43	VAL
17	RF	1	MET
17	RF	2	GLU
17	RF	4	THR
17	RF	13	SER
17	RF	45	VAL
17	RF	73	THR
17	RF	83	LYS
18	FG	6	VAL
18	FG	91	ARG
19	VH	9	SER
19	VH	11	ARG
19	VH	12	ASN
19	VH	55	ARG
19	VH	81	MET
20	TI	5	ARG
20	TI	25	GLN
20	TI	29	ASN
20	TI	30	ASP
20	TI	84	GLN
21	fJ	2	ARG
21	fJ	3	LYS
21	fJ	11	ASP



Mol	Chain	Res	Type
21	fJ	28	THR
21	fJ	29	VAL
21	fJ	33	THR
21	fJ	36	GLU
21	fJ	37	TYR
21	fJ	53	SER
21	fJ	73	PHE
21	fJ	76	ARG
22	HK	12	LYS
22	HK	34	MET
23	OL	18	GLU
23	OL	20	ASP
23	OL	58	MET
23	OL	63	ARG
24	MM	7	VAL
24	MM	18	SER
24	MM	29	THR
24	MM	45	VAL
24	MM	46	SER
24	MM	47	GLN
24	MM	48	LEU
24	MM	53	LEU
24	MM	68	ASP
24	MM	72	GLU
24	MM	75	MET
24	MM	78	LYS
24	MM	87	ARG
24	MM	89	ILE
25	PO	31	VAL
25	PO	33	ARG
25	PO	112	LYS
26	SP	4	SER
26	SP	6	LYS
26	SP	12	ASP
26	SP	29	LYS
26	SP	35	SER
26	SP	37	ARG
26	SP	38	SER
26	SP	41	LEU
26	SP	44	MET
$\overline{26}$	SP	55	ARG
26	SP	67	VAL



Mol	Chain	Res	Type
26	SP	79	THR
27	BQ	34	LYS
28	GR	27	LYS
28	GR	29	LYS
28	GR	42	GLU
28	GR	59	LYS
28	GR	62	MET
28	GR	85	ARG
28	GR	155	GLU
28	GR	176	LYS
28	GR	177	LYS
29	GS	5	ARG
29	GS	11	GLU
29	GS	32	SER
29	GS	97	ARG
29	GS	145	MET
30	CT	14	VAL
30	CT	32	TYR
30	CT	44	ARG
30	CT	48	ASP
30	CT	55	ILE
30	CT	57	ILE
30	CT	59	ARG
30	CT	70	THR
30	CT	76	VAL
30	CT	92	THR
30	CT	93	LYS
30	CT	101	VAL
30	CT	104	GLU
30	CT	107	THR
30	CT	112	ASP
30	CT	122	SER
30	CT	124	LEU
30	CT	149	ILE
30	CT	151	VAL
30	CT	153	LEU
30	CT	154	SER
30	CT	178	LEU
31	KU	26	SER
31	KU	30	THR
32	NV	7	LYS
32	NV	20	LYS



Mol	Chain	Res	Type
32	NV	25	LYS
33	YW	24	LYS
33	YW	53	LEU
34	IX	1	MET
34	IX	45	THR
35	JY	60	ASP
36	QZ	17	ARG
36	QZ	20	SER
36	QZ	26	SER
36	QZ	74	SER
38	Qb	1	MET
38	Qb	79	ARG
39	Nc	66	ASN
39	Nc	101	ARG
39	Nc	103	LYS
41	Je	45	GLU
41	Je	51	ARG
41	Je	53	LYS
41	Je	56	ASP
41	Je	64	ARG
41	Je	80	ASP
41	Je	91	LYS
41	Je	120	GLU
42	Af	5	LEU
42	Af	26	THR
42	Af	29	GLU
42	Af	33	ASN
42	Af	60	ARG
42	Af	94	GLU
42	Af	105	GLU
43	Lg	1	MET
43	Lg	14	LYS
43	Lg	25	SER
43	Lg	26	THR
43	Lg	43	THR
43	Lg	110	SER
44	dh	17	ARG
44	dh	31	HIS
44	dh	52	LYS
45	Oi	3	ASN
45	Oi	6	LEU
45	Oi	19	ARG



Mol	Chain	Res	Type
45	Oi	39	ARG
45	Oi	85	SER
45	Oi	87	GLU
45	Oi	108	LYS
46	Pj	19	VAL
46	Pj	20	VAL
46	Pj	42	LEU
47	bk	18	THR
47	bk	26	MET
47	bk	38	LYS
47	bk	47	GLU
48	Cl	5	LYS
48	Cl	51	THR
48	Cl	110	GLN
48	Cl	147	LYS
48	Cl	177	ARG
48	Cl	186	VAL
48	Cl	245	THR
49	Dm	117	GLN
49	Dm	155	LYS
49	Dm	183	SER
49	Dm	184	LYS
50	Sn	25	SER
50	Sn	28	VAL
50	Sn	35	SER
50	Sn	63	VAL
50	Sn	64	LYS
51	То	53	LYS
51	То	59	ASP
52	ер	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	287	GLN
5	R3	73	ASN
9	F7	10	ASN
9	F7	135	GLN
18	FG	81	ASN
45	Oi	15	GLN
49	Dm	159	GLN



5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	D8	114/115~(99%)	14 (12%)	0
4	Z2	2705/2882~(93%)	387~(14%)	20 (0%)
53	V	75/76~(98%)	26 (34%)	0
54	Y	5/6~(83%)	3~(60%)	0
56	iN	1498/1590~(94%)	266~(17%)	0
All	All	4397/4669~(94%)	696~(15%)	20 (0%)

All (696) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	Z2	10	U
4	Z2	19	G
4	Z2	22	G
4	Z2	30	G
4	Z2	41	U
4	Z2	49	А
4	Z2	53	G
4	Z2	58	G
4	Z2	61	А
4	Z2	62	G
4	Z2	70	А
4	Z2	78	А
4	Z2	81	А
4	Z2	82	G
4	Z2	99	А
4	Z2	124	А
4	Z2	125	А
4	Z2	126	U
4	Z2	137	А
4	Z2	146	А
4	Z2	148	G
4	Z2	161	U
4	Z2	169	С
4	Z2	170	А
4	Z2	173	A
4	Z2	193	A
4	Z2	196	А
4	Z2	202	G
4	Z2	213	А
4	Z2	219	С
4	Z2	222	С



Mol	Chain	Res	Type
4	Z2	226	U
4	Z2	227	G
4	Z2	228	А
4	Z2	245	G
4	Z2	262	А
4	Z2	266	G
4	Z2	267	А
4	Z2	298	A
4	Z2	311	U
4	Z2	314	G
4	Z2	317	A
4	Z2	325	G
4	Z2	333	A
4	Z2	346	A
4	$\overline{Z2}$	354	A
4	Z2	355	G
4	Z2	366	С
4	Z2	369	G
4	Z2	379	G
4	Z2	387	A
4	Z2	394	G
4	Z2	409	С
4	Z2	419	C
4	Z2	431	U
4	Z2	434	U
4	Z2	439	C
4	Z2	440	A
4	Z2	461	A
4	Z2	464	G
4	Z2	473	U
4	Z2	475	A
4	Z2	487	U
4	Z2	488	A
4	Z2	491	A
4	Z2	500	C
4	Z2	514	C
4	Z2	515	А
4	Z2	519	G
4	Z2	526	С
4	Z2	530	U
4	Z2	531	U
4	Z2	532	A


Mol	Chain	Res	Type
4	Z2	533	U
4	Z2	548	А
4	Z2	558	U
4	Z2	559	А
4	Z2	560	А
4	Z2	588	А
4	Z2	589	G
4	Z2	592	U
4	Z2	598	U
4	Z2	599	U
4	Z2	612	А
4	Z2	622	А
4	Z2	630	U
4	Z2	638	C
4	Z2	639	U
4	Z2	640	A
4	Z2	654	G
4	Z2	656	С
4	Z2	662	А
4	Z2	671	U
4	Z2	689	G
4	Z2	702	С
4	Z2	715	A
4	Z2	724	А
4	Z2	732	U
4	Z2	749	A
4	Z2	750	С
4	Z2	760	G
4	Z2	761	G
4	Z2	767	A
4	Z2	769	G
4	Z2	770	G
4	Z2	776	С
4	Z2	777	A
4	Z2	790	G
4	Z2	797	С
4	Z2	812	U
4	Z2	814	A
4	Z2	815	G
4	Z2	844	G
4	Z2	850	С
4	Z2	854	G



Mol	Chain	Res	Type
4	Z2	887	С
4	Z2	890	А
4	Z2	892	G
4	Z2	895	А
4	Z2	900	С
4	Z2	917	U
4	Z2	929	А
4	Z2	930	С
4	Z2	945	С
4	Z2	958	G
4	Z2	967	А
4	Z2	968	A
4	Z2	980	A
4	Z2	983	U
4	Z2	987	G
4	Z2	995	U
4	Z2	996	U
4	Z2	997	С
4	Z2	1001	G
4	Z2	1010	G
4	Z2	1023	А
4	Z2	1025	G
4	Z2	1030	А
4	Z2	1031	G
4	Z2	1044	U
4	Z2	1053	А
4	Z2	1054	А
4	Z2	1055	G
4	Z2	1063	С
4	Z2	1066	U
4	Z2	1072	А
4	Z2	1074	А
4	Z2	1085	U
4	Z2	1095	А
4	Z2	1096	G
4	Z2	1112	G
4	Z2	1113	А
4	Z2	1114	U
4	Z2	1116	U
4	Z2	1119	С
4	Z2	1120	G
4	Z2	1133	G



Mol	Chain	Res	Type
4	Z2	1156	А
4	Z2	1157	С
4	Z2	1158	U
4	Z2	1160	G
4	Z2	1161	U
4	Z2	1162	U
4	Z2	1168	G
4	Z2	1179	G
4	Z2	1190	G
4	Z2	1211	G
4	Z2	1220	G
4	Z2	1225	A
4	Z2	1234	G
4	Z2	1237	A
4	Z2	1240	G
4	Z2	1255	G
4	Z2	1256	А
4	Z2	1257	U
4	Z2	1260	U
4	Z2	1284	G
4	Z2	1285	A
4	Z2	1305	А
4	Z2	1309	U
4	Z2	1313	U
4	Z2	1336	U
4	Z2	1343	А
4	Z2	1349	А
4	Z2	1354	С
4	Z2	1363	U
4	Z2	1367	A
4	Z2	1369	A
4	Z2	1370	U
4	Z2	1379	A
4	Z2	1400	G
4	Z2	1404	U
4	Z2	1405	G
4	Z2	1411	A
4	Z2	1412	С
4	Z2	1419	G
4	Z2	1435	С
4	Z2	1436	G
4	Z2	1466	U



Mol	Chain	Res	Type
4	Z2	1474	А
4	Z2	1477	С
4	Z2	1478	А
4	Z2	1479	А
4	Z2	1489	G
4	Z2	1497	G
4	Z2	1501	А
4	Z2	1515	G
4	Z2	1532	А
4	Z2	1542	U
4	Z2	1551	U
4	Z2	1554	А
4	Z2	1557	А
4	Z2	1566	U
4	Z2	1580	A
4	Z2	1581	А
4	Z2	1596	А
4	Z2	1598	А
4	Z2	1603	С
4	Z2	1604	А
4	Z2	1606	А
4	Z2	1622	А
4	Z2	1635	U
4	Z2	1636	U
4	Z2	1655	G
4	Z2	1662	G
4	Z2	1663	С
4	Z2	1681	U
4	Z2	1684	G
4	Z2	1718	С
4	Z2	1719	U
4	Z2	1724	G
4	Z2	1732	G
4	Z2	1750	G
4	Z2	1759	А
4	Z2	1762	G
4	Z2	1768	U
4	Z2	1770	А
4	Z2	1777	А
4	Z2	1785	G
4	Z2	1786	С
4	Z2	1787	A



Mol	Chain	Res	Type
4	Z2	1796	А
4	Z2	1802	С
4	Z2	1815	А
4	Z2	1819	С
4	Z2	1824	С
4	Z2	1843	G
4	Z2	1848	G
4	Z2	1856	U
4	Z2	1857	А
4	Z2	1870	G
4	Z2	1886	А
4	Z2	1892	G
4	Z2	1893	G
4	Z2	1899	А
4	Z2	1900	С
4	Z2	1913	А
4	Z2	1915	G
4	Z2	1923	А
4	Z2	1924	А
4	Z2	1925	U
4	Z2	1931	G
4	Z2	1941	U
4	Z2	1949	U
4	Z2	1953	С
4	Z2	1956	А
4	Z2	1957	U
4	Z2	1958	G
4	Z2	1968	U
4	Z2	1977	U
4	Z2	1979	U
4	Z2	1983	С
4	Z2	2007	A
4	Z2	2009	С
4	Z2	2016	А
4	Z2	2017	А
4	Z2	2019	А
4	Z2	2022	С
4	Z2	2041	С
4	Z2	2042	G
4	Z2	2046	A
4	Z2	2047	G
4	Z2	2048	А



Mol	Chain	Res	Type
4	Z2	2054	U
4	Z2	2055	G
4	Z2	2079	G
4	Z2	2178	G
4	Z2	2184	А
4	Z2	2189	А
4	Z2	2190	G
4	Z2	2195	А
4	Z2	2197	С
4	Z2	2206	G
4	Z2	2208	А
4	Z2	2221	G
4	Z2	2224	А
4	Z2	2251	А
4	Z2	2256	А
4	Z2	2262	G
4	Z2	2266	U
4	Z2	2270	А
4	Z2	2271	А
4	Z2	2288	U
4	Z2	2294	А
4	Z2	2302	U
4	Z2	2303	А
4	Z2	2305	А
4	Z2	2306	G
4	Z2	2308	А
4	Z2	2309	U
4	Z2	2310	А
4	Z2	2314	G
4	Z2	2327	U
4	Z2	2330	С
4	Z2	2333	С
4	Z2	2337	А
4	Z2	2356	А
4	Z2	2360	A
4	Z2	2365	G
4	Z2	2366	G
4	Z2	2368	С
4	Z2	2374	G
4	Z2	2385	U
4	Z2	2386	С
4	Z2	2389	U



Mol	Chain	Res	Type
4	Z2	2405	С
4	Z2	2406	U
4	Z2	2408	А
4	Z2	2409	А
4	Z2	2412	G
4	Z2	2413	А
4	Z2	2414	U
4	Z2	2417	А
4	Z2	2422	А
4	Z2	2424	U
4	Z2	2431	А
4	Z2	2457	U
4	Z2	2458	С
4	Z2	2459	A
4	Z2	2474	U
4	Z2	2481	С
4	Z2	2485	G
4	Z2	2486	А
4	Z2	2488	G
4	Z2	2501	А
4	Z2	2503	С
4	Z2	2512	G
4	Z2	2530	А
4	Z2	2537	U
4	Z2	2545	U
4	Z2	2549	А
4	Z2	2550	G
4	Z2	2556	С
4	Z2	2561	G
4	Z2	2585	A
4	Z2	2592	U
4	Z2	2596	U
4	Z2	2598	U
4	Z2	2604	G
4	Z2	2612	U
4	Z2	2619	U
4	Z2	2623	G
4	Z2	2644	G
4	Z2	2654	G
4	Z2	2656	G
4	Z2	2658	A
4	Z2	2668	G



Mol	Chain	Res	Type
4	Z2	2672	U
4	Z2	2673	U
4	Z2	2697	G
4	Z2	2709	С
4	Z2	2731	А
4	Z2	2740	А
4	Z2	2748	А
4	Z2	2749	G
4	Z2	2761	А
4	Z2	2762	U
4	Z2	2763	U
4	Z2	2773	U
4	Z2	2774	А
4	Z2	2775	A
4	Z2	2786	А
4	Z2	2787	A
4	Z2	2801	А
4	Z2	2815	G
4	Z2	2839	A
4	Z2	2850	U
10	D8	13	А
10	D8	22	G
10	D8	28	С
10	D8	33	U
10	D8	38	U
10	D8	39	С
10	D8	50	A
10	D8	54	G
10	D8	86	С
10	D8	87	G
10	D8	88	A
10	D8	96	A
10	D8	105	С
10	D8	106	A
53	V	8	U
53	V	14	U
53	V	15	U
53	V	16	U
53	V	17	U
53	V	18	U
53	V	19	U
53	V	20	U



Mol	Chain	Res	Type
53	V	21	U
53	V	23	U
53	V	26	U
53	V	30	U
53	V	32	U
53	V	40	U
53	V	42	U
53	V	46	U
53	V	47	U
53	V	48	U
53	V	49	U
53	V	58	U
53	V	62	U
53	V	68	U
53	V	69	U
53	V	70	U
53	V	71	U
53	V	76	А
54	Y	14	U
54	Y	15	U
54	Y	16	U
56	iN	51	С
56	iN	52	U
56	iN	54	А
56	iN	56	G
56	iN	69	G
56	iN	79	А
56	iN	80	А
56	iN	86	G
56	iN	94	С
56	iN	95	U
56	iN	97	A
56	iN	98	A
$\overline{56}$	iN	116	G
56	iN	118	A
56	iN	122	G
$\overline{56}$	iN	125	G
56	iN	127	A
$\overline{56}$	iN	128	G
56	iN	130	U
56	iN	131	U
56	iN	132	G



Mol	Chain	Res	Type
56	iN	135	U
56	iN	136	С
56	iN	137	U
56	iN	139	G
56	iN	143	А
56	iN	166	U
56	iN	167	А
56	iN	172	G
56	iN	174	А
56	iN	175	А
56	iN	176	U
56	iN	187	G
56	iN	189	G
56	iN	197	G
56	iN	200	С
56	iN	206	A
56	iN	208	С
56	iN	210	С
56	iN	218	U
56	iN	225	U
56	iN	234	С
56	iN	238	А
56	iN	242	А
56	iN	247	G
56	iN	263	G
56	iN	288	U
56	iN	289	А
56	iN	290	G
56	iN	294	G
56	iN	309	G
56	iN	310	C
56	iN	323	С
56	iN	328	U
56	iN	332	G
56	iN	364	A
$\overline{56}$	iN	371	C
56	iN	372	А
56	iN	373	C
56	iN	375	G
56	iN	395	C
56	iN	397	G
56	iN	398	C



Mol	Chain	Res	Type
56	iN	406	А
56	iN	410	U
56	iN	415	С
56	iN	416	А
56	iN	435	С
56	iN	441	U
56	iN	449	G
56	iN	452	U
56	iN	454	А
56	iN	456	G
56	iN	457	А
56	iN	464	U
56	iN	465	U
56	iN	466	U
56	iN	467	G
56	iN	472	U
56	iN	473	А
56	iN	479	С
56	iN	488	G
56	iN	496	G
56	iN	497	А
56	iN	508	А
56	iN	510	U
56	iN	511	А
56	iN	521	G
56	iN	522	А
56	iN	524	G
56	iN	527	А
56	iN	529	U
56	iN	538	А
56	iN	539	A
56	iN	540	U
$\overline{56}$	iN	554	С
56	iN	556	С
56	iN	561	С
$\overline{56}$	iN	567	G
56	iN	570	G
56	iN	574	U
56	iN	575	A
56	iN	576	A
56	iN	578	A
56	iN	582	А



\mathbf{Mol}	Chain	Res	Type
56	iN	590	А
56	iN	602	А
56	iN	607	С
56	iN	615	А
56	iN	616	А
56	iN	619	G
56	iN	620	G
56	iN	622	G
56	iN	631	G
56	iN	639	А
56	iN	650	А
56	iN	658	G
56	iN	675	U
56	iN	686	А
56	iN	697	А
56	iN	709	А
56	iN	730	U
56	iN	739	А
56	iN	747	G
56	iN	761	U
56	iN	765	G
56	iN	767	U
56	iN	768	G
56	iN	773	А
56	iN	777	А
56	iN	789	U
56	iN	798	С
56	iN	799	А
56	iN	804	G
56	iN	821	А
56	iN	825	A
56	iN	837	U
56	iN	838	А
56	iN	843	G
56	iN	853	G
56	iN	856	G
56	iN	859	A
56	iN	861	С
56	iN	872	A
56	iN	873	G
56	iN	880	G
56	iN	891	G



Mol	Chain	Res	Type
56	iN	897	G
56	iN	911	G
56	iN	916	А
56	iN	928	U
56	iN	946	G
56	iN	958	А
56	iN	970	G
56	iN	971	G
56	iN	978	С
56	iN	979	А
56	iN	1002	А
56	iN	1004	U
56	iN	1010	G
56	iN	1011	С
56	iN	1013	А
56	iN	1015	G
56	iN	1019	А
56	iN	1020	G
56	iN	1021	А
56	iN	1036	U
56	iN	1037	G
56	iN	1043	U
56	iN	1044	С
56	iN	1046	А
56	iN	1048	A
56	iN	1050	U
56	iN	1053	U
56	iN	1056	А
56	iN	1070	G
56	iN	1072	С
56	iN	1074	U
56	iN	1075	С
56	iN	1077	G
56	iN	1078	G
56	iN	1080	А
56	iN	1081	U
56	iN	1084	G
56	iN	1085	A
56	iN	1089	C
56	iN	1097	G
56	iN	1109	U
56	iN	1110	С



Mol	Chain	Res	Type
56	iN	1111	А
56	iN	1114	U
56	iN	1129	U
56	iN	1133	G
56	iN	1138	G
56	iN	1139	U
56	iN	1145	А
56	iN	1197	А
56	iN	1202	А
56	iN	1204	U
56	iN	1209	G
56	iN	1213	С
56	iN	1216	А
56	iN	1228	С
56	iN	1240	С
56	iN	1241	А
56	iN	1242	А
56	iN	1257	U
56	iN	1258	А
56	iN	1272	А
56	iN	1273	С
56	iN	1278	G
56	iN	1281	А
56	iN	1283	А
56	iN	1284	А
56	iN	1291	G
56	iN	1302	А
56	iN	1303	G
56	iN	1305	U
56	iN	1323	G
56	iN	1331	А
56	iN	1332	А
56	iN	1333	А
56	iN	1345	G
56	iN	1347	С
56	iN	1348	С
56	iN	1350	G
56	iN	1360	U
56	iN	1362	С
56	iN	1363	A
56	iN	1365	С
56	iN	1367	С



Mol	Chain	Res	Type
56	iN	1377	А
56	iN	1391	А
56	iN	1398	G
56	iN	1408	А
56	iN	1415	G
56	iN	1424	G
56	iN	1425	U
56	iN	1426	U
56	iN	1427	С
56	iN	1439	А
56	iN	1442	С
56	iN	1443	А
56	iN	1445	С
56	iN	1464	G
56	iN	1474	С
56	iN	1477	G
56	iN	1486	А
56	iN	1490	U
56	iN	1491	А
56	iN	1496	U
56	iN	1497	С
56	iN	1520	G
56	iN	1537	А
56	iN	1538	А
56	iN	1542	G
56	iN	1548	А
56	iN	1549	G
56	iN	1551	U
56	iN	1562	G
56	iN	1564	А
56	iN	1565	С
56	iN	1574	G
56	iN	1575	G
56	iN	1577	U
56	iN	1578	С

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	Z2	9	G
4	Z2	169	С
4	Z2	532	А



Mol	Chain	Res	Type
4	Z2	769	G
4	Z2	812	U
4	Z2	886	А
4	Z2	916	А
4	Z2	1224	U
4	Z2	1580	А
4	Z2	1717	U
4	Z2	1856	U
4	Z2	2196	А
4	Z2	2223	U
4	Z2	2355	U
4	Z2	2405	С
4	Z2	2413	А
4	Z2	2456	U
4	Z2	2457	U
4	Z2	2464	G
4	Z2	2739	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19076. 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: 270





Z Index: 270

6.2.2 Raw map



X Index: 270

Y Index: 270



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: 286



Y Index: 272



Z Index: 237

6.3.2 Raw map



X Index: 287

Y Index: 268



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 0.02. 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.



Mask visualisation (i) 6.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

$emd_{19076}_{msk}_{1.map}$ (i) 6.6.1





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 599 $\rm nm^3;$ this corresponds to an approximate mass of 541 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 0.385 \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 0.385 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.91	2.62
Unmasked-calculated*	2.94	3.89	2.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.94 differs from the reported value 2.6 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19076 and PDB model 8RDV. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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 (0.02).



9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7960	0.6270
A4	0.3010	0.5170
Af	0.8940	0.6670
В	0.7040	0.6230
BQ	0.7260	0.6320
Ba	0.9860	0.6950
C1	0.4340	0.5300
CT	0.4160	0.5710
Cl	0.9330	0.6720
D8	0.8340	0.6280
Dm	0.4440	0.5650
E5	0.7520	0.6260
E9	0.7720	0.6430
F	0.3750	0.5310
F7	0.4600	0.5900
FG	0.4350	0.5390
GR	0.5420	0.5910
GS	0.3030	0.4890
Н	0.1710	0.5690
HK	0.3830	0.5170
IX	0.9070	0.6640
JY	0.2900	0.4670
Je	0.8960	0.6650
KU	0.5390	0.5710
Kd	0.8550	0.6530
L6	0.8240	0.6340
Lg	0.8750	0.6510
MB	0.9450	0.6780
MM	0.2540	0.5480
NV	0.4180	0.5520
Nc	0.7180	0.6250
OL	0.7440	0.6140
Oi	0.8800	0.6490
PO	0.9180	0.6760
Рj	0.7080	0.6100



Chain	Atom inclusion	Q-score
QZ	0.6720	0.6010
Qb	0.7370	0.6280
R3	0.6570	0.5770
RF	0.8940	0.6670
SP	0.1690	0.5220
Sn	0.7940	0.6350
TI	0.6060	0.5740
То	0.6900	0.6150
UC	0.7440	0.6300
V	0.5730	0.5220
VH	0.9020	0.6670
WD	0.8370	0.6410
XE	0.5350	0.5690
Y	0.7750	0.5720
YW	0.8920	0.6730
Z2	0.9260	0.6590
aA	0.8840	0.6670
bk	0.8840	0.6610
dh	0.9800	0.6950
ep	0.9240	0.6580
fJ	0.2000	0.5460
iN	0.7790	0.6060

