

May 28, 2025 – 01:59 pm BST

PDB	ID	:	$9 \mathrm{QEG} \ / \ \mathrm{pdb} \ 00009 \mathrm{qeg}$
EMDB	ID	:	EMD-53066
Ti	tle	:	Cryo-EM structure of the 70S ribosome of a MLSb sensitive S. aureus strain
			"KES34" in complex with solithromycin
Auth	ors	:	Rivalta, A.; Yonath, A.
Deposited	on	:	2025-03-10
Resoluti	ion	:	2.21 Å(reported)
Th	is is	a F	full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.21 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	1	52	83%	10% 8%
2	2	45	84%	13% •
3	3	66	91%	8% •
4	4	37	84%	16%
5	В	115	• 57% 36%	6% •
6	С	277	92%	7% •
7	D	220	89%	9% •



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
8	Е	207	87%	12%
9	G	178	83%	7% 10%
10	Н	145	93%	7%
11	Ι	122	88%	12%
12	J	146	94%	6%
13	K	144	89%	6% 5%
14	L	122	84%	13% •
15	М	119	86%	14%
16	Ν	116	85%	10% ·
17	0	118	90%	8% •
18	Р	102	• 90%	10%
19	Q	117	85%	9% 5%
20	R	91	88%	10% •
21	S	105	● 80%	7% • 11%
22	Т	217	37% · 59	%
23	U	94	• 81%	• 16%
24	V	62	8%	15% 19%
25	W	73	78%	10% 12%
26	Х	59	92%	7% •
27	Z	57	• 67% 79	6 26%
28	F	179	28%	11% • 17%
29	11	15	87% 33% 53%	13%
30	A	2923	6 2%	24% • 12%
31	Ae	166	77%	16% • 6%
32	Af	98	80%	17% •



Mol	Chain	Length	Quality of chain	
33	Ag	156	88%	10% ••
34	Ai	132	82%	14% •
35	Al	137	90%	8% •
36	Ao	89	79%	20% •
37	Ар	91	82%	15% ·
38	Aq	87	67% 18%	15%
39	Ar	80	54% 14%	32%
40	At	83	84%	12% ••
41	Aa	1552	^{6%} 57% 33%	• 7%
42	Aj	102	78%	15% • 6%
43	Ac	217	80%	13% 7%
44	Am	121	76%	16% • 6%
45	Ak	129	64% 22%	• 13%
46	Ab	255	21% 36% 5% 59%	
47	Ah	132	82%	16% ••
48	Ad	200	86%	13% •
49	An	61	84%	15% •
50	As	92	79%	10% 11%
51	d	19	5% 42% 53%	5%
52	8	71	69% 58% 31%	11%
53	9	5	40% 60%	
54	13	84	64%	32%



2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 130300 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 Large ribosomal subunit protein bL33A.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
1	1	48	Total 355	C 218	N 70	O 64	${ m S} { m 3}$	0	0

• Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
2	2	44	Total 368	C 225	N 89	O 53	S 1	0	0

• Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	65	Total	C 215	N 109	0	S	0	0
			508	310	108	83	2		

• Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues		Atc	ms	AltConf	Trace		
4	4	37	Total 280	C 175	N 57	O 43	${f S}{5}$	0	0

• Molecule 5 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		At	AltConf	Trace			
5	В	113	Total 2408	C 1076	N 430	0 789	Р 113	0	0

• Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	С	274	Total 2037	C 1271	N 406	O 355	${ m S}{ m 5}$	0	0



• Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues		At	AltConf	Trace			
7	D	215	Total 1582	C 994	N 296	0 287	${ m S}{ m 5}$	0	0

• Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Ε	206	Total 1510	C 955	N 282	0 271	${S \over 2}$	0	0

• Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	G	160	Total 944	C 572	N 191	0 180	S 1	0	0

• Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	Н	145	Total 1140	C 712	N 208	0 217	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	Ι	122	Total 865	C 543	N 163	0 156	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	J	146	Total 1057	C 659	N 213	0 184	S 1	0	0

• Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	К	137	Total 1024	C 660	N 193	0 168	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called Large ribosomal subunit protein bL17.



Mol	Chain	Residues		At	AltConf	Trace			
14	L	118	Total 901	$\begin{array}{c} \mathrm{C} \\ 559 \end{array}$	N 179	O 162	S 1	0	0

• Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
15	М	119	Total 801	C 497	N 162	O 142	0	0

• Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
16	Ν	111	Total 800	C 504	N 159	O 137	0	0

• Molecule 17 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues		At	AltConf	Trace			
17	Ο	116	Total 943	C 593	N 189	0 157	${S \atop 4}$	0	0

• Molecule 18 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues		At	AltConf	Trace			
18	Р	102	Total 752	C 480	N 138	O 133	S 1	0	0

• Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues		At	AltConf	Trace			
19	Q	111	Total 814	C 511	N 158	0 143	${ m S} { m 2}$	0	0

• Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues		At	AltConf	Trace			
20	R	89	Total 664	C 422	N 118	0 120	$\frac{S}{4}$	0	0

• Molecule 21 is a protein called Large ribosomal subunit protein uL24.



Mol	Chain	Residues		At	AltConf	Trace			
21	S	93	Total 635	C 403	N 121	O 110	S 1	0	0

• Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
22	Т	90	Total 600	C 385	N 109	O 106	0	0

• Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
23	U	79	Total 575	C 356	N 115	O 104	0	0

• Molecule 24 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
24	V	50	Total 360	C 223	N 76	O 61	0	0

• Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
25	W	64	Total 473	C 295	N 96	O 82	0	0

• Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues		Atom	ıs	AltConf	Trace	
26	Х	58	Total 438	C 273	N 84	0 81	0	0

• Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
27	Z	42	Total 333	C 205	N 71	O 53	${S \atop 4}$	0	0

• Molecule 28 is a protein called Large ribosomal subunit protein uL5.



Mol	Chain	Residues		At	AltConf	Trace			
28	F	149	Total 914	$\begin{array}{c} \mathrm{C} \\ 580 \end{array}$	N 165	O 166	${ m S} { m 3}$	0	0

• Molecule 29 is a RNA chain called E-site tRNA molecule.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	11	15	Total 322	C 143	N 61	0 103	Р 15	0	0

• Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
30	А	2586	Total	С	Ν	Ο	Р	2	0
		2000	55514	24786	10184	17956	2588	-	0

• Molecule 31 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues		At	AltConf	Trace			
31	Ae	156	Total 1130	C 716	N 211	0 201	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 32 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues		At	AltConf	Trace			
32	Af	95	Total 734	C 466	N 136	O 130	${ m S} { m 2}$	0	0

• Molecule 33 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues		At	AltConf	Trace			
33	Ag	154	Total 1222	C 761	N 234	0 223	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 34 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues		At	AltConf	Trace			
34	Ai	127	Total 975	C 606	N 195	0 173	S 1	0	0

• Molecule 35 is a protein called Small ribosomal subunit protein uS12.



Mol	Chain	Residues		At	AltConf	Trace			
35	Al	134	Total 1011	C 628	N 204	0 177	${ m S} { m 2}$	0	0

• Molecule 36 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues		At	AltConf	Trace			
36	Ao	88	Total 727	C 449	N 150	0 127	S 1	0	0

• Molecule 37 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues		At	AltConf	Trace			
37	Ap	89	Total 679	C 428	N 125	0 125	S 1	0	0

• Molecule 38 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
38	Αα	74	Total	С	Ν	0	0	0
			551	351	106	94	Ŭ	Ŭ

• Molecule 39 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
39	Ar	54	Total 445	C 284	N 86	0 73	S 2	0	0

• Molecule 40 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues		At	Atoms						
40	At	81	Total 593	C 363	N 118	0 110	${ m S} { m 2}$	0	0		

• Molecule 41 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues		A	AltConf	Trace			
41	Aa	1440	Total 30880	C 13790	N 5653	O 9997	Р 1440	0	0

• Molecule 42 is a protein called Small ribosomal subunit protein uS10.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
42	Aj	96	Total 720	$\begin{array}{c} \mathrm{C} \\ 452 \end{array}$	N 133	O 135	0	0

• Molecule 43 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	Ac	202	Total 1477	C 935	N 275	O 266	S 1	0	0

• Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
44	Am	114	Total 845	C 526	N 168	0 150	S 1	0	0

• Molecule 45 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
45	Ak	112	Total 759	C 467	N 146	0 144	${ m S} { m 2}$	0	0

• Molecule 46 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
46	Ab	104	Total 629	C 397	N 117	0 115	0	0

• Molecule 47 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	Ah	131	Total 1032	C 652	N 183	O 193	$\frac{S}{4}$	0	0

• Molecule 48 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
48	Ad	199	Total 1502	C 954	N 283	O 263	${ m S} { m 2}$	0	0

• Molecule 49 is a protein called Small ribosomal subunit protein uS14B.



Mol	Chain	Residues		Ate	oms			AltConf	Trace
49	An	60	Total 502	C 317	N 100	O 80	${ m S}{ m 5}$	0	0

• Molecule 50 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues		At	oms		AltConf	Trace	
50	As	82	Total 617	C 399	N 114	O 102	${ m S} { m 2}$	0	0

• Molecule 51 is a RNA chain called mRNA molecule.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
51	d	19	Total 412	C 184	N 79	O 130	Р 19	0	0

• Molecule 52 is a RNA chain called P-site tRNA molecule.

Mol	Chain	Residues		A	toms			AltConf	Trace
52	8	71	Total 1519	C 677	N 279	0 492	Р 71	0	0

• Molecule 53 is a RNA chain called A-site tRNA molecule.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
53	9	5	Total 106	C 48	N 20	O 33	Р 5	0	0

• Molecule 54 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
54	13	57	Total 382	C 245	N 74	O 63	0	0

• Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	1	1	Total Zn 1 1	0
55	4	1	Total Zn 1 1	0
55	Ζ	1	Total Zn 1 1	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
55	An	1	Total Zn 1 1	0

• Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	С	1	Total Mg 1 1	0
56	D	1	Total Mg 1 1	0
56	А	170	Total Mg 170 170	0
56	Aa	59	Total Mg 59 59	0

• Molecule 57 is $(3aS,4R,7S,9R,10R,11R,13R,15R,15aR)-1-\{4-[4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl]butyl\}-4-ethyl-7-fluoro-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,8,14-tetraox otetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethyl amino)-beta-D-xylo-hexopyranoside (CCD ID: EM1) (formula: C₄₃H₆₅FN₆O₁₀) (labeled as "Ligand of Interest" by depositor).$



Mol	Chain	Residues	Atoms				AltConf	
57	А	1	Total 60	C 43	F 1	N 6	O 10	0

• Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).



Mol	Chain	Residues	Atoms	AltConf
58	А	15	Total K 15 15	0
58	Aa	3	Total K 3 3	0

• Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	С	16	Total O 16 16	0
59	D	2	Total O 2 2	0
59	J	7	Total O 7 7	0
59	Ν	3	Total O 3 3	0
59	О	2	Total O 2 2	0
59	Р	1	Total O 1 1	0
59	R	1	Total O 1 1	0
59	А	574	Total O 574 574	0
59	Aa	15	Total O 15 15	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: Large ribosomal subunit protein bL33A







• Molecule 6: Large ribosomal subunit protein uL2

Chain C:	92%	7%•
MET 42 42 134 134 149 149 149 149	H58 800 800 800 813 181 181 181 181 193 1174	
• Molecule 7: La	rge ribosomal subunit protein uL3	
Chain D:	89%	9% •
MET 12 K3 C4 C4 C4 C4 K3 K3 K3 K7 K7	L 4 1109 1109 1109 1109 1134 1	
• Molecule 8: La	rge ribosomal subunit protein uL4	
Chain E:	87%	12%
MET 42 17 17 17 17 17 17 17 17 13 13 15 13 15 14 13 15 14 14 14 14 14 14 14 14 14 14 14 14 14	P81 V89 V89 V11 V125 V125 F131 F131 F131 F131 F131 F131 F131 F13	
• Molecule 9: La	rge ribosomal subunit protein uL6	
Chain G:	83% 7%	10%
MET 82 83 85 85 85 11 11 11 11 11 11 11 11 11 11 11 11 11	515 V11 V17 V17 V17 V17 V17 V17 V17 F18 ASP	V84 V90 K101 \$110
R149 R160 G161 C162 G164 C174 C174 C174 C174 C174 C174 C174 C17		
• Molecule 10: La	arge ribosomal subunit protein uL13	
Chain H:	93%	7%
M1 R2 Q3 D20 D20 L56 N59 N59	V125 V126 H133 G145 G145	
• Molecule 11: La	arge ribosomal subunit protein uL14	
Chain I:	88%	12%
M1 V24 V34 135 N33 N34 N34 N34 N36 N37 N76	1, 0 186 187 188 188 189 190 190 11, 10 11, 11 11, 12 11, 12	
• Molecule 12: La	arge ribosomal subunit protein uL15	

D W I D E DATA BANK

Chain J:	94%	6%
M N18 N60 N74 E82 E82 K106	K1 10 K1 27 1146	
Molecule 13: Large	ribosomal subunit protein uL16	
• Molecule 15. Large	nbosoniai subunit protein ul 10	
Chain K:	89%	6% 5%
M K22 L34 M54 M58 K60 K60	P99 F104 C17 C118 C17 C17 C17 C17 C17 C17 C17 C17 C17 C17	
• Molecule 14: Large	ribosomal subunit protein bL17	
Chain L:	84%	13% ·
MET MET R13 R13 R13 R13 R13 R13 R36 R36 R36 R36 R36 R36 R36 R36 R36	V44 K52 K55 R55 R57 R57 R57 R57 R97 R92 R92 R92 R92 R92	
• Molecule 15: Large	ribosomal subunit protein uL18	
Chain M:	86%	14%
M1 N19 R11 R11 N13 N13 T52 T52	D60 261 261 165 165 166 176 172 887 887 885 485 628 885 628 885 628 885 628 885 638 885 638 865 1935 1935 1935 1935 1935 1935 1935 193	A109 A112 L117 E118 F119
• Molecule 16: Large	ribosomal subunit protein bL19	
Their N.	-	100
Juan IV.	85%	10% •
T2 72 72 72 72 735 718 718 718 718 718 718 718	043 V44 R52 S68 P77 1102 I112 ARG	
• Molecule 17: Large	ribosomal subunit protein bL20	
Chain O:	90%	8% •
PE RE R3 R6 R6 R70 M74 L79 L79 A86	1100 A116 L17 LYS	
• Molecule 18: Large	ribosomal subunit protein bL21	
Chain P:	90%	10%
M1 112 112 112 112 112 112 112 112 112 1	R67 R78 A102 ♦	

• Molecule 19: Large ribosomal subunit protein uL22 Chain Q: 85% 5% 9% GLU GLU LYS GLU GLU • Molecule 20: Large ribosomal subunit protein uL23 Chain R: 88% 10% • Molecule 21: Large ribosomal subunit protein uL24 Chain S: 80% 7% • 11% THR GLN LEU ASN PRO CLU GLV GLY • Molecule 22: 50S ribosomal protein L25 Chain T: 37% 59% • Molecule 23: Large ribosomal subunit protein bL27 Chain U: 81% 16% MET LEU LYS LLEU ASNN ASNN ASNN PHE PHE PHE SER SER LYS SER LYS GLY • Molecule 24: Large ribosomal subunit protein bL28 8% Chain V: 66% 15% 19% MET GLY GLY GLN GLN CYS CYS PHE VAL VAL VAL VAL THR GLY GLY GLY • Molecule 25: Large ribosomal subunit protein uL29



Chain W:	78%	10%	12%	
MET MET LYS CLN GLN MET K6 L13 S24 S24 S24	KB2 KB2 F59 F663 R64 ALA ALA ALA ALA ALA			
• Molecule 26: 1	Large ribosomal subunit protein uL30			
Chain X:	92%		7% •	
MET A2 42 45 118 718 749 658 858 858	n e			
• Molecule 27: 1	Large ribosomal subunit protein bL32			
Chain Z:	67%	7% 26%		
MET A2 R16 K21 M27 M27 C30 C30	1132 C173 C174 C173 C174			
• Molecule 28: 1	Large ribosomal subunit protein uL5			
Chain F:	28%	11% •	17%	I
MET N2 L4 K5 E5 E6 F8 N9 N9	LIU LIU VIJ2 E14 MI7 MI7 MI7 MI7 MI7 MI7 MI7 MI7	VAL L50 D51 N52 N52 N54 E55 E55	L59 I60	K69 A70 LY7 LY8 SER LY8 A1A A1A A1A A1A A1A A1A A1A
LEU R80 B81 K88 K88 K88 K88 K88 K89 V89 V89 M96	1104 1104 1104 1108 1108 1108 1108 1108 1108 1108 1108 1108 1108 1108 11108 11108 11108 1111 11128 11129 111	0135 1137 1137 1137 1137 1137 1138 1138 1146 1146 1146 1146 1146 1146	ASP LYS V146 \$147 ¥148	V149 H150 G151 1156 V155 V155 T156
D163 R167 E168 L170 A171 A171 A172 F173 F173	M175 P176 ARG LYS			
• Molecule 29: 1	E-site tRNA molecule			
Chain 11:	33% 53%		13%	
G1 C2 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	G71 C72 A73 A76 C74 A76			
• Molecule 30: 2	23S ribosomal RNA			
Chain A:	62%	24% •	12%	
G A U4 A5 A5 G15 G15 G24 C2	42 C30 C31 C30 C31 C31 C32 C32 C32 C32 C32 C32 C32 C32	079 884 931 093 093 093 093	6101 A110 A117	A118 U19 A124 A125









• Molecule 32: Small ribosomal subunit protein bS6



Chain Af:	80%	17% •
M1 R2 R11 L22 L22 K41 W43 G44 V43	455 152 152 152 153 153 153 153 153 153 153 153 153 153	
• Molecule 33:	Small ribosomal subunit protein uS7	
Chain Ag:	88%	10% ••
MET P2 117 117 841 841 871	V75 V75 R92 R92 R10 R10 R10 R10 R10 R10 R10 R10 R10 R10	
• Molecule 34:	Small ribosomal subunit protein uS9	
Chain Ai:	82%	14% •
MET THR LLEU ALA GLN V6 V8 V8 R9 R9 R9 R9 R9	147 148 149 159 159 159 181 181 181 181 181 181 181 181 181 18	
• Molecule 35:	Small ribosomal subunit protein uS12	
Chain Al:	90%	8% •
MET P2 S21 N25 N25 N30 N30 N30 N30 N30 N30 N30 N30 N30 N30	T48 LYS LYS F86 R63 R63 R63 R63 R63 R63 R63 R63 A100 A100 A100 A100 A100	
• Molecule 36:	Small ribosomal subunit protein uS15	
Chain Ao:	79%	20% •
MET A2 K13 F14 E14 F16 R16 F19 E19 E19	N 400 E 41 E 41 K 44 K 46 K 47 K 46 K 47 K 46 K 73 K 73 K 73 K 73 K 73 K 73 K 73 K 73	
• Molecule 37:	Small ribosomal subunit protein bS16	
Chain Ap:	82%	15% ·
MET A2 V3 V3 15 R6 R14 P16 P16	A23 D24 D24 T43 T43 T74 T74 T74 T74 T74 T78 T78 T78 T78 T78 T78 T78 T78 T78 T78	
• Molecule 38:	Small ribosomal subunit protein uS17	
Chain Aq:	67% 18%	15%
MET SER SER CLU R4 R4 D17 LYS LYS ASP ASP	THE THE THE THE THE THE THE THE THE THE	
• Molecule 39:	Small ribosomal subunit protein bS18	



Chain Ar:	54%		14%	32%
MET ALA GLY GLY PRO ARG ARG GLY	GLY ARG ARG ARG LYS LYS LYS VAL CYS TTR PHE TTR ASU ASU GLY	116 124 124 124 124 123 123 133 133 138 169	R66 R66 L173 K77 GLU GLU GLU GLU	
• Molecule	40: Small ribosom	al subunit protein	n bS20	
Chain At:		84%		12% ••
MET A2 E18 N21 I22	K25 130 130 130 130 130 130 150 165 165 165 165	81 N82 LYS		
• Molecule	41: 16S ribosomal	RNA		
Chain Aa:	57	%	33%	• 7%
и А 63 83 83	010 U18 C19 C19 C19 C29 C32 C33 A33 A33 C35 C35 C35 C35	C36 C37 C37 C38 C39 C39 C39 C40 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	G58 G58 U63 C64 C68 C68 G68 G68 G68 G68 G71	072 073 6074 6 6 7 7 4 8 8 8 8 8 9 8 9 0 0 0 0 0 0 0 0 0 0 0 0
	G A 096 098 098 098 098 0198 A1100 A119 C120 C120 C120 C120	U124 A140 A141 C144 U145 C144 C144 C144 C144 C148 C148 A150	A152 C153 U154 U155 C155 C155 C156 C157 C156 C158 A160 A161 A162 A162	C163 C165 C166 C166 A171 A171 A172 A172 A174 A174 A183 A184
U185 U186 U187 U188 G189 A190 A191 C192	C193 C194 C195 C195 C202 A203 A204 A206 A206 C207 C207 C207 C207 C213	d217 0218 0219 0220 0221 0222 0223 0228 0228 0228 0228	A228 1237 12243 1253 1254 1255 1255	0259 0264 0264 0265 0266 0272 0272 0274 0274 0274 0274 0274
A278 C279 A286 A290 G297	C302 C302 C304 C305 C305 C305 C306 C306 C306 C317 C326 C326 C326 C326 C326 C328	A329 (3330 (3332 (3332 (3332) (3332) (3345 (3345) (3345) (3345) (3345) (3345)	U351 U351 A352 C353 C355 C355 C356 C356 C356 C360 C360 C360 C362 C362	U375 C380 C380 C380 A381 C384 A381 C384 C388 C388 C388
(3399 (400 (401 (407 (407 (408 (414	U4 17 04 18 04 19 0 0 04 21 04 29 04 29 04 29 04 31 04 29 04 31 04 32	0436 0437 0437 0437 0439 0441 0445 0446 0446 0446 0446	6455 4456 4457 4458 4459 4459 4460 0461 0462 0462 0468	0469 0471 0471 0473 0475 0475 0484 0482 0483 0484 0487
6492 6493 1494 8495 6496 6496 A499 A500	US01 US02 A503 A503 A505 C504 C509 C509 C510 C512 C512 C512 A518 A518	C519 C526 C526 C527 A521 C530 C530 C533 C533 C533 C533 C533 C533	A540 A547 A547 G548 G549 U550 C553 A554 A555	C563 C563 C565 C565 C565 A567 A567 U557 U577 A580 A580 A581 A581
C584 C586 C586 C586 C588 C588 C588 C588 C588	U602 669 6618 6618 6618 6618 6626 6626 8629 10641	A650 A651 U661 U665 A672 A673 A673	0002 U885 U886 U886 C687 U886 0691 0693 0693 0693	0000 0000 0000 0000 0000 0000 0000 0000 0000
6721 6722 6723 4723 0731 6732	A736 A737 U746 U746 C749 G749 C758 U759 C758 C758	CT63 CT64 UT665 CT72 CT72 CT77 A785 A785	A802 C803 A810 G811 A810 A824 A824 A824 C825 C825 C825 C825	A830 831 833 834 834 834 834 834 834 834 834 834
G C855 C856 U860 A873 A874	C877 A878 A878 A881 A881 C884 C884 C884 C885 C885 C885 C885 C885	C902 C903 A904 A905 A910 C911 C915 A916 A917 A917 A917	A922 A923 U929 G931 C933 C933 C935 C935 C935	C943 A944 A947 G948 G954 G955 G955 G955 G955 G956
(963 1964 1964 1966 1969 1969 1970	(1975 (1976 (1977 (1977) (1986) (1986) (1986) (1986) (1991) (1991)	A992 C3934 A995 A996 A996 A997 A997 C399 U1001 U1001 C1002	A1003 A1005 C 1004 C C C C C C C C C C C C C C C C C C C	C A A C C C C C C C C C C C C C C C C C









• Molecule 50: Sn	nall ribosomal subunit pro	tein uS19		
Chain As:	79%		10% 11%	
MET A 2 8 3 8 4 8 4 7 8 4 0 12 8 35 8 35 8 35	R55 K56 H57 D65 H65 A56 H69 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12			
• Molecule 51: ml	RNA molecule			
Chain d:	42%	53%	5%	
G1 G2 G3 G4 G5 G5 G5 G7 C15 C15 C15 C15 C15 C15 C15 C15 C15 C15	A23 V24 A25			
• Molecule 52: P-	site tRNA molecule			
Chain 8:	59% 58%	31%	11%	
C1 C2 C3 C3 C3 C3 C3 C3 C4 C4 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	A11 612 612 613 613 615 615 623 623 623 633 633 633 633 647	C49 G50 G51 G51 G53 G53 G53 G53 G53 G53 G53 G57 A58 A59	A60 U61 C62 C63 C65 C65 C65	U67 068 069 070 071 071 473 473 473 473 477 477
• Molecule 53: A-	site tRNA molecule			
Chain 9:	40%	60%		
U34 A35 C366 A37 A38				
• Molecule 54: La	rge ribosomal subunit pro	tein bL31B		
Chain 13:	64%	·	32%	
M1 K2 GLY GLY HILE HILE FRD FRD FRD HID H112 (11	113 F14 LEU ASP ASN F21 K22 F23 F23 F23 F23 F23 F23 F23 F23 F23 F	SER SER GLU MET MET M35 E36 E36 E36 E36 C40 C40 C40 C40 C41 C41 C41 C41 C41 C41 C41 C41 C41 C41	P44 V45 ILE ARG LEU D49 I 50	SER SER ASP B54 P56 P56 P1HE T1YR GLIY GLIY R61
162 K63 F64 R81 ASN ASN				



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	408831	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	67.143	Depositor
Minimum map value	-30.208	Depositor
Average map value	0.061	Depositor
Map value standard deviation	1.435	Depositor
Recommended contour level	3	Depositor
Map size (Å)	362.56, 362.56, 362.56	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MG, MG, G7M, EM1, K, 5MC, 5MU, 2MA, OMG, UR3, PSU, ZN, 4OC, H2U

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	l angles
	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5
1	1	0.13	0/360	0.30	0/489
2	2	0.16	0/372	0.33	0/487
3	3	0.17	0/513	0.35	0/678
4	4	0.15	0/283	0.32	0/376
5	В	0.14	0/2692	0.27	0/4193
6	С	0.15	0/2072	0.33	0/2792
7	D	0.16	0/1606	0.39	0/2159
8	Е	0.16	0/1533	0.33	0/2077
9	G	0.14	0/953	0.31	0/1301
10	Н	0.19	0/1162	0.38	0/1566
11	Ι	0.15	0/871	0.33	0/1177
12	J	0.15	0/1071	0.35	0/1433
13	К	0.17	0/1048	0.35	0/1420
14	L	0.18	0/904	0.34	0/1209
15	М	0.15	0/810	0.32	0/1102
16	N	0.13	0/811	0.29	0/1099
17	0	0.19	0/955	0.35	0/1265
18	Р	0.14	0/762	0.31	0/1025
19	Q	0.18	0/822	0.37	0/1113
20	R	0.15	0/671	0.33	0/904
21	S	0.14	0/642	0.31	0/868
22	Т	0.14	0/606	0.32	0/828
23	U	0.15	0/581	0.34	0/776
24	V	0.13	0/363	0.31	0/489
25	W	0.11	0/474	0.24	0/637
26	Х	0.16	0/440	0.34	0/594
27	Ζ	0.17	0/339	0.36	0/451
28	F	0.13	0/923	0.31	0/1260
29	11	0.13	0/358	0.24	0/552
30	А	0.19	0/61919	0.35	0/96529
31	Ae	0.19	0/1144	0.33	0/1547
32	Af	0.16	0/745	0.30	0/1006



Mal	Chain	Bond lengths		Bond	l angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
33	Ag	0.24	0/1240	0.30	0/1668
34	Ai	0.24	0/991	0.31	0/1334
35	Al	0.21	0/1027	0.33	0/1381
36	Ao	0.18	0/736	0.29	0/984
37	Ap	0.24	0/690	0.38	0/934
38	Aq	0.19	0/558	0.36	0/753
39	Ar	0.19	0/452	0.30	0/604
40	At	0.21	0/593	0.26	0/794
41	Aa	0.26	0/34383	0.32	0/53582
42	Aj	0.23	0/729	0.35	0/986
43	Ac	0.25	0/1499	0.31	0/2036
44	Am	0.21	0/851	0.31	0/1145
45	Ak	0.14	0/772	0.28	0/1050
46	Ab	0.10	0/630	0.24	0/858
47	Ah	0.22	0/1044	0.32	0/1401
48	Ad	0.18	0/1532	0.29	0/2071
49	An	0.25	0/512	0.29	0/678
50	As	0.24	0/634	0.29	0/858
51	d	0.15	0/461	0.31	0/715
52	8	0.14	0/1695	0.27	0/2634
53	9	0.14	0/118	0.31	0/181
54	13	0.13	0/386	0.23	0/515
All	All	0.21	0/140338	0.33	0/210564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	355	0	316	4	0
2	2	368	0	409	5	0
3	3	508	0	544	5	0



Continuea from previous page						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	280	0	302	4	0
5	В	2408	0	1217	34	0
6	С	2037	0	2106	11	0
7	D	1582	0	1604	12	0
8	Ε	1510	0	1533	14	0
9	G	944	0	636	10	0
10	Н	1140	0	1130	10	0
11	Ι	865	0	886	9	0
12	J	1057	0	1084	6	0
13	K	1024	0	1023	8	0
14	L	901	0	942	8	0
15	М	801	0	712	12	0
16	N	800	0	767	7	0
17	0	943	0	1014	7	0
18	Р	752	0	761	7	0
19	Q	814	0	854	9	0
20	R	664	0	666	5	0
21	S	635	0	605	6	0
22	Т	600	0	540	5	0
23	U	575	0	568	2	0
24	V	360	0	353	4	0
25	W	473	0	472	4	0
26	Х	438	0	472	2	0
27	Z	333	0	348	2	0
28	F	914	0	695	12	0
29	11	322	0	167	7	0
30	А	55514	0	27922	397	0
31	Ae	1130	0	1188	15	0
32	Af	734	0	705	10	0
33	Ag	1222	0	1255	12	0
34	Ai	975	0	979	12	0
35	Al	1011	0	1036	4	0
36	Ao	727	0	754	8	0
37	Ap	679	0	684	9	0
38	Aq	551	0	528	10	0
39	Ar	445	0	482	5	0
40	At	593	0	634	5	0
41	Aa	30880	0	15569	314	0
42	Aj	720	0	698	9	0
43	Ac	1477	0	1437	20	0
44	Am	845	0	865	17	0
45	Ak	759	0	706	14	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Ab	629	0	463	6	0
47	Ah	1032	0	1082	13	0
48	Ad	1502	0	1440	16	0
49	An	502	0	523	8	0
50	As	617	0	591	7	0
51	d	412	0	207	5	0
52	8	1519	0	775	18	0
53	9	106	0	55	2	0
54	13	382	0	288	2	0
55	1	1	0	0	0	0
55	4	1	0	0	0	0
55	An	1	0	0	0	0
55	Ζ	1	0	0	0	0
56	А	170	0	0	0	0
56	Aa	59	0	0	0	0
56	С	1	0	0	0	0
56	D	1	0	0	0	0
57	А	60	0	65	0	0
58	А	15	0	0	0	0
58	Aa	3	0	0	0	0
59	А	574	0	0	1	0
59	Aa	15	0	0	0	0
59	С	16	0	0	0	0
59	D	2	0	0	0	0
59	J	7	0	0	0	0
59	Ν	3	0	0	0	0
59	0	2	0	0	0	0
59	P	1	0	0	0	0
59	R	1	0	0	0	0
All	All	130300	0	83657	1058	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 5.

All (1058) 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)
44:Am:79:ARG:HH12	50:As:69:HIS:HE1	1.20	0.85
7:D:3:LYS:HD2	7:D:109:THR:HG22	1.58	0.85
30:A:788:A:O2'	30:A:1703:U:OP1	1.96	0.82
10:H:126:TYR:HH	10:H:133:HIS:HE2	1.23	0.81



A 4 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:B:87:U:H3	30:A:1002:U:H3	1.27	0.79
52:8:52:U:H3	52:8:64:G:H1	1.33	0.77
47:Ah:34:LYS:HG2	47:Ah:60:LEU:HD21	1.68	0.75
10:H:1:MET:SD	10:H:1:MET:N	2.51	0.75
41:Aa:1058:G:H21	41:Aa:1223:A:H2	1.33	0.74
30:A:159:U:H3	30:A:169:G:H1	1.35	0.74
41:Aa:672:G:H22	41:Aa:749:G:H1	1.33	0.74
41:Aa:685:U:H3	41:Aa:721:G:H22	1.36	0.73
41:Aa:18:U:H2'	41:Aa:19:C:C6	2.24	0.73
30:A:1886:A:N6	30:A:1910:G:O2'	2.22	0.72
18:P:47:LYS:HD2	18:P:102:ALA:HB1	1.72	0.71
41:Aa:161:A:N1	41:Aa:355:G:O2'	2.22	0.71
43:Ac:94:THR:HG22	43:Ac:96:LYS:HG3	1.73	0.71
52:8:19:G:H21	52:8:59:A:H5'	1.55	0.71
32:Af:2:ARG:HG2	32:Af:93:ARG:HH21	1.55	0.70
14:L:13:ARG:NH2	30:A:2717:A:OP2	2.25	0.70
25:W:52:LYS:NZ	30:A:75:G:O2'	2.22	0.70
44:Am:11:ARG:HA	44:Am:45:VAL:HG22	1.74	0.70
41:Aa:665:U:H3	41:Aa:757:A:H62	1.37	0.70
41:Aa:184:A:N1	41:Aa:207:G:O6	2.24	0.69
30:A:221:G:H22	30:A:238:U:H4'	1.56	0.69
30:A:2355:A:H2'	30:A:2356:A:C8	2.27	0.69
4:4:31:LYS:HE2	30:A:2505:A:H5'	1.75	0.69
31:Ae:115:LEU:HD13	31:Ae:123:ILE:HG21	1.73	0.69
34:Ai:79:GLN:HG2	34:Ai:82:ARG:HH21	1.58	0.69
12:J:18:ARG:NH2	30:A:1288:G:N7	2.41	0.68
41:Aa:955:A:H2'	41:Aa:956:G:C8	2.29	0.68
28:F:35:VAL:HG23	28:F:155:VAL:HB	1.75	0.68
24:V:35:LYS:HD2	24:V:46:LYS:HE3	1.75	0.67
41:Aa:1188:G:N2	41:Aa:1191:G:OP2	2.27	0.67
41:Aa:1058:G:N2	41:Aa:1221:U:O2	2.28	0.67
41:Aa:681:G:H2'	41:Aa:682:G:C8	2.30	0.67
34:Ai:50:LEU:HA	34:Ai:82:ARG:HB2	1.76	0.67
33:Ag:102:ARG:NH2	41:Aa:948:G:OP1	2.28	0.67
41:Aa:1179:A:H2'	41:Aa:1180:A:C8	2.30	0.66
30:A:275:A:H8	30:A:304:G:H21	1.42	0.66
44:Am:16:VAL:HG13	44:Am:34:LEU:HD12	1.76	0.66
5:B:39:G:N7	28:F:69:LYS:NZ	2.40	0.66
30:A:672:A:H61	30:A:682:A:H5"	1.61	0.66
47:Ah:47:LYS:HG3	47:Ah:65:LYS:HG3	1.77	0.66
52:8:63:C:H2'	52:8:64:G:C8	2.31	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:2318:U:H2'	30:A:2319:U:C6	2.31	0.65
41:Aa:1484:G:H2'	41:Aa:1485:G:C8	2.31	0.65
52:8:19:G:N2	52:8:59:A:OP2	2.29	0.65
18:P:67:ARG:NH2	30:A:1261:G:OP1	2.29	0.65
30:A:1916:A:H2'	30:A:1917:A:C8	2.32	0.64
30:A:75:G:H22	30:A:110:A:H2	1.45	0.64
41:Aa:831:G:HO2'	47:Ah:2:THR:N	1.96	0.64
45:Ak:19:GLY:HA2	45:Ak:36:ASP:HA	1.79	0.64
31:Ae:108:GLY:HA2	41:Aa:9:A:H1'	1.79	0.64
41:Aa:1336:U:H2'	41:Aa:1337:A:H8	1.63	0.64
8:E:174:GLN:NE2	8:E:185:ASP:OD2	2.30	0.63
41:Aa:1135:G:N2	41:Aa:1136:U:O4	2.32	0.63
30:A:921:C:H42	30:A:946:A:H61	1.45	0.63
41:Aa:99:U:H2'	41:Aa:100:A:C8	2.34	0.63
41:Aa:1435:A:H2'	41:Aa:1436:A:H8	1.64	0.63
15:M:8:ASN:OD1	15:M:11:ARG:NH2	2.29	0.63
32:Af:69:ASN:O	32:Af:70:ASN:ND2	2.32	0.63
37:Ap:14:ARG:NH2	41:Aa:401:A:OP1	2.32	0.62
41:Aa:721:G:H2'	41:Aa:722:G:C8	2.33	0.62
30:A:291:G:H2'	30:A:292:U:C6	2.35	0.62
50:As:65:ASP:HA	54:13:70:ARG:HG3	1.80	0.62
5:B:38:U:N3	5:B:42:G:OP2	2.20	0.62
17:O:74:MET:HE2	17:O:79:LEU:HA	1.82	0.62
30:A:1442:C:H2'	30:A:1443:A:H8	1.64	0.62
47:Ah:117:GLU:OE1	47:Ah:121:ARG:NH2	2.26	0.62
26:X:18:THR:OG1	26:X:49:LYS:NZ	2.31	0.62
34:Ai:113:LYS:NZ	41:Aa:1381:G:N7	2.48	0.62
41:Aa:148:G:H1	41:Aa:174:A:H61	1.48	0.62
41:Aa:461:C:H5	41:Aa:487:U:H3	1.46	0.62
14:L:24:LEU:HD23	14:L:44:VAL:HG21	1.81	0.61
30:A:631:U:H2'	30:A:632:U:C6	2.34	0.61
30:A:1513:A:H2'	30:A:1514:A:C8	2.36	0.61
28:F:36:VAL:HG22	28:F:154:ILE:HD12	1.82	0.61
30:A:172:U:H2'	30:A:173:A:H8	1.65	0.61
38:Aq:29:THR:HG22	38:Aq:30:TYR:H	1.66	0.61
21:S:92:ARG:HB3	21:S:101:ILE:HG13	1.83	0.61
30:A:830:U:H2'	30:A:831:C:C6	2.36	0.61
28:F:129:THR:HG22	28:F:155:VAL:HG22	1.82	0.61
30:A:702:U:H2'	30:A:703:A:C8	2.36	0.61
41:Aa:147:G:H2'	41:Aa:148:G:C8	2.35	0.61
30:A:787:U:H2'	30:A:788:A:C8	2.36	0.60



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
30:A:172:U:H2'	30:A:173:A:C8	2.36	0.60
44:Am:3:ARG:O	44:Am:57:ARG:NH1	2.34	0.60
9:G:3:ARG:NH2	30:A:1156:G:O3'	2.33	0.60
31:Ae:38:VAL:HG12	31:Ae:117:LEU:HD12	1.83	0.60
41:Aa:1236:C:N4	44:Am:103:LYS:HG3	2.16	0.60
30:A:2618:C:H2'	30:A:2619:G:C8	2.36	0.60
41:Aa:1276:G:N2	41:Aa:1279:A:OP2	2.25	0.60
41:Aa:963:G:H21	41:Aa:1237:A:H62	1.49	0.60
9:G:110:SER:OG	30:A:2694:C:N3	2.33	0.60
30:A:901:G:H2'	30:A:902:A:C8	2.36	0.60
30:A:2825:U:H2'	30:A:2826:U:C6	2.37	0.60
43:Ac:27:ASP:OD2	43:Ac:27:ASP:N	2.35	0.60
41:Aa:1370:A:OP2	49:An:35:ARG:NH2	2.36	0.59
30:A:1675:G:H1'	30:A:1679:A:N6	2.18	0.59
34:Ai:101:LYS:NZ	41:Aa:1188:G:N7	2.42	0.59
30:A:684:U:H2'	30:A:685:C:C6	2.36	0.59
30:A:1594:U:HO2'	30:A:1595:C:H6	1.48	0.59
41:Aa:1490:A:H2'	41:Aa:1491:A:H8	1.65	0.59
5:B:22:G:H4'	5:B:23:U:H5	1.68	0.59
41:Aa:1097:U:H3	41:Aa:1110:G:H22	1.49	0.59
41:Aa:1228:U:H2'	41:Aa:1229:U:C6	2.37	0.59
32:Af:69:ASN:HB2	32:Af:71:LYS:NZ	2.18	0.59
4:4:17:ILE:HD12	4:4:19:ARG:HG3	1.85	0.59
30:A:1823:U:H2'	30:A:1824:C:C6	2.37	0.59
30:A:2260:A:H2'	30:A:2261:G:C8	2.38	0.59
53:9:34:U:H2'	53:9:35:A:C8	2.38	0.58
31:Ae:108:GLY:HA3	41:Aa:10:G:H5'	1.85	0.58
38:Aq:45:LYS:NZ	41:Aa:286:A:OP2	2.36	0.58
12:J:110:LYS:HE2	12:J:127:LYS:HD3	1.83	0.58
30:A:632:U:H2'	30:A:633:A:C8	2.38	0.58
30:A:754:U:H2'	30:A:755:C:C6	2.38	0.58
41:Aa:1025:A:HO2'	41:Aa:1227:U:HO2'	1.50	0.58
41:Aa:1366:G:H2'	41:Aa:1367:A:C8	2.39	0.58
30:A:302:A:H2'	30:A:303:G:H8	1.69	0.58
41:Aa:744:U:H2'	41:Aa:745:U:C6	2.39	0.58
41:Aa:1297:A:H2'	41:Aa:1298:A:C8	2.38	0.58
14:L:52:LYS:NZ	14:L:96:ARG:O	2.37	0.58
30:A:302:A:H2'	30:A:303:G:C8	2.39	0.58
30:A:858:U:H2'	30:A:859:C:C6	2.38	0.58
43:Ac:90:LEU:HD12	43:Ac:100:ILE:HD11	1.85	0.58
30:A:1442:C:H2'	30:A:1443:A:C8	2.37	0.58



A + a 1	At and 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:1829:A:H2'	30:A:1830:A:C8	2.39	0.57
8:E:148:GLN:NE2	8:E:191:SER:OG	2.37	0.57
30:A:1353:A:H2'	30:A:1354:G:C8	2.39	0.57
33:Ag:92:ARG:NH2	41:Aa:1387:A:OP1	2.37	0.57
41:Aa:1133:U:O4	41:Aa:1134:A:N6	2.38	0.57
45:Ak:20:VAL:N	45:Ak:35:THR:O	2.26	0.57
28:F:70:ALA:HB2	28:F:85:ILE:HD11	1.84	0.57
41:Aa:499:A:H2'	41:Aa:500:A:H8	1.69	0.57
41:Aa:777:G:H4'	41:Aa:1524:A:H4'	1.86	0.57
41:Aa:1306:C:H4'	41:Aa:1312:U:O4	2.04	0.57
30:A:221:G:N2	30:A:238:U:H4'	2.19	0.57
41:Aa:1213:C:OP1	49:An:2:ALA:N	2.38	0.57
41:Aa:1497:G:H2'	41:Aa:1498:G:C8	2.40	0.57
8:E:27:GLU:CD	8:E:27:GLU:H	2.12	0.57
32:Af:22:LEU:H	32:Af:22:LEU:HD23	1.68	0.57
41:Aa:824:A:OP1	41:Aa:1537:G:O2'	2.21	0.57
10:H:1:MET:HA	30:A:1039:C:C5	2.40	0.57
21:S:9:VAL:HG12	21:S:70:LEU:HD23	1.87	0.57
41:Aa:991:U:H4'	41:Aa:992:A:H5'	1.87	0.57
13:K:58:MET:HE1	13:K:64:VAL:HG22	1.87	0.57
41:Aa:32:G:O2'	41:Aa:49:C:N4	2.38	0.57
41:Aa:955:A:H2'	41:Aa:956:G:H8	1.69	0.57
28:F:129:THR:HG21	30:A:2330:G:H21	1.70	0.56
30:A:1241:A:H2'	30:A:1242:A:C8	2.40	0.56
41:Aa:186:U:H2'	41:Aa:187:U:C6	2.40	0.56
41:Aa:1058:G:N1	41:Aa:1221:U:N3	2.53	0.56
17:O:105:ALA:HB1	18:P:40:PHE:HZ	1.70	0.56
41:Aa:1333:G:H2'	41:Aa:1334:A:C8	2.41	0.56
9:G:2:SER:HB2	9:G:5:GLY:H	1.70	0.56
24:V:35:LYS:HG3	24:V:48:TRP:CE2	2.40	0.56
30:A:2354:A:H2'	30:A:2355:A:C8	2.41	0.56
30:A:1791:G:N7	59:A:3211:HOH:O	2.33	0.56
16:N:22:PHE:O	16:N:52:ARG:NH1	2.38	0.56
16:N:102:LEU:HD11	16:N:112:ILE:HD11	1.88	0.56
38:Aq:71:ALA:HB2	41:Aa:274:G:H3'	1.88	0.56
41:Aa:345:G:H2'	41:Aa:346:A:C8	2.41	0.56
41:Aa:532:G:H2'	41:Aa:533:C:C6	2.41	0.56
52:8:4:G:H2'	52:8:5:G:H8	1.71	0.56
30:A:687:G:N2	30:A:690:U:OP2	2.36	0.56
41:Aa:736:A:H2'	41:Aa:737:A:C8	2.41	0.56
41:Aa:1435:A:H2'	41:Aa:1436:A:C8	2.40	0.56



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:441:C:H2'	30:A:442:G:H8	1.71	0.56
30:A:1571:G:N2	30:A:1593:G:O6	2.39	0.55
41:Aa:473:U:O2'	41:Aa:475:A:N7	2.27	0.55
50:As:12:ASP:OD2	50:As:35:SER:OG	2.24	0.55
30:A:1357:G:C2	30:A:1366:U:H5"	2.41	0.55
30:A:1712:A:O2'	30:A:1718:G:N7	2.32	0.55
30:A:877:G:H2'	30:A:878:C:C6	2.41	0.55
2:2:2:VAL:N	30:A:1663:G:HO2'	2.05	0.55
18:P:78:ARG:NH2	30:A:606:G:OP2	2.31	0.55
20:R:69:GLN:NE2	20:R:70:GLY:O	2.39	0.55
30:A:1884:G:N2	30:A:1912:A:C2	2.72	0.55
41:Aa:1180:A:H2'	41:Aa:1181:A:O4'	2.06	0.55
11:I:88:ARG:HG2	11:I:94:ARG:HD3	1.89	0.55
30:A:3:U:H2'	30:A:4:U:C6	2.42	0.55
30:A:2618:C:H2'	30:A:2619:G:H8	1.71	0.55
43:Ac:22:TRP:HB3	43:Ac:58:ARG:HB2	1.89	0.55
11:I:113:LYS:HZ2	11:I:117:LEU:HD11	1.72	0.55
30:A:2331:G:H1	30:A:2339:U:H3	1.55	0.55
11:I:35:ILE:HG21	11:I:103:ALA:HB3	1.88	0.55
26:X:5:GLN:HB3	26:X:57:GLU:HG3	1.87	0.55
30:A:1575:A:H2'	30:A:1576:A:C8	2.42	0.55
30:A:259:A:H2'	30:A:260:A:C8	2.42	0.55
30:A:1044:A:H2'	30:A:1045:A:C8	2.41	0.55
41:Aa:1153:G:H2'	41:Aa:1154:G:H8	1.71	0.55
41:Aa:553:C:OP1	48:Ad:54:LYS:NZ	2.39	0.54
41:Aa:1401:U:H2'	41:Aa:1402:G:C8	2.41	0.54
41:Aa:1420:A:H2'	41:Aa:1421:C:C6	2.43	0.54
30:A:2052:C:H2'	30:A:2053:U:C6	2.42	0.54
30:A:2101:U:H2'	30:A:2102:U:C6	2.42	0.54
32:Af:69:ASN:HB2	32:Af:71:LYS:HZ3	1.71	0.54
8:E:174:GLN:HE22	8:E:185:ASP:CG	2.16	0.54
13:K:54:MET:O	13:K:58:MET:HG3	2.08	0.54
30:A:259:A:H2'	30:A:260:A:H8	1.73	0.54
41:Aa:1489:A:H2'	41:Aa:1490:A:C8	2.42	0.54
48:Ad:8:ASN:O	48:Ad:12:SER:OG	2.23	0.54
41:Aa:1082:C:H2'	41:Aa:1083:G:H8	1.71	0.54
41:Aa:1336:U:H2'	41:Aa:1337:A:C8	2.41	0.54
36:Ao:41:GLU:HA	36:Ao:44:ARG:HE	1.71	0.54
41:Aa:390:A:H2'	41:Aa:391:A:C8	2.43	0.54
30:A:525:A:H1'	30:A:526:A:H5"	1.89	0.54
30:A:632:U:H2'	30:A:633:A:H8	1.71	0.54


Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
34:Ai:131:LYS:O	41:Aa:975:2MG:O2'	2.26	0.54
44:Am:79:ARG:HH12	50:As:69:HIS:CE1	2.12	0.54
6:C:150:LYS:HD2	30:A:2231:C:H4'	1.90	0.54
41:Aa:499:A:H2'	41:Aa:500:A:C8	2.43	0.54
45:Ak:35:THR:HB	45:Ak:41:ALA:HA	1.88	0.54
52:8:15:G:N2	52:8:49:C:O2	2.38	0.54
30:A:2232:A:H2'	30:A:2233:C:C6	2.42	0.54
30:A:2654:G:O2'	30:A:2808:A:N1	2.38	0.54
30:A:69:C:H4'	30:A:75:G:N7	2.23	0.54
30:A:156:A:O2'	30:A:157:U:H5"	2.08	0.54
30:A:2705:U:H2'	30:A:2706:A:C8	2.42	0.54
30:A:2817:A:O2'	30:A:2818:A:O5'	2.22	0.54
41:Aa:1161:A:HO2'	41:Aa:1162:A:H8	1.56	0.54
3:3:60:GLN:HE21	3:3:60:GLN:HA	1.73	0.54
6:C:180:GLU:OE2	30:A:1826:G:O2'	2.24	0.54
19:Q:8:ARG:NH1	30:A:539:G:OP1	2.36	0.54
30:A:955:A:H2'	30:A:956:A:C8	2.43	0.54
30:A:1329:G:H2'	30:A:1330:U:C6	2.43	0.54
17:O:66:ASN:O	17:O:70:ARG:HG2	2.09	0.53
19:Q:35:ILE:HG13	27:Z:27:MET:HE1	1.89	0.53
30:A:395:U:H2'	30:A:396:G:H8	1.73	0.53
30:A:1823:U:H2'	30:A:1824:C:H6	1.71	0.53
30:A:2270:U:H2'	30:A:2271:U:C6	2.43	0.53
41:Aa:222:G:H2'	41:Aa:223:C:C6	2.42	0.53
30:A:2817:A:H5"	30:A:2912:A:H2	1.73	0.53
32:Af:45:LYS:HE2	32:Af:59:PHE:CZ	2.44	0.53
41:Aa:917:A:H2'	41:Aa:918:A:C8	2.44	0.53
30:A:422:G:H2'	30:A:423:A:C8	2.44	0.53
30:A:2672:G:H4'	30:A:2759:G:O2'	2.08	0.53
36:Ao:18:HIS:ND1	36:Ao:19:GLU:O	2.41	0.53
41:Aa:302:C:OP1	41:Aa:618:G:O2'	2.22	0.53
9:G:3:ARG:NH1	30:A:2778:G:OP2	2.41	0.53
7:D:156:MET:O	30:A:2079:G:H4'	2.08	0.53
41:Aa:307:G:H2'	41:Aa:308:A:C8	2.44	0.53
41:Aa:1107:C:H2'	41:Aa:1108:C:H6	1.74	0.53
42:Aj:24:LYS:HG2	42:Aj:90:LEU:HD11	1.91	0.53
41:Aa:1137:U:N3	41:Aa:1290:A:OP1	2.40	0.53
6:C:29:PRO:HG2	6:C:34:LEU:HD11	1.90	0.53
41:Aa:1423:A:H61	41:Aa:1498:G:H1	1.54	0.53
47:Ah:43:GLU:HG2	47:Ah:103:ILE:HG21	1.91	0.53
30:A:2220:U:H2'	30:A:2221:U:H6	1.72	0.53



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
9:G:3:ARG:HD2	30:A:2778:G:C8	2.44	0.53
43:Ac:35:ASP:O	43:Ac:39:ARG:HG3	2.08	0.53
30:A:577:A:H4'	30:A:578:G:C8	2.44	0.52
30:A:2232:A:H2'	30:A:2233:C:H6	1.74	0.52
41:Aa:1261:A:H2'	41:Aa:1262:A:C8	2.44	0.52
41:Aa:1488:C:H2'	41:Aa:1489:A:H8	1.73	0.52
15:M:92:ILE:HD13	15:M:117:LEU:HD13	1.91	0.52
30:A:2294:A:H5"	30:A:2295:A:H5'	1.91	0.52
41:Aa:160:A:H2'	41:Aa:161:A:O4'	2.10	0.52
45:Ak:85:THR:HB	45:Ak:113:VAL:HG21	1.91	0.52
1:1:21:ILE:HD13	30:A:2446:U:H5"	1.90	0.52
14:L:59:ARG:HA	14:L:86:PHE:CZ	2.44	0.52
28:F:32:ASP:N	28:F:157:VAL:O	2.42	0.52
5:B:6:U:OP1	15:M:11:ARG:NH1	2.38	0.52
30:A:1337:A:H4'	30:A:1338:U:H5"	1.92	0.52
30:A:1353:A:H2'	30:A:1354:G:H8	1.74	0.52
41:Aa:873:A:H2'	41:Aa:874:A:C8	2.44	0.52
41:Aa:1437:C:H2'	41:Aa:1438:A:H8	1.75	0.52
49:An:42:ILE:O	49:An:46:GLU:HG3	2.09	0.52
51:d:22:U:H2'	51:d:23:A:C8	2.45	0.52
11:I:88:ARG:NE	11:I:90:ASP:OD2	2.41	0.52
30:A:441:C:H2'	30:A:442:G:C8	2.44	0.52
41:Aa:190:A:H2'	41:Aa:191:A:H8	1.75	0.52
15:M:32:ASN:HA	15:M:95:ASP:HB3	1.92	0.52
30:A:200:A:N6	30:A:2457:A:O2'	2.43	0.52
41:Aa:1524:A:H2'	41:Aa:1525:U:C6	2.45	0.52
8:E:205:VAL:HG23	8:E:206:LEU:HD12	1.92	0.52
29:11:72:C:H2'	29:11:73:A:H8	1.75	0.52
30:A:625:G:H2'	30:A:626:G:C8	2.45	0.52
30:A:954:A:H2'	30:A:957:C:C5	2.45	0.52
41:Aa:1107:C:H2'	41:Aa:1108:C:C6	2.45	0.52
41:Aa:1443:A:OP2	41:Aa:1478:G:N1	2.35	0.52
51:d:6:U:H2'	51:d:7:G:C8	2.45	0.52
19:Q:4:LYS:HG3	19:Q:106:VAL:HG22	1.92	0.52
30:A:1880:A:H2'	30:A:1881:A:C8	2.45	0.52
6:C:164:VAL:HA	6:C:174:ILE:HD13	1.92	0.51
30:A:2231:C:H2'	30:A:2232:A:C8	2.45	0.51
30:A:2300:A:H2'	30:A:2301:A:C8	2.45	0.51
34:Ai:7:GLU:OE1	34:Ai:9:ARG:NH2	2.43	0.51
5:B:83:C:H2'	5:B:84:U:O4'	2.09	0.51
19:Q:42:ALA:HB2	30:A:2037:G:H5"	1.92	0.51



A + a 1	At ama 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:78:U:H2'	30:A:79:U:C6	2.45	0.51
30:A:579:U:H2'	30:A:580:C:C6	2.45	0.51
41:Aa:271:A:H2'	41:Aa:272:C:C6	2.45	0.51
43:Ac:39:ARG:NH2	43:Ac:54:VAL:O	2.43	0.51
51:d:23:A:H2'	51:d:24:U:O4'	2.10	0.51
41:Aa:959:U:H2'	41:Aa:960:G:C8	2.45	0.51
43:Ac:174:LEU:HD23	43:Ac:181:ILE:HD13	1.91	0.51
37:Ap:24:ASP:OD2	41:Aa:237:U:O2'	2.26	0.51
15:M:112:ALA:HB1	15:M:117:LEU:HD12	1.91	0.51
30:A:1160:C:H2'	30:A:1161:A:C8	2.45	0.51
41:Aa:1423:A:N1	41:Aa:1498:G:N2	2.54	0.51
30:A:346:A:H2'	30:A:347:U:C6	2.46	0.51
30:A:651:A:H2'	30:A:652:A:C8	2.46	0.51
30:A:1072:A:N6	30:A:1169:G:H2'	2.26	0.51
30:A:1423:C:H2'	30:A:1424:A:C8	2.45	0.51
30:A:1477:U:H2'	30:A:1478:A:C8	2.46	0.51
30:A:2327:A:H2'	30:A:2328:A:C8	2.46	0.51
41:Aa:1434:U:H2'	41:Aa:1435:A:C8	2.45	0.51
25:W:59:THR:O	25:W:63:GLU:HG3	2.11	0.51
30:A:1464:U:H2'	30:A:1465:G:C8	2.45	0.51
41:Aa:190:A:H2'	41:Aa:191:A:C8	2.46	0.51
41:Aa:509:C:H2'	41:Aa:510:C:C6	2.46	0.51
30:A:991:A:H2'	30:A:992:A:C8	2.45	0.51
41:Aa:929:U:H2'	41:Aa:930:U:C6	2.46	0.51
41:Aa:1525:U:H2'	41:Aa:1526:C:C6	2.46	0.51
5:B:40:C:O2	28:F:90:THR:HG22	2.11	0.51
10:H:2:ARG:HB3	10:H:3:GLN:HG3	1.93	0.51
30:A:525:A:N3	30:A:527:G:H5"	2.26	0.51
11:I:88:ARG:NH1	11:I:93:PRO:O	2.44	0.50
30:A:2098:A:H2'	30:A:2099:G:C8	2.45	0.50
41:Aa:155:U:O2	41:Aa:166:G:N2	2.39	0.50
41:Aa:29:G:O2'	41:Aa:304:U:OP1	2.27	0.50
41:Aa:483:C:H2'	41:Aa:484:A:H8	1.76	0.50
41:Aa:995:A:H2'	41:Aa:996:A:C8	2.46	0.50
43:Ac:33:HIS:NE2	49:An:25:GLU:HB2	2.26	0.50
30:A:363:A:H4'	30:A:365:A:C8	2.46	0.50
30:A:1556:G:H2'	30:A:1557:C:C6	2.46	0.50
30:A:618:A:OP2	30:A:2526:C:O2'	2.25	0.50
34:Ai:49:ASP:O	34:Ai:82:ARG:HD3	2.11	0.50
41:Aa:690:U:H2'	41:Aa:691:G:H8	1.76	0.50
41:Aa:917:A:H2'	41:Aa:918:A:H8	1.74	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
41:Aa:1058:G:C2	41:Aa:1221:U:O2	2.64	0.50
45:Ak:47:ALA:HB3	45:Ak:57:LYS:HG2	1.92	0.50
21:S:2:HIS:O	21:S:92:ARG:NH1	2.41	0.50
30:A:766:G:H2'	30:A:767:A:C8	2.47	0.50
30:A:1513:A:H2'	30:A:1514:A:H8	1.77	0.50
30:A:1813:A:H1'	30:A:1965:A:N6	2.27	0.50
2:2:15:LYS:NZ	30:A:124:A:OP1	2.38	0.50
16:N:43:GLN:NE2	41:Aa:354:G:OP1	2.44	0.50
30:A:2231:C:H2'	30:A:2232:A:H8	1.75	0.50
30:A:2539:C:H2'	30:A:2540:A:O4'	2.11	0.50
41:Aa:345:G:H2'	41:Aa:346:A:H8	1.77	0.50
41:Aa:407:G:H2'	41:Aa:408:C:C6	2.46	0.50
41:Aa:650:A:H2'	41:Aa:651:C:H6	1.76	0.50
5:B:4:G:H2'	5:B:5:G:H8	1.76	0.50
30:A:2343:U:H2'	30:A:2344:C:C6	2.47	0.50
52:8:65:C:H2'	52:8:66:C:C6	2.47	0.50
14:L:36:ARG:O	14:L:40:VAL:HG23	2.12	0.50
28:F:32:ASP:H	28:F:158:THR:HA	1.77	0.50
30:A:363:A:H4'	30:A:365:A:N7	2.27	0.50
30:A:5:A:H2'	30:A:6:A:C8	2.47	0.50
41:Aa:73:G:H1	41:Aa:96:U:H3	1.60	0.49
30:A:1238:U:H2'	30:A:1239:C:H6	1.77	0.49
30:A:1238:U:H2'	30:A:1239:C:C6	2.47	0.49
30:A:2356:A:H2'	30:A:2357:G:C8	2.47	0.49
41:Aa:1324:C:H2'	41:Aa:1325:U:C6	2.47	0.49
47:Ah:41:LYS:NZ	47:Ah:47:LYS:O	2.45	0.49
30:A:1390:A:H2'	30:A:1391:A:C8	2.48	0.49
30:A:1969:C:OP2	30:A:1970:U:O2'	2.29	0.49
40:At:30:THR:OG1	41:Aa:1469:C:OP1	2.27	0.49
48:Ad:11:LYS:HE2	48:Ad:59:TYR:CZ	2.47	0.49
30:A:1618:A:H2'	30:A:1619:A:C8	2.48	0.49
41:Aa:704:A:H2'	41:Aa:705:U:H6	1.77	0.49
46:Ab:15:HIS:O	46:Ab:41:ILE:N	2.35	0.49
27:Z:16:ARG:NH2	30:A:1302:G:OP1	2.39	0.49
30:A:903:G:N3	30:A:2295:A:H2'	2.28	0.49
41:Aa:445:U:O2'	48:Ad:116:HIS:ND1	2.33	0.49
41:Aa:1422:C:H2'	41:Aa:1423:A:C8	2.48	0.49
43:Ac:61:ASN:HA	43:Ac:96:LYS:NZ	2.27	0.49
30:A:765:U:H2'	30:A:766:G:C8	2.48	0.49
30:A:841:C:H2'	30:A:842:U:C6	2.48	0.49
30:A:1959:A:H2'	30:A:1960:G:O4'	2.11	0.49



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
41:Aa:716:A:H2'	41:Aa:717:U:C6	2.48	0.49
30:A:460:C:H2'	30:A:461:A:C8	2.48	0.49
30:A:684:U:H2'	30:A:685:C:H6	1.77	0.49
41:Aa:909:A:H2'	41:Aa:910:A:C8	2.47	0.49
11:I:63:VAL:HG12	11:I:106:LEU:HD11	1.95	0.49
41:Aa:470:A:H2'	41:Aa:471:A:C8	2.48	0.49
21:S:24:ILE:N	21:S:34:VAL:O	2.46	0.49
30:A:921:C:H2'	30:A:922:G:C8	2.48	0.49
41:Aa:1083:G:H2'	41:Aa:1084:U:C6	2.48	0.49
7:D:2:THR:HB	7:D:213:THR:HB	1.95	0.48
30:A:398:C:H2'	30:A:399:U:O4'	2.13	0.48
30:A:1876:G:H2'	30:A:1877:G:H8	1.78	0.48
30:A:2705:U:H2'	30:A:2706:A:H8	1.77	0.48
32:Af:11:ARG:HE	32:Af:85:ASP:HA	1.78	0.48
41:Aa:184:A:H2	41:Aa:207:G:H1	1.60	0.48
41:Aa:1441:C:H2'	41:Aa:1442:G:O4'	2.13	0.48
50:As:50:ALA:HB1	50:As:57:HIS:HB3	1.94	0.48
53:9:34:U:H2'	53:9:35:A:H8	1.77	0.48
30:A:422:G:H2'	30:A:423:A:H8	1.78	0.48
30:A:639:U:H2'	30:A:640:G:H8	1.79	0.48
30:A:2313:A:H4'	30:A:2314:A:O4'	2.13	0.48
41:Aa:1337:A:H2'	41:Aa:1338:C:H6	1.79	0.48
41:Aa:1437:C:H2'	41:Aa:1438:A:C8	2.48	0.48
48:Ad:104:ALA:HB1	48:Ad:109:GLN:HB3	1.94	0.48
30:A:2617:A:H2'	30:A:2618:C:H6	1.78	0.48
37:Ap:6:ARG:HB2	41:Aa:384:G:H5"	1.95	0.48
39:Ar:37:PHE:CG	39:Ar:60:LEU:HD21	2.47	0.48
41:Aa:502:C:O2'	41:Aa:504:G:H1'	2.13	0.48
41:Aa:996:A:H2'	41:Aa:997:A:C8	2.48	0.48
41:Aa:1527:G:H2'	41:Aa:1529:MA6:OP2	2.13	0.48
1:1:11:ALA:HB2	1:1:18:ARG:HG3	1.96	0.48
24:V:14:THR:HG21	30:A:192:G:OP2	2.14	0.48
30:A:2431:C:H2'	30:A:2432:G:O4'	2.13	0.48
38:Aq:29:THR:HB	38:Aq:42:TYR:CE1	2.49	0.48
44:Am:15:VAL:HG22	44:Am:43:THR:O	2.13	0.48
45:Ak:29:ASN:OD1	45:Ak:30:THR:N	2.46	0.48
30:A:1518:G:H2'	30:A:1519:U:O4'	2.13	0.48
30:A:2457:A:H2'	30:A:2457:A:N3	2.28	0.48
30:A:2829:A:H2'	30:A:2830:A:C8	2.48	0.48
38:Aq:34:LYS:NZ	38:Aq:35:LEU:HB2	2.29	0.48
41:Aa:331:U:H2'	41:Aa:332:G:O4'	2.13	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
41:Aa:1312:U:C5	44:Am:17:ILE:HG13	2.47	0.48
5:B:48:A:H5'	15:M:68:THR:HG23	1.96	0.48
20:R:19:ALA:HB1	20:R:24:LYS:HB2	1.95	0.48
30:A:2091:C:H2'	30:A:2092:C:C6	2.49	0.48
41:Aa:456:A:H2'	41:Aa:457:A:O4'	2.14	0.48
41:Aa:855:C:H2'	41:Aa:856:C:C6	2.49	0.48
5:B:112:A:H2'	5:B:113:G:H8	1.78	0.48
29:11:3:C:H2'	29:11:4:G:H8	1.78	0.48
30:A:954:A:H2'	30:A:957:C:H5	1.77	0.48
30:A:1160:C:H2'	30:A:1161:A:H8	1.79	0.48
35:Al:63:ARG:NH2	41:Aa:530:C:H41	2.11	0.48
41:Aa:588:C:H2'	41:Aa:589:G:O4'	2.14	0.48
41:Aa:1312:U:C4	44:Am:17:ILE:HG13	2.49	0.48
41:Aa:1366:G:H2'	41:Aa:1367:A:H8	1.79	0.48
17:O:4:VAL:HG22	30:A:1238:U:H1'	1.94	0.48
30:A:317:G:HO2'	30:A:318:A:H8	1.59	0.48
30:A:638:U:H2'	30:A:639:U:C6	2.49	0.48
30:A:1352:C:H2'	30:A:1353:A:C8	2.48	0.48
30:A:2343:U:H2'	30:A:2344:C:H6	1.79	0.48
30:A:2811:U:H2'	30:A:2812:U:C6	2.48	0.48
30:A:250:G:H4'	30:A:432:G:C5	2.48	0.48
30:A:2406:G:H2'	30:A:2407:A:C8	2.49	0.48
30:A:2570:G:H2'	30:A:2571:G:C8	2.49	0.48
41:Aa:436:G:H5"	48:Ad:10:LYS:HG3	1.96	0.48
41:Aa:1325:U:H2'	41:Aa:1326:G:O4'	2.14	0.48
41:Aa:1490:A:H2'	41:Aa:1491:A:C8	2.46	0.48
41:Aa:1260:A:H2'	41:Aa:1261:A:C8	2.49	0.47
52:8:13:C:H2'	52:8:14:A:H5"	1.94	0.47
30:A:127:C:H2'	30:A:128:C:C6	2.49	0.47
30:A:1280:U:H2'	30:A:1281:U:C6	2.49	0.47
41:Aa:153:C:H2'	41:Aa:154:U:C6	2.49	0.47
41:Aa:932:A:H2'	41:Aa:933:C:C6	2.48	0.47
41:Aa:1071:U:H2'	41:Aa:1072:G:H8	1.79	0.47
41:Aa:1433:G:H2'	41:Aa:1434:U:C6	2.49	0.47
41:Aa:1488:C:H2'	41:Aa:1489:A:C8	2.49	0.47
48:Ad:78:LYS:HE2	48:Ad:78:LYS:HB3	1.58	0.47
41:Aa:547:A:H2'	41:Aa:548:G:C8	2.49	0.47
52:8:7:A:H3'	52:8:8:U:H5'	1.95	0.47
41:Aa:963:G:H2'	41:Aa:964:U:C6	2.49	0.47
43:Ac:63:ILE:HD12	43:Ac:94:THR:HG21	1.95	0.47
5:B:4:G:H2'	5:B:5:G:C8	2.49	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:B:36:C:H2'	5:B:37:A:C8	2.49	0.47
6:C:81:ILE:HD11	6:C:110:LEU:HD23	1.95	0.47
30:A:886:A:H2'	30:A:887:A:H8	1.79	0.47
30:A:1326:C:H2'	30:A:1327:C:H6	1.80	0.47
30:A:2676:U:H2'	30:A:2677:C:H6	1.80	0.47
30:A:2856:U:H2'	30:A:2857:A:C8	2.50	0.47
41:Aa:457:A:H2'	41:Aa:458:G:O4'	2.14	0.47
43:Ac:34:GLU:HG2	43:Ac:58:ARG:HH22	1.79	0.47
30:A:318:A:H2'	30:A:319:G:C8	2.50	0.47
30:A:537:A:H2'	30:A:538:G:O4'	2.14	0.47
41:Aa:351:U:O3'	41:Aa:352:A:H8	1.98	0.47
41:Aa:1181:A:H2'	41:Aa:1182:C:C6	2.50	0.47
45:Ak:79:LEU:HD12	45:Ak:105:LEU:HD11	1.97	0.47
46:Ab:95:ARG:HD3	46:Ab:147:PHE:CZ	2.50	0.47
6:C:39:LYS:NZ	6:C:58:HIS:O	2.45	0.47
30:A:55:G:O2'	30:A:126:A:N1	2.41	0.47
30:A:348:C:H2'	30:A:349:U:C6	2.49	0.47
30:A:1362:C:OP1	30:A:1691:G:O2'	2.29	0.47
30:A:2344:C:H3'	30:A:2345:A:H5"	1.96	0.47
33:Ag:109:ARG:HG3	33:Ag:116:MET:HE1	1.95	0.47
41:Aa:904:A:H2'	41:Aa:905:C:C6	2.49	0.47
41:Aa:954:G:C2	41:Aa:955:A:C8	3.03	0.47
41:Aa:967:A:C6	50:As:55:ARG:HG2	2.50	0.47
41:Aa:1337:A:H2'	41:Aa:1338:C:C6	2.50	0.47
41:Aa:1489:A:H2'	41:Aa:1490:A:H8	1.79	0.47
47:Ah:106:VAL:HG13	47:Ah:127:ILE:HD13	1.96	0.47
5:B:3:U:OP1	5:B:60:C:H5'	2.15	0.47
15:M:11:ARG:HG3	15:M:99:TYR:CE1	2.50	0.47
30:A:1907:U:H2'	30:A:1908:A:C8	2.50	0.47
30:A:2885:U:H5"	30:A:2886:G:H2'	1.95	0.47
34:Ai:124:ARG:HG3	41:Aa:1358:U:H4'	1.96	0.47
41:Aa:1159:C:H2'	41:Aa:1160:U:C6	2.50	0.47
11:I:24:VAL:HG13	11:I:33:ALA:HB2	1.97	0.47
30:A:689:A:H4'	30:A:690:U:C5	2.50	0.47
30:A:787:U:H2'	30:A:788:A:H8	1.77	0.47
41:Aa:22:G:H2'	41:Aa:23:G:C8	2.50	0.47
41:Aa:148:G:H1	41:Aa:174:A:N6	2.12	0.47
41:Aa:343:C:H2'	41:Aa:344:A:H8	1.80	0.47
41:Aa:550:U:H5'	48:Ad:34:GLY:HA3	1.97	0.47
42:Aj:24:LYS:HB2	42:Aj:24:LYS:HE2	1.65	0.47
13:K:58:MET:HE1	13:K:64:VAL:CG2	2.45	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
19:Q:82:LEU:HB2	19:Q:98:LYS:HB2	1.95	0.47
41:Aa:155:U:H3	41:Aa:166:G:H1	1.62	0.47
41:Aa:1134:A:O2'	41:Aa:1135:G:H5'	2.15	0.47
41:Aa:1167:A:H62	41:Aa:1188:G:H21	1.61	0.47
47:Ah:107:SER:HB2	47:Ah:128:ILE:HD11	1.96	0.47
51:d:15:C:H2'	51:d:16:A:O4'	2.15	0.47
52:8:4:G:H2'	52:8:5:G:C8	2.50	0.47
22:T:79:PHE:HD1	22:T:86:ILE:HD13	1.80	0.46
29:11:3:C:H2'	29:11:4:G:C8	2.50	0.46
30:A:590:U:OP1	30:A:1257:G:O2'	2.26	0.46
30:A:1617:A:H2'	30:A:1618:A:C8	2.50	0.46
30:A:1648:C:O2'	30:A:1654:A:N1	2.47	0.46
30:A:1817:C:H2'	30:A:1818:A:C5	2.50	0.46
30:A:1857:C:H2'	30:A:1858:G:H8	1.80	0.46
42:Aj:57:LYS:HE3	42:Aj:58:TYR:CZ	2.49	0.46
5:B:58:C:H2'	5:B:59:U:C6	2.50	0.46
34:Ai:67:VAL:HG11	34:Ai:81:ILE:HG12	1.97	0.46
41:Aa:495:A:H2'	41:Aa:496:C:O4'	2.15	0.46
41:Aa:744:U:H2'	41:Aa:745:U:H6	1.79	0.46
41:Aa:759:U:H2'	41:Aa:760:G:O4'	2.15	0.46
30:A:194:A:H2'	30:A:195:C:C6	2.51	0.46
30:A:1873:G:C6	30:A:1874:A:C6	3.04	0.46
36:Ao:69:TYR:CZ	36:Ao:73:LYS:HD3	2.50	0.46
41:Aa:391:A:OP1	41:Aa:462:A:O2'	2.30	0.46
43:Ac:63:ILE:HB	43:Ac:98:VAL:HG22	1.97	0.46
48:Ad:164:TYR:CD2	48:Ad:180:PRO:HB3	2.51	0.46
10:H:1:MET:HA	30:A:1039:C:C4	2.50	0.46
30:A:613:G:H2'	30:A:2057:A:N7	2.30	0.46
30:A:907:G:H2'	30:A:908:A:O4'	2.16	0.46
30:A:1222:A:H2'	30:A:1223:A:C8	2.50	0.46
33:Ag:41:ARG:NH2	41:Aa:1301:U:OP1	2.40	0.46
33:Ag:70:MET:HG2	33:Ag:96:ARG:O	2.15	0.46
36:Ao:79:ARG:HG3	36:Ao:79:ARG:HH11	1.80	0.46
41:Aa:326:G:HO2'	41:Aa:1479:A:HO2'	1.62	0.46
41:Aa:392:G:H2'	41:Aa:393:C:C6	2.51	0.46
41:Aa:455:G:O6	41:Aa:493:G:O2'	2.27	0.46
4:4:4:ARG:O	4:4:36:GLN:HA	2.16	0.46
5:B:25:A:H5"	15:M:39:HIS:CE1	2.51	0.46
10:H:3:GLN:NE2	18:P:13:LYS:O	2.43	0.46
22:T:29:ALA:HA	22:T:89:ILE:O	2.16	0.46
30:A:1053:A:N3	30:A:1197:C:O2'	2.43	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:1157:U:O2'	30:A:1158:G:OP1	2.27	0.46
41:Aa:996:A:H2'	41:Aa:997:A:H8	1.80	0.46
41:Aa:1123:C:O2	43:Ac:178:ARG:HG2	2.16	0.46
30:A:66:C:H2'	30:A:67:G:H8	1.81	0.46
30:A:1072:A:H2'	30:A:1073:A:C8	2.51	0.46
41:Aa:250:C:O2'	41:Aa:253:U:OP1	2.26	0.46
48:Ad:122:ASP:OD1	48:Ad:137:GLN:HG3	2.15	0.46
10:H:126:TYR:OH	10:H:133:HIS:NE2	2.27	0.46
14:L:66:LEU:HD11	14:L:85:LEU:HD22	1.97	0.46
30:A:291:G:O2'	30:A:292:U:OP1	2.28	0.46
30:A:437:A:H1'	30:A:457:G:O4'	2.16	0.46
33:Ag:33:ASP:OD1	41:Aa:1360:A:O2'	2.32	0.46
41:Aa:193:C:H2'	41:Aa:194:G:H8	1.80	0.46
41:Aa:959:U:H2'	41:Aa:960:G:H8	1.81	0.46
8:E:81:PRO:HB3	8:E:89:VAL:HG23	1.98	0.46
30:A:1637:A:H2'	30:A:1638:G:C8	2.51	0.46
30:A:2342:U:H2'	30:A:2343:U:C6	2.51	0.46
31:Ae:93:SER:HB3	31:Ae:128:LEU:O	2.15	0.46
33:Ag:111:ARG:HD2	33:Ag:123:GLU:HG2	1.98	0.46
38:Aq:29:THR:HG22	38:Aq:30:TYR:N	2.28	0.46
41:Aa:171:A:H2'	41:Aa:172:A:C8	2.50	0.46
41:Aa:278:A:H2'	41:Aa:279:C:C6	2.50	0.46
41:Aa:563:C:H2'	41:Aa:564:C:C6	2.50	0.46
41:Aa:771:G:H2'	41:Aa:772:C:C6	2.51	0.46
29:11:73:A:C2'	29:11:74:C:H5'	2.45	0.46
30:A:1723:A:H2	30:A:1791:G:C8	2.33	0.46
37:Ap:79:GLY:O	37:Ap:83:LYS:HG3	2.16	0.46
41:Aa:343:C:H2'	41:Aa:344:A:C8	2.51	0.46
41:Aa:1433:G:H2'	41:Aa:1434:U:H6	1.80	0.46
50:As:4:SER:HB2	50:As:7:LYS:HD3	1.96	0.46
5:B:30:U:C2	5:B:49:G:N2	2.84	0.46
20:R:4:ARG:HG2	25:W:30:PHE:CG	2.51	0.46
29:11:72:C:C2	29:11:73:A:C8	3.04	0.46
30:A:340:C:H2'	30:A:341:G:O4'	2.16	0.46
30:A:391:A:H2'	30:A:392:U:H6	1.81	0.46
30:A:1572:G:C6	30:A:1591:G:C6	3.04	0.46
30:A:2488:C:H2'	30:A:2489:U:C6	2.50	0.46
30:A:2564:U:H2'	30:A:2565:C:C6	2.50	0.46
32:Af:43:TRP:HB2	32:Af:60:TYR:HB2	1.97	0.46
41:Aa:217:G:H2'	41:Aa:218:U:O4'	2.16	0.46
41:Aa:885:A:H2'	41:Aa:886:C:C6	2.50	0.46



A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
41:Aa:1073:U:H2'	41:Aa:1074:C:C6	2.51	0.46
42:Aj:11:LYS:HB2	42:Aj:97:ASP:OD2	2.16	0.46
5:B:65:G:H2'	5:B:66:C:C6	2.51	0.45
9:G:64:ASN:HA	9:G:67:THR:HG22	1.98	0.45
30:A:734:A:H2'	30:A:735:C:C6	2.51	0.45
30:A:1680:U:H2'	30:A:1681:U:C6	2.51	0.45
30:A:1876:G:H2'	30:A:1877:G:C8	2.52	0.45
35:Al:25:ASN:HB2	35:Al:39:ASN:HD22	1.81	0.45
41:Aa:471:A:H2'	41:Aa:472:G:O4'	2.16	0.45
30:A:689:A:H2'	30:A:691:A:C8	2.51	0.45
30:A:1352:C:H2'	30:A:1353:A:H8	1.82	0.45
30:A:2594:G:H2'	30:A:2595:C:C6	2.51	0.45
41:Aa:695:A:C2	41:Aa:712:A:C5	3.05	0.45
41:Aa:1002:G:O2'	41:Aa:1003:A:N7	2.49	0.45
47:Ah:41:LYS:HZ3	47:Ah:48:ASN:HA	1.81	0.45
5:B:58:C:H2'	5:B:59:U:H6	1.80	0.45
30:A:689:A:H4'	30:A:690:U:H5	1.81	0.45
30:A:1240:U:H2'	30:A:1241:A:C8	2.51	0.45
30:A:1674:U:H2'	30:A:1675:G:O4'	2.17	0.45
30:A:1973:U:H2'	30:A:1974:C:C6	2.52	0.45
37:Ap:4:LYS:HB3	37:Ap:4:LYS:HE2	1.75	0.45
41:Aa:1379:C:H2'	41:Aa:1380:G:C8	2.52	0.45
7:D:194:VAL:HG11	16:N:10:VAL:HG11	1.97	0.45
30:A:27:G:N2	30:A:557:G:H1'	2.31	0.45
30:A:279:A:H2'	30:A:280:C:C6	2.52	0.45
30:A:332:A:H2'	30:A:333:C:C6	2.52	0.45
30:A:2495:A:O2'	30:A:2496:A:H8	2.00	0.45
40:At:18:GLU:OE1	41:Aa:330:C:H4'	2.17	0.45
5:B:46:A:H2'	5:B:47:C:C6	2.51	0.45
5:B:106:G:H2'	5:B:107:U:C6	2.52	0.45
7:D:59:TYR:HB3	7:D:74:GLU:OE1	2.17	0.45
30:A:650:U:C5	30:A:665:G:C5	3.04	0.45
30:A:1476:G:H2'	30:A:1477:U:C6	2.52	0.45
30:A:1597:U:H2'	30:A:1598:U:C6	2.52	0.45
30:A:2051:C:H2'	30:A:2052:C:C6	2.51	0.45
30:A:2496:A:N6	30:A:2508:G:O2'	2.49	0.45
30:A:2677:C:H2'	30:A:2678:C:H6	1.82	0.45
30:A:2877:G:N2	30:A:2880:A:OP2	2.36	0.45
31:Ae:37:VAL:HG11	31:Ae:64:VAL:HG22	1.97	0.45
35:Al:83:ILE:HD13	41:Aa:529:G:H4'	1.98	0.45
38:Aq:28:GLU:HA	38:Aq:43:SER:HA	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
40:At:39:VAL:HG11	40:At:81:ALA:HB1	1.98	0.45
41:Aa:265:A:H2'	41:Aa:266:A:C8	2.52	0.45
41:Aa:877:C:H2'	41:Aa:878:A:O4'	2.17	0.45
41:Aa:1082:C:H2'	41:Aa:1083:G:C8	2.51	0.45
42:Aj:40:ILE:HB	42:Aj:73:LEU:HB3	1.98	0.45
44:Am:45:VAL:HA	44:Am:48:LEU:HG	1.98	0.45
28:F:35:VAL:HG21	30:A:2341:A:H5'	1.98	0.45
30:A:901:G:H2'	30:A:902:A:H8	1.79	0.45
30:A:1493:U:H2'	30:A:1494:G:O4'	2.17	0.45
30:A:1821:U:H2'	30:A:1822:C:C6	2.51	0.45
41:Aa:58:G:H2'	41:Aa:59:C:C6	2.51	0.45
41:Aa:398:C:H2'	41:Aa:399:G:C8	2.51	0.45
7:D:5:ILE:HG22	7:D:211:ILE:HB	1.99	0.45
30:A:680:C:O2'	30:A:684:U:OP1	2.27	0.45
30:A:1979:A:N3	30:A:2587:C:O2'	2.46	0.45
41:Aa:381:A:O2'	41:Aa:459:A:N7	2.49	0.45
28:F:54:VAL:HG13	28:F:65:PRO:HG2	1.99	0.45
30:A:946:A:H2'	30:A:947:U:C6	2.52	0.45
30:A:2664:U:H2'	30:A:2665:G:O4'	2.17	0.45
39:Ar:59:MET:HE2	39:Ar:59:MET:HB2	1.85	0.45
41:Aa:1062:G:H2'	41:Aa:1063:U:C6	2.51	0.45
30:A:2260:A:H2'	30:A:2261:G:H8	1.81	0.45
41:Aa:695:A:N6	41:Aa:709:C:O4'	2.50	0.45
47:Ah:34:LYS:O	47:Ah:38:GLU:HG2	2.17	0.45
5:B:59:U:H2'	5:B:60:C:C6	2.51	0.45
30:A:970:U:O2'	30:A:972:A:OP2	2.32	0.45
30:A:1314:A:H2'	30:A:1315:C:C6	2.52	0.45
30:A:2477:A:O2'	52:8:77:A:N1	2.43	0.45
41:Aa:202:C:H2'	41:Aa:203:A:O4'	2.17	0.45
41:Aa:722:G:H2'	41:Aa:723:A:C8	2.52	0.45
41:Aa:1420:A:H2'	41:Aa:1421:C:H6	1.81	0.45
13:K:54:MET:HE1	13:K:104:PHE:CD2	2.52	0.44
30:A:2050:A:H2'	30:A:2051:C:C6	2.52	0.44
30:A:2110:G:H2'	30:A:2111:C:C6	2.52	0.44
30:A:2617:A:H2'	30:A:2618:C:C6	2.51	0.44
41:Aa:63:U:H2'	41:Aa:64:C:C6	2.52	0.44
41:Aa:482:A:H2'	41:Aa:483:C:C6	2.52	0.44
43:Ac:194:LYS:HD3	43:Ac:194:LYS:HĀ	1.78	0.44
44:Am:86:TYR:O	44:Am:90:ARG:HG2	2.17	0.44
52:8:1:C:H2'	52:8:2:G:H8	1.82	0.44
52:8:24:C:H2'	52:8:25:U:C6	2.52	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
52:8:32:G:H2'	52:8:33:C:H6	1.82	0.44
12:J:74:TYR:CZ	12:J:127:LYS:HD2	2.52	0.44
30:A:754:U:H2'	30:A:755:C:H6	1.82	0.44
30:A:1240:U:H2'	30:A:1241:A:H8	1.83	0.44
30:A:2220:U:H2'	30:A:2221:U:C6	2.52	0.44
30:A:2318:U:OP1	30:A:2407:A:O2'	2.35	0.44
30:A:2482:G:H2'	30:A:2483:C:C6	2.52	0.44
37:Ap:78:GLU:HB2	37:Ap:80:ILE:HD12	1.99	0.44
41:Aa:803:C:O2'	45:Ak:128:ARG:O	2.33	0.44
8:E:53:ASN:O	8:E:57:VAL:HG23	2.17	0.44
30:A:1013:U:H2'	30:A:1014:U:C6	2.52	0.44
30:A:1563:U:H2'	30:A:1564:G:C8	2.53	0.44
30:A:1700:C:H2'	30:A:1701:U:H6	1.82	0.44
30:A:2549:U:O2'	30:A:2674:U:OP1	2.29	0.44
41:Aa:317:G:O2'	41:Aa:615:A:N1	2.49	0.44
41:Aa:765:U:H2'	41:Aa:766:G:O4'	2.17	0.44
48:Ad:182:ARG:O	48:Ad:182:ARG:NH1	2.50	0.44
13:K:39:THR:OG1	13:K:99:PRO:HD3	2.18	0.44
30:A:884:U:H2'	30:A:885:C:C6	2.51	0.44
35:Al:25:ASN:HB2	35:Al:39:ASN:ND2	2.32	0.44
38:Aq:65:GLU:OE1	41:Aa:243:C:O2'	2.28	0.44
40:At:25:LYS:HG3	40:At:65:LEU:HD22	1.99	0.44
41:Aa:263:G:H2'	41:Aa:264:U:C6	2.52	0.44
41:Aa:986:A:O2'	41:Aa:988:C:OP2	2.28	0.44
41:Aa:1106:U:H2'	41:Aa:1107:C:C6	2.51	0.44
41:Aa:1131:C:H2'	41:Aa:1132:U:C6	2.52	0.44
48:Ad:120:LEU:HD11	48:Ad:142:ARG:HA	1.98	0.44
9:G:84:VAL:HA	9:G:133:VAL:O	2.18	0.44
13:K:34:LEU:HD13	13:K:118:LEU:HB3	1.98	0.44
14:L:26:ILE:HG13	14:L:71:ILE:HG12	1.99	0.44
30:A:52:A:H2'	30:A:53:A:C8	2.53	0.44
30:A:569:U:H4'	30:A:598:G:H4'	1.99	0.44
30:A:1821:U:H2'	30:A:1822:C:H6	1.82	0.44
30:A:1916:A:H2'	30:A:1917:A:H8	1.80	0.44
41:Aa:697:C:OP2	45:Ak:57:LYS:NZ	2.46	0.44
54:13:63:LYS:HG3	54:13:64:PHE:CD2	2.52	0.44
14:L:22:THR:HG21	14:L:67:ARG:HB2	1.99	0.44
30:A:3:U:H2'	30:A:4:U:H6	1.81	0.44
30:A:622:A:H2'	30:A:623:C:C6	2.52	0.44
30:A:702:U:H2'	30:A:703:A:H8	1.82	0.44
30:A:1045:A:H2'	30:A:1046:G:O4'	2.18	0.44



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:1519:U:H2'	30:A:1520:A:C8	2.53	0.44
41:Aa:692:U:H2'	41:Aa:693:G:O4'	2.18	0.44
41:Aa:1167:A:H61	41:Aa:1190:A:H2'	1.81	0.44
11:I:86:ILE:HG22	11:I:94:ARG:HG3	1.99	0.44
30:A:30:G:H2'	30:A:31:C:C6	2.53	0.44
30:A:766:G:H2'	30:A:767:A:H8	1.82	0.44
30:A:859:C:H2'	30:A:860:U:H6	1.83	0.44
30:A:1158:G:O2'	30:A:1159:A:OP1	2.32	0.44
30:A:2270:U:H2'	30:A:2271:U:H6	1.82	0.44
30:A:2673:C:H2'	30:A:2674:U:O4'	2.18	0.44
41:Aa:441:A:H2'	41:Aa:442:C:C6	2.52	0.44
41:Aa:947:A:N3	41:Aa:1386:U:O2'	2.43	0.44
41:Aa:1081:U:H2'	41:Aa:1082:C:C6	2.52	0.44
30:A:78:U:H2'	30:A:79:U:H6	1.82	0.44
30:A:1521:A:N6	30:A:1559:G:O2'	2.48	0.44
30:A:2494:C:H2'	30:A:2495:A:O4'	2.18	0.44
30:A:2676:U:H2'	30:A:2677:C:C6	2.53	0.44
38:Aq:7:ARG:HB2	38:Aq:64:GLN:HE21	1.83	0.44
41:Aa:36:G:H2'	41:Aa:37:C:C6	2.53	0.44
46:Ab:109:LYS:NZ	46:Ab:109:LYS:HB3	2.33	0.44
8:E:117:LYS:HG3	8:E:192:LEU:HD13	2.00	0.44
30:A:339:A:H2'	30:A:340:C:C6	2.53	0.44
30:A:395:U:H2'	30:A:396:G:C8	2.52	0.44
30:A:725:A:H2'	30:A:726:G:C8	2.52	0.44
41:Aa:166:G:H2'	41:Aa:167:A:H8	1.83	0.44
41:Aa:187:U:H2'	41:Aa:188:U:C6	2.53	0.44
41:Aa:1255:A:H2'	41:Aa:1256:A:H8	1.83	0.44
9:G:90:VAL:O	9:G:160:LYS:HA	2.17	0.43
30:A:1252:A:H4'	30:A:1277:C:H4'	2.00	0.43
41:Aa:123:G:H2'	41:Aa:124:U:C6	2.53	0.43
41:Aa:140:A:H2'	41:Aa:141:A:C8	2.52	0.43
41:Aa:162:A:C5	41:Aa:163:C:H1'	2.53	0.43
41:Aa:225:G:H2'	41:Aa:226:U:C6	2.53	0.43
41:Aa:1423:A:N6	41:Aa:1498:G:H1	2.16	0.43
52:8:1:C:H2'	52:8:2:G:C8	2.53	0.43
25:W:13:LEU:O	25:W:64:ARG:NH2	2.44	0.43
30:A:229:A:O2'	30:A:231:A:N1	2.46	0.43
30:A:349:U:H2'	30:A:350:G:O4'	2.17	0.43
34:Ai:30:ILE:HD13	34:Ai:50:LEU:HD11	2.00	0.43
34:Ai:59:THR:O	34:Ai:62:ASN:HB2	2.18	0.43
36:Ao:39:VAL:HB	36:Ao:56:LEU:HD12	1.99	0.43



Atom 1	Atom 1 Atom 2		Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
41:Aa:1364:U:H2'	41:Aa:1365:A:H8	1.83	0.43
30:A:460:C:H2'	30:A:461:A:H8	1.83	0.43
30:A:464:U:H2'	30:A:465:C:C6	2.54	0.43
30:A:639:U:H2'	30:A:640:G:C8	2.52	0.43
41:Aa:9:A:N6	48:Ad:196:GLU:O	2.51	0.43
41:Aa:417:U:H2'	41:Aa:418:G:O4'	2.18	0.43
41:Aa:1153:G:H2'	41:Aa:1154:G:C8	2.51	0.43
41:Aa:1255:A:H2'	41:Aa:1256:A:C8	2.53	0.43
41:Aa:1265:G:H2'	41:Aa:1289:A:H61	1.82	0.43
6:C:79:ASP:N	6:C:93:LEU:O	2.46	0.43
8:E:154:VAL:HB	8:E:175:VAL:HG22	1.99	0.43
11:I:70:ARG:HB2	11:I:76:TYR:CE2	2.54	0.43
30:A:476:A:H5"	30:A:477:U:OP2	2.18	0.43
30:A:597:U:H2'	30:A:598:G:O4'	2.19	0.43
30:A:878:C:H2'	30:A:879:U:C6	2.53	0.43
30:A:1219:G:O2'	30:A:1220:A:H8	2.00	0.43
30:A:1570:G:H2'	30:A:1571:G:C8	2.53	0.43
30:A:2774:G:O6	30:A:2782:C:H5"	2.19	0.43
41:Aa:1081:U:H2'	41:Aa:1082:C:H6	1.82	0.43
6:C:225:MET:HG2	30:A:827:A:C2	2.53	0.43
30:A:332:A:H2'	30:A:333:C:H6	1.82	0.43
30:A:1208:A:H2'	30:A:1209:U:C6	2.53	0.43
30:A:2495:A:HO2'	30:A:2496:A:H8	1.64	0.43
31:Ae:40:GLY:HA3	31:Ae:117:LEU:HB3	2.01	0.43
36:Ao:13:LYS:HG2	36:Ao:16:ARG:NH2	2.34	0.43
41:Aa:568:A:H4'	41:Aa:569:U:H5"	1.99	0.43
41:Aa:703:A:H2'	41:Aa:704:A:C8	2.53	0.43
41:Aa:984:A:H5'	41:Aa:984:A:H8	1.83	0.43
41:Aa:1122:A:OP1	41:Aa:1193:U:O2'	2.27	0.43
2:2:30:LYS:HB3	2:2:30:LYS:HE3	1.81	0.43
6:C:145:GLU:HG2	6:C:151:GLY:C	2.43	0.43
12:J:73:GLU:O	12:J:106:LYS:HB3	2.18	0.43
18:P:2:PHE:CE1	18:P:42:GLY:HA3	2.53	0.43
19:Q:4:LYS:HB3	19:Q:4:LYS:HE2	1.56	0.43
30:A:886:A:H2'	30:A:887:A:C8	2.54	0.43
30:A:1563:U:H2'	30:A:1564:G:H8	1.83	0.43
30:A:2273:G:H2'	30:A:2274:A:C8	2.54	0.43
31:Ae:95:PHE:O	31:Ae:125:SER:HA	2.18	0.43
7:D:142:SER:OG	30:A:2020:U:H4'	2.19	0.43
8:E:110:LEU:HD23	8:E:110:LEU:HA	1.91	0.43
30:A:637:U:H2'	30:A:638:U:C6	2.53	0.43



	At arra 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:805:G:H2'	30:A:806:A:O4'	2.18	0.43
30:A:1084:U:H2'	30:A:1085:U:O4'	2.17	0.43
41:Aa:1365:A:H2'	41:Aa:1366:G:C8	2.53	0.43
30:A:59:U:H1'	30:A:73:A:H2'	2.00	0.43
30:A:2278:OMG:HM23	30:A:2278:OMG:H1'	1.73	0.43
30:A:2341:A:H2'	30:A:2342:U:C6	2.54	0.43
41:Aa:963:G:H2'	41:Aa:964:U:H6	1.83	0.43
41:Aa:1319:G:N7	44:Am:98:ARG:NH2	2.67	0.43
3:3:41:LYS:HB2	3:3:41:LYS:HE2	1.73	0.43
3:3:60:GLN:NE2	30:A:636:A:O2'	2.32	0.43
16:N:77:PRO:O	16:N:80:THR:HG22	2.19	0.43
41:Aa:271:A:H2'	41:Aa:272:C:C5	2.54	0.43
41:Aa:493:G:O2'	41:Aa:494:U:OP2	2.36	0.43
41:Aa:931:G:H2'	41:Aa:932:A:C8	2.53	0.43
41:Aa:1024:G:H8	41:Aa:1024:G:OP2	2.01	0.43
41:Aa:1487:A:H2'	41:Aa:1488:C:O4'	2.18	0.43
30:A:247:A:H2'	30:A:248:G:O4'	2.18	0.43
30:A:906:A:H2'	30:A:907:G:O4'	2.19	0.43
33:Ag:150:ALA:O	45:Ak:59:THR:HG21	2.18	0.43
41:Aa:150:U:H2'	41:Aa:151:A:H8	1.84	0.43
41:Aa:430:C:P	41:Aa:430:C:H6	2.42	0.43
41:Aa:437:U:H4'	41:Aa:438:A:O5'	2.18	0.43
41:Aa:682:G:H21	45:Ak:118:HIS:HB2	1.84	0.43
41:Aa:847:G:H2'	41:Aa:848:G:C8	2.54	0.43
52:8:19:G:O6	52:8:56:U:O2'	2.36	0.43
8:E:157:GLU:HG2	8:E:201:LYS:HE2	2.00	0.42
12:J:55:LEU:HD23	12:J:60:ARG:HB3	2.01	0.42
30:A:421:C:H2'	30:A:422:G:H8	1.83	0.42
30:A:1185:U:H4'	30:A:1186:A:O4'	2.19	0.42
30:A:1269:A:H2'	30:A:1270:U:C6	2.54	0.42
30:A:1315:C:H2'	30:A:1316:G:H8	1.84	0.42
30:A:1326:C:H2'	30:A:1327:C:C6	2.54	0.42
30:A:1391:A:H2'	30:A:1392:G:O4'	2.19	0.42
30:A:1973:U:H2'	30:A:1974:C:H6	1.84	0.42
30:A:2601:G7M:O5'	30:A:2601:G7M:H8	2.19	0.42
39:Ar:66:ARG:NE	41:Aa:744:U:OP1	2.48	0.42
41:Aa:276:U:H2'	41:Aa:277:U:C6	2.54	0.42
41:Aa:1023:A:C2	41:Aa:1229:U:H1'	2.54	0.42
46:Ab:169:GLU:O	46:Ab:173:ILE:HG12	2.19	0.42
2:2:26:LYS:NZ	30:A:214:G:OP1	2.46	0.42
4:4:10:ILE:HG23	30:A:2504:C:N4	2.34	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:B:11:A:P	23:U:82:ARG:HH11	2.42	0.42
19:Q:94:SER:HB3	30:A:2040:A:O2'	2.19	0.42
23:U:53:ILE:HG12	23:U:85:LYS:HG3	2.01	0.42
39:Ar:37:PHE:CD1	39:Ar:60:LEU:HD21	2.54	0.42
41:Aa:1083:G:H2'	41:Aa:1084:U:H6	1.83	0.42
41:Aa:1189:A:H2'	41:Aa:1190:A:O4'	2.19	0.42
42:Aj:66:GLU:HB3	49:An:59:ALA:HB2	2.01	0.42
48:Ad:18:SER:OG	48:Ad:25:GLU:OE1	2.25	0.42
30:A:65:A:H2'	30:A:66:C:C6	2.54	0.42
30:A:391:A:H2'	30:A:392:U:C6	2.54	0.42
30:A:737:C:H2'	30:A:738:U:C6	2.54	0.42
30:A:1642:C:H2'	30:A:1643:C:H6	1.84	0.42
30:A:2330:G:O6	30:A:2341:A:N6	2.53	0.42
30:A:2529:G:H5"	30:A:2530:2MA:H5"	2.00	0.42
31:Ae:131:ASN:HA	31:Ae:136:MET:HE2	2.00	0.42
41:Aa:1141:A:H2'	41:Aa:1142:U:C6	2.54	0.42
42:Aj:18:ILE:HD13	42:Aj:72:ARG:HG2	2.02	0.42
43:Ac:141:MET:HG3	43:Ac:169:GLU:OE1	2.19	0.42
5:B:65:G:H2'	5:B:66:C:H6	1.85	0.42
22:T:9:ARG:HG2	22:T:42:LYS:HG2	2.01	0.42
30:A:4:U:H2'	30:A:5:A:C8	2.54	0.42
30:A:127:C:H2'	30:A:128:C:H6	1.84	0.42
30:A:266:A:H1'	30:A:476:A:N3	2.34	0.42
30:A:1726:A:H2'	30:A:1727:C:C6	2.55	0.42
38:Aq:53:ASN:N	38:Aq:53:ASN:HD22	2.18	0.42
10:H:43:VAL:HG22	17:O:100:ILE:HG13	2.00	0.42
15:M:19:ARG:NH1	15:M:22:LEU:O	2.49	0.42
30:A:616:G:O6	30:A:2056:G:O2'	2.35	0.42
30:A:920:A:H2'	30:A:921:C:C6	2.55	0.42
30:A:2682:G:N2	30:A:2692:A:OP2	2.38	0.42
44:Am:90:ARG:HB2	44:Am:97:VAL:HG12	2.01	0.42
45:Ak:88:GLY:H	45:Ak:114:THR:HG23	1.84	0.42
8:E:7:LEU:HD23	8:E:13:LYS:HA	2.02	0.42
30:A:296:G:O2'	30:A:297:G:H5'	2.19	0.42
30:A:2038:U:H2'	30:A:2039:G:O4'	2.20	0.42
39:Ar:38:ILE:HD13	39:Ar:73:LEU:HD22	2.01	0.42
41:Aa:439:A:H2'	41:Aa:440:A:O4'	2.20	0.42
47:Ah:104:ALA:HB3	47:Ah:115:ASP:HB3	2.01	0.42
1:1:43:ASN:OD1	30:A:2397:G:O2'	2.37	0.42
8:E:125:VAL:HA	8:E:194:ILE:O	2.20	0.42
9:G:2:SER:O	9:G:6:LYS:N	2.42	0.42



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
22:T:57:ARG:HH21	22:T:77:TYR:HE1	1.67	0.42
29:11:70:G:H2'	29:11:71:G:C8	2.54	0.42
30:A:328:G:N2	30:A:399:U:H1'	2.35	0.42
30:A:396:G:O2'	30:A:397:U:OP1	2.27	0.42
30:A:403:U:H2'	30:A:404:U:C6	2.55	0.42
30:A:544:U:H2'	30:A:545:G:O4'	2.20	0.42
30:A:659:A:H2'	30:A:660:A:C8	2.55	0.42
30:A:786:U:H2'	30:A:787:U:C6	2.55	0.42
30:A:2372:G:N3	30:A:2408:C:H2'	2.34	0.42
41:Aa:1333:G:H2'	41:Aa:1334:A:H8	1.85	0.42
43:Ac:189:ASP:OD1	43:Ac:194:LYS:HE2	2.20	0.42
5:B:59:U:H2'	5:B:60:C:H6	1.85	0.42
30:A:175:C:H2'	30:A:176:A:O4'	2.20	0.42
30:A:2284:U:O2'	30:A:2285:C:H5'	2.20	0.42
30:A:2541:U:H2'	30:A:2542:C:C6	2.54	0.42
31:Ae:126:LYS:NZ	41:Aa:10:G:OP2	2.40	0.42
31:Ae:149:ASN:O	31:Ae:153:VAL:HG13	2.20	0.42
41:Aa:626:C:N4	41:Aa:629:A:OP2	2.52	0.42
41:Aa:899:G:O2'	41:Aa:915:G:O6	2.29	0.42
44:Am:10:PRO:HB2	44:Am:13:LYS:HD2	2.01	0.42
16:N:29:ARG:NH1	16:N:44:VAL:HG11	2.35	0.42
30:A:625:G:H2'	30:A:626:G:H8	1.84	0.42
30:A:2098:A:H2'	30:A:2099:G:H8	1.83	0.42
30:A:2319:U:H2'	30:A:2320:C:C6	2.55	0.42
30:A:2817:A:H5"	30:A:2912:A:C2	2.53	0.42
33:Ag:80:VAL:HG11	33:Ag:154:TYR:CE1	2.55	0.42
37:Ap:74:ILE:O	37:Ap:78:GLU:HG2	2.20	0.42
41:Aa:212:A:H4'	41:Aa:213:G:OP1	2.20	0.42
41:Aa:305:G:H4'	41:Aa:565:G:H4'	2.01	0.42
41:Aa:1101:U:H2'	41:Aa:1102:U:C6	2.55	0.42
41:Aa:1312:U:OP1	44:Am:13:LYS:HE3	2.19	0.42
5:B:112:A:H2'	5:B:113:G:C8	2.55	0.42
20:R:6:ILE:HG23	20:R:33:VAL:HG21	2.02	0.42
41:Aa:511:A:H2'	41:Aa:512:C:C6	2.54	0.42
41:Aa:745:U:H2'	41:Aa:746:U:C6	2.55	0.42
41:Aa:1136:U:HO2'	41:Aa:1137:U:P	2.43	0.42
41:Aa:1324:C:H2'	41:Aa:1325:U:H6	1.82	0.42
47:Ah:94:MET:HE3	47:Ah:124:GLY:HA2	2.02	0.42
15:M:94:PHE:CZ	15:M:109:ALA:HB2	2.55	0.41
21:S:64:HIS:CD2	30:A:371:U:H4'	2.55	0.41
30:A:972:A:H2'	30:A:973:A:C8	2.55	0.41



A 4 1		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
41:Aa:1114:C:H4'	46:Ab:97:LEU:HD13	2.01	0.41	
42:Aj:63:GLU:OE2	49:An:49:TYR:OH	2.27	0.41	
7:D:107:VAL:HG21	7:D:193:LYS:HA	2.00	0.41	
21:S:70:LEU:HD23	21:S:70:LEU:HA	1.89	0.41	
30:A:266:A:H2'	30:A:267:G:O4'	2.20	0.41	
30:A:703:A:H2'	30:A:704:U:C6	2.55	0.41	
30:A:2274:A:H2'	30:A:2275:C:H6	1.85	0.41	
30:A:2400:U:H2'	30:A:2401:C:C6	2.55	0.41	
31:Ae:57:PRO:O	31:Ae:61:LYS:HG2	2.20	0.41	
36:Ao:47:LYS:HB2	36:Ao:47:LYS:HE2	1.70	0.41	
41:Aa:33:A:H2'	41:Aa:34:A:C8	2.55	0.41	
41:Aa:184:A:N1	41:Aa:207:G:C6	2.87	0.41	
46:Ab:14:VAL:C	46:Ab:203:ASN:HB3	2.44	0.41	
28:F:33:LYS:HA	28:F:96:MET:SD	2.61	0.41	
30:A:145:A:H2'	30:A:146:U:C6	2.55	0.41	
30:A:1209:U:H2'	30:A:1210:U:C6	2.55	0.41	
30:A:1237:U:H2'	30:A:1238:U:C6	2.56	0.41	
30:A:2874:A:H2'	30:A:2875:U:C6	2.55	0.41	
31:Ae:149:ASN:OD1	31:Ae:149:ASN:N	2.43	0.41	
41:Aa:23:G:O2'	41:Aa:922:A:N1	2.49	0.41	
41:Aa:1365:A:H2'	41:Aa:1366:G:H8	1.86	0.41	
45:Ak:35:THR:OG1	45:Ak:36:ASP:N	2.53	0.41	
5:B:26:C:H2'	5:B:27:A:O4'	2.20	0.41	
5:B:30:U:H2'	5:B:31:G:H8	1.85	0.41	
5:B:58:C:C2	5:B:59:U:C5	3.09	0.41	
6:C:49:LEU:HD21	6:C:52:ARG:HA	2.02	0.41	
7:D:134:HIS:CD2	7:D:168:LYS:HB3	2.56	0.41	
24:V:49:VAL:HG12	24:V:54:LEU:HG	2.02	0.41	
30:A:2327:A:H2'	30:A:2328:A:H8	1.84	0.41	
31:Ae:120:ILE:HG22	31:Ae:122:ASP:H	1.86	0.41	
36:Ao:14:GLU:HG2	36:Ao:15:TYR:CD2	2.55	0.41	
41:Aa:98:U:H2'	41:Aa:99:U:C6	2.55	0.41	
41:Aa:601:U:H2'	41:Aa:602:U:C6	2.55	0.41	
41:Aa:994:C:H2'	41:Aa:995:A:H8	1.84	0.41	
41:Aa:1248:A:H2	41:Aa:1251:G:N3	2.18	0.41	
41:Aa:1385:A:H2'	41:Aa:1386:U:O4'	2.20	0.41	
47:Ah:52:VAL:HB	47:Ah:59:VAL:HB	2.01	0.41	
5:B:48:A:OP1	15:M:68:THR:HG22	2.20	0.41	
5:B:66:C:H2'	5:B:67:G:O4'	2.20	0.41	
17:O:86:ALA:HB2	17:O:116:ALA:HB2	2.03	0.41	
30:A:1157:U:H2'	30:A:1158:G:H8	1.85	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:2053:U:H2'	30:A:2054:G:O4'	2.20	0.41
30:A:2800:U:H2'	30:A:2801:C:H6	1.85	0.41
32:Af:52:ILE:O	32:Af:55:PHE:HB2	2.20	0.41
41:Aa:1185:G:H2'	41:Aa:1186:A:H8	1.84	0.41
5:B:29:C:O2'	5:B:30:U:H5'	2.20	0.41
8:E:131:PHE:CZ	8:E:138:GLU:HG2	2.55	0.41
20:R:51:ALA:N	20:R:81:THR:O	2.51	0.41
30:A:4:U:H2'	30:A:5:A:H8	1.84	0.41
30:A:753:U:H2'	30:A:754:U:C6	2.55	0.41
30:A:1492:G:H2'	30:A:1493:U:C6	2.55	0.41
30:A:2581:U:H2'	30:A:2582:U:C6	2.56	0.41
31:Ae:77:VAL:HG22	31:Ae:78:GLU:HG2	2.02	0.41
34:Ai:117:LYS:HE2	41:Aa:1197:G:H5'	2.01	0.41
41:Aa:527:C:H2'	41:Aa:528:A:O4'	2.21	0.41
41:Aa:1196:G:H21	49:An:61:TRP:C	2.28	0.41
13:K:54:MET:HE3	13:K:54:MET:HB2	1.91	0.41
30:A:2677:C:H2'	30:A:2678:C:C6	2.56	0.41
32:Af:41:LYS:HB3	32:Af:41:LYS:HE3	1.62	0.41
37:Ap:16:PRO:HD2	37:Ap:43:THR:HG21	2.01	0.41
40:At:21:ASN:HB3	40:At:65:LEU:HD21	2.02	0.41
41:Aa:71:A:H2'	41:Aa:72:C:C6	2.56	0.41
41:Aa:1201:A:OP2	43:Ac:3:GLN:NE2	2.54	0.41
5:B:106:G:H2'	5:B:107:U:H6	1.86	0.41
7:D:159:ASP:HA	7:D:160:ALA:HA	1.81	0.41
10:H:56:ILE:HA	10:H:124:PHE:O	2.20	0.41
30:A:1304:G:O2'	30:A:2039:G:O6	2.36	0.41
30:A:1368:C:H2'	30:A:1370:C:C5	2.55	0.41
37:Ap:5:ILE:HG12	37:Ap:22:VAL:HG22	2.02	0.41
41:Aa:185:U:H2'	41:Aa:186:U:C6	2.56	0.41
41:Aa:407:G:H2'	41:Aa:408:C:H6	1.86	0.41
41:Aa:901:A:H2'	41:Aa:902:C:C6	2.56	0.41
41:Aa:1113:A:H2'	41:Aa:1114:C:C6	2.56	0.41
41:Aa:1236:C:C4	44:Am:103:LYS:HG3	2.56	0.41
41:Aa:1466:G:H2'	41:Aa:1467:A:H8	1.86	0.41
44:Am:14:ARG:HE	44:Am:42:ASP:HA	1.85	0.41
5:B:44:A:C5	5:B:45:C:C5	3.09	0.41
5:B:101:A:H2'	5:B:102:G:O4'	2.21	0.41
15:M:72:LEU:O	15:M:76:VAL:HG23	2.20	0.41
16:N:48:VAL:HG11	16:N:112:ILE:HD12	2.03	0.41
17:O:51:ARG:HD3	30:A:1200:A:C5	2.56	0.41
30:A:463:C:H2'	30:A:464:U:C6	2.56	0.41



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:A:620:G:O2'	30:A:1292:A:OP1	2.36	0.41
30:A:1701:U:H2'	30:A:1702:C:H6	1.85	0.41
30:A:2290:C:H4'	30:A:2356:A:H4'	2.03	0.41
30:A:2322:C:O2'	30:A:2323:U:H5'	2.21	0.41
30:A:2347:A:N6	30:A:2360:A:O2'	2.54	0.41
30:A:2491:C:H2'	30:A:2492:C:O4'	2.20	0.41
33:Ag:41:ARG:HH22	41:Aa:1301:U:P	2.42	0.41
41:Aa:810:A:H2'	41:Aa:811:G:O4'	2.21	0.41
41:Aa:1356:A:N1	41:Aa:1384:A:H5"	2.36	0.41
41:Aa:1397:G:H2'	41:Aa:1398:U:C6	2.56	0.41
43:Ac:107:LYS:HE3	43:Ac:110:LEU:HD12	2.03	0.41
45:Ak:53:LYS:HA	45:Ak:53:LYS:HD3	1.99	0.41
51:d:3:A:H2'	51:d:4:G:C8	2.56	0.41
6:C:173:LEU:HD11	6:C:271:VAL:HG21	2.03	0.41
12:J:82:LEU:HD23	12:J:82:LEU:HA	1.92	0.41
30:A:459:C:H2'	30:A:460:C:C6	2.56	0.41
41:Aa:38:U:O2'	41:Aa:508:G:H4'	2.21	0.41
41:Aa:68:C:H2'	41:Aa:69:G:C8	2.56	0.41
41:Aa:468:G:H2'	41:Aa:469:U:C6	2.56	0.41
41:Aa:686:U:H2'	41:Aa:687:C:C6	2.56	0.41
41:Aa:1165:U:H2'	41:Aa:1166:G:O4'	2.21	0.41
41:Aa:1331:U:H2'	41:Aa:1332:C:C5	2.56	0.41
48:Ad:69:ARG:HD3	48:Ad:198:TYR:CE1	2.56	0.41
13:K:22:LYS:NZ	30:A:909:G:N7	2.62	0.40
19:Q:78:GLU:O	30:A:24:G:O2'	2.39	0.40
29:11:70:G:H2'	29:11:71:G:H8	1.86	0.40
30:A:1919:C:H2'	30:A:1920:C:H6	1.85	0.40
30:A:2051:C:H2'	30:A:2052:C:H6	1.86	0.40
33:Ag:122:ASN:HD22	33:Ag:122:ASN:HA	1.71	0.40
41:Aa:586:C:O2'	41:Aa:736:A:N3	2.47	0.40
41:Aa:1084:U:H2'	41:Aa:1085:G:O4'	2.21	0.40
41:Aa:1124:C:O2'	43:Ac:14:ILE:HD12	2.21	0.40
3:3:53:SER:HB2	30:A:879:U:O3'	2.20	0.40
10:H:20:ASP:OD2	10:H:59:ASN:HB2	2.20	0.40
30:A:1702:C:H2'	30:A:1703:U:C6	2.56	0.40
30:A:2675:G:H2'	30:A:2676:U:C6	2.56	0.40
30:A:2777:A:H1'	30:A:2779:C:N4	2.36	0.40
41:Aa:227:C:H2'	41:Aa:228:A:O4'	2.22	0.40
41:Aa:1435:A:H2	41:Aa:1486:G:H22	1.68	0.40
43:Ac:91:ASN:HD21	43:Ac:98:VAL:HB	1.86	0.40
18:P:64:LYS:HB2	18:P:64:LYS:HE3	1.91	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
19:Q:19:LEU:HD23	19:Q:19:LEU:HA	1.88	0.40
22:T:65:VAL:O	22:T:65:VAL:HG23	2.19	0.40
30:A:226:A:N1	30:A:453:G:O2'	2.46	0.40
30:A:524:A:N1	30:A:545:G:H4'	2.37	0.40
30:A:765:U:H2'	30:A:766:G:H8	1.86	0.40
30:A:1028:G:N3	30:A:1028:G:H2'	2.35	0.40
30:A:2074:C:H2'	30:A:2075:G:H8	1.87	0.40
30:A:2629:A:P	52:8:75:C:H5"	2.61	0.40
33:Ag:92:ARG:O	33:Ag:96:ARG:HG3	2.21	0.40
41:Aa:218:U:H2'	41:Aa:219:C:O4'	2.22	0.40
41:Aa:1278:G:H8	41:Aa:1278:G:OP2	2.04	0.40
41:Aa:1515:G:H4'	41:Aa:1516:G:C4	2.57	0.40
2:2:9:ASN:HB3	2:2:12:LYS:HB3	2.03	0.40
3:3:52:LYS:O	3:3:56:LYS:HG3	2.21	0.40
7:D:67:LYS:HE3	30:A:2850:G:H5'	2.03	0.40
7:D:72:PRO:HG3	30:A:2814:C:H1'	2.04	0.40
30:A:401:U:H2'	30:A:402:C:C6	2.56	0.40
41:Aa:254:A:C2	41:Aa:290:A:C5	3.09	0.40
41:Aa:277:U:H2'	41:Aa:278:A:C8	2.57	0.40
41:Aa:1326:G:H4'	49:An:18:VAL:HG11	2.03	0.40
52:8:51:G:C2'	52:8:52:U:H5'	2.52	0.40
1:1:37:LYS:HA	1:1:37:LYS:HD2	1.96	0.40
9:G:149:ARG:HG3	9:G:162:ILE:O	2.21	0.40
30:A:346:A:H2'	30:A:347:U:H6	1.87	0.40
30:A:2293:A:H4'	30:A:2294:A:N3	2.37	0.40
30:A:2688:G:H2'	30:A:2689:A:C8	2.56	0.40
41:Aa:469:U:H2'	41:Aa:470:A:H8	1.86	0.40
42:Aj:59:LYS:HE2	42:Aj:62:ARG:NH2	2.36	0.40
48:Ad:172:LEU:HD23	48:Ad:172:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	1	46/52~(88%)	45~(98%)	1 (2%)	0	100	100
2	2	42/45~(93%)	42 (100%)	0	0	100	100
3	3	63/66~(96%)	62 (98%)	1 (2%)	0	100	100
4	4	35/37~(95%)	35 (100%)	0	0	100	100
6	С	272/277~(98%)	269 (99%)	3 (1%)	0	100	100
7	D	213/220~(97%)	203 (95%)	10 (5%)	0	100	100
8	Е	204/207~(99%)	201 (98%)	3 (2%)	0	100	100
9	G	152/178~(85%)	133 (88%)	19 (12%)	0	100	100
10	Н	143/145~(99%)	138 (96%)	5 (4%)	0	100	100
11	Ι	120/122~(98%)	117 (98%)	3 (2%)	0	100	100
12	J	144/146~(99%)	140 (97%)	4 (3%)	0	100	100
13	К	135/144 (94%)	133 (98%)	2 (2%)	0	100	100
14	L	114/122~(93%)	112 (98%)	2 (2%)	0	100	100
15	М	117/119~(98%)	111 (95%)	6 (5%)	0	100	100
16	N	107/116~(92%)	105 (98%)	2 (2%)	0	100	100
17	Ο	114/118~(97%)	112 (98%)	2 (2%)	0	100	100
18	Р	100/102~(98%)	99 (99%)	1 (1%)	0	100	100
19	Q	109/117~(93%)	108 (99%)	1 (1%)	0	100	100
20	R	87/91~(96%)	85 (98%)	2 (2%)	0	100	100
21	S	89/105~(85%)	83 (93%)	6 (7%)	0	100	100
22	Т	86/217~(40%)	83 (96%)	3 (4%)	0	100	100
23	U	77/94~(82%)	75 (97%)	2 (3%)	0	100	100
24	V	46/62~(74%)	46 (100%)	0	0	100	100
25	W	62/73~(85%)	59 (95%)	3 (5%)	0	100	100
26	Х	56/59~(95%)	54 (96%)	2 (4%)	0	100	100
27	Z	40/57~(70%)	40 (100%)	0	0	100	100
28	F	139/179~(78%)	130 (94%)	9 (6%)	0	100	100
31	Ae	154/166~(93%)	147 (96%)	7 (4%)	0	100	100
32	Af	93/98~(95%)	89 (96%)	4 (4%)	0	100	100
33	Ag	152/156~(97%)	151 (99%)	1 (1%)	0	100	100
34	Ai	125/132~(95%)	119 (95%)	6 (5%)	0	100	100
35	Al	130/137~(95%)	124 (95%)	6 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
36	Ao	86/89~(97%)	85~(99%)	1 (1%)	0	100	100
37	Ap	87/91~(96%)	82 (94%)	5~(6%)	0	100	100
38	Aq	70/87~(80%)	64 (91%)	6 (9%)	0	100	100
39	Ar	52/80~(65%)	51 (98%)	1 (2%)	0	100	100
40	At	79/83~(95%)	76 (96%)	3 (4%)	0	100	100
42	Aj	90/102~(88%)	86 (96%)	4 (4%)	0	100	100
43	Ac	200/217~(92%)	194 (97%)	6 (3%)	0	100	100
44	Am	112/121 (93%)	109 (97%)	3 (3%)	0	100	100
45	Ak	108/129 (84%)	106 (98%)	2 (2%)	0	100	100
46	Ab	92/255~(36%)	87 (95%)	5 (5%)	0	100	100
47	Ah	129/132~(98%)	124 (96%)	5 (4%)	0	100	100
48	Ad	197/200~(98%)	190 (96%)	7 (4%)	0	100	100
49	An	58/61~(95%)	58 (100%)	0	0	100	100
50	As	80/92~(87%)	79 (99%)	1 (1%)	0	100	100
54	13	43/84 (51%)	42 (98%)	1 (2%)	0	100	100
All	All	5049/5782~(87%)	4883 (97%)	166 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	33/50~(66%)	33 (100%)	0	100 100
2	2	38/40~(95%)	38 (100%)	0	100 100
3	3	51/57~(90%)	51 (100%)	0	100 100
4	4	31/35~(89%)	31 (100%)	0	100 100
6	С	206/224~(92%)	205 (100%)	1 (0%)	86 93
7	D	160/177~(90%)	158 (99%)	2(1%)	65 77



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
8	Е	150/169~(89%)	148 (99%)	2(1%)	65	77
9	G	44/155~(28%)	44 (100%)	0	100	100
10	Η	121/123~(98%)	121 (100%)	0	100	100
11	Ι	85/100~(85%)	85 (100%)	0	100	100
12	J	100/112~(89%)	100 (100%)	0	100	100
13	K	95/119 (80%)	95 (100%)	0	100	100
14	L	88/102 (86%)	87 (99%)	1 (1%)	70	81
15	М	57/95~(60%)	56 (98%)	1 (2%)	54	67
16	Ν	73/102~(72%)	72 (99%)	1 (1%)	62	75
17	О	96/98~(98%)	96 (100%)	0	100	100
18	Р	73/86~(85%)	72 (99%)	1 (1%)	62	75
19	Q	80/94~(85%)	79~(99%)	1 (1%)	65	77
20	R	66/82~(80%)	66 (100%)	0	100	100
21	S	54/90~(60%)	51 (94%)	3 (6%)	17	20
22	Т	49/190~(26%)	48 (98%)	1 (2%)	50	63
23	U	53/75~(71%)	53 (100%)	0	100	100
24	V	32/52~(62%)	29 (91%)	3(9%)	7	6
25	W	42/66~(64%)	41 (98%)	1 (2%)	44	56
26	Х	49/53~(92%)	49 (100%)	0	100	100
27	Ζ	37/50~(74%)	35~(95%)	2(5%)	18	21
28	F	54/158~(34%)	48 (89%)	6 (11%)	5	4
31	Ae	114/131 (87%)	107 (94%)	7 (6%)	15	17
32	Af	68/86~(79%)	66~(97%)	2(3%)	37	48
33	Ag	129/132~(98%)	125 (97%)	4 (3%)	35	45
34	Ai	97/109~(89%)	94 (97%)	3 (3%)	35	45
35	Al	106/119~(89%)	99~(93%)	7 (7%)	14	15
36	Ao	78/81~(96%)	74 (95%)	4(5%)	20	24
37	Ар	69/77~(90%)	68~(99%)	1 (1%)	62	75
38	Aq	50/82~(61%)	47 (94%)	3(6%)	16	18
39	Ar	48/68~(71%)	43 (90%)	5 (10%)	5	5
40	At	61/69~(88%)	56 (92%)	5 (8%)	9	8



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
42	Aj	72/91~(79%)	69~(96%)	3~(4%)	25	32
43	Ac	135/175~(77%)	134~(99%)	1 (1%)	81	89
44	Am	82/104~(79%)	77~(94%)	5~(6%)	15	17
45	Ak	70/104~(67%)	58~(83%)	12 (17%)	1	1
46	Ab	32/221~(14%)	30~(94%)	2~(6%)	15	16
47	Ah	112/113~(99%)	109~(97%)	3~(3%)	40	51
48	Ad	142/175~(81%)	136~(96%)	6 (4%)	25	32
49	An	52/53~(98%)	52 (100%)	0	100	100
50	As	59/80~(74%)	59~(100%)	0	100	100
54	13	22/75~(29%)	22 (100%)	0	100	100
All	All	3615/4899 (74%)	3516 (97%)	99~(3%)	41	51

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
6	С	101	LYS
7	D	107	VAL
7	D	200	ASN
8	Е	124	THR
8	Е	191	SER
14	L	92	ARG
15	М	52	THR
16	N	68	SER
18	Р	12	ILE
19	Q	11	ARG
21	S	66	SER
21	S	92	ARG
21	S	101	ILE
22	Т	42	LYS
24	V	38	ILE
24	V	50	SER
24	V	55	LYS
25	W	24	SER
27	Z	21	LYS
27	Z	30	CYS
28	F	35	VAL
28	F	88	LYS
28	F	89	VAL



Mol	Chain	Res	Type
28	F	130	LEU
28	F	137	ILE
28	F	172	ASN
31	Ae	17	THR
31	Ae	34	THR
31	Ae	73	VAL
31	Ae	77	VAL
31	Ae	80	THR
31	Ae	127	SER
31	Ae	153	VAL
32	Af	73	THR
32	Af	83	SER
33	Ag	17	ILE
33	Ag	72	VAL
33	Ag	75	VAL
33	Ag	80	VAL
34	Ai	47	ILE
34	Ai	99	SER
34	Ai	130	SER
35	Al	21	SER
35	Al	30	SER
35	Al	36	THR
35	Al	48	THR
35	Al	75	GLU
35	Al	91	SER
35	Al	100	VAL
36	Ao	48	LYS
36	Ao	58	LYS
36	Ao	84	SER
36	Ao	88	ARG
37	Ap	27	SER
38	Aq	54	SER
38	Aq	69	LEU
38	Aq	78	VAL
39	Ar	24	THR
39	Ar	25	HIS
39	Ar	31	THR
39	Ar	33	LEU
39	Ar	67	SER
40	At	22	ILE
40	At	33	LYS
40	At	39	VAL



Mol	Chain	Res	Type
40	At	51	SER
40	At	76	SER
42	Aj	6	ILE
42	Aj	18	ILE
42	Aj	77	VAL
43	Ac	171	THR
44	Am	7	VAL
44	Am	15	VAL
44	Am	16	VAL
44	Am	45	VAL
44	Am	114	LYS
45	Ak	26	THR
45	Ak	33	THR
45	Ak	43	SER
45	Ak	67	SER
45	Ak	73	SER
45	Ak	76	GLU
45	Ak	82	VAL
45	Ak	86	VAL
45	Ak	95	SER
45	Ak	113	VAL
45	Ak	116	VAL
45	Ak	119	ASN
46	Ab	106	THR
46	Ab	199	VAL
47	Ah	34	LYS
47	Ah	43	GLU
47	Ah	120	LYS
48	Ad	12	SER
48	Ad	77	LYS
48	Ad	89	LEU
48	Ad	92	SER
48	Ad	137	GLN
48	Ad	140	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	27	ASN
3	3	21	GLN
3	3	35	ASN
3	3	60	GLN



Mol	Chain	Res	Type
7	D	134	HIS
7	D	136	GLN
7	D	167	GLN
7	D	200	ASN
8	Е	148	GLN
8	Е	174	GLN
9	G	111	HIS
11	Ι	45	ASN
12	J	104	ASN
13	K	35	GLN
14	L	106	GLN
15	М	37	ASN
15	М	39	HIS
16	Ν	113	GLN
17	0	52	GLN
17	0	108	GLN
19	Q	65	ASN
20	R	47	ASN
23	U	58	ASN
23	U	86	GLN
24	V	30	ASN
25	W	40	GLN
28	F	63	GLN
28	F	127	ASN
33	Ag	19	ASN
33	Ag	130	ASN
34	Ai	29	ASN
34	Ai	52	GLN
34	Ai	128	GLN
35	Al	39	ASN
36	Ao	5	GLN
36	Ao	9	ASN
38	Aq	53	ASN
40	At	3	ASN
43	Ac	3	GLN
43	Ac	91	ASN
43	Ac	101	ASN
44	Am	104	ASN
45	Ak	18	ASN
45	Ak	119	ASN
47	Ah	18	ASN
47	Ah	22	HIS



Continued from previous page...

Mol	Chain	Res	Type
48	Ad	146	GLN
50	As	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	11	13/15~(86%)	5~(38%)	0
30	А	2562/2923~(87%)	303~(11%)	9~(0%)
41	Aa	1423/1552~(91%)	171 (12%)	0
5	В	112/115~(97%)	15 (13%)	0
51	d	17/19~(89%)	3~(17%)	0
52	8	67/71~(94%)	13 (19%)	0
53	9	4/5~(80%)	1 (25%)	0
All	All	4198/4700~(89%)	511 (12%)	9~(0%)

All (511) RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
5	В	10	U
5	В	11	А
5	В	23	U
5	В	30	U
5	В	33	U
5	В	34	С
5	В	39	G
5	В	49	G
5	В	50	А
5	В	54	U
5	В	55	А
5	В	64	А
5	В	87	U
5	В	88	G
5	В	106	G
29	11	2	С
29	11	5	G
29	11	71	G
29	11	74	С
29	11	76	А
30	А	15	G
30	А	34	U
30	A	63	U



Mol	Chain	Res	Type
30	А	71	А
30	А	75	G
30	А	84	А
30	А	91	А
30	А	93	U
30	А	96	G
30	А	101	G
30	А	117	А
30	А	118	А
30	А	119	U
30	А	130	А
30	А	136	А
30	А	153	G
30	А	161	А
30	А	164	А
30	А	177	G
30	А	184	С
30	А	185	А
30	А	199	А
30	А	202	А
30	А	216	А
30	А	218	G
30	А	219	А
30	А	225	А
30	А	226	А
30	А	251	G
30	А	269	G
30	А	272	С
30	А	279	А
30	А	292	U
30	А	294	G
30	А	295	G
30	A	318	A
30	А	321	U
30	A	324	А
30	A	327	G
30	А	328	G
30	А	354	А
30	A	364	А
30	A	373	А
30	А	381	G
30	А	389	А



Mol	Chain	Res	Type
30	А	393	G
30	А	397	U
30	А	401	U
30	А	402	С
30	А	412	U
30	А	429	С
30	А	432	G
30	А	445	G
30	А	450	С
30	А	457	G
30	А	470	G
30	А	474	A
30	А	476	А
30	А	481	С
30	А	482	U
30	А	526	A
30	А	527	G
30	А	549	U
30	А	550	A
30	А	552	А
30	А	553	A
30	А	567	G
30	А	576	U
30	А	577	А
30	А	578	G
30	А	583	А
30	А	593	U
30	А	594	G
30	А	606	G
30	А	616	G
30	A	617	A
30	A	618	A
30	А	630	G
30	A	646	A
30	A	650	U
30	A	682	A
30	A	690	U
30	A	699	U
30	A	700	A
30	A	731	U
30	A	762	С
30	A	775	A



Mol	Chain	Res	Type
30	А	792	5MU
30	А	793	G
30	А	820	G
30	А	827	А
30	А	829	U
30	А	837	G
30	А	850	G
30	А	857	С
30	А	872	U
30	А	873	U
30	А	888	G
30	А	892	U
30	А	904	G
30	А	911	А
30	А	919	G
30	А	955	А
30	А	962	А
30	А	977	A
30	А	989	А
30	А	990	G
30	А	1005	G
30	А	1018	А
30	А	1027	А
30	А	1040	А
30	А	1049	C
30	А	1056	U
30	А	1057	A
30	А	1070	A
30	А	1077	U
30	А	1078	G
30	А	1083	G
30	А	1158	G
30	А	1159	А
30	A	1161	A
30	A	1173	A
30	A	$117\overline{6}$	U
30	A	1177	A
30	A	1178	С
30	A	1179	C
30	A	1186	A
30	A	1199	A
30	А	1201	G



Mol	Chain	Res	Type
30	А	1212	U
30	А	1219	G
30	А	1220	А
30	А	1221	С
30	А	1291	А
30	А	1294	G
30	А	1309	G
30	А	1310	А
30	А	1312	А
30	А	1337	А
30	А	1338	U
30	А	1389	U
30	А	1402	А
30	А	1416	U
30	А	1449	А
30	А	1465	G
30	А	1467	G
30	А	1472	С
30	А	1489	А
30	А	1490	G
30	А	1494	G
30	А	1498	U
30	А	1500	G
30	А	1511	С
30	А	1517	А
30	А	1522	G
30	А	1560	А
30	А	1568	U
30	А	1569	G
30	А	1572	G
30	А	1573	А
30	А	1574	G
30	А	1591	G
30	А	1592	A
30	А	1593	G
30	A	1595	C
30	A	1606	C
30	A	1613	G
30	A	1616	A
30	A	1651	C
30	A	1652	A
30	А	1690	A



Mol	Chain	Res	Type
30	А	1691	G
30	А	1692	С
30	А	1718	G
30	А	1740	G
30	А	1747	G
30	А	1783	G
30	А	1790	G
30	А	1791	G
30	А	1800	А
30	А	1809	С
30	А	1818	А
30	А	1827	С
30	А	1828	U
30	А	1843	U
30	А	1856	А
30	А	1862	G
30	А	1875	А
30	А	1885	G
30	А	1886	А
30	А	1892	U
30	А	1904	А
30	А	1906	С
30	А	1911	А
30	А	1933	G
30	А	1954	А
30	А	1956	G
30	А	1957	G
30	А	1964	А
30	А	1965	А
30	А	1969	С
30	А	1982	U
30	А	1994	С
30	А	1997	А
30	А	1998	А
30	А	1999	G
30	А	2018	U
30	А	2020	U
30	А	2024	А
30	А	2047	А
30	А	2050	А
30	А	2058	А
30	А	2059	G



Mol	Chain	Res	Type
30	А	2060	А
30	А	2070	С
30	А	2082	С
30	А	2083	G
30	А	2087	А
30	А	2088	G
30	А	2096	G
30	А	2120	G
30	А	2225	А
30	А	2231	С
30	А	2238	U
30	А	2239	А
30	А	2252	А
30	А	2253	С
30	А	2265	G
30	А	2266	G
30	А	2295	А
30	А	2310	С
30	А	2314	А
30	А	2315	А
30	А	2316	G
30	А	2345	А
30	А	2347	А
30	А	2349	А
30	А	2352	G
30	А	2354	А
30	А	2362	А
30	А	2374	С
30	А	2377	С
30	А	2399	G
30	А	2410	G
30	А	2412	С
30	А	2429	U
30	А	2433	С
30	А	2450	U
30	A	2452	А
30	А	2456	G
30	A	2457	A
30	А	2462	А
30	A	2468	С
30	A	2475	A
30	А	2505	A



Mol	Chain	Res	Type
30	А	2529	G
30	А	2532	G
30	А	2545	А
30	А	2556	G
30	А	2561	С
30	А	2575	G
30	А	2581	U
30	А	2593	А
30	А	2594	G
30	А	2600	С
30	А	2612	U
30	А	2629	А
30	А	2630	G
30	А	2636	U
30	А	2640	U
30	А	2656	А
30	А	2657	G
30	А	2682	G
30	А	2687	А
30	А	2695	G
30	А	2700	G
30	А	2709	U
30	А	2716	U
30	А	2717	А
30	А	2718	С
30	А	2741	G
30	А	2753	U
30	А	2775	А
30	А	2778	G
30	А	2784	А
30	А	2792	А
30	А	2793	G
30	A	2805	А
30	А	2807	G
30	А	2816	С
30	A	2817	А
30	А	2818	А
30	А	2828	U
30	А	2833	U
30	A	2855	А
30	А	2887	G
30	А	2892	G


Mol	Chain	Res	Type
30	А	2903	А
30	А	2906	G
30	А	2911	А
30	А	2913	G
30	А	2918	А
30	А	2920	U
41	Aa	10	G
41	Aa	33	А
41	Aa	40	G
41	Aa	45	G
41	Aa	48	С
41	Aa	49	С
41	Aa	51	А
41	Aa	52	А
41	Aa	108	А
41	Aa	119	А
41	Aa	120	С
41	Aa	144	С
41	Aa	146	G
41	Aa	157	G
41	Aa	158	G
41	Aa	163	С
41	Aa	168	G
41	Aa	182	А
41	Aa	183	U
41	Aa	184	А
41	Aa	185	U
41	Aa	189	G
41	Aa	195	С
41	Aa	196	А
41	Aa	203	A
41	Aa	204	A
41	Aa	205	A
41	Aa	207	G
41	Aa	213	G
41	Aa	221	U
41	Aa	253	U
41	Aa	255	G
41	Aa	259	G
41	Aa	274	G
41	Aa	275	С
41	Aa	297	G



Mol	Chain	Res	Type
41	Aa	328	А
41	Aa	336	С
41	Aa	340	G
41	Aa	353	С
41	Aa	355	G
41	Aa	356	G
41	Aa	360	С
41	Aa	362	G
41	Aa	375	U
41	Aa	380	С
41	Aa	381	А
41	Aa	392	G
41	Aa	414	G
41	Aa	419	A
41	Aa	424	G
41	Aa	429	U
41	Aa	430	С
41	Aa	432	G
41	Aa	437	U
41	Aa	443	U
41	Aa	447	U
41	Aa	456	А
41	Aa	460	А
41	Aa	461	С
41	Aa	467	U
41	Aa	474	А
41	Aa	492	G
41	Aa	493	G
41	Aa	503	A
41	Aa	505	А
41	Aa	517	A
41	Aa	519	С
41	Aa	526	С
41	Aa	529	G
41	Aa	532	G
41	Aa	535	G7M
41	Aa	540	А
41	Aa	555	А
41	Aa	567	A
41	Aa	570	U
41	Aa	572	U
41	Aa	580	А



Mol	Chain	Res	Type
41	Aa	581	А
41	Aa	584	С
41	Aa	609	G
41	Aa	641	U
41	Aa	642	С
41	Aa	661	U
41	Aa	673	А
41	Aa	695	А
41	Aa	696	G
41	Aa	703	А
41	Aa	711	G
41	Aa	731	U
41	Aa	732	G
41	Aa	757	А
41	Aa	763	G
41	Aa	785	А
41	Aa	801	U
41	Aa	802	А
41	Aa	823	А
41	Aa	825	С
41	Aa	829	G
41	Aa	836	А
41	Aa	844	G
41	Aa	860	U
41	Aa	881	А
41	Aa	883	G
41	Aa	911	G
41	Aa	923	А
41	Aa	935	G
41	Aa	943	С
41	Aa	944	A
41	Aa	969	U
41	Aa	977	A
41	Aa	978	A
41	Aa	980	G
41	Aa	984	A
41	Aa	986	A
41	Aa	992	A
41	Aa	1001	U
41	Aa	1002	G
41	Aa	1003	A
41	Aa	1024	G



Mol	Chain	Res	Type
41	Aa	1027	А
41	Aa	1076	U
41	Aa	1096	U
41	Aa	1097	U
41	Aa	1099	G
41	Aa	1105	G
41	Aa	1106	U
41	Aa	1112	А
41	Aa	1123	С
41	Aa	1150	U
41	Aa	1152	G
41	Aa	1165	U
41	Aa	1167	A
41	Aa	1191	G
41	Aa	1193	U
41	Aa	1194	G
41	Aa	1206	A
41	Aa	1207	A
41	Aa	1219	С
41	Aa	1220	С
41	Aa	1224	U
41	Aa	1237	А
41	Aa	1263	G
41	Aa	1267	А
41	Aa	1278	G
41	Aa	1289	А
41	Aa	1290	А
41	Aa	1309	А
41	Aa	1310	G
41	Aa	1312	U
41	Aa	1315	G
41	Aa	1330	С
41	Aa	1346	U
41	Aa	1356	A
41	Aa	1363	G
41	Aa	1374	U
41	Aa	1380	G
41	Aa	1388	С
41	Aa	1391	U
41	Aa	1404	A
41	Aa	1407	С
41	Aa	1505	G



Mol	Chain	Res	Type
41	Aa	1508	G
41	Aa	1510	А
41	Aa	1513	А
41	Aa	1514	А
41	Aa	1517	U
41	Aa	1528	G
41	Aa	1540	G
41	Aa	1541	G
41	Aa	1548	U
51	d	21	А
51	d	22	U
51	d	25	А
52	8	4	G
52	8	8	U
52	8	9	G
52	8	14	А
52	8	23	G
52	8	24	С
52	8	50	G
52	8	52	U
52	8	54	G
52	8	59	А
52	8	75	С
52	8	76	С
52	8	77	А
53	9	36	С

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	А	291	G
30	А	396	G
30	А	525	А
30	А	793	G
30	А	809	А
30	А	1157	U
30	А	1158	G
30	А	1905	G
30	А	2783	U



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

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

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

Mal	Tuno	Chain	Dog	Link	Box Link Bond lengths		В	ond ang	les	
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
41	5MC	Aa	976	41	18,22,23	0.28	0	$26,\!32,\!35$	0.43	0
41	4OC	Aa	1412	41	20,23,24	0.32	0	$26,\!32,\!35$	0.54	0
30	OMG	А	2278	52,30	18,26,27	0.94	1 (5%)	19,38,41	0.59	0
30	G7M	А	2601	56,30	20,26,27	0.55	0	17,39,42	0.33	0
30	PSU	А	2484	30	18,21,22	0.52	0	22,30,33	0.59	0
30	H2U	А	2476	30	18,21,22	0.49	0	21,30,33	0.86	1 (4%)
30	5MU	А	1966	30	19,22,23	0.51	0	28,32,35	0.49	0
41	MA6	Aa	1530	41	18,26,27	0.75	0	19,38,41	0.73	0
30	2MA	А	2530	56,30	19,25,26	1.06	2 (10%)	21,37,40	3.02	4 (19%)
30	PSU	А	2632	30	18,21,22	0.48	0	22,30,33	0.61	0
30	PSU	А	2607	30	18,21,22	0.61	1 (5%)	22,30,33	0.75	1 (4%)
41	2MG	Aa	975	41	18,26,27	0.98	2 (11%)	16,38,41	0.67	0
41	G7M	Aa	535	41	20,26,27	0.59	0	17,39,42	0.48	0
30	5MU	А	792	30	19,22,23	0.44	0	28,32,35	0.65	0
30	2MG	А	2472	30	18,26,27	0.92	1 (5%)	16,38,41	0.66	0
41	MA6	Aa	1529	41	18,26,27	0.77	0	19,38,41	0.75	0
41	UR3	Aa	1509	41	19,22,23	0.30	0	$26,\!32,\!35$	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	5MC	Aa	976	41	-	0/7/25/26	0/2/2/2
41	4OC	Aa	1412	41	-	0/9/29/30	0/2/2/2
30	OMG	А	2278	52,30	-	1/5/27/28	0/3/3/3
30	G7M	А	2601	56,30	-	0/3/25/26	0/3/3/3
30	PSU	А	2484	30	-	0/7/25/26	0/2/2/2
30	H2U	A	2476	30	-	0/7/38/39	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	5MU	А	1966	30	-	0/7/25/26	0/2/2/2
41	MA6	Aa	1530	41	-	2/7/29/30	0/3/3/3
30	2MA	А	2530	$56,\!30$	-	2/3/25/26	0/3/3/3
30	PSU	А	2632	30	-	0/7/25/26	0/2/2/2
30	PSU	А	2607	30	-	0/7/25/26	0/2/2/2
41	2MG	Aa	975	41	-	0/5/27/28	0/3/3/3
41	G7M	Aa	535	41	-	2/3/25/26	0/3/3/3
30	5MU	А	792	30	-	0/7/25/26	0/2/2/2
30	2MG	А	2472	30	-	0/5/27/28	0/3/3/3
41	MA6	Aa	1529	41	-	0/7/29/30	0/3/3/3
41	UR3	Aa	1509	41	-	0/7/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
41	Aa	975	2MG	C5-C6	-2.51	1.42	1.47
30	А	2530	2MA	C6-N6	-2.35	1.25	1.34
30	А	2278	OMG	C5-C6	-2.32	1.42	1.47
30	А	2607	PSU	O4'-C1'	-2.17	1.40	1.43
30	А	2530	2MA	C6-N1	2.11	1.37	1.33
30	А	2472	2MG	C5-C6	-2.11	1.43	1.47
41	Aa	975	2MG	C8-N7	-2.07	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
30	А	2530	2MA	C5-C6-N1	-12.10	113.06	121.01
30	А	2530	2MA	C2-N3-C4	-4.06	112.22	115.52
30	А	2530	2MA	C2-N1-C6	3.60	123.70	118.08
30	А	2607	PSU	O4'-C1'-C2'	2.57	108.77	105.14
30	А	2530	2MA	N6-C6-N1	2.50	123.87	117.07
30	А	2476	H2U	C5-C4-N3	-2.36	114.00	116.65

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	Aa	535	G7M	O4'-C4'-C5'-O5'
41	Aa	535	G7M	C3'-C4'-C5'-O5'
30	А	2278	OMG	C1'-C2'-O2'-CM2



Mol	Chain	Res	Type	Atoms
41	Aa	1530	MA6	O4'-C4'-C5'-O5'
41	Aa	1530	MA6	C3'-C4'-C5'-O5'
30	А	2530	2MA	C4'-C5'-O5'-P
30	А	2530	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	А	2278	OMG	1	0
30	А	2601	G7M	1	0
30	А	2530	2MA	1	0
41	Aa	975	2MG	1	0
41	Aa	1529	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 254 ligands modelled in this entry, 253 are monoatomic - leaving 1 for Mogul analysis.

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

Mal	al Tuna Chain Dag Lin		Tink	Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
57	EM1	А	3001	-	58,64,64	0.51	0	$71,\!97,\!97$	0.42	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	EM1	А	3001	-	-	1/71/112/112	0/4/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	А	3001	EM1	C84-C83-N80-N81

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	8	3
51	d	1
29	11	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	8:A	O3'	15:C	Р	14.91
1	11	6:A	O3'	68:C	Р	14.41
1	8	19:G	O3'	22:A	Р	10.42
1	8	15:G	O3'	19:G	Р	8.49
1	8	47:G	O3'	49:C	Р	6.61



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-53066. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 220

Y Index: 220

Z Index: 220



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: 192

Y Index: 235

Z Index: 318

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



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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 955 nm^3 ; this corresponds to an approximate mass of 863 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 0.452 \AA^{-1}



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-53066 and PDB model 9QEG. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 3.0 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 (3).



9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9320	0.7030
1	0.8840	0.6800
11	0.2360	0.4530
13	0.6190	0.5520
2	0.9910	0.8090
3	0.9960	0.7950
4	0.9750	0.7430
8	0.3500	0.4210
9	0.5470	0.4800
А	0.9580	0.7340
Aa	0.9110	0.6620
Ab	0.4820	0.5090
Ac	0.9930	0.6940
Ad	0.9880	0.6740
Ae	0.9710	0.6700
Af	0.9590	0.6110
Ag	0.9770	0.6760
Ah	0.9850	0.7030
Ai	0.9950	0.7020
Aj	0.9890	0.6800
Ak	0.9560	0.5860
Al	0.9910	0.7080
Am	0.9900	0.7040
An	0.9920	0.7280
Ao	0.9800	0.6920
Ap	0.9830	0.7060
Aq	0.9890	0.6450
Ar	0.9910	0.6890
As	0.9980	0.7180
At	0.9900	0.6940
В	0.8760	0.6300
C	0.9890	0.7810
D	0.9890	0.7830
E	0.9670	0.7630
F	0.5770	0.5070



Chain	Atom inclusion	Q-score
G	0.7990	0.6130
Н	0.9750	0.7770
Ι	0.9800	0.7680
J	0.9640	0.7500
K	0.9810	0.7680
L	0.9860	0.7830
М	0.8780	0.6560
N	0.9760	0.7650
0	0.9870	0.7910
Р	0.9740	0.7720
Q	0.9790	0.7880
R	0.9680	0.7520
S	0.9220	0.6950
Т	0.8980	0.6790
U	0.9780	0.7810
V	0.8850	0.7030
W	0.9300	0.7170
Х	0.9650	0.7680
Z	0.9350	0.7500
d	0.7430	0.4670

